



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:36 am BST

PDB ID : 6HIF  
Title : Kuenenia stuttgartiensis hydrazine dehydrogenase complex  
Authors : Akram, M.; Dietl, A.; Mersdorf, U.; Prinz, S.; Maalcke, W.; Keltjens, J.; Ferousi, C.; de Almeida, N.M.; Reimann, J.; Kartal, B.; Jetten, M.S.M.; Parey, K.; Barends, T.R.M.  
Deposited on : 2018-08-29  
Resolution : 2.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

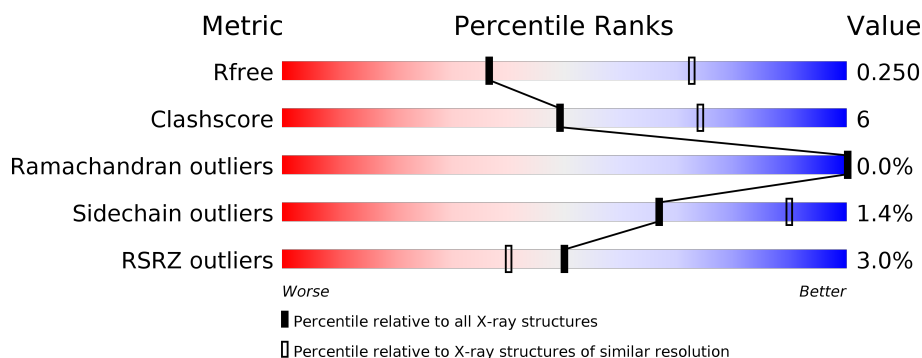
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	582	<div> <div>2%</div> <div>80% 11% 9%</div> </div>
1	B	582	<div> <div>2%</div> <div>82% 9% 9%</div> </div>
1	C	582	<div> <div>82% 10% 9%</div> </div>
1	D	582	<div> <div>74% 17% 9%</div> </div>
1	E	582	<div> <div>2%</div> <div>81% 10% 9%</div> </div>
1	F	582	<div> <div>2%</div> <div>80% 11% 9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	582	
1	H	582	
1	I	582	
1	J	582	
1	K	582	
1	L	582	
1	M	582	
1	N	582	
1	O	582	
1	P	582	
1	Q	582	
1	R	582	
1	S	582	
1	T	582	
1	U	582	
1	V	582	
1	W	582	
1	X	582	
2	Y	114	
2	Z	114	
2	a	114	
2	b	114	
2	c	114	
2	d	114	
2	e	114	

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Mol	Chain	Length	Quality of chain
2	f	114	
2	g	114	
2	h	114	
2	i	114	
2	j	114	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	G	610	-	-	X	-
4	SO4	G	611	-	-	-	X
4	SO4	J	611	-	-	X	-
5	GOL	H	614	-	-	X	-
5	GOL	H	615	-	-	X	X
5	GOL	I	614	-	-	X	-
5	GOL	K	614	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 118753 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 Hydrazine dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	A	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	B	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	C	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	D	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	E	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	F	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	H	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	I	527	Total	C	N	O	S	0	0	0
			4201	2633	739	793	36			
1	J	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	K	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	L	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	M	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	N	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	O	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	P	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	R	531	Total	C	N	O	S	0	1	0
			4237	2653	749	799	36			
1	S	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	T	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	U	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	V	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	W	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	X	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			

- Molecule 2 is a protein called hdh assembly factor Kustc1130.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	Z	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	a	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	b	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	c	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	d	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	e	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	f	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	g	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	h	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	i	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	j	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			

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- The chemical structure of HEC (Hydroxyethylchlorin) is shown. It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The structure includes various side chains and a central hydrogen atom (H). The atoms are labeled with green and red text, and the bonds are color-coded: green for the main ring and side chains, and red for the hydroxyl groups.

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



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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	M	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	M	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	M	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	M	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	M	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	M	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	M	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	M	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	O	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	O	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	O	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	O	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	O	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	O	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	O	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	O	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	R	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	R	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	R	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	R	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	R	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	R	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	R	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	R	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	S	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	S	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	S	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	S	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	S	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	S	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	S	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	S	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	T	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	T	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	T	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	T	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	T	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	T	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	T	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	T	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	U	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	U	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	U	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	U	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	U	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	U	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	U	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	U	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	U	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	W	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	W	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	W	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	W	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	W	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	W	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	W	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	W	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	X	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	X	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	X	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	X	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	X	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	X	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	X	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	X	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		

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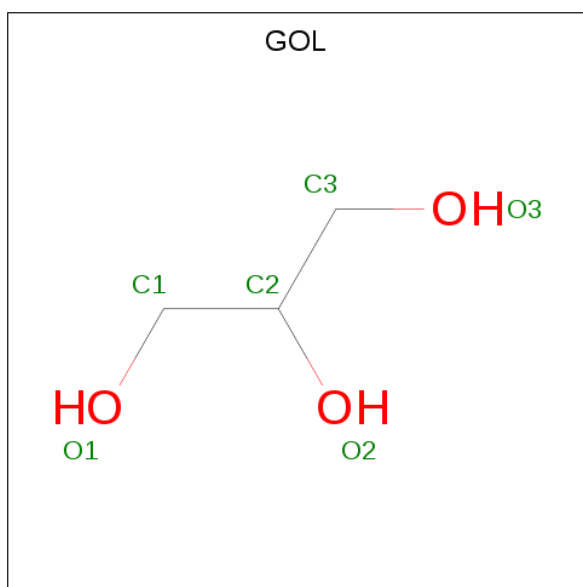
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total 5	O 4	S 1	0	0
4	L	1	Total 5	O 4	S 1	0	0
4	L	1	Total 5	O 4	S 1	0	0
4	M	1	Total 5	O 4	S 1	0	0
4	M	1	Total 5	O 4	S 1	0	0
4	M	1	Total 5	O 4	S 1	0	0
4	M	1	Total 5	O 4	S 1	0	0
4	N	1	Total 5	O 4	S 1	0	0
4	N	1	Total 5	O 4	S 1	0	0
4	N	1	Total 5	O 4	S 1	0	0
4	O	1	Total 5	O 4	S 1	0	0
4	O	1	Total 5	O 4	S 1	0	0
4	O	1	Total 5	O 4	S 1	0	0
4	P	1	Total 5	O 4	S 1	0	0
4	Q	1	Total 5	O 4	S 1	0	0
4	Q	1	Total 5	O 4	S 1	0	0
4	Q	1	Total 5	O 4	S 1	0	0
4	R	1	Total 5	O 4	S 1	0	0
4	R	1	Total 5	O 4	S 1	0	0
4	R	1	Total 5	O 4	S 1	0	0
4	S	1	Total 5	O 4	S 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	S	1	Total	O	S	0	0
			5	4	1		
4	T	1	Total	O	S	0	0
			5	4	1		
4	U	1	Total	O	S	0	0
			5	4	1		
4	U	1	Total	O	S	0	0
			5	4	1		
4	U	1	Total	O	S	0	0
			5	4	1		
4	V	1	Total	O	S	0	0
			5	4	1		
4	V	1	Total	O	S	0	0
			5	4	1		
4	V	1	Total	O	S	0	0
			5	4	1		
4	W	1	Total	O	S	0	0
			5	4	1		
4	X	1	Total	O	S	0	0
			5	4	1		
4	X	1	Total	O	S	0	0
			5	4	1		
4	X	1	Total	O	S	0	0
			5	4	1		
4	Y	1	Total	O	S	0	0
			5	4	1		
4	Y	1	Total	O	S	0	0
			5	4	1		
4	a	1	Total	O	S	0	0
			5	4	1		
4	c	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	C	O	0	0
			6	3	3		
5	G	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		
5	I	1	Total	C	O	0	0
			6	3	3		
5	I	1	Total	C	O	0	0
			6	3	3		
5	I	1	Total	C	O	0	0
			6	3	3		
5	J	1	Total	C	O	0	0
			6	3	3		
5	J	1	Total	C	O	0	0
			6	3	3		
5	K	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	K	1	Total	C	O	0	0
			6	3	3		
5	K	1	Total	C	O	0	0
			6	3	3		
5	K	1	Total	C	O	0	0
			6	3	3		
5	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	1	Total	K	0	0
			1	1		
6	X	1	Total	K	0	0
			1	1		
6	Q	1	Total	K	0	0
			1	1		
6	K	1	Total	K	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	78	Total	O	0	0
			78	78		
7	A	33	Total	O	0	0
			33	33		
7	B	40	Total	O	0	0
			40	40		
7	C	36	Total	O	0	0
			36	36		
7	D	21	Total	O	0	0
			21	21		
7	E	21	Total	O	0	0
			21	21		
7	F	24	Total	O	0	0
			24	24		
7	H	70	Total	O	0	0
			70	70		
7	I	62	Total	O	0	0
			62	62		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	J	78	Total O 78 78	0	0
7	K	57	Total O 57 57	0	0
7	L	69	Total O 69 69	0	0
7	M	27	Total O 27 27	0	0
7	N	37	Total O 37 37	0	0
7	O	40	Total O 40 40	0	0
7	P	50	Total O 50 50	0	0
7	Q	48	Total O 48 48	0	0
7	R	49	Total O 49 49	0	0
7	S	4	Total O 4 4	0	0
7	T	15	Total O 15 15	0	0
7	U	15	Total O 15 15	0	0
7	V	17	Total O 17 17	0	0
7	W	12	Total O 12 12	0	0
7	X	13	Total O 13 13	0	0
7	Y	2	Total O 2 2	0	0
7	Z	1	Total O 1 1	0	0
7	a	2	Total O 2 2	0	0
7	b	2	Total O 2 2	0	0
7	c	2	Total O 2 2	0	0
7	d	2	Total O 2 2	0	0

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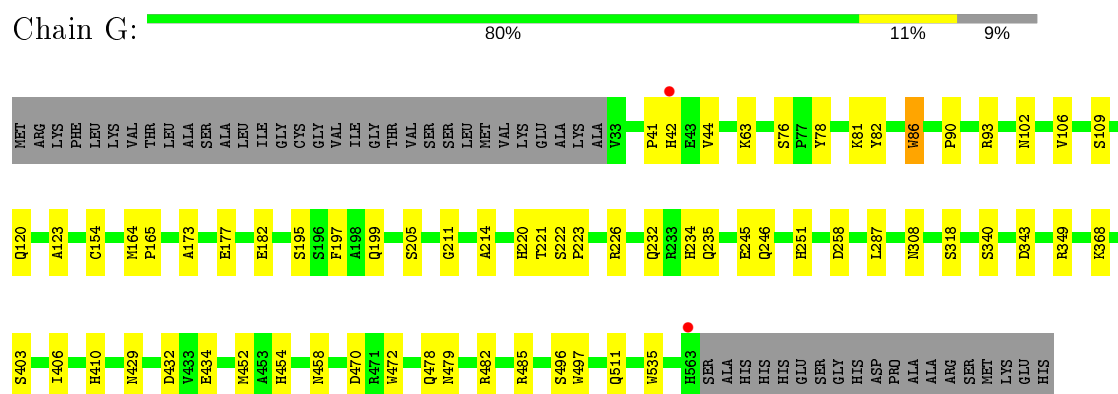
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	e	2	Total 2	O 2	0	0
7	f	2	Total 2	O 2	0	0
7	g	1	Total 1	O 1	0	0
7	i	2	Total 2	O 2	0	0
7	j	1	Total 1	O 1	0	0

