



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2020 – 03:49 am BST

PDB ID : 4RKM
Title : Wolinella succinogenes octaheme sulfite reductase MccA, form I
Authors : Hermann, B.; Kern, M.; La Pietra, L.; Simon, J.; Einsle, O.
Deposited on : 2014-10-13
Resolution : 2.20 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)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

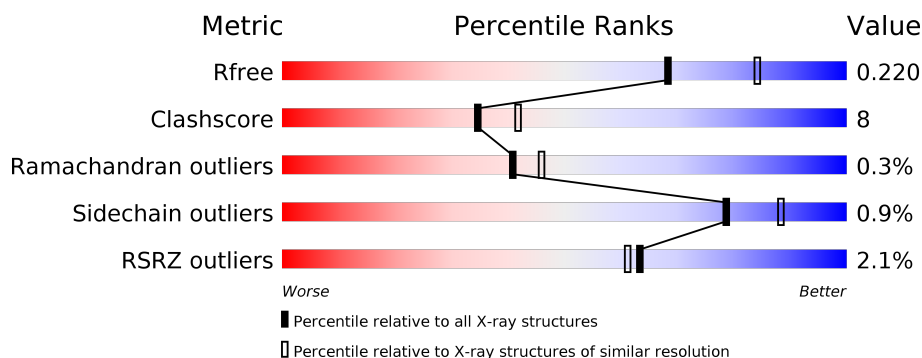
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	732	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>5%</div> <div>10%</div> </div> </div>
1	B	732	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>5%</div> <div>10%</div> </div> </div>
1	C	732	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>5%</div> <div>10%</div> </div> </div>
1	D	732	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>5%</div> <div>10%</div> </div> </div>
1	E	732	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>6%</div> <div>10%</div> </div> </div>
1	F	732	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>6%</div> <div>10%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	732	<div> <div></div> <div>2%</div> <div>84%</div> <div>5%</div> <div>10%</div> </div>
1	H	732	<div> <div></div> <div>%</div> <div>86%</div> <div>5%</div> <div>10%</div> </div>
1	I	732	<div> <div></div> <div>2%</div> <div>84%</div> <div>6%</div> <div>10%</div> </div>
1	J	732	<div> <div></div> <div>2%</div> <div>84%</div> <div>6%</div> <div>10%</div> </div>
1	K	732	<div> <div></div> <div>%</div> <div>85%</div> <div>5%</div> <div>10%</div> </div>
1	L	732	<div> <div></div> <div>5%</div> <div>84%</div> <div>6%</div> <div>10%</div> </div>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 70014 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 MccA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	659	Total	C	N	O	S	0	0	0
			5224	3283	919	987	35			
1	B	660	Total	C	N	O	S	0	0	0
			5232	3289	920	988	35			
1	C	659	Total	C	N	O	S	0	0	0
			5224	3283	919	987	35			
1	D	659	Total	C	N	O	S	0	0	0
			5224	3283	919	987	35			
1	E	659	Total	C	N	O	S	0	0	0
			5224	3283	919	987	35			
1	F	659	Total	C	N	O	S	0	0	0
			5224	3283	919	987	35			
1	H	660	Total	C	N	O	S	0	0	0
			5232	3289	920	988	35			
1	I	659	Total	C	N	O	S	0	0	0
			5224	3283	919	987	35			
1	J	659	Total	C	N	O	S	0	0	0
			5224	3283	919	987	35			
1	K	659	Total	C	N	O	S	0	0	0
			5224	3283	919	987	35			
1	L	659	Total	C	N	O	S	0	0	0
			5224	3283	919	987	35			
1	G	658	Total	C	N	O	S	0	0	0
			5218	3280	918	985	35			

There are 360 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	691	SER	-	EXPRESSION TAG	UNP Q7MSJ8
A	692	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
A	693	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
A	694	SER	-	EXPRESSION TAG	UNP Q7MSJ8
A	695	HIS	-	EXPRESSION TAG	UNP Q7MSJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	696	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
A	697	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
A	698	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
A	699	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
A	700	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
A	701	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
A	702	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
A	703	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
A	704	SER	-	EXPRESSION TAG	UNP Q7MSJ8
A	705	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
A	706	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
A	707	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
A	708	SER	-	EXPRESSION TAG	UNP Q7MSJ8
A	709	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
A	710	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
A	711	SER	-	EXPRESSION TAG	UNP Q7MSJ8
A	712	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
A	713	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
A	714	SER	-	EXPRESSION TAG	UNP Q7MSJ8
A	715	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
A	716	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
A	717	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
A	718	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
A	719	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
A	720	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
B	691	SER	-	EXPRESSION TAG	UNP Q7MSJ8
B	692	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
B	693	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
B	694	SER	-	EXPRESSION TAG	UNP Q7MSJ8
B	695	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
B	696	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
B	697	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
B	698	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
B	699	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
B	700	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
B	701	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
B	702	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
B	703	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
B	704	SER	-	EXPRESSION TAG	UNP Q7MSJ8
B	705	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
B	706	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
B	707	GLY	-	EXPRESSION TAG	UNP Q7MSJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	708	SER	-	EXPRESSION TAG	UNP Q7MSJ8
B	709	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
B	710	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
B	711	SER	-	EXPRESSION TAG	UNP Q7MSJ8
B	712	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
B	713	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
B	714	SER	-	EXPRESSION TAG	UNP Q7MSJ8
B	715	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
B	716	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
B	717	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
B	718	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
B	719	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
B	720	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
C	691	SER	-	EXPRESSION TAG	UNP Q7MSJ8
C	692	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
C	693	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
C	694	SER	-	EXPRESSION TAG	UNP Q7MSJ8
C	695	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
C	696	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
C	697	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
C	698	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
C	699	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
C	700	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
C	701	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
C	702	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
C	703	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
C	704	SER	-	EXPRESSION TAG	UNP Q7MSJ8
C	705	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
C	706	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
C	707	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
C	708	SER	-	EXPRESSION TAG	UNP Q7MSJ8
C	709	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
C	710	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
C	711	SER	-	EXPRESSION TAG	UNP Q7MSJ8
C	712	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
C	713	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
C	714	SER	-	EXPRESSION TAG	UNP Q7MSJ8
C	715	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
C	716	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
C	717	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
C	718	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
C	719	GLU	-	EXPRESSION TAG	UNP Q7MSJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	720	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
D	691	SER	-	EXPRESSION TAG	UNP Q7MSJ8
D	692	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
D	693	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
D	694	SER	-	EXPRESSION TAG	UNP Q7MSJ8
D	695	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
D	696	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
D	697	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
D	698	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
D	699	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
D	700	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
D	701	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
D	702	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
D	703	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
D	704	SER	-	EXPRESSION TAG	UNP Q7MSJ8
D	705	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
D	706	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
D	707	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
D	708	SER	-	EXPRESSION TAG	UNP Q7MSJ8
D	709	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
D	710	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
D	711	SER	-	EXPRESSION TAG	UNP Q7MSJ8
D	712	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
D	713	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
D	714	SER	-	EXPRESSION TAG	UNP Q7MSJ8
D	715	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
D	716	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
D	717	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
D	718	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
D	719	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
D	720	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
E	691	SER	-	EXPRESSION TAG	UNP Q7MSJ8
E	692	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
E	693	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
E	694	SER	-	EXPRESSION TAG	UNP Q7MSJ8
E	695	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
E	696	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
E	697	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
E	698	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
E	699	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
E	700	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
E	701	GLY	-	EXPRESSION TAG	UNP Q7MSJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	702	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
E	703	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
E	704	SER	-	EXPRESSION TAG	UNP Q7MSJ8
E	705	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
E	706	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
E	707	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
E	708	SER	-	EXPRESSION TAG	UNP Q7MSJ8
E	709	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
E	710	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
E	711	SER	-	EXPRESSION TAG	UNP Q7MSJ8
E	712	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
E	713	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
E	714	SER	-	EXPRESSION TAG	UNP Q7MSJ8
E	715	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
E	716	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
E	717	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
E	718	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
E	719	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
E	720	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
F	691	SER	-	EXPRESSION TAG	UNP Q7MSJ8
F	692	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
F	693	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
F	694	SER	-	EXPRESSION TAG	UNP Q7MSJ8
F	695	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
F	696	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
F	697	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
F	698	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
F	699	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
F	700	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
F	701	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
F	702	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
F	703	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
F	704	SER	-	EXPRESSION TAG	UNP Q7MSJ8
F	705	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
F	706	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
F	707	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
F	708	SER	-	EXPRESSION TAG	UNP Q7MSJ8
F	709	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
F	710	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
F	711	SER	-	EXPRESSION TAG	UNP Q7MSJ8
F	712	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
F	713	TRP	-	EXPRESSION TAG	UNP Q7MSJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	714	SER	-	EXPRESSION TAG	UNP Q7MSJ8
F	715	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
F	716	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
F	717	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
F	718	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
F	719	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
F	720	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
H	691	SER	-	EXPRESSION TAG	UNP Q7MSJ8
H	692	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
H	693	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
H	694	SER	-	EXPRESSION TAG	UNP Q7MSJ8
H	695	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
H	696	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
H	697	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
H	698	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
H	699	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
H	700	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
H	701	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
H	702	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
H	703	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
H	704	SER	-	EXPRESSION TAG	UNP Q7MSJ8
H	705	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
H	706	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
H	707	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
H	708	SER	-	EXPRESSION TAG	UNP Q7MSJ8
H	709	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
H	710	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
H	711	SER	-	EXPRESSION TAG	UNP Q7MSJ8
H	712	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
H	713	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
H	714	SER	-	EXPRESSION TAG	UNP Q7MSJ8
H	715	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
H	716	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
H	717	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
H	718	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
H	719	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
H	720	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
I	691	SER	-	EXPRESSION TAG	UNP Q7MSJ8
I	692	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
I	693	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
I	694	SER	-	EXPRESSION TAG	UNP Q7MSJ8
I	695	HIS	-	EXPRESSION TAG	UNP Q7MSJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
I	696	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
I	697	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
I	698	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
I	699	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
I	700	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
I	701	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
I	702	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
I	703	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
I	704	SER	-	EXPRESSION TAG	UNP Q7MSJ8
I	705	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
I	706	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
I	707	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
I	708	SER	-	EXPRESSION TAG	UNP Q7MSJ8
I	709	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
I	710	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
I	711	SER	-	EXPRESSION TAG	UNP Q7MSJ8
I	712	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
I	713	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
I	714	SER	-	EXPRESSION TAG	UNP Q7MSJ8
I	715	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
I	716	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
I	717	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
I	718	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
I	719	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
I	720	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
J	691	SER	-	EXPRESSION TAG	UNP Q7MSJ8
J	692	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
J	693	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
J	694	SER	-	EXPRESSION TAG	UNP Q7MSJ8
J	695	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
J	696	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
J	697	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
J	698	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
J	699	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
J	700	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
J	701	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
J	702	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
J	703	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
J	704	SER	-	EXPRESSION TAG	UNP Q7MSJ8
J	705	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
J	706	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
J	707	GLY	-	EXPRESSION TAG	UNP Q7MSJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
J	708	SER	-	EXPRESSION TAG	UNP Q7MSJ8
J	709	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
J	710	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
J	711	SER	-	EXPRESSION TAG	UNP Q7MSJ8
J	712	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
J	713	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
J	714	SER	-	EXPRESSION TAG	UNP Q7MSJ8
J	715	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
J	716	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
J	717	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
J	718	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
J	719	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
J	720	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
K	691	SER	-	EXPRESSION TAG	UNP Q7MSJ8
K	692	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
K	693	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
K	694	SER	-	EXPRESSION TAG	UNP Q7MSJ8
K	695	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
K	696	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
K	697	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
K	698	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
K	699	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
K	700	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
K	701	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
K	702	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
K	703	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
K	704	SER	-	EXPRESSION TAG	UNP Q7MSJ8
K	705	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
K	706	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
K	707	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
K	708	SER	-	EXPRESSION TAG	UNP Q7MSJ8
K	709	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
K	710	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
K	711	SER	-	EXPRESSION TAG	UNP Q7MSJ8
K	712	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
K	713	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
K	714	SER	-	EXPRESSION TAG	UNP Q7MSJ8
K	715	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
K	716	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
K	717	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
K	718	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
K	719	GLU	-	EXPRESSION TAG	UNP Q7MSJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
K	720	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
L	691	SER	-	EXPRESSION TAG	UNP Q7MSJ8
L	692	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
L	693	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
L	694	SER	-	EXPRESSION TAG	UNP Q7MSJ8
L	695	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
L	696	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
L	697	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
L	698	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
L	699	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
L	700	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
L	701	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
L	702	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
L	703	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
L	704	SER	-	EXPRESSION TAG	UNP Q7MSJ8
L	705	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
L	706	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
L	707	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
L	708	SER	-	EXPRESSION TAG	UNP Q7MSJ8
L	709	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
L	710	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
L	711	SER	-	EXPRESSION TAG	UNP Q7MSJ8
L	712	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
L	713	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
L	714	SER	-	EXPRESSION TAG	UNP Q7MSJ8
L	715	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
L	716	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
L	717	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
L	718	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
L	719	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
L	720	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
G	691	SER	-	EXPRESSION TAG	UNP Q7MSJ8
G	692	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
G	693	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
G	694	SER	-	EXPRESSION TAG	UNP Q7MSJ8
G	695	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
G	696	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
G	697	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
G	698	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
G	699	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
G	700	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
G	701	GLY	-	EXPRESSION TAG	UNP Q7MSJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	702	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
G	703	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
G	704	SER	-	EXPRESSION TAG	UNP Q7MSJ8
G	705	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
G	706	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
G	707	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
G	708	SER	-	EXPRESSION TAG	UNP Q7MSJ8
G	709	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
G	710	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
G	711	SER	-	EXPRESSION TAG	UNP Q7MSJ8
G	712	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
G	713	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
G	714	SER	-	EXPRESSION TAG	UNP Q7MSJ8
G	715	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
G	716	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
G	717	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
G	718	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
G	719	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
G	720	LYS	-	EXPRESSION TAG	UNP Q7MSJ8

- Molecule 2 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

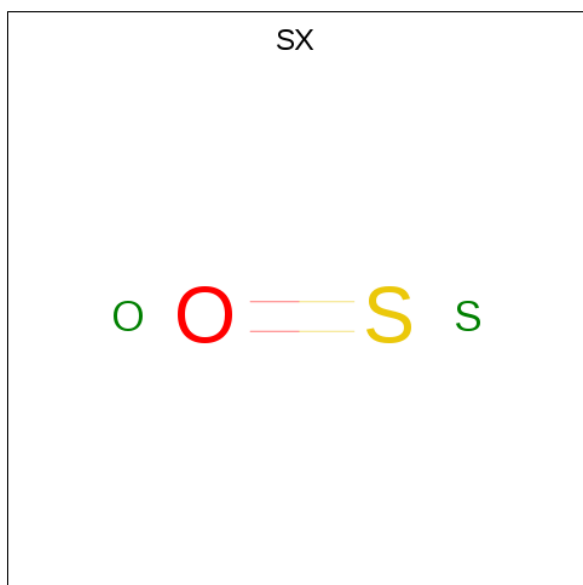
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Cu 1 1	0	0
2	J	1	Total Cu 1 1	0	0
2	D	1	Total Cu 1 1	0	0
2	K	1	Total Cu 1 1	0	0
2	E	1	Total Cu 1 1	0	0
2	H	1	Total Cu 1 1	0	0
2	B	1	Total Cu 1 1	0	0
2	I	1	Total Cu 1 1	0	0
2	C	1	Total Cu 1 1	0	0
2	A	1	Total Cu 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	L	1	Total	Cu	0	0
			1	1		
2	F	1	Total	Cu	0	0
			1	1		

- Molecule 3 is SULFUR OXIDE (three-letter code: SX) (formula: OS).



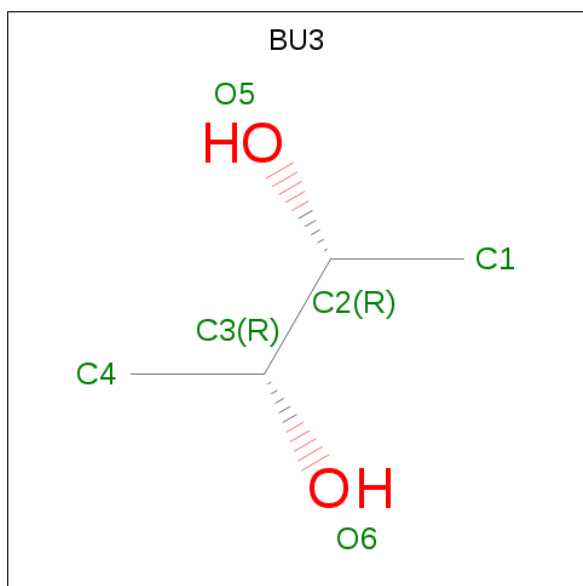
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			2	1	1		
3	B	1	Total	O	S	0	0
			2	1	1		
3	C	1	Total	O	S	0	0
			2	1	1		
3	E	1	Total	O	S	0	0
			2	1	1		
3	F	1	Total	O	S	0	0
			2	1	1		
3	H	1	Total	O	S	0	0
			2	1	1		
3	J	1	Total	O	S	0	0
			2	1	1		
3	K	1	Total	O	S	0	0
			2	1	1		
3	L	1	Total	O	S	0	0
			2	1	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	O	S	0	0
			2	1	1		

- Molecule 4 is (R,R)-2,3-BUTANEDIOL (three-letter code: BU3) (formula: C₄H₁₀O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	4	2		
4	A	1	Total	C	O	0	0
			6	4	2		
4	B	1	Total	C	O	0	0
			6	4	2		
4	B	1	Total	C	O	0	0
			6	4	2		
4	B	1	Total	C	O	0	0
			6	4	2		
4	C	1	Total	C	O	0	0
			6	4	2		
4	C	1	Total	C	O	0	0
			6	4	2		
4	D	1	Total	C	O	0	0
			6	4	2		
4	D	1	Total	C	O	0	0
			6	4	2		
4	E	1	Total	C	O	0	0
			6	4	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			6	4	2		
4	F	1	Total	C	O	0	0
			6	4	2		
4	F	1	Total	C	O	0	0
			6	4	2		
4	F	1	Total	C	O	0	0
			6	4	2		
4	H	1	Total	C	O	0	0
			6	4	2		
4	H	1	Total	C	O	0	0
			6	4	2		
4	H	1	Total	C	O	0	0
			6	4	2		
4	I	1	Total	C	O	0	0
			6	4	2		
4	I	1	Total	C	O	0	0
			6	4	2		
4	J	1	Total	C	O	0	0
			6	4	2		
4	J	1	Total	C	O	0	0
			6	4	2		
4	K	1	Total	C	O	0	0
			6	4	2		
4	K	1	Total	C	O	0	0
			6	4	2		
4	L	1	Total	C	O	0	0
			6	4	2		
4	L	1	Total	C	O	0	0
			6	4	2		
4	G	1	Total	C	O	0	0
			6	4	2		
4	G	1	Total	C	O	0	0
			6	4	2		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	I	1	Total	C	O	0	0
			4	2	2		
5	J	1	Total	C	O	0	0
			4	2	2		
5	K	1	Total	C	O	0	0
			4	2	2		
5	L	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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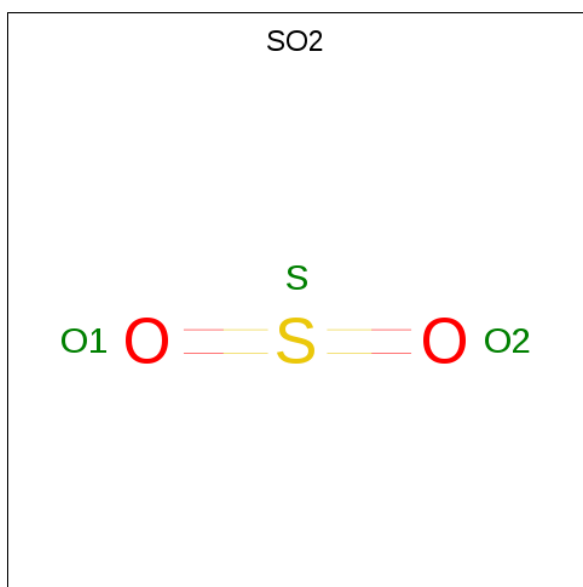
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 7 is SULFUR DIOXIDE (three-letter code: SO2) (formula: O₂S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			3	2	1		
7	D	1	Total	O	S	0	0
			3	2	1		
7	I	1	Total	O	S	0	0
			3	2	1		
7	G	1	Total	O	S	0	0
			3	2	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	416	Total	O	0	0
			416	416		
8	B	298	Total	O	0	0
			298	298		
8	C	285	Total	O	0	0
			285	285		
8	D	307	Total	O	0	0
			307	307		
8	E	219	Total	O	0	0
			219	219		
8	F	245	Total	O	0	0
			245	245		
8	H	250	Total	O	0	0
			250	250		
8	I	218	Total	O	0	0
			218	218		

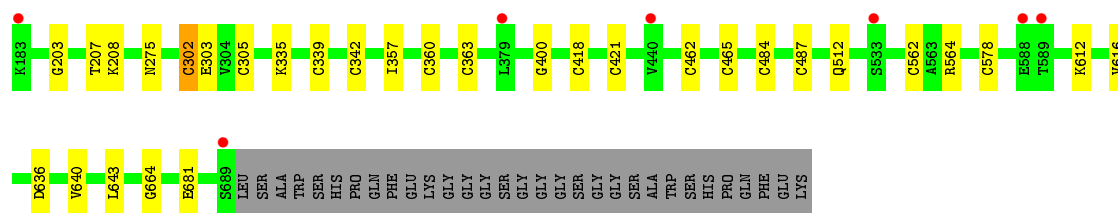
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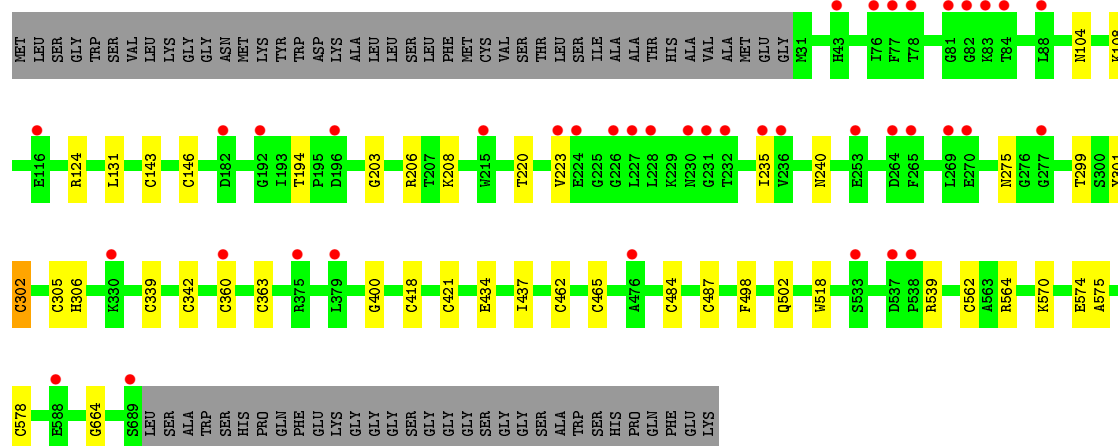
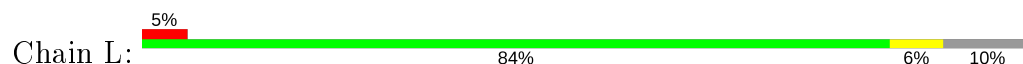
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	180	Total 180	O 180	0	0
8	K	158	Total 158	O 158	0	0
8	L	126	Total 126	O 126	0	0
8	G	232	Total 232	O 232	0	0

- Molecule 1: MccA

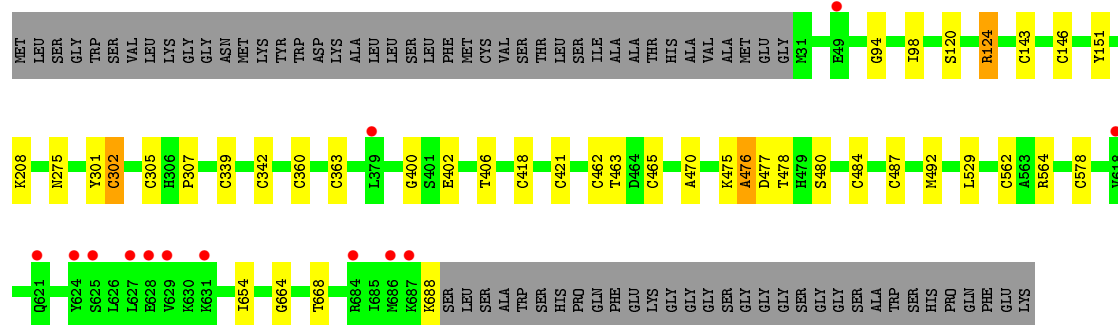
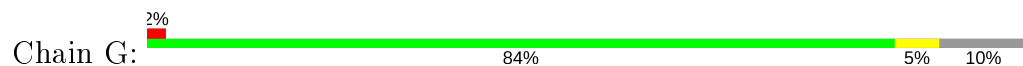




• Molecule 1: MccA



• Molecule 1: MccA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	211.12Å 103.04Å 233.07Å 90.00° 98.46° 90.00°	Depositor
Resolution (Å)	49.37 – 2.20 49.38 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.37-2.20) 99.8 (49.38-2.20)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.184 , 0.220 0.187 , 0.220	Depositor DCC
R_{free} test set	24857 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	70014	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SX, CU1, BU3, SO2, ACT, 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.34	0/5354	0.57	0/7212
1	B	0.32	0/5362	0.54	0/7223
1	C	0.32	0/5354	0.54	0/7212
1	D	0.32	0/5354	0.55	0/7212
1	E	0.31	0/5354	0.52	0/7212
1	F	0.31	0/5354	0.53	0/7212
1	G	0.31	0/5348	0.54	0/7204
1	H	0.31	0/5362	0.52	0/7223
1	I	0.32	0/5354	0.53	0/7212
1	J	0.30	0/5354	0.52	0/7212
1	K	0.31	0/5354	0.52	0/7212
1	L	0.30	0/5354	0.52	0/7212
All	All	0.31	0/64258	0.53	0/86558

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	5224	0	5051	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5232	0	5063	83	0
1	C	5224	0	5052	84	0
1	D	5224	0	5054	90	0
1	E	5224	0	5052	93	0
1	F	5224	0	5052	88	0
1	G	5218	0	5048	92	0
1	H	5232	0	5064	85	0
1	I	5224	0	5053	91	0
1	J	5224	0	5054	87	0
1	K	5224	0	5053	84	0
1	L	5224	0	5054	83	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
4	A	12	0	20	0	0
4	B	18	0	30	0	0
4	C	12	0	20	0	0
4	D	12	0	20	0	0
4	E	12	0	20	2	0
4	F	18	0	30	0	0
4	G	12	0	20	0	0
4	H	18	0	30	1	0
4	I	12	0	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	12	0	20	0	0
4	K	12	0	20	1	0
4	L	12	0	20	0	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
5	C	4	0	3	1	0
5	D	4	0	3	0	0
5	E	4	0	3	1	0
5	F	4	0	3	1	0
5	G	4	0	3	0	0
5	H	4	0	3	0	0
5	I	4	0	3	0	0
5	J	4	0	3	0	0
5	K	4	0	3	0	0
5	L	4	0	3	0	0
6	A	344	0	240	80	0
6	B	344	0	240	79	0
6	C	344	0	240	78	0
6	D	344	0	240	85	0
6	E	344	0	240	79	0
6	F	344	0	240	78	0
6	G	344	0	240	82	0
6	H	344	0	240	85	0
6	I	344	0	240	83	0
6	J	344	0	240	80	0
6	K	344	0	240	80	0
6	L	344	0	240	85	0
7	A	3	0	0	1	0
7	D	3	0	0	0	0
7	G	3	0	0	0	0
7	I	3	0	0	0	0
8	A	416	0	0	3	0
8	B	298	0	0	0	0
8	C	285	0	0	0	0
8	D	307	0	0	1	0
8	E	219	0	0	2	0
8	F	245	0	0	0	0
8	G	232	0	0	0	0
8	H	250	0	0	0	0
8	I	218	0	0	0	0
8	J	180	0	0	0	0
8	K	158	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	L	126	0	0	0	0
All	All	70014	0	63836	1090	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 8.

All (1090) 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:A:462:CYS:SG	6:A:811:HEM:HAB	1.41	1.55
1:J:143:CYS:SG	6:J:806:HEM:HAB	1.47	1.51
1:A:339:CYS:SG	6:A:808:HEM:CAB	2.04	1.46
1:A:462:CYS:SG	6:A:811:HEM:CAB	2.02	1.46
1:F:462:CYS:SG	6:F:812:HEM:CAB	2.03	1.46
1:A:484:CYS:SG	6:A:812:HEM:CAB	2.05	1.45
1:F:484:CYS:SG	6:F:813:HEM:CAB	2.04	1.45
1:C:462:CYS:SG	6:C:811:HEM:CAB	2.03	1.45
1:B:339:CYS:SG	6:B:809:HEM:CAB	2.05	1.44
1:I:462:CYS:SG	6:I:811:HEM:CAB	2.06	1.44
1:K:418:CYS:SG	6:K:810:HEM:CAB	2.06	1.44
1:C:418:CYS:SG	6:C:810:HEM:CAB	2.03	1.44
1:H:484:CYS:SG	6:H:813:HEM:CAB	2.04	1.44
1:G:462:CYS:SG	6:G:811:HEM:CAB	2.06	1.43
1:E:339:CYS:SG	6:E:808:HEM:CAB	2.06	1.43
1:B:484:CYS:SG	6:B:813:HEM:CAB	2.05	1.43
1:E:462:CYS:SG	6:E:811:HEM:CAB	2.05	1.43
1:D:484:CYS:SG	6:D:812:HEM:CAB	2.07	1.43
1:F:562:CYS:SG	6:F:814:HEM:CAB	2.07	1.43
1:K:143:CYS:SG	6:K:806:HEM:HAB	1.57	1.43
1:A:143:CYS:SG	6:A:806:HEM:CAB	2.07	1.42
1:D:418:CYS:SG	6:D:810:HEM:CAB	2.07	1.42
1:I:339:CYS:SG	6:I:808:HEM:CAB	2.07	1.42
1:F:143:CYS:SG	6:F:807:HEM:CAB	2.07	1.42
1:C:562:CYS:SG	6:C:813:HEM:CAB	2.08	1.42
1:E:484:CYS:SG	6:E:812:HEM:CAB	2.08	1.41
1:C:339:CYS:SG	6:C:808:HEM:CAB	2.08	1.41
1:G:418:CYS:SG	6:G:810:HEM:CAB	2.06	1.41
1:K:462:CYS:SG	6:K:811:HEM:CAB	2.09	1.41
1:D:562:CYS:SG	6:D:813:HEM:CAB	2.08	1.41
1:A:418:CYS:SG	6:A:810:HEM:CAB	2.07	1.41
1:C:360:CYS:SG	6:C:809:HEM:CAB	2.09	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:339:CYS:SG	6:G:808:HEM:CAB	2.09	1.40
1:A:562:CYS:SG	6:A:813:HEM:CAB	2.08	1.40
1:C:484:CYS:SG	6:C:812:HEM:CAB	2.09	1.40
1:E:418:CYS:SG	6:E:810:HEM:CAB	2.09	1.40
1:D:462:CYS:SG	6:D:811:HEM:CAB	2.09	1.40
1:B:562:CYS:SG	6:B:814:HEM:CAB	2.08	1.40
1:I:484:CYS:SG	6:I:812:HEM:CAB	2.10	1.40
1:L:339:CYS:SG	6:L:808:HEM:CAB	2.10	1.40
1:B:418:CYS:SG	6:B:811:HEM:CAB	2.08	1.39
1:G:562:CYS:SG	6:G:813:HEM:CAB	2.11	1.39
1:G:484:CYS:SG	6:G:812:HEM:CAB	2.11	1.39
1:B:143:CYS:SG	6:B:807:HEM:CAB	2.10	1.39
1:D:339:CYS:SG	6:D:808:HEM:CAB	2.09	1.39
1:H:562:CYS:SG	6:H:814:HEM:CAB	2.10	1.39
1:J:462:CYS:SG	6:J:811:HEM:CAB	2.10	1.39
1:B:462:CYS:SG	6:B:812:HEM:CAB	2.11	1.39
1:F:339:CYS:SG	6:F:809:HEM:CAB	2.10	1.39
1:G:143:CYS:HG	6:G:806:HEM:CAB	1.36	1.39
1:I:418:CYS:SG	6:I:810:HEM:CAB	2.09	1.39
1:J:339:CYS:SG	6:J:808:HEM:CAB	2.11	1.39
1:A:305:CYS:SG	6:A:807:HEM:CAC	2.11	1.39
1:I:363:CYS:SG	6:I:809:HEM:CAC	2.11	1.39
1:J:562:CYS:SG	6:J:813:HEM:CAB	2.11	1.39
1:E:562:CYS:SG	6:E:813:HEM:CAB	2.09	1.38
1:L:562:CYS:SG	6:L:813:HEM:CAB	2.11	1.38
1:K:339:CYS:SG	6:K:808:HEM:CAB	2.10	1.38
1:K:484:CYS:SG	6:K:812:HEM:CAB	2.11	1.38
1:G:143:CYS:SG	6:G:806:HEM:CAB	2.10	1.38
1:H:462:CYS:SG	6:H:812:HEM:CAB	2.09	1.38
1:D:143:CYS:SG	6:D:806:HEM:CAB	2.11	1.38
1:F:418:CYS:SG	6:F:811:HEM:CAB	2.12	1.38
1:H:562:CYS:HG	6:H:814:HEM:CAB	1.33	1.38
1:J:484:CYS:SG	6:J:812:HEM:CAB	2.12	1.37
1:I:562:CYS:SG	6:I:813:HEM:CAB	2.12	1.37
1:H:418:CYS:SG	6:H:811:HEM:CAB	2.11	1.37
1:J:418:CYS:SG	6:J:810:HEM:CAB	2.10	1.37
1:K:143:CYS:SG	6:K:806:HEM:CAB	2.10	1.37
1:C:143:CYS:SG	6:C:806:HEM:CAB	2.13	1.36
1:C:363:CYS:SG	6:C:809:HEM:CAC	2.14	1.36
1:A:363:CYS:SG	6:A:809:HEM:CAC	2.13	1.36
1:H:339:CYS:SG	6:H:809:HEM:CAB	2.14	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:363:CYS:SG	6:H:810:HEM:CAC	2.14	1.35
1:J:143:CYS:SG	6:J:806:HEM:CAB	2.12	1.35
1:K:562:CYS:SG	6:K:813:HEM:CAB	2.12	1.35
1:D:363:CYS:SG	6:D:809:HEM:CAC	2.14	1.35
1:L:484:CYS:SG	6:L:812:HEM:CAB	2.14	1.35
1:E:360:CYS:SG	6:E:809:HEM:CAB	2.13	1.35
1:B:360:CYS:SG	6:B:810:HEM:CAB	2.15	1.35
1:D:360:CYS:SG	6:D:809:HEM:CAB	2.15	1.34
1:L:418:CYS:SG	6:L:810:HEM:CAB	2.15	1.34
1:F:363:CYS:SG	6:F:810:HEM:CAC	2.14	1.34
1:L:143:CYS:SG	6:L:806:HEM:CAB	2.15	1.34
1:A:578:CYS:SG	6:A:813:HEM:CAC	2.15	1.34
1:E:363:CYS:SG	6:E:809:HEM:CAC	2.16	1.34
1:G:363:CYS:SG	6:G:809:HEM:CAC	2.16	1.34
1:H:143:CYS:SG	6:H:807:HEM:CAB	2.15	1.33
1:C:305:CYS:SG	6:C:807:HEM:CAC	2.16	1.33
1:K:363:CYS:SG	6:K:809:HEM:CAC	2.16	1.33
1:L:360:CYS:SG	6:L:809:HEM:CAB	2.17	1.33
1:B:363:CYS:SG	6:B:810:HEM:CAC	2.16	1.33
1:E:418:CYS:HG	6:E:810:HEM:CAB	1.40	1.32
1:E:143:CYS:SG	6:E:806:HEM:CAB	2.17	1.32
1:L:363:CYS:SG	6:L:809:HEM:CAC	2.16	1.32
1:E:305:CYS:SG	6:E:807:HEM:CAC	2.17	1.32
1:J:360:CYS:SG	6:J:809:HEM:CAB	2.18	1.31
1:K:360:CYS:SG	6:K:809:HEM:CAB	2.18	1.31
1:H:487:CYS:SG	6:H:813:HEM:CAC	2.18	1.31
1:F:360:CYS:SG	6:F:810:HEM:CAB	2.18	1.31
1:H:360:CYS:SG	6:H:810:HEM:CAB	2.18	1.31
1:A:487:CYS:SG	6:A:812:HEM:CAC	2.18	1.31
1:I:143:CYS:SG	6:I:806:HEM:CAB	2.18	1.31
1:J:305:CYS:SG	6:J:807:HEM:CAC	2.19	1.31
1:L:462:CYS:SG	6:L:811:HEM:CAB	2.19	1.31
1:A:360:CYS:SG	6:A:809:HEM:CAB	2.18	1.31
1:G:360:CYS:SG	6:G:809:HEM:CAB	2.19	1.31
1:H:305:CYS:SG	6:H:808:HEM:CAC	2.19	1.30
1:I:305:CYS:SG	6:I:807:HEM:CAC	2.19	1.30
1:I:360:CYS:SG	6:I:809:HEM:CAB	2.19	1.30
1:G:146:CYS:SG	6:G:806:HEM:CAC	2.18	1.30
1:J:363:CYS:SG	6:J:809:HEM:CAC	2.19	1.30
1:D:305:CYS:SG	6:D:807:HEM:CAC	2.19	1.30
1:F:578:CYS:SG	6:F:814:HEM:CAC	2.19	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:305:CYS:SG	6:K:807:HEM:CAC	2.20	1.30
1:D:487:CYS:SG	6:D:812:HEM:CAC	2.20	1.30
1:C:342:CYS:SG	6:C:808:HEM:CAC	2.19	1.30
1:E:578:CYS:SG	6:E:813:HEM:CAC	2.19	1.29
1:F:342:CYS:SG	6:F:809:HEM:CAC	2.19	1.29
1:I:342:CYS:SG	6:I:808:HEM:CAC	2.20	1.29
1:C:146:CYS:SG	6:C:806:HEM:CAC	2.20	1.29
1:F:146:CYS:SG	6:F:807:HEM:CAC	2.20	1.29
1:B:305:CYS:SG	6:B:808:HEM:CAC	2.18	1.29
1:G:487:CYS:SG	6:G:812:HEM:CAC	2.21	1.29
1:E:487:CYS:SG	6:E:812:HEM:CAC	2.20	1.29
1:I:465:CYS:SG	6:I:811:HEM:CAC	2.21	1.29
1:K:487:CYS:SG	6:K:812:HEM:CAC	2.21	1.29
1:B:487:CYS:SG	6:B:813:HEM:CAC	2.21	1.29
1:H:465:CYS:SG	6:H:812:HEM:CAC	2.21	1.28
1:F:487:CYS:SG	6:F:813:HEM:CAC	2.22	1.28
1:A:146:CYS:SG	6:A:806:HEM:CAC	2.22	1.28
1:C:487:CYS:SG	6:C:812:HEM:CAC	2.20	1.28
1:H:578:CYS:HG	6:H:814:HEM:CAC	1.46	1.28
1:E:146:CYS:SG	6:E:806:HEM:CAC	2.22	1.28
1:G:465:CYS:SG	6:G:811:HEM:CAC	2.22	1.28
1:H:578:CYS:SG	6:H:814:HEM:CAC	2.20	1.28
1:J:578:CYS:SG	6:J:813:HEM:CAC	2.22	1.28
1:D:342:CYS:SG	6:D:808:HEM:CAC	2.22	1.28
1:D:363:CYS:HG	6:D:809:HEM:CAC	1.47	1.28
1:K:363:CYS:HG	6:K:809:HEM:CAC	1.42	1.28
1:B:465:CYS:SG	6:B:812:HEM:CAC	2.22	1.28
1:B:342:CYS:SG	6:B:809:HEM:CAC	2.22	1.27
1:E:363:CYS:HG	6:E:809:HEM:CAC	1.46	1.27
1:J:487:CYS:SG	6:J:812:HEM:CAC	2.22	1.27
1:K:578:CYS:SG	6:K:813:HEM:CAC	2.21	1.27
1:L:487:CYS:SG	6:L:812:HEM:CAC	2.22	1.27
1:K:465:CYS:SG	6:K:811:HEM:CAC	2.21	1.27
1:C:465:CYS:SG	6:C:811:HEM:CAC	2.23	1.27
1:K:146:CYS:SG	6:K:806:HEM:CAC	2.22	1.27
1:E:465:CYS:SG	6:E:811:HEM:CAC	2.23	1.27
1:I:487:CYS:SG	6:I:812:HEM:CAC	2.22	1.27
1:I:421:CYS:SG	6:I:810:HEM:CAC	2.23	1.27
1:A:421:CYS:SG	6:A:810:HEM:CAC	2.22	1.27
1:H:421:CYS:HG	6:H:811:HEM:CAC	1.45	1.27
1:J:146:CYS:SG	6:J:806:HEM:CAC	2.22	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:578:CYS:SG	6:D:813:HEM:CAC	2.21	1.27
1:D:146:CYS:SG	6:D:806:HEM:CAC	2.22	1.26
1:L:578:CYS:SG	6:L:813:HEM:HAC	1.73	1.26
1:L:146:CYS:SG	6:L:806:HEM:CAC	2.23	1.26
1:F:305:CYS:SG	6:F:808:HEM:CAC	2.23	1.26
1:L:342:CYS:SG	6:L:808:HEM:CAC	2.23	1.26
1:J:342:CYS:SG	6:J:808:HEM:CAC	2.22	1.26
1:L:305:CYS:SG	6:L:807:HEM:CAC	2.22	1.26
1:B:578:CYS:SG	6:B:814:HEM:CAC	2.24	1.26
1:L:578:CYS:SG	6:L:813:HEM:CAC	2.22	1.26
1:D:465:CYS:SG	6:D:811:HEM:CAC	2.24	1.26
1:K:342:CYS:SG	6:K:808:HEM:CAC	2.22	1.26
1:G:305:CYS:SG	6:G:807:HEM:CAC	2.23	1.25
1:B:146:CYS:SG	6:B:807:HEM:CAC	2.22	1.25
1:G:342:CYS:SG	6:G:808:HEM:CAC	2.23	1.25
1:I:146:CYS:SG	6:I:806:HEM:CAC	2.23	1.25
1:D:421:CYS:SG	6:D:810:HEM:CAC	2.24	1.25
1:I:578:CYS:SG	6:I:813:HEM:CAC	2.23	1.25
1:L:465:CYS:SG	6:L:811:HEM:CAC	2.24	1.25
1:F:465:CYS:SG	6:F:812:HEM:CAC	2.24	1.25
1:H:342:CYS:SG	6:H:809:HEM:CAC	2.24	1.25
1:H:421:CYS:SG	6:H:811:HEM:CAC	2.25	1.25
1:F:421:CYS:SG	6:F:811:HEM:CAC	2.25	1.24
1:J:465:CYS:SG	6:J:811:HEM:CAC	2.24	1.24
1:A:342:CYS:SG	6:A:808:HEM:CAC	2.24	1.24
1:L:421:CYS:SG	6:L:810:HEM:CAC	2.25	1.23
7:A:814:SO2:O1	8:A:1232:HOH:O	1.55	1.23
1:E:342:CYS:SG	6:E:808:HEM:CAC	2.26	1.23
1:H:146:CYS:SG	6:H:807:HEM:CAC	2.26	1.23
1:J:421:CYS:SG	6:J:810:HEM:CAC	2.27	1.23
1:A:465:CYS:SG	6:A:811:HEM:CAC	2.26	1.23
1:C:578:CYS:SG	6:C:813:HEM:CAC	2.25	1.23
1:A:487:CYS:HG	6:A:812:HEM:CAC	1.47	1.22
1:E:421:CYS:SG	6:E:810:HEM:CAC	2.27	1.22
1:G:578:CYS:SG	6:G:813:HEM:CAC	2.27	1.22
1:G:421:CYS:SG	6:G:810:HEM:CAC	2.27	1.22
1:C:421:CYS:SG	6:C:810:HEM:CAC	2.27	1.22
1:B:421:CYS:SG	6:B:811:HEM:CAC	2.27	1.22
1:K:302:CYS:SG	6:K:807:HEM:CAB	2.27	1.21
1:K:421:CYS:SG	6:K:810:HEM:CAC	2.29	1.21
1:H:487:CYS:HG	6:H:813:HEM:CAC	1.51	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:462:CYS:HG	6:L:811:HEM:CAB	1.50	1.19
1:H:302:CYS:SG	6:H:808:HEM:CAB	2.30	1.19
1:J:487:CYS:SG	6:J:812:HEM:CBC	2.31	1.19
1:K:462:CYS:HG	6:K:811:HEM:CAB	1.47	1.19
1:D:302:CYS:SG	6:D:807:HEM:CAB	2.31	1.18
1:L:302:CYS:SG	6:L:807:HEM:CAB	2.31	1.18
1:K:302:CYS:SG	6:K:807:HEM:C3B	2.37	1.18
1:D:339:CYS:SG	6:D:808:HEM:HAB	1.73	1.18
1:J:360:CYS:HG	6:J:809:HEM:CAB	1.55	1.18
1:G:360:CYS:HG	6:G:809:HEM:CAB	1.54	1.17
1:J:302:CYS:SG	6:J:807:HEM:CAB	2.33	1.17
1:E:562:CYS:HG	6:E:813:HEM:CAB	1.47	1.17
1:F:302:CYS:SG	6:F:808:HEM:CAB	2.34	1.16
1:C:339:CYS:HG	6:C:808:HEM:CAB	1.53	1.16
1:C:302:CYS:SG	6:C:807:HEM:CAB	2.33	1.16
1:F:418:CYS:HG	6:F:811:HEM:CAB	1.55	1.15
1:A:302:CYS:SG	6:A:807:HEM:CAB	2.34	1.15
1:B:302:CYS:SG	6:B:808:HEM:CAB	2.35	1.15
1:A:363:CYS:HG	6:A:809:HEM:CAC	1.55	1.14
1:A:562:CYS:HG	6:A:813:HEM:CAB	1.53	1.14
1:E:302:CYS:SG	6:E:807:HEM:CAB	2.36	1.13
1:I:302:CYS:SG	6:I:807:HEM:CAB	2.37	1.13
1:K:418:CYS:SG	6:K:810:HEM:CBB	2.36	1.12
1:J:562:CYS:HG	6:J:813:HEM:CAB	1.52	1.12
1:F:143:CYS:SG	6:F:807:HEM:CBB	2.36	1.12
1:H:578:CYS:SG	6:H:814:HEM:CBC	2.39	1.11
1:C:339:CYS:SG	6:C:808:HEM:HAB	1.83	1.11
1:I:418:CYS:HG	6:I:810:HEM:CAB	1.50	1.11
1:G:302:CYS:SG	6:G:807:HEM:CAB	2.39	1.11
1:I:465:CYS:HG	6:I:811:HEM:CAC	1.57	1.09
1:H:462:CYS:SG	6:H:812:HEM:CBB	2.41	1.08
1:J:363:CYS:HG	6:J:809:HEM:CAC	1.61	1.08
1:K:462:CYS:SG	6:K:811:HEM:CBB	2.41	1.08
1:K:578:CYS:SG	6:K:813:HEM:CBC	2.42	1.07
1:C:462:CYS:SG	6:C:811:HEM:CBB	2.43	1.07
1:H:484:CYS:SG	6:H:813:HEM:CBB	2.43	1.07
1:L:487:CYS:SG	6:L:812:HEM:CBC	2.43	1.06
1:L:462:CYS:SG	6:L:811:HEM:HAB	1.94	1.06
1:E:360:CYS:HG	6:E:809:HEM:CAB	1.57	1.06
1:F:484:CYS:SG	6:F:813:HEM:HAB	1.92	1.05
1:B:360:CYS:HG	6:B:810:HEM:CAB	1.60	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:CYS:SG	6:B:814:HEM:CBC	2.44	1.05
1:C:418:CYS:SG	6:C:810:HEM:CBB	2.44	1.05
1:I:339:CYS:HG	6:I:808:HEM:CAB	1.56	1.05
1:J:302:CYS:SG	6:J:807:HEM:C3B	2.50	1.05
1:L:570:LYS:NZ	1:L:574:GLU:OE2	1.87	1.05
1:F:462:CYS:SG	6:F:812:HEM:CBB	2.44	1.04
1:C:562:CYS:SG	6:C:813:HEM:CBB	2.45	1.04
1:J:305:CYS:SG	6:J:807:HEM:CBC	2.45	1.04
1:J:462:CYS:SG	6:J:811:HEM:CBB	2.46	1.04
1:L:146:CYS:SG	6:L:806:HEM:CBC	2.44	1.04
1:B:305:CYS:SG	6:B:808:HEM:CBC	2.46	1.04
1:D:360:CYS:HG	6:D:809:HEM:CAB	1.61	1.04
1:I:462:CYS:SG	6:I:811:HEM:CBB	2.44	1.04
1:L:562:CYS:SG	6:L:813:HEM:CBB	2.45	1.03
1:D:339:CYS:HG	6:D:808:HEM:CAB	1.59	1.03
1:H:302:CYS:SG	6:H:808:HEM:C3B	2.50	1.03
1:K:484:CYS:SG	6:K:812:HEM:CBB	2.46	1.03
1:K:562:CYS:SG	6:K:813:HEM:CBB	2.46	1.03
1:J:146:CYS:SG	6:J:806:HEM:CBC	2.47	1.02
1:I:562:CYS:SG	6:I:813:HEM:CBB	2.47	1.02
1:A:143:CYS:SG	6:A:806:HEM:HAB	1.93	1.02
1:D:302:CYS:SG	6:D:807:HEM:C3B	2.52	1.02
1:I:302:CYS:SG	6:I:807:HEM:C3B	2.53	1.02
1:L:302:CYS:SG	6:L:807:HEM:C3B	2.52	1.02
1:I:339:CYS:SG	6:I:808:HEM:HAB	2.00	1.02
1:L:305:CYS:SG	6:L:807:HEM:CBC	2.47	1.02
1:D:487:CYS:SG	6:D:812:HEM:CBC	2.48	1.01
1:F:360:CYS:HG	6:F:810:HEM:CAB	1.69	1.01
1:E:484:CYS:SG	6:E:812:HEM:CBB	2.47	1.01
1:E:418:CYS:SG	6:E:810:HEM:CBB	2.49	1.01
1:J:418:CYS:SG	6:J:810:HEM:CBB	2.48	1.01
1:I:363:CYS:HG	6:I:809:HEM:CAC	1.69	1.01
1:C:302:CYS:SG	6:C:807:HEM:C3B	2.53	1.01
1:B:462:CYS:SG	6:B:812:HEM:CBB	2.48	1.01
1:A:418:CYS:SG	6:A:810:HEM:HAB	1.95	1.00
1:I:418:CYS:SG	6:I:810:HEM:CBB	2.48	1.00
1:F:339:CYS:SG	6:F:809:HEM:HAB	1.96	1.00
1:D:562:CYS:SG	6:D:813:HEM:CBB	2.49	1.00
1:B:562:CYS:SG	6:B:814:HEM:CBB	2.50	1.00
1:C:363:CYS:HG	6:C:809:HEM:CAC	1.63	1.00
1:G:487:CYS:SG	6:G:812:HEM:CBC	2.49	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:462:CYS:SG	6:G:811:HEM:CBB	2.50	1.00
1:E:462:CYS:SG	6:E:811:HEM:CBB	2.48	1.00
1:L:418:CYS:SG	6:L:810:HEM:CBB	2.49	0.99
1:C:143:CYS:SG	6:C:806:HEM:HAB	1.99	0.99
1:E:305:CYS:SG	6:E:807:HEM:CBC	2.50	0.99
1:F:418:CYS:SG	6:F:811:HEM:HAB	2.01	0.99
1:B:302:CYS:SG	6:B:808:HEM:C3B	2.55	0.99
1:E:465:CYS:SG	6:E:811:HEM:CBC	2.50	0.99
1:C:305:CYS:SG	6:C:807:HEM:CBC	2.51	0.99
1:D:418:CYS:SG	6:D:810:HEM:HAB	2.01	0.99
1:H:578:CYS:HG	6:H:814:HEM:CBC	1.74	0.99
1:L:339:CYS:SG	6:L:808:HEM:CBB	2.51	0.99
1:H:487:CYS:SG	6:H:813:HEM:CBC	2.51	0.99
1:A:484:CYS:SG	6:A:812:HEM:CBB	2.51	0.99
1:A:578:CYS:SG	6:A:813:HEM:CBC	2.51	0.99
1:B:484:CYS:SG	6:B:813:HEM:CBB	2.49	0.99
1:E:302:CYS:SG	6:E:807:HEM:C3B	2.56	0.99
1:G:562:CYS:SG	6:G:813:HEM:CBB	2.51	0.99
1:A:339:CYS:SG	6:A:808:HEM:HAB	1.99	0.98
1:L:363:CYS:HG	6:L:809:HEM:CAC	1.65	0.98
1:B:339:CYS:SG	6:B:809:HEM:HAB	2.02	0.98
1:K:342:CYS:SG	6:K:808:HEM:CBC	2.51	0.98
1:A:418:CYS:HG	6:A:810:HEM:CAB	1.63	0.98
1:E:487:CYS:SG	6:E:812:HEM:CBC	2.51	0.97
1:G:146:CYS:SG	6:G:806:HEM:CBC	2.51	0.97
1:H:418:CYS:HG	6:H:811:HEM:CAB	1.66	0.97
1:H:360:CYS:HG	6:H:810:HEM:CAB	1.69	0.97
1:I:360:CYS:HG	6:I:809:HEM:CAB	1.69	0.97
1:B:418:CYS:SG	6:B:811:HEM:HAB	2.02	0.97
1:D:484:CYS:SG	6:D:812:HEM:CBB	2.53	0.97
1:E:339:CYS:SG	6:E:808:HEM:CBB	2.53	0.97
1:G:418:CYS:SG	6:G:810:HEM:HAB	2.03	0.97
1:H:339:CYS:SG	6:H:809:HEM:HAB	2.05	0.97
1:K:339:CYS:SG	6:K:808:HEM:HAB	2.05	0.97
1:F:562:CYS:SG	6:F:814:HEM:CBB	2.51	0.96
1:G:339:CYS:SG	6:G:808:HEM:CBB	2.53	0.96
1:B:487:CYS:SG	6:B:813:HEM:CBC	2.53	0.96
1:F:578:CYS:SG	6:F:814:HEM:CBC	2.53	0.96
1:A:484:CYS:SG	6:A:812:HEM:HAB	2.03	0.96
1:L:360:CYS:HG	6:L:809:HEM:CAB	1.70	0.96
1:D:462:CYS:SG	6:D:811:HEM:CBB	2.54	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:302:CYS:SG	6:F:808:HEM:C3B	2.59	0.95
1:G:143:CYS:SG	6:G:806:HEM:HAB	2.06	0.95
1:H:484:CYS:SG	6:H:813:HEM:HAB	2.06	0.95
1:L:421:CYS:SG	6:L:810:HEM:CBC	2.53	0.95
1:D:146:CYS:SG	6:D:806:HEM:CBC	2.54	0.95
1:I:484:CYS:SG	6:I:812:HEM:HAB	2.04	0.95
1:K:305:CYS:SG	6:K:807:HEM:CBC	2.53	0.95
1:G:484:CYS:SG	6:G:812:HEM:CBB	2.54	0.95
1:G:418:CYS:SG	6:G:810:HEM:CBB	2.53	0.95
1:H:487:CYS:HG	6:H:813:HEM:CBC	1.78	0.95
1:J:339:CYS:SG	6:J:808:HEM:HAB	2.07	0.95
1:L:484:CYS:SG	6:L:812:HEM:CBB	2.54	0.95
1:B:465:CYS:SG	6:B:812:HEM:CBC	2.54	0.95
1:E:578:CYS:SG	6:E:813:HEM:CBC	2.54	0.95
1:A:305:CYS:SG	6:A:807:HEM:C3C	2.60	0.95
1:A:302:CYS:SG	6:A:807:HEM:C3B	2.59	0.95
1:C:462:CYS:SG	6:C:811:HEM:HAB	2.06	0.95
1:J:484:CYS:SG	6:J:812:HEM:CBB	2.54	0.95
1:A:339:CYS:SG	6:A:808:HEM:CBB	2.55	0.95
1:C:465:CYS:SG	6:C:811:HEM:CBC	2.54	0.95
1:D:418:CYS:HG	6:D:810:HEM:CAB	1.59	0.95
1:B:484:CYS:SG	6:B:813:HEM:HAB	2.05	0.94
1:D:484:CYS:SG	6:D:812:HEM:HAB	2.03	0.94
1:G:339:CYS:SG	6:G:808:HEM:HAB	2.05	0.94
1:B:143:CYS:SG	6:B:807:HEM:HAB	2.05	0.94
1:F:487:CYS:SG	6:F:813:HEM:CBC	2.55	0.94
1:C:484:CYS:SG	6:C:812:HEM:HAB	2.05	0.94
1:D:578:CYS:SG	6:D:813:HEM:CBC	2.54	0.94
1:B:363:CYS:SG	6:B:810:HEM:CBC	2.55	0.94
1:D:143:CYS:SG	6:D:806:HEM:HAB	2.05	0.94
1:H:418:CYS:SG	6:H:811:HEM:CBB	2.55	0.94
1:J:562:CYS:SG	6:J:813:HEM:CBB	2.54	0.94
1:K:487:CYS:SG	6:K:812:HEM:CBC	2.56	0.94
1:B:418:CYS:HG	6:B:811:HEM:CAB	1.62	0.94
1:L:339:CYS:SG	6:L:808:HEM:HAB	2.06	0.93
1:C:418:CYS:SG	6:C:810:HEM:HAB	2.06	0.93
1:F:462:CYS:SG	6:F:812:HEM:HAB	2.05	0.93
1:A:360:CYS:HG	6:A:809:HEM:CAB	1.68	0.93
1:E:143:CYS:SG	6:E:806:HEM:HAB	2.09	0.93
1:G:305:CYS:SG	6:G:807:HEM:CBC	2.56	0.93
1:G:462:CYS:SG	6:G:811:HEM:HAB	2.08	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:339:CYS:SG	6:E:808:HEM:HAB	2.06	0.93
1:J:578:CYS:SG	6:J:813:HEM:CBC	2.56	0.92
1:D:305:CYS:SG	6:D:807:HEM:CBC	2.57	0.92
1:F:562:CYS:SG	6:F:814:HEM:HAB	2.07	0.92
1:H:421:CYS:HG	6:H:811:HEM:CBC	1.80	0.92
1:I:578:CYS:SG	6:I:813:HEM:CBC	2.57	0.92
1:H:143:CYS:SG	6:H:807:HEM:HAB	2.06	0.92
1:I:146:CYS:SG	6:I:806:HEM:CBC	2.57	0.92
1:H:146:CYS:SG	6:H:807:HEM:CBC	2.58	0.92
1:J:484:CYS:SG	6:J:812:HEM:HAB	2.09	0.92
1:H:360:CYS:SG	6:H:810:HEM:CBB	2.58	0.92
1:H:418:CYS:SG	6:H:811:HEM:HAB	2.10	0.92
1:B:421:CYS:SG	6:B:811:HEM:CBC	2.58	0.92
1:C:305:CYS:SG	6:C:807:HEM:C3C	2.63	0.92
1:A:305:CYS:SG	6:A:807:HEM:CBC	2.57	0.91
1:B:143:CYS:SG	6:B:807:HEM:CBB	2.58	0.91
1:C:578:CYS:SG	6:C:813:HEM:CBC	2.57	0.91
1:H:363:CYS:SG	6:H:810:HEM:CBC	2.58	0.91
1:I:339:CYS:SG	6:I:808:HEM:CBB	2.57	0.91
1:F:465:CYS:SG	6:F:812:HEM:CBC	2.57	0.91
1:G:143:CYS:SG	6:G:806:HEM:CBB	2.58	0.91
1:G:484:CYS:SG	6:G:812:HEM:HAB	2.09	0.91
1:I:484:CYS:SG	6:I:812:HEM:CBB	2.57	0.91
1:B:339:CYS:SG	6:B:809:HEM:CBB	2.57	0.91
1:H:465:CYS:SG	6:H:812:HEM:CBC	2.59	0.91
1:F:305:CYS:SG	6:F:808:HEM:CBC	2.59	0.91
1:H:305:CYS:SG	6:H:808:HEM:C3C	2.64	0.91
1:E:562:CYS:SG	6:E:813:HEM:CBB	2.58	0.91
1:I:487:CYS:SG	6:I:812:HEM:CBC	2.59	0.91
1:A:487:CYS:SG	6:A:812:HEM:CBC	2.58	0.90
1:D:465:CYS:SG	6:D:811:HEM:CBC	2.59	0.90
1:B:418:CYS:SG	6:B:811:HEM:CBB	2.60	0.90
1:D:418:CYS:SG	6:D:810:HEM:CBB	2.59	0.90
1:J:339:CYS:SG	6:J:808:HEM:CBB	2.58	0.90
1:C:342:CYS:SG	6:C:808:HEM:CBC	2.59	0.90
1:K:360:CYS:HG	6:K:809:HEM:CAB	1.74	0.90
1:D:562:CYS:SG	6:D:813:HEM:HAB	2.12	0.90
1:C:487:CYS:SG	6:C:812:HEM:CBC	2.59	0.90
1:E:462:CYS:SG	6:E:811:HEM:HAB	2.10	0.90
1:E:562:CYS:SG	6:E:813:HEM:HAB	2.11	0.90
1:I:143:CYS:SG	6:I:806:HEM:CBB	2.60	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:342:CYS:SG	6:L:808:HEM:CBC	2.58	0.90
1:G:478:THR:O	6:G:813:HEM:O2D	1.88	0.90
1:K:339:CYS:SG	6:K:808:HEM:CBB	2.58	0.89
1:H:562:CYS:SG	6:H:814:HEM:CBB	2.60	0.89
1:K:143:CYS:HG	6:K:806:HEM:HAB	1.12	0.89
1:K:465:CYS:SG	6:K:811:HEM:CBC	2.60	0.89
1:A:562:CYS:SG	6:A:813:HEM:CBB	2.60	0.89
1:I:305:CYS:SG	6:I:807:HEM:CBC	2.60	0.89
1:I:418:CYS:SG	6:I:810:HEM:HAB	2.12	0.89
1:A:465:CYS:SG	6:A:811:HEM:CBC	2.59	0.89
1:D:143:CYS:SG	6:D:806:HEM:CBB	2.59	0.89
1:H:421:CYS:SG	6:H:811:HEM:CBC	2.61	0.89
1:I:363:CYS:SG	6:I:809:HEM:C3C	2.65	0.89
1:J:462:CYS:SG	6:J:811:HEM:HAB	2.13	0.89
1:C:363:CYS:SG	6:C:809:HEM:HAC	2.12	0.89
1:E:146:CYS:SG	6:E:806:HEM:CBC	2.61	0.89
1:I:462:CYS:SG	6:I:811:HEM:HAB	2.11	0.89
1:J:418:CYS:SG	6:J:810:HEM:HAB	2.09	0.89
1:L:143:CYS:SG	6:L:806:HEM:CBB	2.61	0.89
1:E:421:CYS:SG	6:E:810:HEM:CBC	2.61	0.88
1:G:302:CYS:SG	6:G:807:HEM:C3B	2.66	0.88
1:D:360:CYS:SG	6:D:809:HEM:CBB	2.61	0.88
1:F:418:CYS:SG	6:F:811:HEM:CBB	2.62	0.88
1:E:484:CYS:SG	6:E:812:HEM:HAB	2.09	0.88
1:D:462:CYS:SG	6:D:811:HEM:HAB	2.11	0.88
1:H:562:CYS:HG	6:H:814:HEM:CBB	1.87	0.88
1:D:363:CYS:SG	6:D:809:HEM:CBC	2.60	0.88
1:E:418:CYS:SG	6:E:810:HEM:HAB	2.10	0.88
1:A:487:CYS:HG	6:A:812:HEM:CBC	1.88	0.88
1:I:363:CYS:SG	6:I:809:HEM:HAC	2.14	0.88
1:B:146:CYS:SG	6:B:807:HEM:CBC	2.62	0.87
1:G:143:CYS:HG	6:G:806:HEM:CBB	1.87	0.87
1:G:421:CYS:SG	6:G:810:HEM:CBC	2.61	0.87
1:H:462:CYS:SG	6:H:812:HEM:HAB	2.13	0.87
1:K:146:CYS:SG	6:K:806:HEM:CBC	2.61	0.87
1:F:146:CYS:SG	6:F:807:HEM:CBC	2.62	0.87
1:G:562:CYS:SG	6:G:813:HEM:HAB	2.14	0.87
1:D:305:CYS:SG	6:D:807:HEM:C3C	2.68	0.87
1:I:562:CYS:SG	6:I:813:HEM:HAB	2.15	0.87
1:L:143:CYS:SG	6:L:806:HEM:HAB	2.11	0.87
1:B:305:CYS:SG	6:B:808:HEM:C3C	2.68	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:339:CYS:HG	6:I:808:HEM:CBB	1.86	0.87
1:A:562:CYS:SG	6:A:813:HEM:HAB	2.11	0.87
1:A:143:CYS:SG	6:A:806:HEM:CBB	2.62	0.87
1:E:305:CYS:SG	6:E:807:HEM:C3C	2.68	0.86
1:H:363:CYS:SG	6:H:810:HEM:C3C	2.68	0.86
1:J:305:CYS:SG	6:J:807:HEM:C3C	2.67	0.86
1:A:363:CYS:SG	6:A:809:HEM:CBC	2.62	0.86
1:H:143:CYS:SG	6:H:807:HEM:CBB	2.62	0.86
1:J:421:CYS:SG	6:J:810:HEM:CBC	2.64	0.86
1:C:146:CYS:SG	6:C:806:HEM:CBC	2.63	0.86
1:F:484:CYS:SG	6:F:813:HEM:CBB	2.63	0.86
1:I:305:CYS:SG	6:I:807:HEM:C3C	2.68	0.86
1:A:342:CYS:SG	6:A:808:HEM:CBC	2.62	0.86
1:G:578:CYS:SG	6:G:813:HEM:CBC	2.64	0.86
1:J:342:CYS:SG	6:J:808:HEM:CBC	2.64	0.86
1:D:302:CYS:HG	6:D:807:HEM:CAB	1.83	0.86
1:G:342:CYS:SG	6:G:808:HEM:CBC	2.63	0.86
1:E:418:CYS:HG	6:E:810:HEM:CBB	1.85	0.86
1:G:465:CYS:SG	6:G:811:HEM:C3C	2.69	0.86
1:K:484:CYS:SG	6:K:812:HEM:HAB	2.15	0.86
1:F:363:CYS:SG	6:F:810:HEM:CBC	2.64	0.85
1:H:562:CYS:SG	6:H:814:HEM:HAB	2.11	0.85
1:K:305:CYS:SG	6:K:807:HEM:C3C	2.69	0.85
1:A:363:CYS:HG	6:A:809:HEM:CBC	1.88	0.85
1:F:305:CYS:SG	6:F:808:HEM:C3C	2.70	0.85
1:B:342:CYS:SG	6:B:809:HEM:CBC	2.64	0.85
1:C:360:CYS:SG	6:C:809:HEM:HAB	2.17	0.85
1:B:562:CYS:SG	6:B:814:HEM:HAB	2.16	0.85
1:D:342:CYS:SG	6:D:808:HEM:CBC	2.63	0.85
1:L:360:CYS:SG	6:L:809:HEM:CBB	2.64	0.85
1:A:418:CYS:SG	6:A:810:HEM:CBB	2.65	0.84
1:K:360:CYS:SG	6:K:809:HEM:CBB	2.64	0.84
1:C:360:CYS:SG	6:C:809:HEM:CBB	2.65	0.84
1:F:363:CYS:SG	6:F:810:HEM:HAC	2.16	0.84
1:C:562:CYS:SG	6:C:813:HEM:HAB	2.15	0.84
1:B:302:CYS:HG	6:B:808:HEM:CAB	1.84	0.84
1:E:360:CYS:SG	6:E:809:HEM:CBB	2.64	0.84
1:F:360:CYS:SG	6:F:810:HEM:CBB	2.64	0.84
1:H:305:CYS:SG	6:H:808:HEM:CBC	2.65	0.84
1:L:465:CYS:SG	6:L:811:HEM:CBC	2.65	0.84
1:D:363:CYS:SG	6:D:809:HEM:C3C	2.68	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:363:CYS:SG	6:L:809:HEM:C3C	2.68	0.84
1:L:484:CYS:SG	6:L:812:HEM:HAB	2.18	0.84
1:C:484:CYS:SG	6:C:812:HEM:CBB	2.64	0.84
1:I:465:CYS:SG	6:I:811:HEM:CBC	2.65	0.84
1:E:363:CYS:SG	6:E:809:HEM:CBC	2.66	0.83
1:A:146:CYS:SG	6:A:806:HEM:CBC	2.66	0.83
1:D:363:CYS:HG	6:D:809:HEM:CBC	1.90	0.83
1:C:363:CYS:SG	6:C:809:HEM:C3C	2.70	0.83
1:G:363:CYS:SG	6:G:809:HEM:C3C	2.70	0.83
1:A:421:CYS:SG	6:A:810:HEM:CBC	2.66	0.83
1:G:302:CYS:HG	6:G:807:HEM:CAB	1.88	0.83
1:J:465:CYS:SG	6:J:811:HEM:CBC	2.65	0.83
1:L:418:CYS:SG	6:L:810:HEM:HAB	2.16	0.83
1:E:363:CYS:SG	6:E:809:HEM:C3C	2.70	0.83
1:B:462:CYS:SG	6:B:812:HEM:HAB	2.14	0.83
1:F:421:CYS:SG	6:F:811:HEM:CBC	2.68	0.82
1:F:342:CYS:SG	6:F:809:HEM:CBC	2.67	0.82
1:A:360:CYS:SG	6:A:809:HEM:CBB	2.67	0.82
1:C:360:CYS:SG	6:C:809:HEM:C3B	2.66	0.82
1:H:342:CYS:SG	6:H:809:HEM:CBC	2.67	0.82
1:B:360:CYS:SG	6:B:810:HEM:CBB	2.66	0.82
1:F:143:CYS:SG	6:F:807:HEM:HAB	2.17	0.82
1:H:339:CYS:SG	6:H:809:HEM:CBB	2.67	0.82
1:D:421:CYS:SG	6:D:810:HEM:CBC	2.68	0.82
1:I:421:CYS:SG	6:I:810:HEM:C3C	2.72	0.82
1:B:478:THR:O	6:B:814:HEM:O2D	1.97	0.82
1:C:360:CYS:HG	6:C:809:HEM:CAB	1.76	0.82
1:H:302:CYS:HG	6:H:808:HEM:CAB	1.88	0.82
1:I:143:CYS:SG	6:I:806:HEM:HAB	2.18	0.82
1:J:363:CYS:SG	6:J:809:HEM:CBC	2.68	0.82
1:A:363:CYS:SG	6:A:809:HEM:HAC	2.19	0.81
1:I:421:CYS:SG	6:I:810:HEM:CBC	2.68	0.81
1:E:363:CYS:HG	6:E:809:HEM:CBC	1.94	0.81
1:J:143:CYS:HG	6:J:806:HEM:HAB	0.99	0.81
1:I:342:CYS:SG	6:I:808:HEM:CBC	2.68	0.81
1:F:146:CYS:SG	6:F:807:HEM:C3C	2.73	0.81
1:L:305:CYS:SG	6:L:807:HEM:C3C	2.72	0.81
1:C:421:CYS:SG	6:C:810:HEM:CBC	2.68	0.81
1:J:360:CYS:SG	6:J:809:HEM:CBB	2.69	0.81
1:K:363:CYS:SG	6:K:809:HEM:C3C	2.69	0.81
1:H:465:CYS:SG	6:H:812:HEM:C3C	2.73	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:360:CYS:SG	6:I:809:HEM:C3B	2.69	0.81
1:L:421:CYS:SG	6:L:810:HEM:C3C	2.74	0.81
1:E:342:CYS:SG	6:E:808:HEM:CBC	2.69	0.80
1:A:363:CYS:SG	6:A:809:HEM:C3C	2.74	0.80
1:K:418:CYS:SG	6:K:810:HEM:HAB	2.16	0.80
1:G:305:CYS:SG	6:G:807:HEM:C3C	2.74	0.80
1:I:465:CYS:HG	6:I:811:HEM:CBC	1.95	0.80
1:J:465:CYS:SG	6:J:811:HEM:C3C	2.75	0.80
1:K:465:CYS:SG	6:K:811:HEM:C3C	2.74	0.80
1:A:146:CYS:SG	6:A:806:HEM:C3C	2.75	0.80
1:B:360:CYS:SG	6:B:810:HEM:HAB	2.21	0.80
1:E:146:CYS:SG	6:E:806:HEM:C3C	2.74	0.80
1:L:562:CYS:SG	6:L:813:HEM:HAB	2.20	0.80
1:E:143:CYS:SG	6:E:806:HEM:CBB	2.69	0.80
1:G:360:CYS:SG	6:G:809:HEM:CBB	2.69	0.80
1:J:562:CYS:HG	6:J:813:HEM:CBB	1.95	0.80
1:E:562:CYS:HG	6:E:813:HEM:CBB	1.94	0.79
1:G:363:CYS:SG	6:G:809:HEM:HAC	2.22	0.79
1:J:363:CYS:SG	6:J:809:HEM:C3C	2.75	0.79
1:B:363:CYS:SG	6:B:810:HEM:C3C	2.75	0.79
1:F:339:CYS:SG	6:F:809:HEM:CBB	2.71	0.79
1:K:363:CYS:HG	6:K:809:HEM:CBC	1.94	0.79
1:K:363:CYS:SG	6:K:809:HEM:CBC	2.71	0.79
1:I:465:CYS:SG	6:I:811:HEM:C3C	2.74	0.79
1:A:360:CYS:SG	6:A:809:HEM:HAB	2.22	0.79
6:L:807:HEM:HMD1	6:L:807:HEM:CGD	2.12	0.79
6:J:807:HEM:HMD1	6:J:807:HEM:CGD	2.13	0.79
1:K:462:CYS:SG	6:K:811:HEM:HAB	2.20	0.79
1:B:146:CYS:SG	6:B:807:HEM:C3C	2.77	0.78
1:G:363:CYS:SG	6:G:809:HEM:CBC	2.72	0.78
1:D:146:CYS:SG	6:D:806:HEM:C3C	2.77	0.78
1:E:360:CYS:SG	6:E:809:HEM:HAB	2.20	0.78
1:K:363:CYS:SG	6:K:809:HEM:HAC	2.24	0.78
6:C:807:HEM:HMD1	6:C:807:HEM:CGD	2.14	0.78
1:I:418:CYS:HG	6:I:810:HEM:CBB	1.94	0.78
1:I:146:CYS:SG	6:I:806:HEM:C3C	2.77	0.78
1:E:462:CYS:SG	6:E:811:HEM:C3B	2.77	0.78
1:E:465:CYS:SG	6:E:811:HEM:C3C	2.77	0.78
1:B:339:CYS:SG	6:B:809:HEM:C3B	2.78	0.77
1:L:363:CYS:SG	6:L:809:HEM:HAC	2.24	0.77
1:A:562:CYS:SG	6:A:813:HEM:C3B	2.75	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:487:CYS:SG	6:E:812:HEM:C3C	2.76	0.77
1:L:360:CYS:SG	6:L:809:HEM:C3B	2.73	0.77
1:G:465:CYS:SG	6:G:811:HEM:CBC	2.72	0.77
1:K:487:CYS:SG	6:K:812:HEM:C3C	2.76	0.77
1:C:484:CYS:SG	6:C:812:HEM:C3B	2.78	0.77
1:F:418:CYS:HG	6:F:811:HEM:CBB	1.95	0.77
1:I:363:CYS:SG	6:I:809:HEM:CBC	2.73	0.77
1:F:342:CYS:SG	6:F:809:HEM:C3C	2.78	0.77
1:D:421:CYS:SG	6:D:810:HEM:C3C	2.79	0.76
1:C:146:CYS:SG	6:C:806:HEM:C3C	2.78	0.76
6:I:807:HEM:CGD	6:I:807:HEM:HMD1	2.14	0.76
6:K:807:HEM:HMD1	6:K:807:HEM:CGD	2.15	0.76
1:A:578:CYS:SG	6:A:813:HEM:C3C	2.78	0.76
1:G:146:CYS:SG	6:G:806:HEM:C3C	2.77	0.76
1:L:363:CYS:SG	6:L:809:HEM:CBC	2.73	0.76
1:A:465:CYS:SG	6:A:811:HEM:C3C	2.79	0.76
6:D:807:HEM:HMD1	6:D:807:HEM:CGD	2.14	0.76
1:J:562:CYS:SG	6:J:813:HEM:HAB	2.22	0.76
1:J:360:CYS:SG	6:J:809:HEM:C3B	2.71	0.76
1:L:146:CYS:SG	6:L:806:HEM:C3C	2.78	0.76
1:K:421:CYS:SG	6:K:810:HEM:CBC	2.73	0.76
1:E:339:CYS:SG	6:E:808:HEM:C3B	2.78	0.76
1:H:421:CYS:SG	6:H:811:HEM:C3C	2.76	0.76
1:H:146:CYS:SG	6:H:807:HEM:C3C	2.78	0.76
1:I:342:CYS:SG	6:I:808:HEM:C3C	2.79	0.76
1:J:421:CYS:SG	6:J:810:HEM:C3C	2.79	0.76
1:F:302:CYS:HG	6:F:808:HEM:CAB	1.99	0.76
1:F:363:CYS:SG	6:F:810:HEM:C3C	2.78	0.76
1:B:465:CYS:SG	6:B:812:HEM:C3C	2.79	0.75
1:B:562:CYS:SG	6:B:814:HEM:C3B	2.79	0.75
1:J:562:CYS:SG	6:J:813:HEM:C3B	2.74	0.75
1:E:421:CYS:SG	6:E:810:HEM:C3C	2.79	0.75
1:L:465:CYS:SG	6:L:811:HEM:C3C	2.79	0.75
1:F:421:CYS:SG	6:F:811:HEM:C3C	2.78	0.75
1:G:360:CYS:SG	6:G:809:HEM:HAB	2.25	0.75
1:E:302:CYS:HG	6:E:807:HEM:CAB	1.89	0.75
1:A:421:CYS:SG	6:A:810:HEM:C3C	2.79	0.75
1:C:143:CYS:SG	6:C:806:HEM:CBB	2.73	0.75
1:B:360:CYS:SG	6:B:810:HEM:C3B	2.74	0.75
1:B:342:CYS:SG	6:B:809:HEM:C3C	2.79	0.75
1:D:465:CYS:SG	6:D:811:HEM:C3C	2.80	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:342:CYS:SG	6:L:808:HEM:C3C	2.80	0.75
1:B:421:CYS:SG	6:B:811:HEM:C3C	2.79	0.74
1:F:342:CYS:SG	6:F:809:HEM:HAC	2.25	0.74
1:K:421:CYS:SG	6:K:810:HEM:C3C	2.80	0.74
1:A:562:CYS:HG	6:A:813:HEM:CBB	1.99	0.74
1:C:462:CYS:SG	6:C:811:HEM:C3B	2.80	0.74
1:D:360:CYS:SG	6:D:809:HEM:HAB	2.26	0.74
1:E:360:CYS:SG	6:E:809:HEM:C3B	2.73	0.74
1:F:462:CYS:SG	6:F:812:HEM:C3B	2.79	0.74
1:C:421:CYS:SG	6:C:810:HEM:C3C	2.81	0.74
1:H:360:CYS:SG	6:H:810:HEM:C3B	2.77	0.74
1:A:339:CYS:SG	6:A:808:HEM:C3B	2.81	0.74
1:J:302:CYS:HG	6:J:807:HEM:CAB	1.91	0.73
1:G:462:CYS:SG	6:G:811:HEM:C3B	2.81	0.73
1:F:465:CYS:SG	6:F:812:HEM:C3C	2.81	0.73
1:C:465:CYS:SG	6:C:811:HEM:C3C	2.81	0.73
6:A:807:HEM:HMD1	6:A:807:HEM:CGD	2.18	0.73
6:L:810:HEM:HMC1	6:L:810:HEM:HBC2	1.71	0.73
1:F:484:CYS:SG	6:F:813:HEM:C3B	2.82	0.73
1:F:360:CYS:SG	6:F:810:HEM:HAB	2.26	0.72
1:K:462:CYS:HG	6:K:811:HEM:CBB	1.90	0.72
1:I:360:CYS:SG	6:I:809:HEM:HAB	2.25	0.72
1:G:487:CYS:SG	6:G:812:HEM:C3C	2.82	0.72
1:I:360:CYS:SG	6:I:809:HEM:CBB	2.78	0.72
1:C:562:CYS:SG	6:C:813:HEM:C3B	2.82	0.72
1:H:487:CYS:SG	6:H:813:HEM:C3C	2.79	0.72
1:K:562:CYS:SG	6:K:813:HEM:C3B	2.82	0.72
1:D:462:CYS:SG	6:D:811:HEM:C3B	2.81	0.72
1:K:562:CYS:SG	6:K:813:HEM:HAB	2.24	0.72
1:C:418:CYS:SG	6:C:810:HEM:C3B	2.81	0.72
1:F:578:CYS:SG	6:F:814:HEM:C3C	2.83	0.72
1:H:342:CYS:SG	6:H:809:HEM:C3C	2.82	0.72
1:K:418:CYS:SG	6:K:810:HEM:C3B	2.82	0.72
1:F:562:CYS:SG	6:F:814:HEM:C3B	2.83	0.71
1:D:342:CYS:SG	6:D:808:HEM:HAC	2.30	0.71
1:I:462:CYS:SG	6:I:811:HEM:C3B	2.81	0.71
1:I:342:CYS:SG	6:I:808:HEM:HAC	2.27	0.71
1:D:339:CYS:SG	6:D:808:HEM:C3B	2.84	0.71
1:A:484:CYS:SG	6:A:812:HEM:C3B	2.83	0.71
1:C:363:CYS:SG	6:C:809:HEM:CBC	2.78	0.71
1:D:562:CYS:SG	6:D:813:HEM:C3B	2.82	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:146:CYS:SG	6:K:806:HEM:C3C	2.82	0.71
1:C:342:CYS:SG	6:C:808:HEM:HAC	2.28	0.71
1:K:360:CYS:SG	6:K:809:HEM:HAB	2.27	0.71
1:C:487:CYS:SG	6:C:812:HEM:C3C	2.84	0.70
1:C:487:CYS:SG	6:C:812:HEM:HAC	2.30	0.70
1:D:342:CYS:SG	6:D:808:HEM:C3C	2.83	0.70
1:D:487:CYS:SG	6:D:812:HEM:C3C	2.83	0.70
1:G:342:CYS:SG	6:G:808:HEM:HAC	2.30	0.70
1:G:418:CYS:SG	6:G:810:HEM:C3B	2.83	0.70
1:I:339:CYS:SG	6:I:808:HEM:C3B	2.84	0.70
1:J:146:CYS:SG	6:J:806:HEM:C3C	2.83	0.70
1:J:578:CYS:SG	6:J:813:HEM:C3C	2.83	0.70
1:L:462:CYS:SG	6:L:811:HEM:C3B	2.79	0.70
1:C:342:CYS:SG	6:C:808:HEM:C3C	2.83	0.70
1:C:578:CYS:SG	6:C:813:HEM:C3C	2.84	0.70
1:I:302:CYS:HG	6:I:807:HEM:CAB	1.91	0.70
1:B:487:CYS:SG	6:B:813:HEM:C3C	2.83	0.70
1:F:360:CYS:SG	6:F:810:HEM:C3B	2.78	0.70
1:A:487:CYS:SG	6:A:812:HEM:C3C	2.81	0.70
1:G:562:CYS:SG	6:G:813:HEM:C3B	2.85	0.70
1:G:421:CYS:SG	6:G:810:HEM:C3C	2.84	0.70
1:H:484:CYS:SG	6:H:813:HEM:C3B	2.84	0.70
1:J:363:CYS:HG	6:J:809:HEM:CBC	2.05	0.70
1:J:487:CYS:SG	6:J:812:HEM:C3C	2.84	0.70
1:E:578:CYS:SG	6:E:813:HEM:C3C	2.85	0.69
1:C:339:CYS:SG	6:C:808:HEM:C3B	2.83	0.69
1:A:578:CYS:SG	6:A:813:HEM:HAC	2.30	0.69
1:K:578:CYS:SG	6:K:813:HEM:C3C	2.84	0.69
1:L:562:CYS:SG	6:L:813:HEM:C3B	2.84	0.69
1:I:487:CYS:SG	6:I:812:HEM:C3C	2.85	0.69
1:K:360:CYS:SG	6:K:809:HEM:C3B	2.77	0.69
1:B:484:CYS:SG	6:B:813:HEM:C3B	2.84	0.69
1:E:578:CYS:SG	6:E:813:HEM:HAC	2.31	0.69
6:E:807:HEM:HMD1	6:E:807:HEM:CGD	2.23	0.69
1:A:208:LYS:HG3	6:A:807:HEM:HMA2	1.73	0.69
1:F:143:CYS:SG	6:F:807:HEM:C3B	2.85	0.69
1:F:143:CYS:HG	6:F:807:HEM:CAB	2.05	0.69
6:F:808:HEM:HMD1	6:F:808:HEM:CGD	2.23	0.69
1:I:578:CYS:SG	6:I:813:HEM:C3C	2.86	0.69
1:D:578:CYS:SG	6:D:813:HEM:C3C	2.85	0.68
1:A:487:CYS:SG	6:A:812:HEM:HAC	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:363:CYS:SG	6:J:809:HEM:HAC	2.28	0.68
1:L:487:CYS:SG	6:L:812:HEM:C3C	2.86	0.68
1:F:339:CYS:SG	6:F:809:HEM:C3B	2.85	0.68
6:G:807:HEM:HMD1	6:G:807:HEM:CGD	2.22	0.68
1:A:342:CYS:SG	6:A:808:HEM:HAC	2.32	0.68
1:K:342:CYS:SG	6:K:808:HEM:C3C	2.86	0.68
1:B:418:CYS:SG	6:B:811:HEM:C3B	2.85	0.68
1:J:339:CYS:SG	6:J:808:HEM:C3B	2.87	0.68
1:E:363:CYS:SG	6:E:809:HEM:HAC	2.26	0.68
6:H:808:HEM:HMD1	6:H:808:HEM:CGD	2.24	0.68
1:L:302:CYS:HG	6:L:807:HEM:CAB	2.06	0.68
1:E:342:CYS:SG	6:E:808:HEM:C3C	2.86	0.68
1:J:342:CYS:SG	6:J:808:HEM:C3C	2.85	0.68
1:A:302:CYS:HG	6:A:807:HEM:CAB	1.97	0.67
1:E:562:CYS:SG	6:E:813:HEM:C3B	2.78	0.67
1:F:487:CYS:SG	6:F:813:HEM:C3C	2.88	0.67
1:K:339:CYS:SG	6:K:808:HEM:C3B	2.88	0.67
1:H:360:CYS:SG	6:H:810:HEM:HAB	2.31	0.67
1:H:363:CYS:SG	6:H:810:HEM:HAC	2.31	0.67
6:B:808:HEM:HMD1	6:B:808:HEM:CGD	2.25	0.67
1:G:342:CYS:SG	6:G:808:HEM:C3C	2.88	0.67
1:D:363:CYS:SG	6:D:809:HEM:HAC	2.27	0.67
1:E:143:CYS:HG	6:E:806:HEM:CAB	2.03	0.67
1:E:143:CYS:HG	6:E:806:HEM:HAB	1.58	0.67
1:B:143:CYS:SG	6:B:807:HEM:C3B	2.88	0.67
1:E:342:CYS:SG	6:E:808:HEM:HAC	2.34	0.66
1:G:484:CYS:SG	6:G:812:HEM:C3B	2.88	0.66
1:J:342:CYS:SG	6:J:808:HEM:HAC	2.29	0.66
1:D:418:CYS:SG	6:D:810:HEM:C3B	2.84	0.66
1:G:578:CYS:SG	6:G:813:HEM:C3C	2.88	0.66
1:L:360:CYS:SG	6:L:809:HEM:HAB	2.28	0.66
1:J:360:CYS:SG	6:J:809:HEM:HAB	2.29	0.66
1:A:418:CYS:SG	6:A:810:HEM:C3B	2.85	0.66
1:H:339:CYS:SG	6:H:809:HEM:C3B	2.89	0.65
1:I:562:CYS:SG	6:I:813:HEM:C3B	2.90	0.65
1:I:484:CYS:SG	6:I:812:HEM:C3B	2.88	0.65
1:C:339:CYS:SG	6:C:808:HEM:CBB	2.84	0.65
1:J:462:CYS:SG	6:J:811:HEM:C3B	2.88	0.65
1:A:342:CYS:SG	6:A:808:HEM:C3C	2.89	0.65
1:K:146:CYS:SG	6:K:806:HEM:HAC	2.35	0.65
1:C:363:CYS:HG	6:C:809:HEM:CBC	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:120:SER:OG	1:G:124:ARG:HG3	1.97	0.65
1:B:363:CYS:SG	6:B:810:HEM:HAC	2.31	0.64
1:B:418:CYS:HG	6:B:811:HEM:CBB	2.05	0.64
1:I:487:CYS:SG	6:I:812:HEM:HAC	2.35	0.64
1:A:421:CYS:SG	6:A:810:HEM:HAC	2.33	0.64
1:D:484:CYS:SG	6:D:812:HEM:C3B	2.87	0.64
1:E:484:CYS:SG	6:E:812:HEM:C3B	2.88	0.64
1:L:484:CYS:SG	6:L:812:HEM:C3B	2.88	0.64
1:B:462:CYS:SG	6:B:812:HEM:C3B	2.89	0.64
1:C:143:CYS:SG	6:C:806:HEM:C3B	2.91	0.64
6:B:811:HEM:HMC1	6:B:811:HEM:HBC2	1.80	0.63
1:C:339:CYS:HG	6:C:808:HEM:CBB	2.10	0.63
1:H:342:CYS:SG	6:H:809:HEM:HAC	2.33	0.63
1:H:562:CYS:SG	6:H:814:HEM:C3B	2.80	0.63
1:C:146:CYS:SG	6:C:806:HEM:HAC	2.30	0.63
1:C:302:CYS:HG	6:C:807:HEM:CAB	2.08	0.63
1:G:339:CYS:SG	6:G:808:HEM:C3B	2.89	0.63
1:K:484:CYS:SG	6:K:812:HEM:C3B	2.90	0.63
1:I:465:CYS:SG	6:I:811:HEM:HAC	2.35	0.63
1:D:360:CYS:SG	6:D:809:HEM:C3B	2.74	0.63
1:D:143:CYS:SG	6:D:806:HEM:C3B	2.89	0.63
1:L:143:CYS:SG	6:L:806:HEM:C3B	2.91	0.63
1:A:305:CYS:SG	6:A:807:HEM:HAC	2.31	0.62
1:G:208:LYS:HG3	6:G:807:HEM:HMA3	1.82	0.62
1:F:487:CYS:SG	6:F:813:HEM:HAC	2.33	0.62
1:L:578:CYS:SG	6:L:813:HEM:C3C	2.93	0.62
1:E:143:CYS:SG	6:E:806:HEM:C3B	2.91	0.62
1:G:475:LYS:O	1:G:476:ALA:O	2.17	0.62
1:D:375:ARG:NH1	8:D:1036:HOH:O	2.31	0.62
1:J:484:CYS:SG	6:J:812:HEM:C3B	2.91	0.62
1:H:462:CYS:SG	6:H:812:HEM:C3B	2.91	0.61
1:B:689:SER:O	1:B:690:LEU:HB2	2.01	0.61
1:F:418:CYS:SG	6:F:811:HEM:C3B	2.92	0.61
1:H:418:CYS:SG	6:H:811:HEM:C3B	2.89	0.61
1:B:578:CYS:SG	6:B:814:HEM:C3C	2.92	0.61
1:B:487:CYS:SG	6:B:813:HEM:HAC	2.36	0.61
1:A:360:CYS:SG	6:A:809:HEM:C3B	2.80	0.61
1:D:421:CYS:SG	6:D:810:HEM:HAC	2.37	0.61
1:J:418:CYS:SG	6:J:810:HEM:C3B	2.92	0.61
1:B:342:CYS:SG	6:B:809:HEM:HAC	2.34	0.60
1:I:418:CYS:SG	6:I:810:HEM:C3B	2.86	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:502:GLN:O	1:L:539:ARG:NH2	2.35	0.60
1:G:360:CYS:SG	6:G:809:HEM:C3B	2.78	0.60
1:D:418:CYS:HG	6:D:810:HEM:CBB	2.07	0.60
1:A:143:CYS:SG	6:A:806:HEM:C3B	2.91	0.59
1:C:302:CYS:SG	6:C:807:HEM:CBB	2.89	0.59
1:H:418:CYS:HG	6:H:811:HEM:CBB	2.06	0.59
1:I:143:CYS:SG	6:I:806:HEM:C3B	2.93	0.59
1:L:339:CYS:SG	6:L:808:HEM:C3B	2.93	0.59
1:J:650:THR:HG23	1:J:671:ARG:HG2	1.84	0.59
1:E:418:CYS:SG	6:E:810:HEM:C3B	2.87	0.59
1:K:302:CYS:SG	6:K:807:HEM:C2B	2.95	0.58
1:L:418:CYS:SG	6:L:810:HEM:C3B	2.95	0.58
1:J:305:CYS:CB	6:J:807:HEM:C3C	2.86	0.58
1:K:302:CYS:SG	6:K:807:HEM:HAB	2.39	0.58
1:I:363:CYS:HG	6:I:809:HEM:CBC	2.14	0.58
1:I:208:LYS:HG3	6:I:807:HEM:HMA3	1.86	0.58
1:F:578:CYS:SG	6:F:814:HEM:HAC	2.34	0.58
1:G:465:CYS:SG	6:G:811:HEM:HAC	2.36	0.57
1:I:578:CYS:SG	6:I:813:HEM:HAC	2.37	0.57
1:B:146:CYS:SG	6:B:807:HEM:HAC	2.38	0.56
1:K:465:CYS:SG	6:K:811:HEM:HAC	2.40	0.56
1:F:146:CYS:SG	6:F:807:HEM:HAC	2.37	0.56
1:A:434:GLU:HB2	1:A:437:ILE:HD12	1.86	0.56
1:H:578:CYS:SG	6:H:814:HEM:C3C	2.86	0.56
6:L:812:HEM:HMC2	6:L:812:HEM:HBC2	1.88	0.56
1:H:143:CYS:SG	6:H:807:HEM:C3B	2.96	0.56
1:K:462:CYS:SG	6:K:811:HEM:C3B	2.80	0.56
1:A:302:CYS:SG	6:A:807:HEM:CBB	2.93	0.55
1:K:143:CYS:SG	6:K:806:HEM:CBB	2.90	0.55
1:L:575:ALA:HB3	6:L:813:HEM:HBC1	1.88	0.55
1:A:146:CYS:SG	6:A:806:HEM:HAC	2.36	0.55
1:D:302:CYS:SG	6:D:807:HEM:CBB	2.93	0.55
1:L:575:ALA:HB3	6:L:813:HEM:CBC	2.36	0.55
1:J:612:LYS:HE3	1:J:676:VAL:HG21	1.88	0.55
6:J:813:HEM:HBB2	6:J:813:HEM:HMB1	1.88	0.55
1:I:421:CYS:SG	6:I:810:HEM:HAC	2.38	0.54
1:K:305:CYS:CB	6:K:807:HEM:C3C	2.90	0.54
1:D:208:LYS:HG3	6:D:807:HEM:HMA2	1.88	0.54
1:A:402:GLU:O	1:A:406:THR:HG23	2.08	0.54
1:D:402:GLU:O	1:D:406:THR:HG23	2.07	0.54
1:G:578:CYS:SG	6:G:813:HEM:HAC	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:302:CYS:SG	6:E:807:HEM:CBB	2.95	0.54
1:G:476:ALA:O	1:G:480:SER:HB3	2.06	0.54
1:A:305:CYS:CB	6:A:807:HEM:C3C	2.90	0.53
1:B:146:CYS:CB	6:B:807:HEM:C3C	2.91	0.53
1:D:487:CYS:SG	6:D:812:HEM:HAC	2.39	0.53
1:D:578:CYS:SG	6:D:813:HEM:HAC	2.36	0.53
1:C:578:CYS:SG	6:C:813:HEM:HAC	2.42	0.53
1:A:462:CYS:SG	6:A:811:HEM:C3B	2.91	0.53
6:K:810:HEM:HMB1	6:K:810:HEM:HBB2	1.90	0.53
1:D:305:CYS:CB	6:D:807:HEM:C3C	2.92	0.53
1:H:400:GLY:HA3	6:H:808:HEM:HMD2	1.89	0.53
1:C:612:LYS:HE3	1:C:676:VAL:HG21	1.91	0.53
1:B:305:CYS:CB	6:B:808:HEM:C3C	2.92	0.53
1:H:487:CYS:SG	6:H:813:HEM:HAC	2.36	0.53
1:B:302:CYS:SG	6:B:808:HEM:CBB	2.95	0.52
1:E:208:LYS:HG3	6:E:807:HEM:HMA2	1.92	0.52
1:A:418:CYS:HG	6:A:810:HEM:CBB	2.13	0.52
1:E:484:CYS:CB	6:E:812:HEM:CAB	2.87	0.52
1:E:540:ASP:O	4:E:804:BU3:H3	2.10	0.52
1:F:146:CYS:CB	6:F:807:HEM:C3C	2.93	0.52
1:G:302:CYS:SG	6:G:807:HEM:CBB	2.98	0.52
1:F:302:CYS:SG	6:F:808:HEM:CBB	2.98	0.52
1:H:302:CYS:SG	6:H:808:HEM:CBB	2.96	0.52
1:F:208:LYS:HG3	6:F:808:HEM:HMA3	1.92	0.51
1:H:305:CYS:CB	6:H:808:HEM:C3C	2.93	0.51
1:L:208:LYS:HG3	6:L:807:HEM:HMA3	1.91	0.51
1:G:146:CYS:SG	6:G:806:HEM:HAC	2.38	0.51
1:B:208:LYS:HG3	6:B:808:HEM:HMA3	1.93	0.51
1:L:305:CYS:CB	6:L:807:HEM:C3C	2.94	0.51
1:L:400:GLY:HA3	6:L:807:HEM:HMD2	1.92	0.51
1:G:146:CYS:CB	6:G:806:HEM:C3C	2.93	0.51
1:L:146:CYS:CB	6:L:806:HEM:C3C	2.94	0.51
1:L:575:ALA:CB	6:L:813:HEM:CBC	2.89	0.51
1:J:578:CYS:SG	6:J:813:HEM:HAC	2.37	0.51
1:A:435:LYS:NZ	1:A:445:GLU:OE1	2.43	0.51
1:C:146:CYS:CB	6:C:806:HEM:C3C	2.94	0.51
1:D:146:CYS:CB	6:D:806:HEM:C3C	2.94	0.51
1:F:305:CYS:CB	6:F:808:HEM:C3C	2.94	0.51
1:G:484:CYS:CB	6:G:812:HEM:CAB	2.89	0.51
1:D:339:CYS:HG	6:D:808:HEM:CBB	2.22	0.51
1:C:395:MET:HG2	1:C:544:TRP:CE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:305:CYS:CB	6:I:807:HEM:C3C	2.93	0.50
1:A:49:GLU:HG2	8:A:1274:HOH:O	2.11	0.50
1:A:629:VAL:HG12	1:A:629:VAL:O	2.11	0.50
1:F:363:CYS:CB	6:F:810:HEM:C3C	2.95	0.50
1:L:465:CYS:SG	6:L:811:HEM:HAC	2.39	0.50
1:L:518:TRP:HE1	6:L:811:HEM:HBB2	1.76	0.50
1:E:146:CYS:CB	6:E:806:HEM:C3C	2.95	0.50
1:D:339:CYS:SG	6:D:808:HEM:CBB	2.95	0.49
1:I:484:CYS:HB3	6:I:812:HEM:C3B	2.48	0.49
1:D:632:LEU:HD13	1:D:636:ASP:CB	2.43	0.49
6:H:811:HEM:HBB2	6:H:811:HEM:HMB1	1.94	0.49
1:J:146:CYS:CB	6:J:806:HEM:C3C	2.96	0.49
1:L:104:ASN:O	1:L:108:LYS:HG2	2.12	0.49
1:L:342:CYS:SG	6:L:808:HEM:HAC	2.40	0.49
6:B:809:HEM:HBC1	6:B:810:HEM:CHC	2.42	0.49
1:C:421:CYS:SG	6:C:810:HEM:HAC	2.41	0.49
1:C:208:LYS:HG3	6:C:807:HEM:HMA3	1.95	0.49
1:L:363:CYS:HG	6:L:809:HEM:CBC	2.17	0.49
1:H:84:THR:OG1	1:H:86:GLY:O	2.25	0.49
1:B:465:CYS:SG	6:B:812:HEM:HAC	2.43	0.49
1:A:410:ALA:O	1:A:414:LYS:HG2	2.12	0.48
6:J:812:HEM:HMC2	6:J:812:HEM:HBC2	1.95	0.48
1:K:421:CYS:SG	6:K:810:HEM:HAC	2.43	0.48
1:J:360:CYS:HG	6:J:809:HEM:CBB	2.21	0.48
1:A:146:CYS:CB	6:A:806:HEM:C3C	2.96	0.48
1:K:342:CYS:SG	6:K:808:HEM:HAC	2.39	0.48
1:C:486:SER:HB2	6:C:813:HEM:HBC2	1.96	0.48
1:F:223:VAL:CG2	1:F:235:ILE:HD13	2.43	0.48
1:I:146:CYS:CB	6:I:806:HEM:C3C	2.96	0.48
1:G:487:CYS:SG	6:G:812:HEM:HAC	2.40	0.48
1:I:484:CYS:CB	6:I:812:HEM:CAB	2.89	0.48
6:L:806:HEM:HMC2	6:L:806:HEM:HBC2	1.96	0.48
1:I:146:CYS:SG	6:I:806:HEM:HAC	2.44	0.48
1:A:462:CYS:SG	6:A:811:HEM:CBB	2.94	0.47
1:D:360:CYS:HG	6:D:809:HEM:CBB	2.20	0.47
1:J:84:THR:HG21	1:J:88:LEU:HD21	1.95	0.47
1:E:146:CYS:SG	6:E:806:HEM:HAC	2.40	0.47
1:J:463:THR:HG22	1:J:470:ALA:HB2	1.96	0.47
1:G:484:CYS:HB3	6:G:812:HEM:C3B	2.49	0.47
1:I:681:GLU:O	1:I:685:ILE:HD12	2.14	0.47
1:J:421:CYS:SG	6:J:810:HEM:HAC	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:465:CYS:SG	6:J:811:HEM:HAC	2.41	0.47
1:K:165:PHE:CZ	1:K:335:LYS:HD3	2.49	0.47
1:C:465:CYS:SG	6:C:811:HEM:HAC	2.43	0.47
1:E:305:CYS:CB	6:E:807:HEM:C3C	2.97	0.47
1:K:487:CYS:SG	6:K:812:HEM:HAC	2.41	0.47
1:E:607:THR:HB	1:E:608:PRO:HD3	1.96	0.47
1:G:305:CYS:C	1:G:307:PRO:HD3	2.35	0.47
1:G:143:CYS:SG	6:G:806:HEM:C3B	2.87	0.47
1:I:400:GLY:HA3	6:I:807:HEM:HMD2	1.97	0.47
1:A:547:GLU:HG3	8:A:1296:HOH:O	2.15	0.47
1:G:305:CYS:CB	6:G:807:HEM:C3C	2.98	0.47
1:C:400:GLY:HA3	6:C:807:HEM:HMD2	1.98	0.47
1:C:623:LEU:O	1:C:627:LEU:HG	2.15	0.46
1:F:421:CYS:SG	6:F:811:HEM:HAC	2.40	0.46
1:K:208:LYS:HG3	6:K:807:HEM:HMA3	1.95	0.46
1:L:302:CYS:SG	6:L:807:HEM:CBB	2.99	0.46
6:I:810:HEM:HBB2	6:I:810:HEM:HMB1	1.96	0.46
1:C:305:CYS:CB	6:C:807:HEM:C3C	2.99	0.46
1:F:491:PHE:O	1:F:511:THR:HB	2.16	0.46
1:J:684:ARG:O	1:J:688:LYS:NZ	2.48	0.46
1:K:305:CYS:HB2	6:K:807:HEM:C3C	2.50	0.46
1:B:243:GLN:HB3	1:B:496:GLU:OE2	2.14	0.46
1:E:646:LYS:NZ	8:E:1118:HOH:O	2.49	0.46
1:H:146:CYS:CB	6:H:807:HEM:C3C	2.99	0.46
6:H:807:HEM:HBC2	6:H:807:HEM:HMC2	1.97	0.46
1:I:372:ASP:OD1	1:I:375:ARG:NH2	2.48	0.46
1:A:363:CYS:CB	6:A:809:HEM:C3C	2.99	0.46
6:L:808:HEM:HBC1	6:L:809:HEM:CHC	2.46	0.46
1:C:301:TYR:CD2	6:C:807:HEM:HAB	2.51	0.46
1:D:465:CYS:HG	6:D:811:HEM:CAC	2.26	0.46
1:I:289:TYR:CE2	1:I:290:LYS:HE2	2.51	0.46
1:J:146:CYS:SG	6:J:806:HEM:HAC	2.45	0.46
6:K:808:HEM:CMC	6:K:808:HEM:HBC2	2.46	0.46
6:L:807:HEM:HBC2	6:L:807:HEM:HMC2	1.97	0.46
1:D:484:CYS:CB	6:D:812:HEM:CAB	2.91	0.45
1:E:112:ARG:HB2	1:K:151:TYR:CE1	2.51	0.45
1:F:365:GLN:NE2	5:F:806:ACT:O	2.48	0.45
1:G:654:ILE:HD12	1:G:668:THR:HG23	1.98	0.45
1:I:305:CYS:SG	6:I:807:HEM:HAC	2.39	0.45
1:A:484:CYS:CB	6:A:812:HEM:CAB	2.93	0.45
1:B:675:ALA:HA	1:B:678:TYR:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:302:CYS:HG	6:K:807:HEM:CAB	2.10	0.45
1:C:650:THR:HG23	1:C:671:ARG:HG2	1.98	0.45
1:C:365:GLN:OE1	5:C:805:ACT:H1	2.17	0.45
1:F:143:CYS:CB	6:F:807:HEM:CAB	2.92	0.45
1:F:486:SER:HB2	6:F:814:HEM:HBC2	1.98	0.45
1:G:402:GLU:O	1:G:406:THR:HG23	2.16	0.45
1:A:305:CYS:HB2	6:A:807:HEM:C3C	2.51	0.45
1:G:487:CYS:HG	6:G:812:HEM:CAC	2.22	0.45
1:E:305:CYS:SG	6:E:807:HEM:HAC	2.43	0.45
1:E:659:SER:HB3	1:E:663:HIS:CE1	2.52	0.45
1:G:360:CYS:HG	6:G:809:HEM:CBB	2.16	0.45
1:I:499:TYR:O	1:I:539:ARG:NH2	2.50	0.45
1:G:208:LYS:HG3	6:G:807:HEM:CMA	2.48	0.44
6:I:806:HEM:HBC2	6:I:806:HEM:HMC2	1.99	0.44
1:K:146:CYS:CB	6:K:806:HEM:C3C	3.00	0.44
1:E:654:ILE:HD12	1:E:668:THR:HG23	1.99	0.44
1:K:357:ILE:HB	4:K:803:BU3:H11	1.99	0.44
1:F:363:CYS:HB2	6:F:810:HEM:C3C	2.51	0.44
1:G:94:GLY:O	1:G:98:ILE:HB	2.16	0.44
1:L:220:THR:HA	1:L:240:ASN:ND2	2.33	0.44
1:D:146:CYS:SG	6:D:806:HEM:HAC	2.44	0.44
1:D:465:CYS:SG	6:D:811:HEM:HAC	2.44	0.44
1:D:486:SER:HB2	6:D:813:HEM:HBC2	1.99	0.44
1:G:688:LYS:N	1:G:688:LYS:HD3	2.33	0.44
6:J:813:HEM:HBD1	6:J:813:HEM:HMD2	1.98	0.44
1:F:223:VAL:HG22	1:F:235:ILE:HD13	1.99	0.44
1:F:659:SER:HB3	1:F:663:HIS:CE1	2.53	0.44
1:A:243:GLN:HB3	1:A:496:GLU:OE2	2.18	0.44
1:E:402:GLU:O	1:E:406:THR:HG23	2.16	0.44
1:G:421:CYS:SG	6:G:810:HEM:HAC	2.45	0.44
1:B:305:CYS:C	1:B:307:PRO:HD3	2.37	0.44
1:J:208:LYS:HG3	6:J:807:HEM:HMA3	1.99	0.44
6:C:807:HEM:HBB2	6:C:807:HEM:HMB2	2.00	0.44
6:D:811:HEM:HMC2	6:D:811:HEM:HBC2	1.99	0.44
1:E:484:CYS:HB3	6:E:812:HEM:C3B	2.53	0.44
1:F:633:ALA:O	1:F:636:ASP:N	2.44	0.44
1:J:143:CYS:HG	6:J:806:HEM:CAB	1.88	0.44
1:B:578:CYS:SG	6:B:814:HEM:HAC	2.43	0.43
1:C:104:ASN:O	1:C:108:LYS:HG2	2.17	0.43
6:C:810:HEM:HMB1	6:C:810:HEM:HBB2	2.00	0.43
1:H:123:TYR:CE1	6:H:808:HEM:HBC2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:305:CYS:HB2	6:J:807:HEM:C3C	2.53	0.43
1:J:402:GLU:O	1:J:406:THR:HG23	2.19	0.43
1:K:400:GLY:HA3	6:K:807:HEM:HMD2	2.00	0.43
1:B:270:GLU:HG2	1:B:271:GLU:N	2.33	0.43
1:B:143:CYS:HG	6:B:807:HEM:CAB	2.21	0.43
1:F:453:TYR:CD2	1:F:570:LYS:HG2	2.54	0.43
1:H:305:CYS:SG	6:H:808:HEM:HAC	2.39	0.43
1:H:203:GLY:HA3	6:H:808:HEM:HMA1	2.01	0.43
1:D:410:ALA:O	1:D:414:LYS:HG2	2.19	0.43
1:E:343:HIS:CE1	6:E:808:HEM:ND	2.86	0.43
1:K:207:THR:HG23	1:K:512:GLN:HG3	2.00	0.43
1:J:302:CYS:SG	6:J:807:HEM:CBB	3.04	0.43
1:D:305:CYS:HB2	6:D:807:HEM:C3C	2.53	0.43
1:D:659:SER:HB3	1:D:663:HIS:CE1	2.54	0.43
1:F:484:CYS:CB	6:F:813:HEM:CAB	2.95	0.43
6:H:814:HEM:HMC2	6:H:814:HEM:HBC2	1.99	0.43
1:D:151:TYR:CE1	1:K:112:ARG:HB2	2.54	0.43
1:D:305:CYS:SG	6:D:807:HEM:HAC	2.43	0.43
1:F:151:TYR:CE1	1:I:112:ARG:HB2	2.53	0.43
1:G:400:GLY:HA3	6:G:807:HEM:HMD2	2.00	0.43
1:L:131:LEU:HD21	1:L:299:THR:HG21	2.01	0.43
1:L:434:GLU:HB2	1:L:437:ILE:HD12	2.01	0.43
6:D:808:HEM:HBC1	6:D:809:HEM:CHC	2.48	0.43
1:H:493:MET:HB2	1:H:513:ARG:HB2	2.01	0.43
1:I:402:GLU:O	1:I:406:THR:HG23	2.18	0.43
1:I:453:TYR:CD2	1:I:570:LYS:HD2	2.54	0.43
1:I:151:TYR:CE1	1:J:112:ARG:HB2	2.53	0.43
6:D:806:HEM:HBC2	6:D:806:HEM:HMC2	2.01	0.43
1:H:302:CYS:SG	6:H:808:HEM:HAB	2.48	0.43
6:A:808:HEM:HBC1	6:A:809:HEM:CHC	2.49	0.43
1:E:223:VAL:HG22	1:E:235:ILE:HD13	2.01	0.43
1:F:143:CYS:HG	6:F:807:HEM:CBB	2.19	0.43
1:K:143:CYS:SG	6:K:806:HEM:C3B	3.00	0.43
6:G:806:HEM:HMC2	6:G:806:HEM:HBC2	2.01	0.42
1:H:395:MET:HG2	1:H:544:TRP:CE2	2.54	0.42
1:K:84:THR:OG1	1:K:86:GLY:O	2.37	0.42
1:L:339:CYS:HA	6:L:808:HEM:CHC	2.49	0.42
6:L:807:HEM:HBB2	6:L:807:HEM:HMB2	2.00	0.42
1:B:487:CYS:HG	6:B:813:HEM:CAC	2.22	0.42
1:H:484:CYS:CB	6:H:813:HEM:CAB	2.95	0.42
1:K:612:LYS:O	1:K:616:VAL:HG23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:223:VAL:HG22	1:L:235:ILE:HD13	2.01	0.42
6:K:808:HEM:HBC2	6:K:808:HEM:HMC2	2.01	0.42
1:L:305:CYS:HB2	6:L:807:HEM:C3C	2.55	0.42
1:E:499:TYR:CD1	4:E:804:BU3:H43	2.54	0.42
1:E:360:CYS:HG	6:E:809:HEM:CBB	2.19	0.42
1:G:363:CYS:CB	6:G:809:HEM:C3C	3.03	0.42
6:J:813:HEM:HBD1	6:J:813:HEM:CMD	2.50	0.42
1:B:191:GLN:HG2	1:B:223:VAL:O	2.19	0.42
6:B:808:HEM:HMB2	6:B:808:HEM:HBB2	2.00	0.42
6:C:807:HEM:HMD1	6:C:807:HEM:CBD	2.50	0.42
1:D:607:THR:HB	1:D:608:PRO:HD3	2.01	0.42
1:A:264:ASP:OD1	1:A:264:ASP:N	2.51	0.42
1:F:302:CYS:SG	6:F:808:HEM:HAB	2.50	0.42
6:H:807:HEM:HBC2	6:H:807:HEM:CMC	2.50	0.42
1:J:197:VAL:O	1:J:214:ALA:N	2.53	0.42
1:L:301:TYR:CD2	6:L:807:HEM:HAB	2.55	0.42
1:G:492:MET:CE	1:G:529:LEU:HD21	2.49	0.42
1:H:374:MET:CE	1:H:384:PRO:HA	2.50	0.42
6:L:812:HEM:HBC2	6:L:812:HEM:CMC	2.50	0.42
1:F:471:TYR:O	1:F:474:SER:OG	2.33	0.42
6:K:808:HEM:HBC1	6:K:809:HEM:CHC	2.49	0.42
1:G:402:GLU:HB2	6:G:810:HEM:HMB3	2.01	0.41
1:J:259:LYS:HA	1:J:262:VAL:O	2.20	0.41
1:J:654:ILE:CD1	1:J:672:LEU:HG	2.50	0.41
1:L:302:CYS:SG	6:L:807:HEM:HAB	2.47	0.41
1:C:607:THR:HB	1:C:608:PRO:HD3	2.02	0.41
1:E:395:MET:HG2	1:E:544:TRP:CE2	2.55	0.41
5:E:805:ACT:H1	8:E:1105:HOH:O	2.19	0.41
1:G:476:ALA:O	1:G:477:ASP:CB	2.68	0.41
1:G:484:CYS:CB	6:G:812:HEM:C3B	3.03	0.41
6:H:809:HEM:HBC1	6:H:810:HEM:CHC	2.50	0.41
1:I:302:CYS:SG	6:I:807:HEM:C2B	3.12	0.41
1:I:62:GLU:OE1	1:I:129:SER:OG	2.25	0.41
1:L:203:GLY:HA2	6:L:807:HEM:HBA2	2.02	0.41
1:C:305:CYS:C	1:C:307:PRO:HD3	2.40	0.41
1:E:628:GLU:O	1:E:629:VAL:HG22	2.19	0.41
1:A:642:GLU:OE2	1:C:646:LYS:HE3	2.21	0.41
1:D:642:GLU:HG3	1:E:646:LYS:HE3	2.03	0.41
1:F:400:GLY:HA3	6:F:808:HEM:HMD2	2.03	0.41
1:L:306:HIS:CE1	6:L:809:HEM:HMD2	2.56	0.41
1:B:418:CYS:CA	6:B:811:HEM:HAB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:GLU:O	1:C:406:THR:HG23	2.21	0.41
1:F:184:ASP:OD1	1:F:184:ASP:N	2.52	0.41
1:G:463:THR:HG22	1:G:470:ALA:HB2	2.03	0.41
1:H:112:ARG:HB2	1:G:151:TYR:CE1	2.56	0.41
1:K:636:ASP:O	1:K:640:VAL:HG23	2.21	0.41
1:D:301:TYR:CD2	6:D:807:HEM:HAB	2.56	0.41
1:I:305:CYS:C	1:I:307:PRO:HD3	2.40	0.41
1:I:484:CYS:CB	6:I:812:HEM:C3B	3.04	0.41
1:J:302:CYS:SG	6:J:807:HEM:C2B	3.10	0.41
1:K:643:LEU:HD11	1:K:681:GLU:HG2	2.02	0.41
1:B:143:CYS:HG	6:B:807:HEM:HAB	1.81	0.41
1:J:143:CYS:SG	6:J:806:HEM:C3B	3.03	0.41
1:E:311:ASP:C	1:E:311:ASP:OD1	2.59	0.41
1:G:475:LYS:O	1:G:476:ALA:C	2.60	0.41
1:J:94:GLY:O	1:J:98:ILE:HB	2.21	0.41
1:B:305:CYS:HB2	6:B:808:HEM:C3C	2.55	0.41
1:D:84:THR:HG21	1:D:88:LEU:HD21	2.03	0.41
1:E:434:GLU:HB2	1:E:437:ILE:HD12	2.03	0.41
1:F:175:LYS:HE3	1:F:178:ASP:OD2	2.21	0.41
1:B:196:ASP:N	1:B:196:ASP:OD1	2.54	0.40
1:B:659:SER:HB3	1:B:663:HIS:CE1	2.56	0.40
6:G:812:HEM:HMC2	6:G:812:HEM:HBC2	2.03	0.40
1:H:357:ILE:HB	4:H:803:BU3:H11	2.02	0.40
1:I:94:GLY:O	1:I:98:ILE:HB	2.20	0.40
1:B:203:GLY:HA3	6:B:808:HEM:HMA1	2.03	0.40
1:H:421:CYS:SG	6:H:811:HEM:HAC	2.45	0.40
1:J:147:HIS:CE1	6:J:806:HEM:ND	2.89	0.40
1:J:605:TRP:HE3	1:J:662:MET:SD	2.44	0.40
1:D:513:ARG:NH1	6:D:810:HEM:O1A	2.55	0.40
1:E:484:CYS:CB	6:E:812:HEM:C3B	3.05	0.40
1:E:650:THR:HG23	1:E:671:ARG:HB3	2.04	0.40
1:K:203:GLY:HA3	6:K:807:HEM:HMA1	2.03	0.40
6:L:809:HEM:HMB2	6:L:809:HEM:HBB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	657/732 (90%)	632 (96%)	24 (4%)	1 (0%)	47	55
1	B	658/732 (90%)	628 (95%)	29 (4%)	1 (0%)	47	55
1	C	657/732 (90%)	632 (96%)	23 (4%)	2 (0%)	41	46
1	D	657/732 (90%)	624 (95%)	32 (5%)	1 (0%)	47	55
1	E	657/732 (90%)	625 (95%)	30 (5%)	2 (0%)	41	46
1	F	657/732 (90%)	626 (95%)	29 (4%)	2 (0%)	41	46
1	G	656/732 (90%)	625 (95%)	28 (4%)	3 (0%)	29	31
1	H	658/732 (90%)	631 (96%)	26 (4%)	1 (0%)	47	55
1	I	657/732 (90%)	626 (95%)	29 (4%)	2 (0%)	41	46
1	J	657/732 (90%)	623 (95%)	32 (5%)	2 (0%)	41	46
1	K	657/732 (90%)	625 (95%)	31 (5%)	1 (0%)	47	55
1	L	657/732 (90%)	628 (96%)	27 (4%)	2 (0%)	41	46
All	All	7885/8784 (90%)	7525 (95%)	340 (4%)	20 (0%)	41	46

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	476	ALA
1	K	664	GLY
1	L	664	GLY
1	C	301	TYR
1	F	301	TYR
1	J	301	TYR
1	G	301	TYR
1	E	301	TYR
1	I	301	TYR
1	L	206	ARG
1	I	664	GLY
1	B	664	GLY

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Mol	Chain	Res	Type
1	D	664	GLY
1	A	664	GLY
1	F	664	GLY
1	H	664	GLY
1	G	664	GLY
1	C	664	GLY
1	E	664	GLY
1	J	664	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	559/613 (91%)	553 (99%)	6 (1%)	73	85
1	B	560/613 (91%)	555 (99%)	5 (1%)	78	88
1	C	559/613 (91%)	554 (99%)	5 (1%)	78	88
1	D	559/613 (91%)	553 (99%)	6 (1%)	73	85
1	E	559/613 (91%)	555 (99%)	4 (1%)	84	91
1	F	559/613 (91%)	552 (99%)	7 (1%)	69	81
1	G	558/613 (91%)	554 (99%)	4 (1%)	84	91
1	H	560/613 (91%)	555 (99%)	5 (1%)	78	88
1	I	559/613 (91%)	553 (99%)	6 (1%)	73	85
1	J	559/613 (91%)	555 (99%)	4 (1%)	84	91
1	K	559/613 (91%)	554 (99%)	5 (1%)	78	88
1	L	559/613 (91%)	553 (99%)	6 (1%)	73	85
All	All	6709/7356 (91%)	6646 (99%)	63 (1%)	78	88

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	ARG
1	A	250	LEU

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Mol	Chain	Res	Type
1	A	275	ASN
1	A	302	CYS
1	A	498	PHE
1	A	564	ARG
1	B	124	ARG
1	B	270	GLU
1	B	275	ASN
1	B	302	CYS
1	B	564	ARG
1	C	124	ARG
1	C	275	ASN
1	C	302	CYS
1	C	564	ARG
1	C	651	VAL
1	D	124	ARG
1	D	275	ASN
1	D	302	CYS
1	D	498	PHE
1	D	564	ARG
1	D	645	GLU
1	E	124	ARG
1	E	275	ASN
1	E	302	CYS
1	E	564	ARG
1	F	124	ARG
1	F	129	SER
1	F	194	THR
1	F	275	ASN
1	F	302	CYS
1	F	498	PHE
1	F	564	ARG
1	H	124	ARG
1	H	275	ASN
1	H	302	CYS
1	H	564	ARG
1	H	690	LEU
1	I	124	ARG
1	I	275	ASN
1	I	290	LYS
1	I	302	CYS
1	I	498	PHE
1	I	564	ARG

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Mol	Chain	Res	Type
1	J	124	ARG
1	J	275	ASN
1	J	302	CYS
1	J	564	ARG
1	K	124	ARG
1	K	275	ASN
1	K	302	CYS
1	K	303	GLU
1	K	564	ARG
1	L	124	ARG
1	L	194	THR
1	L	275	ASN
1	L	302	CYS
1	L	498	PHE
1	L	564	ARG
1	G	124	ARG
1	G	275	ASN
1	G	302	CYS
1	G	564	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	683	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 161 ligands modelled in this entry, 12 are monoatomic - leaving 149 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
3	SX	L	802	6	0,1,1	0.00	-	-		
6	HEM	L	806	1	27,50,50	1.16	3 (11%)	17,82,82	1.60	4 (23%)
6	HEM	D	808	1	27,50,50	1.25	4 (14%)	17,82,82	1.99	5 (29%)
4	BU3	H	803	-	4,5,5	0.30	0	6,6,6	0.23	0
6	HEM	I	809	1	27,50,50	1.09	4 (14%)	17,82,82	1.53	3 (17%)
6	HEM	E	810	1	27,50,50	1.15	4 (14%)	17,82,82	1.75	4 (23%)
6	HEM	F	814	1	27,50,50	1.14	4 (14%)	17,82,82	1.64	2 (11%)
5	ACT	I	805	-	1,3,3	1.37	0	0,3,3	0.00	-
6	HEM	D	807	1,7	27,50,50	1.12	4 (14%)	17,82,82	1.93	6 (35%)
4	BU3	L	804	-	4,5,5	0.41	0	6,6,6	0.37	0
6	HEM	A	810	1	27,50,50	1.18	4 (14%)	17,82,82	1.78	4 (23%)
6	HEM	H	812	1	27,50,50	1.18	4 (14%)	17,82,82	1.86	6 (35%)
7	SO2	D	802	6	2,2,2	1.88	0	1,1,1	1.82	0
6	HEM	E	809	1	27,50,50	1.13	3 (11%)	17,82,82	1.68	4 (23%)
4	BU3	I	804	-	4,5,5	0.50	0	6,6,6	0.33	0
5	ACT	H	806	-	1,3,3	1.35	0	0,3,3	0.00	-
6	HEM	B	809	1	27,50,50	1.12	3 (11%)	17,82,82	2.08	5 (29%)
6	HEM	C	806	1	27,50,50	1.19	4 (14%)	17,82,82	1.58	4 (23%)
6	HEM	L	809	1	27,50,50	1.13	4 (14%)	17,82,82	1.58	2 (11%)
6	HEM	C	807	1,3	27,50,50	1.14	4 (14%)	17,82,82	1.81	3 (17%)
4	BU3	B	803	-	4,5,5	0.39	0	6,6,6	0.20	0
6	HEM	H	813	1	27,50,50	1.16	4 (14%)	17,82,82	1.63	3 (17%)
3	SX	G	802	6	0,1,1	0.00	-	-		
6	HEM	L	810	1	27,50,50	1.10	4 (14%)	17,82,82	1.76	6 (35%)
6	HEM	D	813	1	27,50,50	1.14	4 (14%)	17,82,82	1.67	3 (17%)
5	ACT	B	806	-	1,3,3	1.73	0	0,3,3	0.00	-
6	HEM	C	808	1	27,50,50	1.19	4 (14%)	17,82,82	2.12	6 (35%)
6	HEM	C	810	1	27,50,50	1.16	4 (14%)	17,82,82	1.72	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	HEM	A	813	1	27,50,50	1.16	3 (11%)	17,82,82	1.80	6 (35%)
6	HEM	G	813	1	27,50,50	1.13	4 (14%)	17,82,82	1.67	5 (29%)
6	HEM	L	808	1	27,50,50	1.14	4 (14%)	17,82,82	1.81	4 (23%)
3	SX	A	802	6	0,1,1	0.00	-	-		
3	SX	K	802	6	0,1,1	0.00	-	-		
6	HEM	K	809	1	27,50,50	1.14	3 (11%)	17,82,82	1.79	3 (17%)
5	ACT	A	805	-	1,3,3	1.63	0	0,3,3	0.00	-
4	BU3	C	804	-	4,5,5	0.32	0	6,6,6	0.30	0
6	HEM	J	806	1	27,50,50	1.25	3 (11%)	17,82,82	1.81	3 (17%)
4	BU3	E	803	-	4,5,5	0.31	0	6,6,6	0.27	0
4	BU3	I	803	-	4,5,5	0.38	0	6,6,6	0.19	0
6	HEM	F	813	1	27,50,50	1.18	4 (14%)	17,82,82	1.74	3 (17%)
6	HEM	E	812	1	27,50,50	1.20	4 (14%)	17,82,82	1.61	4 (23%)
6	HEM	I	810	1	27,50,50	1.10	4 (14%)	17,82,82	1.80	4 (23%)
6	HEM	E	811	1	27,50,50	1.18	3 (11%)	17,82,82	2.06	5 (29%)
6	HEM	J	809	1	27,50,50	1.17	3 (11%)	17,82,82	1.73	4 (23%)
6	HEM	D	810	1	27,50,50	1.18	4 (14%)	17,82,82	1.67	3 (17%)
6	HEM	D	806	1	27,50,50	1.15	4 (14%)	17,82,82	1.59	3 (17%)
3	SX	C	802	6	0,1,1	0.00	-	-		
4	BU3	A	804	-	4,5,5	0.36	0	6,6,6	0.39	0
6	HEM	B	810	1	27,50,50	1.16	4 (14%)	17,82,82	1.70	5 (29%)
5	ACT	F	806	-	1,3,3	1.26	0	0,3,3	0.00	-
6	HEM	J	811	1	27,50,50	1.15	3 (11%)	17,82,82	1.87	4 (23%)
6	HEM	L	812	1	27,50,50	1.13	4 (14%)	17,82,82	1.49	2 (11%)
6	HEM	A	807	1,3,7	27,50,50	1.16	4 (14%)	17,82,82	1.91	5 (29%)
4	BU3	F	803	-	4,5,5	0.37	0	6,6,6	0.43	0
4	BU3	K	804	-	4,5,5	0.49	0	6,6,6	0.29	0
4	BU3	J	804	-	4,5,5	0.45	0	6,6,6	0.24	0
6	HEM	K	810	1	27,50,50	1.15	4 (14%)	17,82,82	1.75	4 (23%)
6	HEM	B	813	1	27,50,50	1.17	4 (14%)	17,82,82	1.67	3 (17%)
6	HEM	G	809	1	27,50,50	1.13	4 (14%)	17,82,82	1.60	3 (17%)
6	HEM	H	811	1	27,50,50	1.15	4 (14%)	17,82,82	1.88	6 (35%)
6	HEM	I	808	1	27,50,50	1.11	4 (14%)	17,82,82	1.91	8 (47%)
4	BU3	D	804	-	4,5,5	0.46	0	6,6,6	0.38	0
4	BU3	L	803	-	4,5,5	0.44	0	6,6,6	0.19	0
3	SX	B	802	6	0,1,1	0.00	-	-		
4	BU3	G	803	-	4,5,5	0.43	0	6,6,6	0.29	0
4	BU3	D	803	-	4,5,5	0.37	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	HEM	D	809	1	27,50,50	1.14	4 (14%)	17,82,82	1.65	3 (17%)
5	ACT	E	805	-	1,3,3	1.39	0	0,3,3	0.00	-
6	HEM	H	814	1	27,50,50	1.17	4 (14%)	17,82,82	1.72	4 (23%)
4	BU3	B	804	-	4,5,5	0.38	0	6,6,6	0.33	0
6	HEM	E	808	1	27,50,50	1.18	4 (14%)	17,82,82	1.98	5 (29%)
4	BU3	F	804	-	4,5,5	0.43	0	6,6,6	0.32	0
6	HEM	C	813	1	27,50,50	1.13	3 (11%)	17,82,82	1.71	4 (23%)
6	HEM	I	812	1	27,50,50	1.16	4 (14%)	17,82,82	1.68	4 (23%)
6	HEM	E	813	1	27,50,50	1.15	4 (14%)	17,82,82	1.69	4 (23%)
6	HEM	L	811	1	27,50,50	1.15	4 (14%)	17,82,82	1.84	5 (29%)
5	ACT	D	805	-	1,3,3	1.54	0	0,3,3	0.00	-
4	BU3	A	803	-	4,5,5	0.36	0	6,6,6	0.34	0
6	HEM	G	806	1	27,50,50	1.14	3 (11%)	17,82,82	1.51	2 (11%)
6	HEM	E	806	1	27,50,50	1.15	3 (11%)	17,82,82	1.59	3 (17%)
3	SX	H	802	6	0,1,1	0.00	-	-	-	-
6	HEM	B	807	1	27,50,50	1.17	4 (14%)	17,82,82	1.62	5 (29%)
4	BU3	B	805	-	4,5,5	0.32	0	6,6,6	0.26	0
6	HEM	J	808	1	27,50,50	1.16	3 (11%)	17,82,82	1.90	5 (29%)
6	HEM	I	807	1,7	27,50,50	1.12	4 (14%)	17,82,82	1.89	4 (23%)
3	SX	E	802	6	0,1,1	0.00	-	-	-	-
6	HEM	F	812	1	27,50,50	1.18	4 (14%)	17,82,82	2.03	5 (29%)
3	SX	J	802	6	0,1,1	0.00	-	-	-	-
5	ACT	L	805	-	1,3,3	1.42	0	0,3,3	0.00	-
6	HEM	H	807	1	27,50,50	1.17	3 (11%)	17,82,82	1.69	4 (23%)
6	HEM	H	809	1	27,50,50	1.16	3 (11%)	17,82,82	1.83	5 (29%)
4	BU3	F	805	-	4,5,5	0.41	0	6,6,6	0.23	0
6	HEM	F	810	1	27,50,50	1.14	3 (11%)	17,82,82	1.63	3 (17%)
5	ACT	C	805	-	1,3,3	1.49	0	0,3,3	0.00	-
6	HEM	B	811	1	27,50,50	1.17	4 (14%)	17,82,82	1.73	5 (29%)
6	HEM	I	806	1	27,50,50	1.13	4 (14%)	17,82,82	1.55	3 (17%)
6	HEM	L	813	1	27,50,50	1.18	4 (14%)	17,82,82	1.71	5 (29%)
5	ACT	G	805	-	1,3,3	1.23	0	0,3,3	0.00	-
6	HEM	L	807	1,3	27,50,50	1.15	3 (11%)	17,82,82	1.80	4 (23%)
6	HEM	G	811	1	27,50,50	1.17	3 (11%)	17,82,82	1.91	6 (35%)
6	HEM	F	809	1	27,50,50	1.16	3 (11%)	17,82,82	1.96	5 (29%)
6	HEM	F	807	1	27,50,50	1.15	3 (11%)	17,82,82	1.66	3 (17%)
6	HEM	G	810	1	27,50,50	1.18	4 (14%)	17,82,82	1.72	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	HEM	B	814	1	27,50,50	1.15	4 (14%)	17,82,82	1.63	3 (17%)
6	HEM	B	808	1,3	27,50,50	1.10	4 (14%)	17,82,82	1.94	5 (29%)
6	HEM	G	812	1	27,50,50	1.16	4 (14%)	17,82,82	1.76	5 (29%)
6	HEM	K	812	1	27,50,50	1.09	4 (14%)	17,82,82	1.58	4 (23%)
6	HEM	F	811	1	27,50,50	1.16	4 (14%)	17,82,82	1.83	4 (23%)
4	BU3	C	803	-	4,5,5	0.34	0	6,6,6	0.34	0
6	HEM	D	812	1	27,50,50	1.23	4 (14%)	17,82,82	1.65	2 (11%)
4	BU3	K	803	-	4,5,5	0.35	0	6,6,6	0.38	0
6	HEM	J	807	1,3	27,50,50	1.12	4 (14%)	17,82,82	1.96	6 (35%)
6	HEM	I	813	1	27,50,50	1.14	4 (14%)	17,82,82	1.82	6 (35%)
6	HEM	G	807	1,3,7	27,50,50	1.15	4 (14%)	17,82,82	1.94	5 (29%)
6	HEM	G	808	1	27,50,50	1.13	4 (14%)	17,82,82	1.91	3 (17%)
6	HEM	K	808	1	27,50,50	1.11	4 (14%)	17,82,82	1.76	3 (17%)
6	HEM	A	809	1	27,50,50	1.17	4 (14%)	17,82,82	1.62	5 (29%)
5	ACT	J	805	-	1,3,3	1.38	0	0,3,3	0.00	-
6	HEM	I	811	1	27,50,50	1.15	4 (14%)	17,82,82	2.02	6 (35%)
6	HEM	A	812	1	27,50,50	1.19	4 (14%)	17,82,82	1.96	7 (41%)
4	BU3	E	804	-	4,5,5	0.30	0	6,6,6	0.28	0
4	BU3	G	804	-	4,5,5	0.39	0	6,6,6	0.27	0
6	HEM	K	807	1,3	27,50,50	1.14	4 (14%)	17,82,82	1.98	6 (35%)
7	SO2	I	802	6	2,2,2	1.90	0	1,1,1	1.79	0
7	SO2	G	814	6	2,2,2	1.80	0	1,1,1	1.88	0
5	ACT	K	805	-	1,3,3	1.48	0	0,3,3	0.00	-
6	HEM	K	806	1	27,50,50	1.25	4 (14%)	17,82,82	1.75	2 (11%)
6	HEM	J	813	1	27,50,50	1.16	4 (14%)	17,82,82	1.71	4 (23%)
6	HEM	J	810	1	27,50,50	1.16	3 (11%)	17,82,82	1.69	4 (23%)
6	HEM	H	810	1	27,50,50	1.10	3 (11%)	17,82,82	1.63	4 (23%)
6	HEM	E	807	1,3	27,50,50	1.13	4 (14%)	17,82,82	1.88	4 (23%)
6	HEM	J	812	1	27,50,50	1.14	3 (11%)	17,82,82	1.73	5 (29%)
6	HEM	H	808	1,3	27,50,50	1.09	4 (14%)	17,82,82	1.91	5 (29%)
6	HEM	B	812	1	27,50,50	1.14	4 (14%)	17,82,82	1.78	6 (35%)
7	SO2	A	814	6	2,2,2	1.81	0	1,1,1	1.71	0
3	SX	F	802	6	0,1,1	0.00	-	-	-	-
6	HEM	K	811	1	27,50,50	1.14	3 (11%)	17,82,82	1.78	5 (29%)
6	HEM	F	808	1,3	27,50,50	1.13	4 (14%)	17,82,82	2.06	6 (35%)
6	HEM	K	813	1	27,50,50	1.13	4 (14%)	17,82,82	1.88	6 (35%)
4	BU3	H	804	-	4,5,5	0.38	0	6,6,6	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BU3	J	803	-	4,5,5	0.32	0	6,6,6	0.30	0
6	HEM	C	809	1	27,50,50	1.17	4 (14%)	17,82,82	1.59	3 (17%)
6	HEM	C	812	1	27,50,50	1.18	4 (14%)	17,82,82	1.66	4 (23%)
6	HEM	C	811	1	27,50,50	1.20	4 (14%)	17,82,82	1.82	3 (17%)
6	HEM	A	811	1	27,50,50	1.24	5 (18%)	17,82,82	1.97	3 (17%)
4	BU3	H	805	-	4,5,5	0.27	0	6,6,6	0.62	0
6	HEM	A	806	1	27,50,50	1.15	3 (11%)	17,82,82	1.72	4 (23%)
6	HEM	A	808	1	27,50,50	1.15	3 (11%)	17,82,82	1.78	5 (29%)
6	HEM	D	811	1	27,50,50	1.18	4 (14%)	17,82,82	1.80	5 (29%)

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
6	HEM	L	806	1	-	1/6/54/54	-
6	HEM	D	808	1	-	0/6/54/54	-
4	BU3	H	803	-	-	0/4/4/4	-
6	HEM	I	809	1	-	0/6/54/54	-
6	HEM	E	810	1	-	0/6/54/54	-
6	HEM	F	814	1	-	0/6/54/54	-
6	HEM	D	807	1,7	-	2/6/54/54	-
4	BU3	L	804	-	-	4/4/4/4	-
6	HEM	A	810	1	-	0/6/54/54	-
6	HEM	H	812	1	-	0/6/54/54	-
6	HEM	E	809	1	-	0/6/54/54	-
4	BU3	I	804	-	-	4/4/4/4	-
6	HEM	B	809	1	-	0/6/54/54	-
6	HEM	C	806	1	-	1/6/54/54	-
6	HEM	L	809	1	-	0/6/54/54	-
6	HEM	C	807	1,3	-	2/6/54/54	-
4	BU3	B	803	-	-	4/4/4/4	-
6	HEM	H	813	1	-	0/6/54/54	-
6	HEM	L	810	1	-	0/6/54/54	-
6	HEM	D	813	1	-	0/6/54/54	-
6	HEM	C	808	1	-	1/6/54/54	-
6	HEM	C	810	1	-	0/6/54/54	-
6	HEM	A	813	1	-	0/6/54/54	-
6	HEM	G	813	1	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HEM	L	808	1	-	1/6/54/54	-
6	HEM	K	809	1	-	0/6/54/54	-
6	HEM	A	807	1,3,7	-	2/6/54/54	-
4	BU3	C	804	-	-	4/4/4/4	-
6	HEM	J	806	1	-	1/6/54/54	-
4	BU3	E	803	-	-	2/4/4/4	-
4	BU3	I	803	-	-	4/4/4/4	-
6	HEM	F	813	1	-	0/6/54/54	-
6	HEM	E	812	1	-	0/6/54/54	-
6	HEM	I	810	1	-	0/6/54/54	-
6	HEM	E	811	1	-	0/6/54/54	-
6	HEM	J	809	1	-	0/6/54/54	-
6	HEM	D	810	1	-	0/6/54/54	-
6	HEM	D	806	1	-	1/6/54/54	-
4	BU3	A	804	-	-	4/4/4/4	-
6	HEM	B	810	1	-	0/6/54/54	-
6	HEM	J	811	1	-	0/6/54/54	-
6	HEM	L	812	1	-	0/6/54/54	-
4	BU3	F	803	-	-	4/4/4/4	-
4	BU3	K	804	-	-	4/4/4/4	-
4	BU3	J	804	-	-	4/4/4/4	-
6	HEM	K	810	1	-	0/6/54/54	-
6	HEM	B	813	1	-	0/6/54/54	-
6	HEM	G	809	1	-	0/6/54/54	-
6	HEM	H	811	1	-	0/6/54/54	-
6	HEM	I	808	1	-	1/6/54/54	-
4	BU3	D	804	-	-	4/4/4/4	-
4	BU3	L	803	-	-	4/4/4/4	-
4	BU3	G	803	-	-	4/4/4/4	-
4	BU3	D	803	-	-	0/4/4/4	-
6	HEM	D	809	1	-	0/6/54/54	-
6	HEM	H	814	1	-	0/6/54/54	-
4	BU3	B	804	-	-	4/4/4/4	-
6	HEM	E	808	1	-	1/6/54/54	-
4	BU3	F	804	-	-	4/4/4/4	-
6	HEM	C	813	1	-	0/6/54/54	-
6	HEM	I	812	1	-	0/6/54/54	-
6	HEM	E	813	1	-	0/6/54/54	-
6	HEM	L	811	1	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BU3	A	803	-	-	4/4/4/4	-
6	HEM	G	806	1	-	1/6/54/54	-
6	HEM	E	806	1	-	1/6/54/54	-
6	HEM	B	807	1	-	1/6/54/54	-
4	BU3	B	805	-	-	0/4/4/4	-
6	HEM	J	808	1	-	1/6/54/54	-
6	HEM	I	807	1,7	-	2/6/54/54	-
6	HEM	F	812	1	-	0/6/54/54	-
6	HEM	H	807	1	-	1/6/54/54	-
6	HEM	H	809	1	-	0/6/54/54	-
4	BU3	F	805	-	-	4/4/4/4	-
6	HEM	F	810	1	-	0/6/54/54	-
6	HEM	B	811	1	-	0/6/54/54	-
6	HEM	I	806	1	-	1/6/54/54	-
6	HEM	L	813	1	-	0/6/54/54	-
6	HEM	L	807	1,3	-	2/6/54/54	-
6	HEM	G	811	1	-	0/6/54/54	-
6	HEM	F	809	1	-	1/6/54/54	-
6	HEM	F	807	1	-	1/6/54/54	-
6	HEM	G	810	1	-	0/6/54/54	-
6	HEM	B	814	1	-	0/6/54/54	-
6	HEM	B	808	1,3	-	3/6/54/54	-
6	HEM	G	812	1	-	0/6/54/54	-
6	HEM	K	812	1	-	0/6/54/54	-
6	HEM	F	811	1	-	0/6/54/54	-
4	BU3	C	803	-	-	4/4/4/4	-
6	HEM	D	812	1	-	0/6/54/54	-
4	BU3	K	803	-	-	0/4/4/4	-
6	HEM	J	807	1,3	-	2/6/54/54	-
6	HEM	I	813	1	-	0/6/54/54	-
6	HEM	G	807	1,3,7	-	2/6/54/54	-
6	HEM	G	808	1	-	2/6/54/54	-
6	HEM	K	808	1	-	1/6/54/54	-
6	HEM	A	809	1	-	0/6/54/54	-
6	HEM	I	811	1	-	0/6/54/54	-
6	HEM	A	812	1	-	0/6/54/54	-
4	BU3	E	804	-	-	0/4/4/4	-
4	BU3	G	804	-	-	0/4/4/4	-
6	HEM	K	807	1,3	-	2/6/54/54	-
6	HEM	K	806	1	-	1/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HEM	J	813	1	-	2/6/54/54	-
6	HEM	J	810	1	-	0/6/54/54	-
6	HEM	H	810	1	-	0/6/54/54	-
6	HEM	E	807	1,3	-	2/6/54/54	-
6	HEM	J	812	1	-	0/6/54/54	-
6	HEM	H	808	1,3	-	2/6/54/54	-
6	HEM	B	812	1	-	0/6/54/54	-
6	HEM	K	811	1	-	0/6/54/54	-
6	HEM	F	808	1,3	-	2/6/54/54	-
6	HEM	K	813	1	-	0/6/54/54	-
4	BU3	H	804	-	-	4/4/4/4	-
4	BU3	J	803	-	-	4/4/4/4	-
6	HEM	C	809	1	-	0/6/54/54	-
6	HEM	C	812	1	-	0/6/54/54	-
6	HEM	C	811	1	-	0/6/54/54	-
6	HEM	A	811	1	-	0/6/54/54	-
4	BU3	H	805	-	-	0/4/4/4	-
6	HEM	A	806	1	-	1/6/54/54	-
6	HEM	A	808	1	-	1/6/54/54	-
6	HEM	D	811	1	-	0/6/54/54	-

All (359) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	812	HEM	C4B-NB	-3.19	1.29	1.36
6	D	812	HEM	C4B-NB	-3.14	1.29	1.36
6	K	806	HEM	C3B-C2B	-3.10	1.36	1.40
6	E	812	HEM	C4B-NB	-3.04	1.29	1.36
6	G	810	HEM	CBB-CAB	2.99	1.49	1.29
6	H	810	HEM	CBC-CAC	2.97	1.49	1.29
6	L	812	HEM	CBB-CAB	2.96	1.48	1.29
6	J	810	HEM	CBB-CAB	2.96	1.48	1.29
6	G	806	HEM	CBC-CAC	2.95	1.48	1.29
6	G	811	HEM	CBC-CAC	2.94	1.48	1.29
6	L	806	HEM	CBC-CAC	2.94	1.48	1.29
6	C	813	HEM	CBB-CAB	2.94	1.48	1.29
6	C	809	HEM	CBB-CAB	2.94	1.48	1.29
6	F	813	HEM	CBB-CAB	2.93	1.48	1.29
6	G	809	HEM	CBB-CAB	2.93	1.48	1.29
6	K	806	HEM	CBC-CAC	2.93	1.48	1.29
6	F	809	HEM	CBB-CAB	2.93	1.48	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	809	HEM	CBC-CAC	2.92	1.48	1.29
6	C	811	HEM	CBC-CAC	2.92	1.48	1.29
6	H	807	HEM	CBC-CAC	2.92	1.48	1.29
6	B	813	HEM	CBB-CAB	2.92	1.48	1.29
6	A	809	HEM	CBC-CAC	2.92	1.48	1.29
6	C	810	HEM	CBB-CAB	2.92	1.48	1.29
6	I	811	HEM	CBC-CAC	2.92	1.48	1.29
6	E	813	HEM	CBC-CAC	2.91	1.48	1.29
6	I	806	HEM	CBC-CAC	2.91	1.48	1.29
6	F	807	HEM	CBC-CAC	2.91	1.48	1.29
6	F	814	HEM	CBB-CAB	2.91	1.48	1.29
6	G	811	HEM	CBB-CAB	2.91	1.48	1.29
6	H	814	HEM	C4B-NB	-2.91	1.30	1.36
6	E	812	HEM	CBC-CAC	2.91	1.48	1.29
6	L	811	HEM	CBC-CAC	2.91	1.48	1.29
6	H	812	HEM	CBC-CAC	2.91	1.48	1.29
6	K	810	HEM	CBB-CAB	2.91	1.48	1.29
6	L	809	HEM	CBB-CAB	2.91	1.48	1.29
6	D	811	HEM	CBC-CAC	2.90	1.48	1.29
6	C	806	HEM	CBB-CAB	2.90	1.48	1.29
6	J	813	HEM	CBC-CAC	2.90	1.48	1.29
6	B	812	HEM	CBC-CAC	2.90	1.48	1.29
6	J	813	HEM	CBB-CAB	2.90	1.48	1.29
6	E	811	HEM	CBB-CAB	2.90	1.48	1.29
6	E	811	HEM	CBC-CAC	2.90	1.48	1.29
6	H	814	HEM	CBB-CAB	2.90	1.48	1.29
6	B	812	HEM	CBB-CAB	2.90	1.48	1.29
6	J	809	HEM	CBB-CAB	2.90	1.48	1.29
6	H	807	HEM	CBB-CAB	2.90	1.48	1.29
6	J	806	HEM	CBC-CAC	2.90	1.48	1.29
6	L	810	HEM	CBB-CAB	2.89	1.48	1.29
6	D	808	HEM	C4B-NB	-2.89	1.30	1.36
6	B	814	HEM	CBB-CAB	2.89	1.48	1.29
6	J	812	HEM	CBB-CAB	2.89	1.48	1.29
6	A	812	HEM	CBB-CAB	2.89	1.48	1.29
6	K	813	HEM	CBB-CAB	2.89	1.48	1.29
6	K	811	HEM	CBB-CAB	2.89	1.48	1.29
6	L	813	HEM	CBB-CAB	2.88	1.48	1.29
6	G	806	HEM	CBB-CAB	2.88	1.48	1.29
6	I	813	HEM	CBB-CAB	2.88	1.48	1.29
6	E	806	HEM	CBB-CAB	2.88	1.48	1.29
6	F	808	HEM	CBB-CAB	2.88	1.48	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	808	HEM	CBB-CAB	2.88	1.48	1.29
6	G	813	HEM	CBB-CAB	2.88	1.48	1.29
6	C	807	HEM	CBC-CAC	2.88	1.48	1.29
6	B	810	HEM	CBC-CAC	2.88	1.48	1.29
6	J	811	HEM	CBB-CAB	2.88	1.48	1.29
6	C	808	HEM	CBB-CAB	2.88	1.48	1.29
6	K	813	HEM	CBC-CAC	2.87	1.48	1.29
6	J	812	HEM	CBC-CAC	2.87	1.48	1.29
6	J	806	HEM	C3B-C2B	-2.87	1.36	1.40
6	J	809	HEM	CBC-CAC	2.87	1.48	1.29
6	J	807	HEM	CBC-CAC	2.87	1.48	1.29
6	E	810	HEM	CBB-CAB	2.87	1.48	1.29
6	E	809	HEM	CBC-CAC	2.87	1.48	1.29
6	D	806	HEM	CBC-CAC	2.87	1.48	1.29
6	I	806	HEM	CBB-CAB	2.87	1.48	1.29
6	A	807	HEM	CBC-CAC	2.87	1.48	1.29
6	E	807	HEM	CBC-CAC	2.87	1.48	1.29
6	G	812	HEM	CBB-CAB	2.86	1.48	1.29
6	H	812	HEM	C4B-NB	-2.86	1.30	1.36
6	J	811	HEM	CBC-CAC	2.86	1.48	1.29
6	G	807	HEM	CBB-CAB	2.86	1.48	1.29
6	E	806	HEM	CBC-CAC	2.86	1.48	1.29
6	K	809	HEM	CBC-CAC	2.86	1.48	1.29
6	A	813	HEM	CBC-CAC	2.86	1.48	1.29
6	E	811	HEM	C4B-NB	-2.86	1.30	1.36
6	G	809	HEM	CBC-CAC	2.86	1.48	1.29
6	D	813	HEM	CBC-CAC	2.86	1.48	1.29
6	I	813	HEM	CBC-CAC	2.85	1.48	1.29
6	G	812	HEM	CBC-CAC	2.85	1.48	1.29
6	K	812	HEM	CBB-CAB	2.85	1.48	1.29
6	J	807	HEM	CBB-CAB	2.85	1.48	1.29
6	G	813	HEM	CBC-CAC	2.85	1.48	1.29
6	B	810	HEM	CBB-CAB	2.85	1.48	1.29
6	L	812	HEM	CBC-CAC	2.85	1.48	1.29
6	H	814	HEM	CBC-CAC	2.85	1.48	1.29
6	D	813	HEM	CBB-CAB	2.85	1.48	1.29
6	F	810	HEM	CBC-CAC	2.85	1.48	1.29
6	K	808	HEM	CBC-CAC	2.85	1.48	1.29
6	D	811	HEM	CBB-CAB	2.84	1.48	1.29
6	A	810	HEM	CBB-CAB	2.84	1.48	1.29
6	D	812	HEM	CBC-CAC	2.84	1.48	1.29
6	A	812	HEM	CBC-CAC	2.84	1.48	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	814	HEM	CBC-CAC	2.84	1.48	1.29
6	K	811	HEM	CBC-CAC	2.84	1.48	1.29
6	I	809	HEM	CBC-CAC	2.84	1.48	1.29
6	F	807	HEM	C4B-NB	-2.84	1.30	1.36
6	L	806	HEM	CBB-CAB	2.84	1.48	1.29
6	C	813	HEM	CBC-CAC	2.84	1.48	1.29
6	I	807	HEM	CBC-CAC	2.83	1.48	1.29
6	E	809	HEM	CBB-CAB	2.83	1.48	1.29
6	A	813	HEM	CBB-CAB	2.83	1.48	1.29
6	F	808	HEM	CBC-CAC	2.83	1.48	1.29
6	H	809	HEM	CBB-CAB	2.83	1.48	1.29
6	L	807	HEM	CBC-CAC	2.83	1.48	1.29
6	F	814	HEM	CBC-CAC	2.83	1.48	1.29
6	E	813	HEM	CBB-CAB	2.83	1.48	1.29
6	J	810	HEM	CBC-CAC	2.83	1.48	1.29
6	L	807	HEM	CBB-CAB	2.83	1.48	1.29
6	H	811	HEM	CBB-CAB	2.83	1.48	1.29
6	A	806	HEM	CBC-CAC	2.83	1.48	1.29
6	D	809	HEM	CBC-CAC	2.83	1.48	1.29
6	H	813	HEM	CBC-CAC	2.83	1.48	1.29
6	A	811	HEM	CBC-CAC	2.82	1.48	1.29
6	D	810	HEM	CBB-CAB	2.82	1.48	1.29
6	C	809	HEM	CBC-CAC	2.82	1.48	1.29
6	H	812	HEM	CBB-CAB	2.82	1.48	1.29
6	C	813	HEM	C4B-NB	-2.82	1.30	1.36
6	A	812	HEM	C4B-NB	-2.82	1.30	1.36
6	D	810	HEM	CBC-CAC	2.82	1.47	1.29
6	C	811	HEM	CBB-CAB	2.82	1.47	1.29
6	B	809	HEM	CBB-CAB	2.81	1.47	1.29
6	I	812	HEM	CBB-CAB	2.81	1.47	1.29
6	G	807	HEM	CBC-CAC	2.81	1.47	1.29
6	L	808	HEM	CBC-CAC	2.81	1.47	1.29
6	L	811	HEM	CBB-CAB	2.81	1.47	1.29
6	I	812	HEM	CBC-CAC	2.81	1.47	1.29
6	B	811	HEM	CBB-CAB	2.81	1.47	1.29
6	C	812	HEM	CBC-CAC	2.81	1.47	1.29
6	D	809	HEM	CBB-CAB	2.81	1.47	1.29
6	H	809	HEM	C4B-NB	-2.81	1.30	1.36
6	I	810	HEM	CBB-CAB	2.81	1.47	1.29
6	H	813	HEM	CBB-CAB	2.81	1.47	1.29
6	K	808	HEM	CBB-CAB	2.80	1.47	1.29
6	F	811	HEM	CBC-CAC	2.80	1.47	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	811	HEM	C4B-NB	-2.80	1.30	1.36
6	B	807	HEM	CBC-CAC	2.80	1.47	1.29
6	C	806	HEM	CBC-CAC	2.80	1.47	1.29
6	H	809	HEM	CBC-CAC	2.80	1.47	1.29
6	J	808	HEM	C4B-NB	-2.80	1.30	1.36
6	B	807	HEM	C4B-NB	-2.80	1.30	1.36
6	F	810	HEM	CBB-CAB	2.80	1.47	1.29
6	I	811	HEM	C4B-NB	-2.80	1.30	1.36
6	B	808	HEM	CBC-CAC	2.79	1.47	1.29
6	I	808	HEM	CBB-CAB	2.79	1.47	1.29
6	A	808	HEM	C4B-NB	-2.79	1.30	1.36
6	F	813	HEM	CBC-CAC	2.79	1.47	1.29
6	H	808	HEM	CBB-CAB	2.79	1.47	1.29
6	C	812	HEM	CBB-CAB	2.79	1.47	1.29
6	G	808	HEM	CBC-CAC	2.79	1.47	1.29
6	A	806	HEM	CBB-CAB	2.79	1.47	1.29
6	C	808	HEM	CBC-CAC	2.79	1.47	1.29
6	C	810	HEM	C4B-NB	-2.79	1.30	1.36
6	K	809	HEM	CBB-CAB	2.79	1.47	1.29
6	E	812	HEM	CBB-CAB	2.79	1.47	1.29
6	A	809	HEM	CBB-CAB	2.79	1.47	1.29
6	D	808	HEM	CBB-CAB	2.79	1.47	1.29
6	J	808	HEM	CBB-CAB	2.78	1.47	1.29
6	C	812	HEM	C4B-NB	-2.78	1.30	1.36
6	F	813	HEM	C4B-NB	-2.78	1.30	1.36
6	I	810	HEM	CBC-CAC	2.78	1.47	1.29
6	E	807	HEM	CBB-CAB	2.78	1.47	1.29
6	F	812	HEM	CBC-CAC	2.78	1.47	1.29
6	I	811	HEM	CBB-CAB	2.78	1.47	1.29
6	A	806	HEM	C4B-NB	-2.78	1.30	1.36
6	C	806	HEM	C4B-NB	-2.77	1.30	1.36
6	D	807	HEM	CBC-CAC	2.77	1.47	1.29
6	A	808	HEM	CBB-CAB	2.77	1.47	1.29
6	F	811	HEM	CBB-CAB	2.77	1.47	1.29
6	K	807	HEM	CBC-CAC	2.77	1.47	1.29
6	L	808	HEM	CBB-CAB	2.77	1.47	1.29
6	G	810	HEM	CBC-CAC	2.77	1.47	1.29
6	K	812	HEM	CBC-CAC	2.76	1.47	1.29
6	L	810	HEM	CBC-CAC	2.76	1.47	1.29
6	D	807	HEM	CBB-CAB	2.76	1.47	1.29
6	H	810	HEM	CBB-CAB	2.76	1.47	1.29
6	A	813	HEM	C4B-NB	-2.76	1.30	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	808	HEM	CBB-CAB	2.76	1.47	1.29
6	E	808	HEM	CBC-CAC	2.76	1.47	1.29
6	H	811	HEM	CBC-CAC	2.76	1.47	1.29
6	B	807	HEM	CBB-CAB	2.76	1.47	1.29
6	C	808	HEM	C4B-NB	-2.76	1.30	1.36
6	B	813	HEM	C4B-NB	-2.76	1.30	1.36
6	H	808	HEM	CBC-CAC	2.76	1.47	1.29
6	A	807	HEM	CBB-CAB	2.75	1.47	1.29
6	I	809	HEM	CBB-CAB	2.75	1.47	1.29
6	A	811	HEM	C3B-C2B	-2.75	1.36	1.40
6	B	813	HEM	CBC-CAC	2.75	1.47	1.29
6	D	812	HEM	CBB-CAB	2.75	1.47	1.29
6	I	807	HEM	CBB-CAB	2.74	1.47	1.29
6	C	807	HEM	CBB-CAB	2.74	1.47	1.29
6	B	811	HEM	C4B-NB	-2.74	1.30	1.36
6	D	811	HEM	C4B-NB	-2.74	1.30	1.36
6	K	811	HEM	C4B-NB	-2.74	1.30	1.36
6	J	806	HEM	CBB-CAB	2.73	1.47	1.29
6	E	810	HEM	CBC-CAC	2.73	1.47	1.29
6	B	808	HEM	CBB-CAB	2.73	1.47	1.29
6	K	810	HEM	CBC-CAC	2.72	1.47	1.29
6	J	811	HEM	C4B-NB	-2.72	1.30	1.36
6	F	809	HEM	CBC-CAC	2.72	1.47	1.29
6	H	813	HEM	C4B-NB	-2.72	1.30	1.36
6	F	807	HEM	CBB-CAB	2.72	1.47	1.29
6	A	809	HEM	C4B-NB	-2.72	1.30	1.36
6	A	808	HEM	CBC-CAC	2.72	1.47	1.29
6	B	811	HEM	CBC-CAC	2.71	1.47	1.29
6	C	810	HEM	CBC-CAC	2.71	1.47	1.29
6	A	810	HEM	C4B-NB	-2.71	1.30	1.36
6	A	811	HEM	CBB-CAB	2.71	1.47	1.29
6	K	806	HEM	CBB-CAB	2.71	1.47	1.29
6	I	808	HEM	CBC-CAC	2.71	1.47	1.29
6	G	808	HEM	C4B-NB	-2.71	1.30	1.36
6	K	807	HEM	CBB-CAB	2.71	1.47	1.29
6	J	808	HEM	CBC-CAC	2.70	1.47	1.29
6	G	811	HEM	C4B-NB	-2.69	1.30	1.36
6	A	810	HEM	CBC-CAC	2.69	1.47	1.29
6	D	808	HEM	CBC-CAC	2.69	1.47	1.29
6	I	812	HEM	C4B-NB	-2.68	1.30	1.36
6	A	807	HEM	C4B-NB	-2.68	1.30	1.36
6	I	808	HEM	C4B-NB	-2.67	1.30	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	809	HEM	CBC-CAC	2.67	1.47	1.29
6	F	812	HEM	CBB-CAB	2.67	1.46	1.29
6	F	809	HEM	C4B-NB	-2.65	1.30	1.36
6	G	812	HEM	C4B-NB	-2.65	1.30	1.36
6	E	808	HEM	C4B-NB	-2.64	1.30	1.36
6	B	814	HEM	C4B-NB	-2.63	1.30	1.36
6	D	810	HEM	C4B-NB	-2.62	1.30	1.36
6	G	810	HEM	C4B-NB	-2.61	1.30	1.36
6	D	806	HEM	CBB-CAB	2.60	1.46	1.29
6	D	806	HEM	C4B-NB	-2.60	1.30	1.36
6	J	813	HEM	C4B-NB	-2.60	1.30	1.36
6	E	806	HEM	C4B-NB	-2.59	1.30	1.36
6	F	811	HEM	C4B-NB	-2.59	1.30	1.36
6	L	806	HEM	C4B-NB	-2.59	1.30	1.36
6	K	810	HEM	C4B-NB	-2.59	1.30	1.36
6	J	810	HEM	C4B-NB	-2.58	1.30	1.36
6	E	813	HEM	C4B-NB	-2.57	1.30	1.36
6	L	808	HEM	C4B-NB	-2.57	1.30	1.36
6	E	810	HEM	C4B-NB	-2.56	1.30	1.36
6	D	807	HEM	C4D-C3D	2.56	1.48	1.42
6	H	807	HEM	C4B-NB	-2.55	1.30	1.36
6	F	814	HEM	C4B-NB	-2.54	1.30	1.36
6	C	807	HEM	C4B-NB	-2.54	1.30	1.36
6	D	813	HEM	C4B-NB	-2.54	1.30	1.36
6	K	807	HEM	C4B-NB	-2.53	1.30	1.36
6	E	807	HEM	C4B-NB	-2.53	1.30	1.36
6	G	807	HEM	C4B-NB	-2.52	1.31	1.36
6	J	812	HEM	C4B-NB	-2.50	1.31	1.36
6	D	807	HEM	C4B-NB	-2.50	1.31	1.36
6	B	809	HEM	C4B-NB	-2.49	1.31	1.36
6	L	813	HEM	CBC-CAC	2.49	1.45	1.29
6	G	806	HEM	C4B-NB	-2.48	1.31	1.36
6	D	810	HEM	C4D-C3D	2.45	1.48	1.42
6	L	813	HEM	C4B-NB	-2.44	1.31	1.36
6	F	808	HEM	C4D-C3D	2.44	1.48	1.42
6	K	808	HEM	C4B-NB	-2.44	1.31	1.36
6	K	809	HEM	C4B-NB	-2.44	1.31	1.36
6	I	807	HEM	C4B-NB	-2.43	1.31	1.36
6	L	812	HEM	C4B-NB	-2.43	1.31	1.36
6	E	809	HEM	C4B-NB	-2.42	1.31	1.36
6	E	807	HEM	C4D-C3D	2.42	1.48	1.42
6	D	809	HEM	C4B-NB	-2.42	1.31	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	813	HEM	C4B-NB	-2.41	1.31	1.36
6	L	811	HEM	C4B-NB	-2.41	1.31	1.36
6	G	813	HEM	C4D-C3D	2.40	1.48	1.42
6	E	812	HEM	C4D-C3D	2.40	1.48	1.42
6	H	811	HEM	C4B-NB	-2.39	1.31	1.36
6	B	813	HEM	C4D-C3D	2.38	1.48	1.42
6	L	807	HEM	C4B-NB	-2.38	1.31	1.36
6	B	812	HEM	C4B-NB	-2.37	1.31	1.36
6	K	810	HEM	C4D-C3D	2.37	1.47	1.42
6	B	808	HEM	C4D-C3D	2.37	1.47	1.42
6	I	809	HEM	C4B-NB	-2.37	1.31	1.36
6	I	813	HEM	C4B-NB	-2.37	1.31	1.36
6	B	808	HEM	C4B-NB	-2.37	1.31	1.36
6	G	807	HEM	C4D-C3D	2.36	1.47	1.42
6	H	811	HEM	C4D-C3D	2.36	1.47	1.42
6	I	810	HEM	C4B-NB	-2.35	1.31	1.36
6	B	814	HEM	C4D-C3D	2.35	1.47	1.42
6	I	806	HEM	C4B-NB	-2.35	1.31	1.36
6	I	812	HEM	C4D-C3D	2.34	1.47	1.42
6	C	809	HEM	C4B-NB	-2.33	1.31	1.36
6	F	810	HEM	C4B-NB	-2.33	1.31	1.36
6	L	810	HEM	C4B-NB	-2.31	1.31	1.36
6	J	807	HEM	C4B-NB	-2.31	1.31	1.36
6	C	810	HEM	C4D-C3D	2.31	1.47	1.42
6	L	811	HEM	C4D-C3D	2.31	1.47	1.42
6	G	810	HEM	C4D-C3D	2.31	1.47	1.42
6	C	812	HEM	C4D-C3D	2.30	1.47	1.42
6	H	808	HEM	C4B-NB	-2.30	1.31	1.36
6	B	811	HEM	C4D-C3D	2.30	1.47	1.42
6	J	813	HEM	C4D-C3D	2.28	1.47	1.42
6	J	807	HEM	C4D-C3D	2.27	1.47	1.42
6	H	808	HEM	C4D-C3D	2.27	1.47	1.42
6	A	810	HEM	C4D-C3D	2.27	1.47	1.42
6	D	811	HEM	C4D-C3D	2.27	1.47	1.42
6	D	808	HEM	C4D-C3D	2.25	1.47	1.42
6	K	807	HEM	C4D-C3D	2.25	1.47	1.42
6	C	809	HEM	C4D-C3D	2.25	1.47	1.42
6	B	810	HEM	C4B-NB	-2.24	1.31	1.36
6	L	812	HEM	C4D-C3D	2.24	1.47	1.42
6	H	813	HEM	C4D-C3D	2.23	1.47	1.42
6	F	808	HEM	C4B-NB	-2.23	1.31	1.36
6	F	813	HEM	C4D-C3D	2.23	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	810	HEM	C4B-NB	-2.22	1.31	1.36
6	I	811	HEM	C4D-C3D	2.22	1.47	1.42
6	K	813	HEM	C4B-NB	-2.22	1.31	1.36
6	D	813	HEM	C4D-C3D	2.22	1.47	1.42
6	J	809	HEM	C4B-NB	-2.22	1.31	1.36
6	D	809	HEM	C4D-C3D	2.21	1.47	1.42
6	A	811	HEM	C4B-NB	-2.21	1.31	1.36
6	G	809	HEM	C4D-C3D	2.19	1.47	1.42
6	E	808	HEM	C4D-C3D	2.19	1.47	1.42
6	K	812	HEM	C4B-NB	-2.18	1.31	1.36
6	K	812	HEM	C4D-C3D	2.17	1.47	1.42
6	B	812	HEM	C4D-C3D	2.17	1.47	1.42
6	L	810	HEM	C4D-C3D	2.16	1.47	1.42
6	A	807	HEM	C4D-C3D	2.15	1.47	1.42
6	B	810	HEM	C4D-C3D	2.15	1.47	1.42
6	L	808	HEM	C4D-C3D	2.14	1.47	1.42
6	D	806	HEM	C4D-C3D	2.14	1.47	1.42
6	I	813	HEM	C4D-C3D	2.12	1.47	1.42
6	I	808	HEM	C4D-C3D	2.12	1.47	1.42
6	E	810	HEM	C4D-C3D	2.11	1.47	1.42
6	G	809	HEM	C4B-NB	-2.10	1.31	1.36
6	I	809	HEM	C4D-C3D	2.10	1.47	1.42
6	B	807	HEM	C4D-C3D	2.10	1.47	1.42
6	D	812	HEM	C4D-C3D	2.09	1.47	1.42
6	C	811	HEM	C4D-C3D	2.09	1.47	1.42
6	F	814	HEM	C4D-C3D	2.09	1.47	1.42
6	A	809	HEM	C4D-C3D	2.08	1.47	1.42
6	G	812	HEM	C4D-C3D	2.08	1.47	1.42
6	G	808	HEM	C4D-C3D	2.07	1.47	1.42
6	K	808	HEM	C4D-C3D	2.07	1.47	1.42
6	K	813	HEM	C4D-C3D	2.06	1.47	1.42
6	F	812	HEM	C4D-C3D	2.06	1.47	1.42
6	C	807	HEM	C4D-C3D	2.05	1.47	1.42
6	C	808	HEM	C4D-C3D	2.05	1.47	1.42
6	L	809	HEM	C4D-C3D	2.05	1.47	1.42
6	C	806	HEM	C4D-C3D	2.03	1.47	1.42
6	L	809	HEM	C4B-NB	-2.03	1.32	1.36
6	A	812	HEM	C4D-C3D	2.02	1.47	1.42
6	L	813	HEM	C4D-C3D	2.02	1.47	1.42
6	I	810	HEM	C4D-C3D	2.02	1.47	1.42
6	I	806	HEM	C4D-C3D	2.02	1.47	1.42
6	A	811	HEM	C4D-C3D	2.02	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	806	HEM	C4D-C3D	2.01	1.47	1.42
6	E	813	HEM	C4D-C3D	2.01	1.47	1.42
6	F	811	HEM	C4D-C3D	2.01	1.47	1.42
6	H	812	HEM	C4D-C3D	2.01	1.47	1.42
6	I	807	HEM	C4D-C3D	2.01	1.47	1.42
6	H	814	HEM	C4D-C3D	2.00	1.47	1.42

All (409) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	806	HEM	C3B-C4B-NB	-5.88	101.61	109.21
6	A	811	HEM	C3B-C4B-NB	-5.75	101.77	109.21
6	J	806	HEM	C3B-C4B-NB	-5.74	101.79	109.21
6	F	813	HEM	C3B-C4B-NB	-5.05	102.68	109.21
6	I	811	HEM	C3B-C4B-NB	-4.95	102.81	109.21
6	B	809	HEM	C3B-C4B-NB	-4.91	102.86	109.21
6	F	812	HEM	C3B-C4B-NB	-4.90	102.88	109.21
6	E	811	HEM	C3B-C4B-NB	-4.88	102.90	109.21
6	C	811	HEM	C3B-C4B-NB	-4.88	102.90	109.21
6	D	808	HEM	C3B-C4B-NB	-4.85	102.94	109.21
6	A	812	HEM	C3B-C4B-NB	-4.75	103.06	109.21
6	J	811	HEM	C3B-C4B-NB	-4.74	103.08	109.21
6	A	806	HEM	C3B-C4B-NB	-4.64	103.21	109.21
6	C	808	HEM	C3B-C4B-NB	-4.61	103.26	109.21
6	J	812	HEM	C3B-C4B-NB	-4.60	103.26	109.21
6	G	811	HEM	C3B-C4B-NB	-4.59	103.28	109.21
6	D	810	HEM	C3B-C4B-NB	-4.58	103.28	109.21
6	C	812	HEM	C3B-C4B-NB	-4.58	103.29	109.21
6	D	811	HEM	C3B-C4B-NB	-4.57	103.31	109.21
6	G	806	HEM	C3B-C4B-NB	-4.56	103.31	109.21
6	H	807	HEM	C3B-C4B-NB	-4.54	103.34	109.21
6	D	807	HEM	C3B-C4B-NB	-4.54	103.34	109.21
6	F	807	HEM	C3B-C4B-NB	-4.54	103.34	109.21
6	A	810	HEM	C3B-C4B-NB	-4.53	103.35	109.21
6	D	812	HEM	C3B-C4B-NB	-4.52	103.37	109.21
6	F	809	HEM	C3B-C4B-NB	-4.50	103.39	109.21
6	L	807	HEM	C3B-C4B-NB	-4.50	103.39	109.21
6	E	808	HEM	C3B-C4B-NB	-4.50	103.39	109.21
6	H	811	HEM	C3B-C4B-NB	-4.49	103.41	109.21
6	I	807	HEM	C3B-C4B-NB	-4.48	103.41	109.21
6	I	812	HEM	C3B-C4B-NB	-4.48	103.42	109.21
6	H	813	HEM	C3B-C4B-NB	-4.48	103.42	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	811	HEM	C3B-C4B-NB	-4.47	103.43	109.21
6	G	807	HEM	C3B-C4B-NB	-4.47	103.43	109.21
6	K	807	HEM	C3B-C4B-NB	-4.46	103.44	109.21
6	C	806	HEM	C3B-C4B-NB	-4.43	103.48	109.21
6	H	808	HEM	C3B-C4B-NB	-4.43	103.48	109.21
6	F	814	HEM	C3B-C4B-NB	-4.42	103.50	109.21
6	E	810	HEM	C3B-C4B-NB	-4.42	103.50	109.21
6	G	810	HEM	C3B-C4B-NB	-4.41	103.50	109.21
6	J	807	HEM	C3B-C4B-NB	-4.40	103.52	109.21
6	B	813	HEM	C3B-C4B-NB	-4.40	103.52	109.21
6	E	807	HEM	C3B-C4B-NB	-4.40	103.52	109.21
6	C	810	HEM	C3B-C4B-NB	-4.39	103.53	109.21
6	B	807	HEM	C3B-C4B-NB	-4.39	103.53	109.21
6	K	811	HEM	C3B-C4B-NB	-4.37	103.56	109.21
6	B	812	HEM	C3B-C4B-NB	-4.35	103.59	109.21
6	C	808	HEM	CBA-CAA-C2A	-4.33	104.50	112.49
6	B	808	HEM	C3B-C4B-NB	-4.32	103.63	109.21
6	A	807	HEM	C3B-C4B-NB	-4.32	103.63	109.21
6	H	809	HEM	CBA-CAA-C2A	-4.31	104.53	112.49
6	E	812	HEM	C3B-C4B-NB	-4.29	103.66	109.21
6	E	811	HEM	CAD-CBD-CGD	-4.29	105.47	112.67
6	D	813	HEM	C3B-C4B-NB	-4.29	103.67	109.21
6	J	810	HEM	C3B-C4B-NB	-4.29	103.67	109.21
6	A	808	HEM	C3B-C4B-NB	-4.27	103.68	109.21
6	I	813	HEM	C3B-C4B-NB	-4.27	103.69	109.21
6	K	812	HEM	C3B-C4B-NB	-4.26	103.70	109.21
6	G	808	HEM	CBA-CAA-C2A	-4.26	104.63	112.49
6	G	812	HEM	C3B-C4B-NB	-4.26	103.71	109.21
6	E	806	HEM	C3B-C4B-NB	-4.26	103.71	109.21
6	C	813	HEM	C3B-C4B-NB	-4.25	103.71	109.21
6	L	808	HEM	C3B-C4B-NB	-4.23	103.74	109.21
6	K	810	HEM	C3B-C4B-NB	-4.22	103.75	109.21
6	E	813	HEM	C3B-C4B-NB	-4.22	103.75	109.21
6	D	806	HEM	C3B-C4B-NB	-4.20	103.78	109.21
6	F	808	HEM	C3B-C4B-NB	-4.19	103.80	109.21
6	I	810	HEM	C3B-C4B-NB	-4.18	103.80	109.21
6	H	812	HEM	C3B-C4B-NB	-4.18	103.80	109.21
6	K	808	HEM	C3B-C4B-NB	-4.16	103.83	109.21
6	B	811	HEM	C3B-C4B-NB	-4.16	103.84	109.21
6	I	808	HEM	C3B-C4B-NB	-4.14	103.86	109.21
6	K	813	HEM	C3B-C4B-NB	-4.13	103.87	109.21
6	G	808	HEM	C3B-C4B-NB	-4.11	103.89	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	808	HEM	CBA-CAA-C2A	-4.11	104.91	112.49
6	E	808	HEM	CBA-CAA-C2A	-4.11	104.91	112.49
6	C	807	HEM	C3B-C4B-NB	-4.10	103.90	109.21
6	L	808	HEM	CBA-CAA-C2A	-4.09	104.95	112.49
6	L	810	HEM	C3B-C4B-NB	-4.08	103.94	109.21
6	L	812	HEM	C3B-C4B-NB	-3.99	104.05	109.21
6	H	810	HEM	C3B-C4B-NB	-3.97	104.08	109.21
6	I	806	HEM	C3B-C4B-NB	-3.96	104.09	109.21
6	H	814	HEM	C3B-C4B-NB	-3.96	104.10	109.21
6	D	808	HEM	CBA-CAA-C2A	-3.95	105.21	112.49
6	B	810	HEM	C3B-C4B-NB	-3.94	104.11	109.21
6	K	809	HEM	CBD-CAD-C3D	-3.94	105.22	112.48
6	A	813	HEM	C3B-C4B-NB	-3.94	104.12	109.21
6	H	809	HEM	C3B-C4B-NB	-3.91	104.15	109.21
6	L	806	HEM	C3B-C4B-NB	-3.89	104.18	109.21
6	B	809	HEM	CBA-CAA-C2A	-3.89	105.31	112.49
6	C	809	HEM	C3B-C4B-NB	-3.88	104.19	109.21
6	F	812	HEM	CAD-CBD-CGD	-3.87	106.19	112.67
6	L	809	HEM	C3B-C4B-NB	-3.86	104.22	109.21
6	D	809	HEM	C3B-C4B-NB	-3.86	104.22	109.21
6	J	808	HEM	C3B-C4B-NB	-3.86	104.22	109.21
6	K	808	HEM	CBA-CAA-C2A	-3.84	105.41	112.49
6	A	811	HEM	CAD-CBD-CGD	-3.83	106.24	112.67
6	G	813	HEM	C3B-C4B-NB	-3.83	104.26	109.21
6	I	811	HEM	CAD-CBD-CGD	-3.82	106.26	112.67
6	F	809	HEM	CBA-CAA-C2A	-3.80	105.48	112.49
6	L	811	HEM	CAD-CBD-CGD	-3.80	106.30	112.67
6	J	813	HEM	C3B-C4B-NB	-3.78	104.32	109.21
6	J	809	HEM	CBD-CAD-C3D	-3.78	105.51	112.48
6	B	814	HEM	C3B-C4B-NB	-3.77	104.33	109.21
6	A	808	HEM	CBA-CAA-C2A	-3.76	105.56	112.49
6	L	811	HEM	C3B-C4B-NB	-3.73	104.38	109.21
6	E	809	HEM	C3B-C4B-NB	-3.65	104.48	109.21
6	G	809	HEM	C3B-C4B-NB	-3.60	104.55	109.21
6	F	808	HEM	CMA-C3A-C4A	-3.56	122.99	128.46
6	I	809	HEM	C3B-C4B-NB	-3.54	104.63	109.21
6	A	809	HEM	C3B-C4B-NB	-3.53	104.64	109.21
6	F	810	HEM	C3B-C4B-NB	-3.52	104.66	109.21
6	J	809	HEM	C3B-C4B-NB	-3.50	104.69	109.21
6	J	811	HEM	CAD-CBD-CGD	-3.48	106.83	112.67
6	B	808	HEM	CMA-C3A-C4A	-3.46	123.15	128.46
6	H	812	HEM	CAD-CBD-CGD	-3.45	106.88	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	807	HEM	CMA-C3A-C4A	-3.37	123.28	128.46
6	J	807	HEM	CMA-C3A-C4A	-3.37	123.29	128.46
6	I	813	HEM	CAD-CBD-CGD	-3.36	107.03	112.67
6	K	809	HEM	C3B-C4B-NB	-3.34	104.89	109.21
6	C	811	HEM	CAD-CBD-CGD	-3.32	107.10	112.67
6	L	813	HEM	C3B-C4B-NB	-3.26	105.00	109.21
6	F	808	HEM	C4A-C3A-C2A	3.26	109.26	107.00
6	A	812	HEM	CAD-CBD-CGD	-3.24	107.23	112.67
6	G	812	HEM	CMA-C3A-C4A	-3.22	123.52	128.46
6	H	814	HEM	CAA-CBA-CGA	-3.20	107.30	112.67
6	I	810	HEM	CAA-CBA-CGA	-3.18	107.33	112.67
6	H	808	HEM	CMA-C3A-C4A	-3.18	123.58	128.46
6	G	813	HEM	CAA-CBA-CGA	-3.16	107.38	112.67
6	K	810	HEM	CAA-CBA-CGA	-3.15	107.38	112.67
6	G	807	HEM	CMA-C3A-C4A	-3.15	123.63	128.46
6	L	813	HEM	CAA-CBA-CGA	-3.14	107.40	112.67
6	F	811	HEM	CAA-CBA-CGA	-3.13	107.42	112.67
6	A	807	HEM	CMA-C3A-C4A	-3.02	123.82	128.46
6	J	810	HEM	C4A-C3A-C2A	3.01	109.09	107.00
6	C	813	HEM	CBD-CAD-C3D	-2.98	106.98	112.48
6	C	807	HEM	CMA-C3A-C4A	-2.97	123.90	128.46
6	C	810	HEM	C4A-C3A-C2A	2.96	109.06	107.00
6	D	811	HEM	CAD-CBD-CGD	-2.92	107.78	112.67
6	E	807	HEM	CMA-C3A-C4A	-2.91	124.00	128.46
6	D	807	HEM	CMA-C3A-C4A	-2.90	124.01	128.46
6	G	811	HEM	CAD-CBD-CGD	-2.87	107.86	112.67
6	E	809	HEM	CBD-CAD-C3D	-2.85	107.22	112.48
6	I	806	HEM	C4A-C3A-C2A	2.85	108.98	107.00
6	B	814	HEM	C4A-C3A-C2A	2.84	108.97	107.00
6	B	810	HEM	CBD-CAD-C3D	-2.83	107.27	112.48
6	K	813	HEM	C4A-C3A-C2A	2.82	108.96	107.00
6	C	809	HEM	CMA-C3A-C4A	-2.82	124.13	128.46
6	I	807	HEM	CMA-C3A-C4A	-2.82	124.14	128.46
6	J	809	HEM	C4A-C3A-C2A	2.81	108.95	107.00
6	L	809	HEM	CBD-CAD-C3D	-2.81	107.30	112.48
6	I	808	HEM	CBA-CAA-C2A	-2.79	107.33	112.49
6	H	811	HEM	CBD-CAD-C3D	-2.78	107.35	112.48
6	K	813	HEM	CBD-CAD-C3D	-2.77	107.38	112.48
6	E	811	HEM	C4A-C3A-C2A	2.77	108.92	107.00
6	E	810	HEM	C4A-C3A-C2A	2.76	108.92	107.00
6	J	813	HEM	C4A-C3A-C2A	2.75	108.91	107.00
6	A	812	HEM	CMB-C2B-C3B	2.74	129.81	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	811	HEM	C4A-C3A-C2A	2.74	108.90	107.00
6	B	808	HEM	CMD-C2D-C1D	-2.73	124.27	128.46
6	F	809	HEM	CMA-C3A-C4A	-2.71	124.29	128.46
6	C	808	HEM	CMA-C3A-C4A	-2.71	124.30	128.46
6	F	808	HEM	CBD-CAD-C3D	2.70	117.46	112.48
6	G	810	HEM	CAA-CBA-CGA	-2.69	108.15	112.67
6	A	807	HEM	CBD-CAD-C3D	2.69	117.43	112.48
6	E	806	HEM	C4A-C3A-C2A	2.69	108.86	107.00
6	K	813	HEM	CAD-CBD-CGD	-2.68	108.17	112.67
6	A	810	HEM	CMB-C2B-C3B	2.68	129.69	124.68
6	A	809	HEM	CMA-C3A-C4A	-2.67	124.36	128.46
6	G	809	HEM	CMA-C3A-C4A	-2.66	124.37	128.46
6	E	807	HEM	CBD-CAD-C3D	2.65	117.37	112.48
6	L	810	HEM	CBD-CAD-C3D	-2.65	107.59	112.48
6	B	812	HEM	CBA-CAA-C2A	-2.65	107.60	112.49
6	F	812	HEM	CMB-C2B-C3B	2.65	129.63	124.68
6	B	812	HEM	CAD-CBD-CGD	-2.64	108.24	112.67
6	D	812	HEM	CMB-C2B-C3B	2.62	129.58	124.68
6	E	810	HEM	CMB-C2B-C3B	2.61	129.57	124.68
6	B	809	HEM	C4A-C3A-C2A	2.61	108.81	107.00
6	C	808	HEM	CMB-C2B-C3B	2.61	129.56	124.68
6	B	813	HEM	CMB-C2B-C3B	2.61	129.55	124.68
6	K	810	HEM	C4A-C3A-C2A	2.60	108.81	107.00
6	K	807	HEM	CBD-CAD-C3D	2.60	117.27	112.48
6	E	813	HEM	CAD-CBD-CGD	-2.60	108.31	112.67
6	L	807	HEM	CMA-C3A-C4A	-2.59	124.48	128.46
6	K	809	HEM	CMA-C3A-C4A	-2.59	124.49	128.46
6	A	810	HEM	CAA-CBA-CGA	-2.59	108.33	112.67
6	B	811	HEM	CAA-CBA-CGA	-2.57	108.35	112.67
6	F	811	HEM	CMB-C2B-C3B	2.57	129.49	124.68
6	E	809	HEM	C4A-C3A-C2A	2.57	108.78	107.00
6	C	812	HEM	CMB-C2B-C3B	2.56	129.46	124.68
6	I	812	HEM	CMB-C2B-C3B	2.56	129.46	124.68
6	H	808	HEM	CBD-CAD-C3D	2.55	117.18	112.48
6	I	808	HEM	CMB-C2B-C3B	2.55	129.45	124.68
6	F	807	HEM	CMB-C2B-C3B	2.55	129.44	124.68
6	E	812	HEM	CMB-C2B-C3B	2.55	129.44	124.68
6	C	809	HEM	C4A-C3A-C2A	2.52	108.75	107.00
6	B	811	HEM	C4A-C3A-C2A	2.51	108.75	107.00
6	G	811	HEM	CMA-C3A-C4A	-2.51	124.61	128.46
6	D	810	HEM	C4A-C3A-C2A	2.51	108.74	107.00
6	G	810	HEM	C4A-C3A-C2A	2.51	108.74	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	806	HEM	C4A-C3A-C2A	2.50	108.74	107.00
6	L	813	HEM	C3C-C4C-NC	-2.50	106.22	110.94
6	J	812	HEM	CMA-C3A-C4A	-2.49	124.63	128.46
6	I	811	HEM	CMB-C2B-C3B	2.49	129.34	124.68
6	K	811	HEM	CMA-C3A-C4A	-2.49	124.64	128.46
6	B	808	HEM	CMD-C2D-C3D	2.49	129.63	124.94
6	A	813	HEM	CAD-CBD-CGD	-2.48	108.50	112.67
6	H	810	HEM	CMA-C3A-C4A	-2.48	124.66	128.46
6	H	807	HEM	C4A-C3A-C2A	2.47	108.72	107.00
6	G	807	HEM	CMB-C2B-C3B	2.47	129.30	124.68
6	C	807	HEM	CBD-CAD-C3D	2.46	117.01	112.48
6	H	807	HEM	CMA-C3A-C4A	-2.46	124.68	128.46
6	J	808	HEM	CMA-C3A-C4A	-2.46	124.69	128.46
6	I	808	HEM	CMA-C3A-C4A	-2.46	124.69	128.46
6	I	807	HEM	C4A-C3A-C2A	2.46	108.70	107.00
6	E	811	HEM	CMA-C3A-C4A	-2.45	124.69	128.46
6	L	810	HEM	C4A-C3A-C2A	2.45	108.70	107.00
6	G	812	HEM	C4A-C3A-C2A	2.44	108.69	107.00
6	G	811	HEM	C4A-C3A-C2A	2.43	108.69	107.00
6	B	809	HEM	CMA-C3A-C4A	-2.43	124.72	128.46
6	H	810	HEM	C4A-C3A-C2A	2.43	108.69	107.00
6	H	812	HEM	C4A-C3A-C2A	2.43	108.69	107.00
6	L	806	HEM	C4A-C3A-C2A	2.42	108.68	107.00
6	D	811	HEM	CMB-C2B-C3B	2.41	129.19	124.68
6	A	813	HEM	CBD-CAD-C3D	-2.41	108.04	112.48
6	E	807	HEM	C4A-C3A-C2A	2.41	108.67	107.00
6	D	809	HEM	CBD-CAD-C3D	-2.41	108.04	112.48
6	L	808	HEM	CMB-C2B-C3B	2.41	129.18	124.68
6	B	810	HEM	C4A-C3A-C2A	2.41	108.67	107.00
6	A	811	HEM	CBA-CAA-C2A	-2.40	108.06	112.49
6	H	810	HEM	CBD-CAD-C3D	-2.39	108.08	112.48
6	H	814	HEM	CMB-C2B-C3B	2.39	129.14	124.68
6	C	806	HEM	CMB-C2B-C3B	2.38	129.12	124.68
6	J	811	HEM	C4A-C3A-C2A	2.38	108.65	107.00
6	G	807	HEM	C4A-C3A-C2A	2.37	108.65	107.00
6	A	813	HEM	C4A-C3A-C2A	2.37	108.65	107.00
6	D	807	HEM	CBD-CAD-C3D	2.37	116.85	112.48
6	A	807	HEM	CMB-C2B-C3B	2.37	129.11	124.68
6	D	809	HEM	CMA-C3A-C4A	-2.37	124.82	128.46
6	I	811	HEM	C4A-C3A-C2A	2.37	108.64	107.00
6	B	814	HEM	CMA-C3A-C4A	-2.36	124.83	128.46
6	D	807	HEM	CMB-C2B-C3B	2.36	129.09	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	806	HEM	CBA-CAA-C2A	-2.36	108.13	112.49
6	F	813	HEM	CMB-C2B-C3B	2.36	129.09	124.68
6	E	809	HEM	CMB-C2B-C3B	2.36	129.09	124.68
6	I	811	HEM	CMA-C3A-C4A	-2.35	124.86	128.46
6	F	812	HEM	C4A-C3A-C2A	2.35	108.63	107.00
6	A	810	HEM	CMA-C3A-C4A	-2.34	124.86	128.46
6	J	806	HEM	CMA-C3A-C4A	-2.34	124.86	128.46
6	J	812	HEM	CMB-C2B-C3B	2.33	129.04	124.68
6	A	806	HEM	CMB-C2B-C3B	2.33	129.04	124.68
6	L	807	HEM	CBA-CAA-C2A	-2.32	108.20	112.49
6	J	808	HEM	C4A-C3A-C2A	2.32	108.61	107.00
6	H	811	HEM	CAA-CBA-CGA	-2.31	108.79	112.67
6	C	811	HEM	CMB-C2B-C3B	2.31	129.00	124.68
6	G	809	HEM	C4A-C3A-C2A	2.31	108.60	107.00
6	L	811	HEM	CMA-C3A-C4A	-2.30	124.92	128.46
6	I	809	HEM	CMB-C2B-C3B	2.30	128.99	124.68
6	B	807	HEM	CMB-C2B-C3B	2.30	128.98	124.68
6	I	810	HEM	C4A-C3A-C2A	2.30	108.59	107.00
6	I	808	HEM	C4A-C3A-C2A	2.30	108.59	107.00
6	A	808	HEM	CMA-C3A-C4A	-2.30	124.93	128.46
6	I	813	HEM	CAA-CBA-CGA	-2.29	108.82	112.67
6	B	812	HEM	C4A-C3A-C2A	2.29	108.59	107.00
6	K	812	HEM	CMB-C2B-C3B	2.29	128.97	124.68
6	J	813	HEM	CMA-C3A-C4A	-2.29	124.95	128.46
6	F	809	HEM	CMB-C2B-C3B	2.28	128.95	124.68
6	A	806	HEM	CMA-C3A-C4A	-2.28	124.95	128.46
6	B	808	HEM	C4A-C3A-C2A	2.27	108.58	107.00
6	F	808	HEM	CMB-C2B-C3B	2.26	128.91	124.68
6	L	813	HEM	CAD-CBD-CGD	-2.26	108.88	112.67
6	A	812	HEM	CMA-C3A-C4A	-2.26	124.99	128.46
6	H	809	HEM	CMC-C2C-C3C	2.25	128.90	124.68
6	D	806	HEM	CMB-C2B-C3B	2.25	128.90	124.68
6	I	813	HEM	C4A-C3A-C2A	2.25	108.56	107.00
6	K	811	HEM	CAD-CBD-CGD	-2.25	108.89	112.67
6	I	808	HEM	CMC-C2C-C3C	2.25	128.89	124.68
6	A	809	HEM	C4A-C3A-C2A	2.25	108.56	107.00
6	F	809	HEM	C3C-C4C-NC	-2.25	106.70	110.94
6	G	807	HEM	CBD-CAD-C3D	2.25	116.62	112.48
6	I	807	HEM	CMD-C2D-C1D	-2.24	125.02	128.46
6	D	813	HEM	CMB-C2B-C3B	2.24	128.86	124.68
6	A	812	HEM	C1D-C2D-C3D	-2.23	105.44	107.00
6	C	813	HEM	CMB-C2B-C3B	2.23	128.85	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	813	HEM	CMA-C3A-C4A	-2.23	125.04	128.46
6	G	811	HEM	CBD-CAD-C3D	-2.22	108.38	112.48
6	H	813	HEM	C4A-C3A-C2A	2.22	108.54	107.00
6	I	809	HEM	CBD-CAD-C3D	-2.22	108.38	112.48
6	K	810	HEM	CMB-C2B-C3B	2.22	128.84	124.68
6	G	813	HEM	CMA-C3A-C4A	-2.22	125.05	128.46
6	C	810	HEM	CMC-C2C-C3C	2.22	128.83	124.68
6	L	812	HEM	CMA-C3A-C4A	-2.22	125.06	128.46
6	I	812	HEM	CMA-C3A-C4A	-2.21	125.07	128.46
6	H	812	HEM	CMA-C3A-C4A	-2.21	125.07	128.46
6	H	811	HEM	CMB-C2B-C3B	2.21	128.80	124.68
6	D	807	HEM	C4A-C3A-C2A	2.20	108.53	107.00
6	K	807	HEM	C4A-C3A-C2A	2.19	108.52	107.00
6	H	812	HEM	CMB-C2B-C3B	2.19	128.78	124.68
6	K	807	HEM	CMD-C2D-C1D	-2.19	125.10	128.46
6	G	812	HEM	CMB-C2B-C3B	2.19	128.77	124.68
6	C	813	HEM	C4A-C3A-C2A	2.19	108.52	107.00
6	D	808	HEM	CMA-C3A-C4A	-2.18	125.11	128.46
6	D	813	HEM	C4A-C3A-C2A	2.17	108.51	107.00
6	D	810	HEM	CMB-C2B-C3B	2.17	128.74	124.68
6	F	810	HEM	CMA-C3A-C4A	-2.17	125.13	128.46
6	K	812	HEM	C4A-C3A-C2A	2.17	108.50	107.00
6	C	812	HEM	CMA-C3A-C4A	-2.17	125.13	128.46
6	G	806	HEM	CMB-C2B-C3B	2.17	128.73	124.68
6	L	808	HEM	CMA-C3A-C4A	-2.17	125.13	128.46
6	B	810	HEM	CMA-C3A-C4A	-2.16	125.14	128.46
6	E	808	HEM	CAD-CBD-CGD	-2.16	109.05	112.67
6	L	807	HEM	CMD-C2D-C1D	-2.16	125.15	128.46
6	G	811	HEM	CMB-C2B-C3B	2.16	128.71	124.68
6	F	810	HEM	CBD-CAD-C3D	-2.16	108.51	112.48
6	B	810	HEM	CMB-C2B-C3B	2.16	128.71	124.68
6	K	808	HEM	CMA-C3A-C4A	-2.15	125.15	128.46
6	J	812	HEM	C4A-C3A-C2A	2.15	108.49	107.00
6	B	811	HEM	CMB-C2B-C3B	2.15	128.71	124.68
6	E	811	HEM	CMB-C2B-C3B	2.15	128.70	124.68
6	L	810	HEM	CMA-C3A-C4A	-2.15	125.16	128.46
6	C	810	HEM	CMB-C2B-C3B	2.15	128.70	124.68
6	I	811	HEM	CBA-CAA-C2A	-2.15	108.53	112.49
6	F	811	HEM	CMC-C2C-C3C	2.15	128.69	124.68
6	D	806	HEM	CBA-CAA-C2A	-2.15	108.53	112.49
6	C	808	HEM	C4A-C3A-C2A	2.14	108.49	107.00
6	H	808	HEM	C4A-C3A-C2A	2.14	108.49	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	807	HEM	CMB-C2B-C3B	2.14	128.68	124.68
6	F	807	HEM	C4A-C3A-C2A	2.14	108.48	107.00
6	A	812	HEM	CMC-C2C-C3C	2.14	128.68	124.68
6	E	806	HEM	CMB-C2B-C3B	2.14	128.67	124.68
6	B	807	HEM	C4A-C3A-C2A	2.13	108.48	107.00
6	D	808	HEM	C4A-C3A-C2A	2.13	108.48	107.00
6	L	811	HEM	C4A-C3A-C2A	2.13	108.48	107.00
6	K	806	HEM	CMA-C3A-C4A	-2.13	125.20	128.46
6	H	809	HEM	CMB-C2B-C3B	2.12	128.65	124.68
6	B	812	HEM	CMA-C3A-C4A	-2.12	125.20	128.46
6	B	809	HEM	CMB-C2B-C3B	2.12	128.65	124.68
6	E	808	HEM	C4A-C3A-C2A	2.11	108.47	107.00
6	J	807	HEM	C4A-C3A-C2A	2.11	108.47	107.00
6	K	813	HEM	C1D-C2D-C3D	-2.11	105.53	107.00
6	A	812	HEM	CAA-CBA-CGA	-2.11	109.13	112.67
6	F	814	HEM	C4A-C3A-C2A	2.11	108.46	107.00
6	J	808	HEM	CMC-C2C-C3C	2.10	128.62	124.68
6	A	808	HEM	CMB-C2B-C3B	2.10	128.62	124.68
6	A	809	HEM	CBD-CAD-C3D	-2.10	108.60	112.48
6	D	807	HEM	CMD-C2D-C1D	-2.10	125.23	128.46
6	I	810	HEM	CMB-C2B-C3B	2.10	128.61	124.68
6	F	808	HEM	CMD-C2D-C1D	-2.10	125.23	128.46
6	A	813	HEM	C1D-C2D-C3D	-2.10	105.53	107.00
6	A	813	HEM	CMB-C2B-C3B	2.10	128.61	124.68
6	B	811	HEM	CMA-C3A-C4A	-2.10	125.24	128.46
6	I	808	HEM	C4C-C3C-C2C	2.10	108.36	106.90
6	J	812	HEM	CAA-CBA-CGA	-2.10	109.15	112.67
6	J	807	HEM	CMB-C2B-C3B	2.09	128.59	124.68
6	E	812	HEM	C4A-C3A-C2A	2.09	108.45	107.00
6	I	812	HEM	C4A-C3A-C2A	2.08	108.45	107.00
6	G	813	HEM	C1D-C2D-C3D	-2.08	105.55	107.00
6	C	812	HEM	C4A-C3A-C2A	2.08	108.44	107.00
6	I	808	HEM	C3C-C4C-NC	-2.08	107.02	110.94
6	D	811	HEM	CBA-CAA-C2A	-2.08	108.65	112.49
6	J	811	HEM	CMB-C2B-C3B	2.08	128.57	124.68
6	L	806	HEM	CMA-C3A-C4A	-2.08	125.27	128.46
6	E	813	HEM	CMB-C2B-C3B	2.08	128.56	124.68
6	B	812	HEM	CMB-C2B-C3B	2.07	128.56	124.68
6	I	806	HEM	CMA-C3A-C4A	-2.07	125.28	128.46
6	F	812	HEM	CBA-CAA-C2A	-2.07	108.67	112.49
6	G	812	HEM	CAA-CBA-CGA	-2.07	109.20	112.67
6	A	809	HEM	CMB-C2B-C3B	2.07	128.55	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	813	HEM	CAA-CBA-CGA	-2.07	109.20	112.67
6	L	810	HEM	CMC-C2C-C3C	2.07	128.54	124.68
6	I	813	HEM	CMB-C2B-C3B	2.06	128.54	124.68
6	D	811	HEM	CMA-C3A-C4A	-2.06	125.30	128.46
6	C	810	HEM	CAA-CBA-CGA	-2.06	109.21	112.67
6	C	808	HEM	CMC-C2C-C3C	2.06	128.53	124.68
6	K	811	HEM	CMB-C2B-C3B	2.05	128.52	124.68
6	J	807	HEM	CBA-CAA-C2A	-2.05	108.71	112.49
6	K	813	HEM	CMB-C2B-C3B	2.05	128.51	124.68
6	H	811	HEM	CMA-C3A-C4A	-2.05	125.32	128.46
6	H	809	HEM	C3C-C4C-NC	-2.05	107.08	110.94
6	J	813	HEM	CBD-CAD-C3D	2.04	116.25	112.48
6	K	812	HEM	CMA-C3A-C4A	-2.04	125.32	128.46
6	B	813	HEM	CMA-C3A-C4A	-2.04	125.33	128.46
6	E	812	HEM	CMA-C3A-C4A	-2.04	125.33	128.46
6	H	808	HEM	CMD-C2D-C1D	-2.03	125.34	128.46
6	G	808	HEM	CMB-C2B-C3B	2.03	128.47	124.68
6	K	807	HEM	CMB-C2B-C3B	2.03	128.47	124.68
6	J	810	HEM	CMB-C2B-C3B	2.03	128.47	124.68
6	J	807	HEM	CMD-C2D-C1D	-2.03	125.35	128.46
6	H	812	HEM	CBA-CAA-C2A	-2.02	108.76	112.49
6	K	811	HEM	C4A-C3A-C2A	2.02	108.40	107.00
6	B	807	HEM	CAA-CBA-CGA	2.02	116.06	112.67
6	J	810	HEM	CMA-C3A-C4A	-2.02	125.36	128.46
6	B	807	HEM	CMA-C3A-C4A	-2.02	125.36	128.46
6	H	814	HEM	CAD-CBD-CGD	-2.02	109.29	112.67
6	A	808	HEM	C3C-C4C-NC	-2.01	107.14	110.94
6	E	810	HEM	CBD-CAD-C3D	-2.01	108.77	112.48
6	C	806	HEM	C4A-C3A-C2A	2.01	108.40	107.00
6	I	813	HEM	CMA-C3A-C4A	-2.01	125.38	128.46
6	L	810	HEM	CMB-C2B-C3B	2.01	128.44	124.68
6	A	807	HEM	CMD-C2D-C1D	-2.01	125.38	128.46
6	L	811	HEM	CBA-CAA-C2A	-2.01	108.78	112.49
6	J	809	HEM	CMA-C3A-C4A	-2.01	125.38	128.46
6	H	813	HEM	CAD-CBD-CGD	-2.01	109.31	112.67
6	E	808	HEM	CMA-C3A-C4A	-2.00	125.38	128.46
6	J	806	HEM	CAD-CBD-CGD	-2.00	109.31	112.67
6	C	806	HEM	CMA-C3A-C4A	-2.00	125.39	128.46
6	G	813	HEM	CMB-C2B-C3B	2.00	128.42	124.68
6	D	808	HEM	C3C-C4C-NC	-2.00	107.17	110.94
6	F	813	HEM	CAD-CBD-CGD	-2.00	109.31	112.67

There are no chirality outliers.