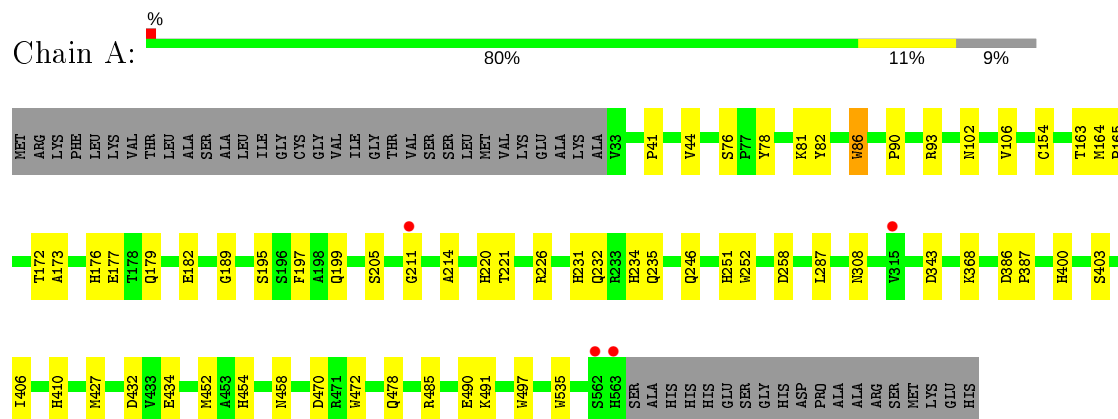
### 3 Residue-property plots

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

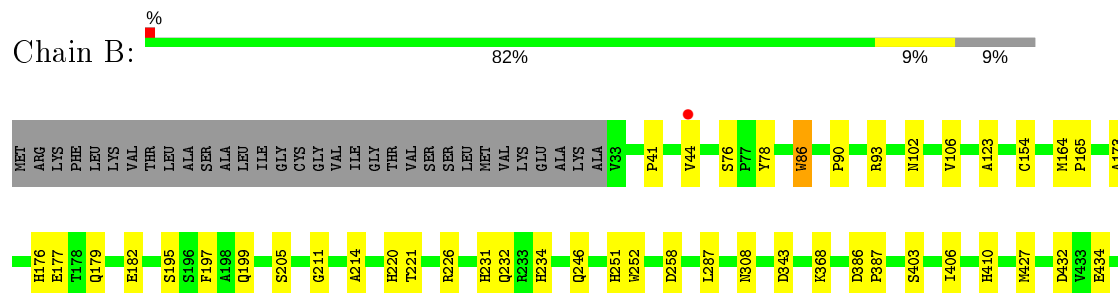
- Molecule 1: Hydrazine dehydrogenase

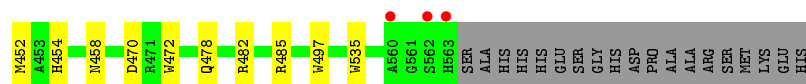


- Molecule 1: Hydrazine dehydrogenase



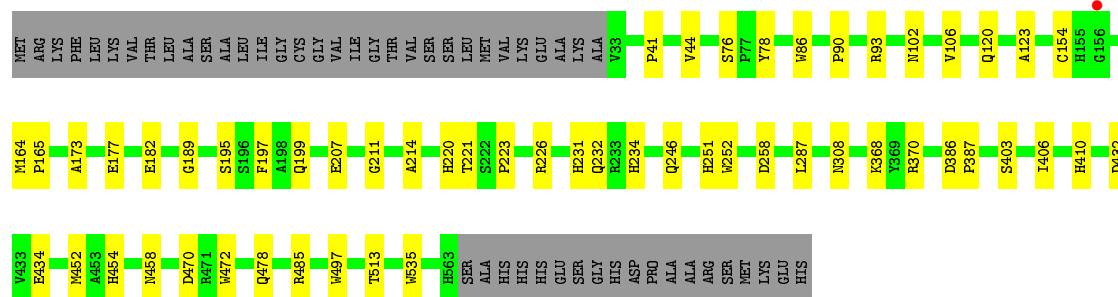
- Molecule 1: Hydrazine dehydrogenase





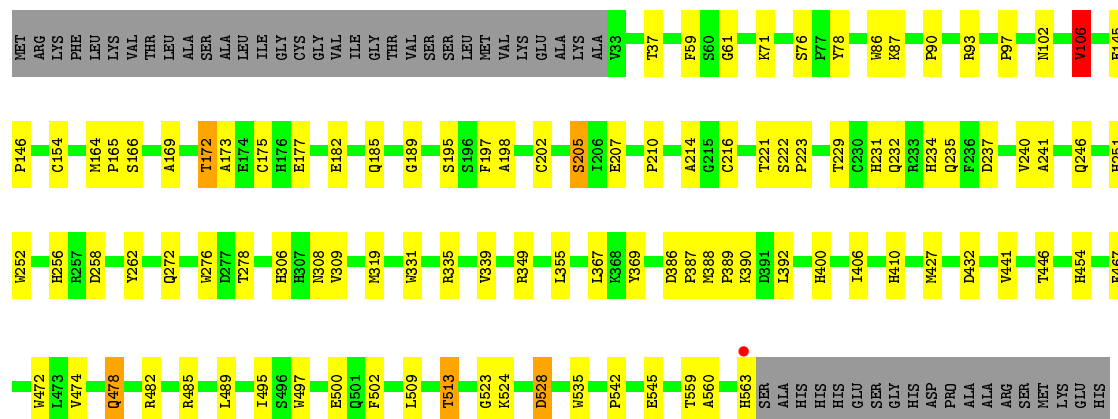
• Molecule 1: Hydrazine dehydrogenase

Chain C: 82% 10% 9%



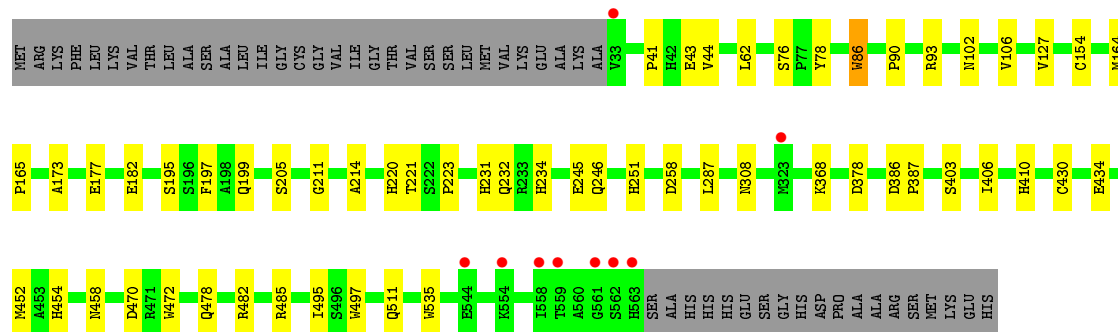
• Molecule 1: Hydrazine dehydrogenase

Chain D: 74% 17% 9%



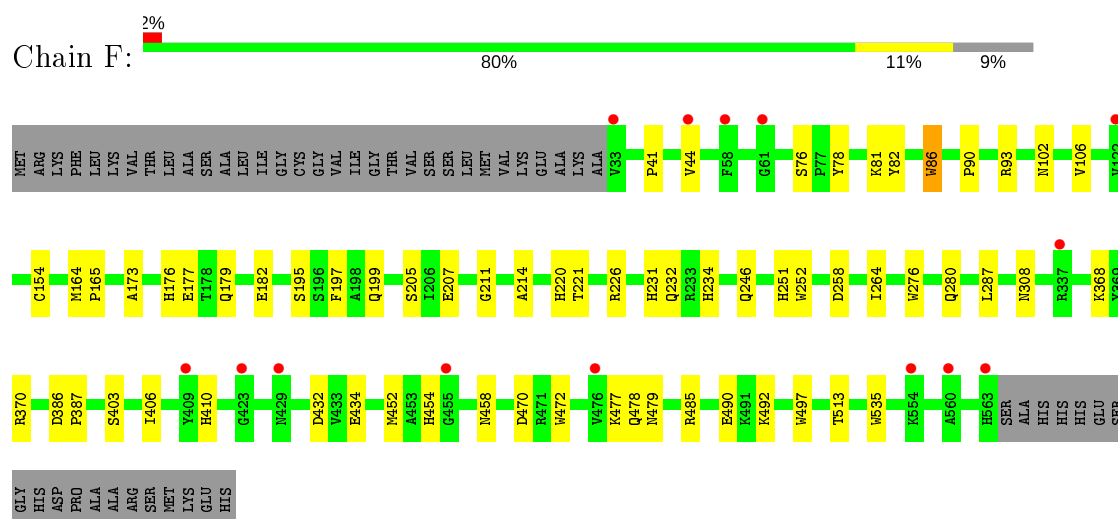
• Molecule 1: Hydrazine dehydrogenase

Chain E: 2% 81% 10% 9%

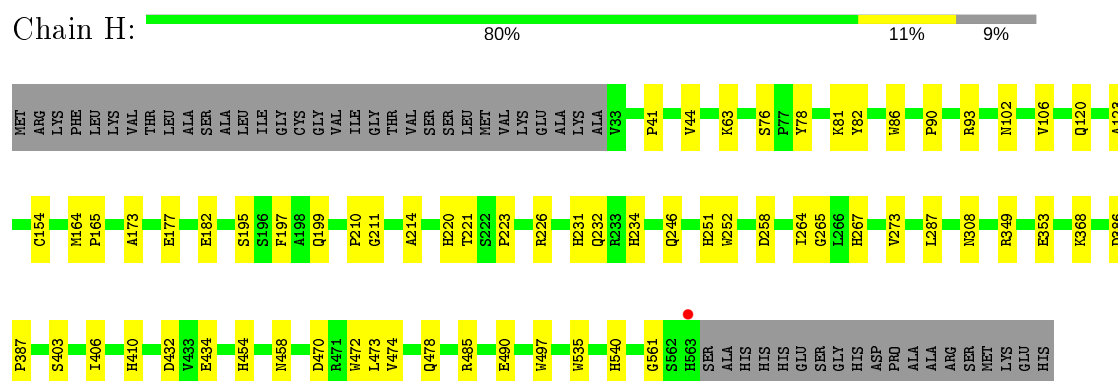


• Molecule 1: Hydrazine dehydrogenase

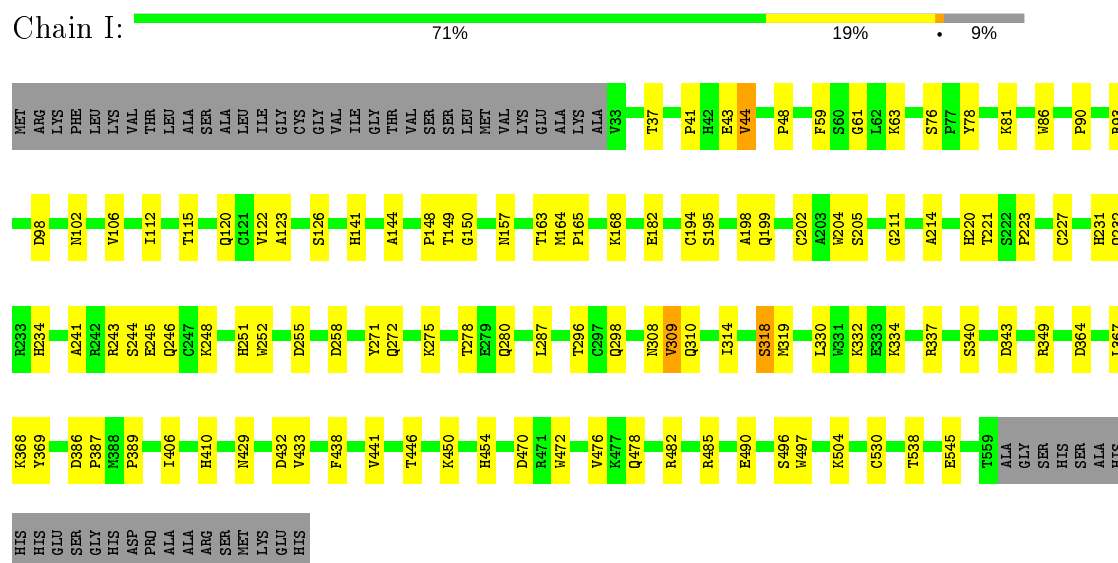





- Molecule 1: Hydrazine dehydrogenase

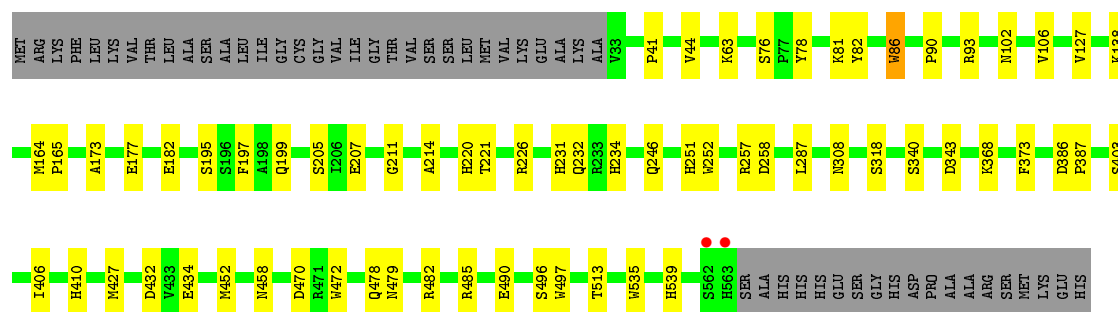


- Molecule 1: Hydrazine dehydrogenase




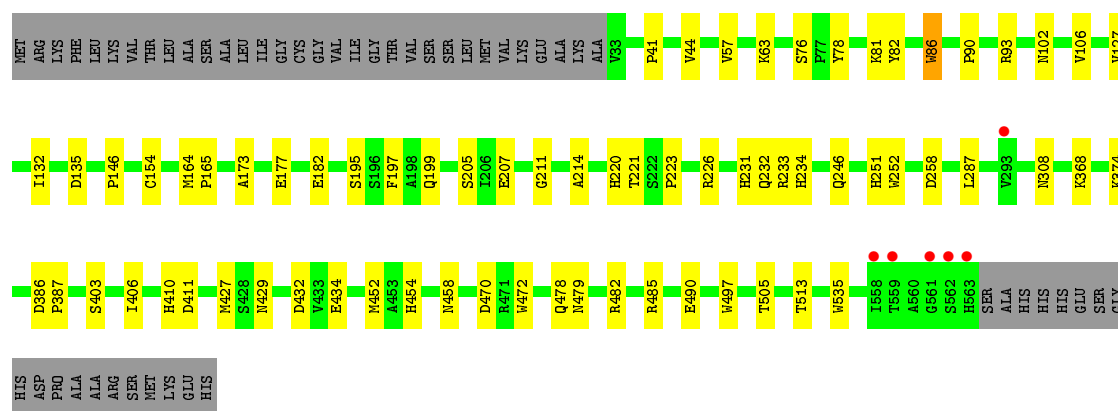
- Molecule 1: Hydrazine dehydrogenase

Chain J: 




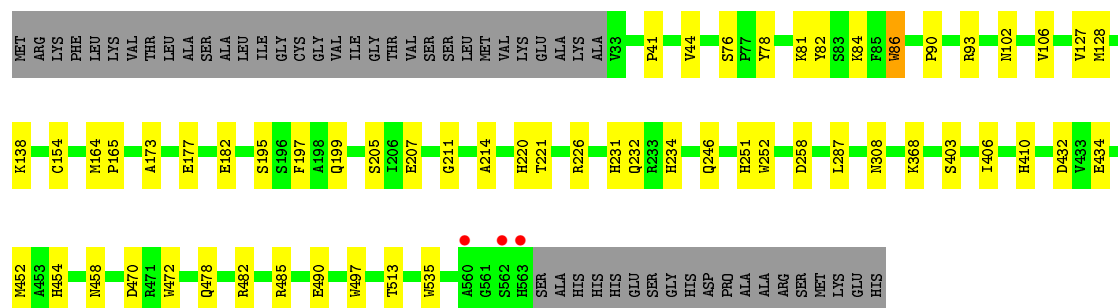
• Molecule 1: Hydrazine dehydrogenase

Chain K: 




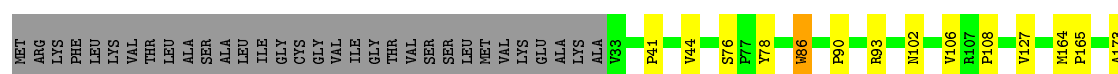
• Molecule 1: Hydrazine dehydrogenase

Chain L: 

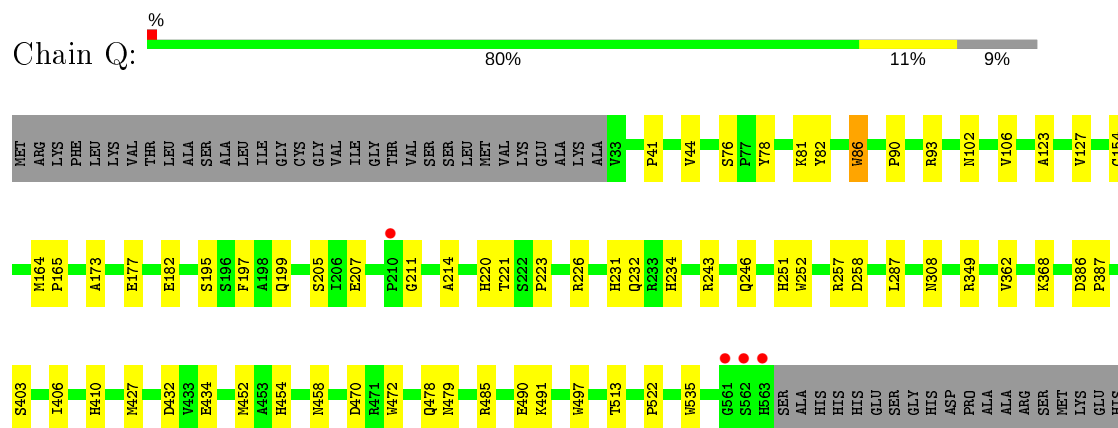


• Molecule 1: Hydrazine dehydrogenase

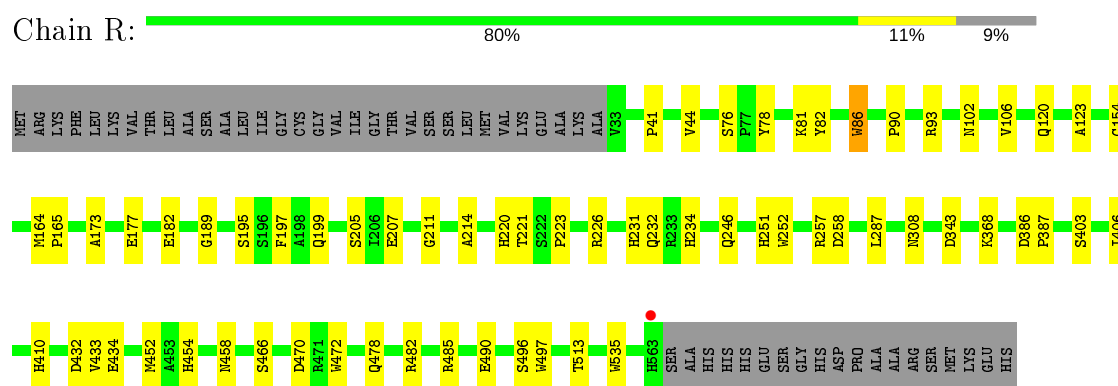
Chain M: 



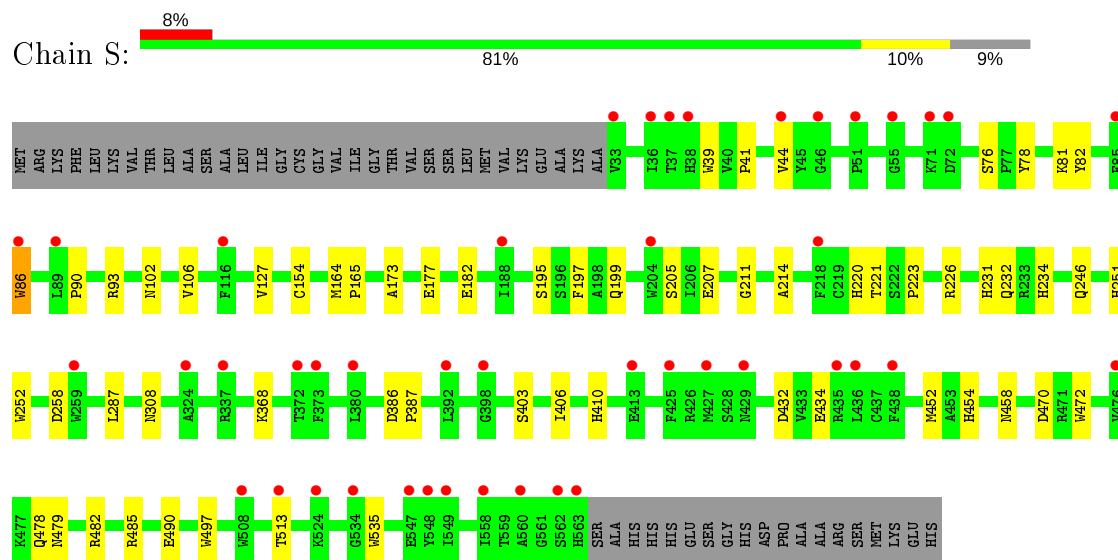




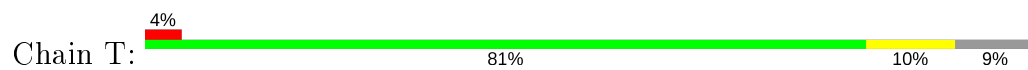
• Molecule 1: Hydrazine dehydrogenase

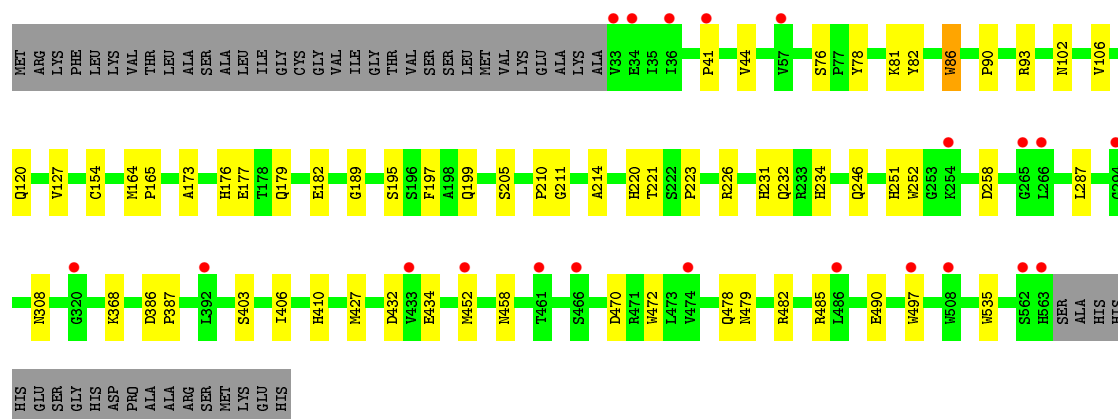


• Molecule 1: Hydrazine dehydrogenase

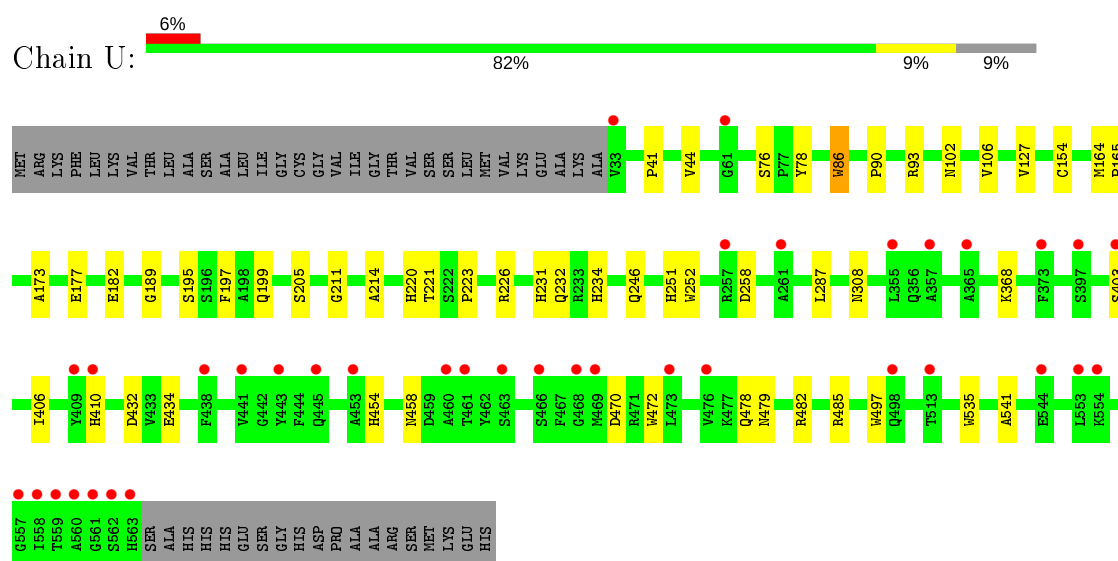


• Molecule 1: Hydrazine dehydrogenase

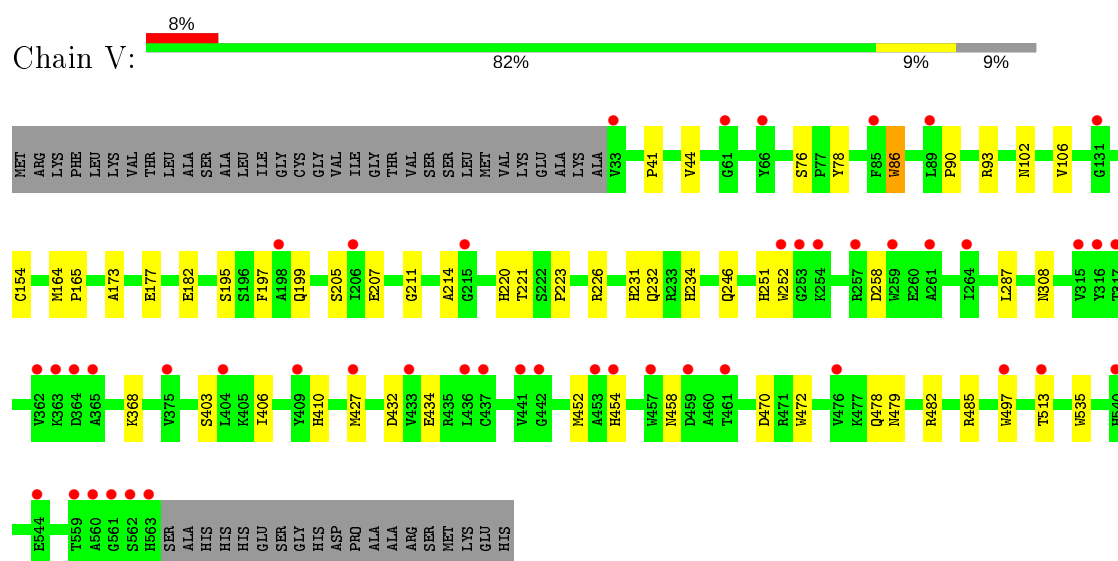




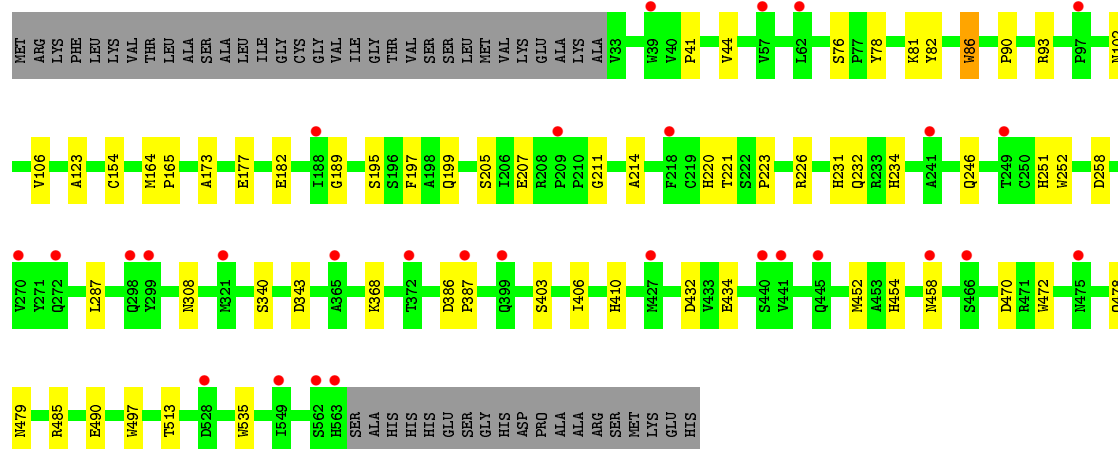
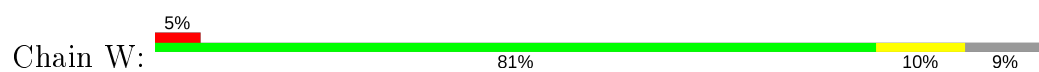
• Molecule 1: Hydrazine dehydrogenase



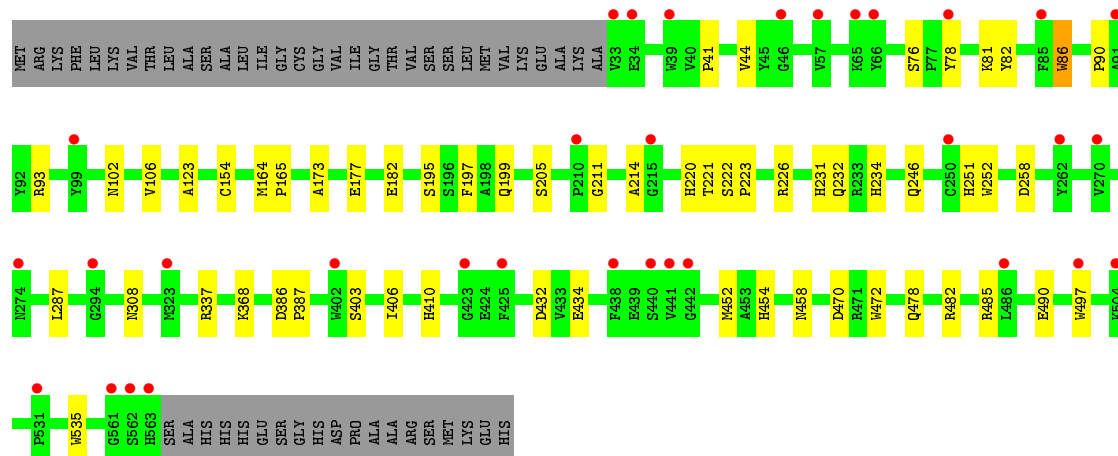
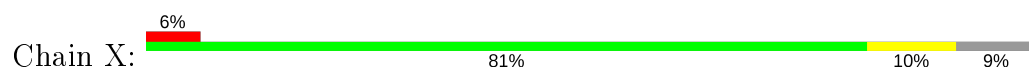
• Molecule 1: Hydrazine dehydrogenase