All (127) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	806	HEM	C2A-CAA-CBA-CGA
6	D	807	HEM	C2D-C3D-CAD-CBD
6	D	807	HEM	C4D-C3D-CAD-CBD
4	L	804	BU3	O5-C2-C3-O6
4	L	804	BU3	C1-C2-C3-C4
4	I	804	BU3	O5-C2-C3-O6
6	C	806	HEM	C2A-CAA-CBA-CGA
6	C	807	HEM	C2D-C3D-CAD-CBD
6	C	807	HEM	C4D-C3D-CAD-CBD
4	B	803	BU3	C1-C2-C3-O6
4	B	803	BU3	O5-C2-C3-C4
4	B	803	BU3	C1-C2-C3-C4
4	C	804	BU3	O5-C2-C3-O6
4	C	804	BU3	C1-C2-C3-O6
4	C	804	BU3	O5-C2-C3-C4
4	C	804	BU3	C1-C2-C3-C4
6	J	806	HEM	C2A-CAA-CBA-CGA
4	E	803	BU3	C1-C2-C3-C4
4	I	803	BU3	O5-C2-C3-O6
4	I	803	BU3	C1-C2-C3-O6
4	I	803	BU3	O5-C2-C3-C4
4	I	803	BU3	C1-C2-C3-C4
6	D	806	HEM	C2A-CAA-CBA-CGA
4	A	804	BU3	O5-C2-C3-O6
4	A	804	BU3	C1-C2-C3-O6
4	A	804	BU3	O5-C2-C3-C4
4	A	804	BU3	C1-C2-C3-C4
6	A	807	HEM	C2D-C3D-CAD-CBD
6	A	807	HEM	C4D-C3D-CAD-CBD
4	F	803	BU3	O5-C2-C3-O6
4	K	804	BU3	O5-C2-C3-O6
4	K	804	BU3	C1-C2-C3-C4
4	J	804	BU3	C1-C2-C3-O6
4	J	804	BU3	O5-C2-C3-C4
4	J	804	BU3	C1-C2-C3-C4
4	D	804	BU3	O5-C2-C3-O6
4	L	803	BU3	O5-C2-C3-O6
4	L	803	BU3	C1-C2-C3-O6
4	L	803	BU3	O5-C2-C3-C4
4	L	803	BU3	C1-C2-C3-C4
4	G	803	BU3	O5-C2-C3-O6
4	B	804	BU3	O5-C2-C3-O6

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Mol	Chain	Res	Type	Atoms
4	B	804	BU3	O5-C2-C3-C4
4	B	804	BU3	C1-C2-C3-C4
4	A	803	BU3	O5-C2-C3-O6
4	A	803	BU3	C1-C2-C3-O6
4	A	803	BU3	O5-C2-C3-C4
6	G	806	HEM	C2A-CAA-CBA-CGA
6	B	807	HEM	C2A-CAA-CBA-CGA
4	F	804	BU3	O5-C2-C3-O6
4	F	804	BU3	C1-C2-C3-C4
6	I	807	HEM	C2D-C3D-CAD-CBD
6	I	807	HEM	C4D-C3D-CAD-CBD
4	F	805	BU3	O5-C2-C3-O6
4	F	805	BU3	C1-C2-C3-O6
4	F	805	BU3	O5-C2-C3-C4
4	F	805	BU3	C1-C2-C3-C4
6	I	806	HEM	C2A-CAA-CBA-CGA
6	L	807	HEM	C2D-C3D-CAD-CBD
6	L	807	HEM	C4D-C3D-CAD-CBD
6	F	807	HEM	C2A-CAA-CBA-CGA
6	B	808	HEM	C2D-C3D-CAD-CBD
6	B	808	HEM	C4D-C3D-CAD-CBD
4	C	803	BU3	O5-C2-C3-O6
4	C	803	BU3	C1-C2-C3-C4
6	J	807	HEM	C2D-C3D-CAD-CBD
6	J	807	HEM	C4D-C3D-CAD-CBD
6	G	807	HEM	C2D-C3D-CAD-CBD
6	G	807	HEM	C4D-C3D-CAD-CBD
6	K	807	HEM	C2D-C3D-CAD-CBD
6	K	807	HEM	C4D-C3D-CAD-CBD
6	J	813	HEM	C2D-C3D-CAD-CBD
6	J	813	HEM	C4D-C3D-CAD-CBD
6	E	807	HEM	C2D-C3D-CAD-CBD
6	E	807	HEM	C4D-C3D-CAD-CBD
6	H	808	HEM	C2D-C3D-CAD-CBD
6	H	808	HEM	C4D-C3D-CAD-CBD
6	F	808	HEM	C2D-C3D-CAD-CBD
6	F	808	HEM	C4D-C3D-CAD-CBD
4	H	804	BU3	O5-C2-C3-O6
4	H	804	BU3	C1-C2-C3-C4
4	J	803	BU3	C1-C2-C3-O6
4	J	803	BU3	O5-C2-C3-C4
4	J	803	BU3	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
6	A	806	HEM	C2A-CAA-CBA-CGA
4	B	803	BU3	O5-C2-C3-O6
4	J	803	BU3	O5-C2-C3-O6
6	E	806	HEM	C2A-CAA-CBA-CGA
6	H	807	HEM	C2A-CAA-CBA-CGA
6	F	809	HEM	C3D-CAD-CBD-CGD
4	L	804	BU3	C1-C2-C3-O6
4	L	804	BU3	O5-C2-C3-C4
4	I	804	BU3	C1-C2-C3-O6
4	I	804	BU3	O5-C2-C3-C4
4	F	803	BU3	C1-C2-C3-O6
4	F	803	BU3	O5-C2-C3-C4
4	K	804	BU3	C1-C2-C3-O6
4	K	804	BU3	O5-C2-C3-C4
4	D	804	BU3	C1-C2-C3-O6
4	D	804	BU3	O5-C2-C3-C4
4	G	803	BU3	C1-C2-C3-O6
4	G	803	BU3	O5-C2-C3-C4
4	B	804	BU3	C1-C2-C3-O6
4	F	804	BU3	C1-C2-C3-O6
4	F	804	BU3	O5-C2-C3-C4
4	C	803	BU3	C1-C2-C3-O6
4	C	803	BU3	O5-C2-C3-C4
4	H	804	BU3	C1-C2-C3-O6
4	H	804	BU3	O5-C2-C3-C4
4	I	804	BU3	C1-C2-C3-C4
4	F	803	BU3	C1-C2-C3-C4
4	D	804	BU3	C1-C2-C3-C4
4	G	803	BU3	C1-C2-C3-C4
4	A	803	BU3	C1-C2-C3-C4
6	E	808	HEM	C2D-C3D-CAD-CBD
6	G	808	HEM	C2D-C3D-CAD-CBD
4	J	804	BU3	O5-C2-C3-O6
6	K	808	HEM	C3D-CAD-CBD-CGD
6	K	806	HEM	C2A-CAA-CBA-CGA
6	L	808	HEM	C3D-CAD-CBD-CGD
6	I	808	HEM	C3D-CAD-CBD-CGD
6	B	808	HEM	C3D-CAD-CBD-CGD
6	G	808	HEM	C3D-CAD-CBD-CGD
4	E	803	BU3	O5-C2-C3-O6
6	C	808	HEM	C3D-CAD-CBD-CGD
6	J	808	HEM	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
6	A	808	HEM	C3D-CAD-CBD-CGD

There are no ring outliers.

103 monomers are involved in 982 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	806	HEM	9	0
6	D	808	HEM	11	0
4	H	803	BU3	1	0
6	I	809	HEM	11	0
6	E	810	HEM	9	0
6	F	814	HEM	9	0
6	D	807	HEM	13	0
6	A	810	HEM	10	0
6	H	812	HEM	7	0
6	E	809	HEM	12	0
6	B	809	HEM	9	0
6	C	806	HEM	9	0
6	L	809	HEM	14	0
6	C	807	HEM	14	0
6	H	813	HEM	11	0
6	L	810	HEM	8	0
6	D	813	HEM	9	0
6	C	808	HEM	10	0
6	C	810	HEM	9	0
6	A	813	HEM	10	0
6	G	813	HEM	9	0
6	L	808	HEM	10	0
6	K	809	HEM	12	0
6	J	806	HEM	11	0
6	F	813	HEM	9	0
6	E	812	HEM	10	0
6	I	810	HEM	11	0
6	E	811	HEM	7	0
6	J	809	HEM	12	0
6	D	810	HEM	11	0
6	D	806	HEM	10	0
6	B	810	HEM	10	0
5	F	806	ACT	1	0
6	J	811	HEM	8	0
6	L	812	HEM	9	0
6	A	807	HEM	12	0

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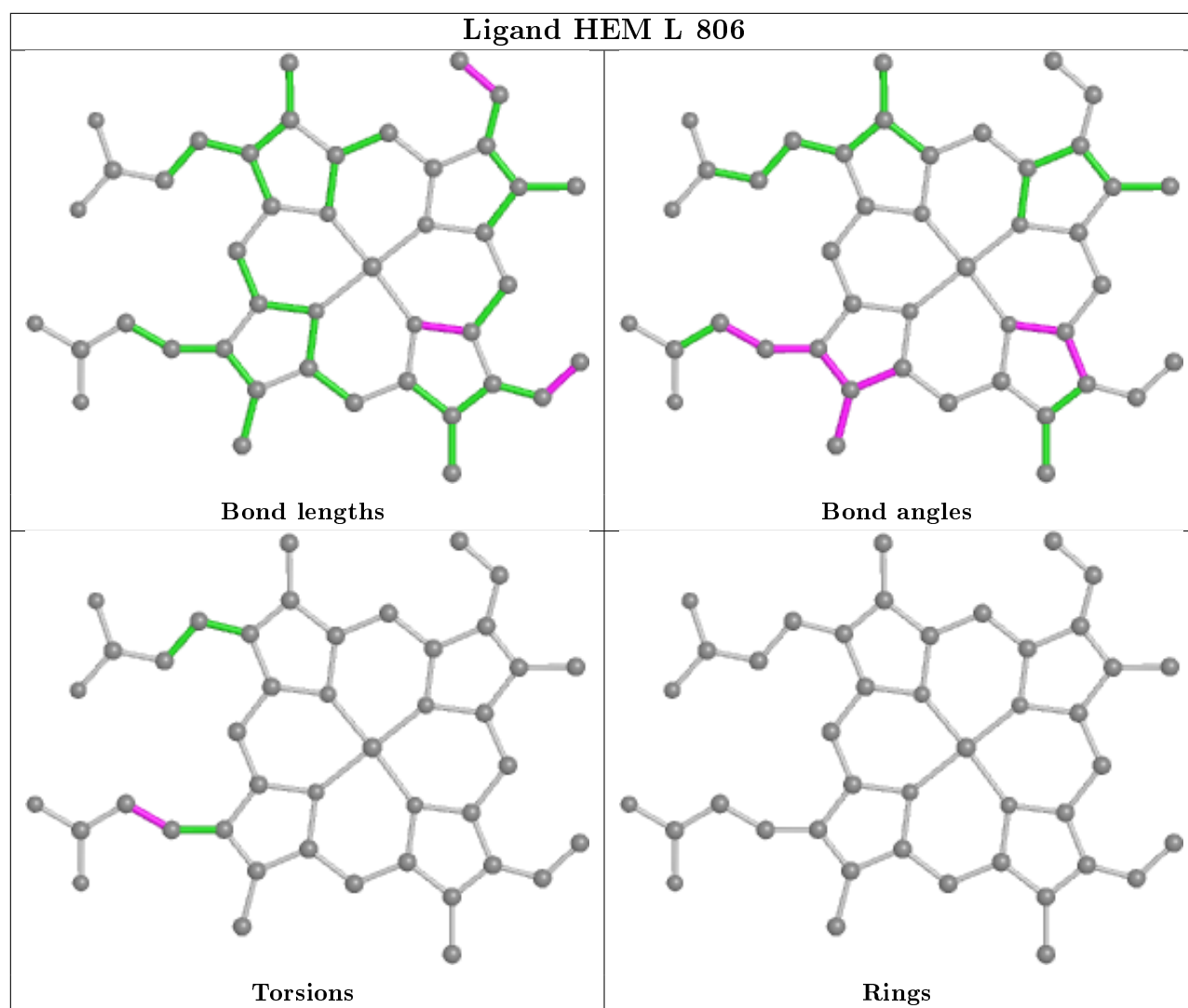
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	810	HEM	9	0
6	B	813	HEM	9	0
6	G	809	HEM	11	0
6	H	811	HEM	13	0
6	I	808	HEM	10	0
6	D	809	HEM	13	0
5	E	805	ACT	1	0
6	H	814	HEM	12	0
6	E	808	HEM	9	0
6	C	813	HEM	9	0
6	I	812	HEM	11	0
6	E	813	HEM	10	0
6	L	811	HEM	9	0
6	G	806	HEM	12	0
6	E	806	HEM	11	0
6	B	807	HEM	11	0
6	J	808	HEM	8	0
6	I	807	HEM	12	0
6	F	812	HEM	7	0
6	H	807	HEM	10	0
6	H	809	HEM	9	0
6	F	810	HEM	11	0
5	C	805	ACT	1	0
6	B	811	HEM	11	0
6	I	806	HEM	10	0
6	L	813	HEM	10	0
6	L	807	HEM	17	0
6	G	811	HEM	8	0
6	F	809	HEM	8	0
6	F	807	HEM	12	0
6	G	810	HEM	9	0
6	B	814	HEM	9	0
6	B	808	HEM	13	0
6	G	812	HEM	13	0
6	K	812	HEM	8	0
6	F	811	HEM	10	0
6	D	812	HEM	9	0
4	K	803	BU3	1	0
6	J	807	HEM	12	0
6	I	813	HEM	8	0
6	G	807	HEM	12	0
6	G	808	HEM	8	0

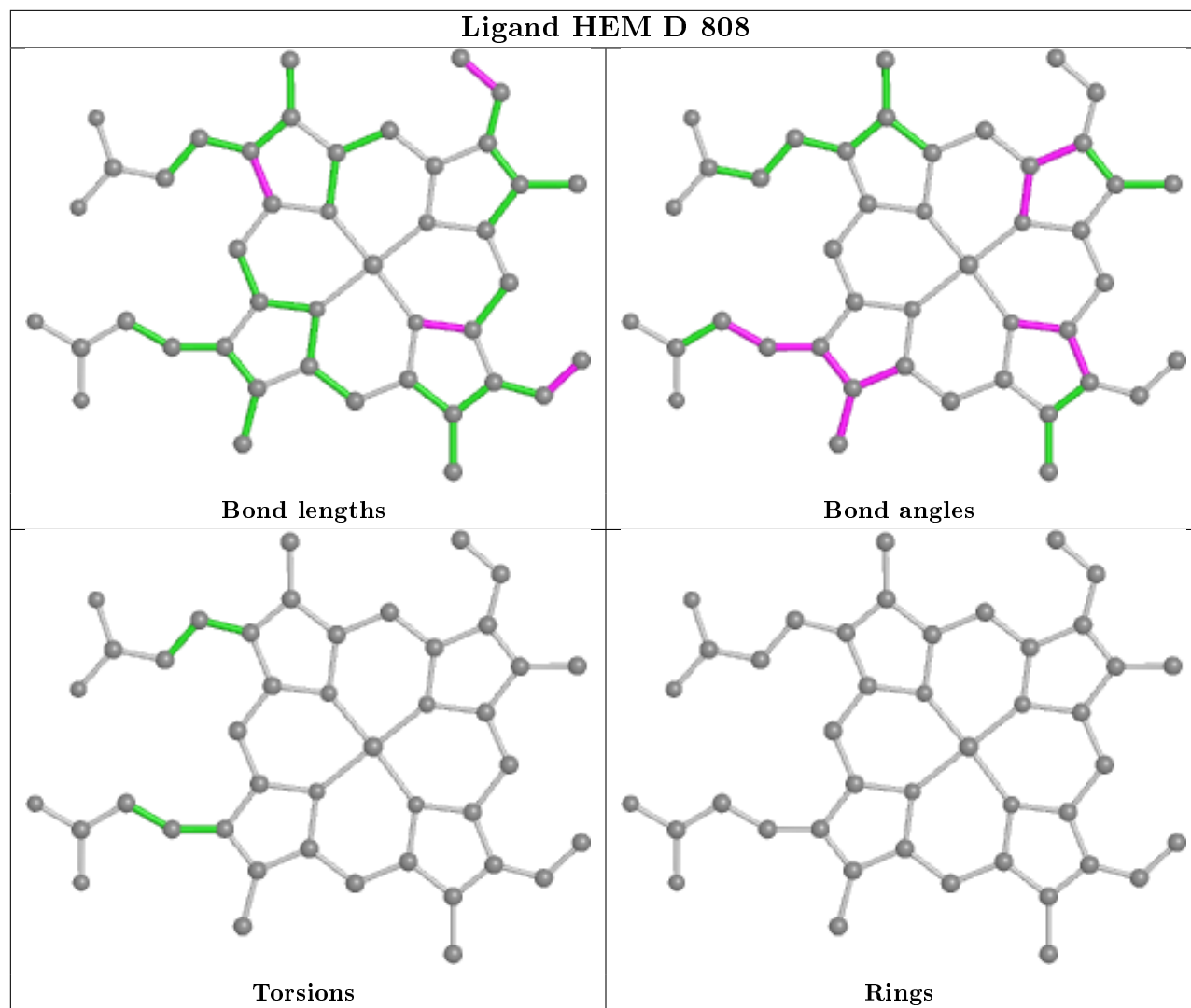
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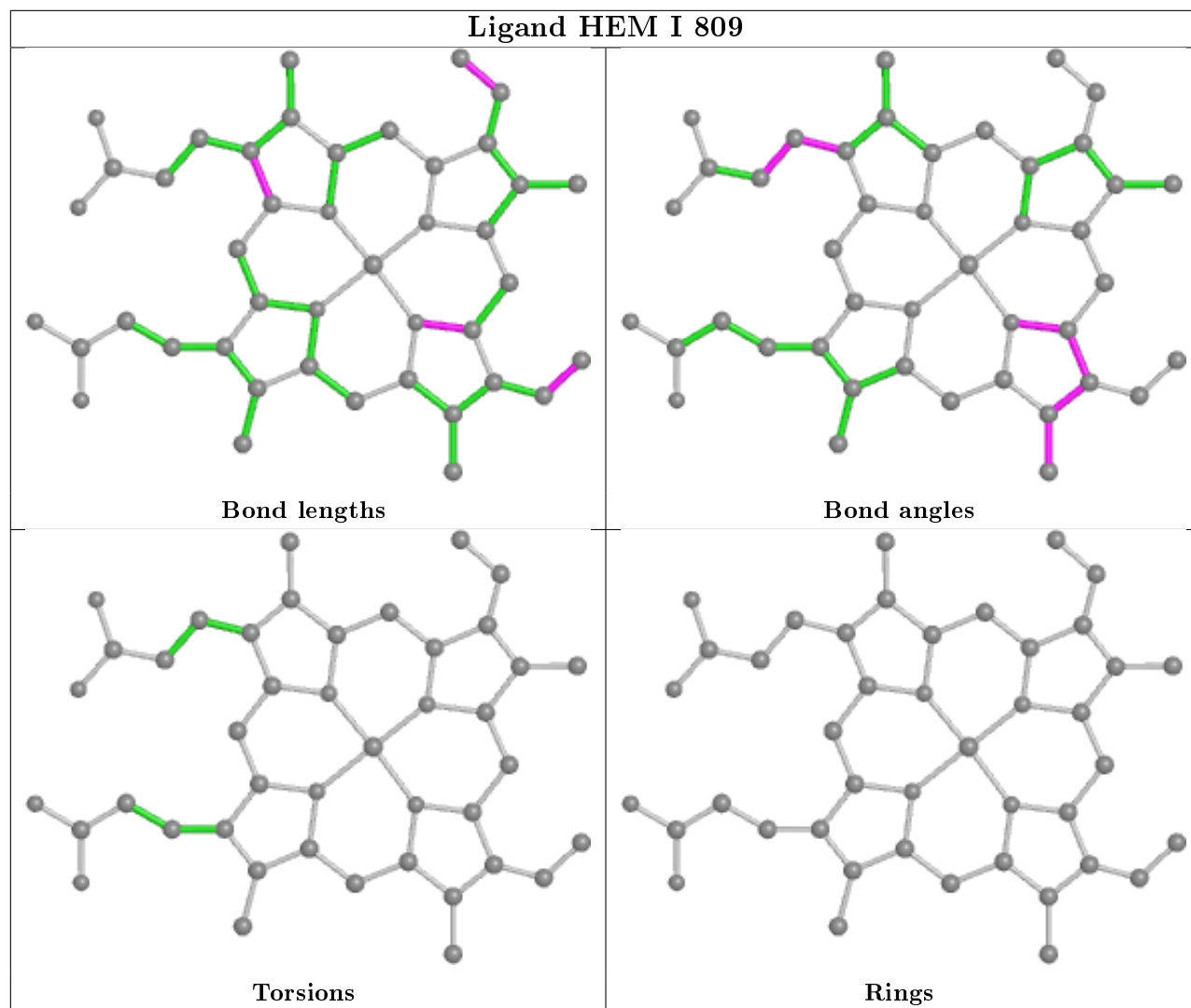
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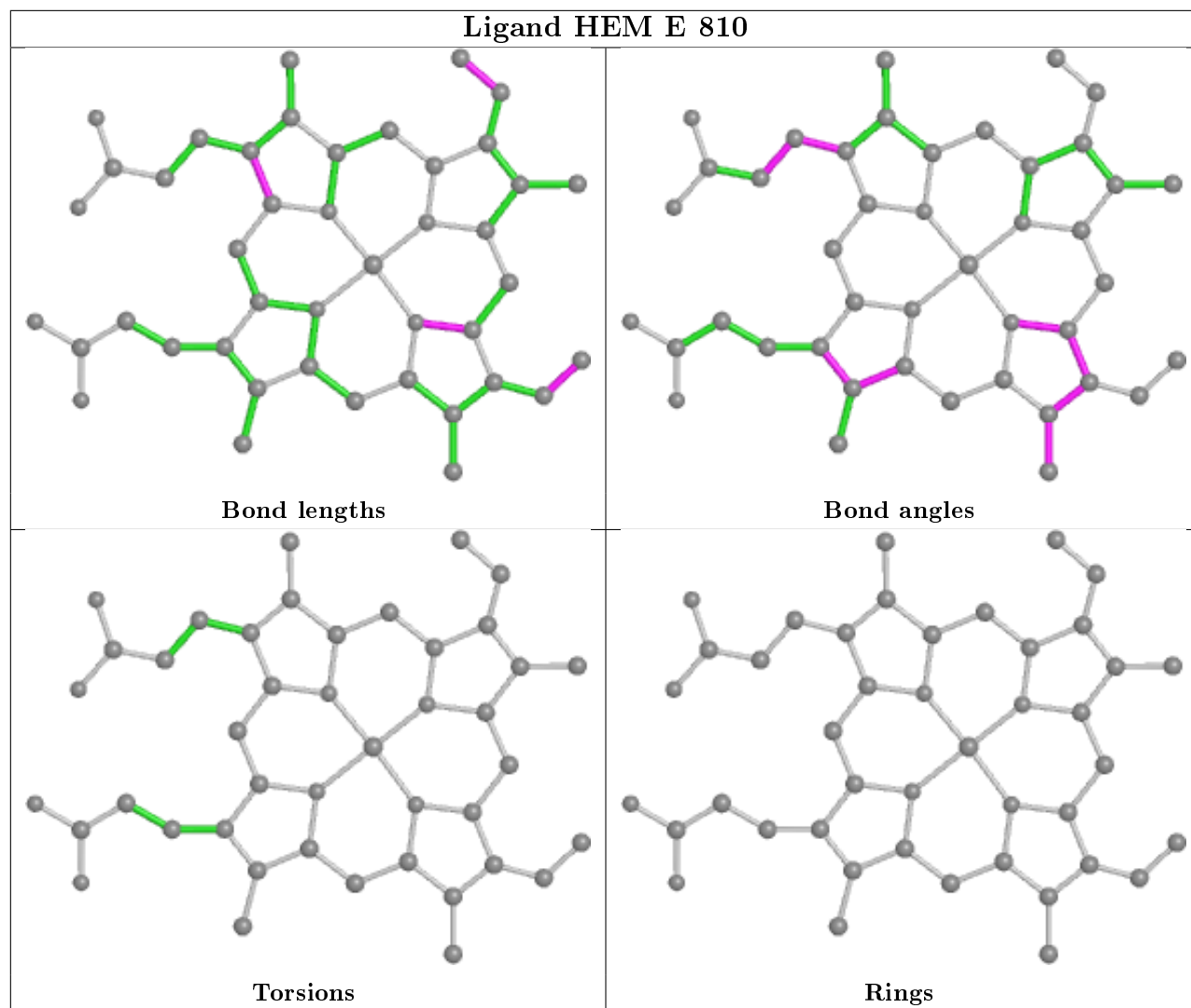
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	808	HEM	11	0
6	A	809	HEM	13	0
6	I	811	HEM	10	0
6	A	812	HEM	11	0
4	E	804	BU3	2	0
6	K	807	HEM	14	0
6	K	806	HEM	10	0
6	J	813	HEM	13	0
6	J	810	HEM	8	0
6	H	810	HEM	10	0
6	E	807	HEM	11	0
6	J	812	HEM	8	0
6	H	808	HEM	14	0
6	B	812	HEM	8	0
7	A	814	SO2	1	0
6	K	811	HEM	10	0
6	F	808	HEM	12	0
6	K	813	HEM	7	0
6	C	809	HEM	11	0
6	C	812	HEM	8	0
6	C	811	HEM	8	0
6	A	811	HEM	7	0
6	A	806	HEM	9	0
6	A	808	HEM	9	0
6	D	811	HEM	10	0

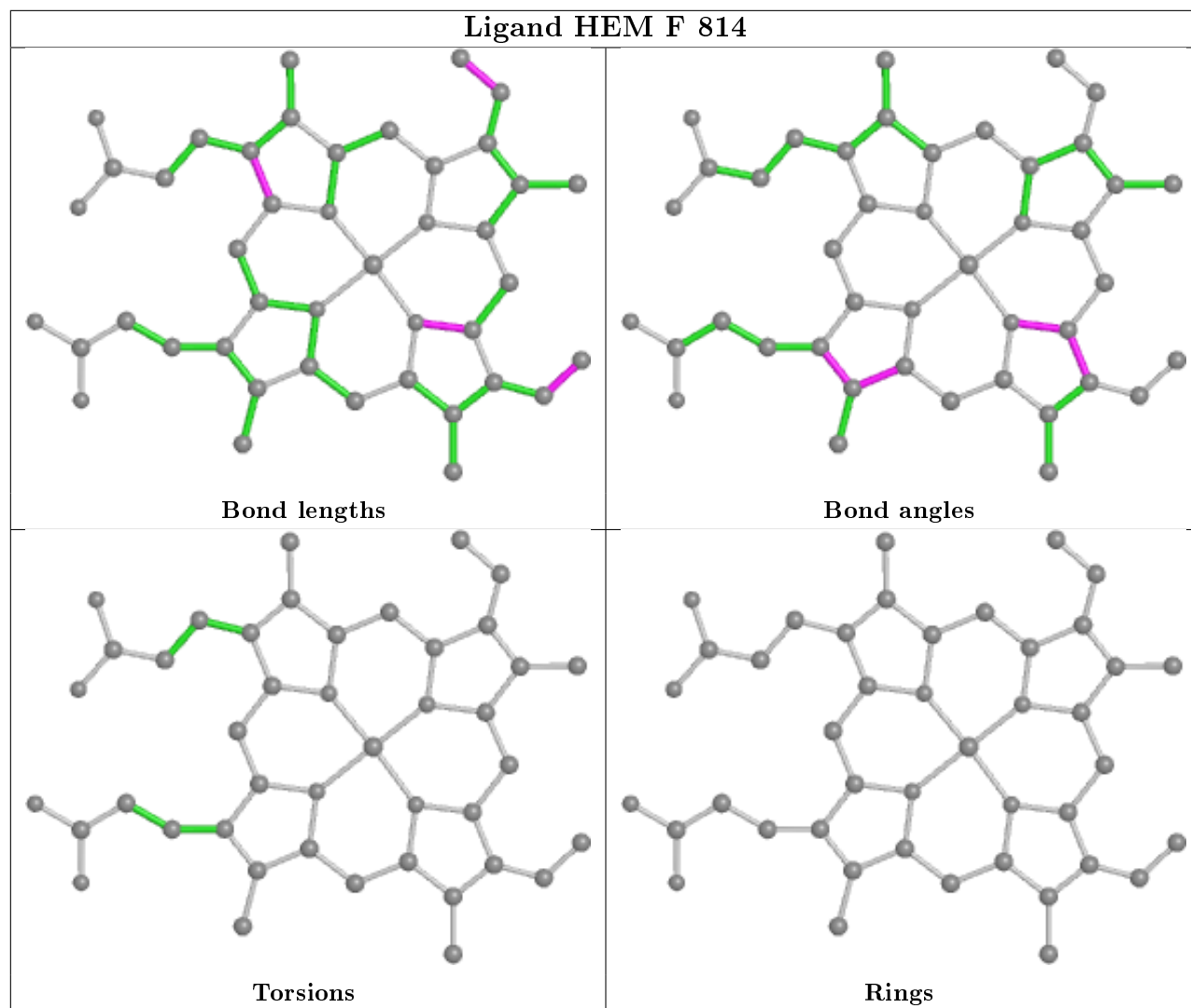
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

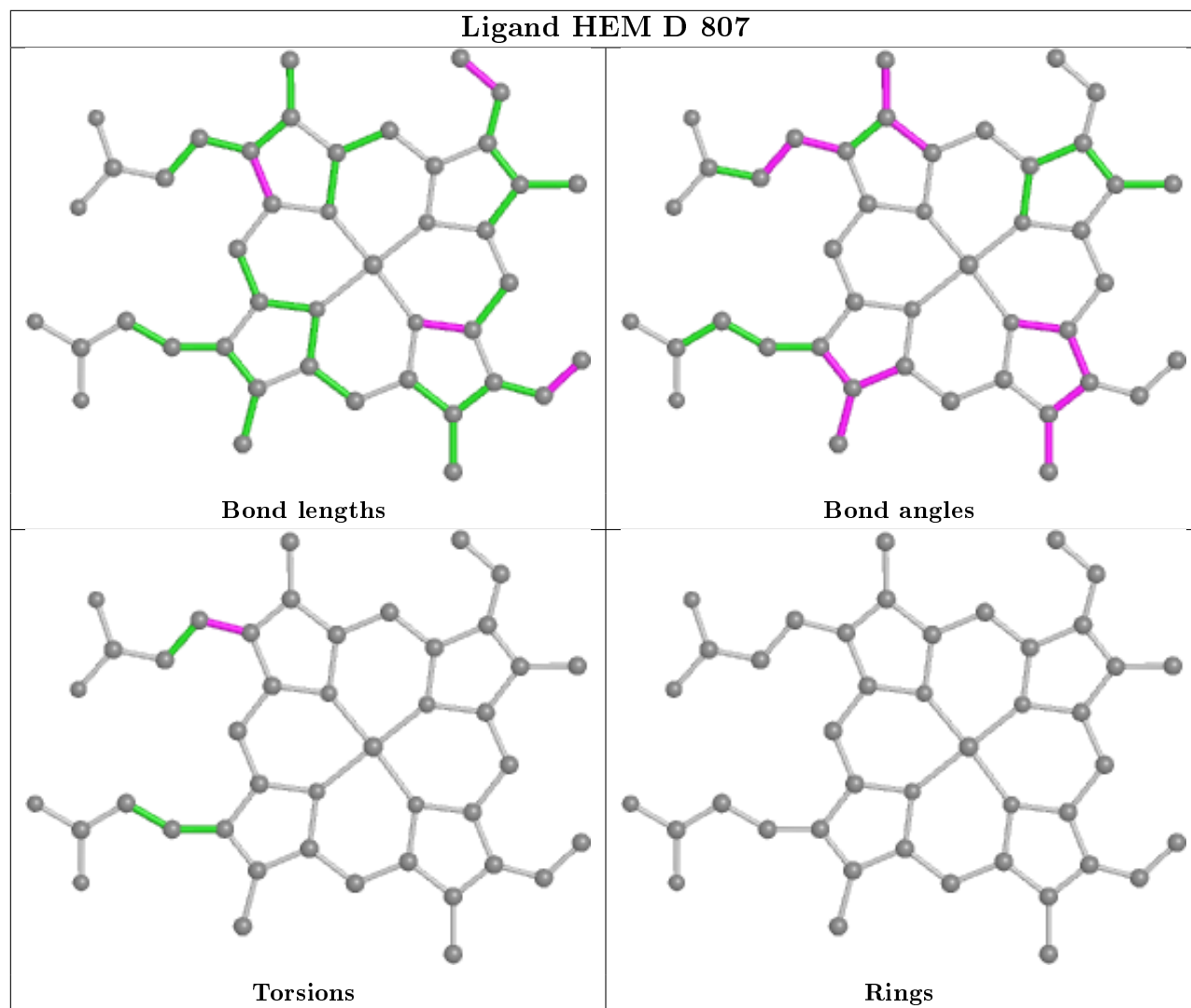


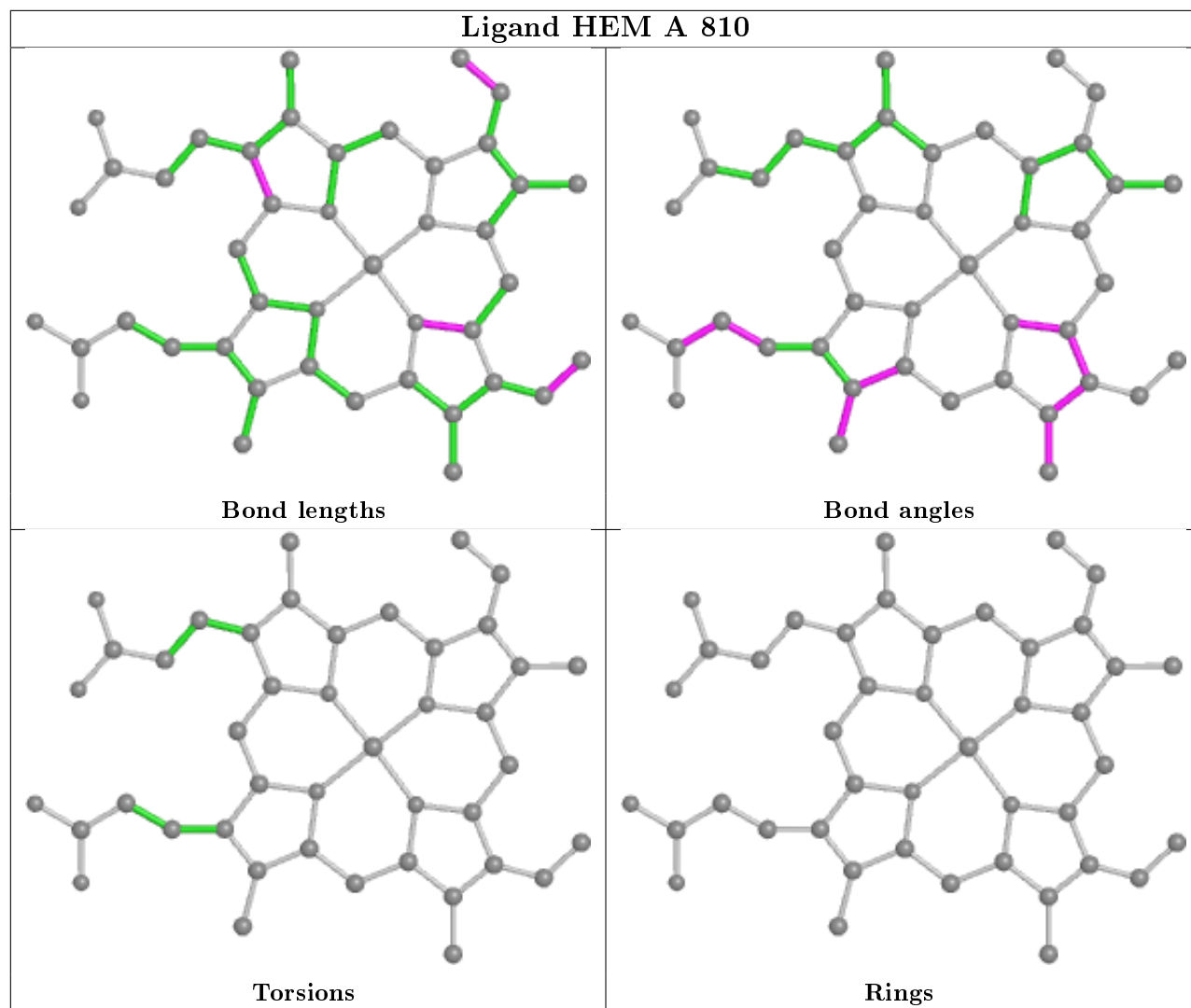


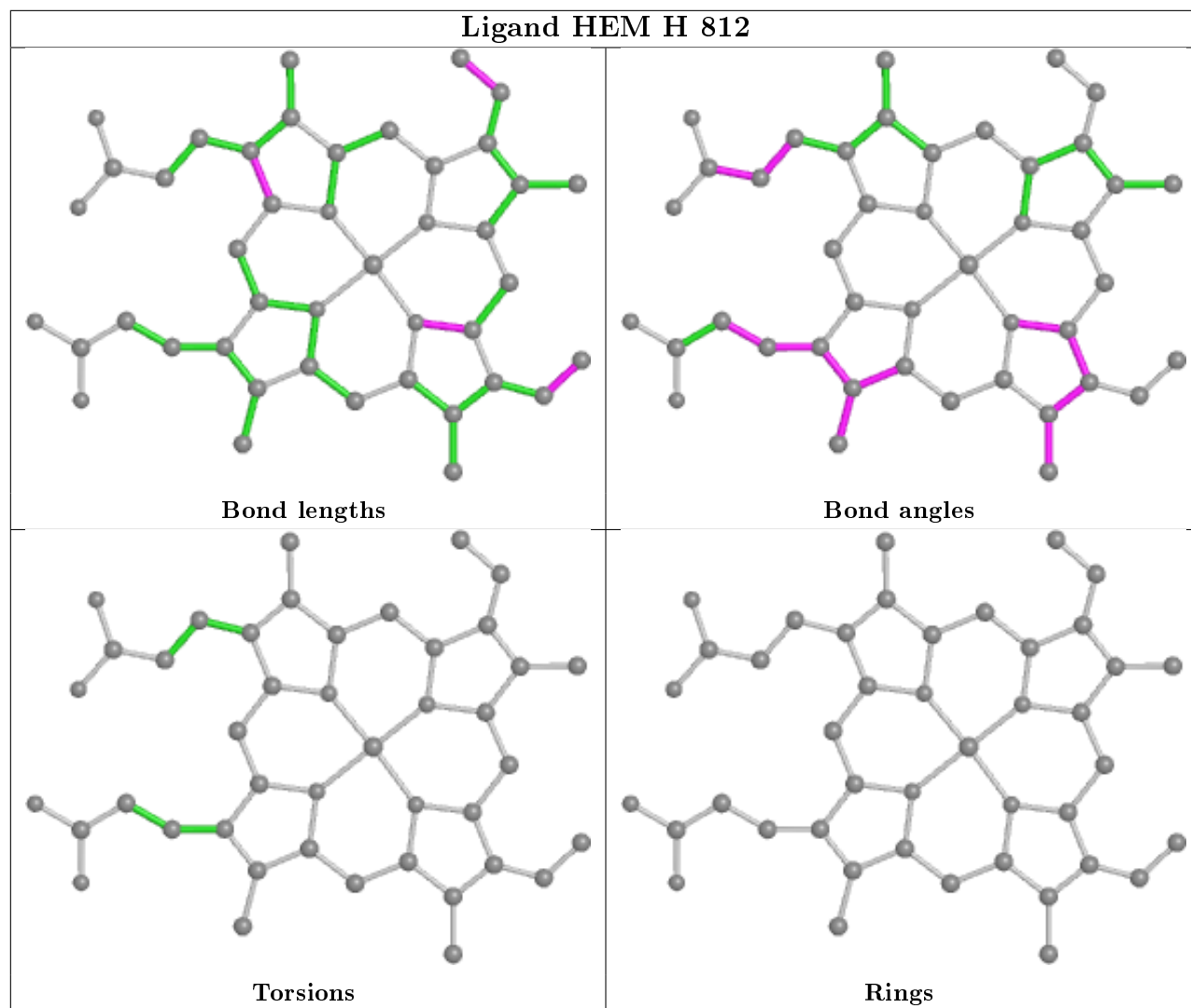


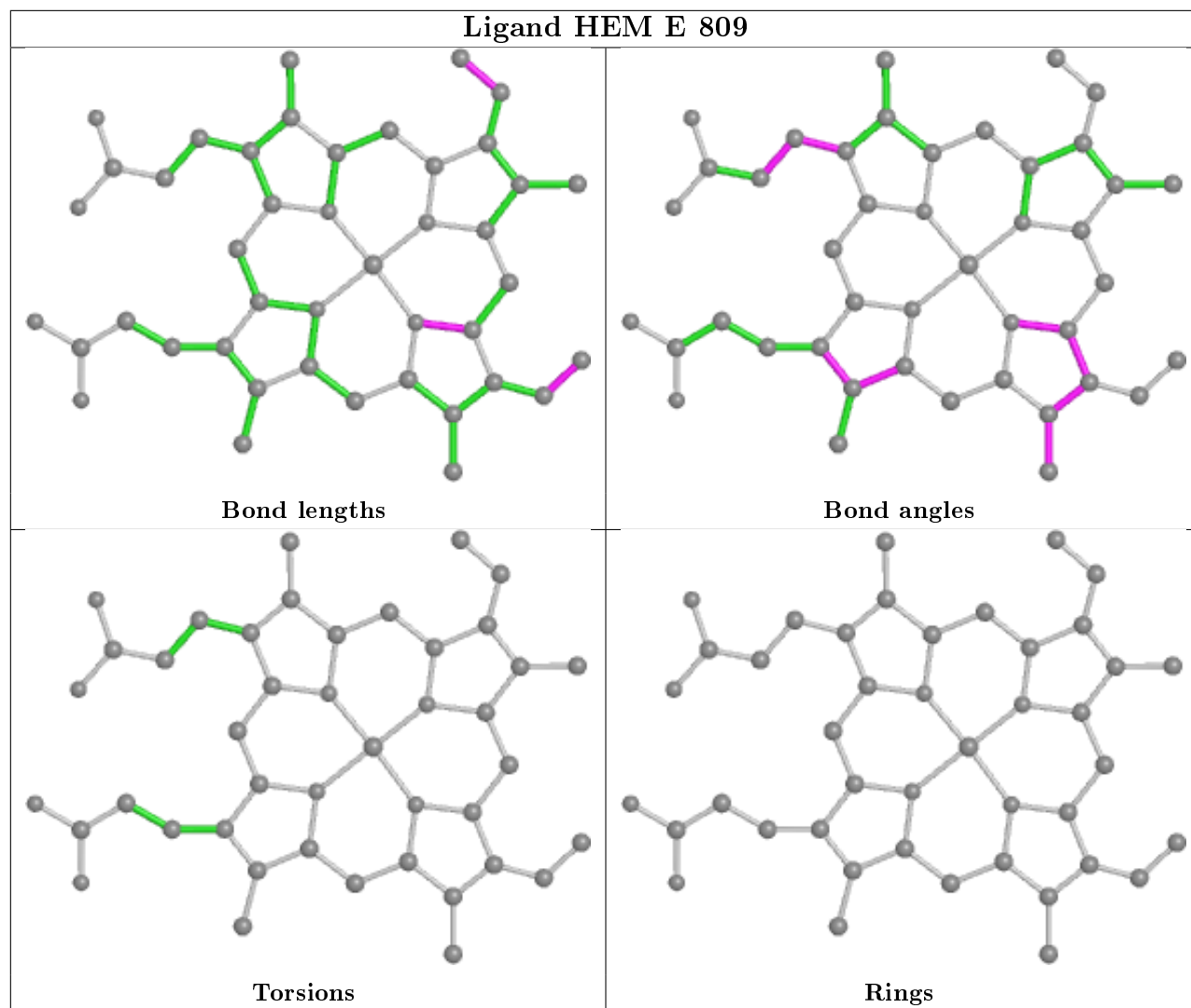


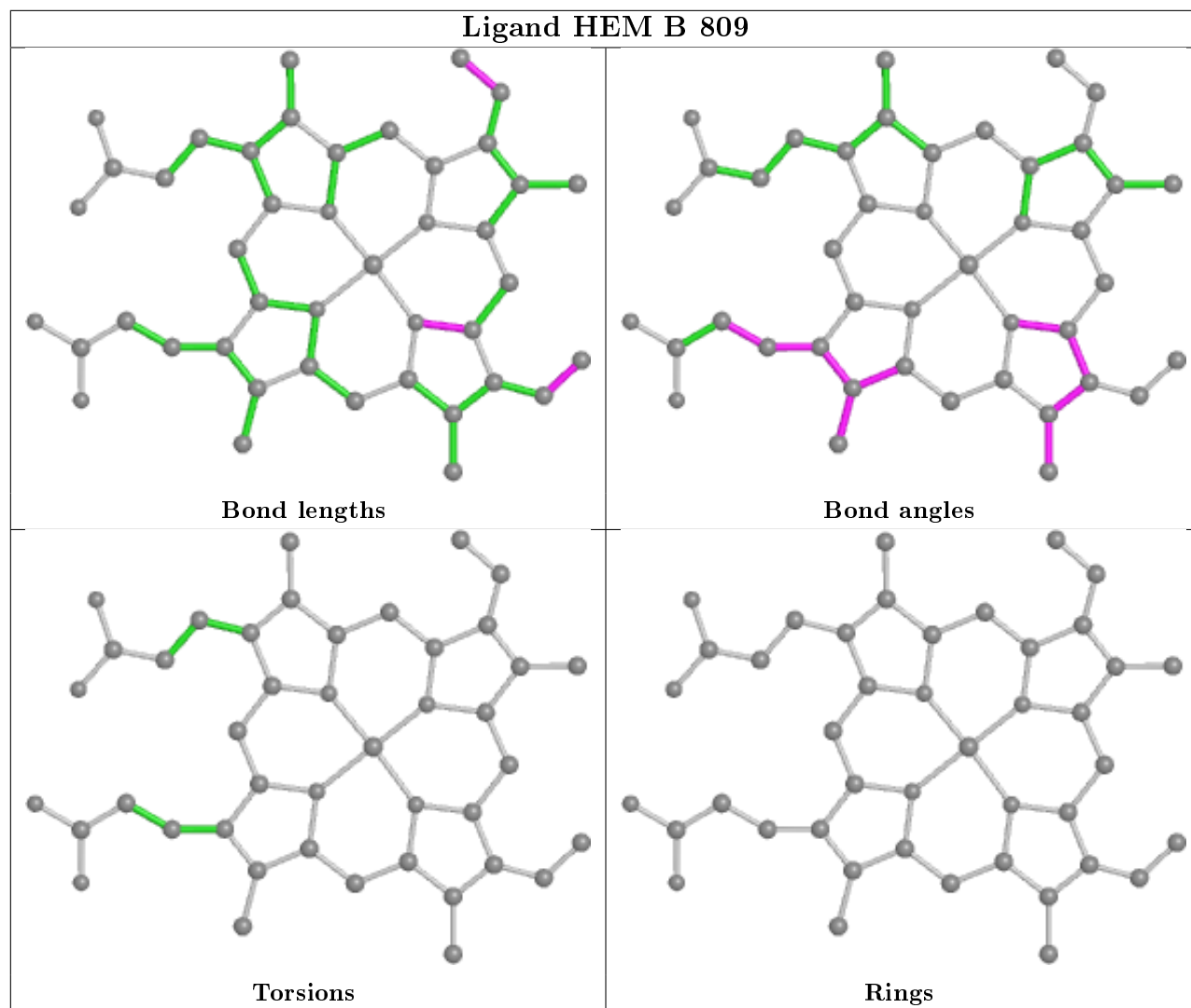


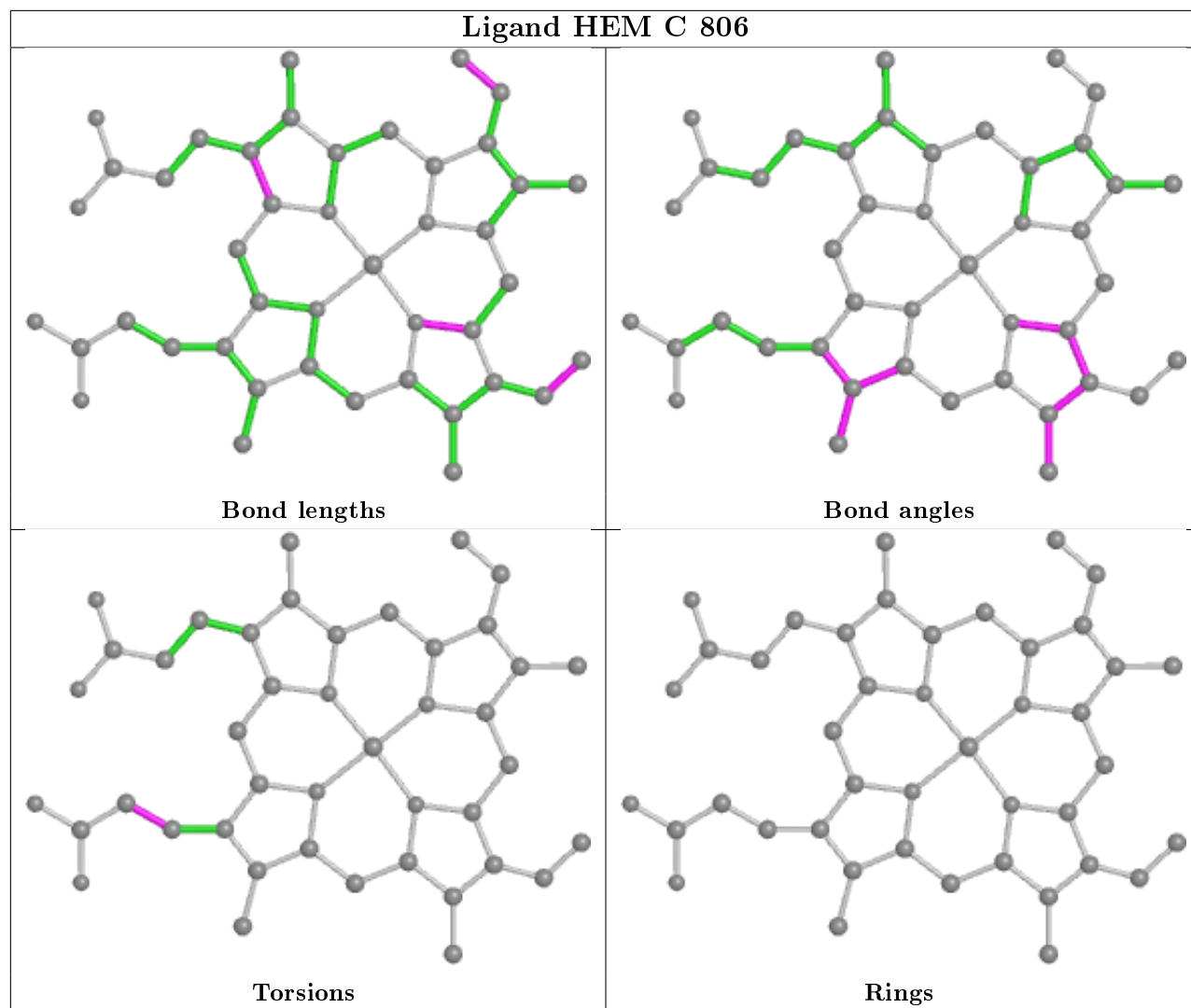


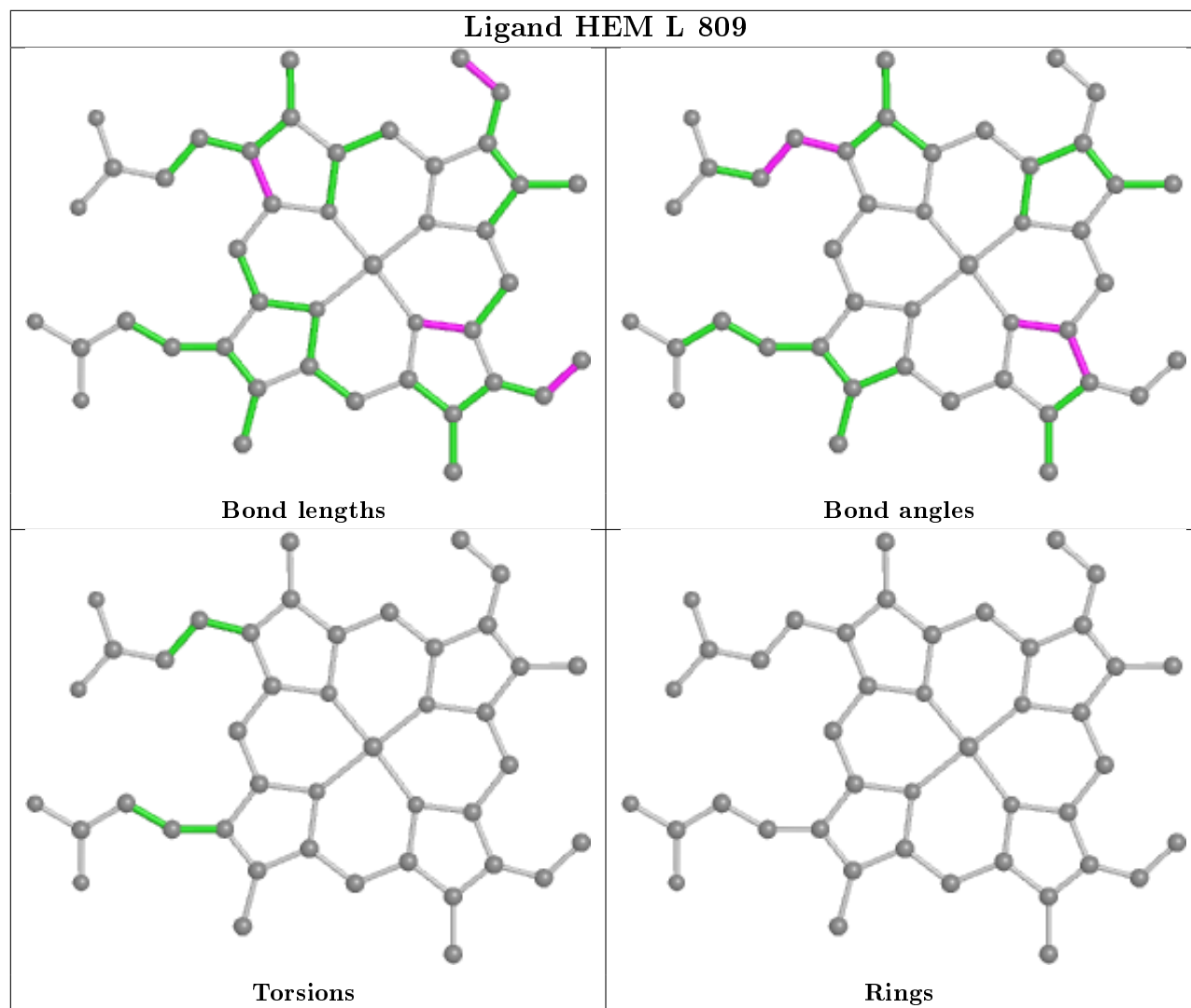


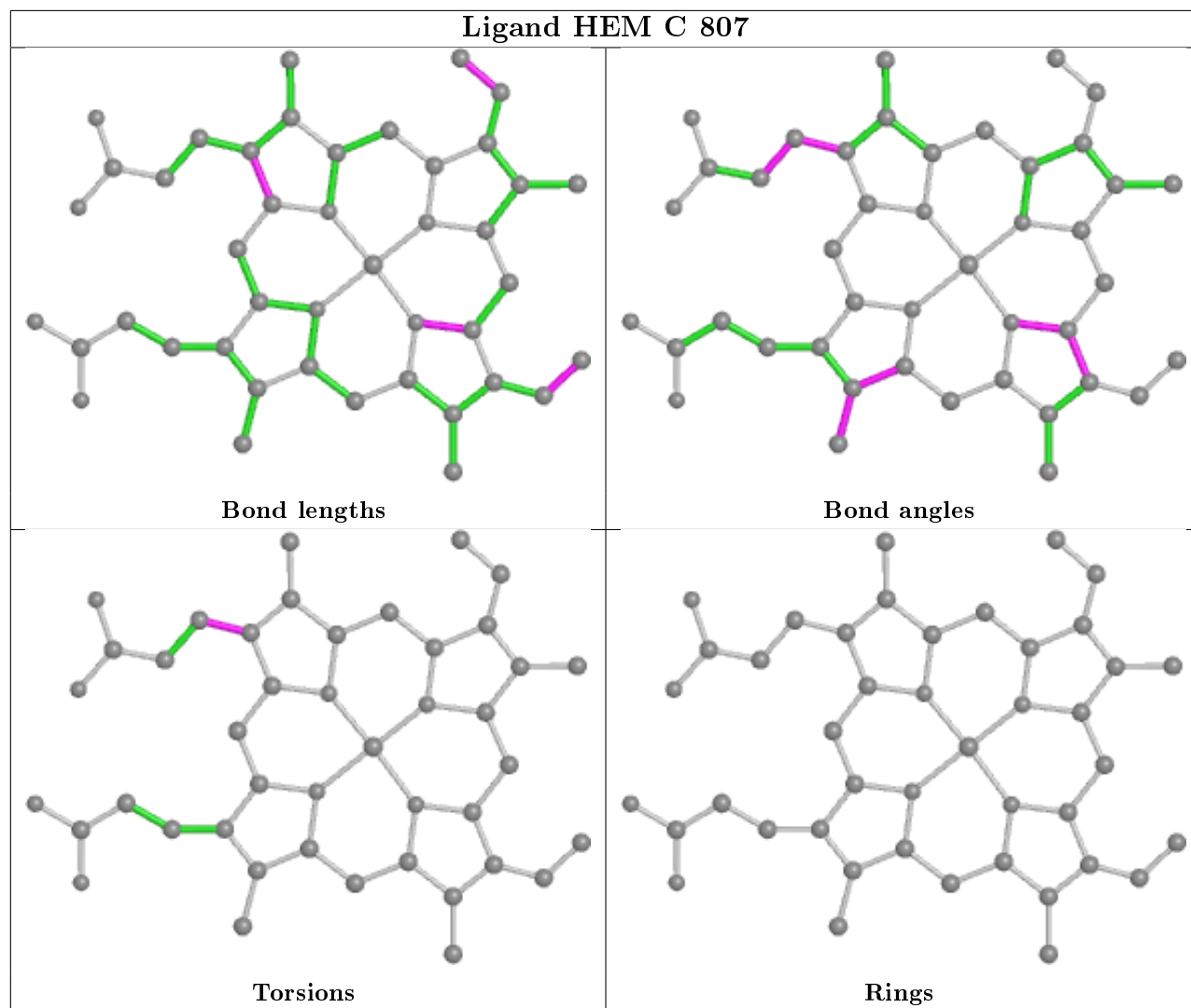


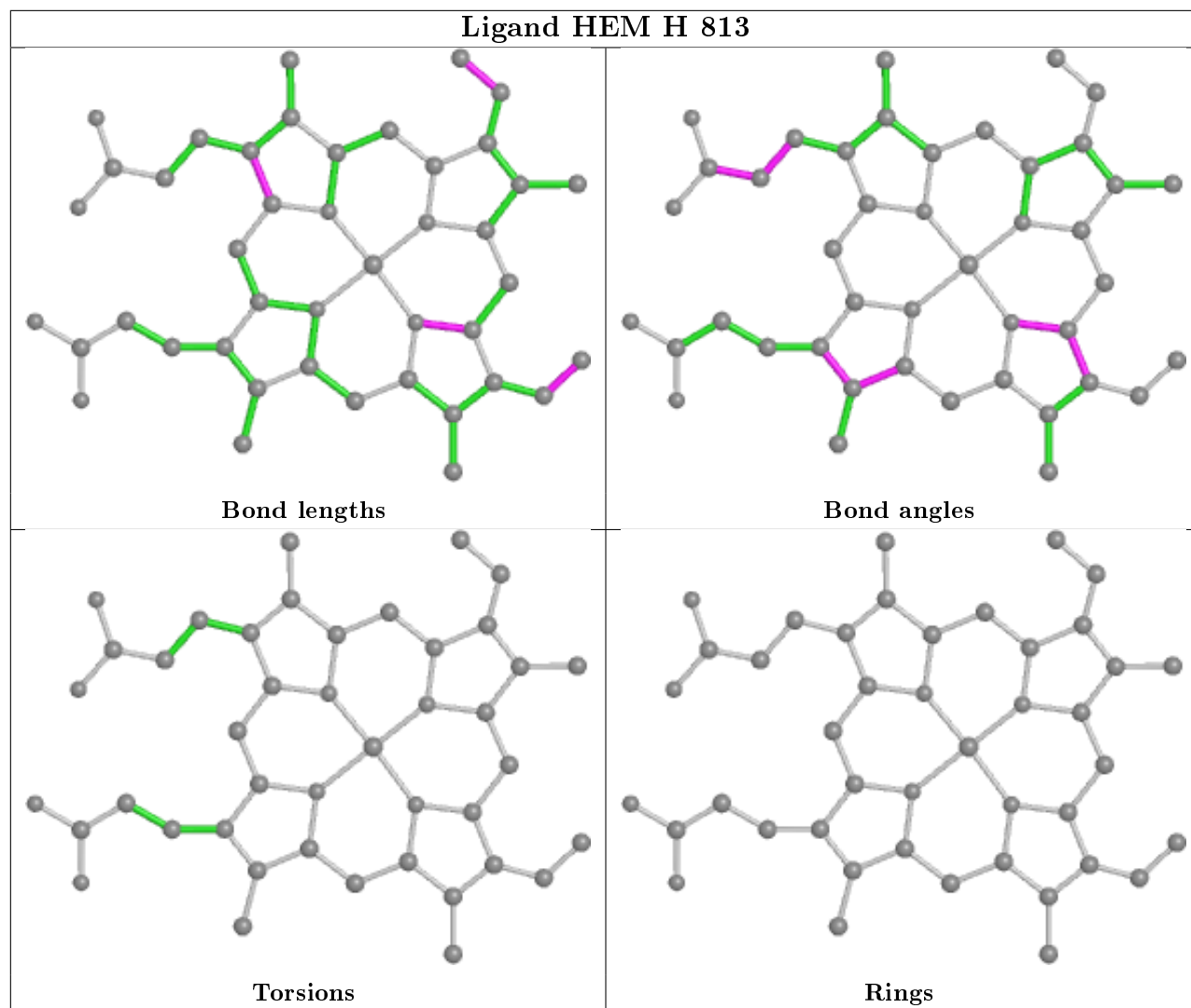


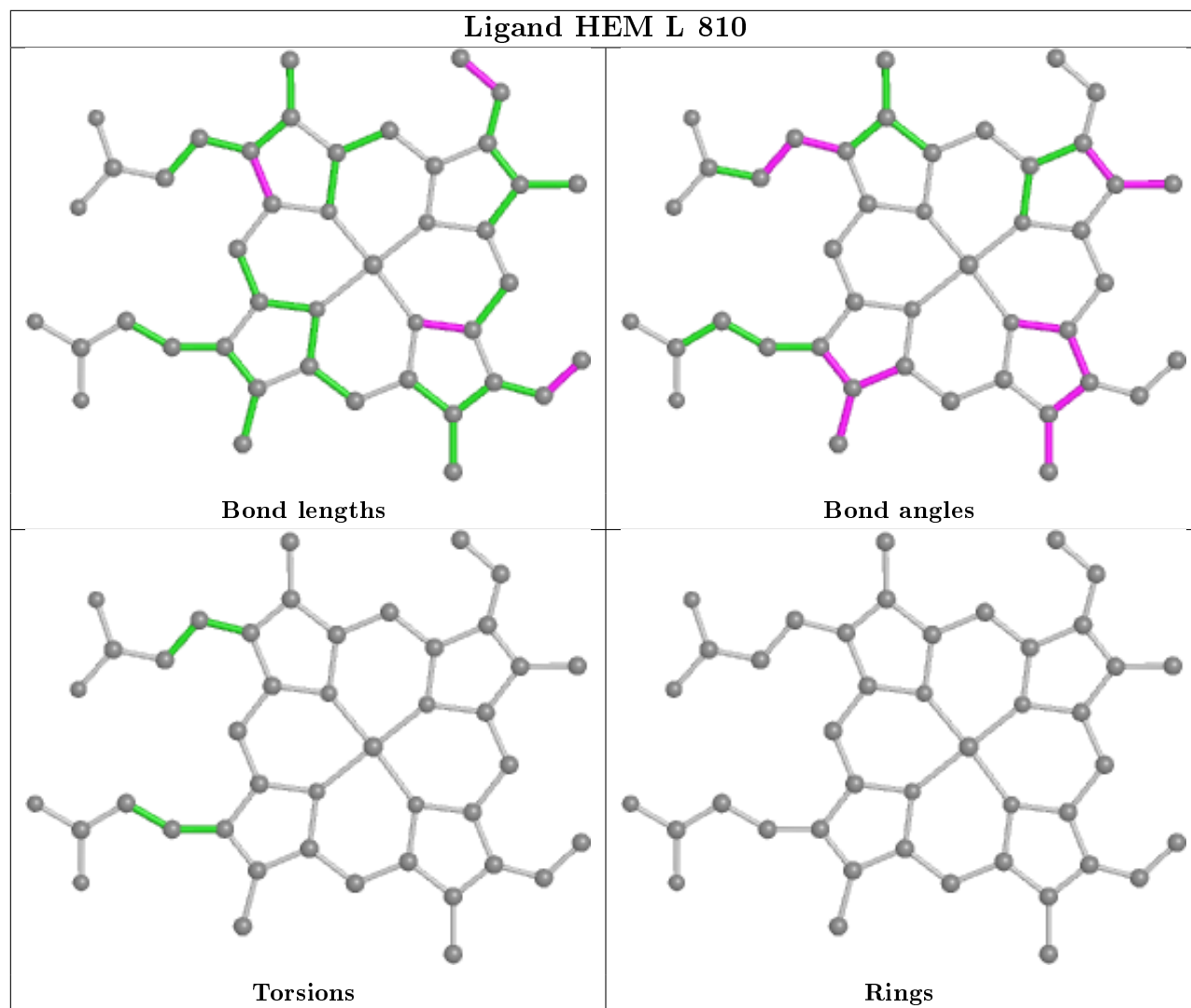


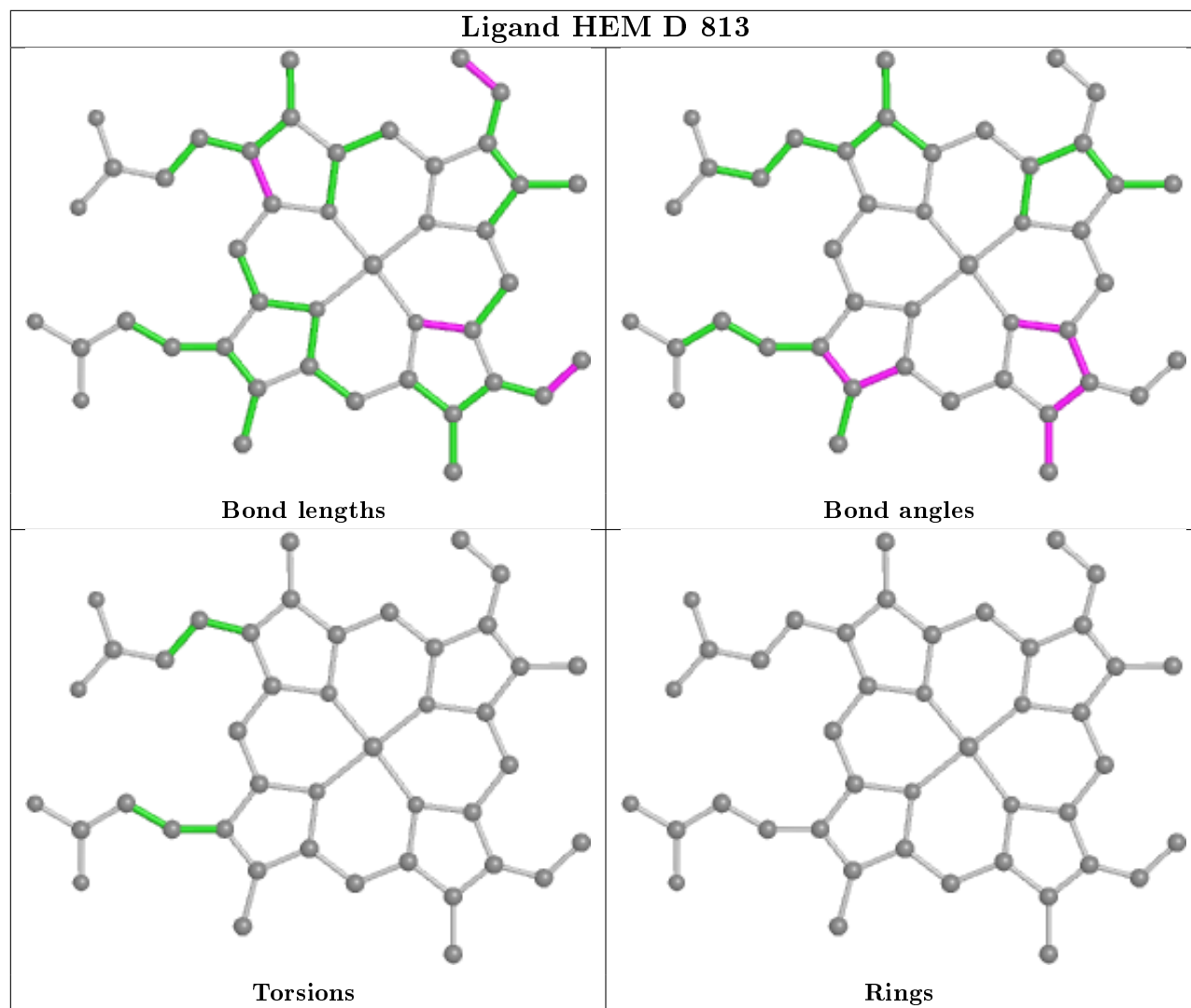


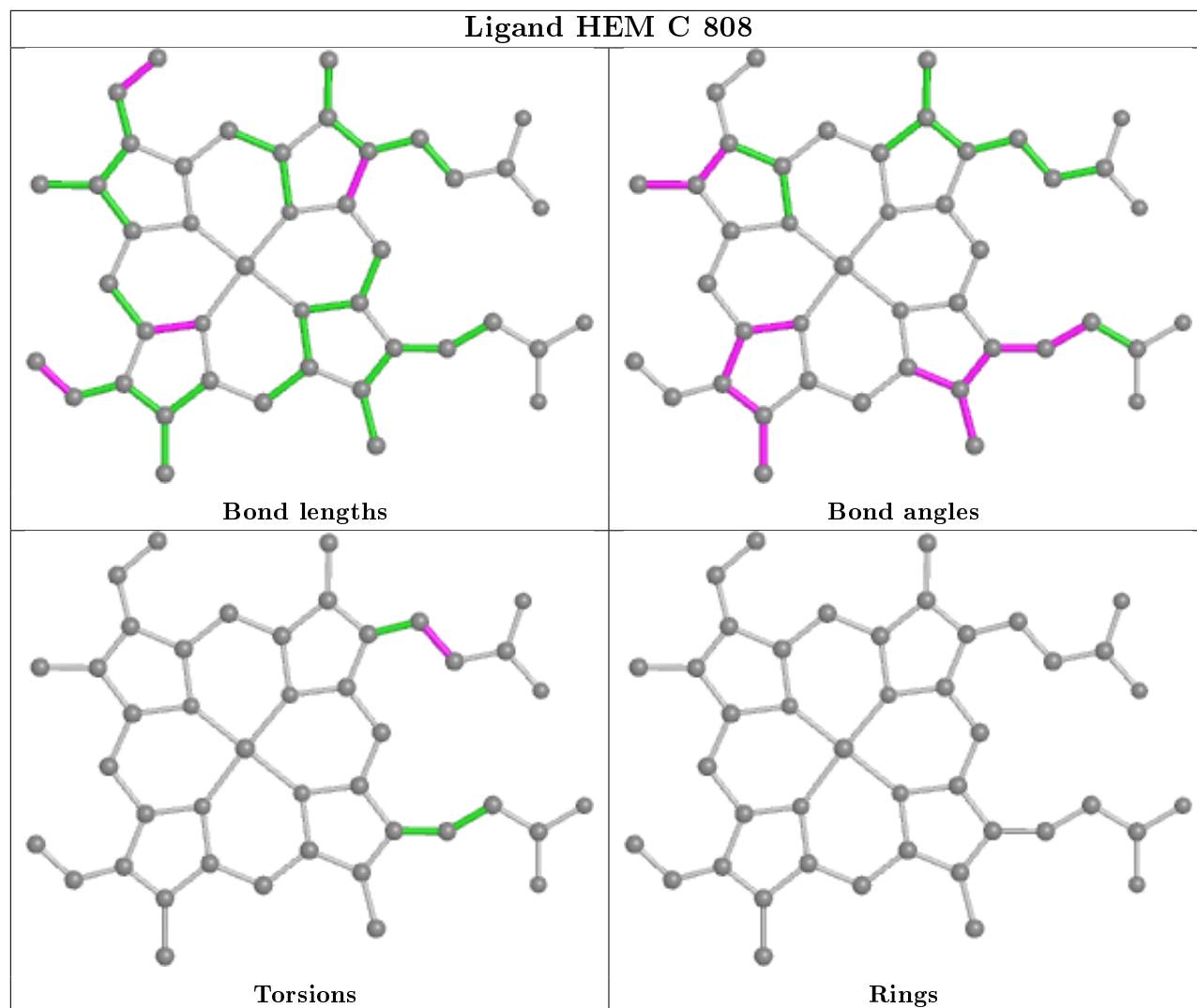


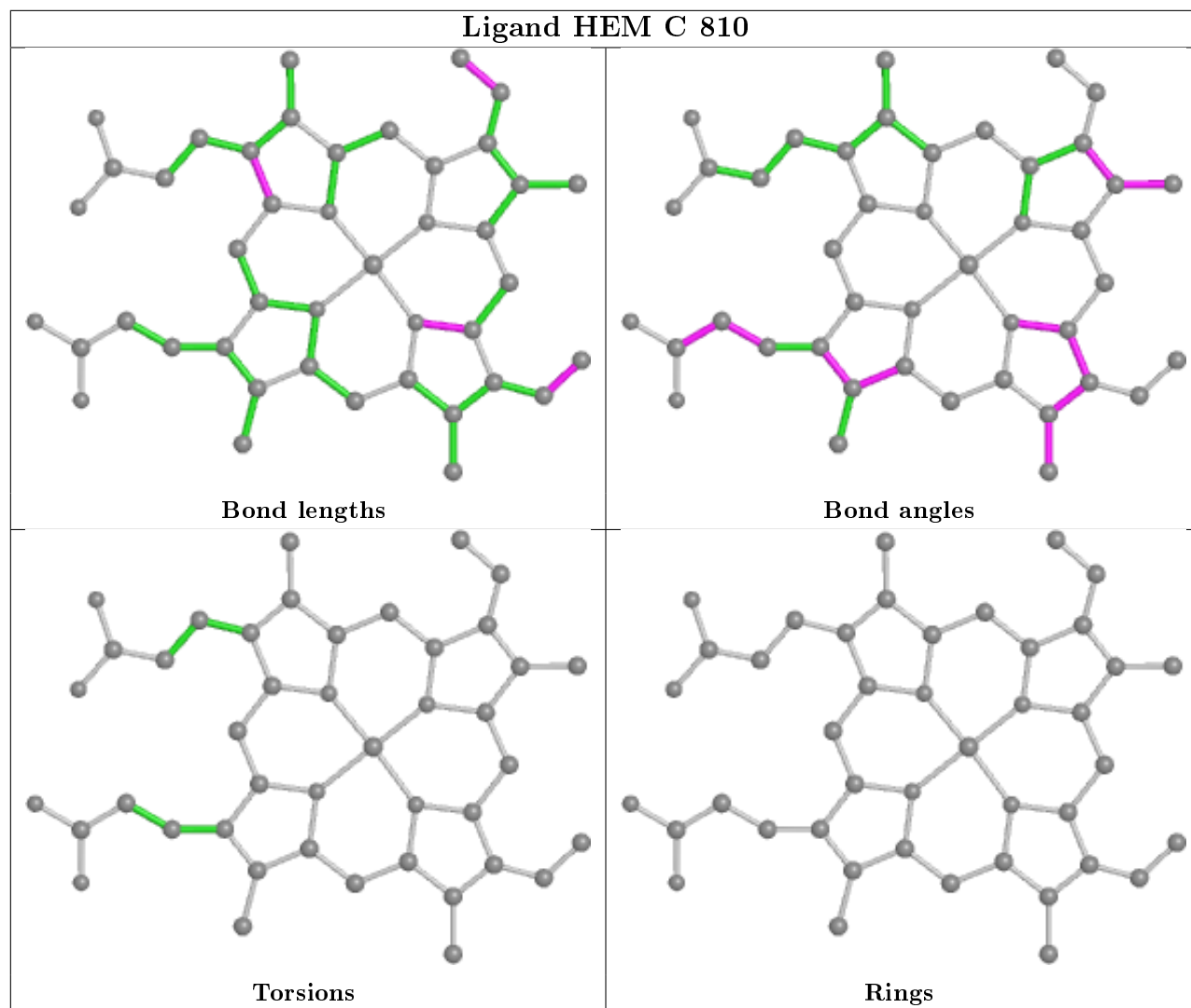


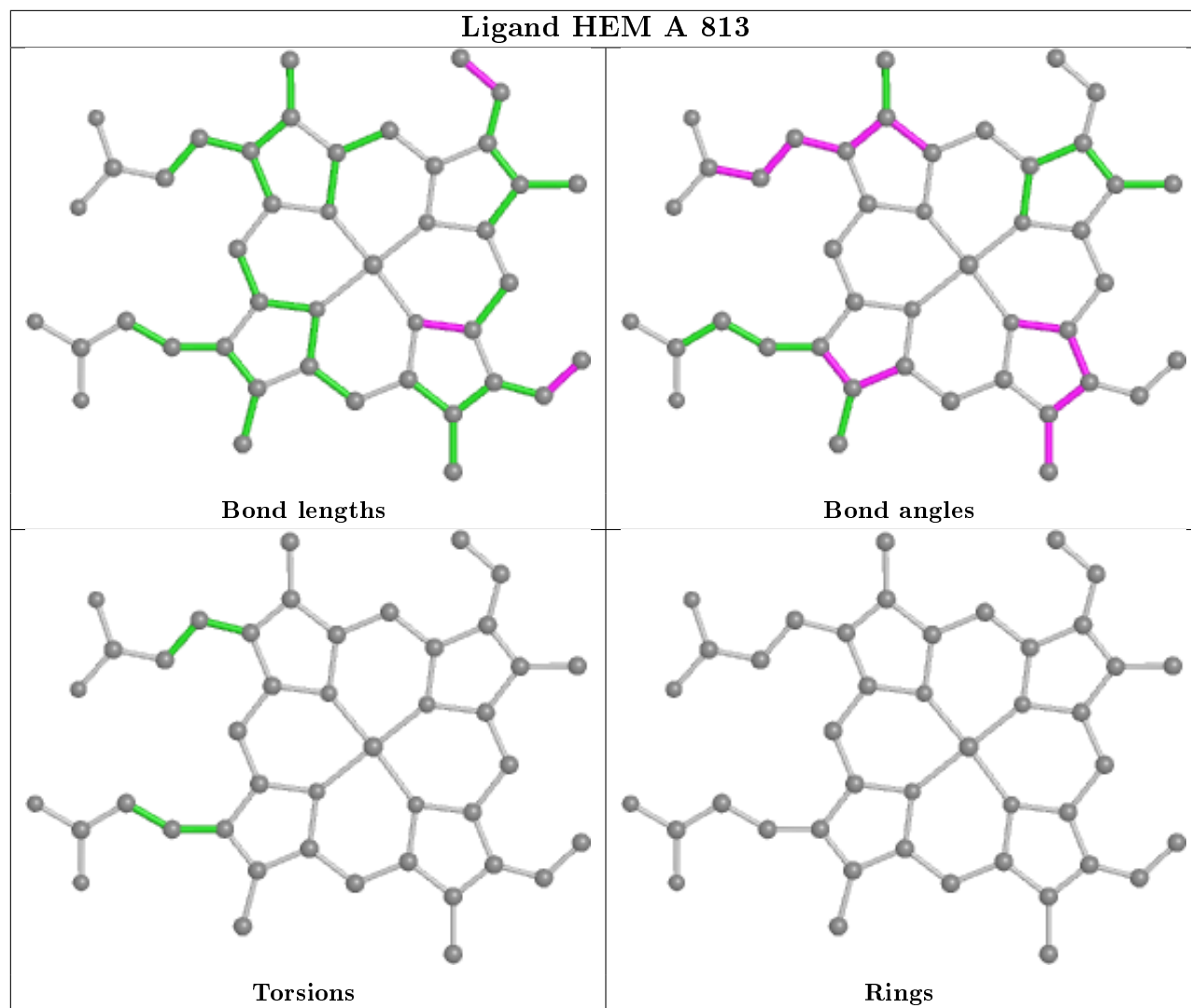


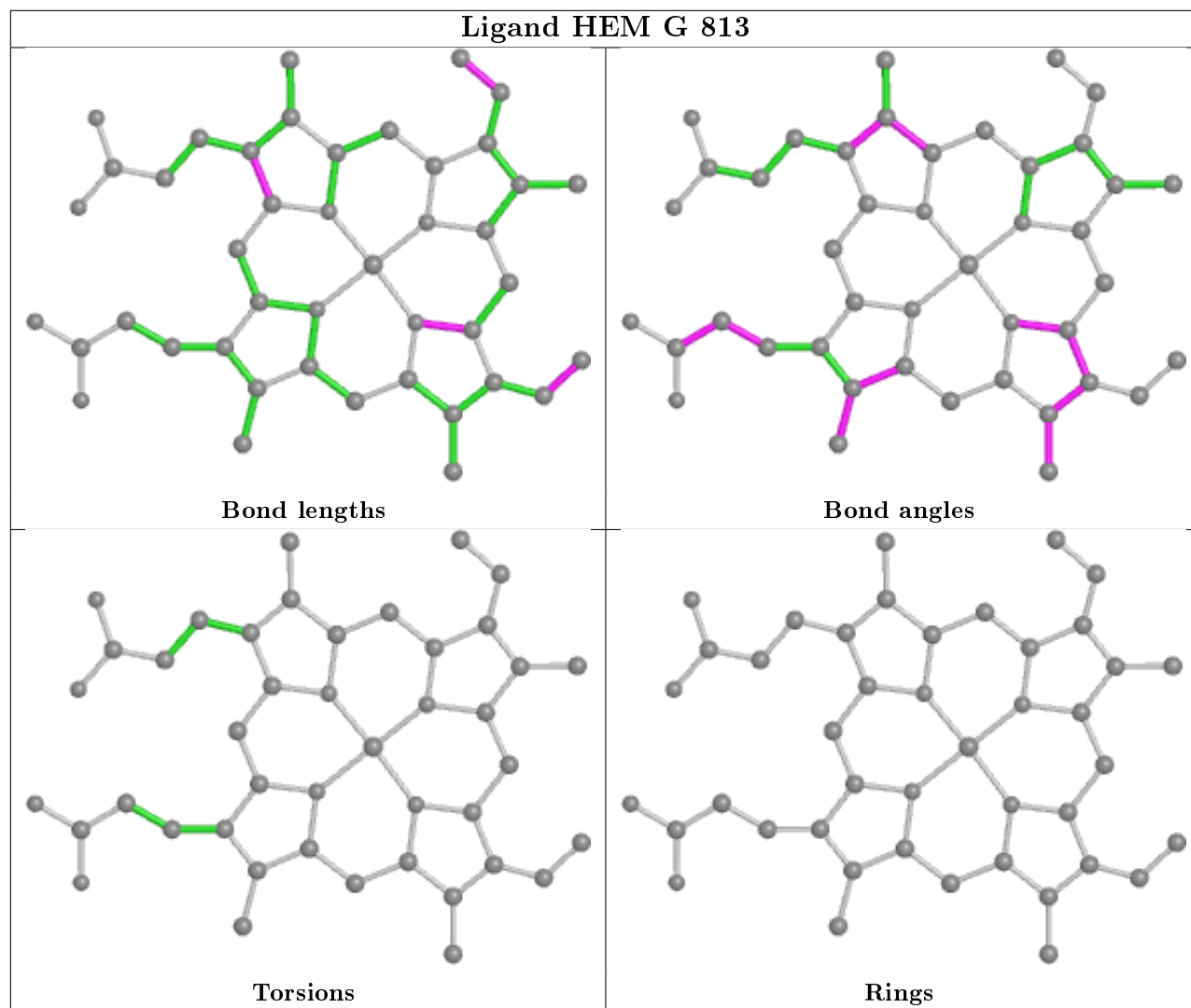


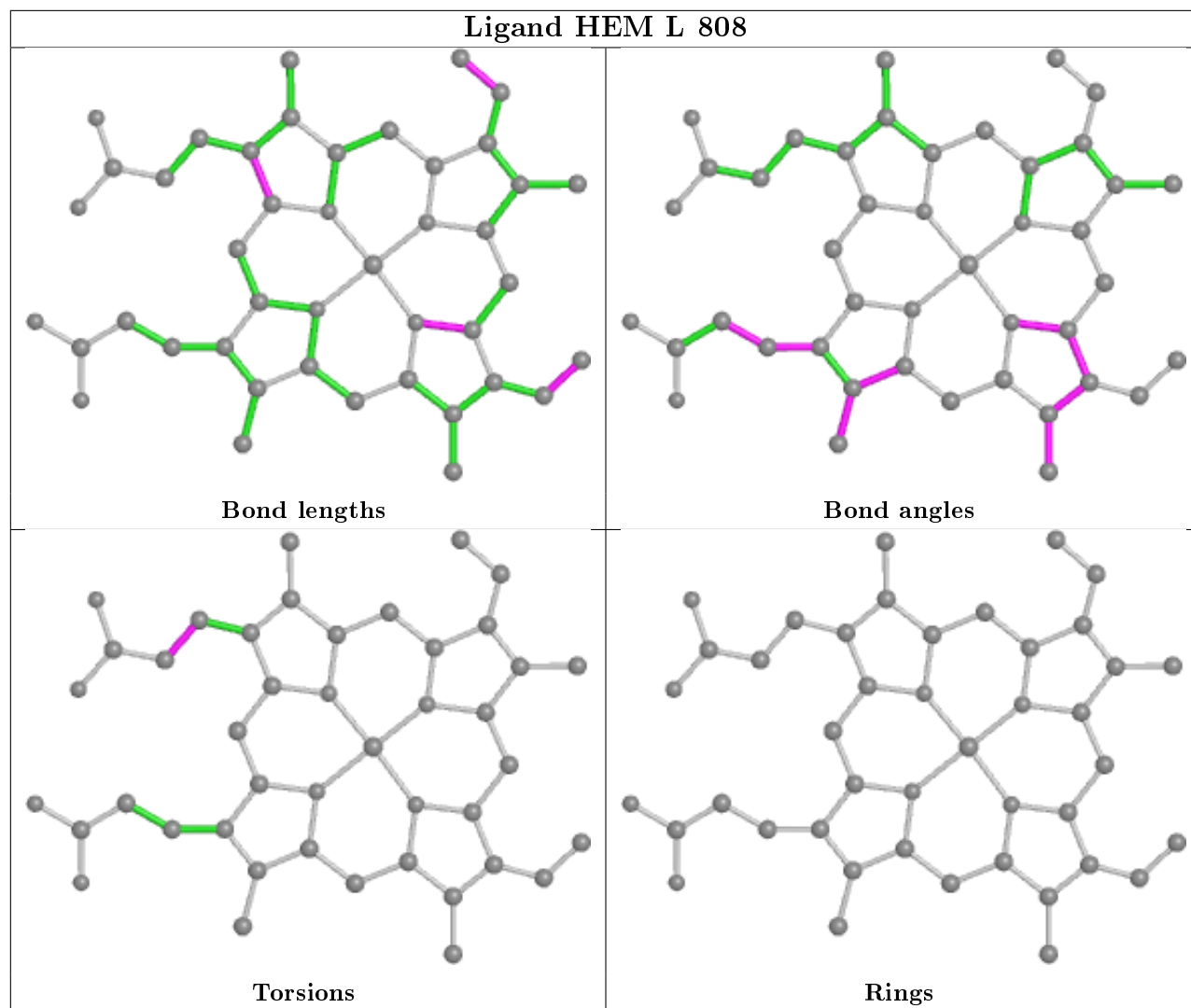


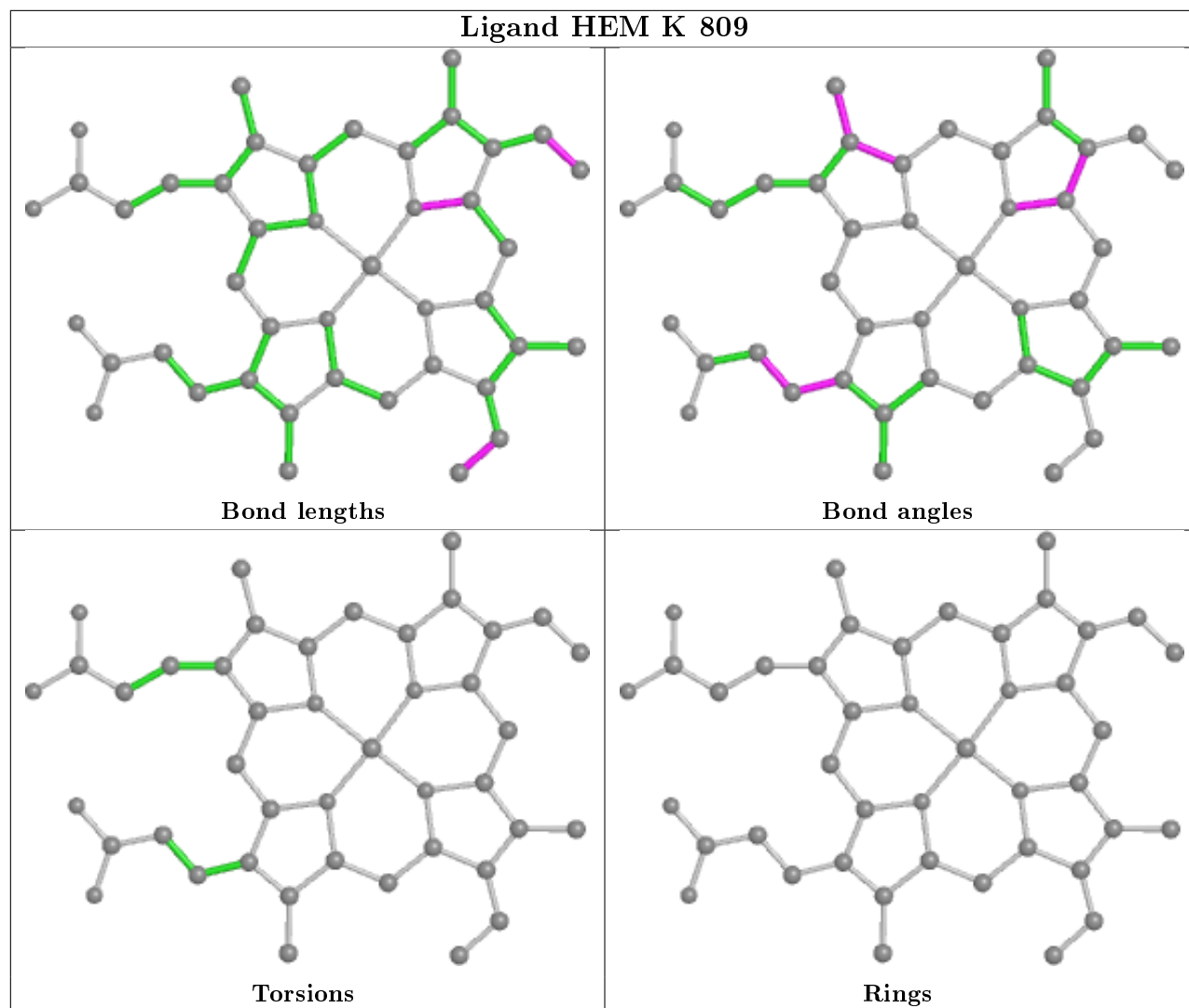


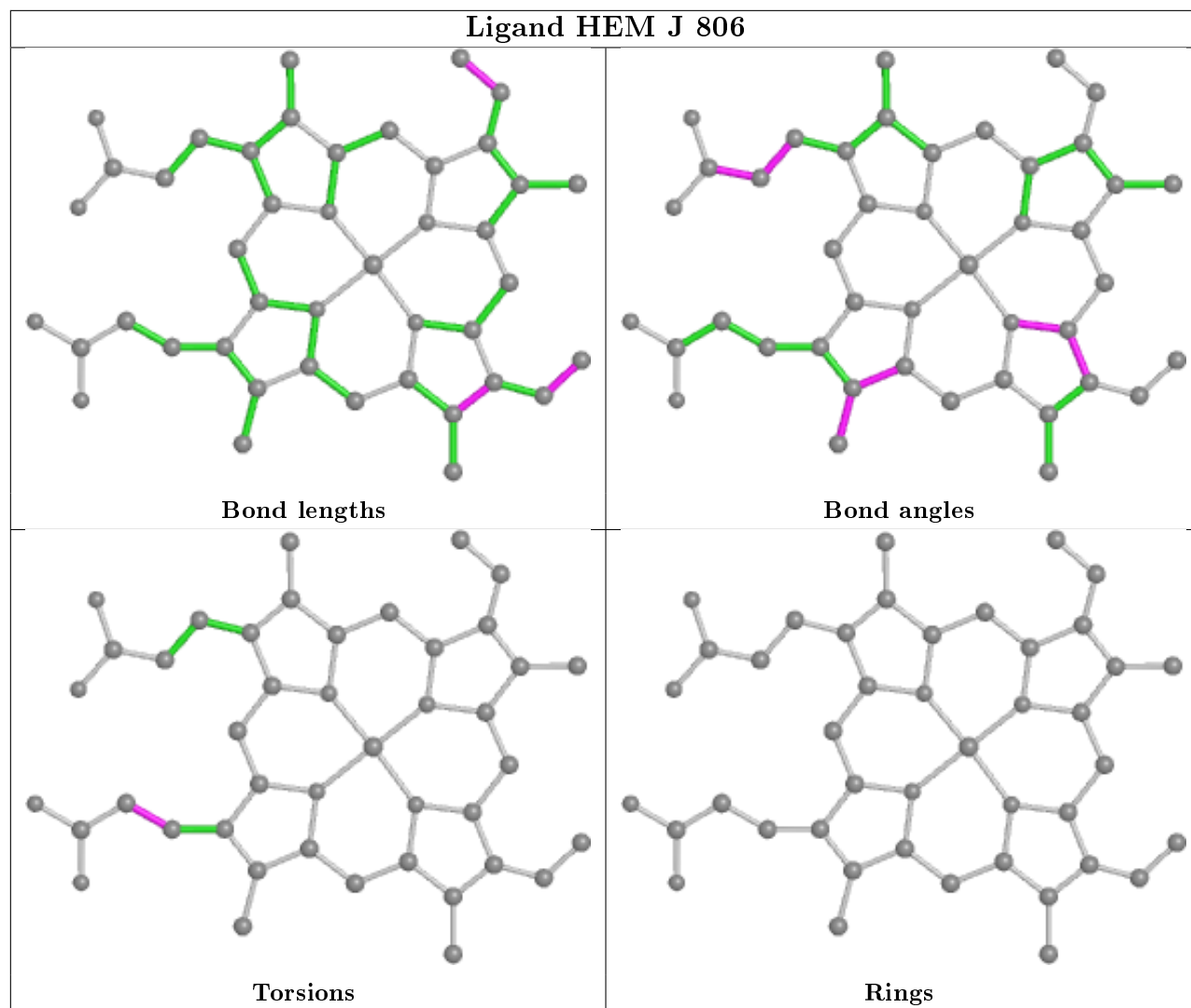


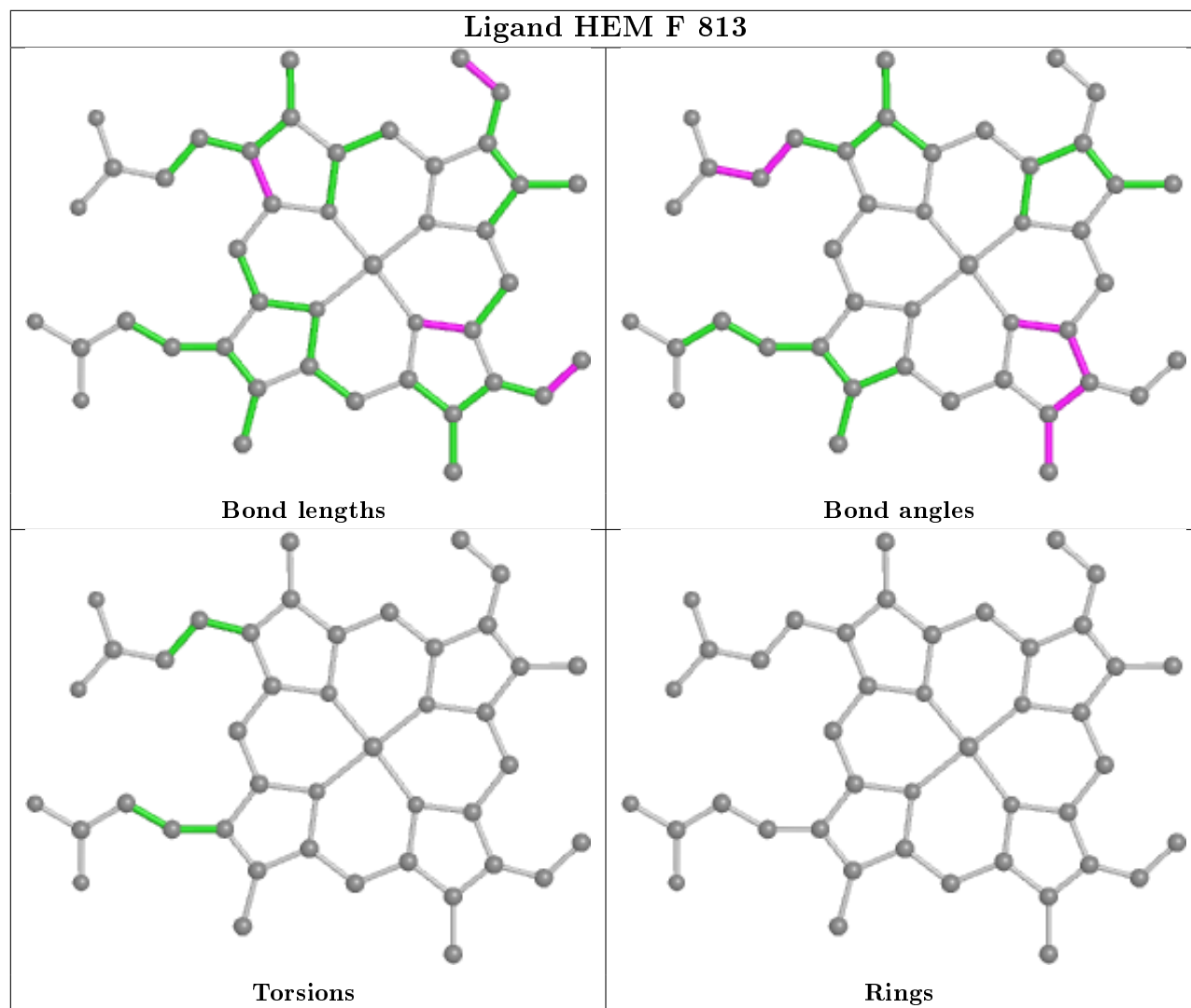


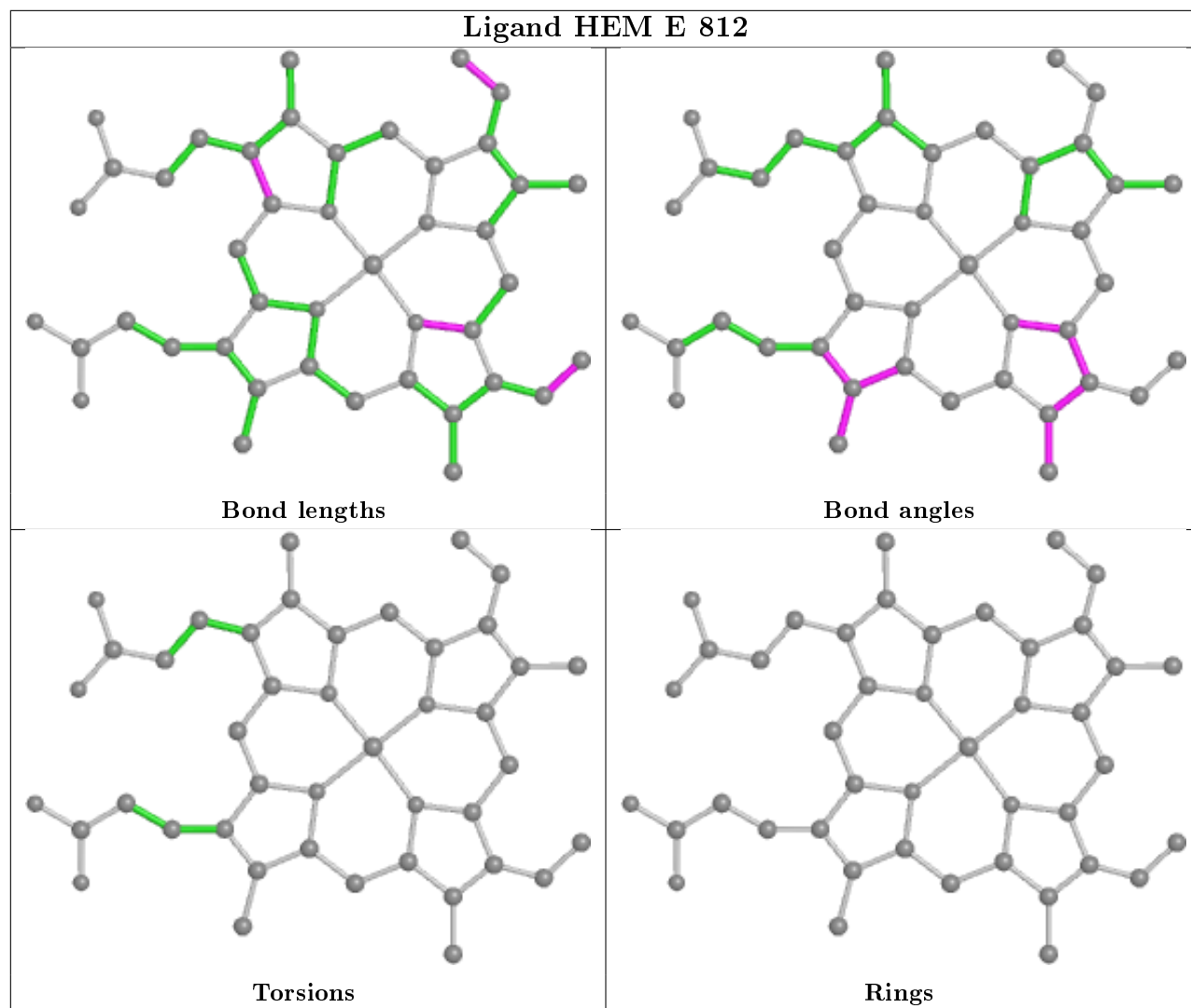




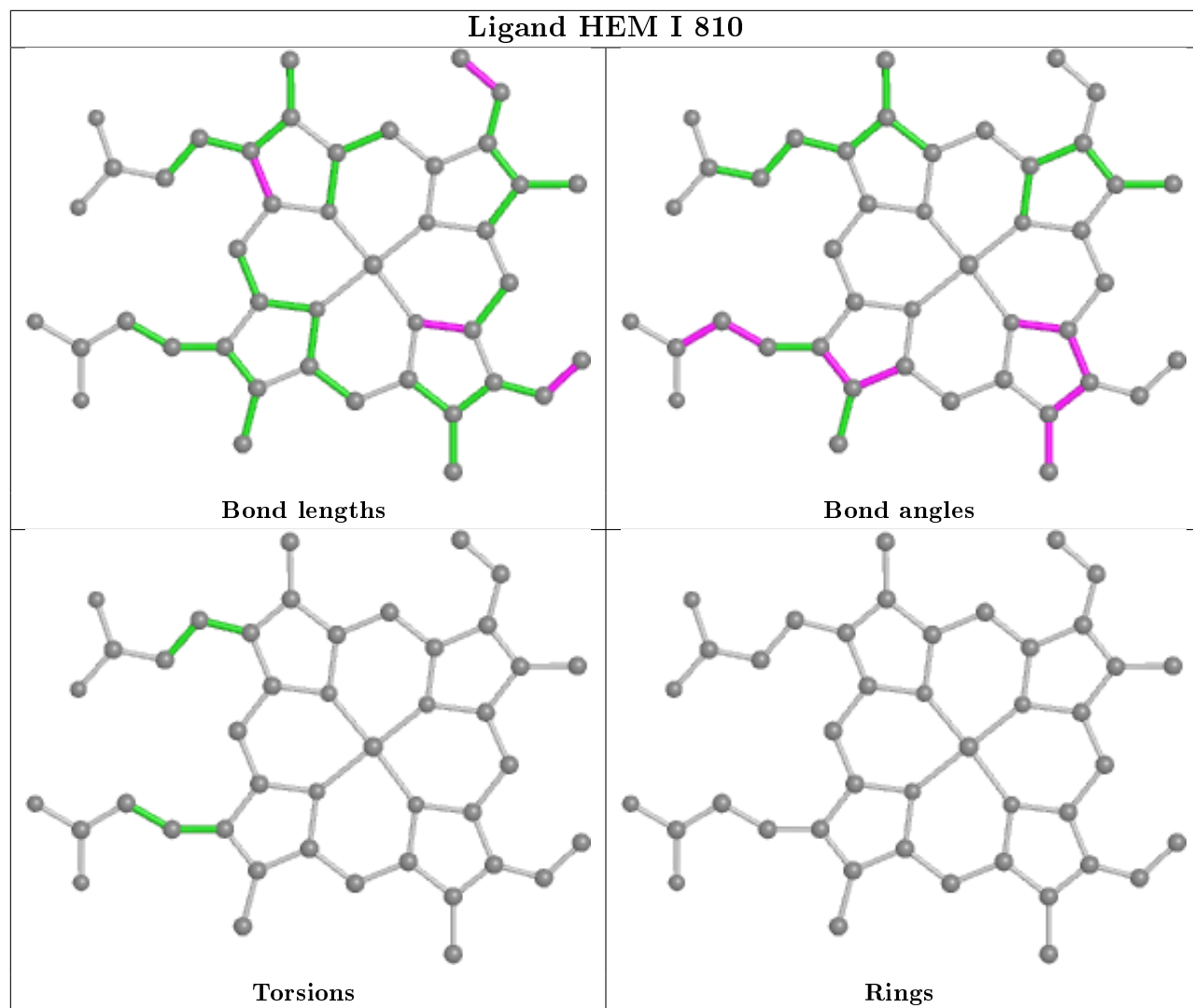


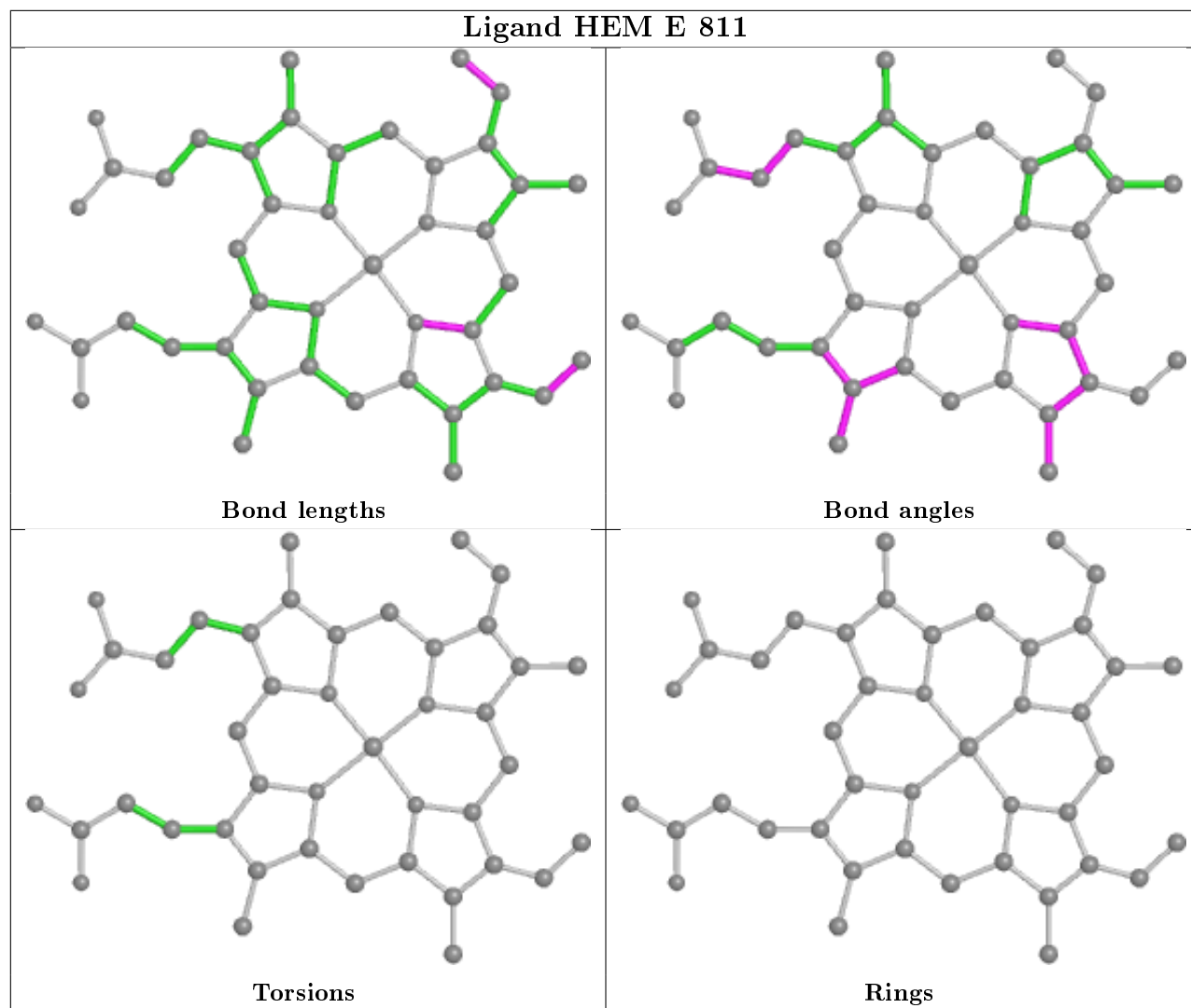


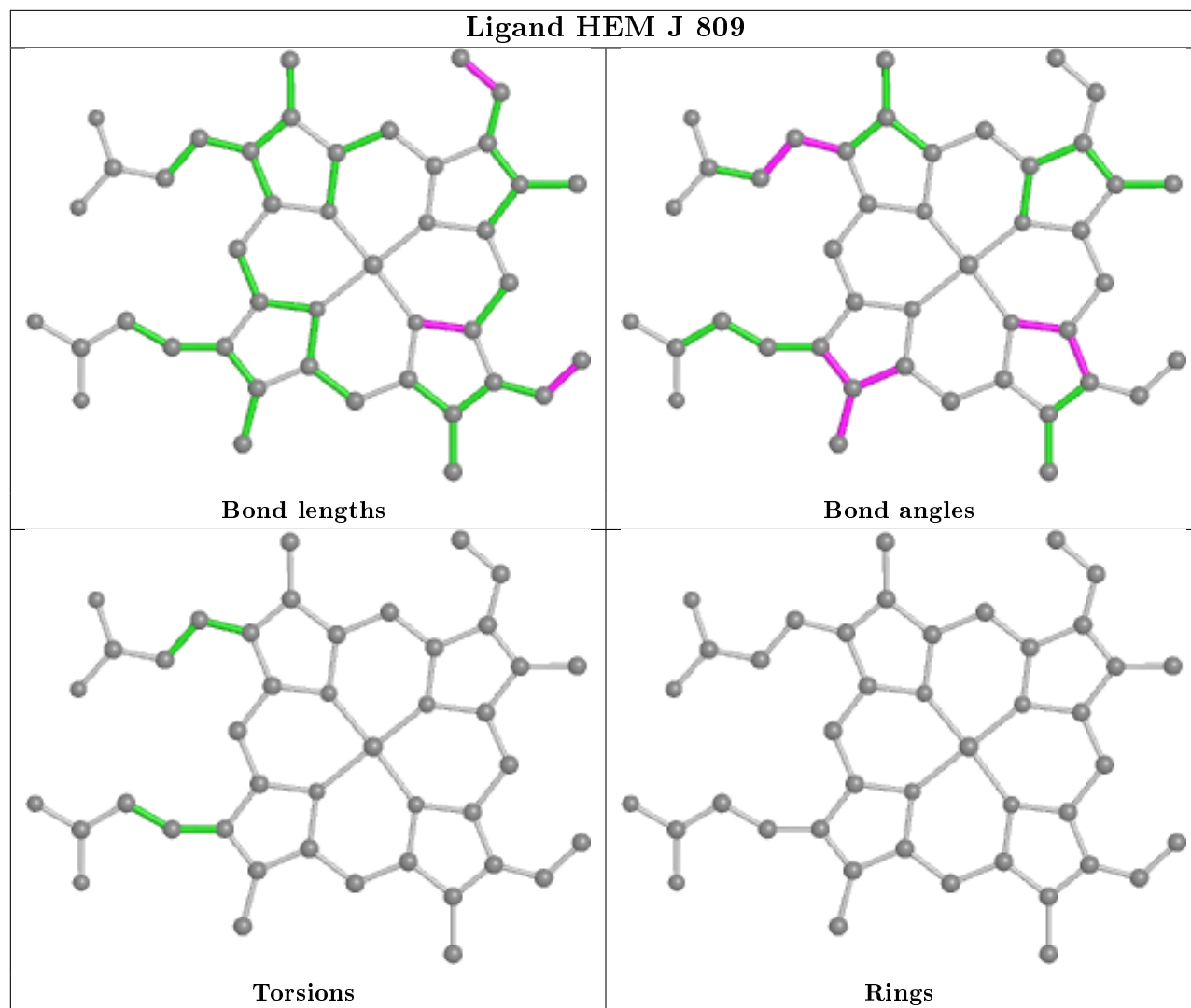


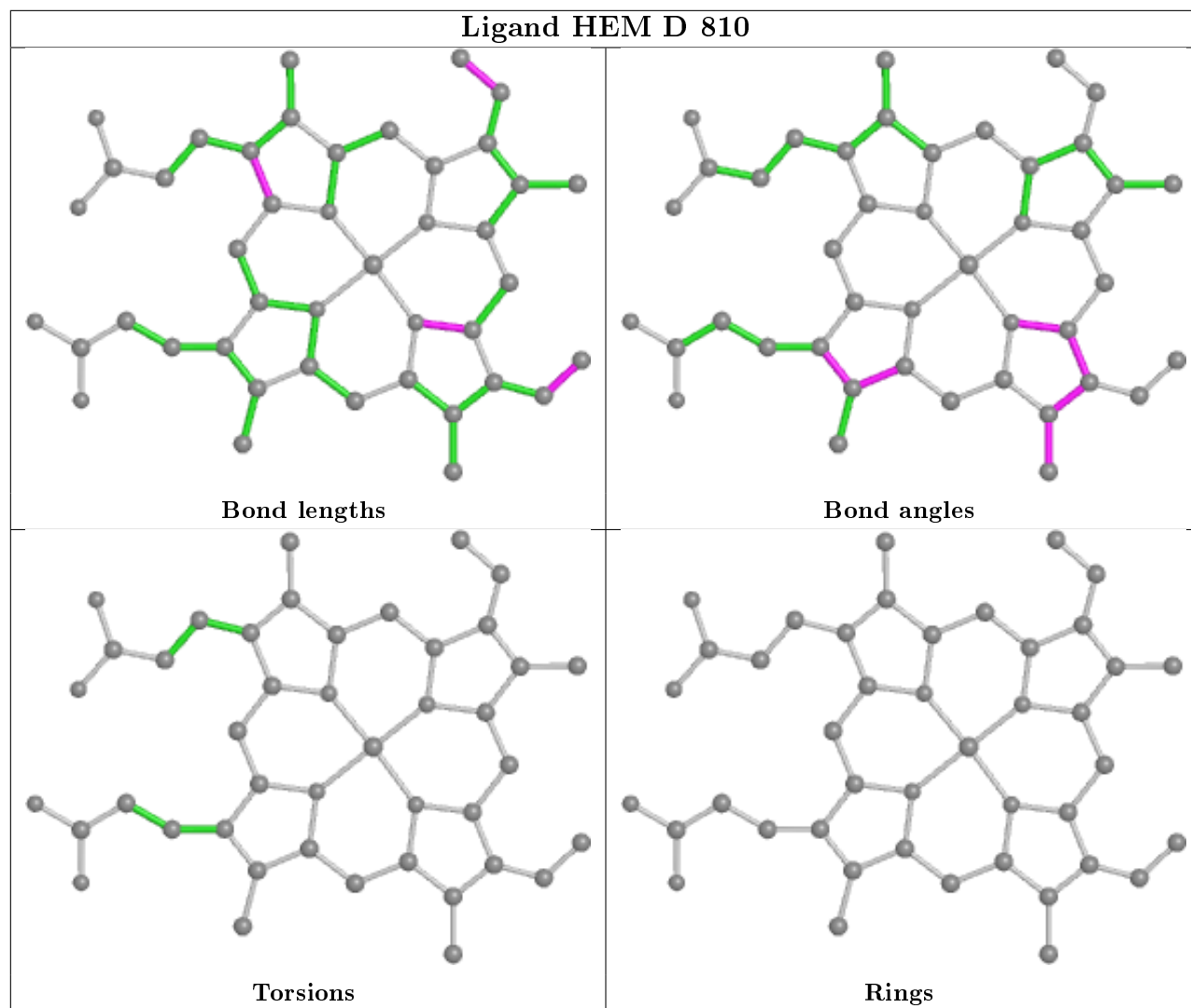


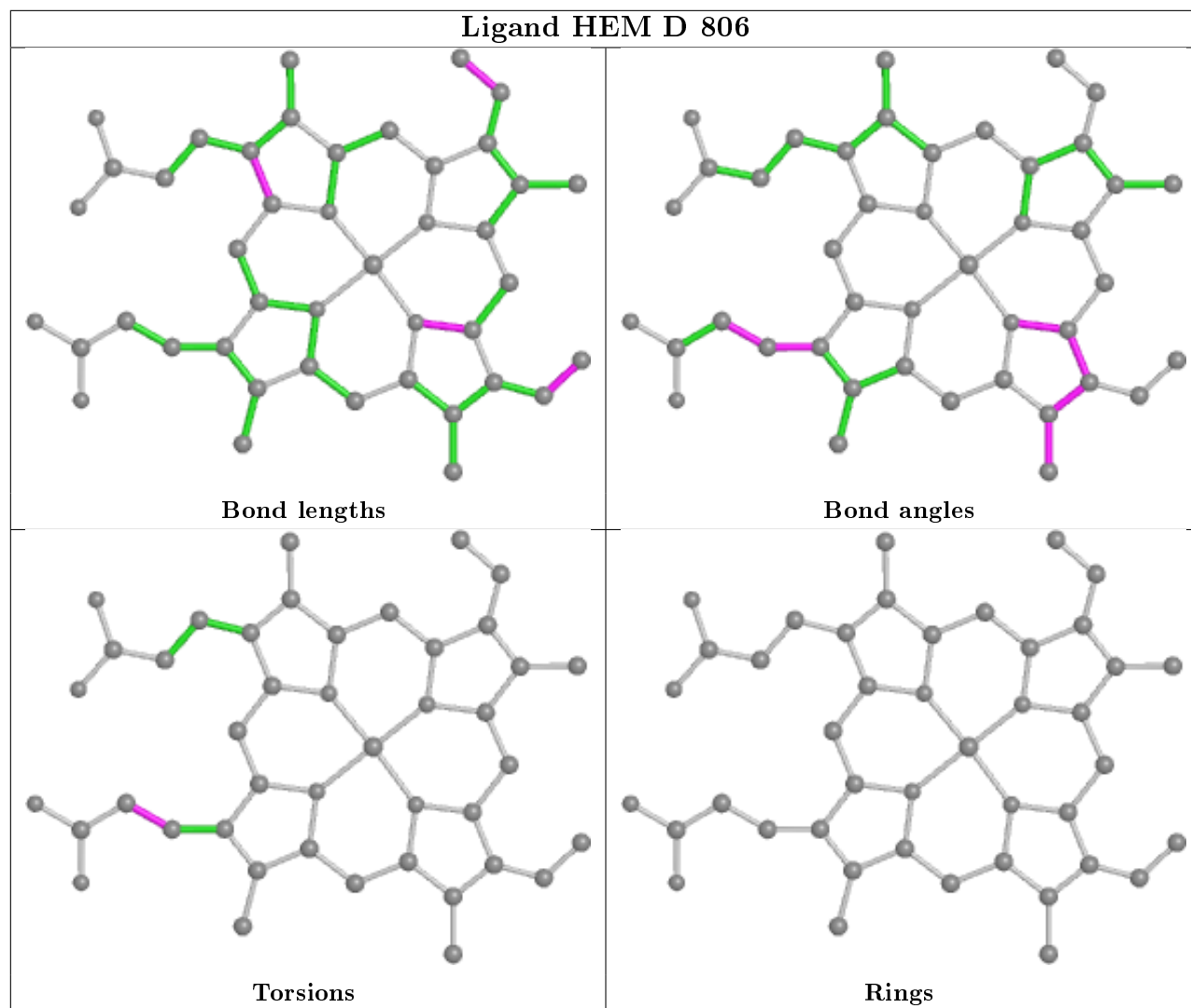
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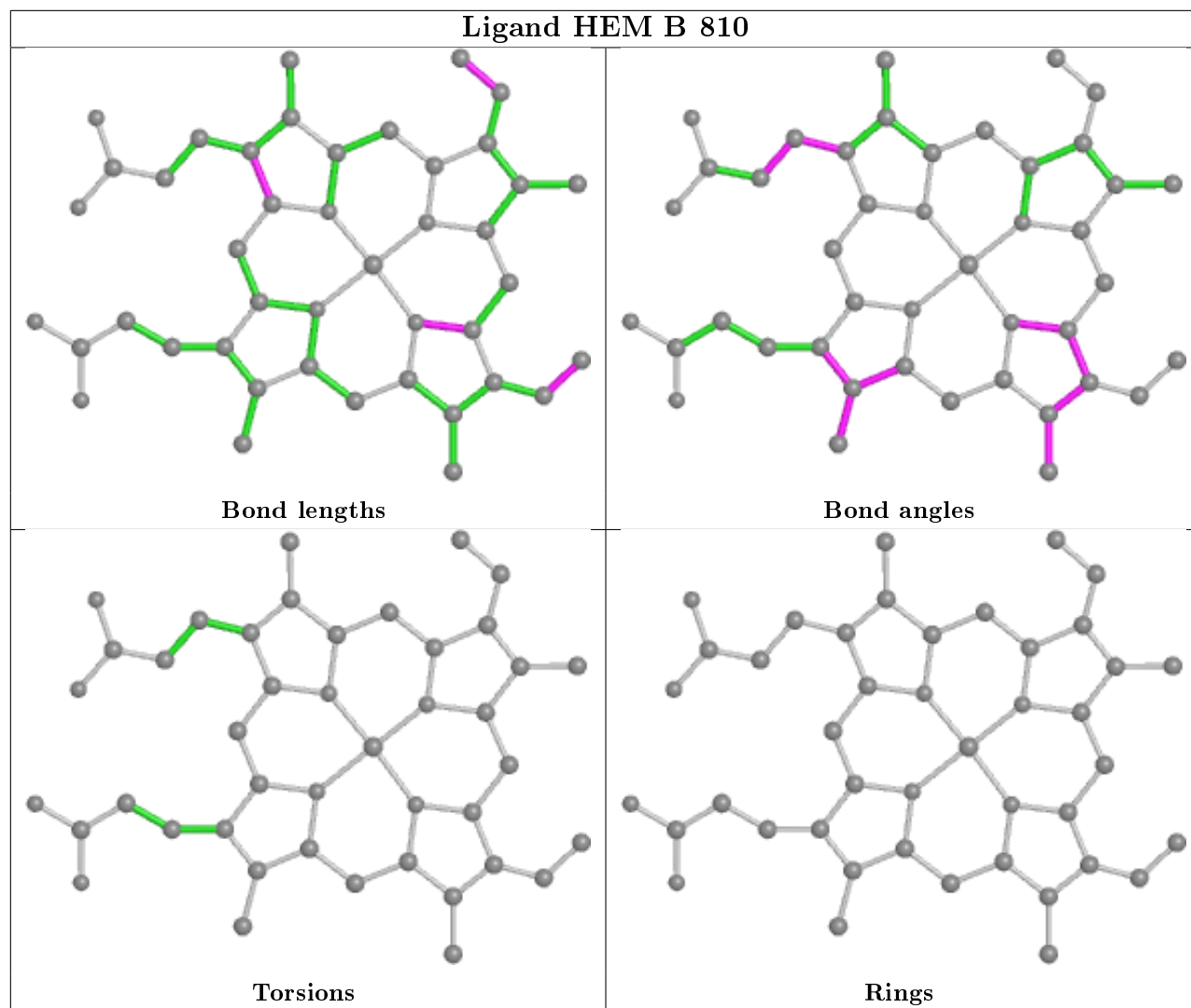


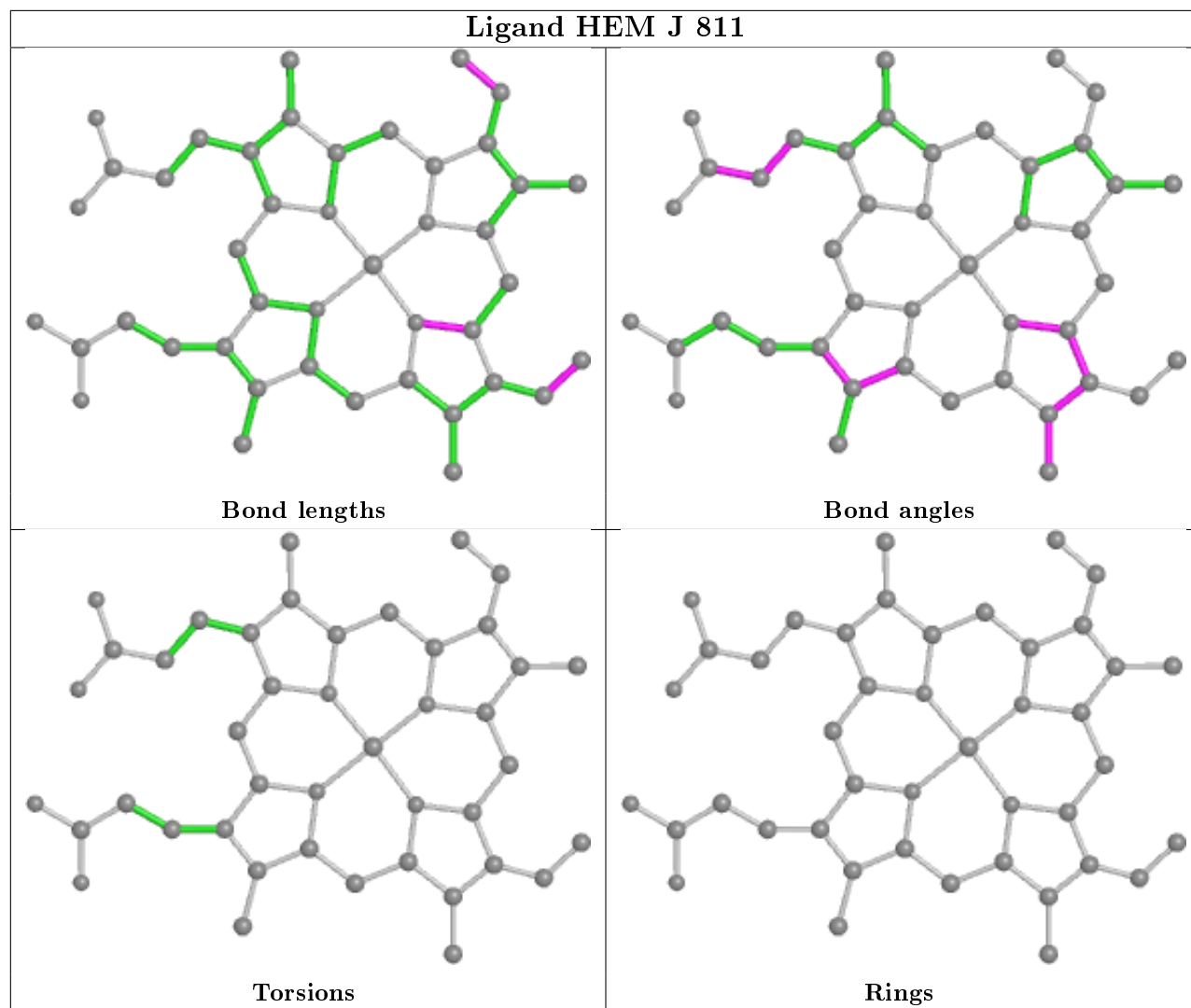


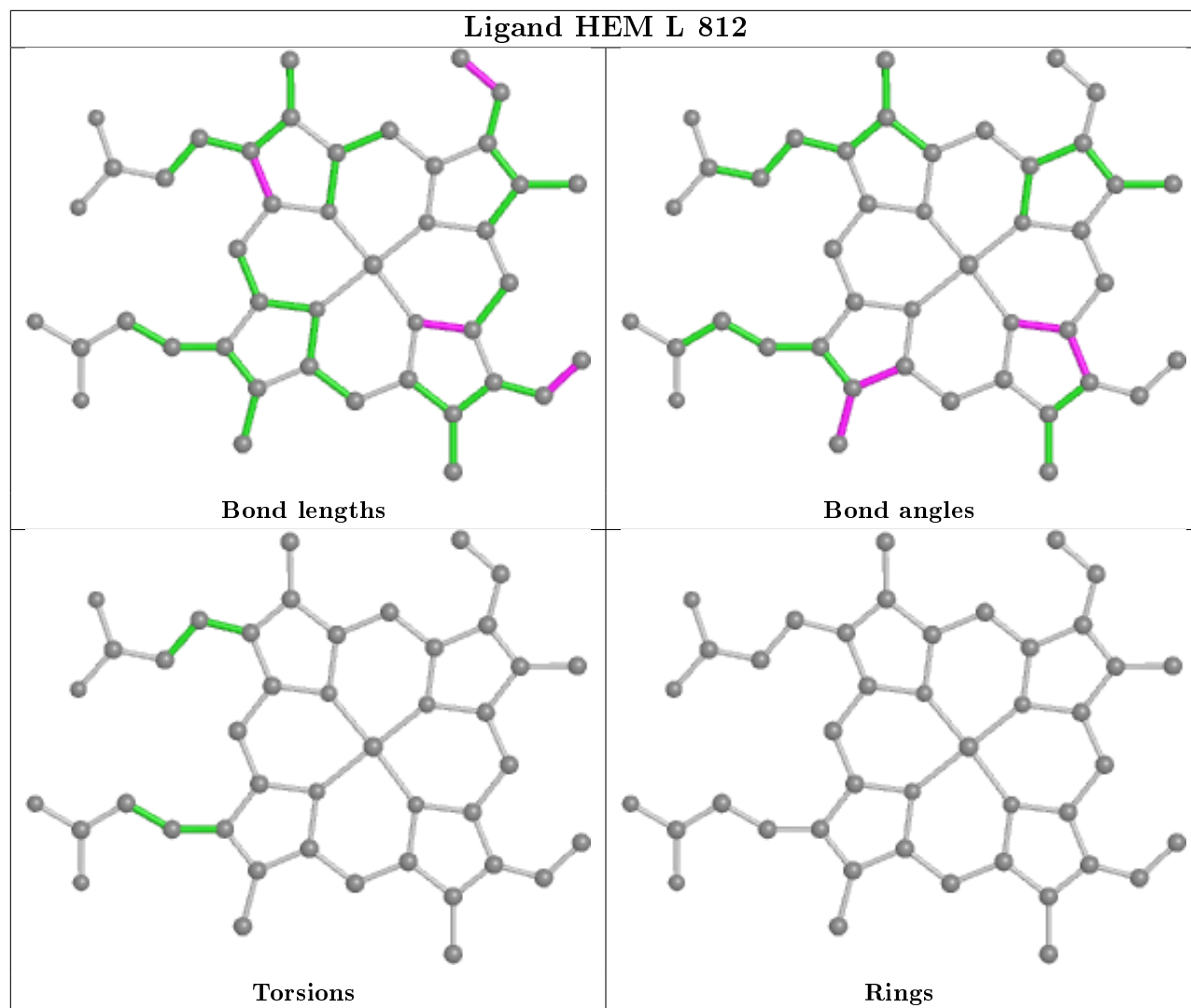


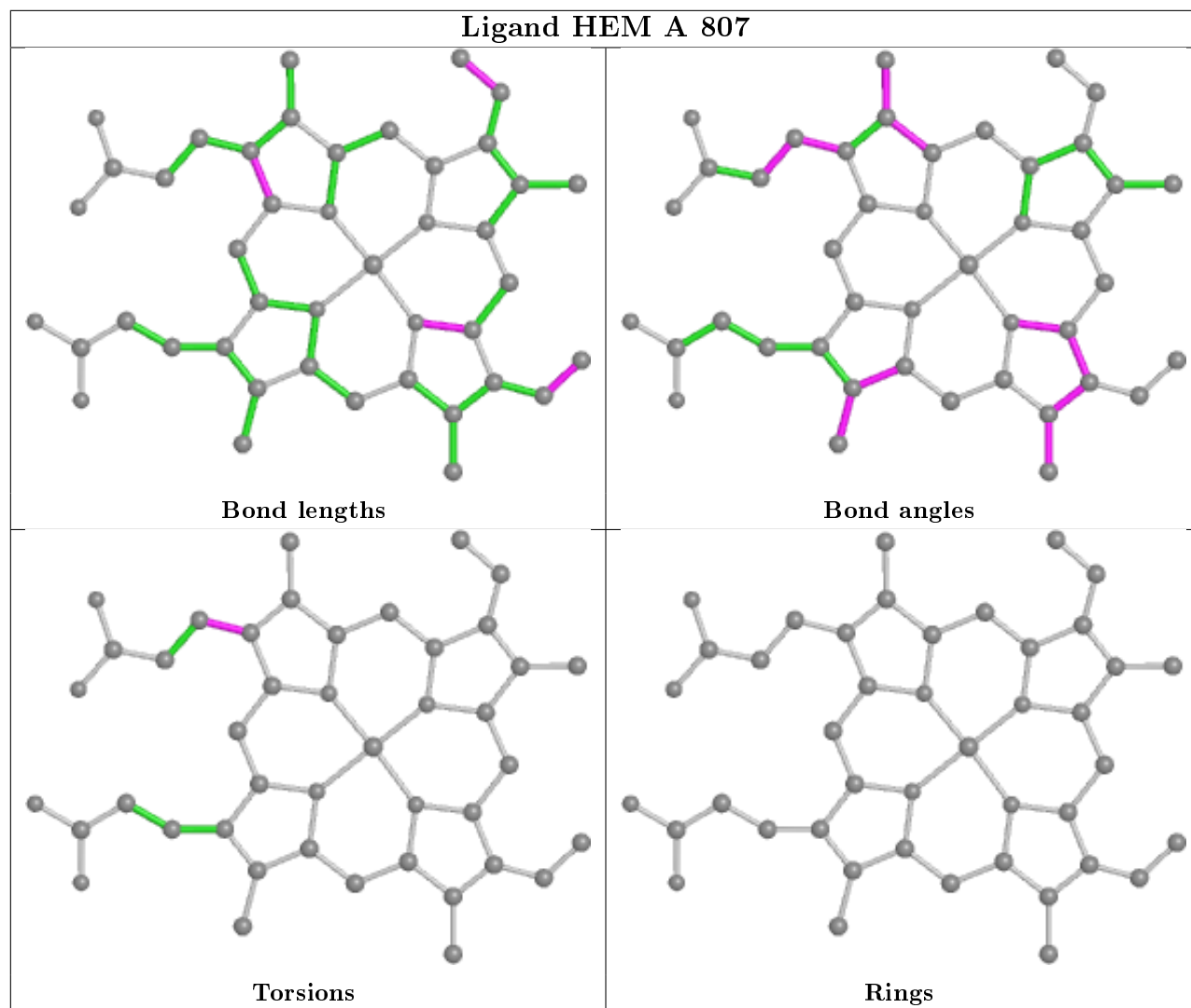


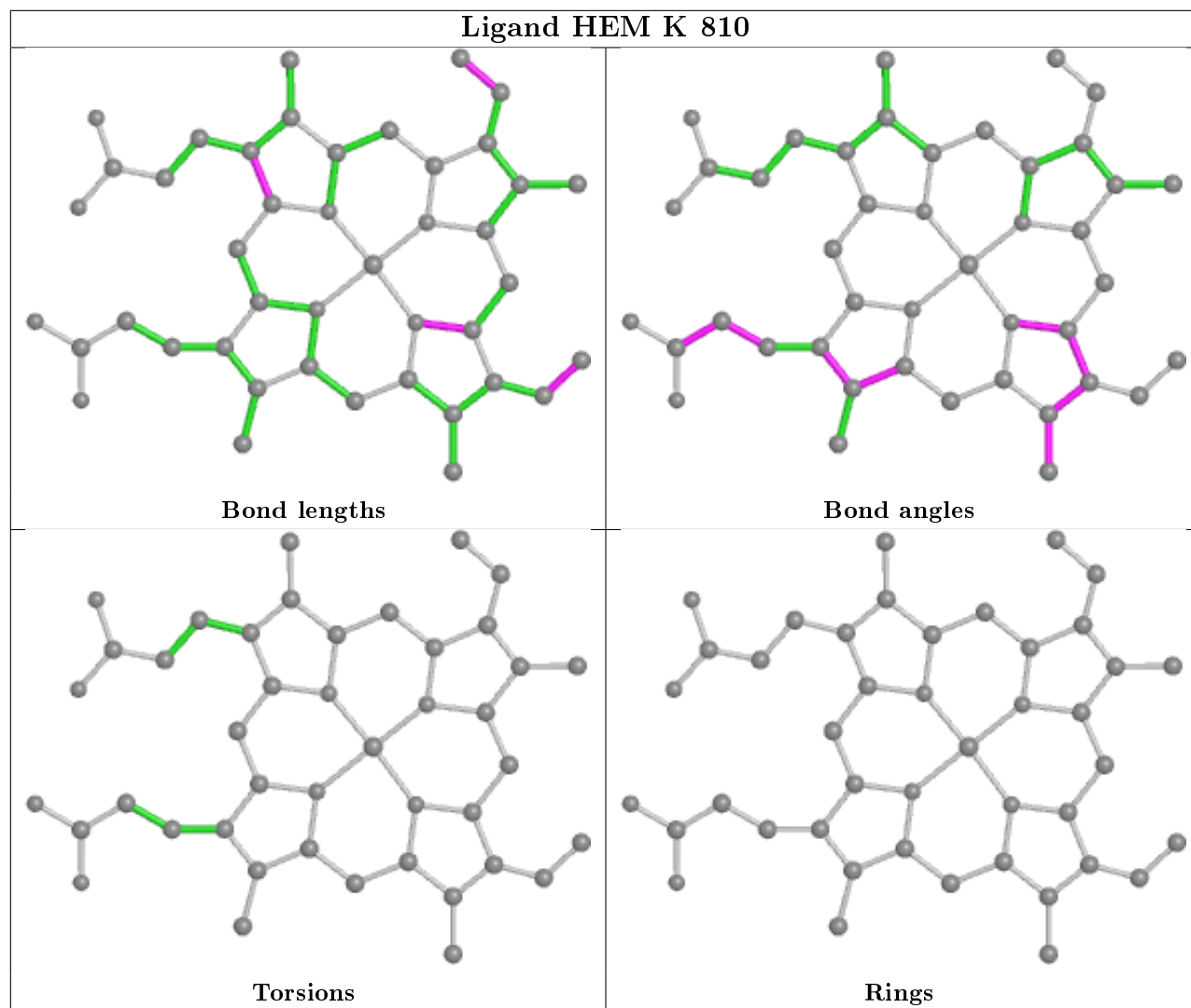


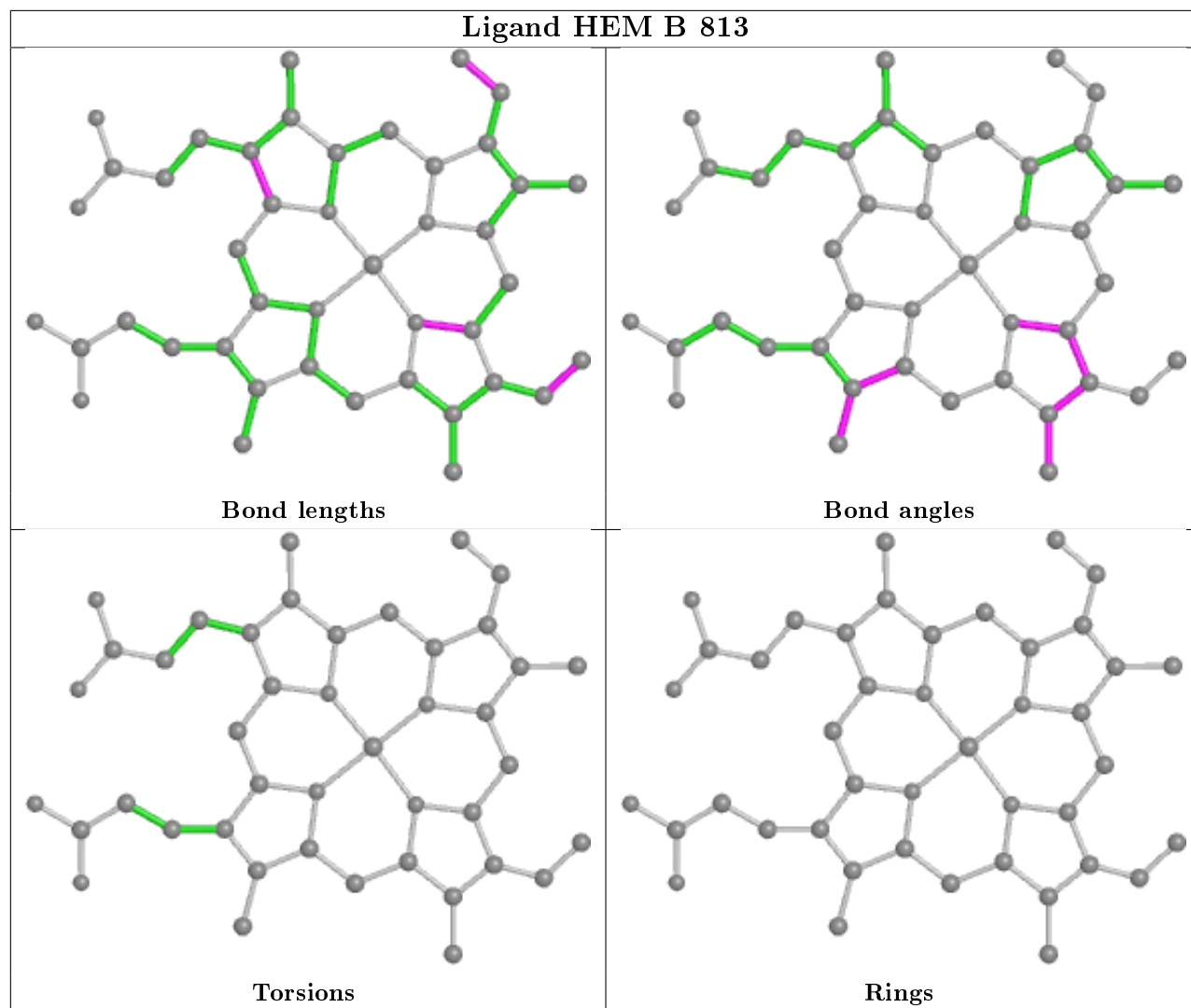


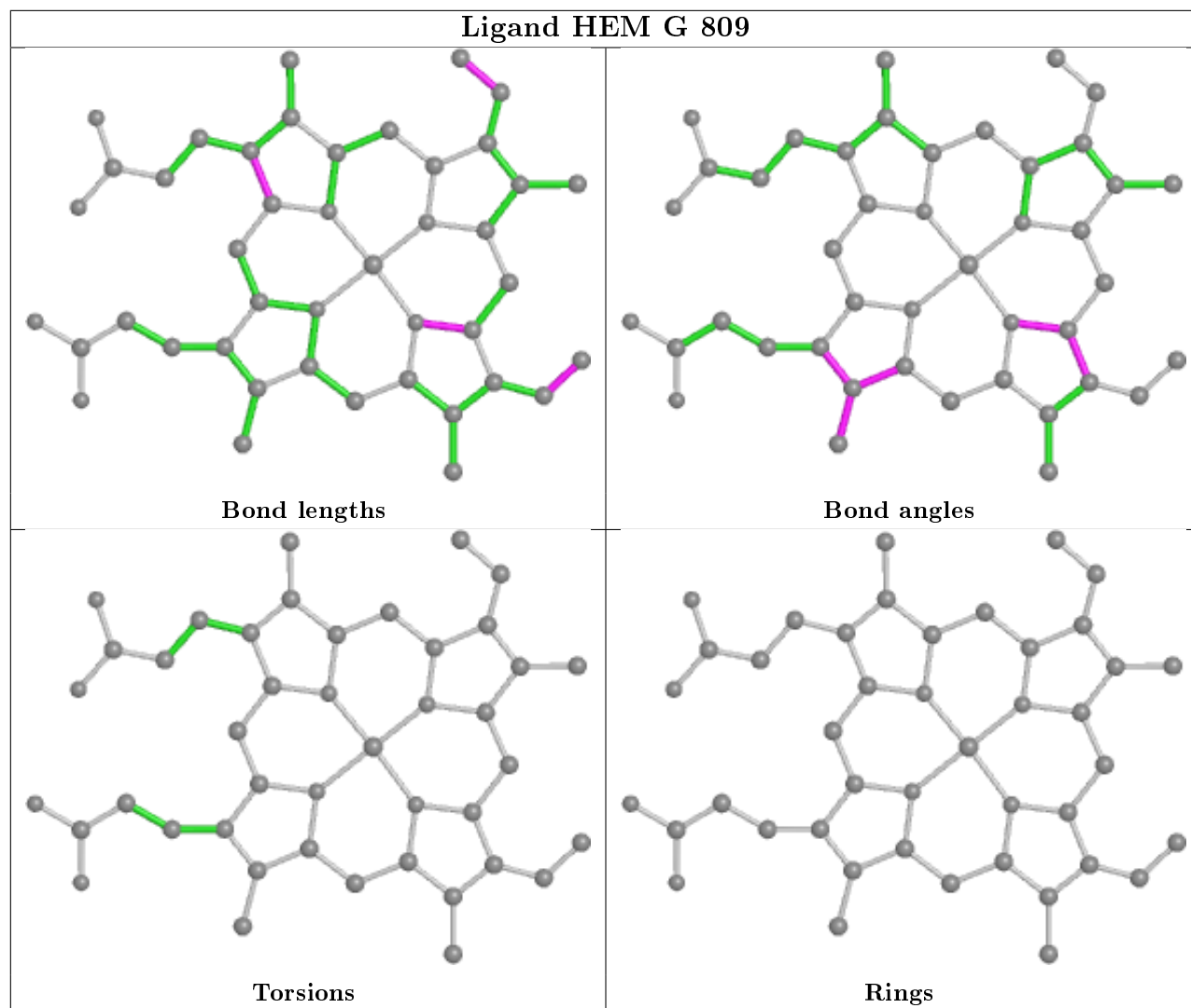


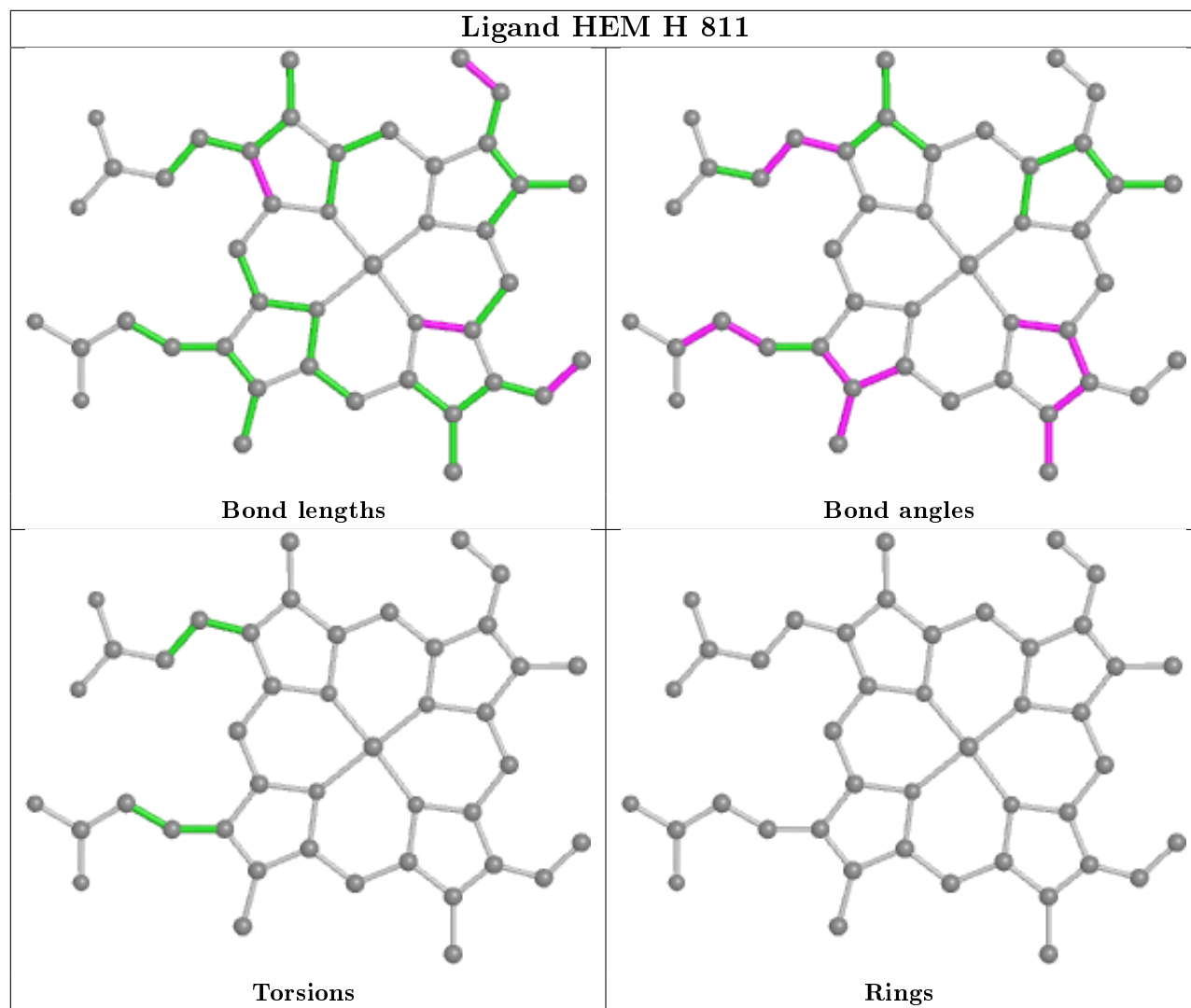




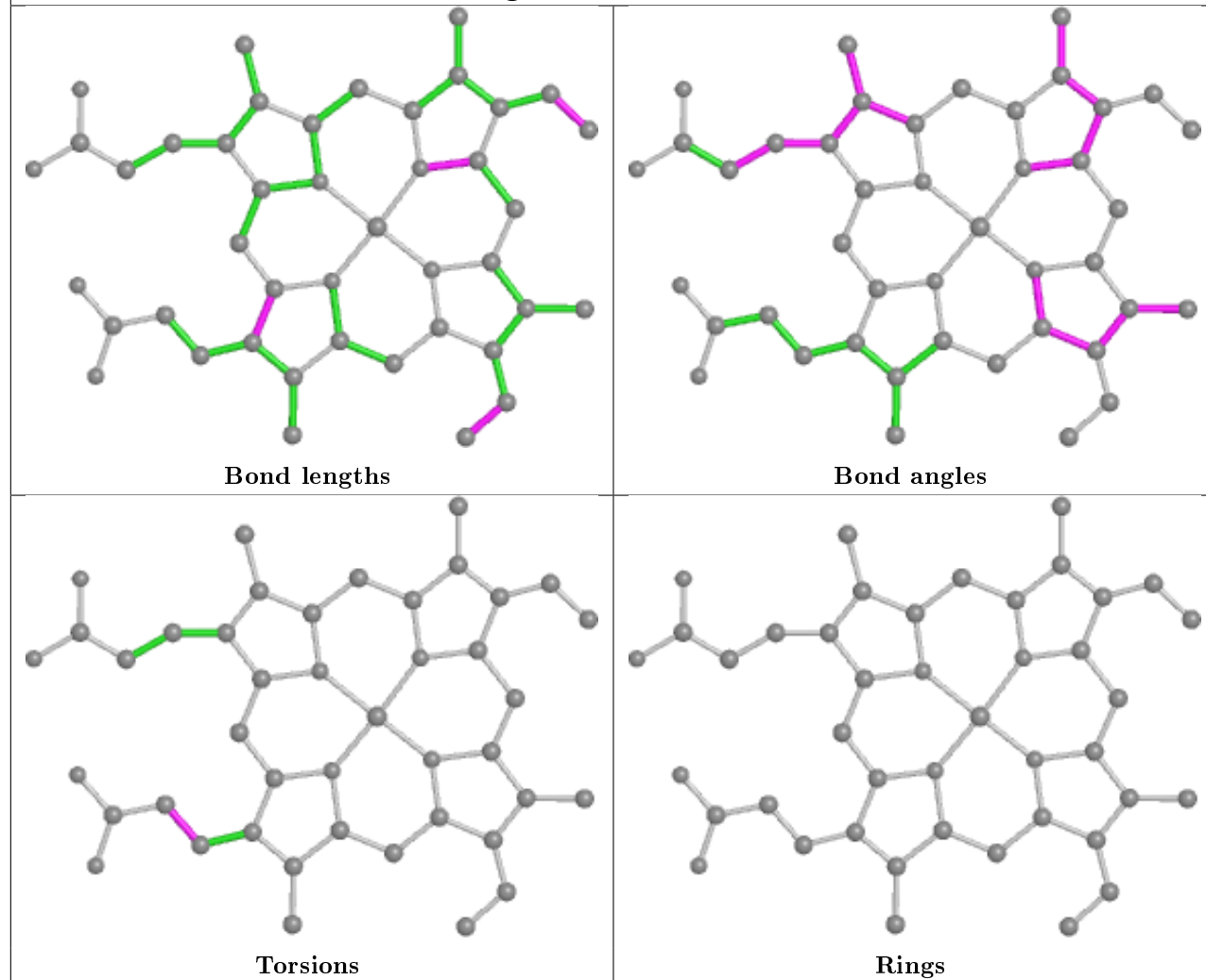


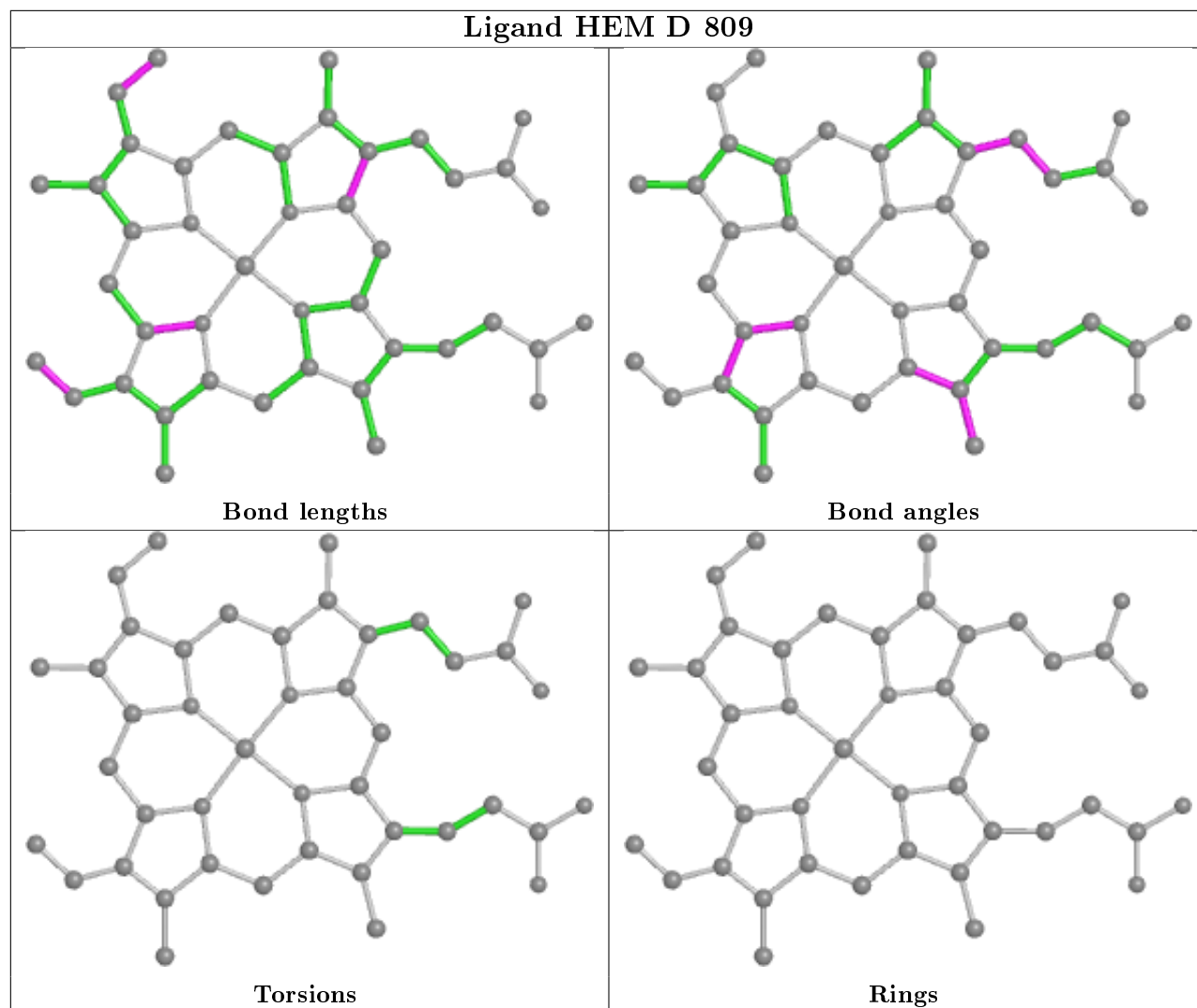


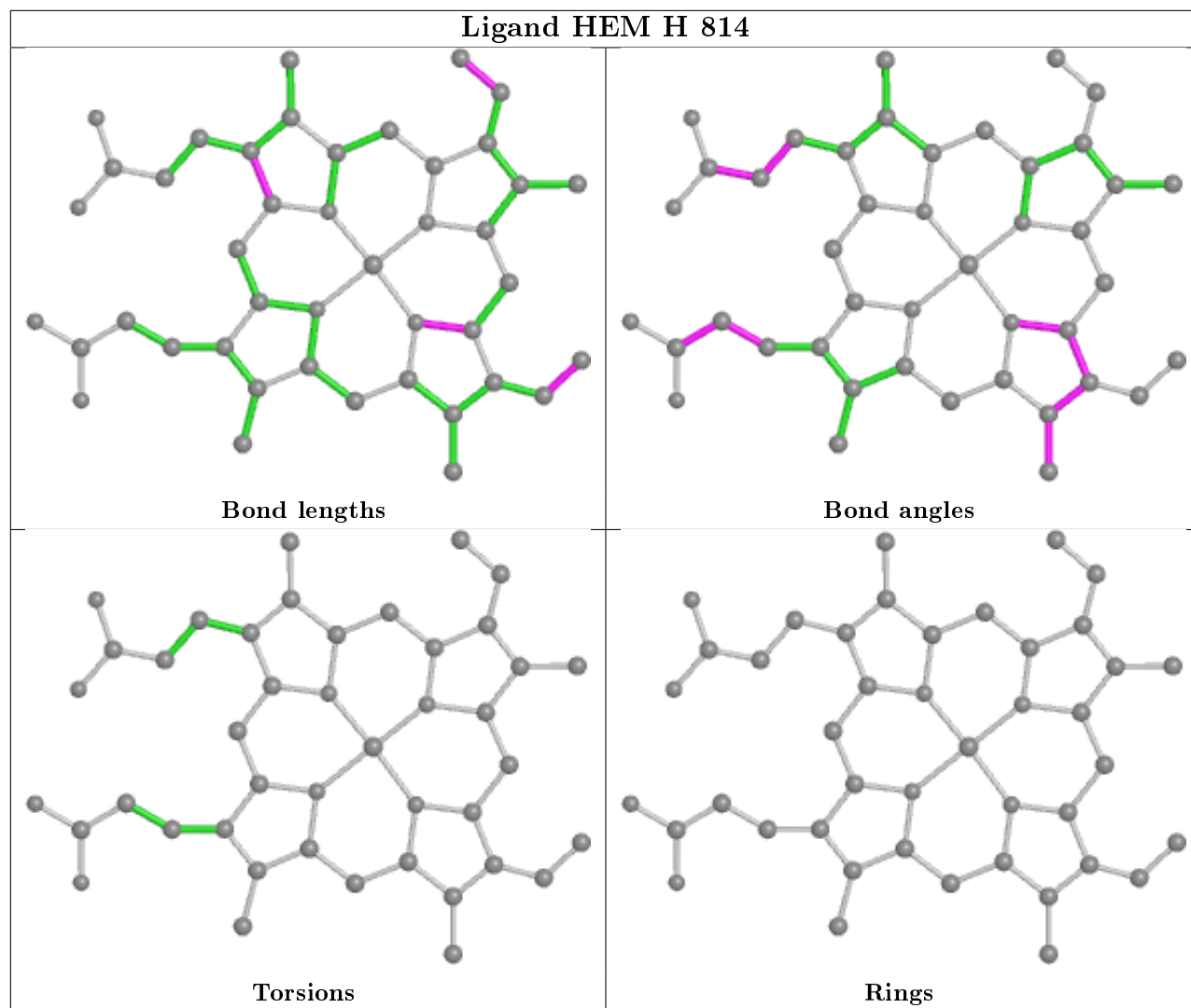


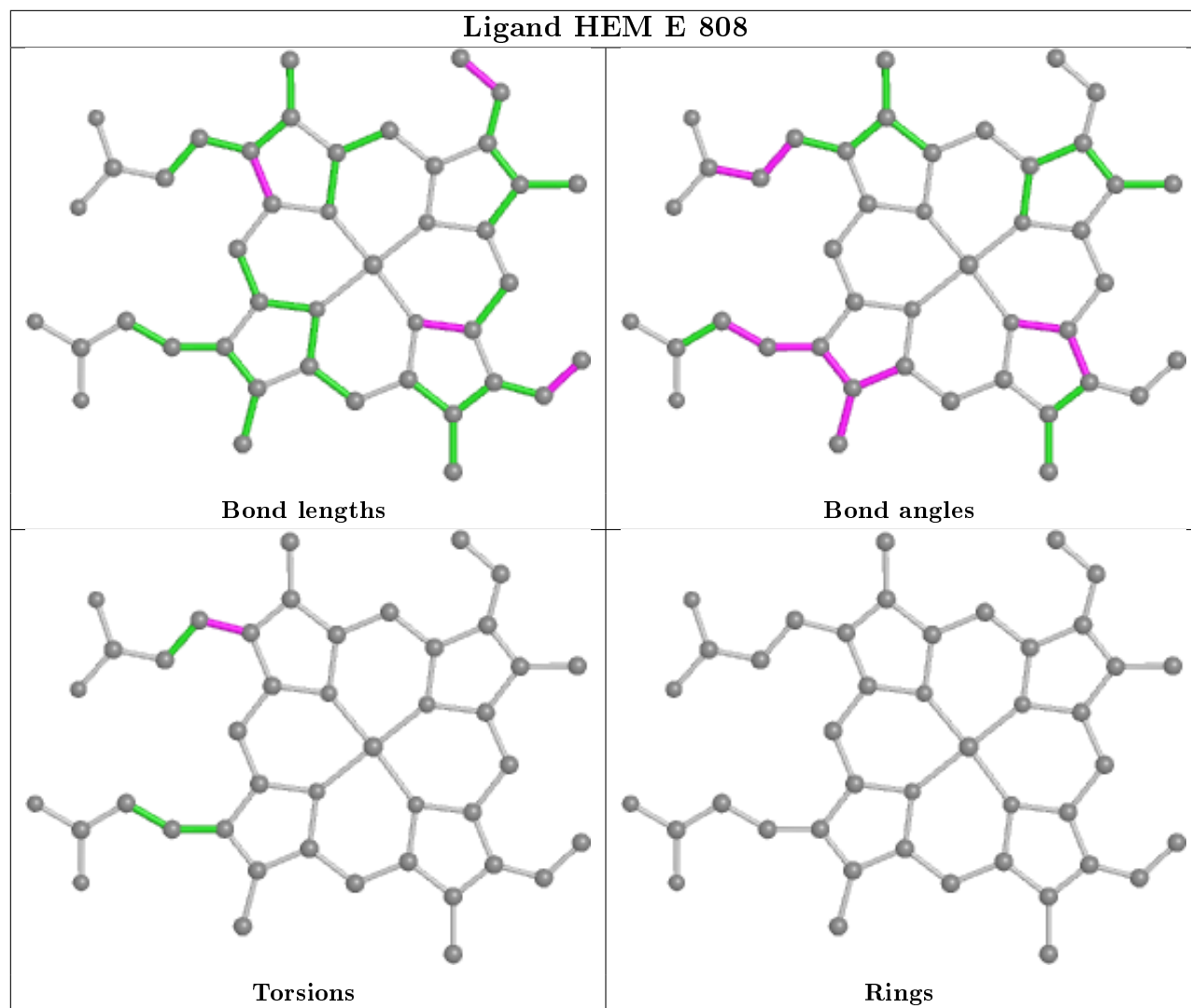


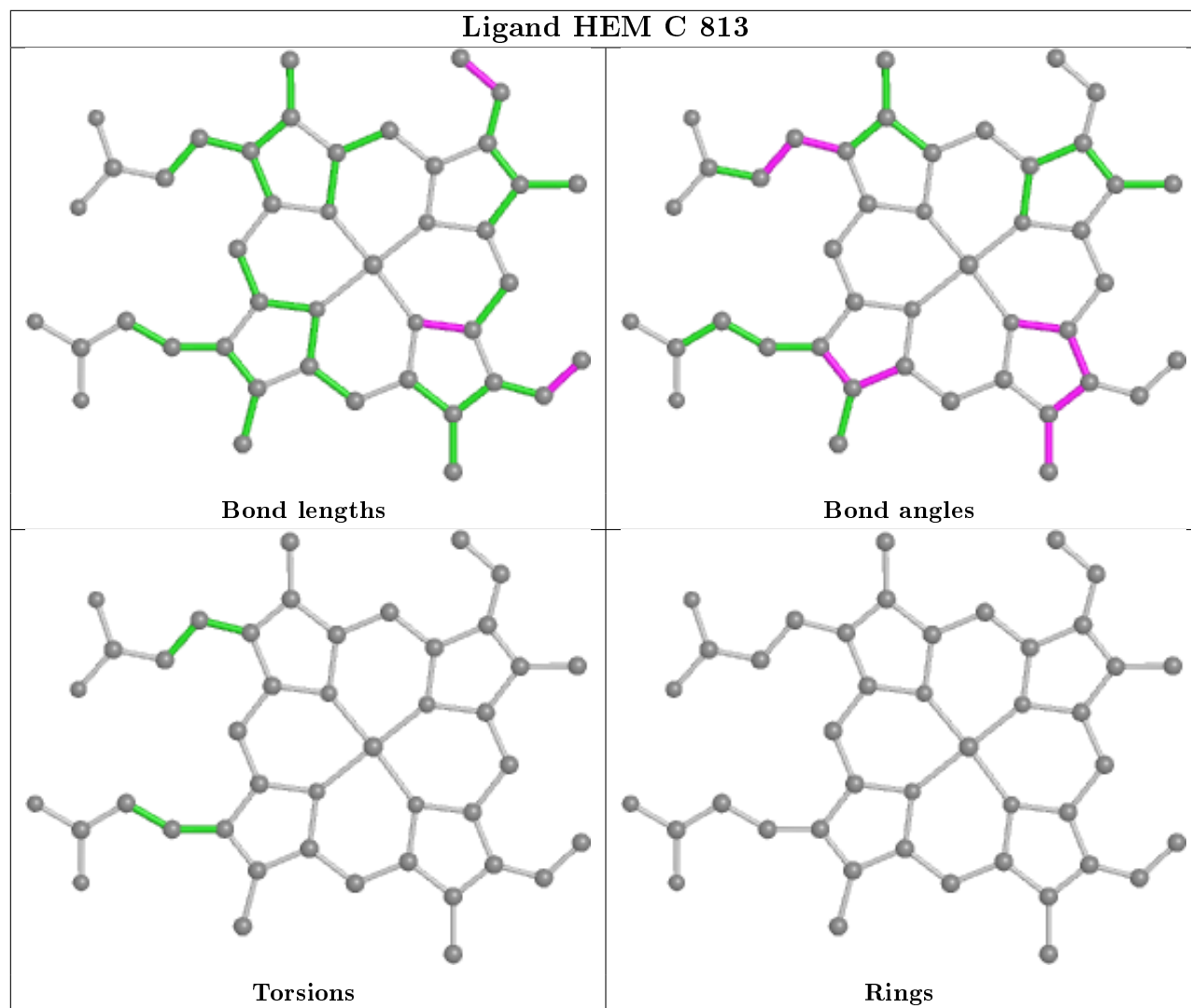
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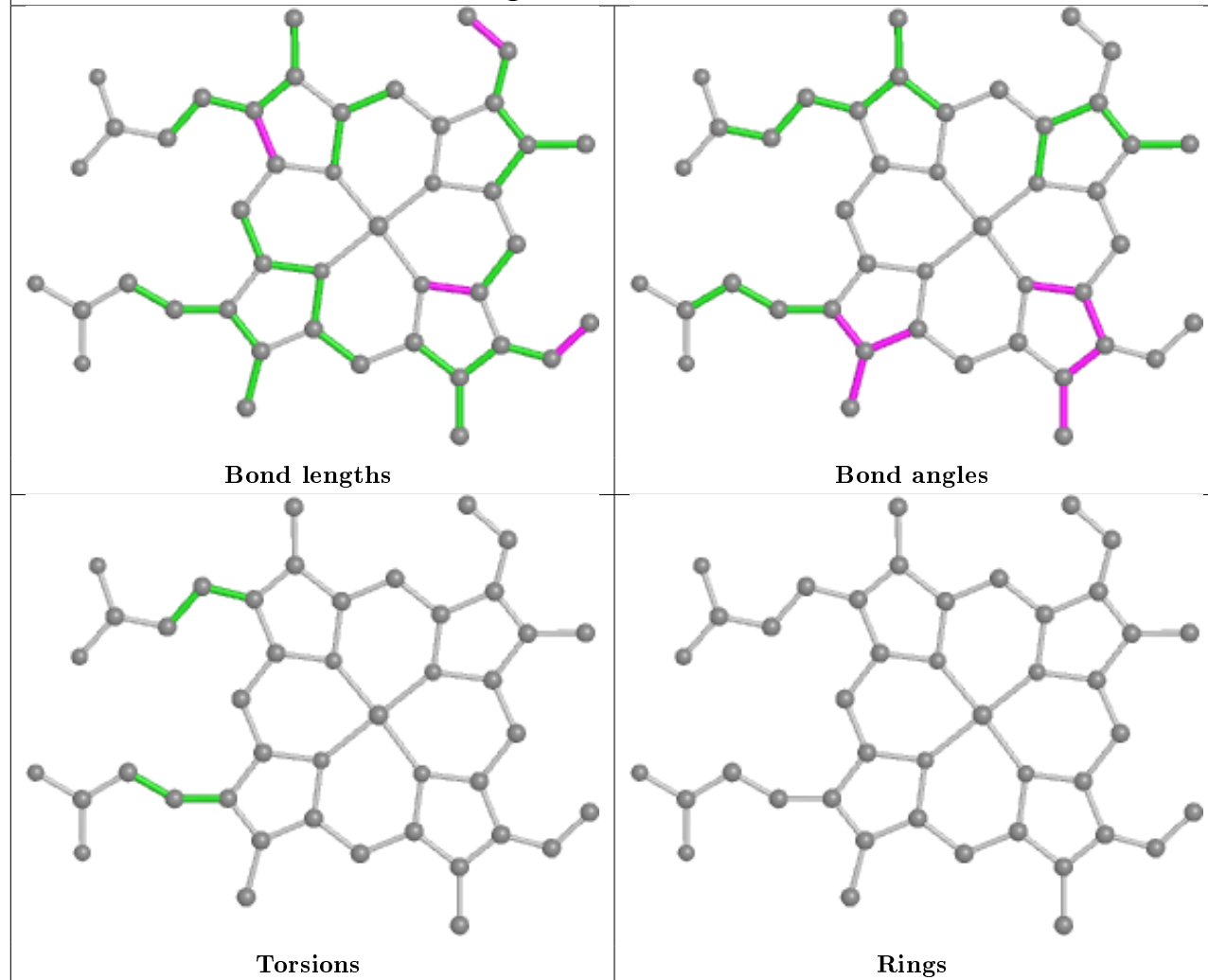