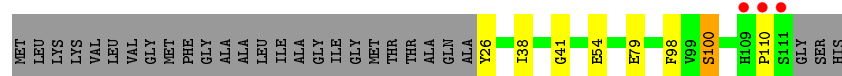
• Molecule 1: Hydrazine dehydrogenase



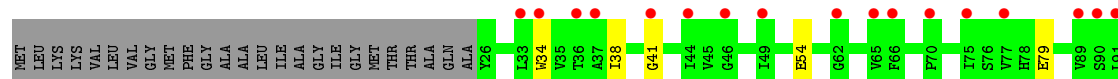
• Molecule 1: Hydrazine dehydrogenase

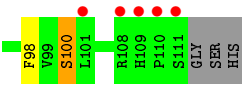


• Molecule 2: hdh assembly factor Kustc1130



• Molecule 2: hdh assembly factor Kustc1130

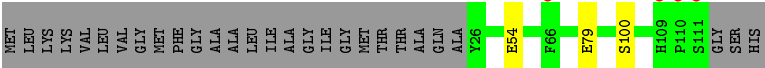




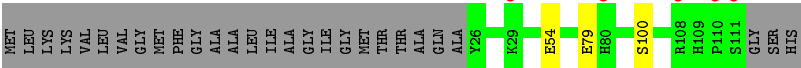
• Molecule 2: hdh assembly factor Kustc1130



• Molecule 2: hdh assembly factor Kustc1130



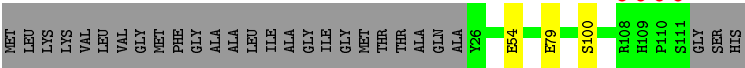
• Molecule 2: hdh assembly factor Kustc1130



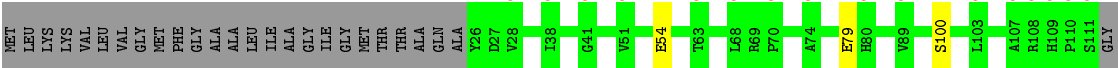
• Molecule 2: hdh assembly factor Kustc1130



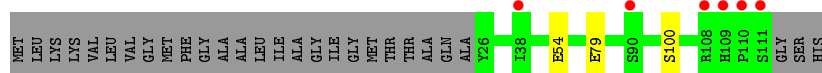
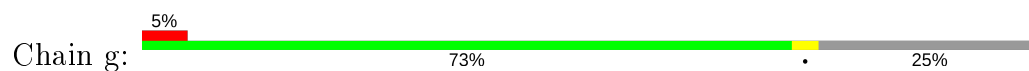
• Molecule 2: hdh assembly factor Kustc1130



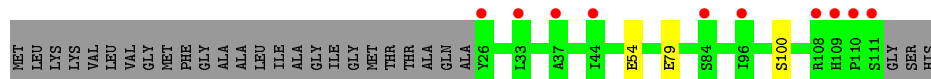
• Molecule 2: hdh assembly factor Kustc1130



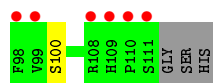
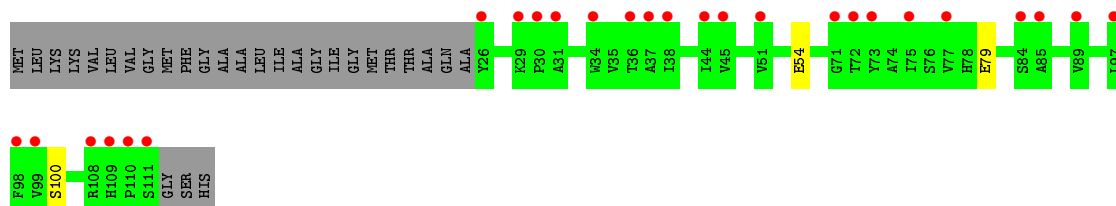
- Molecule 2: hdh assembly factor Kustc1130



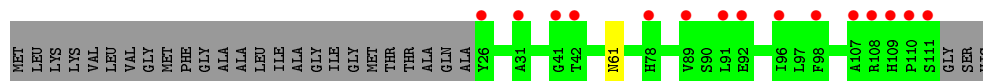
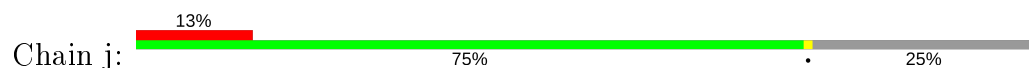
- Molecule 2: hdh assembly factor Kustc1130



- Molecule 2: hdh assembly factor Kustc1130



- Molecule 2: hdh assembly factor Kustc1130





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.86Å 211.86Å 398.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	93.71 – 2.80 93.54 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.6 (93.71-2.80) 96.6 (93.54-2.80)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, $R_{free}$	0.221 , 0.238 0.220 , 0.250	Depositor DCC
$R_{free}$ test set	30022 reflections (6.31%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.7	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.000 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	118753	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, K, SO4, HEC

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	0.26	0/4355	0.49	0/5901
1	B	0.26	0/4355	0.49	0/5901
1	C	0.26	0/4355	0.49	0/5901
1	D	0.26	0/4355	0.52	0/5901
1	E	0.26	0/4355	0.49	0/5901
1	F	0.26	0/4355	0.49	0/5901
1	G	0.27	0/4355	0.50	0/5901
1	H	0.27	0/4355	0.49	0/5901
1	I	0.28	0/4329	0.55	0/5866
1	J	0.28	0/4355	0.49	0/5901
1	K	0.27	0/4355	0.49	0/5901
1	L	0.27	0/4355	0.49	0/5901
1	M	0.26	0/4355	0.49	0/5901
1	N	0.26	0/4355	0.49	0/5901
1	O	0.27	0/4355	0.49	0/5901
1	P	0.27	0/4355	0.49	0/5901
1	Q	0.27	0/4355	0.49	0/5901
1	R	0.27	0/4366	0.49	0/5915
1	S	0.26	0/4355	0.49	0/5901
1	T	0.26	0/4355	0.49	0/5901
1	U	0.26	0/4355	0.49	0/5901
1	V	0.26	0/4355	0.49	0/5901
1	W	0.26	0/4355	0.49	0/5901
1	X	0.26	0/4355	0.49	0/5901
2	Y	0.27	0/653	0.54	0/887
2	Z	0.27	0/653	0.54	0/887
2	a	0.27	0/653	0.53	0/887
2	b	0.27	0/653	0.54	0/887
2	c	0.27	0/653	0.54	0/887
2	d	0.27	0/653	0.54	0/887
2	e	0.27	0/653	0.54	0/887
2	f	0.27	0/653	0.54	0/887

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	g	0.27	0/653	0.54	0/887
2	h	0.27	0/653	0.54	0/887
2	i	0.27	0/653	0.54	0/887
2	j	0.27	0/653	0.53	0/887
All	All	0.27	0/112341	0.50	0/152247

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4226	0	3941	48	1
1	B	4226	0	3941	44	0
1	C	4226	0	3941	46	0
1	D	4226	0	3941	69	0
1	E	4226	0	3941	46	0
1	F	4226	0	3941	45	0
1	G	4226	0	3941	63	2
1	H	4226	0	3941	71	0
1	I	4201	0	3921	92	0
1	J	4226	0	3941	58	1
1	K	4226	0	3941	67	0
1	L	4226	0	3941	49	0
1	M	4226	0	3941	42	0
1	N	4226	0	3941	47	0
1	O	4226	0	3941	49	0
1	P	4226	0	3941	49	0
1	Q	4226	0	3941	50	1
1	R	4237	0	3953	52	1
1	S	4226	0	3941	41	0
1	T	4226	0	3941	44	0
1	U	4226	0	3941	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	V	4226	0	3941	38	0
1	W	4226	0	3941	45	0
1	X	4226	0	3941	43	0
2	Y	640	0	627	5	0
2	Z	640	0	627	4	0
2	a	640	0	627	0	0
2	b	640	0	627	0	0
2	c	640	0	627	0	0
2	d	640	0	627	0	0
2	e	640	0	627	0	0
2	f	640	0	627	0	0
2	g	640	0	627	0	0
2	h	640	0	627	0	0
2	i	640	0	627	0	0
2	j	640	0	627	0	0
3	A	344	0	236	15	0
3	B	344	0	236	15	0
3	C	344	0	236	18	0
3	D	344	0	237	20	0
3	E	344	0	236	15	0
3	F	344	0	236	14	0
3	G	344	0	236	15	0
3	H	344	0	236	16	0
3	I	344	0	237	27	0
3	J	344	0	236	14	0
3	K	344	0	236	19	0
3	L	344	0	236	15	0
3	M	344	0	236	14	0
3	N	344	0	236	16	0
3	O	344	0	236	17	0
3	P	344	0	236	16	0
3	Q	344	0	236	17	0
3	R	344	0	236	17	0
3	S	344	0	236	15	0
3	T	344	0	236	15	0
3	U	344	0	236	17	0
3	V	344	0	236	16	0
3	W	344	0	236	18	0
3	X	344	0	236	16	0
4	A	15	0	0	0	0
4	B	10	0	0	1	0
4	C	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	5	0	0	0	0
4	E	10	0	0	0	0
4	F	10	0	0	0	0
4	G	30	0	0	3	0
4	H	25	0	0	1	0
4	I	20	0	0	0	0
4	J	15	0	0	2	0
4	K	15	0	0	0	0
4	L	20	0	0	1	0
4	M	20	0	0	0	0
4	N	15	0	0	1	0
4	O	15	0	0	0	0
4	P	5	0	0	0	0
4	Q	15	0	0	1	0
4	R	15	0	0	0	0
4	S	10	0	0	0	0
4	T	5	0	0	0	0
4	U	15	0	0	0	0
4	V	15	0	0	0	0
4	W	5	0	0	0	0
4	X	15	0	0	1	0
4	Y	10	0	0	0	0
4	a	5	0	0	0	0
4	c	5	0	0	0	0
5	A	18	0	24	2	0
5	D	6	0	8	0	0
5	G	12	0	16	2	0
5	H	12	0	16	20	0
5	I	18	0	24	5	0
5	J	12	0	16	3	0
5	K	24	0	32	14	0
5	L	6	0	8	1	0
6	H	1	0	0	0	0
6	K	1	0	0	0	0
6	Q	1	0	0	0	0
6	X	1	0	0	0	0
7	A	33	0	0	3	0
7	B	40	0	0	2	0
7	C	36	0	0	0	0
7	D	21	0	0	0	0
7	E	21	0	0	2	0
7	F	24	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	78	0	0	8	0
7	H	70	0	0	4	0
7	I	62	0	0	1	0
7	J	78	0	0	4	0
7	K	57	0	0	5	0
7	L	69	0	0	1	0
7	M	27	0	0	1	0
7	N	37	0	0	0	0
7	O	40	0	0	0	0
7	P	50	0	0	3	0
7	Q	48	0	0	4	0
7	R	49	0	0	5	0
7	S	4	0	0	0	0
7	T	15	0	0	1	0
7	U	15	0	0	0	0
7	V	17	0	0	0	0
7	W	12	0	0	0	0
7	X	13	0	0	0	0
7	Y	2	0	0	0	0
7	Z	1	0	0	0	0
7	a	2	0	0	0	0
7	b	2	0	0	0	0
7	c	2	0	0	0	0
7	d	2	0	0	0	0
7	e	2	0	0	0	0
7	f	2	0	0	0	0
7	g	1	0	0	0	0
7	i	2	0	0	0	0
7	j	1	0	0	0	0
All	All	118753	0	107910	1271	3