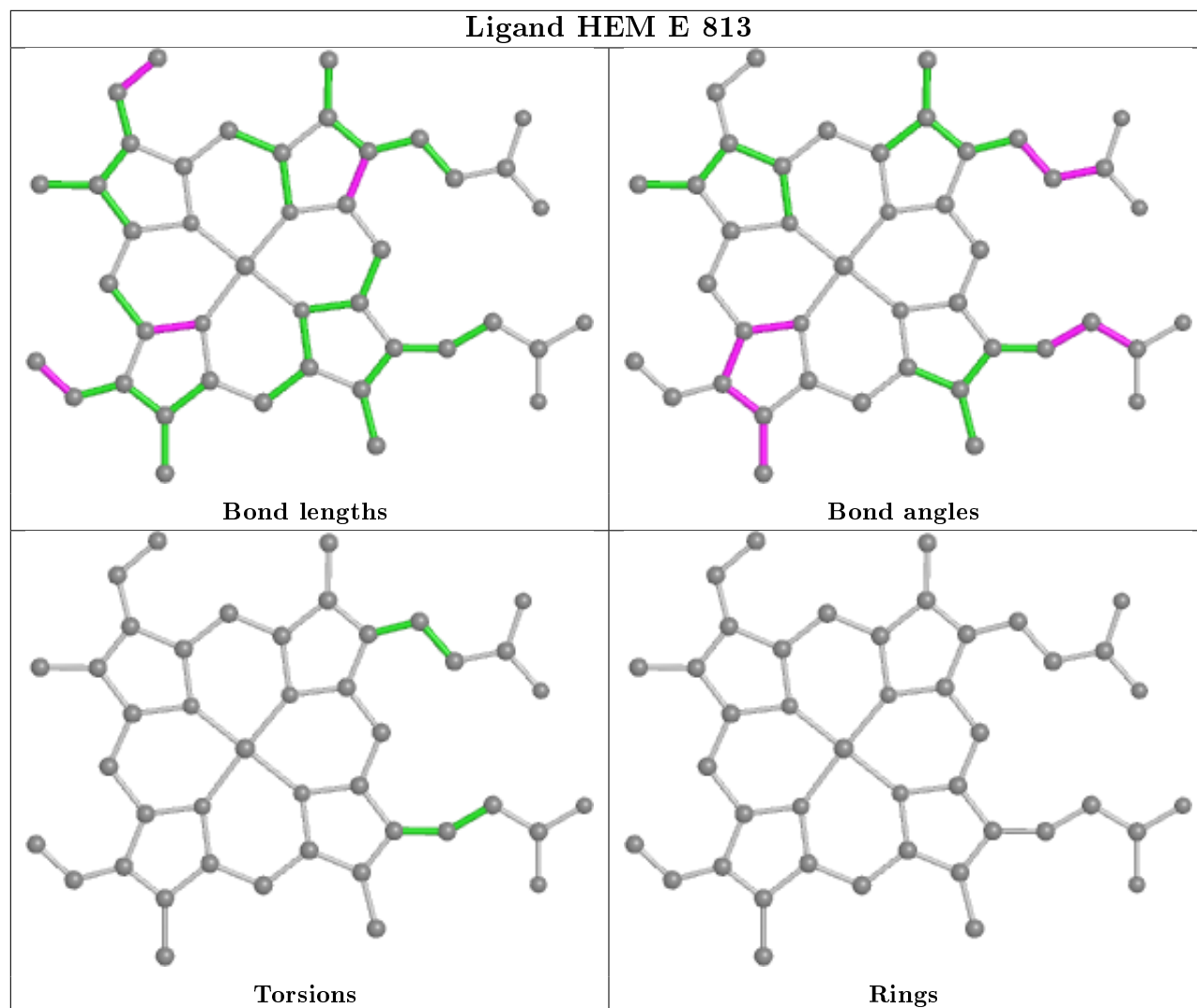


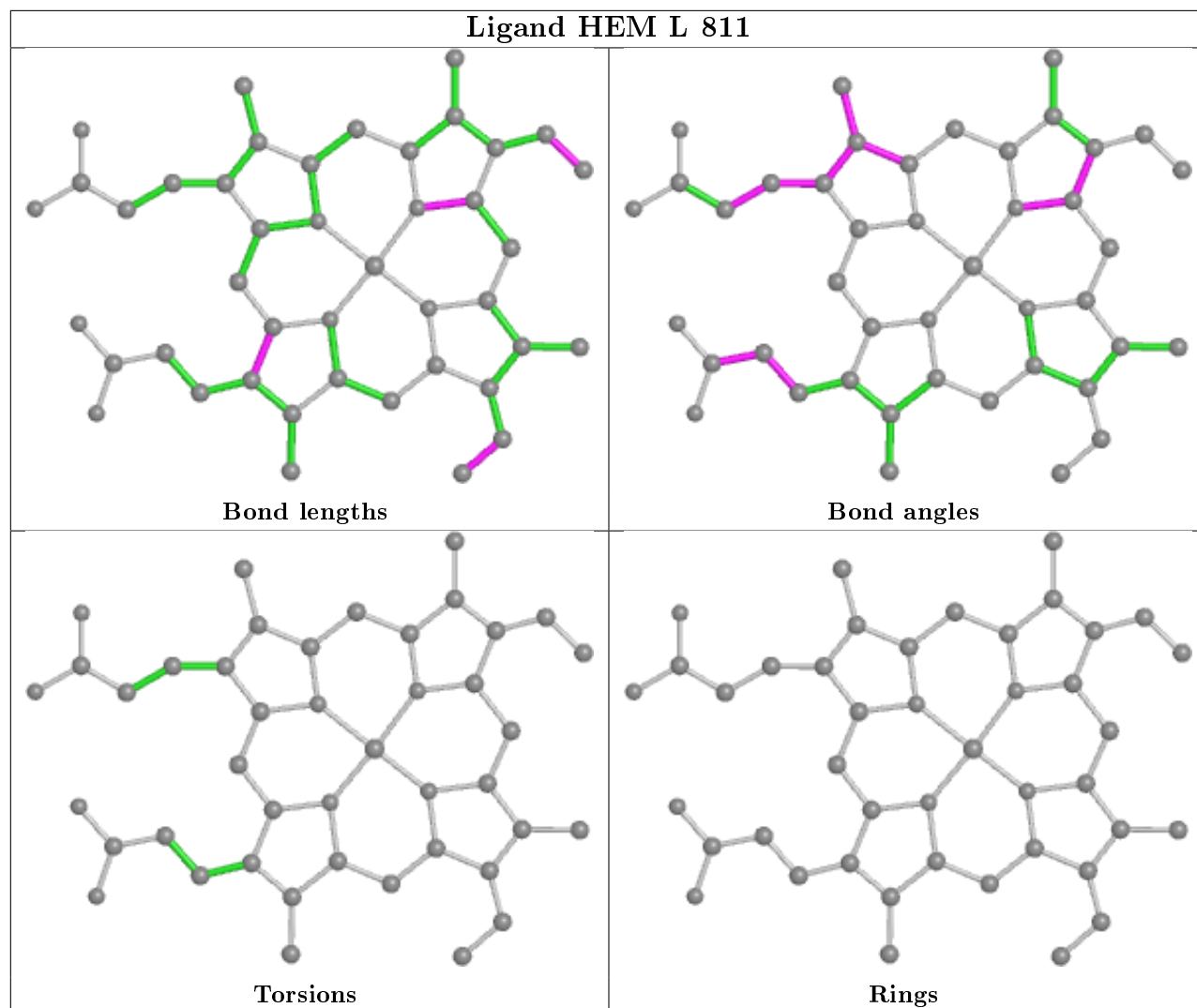


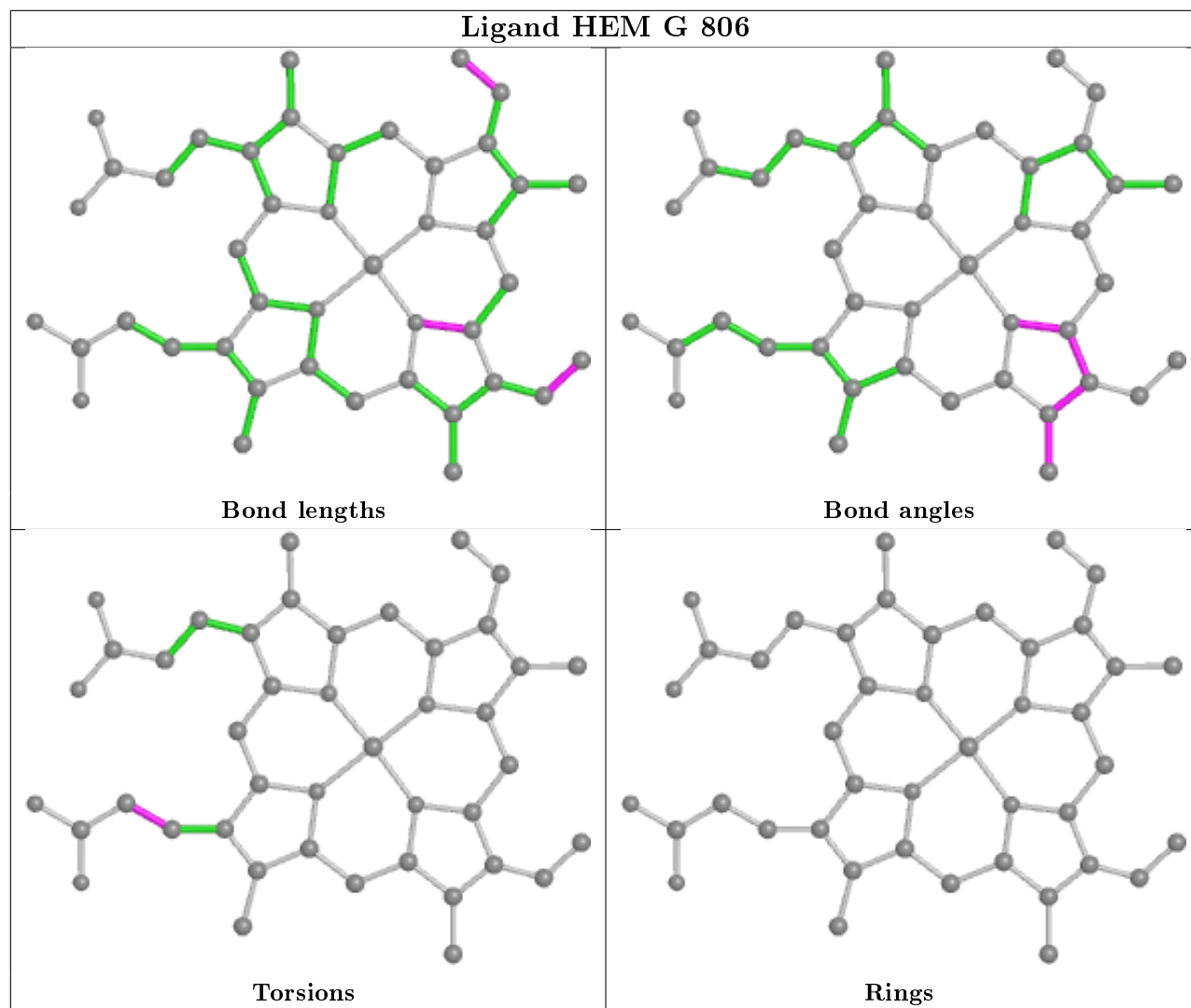


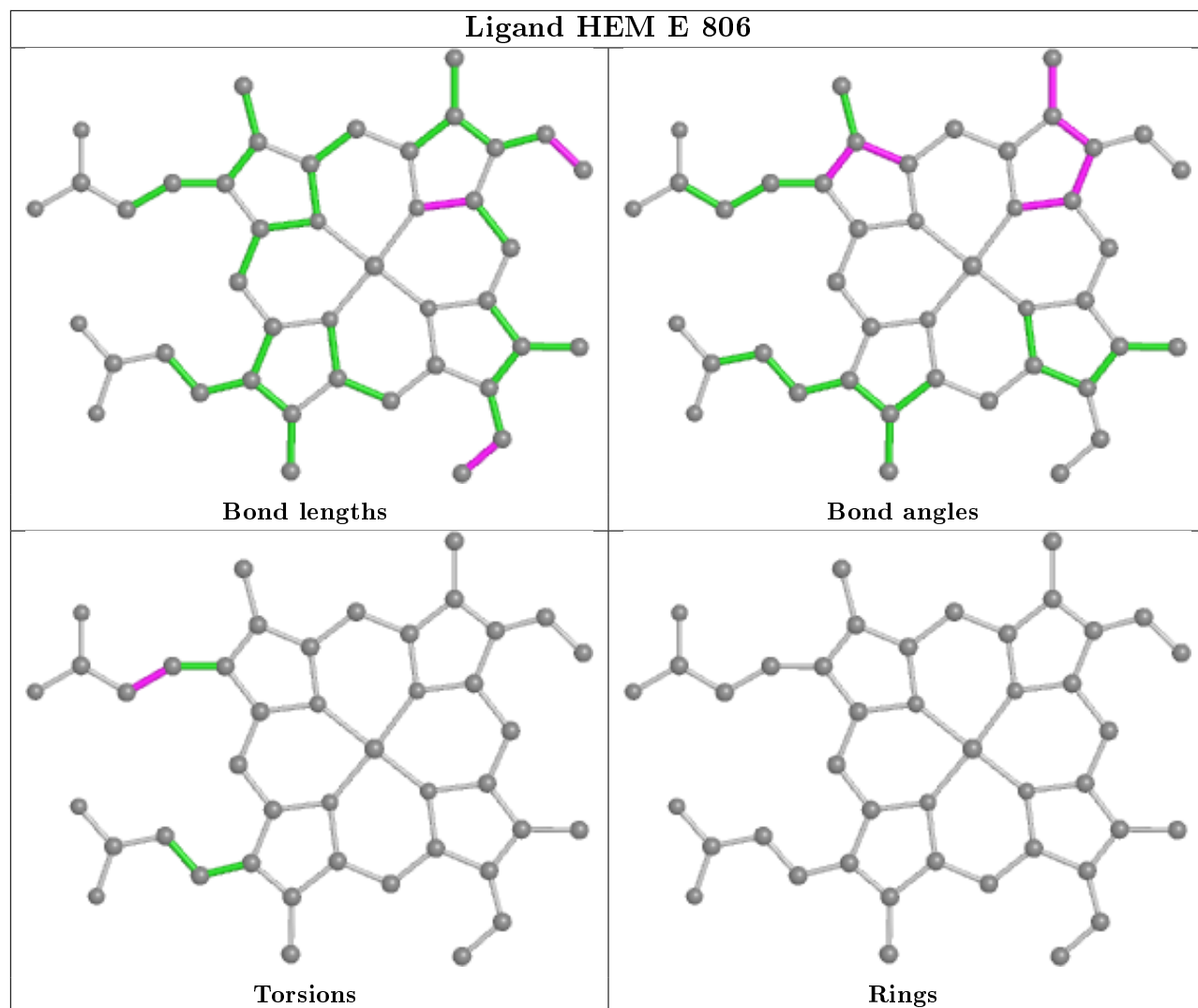
Ligand HEM I 812

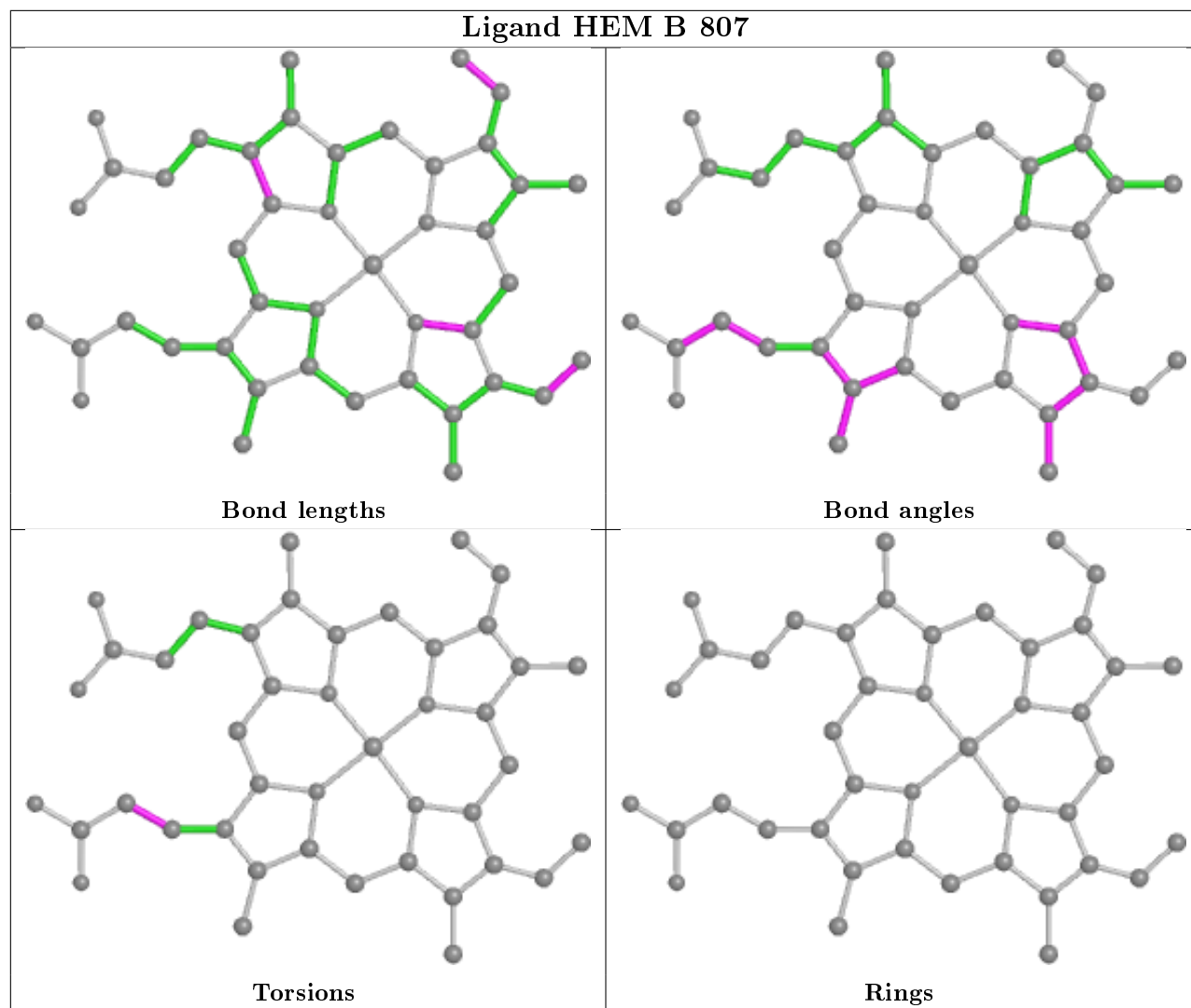


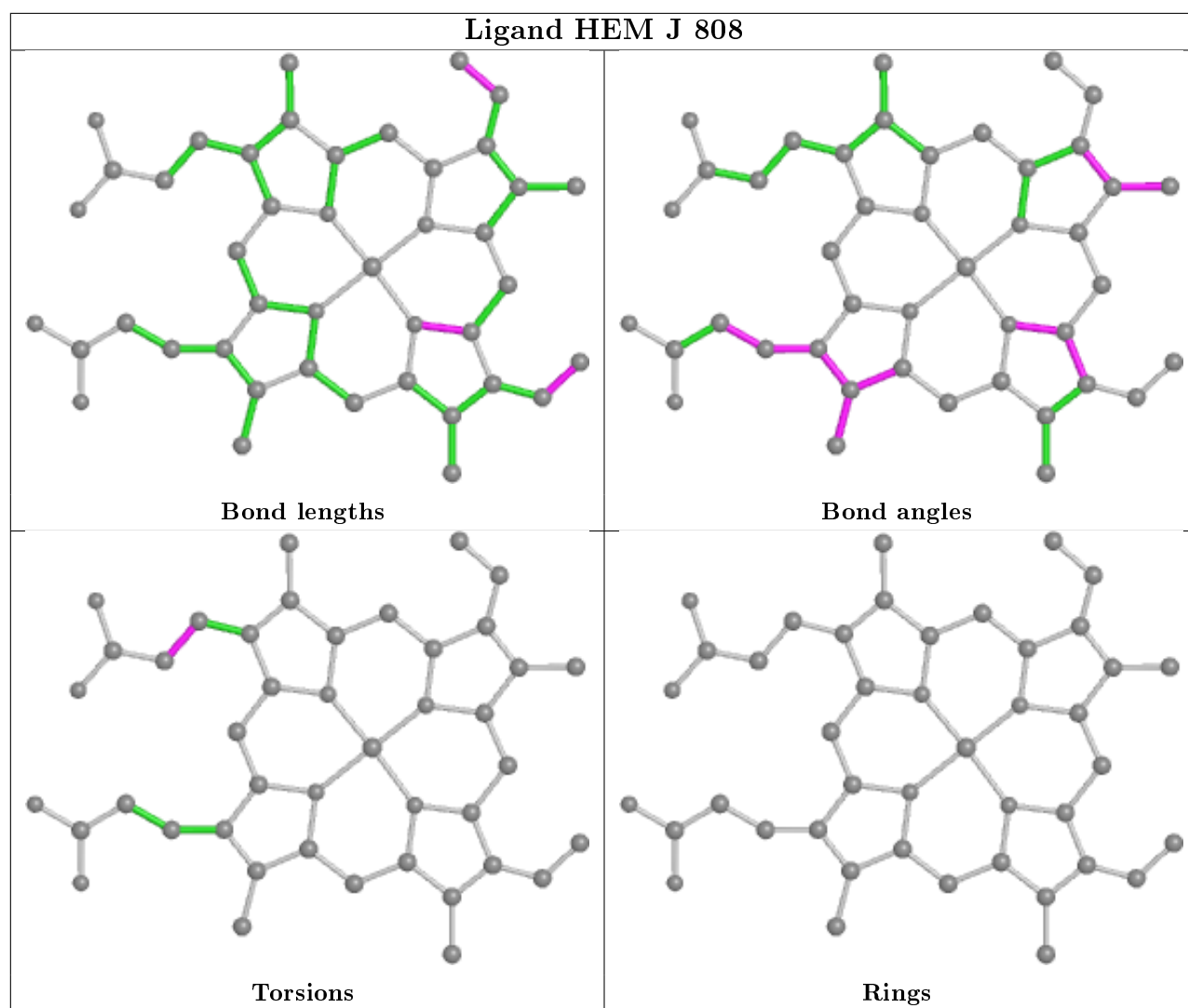




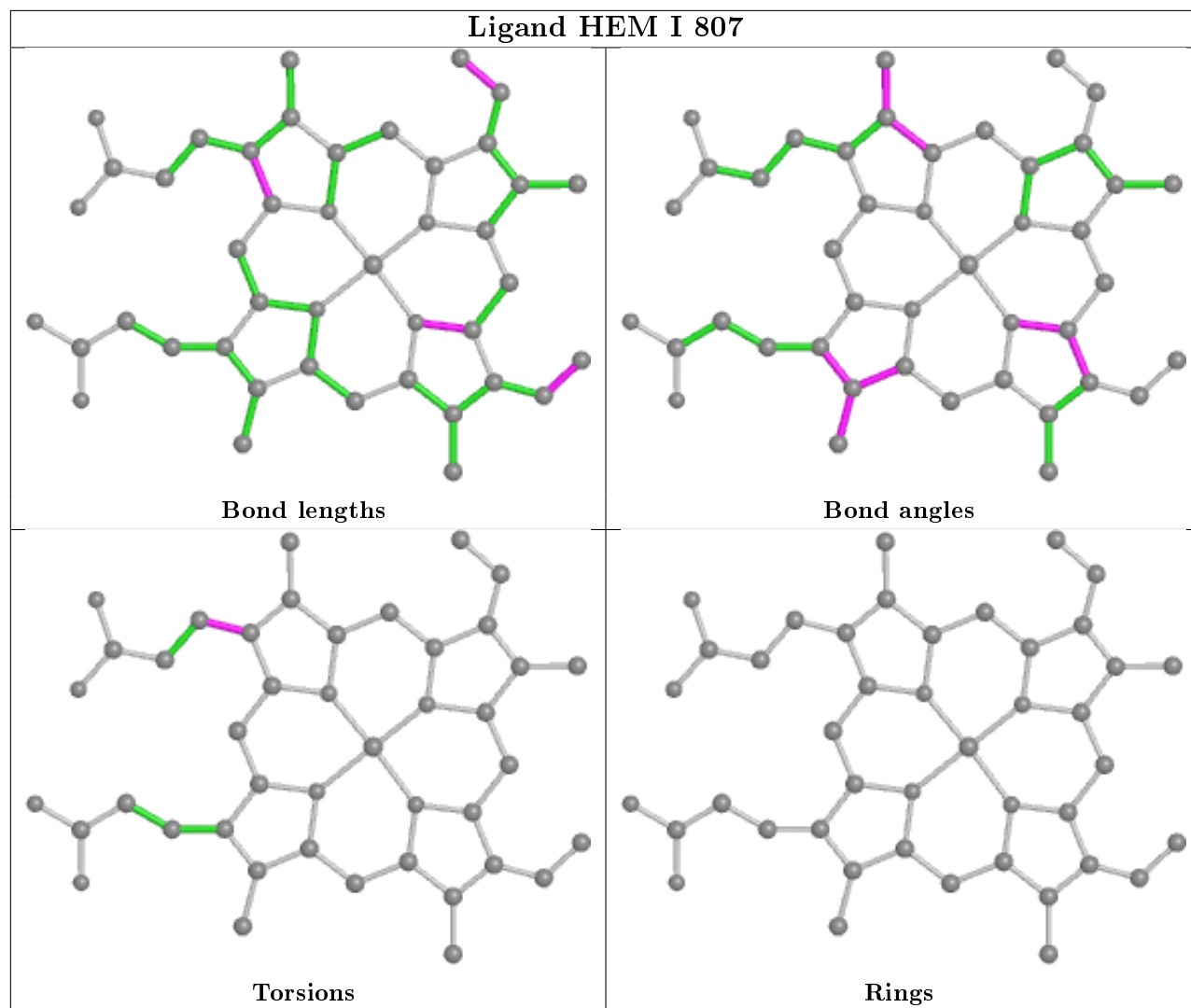


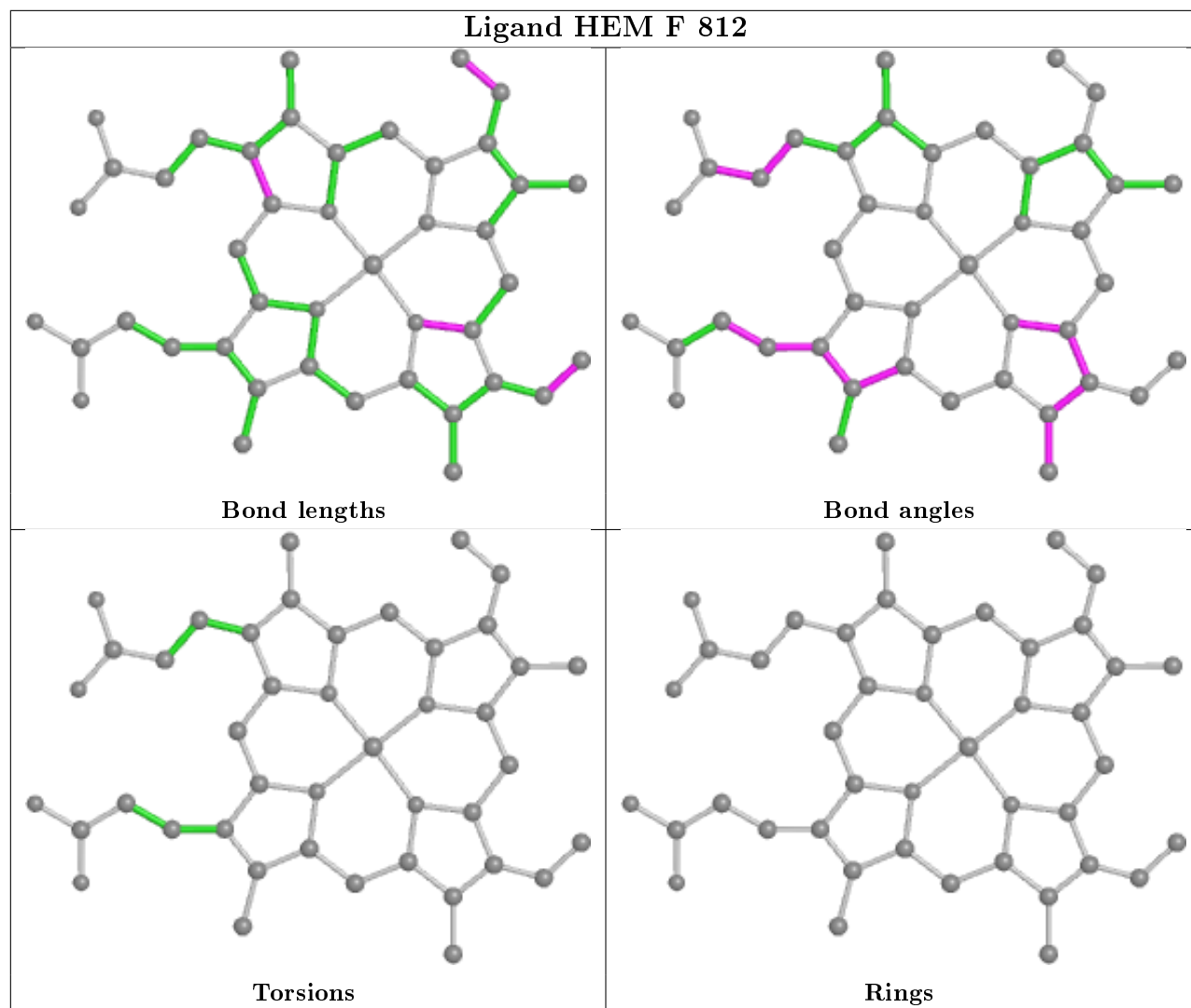


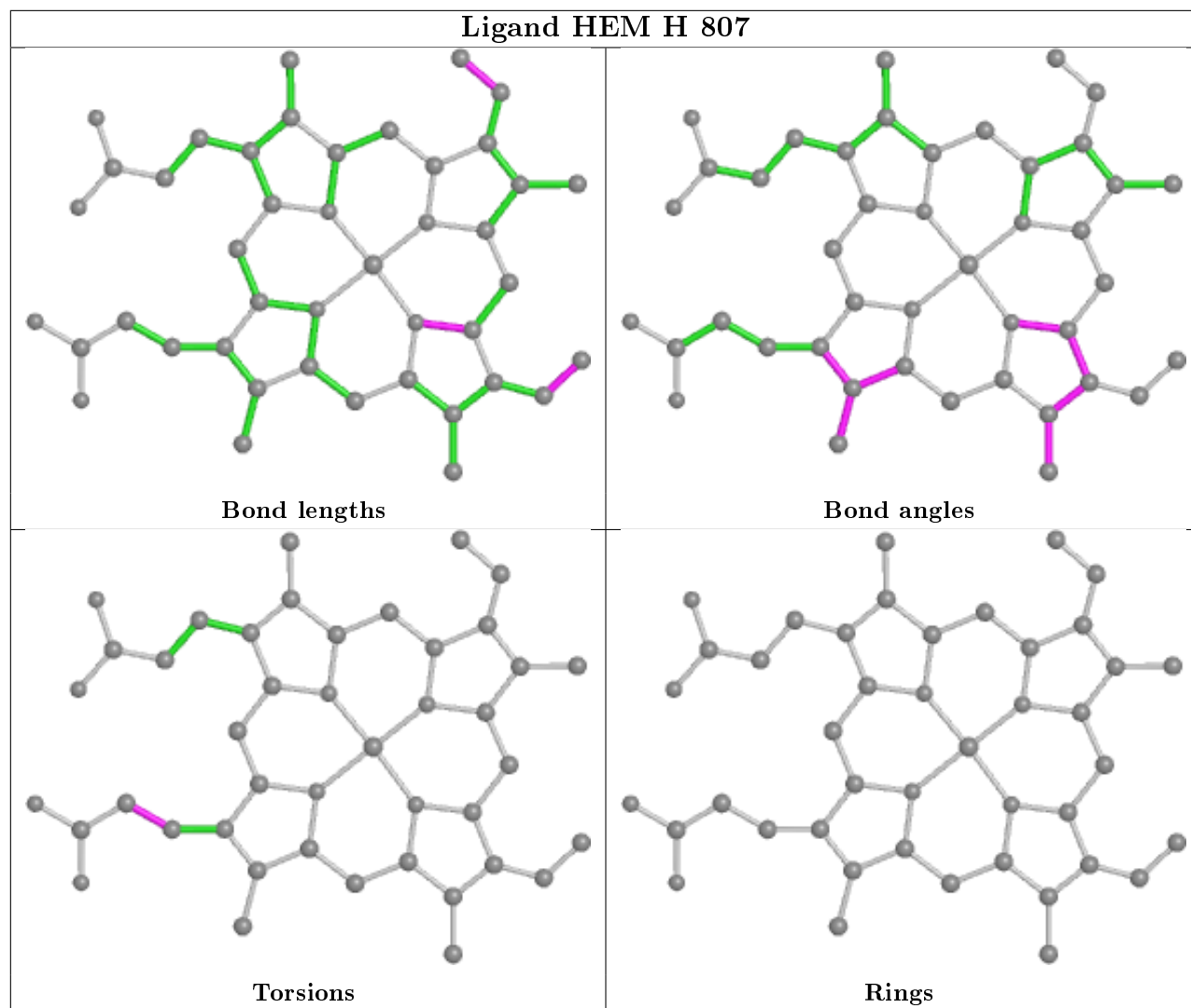


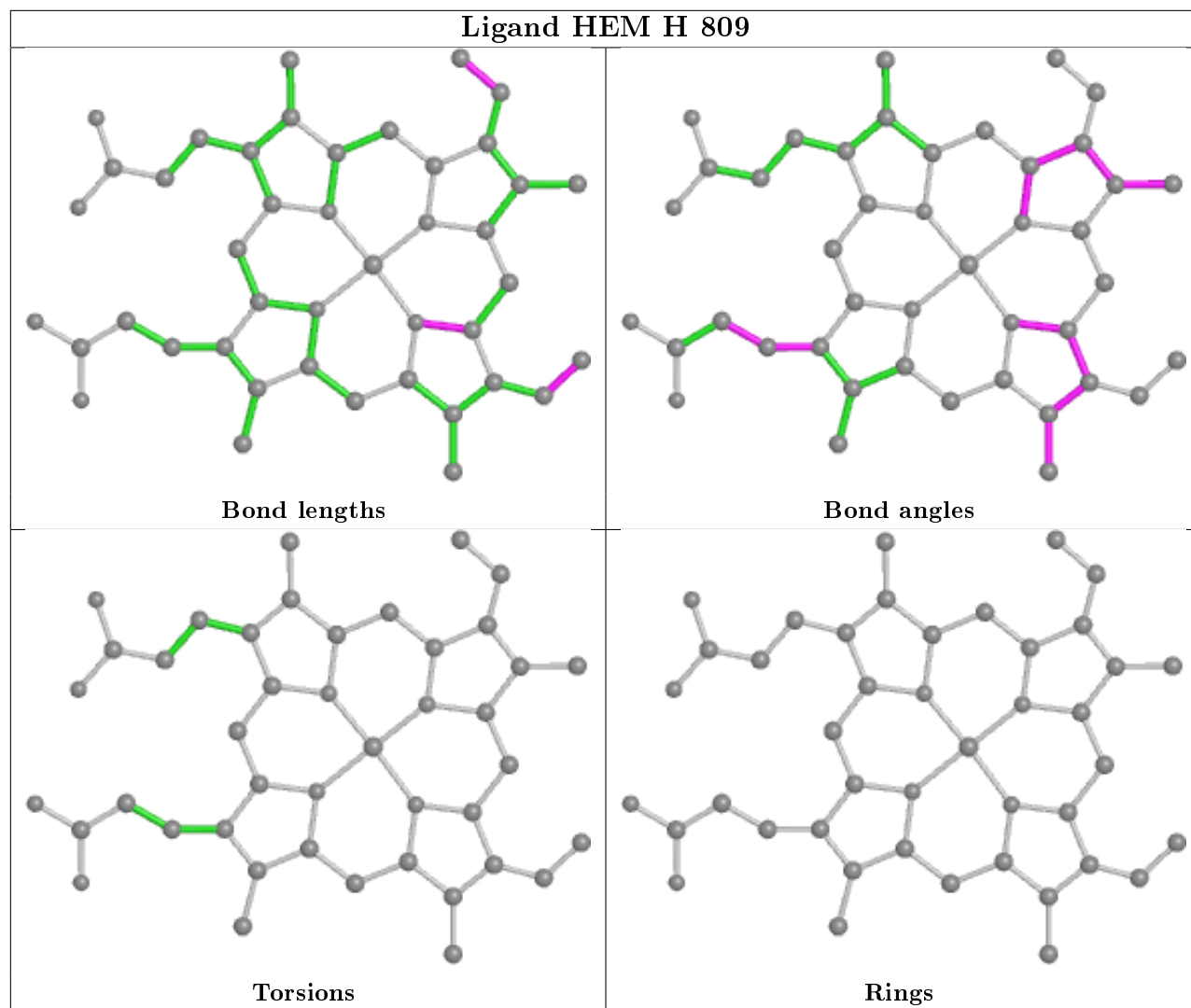


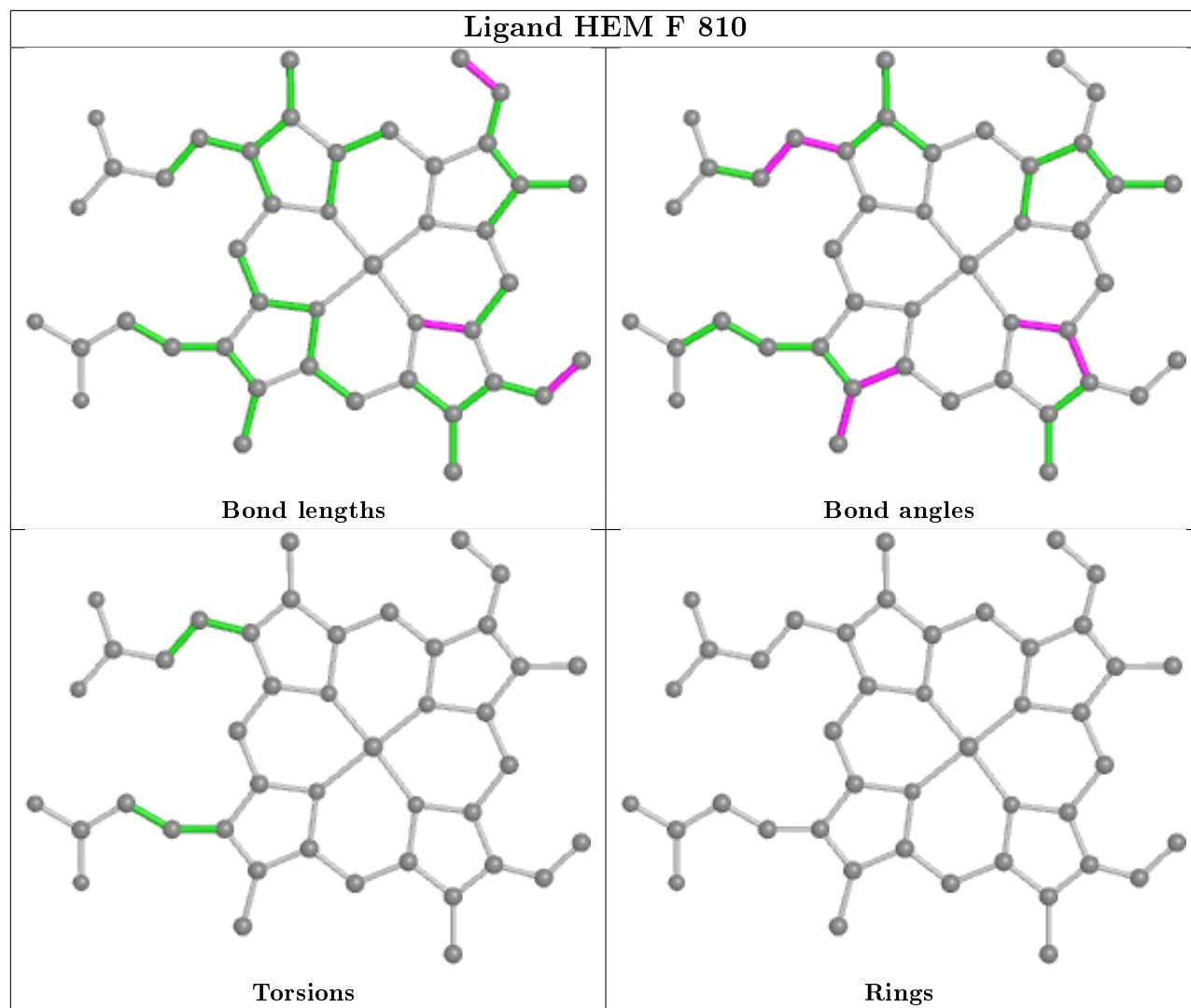
Ligand HEM I 807

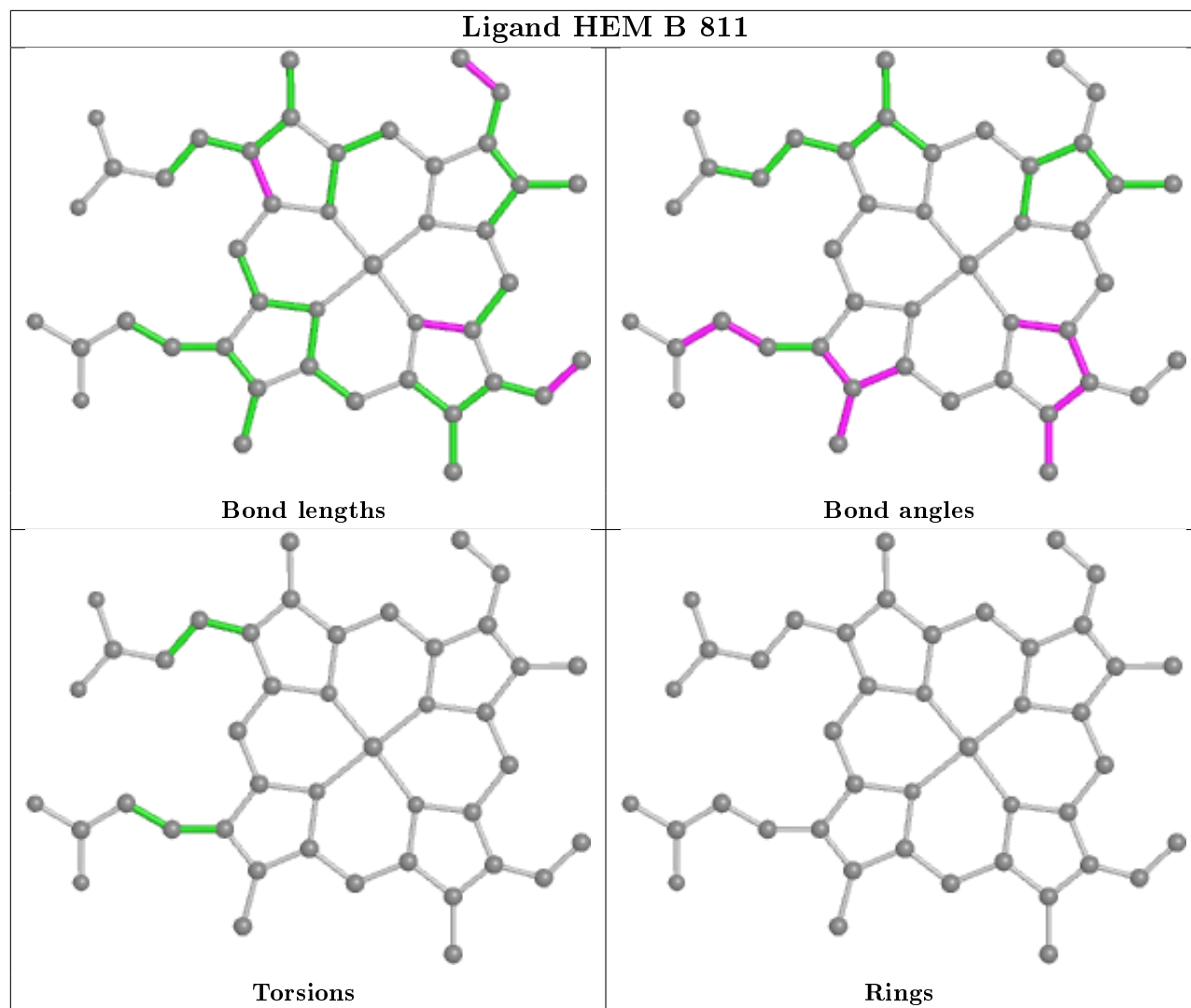




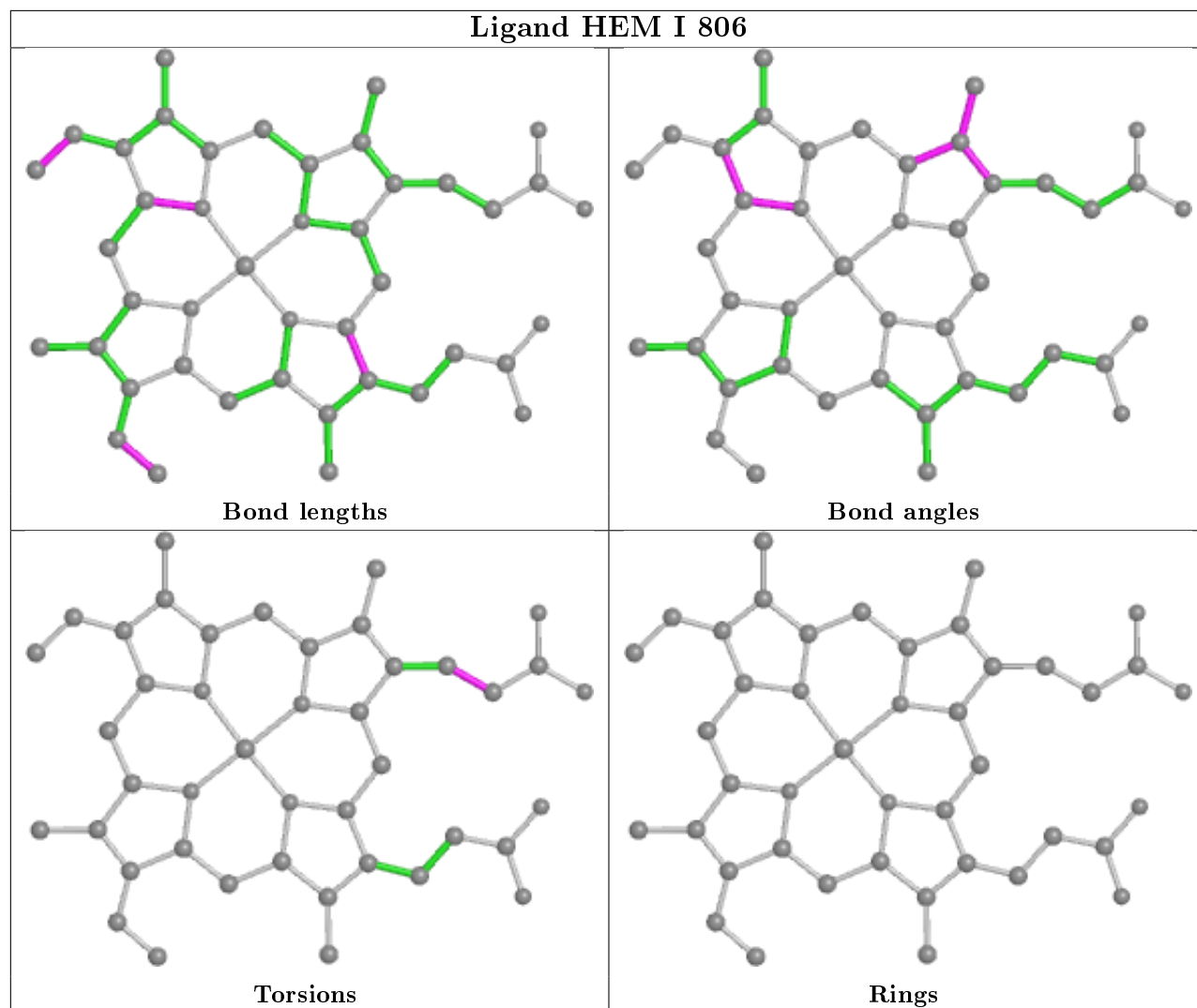


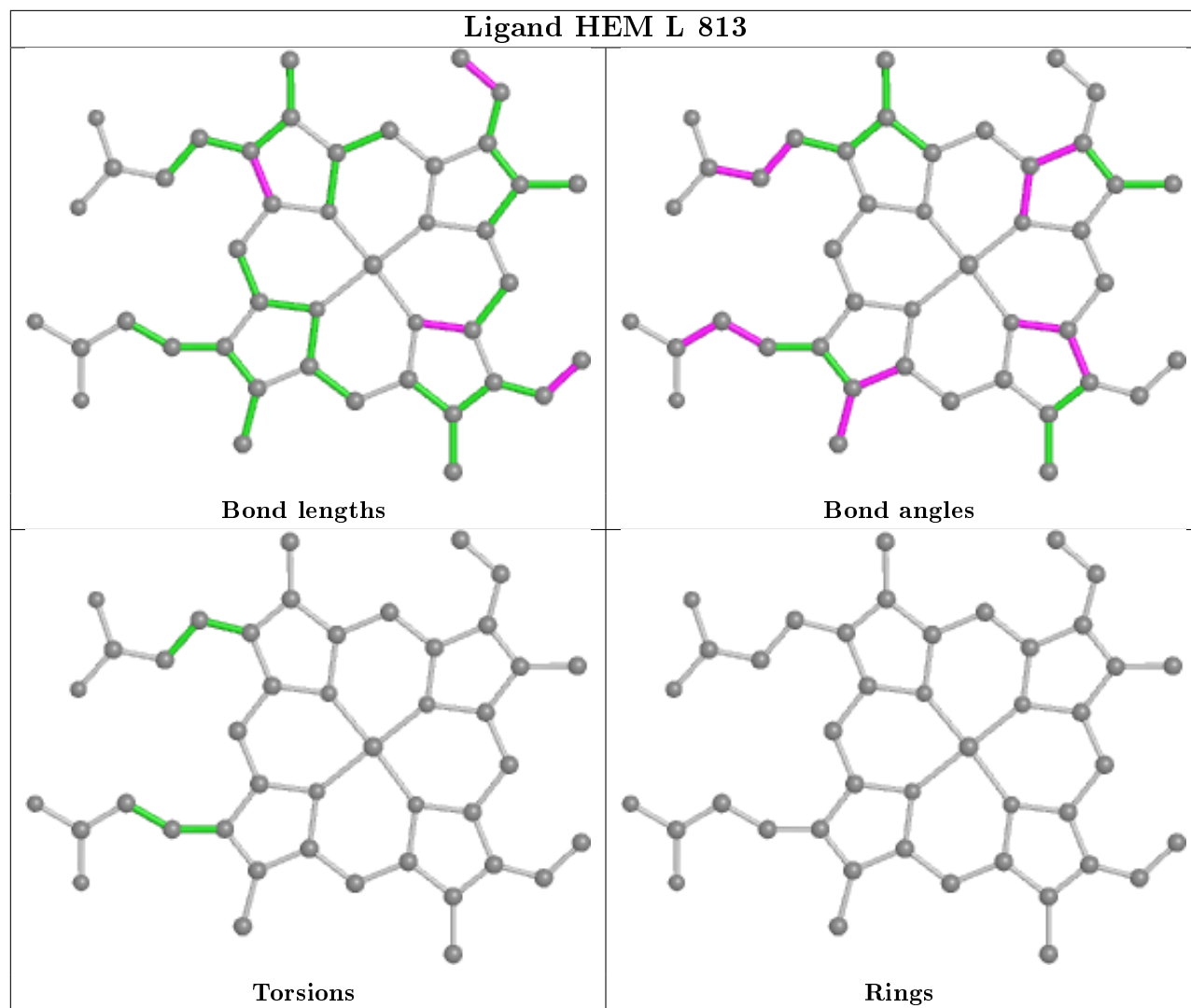


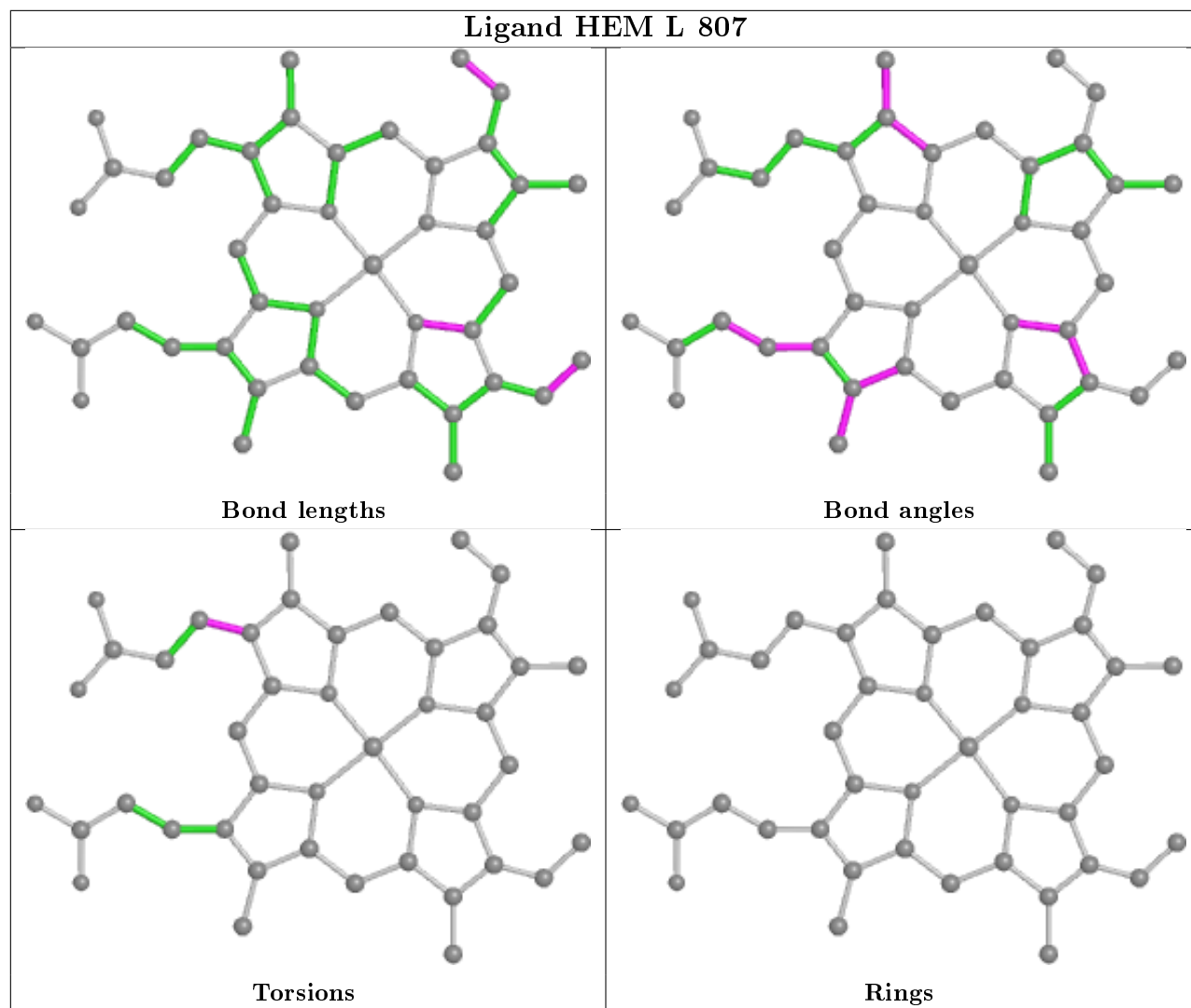


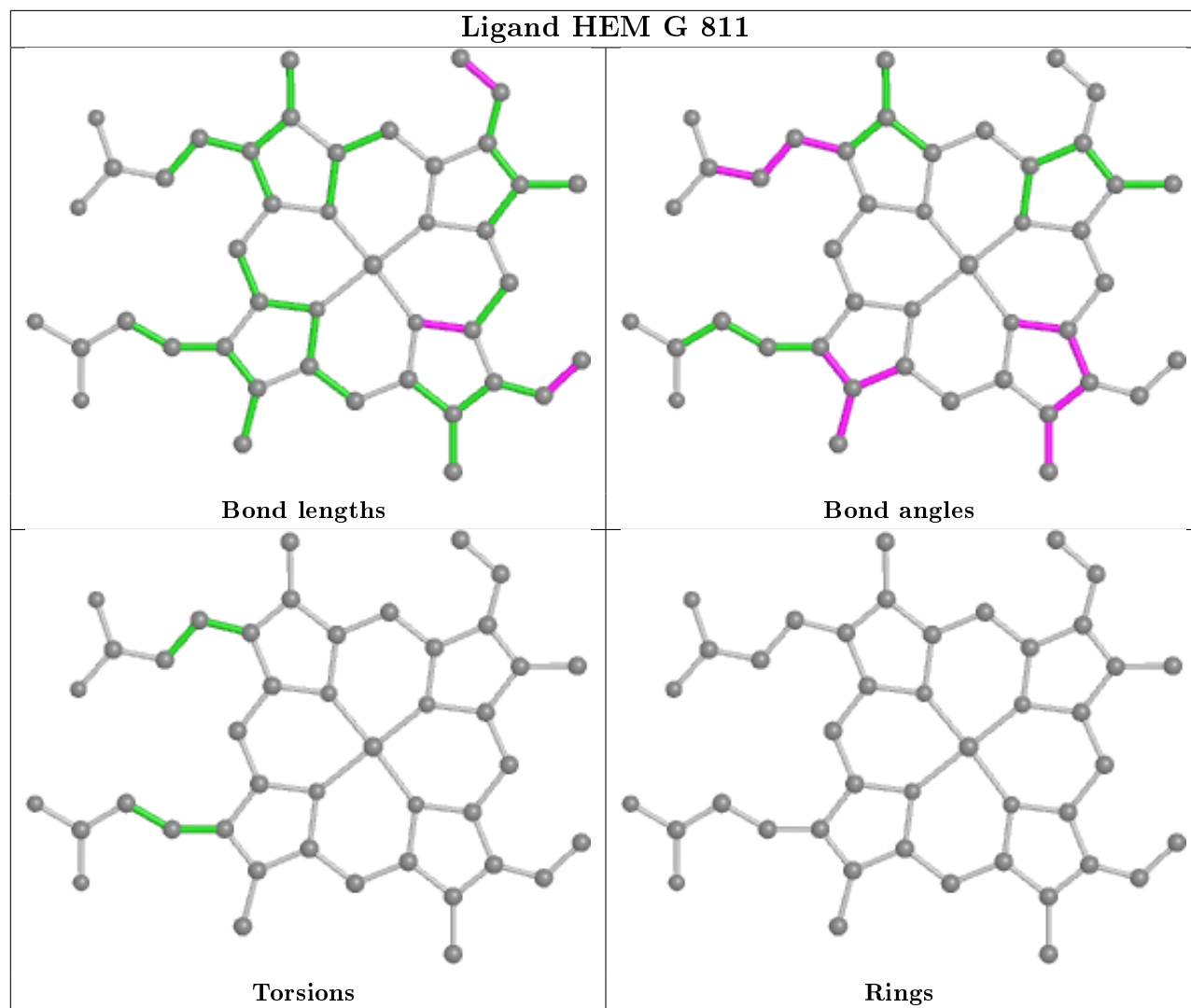


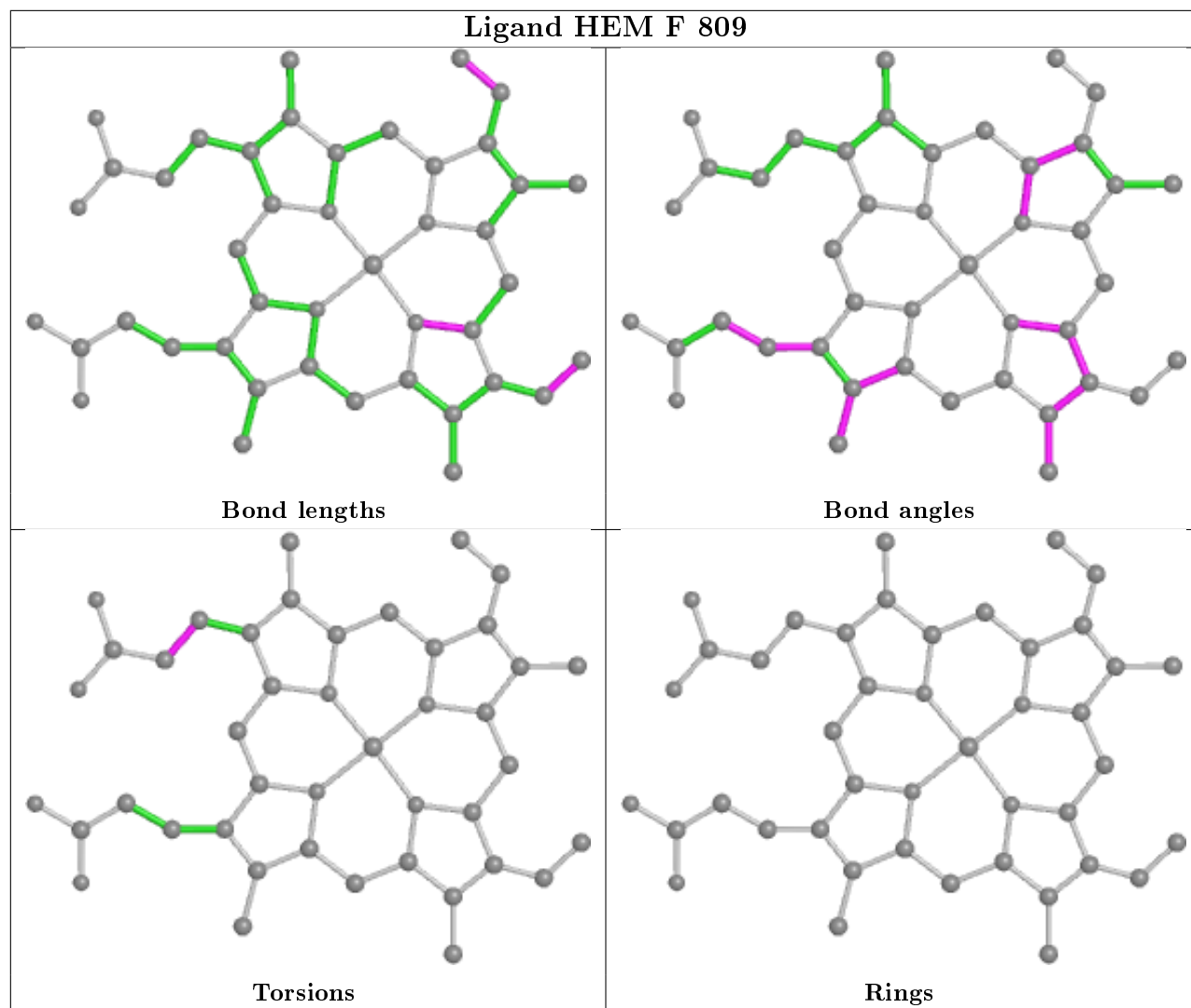
Ligand HEM I 806

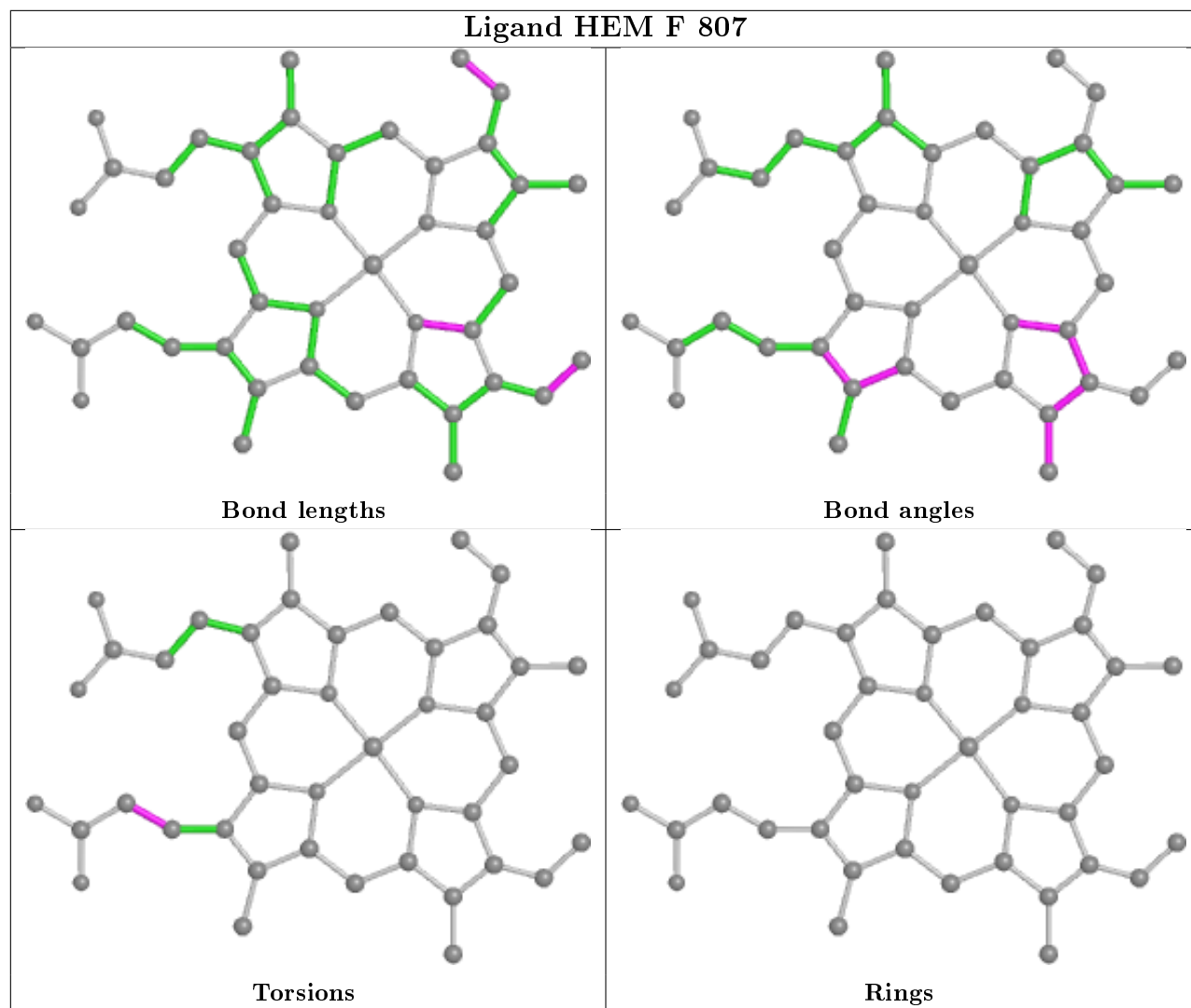


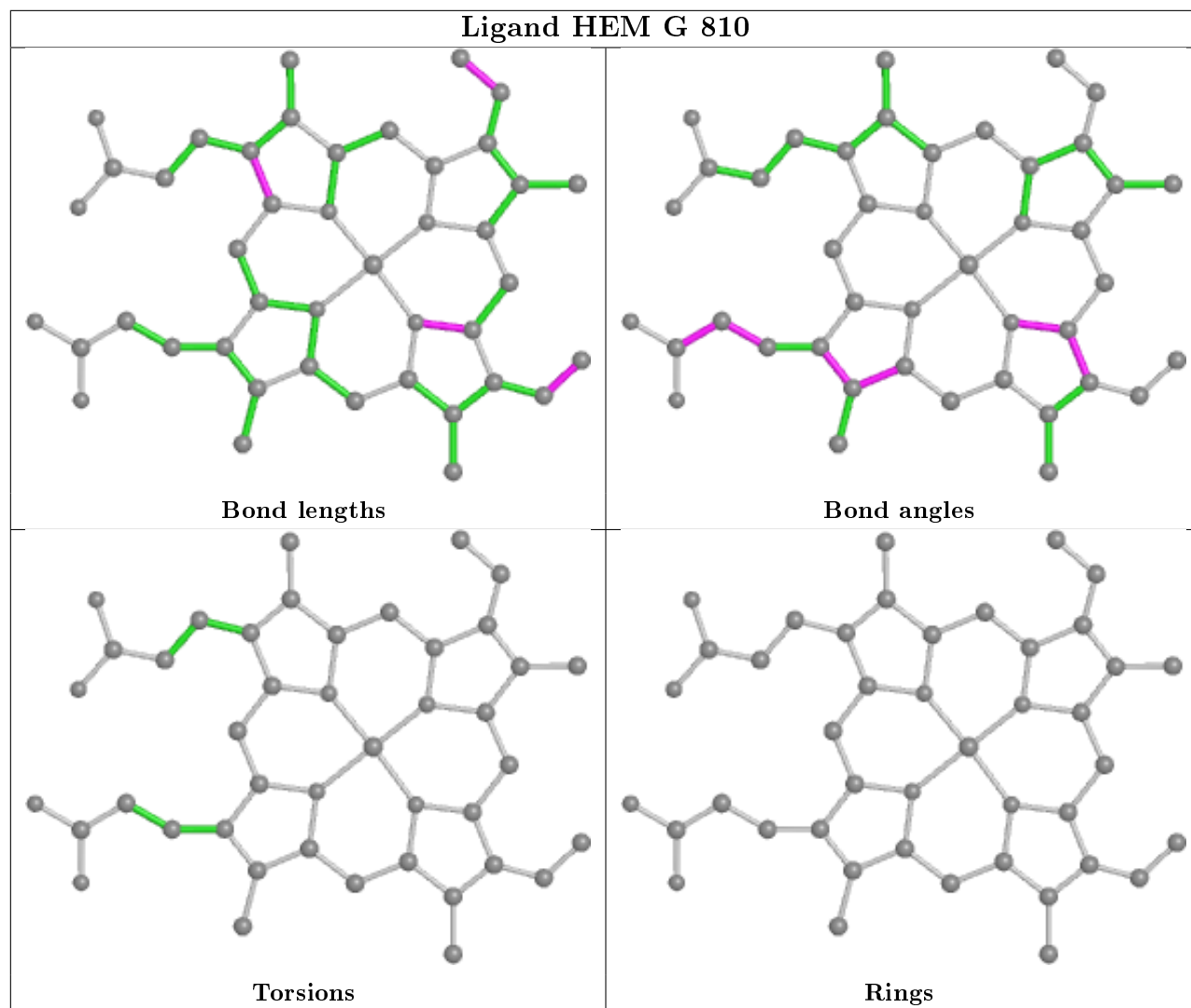


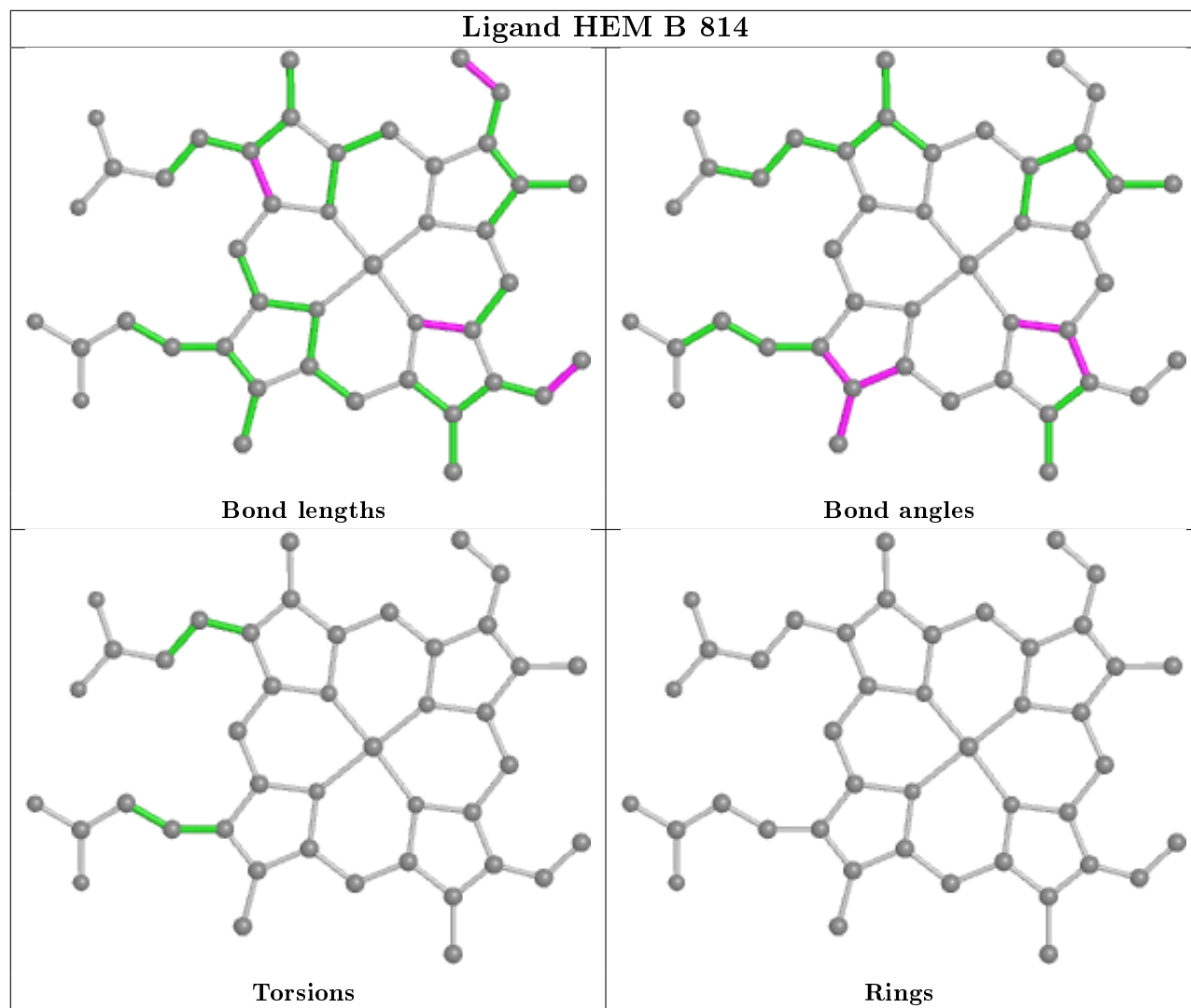


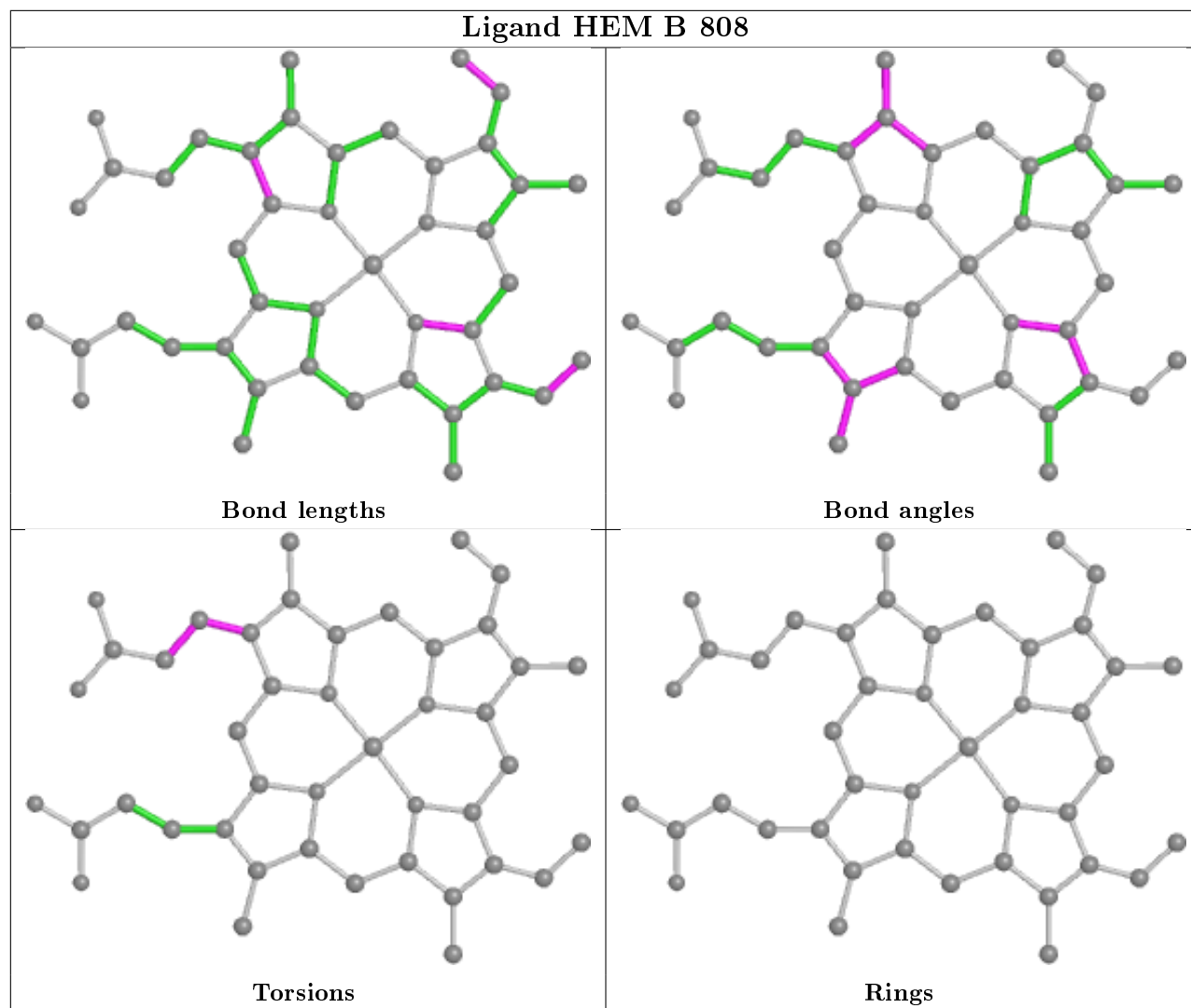


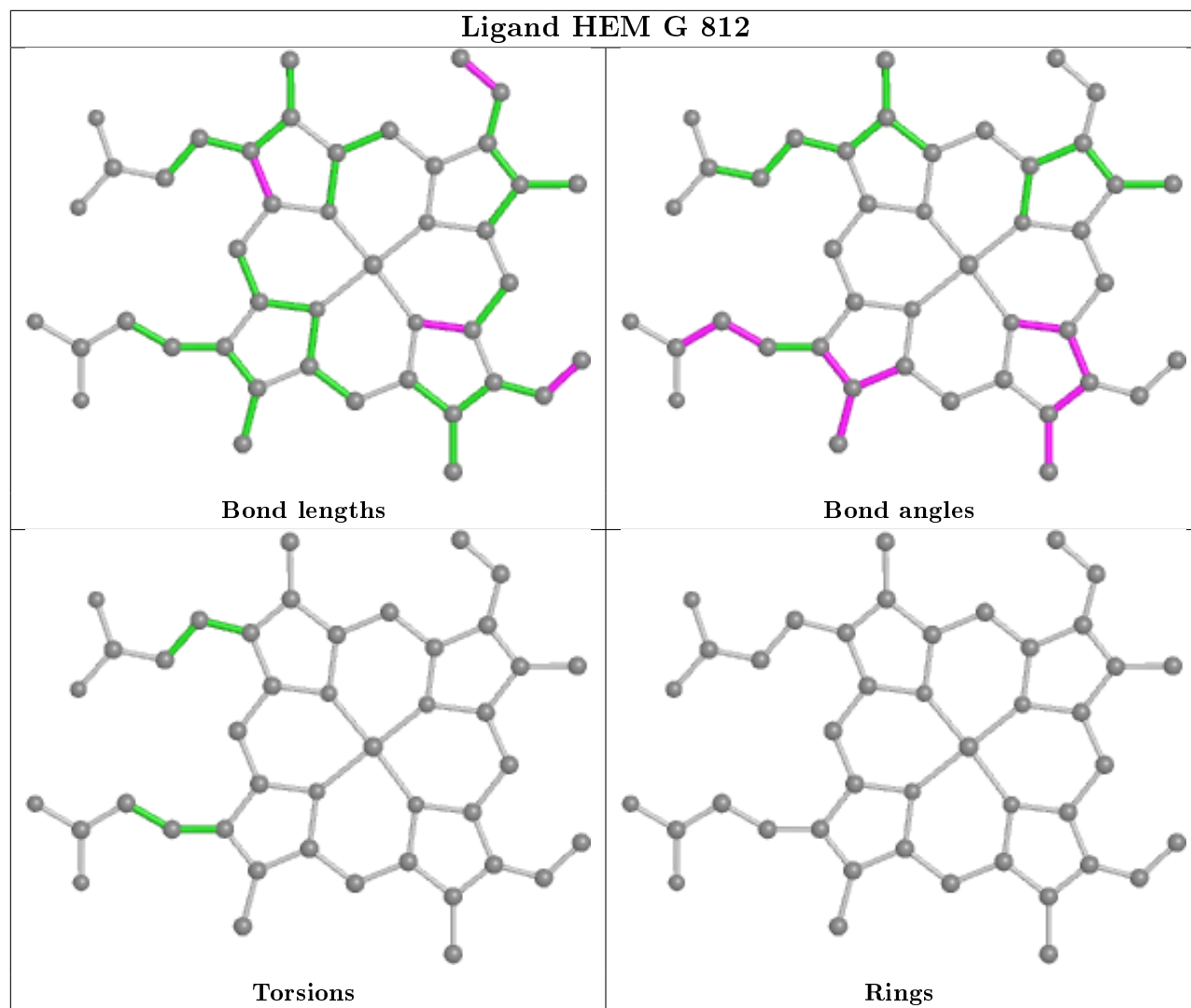


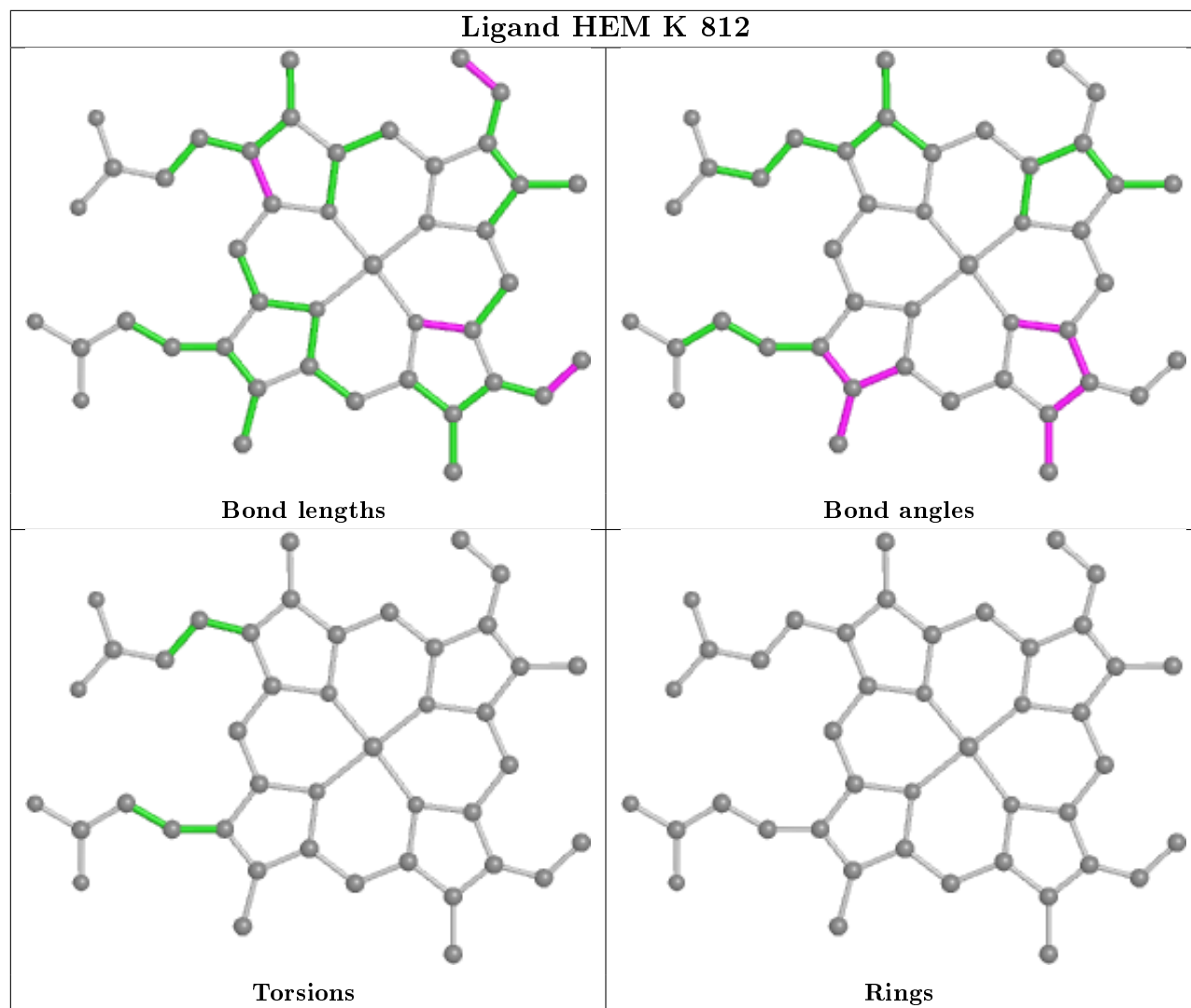


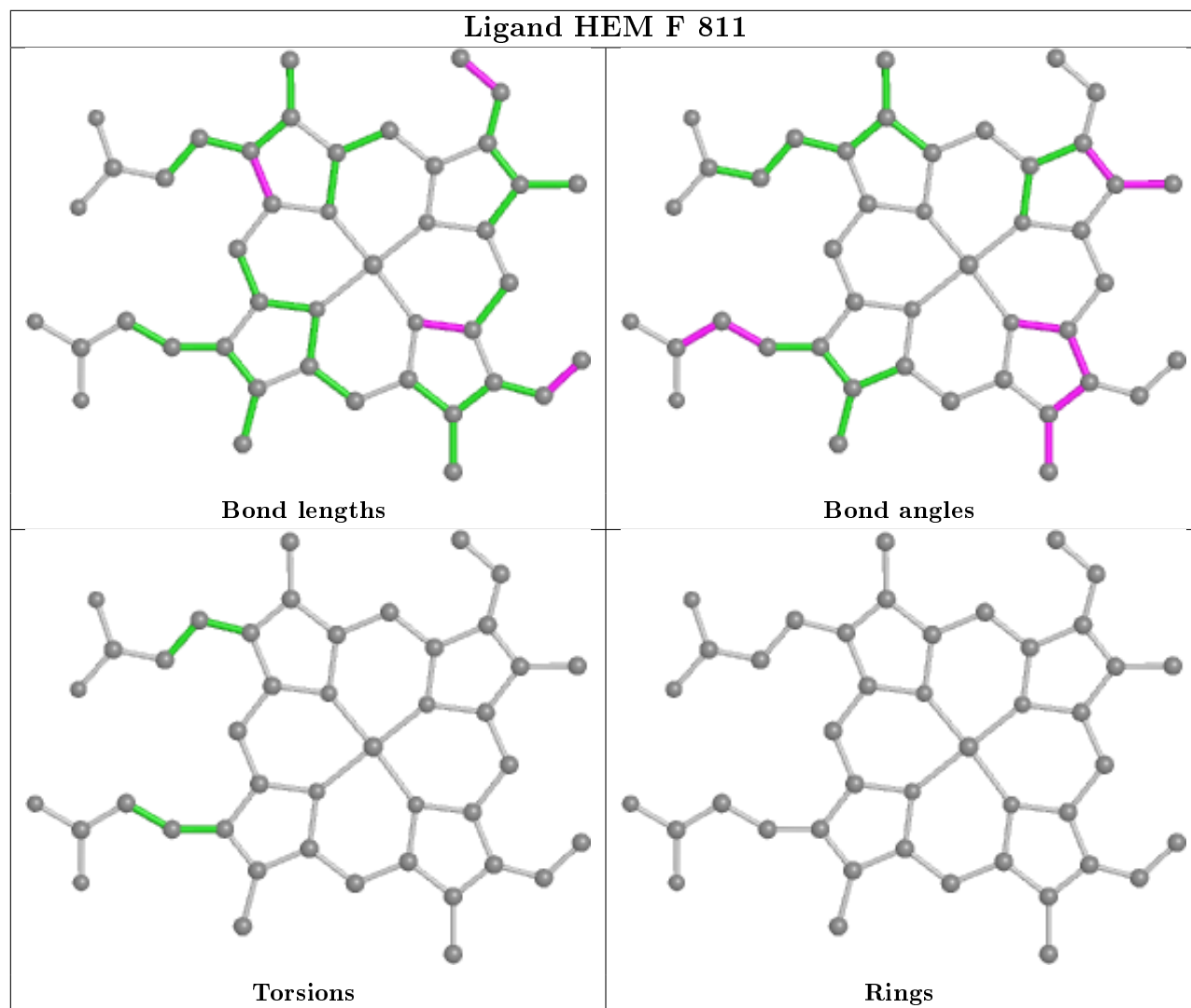


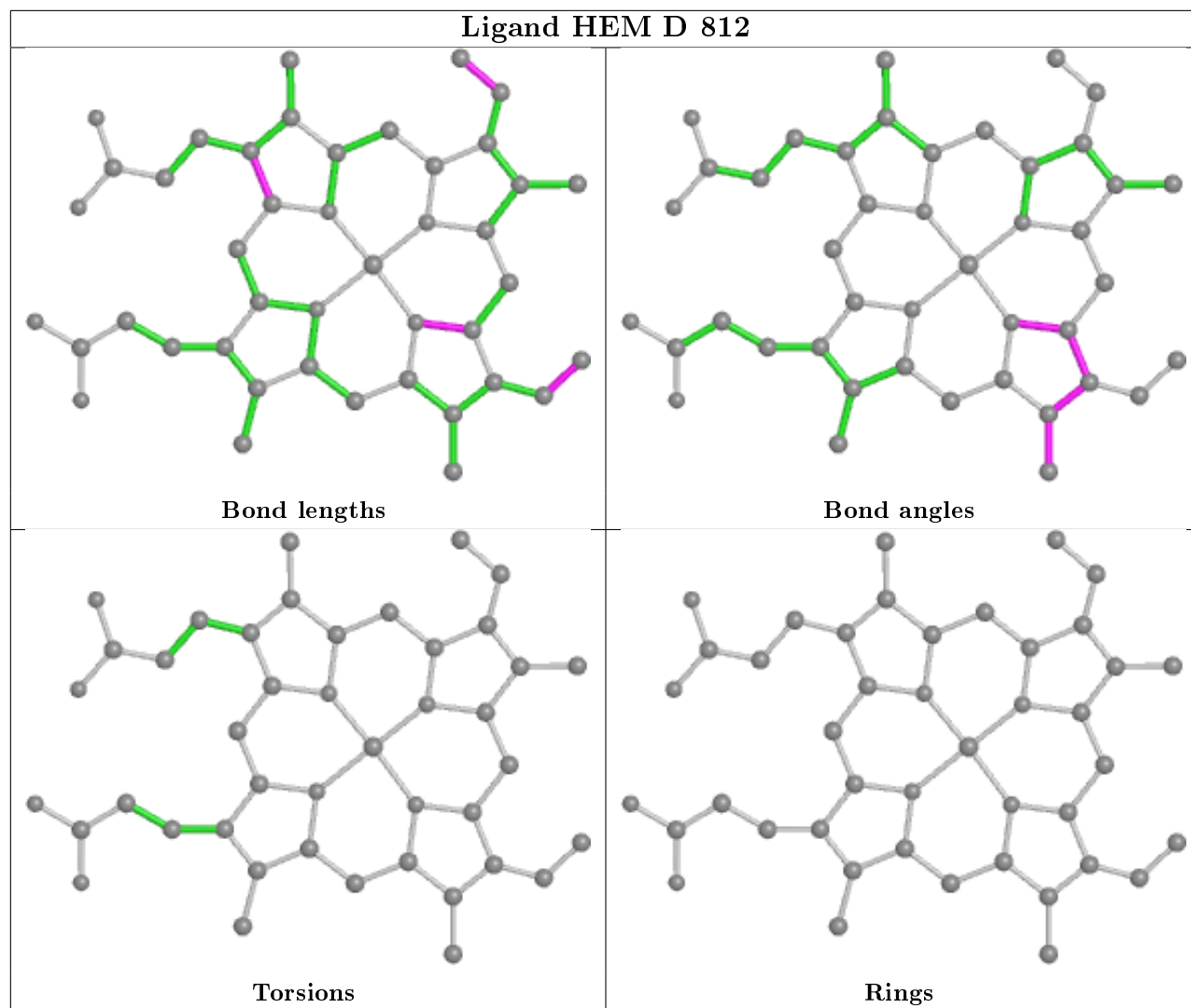


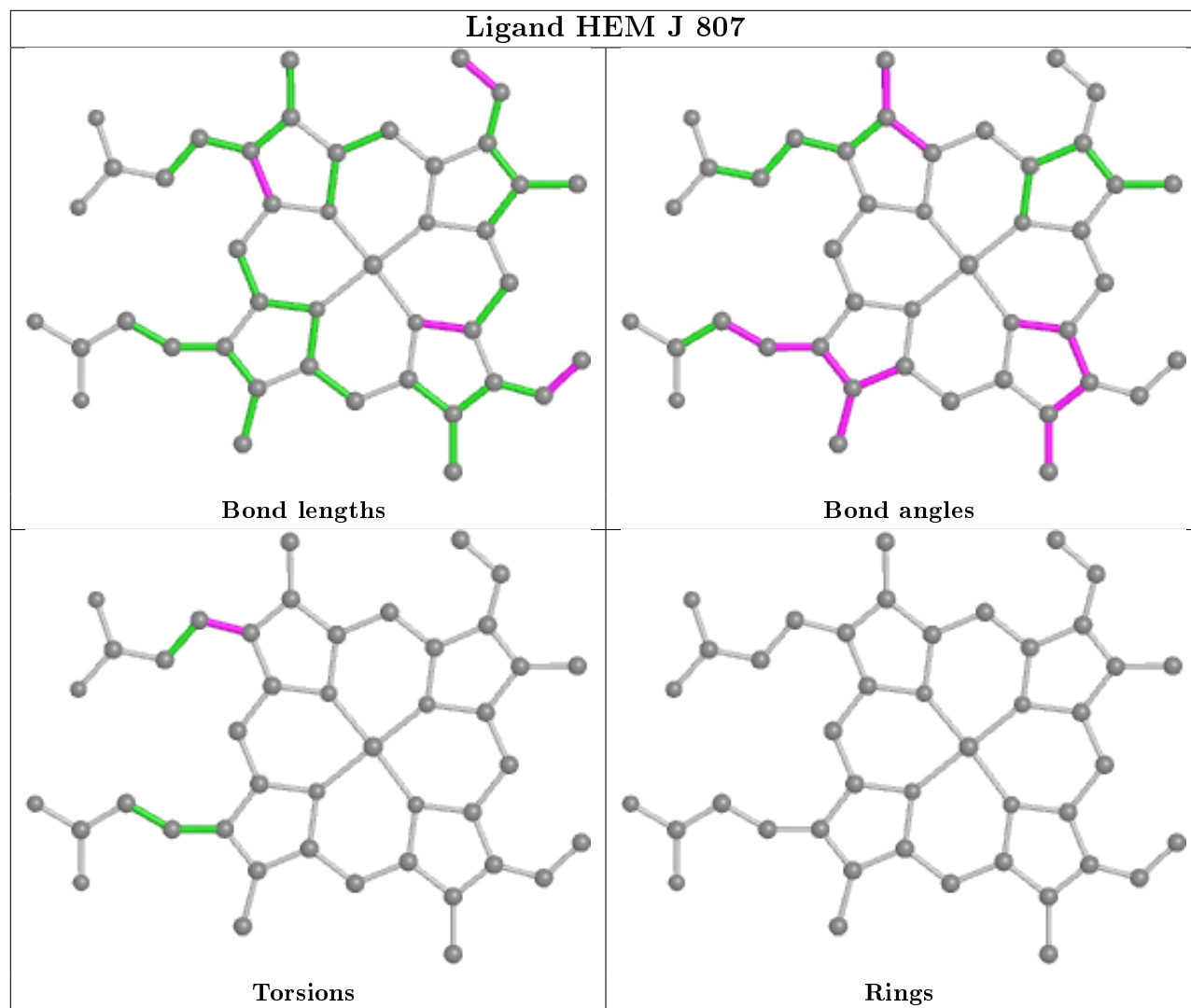




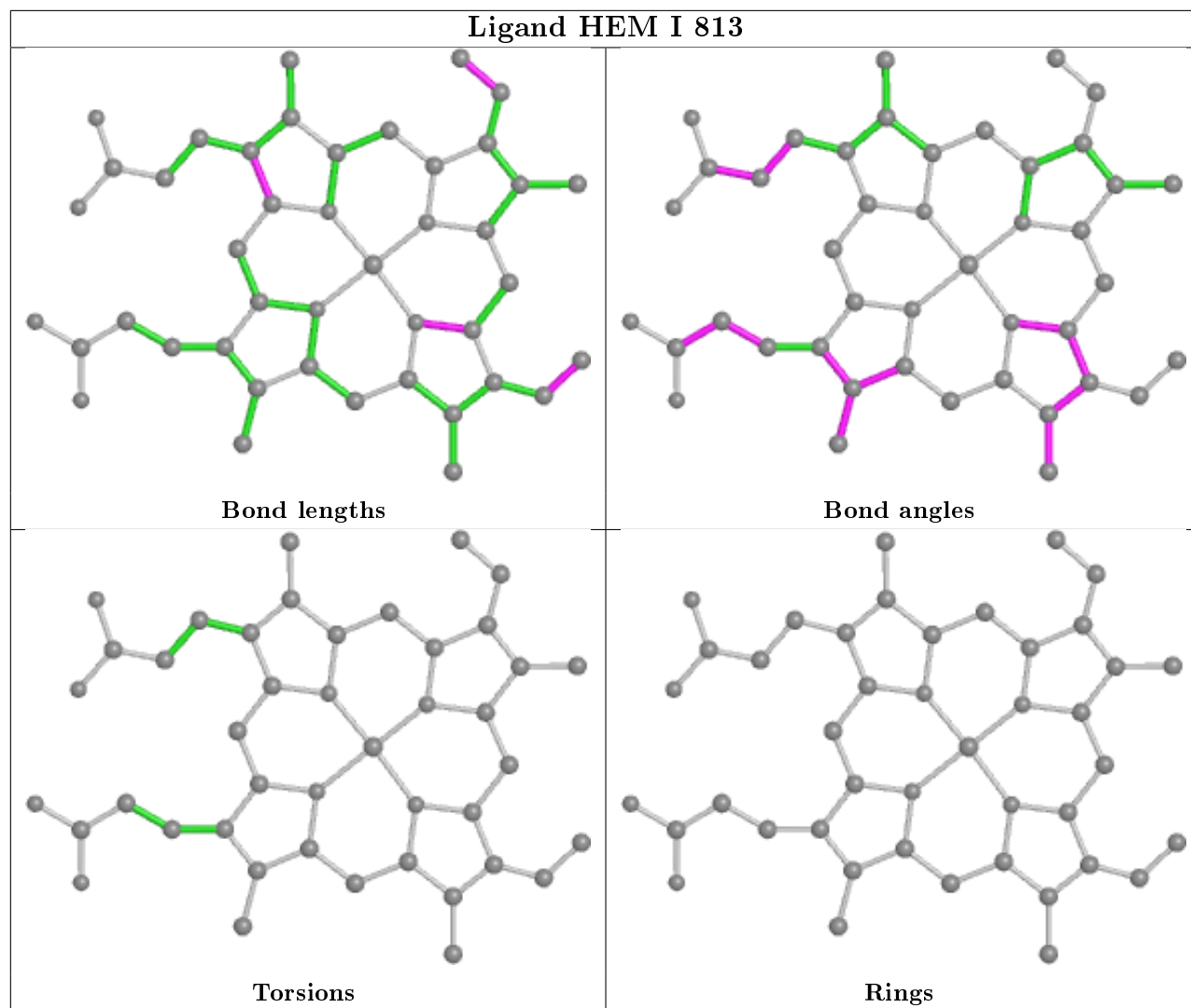


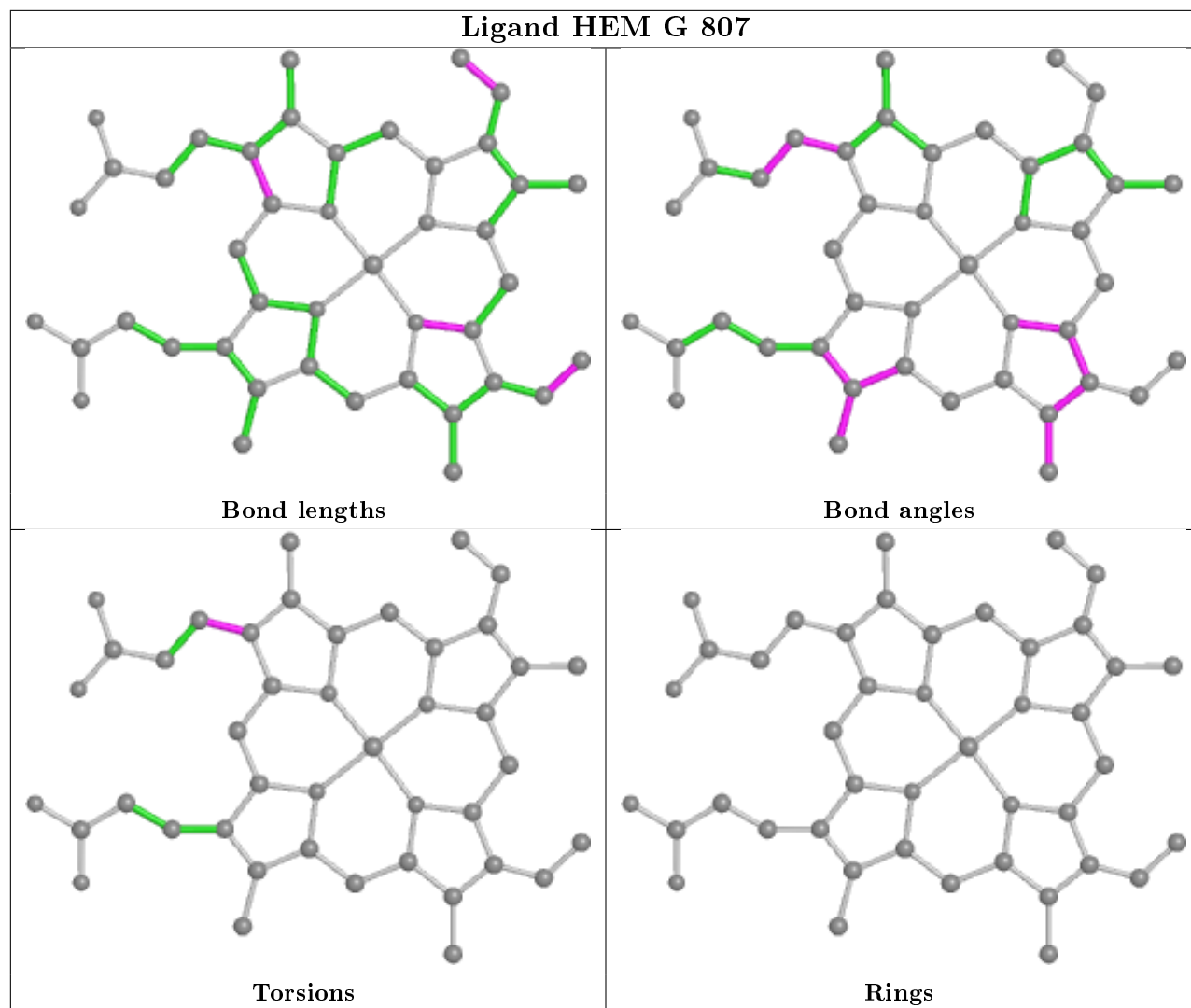


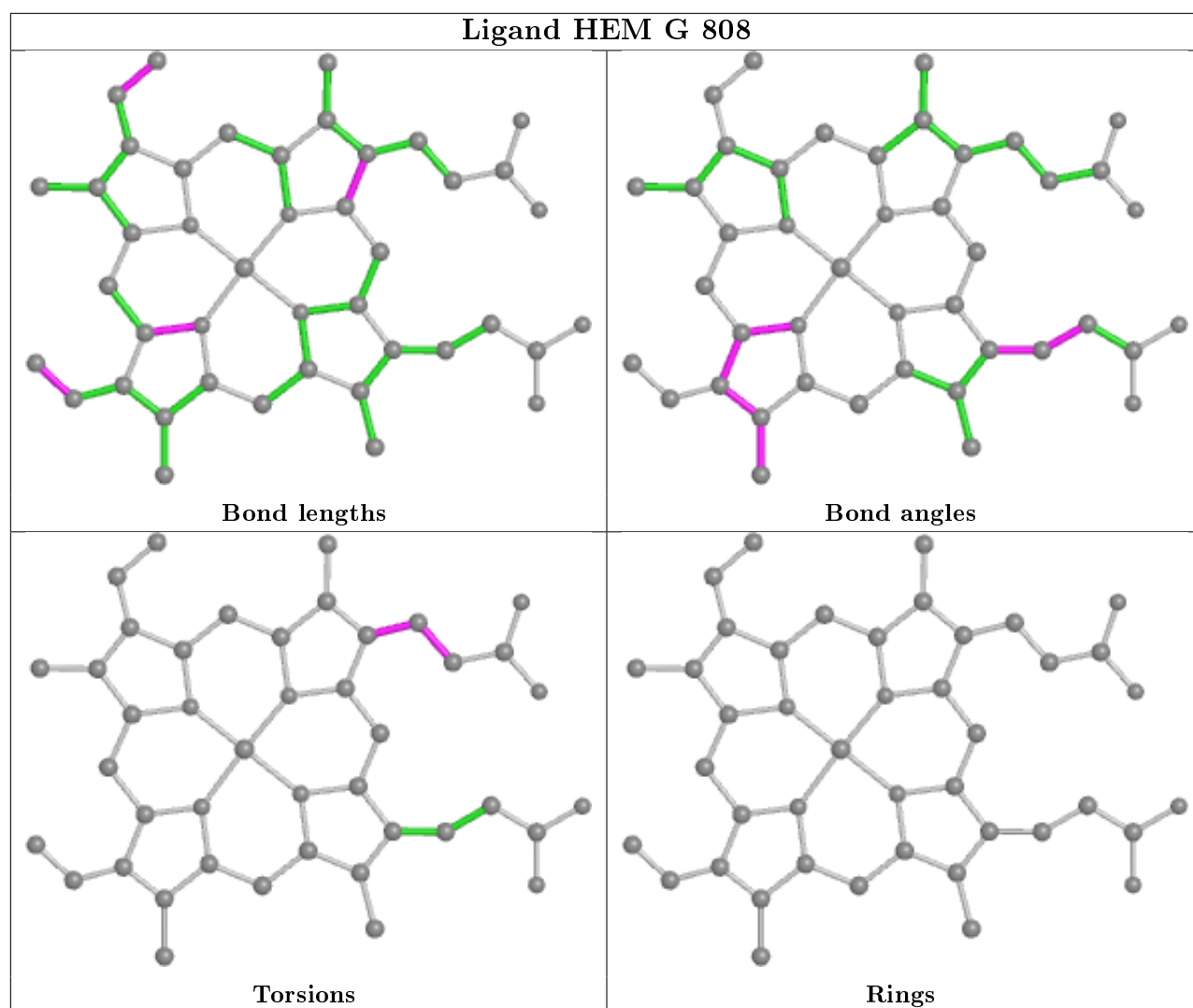


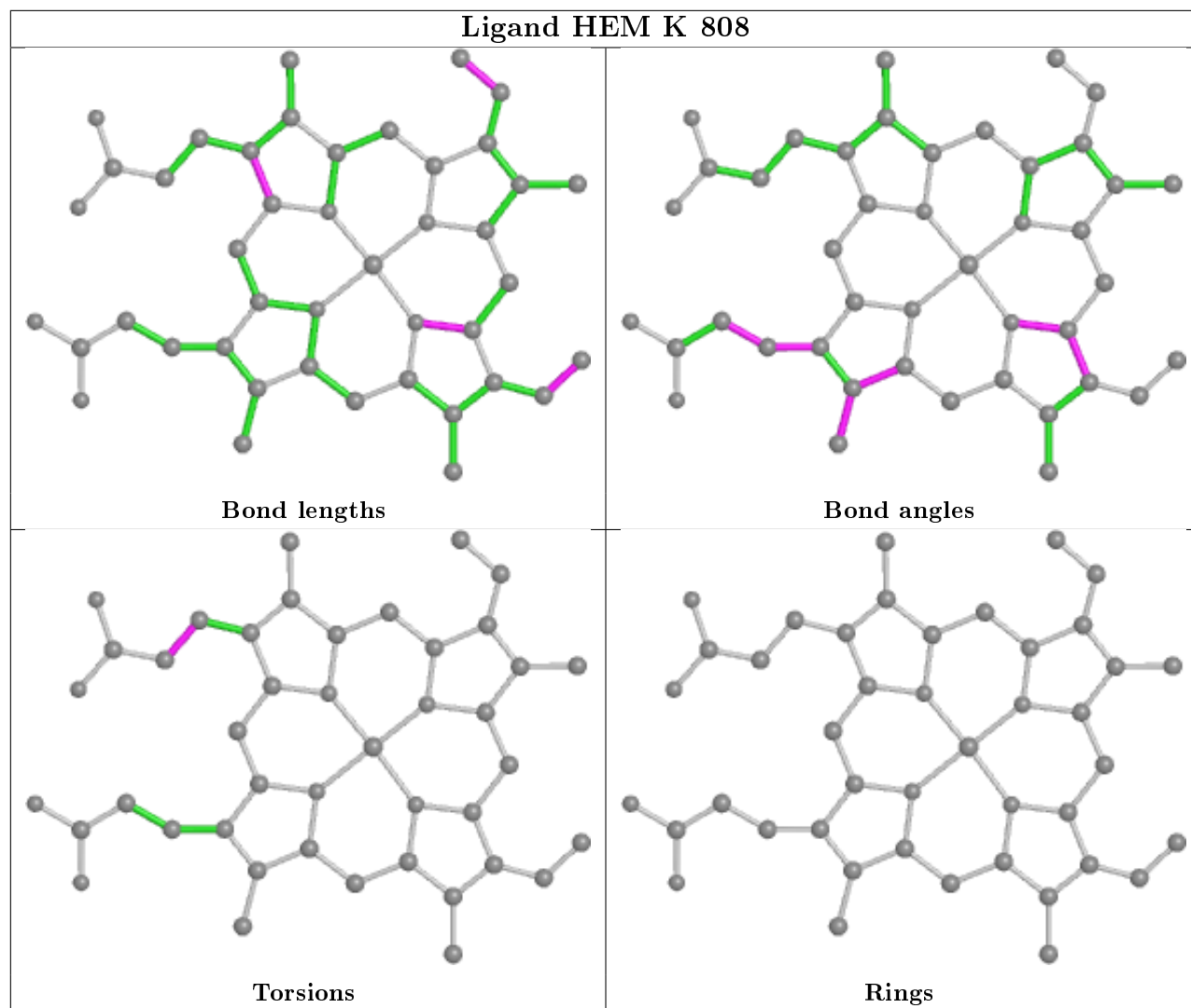


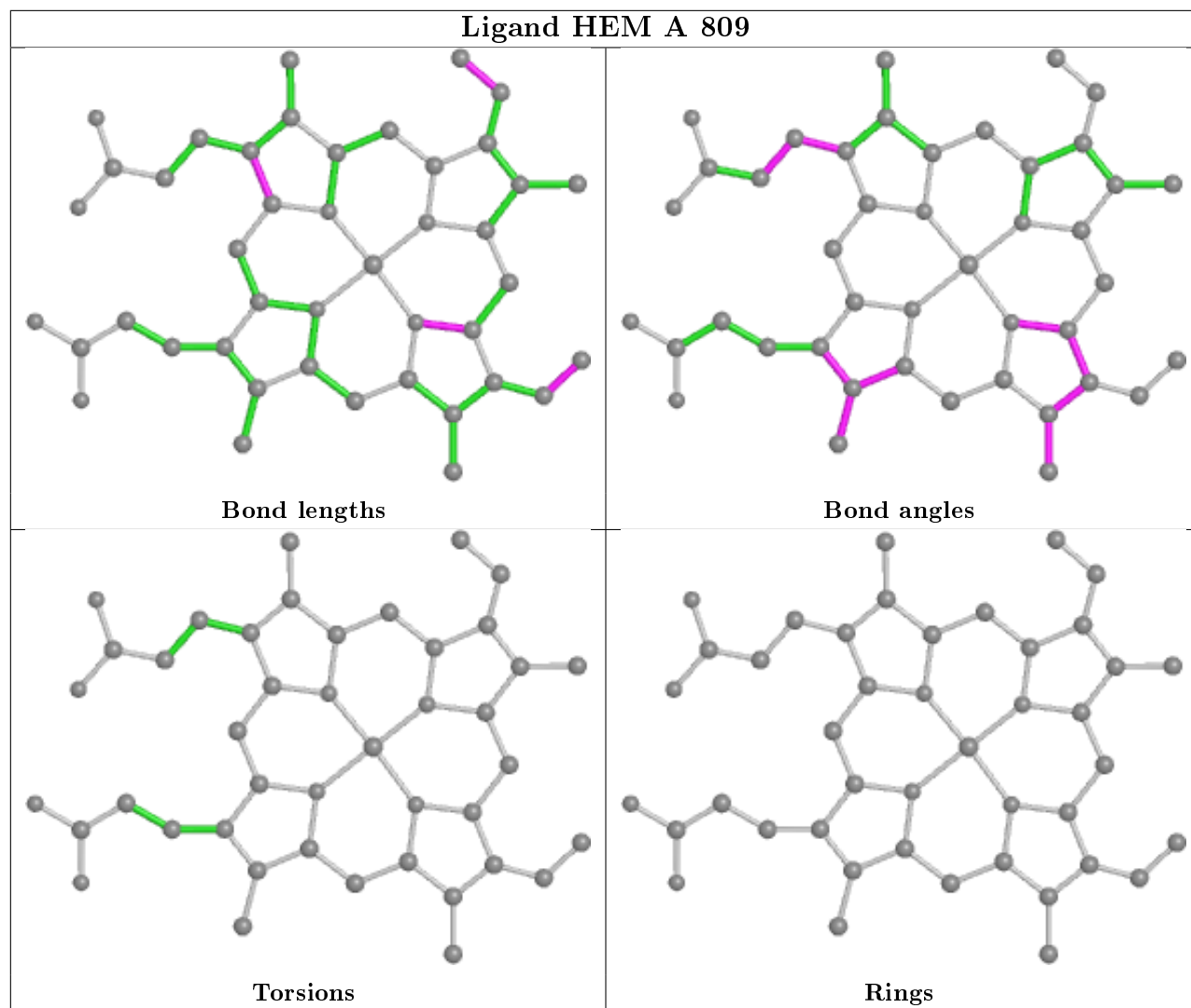
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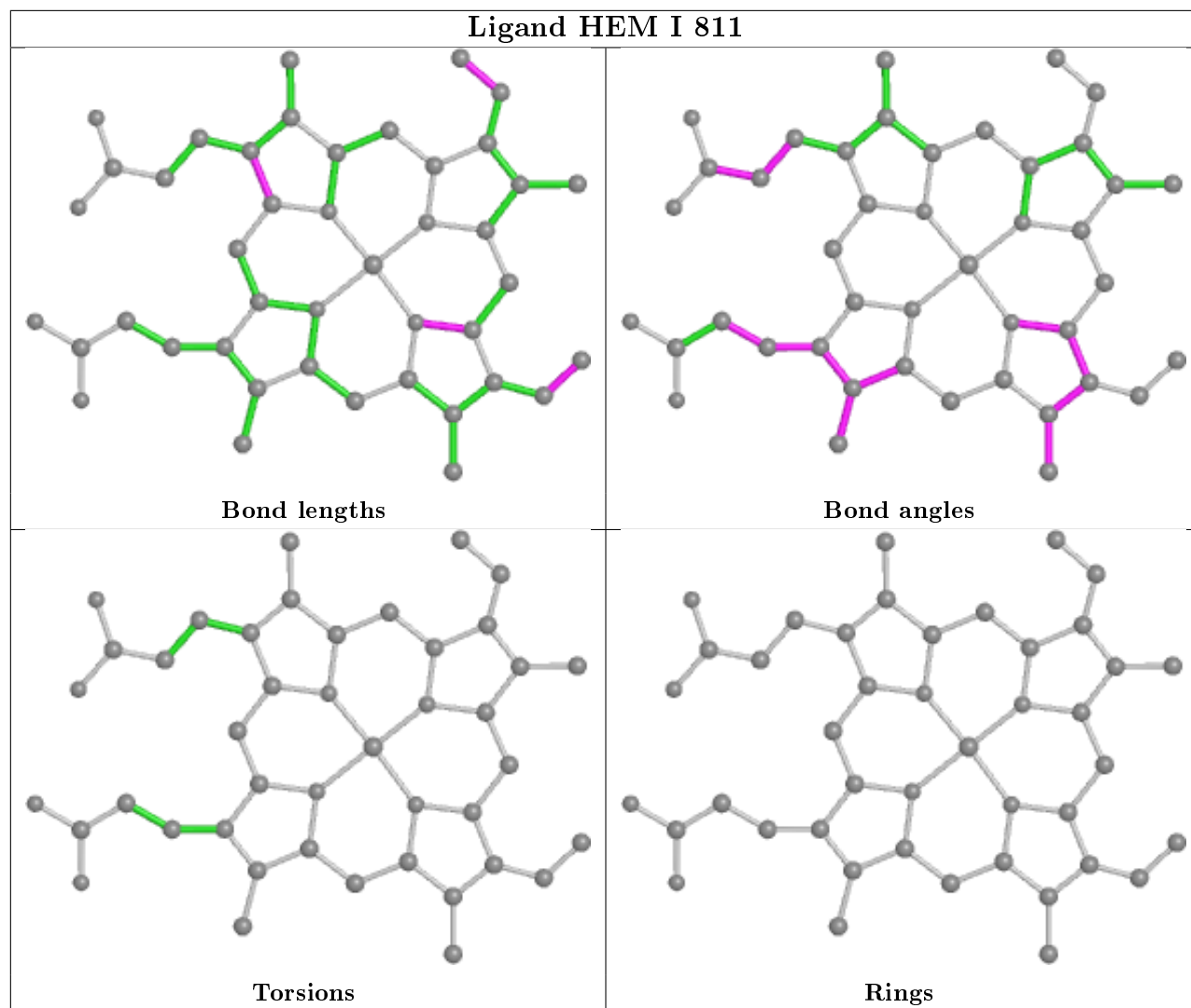