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

All (1271) 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:H:267:HIS:HD1	5:H:614:GOL:H11	1.06	1.14
1:H:267:HIS:ND1	5:H:614:GOL:H11	1.65	1.12
1:H:267:HIS:HD1	5:H:614:GOL:C1	1.74	1.01
1:H:267:HIS:CE1	5:H:614:GOL:H31	2.01	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:406:ILE:H	1:I:410:HIS:HD2	1.14	0.95
1:B:406:ILE:H	1:B:410:HIS:HD2	1.16	0.93
5:H:615:GOL:H12	1:I:429:ASN:H	1.32	0.93
1:R:406:ILE:H	1:R:410:HIS:HD2	1.17	0.93
1:H:267:HIS:HE1	5:H:614:GOL:H31	1.32	0.92
1:N:406:ILE:H	1:N:410:HIS:HD2	1.17	0.92
1:G:406:ILE:H	1:G:410:HIS:HD2	1.16	0.92
1:Q:406:ILE:H	1:Q:410:HIS:HD2	1.17	0.92
1:A:406:ILE:H	1:A:410:HIS:HD2	1.16	0.91
1:H:474:VAL:HG22	5:H:615:GOL:H32	1.49	0.91
1:J:406:ILE:H	1:J:410:HIS:HD2	1.18	0.91
1:M:406:ILE:H	1:M:410:HIS:HD2	1.18	0.91
1:D:232:GLN:HE22	1:D:246:GLN:HE22	1.13	0.90
1:H:406:ILE:H	1:H:410:HIS:HD2	1.17	0.90
1:G:410:HIS:HA	5:G:616:GOL:H31	1.54	0.89
1:T:406:ILE:H	1:T:410:HIS:HD2	1.19	0.89
1:L:406:ILE:H	1:L:410:HIS:HD2	1.17	0.89
1:J:138:LYS:HE3	7:L:724:HOH:O	1.72	0.88
1:K:406:ILE:H	1:K:410:HIS:HD2	1.18	0.88
1:U:406:ILE:H	1:U:410:HIS:HD2	1.19	0.88
1:S:406:ILE:H	1:S:410:HIS:HD2	1.19	0.88
1:C:406:ILE:H	1:C:410:HIS:HD2	1.19	0.88
1:X:406:ILE:H	1:X:410:HIS:HD2	1.19	0.87
1:E:406:ILE:H	1:E:410:HIS:HD2	1.20	0.87
1:W:406:ILE:H	1:W:410:HIS:HD2	1.20	0.86
1:V:406:ILE:H	1:V:410:HIS:HD2	1.18	0.86
1:K:232:GLN:HE22	1:K:246:GLN:HE22	1.24	0.86
1:P:406:ILE:H	1:P:410:HIS:HD2	1.19	0.85
1:F:406:ILE:H	1:F:410:HIS:HD2	1.19	0.85
1:I:211:GLY:HA2	1:I:214:ALA:HB2	1.56	0.85
1:I:438:PHE:HZ	5:I:614:GOL:H31	1.41	0.84
1:O:406:ILE:H	1:O:410:HIS:HD2	1.18	0.84
1:L:232:GLN:HE22	1:L:246:GLN:HE22	1.26	0.84
1:W:232:GLN:HE22	1:W:246:GLN:HE22	1.27	0.82
1:R:232:GLN:HE22	1:R:246:GLN:HE22	1.27	0.81
1:J:232:GLN:HE22	1:J:246:GLN:HE22	1.27	0.81
1:E:232:GLN:HE22	1:E:246:GLN:HE22	1.27	0.81
1:X:232:GLN:HE22	1:X:246:GLN:HE22	1.29	0.81
1:D:207:GLU:HA	1:D:513:THR:OG1	1.79	0.81
1:J:76:SER:HB2	1:J:106:VAL:HG11	1.62	0.81
1:P:232:GLN:HE22	1:P:246:GLN:HE22	1.29	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:232:GLN:HE22	1:G:246:GLN:HE22	1.29	0.80
1:U:232:GLN:HE22	1:U:246:GLN:HE22	1.29	0.80
1:D:497:TRP:CD1	1:F:485:ARG:HD3	2.15	0.80
1:F:232:GLN:HE22	1:F:246:GLN:HE22	1.29	0.80
1:T:232:GLN:HE22	1:T:246:GLN:HE22	1.29	0.80
1:S:232:GLN:HE22	1:S:246:GLN:HE22	1.27	0.80
1:V:232:GLN:HE22	1:V:246:GLN:HE22	1.28	0.80
1:G:76:SER:HB2	1:G:106:VAL:HG11	1.64	0.80
1:Q:232:GLN:HE22	1:Q:246:GLN:HE22	1.30	0.80
1:B:76:SER:HB2	1:B:106:VAL:HG11	1.63	0.79
1:D:102:ASN:HD21	1:D:164:MET:H	1.27	0.79
1:N:232:GLN:HE22	1:N:246:GLN:HE22	1.30	0.79
1:E:76:SER:HB2	1:E:106:VAL:HG11	1.64	0.79
1:H:454:HIS:HA	5:H:614:GOL:H2	1.61	0.79
1:C:232:GLN:HE22	1:C:246:GLN:HE22	1.31	0.79
1:C:76:SER:HB2	1:C:106:VAL:HG11	1.65	0.79
7:K:721:HOH:O	1:L:138:LYS:HE3	1.82	0.78
1:K:76:SER:HB2	1:K:106:VAL:HG11	1.65	0.78
1:O:232:GLN:HE22	1:O:246:GLN:HE22	1.32	0.78
1:N:76:SER:HB2	1:N:106:VAL:HG11	1.65	0.78
1:H:76:SER:HB2	1:H:106:VAL:HG11	1.65	0.78
1:B:232:GLN:HE22	1:B:246:GLN:HE22	1.30	0.78
1:X:76:SER:HB2	1:X:106:VAL:HG11	1.66	0.77
1:F:76:SER:HB2	1:F:106:VAL:HG11	1.65	0.77
1:L:76:SER:HB2	1:L:106:VAL:HG11	1.63	0.77
1:S:76:SER:HB2	1:S:106:VAL:HG11	1.64	0.77
1:H:474:VAL:HG23	5:H:615:GOL:H11	1.66	0.77
1:M:232:GLN:HE22	1:M:246:GLN:HE22	1.29	0.77
1:G:235:GLN:HE22	1:I:280:GLN:HE22	1.31	0.77
1:O:76:SER:HB2	1:O:106:VAL:HG11	1.65	0.77
1:D:232:GLN:NE2	1:D:246:GLN:HE22	1.83	0.77
1:U:76:SER:HB2	1:U:106:VAL:HG11	1.67	0.77
1:M:76:SER:HB2	1:M:106:VAL:HG11	1.65	0.77
1:H:232:GLN:HE22	1:H:246:GLN:HE22	1.31	0.76
1:G:432:ASP:H	1:I:478:GLN:HE21	1.32	0.76
1:P:76:SER:HB2	1:P:106:VAL:HG11	1.67	0.76
1:H:267:HIS:CE1	5:H:614:GOL:H11	2.21	0.75
1:T:76:SER:HB2	1:T:106:VAL:HG11	1.65	0.75
1:I:102:ASN:HD21	1:I:164:MET:H	1.32	0.75
1:G:235:GLN:HE22	1:I:280:GLN:NE2	1.85	0.75
1:W:76:SER:HB2	1:W:106:VAL:HG11	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:232:GLN:HE22	1:I:246:GLN:HE22	1.33	0.75
1:A:76:SER:HB2	1:A:106:VAL:HG11	1.68	0.74
1:C:123:ALA:HB2	1:L:127:VAL:HG21	1.69	0.74
1:Q:76:SER:HB2	1:Q:106:VAL:HG11	1.67	0.74
1:R:76:SER:HB2	1:R:106:VAL:HG11	1.68	0.74
1:V:102:ASN:HD21	1:V:164:MET:H	1.36	0.74
1:A:232:GLN:HE22	1:A:246:GLN:HE22	1.33	0.74
1:H:540:HIS:HB2	7:H:770:HOH:O	1.87	0.74
1:V:76:SER:HB2	1:V:106:VAL:HG11	1.67	0.74
1:A:400:HIS:H	5:A:613:GOL:H2	1.53	0.73
1:J:102:ASN:HD21	1:J:164:MET:H	1.34	0.73
1:P:102:ASN:HD21	1:P:164:MET:H	1.36	0.73
1:R:102:ASN:HD21	1:R:164:MET:H	1.36	0.73
1:O:102:ASN:HD21	1:O:164:MET:H	1.36	0.73
1:D:232:GLN:HE22	1:D:246:GLN:NE2	1.87	0.73
1:K:132:ILE:HG12	5:K:614:GOL:H31	1.70	0.73
1:K:102:ASN:HD21	1:K:164:MET:H	1.35	0.73
1:Q:102:ASN:HD21	1:Q:164:MET:H	1.36	0.73
1:G:343:ASP:HB2	7:G:701:HOH:O	1.89	0.72
1:H:123:ALA:HB2	1:K:127:VAL:HG21	1.71	0.72
1:C:102:ASN:HD21	1:C:164:MET:H	1.36	0.72
3:I:605:HEC:HMD1	3:I:605:HEC:HBD1	1.72	0.72
1:M:102:ASN:HD21	1:M:164:MET:H	1.37	0.71
1:H:102:ASN:HD21	1:H:164:MET:H	1.35	0.71
1:P:318:SER:HB2	7:P:717:HOH:O	1.91	0.71
1:S:102:ASN:HD21	1:S:164:MET:H	1.38	0.71
1:N:127:VAL:HG21	1:R:123:ALA:HB2	1.71	0.71
1:I:163:THR:HG21	2:Y:98:PHE:HB2	1.73	0.70
1:G:102:ASN:HD21	1:G:164:MET:H	1.39	0.70
1:T:102:ASN:HD21	1:T:164:MET:H	1.37	0.70
1:I:406:ILE:H	1:I:410:HIS:CD2	2.04	0.70
1:I:438:PHE:CZ	5:I:614:GOL:H31	2.26	0.70
1:F:102:ASN:HD21	1:F:164:MET:H	1.37	0.70
1:J:127:VAL:HG21	1:P:123:ALA:HB2	1.73	0.70
1:G:343:ASP:CB	7:G:701:HOH:O	2.40	0.70
1:A:102:ASN:HD21	1:A:164:MET:H	1.39	0.70
3:D:600:HEC:HAA2	3:D:601:HEC:HMA3	1.74	0.70
1:L:102:ASN:HD21	1:L:164:MET:H	1.40	0.70
1:E:102:ASN:HD21	1:E:164:MET:H	1.40	0.69
1:G:340:SER:O	7:G:701:HOH:O	2.10	0.69
1:B:102:ASN:HD21	1:B:164:MET:H	1.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:600:HEC:HAA2	3:Q:601:HEC:HMA3	1.75	0.69
1:U:102:ASN:HD21	1:U:164:MET:H	1.39	0.69
3:J:600:HEC:HAA2	3:J:601:HEC:HMA3	1.75	0.68
3:O:600:HEC:HHH	3:O:600:HEC:HBC3	1.75	0.68
1:J:76:SER:HB2	1:J:106:VAL:CG1	2.23	0.68
3:L:600:HEC:HAA2	3:L:601:HEC:HMA3	1.76	0.68
1:X:102:ASN:HD21	1:X:164:MET:H	1.39	0.68
1:H:474:VAL:CG2	5:H:615:GOL:H32	2.22	0.68
3:I:600:HEC:HBC3	3:I:600:HEC:HHH	1.75	0.68
3:K:600:HEC:HAA2	3:K:601:HEC:HMA3	1.75	0.68
3:B:605:HEC:HBD1	3:B:605:HEC:HMD1	1.76	0.68
1:G:76:SER:HB2	1:G:106:VAL:CG1	2.24	0.68
3:I:604:HEC:HBC1	3:I:605:HEC:HBB2	1.76	0.67
3:Q:605:HEC:HBD1	3:Q:605:HEC:HMD1	1.76	0.67
1:D:272:GLN:OE1	1:E:245:GLU:HG2	1.93	0.67
1:W:102:ASN:HD21	1:W:164:MET:H	1.40	0.67
1:B:76:SER:HB2	1:B:106:VAL:CG1	2.25	0.67
5:H:615:GOL:H12	1:I:429:ASN:N	2.08	0.67
3:R:605:HEC:HMD1	3:R:605:HEC:HBD1	1.76	0.67
3:F:600:HEC:HBC3	3:F:600:HEC:HHH	1.77	0.67
1:L:76:SER:HB2	1:L:106:VAL:CG1	2.24	0.67
3:G:600:HEC:HBC3	3:G:600:HEC:HHH	1.76	0.66
1:N:102:ASN:HD21	1:N:164:MET:H	1.41	0.66
3:V:600:HEC:HAA2	3:V:601:HEC:HMA3	1.78	0.66
3:E:605:HEC:HBD1	3:E:605:HEC:HMD1	1.75	0.66
3:D:604:HEC:HBC1	3:D:605:HEC:HBB2	1.76	0.66
3:A:600:HEC:HAA2	3:A:601:HEC:HMA3	1.77	0.66
1:D:172:THR:HG23	1:D:175:CYS:HB2	1.77	0.66
3:V:605:HEC:HBD1	3:V:605:HEC:HMD1	1.78	0.66
1:C:76:SER:HB2	1:C:106:VAL:CG1	2.26	0.66
1:K:234:HIS:HD1	5:K:614:GOL:H11	1.61	0.66
3:L:605:HEC:HMD1	3:L:605:HEC:HBD1	1.78	0.66
3:J:604:HEC:HBC1	3:J:605:HEC:HBB2	1.78	0.66
1:T:76:SER:HB2	1:T:106:VAL:CG1	2.26	0.66
1:V:76:SER:HB2	1:V:106:VAL:CG1	2.26	0.66
3:X:605:HEC:HMD1	3:X:605:HEC:HBD1	1.78	0.66
3:L:600:HEC:HBC3	3:L:600:HEC:HHH	1.78	0.66
3:V:604:HEC:HBC1	3:V:605:HEC:HBB2	1.78	0.66
1:D:234:HIS:HD2	3:D:601:HEC:NC	1.93	0.65
1:D:182:GLU:O	1:D:308:ASN:HB2	1.97	0.65
1:I:255:ASP:HB2	1:I:319:MET:HE1	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:605:HEC:HMD1	3:M:605:HEC:HBD1	1.78	0.65
1:G:235:GLN:NE2	1:I:280:GLN:HE22	1.94	0.65
1:M:76:SER:HB2	1:M:106:VAL:CG1	2.26	0.65
1:N:76:SER:HB2	1:N:106:VAL:CG1	2.27	0.65
2:Y:38:ILE:HD11	2:Y:100:SER:OG	1.97	0.65
3:G:605:HEC:HBD1	3:G:605:HEC:HMD1	1.78	0.65
1:F:76:SER:HB2	1:F:106:VAL:CG1	2.26	0.65
1:J:539:HIS:HE1	7:J:774:HOH:O	1.80	0.65
1:S:76:SER:HB2	1:S:106:VAL:CG1	2.26	0.65
3:W:604:HEC:HBC1	3:W:605:HEC:HBB2	1.79	0.65
1:G:226:ARG:NH2	3:I:607:HEC:O2A	2.30	0.65
3:M:600:HEC:HAA2	3:M:601:HEC:HMA3	1.79	0.65
3:W:600:HEC:HAA2	3:W:601:HEC:HMA3	1.79	0.65
3:F:605:HEC:HBD1	3:F:605:HEC:HMD1	1.78	0.65
3:H:600:HEC:HHH	3:H:600:HEC:HBC3	1.79	0.65
1:H:76:SER:HB2	1:H:106:VAL:CG1	2.26	0.65
3:K:600:HEC:HHH	3:K:600:HEC:HBC3	1.77	0.65
3:P:600:HEC:HAA2	3:P:601:HEC:HMA3	1.79	0.65
1:I:271:TYR:O	1:I:275:LYS:HB3	1.97	0.65
3:U:605:HEC:HBD1	3:U:605:HEC:HMD1	1.79	0.65
3:M:600:HEC:HHH	3:M:600:HEC:HBC3	1.80	0.64
1:O:76:SER:HB2	1:O:106:VAL:CG1	2.26	0.64
3:H:600:HEC:HAA2	3:H:601:HEC:HMA3	1.79	0.64
3:H:605:HEC:HBD1	3:H:605:HEC:HMD1	1.79	0.64
3:J:600:HEC:HBC3	3:J:600:HEC:HHH	1.79	0.64
3:S:605:HEC:HBD1	3:S:605:HEC:HMD1	1.78	0.64
1:R:76:SER:HB2	1:R:106:VAL:CG1	2.27	0.64
3:U:604:HEC:HBC1	3:U:605:HEC:HBB2	1.79	0.64
3:J:605:HEC:HBD1	3:J:605:HEC:HMD1	1.79	0.64
1:Q:76:SER:HB2	1:Q:106:VAL:CG1	2.27	0.64
3:A:605:HEC:HMD1	3:A:605:HEC:HBD1	1.80	0.64
1:G:123:ALA:HB2	1:E:127:VAL:HG21	1.80	0.64
1:E:76:SER:HB2	1:E:106:VAL:CG1	2.26	0.64
3:R:604:HEC:HBC1	3:R:605:HEC:HBB2	1.80	0.64
3:U:600:HEC:HAA2	3:U:601:HEC:HMA3	1.80	0.64
3:G:600:HEC:HAA2	3:G:601:HEC:HMA3	1.80	0.64
1:K:76:SER:HB2	1:K:106:VAL:CG1	2.26	0.64
1:K:411:ASP:H	5:K:613:GOL:H31	1.62	0.64
1:P:76:SER:HB2	1:P:106:VAL:CG1	2.27	0.64
3:B:604:HEC:HBC1	3:B:605:HEC:HBB2	1.79	0.64
1:W:76:SER:HB2	1:W:106:VAL:CG1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:605:HEC:HBD1	3:W:605:HEC:HMD1	1.78	0.64
3:X:600:HEC:HHH	3:X:600:HEC:HBC3	1.78	0.64
1:D:454:HIS:CD2	3:D:606:HEC:NC	2.66	0.64
3:E:600:HEC:HAA2	3:E:601:HEC:HMA3	1.78	0.64
1:A:76:SER:HB2	1:A:106:VAL:CG1	2.28	0.64
3:F:604:HEC:HBC1	3:F:605:HEC:HBB2	1.79	0.63
3:T:600:HEC:HBC3	3:T:600:HEC:HHH	1.81	0.63
1:I:165:PRO:HG2	3:I:601:HEC:HMD3	1.79	0.63
3:K:605:HEC:HMD1	3:K:605:HEC:HBD1	1.80	0.63
3:W:600:HEC:HBC3	3:W:600:HEC:HHH	1.81	0.63
1:X:76:SER:HB2	1:X:106:VAL:CG1	2.27	0.63
1:G:432:ASP:H	1:I:478:GLN:NE2	1.96	0.63
3:T:605:HEC:HMD1	3:T:605:HEC:HBD1	1.80	0.63
1:U:76:SER:HB2	1:U:106:VAL:CG1	2.28	0.63
3:A:600:HEC:HBC3	3:A:600:HEC:HHH	1.81	0.63
1:J:226:ARG:HD3	7:J:708:HOH:O	1.99	0.63
3:N:600:HEC:HAA2	3:N:601:HEC:HMA3	1.80	0.63
3:V:600:HEC:HHH	3:V:600:HEC:HBC3	1.81	0.63
3:L:604:HEC:HBC1	3:L:605:HEC:HBB2	1.81	0.63
3:N:605:HEC:HBD1	3:N:605:HEC:HMD1	1.79	0.63
3:R:600:HEC:HAA2	3:R:601:HEC:HMA3	1.81	0.63
3:B:600:HEC:HAA2	3:B:601:HEC:HMA3	1.81	0.63
3:B:600:HEC:HBC3	3:B:600:HEC:HHH	1.80	0.63
1:G:226:ARG:HH22	3:I:607:HEC:CGA	2.11	0.63
1:I:340:SER:O	1:I:343:ASP:HB2	1.99	0.63
1:G:497:TRP:CD1	1:I:485:ARG:HD3	2.34	0.63
3:X:604:HEC:HBC1	3:X:605:HEC:HBB2	1.79	0.63
3:Q:600:HEC:HHH	3:Q:600:HEC:HBC3	1.81	0.63
3:O:600:HEC:HAA2	3:O:601:HEC:HMA3	1.81	0.62
3:S:600:HEC:HBC3	3:S:600:HEC:HHH	1.80	0.62
1:H:406:ILE:H	1:H:410:HIS:CD2	2.09	0.62
3:T:604:HEC:HBC1	3:T:605:HEC:HBB2	1.81	0.62
1:V:406:ILE:H	1:V:410:HIS:CD2	2.10	0.62
2:Z:38:ILE:HD11	2:Z:100:SER:OG	1.98	0.62
3:C:600:HEC:HHH	3:C:600:HEC:HBC3	1.80	0.62
3:C:605:HEC:HMD1	3:C:605:HEC:HBD1	1.81	0.62
1:I:182:GLU:O	1:I:308:ASN:HB2	1.99	0.62
3:R:600:HEC:HBC3	3:R:600:HEC:HHH	1.81	0.62
3:T:600:HEC:HAA2	3:T:601:HEC:HMA3	1.80	0.62
3:U:600:HEC:HBC3	3:U:600:HEC:HHH	1.81	0.62
3:P:605:HEC:HBD1	3:P:605:HEC:HMD1	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:ILE:H	1:B:410:HIS:CD2	2.09	0.62
3:O:605:HEC:HBD1	3:O:605:HEC:HMD1	1.82	0.62
3:D:600:HEC:HHH	3:D:600:HEC:HBC3	1.82	0.62
3:E:604:HEC:HBC1	3:E:605:HEC:HBB2	1.81	0.62
3:C:604:HEC:HBC1	3:C:605:HEC:HBB2	1.80	0.62
3:C:600:HEC:HAA2	3:C:601:HEC:HMA3	1.79	0.61
3:N:600:HEC:HHH	3:N:600:HEC:HBC3	1.82	0.61
3:D:605:HEC:HBD1	3:D:605:HEC:HMD1	1.81	0.61
1:H:474:VAL:HG22	5:H:615:GOL:C3	2.24	0.61
3:E:600:HEC:HBC3	3:E:600:HEC:HHH	1.81	0.61
1:H:454:HIS:CA	5:H:614:GOL:H2	2.29	0.61
1:I:98:ASP:OD2	1:I:168:LYS:HD2	2.00	0.61
1:M:165:PRO:HG2	3:M:601:HEC:HMD3	1.82	0.61
1:L:84:LYS:HE2	4:L:610:SO4:S	2.41	0.61
3:S:600:HEC:HAA2	3:S:601:HEC:HMA3	1.81	0.61
1:L:406:ILE:H	1:L:410:HIS:CD2	2.09	0.61
1:R:406:ILE:H	1:R:410:HIS:CD2	2.09	0.61
3:P:604:HEC:HBC1	3:P:605:HEC:HBB2	1.82	0.60
3:S:604:HEC:HBC1	3:S:605:HEC:HBB2	1.81	0.60
3:X:600:HEC:HAA2	3:X:601:HEC:HMA3	1.82	0.60
3:F:600:HEC:HAA2	3:F:601:HEC:HMA3	1.82	0.60
1:I:251:HIS:HB3	1:I:258:ASP:HB2	1.81	0.60
1:X:234:HIS:HD2	3:X:601:HEC:NC	1.99	0.60
3:A:604:HEC:HBC1	3:A:605:HEC:HBB2	1.83	0.60
3:P:600:HEC:HHH	3:P:600:HEC:HBC3	1.81	0.60
3:Q:604:HEC:HBC1	3:Q:605:HEC:HBB2	1.81	0.60
1:T:210:PRO:HA	7:T:707:HOH:O	2.01	0.60
1:U:234:HIS:HD2	3:U:601:HEC:NC	2.00	0.60
1:W:234:HIS:HD2	3:W:601:HEC:NC	1.99	0.60
1:G:485:ARG:HD3	1:H:497:TRP:CD1	2.37	0.60
1:G:479:ASN:HD22	1:I:482:ARG:HH12	1.50	0.60
1:D:251:HIS:HB3	1:D:258:ASP:HB2	1.83	0.60
1:D:478:GLN:O	1:D:482:ARG:HG2	2.02	0.60
1:C:120:GLN:HA	1:L:127:VAL:HG11	1.82	0.59
1:N:211:GLY:HA2	1:N:214:ALA:HB2	1.84	0.59
1:N:234:HIS:HD2	3:N:601:HEC:NC	2.00	0.59
1:A:211:GLY:HA2	1:A:214:ALA:HB2	1.84	0.59
3:K:604:HEC:HBC1	3:K:605:HEC:HBB2	1.82	0.59
1:P:234:HIS:HD2	3:P:601:HEC:NC	2.00	0.59
1:G:182:GLU:O	1:G:308:ASN:HB2	2.03	0.59
3:N:604:HEC:HBC1	3:N:605:HEC:HBB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:234:HIS:HD2	3:E:601:HEC:NC	2.00	0.59
1:D:102:ASN:ND2	1:D:164:MET:H	1.99	0.59
1:G:234:HIS:HD2	3:G:601:HEC:NC	2.00	0.59
1:P:211:GLY:HA2	1:P:214:ALA:HB2	1.84	0.59
1:X:406:ILE:H	1:X:410:HIS:CD2	2.11	0.59
1:F:406:ILE:H	1:F:410:HIS:CD2	2.11	0.59
1:J:482:ARG:NH1	4:J:611:SO4:O3	2.36	0.59
1:J:234:HIS:HD2	3:J:601:HEC:NC	2.00	0.59
1:K:374:LYS:NZ	7:K:701:HOH:O	2.25	0.59
1:T:234:HIS:HD2	3:T:601:HEC:NC	1.99	0.59
1:H:234:HIS:HD2	3:H:601:HEC:NC	2.01	0.59
1:K:406:ILE:H	1:K:410:HIS:CD2	2.10	0.59
1:L:234:HIS:HD2	3:L:601:HEC:NC	2.00	0.59
1:A:406:ILE:H	1:A:410:HIS:CD2	2.09	0.58
1:X:211:GLY:HA2	1:X:214:ALA:HB2	1.84	0.58
3:I:605:HEC:HBC3	3:I:605:HEC:HMC1	1.84	0.58
1:Q:234:HIS:HD2	3:Q:601:HEC:NC	2.00	0.58
1:V:234:HIS:HD2	3:V:601:HEC:NC	1.98	0.58
1:M:234:HIS:HD2	3:M:601:HEC:NC	1.99	0.58
1:C:406:ILE:H	1:C:410:HIS:CD2	2.11	0.58
1:Q:406:ILE:H	1:Q:410:HIS:CD2	2.09	0.58
1:W:211:GLY:HA2	1:W:214:ALA:HB2	1.86	0.58
1:I:211:GLY:HA2	1:I:214:ALA:CB	2.30	0.58
1:A:343:ASP:HB3	7:A:715:HOH:O	2.02	0.58
1:B:211:GLY:HA2	1:B:214:ALA:HB2	1.86	0.58
1:S:211:GLY:HA2	1:S:214:ALA:HB2	1.85	0.58
1:F:234:HIS:HD2	3:F:601:HEC:NC	2.01	0.58
3:I:600:HEC:HAA2	3:I:601:HEC:HMA3	1.85	0.58
1:J:211:GLY:HA2	1:J:214:ALA:HB2	1.86	0.58
1:U:182:GLU:O	1:U:308:ASN:HB2	2.03	0.58
3:H:604:HEC:HBC1	3:H:605:HEC:HBB2	1.84	0.58
1:K:234:HIS:HD2	3:K:601:HEC:NC	2.02	0.58
1:W:406:ILE:H	1:W:410:HIS:CD2	2.12	0.58
1:R:211:GLY:HA2	1:R:214:ALA:HB2	1.86	0.57
1:K:211:GLY:HA2	1:K:214:ALA:HB2	1.85	0.57
1:U:211:GLY:HA2	1:U:214:ALA:HB2	1.85	0.57
1:C:211:GLY:HA2	1:C:214:ALA:HB2	1.87	0.57
1:E:211:GLY:HA2	1:E:214:ALA:HB2	1.86	0.57
1:H:182:GLU:O	1:H:308:ASN:HB2	2.03	0.57
1:S:234:HIS:HD2	3:S:601:HEC:NC	2.01	0.57
1:A:182:GLU:O	1:A:308:ASN:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:273:VAL:HG13	1:I:243:ARG:HG3	1.87	0.57
1:O:165:PRO:HG2	3:O:601:HEC:HMD3	1.86	0.57
1:B:123:ALA:HB2	1:U:127:VAL:HG21	1.86	0.57
1:B:234:HIS:HD2	3:B:601:HEC:NC	2.02	0.57
1:O:211:GLY:HA2	1:O:214:ALA:HB2	1.86	0.57
1:A:234:HIS:HD2	3:A:601:HEC:NC	2.01	0.57
1:D:237:ASP:HB3	1:D:240:VAL:HG22	1.85	0.57
1:F:211:GLY:HA2	1:F:214:ALA:HB2	1.86	0.57
1:A:226:ARG:HD3	7:A:702:HOH:O	2.04	0.57
1:R:234:HIS:HD2	3:R:601:HEC:NC	2.02	0.57
1:E:182:GLU:O	1:E:308:ASN:HB2	2.03	0.57
1:W:182:GLU:O	1:W:308:ASN:HB2	2.04	0.57
1:C:234:HIS:HD2	3:C:601:HEC:NC	2.00	0.56
1:I:245:GLU:O	1:I:248:LYS:HG2	2.05	0.56
1:S:182:GLU:O	1:S:308:ASN:HB2	2.05	0.56
1:G:406:ILE:H	1:G:410:HIS:CD2	2.09	0.56
1:N:406:ILE:H	1:N:410:HIS:CD2	2.09	0.56
1:O:234:HIS:HD2	3:O:601:HEC:NC	2.02	0.56
1:P:406:ILE:H	1:P:410:HIS:CD2	2.11	0.56
1:Q:182:GLU:O	1:Q:308:ASN:HB2	2.05	0.56
1:M:211:GLY:HA2	1:M:214:ALA:HB2	1.87	0.56
1:V:211:GLY:HA2	1:V:214:ALA:HB2	1.86	0.56
1:G:251:HIS:HB3	1:G:258:ASP:HB2	1.88	0.56
1:H:195:SER:HB2	1:H:221:THR:HA	1.87	0.56
1:J:251:HIS:HB3	1:J:258:ASP:HB2	1.87	0.56
1:K:182:GLU:O	1:K:308:ASN:HB2	2.05	0.56
1:Q:211:GLY:HA2	1:Q:214:ALA:HB2	1.87	0.56
1:U:251:HIS:HB3	1:U:258:ASP:HB2	1.88	0.56
1:H:211:GLY:HA2	1:H:214:ALA:HB2	1.86	0.56
1:J:127:VAL:HG11	1:P:120:GLN:HA	1.87	0.56
1:R:195:SER:HB2	1:R:221:THR:HA	1.88	0.56
3:G:604:HEC:HBC1	3:G:605:HEC:HBB2	1.88	0.56
1:I:81:LYS:NZ	1:I:530:CYS:O	2.36	0.56
1:J:182:GLU:O	1:J:308:ASN:HB2	2.05	0.56
1:L:182:GLU:O	1:L:308:ASN:HB2	2.05	0.56
1:V:182:GLU:O	1:V:308:ASN:HB2	2.05	0.56
1:X:251:HIS:HB3	1:X:258:ASP:HB2	1.88	0.56
1:N:182:GLU:O	1:N:308:ASN:HB2	2.06	0.56
1:J:368:LYS:HE2	1:J:470:ASP:OD1	2.06	0.56
3:O:604:HEC:HBC1	3:O:605:HEC:HBB2	1.86	0.56
1:S:251:HIS:HB3	1:S:258:ASP:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:211:GLY:HA2	1:G:214:ALA:HB2	1.86	0.56
1:C:165:PRO:HG2	3:C:601:HEC:HMD3	1.88	0.55
1:G:226:ARG:HD3	7:G:724:HOH:O	2.05	0.55
1:L:251:HIS:HB3	1:L:258:ASP:HB2	1.89	0.55
1:O:406:ILE:H	1:O:410:HIS:CD2	2.10	0.55
1:T:182:GLU:O	1:T:308:ASN:HB2	2.06	0.55
1:E:368:LYS:HE2	1:E:470:ASP:OD1	2.07	0.55
1:W:251:HIS:HB3	1:W:258:ASP:HB2	1.87	0.55
1:K:485:ARG:HD3	1:L:497:TRP:CD1	2.42	0.55
1:O:251:HIS:HB3	1:O:258:ASP:HB2	1.88	0.55
1:P:165:PRO:HG2	3:P:601:HEC:HMD3	1.88	0.55
1:X:182:GLU:O	1:X:308:ASN:HB2	2.07	0.55
1:O:306:HIS:HD2	2:Y:26:TYR:CD2	2.25	0.55
1:K:251:HIS:HB3	1:K:258:ASP:HB2	1.88	0.55
1:C:182:GLU:O	1:C:308:ASN:HB2	2.07	0.55
1:F:182:GLU:O	1:F:308:ASN:HB2	2.06	0.55
1:G:479:ASN:ND2	1:I:482:ARG:HH12	2.04	0.55
1:I:150:GLY:C	3:I:601:HEC:HMC3	2.26	0.55
3:K:601:HEC:O1A	5:K:614:GOL:H32	2.06	0.55
1:L:211:GLY:HA2	1:L:214:ALA:HB2	1.87	0.55
1:M:182:GLU:O	1:M:308:ASN:HB2	2.07	0.55
1:D:214:ALA:HB3	1:F:452:MET:HE1	1.88	0.55
1:R:182:GLU:O	1:R:308:ASN:HB2	2.07	0.55
1:B:485:ARG:HD3	1:C:497:TRP:CD1	2.42	0.55
1:K:132:ILE:HG12	5:K:614:GOL:H11	1.88	0.55
1:Q:251:HIS:HB3	1:Q:258:ASP:HB2	1.89	0.55
1:R:165:PRO:HG2	3:R:601:HEC:HMD3	1.88	0.55
1:I:195:SER:HB2	1:I:221:THR:HA	1.89	0.55
1:J:165:PRO:HG2	3:J:601:HEC:HMD3	1.89	0.55
1:T:251:HIS:HB3	1:T:258:ASP:HB2	1.88	0.55
1:V:251:HIS:HB3	1:V:258:ASP:HB2	1.89	0.55
1:I:232:GLN:HE22	1:I:246:GLN:NE2	2.02	0.55
1:Q:123:ALA:HB2	1:T:127:VAL:HG21	1.89	0.55
1:T:406:ILE:H	1:T:410:HIS:CD2	2.11	0.55
1:W:165:PRO:HG2	3:W:601:HEC:HMD3	1.88	0.54
1:I:504:LYS:HG3	7:I:734:HOH:O	2.05	0.54
1:P:182:GLU:O	1:P:308:ASN:HB2	2.07	0.54
1:P:251:HIS:HB3	1:P:258:ASP:HB2	1.89	0.54
1:B:251:HIS:HB3	1:B:258:ASP:HB2	1.90	0.54
1:M:251:HIS:HB3	1:M:258:ASP:HB2	1.88	0.54
1:N:251:HIS:HB3	1:N:258:ASP:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:THR:HG21	2:Z:98:PHE:HB2	1.89	0.54
1:H:251:HIS:HB3	1:H:258:ASP:HB2	1.90	0.54
1:I:337:ARG:O	1:I:340:SER:HB2	2.07	0.54
1:P:195:SER:HB2	1:P:221:THR:HA	1.90	0.54
1:W:195:SER:HB2	1:W:221:THR:HA	1.90	0.54
1:U:165:PRO:HG2	3:U:601:HEC:HMD3	1.90	0.54
1:F:251:HIS:HB3	1:F:258:ASP:HB2	1.89	0.54