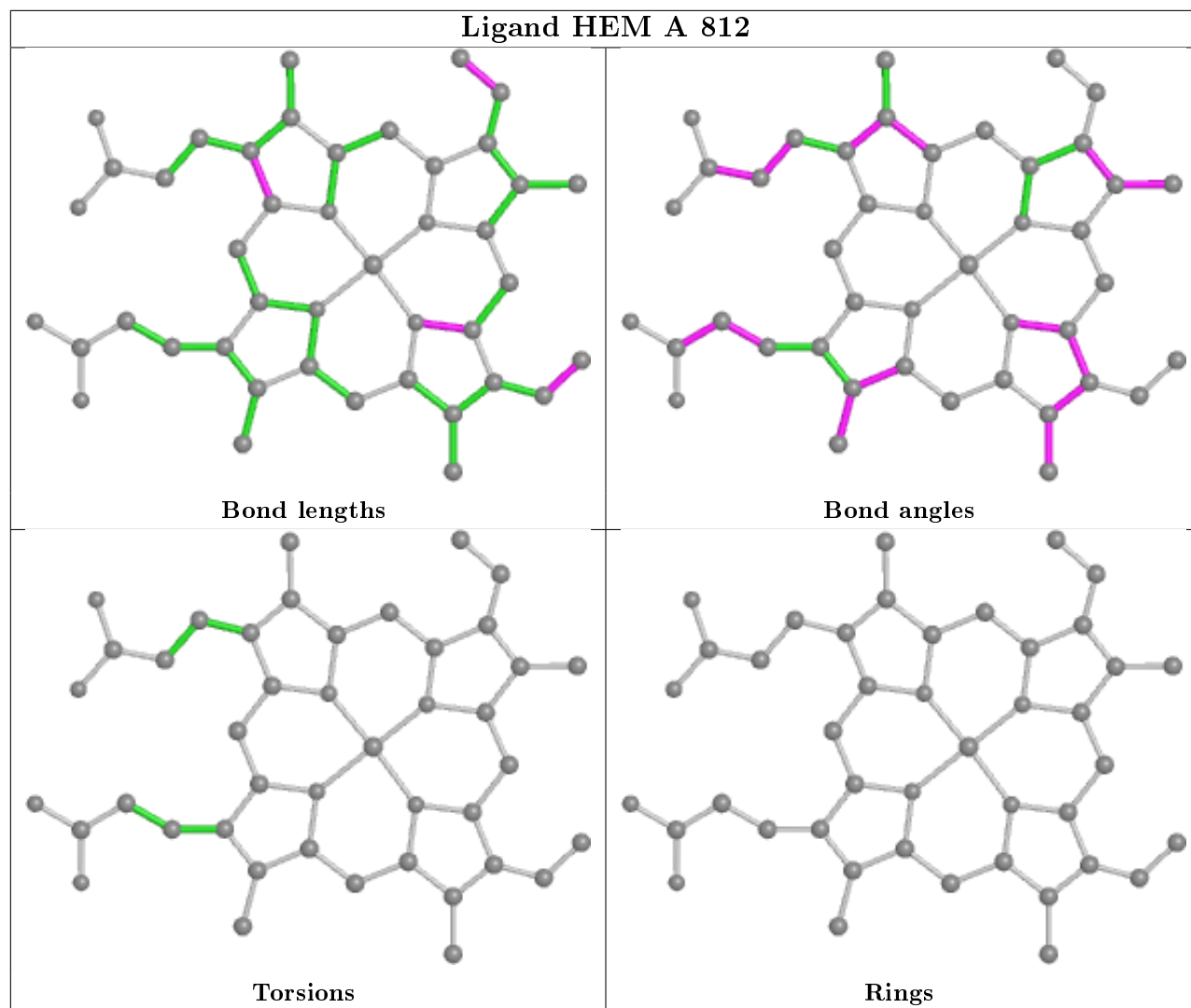


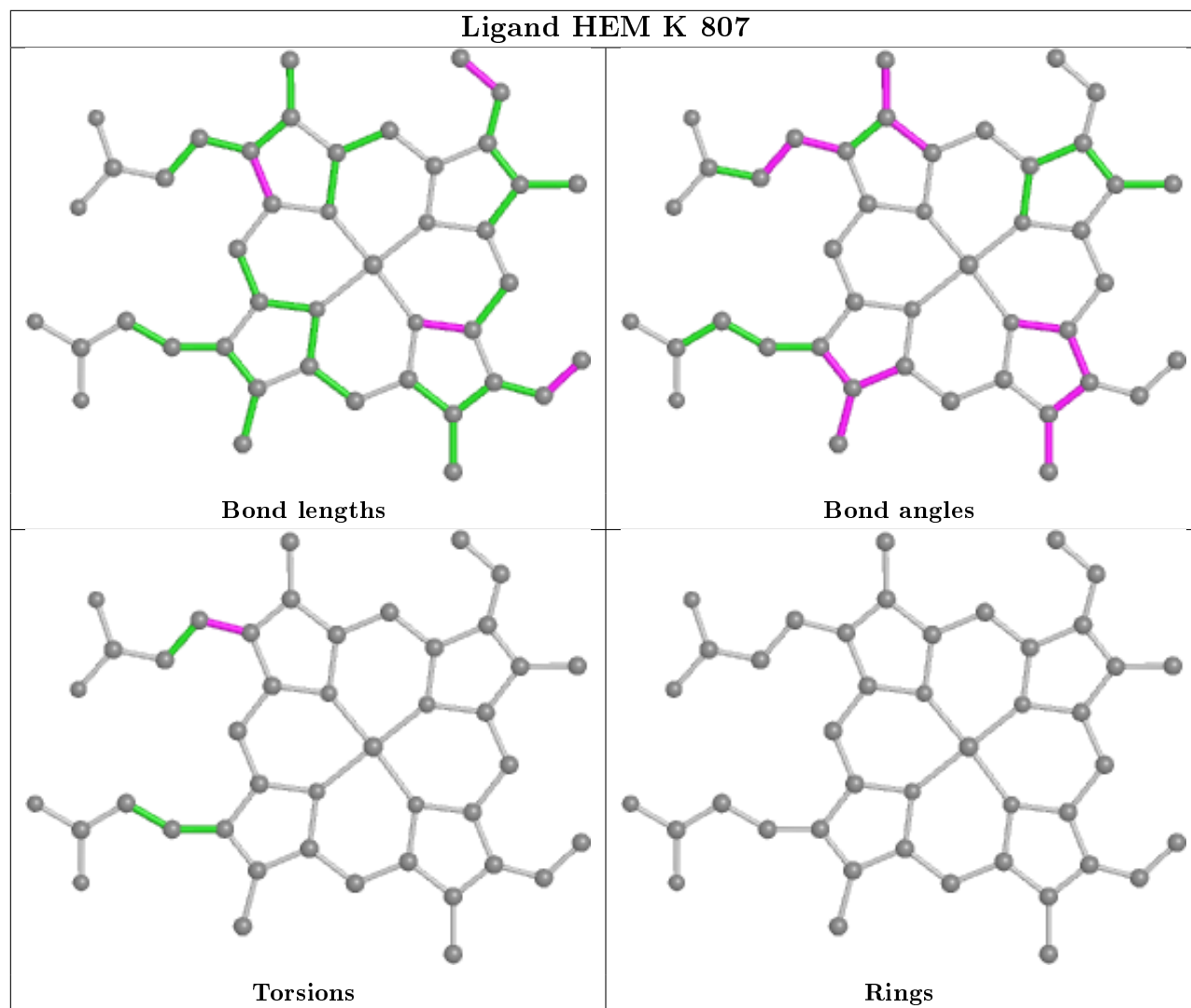


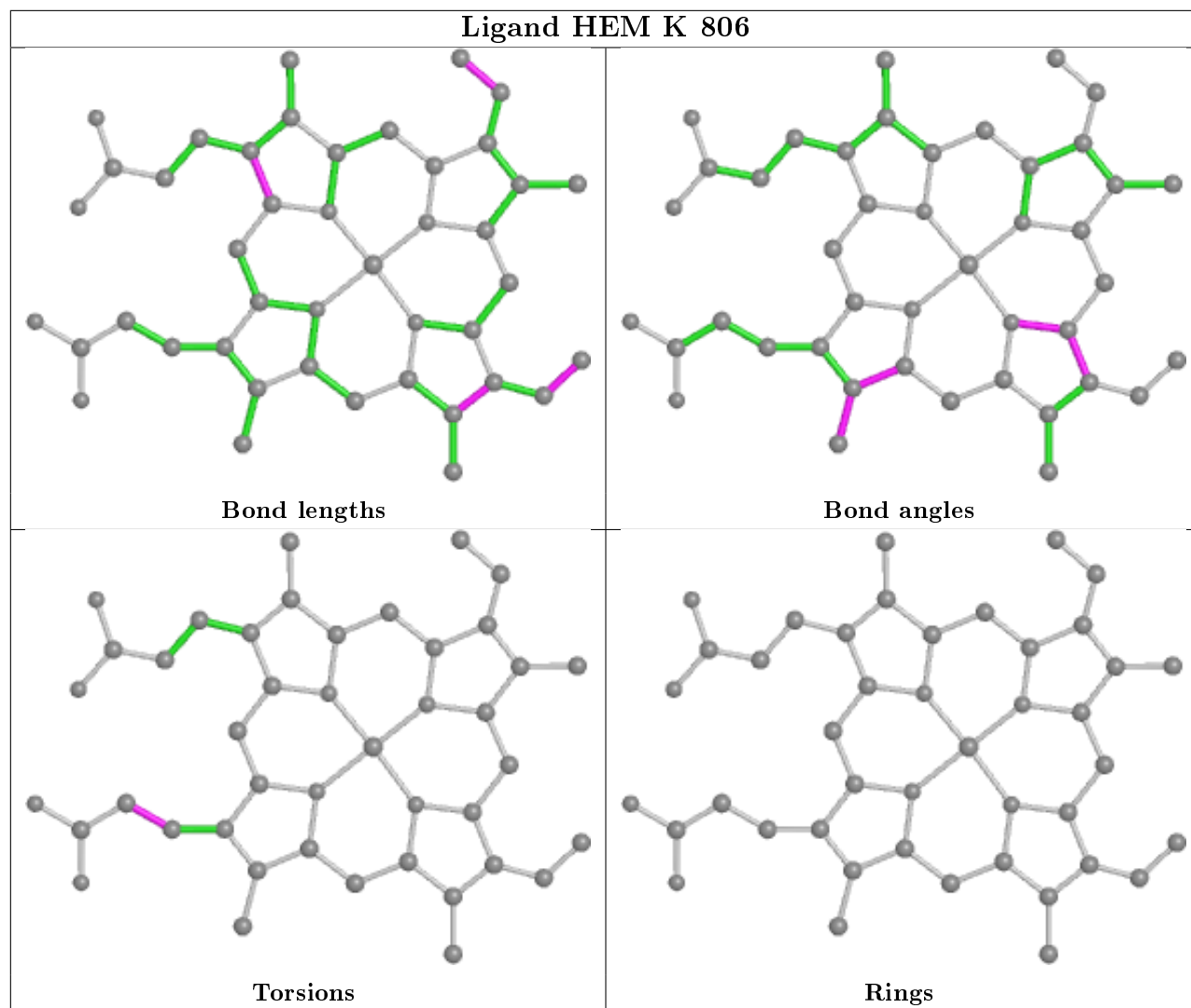


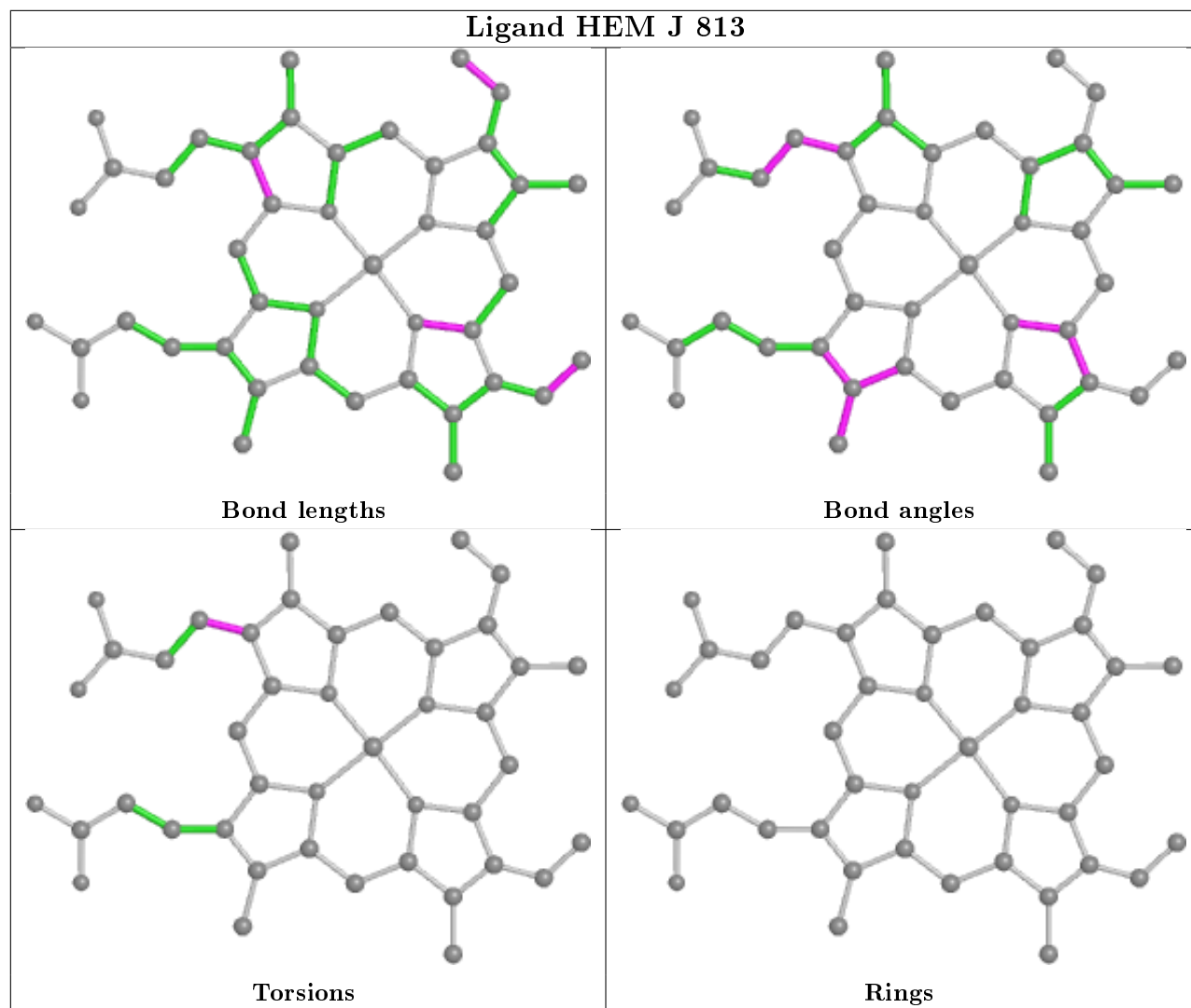
Ligand HEM I 811

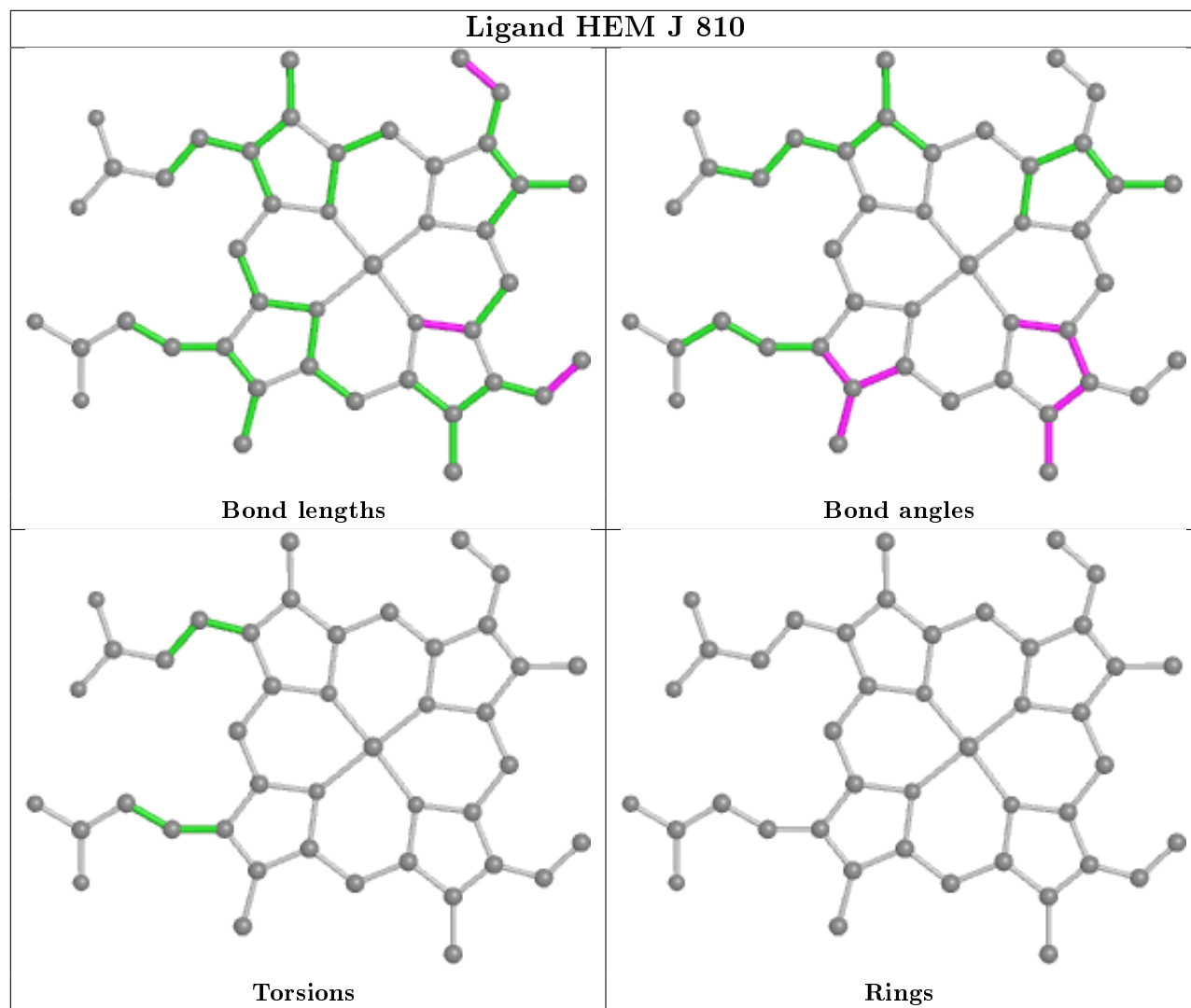


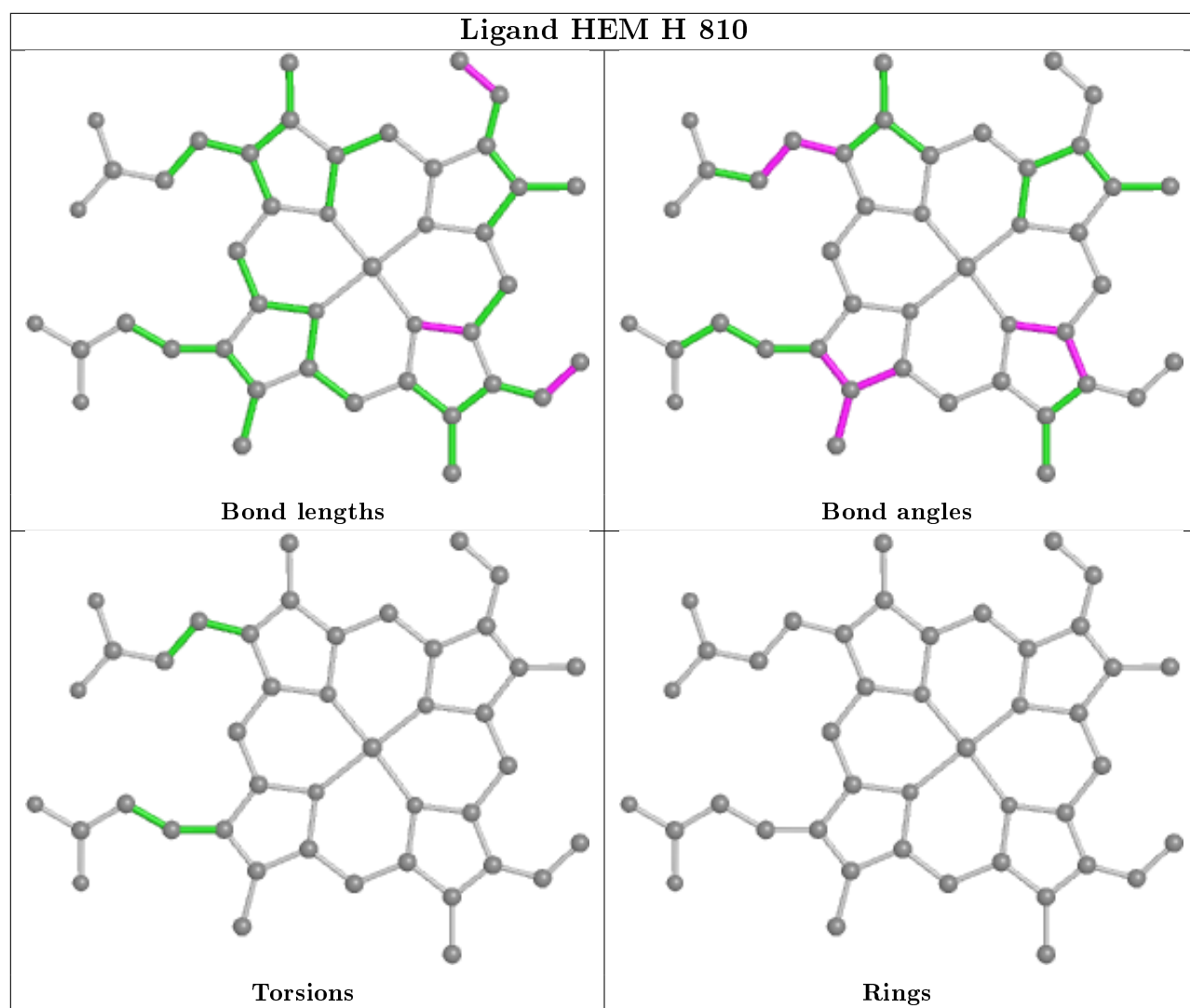


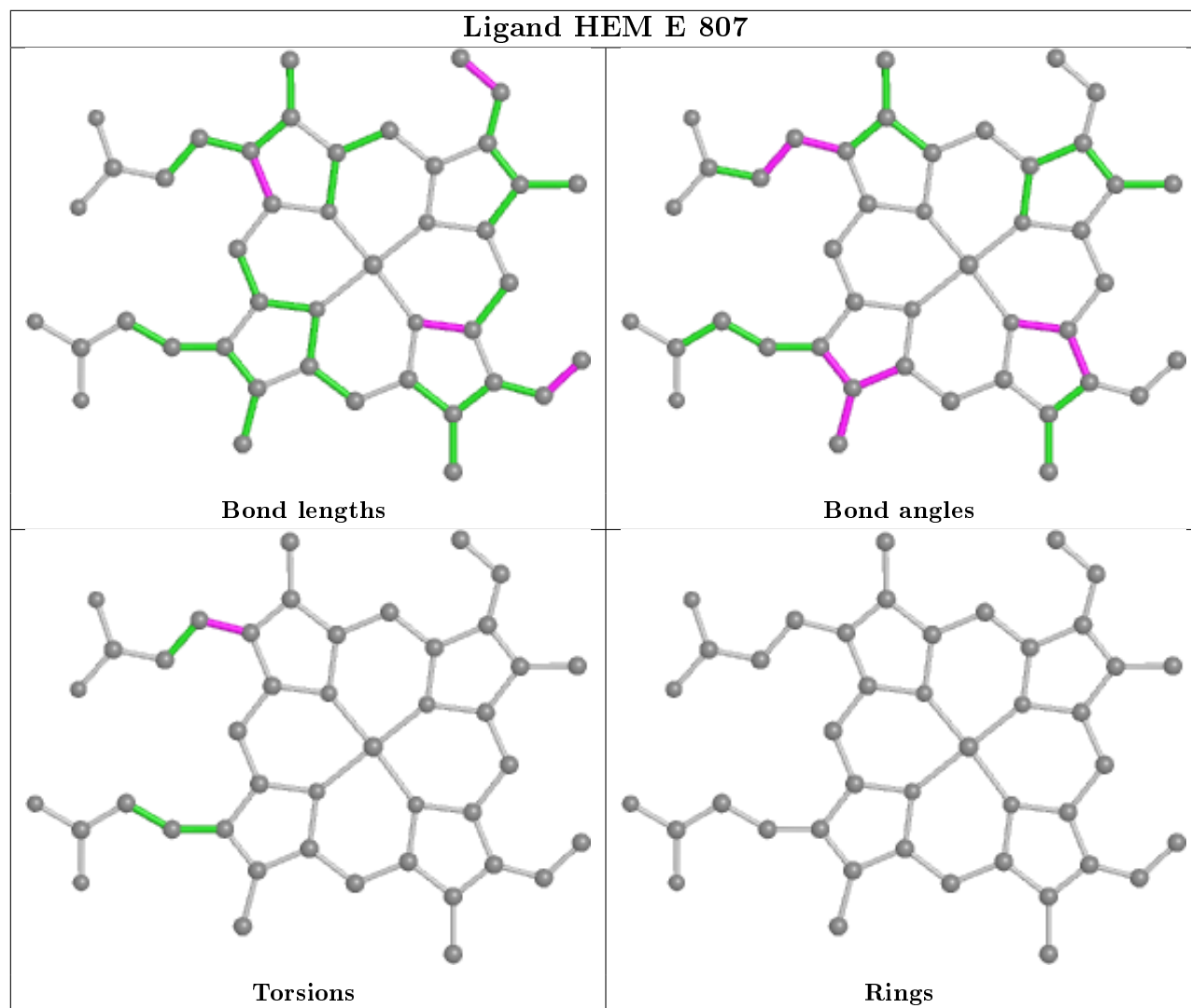


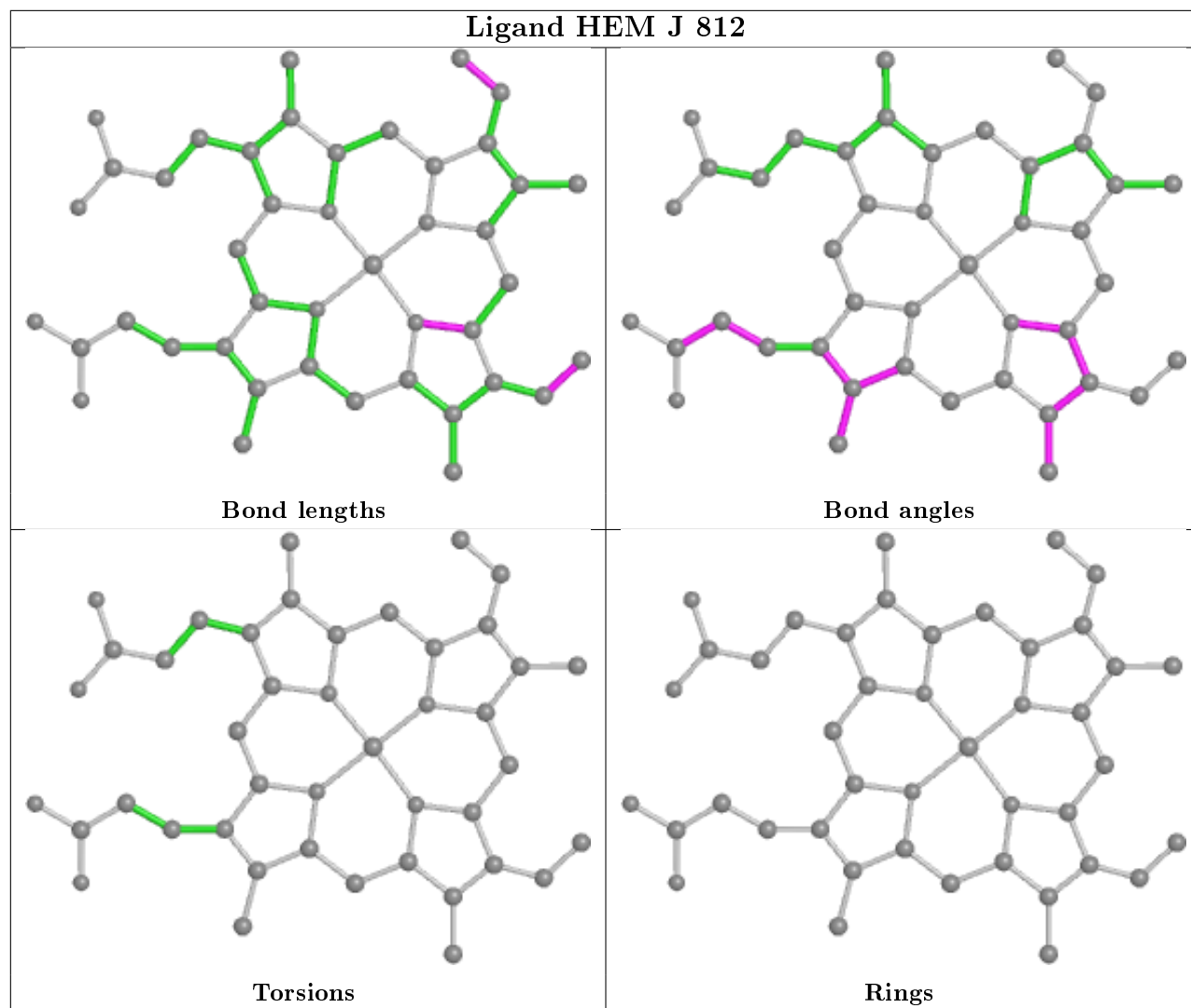


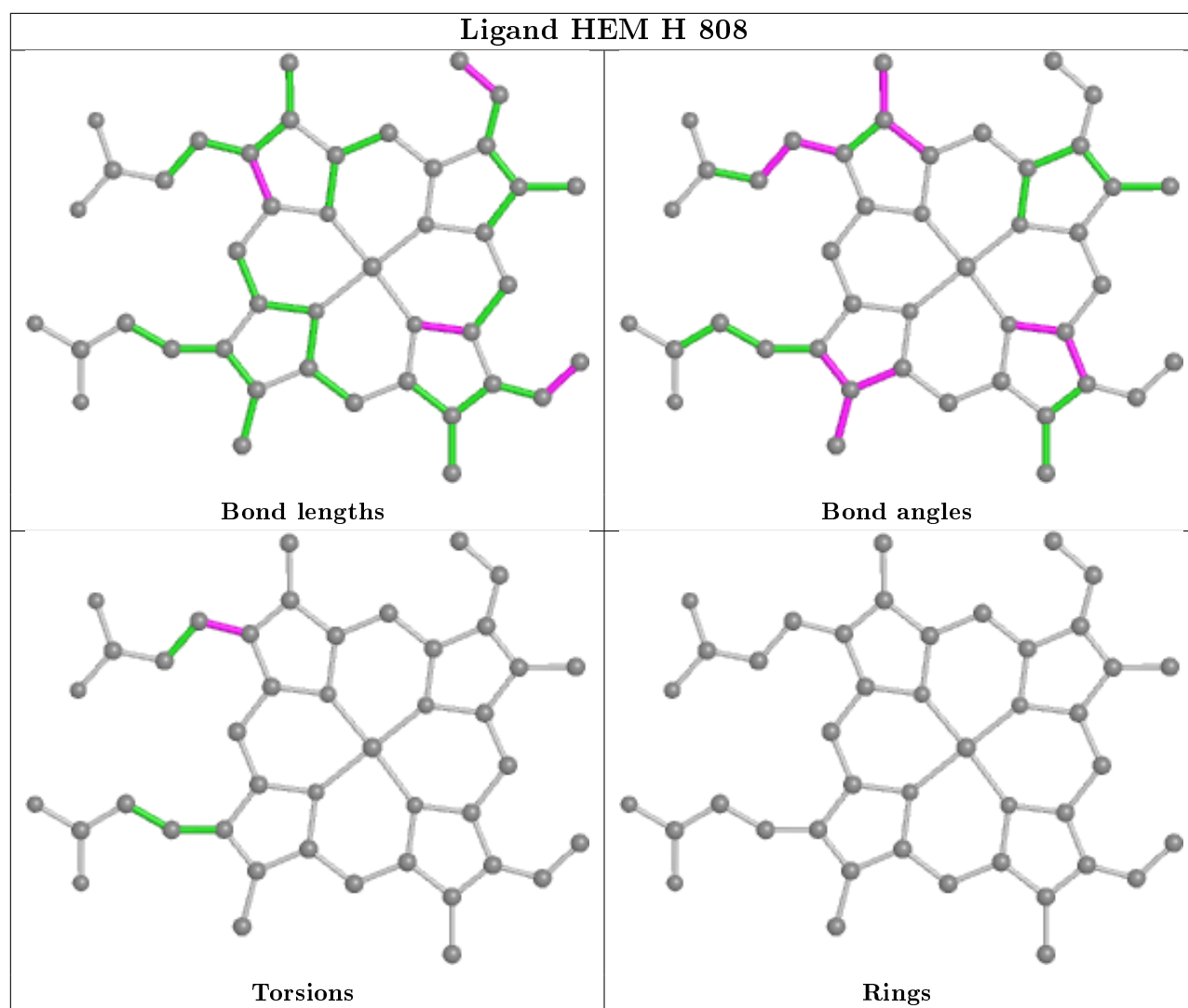


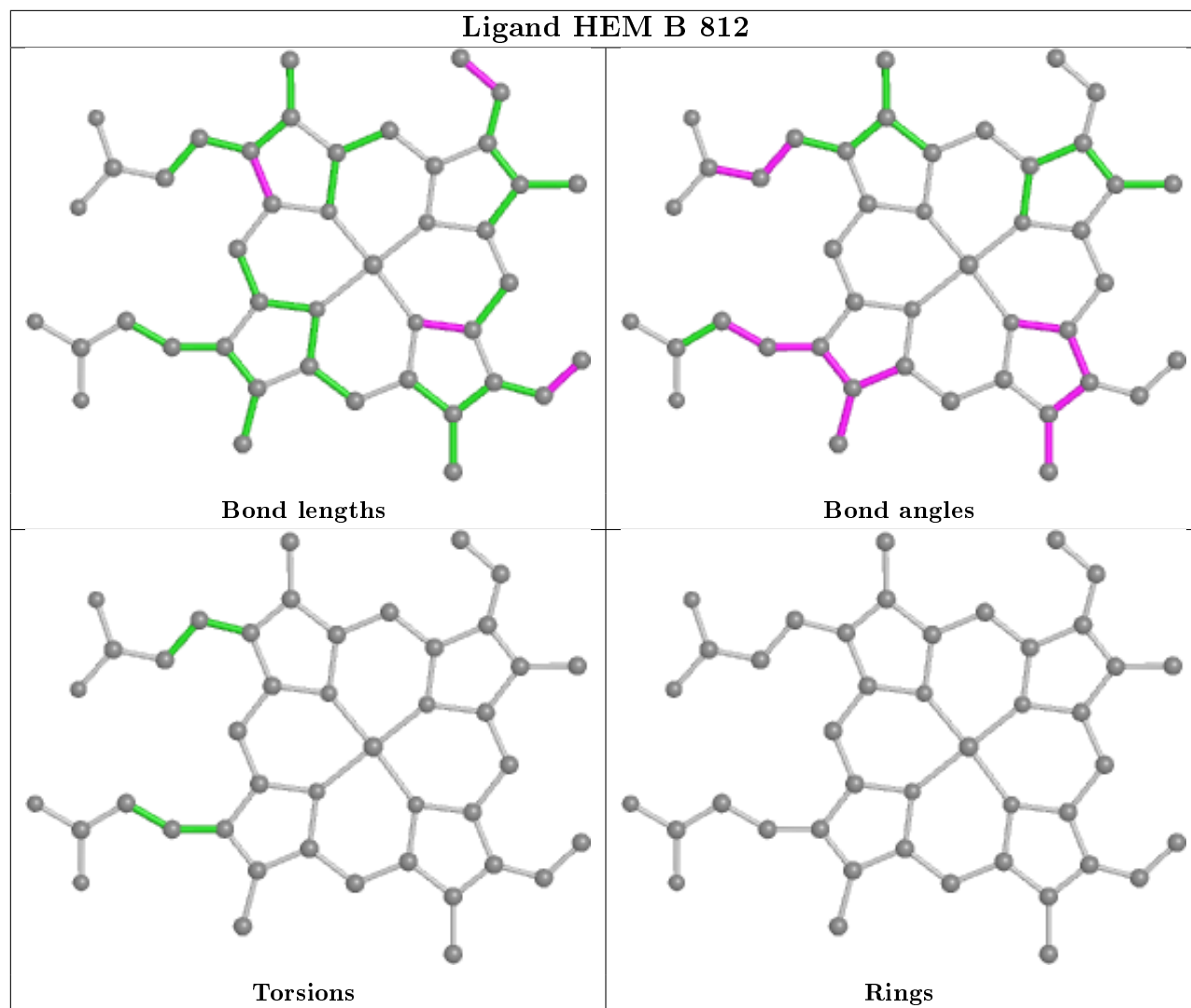


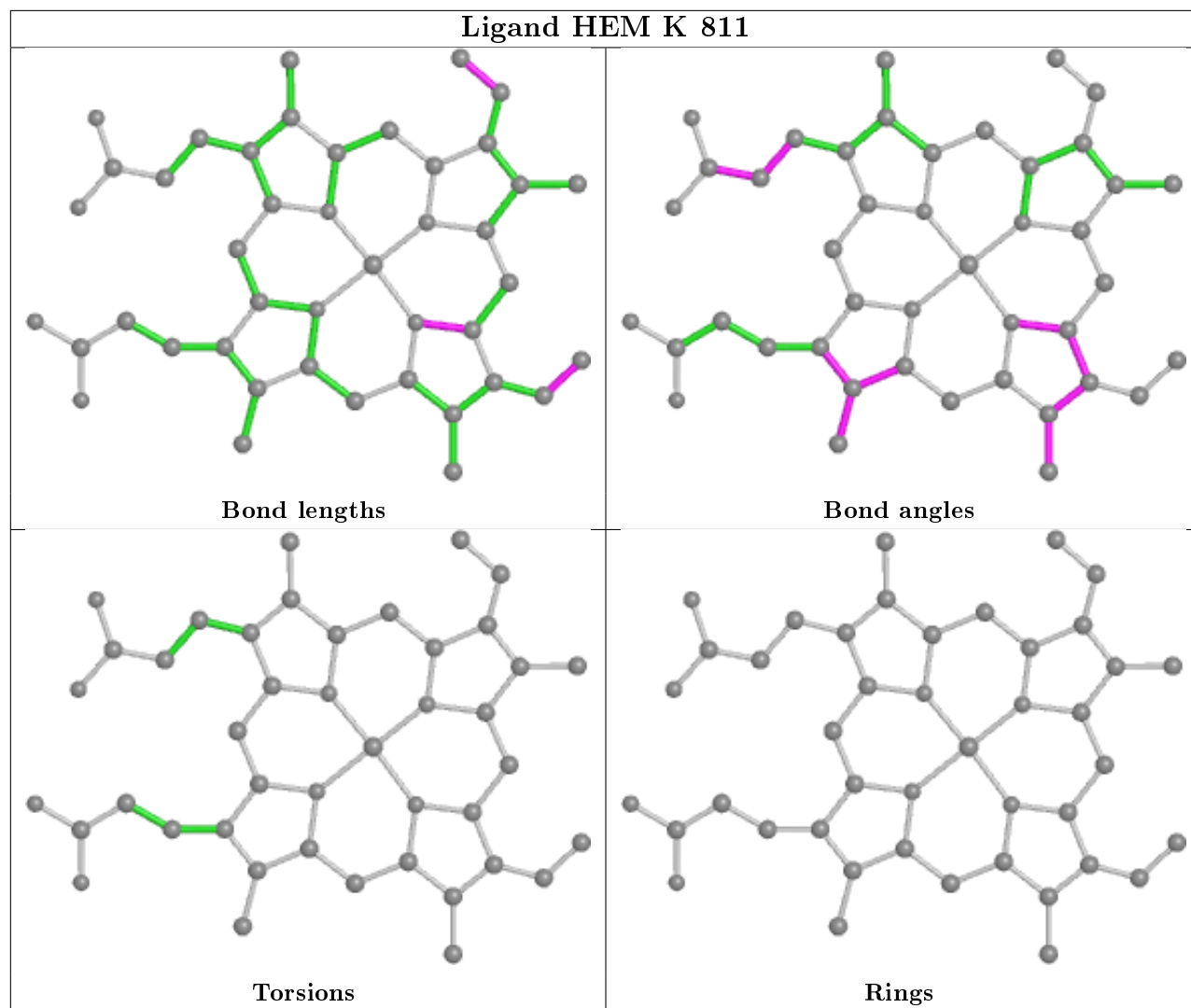


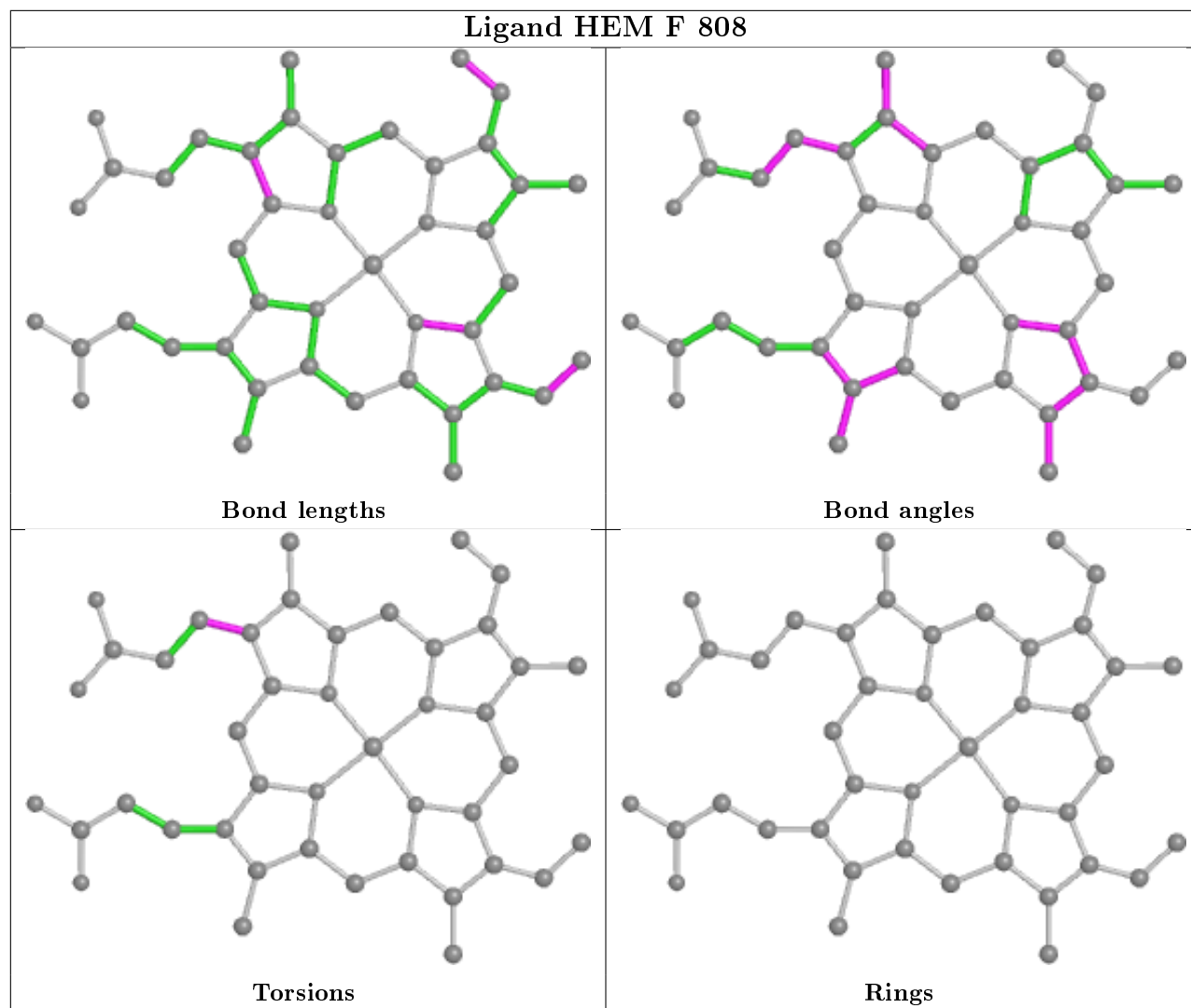


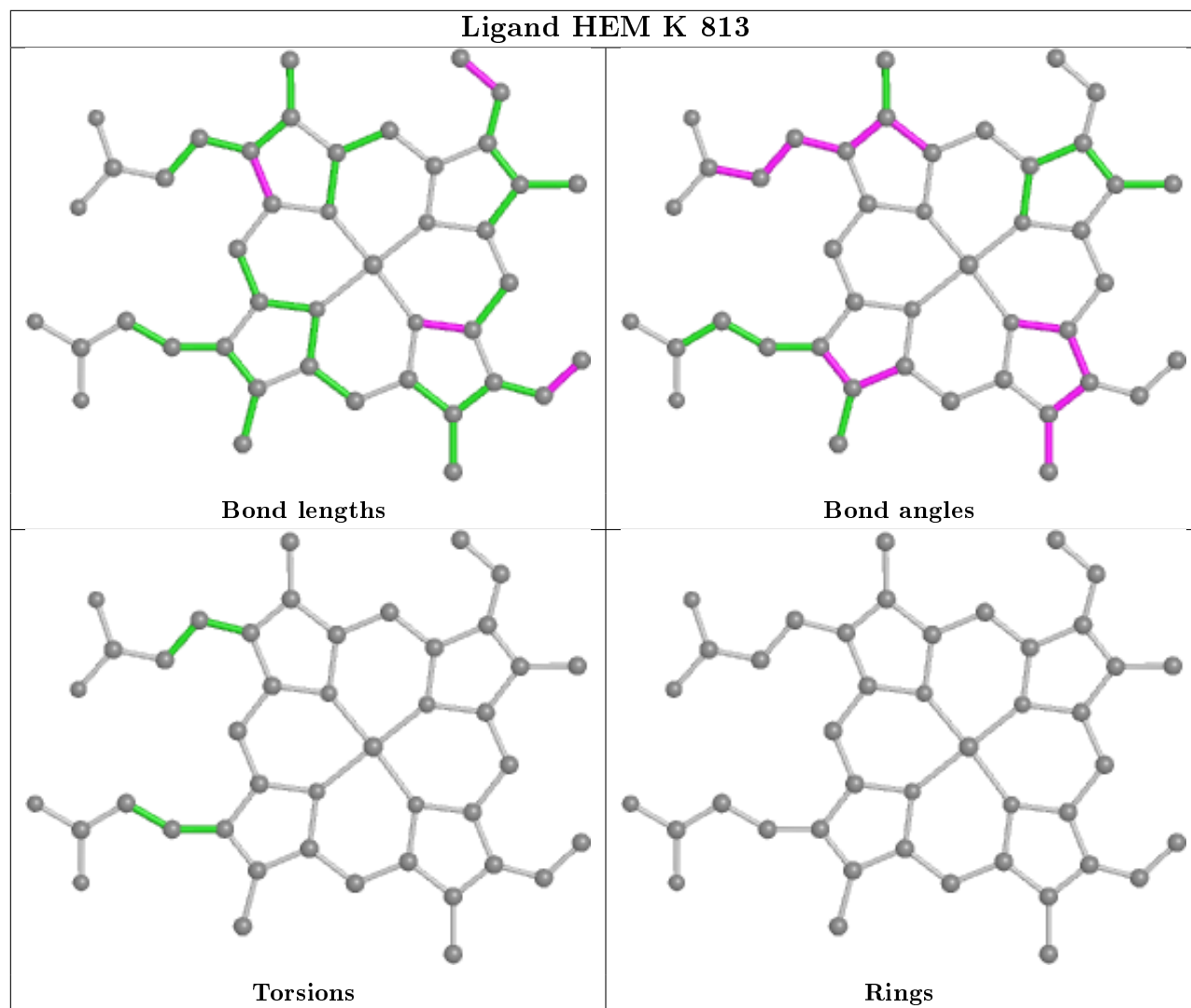


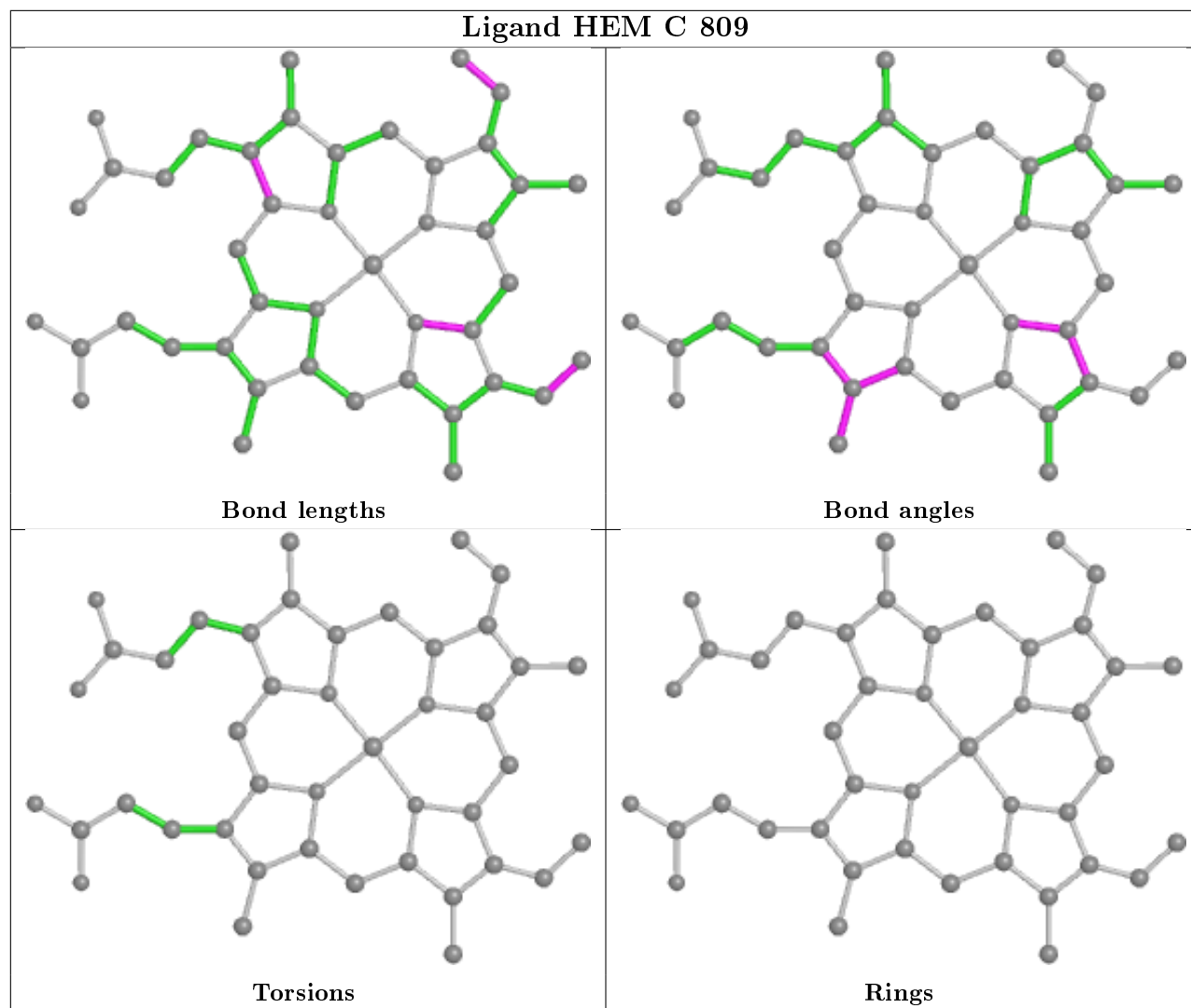


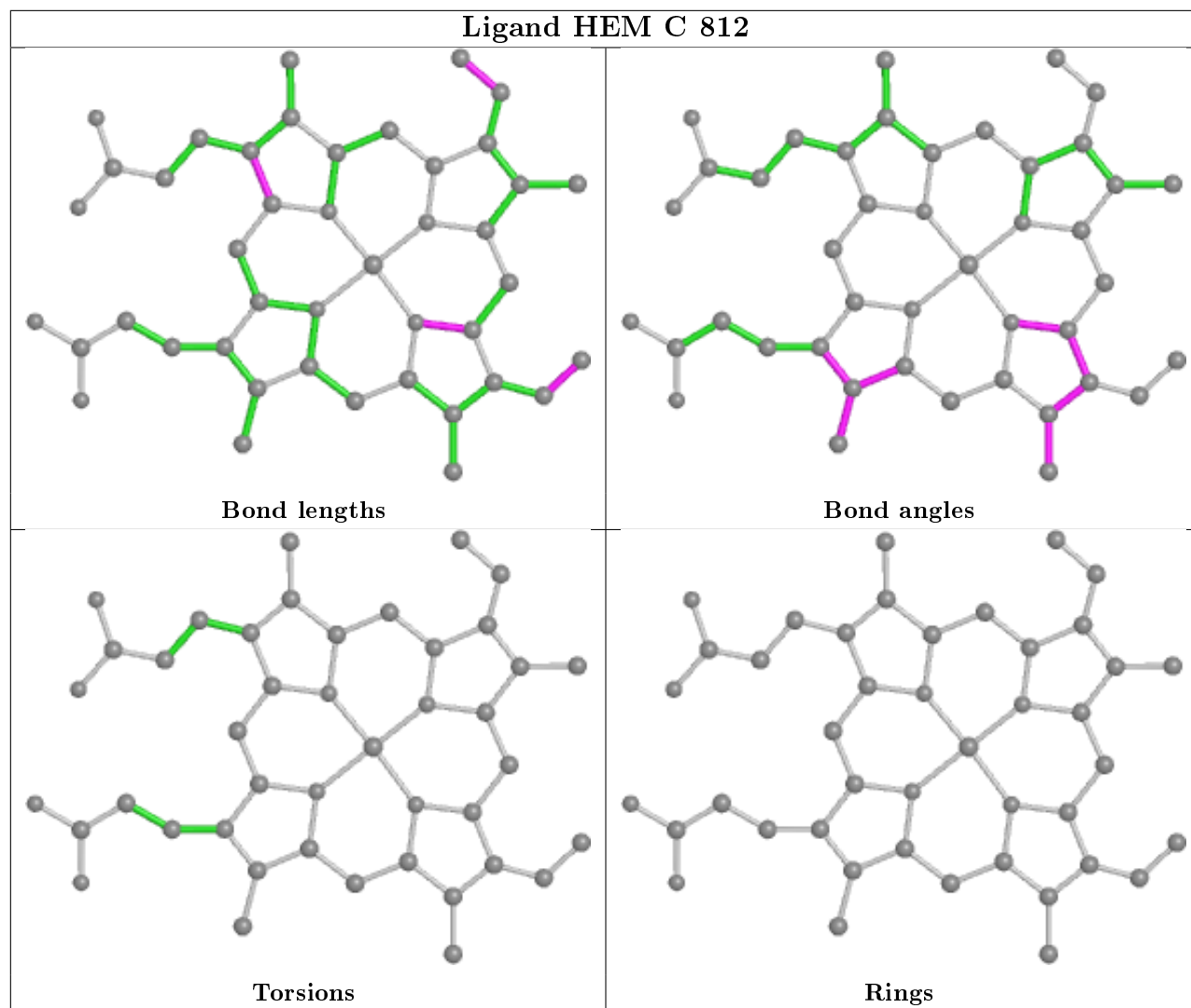


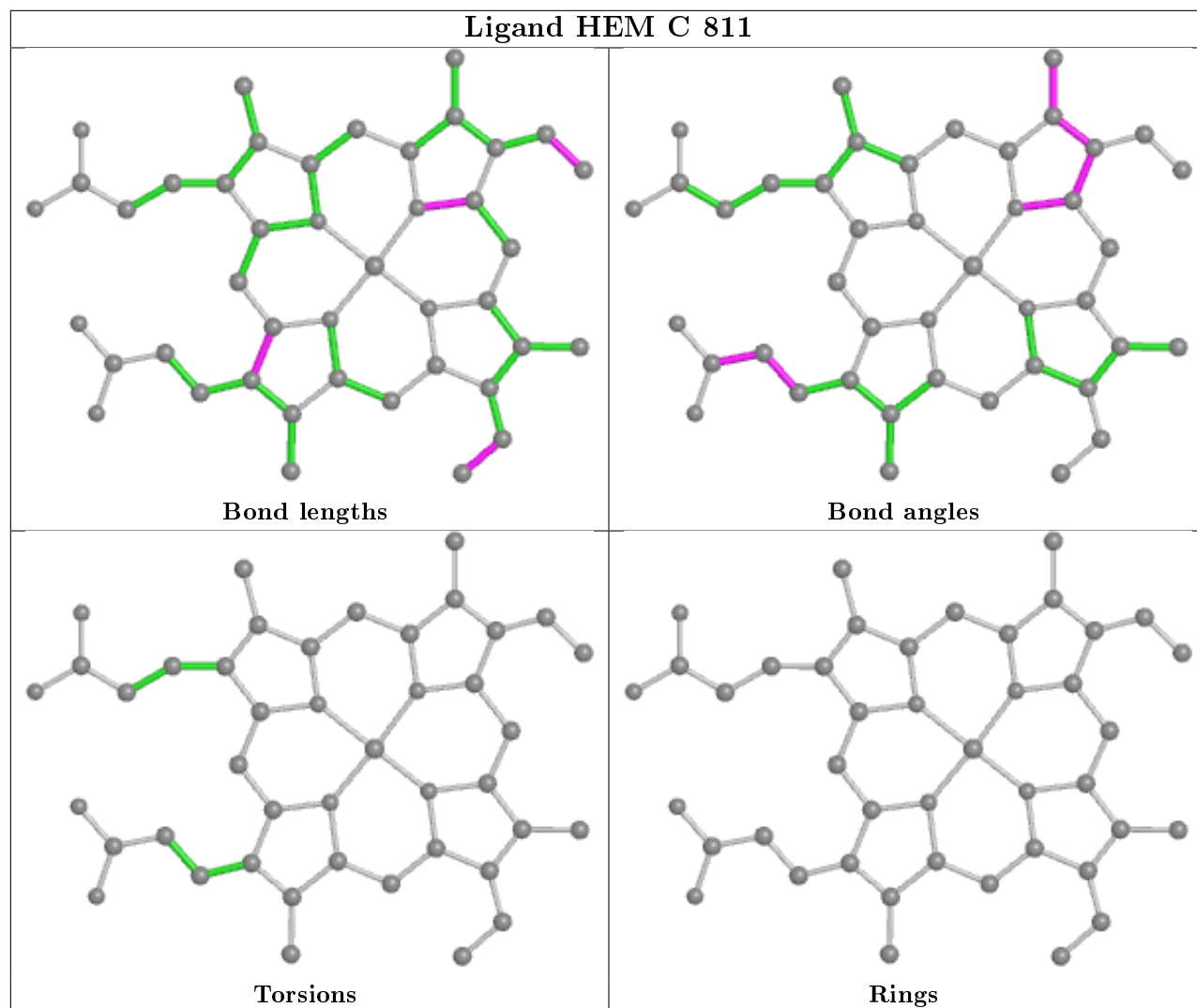


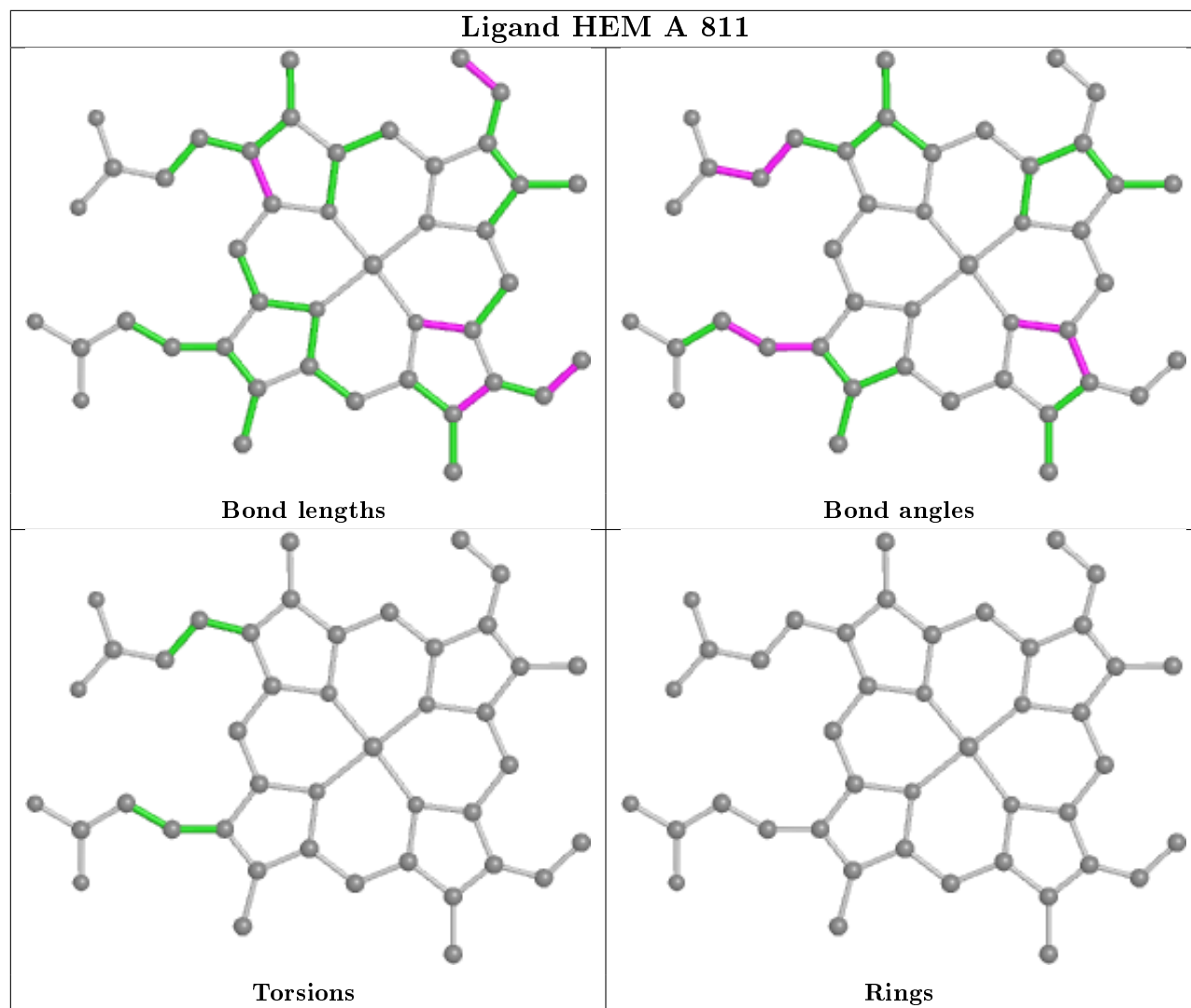


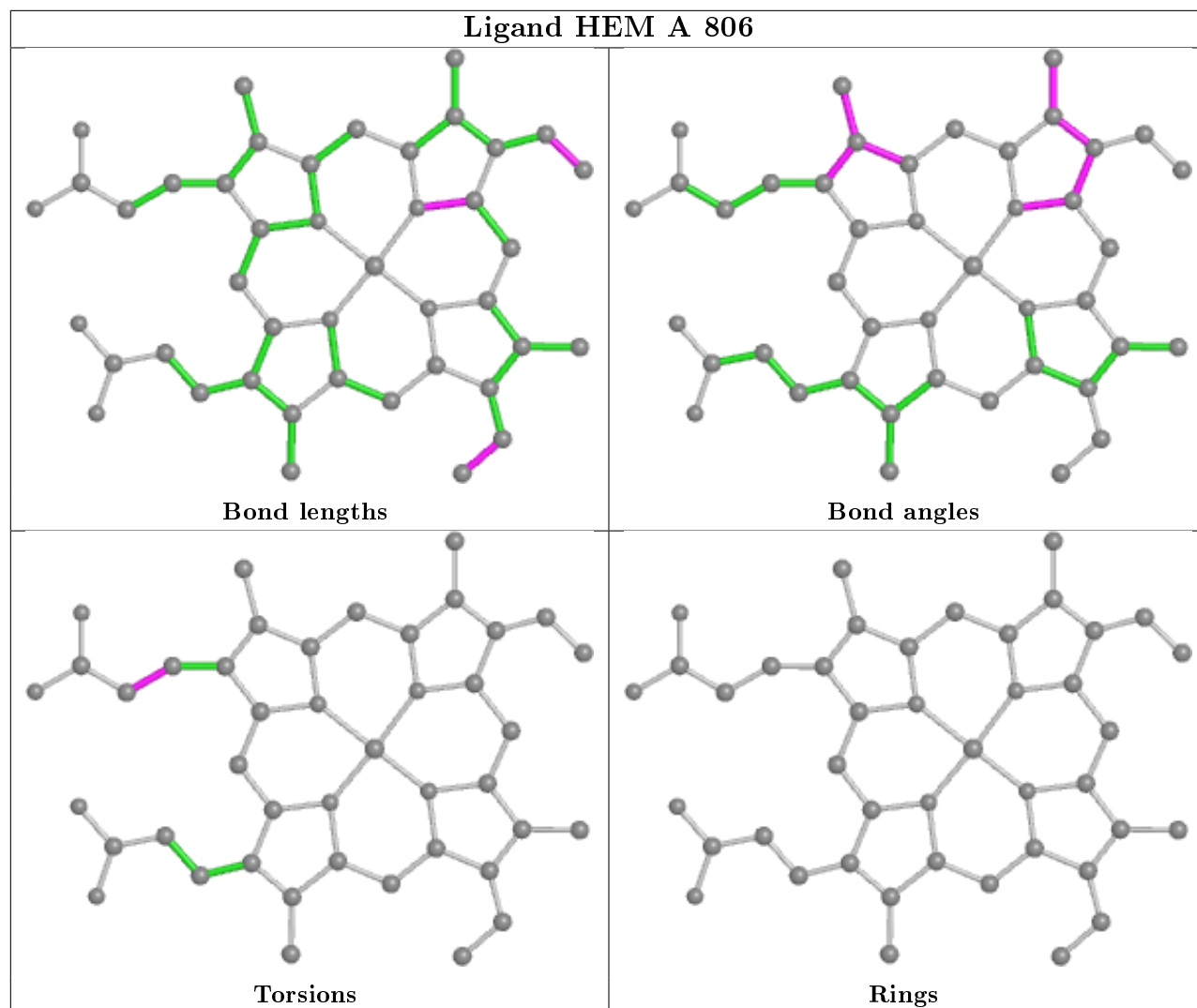


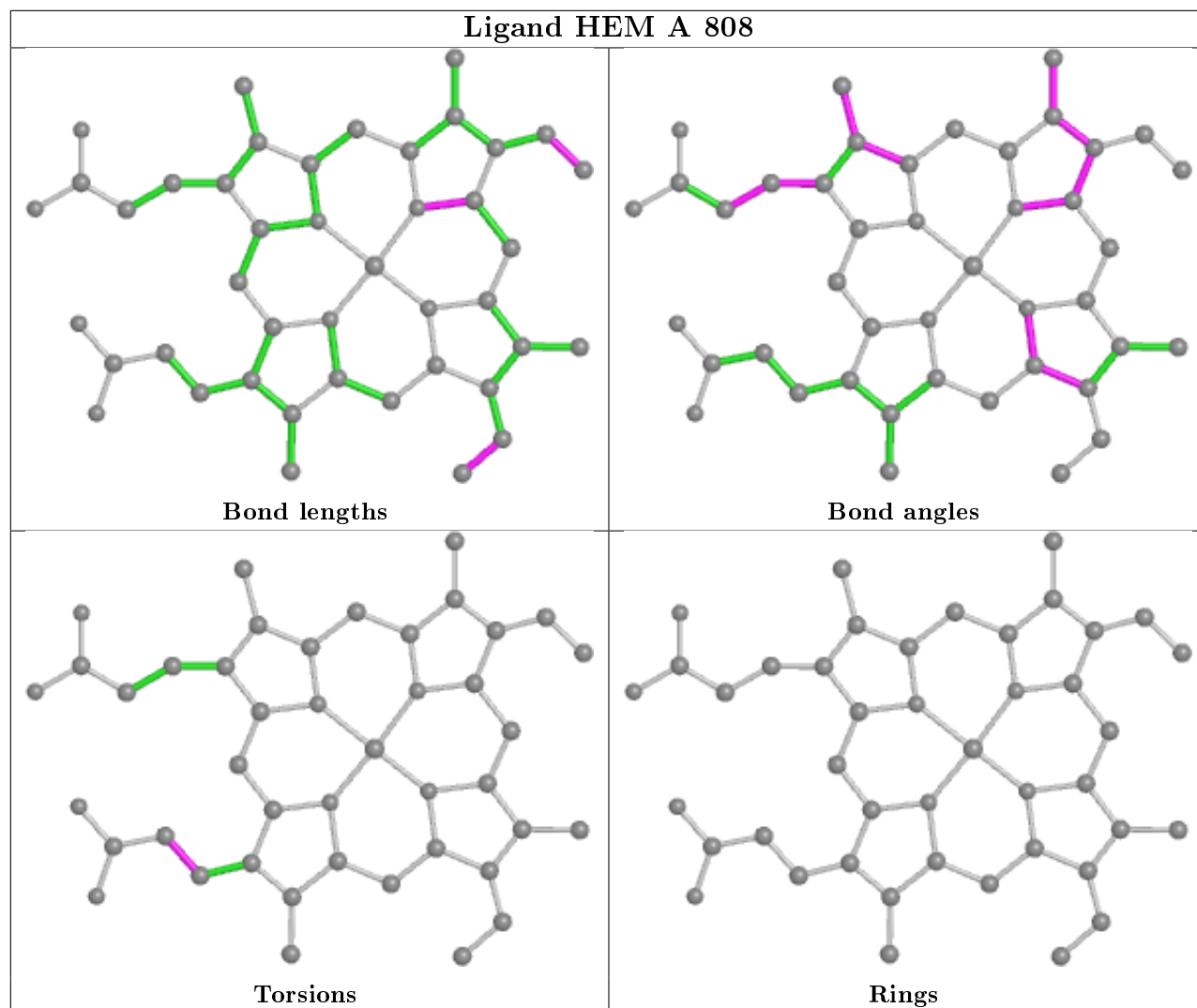


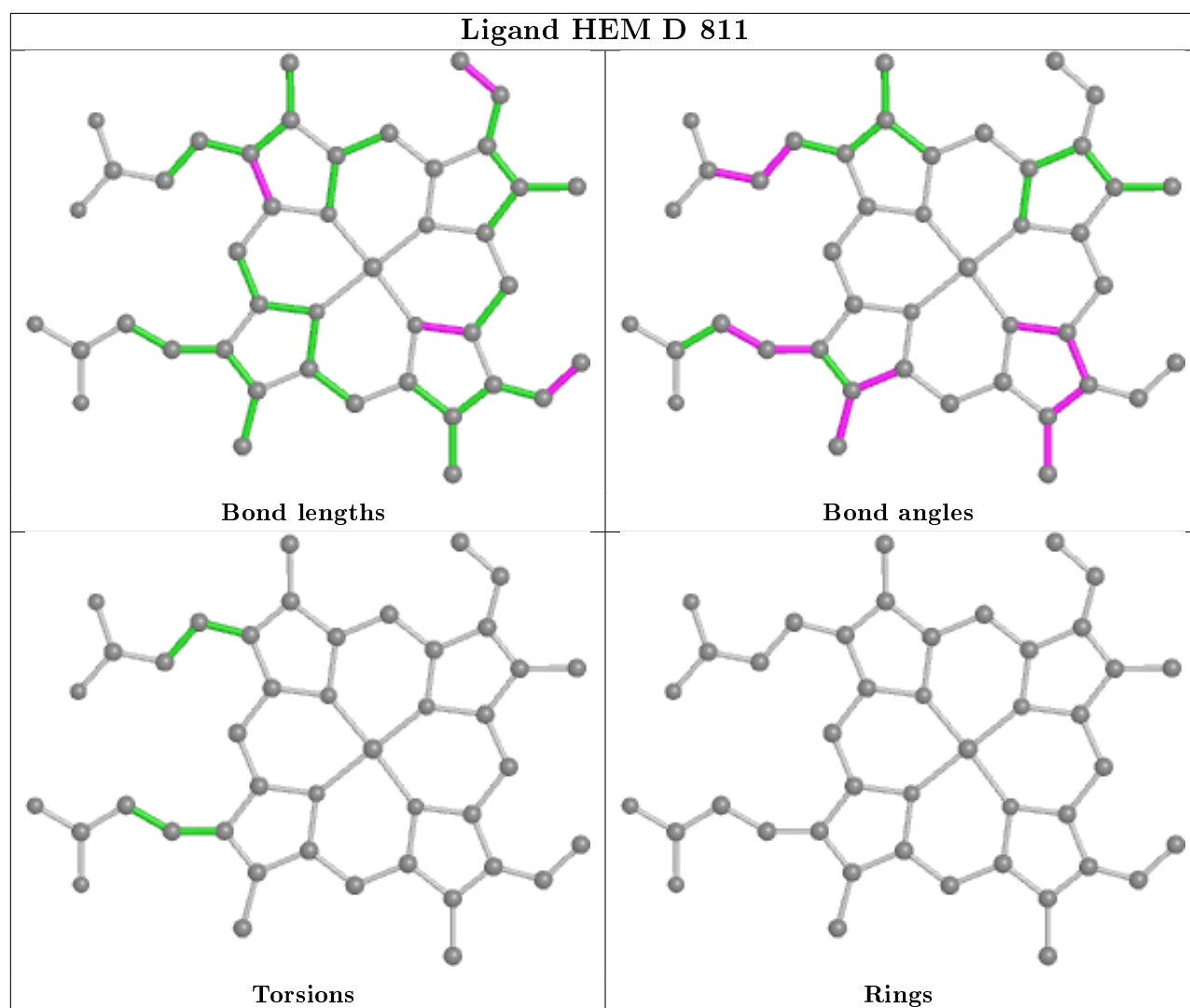












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	659/732 (90%)	-0.24	12 (1%) 68 66	16, 24, 45, 95	0
1	B	660/732 (90%)	-0.29	6 (0%) 84 83	20, 33, 49, 82	0
1	C	659/732 (90%)	-0.23	4 (0%) 89 88	18, 32, 54, 86	0
1	D	659/732 (90%)	-0.23	19 (2%) 51 49	21, 32, 56, 102	0
1	E	659/732 (90%)	-0.15	10 (1%) 73 72	23, 38, 59, 104	0
1	F	659/732 (90%)	-0.07	13 (1%) 65 63	21, 38, 63, 107	0
1	G	658/732 (89%)	-0.25	13 (1%) 65 63	25, 37, 57, 93	0
1	H	660/732 (90%)	-0.20	7 (1%) 80 79	25, 37, 61, 95	0
1	I	659/732 (90%)	0.02	18 (2%) 54 52	26, 39, 58, 76	0
1	J	659/732 (90%)	0.02	18 (2%) 54 52	27, 46, 69, 96	0
1	K	659/732 (90%)	-0.01	7 (1%) 80 79	25, 46, 68, 85	0
1	L	659/732 (90%)	0.39	40 (6%) 21 20	30, 51, 76, 89	0
All	All	7909/8784 (90%)	-0.10	167 (2%) 63 61	16, 37, 65, 107	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	629	VAL	7.4
1	F	629	VAL	7.3
1	A	629	VAL	6.5
1	G	379	LEU	5.2
1	H	629	VAL	5.2
1	F	628	GLU	4.8
1	H	628	GLU	4.8
1	G	629	VAL	4.6
1	L	81	GLY	4.6
1	H	631	LYS	4.4
1	D	628	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	624	TYR	4.2
1	L	231	GLY	4.2
1	G	625	SER	4.0
1	A	688	LYS	4.0
1	L	379	LEU	4.0
1	G	627	LEU	4.0
1	L	223	VAL	4.0
1	F	687	LYS	3.9
1	D	629	VAL	3.8
1	L	78	THR	3.8
1	A	624	TYR	3.8
1	D	634	PRO	3.8
1	L	537	ASP	3.8
1	E	634	PRO	3.7
1	J	689	SER	3.7
1	D	641	TYR	3.6
1	L	689	SER	3.6
1	B	435	LYS	3.6
1	E	629	VAL	3.6
1	D	621	GLN	3.5
1	L	82	GLY	3.4
1	L	277	GLY	3.4
1	H	690	LEU	3.4
1	F	631	LYS	3.4
1	J	688	LYS	3.4
1	A	625	SER	3.3
1	A	630	LYS	3.3
1	L	538	PRO	3.3
1	L	235	ILE	3.3
1	G	628	GLU	3.2
1	I	357	ILE	3.2
1	D	623	LEU	3.2
1	G	687	LYS	3.2
1	E	689	SER	3.2
1	J	627	LEU	3.1
1	G	624	TYR	3.1
1	K	689	SER	3.1
1	E	638	THR	3.1
1	L	227	LEU	3.0
1	K	589	THR	3.0
1	E	635	SER	3.0
1	H	630	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	689	SER	3.0
1	A	641	TYR	3.0
1	B	690	LEU	3.0
1	I	35	LYS	3.0
1	E	633	ALA	3.0
1	D	625	SER	2.9
1	L	228	LEU	2.9
1	L	230	ASN	2.9
1	H	626	LEU	2.9
1	I	379	LEU	2.9
1	F	688	LYS	2.9
1	D	632	LEU	2.8
1	I	39	GLU	2.8
1	L	196	ASP	2.8
1	B	476	ALA	2.8
1	C	438	LYS	2.8
1	L	236	VAL	2.8
1	L	226	GLY	2.8
1	A	438	LYS	2.8
1	I	360	CYS	2.8
1	L	84	THR	2.7
1	L	264	ASP	2.7
1	I	378	PRO	2.7
1	J	628	GLU	2.7
1	L	476	ALA	2.7
1	D	687	LYS	2.7
1	D	688	LYS	2.7
1	L	215	TRP	2.7
1	L	83	LYS	2.6
1	G	618	VAL	2.6
1	D	438	LYS	2.6
1	K	183	LYS	2.6
1	D	622	GLY	2.6
1	D	626	LEU	2.6
1	B	536	LYS	2.6
1	L	76	ILE	2.6
1	F	622	GLY	2.5
1	A	628	GLU	2.5
1	L	43	HIS	2.5
1	I	363	CYS	2.5
1	F	634	PRO	2.5
1	G	621	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	225	GLY	2.5
1	F	632	LEU	2.5
1	K	379	LEU	2.5
1	D	631	LYS	2.5
1	C	629	VAL	2.5
1	I	375	ARG	2.5
1	J	184	ASP	2.5
1	A	687	LYS	2.4
1	L	232	THR	2.4
1	L	330	LYS	2.4
1	F	226	GLY	2.4
1	L	224	GLU	2.4
1	G	631	LYS	2.4
1	D	630	LYS	2.4
1	F	438	LYS	2.4
1	L	360	CYS	2.4
1	A	686	MET	2.4
1	J	31	MET	2.4
1	L	375	ARG	2.3
1	J	43	HIS	2.3
1	C	379	LEU	2.3
1	L	116	GLU	2.3
1	J	588	GLU	2.3
1	F	183	LYS	2.3
1	I	87	LYS	2.3
1	I	438	LYS	2.3
1	L	265	PHE	2.3
1	E	43	HIS	2.3
1	B	438	LYS	2.3
1	B	689	SER	2.3
1	I	337	VAL	2.2
1	I	427	VAL	2.2
1	L	77	PHE	2.2
1	G	49	GLU	2.2
1	I	534	THR	2.2
1	I	43	HIS	2.2
1	J	618	VAL	2.2
1	A	689	SER	2.2
1	D	686	MET	2.2
1	C	689	SER	2.2
1	I	476	ALA	2.2
1	E	631	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	358	SER	2.2
1	K	533	SER	2.2
1	L	88	LEU	2.2
1	D	636	ASP	2.2
1	J	223	VAL	2.1
1	L	533	SER	2.1
1	J	225	GLY	2.1
1	J	631	LYS	2.1
1	L	270	GLU	2.1
1	E	632	LEU	2.1
1	J	687	LYS	2.1
1	L	182	ASP	2.1
1	K	440	VAL	2.1
1	J	272	TYR	2.1
1	J	624	TYR	2.1
1	J	611	ASP	2.1
1	I	359	ASN	2.1
1	E	536	LYS	2.1
1	K	588	GLU	2.0
1	F	72	LYS	2.0
1	H	686	MET	2.0
1	J	259	LYS	2.0
1	L	253	GLU	2.0
1	G	684	ARG	2.0
1	G	686	MET	2.0
1	A	684	ARG	2.0
1	L	269	LEU	2.0
1	L	588	GLU	2.0
1	L	192	GLY	2.0
1	I	68	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BU3	K	803	6/6	0.72	0.33	56,58,59,60	0
5	ACT	K	805	4/4	0.76	0.21	58,58,58,59	0
4	BU3	K	804	6/6	0.77	0.31	74,77,78,79	0
5	ACT	H	806	4/4	0.80	0.28	59,63,64,64	0
5	ACT	D	805	4/4	0.80	0.28	59,62,62,63	0
5	ACT	B	806	4/4	0.81	0.29	46,47,48,49	0
5	ACT	A	805	4/4	0.81	0.28	47,50,50,51	0
4	BU3	C	804	6/6	0.82	0.24	48,49,49,50	0
5	ACT	E	805	4/4	0.84	0.23	58,60,61,61	0
4	BU3	H	805	6/6	0.84	0.25	49,50,51,53	0
7	SO2	I	802	3/3	0.85	0.18	63,63,64,71	0
4	BU3	F	805	6/6	0.85	0.30	58,60,61,62	0
5	ACT	J	805	4/4	0.85	0.26	62,62,62,63	0
4	BU3	D	803	6/6	0.86	0.28	50,54,54,55	0
4	BU3	F	803	6/6	0.86	0.26	49,50,50,50	0
4	BU3	E	804	6/6	0.86	0.30	77,79,79,79	0
4	BU3	J	804	6/6	0.86	0.21	64,65,66,66	0
5	ACT	L	805	4/4	0.86	0.34	61,63,63,64	0
4	BU3	L	803	6/6	0.86	0.33	57,58,58,60	0
4	BU3	I	804	6/6	0.87	0.29	60,61,62,62	0
4	BU3	A	804	6/6	0.87	0.20	40,41,42,43	0
5	ACT	C	805	4/4	0.87	0.25	58,59,61,61	0
4	BU3	C	803	6/6	0.87	0.33	52,53,54,55	0
4	BU3	J	803	6/6	0.87	0.33	55,57,58,58	0
4	BU3	H	803	6/6	0.87	0.29	62,63,64,65	0
4	BU3	B	803	6/6	0.88	0.29	50,51,52,52	0
3	SX	B	802	2/2	0.88	0.18	51,51,51,52	0
4	BU3	A	803	6/6	0.89	0.34	47,47,48,48	0
4	BU3	B	805	6/6	0.89	0.26	55,59,59,60	0
3	SX	E	802	2/2	0.89	0.16	66,66,66,68	0
4	BU3	L	804	6/6	0.89	0.18	69,70,70,72	0
5	ACT	G	805	4/4	0.89	0.20	51,51,52,52	0
3	SX	C	802	2/2	0.90	0.16	55,55,55,56	0
3	SX	H	802	2/2	0.90	0.14	58,58,58,61	0
4	BU3	H	804	6/6	0.90	0.18	61,62,62,64	0
4	BU3	B	804	6/6	0.90	0.22	50,52,53,53	0
4	BU3	I	803	6/6	0.90	0.44	48,50,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	BU3	G	803	6/6	0.91	0.29	49,50,51,52	0
5	ACT	F	806	4/4	0.92	0.19	54,56,56,56	0
4	BU3	E	803	6/6	0.92	0.29	50,51,54,55	0
4	BU3	F	804	6/6	0.93	0.15	62,63,64,65	0
3	SX	A	802	2/2	0.94	0.10	45,45,45,50	2
4	BU3	G	804	6/6	0.94	0.18	58,59,61,61	0
6	HEM	L	813	43/43	0.94	0.17	46,48,58,65	0
2	CU1	J	801	1/1	0.94	0.08	51,51,51,51	0
4	BU3	D	804	6/6	0.94	0.13	45,46,47,47	0
2	CU1	L	801	1/1	0.94	0.06	55,55,55,55	0
5	ACT	I	805	4/4	0.94	0.24	50,50,52,52	0
3	SX	K	802	2/2	0.94	0.13	67,67,67,71	0
6	HEM	I	813	43/43	0.95	0.14	33,35,46,49	0
3	SX	F	802	2/2	0.95	0.16	69,69,69,73	0
6	HEM	K	813	43/43	0.95	0.13	39,41,52,55	0
6	HEM	I	810	43/43	0.96	0.15	24,26,30,35	0
6	HEM	J	807	43/43	0.96	0.12	34,36,38,39	0
6	HEM	H	812	43/43	0.96	0.12	23,26,35,43	0
6	HEM	C	813	43/43	0.96	0.14	30,32,45,50	0
6	HEM	I	811	43/43	0.96	0.13	25,26,35,43	0
6	HEM	F	812	43/43	0.96	0.12	21,23,32,42	0
6	HEM	J	811	43/43	0.96	0.12	29,31,41,51	0
6	HEM	L	812	43/43	0.96	0.14	37,39,41,42	0
3	SX	J	802	2/2	0.96	0.10	57,57,57,62	0
6	HEM	L	810	43/43	0.96	0.17	31,32,39,43	0
6	HEM	G	813	43/43	0.96	0.11	28,31,38,45	0
2	CU1	E	801	1/1	0.96	0.08	37,37,37,37	0
7	SO2	A	814	3/3	0.96	0.12	16,16,16,16	3
6	HEM	E	813	43/43	0.96	0.14	30,32,44,55	0
6	HEM	L	811	43/43	0.96	0.12	34,37,45,49	0
6	HEM	B	814	43/43	0.96	0.15	29,31,43,46	0
6	HEM	K	812	43/43	0.96	0.11	31,34,36,37	0
6	HEM	I	809	43/43	0.96	0.21	26,27,30,32	0
6	HEM	L	809	43/43	0.97	0.20	32,34,38,40	0
6	HEM	F	813	43/43	0.97	0.10	21,23,24,26	0
6	HEM	E	812	43/43	0.97	0.11	26,28,31,32	0
6	HEM	G	806	43/43	0.97	0.12	27,28,29,29	0
2	CU1	D	801	1/1	0.97	0.10	33,33,33,33	0
6	HEM	B	807	43/43	0.97	0.14	21,22,23,24	0
6	HEM	E	811	43/43	0.97	0.11	27,29,36,43	0
6	HEM	D	810	43/43	0.97	0.12	21,22,25,28	0
6	HEM	I	807	43/43	0.97	0.15	29,32,33,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	HEM	D	806	43/43	0.97	0.12	28,30,32,33	0
2	CU1	H	801	1/1	0.97	0.17	45,45,45,45	0
6	HEM	L	806	43/43	0.97	0.14	24,30,33,34	0
6	HEM	H	813	43/43	0.97	0.11	26,27,28,29	0
6	HEM	H	807	43/43	0.97	0.18	32,33,35,36	0
6	HEM	H	809	43/43	0.97	0.16	29,31,34,39	0
6	HEM	A	810	43/43	0.97	0.14	16,17,21,24	0
6	HEM	E	810	43/43	0.97	0.14	24,25,29,34	0
6	HEM	B	811	43/43	0.97	0.15	21,22,28,34	0
6	HEM	I	806	43/43	0.97	0.16	27,30,32,32	0
6	HEM	D	813	43/43	0.97	0.12	25,26,34,36	0
6	HEM	L	807	43/43	0.97	0.20	37,39,42,44	0
6	HEM	G	811	43/43	0.97	0.12	28,31,43,49	0
6	HEM	F	809	43/43	0.97	0.19	28,29,30,31	0
6	HEM	F	807	43/43	0.97	0.20	25,29,32,33	0
6	HEM	G	810	43/43	0.97	0.12	24,24,29,31	0
2	CU1	C	801	1/1	0.97	0.07	31,31,31,31	0
6	HEM	A	807	43/43	0.97	0.14	16,16,17,17	0
6	HEM	A	812	43/43	0.97	0.13	18,19,22,25	0
7	SO2	D	802	3/3	0.97	0.09	51,51,53,54	0
6	HEM	C	810	43/43	0.97	0.14	20,21,24,28	0
6	HEM	A	813	43/43	0.97	0.13	21,23,31,34	0
6	HEM	K	810	43/43	0.97	0.12	27,29,33,37	0
6	HEM	B	813	43/43	0.97	0.12	24,26,29,30	0
6	HEM	G	808	43/43	0.97	0.13	25,26,28,30	0
6	HEM	K	808	43/43	0.97	0.14	27,27,29,31	0
6	HEM	G	809	43/43	0.97	0.14	24,27,28,28	0
6	HEM	H	811	43/43	0.97	0.13	25,27,30,33	0
6	HEM	I	808	43/43	0.97	0.21	27,28,30,30	0
6	HEM	G	812	43/43	0.97	0.10	26,28,32,33	0
6	HEM	L	808	43/43	0.97	0.16	31,33,35,38	0
6	HEM	K	807	43/43	0.97	0.14	38,41,45,49	0
6	HEM	E	809	43/43	0.97	0.17	24,25,26,26	0
7	SO2	G	814	3/3	0.97	0.15	74,74,74,76	3
6	HEM	K	809	43/43	0.97	0.13	28,31,34,35	0
6	HEM	F	814	43/43	0.97	0.13	24,26,34,39	0
6	HEM	K	806	43/43	0.97	0.18	26,28,31,32	0
6	HEM	J	813	43/43	0.97	0.14	37,40,53,62	0
6	HEM	J	810	43/43	0.97	0.13	26,28,33,37	0
6	HEM	H	810	43/43	0.97	0.12	28,30,31,32	0
6	HEM	D	808	43/43	0.97	0.12	25,27,31,35	0
6	HEM	E	807	43/43	0.97	0.17	28,29,31,33	0

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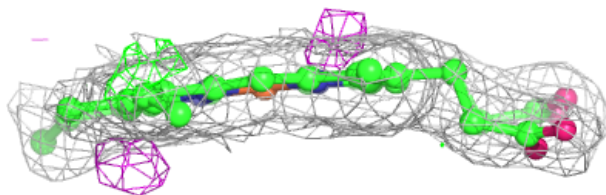
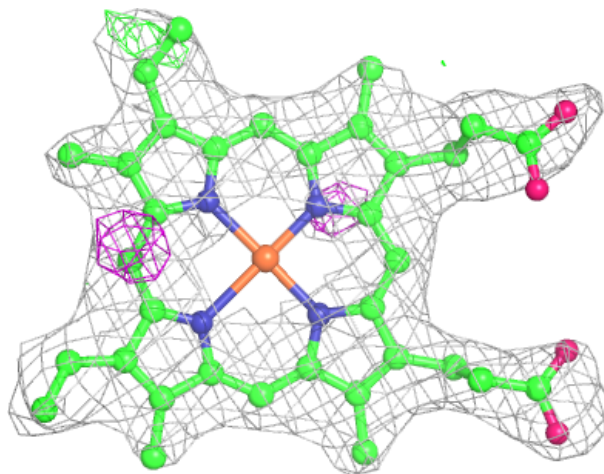
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	HEM	J	812	43/43	0.97	0.10	34,36,37,39	0
6	HEM	H	808	43/43	0.97	0.11	24,29,31,33	0
6	HEM	B	812	43/43	0.97	0.14	23,24,33,43	0
6	HEM	H	814	43/43	0.97	0.12	25,26,36,40	0
6	HEM	J	806	43/43	0.97	0.14	28,30,32,34	0
6	HEM	K	811	43/43	0.97	0.12	27,30,39,47	0
6	HEM	F	808	43/43	0.97	0.13	25,28,32,35	0
6	HEM	E	808	43/43	0.97	0.18	23,24,25,27	0
6	HEM	J	808	43/43	0.97	0.13	27,28,29,30	0
6	HEM	D	807	43/43	0.97	0.11	21,22,24,25	0
6	HEM	C	812	43/43	0.97	0.11	23,25,28,31	0
6	HEM	C	811	43/43	0.97	0.12	24,26,36,46	0