3:K:607:HEC:CGA	1:L:226:ARG:HH22	2.21	0.54
1:G:165:PRO:HG2	3:G:601:HEC:HMD3	1.89	0.54
3:I:601:HEC:HHA	3:I:601:HEC:HBA1	1.90	0.54
1:O:182:GLU:O	1:O:308:ASN:HB2	2.08	0.54
1:R:251:HIS:HB3	1:R:258:ASP:HB2	1.89	0.54
1:V:165:PRO:HG2	3:V:601:HEC:HMD3	1.90	0.54
3:V:607:HEC:CGA	1:W:226:ARG:HH22	2.21	0.54
1:E:251:HIS:HB3	1:E:258:ASP:HB2	1.90	0.53
3:E:605:HEC:CBD	3:E:605:HEC:HMD1	2.37	0.53
1:A:368:LYS:HE2	1:A:470:ASP:OD1	2.07	0.53
1:K:132:ILE:CG1	5:K:614:GOL:H31	2.38	0.53
1:R:368:LYS:HE2	1:R:470:ASP:OD1	2.08	0.53
1:J:485:ARG:HD3	1:K:497:TRP:CD1	2.43	0.53
3:K:600:HEC:CAA	3:K:601:HEC:HMA3	2.39	0.53
3:M:604:HEC:HBC1	3:M:605:HEC:HBB2	1.89	0.53
1:T:211:GLY:HA2	1:T:214:ALA:HB2	1.89	0.53
1:B:195:SER:HB2	1:B:221:THR:HA	1.91	0.53
1:J:497:TRP:CD1	1:L:485:ARG:HD3	2.43	0.53
1:F:165:PRO:HG2	3:F:601:HEC:HMD3	1.91	0.53
3:I:600:HEC:HHD	3:I:600:HEC:CBC	2.39	0.53
1:U:406:ILE:H	1:U:410:HIS:CD2	2.11	0.53
1:E:165:PRO:HG2	3:E:601:HEC:HMD3	1.90	0.53
1:P:485:ARG:HD3	1:Q:497:TRP:CD1	2.44	0.53
1:S:406:ILE:H	1:S:410:HIS:CD2	2.11	0.53
1:V:195:SER:HB2	1:V:221:THR:HA	1.91	0.53
1:G:195:SER:HB2	1:G:221:THR:HA	1.91	0.53
1:K:146:PRO:HD2	7:K:735:HOH:O	2.09	0.53
1:M:485:ARG:HD3	1:N:497:TRP:CD1	2.44	0.53
1:T:368:LYS:HE2	1:T:470:ASP:OD1	2.09	0.53
1:T:165:PRO:HG2	3:T:601:HEC:HMD3	1.90	0.53
1:T:478:GLN:HE21	1:U:432:ASP:HB2	1.74	0.53
1:B:165:PRO:HG2	3:B:601:HEC:HMD3	1.90	0.53
1:C:251:HIS:HB3	1:C:258:ASP:HB2	1.91	0.53
3:D:605:HEC:HBA2	3:D:606:HEC:HMA3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:226:ARG:HH22	3:L:607:HEC:CGA	2.22	0.53
1:Q:485:ARG:HD3	1:R:497:TRP:CD1	2.44	0.53
3:D:607:HEC:HBC3	3:D:607:HEC:HMC1	1.91	0.53
3:Q:605:HEC:CBD	3:Q:605:HEC:HMD1	2.39	0.53
1:R:343:ASP:CB	7:R:701:HOH:O	2.57	0.53
1:S:165:PRO:HG2	3:S:601:HEC:HMD3	1.90	0.53
1:A:497:TRP:CD1	1:C:485:ARG:HD3	2.44	0.52
3:B:605:HEC:CBD	3:B:605:HEC:HMD1	2.39	0.52
1:I:255:ASP:HB3	5:I:614:GOL:H2	1.91	0.52
1:K:234:HIS:HE1	5:K:614:GOL:O3	1.92	0.52
1:M:406:ILE:H	1:M:410:HIS:CD2	2.10	0.52
1:T:195:SER:HB2	1:T:221:THR:HA	1.91	0.52
1:V:368:LYS:HE2	1:V:470:ASP:OD1	2.09	0.52
1:X:165:PRO:HG2	3:X:601:HEC:HMD3	1.89	0.52
1:A:251:HIS:HB3	1:A:258:ASP:HB2	1.90	0.52
1:D:173:ALA:HA	1:D:177:GLU:HB2	1.90	0.52
1:D:406:ILE:H	1:D:410:HIS:HD2	1.57	0.52
1:H:368:LYS:HE2	1:H:470:ASP:OD1	2.08	0.52
1:K:165:PRO:HG2	3:K:601:HEC:HMD3	1.90	0.52
1:X:368:LYS:HE2	1:X:470:ASP:OD1	2.09	0.52
1:D:90:PRO:O	1:D:93:ARG:HG2	2.09	0.52
3:J:600:HEC:CAA	3:J:601:HEC:HMA3	2.40	0.52
3:L:600:HEC:CAA	3:L:601:HEC:HMA3	2.39	0.52
1:N:485:ARG:HD3	1:O:497:TRP:CD1	2.44	0.52
3:Q:600:HEC:CAA	3:Q:601:HEC:HMA3	2.38	0.52
1:J:406:ILE:H	1:J:410:HIS:CD2	2.10	0.52
1:L:165:PRO:HG2	3:L:601:HEC:HMD3	1.91	0.52
1:W:368:LYS:HE2	1:W:470:ASP:OD1	2.09	0.52
1:B:182:GLU:O	1:B:308:ASN:HB2	2.10	0.52
3:F:605:HEC:CBD	3:F:605:HEC:HMD1	2.40	0.52
3:J:607:HEC:CGA	1:K:226:ARG:HH22	2.22	0.52
3:A:600:HEC:CAA	3:A:601:HEC:HMA3	2.40	0.52
1:A:165:PRO:HG2	3:A:601:HEC:HMD3	1.92	0.52
1:H:165:PRO:HG2	3:H:601:HEC:HMD3	1.90	0.52
1:M:497:TRP:CD1	1:O:485:ARG:HD3	2.45	0.52
3:D:600:HEC:CAA	3:D:601:HEC:HMA3	2.38	0.52
1:I:368:LYS:HE2	1:I:470:ASP:OD1	2.10	0.52
1:J:90:PRO:O	1:J:93:ARG:HG2	2.10	0.52
1:P:368:LYS:HE2	1:P:470:ASP:OD1	2.09	0.52
1:Q:165:PRO:HG2	3:Q:601:HEC:HMD3	1.91	0.52
1:V:485:ARG:HD3	1:W:497:TRP:CD1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:485:ARG:HD3	1:H:497:TRP:CG	2.45	0.52
1:M:195:SER:HB2	1:M:221:THR:HA	1.92	0.52
1:D:406:ILE:HD12	1:E:62:LEU:HD12	1.91	0.52
1:N:368:LYS:HE2	1:N:470:ASP:OD1	2.09	0.52
3:C:600:HEC:CAA	3:C:601:HEC:HMA3	2.40	0.51
1:D:154:CYS:HB3	1:D:165:PRO:HG3	1.91	0.51
3:V:600:HEC:CAA	3:V:601:HEC:HMA3	2.39	0.51
3:G:605:HEC:CBD	3:G:605:HEC:HMD1	2.40	0.51
1:I:318:SER:O	1:I:319:MET:HB2	2.09	0.51
1:V:432:ASP:HB2	1:X:478:GLN:HE21	1.76	0.51
3:W:600:HEC:CAA	3:W:601:HEC:HMA3	2.41	0.51
1:G:497:TRP:CG	1:I:485:ARG:HD3	2.46	0.51
1:Q:368:LYS:HE2	1:Q:470:ASP:OD1	2.10	0.51
3:D:604:HEC:CBC	3:D:605:HEC:HBB2	2.40	0.51
1:M:287:LEU:HD12	3:M:604:HEC:HBD2	1.92	0.51
1:Q:287:LEU:HD12	3:Q:604:HEC:HBD2	1.92	0.51
3:D:601:HEC:HBA1	3:D:601:HEC:HHA	1.91	0.51
1:I:199:GLN:HB2	1:I:220:HIS:HB3	1.93	0.51
1:K:195:SER:HB2	1:K:221:THR:HA	1.93	0.51
3:P:600:HEC:CAA	3:P:601:HEC:HMA3	2.40	0.51
1:F:287:LEU:HD12	3:F:604:HEC:HBD2	1.91	0.51
3:N:607:HEC:CGA	1:O:226:ARG:HH22	2.23	0.51
1:P:497:TRP:CD1	1:R:485:ARG:HD3	2.46	0.51
1:Q:257:ARG:HD3	7:Q:729:HOH:O	2.08	0.51
3:A:607:HEC:CGA	1:B:226:ARG:HH22	2.24	0.51
1:K:135:ASP:OD2	5:K:614:GOL:O1	2.28	0.51
1:V:287:LEU:HD12	3:V:604:HEC:HBD2	1.93	0.51
1:A:485:ARG:HD3	1:B:497:TRP:CD1	2.45	0.51
1:F:195:SER:HB2	1:F:221:THR:HA	1.92	0.51
3:G:607:HEC:CGA	1:H:226:ARG:HH22	2.24	0.51
3:K:605:HEC:CBD	3:K:605:HEC:HMD1	2.41	0.51
1:O:368:LYS:HE2	1:O:470:ASP:OD1	2.10	0.51
1:C:368:LYS:HE2	1:C:470:ASP:OD1	2.11	0.51
1:D:195:SER:HB2	1:D:221:THR:HA	1.93	0.51
1:L:195:SER:HB2	1:L:221:THR:HA	1.93	0.51
1:L:368:LYS:HE2	1:L:470:ASP:OD1	2.11	0.51
1:E:195:SER:HB2	1:E:221:THR:HA	1.92	0.51
3:E:600:HEC:CAA	3:E:601:HEC:HMA3	2.41	0.51
1:I:433:VAL:HG13	1:I:476:VAL:HG13	1.92	0.51
3:M:605:HEC:CBD	3:M:605:HEC:HMD1	2.40	0.51
3:S:605:HEC:CBD	3:S:605:HEC:HMD1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:485:ARG:HD3	1:T:497:TRP:CD1	2.46	0.50
3:H:600:HEC:CAA	3:H:601:HEC:HMA3	2.41	0.50
1:H:63:LYS:NZ	7:H:703:HOH:O	2.43	0.50
3:X:605:HEC:CBD	3:X:605:HEC:HMD1	2.42	0.50
1:D:388:MET:HB3	1:D:389:PRO:HD2	1.93	0.50
1:S:368:LYS:HE2	1:S:470:ASP:OD1	2.11	0.50
1:D:331:TRP:CZ2	1:E:44:VAL:HG21	2.46	0.50
3:H:605:HEC:CBD	3:H:605:HEC:HMD1	2.42	0.50
1:I:234:HIS:HD2	3:I:601:HEC:NC	2.06	0.50
3:M:607:HEC:CGA	1:N:226:ARG:HH22	2.23	0.50
1:A:195:SER:HB2	1:A:221:THR:HA	1.93	0.50
3:Q:607:HEC:CGA	1:R:226:ARG:HH22	2.24	0.50
1:W:287:LEU:HD12	3:W:604:HEC:HBD2	1.94	0.50
1:C:123:ALA:HB2	1:L:127:VAL:CG2	2.41	0.50
1:D:165:PRO:HG2	3:D:601:HEC:HMD3	1.93	0.50
1:O:127:VAL:HG21	1:W:123:ALA:HB2	1.93	0.50
1:P:226:ARG:HD3	7:P:718:HOH:O	2.09	0.50
3:R:600:HEC:CAA	3:R:601:HEC:HMA3	2.42	0.50
1:X:287:LEU:HD12	3:X:604:HEC:HBD2	1.92	0.50
1:I:48:PRO:HG3	1:I:63:LYS:HD2	1.92	0.50
3:J:605:HEC:HMD1	3:J:605:HEC:CBD	2.40	0.50
3:R:605:HEC:HMD1	3:R:605:HEC:CBD	2.41	0.50
3:T:600:HEC:CAA	3:T:601:HEC:HMA3	2.42	0.50
1:V:226:ARG:HH22	3:X:607:HEC:CGA	2.24	0.50
1:C:195:SER:HB2	1:C:221:THR:HA	1.93	0.50
1:D:197:PHE:HB2	1:D:535:TRP:CD2	2.46	0.50
1:E:406:ILE:H	1:E:410:HIS:CD2	2.12	0.50
1:H:210:PRO:HA	7:H:709:HOH:O	2.12	0.50
1:P:287:LEU:HD12	3:P:604:HEC:HBD2	1.94	0.50
1:G:287:LEU:HD12	3:G:604:HEC:HBD2	1.93	0.50
1:S:432:ASP:HB2	1:U:478:GLN:HE21	1.77	0.50
1:I:194:CYS:HA	3:I:605:HEC:O1D	2.12	0.49
1:K:234:HIS:CE1	5:K:614:GOL:O3	2.65	0.49
1:J:63:LYS:HD3	5:L:613:GOL:H12	1.94	0.49
3:U:600:HEC:CAA	3:U:601:HEC:HMA3	2.41	0.49
1:U:287:LEU:HD12	3:U:604:HEC:HBD2	1.93	0.49
1:D:495:ILE:HG12	1:F:492:LYS:HD3	1.93	0.49
1:I:144:ALA:HB3	1:I:148:PRO:HA	1.95	0.49
3:T:605:HEC:CBD	3:T:605:HEC:HMD1	2.43	0.49
1:D:182:GLU:O	1:D:185:GLN:HB2	2.12	0.49
3:G:600:HEC:CAA	3:G:601:HEC:HMA3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:195:SER:HB2	1:Q:221:THR:HA	1.95	0.49
1:G:429:ASN:ND2	7:G:706:HOH:O	2.46	0.49
1:K:368:LYS:HE2	1:K:470:ASP:OD1	2.12	0.49
1:O:195:SER:HB2	1:O:221:THR:HA	1.94	0.49
1:G:343:ASP:HB3	7:G:701:HOH:O	2.09	0.49
1:I:310:GLN:O	1:I:310:GLN:HG2	2.12	0.49
3:L:605:HEC:HMD1	3:L:605:HEC:CBD	2.41	0.49
2:Y:38:ILE:HG22	2:Y:41:GLY:H	1.77	0.49
1:B:343:ASP:HB3	7:B:709:HOH:O	2.12	0.49
1:G:368:LYS:HE2	1:G:470:ASP:OD1	2.13	0.49
3:I:603:HEC:HBC3	3:I:603:HEC:HMC1	1.95	0.49
3:W:605:HEC:CBD	3:W:605:HEC:HMD1	2.41	0.49
1:B:368:LYS:HE2	1:B:470:ASP:OD1	2.13	0.49
3:C:605:HEC:HMD1	3:C:605:HEC:CBD	2.42	0.49
3:U:605:HEC:CBD	3:U:605:HEC:HMD1	2.42	0.49
3:I:600:HEC:CAA	3:I:601:HEC:HMA3	2.43	0.49
1:K:232:GLN:HE22	1:K:246:GLN:NE2	2.03	0.49
3:N:605:HEC:CBD	3:N:605:HEC:HMD1	2.42	0.49
1:U:195:SER:HB2	1:U:221:THR:HA	1.94	0.49
3:W:607:HEC:CGA	1:X:226:ARG:HH22	2.25	0.49
1:A:497:TRP:CG	1:C:485:ARG:HD3	2.48	0.49
1:I:538:THR:HA	2:Y:110:PRO:HA	1.94	0.49
1:N:287:LEU:HD12	3:N:604:HEC:HBD2	1.94	0.49
1:Q:522:PRO:HD2	7:Q:728:HOH:O	2.12	0.49
1:S:195:SER:HB2	1:S:221:THR:HA	1.94	0.49
3:M:600:HEC:CAA	3:M:601:HEC:HMA3	2.41	0.48
1:S:90:PRO:O	1:S:93:ARG:HG2	2.13	0.48
1:H:349:ARG:NH2	4:H:609:SO4:O2	2.46	0.48
1:H:485:ARG:NH1	1:I:490:GLU:OE1	2.46	0.48
1:J:287:LEU:HD12	3:J:604:HEC:HBD2	1.95	0.48
1:K:233:ARG:NE	5:K:614:GOL:O3	2.43	0.48
3:O:605:HEC:CBD	3:O:605:HEC:HMD1	2.43	0.48
1:P:226:ARG:HH22	3:R:607:HEC:CGA	2.26	0.48
3:T:605:HEC:HBA2	3:T:606:HEC:HMA3	1.95	0.48
1:D:560:ALA:HB1	1:E:43:GLU:HA	1.93	0.48
1:I:389:PRO:HB2	5:I:615:GOL:H32	1.95	0.48
1:P:432:ASP:HB2	1:R:478:GLN:HE21	1.78	0.48
3:S:600:HEC:CAA	3:S:601:HEC:HMA3	2.43	0.48
1:V:479:ASN:HD22	1:X:482:ARG:HH22	1.60	0.48
3:V:605:HEC:HMD1	3:V:605:HEC:CBD	2.42	0.48
1:C:287:LEU:HD12	3:C:604:HEC:HBD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:CYS:HA	3:D:603:HEC:HMC3	1.94	0.48
1:I:76:SER:HB2	1:I:106:VAL:CG1	2.43	0.48
1:J:497:TRP:CG	1:L:485:ARG:HD3	2.48	0.48
1:K:485:ARG:HD3	1:L:497:TRP:CG	2.48	0.48
1:N:127:VAL:HG11	1:R:120:GLN:HA	1.95	0.48
1:V:452:MET:HE1	1:W:214:ALA:HB3	1.95	0.48
1:A:226:ARG:HH22	3:C:607:HEC:CGA	2.27	0.48
1:A:287:LEU:HD12	3:A:604:HEC:HBD2	1.93	0.48
1:B:485:ARG:HD3	1:C:497:TRP:CG	2.48	0.48
1:E:478:GLN:HE21	1:F:432:ASP:HB2	1.79	0.48
1:L:199:GLN:HB2	1:L:220:HIS:HB3	1.96	0.48
1:M:368:LYS:HE2	1:M:470:ASP:OD1	2.14	0.48
1:N:165:PRO:HG2	3:N:601:HEC:HMD3	1.94	0.48
1:W:485:ARG:HD3	1:X:497:TRP:CD1	2.48	0.48
3:A:605:HEC:HMD1	3:A:605:HEC:CBD	2.43	0.48
1:H:123:ALA:HB2	1:K:127:VAL:CG2	2.40	0.48
1:I:76:SER:HB2	1:I:106:VAL:HG13	1.96	0.48
1:J:452:MET:HE3	1:K:214:ALA:HB3	1.94	0.48
1:V:90:PRO:O	1:V:93:ARG:HG2	2.14	0.48
3:B:607:HEC:CGA	1:C:226:ARG:HH22	2.27	0.48
1:D:37:THR:HA	1:D:59:PHE:CE1	2.49	0.48
3:F:600:HEC:CAA	3:F:601:HEC:HMA3	2.44	0.48
1:N:195:SER:HB2	1:N:221:THR:HA	1.96	0.48
1:X:195:SER:HB2	1:X:221:THR:HA	1.96	0.48
1:E:199:GLN:HB2	1:E:220:HIS:HB3	1.95	0.48
1:I:120:GLN:HA	1:M:127:VAL:HG11	1.96	0.48
1:C:90:PRO:O	1:C:93:ARG:HG2	2.13	0.48
1:K:478:GLN:HE21	1:L:432:ASP:HB2	1.79	0.48
3:W:605:HEC:HBA2	3:W:606:HEC:HMA3	1.96	0.48
1:P:214:ALA:HB3	1:R:452:MET:HE3	1.96	0.48
1:T:485:ARG:HD3	1:U:497:TRP:CD1	2.49	0.48
1:S:479:ASN:HD22	1:U:482:ARG:HH22	1.62	0.48
1:I:90:PRO:O	1:I:93:ARG:HG2	2.14	0.47
1:J:195:SER:HB2	1:J:221:THR:HA	1.95	0.47
1:A:478:GLN:HE21	1:B:432:ASP:HB2	1.79	0.47
1:B:452:MET:HE3	1:C:214:ALA:HB3	1.96	0.47
1:D:231:HIS:HB3	1:D:241:ALA:HB2	1.96	0.47
1:G:454:HIS:HD2	3:G:606:HEC:NC	2.12	0.47
3:H:605:HEC:HBA2	3:H:606:HEC:HMA3	1.96	0.47
1:S:458:ASN:HB3	1:T:252:TRP:CZ2	2.49	0.47
1:U:368:LYS:HE2	1:U:470:ASP:OD1	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:90:PRO:O	1:X:93:ARG:HG2	2.14	0.47
1:D:524:LYS:HG2	1:D:528:ASP:HB3	1.96	0.47
1:N:478:GLN:HE21	1:O:432:ASP:HB2	1.79	0.47
3:X:600:HEC:CAA	3:X:601:HEC:HMA3	2.44	0.47
1:D:390:LYS:HA	1:D:400:HIS:HB3	1.96	0.47
1:G:120:GLN:HA	1:E:127:VAL:HG11	1.96	0.47
4:G:610:SO4:O4	1:I:482:ARG:HG3	2.15	0.47
1:G:44:VAL:HG23	1:I:330:LEU:HD21	1.96	0.47
1:J:199:GLN:HB2	1:J:220:HIS:HB3	1.96	0.47
1:M:226:ARG:HH22	3:O:607:HEC:CGA	2.27	0.47
1:V:214:ALA:HB3	1:X:452:MET:HE1	1.97	0.47
1:D:198:ALA:O	3:D:603:HEC:HHB	2.15	0.47
1:S:287:LEU:HD12	3:S:604:HEC:HBD2	1.96	0.47
1:U:90:PRO:O	1:U:93:ARG:HG2	2.14	0.47
1:D:500:GLU:N	1:D:500:GLU:OE1	2.46	0.47
3:E:607:HEC:CGA	1:F:226:ARG:HH22	2.27	0.47
1:P:223:PRO:HG3	3:P:605:HEC:HBC2	1.97	0.47
1:R:343:ASP:HB2	7:R:701:HOH:O	2.15	0.47
1:R:287:LEU:HD12	3:R:604:HEC:HBD2	1.97	0.47
1:A:452:MET:HE1	1:B:214:ALA:HB3	1.97	0.47
1:D:97:PRO:HG2	1:D:166:SER:HB3	1.96	0.47
1:E:287:LEU:HD12	3:E:604:HEC:HBD2	1.95	0.47
3:Q:605:HEC:HBA2	3:Q:606:HEC:HMA3	1.97	0.47
1:B:287:LEU:HD12	3:B:604:HEC:HBD2	1.96	0.47
1:D:542:PRO:HG2	1:D:545:GLU:HB2	1.96	0.47
1:G:199:GLN:HB2	1:G:220:HIS:HB3	1.97	0.47
1:J:485:ARG:HD3	1:K:497:TRP:CG	2.49	0.47
4:J:611:SO4:O2	1:K:482:ARG:NH1	2.48	0.47
1:M:432:ASP:HB2	1:O:478:GLN:HE21	1.80	0.47
1:R:199:GLN:HB2	1:R:220:HIS:HB3	1.97	0.47
3:X:604:HEC:CBC	3:X:605:HEC:HBB2	2.45	0.47
1:A:172:THR:HG21	2:Z:34:TRP:CH2	2.50	0.47
1:C:207:GLU:HA	1:C:513:THR:OG1	2.15	0.47
1:D:523:GLY:O	1:D:524:LYS:HG3	2.14	0.47
1:S:485:ARG:HD2	1:T:490:GLU:OE2	2.13	0.47
1:G:109:SER:HA	7:G:745:HOH:O	2.15	0.47
1:H:90:PRO:O	1:H:93:ARG:HG2	2.15	0.47
1:K:452:MET:HE3	1:L:214:ALA:HB3	1.97	0.47
3:P:605:HEC:HBA2	3:P:606:HEC:HMA3	1.97	0.47
1:X:386:ASP:HA	1:X:387:PRO:HA	1.73	0.47
1:C:232:GLN:HE22	1:C:246:GLN:NE2	2.07	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:GLY:O	1:F:370:ARG:NH1	2.46	0.47
1:H:485:ARG:HD2	1:I:490:GLU:OE2	2.14	0.47
1:M:252:TRP:CZ2	1:O:458:ASN:HB3	2.50	0.47
3:O:600:HEC:CAA	3:O:601:HEC:HMA3	2.43	0.47
1:O:287:LEU:HD12	3:O:604:HEC:HBD2	1.96	0.47
1:U:199:GLN:HB2	1:U:220:HIS:HB3	1.97	0.47
1:D:87:LYS:HB2	1:D:210:PRO:HD3	1.97	0.46
1:G:452:MET:HE3	1:H:214:ALA:HB3	1.97	0.46
1:J:403:SER:HB3	1:J:434:GLU:OE2	2.15	0.46
3:P:605:HEC:HMD1	3:P:605:HEC:CBD	2.43	0.46
1:R:343:ASP:HB3	7:R:701:HOH:O	2.15	0.46
1:F:173:ALA:HA	1:F:177:GLU:HB2	1.97	0.46
1:Q:386:ASP:HA	1:Q:387:PRO:HA	1.73	0.46
1:S:199:GLN:HB2	1:S:220:HIS:HB3	1.98	0.46
1:T:287:LEU:HD12	3:T:604:HEC:HBD2	1.96	0.46
1:T:90:PRO:O	1:T:93:ARG:HG2	2.15	0.46
1:S:252:TRP:CZ2	1:U:458:ASN:HB3	2.50	0.46
1:T:482:ARG:HH22	1:U:479:ASN:HD22	1.62	0.46
1:W:199:GLN:HB2	1:W:220:HIS:HB3	1.97	0.46
1:A:485:ARG:HD3	1:B:497:TRP:CG	2.50	0.46
1:K:403:SER:HB3	1:K:434:GLU:OE2	2.15	0.46
1:Q:173:ALA:HA	1:Q:177:GLU:HB2	1.97	0.46
3:R:605:HEC:HBA2	3:R:606:HEC:HMA3	1.98	0.46
1:D:306:HIS:CE1	1:D:308:ASN:HB3	2.50	0.46
1:G:349:ARG:NH2	4:G:609:SO4:O3	2.48	0.46
1:H:199:GLN:HB2	1:H:220:HIS:HB3	1.98	0.46
1:H:473:LEU:HG	5:H:615:GOL:H2	1.97	0.46
1:G:511:GLN:HG3	1:I:367:LEU:HD21	1.98	0.46
1:I:227:CYS:HB2	3:I:602:HEC:HMB1	1.98	0.46
1:N:199:GLN:HB2	1:N:220:HIS:HB3	1.96	0.46
1:P:478:GLN:HE21	1:Q:432:ASP:HB2	1.80	0.46
1:Q:485:ARG:HD3	1:R:497:TRP:CG	2.50	0.46
1:B:482:ARG:HG3	4:B:609:SO4:O1	2.16	0.46
1:A:432:ASP:H	1:C:478:GLN:NE2	2.14	0.46
1:F:368:LYS:HE2	1:F:470:ASP:OD1	2.15	0.46
1:D:432:ASP:HB2	1:F:478:GLN:HE21	1.81	0.46
3:N:600:HEC:CAA	3:N:601:HEC:HMA3	2.44	0.46
1:S:226:ARG:HH22	3:U:607:HEC:CGA	2.28	0.46
1:V:199:GLN:HB2	1:V:220:HIS:HB3	1.98	0.46
1:A:199:GLN:HB2	1:A:220:HIS:HB3	1.97	0.46
1:J:318:SER:HB2	5:K:615:GOL:O3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:605:HEC:HBA2	3:O:606:HEC:HMA3	1.97	0.46
1:P:252:TRP:CZ2	1:R:458:ASN:HB3	2.51	0.46
3:U:604:HEC:CBC	3:U:605:HEC:HBB2	2.45	0.46
1:V:252:TRP:CZ2	1:X:458:ASN:HB3	2.51	0.46
1:C:199:GLN:HB2	1:C:220:HIS:HB3	1.97	0.46
1:F:199:GLN:HB2	1:F:220:HIS:HB3	1.98	0.46
1:I:123:ALA:HB2	1:M:127:VAL:HG21	1.98	0.46
1:I:255:ASP:HB2	1:I:319:MET:CE	2.46	0.46
1:J:214:ALA:HB3	1:L:452:MET:HE1	1.98	0.46
3:P:607:HEC:CGA	1:Q:226:ARG:HH22	2.27	0.46
1:S:127:VAL:HG21	1:X:123:ALA:HB2	1.97	0.46
3:B:600:HEC:CAA	3:B:601:HEC:HMA3	2.45	0.46
3:B:605:HEC:HBA2	3:B:606:HEC:HMA3	1.97	0.46
1:H:123:ALA:CB	1:K:127:VAL:HB	2.46	0.46
1:H:458:ASN:HB3	1:I:252:TRP:CZ2	2.51	0.46
2:Z:38:ILE:HG22	2:Z:41:GLY:H	1.81	0.46
1:H:173:ALA:HA	1:H:177:GLU:HB2	1.98	0.46
3:I:604:HEC:CBC	3:I:605:HEC:HBB2	2.45	0.46
3:J:605:HEC:HBA2	3:J:606:HEC:HMA3	1.98	0.46
1:K:90:PRO:O	1:K:93:ARG:HG2	2.16	0.46
1:M:485:ARG:HD3	1:N:497:TRP:CG	2.51	0.46
3:C:605:HEC:HBA2	3:C:606:HEC:HMA3	1.98	0.46
1:H:485:ARG:HD3	1:I:497:TRP:CG	2.51	0.46
1:K:223:PRO:HG3	3:K:605:HEC:HBC2	1.98	0.46
1:N:485:ARG:HD3	1:O:497:TRP:CG	2.51	0.46
1:O:386:ASP:HA	1:O:387:PRO:HA	1.73	0.46
1:O:403:SER:HB3	1:O:434:GLU:OE2	2.16	0.46
1:M:497:TRP:CG	1:O:485:ARG:HD3	2.51	0.46
1:O:207:GLU:HA	1:O:513:THR:OG1	2.16	0.46
1:T:458:ASN:HB3	1:U:252:TRP:CZ2	2.51	0.46
1:S:497:TRP:CD1	1:U:485:ARG:HD3	2.50	0.46
3:U:605:HEC:HBA2	3:U:606:HEC:HMA3	1.98	0.46
1:A:432:ASP:HB2	1:C:478:GLN:HE21	1.81	0.45
1:D:367:LEU:HD21	1:E:511:GLN:HG3	1.97	0.45
1:G:63:LYS:NZ	5:G:615:GOL:O3	2.49	0.45
1:H:386:ASP:HA	1:H:387:PRO:HA	1.74	0.45
1:O:199:GLN:HB2	1:O:220:HIS:HB3	1.97	0.45
1:R:257:ARG:HD3	7:R:720:HOH:O	2.16	0.45
1:T:199:GLN:HB2	1:T:220:HIS:HB3	1.98	0.45
1:W:485:ARG:HD2	1:X:490:GLU:OE2	2.16	0.45
1:E:90:PRO:O	1:E:93:ARG:HG2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:TRP:CZ2	1:F:458:ASN:HB3	2.51	0.45
1:G:403:SER:HB3	1:G:434:GLU:OE2	2.16	0.45
1:H:454:HIS:HA	5:H:614:GOL:C2	2.38	0.45
1:K:173:ALA:HA	1:K:177:GLU:HB2	1.98	0.45
1:J:127:VAL:CG2	1:P:123:ALA:HB2	2.45	0.45
1:V:173:ALA:HA	1:V:177:GLU:HB2	1.98	0.45
1:E:482:ARG:HH22	1:F:479:ASN:HD22	1.65	0.45
3:G:605:HEC:HBA2	3:G:606:HEC:HMA3	1.98	0.45
3:J:604:HEC:CBC	3:J:605:HEC:HBB2	2.46	0.45
1:K:478:GLN:NE2	1:L:432:ASP:H	2.13	0.45
1:M:199:GLN:HB2	1:M:220:HIS:HB3	1.97	0.45
1:P:199:GLN:HB2	1:P:220:HIS:HB3	1.97	0.45
1:P:90:PRO:O	1:P:93:ARG:HG2	2.17	0.45
1:Q:452:MET:HE3	1:R:214:ALA:HB3	1.98	0.45
3:T:607:HEC:CGA	1:U:226:ARG:HH22	2.30	0.45
1:T:452:MET:HE1	1:U:214:ALA:HB3	1.98	0.45
3:D:605:HEC:HMD1	3:D:605:HEC:CBD	2.45	0.45
1:G:482:ARG:HG3	4:G:610:SO4:O1	2.15	0.45
1:G:478:GLN:NE2	1:H:432:ASP:H	2.13	0.45
1:W:90:PRO:O	1:W:93:ARG:HG2	2.17	0.45
3:A:605:HEC:HBA2	3:A:606:HEC:HMA3	1.99	0.45
3:K:606:HEC:HBC1	3:K:607:HEC:HHC	1.99	0.45
1:L:287:LEU:HD12	3:L:604:HEC:HBD2	1.98	0.45
1:P:458:ASN:HB3	1:Q:252:TRP:CZ2	2.51	0.45
1:A:403:SER:HB3	1:A:434:GLU:OE2	2.16	0.45
1:G:245:GLU:HG2	1:I:272:GLN:OE1	2.17	0.45
1:J:432:ASP:HB2	1:L:478:GLN:HE21	1.81	0.45
3:T:606:HEC:HBC1	3:T:607:HEC:HHC	1.99	0.45
1:V:454:HIS:HD2	3:V:606:HEC:NC	2.13	0.45
1:X:173:ALA:HA	1:X:177:GLU:HB2	1.98	0.45
1:A:490:GLU:OE2	1:C:485:ARG:HD2	2.17	0.45
1:G:90:PRO:O	1:G:93:ARG:HG2	2.16	0.45
5:J:613:GOL:O1	1:K:63:LYS:NZ	2.49	0.45
3:L:605:HEC:HBA2	3:L:606:HEC:HMA3	1.99	0.45
1:N:90:PRO:O	1:N:93:ARG:HG2	2.16	0.45
3:R:604:HEC:CBC	3:R:605:HEC:HBB2	2.47	0.45
3:S:605:HEC:HBA2	3:S:606:HEC:HMA3	1.98	0.45
3:S:607:HEC:CGA	1:T:226:ARG:HH22	2.29	0.45
1:U:173:ALA:HA	1:U:177:GLU:HB2	1.99	0.45
1:V:478:GLN:HE21	1:W:432:ASP:HB2	1.81	0.45
1:A:90:PRO:O	1:A:93:ARG:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:GLN:HB2	1:B:220:HIS:HB3	1.98	0.45
1:A:252:TRP:CZ2	1:C:458:ASN:HB3	2.52	0.45
1:E:485:ARG:HD3	1:F:497:TRP:CD1	2.52	0.45
1:D:489:LEU:HD23	1:E:495:ILE:HD12	1.99	0.45
3:E:605:HEC:HBA2	3:E:606:HEC:HMA3	1.98	0.45
3:F:604:HEC:CBC	3:F:605:HEC:HBB2	2.46	0.45
1:I:369:TYR:CE1	1:I:441:VAL:HB	2.52	0.45
1:J:386:ASP:HA	1:J:387:PRO:HA	1.73	0.45
1:N:154:CYS:HB3	1:N:165:PRO:HG3	1.98	0.45
3:N:605:HEC:HBA2	3:N:606:HEC:HMA3	1.99	0.45
1:Q:199:GLN:HB2	1:Q:220:HIS:HB3	1.98	0.45
1:Q:478:GLN:HE21	1:R:432:ASP:HB2	1.82	0.45
3:R:606:HEC:HBC1	3:R:607:HEC:HHC	1.99	0.45
3:V:604:HEC:CBC	3:V:605:HEC:HBB2	2.46	0.45
1:V:497:TRP:CD1	1:X:485:ARG:HD3	2.52	0.45
1:B:458:ASN:HB3	1:C:252:TRP:CZ2	2.52	0.45
1:E:458:ASN:HB3	1:F:252:TRP:CZ2	2.52	0.45
3:F:605:HEC:HBA2	3:F:606:HEC:HMA3	1.98	0.45
1:F:90:PRO:O	1:F:93:ARG:HG2	2.16	0.45
1:G:41:PRO:O	1:G:44:VAL:HG12	2.17	0.45
1:K:199:GLN:HB2	1:K:220:HIS:HB3	1.98	0.45
1:M:403:SER:HB3	1:M:434:GLU:OE2	2.17	0.45
1:P:432:ASP:H	1:R:478:GLN:NE2	2.15	0.45
3:W:604:HEC:CBC	3:W:605:HEC:HBB2	2.46	0.45
1:X:199:GLN:HB2	1:X:220:HIS:HB3	1.98	0.45
1:B:343:ASP:CB	7:B:709:HOH:O	2.64	0.45
1:M:478:GLN:HE21	1:N:432:ASP:HB2	1.82	0.45
1:N:403:SER:HB3	1:N:434:GLU:OE2	2.16	0.45
1:M:490:GLU:OE2	1:O:485:ARG:HD2	2.17	0.45
1:P:403:SER:HB3	1:P:434:GLU:OE2	2.17	0.45
1:Q:90:PRO:O	1:Q:93:ARG:HG2	2.16	0.45
3:X:605:HEC:HBA2	3:X:606:HEC:HMA3	1.99	0.45
1:A:458:ASN:HB3	1:B:252:TRP:CZ2	2.52	0.44
3:F:606:HEC:HBC1	3:F:607:HEC:HHC	2.00	0.44
1:I:241:ALA:O	1:I:298:GLN:NE2	2.50	0.44
1:L:90:PRO:O	1:L:93:ARG:HG2	2.17	0.44
1:M:452:MET:HE1	1:N:214:ALA:HB3	1.99	0.44
1:M:432:ASP:H	1:O:478:GLN:NE2	2.16	0.44
1:S:41:PRO:O	1:S:44:VAL:HG12	2.17	0.44
1:W:452:MET:HE1	1:X:214:ALA:HB3	1.97	0.44
1:C:403:SER:HB3	1:C:434:GLU:OE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:ALA:HA	1:E:177:GLU:HB2	2.00	0.44
1:J:340:SER:O	1:J:343:ASP:HB2	2.17	0.44
3:M:605:HEC:HBA2	3:M:606:HEC:HMA3	1.98	0.44
1:N:454:HIS:HD2	3:N:606:HEC:NC	2.15	0.44
3:V:606:HEC:HBC1	3:V:607:HEC:HHC	1.99	0.44
1:A:154:CYS:HB3	1:A:165:PRO:HG3	2.00	0.44
1:E:154:CYS:HB3	1:E:165:PRO:HG3	1.98	0.44
1:H:287:LEU:HD12	3:H:604:HEC:HBD2	1.98	0.44
1:J:485:ARG:HD2	1:K:490:GLU:OE2	2.17	0.44
1:K:287:LEU:HD12	3:K:604:HEC:HBD2	1.98	0.44
1:J:318:SER:HB2	5:K:615:GOL:C3	2.48	0.44
1:P:485:ARG:HD3	1:Q:497:TRP:CG	2.51	0.44
1:T:173:ALA:HA	1:T:177:GLU:HB2	1.97	0.44
1:B:154:CYS:HB3	1:B:165:PRO:HG3	1.99	0.44
3:B:606:HEC:HBC1	3:B:607:HEC:HHC	2.00	0.44
1:H:223:PRO:HG3	3:H:605:HEC:HBC2	1.99	0.44
3:I:605:HEC:HBA2	3:I:606:HEC:HMA3	1.99	0.44
3:K:605:HEC:HBA2	3:K:606:HEC:HMA3	1.99	0.44
1:M:214:ALA:HB3	1:O:452:MET:HE1	1.99	0.44
1:D:222:SER:HB2	1:D:223:PRO:HD3	1.99	0.44
1:F:154:CYS:HB3	1:F:165:PRO:HG3	2.00	0.44
1:G:478:GLN:HE21	1:H:432:ASP:HB2	1.81	0.44
1:J:197:PHE:HB2	1:J:535:TRP:CD2	2.53	0.44
1:H:120:GLN:HA	1:K:127:VAL:HG11	1.99	0.44
1:J:490:GLU:OE2	1:L:485:ARG:HD2	2.17	0.44
1:S:403:SER:HB3	1:S:434:GLU:OE2	2.18	0.44
1:U:403:SER:HB3	1:U:434:GLU:OE2	2.17	0.44
1:B:173:ALA:HA	1:B:177:GLU:HB2	2.00	0.44
1:I:59:PHE:C	1:I:61:GLY:H	2.20	0.44
3:K:607:HEC:O2A	1:L:226:ARG:NH2	2.51	0.44
1:L:403:SER:HB3	1:L:434:GLU:OE2	2.18	0.44
1:Q:458:ASN:HB3	1:R:252:TRP:CZ2	2.53	0.44
1:V:223:PRO:HG3	3:V:605:HEC:HBC2	2.00	0.44
1:W:403:SER:HB3	1:W:434:GLU:OE2	2.17	0.44
1:E:386:ASP:HA	1:E:387:PRO:HA	1.73	0.44
1:D:331:TRP:HZ2	1:E:44:VAL:HG21	1.83	0.44
1:G:197:PHE:HB2	1:G:535:TRP:CD2	2.53	0.44
1:H:474:VAL:CG2	5:H:615:GOL:C3	2.93	0.44
1:J:478:GLN:HE21	1:K:432:ASP:HB2	1.83	0.44
1:T:197:PHE:HB2	1:T:535:TRP:CD2	2.53	0.44
1:W:386:ASP:HA	1:W:387:PRO:HA	1.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:223:PRO:HG3	3:W:605:HEC:HBC2	1.99	0.44
1:B:86:TRP:CH2	1:B:205:SER:HB3	2.53	0.44
1:B:403:SER:HB3	1:B:434:GLU:OE2	2.17	0.44
1:B:90:PRO:O	1:B:93:ARG:HG2	2.17	0.44
1:I:241:ALA:HA	1:I:246:GLN:HG3	1.99	0.44
1:J:373:PHE:CD1	5:J:613:GOL:H11	2.52	0.44
3:V:607:HEC:O2A	1:W:226:ARG:NH2	2.51	0.44
1:W:207:GLU:HA	1:W:513:THR:OG1	2.18	0.44
1:A:173:ALA:HA	1:A:177:GLU:HB2	1.98	0.44
1:D:389:PRO:HA	1:D:392:LEU:HD12	1.99	0.44
1:E:223:PRO:HG3	3:E:605:HEC:HBC2	2.00	0.44
1:H:154:CYS:HB3	1:H:165:PRO:HG3	2.00	0.44
1:H:403:SER:HB3	1:H:434:GLU:OE2	2.17	0.44
1:J:173:ALA:HA	1:J:177:GLU:HB2	1.99	0.44
1:L:81:LYS:HD3	1:L:82:TYR:CZ	2.53	0.44
1:O:90:PRO:O	1:O:93:ARG:HG2	2.17	0.44
3:Q:604:HEC:CBC	3:Q:605:HEC:HBB2	2.48	0.44
1:R:403:SER:HB3	1:R:434:GLU:OE2	2.18	0.44
1:Q:485:ARG:HD2	1:R:490:GLU:OE2	2.18	0.44
1:W:478:GLN:HE21	1:X:432:ASP:HB2	1.83	0.44
1:H:265:GLY:HA3	7:H:732:HOH:O	2.18	0.43
1:Q:41:PRO:O	1:Q:44:VAL:HG12	2.18	0.43
1:P:497:TRP:CG	1:R:485:ARG:HD3	2.52	0.43
1:B:41:PRO:O	1:B:44:VAL:HG12	2.18	0.43
1:L:173:ALA:HA	1:L:177:GLU:HB2	2.00	0.43
3:M:606:HEC:HBC1	3:M:607:HEC:HHC	2.00	0.43
1:N:173:ALA:HA	1:N:177:GLU:HB2	2.00	0.43
1:U:86:TRP:CH2	1:U:205:SER:HB3	2.54	0.43
3:U:606:HEC:HBC1	3:U:607:HEC:HHC	2.00	0.43
3:V:605:HEC:HBA2	3:V:606:HEC:HMA3	2.01	0.43
1:V:458:ASN:HB3	1:W:252:TRP:CZ2	2.53	0.43
1:X:232:GLN:HE22	1:X:246:GLN:NE2	2.07	0.43
1:D:76:SER:HB2	1:D:106:VAL:HG13	2.00	0.43
1:F:41:PRO:O	1:F:44:VAL:HG12	2.18	0.43
1:G:458:ASN:HB3	1:H:252:TRP:CZ2	2.53	0.43
1:H:454:HIS:C	5:H:614:GOL:H2	2.39	0.43
1:I:309:VAL:HG13	3:I:605:HEC:C3A	2.48	0.43
1:J:478:GLN:NE2	1:K:432:ASP:H	2.16	0.43
3:L:604:HEC:CBC	3:L:605:HEC:HBB2	2.47	0.43
1:Q:362:VAL:HG13	7:Q:736:HOH:O	2.17	0.43
1:P:485:ARG:HD2	1:Q:490:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:478:GLN:NE2	1:U:432:ASP:H	2.15	0.43
1:V:485:ARG:HD2	1:W:490:GLU:OE2	2.17	0.43
1:E:86:TRP:CH2	1:E:205:SER:HB3	2.54	0.43
1:E:452:MET:HE1	1:F:214:ALA:HB3	2.00	0.43
1:I:244:SER:OG	1:I:296:THR:HB	2.18	0.43
1:N:452:MET:HE3	1:O:214:ALA:HB3	2.01	0.43
1:Q:127:VAL:HG13	1:T:120:GLN:NE2	2.33	0.43
1:X:86:TRP:CH2	1:X:205:SER:HB3	2.53	0.43
1:X:223:PRO:HG3	3:X:605:HEC:HBC2	2.01	0.43
1:E:197:PHE:HB2	1:E:535:TRP:CD2	2.53	0.43
1:G:173:ALA:HA	1:G:177:GLU:HB2	2.00	0.43
3:H:606:HEC:HBC1	3:H:607:HEC:HHC	1.99	0.43
1:J:432:ASP:H	1:L:478:GLN:NE2	2.16	0.43
1:N:485:ARG:HD2	1:O:490:GLU:OE2	2.19	0.43
1:D:467:PHE:N	1:D:467:PHE:CD1	2.86	0.43
1:G:318:SER:HB2	7:G:703:HOH:O	2.18	0.43
3:J:606:HEC:HBC1	3:J:607:HEC:HHC	2.00	0.43
1:K:76:SER:CB	1:K:106:VAL:HG11	2.44	0.43
1:M:173:ALA:HA	1:M:177:GLU:HB2	1.99	0.43
1:T:403:SER:HB3	1:T:434:GLU:OE2	2.18	0.43
1:W:173:ALA:HA	1:W:177:GLU:HB2	1.99	0.43
1:X:197:PHE:HB2	1:X:535:TRP:CD2	2.54	0.43
1:B:478:GLN:HE21	1:C:432:ASP:HB2	1.83	0.43
1:E:454:HIS:HD2	3:E:606:HEC:NC	2.16	0.43
1:J:41:PRO:O	1:J:44:VAL:HG12	2.19	0.43
3:J:607:HEC:O2A	1:K:226:ARG:NH2	2.52	0.43
3:L:606:HEC:HBC1	3:L:607:HEC:HHC	2.01	0.43
3:P:604:HEC:CB	3:P:605:HEC:HBB2	2.49	0.43
1:S:207:GLU:HA	1:S:513:THR:OG1	2.19	0.43
3:W:606:HEC:HBC1	3:W:607:HEC:HHC	2.00	0.43
1:E:403:SER:HB3	1:E:434:GLU:OE2	2.17	0.43
1:I:204:TRP:HH2	5:I:614:GOL:H31	1.84	0.43
1:K:197:PHE:HB2	1:K:535:TRP:CD2	2.54	0.43
1:J:226:ARG:NH2	3:L:607:HEC:O2A	2.52	0.43
3:Q:606:HEC:HBC1	3:Q:607:HEC:HHC	1.99	0.43
1:S:173:ALA:HA	1:S:177:GLU:HB2	2.00	0.43
1:S:86:TRP:CH2	1:S:205:SER:HB3	2.53	0.43
1:W:454:HIS:HD2	3:W:606:HEC:NC	2.14	0.43
1:C:454:HIS:HD2	3:C:606:HEC:NC	2.16	0.43
1:C:223:PRO:HG3	3:C:605:HEC:HBC2	2.00	0.43
1:D:509:LEU:HD11	1:F:477:LYS:NZ	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:PRO:O	1:E:44:VAL:HG12	2.19	0.43
1:F:86:TRP:CH2	1:F:205:SER:HB3	2.54	0.43
1:H:232:GLN:HE22	1:H:246:GLN:NE2	2.08	0.43
1:K:458:ASN:HB3	1:L:252:TRP:CZ2	2.54	0.43
1:L:41:PRO:O	1:L:44:VAL:HG12	2.19	0.43
1:L:197:PHE:HB2	1:L:535:TRP:CD2	2.54	0.43
1:M:223:PRO:HG3	3:M:605:HEC:HBC2	2.00	0.43
1:R:41:PRO:O	1:R:44:VAL:HG12	2.18	0.43
1:C:41:PRO:O	1:C:44:VAL:HG12	2.19	0.43
3:Q:607:HEC:O2A	1:R:226:ARG:NH2	2.51	0.43
1:S:478:GLN:HE21	1:T:432:ASP:HB2	1.83	0.43
1:U:197:PHE:HB2	1:U:535:TRP:CD2	2.54	0.43
1:A:197:PHE:HB2	1:A:535:TRP:CD2	2.54	0.42
1:B:232:GLN:HE22	1:B:246:GLN:NE2	2.09	0.42
1:A:214:ALA:HB3	1:C:452:MET:HE3	2.00	0.42
1:D:276:TRP:CE2	1:F:276:TRP:HB2	2.54	0.42
1:F:197:PHE:HB2	1:F:535:TRP:CD2	2.54	0.42
1:G:81:LYS:HD3	1:G:82:TYR:CZ	2.54	0.42
1:I:454:HIS:HD2	3:I:606:HEC:C1C	2.32	0.42
1:J:81:LYS:HD3	1:J:82:TYR:CZ	2.53	0.42
1:K:454:HIS:HD2	3:K:606:HEC:NC	2.14	0.42
1:O:173:ALA:HA	1:O:177:GLU:HB2	2.00	0.42
3:T:604:HEC:CBC	3:T:605:HEC:HBB2	2.47	0.42
1:B:197:PHE:HB2	1:B:535:TRP:CD2	2.54	0.42
1:C:173:ALA:HA	1:C:177:GLU:HB2	2.00	0.42
1:D:145:GLU:HA	1:D:146:PRO:C	2.39	0.42
1:I:122:VAL:O	1:I:126:SER:HB3	2.19	0.42
1:I:386:ASP:HA	1:I:387:PRO:HA	1.68	0.42
3:I:603:HEC:HAD2	3:I:603:HEC:HHA	1.89	0.42
1:I:287:LEU:HD12	3:I:604:HEC:HBD2	2.01	0.42
1:M:90:PRO:O	1:M:93:ARG:HG2	2.19	0.42
1:M:458:ASN:HB3	1:N:252:TRP:CZ2	2.53	0.42
1:Q:223:PRO:HG3	3:Q:605:HEC:HBC2	2.01	0.42
1:R:173:ALA:HA	1:R:177:GLU:HB2	1.99	0.42
1:R:86:TRP:CH2	1:R:205:SER:HB3	2.54	0.42
1:A:41:PRO:O	1:A:44:VAL:HG12	2.20	0.42
3:E:604:HEC:CBC	3:E:605:HEC:HBB2	2.47	0.42
3:G:607:HEC:O2A	1:H:226:ARG:NH2	2.52	0.42
1:K:41:PRO:O	1:K:44:VAL:HG12	2.19	0.42
3:C:600:HEC:HMC1	1:L:128:MET:HE1	2.01	0.42
1:P:173:ALA:HA	1:P:177:GLU:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:606:HEC:HBC1	3:C:607:HEC:HHC	2.01	0.42
1:F:81:LYS:HD3	1:F:82:TYR:CZ	2.55	0.42
1:K:207:GLU:HA	1:K:513:THR:OG1	2.20	0.42
1:R:386:ASP:HA	1:R:387:PRO:HA	1.73	0.42
1:S:197:PHE:HB2	1:S:535:TRP:CD2	2.54	0.42
3:U:601:HEC:HBA1	3:U:601:HEC:HHA	2.02	0.42
1:V:482:ARG:HH22	1:W:479:ASN:HD22	1.67	0.42
1:F:386:ASP:HA	1:F:387:PRO:HA	1.73	0.42
1:F:403:SER:HB3	1:F:434:GLU:OE2	2.18	0.42
1:G:232:GLN:HE22	1:G:246:GLN:NE2	2.07	0.42
1:H:264:ILE:HG12	1:I:252:TRP:CE2	2.54	0.42
1:T:86:TRP:CH2	1:T:205:SER:HB3	2.54	0.42
1:V:403:SER:HB3	1:V:434:GLU:OE2	2.20	0.42
3:X:606:HEC:HBC1	3:X:607:HEC:HHC	2.02	0.42
3:A:607:HEC:O2A	1:B:226:ARG:NH2	2.53	0.42
1:B:478:GLN:NE2	1:C:432:ASP:H	2.18	0.42
1:C:189:GLY:HA2	3:C:605:HEC:CGD	2.50	0.42
1:D:485:ARG:HD3	1:E:497:TRP:CD2	2.55	0.42
1:F:454:HIS:HD2	3:F:606:HEC:NC	2.14	0.42
1:H:353:GLU:OE2	1:I:93:ARG:NH1	2.53	0.42
1:I:364:ASP:O	1:I:367:LEU:HB3	2.20	0.42
1:I:37:THR:HA	1:I:59:PHE:CE1	2.55	0.42
1:K:429:ASN:ND2	7:K:706:HOH:O	2.50	0.42
1:P:454:HIS:HD2	3:P:606:HEC:NC	2.14	0.42
1:R:189:GLY:HA2	3:R:605:HEC:CGD	2.50	0.42
1:X:222:SER:HB2	1:X:223:PRO:HD3	2.02	0.42
3:A:606:HEC:HBC1	3:A:607:HEC:HHC	2.01	0.42
3:C:604:HEC:CBC	3:C:605:HEC:HBB2	2.48	0.42
1:L:86:TRP:CH2	1:L:205:SER:HB3	2.54	0.42
1:M:41:PRO:O	1:M:44:VAL:HG12	2.19	0.42
1:M:482:ARG:HH22	1:N:479:ASN:HD22	1.67	0.42
1:M:485:ARG:HD2	1:N:490:GLU:OE2	2.19	0.42
1:N:197:PHE:HB2	1:N:535:TRP:CD2	2.55	0.42
3:O:606:HEC:HBC1	3:O:607:HEC:HHC	2.01	0.42
1:N:127:VAL:CG2	1:R:123:ALA:HB2	2.43	0.42
1:W:197:PHE:HB2	1:W:535:TRP:CD2	2.55	0.42
3:H:604:HEC:CBC	3:H:605:HEC:HBB2	2.49	0.42
1:H:478:GLN:NE2	1:I:432:ASP:H	2.18	0.42
3:N:607:HEC:O2A	1:O:226:ARG:NH2	2.52	0.42
1:N:458:ASN:HB3	1:O:252:TRP:CZ2	2.55	0.42
1:O:454:HIS:HD2	3:O:606:HEC:NC	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:403:SER:HB3	1:Q:434:GLU:OE2	2.19	0.42
1:R:197:PHE:HB2	1:R:535:TRP:CD2	2.55	0.42
1:W:86:TRP:CH2	1:W:205:SER:HB3	2.55	0.42
1:W:189:GLY:HA2	3:W:605:HEC:CGD	2.50	0.42
1:X:41:PRO:O	1:X:44:VAL:HG12	2.19	0.42
1:D:229:THR:HB	3:D:604:HEC:HMC3	2.02	0.42
1:E:76:SER:CB	1:E:106:VAL:HG11	2.43	0.42
1:H:561:GLY:H	1:I:43:GLU:HA	1.85	0.42
1:K:505:THR:HG22	7:K:707:HOH:O	2.18	0.42
1:P:86:TRP:CH2	1:P:205:SER:HB3	2.55	0.42
1:Q:81:LYS:HD3	1:Q:82:TYR:CZ	2.55	0.42
1:S:454:HIS:HD2	3:S:606:HEC:NC	2.15	0.42
1:S:482:ARG:HH22	1:T:479:ASN:HD22	1.68	0.42
1:U:454:HIS:HD2	3:U:606:HEC:NC	2.14	0.42
1:A:235:GLN:HG2	7:A:723:HOH:O	2.19	0.42
1:C:386:ASP:HA	1:C:387:PRO:HA	1.73	0.42
3:D:602:HEC:HBB3	3:D:602:HEC:HMB1	2.01	0.42
3:G:606:HEC:HBC1	3:G:607:HEC:HHC	2.01	0.42
1:J:482:ARG:HH22	1:K:479:ASN:HD22	1.68	0.42
1:N:207:GLU:HA	1:N:513:THR:OG1	2.20	0.42
1:O:86:TRP:CH2	1:O:205:SER:HB3	2.55	0.42
1:O:223:PRO:HG3	3:O:605:HEC:HBC2	2.01	0.42
1:P:197:PHE:HB2	1:P:535:TRP:CD2	2.55	0.42
1:Q:154:CYS:HB3	1:Q:165:PRO:HG3	2.02	0.42
1:S:223:PRO:HG3	3:S:605:HEC:HBC2	2.01	0.42
1:S:490:GLU:OE2	1:U:485:ARG:HD2	2.20	0.42
1:D:235:GLN:HE22	1:F:280:GLN:NE2	2.18	0.41
1:D:262:TYR:CB	3:D:606:HEC:HBB2	2.50	0.41
1:H:41:PRO:O	1:H:44:VAL:HG12	2.19	0.41
1:G:485:ARG:HD2	1:H:490:GLU:OE2	2.20	0.41
1:I:450:LYS:HE2	3:I:606:HEC:HAA1	2.01	0.41
1:J:458:ASN:HB3	1:K:252:TRP:CZ2	2.54	0.41
1:N:41:PRO:O	1:N:44:VAL:HG12	2.20	0.41
1:N:86:TRP:CH2	1:N:205:SER:HB3	2.55	0.41
1:O:176:HIS:HB3	1:O:179:GLN:HE21	1.85	0.41
1:O:41:PRO:O	1:O:44:VAL:HG12	2.20	0.41
1:O:197:PHE:HB2	1:O:535:TRP:CD2	2.55	0.41
1:Q:86:TRP:CH2	1:Q:205:SER:HB3	2.54	0.41
1:R:223:PRO:HG3	3:R:605:HEC:HBC2	2.02	0.41
1:R:90:PRO:O	1:R:93:ARG:HG2	2.19	0.41
1:T:189:GLY:HA2	3:T:605:HEC:CGD	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:378:ASP:HB2	7:E:711:HOH:O	2.20	0.41
1:F:232:GLN:HE22	1:F:246:GLN:NE2	2.08	0.41
1:H:197:PHE:HB2	1:H:535:TRP:CD2	2.55	0.41
3:K:604:HEC:CBC	3:K:605:HEC:HBB2	2.48	0.41
1:R:81:LYS:HD3	1:R:82:TYR:CZ	2.55	0.41
1:T:386:ASP:HA	1:T:387:PRO:HA	1.73	0.41
1:A:478:GLN:NE2	1:B:432:ASP:H	2.18	0.41
3:E:601:HEC:HHA	3:E:601:HEC:HBA1	2.02	0.41
1:G:223:PRO:HG3	3:G:605:HEC:HBC2	2.02	0.41
1:H:81:LYS:HD3	1:H:82:TYR:CZ	2.55	0.41
1:H:485:ARG:HD3	1:I:497:TRP:CD1	2.55	0.41
3:K:601:HEC:HBC1	3:K:602:HEC:CHC	2.50	0.41
1:K:57:VAL:HG11	5:K:615:GOL:O2	2.21	0.41
1:K:81:LYS:HD3	1:K:82:TYR:CZ	2.56	0.41
1:L:154:CYS:HB3	1:L:165:PRO:HG3	2.02	0.41
1:R:433:VAL:HG23	7:R:709:HOH:O	2.19	0.41
1:R:454:HIS:HD2	3:R:606:HEC:NC	2.15	0.41
1:S:154:CYS:HB3	1:S:165:PRO:HG3	2.02	0.41
1:V:86:TRP:CH2	1:V:205:SER:HB3	2.55	0.41
1:V:197:PHE:HB2	1:V:535:TRP:CD2	2.55	0.41
1:A:81:LYS:HD3	1:A:82:TYR:CZ	2.56	0.41
1:D:355:LEU:HD23	1:D:355:LEU:HA	1.92	0.41
1:I:141:HIS:CD2	1:I:149:THR:HB	2.56	0.41
1:M:86:TRP:CH2	1:M:205:SER:HB3	2.55	0.41
1:O:232:GLN:HE22	1:O:246:GLN:NE2	2.10	0.41
1:Q:197:PHE:HB2	1:Q:535:TRP:CD2	2.55	0.41
1:T:154:CYS:HB3	1:T:165:PRO:HG3	2.01	0.41
1:X:154:CYS:HB3	1:X:165:PRO:HG3	2.02	0.41
1:A:86:TRP:CH2	1:A:205:SER:HB3	2.54	0.41
1:A:386:ASP:HA	1:A:387:PRO:HA	1.74	0.41
1:B:454:HIS:HD2	3:B:606:HEC:NC	2.13	0.41
1:C:154:CYS:HB3	1:C:165:PRO:HG3	2.03	0.41
1:C:197:PHE:HB2	1:C:535:TRP:CD2	2.55	0.41
1:A:226:ARG:NH2	3:C:607:HEC:O2A	2.53	0.41
1:D:335:ARG:O	1:D:339:VAL:HG23	2.21	0.41
1:K:132:ILE:HG12	5:K:614:GOL:C1	2.50	0.41
1:J:479:ASN:HD22	1:L:482:ARG:HH22	1.69	0.41
1:M:479:ASN:HD22	1:O:482:ARG:HH22	1.69	0.41
1:T:81:LYS:HD3	1:T:82:TYR:CZ	2.55	0.41
1:U:223:PRO:HG3	3:U:605:HEC:HBC2	2.01	0.41
1:V:41:PRO:O	1:V:44:VAL:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:485:ARG:HD3	1:W:497:TRP:CG	2.55	0.41
3:W:607:HEC:O2A	1:X:226:ARG:NH2	2.54	0.41
1:A:454:HIS:HD2	3:A:606:HEC:NC	2.14	0.41
1:E:378:ASP:CB	7:E:711:HOH:O	2.69	0.41
1:D:474:VAL:HG13	1:E:430:CYS:O	2.20	0.41
1:G:154:CYS:HB3	1:G:165:PRO:HG3	2.02	0.41
1:I:198:ALA:O	1:I:202:CYS:HB2	2.20	0.41
1:I:41:PRO:O	1:I:44:VAL:HG12	2.20	0.41
1:J:76:SER:CB	1:J:106:VAL:HG11	2.43	0.41
1:L:454:HIS:HD2	3:L:606:HEC:NC	2.15	0.41
3:M:607:HEC:O2A	1:N:226:ARG:NH2	2.53	0.41
1:N:349:ARG:NH2	4:N:610:SO4:S	2.94	0.41
1:P:207:GLU:HA	1:P:513:THR:OG1	2.20	0.41
1:Q:207:GLU:HA	1:Q:513:THR:OG1	2.20	0.41
1:R:207:GLU:HA	1:R:513:THR:OG1	2.21	0.41
3:S:601:HEC:HHA	3:S:601:HEC:HBA1	2.02	0.41
1:S:452:MET:HE1	1:T:214:ALA:HB3	2.01	0.41
1:W:340:SER:O	1:W:343:ASP:HB2	2.20	0.41
1:W:41:PRO:O	1:W:44:VAL:HG12	2.20	0.41
1:X:454:HIS:HD2	3:X:606:HEC:NC	2.15	0.41
1:I:48:PRO:HA	1:I:63:LYS:HB3	2.02	0.41
3:K:601:HEC:HBA1	3:K:601:HEC:HHA	2.03	0.41
3:O:601:HEC:HHA	3:O:601:HEC:HBA1	2.02	0.41
1:P:154:CYS:HB3	1:P:165:PRO:HG3	2.03	0.41
1:P:479:ASN:HD22	1:R:482:ARG:HH22	1.68	0.41
1:W:458:ASN:HB3	1:X:252:TRP:CZ2	2.56	0.41
1:D:485:ARG:HD3	1:E:497:TRP:CE2	2.56	0.41
1:J:207:GLU:HA	1:J:513:THR:OG1	2.21	0.41
1:K:86:TRP:CH2	1:K:205:SER:HB3	2.55	0.41
1:M:108:PRO:HD3	7:M:712:HOH:O	2.19	0.41
3:O:605:HEC:HMC1	3:O:605:HEC:HBC3	2.03	0.41
1:P:98:ASP:HB2	7:P:701:HOH:O	2.20	0.41
1:U:154:CYS:HB3	1:U:165:PRO:HG3	2.02	0.41
1:U:41:PRO:O	1:U:44:VAL:HG12	2.20	0.41
1:D:169:ALA:O	1:D:172:THR:HG22	2.21	0.41
1:D:223:PRO:HG3	3:D:605:HEC:HBC2	2.02	0.41
1:E:485:ARG:HD2	1:F:490:GLU:OE2	2.20	0.41
1:I:319:MET:SD	3:I:603:HEC:HBA1	2.61	0.41
1:J:410:HIS:HE1	5:J:613:GOL:O1	2.04	0.41
1:K:386:ASP:HA	1:K:387:PRO:HA	1.72	0.41
1:L:232:GLN:HE22	1:L:246:GLN:NE2	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:478:GLN:NE2	1:N:432:ASP:H	2.18	0.41
1:N:482:ARG:HH22	1:O:479:ASN:HD22	1.68	0.41
3:O:600:HEC:CBC	3:O:600:HEC:HHD	2.48	0.41
1:Q:349:ARG:NH2	4:Q:609:SO4:O1	2.53	0.41
1:S:386:ASP:HA	1:S:387:PRO:HA	1.73	0.41
1:S:81:LYS:HD3	1:S:82:TYR:CZ	2.56	0.41
1:Q:127:VAL:HG13	1:T:120:GLN:HE21	1.85	0.41
1:T:223:PRO:HG3	3:T:605:HEC:HBC2	2.02	0.41
3:X:601:HEC:HHA	3:X:601:HEC:HBA1	2.03	0.41
1:D:202:CYS:HB3	1:D:205:SER:HB2	2.01	0.41
3:F:600:HEC:CBC	3:F:600:HEC:HHD	2.49	0.41
1:G:86:TRP:CH2	1:G:205:SER:HB3	2.56	0.41
1:I:232:GLN:NE2	1:I:246:GLN:HE22	2.10	0.41
1:J:252:TRP:CZ2	1:L:458:ASN:HB3	2.56	0.41
1:T:176:HIS:HB3	1:T:179:GLN:HE21	1.86	0.41
1:D:386:ASP:HA	1:D:387:PRO:HA	1.76	0.41
3:H:606:HEC:CBC	5:H:614:GOL:H12	2.51	0.41
1:O:76:SER:CB	1:O:106:VAL:HG11	2.44	0.41
1:N:478:GLN:NE2	1:O:432:ASP:H	2.19	0.41
1:Q:243:ARG:NH1	7:Q:702:HOH:O	2.47	0.41
3:Q:601:HEC:HBA1	3:Q:601:HEC:HHA	2.02	0.41
1:R:154:CYS:HB3	1:R:165:PRO:HG3	2.03	0.41
1:S:39:TRP:CZ2	1:U:541:ALA:HA	2.56	0.41
3:S:604:HEC:CBC	3:S:605:HEC:HBB2	2.48	0.41
1:V:154:CYS:HB3	1:V:165:PRO:HG3	2.02	0.41
1:A:176:HIS:HB3	1:A:179:GLN:HE21	1.86	0.40
3:B:604:HEC:CBC	3:B:605:HEC:HBB2	2.46	0.40
1:G:222:SER:HB2	1:G:223:PRO:HD3	2.03	0.40
1:H:454:HIS:HD2	3:H:606:HEC:NC	2.15	0.40
1:I:314:ILE:HA	1:I:334:LYS:HD3	2.03	0.40
3:I:605:HEC:CBD	3:I:605:HEC:HMD1	2.46	0.40
1:M:207:GLU:HA	1:M:513:THR:OG1	2.21	0.40
1:O:81:LYS:HD3	1:O:82:TYR:CZ	2.56	0.40
1:P:482:ARG:HH22	1:Q:479:ASN:HD22	1.69	0.40
1:P:189:GLY:HA2	3:P:605:HEC:CGD	2.51	0.40
1:P:478:GLN:NE2	1:Q:432:ASP:H	2.18	0.40
1:R:368:LYS:NZ	1:R:466:SER:OG	2.54	0.40
1:V:207:GLU:HA	1:V:513:THR:OG1	2.21	0.40
1:W:154:CYS:HB3	1:W:165:PRO:HG3	2.02	0.40
3:W:601:HEC:HHA	3:W:601:HEC:HBA1	2.02	0.40
1:X:403:SER:HB3	1:X:434:GLU:OE2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:485:ARG:HD3	1:X:497:TRP:CG	2.56	0.40
1:X:337:ARG:NH2	4:X:610:SO4:S	2.91	0.40
1:X:81:LYS:HD3	1:X:82:TYR:CZ	2.56	0.40
1:B:386:ASP:HA	1:B:387:PRO:HA	1.72	0.40
1:D:369:TYR:CE1	1:D:441:VAL:HB	2.56	0.40
1:F:176:HIS:HB3	1:F:179:GLN:HE21	1.86	0.40
3:H:605:HEC:HMC1	3:H:605:HEC:HBC3	2.03	0.40
1:I:112:ILE:HG13	3:I:600:HEC:HMD2	2.02	0.40
1:K:485:ARG:HD2	1:L:490:GLU:OE2	2.21	0.40
3:N:604:HEC:CBC	3:N:605:HEC:HBB2	2.50	0.40
1:U:189:GLY:HA2	3:U:605:HEC:CGD	2.50	0.40
1:D:189:GLY:HA2	3:D:605:HEC:O2D	2.22	0.40
1:F:207:GLU:HA	1:F:513:THR:OG1	2.21	0.40
1:H:473:LEU:HD23	5:H:615:GOL:O1	2.21	0.40
1:I:220:HIS:O	1:I:223:PRO:HD2	2.21	0.40
1:I:314:ILE:HD12	3:I:606:HEC:O2D	2.21	0.40
1:J:86:TRP:CH2	1:J:205:SER:HB3	2.56	0.40
1:J:257:ARG:HD3	7:J:763:HOH:O	2.20	0.40
1:K:154:CYS:HB3	1:K:165:PRO:HG3	2.03	0.40
1:L:207:GLU:HA	1:L:513:THR:OG1	2.22	0.40
1:P:226:ARG:NH2	3:R:607:HEC:O2A	2.55	0.40
3:P:606:HEC:HBC1	3:P:607:HEC:HHC	2.02	0.40
1:P:81:LYS:HD3	1:P:82:TYR:CZ	2.56	0.40
1:T:41:PRO:O	1:T:44:VAL:HG12	2.21	0.40
5:A:612:GOL:H11	1:C:370:ARG:HG2	2.03	0.40
3:B:605:HEC:HMC1	3:B:605:HEC:HBC3	2.03	0.40
1:D:252:TRP:CE2	1:F:264:ILE:HG12	2.57	0.40
1:G:235:GLN:NE2	1:I:280:GLN:NE2	2.60	0.40
1:J:427:MET:CE	7:J:747:HOH:O	2.70	0.40
1:N:189:GLY:HA2	3:N:605:HEC:CGD	2.51	0.40
1:P:452:MET:HE1	1:Q:214:ALA:HB3	2.02	0.40
1:A:189:GLY:HA2	3:A:605:HEC:CGD	2.51	0.40
1:B:176:HIS:HB3	1:B:179:GLN:HE21	1.85	0.40
1:C:76:SER:CB	1:C:106:VAL:HG11	2.44	0.40
3:N:606:HEC:HBC1	3:N:607:HEC:HHC	2.03	0.40
1:Q:454:HIS:HD2	3:Q:606:HEC:NC	2.14	0.40
1:W:81:LYS:HD3	1:W:82:TYR:CZ	2.56	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:LYS:O	1:R:496:SER:OG[1_545]	1.83	0.37
1:G:42:HIS:NE2	1:J:496:SER:CB[2_555]	2.03	0.17
1:G:496:SER:OG	1:Q:491:LYS:O[1_655]	2.18	0.02