6	HEM	A	811	43/43	0.97	0.14	19,20,28,33	0
6	HEM	I	812	43/43	0.97	0.11	27,28,31,33	0
6	HEM	A	806	43/43	0.97	0.14	19,20,21,21	0
6	HEM	D	811	43/43	0.97	0.13	21,23,33,42	0
6	HEM	D	812	43/43	0.98	0.12	20,22,24,27	0
6	HEM	F	810	43/43	0.98	0.15	25,27,27,27	0
6	HEM	E	806	43/43	0.98	0.16	23,24,26,26	0
6	HEM	C	807	43/43	0.98	0.17	21,23,23,24	0
6	HEM	G	807	43/43	0.98	0.11	25,26,28,29	0
2	CU1	F	801	1/1	0.98	0.12	38,38,38,38	0
3	SX	L	802	2/2	0.98	0.15	65,65,65,68	0
6	HEM	A	809	43/43	0.98	0.16	14,15,17,19	0
6	HEM	B	810	43/43	0.98	0.15	20,23,25,27	0
6	HEM	B	809	43/43	0.98	0.16	20,22,23,27	0
6	HEM	C	808	43/43	0.98	0.16	18,19,21,23	0
2	CU1	K	801	1/1	0.98	0.14	53,53,53,53	0
6	HEM	C	806	43/43	0.98	0.15	16,17,18,19	0
6	HEM	J	809	43/43	0.98	0.13	29,31,33,35	0
6	HEM	C	809	43/43	0.98	0.16	18,20,21,21	0
3	SX	G	802	2/2	0.98	0.13	31,31,31,32	2
6	HEM	B	808	43/43	0.98	0.14	24,25,26,28	0
2	CU1	B	801	1/1	0.98	0.08	35,35,35,35	0
2	CU1	G	801	1/1	0.98	0.12	34,34,34,34	0
6	HEM	F	811	43/43	0.98	0.14	21,22,26,31	0
6	HEM	A	808	43/43	0.98	0.16	17,18,20,23	0
6	HEM	D	809	43/43	0.98	0.12	21,22,23,25	0
2	CU1	A	801	1/1	0.99	0.08	26,26,26,26	0
2	CU1	I	801	1/1	0.99	0.10	39,39,39,39	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

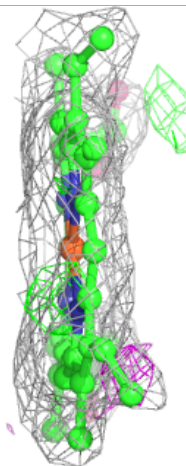
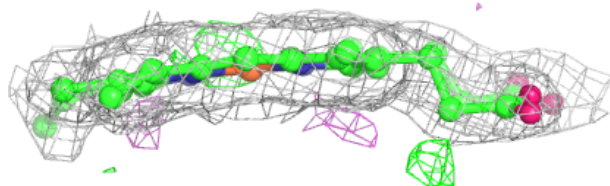
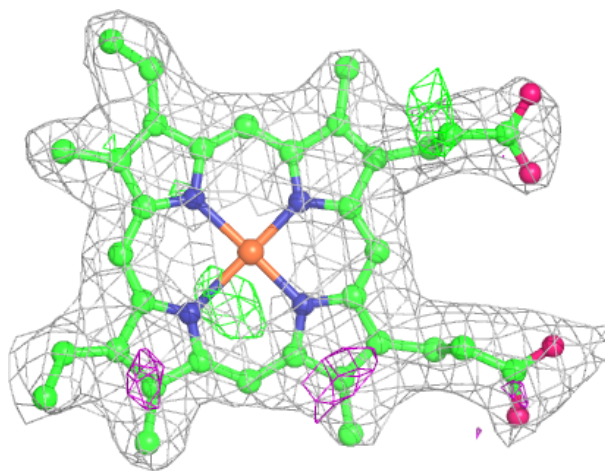
Electron density around HEM L 813:

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



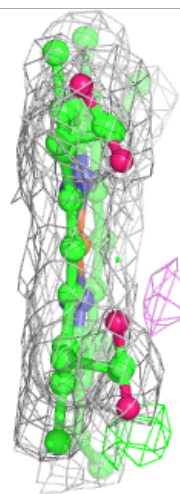
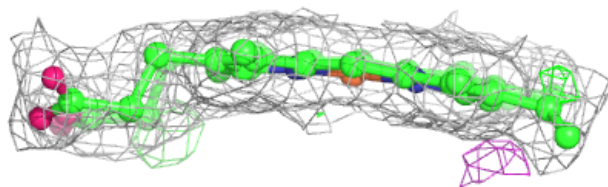
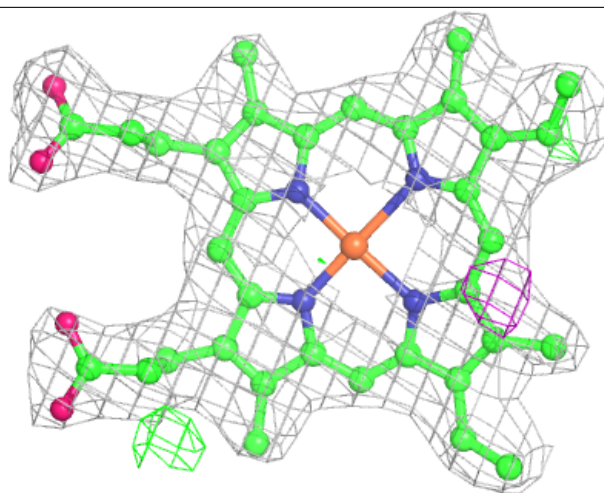
Electron density around HEM I 813:

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



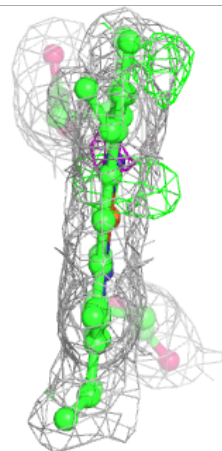
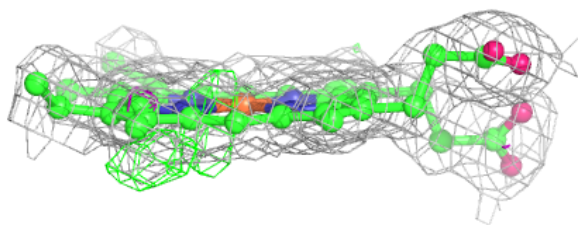
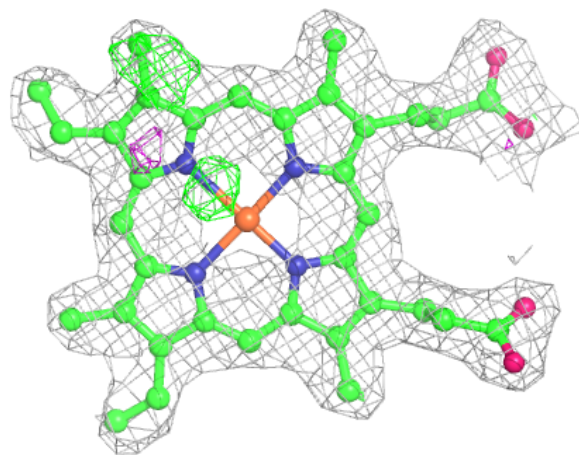
Electron density around HEM K 813:

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



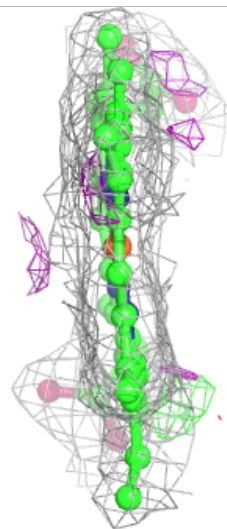
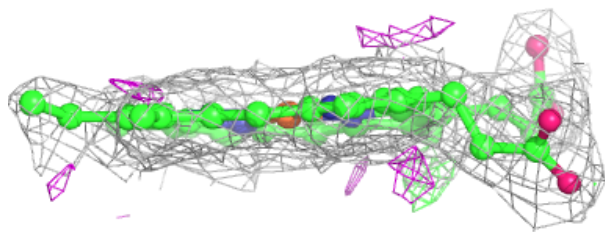
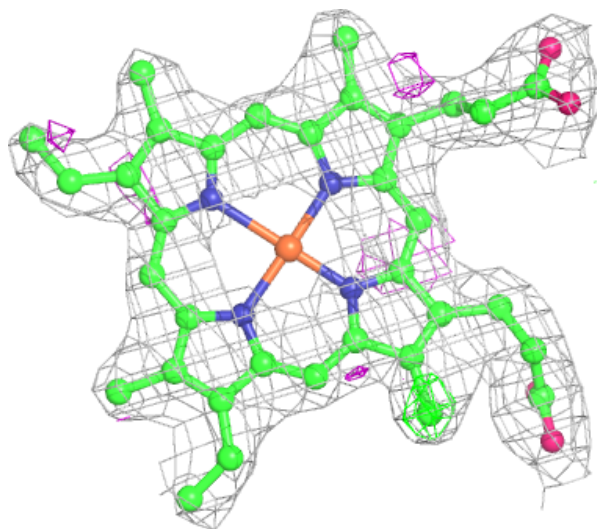
Electron density around HEM I 810:

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



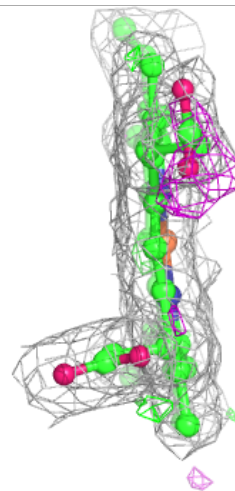
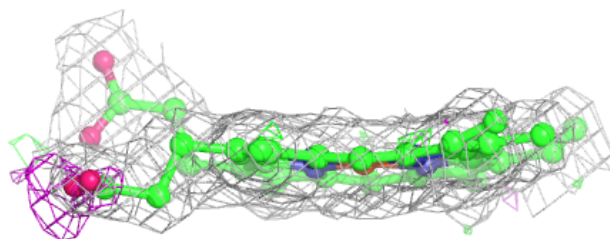
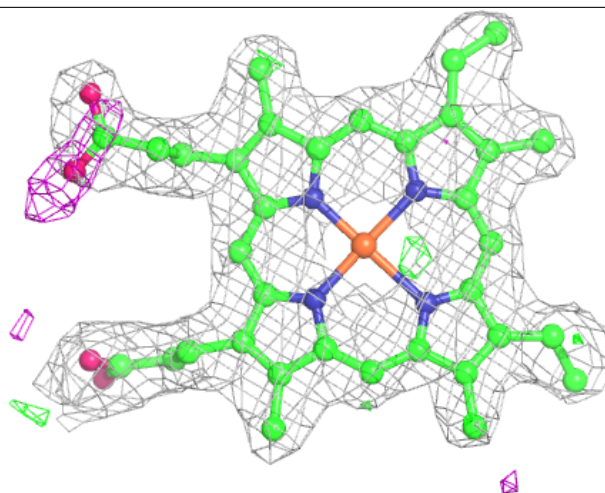
Electron density around HEM J 807:

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



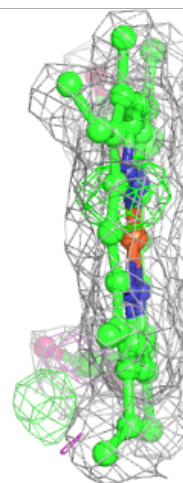
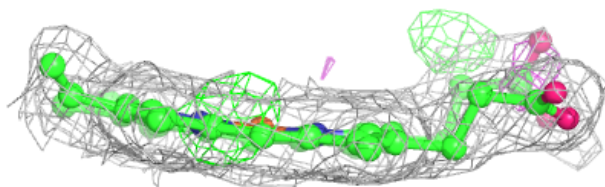
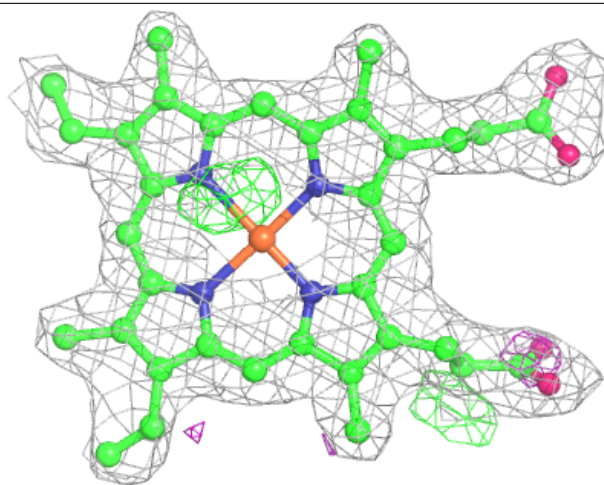
Electron density around HEM H 812:

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



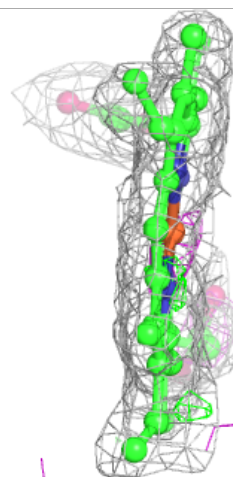
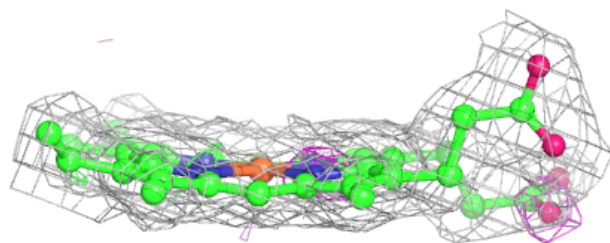
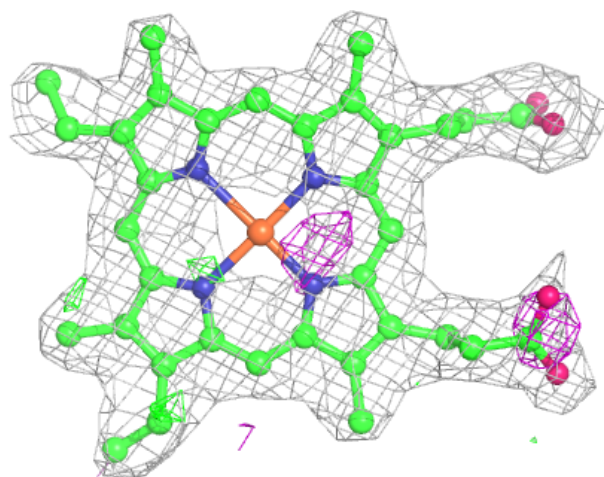
Electron density around HEM C 813:

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



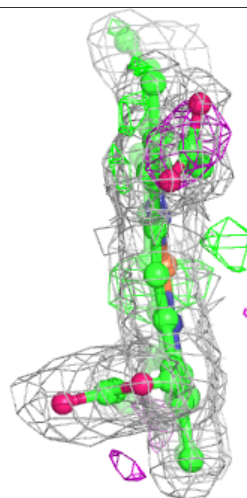
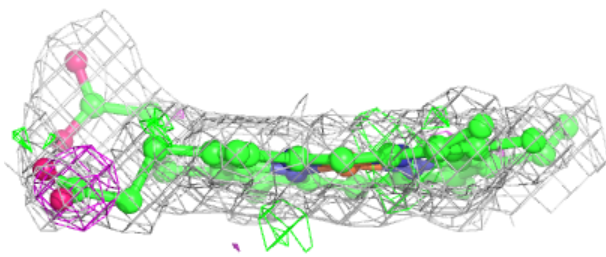
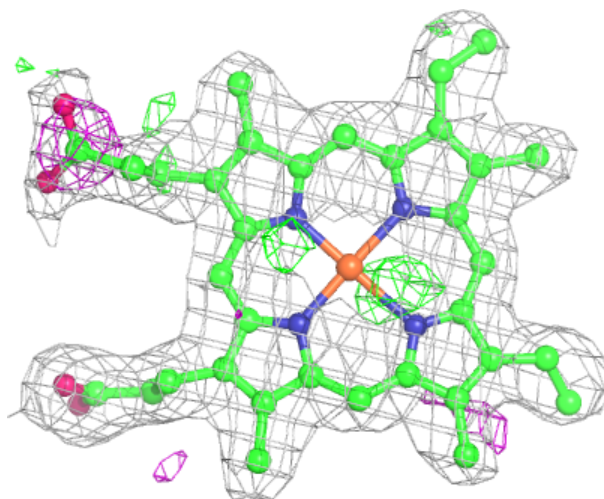
Electron density around HEM I 811:

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



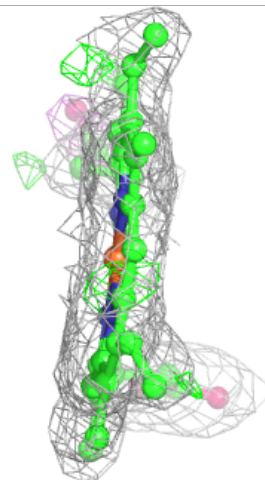
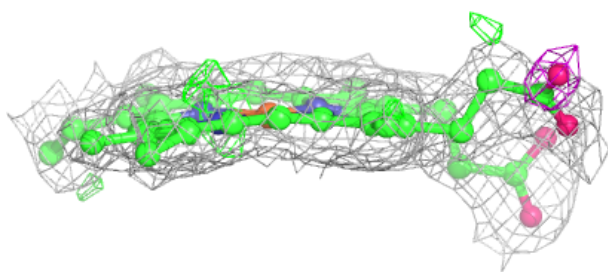
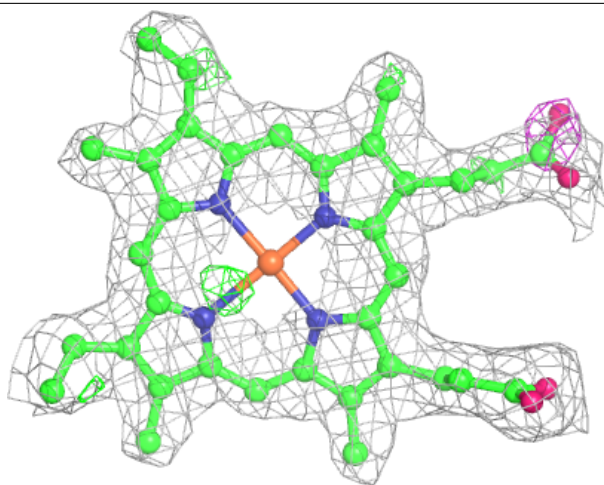
Electron density around HEM F 812:

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



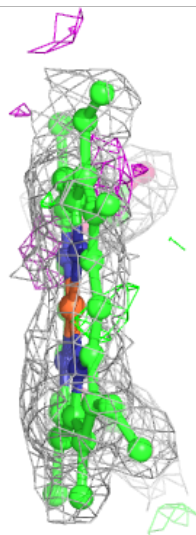
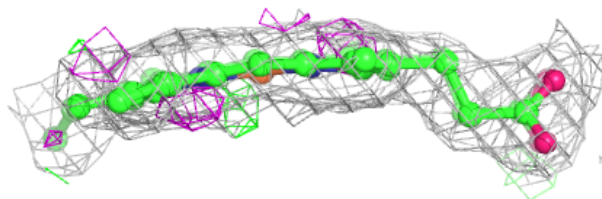
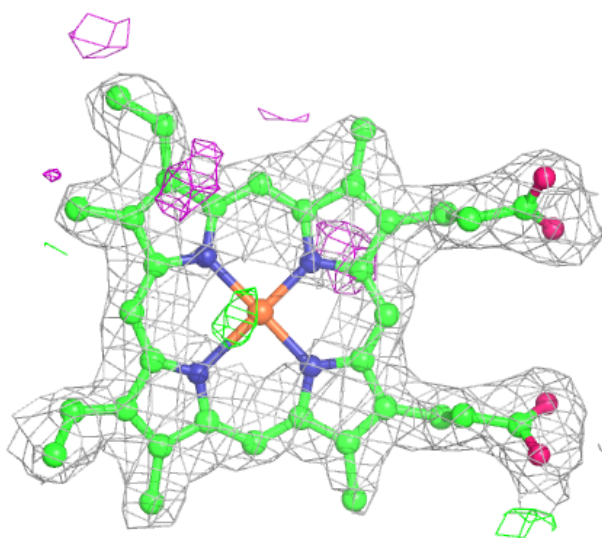
Electron density around HEM J 811:

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



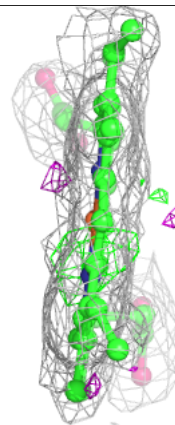
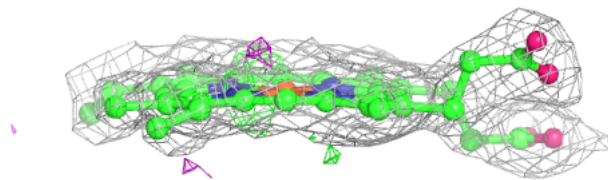
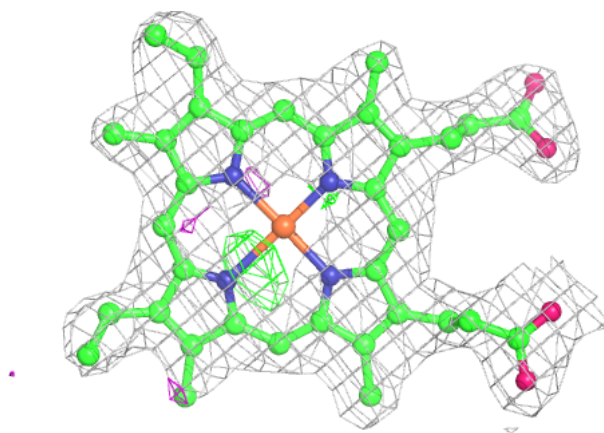
Electron density around HEM L 812:

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



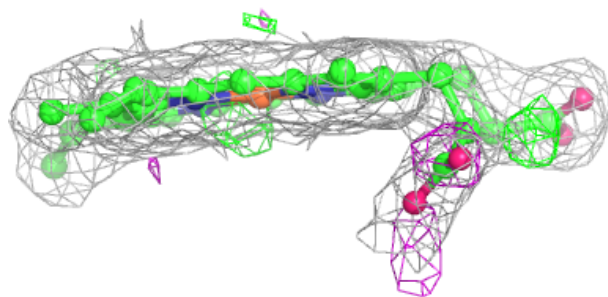
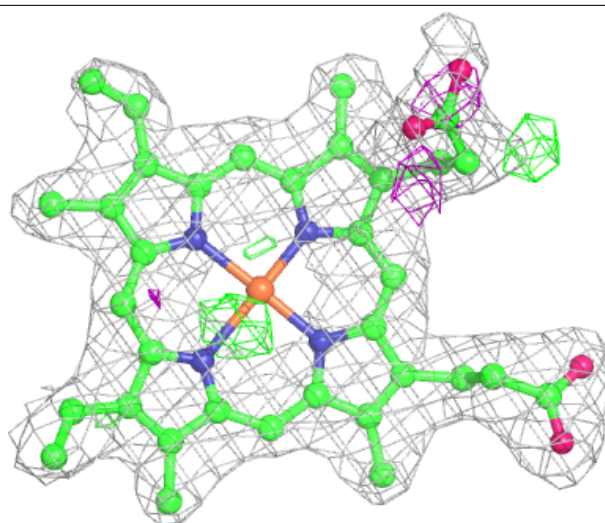
Electron density around HEM L 810:

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



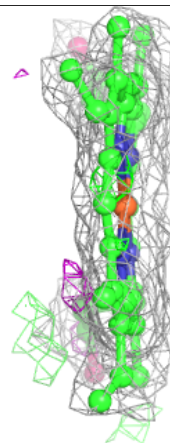
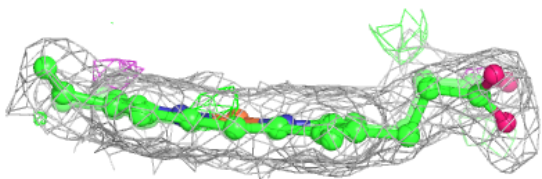
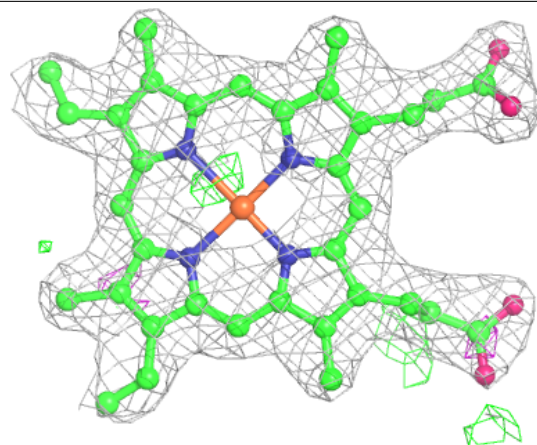
Electron density around HEM G 813:

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



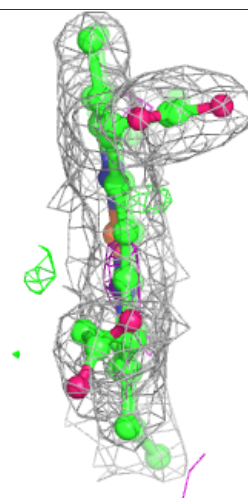
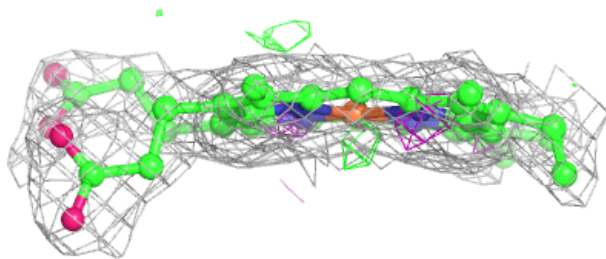
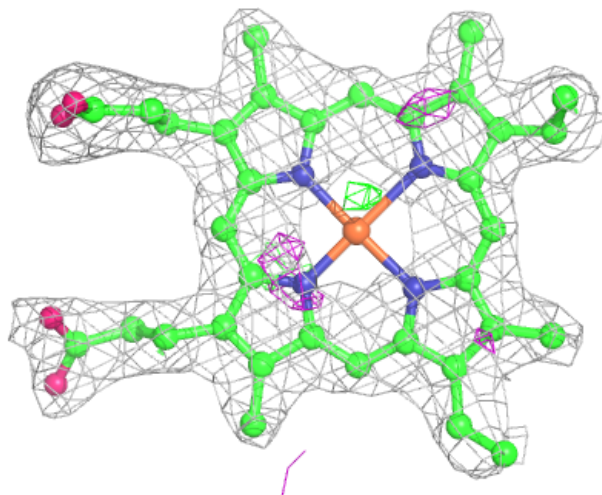
Electron density around HEM E 813:

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



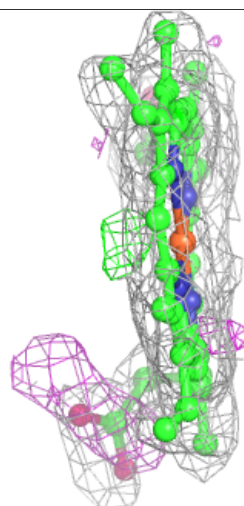
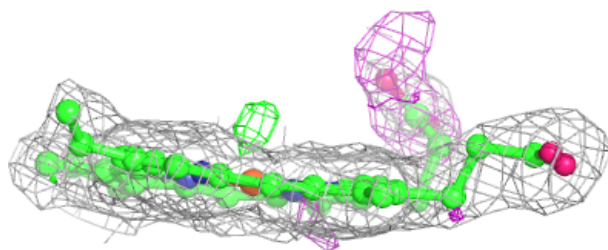
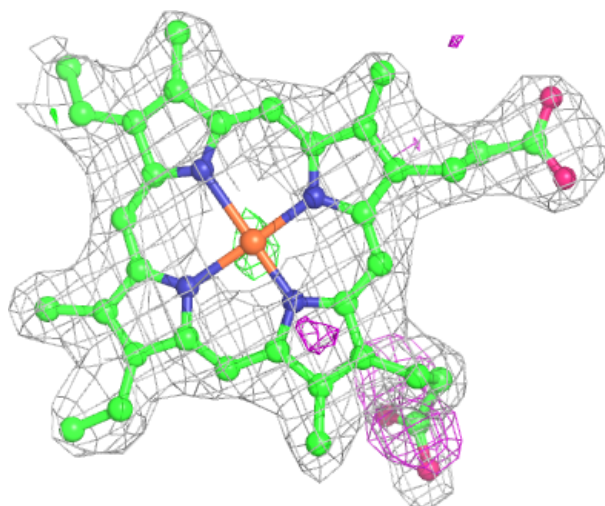
Electron density around HEM L 811:

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



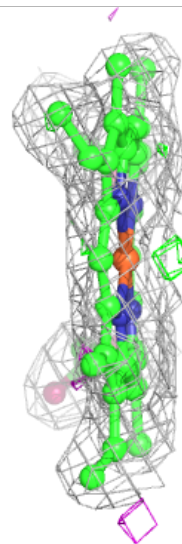
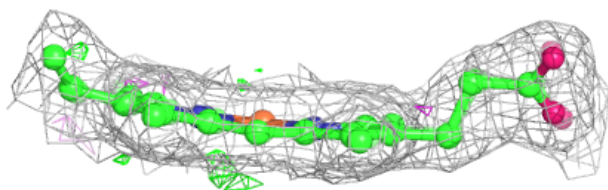
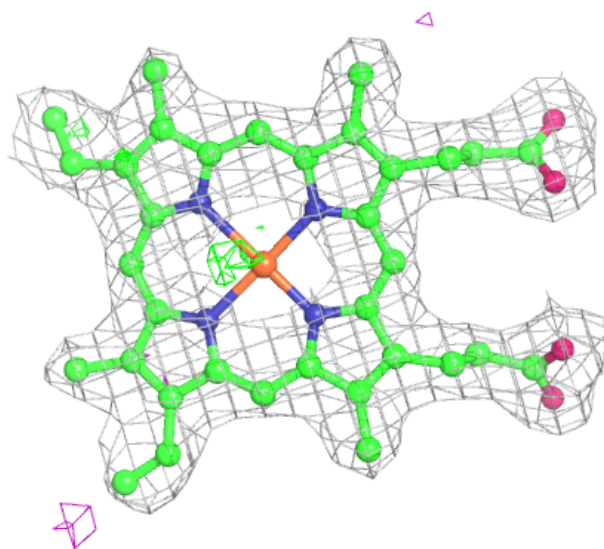
Electron density around HEM B 814:

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



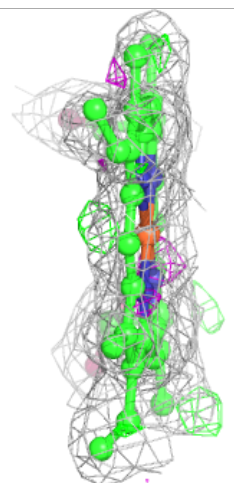
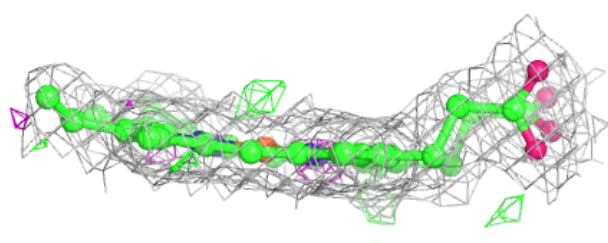
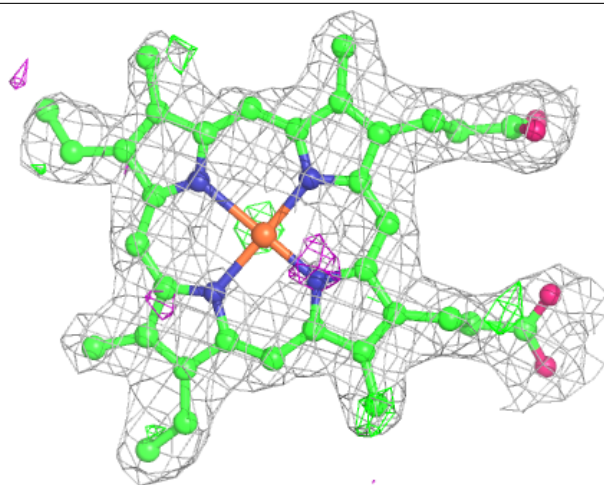
Electron density around HEM K 812:

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



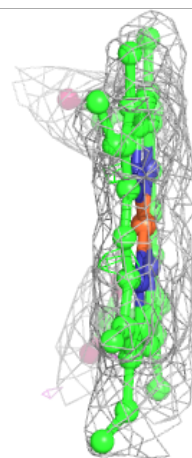
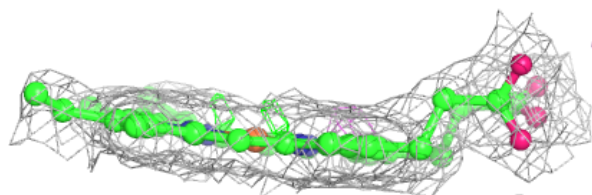
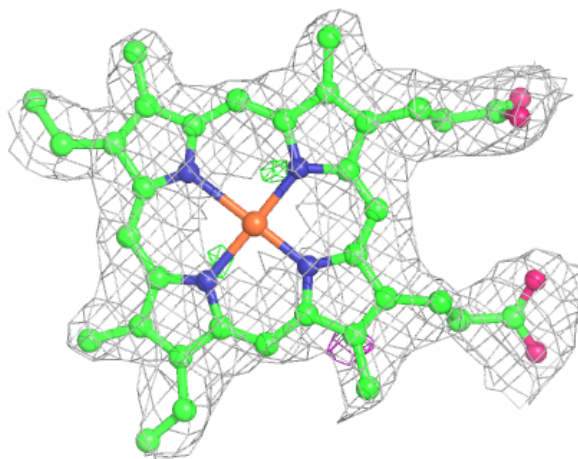
Electron density around HEM I 809:

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



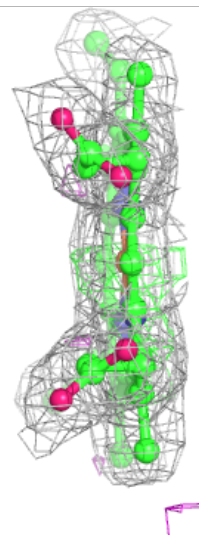
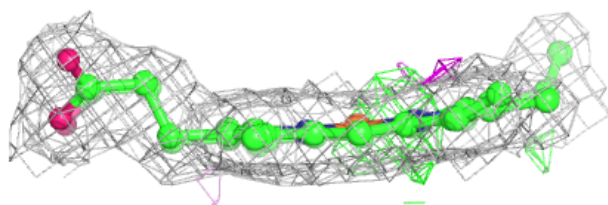
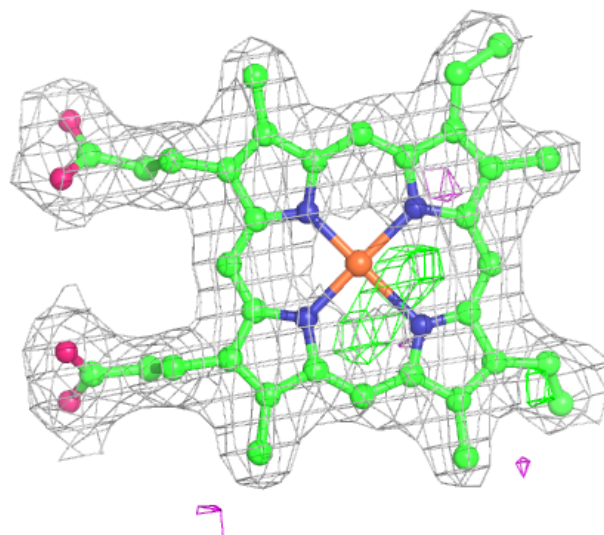
Electron density around HEM L 809:

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



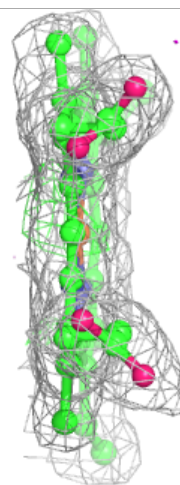
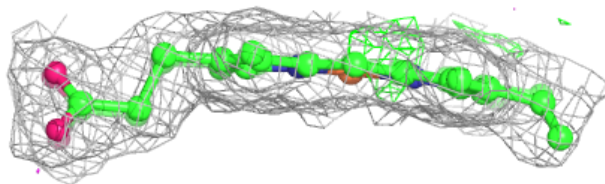
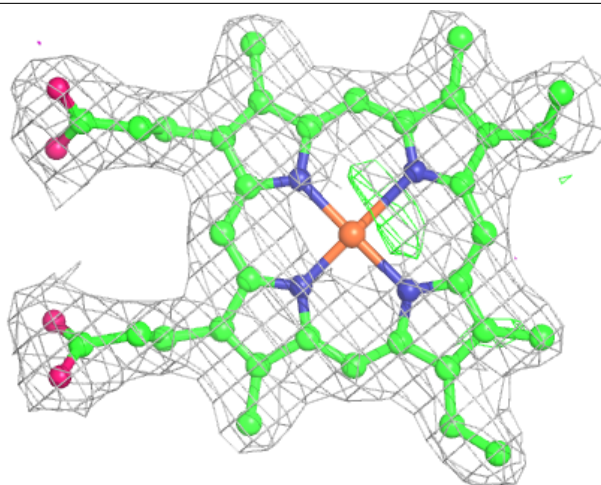
Electron density around HEM F 813:

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



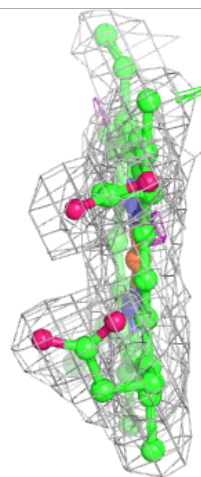
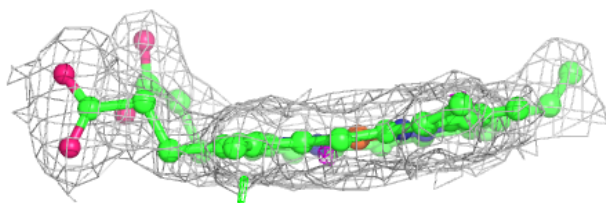
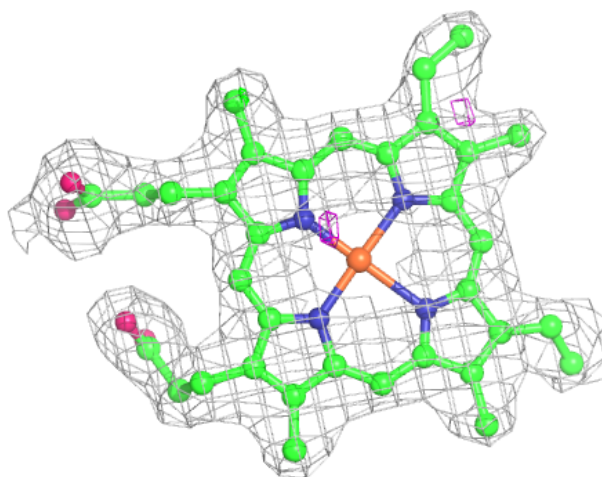
Electron density around HEM E 812:

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



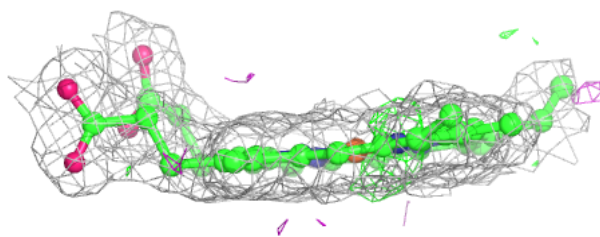
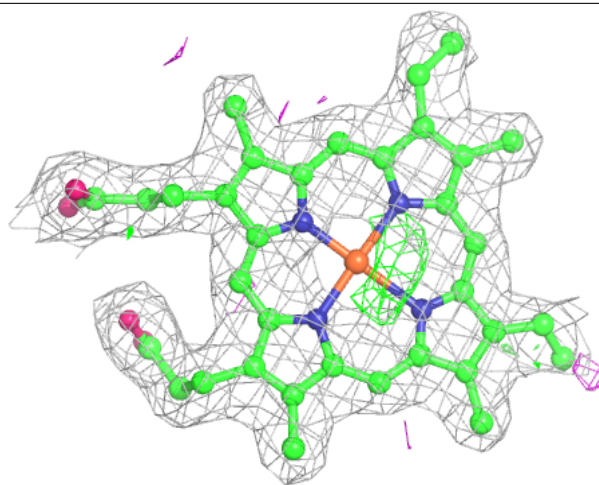
Electron density around HEM G 806:

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



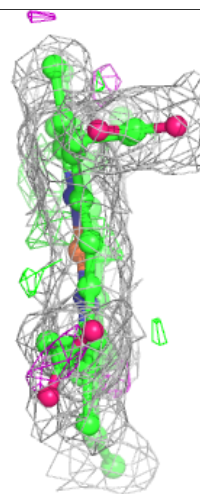
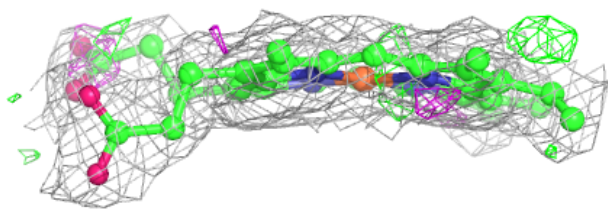
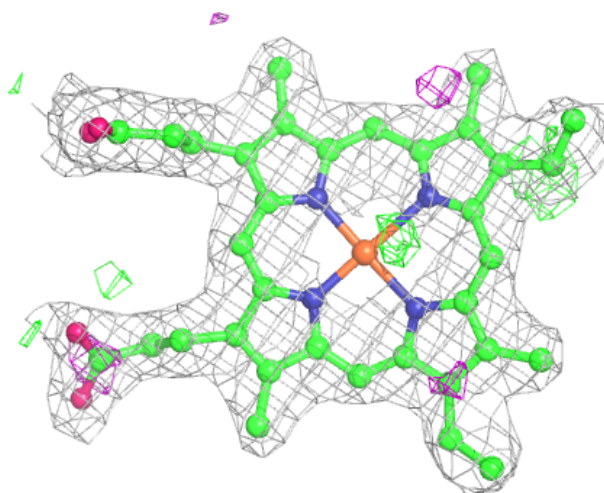
Electron density around HEM B 807:

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



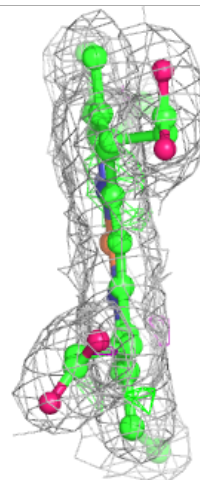
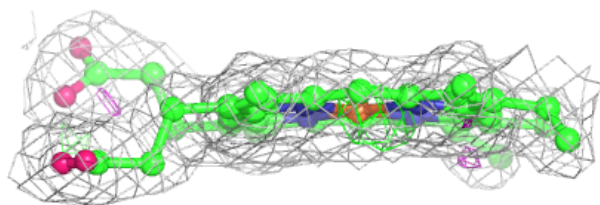
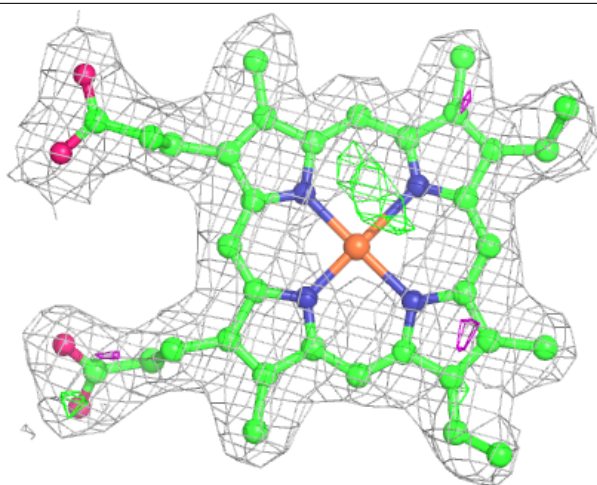
Electron density around HEM E 811:

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



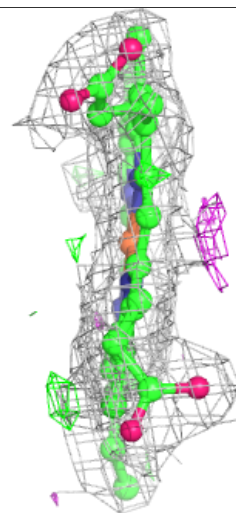
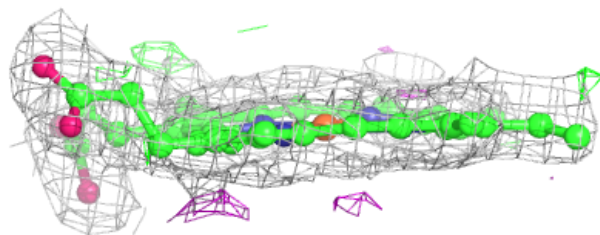
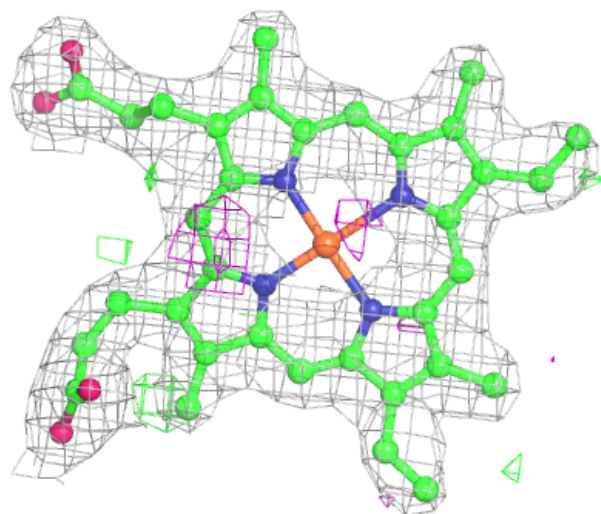
Electron density around HEM D 810:

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



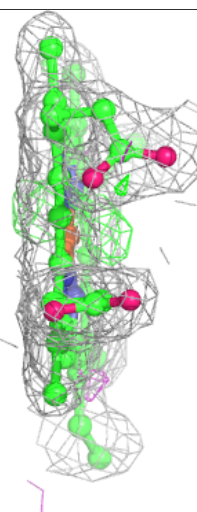
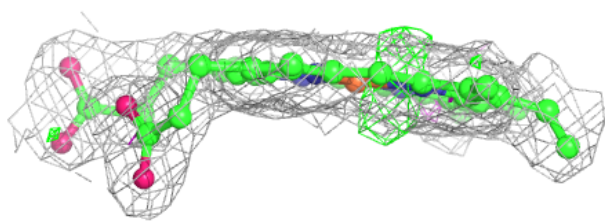
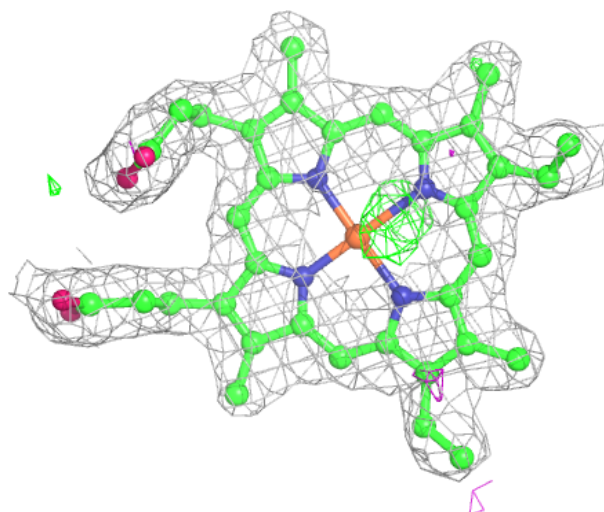
Electron density around HEM I 807:

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



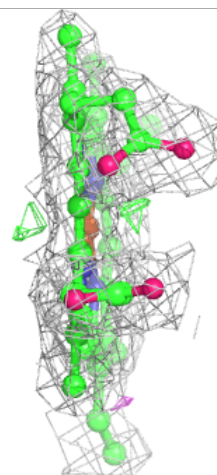
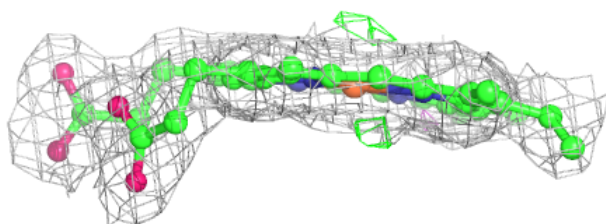
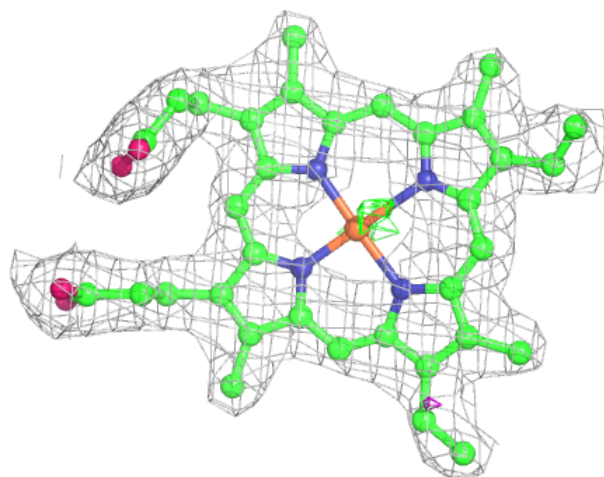
Electron density around HEM D 806:

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



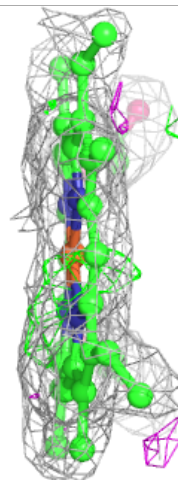
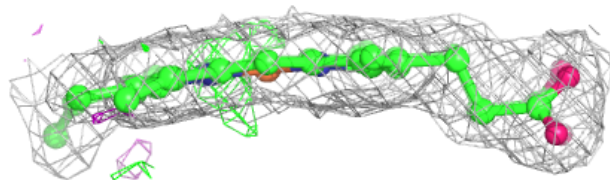
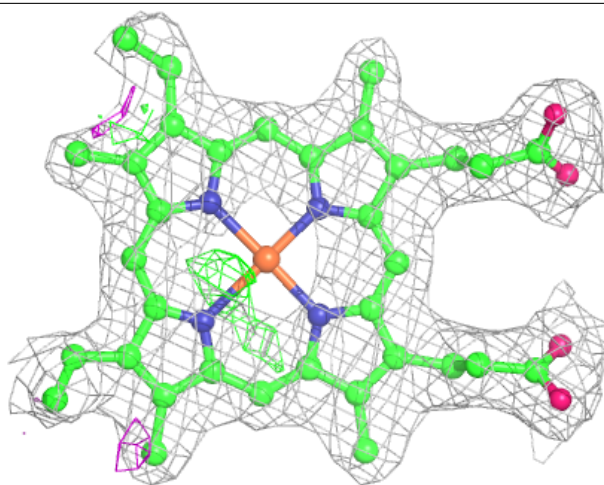
Electron density around HEM L 806:

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



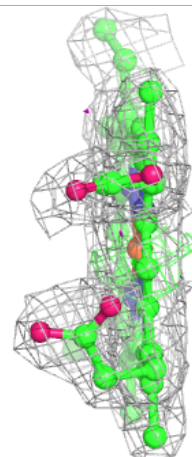
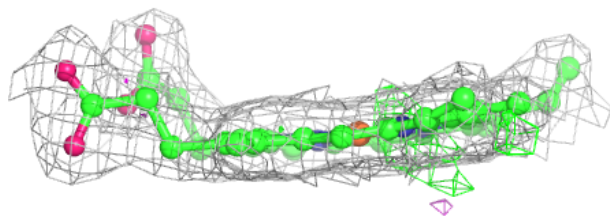
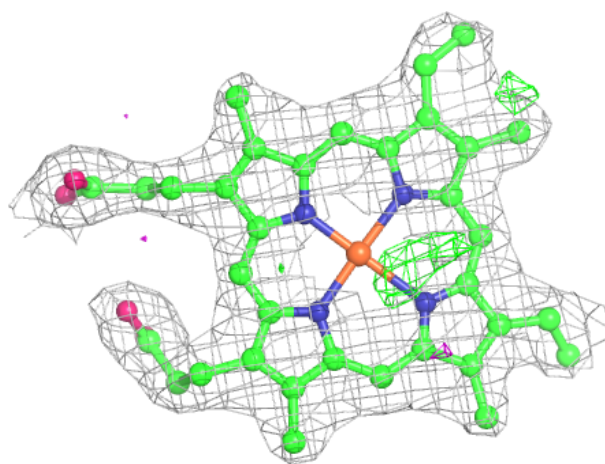
Electron density around HEM H 813:

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



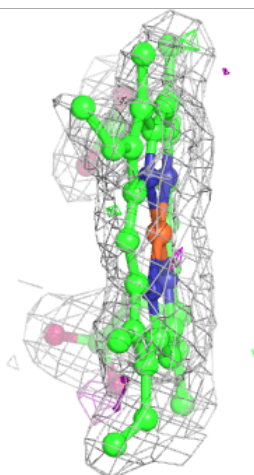
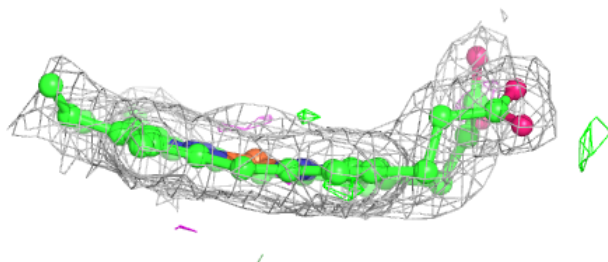
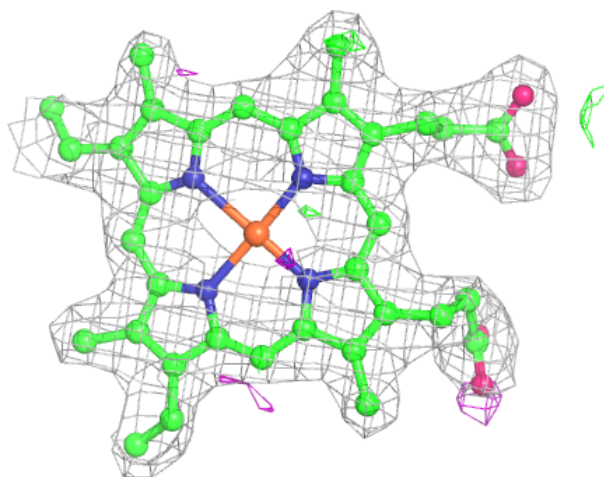
Electron density around HEM H 807:

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



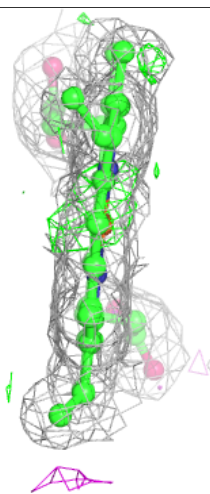
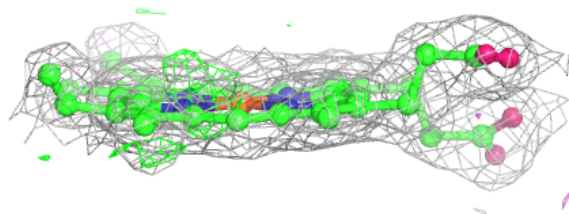
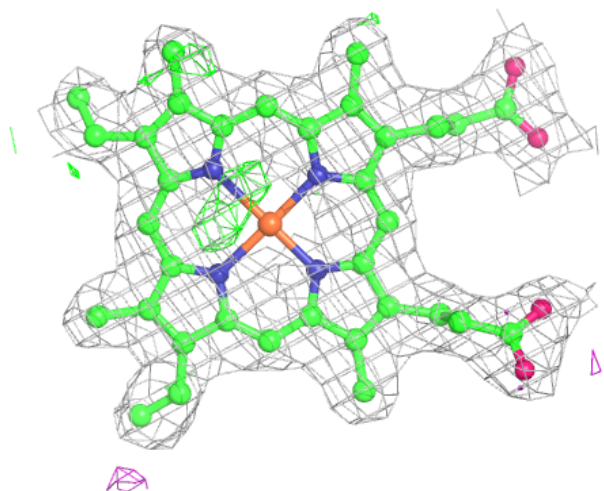
Electron density around HEM H 809:

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



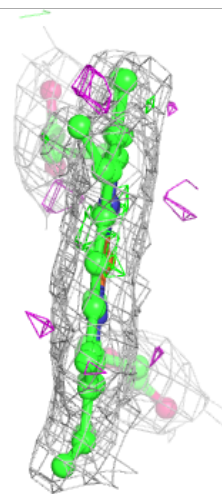
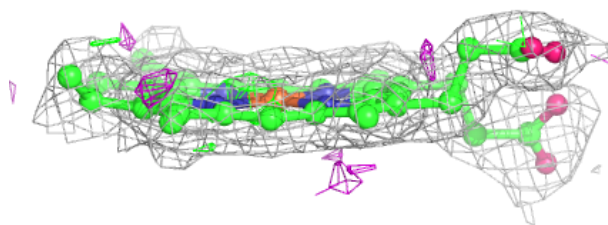
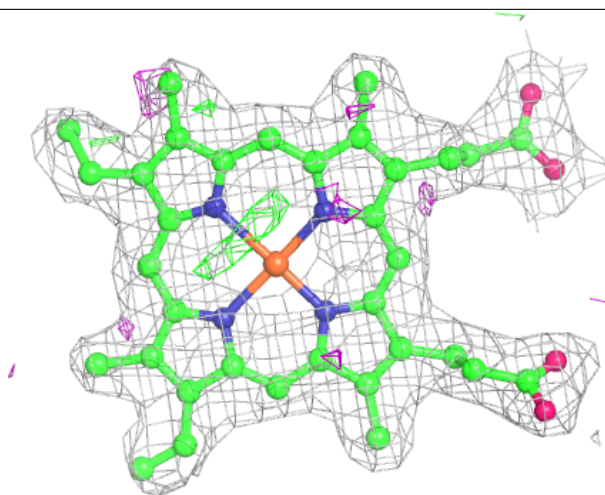
Electron density around HEM A 810:

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



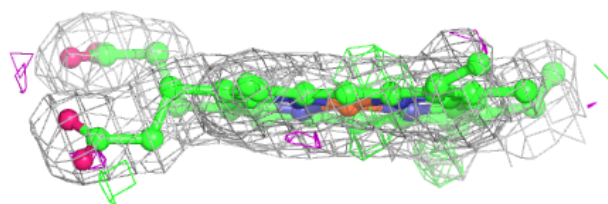
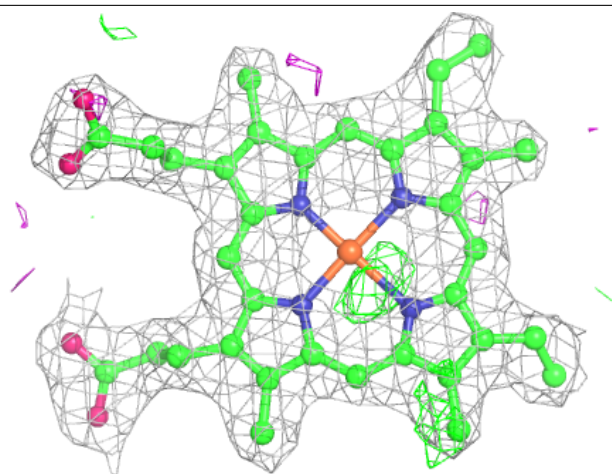
Electron density around HEM E 810:

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



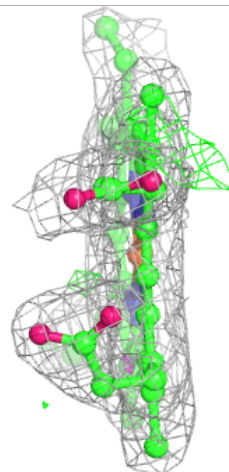
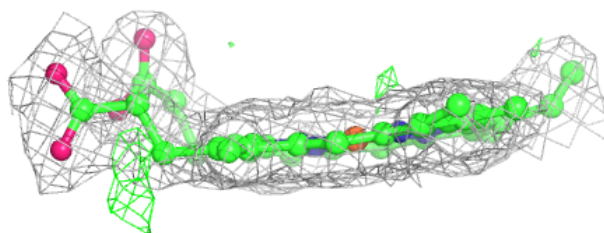
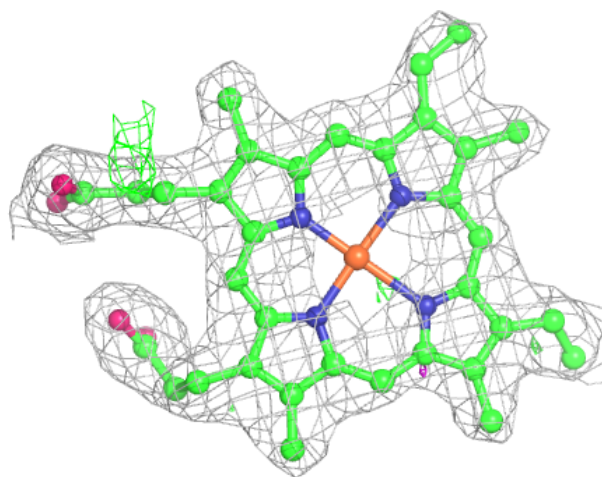
Electron density around HEM B 811:

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



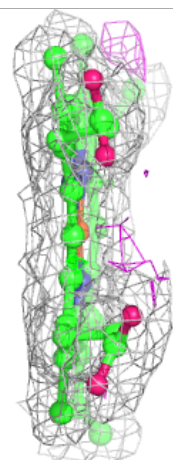
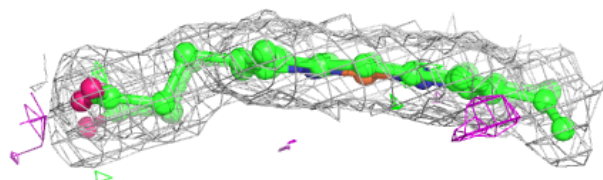
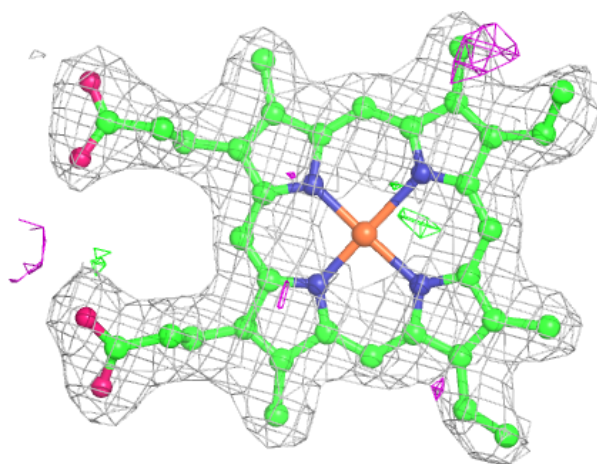
Electron density around HEM I 806:

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



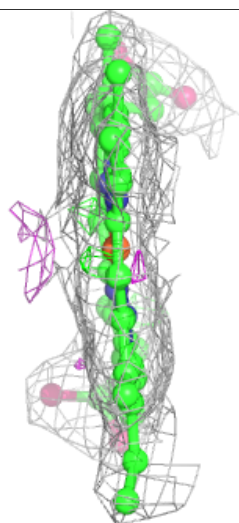
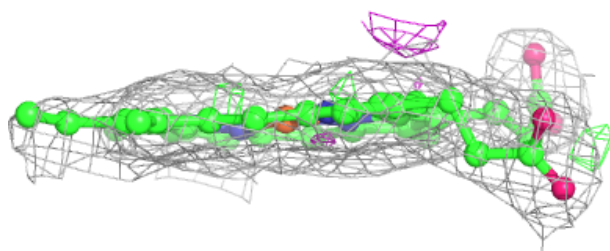
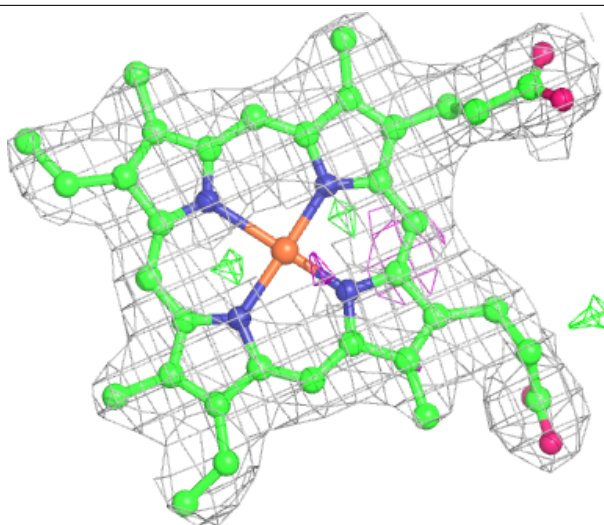
Electron density around HEM D 813:

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



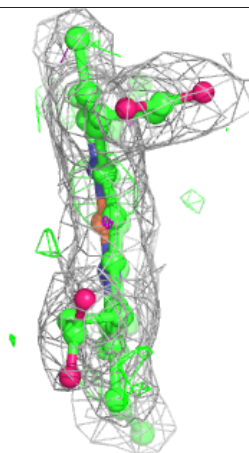
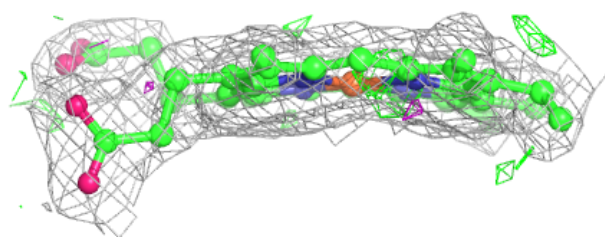
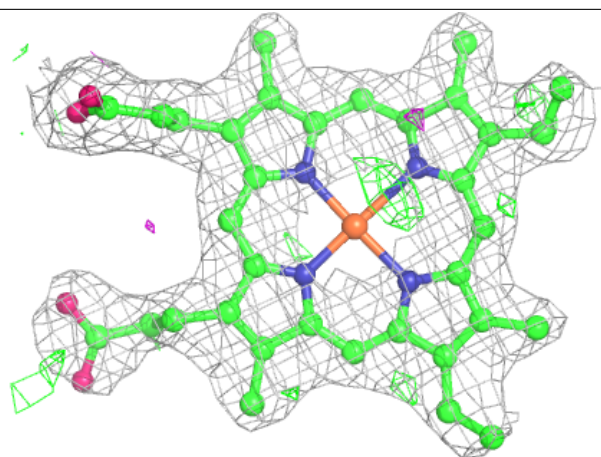
Electron density around HEM L 807:

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



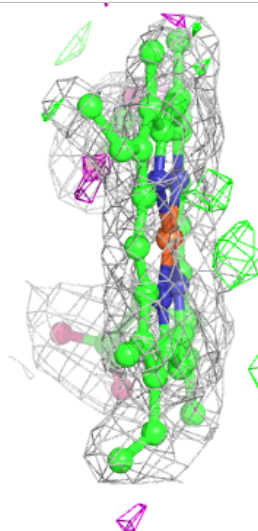
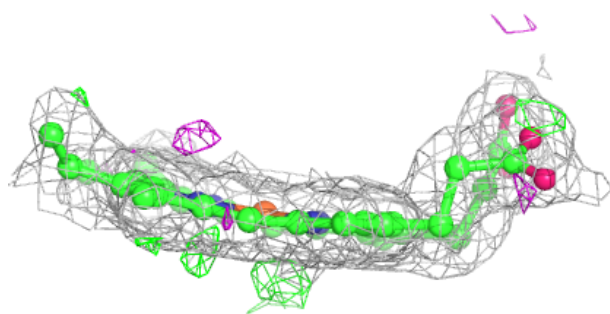
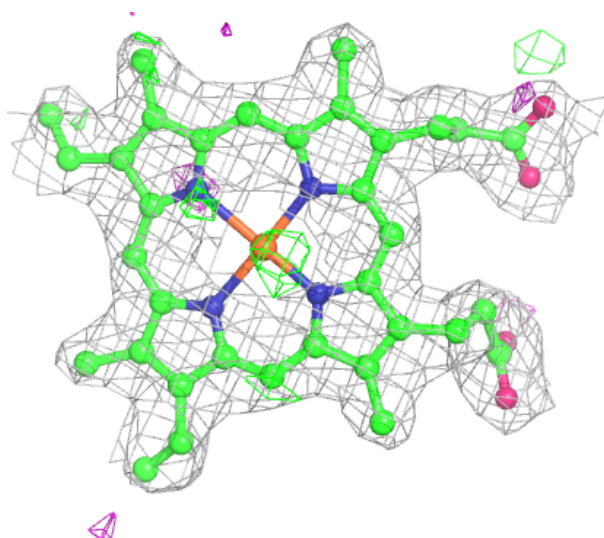
Electron density around HEM G 811:

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



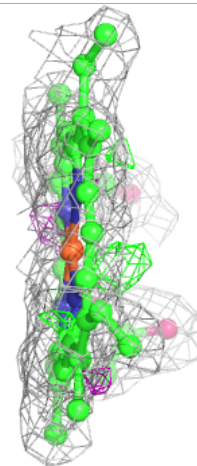
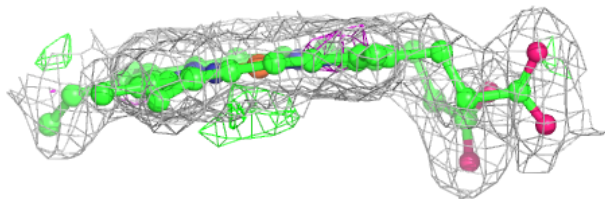
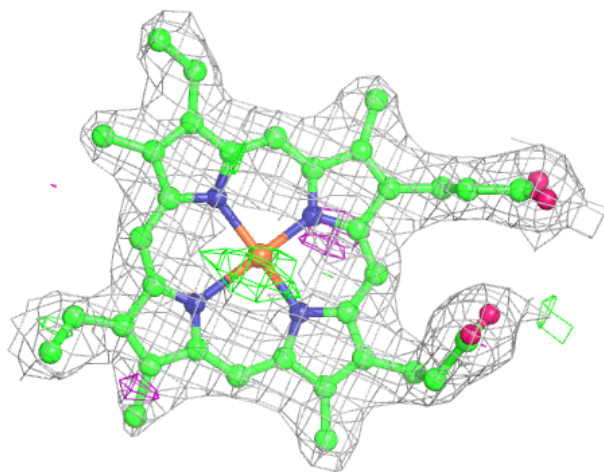
Electron density around HEM F 809:

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



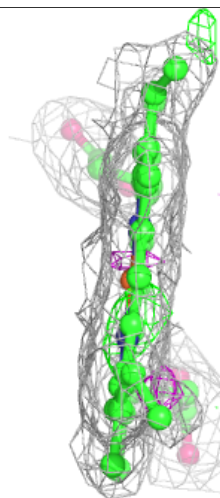
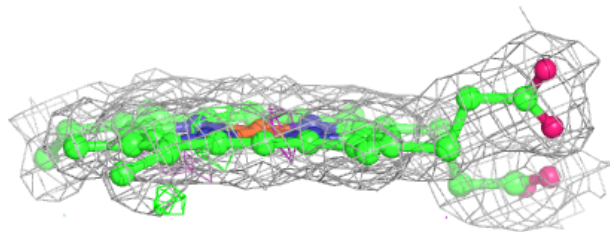
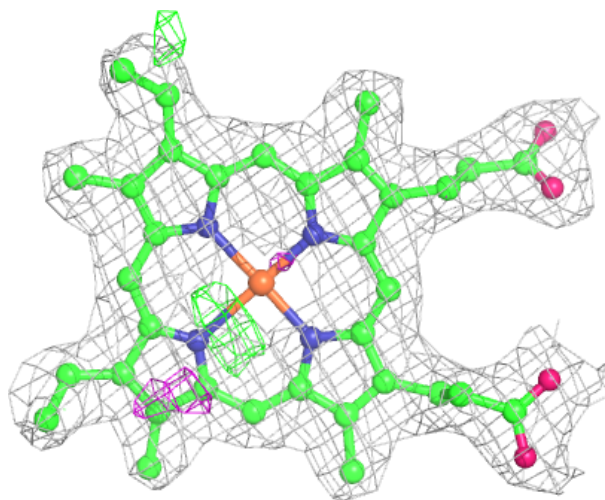
Electron density around HEM F 807:

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



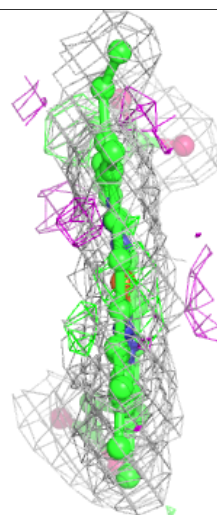
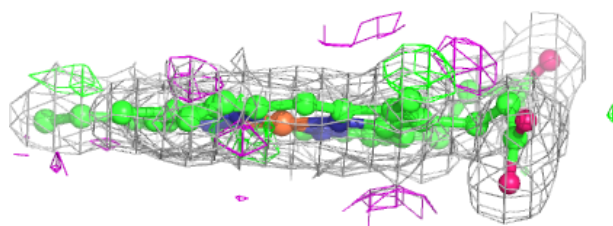
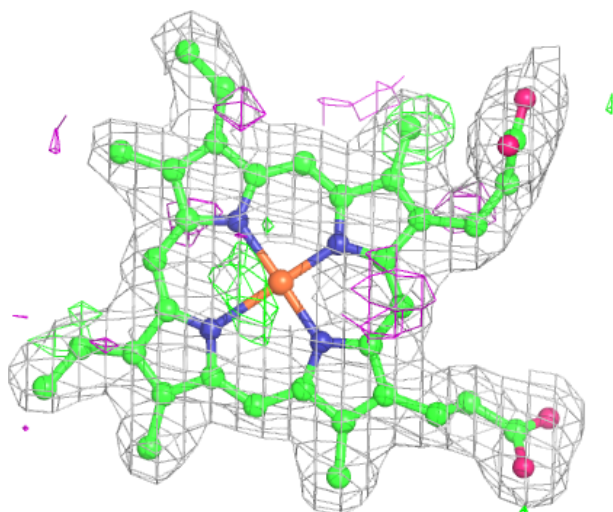
Electron density around HEM G 810:

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



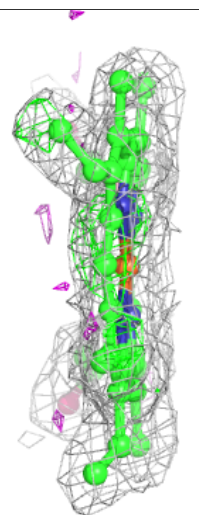
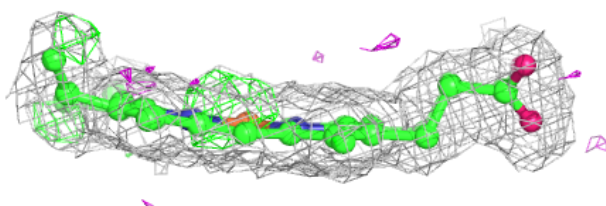
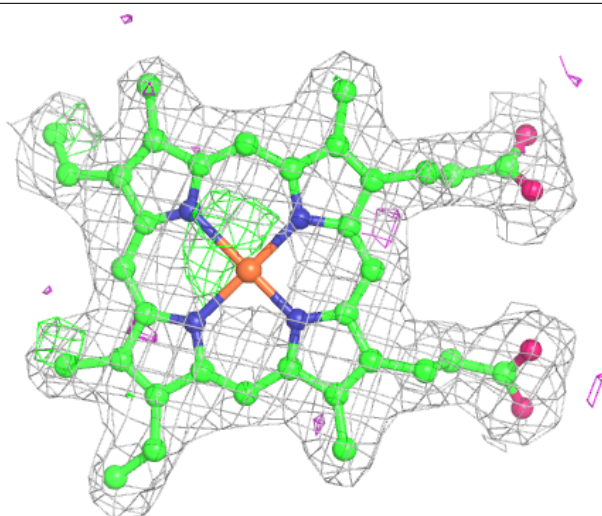
Electron density around HEM A 807:

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



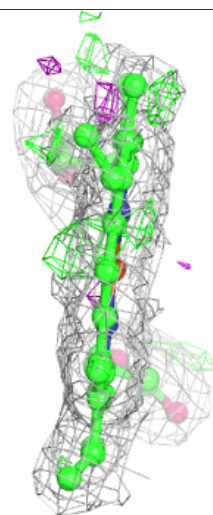
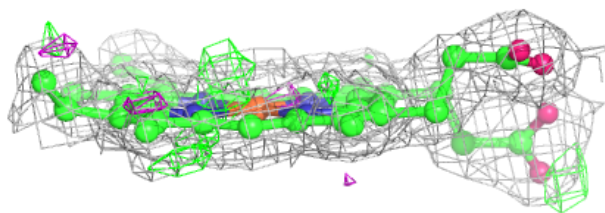
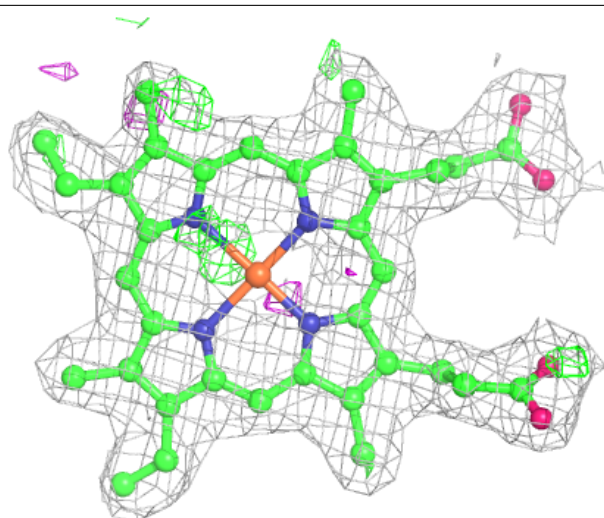
Electron density around HEM A 812:

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



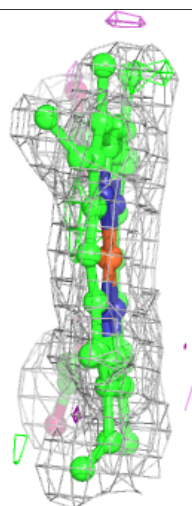
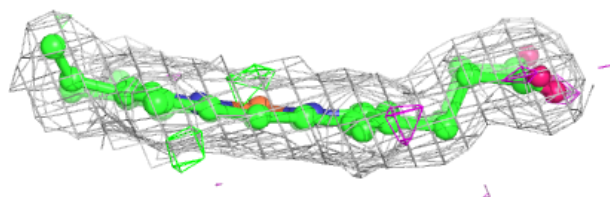
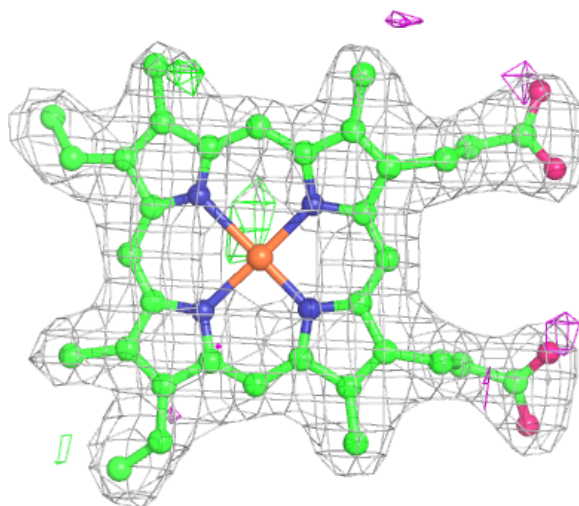
Electron density around HEM C 810:

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



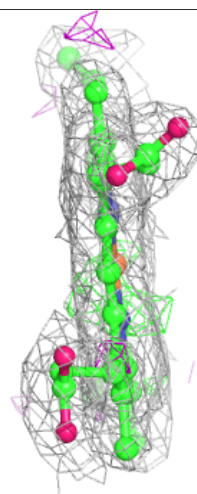
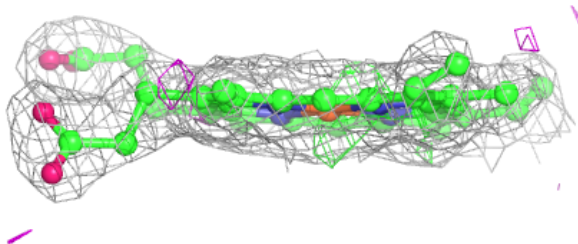
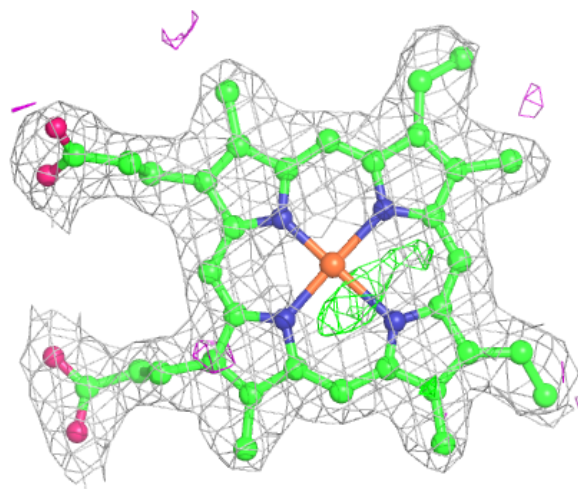
Electron density around HEM A 813:

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



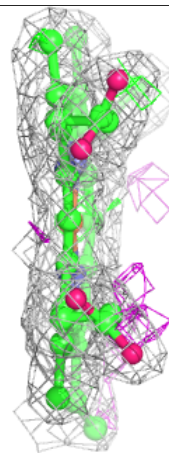
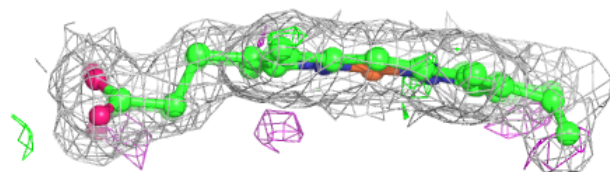
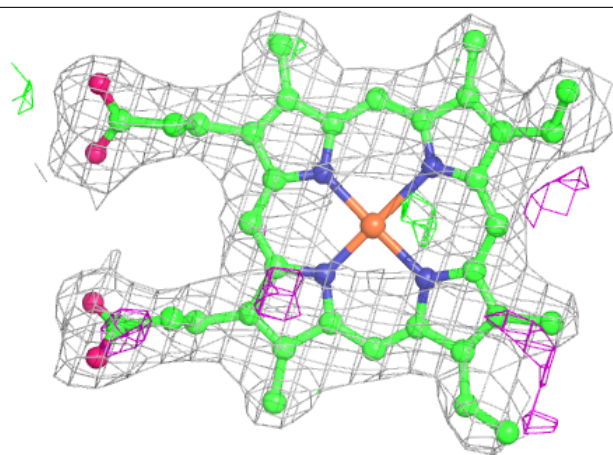
Electron density around HEM K 810:

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



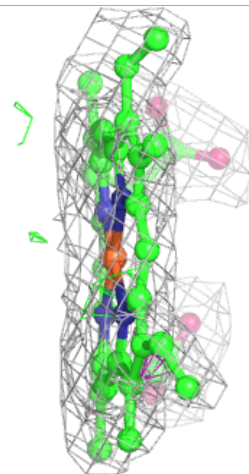
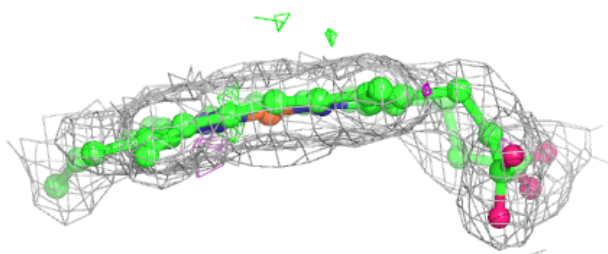
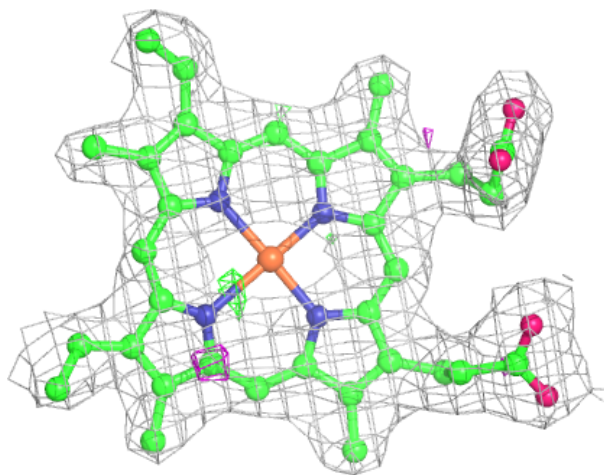
Electron density around HEM B 813:

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



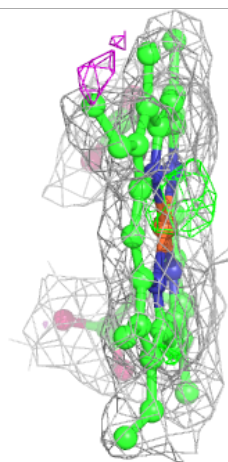
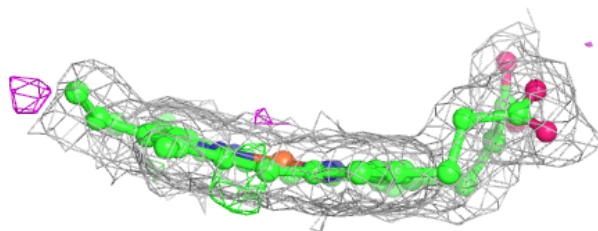
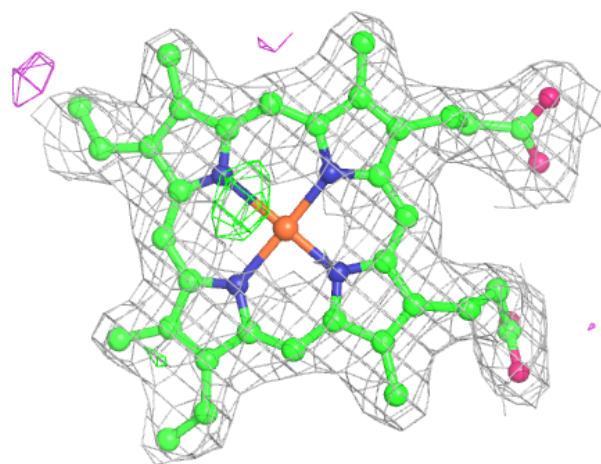
Electron density around HEM G 808:

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



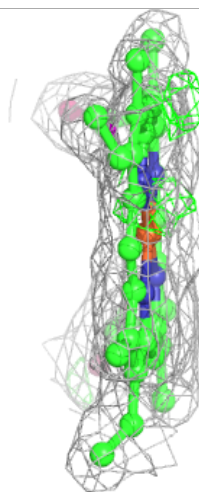
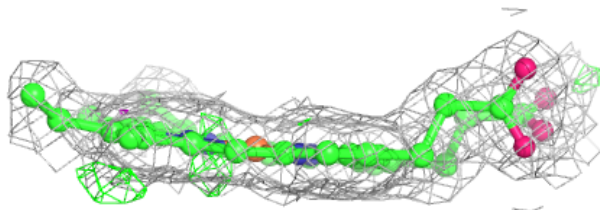
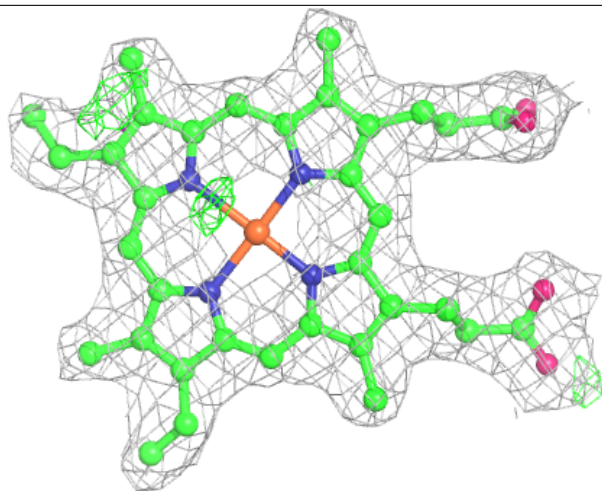
Electron density around HEM K 808:

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



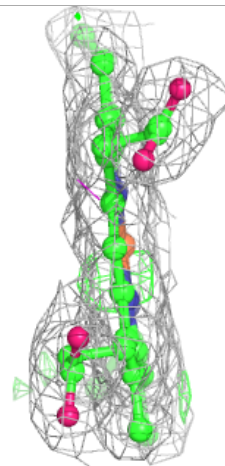
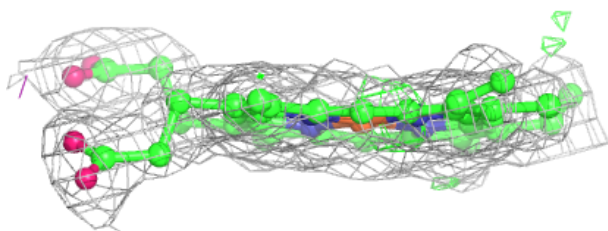
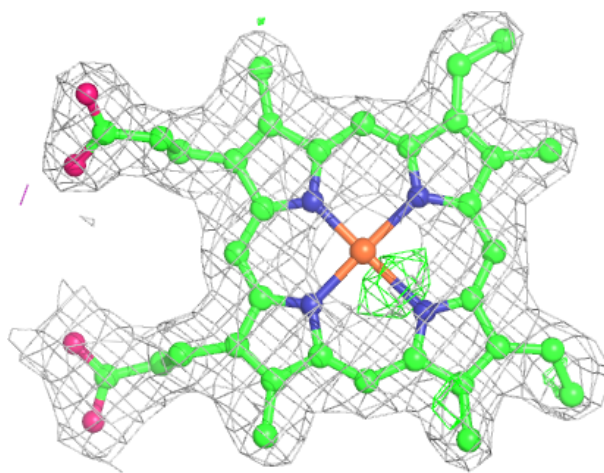
Electron density around HEM G 809:

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



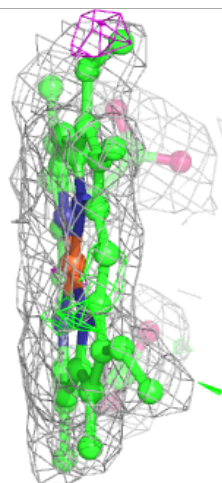
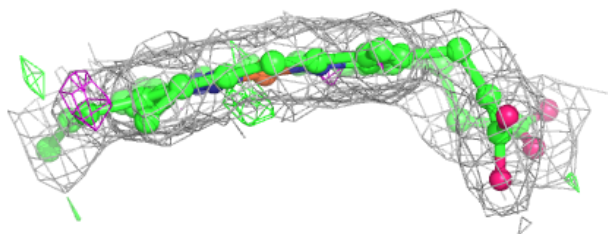
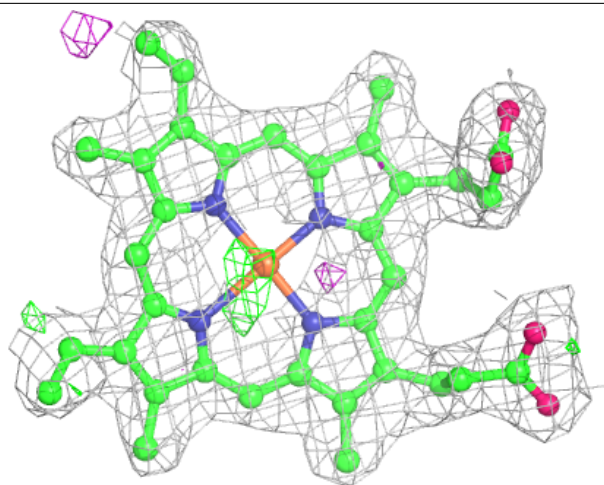
Electron density around HEM H 811:

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



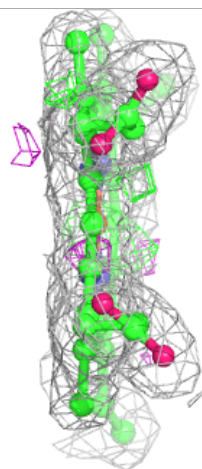
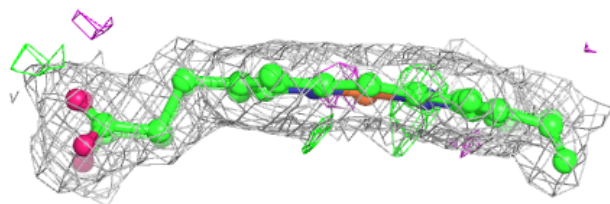
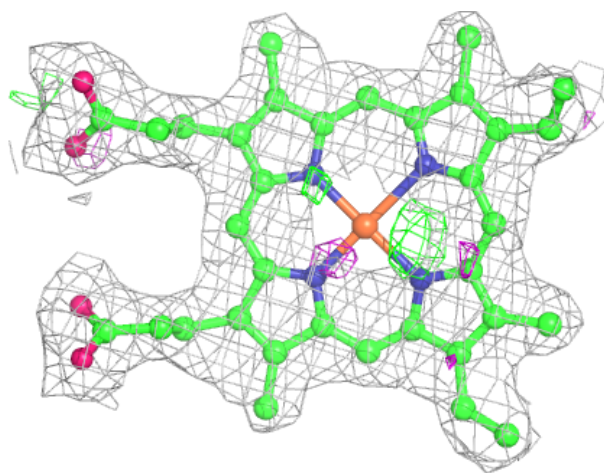
Electron density around HEM I 808:

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



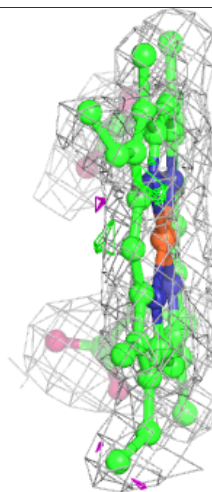
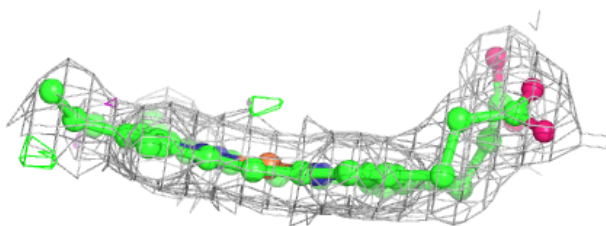
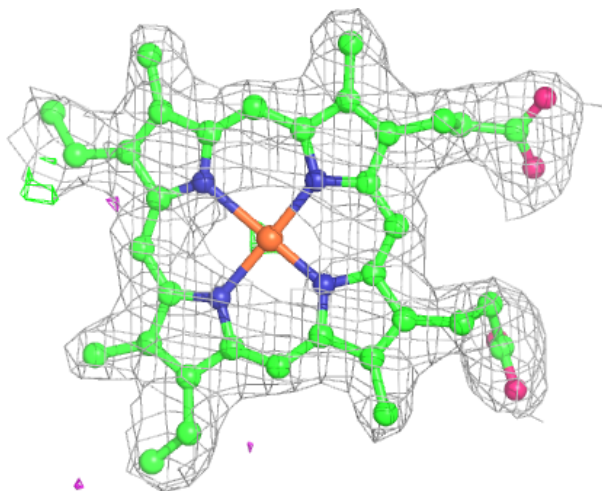
Electron density around HEM G 812:

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



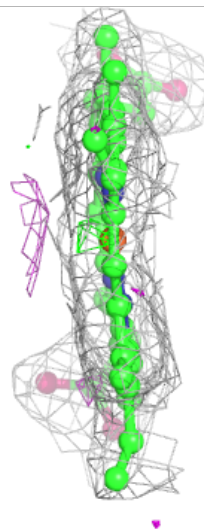
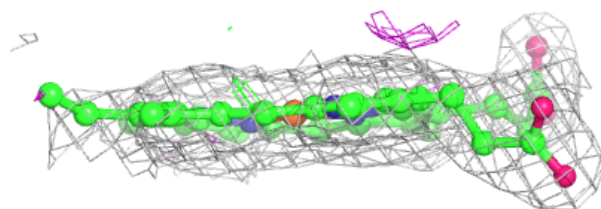
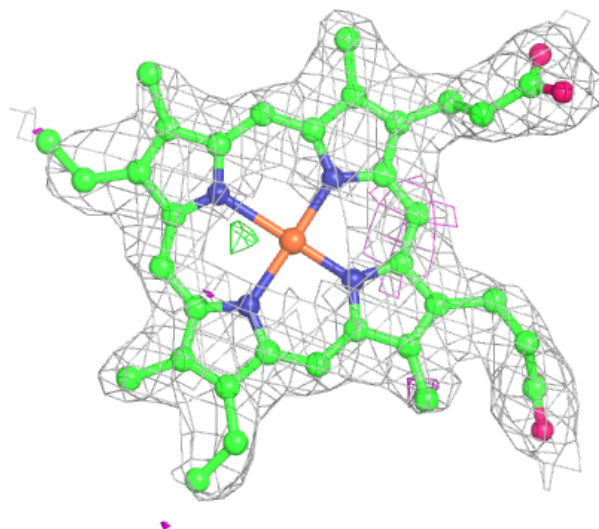
Electron density around HEM L 808:

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



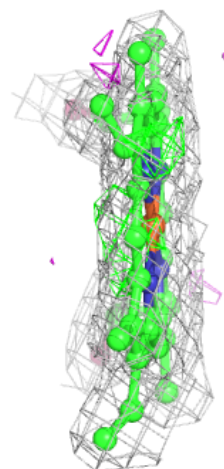
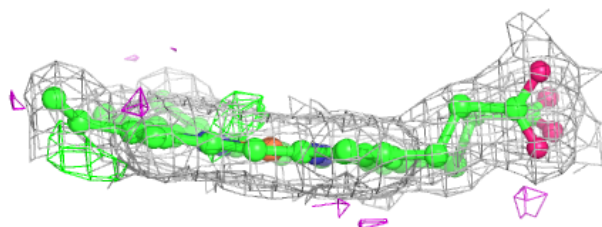
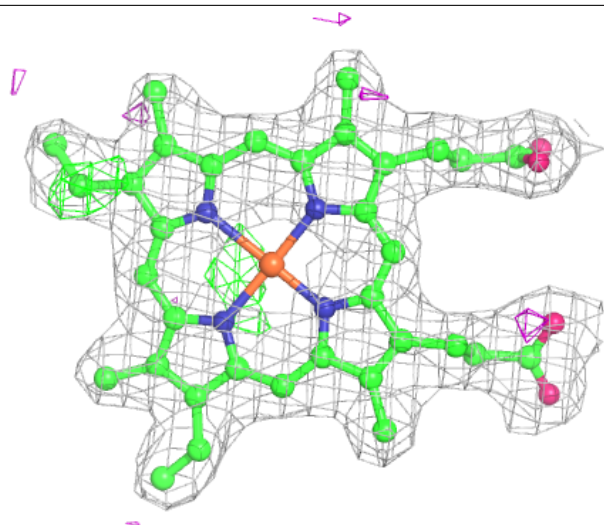
Electron density around HEM K 807:

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



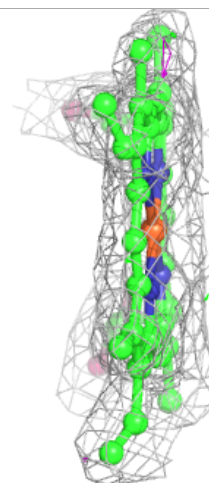
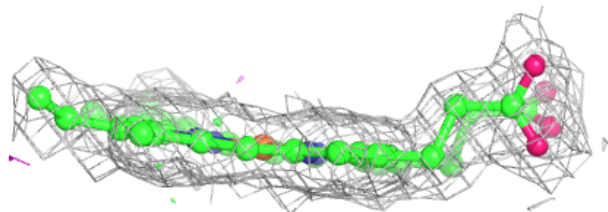
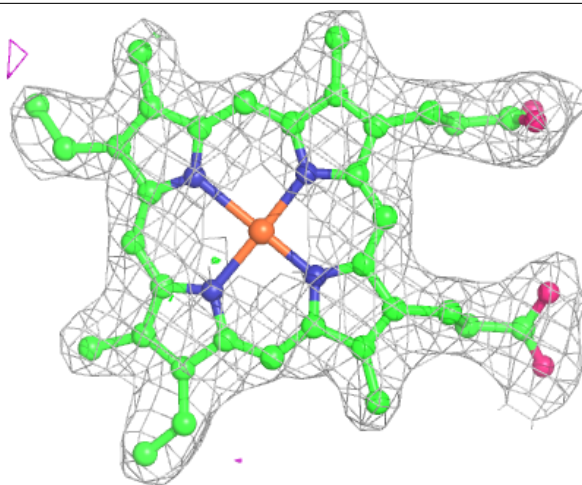
Electron density around HEM E 809:

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



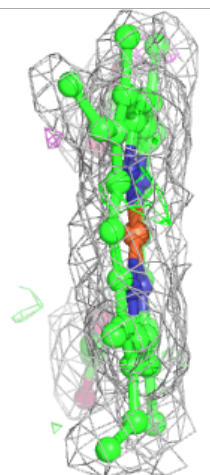
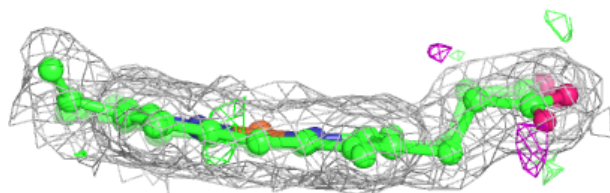
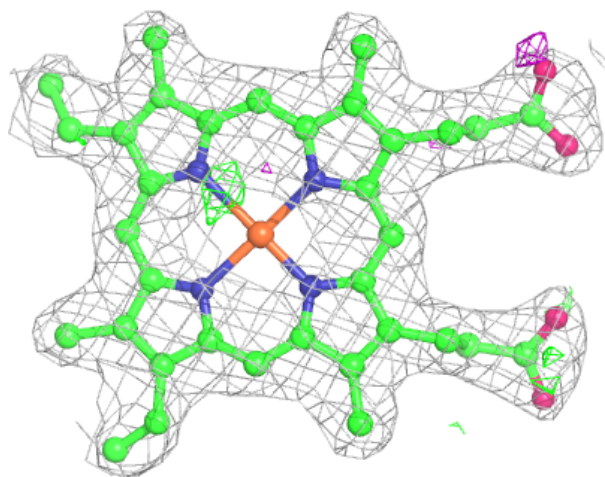
Electron density around HEM K 809:

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



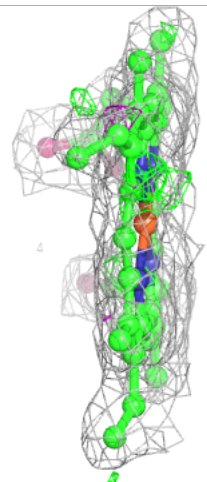
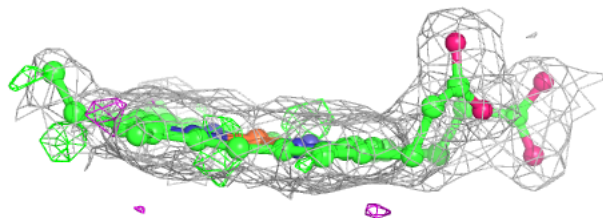
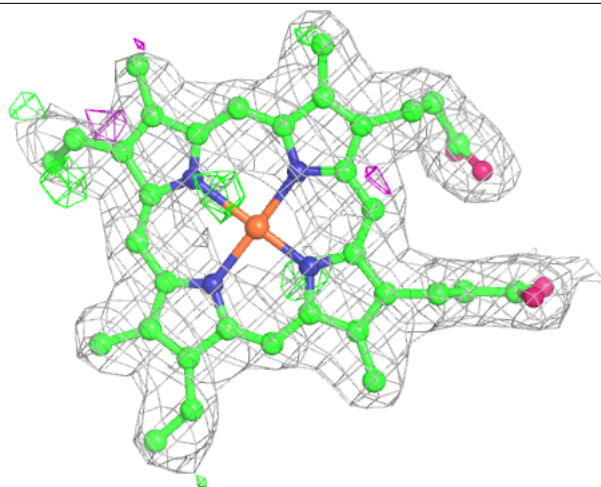
Electron density around HEM F 814:

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



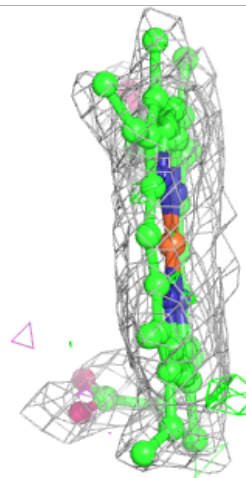
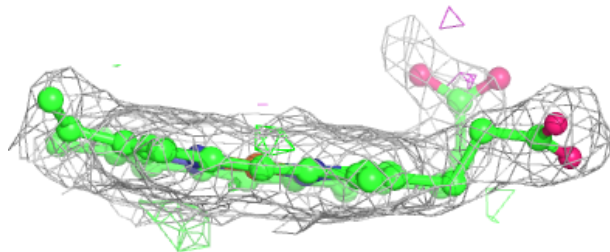
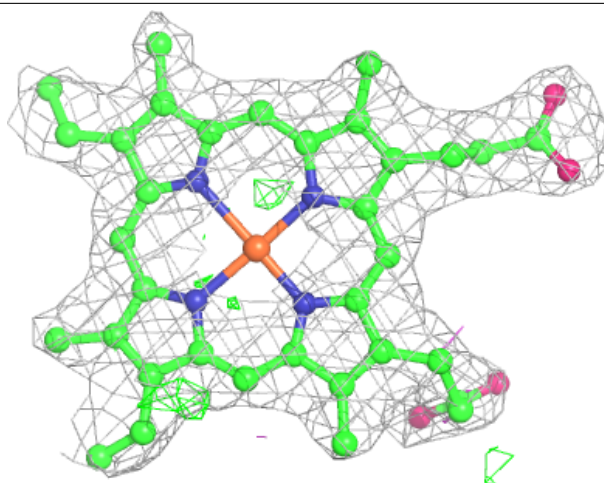
Electron density around HEM K 806:

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



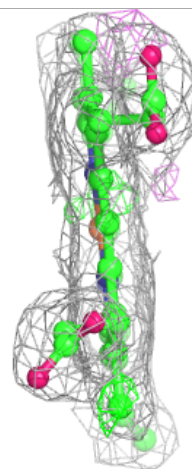
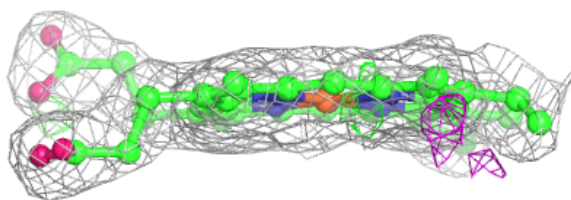
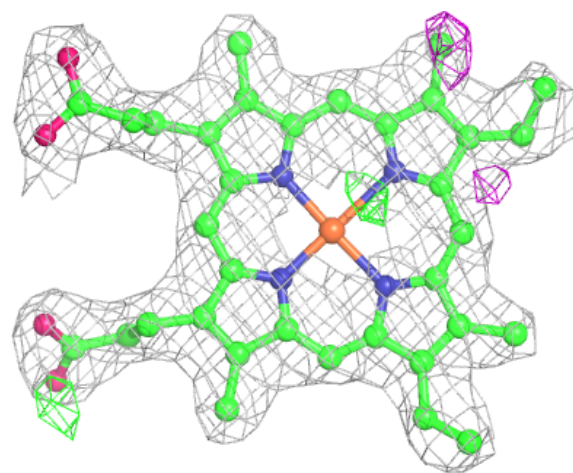
Electron density around HEM J 813:

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



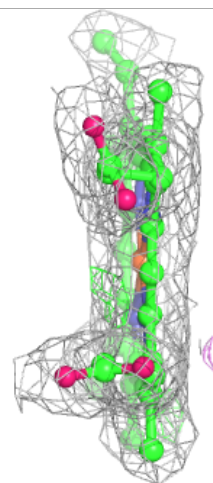
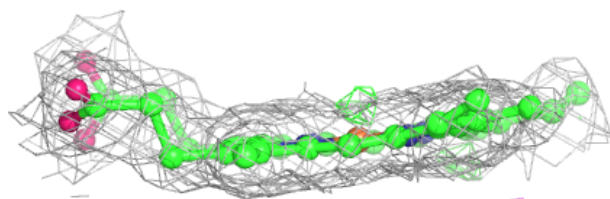
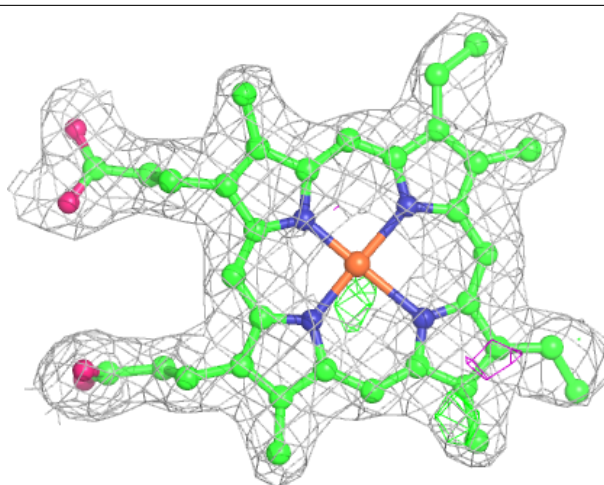
Electron density around HEM J 810:

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



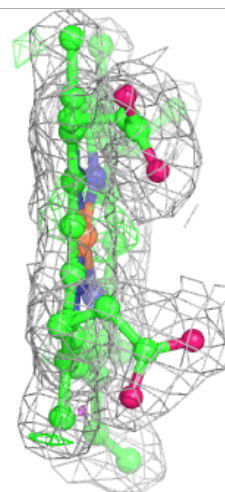
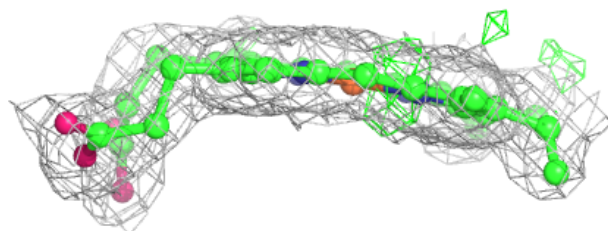
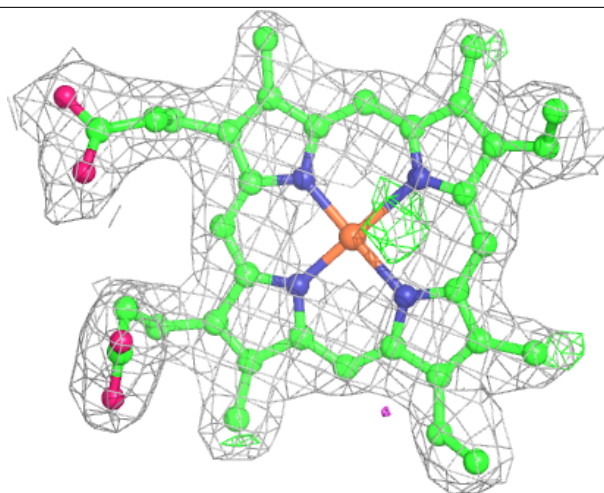
Electron density around HEM H 810:

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



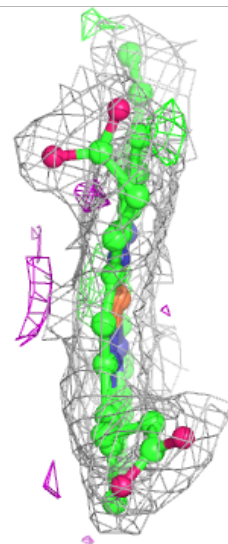
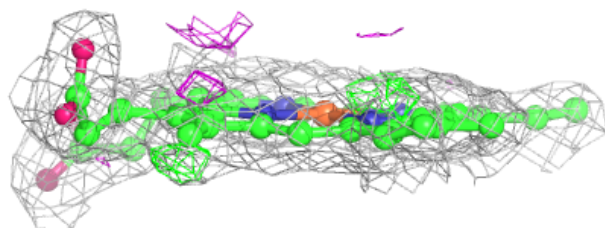
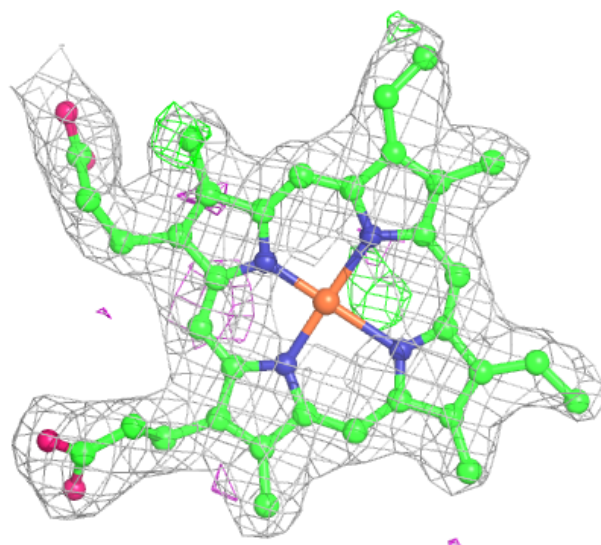
Electron density around HEM D 808:

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



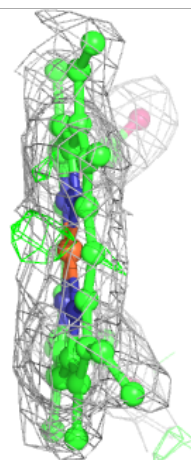
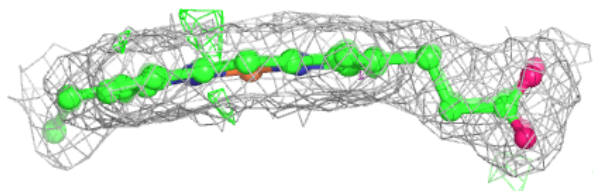
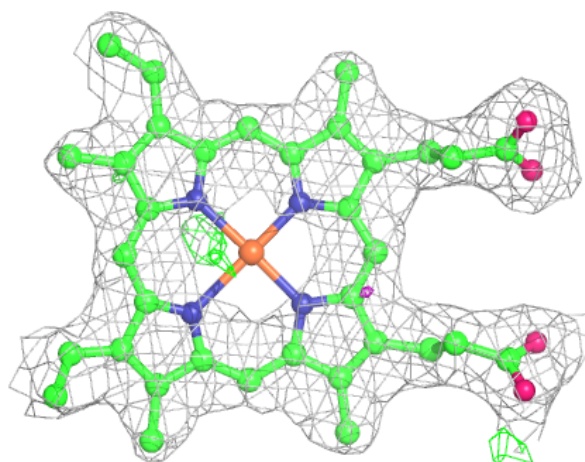
Electron density around HEM E 807:

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



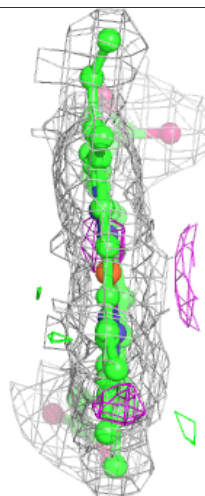
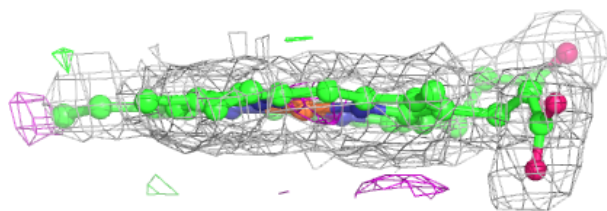
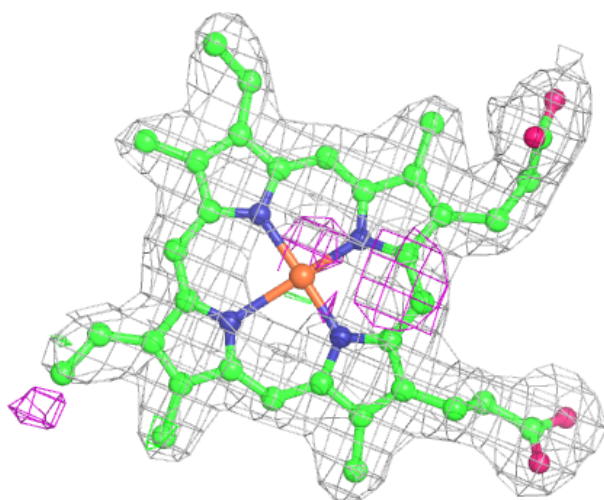
Electron density around HEM J 812:

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



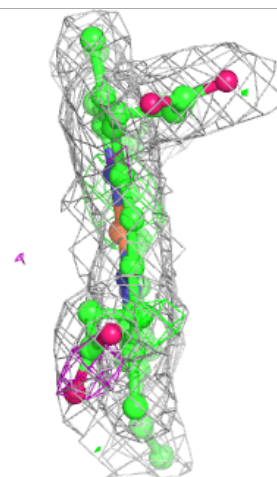
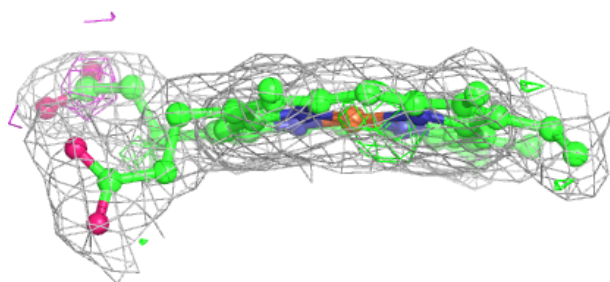
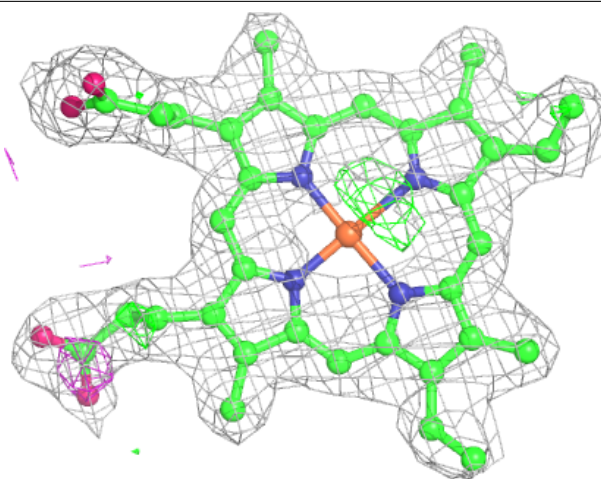
Electron density around HEM H 808:

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



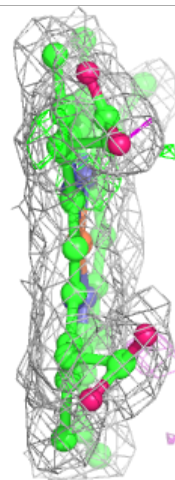
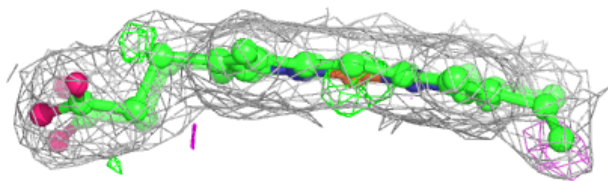
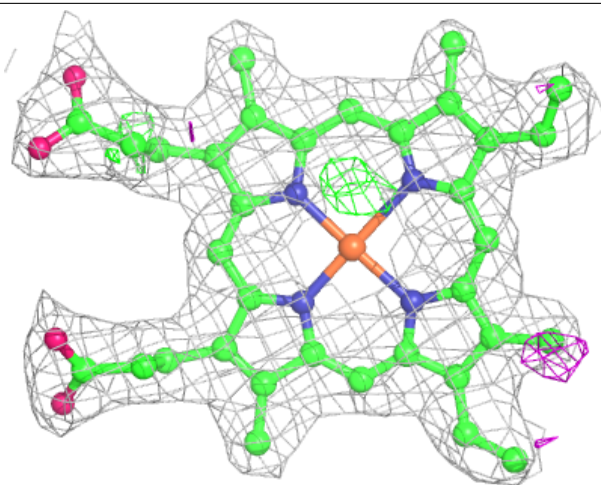
Electron density around HEM B 812:

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



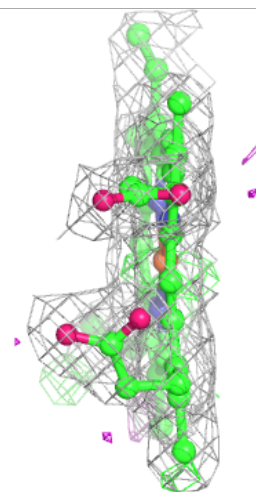
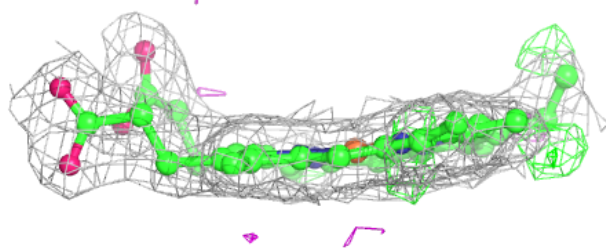
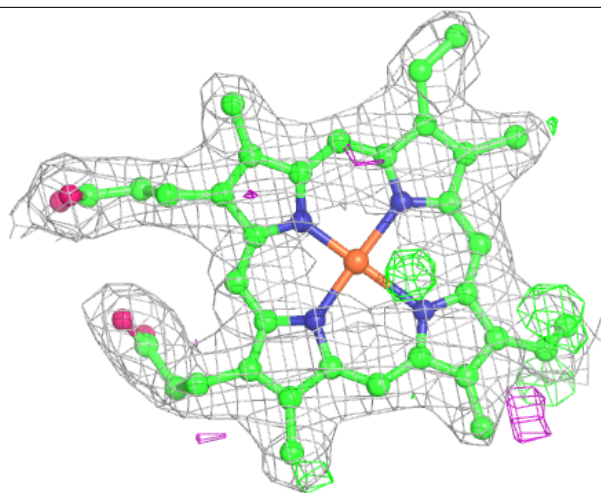
Electron density around HEM H 814:

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



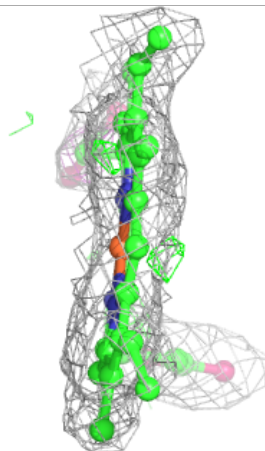
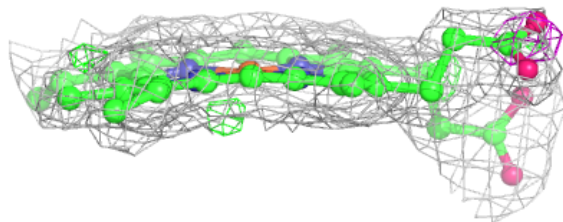
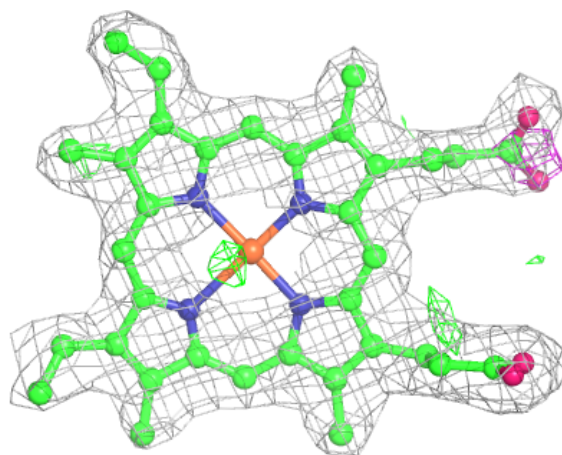
Electron density around HEM J 806:

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



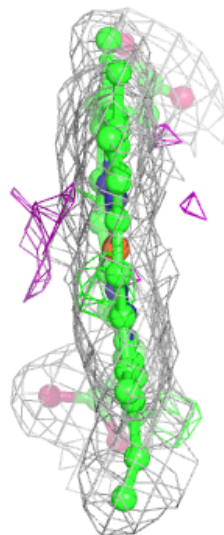
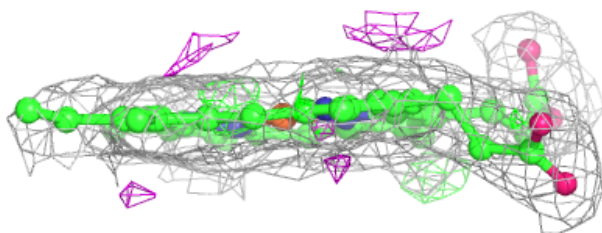
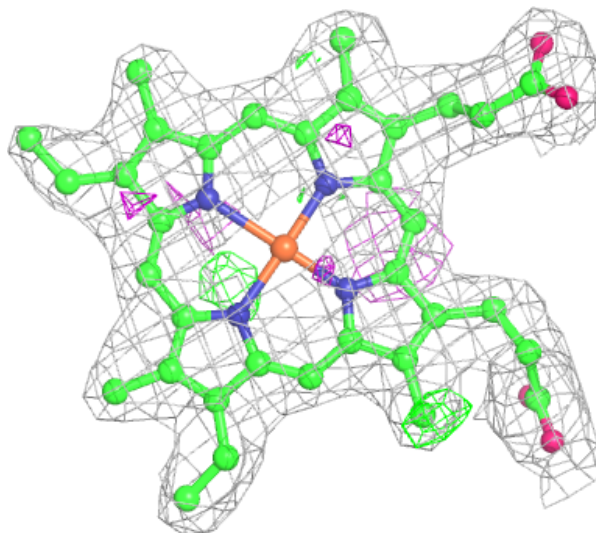
Electron density around HEM K 811:

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



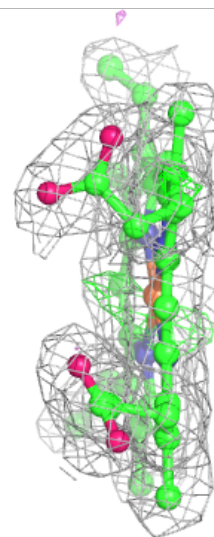
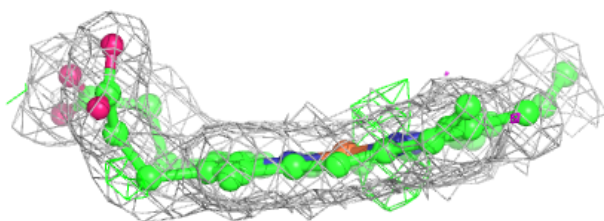
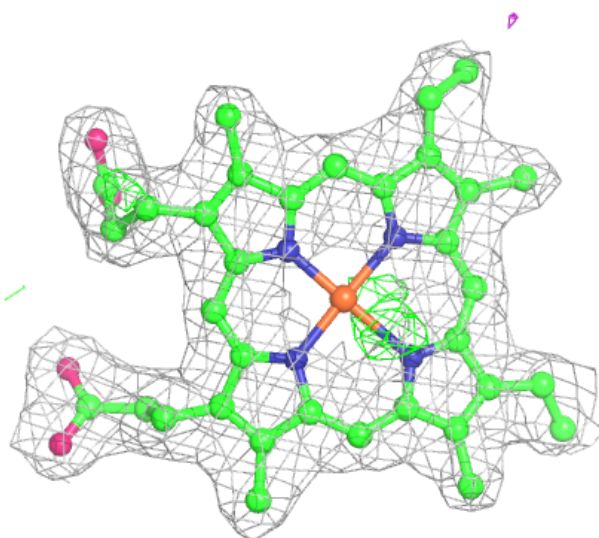
Electron density around HEM F 808:

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



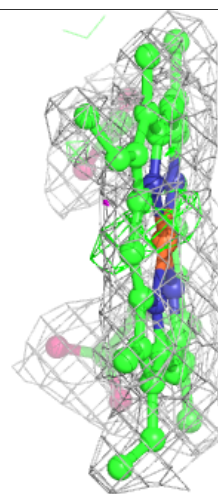
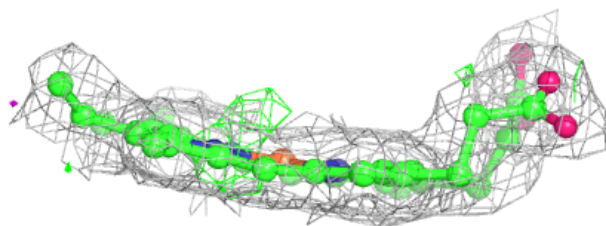
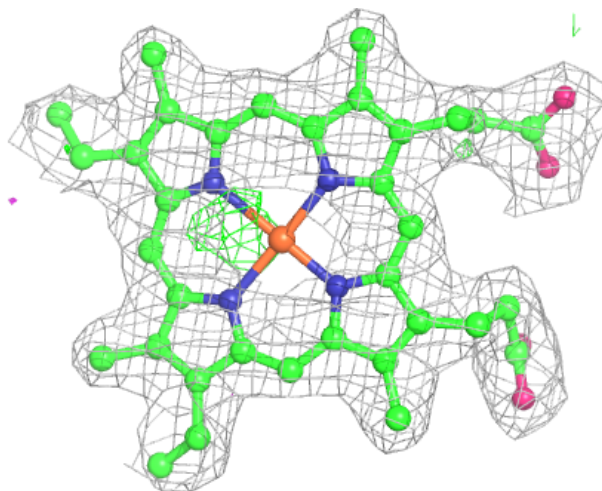
Electron density around HEM E 808:

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



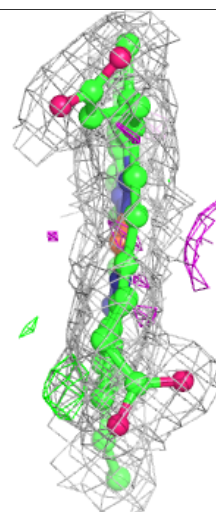
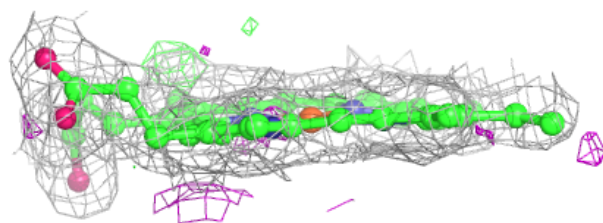
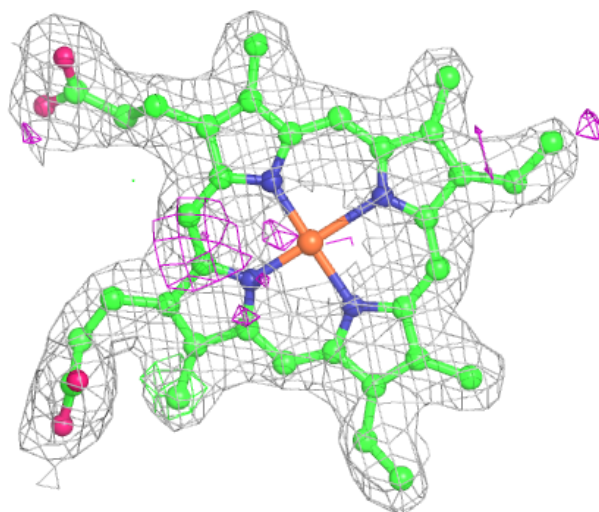
Electron density around HEM J 808:

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



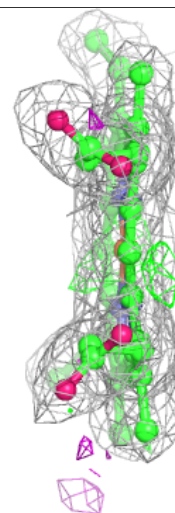
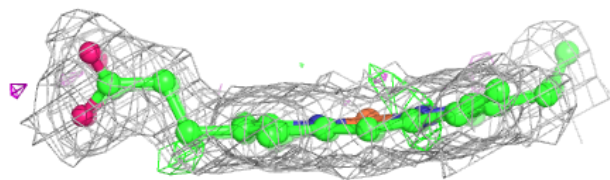
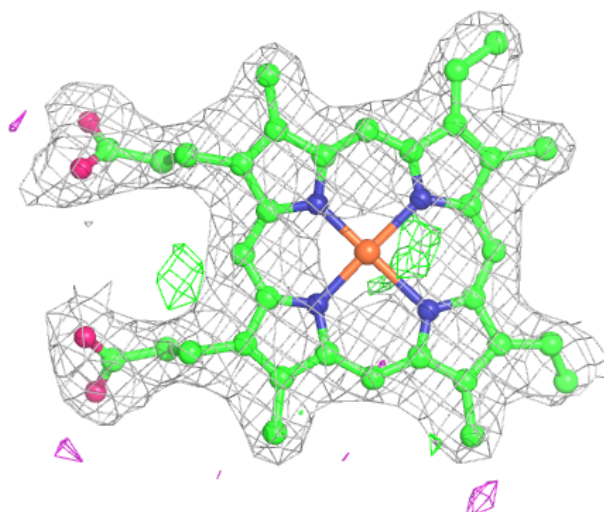
Electron density around HEM D 807:

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



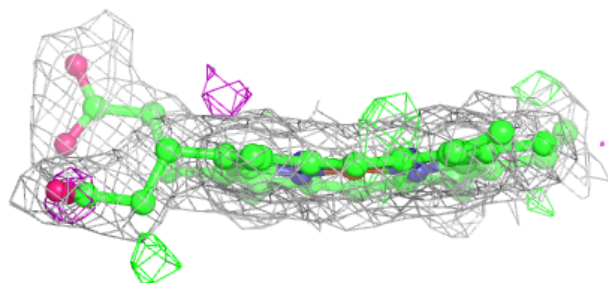
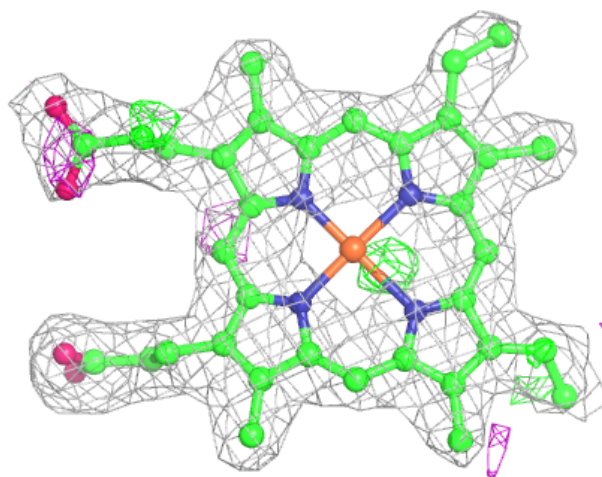
Electron density around HEM C 812:

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



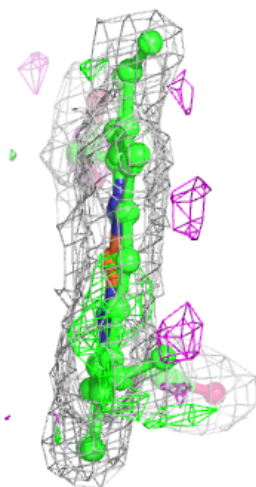
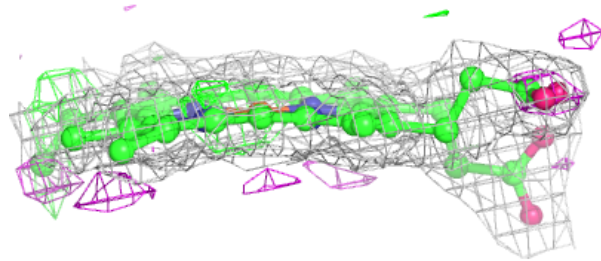
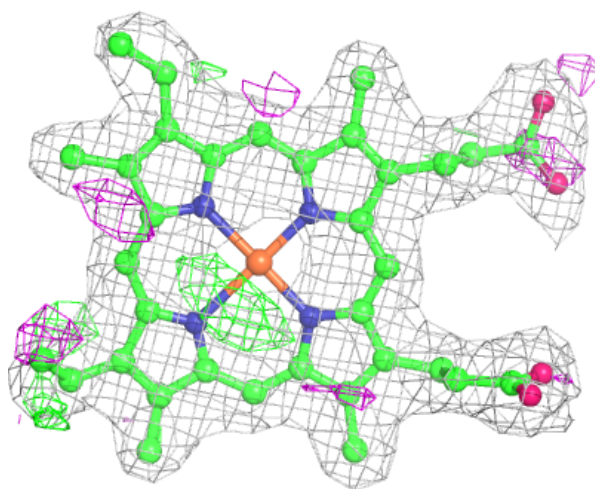
Electron density around HEM C 811:

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



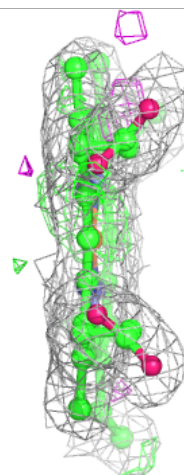
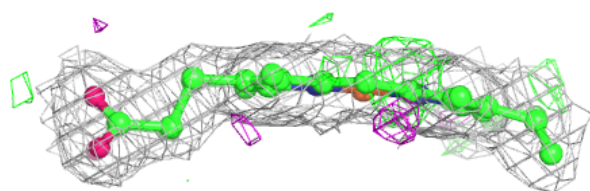
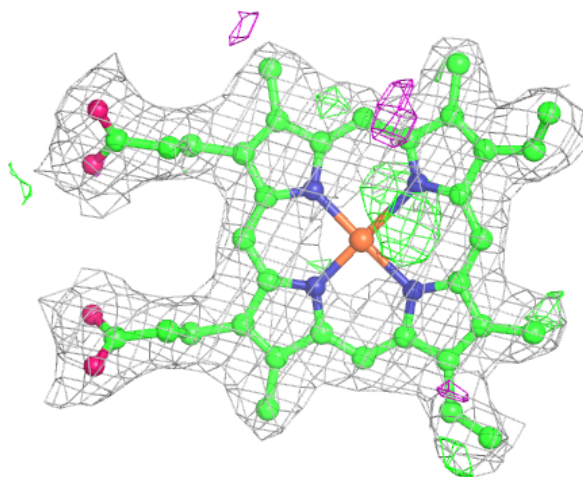
Electron density around HEM A 811:

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



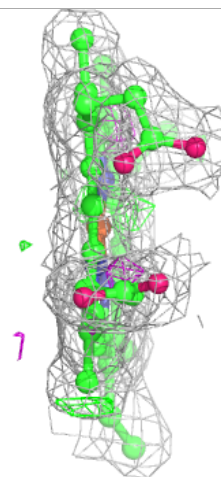
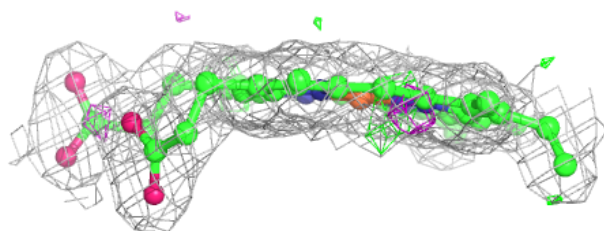
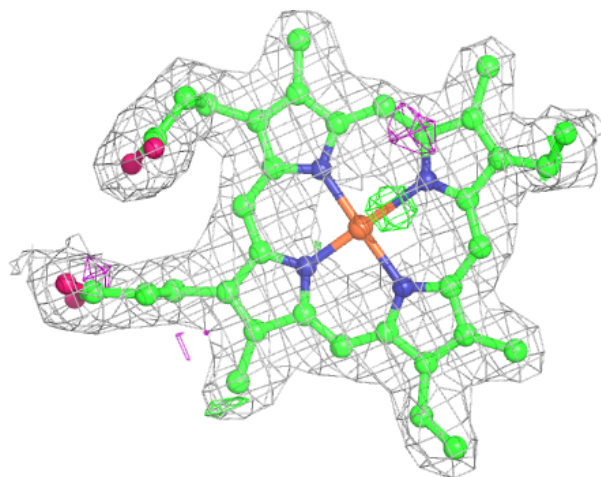
Electron density around HEM I 812:

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



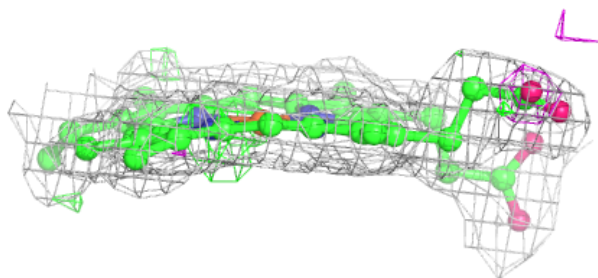
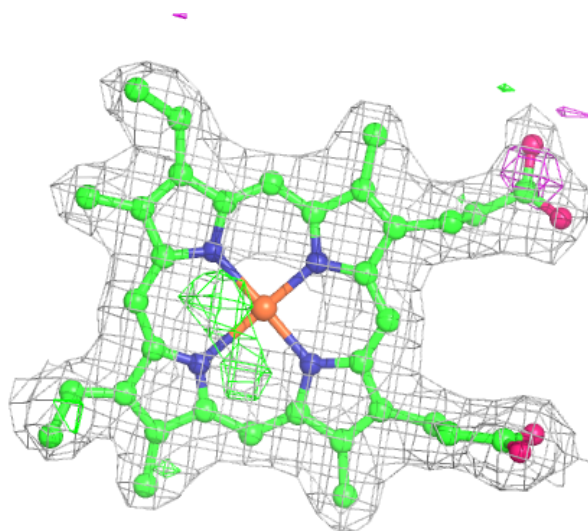
Electron density around HEM A 806:

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



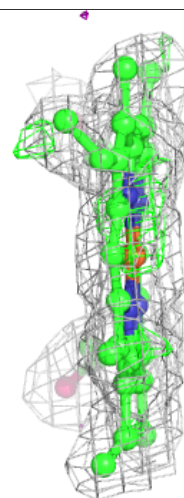
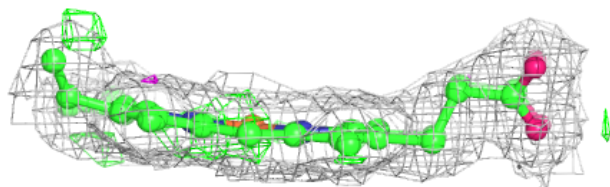
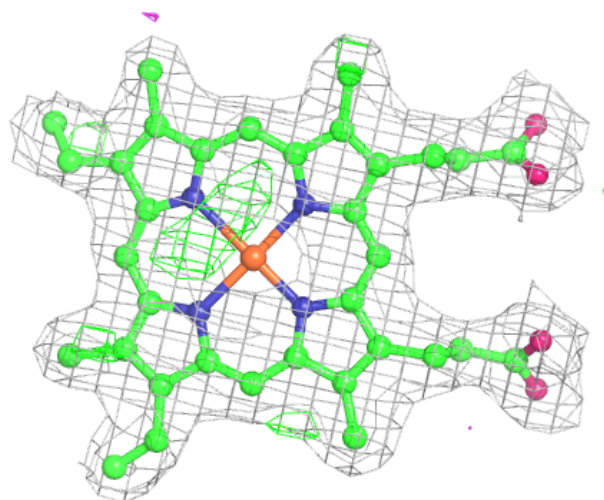
Electron density around HEM D 811:

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



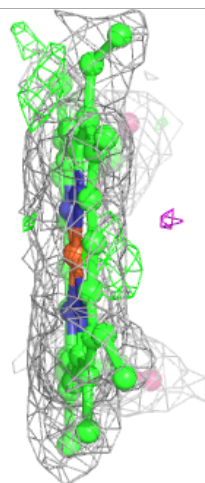
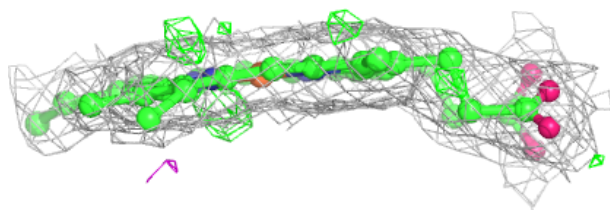
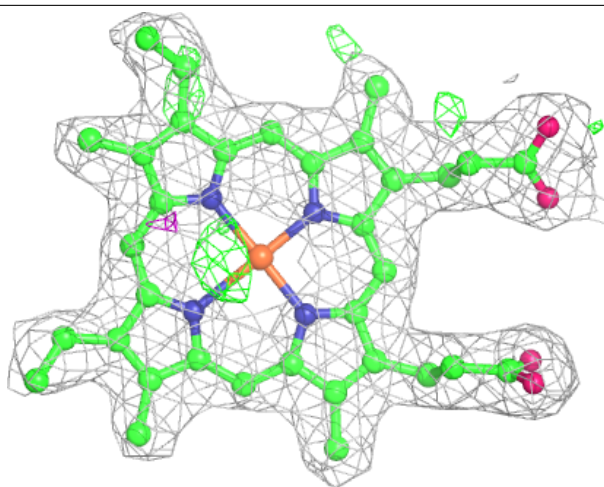
Electron density around HEM D 812:

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



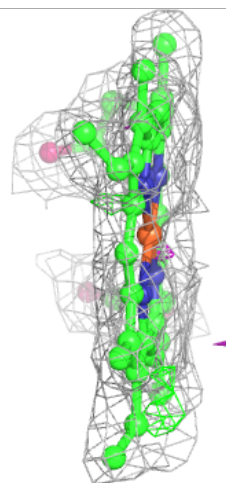
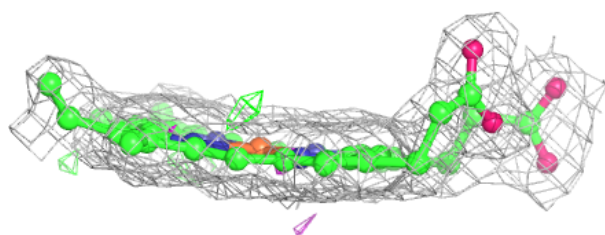
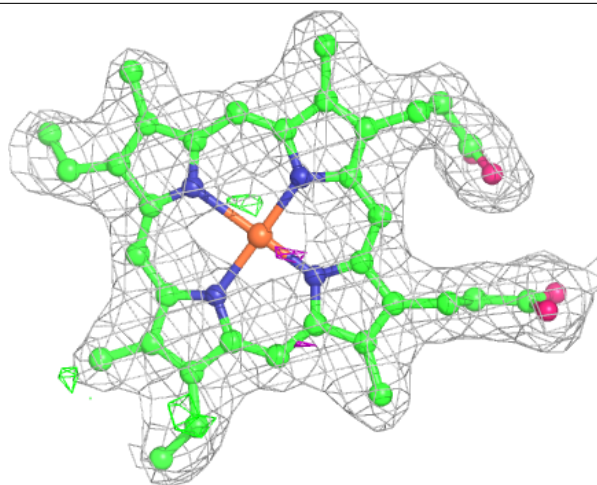
Electron density around HEM F 810:

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



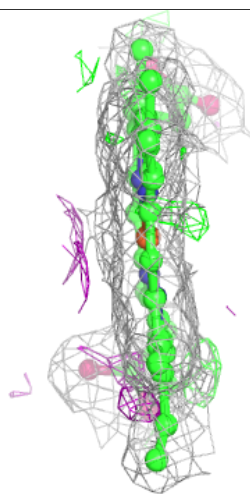
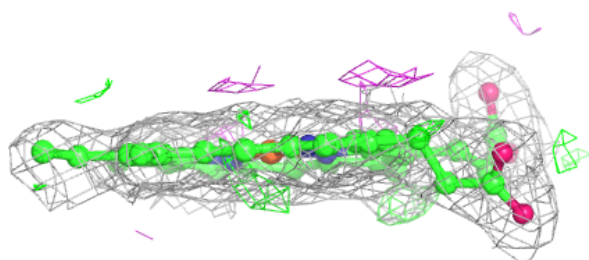
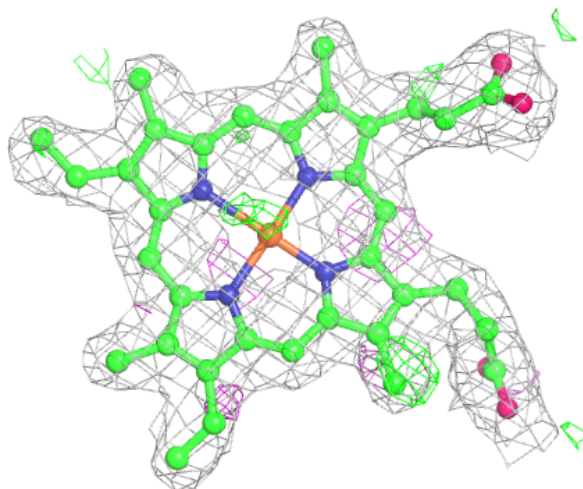
Electron density around HEM E 806:

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



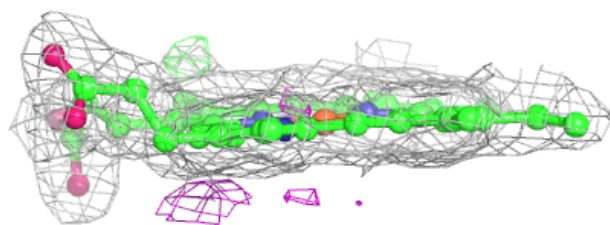
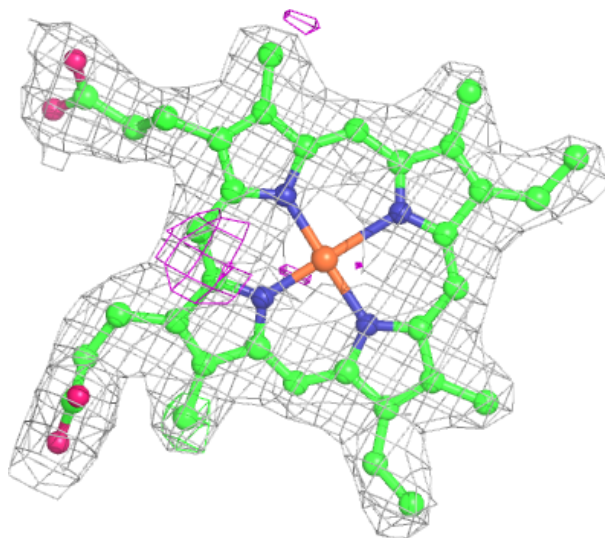
Electron density around HEM C 807:

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



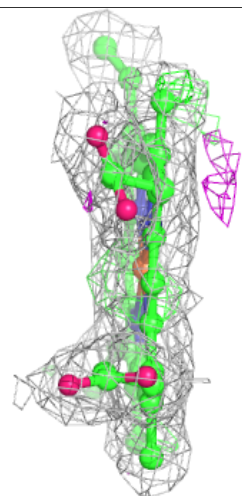
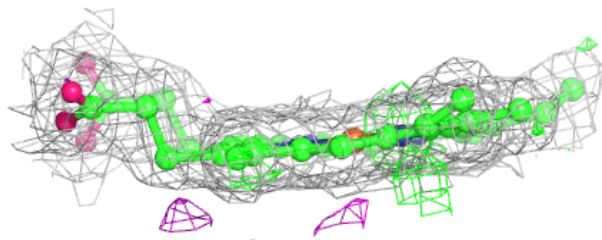
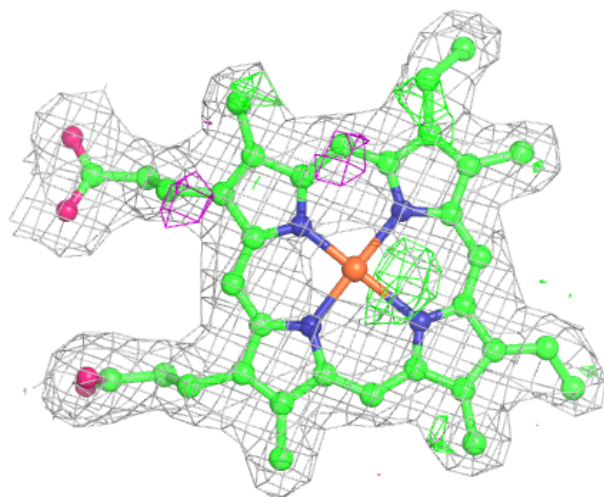
Electron density around HEM G 807:

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



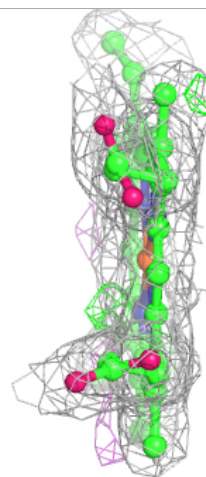
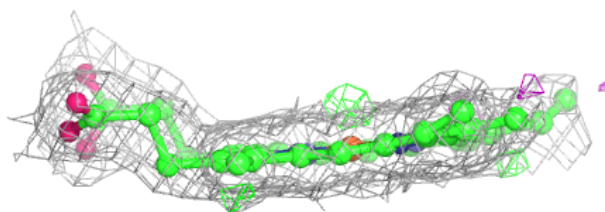
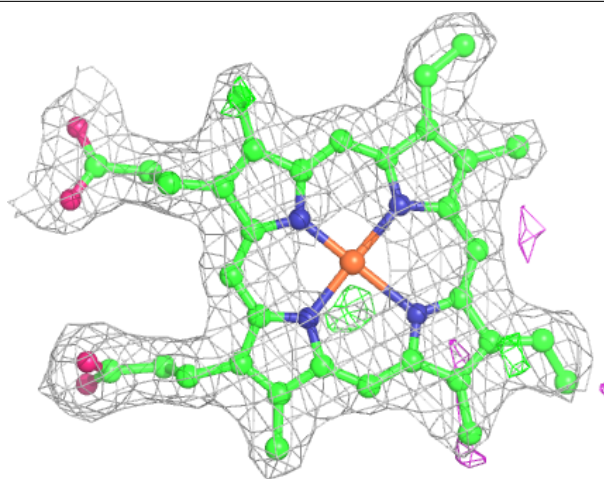
Electron density around HEM A 809:

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



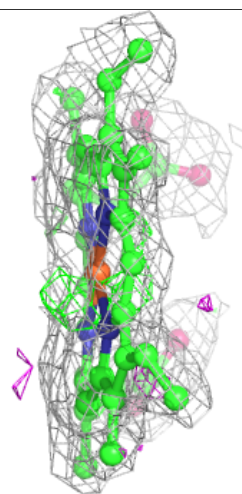
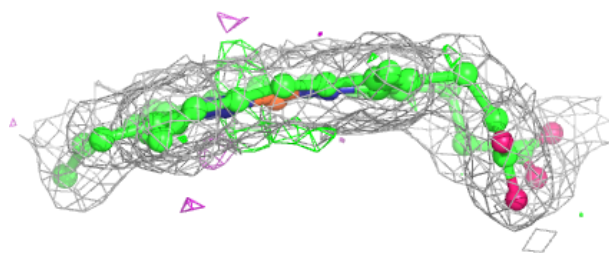
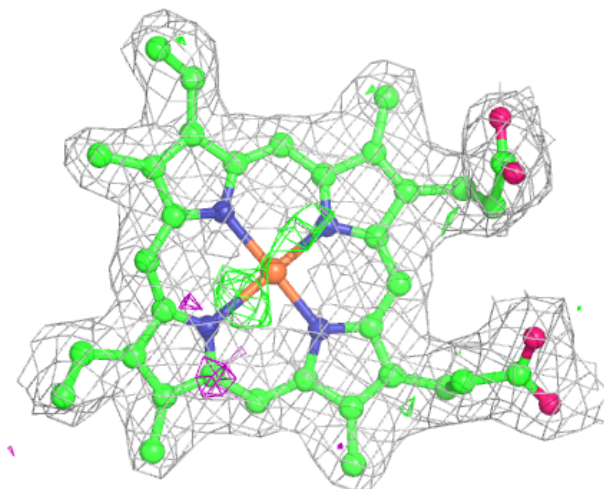
Electron density around HEM B 810:

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



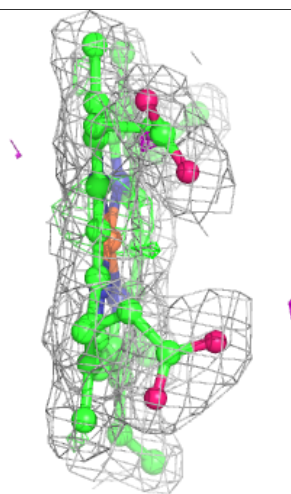
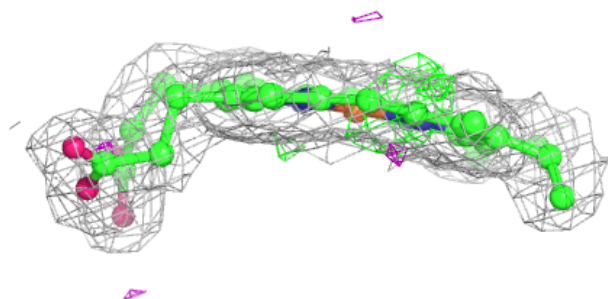
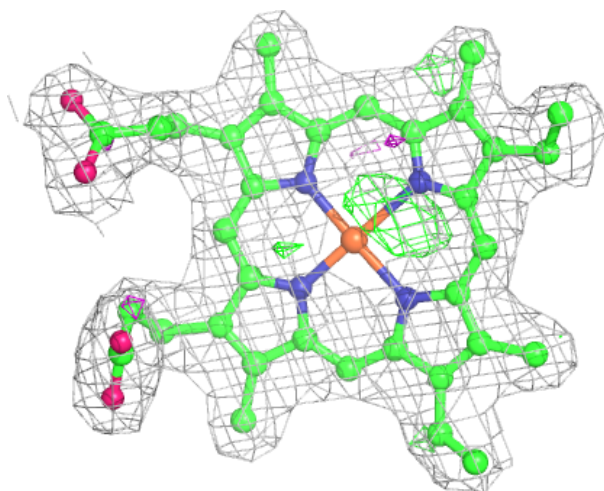
Electron density around HEM B 809:

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



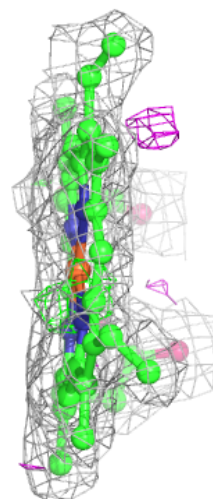
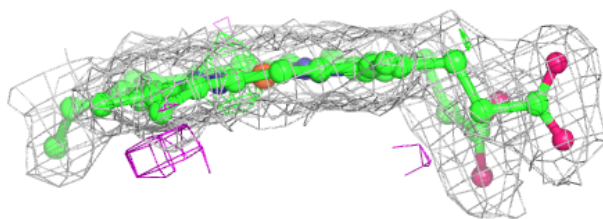
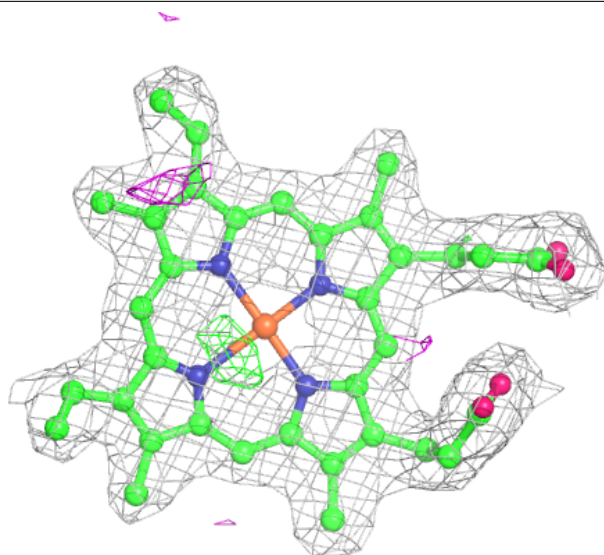
Electron density around HEM C 808:

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



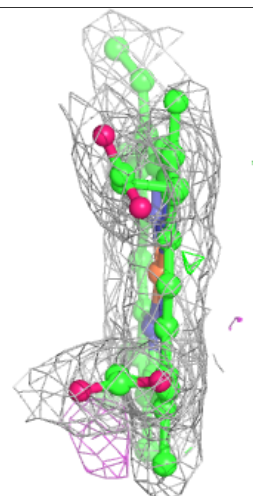
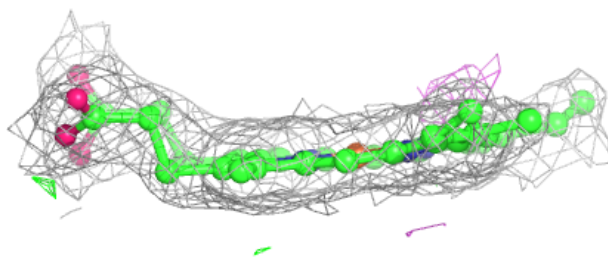
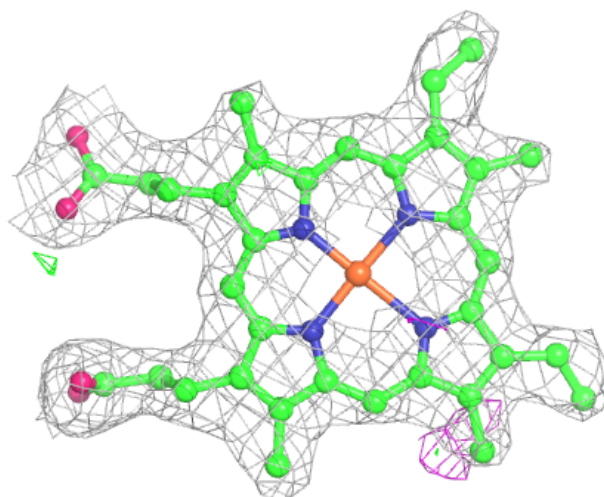
Electron density around HEM C 806:

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



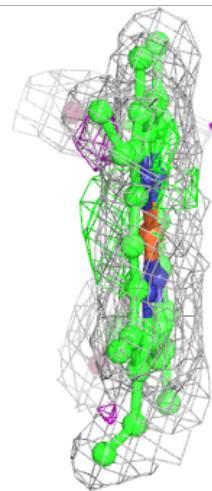
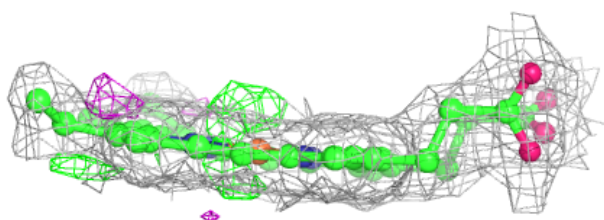
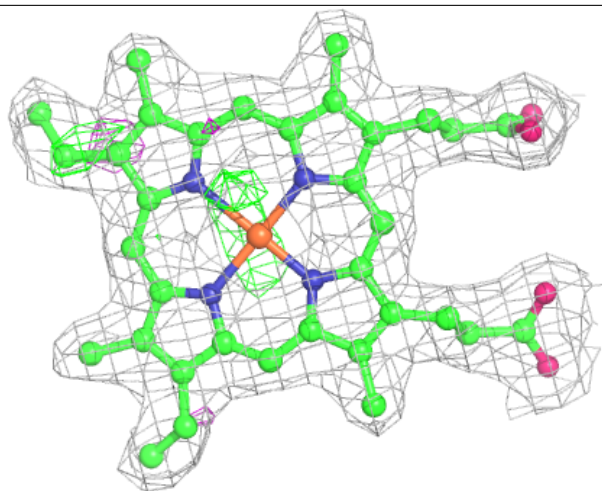
Electron density around HEM J 809:

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



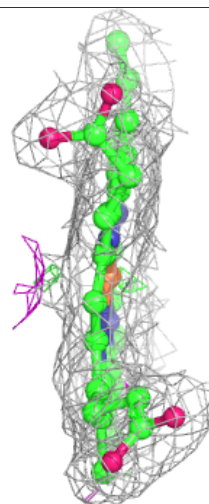
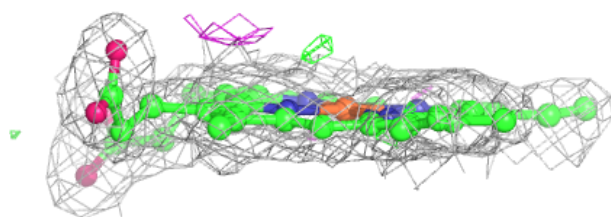
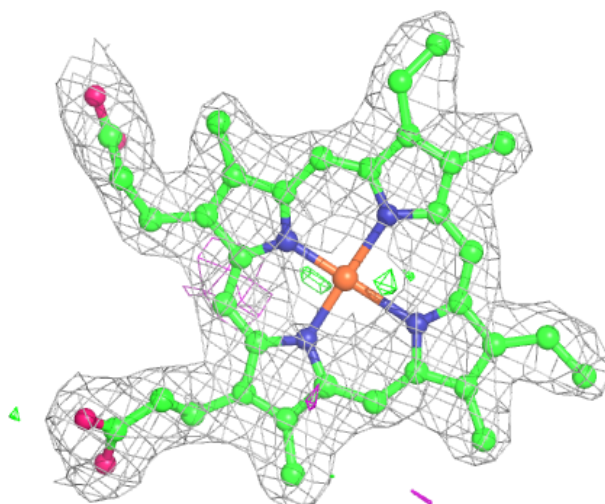
Electron density around HEM C 809:

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



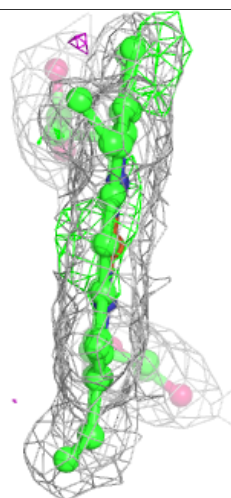
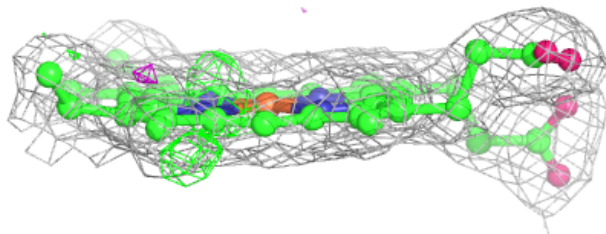
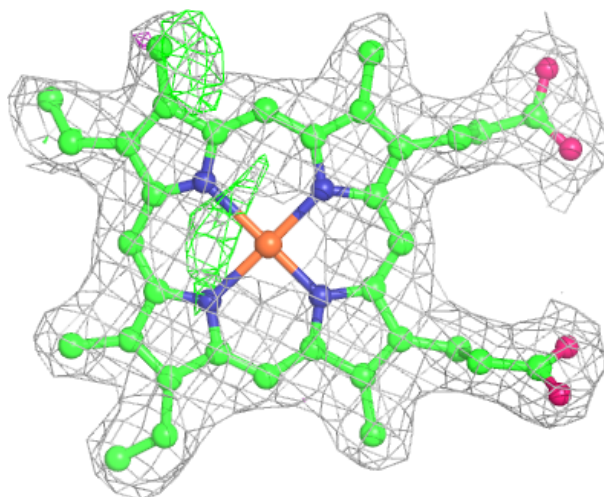
Electron density around HEM B 808:

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



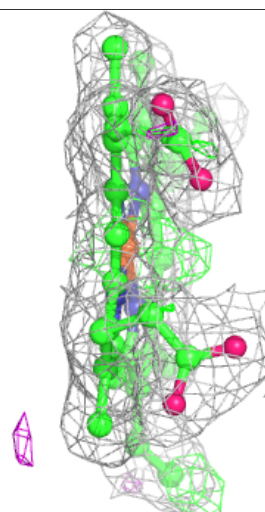
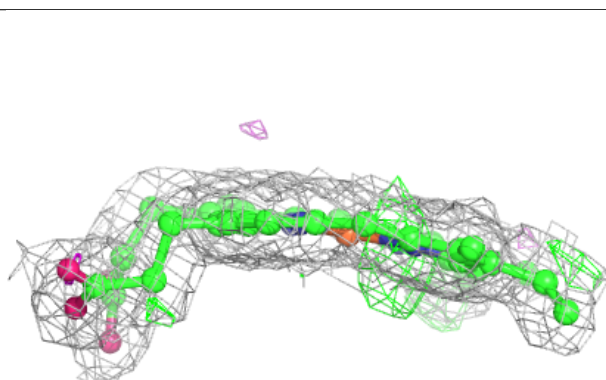
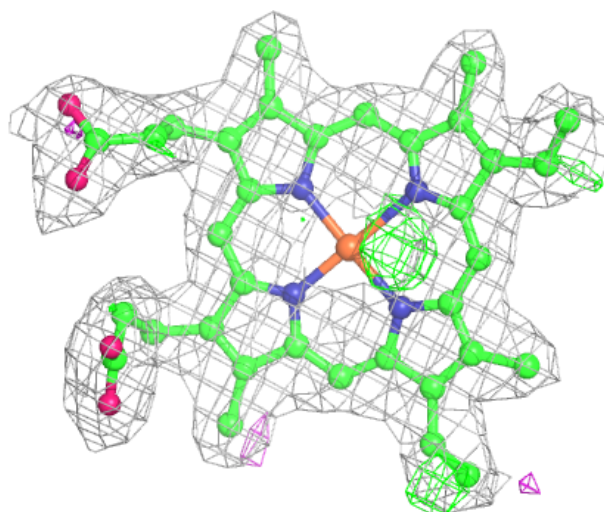
Electron density around HEM F 811:

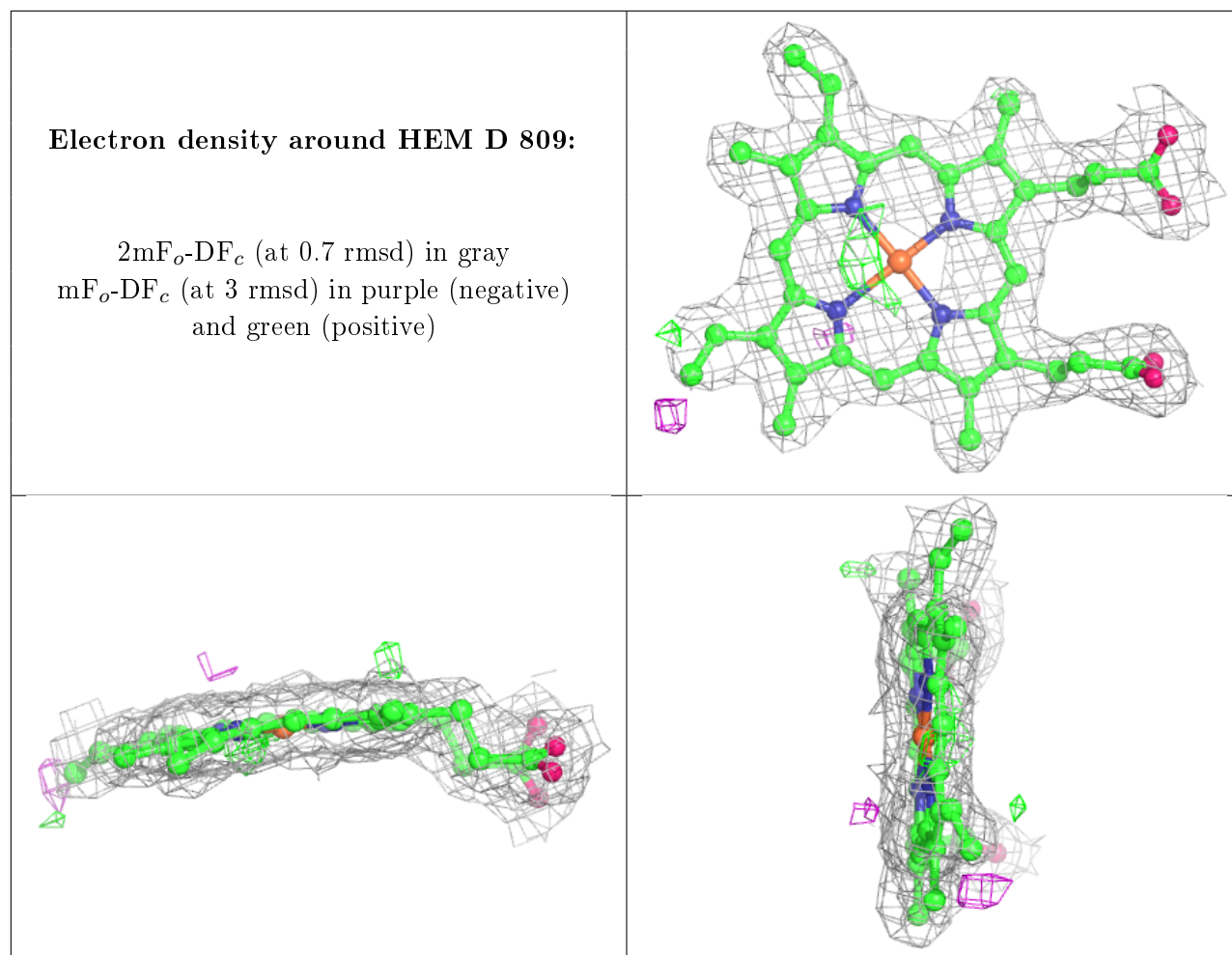
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 808:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.