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	529/582 (91%)	513 (97%)	16 (3%)	0	100	100
1	B	529/582 (91%)	514 (97%)	15 (3%)	0	100	100
1	C	529/582 (91%)	512 (97%)	17 (3%)	0	100	100
1	D	529/582 (91%)	491 (93%)	36 (7%)	2 (0%)	34	66
1	E	529/582 (91%)	512 (97%)	17 (3%)	0	100	100
1	F	529/582 (91%)	515 (97%)	14 (3%)	0	100	100
1	G	529/582 (91%)	516 (98%)	13 (2%)	0	100	100
1	H	529/582 (91%)	513 (97%)	16 (3%)	0	100	100
1	I	525/582 (90%)	502 (96%)	23 (4%)	0	100	100
1	J	529/582 (91%)	516 (98%)	13 (2%)	0	100	100
1	K	529/582 (91%)	513 (97%)	16 (3%)	0	100	100
1	L	529/582 (91%)	513 (97%)	16 (3%)	0	100	100
1	M	529/582 (91%)	515 (97%)	14 (3%)	0	100	100
1	N	529/582 (91%)	513 (97%)	16 (3%)	0	100	100
1	O	529/582 (91%)	513 (97%)	16 (3%)	0	100	100
1	P	529/582 (91%)	513 (97%)	16 (3%)	0	100	100
1	Q	529/582 (91%)	514 (97%)	15 (3%)	0	100	100
1	R	530/582 (91%)	515 (97%)	15 (3%)	0	100	100
1	S	529/582 (91%)	513 (97%)	16 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	T	529/582 (91%)	511 (97%)	18 (3%)	0	100	100
1	U	529/582 (91%)	513 (97%)	16 (3%)	0	100	100
1	V	529/582 (91%)	512 (97%)	17 (3%)	0	100	100
1	W	529/582 (91%)	512 (97%)	17 (3%)	0	100	100
1	X	529/582 (91%)	515 (97%)	14 (3%)	0	100	100
2	Y	84/114 (74%)	83 (99%)	1 (1%)	0	100	100
2	Z	84/114 (74%)	82 (98%)	2 (2%)	0	100	100
2	a	84/114 (74%)	83 (99%)	1 (1%)	0	100	100
2	b	84/114 (74%)	83 (99%)	1 (1%)	0	100	100
2	c	84/114 (74%)	83 (99%)	1 (1%)	0	100	100
2	d	84/114 (74%)	83 (99%)	1 (1%)	0	100	100
2	e	84/114 (74%)	82 (98%)	2 (2%)	0	100	100
2	f	84/114 (74%)	83 (99%)	1 (1%)	0	100	100
2	g	84/114 (74%)	83 (99%)	1 (1%)	0	100	100
2	h	84/114 (74%)	83 (99%)	1 (1%)	0	100	100
2	i	84/114 (74%)	83 (99%)	1 (1%)	0	100	100
2	j	84/114 (74%)	79 (94%)	5 (6%)	0	100	100
All	All	13701/15336 (89%)	13279 (97%)	420 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	256	HIS
1	D	106	VAL

### 5.3.2 Protein sidechains ⓘ

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	451/491 (92%)	446 (99%)	5 (1%)	73	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	451/491 (92%)	446 (99%)	5 (1%)	73	92
1	C	451/491 (92%)	447 (99%)	4 (1%)	78	94
1	D	451/491 (92%)	432 (96%)	19 (4%)	30	63
1	E	451/491 (92%)	447 (99%)	4 (1%)	78	94
1	F	451/491 (92%)	447 (99%)	4 (1%)	78	94
1	G	451/491 (92%)	448 (99%)	3 (1%)	84	95
1	H	451/491 (92%)	447 (99%)	4 (1%)	78	94
1	I	449/491 (91%)	433 (96%)	16 (4%)	35	69
1	J	451/491 (92%)	447 (99%)	4 (1%)	78	94
1	K	451/491 (92%)	446 (99%)	5 (1%)	73	92
1	L	451/491 (92%)	447 (99%)	4 (1%)	78	94
1	M	451/491 (92%)	447 (99%)	4 (1%)	78	94
1	N	451/491 (92%)	446 (99%)	5 (1%)	73	92
1	O	451/491 (92%)	446 (99%)	5 (1%)	73	92
1	P	451/491 (92%)	447 (99%)	4 (1%)	78	94
1	Q	451/491 (92%)	446 (99%)	5 (1%)	73	92
1	R	452/491 (92%)	448 (99%)	4 (1%)	78	94
1	S	451/491 (92%)	447 (99%)	4 (1%)	78	94
1	T	451/491 (92%)	446 (99%)	5 (1%)	73	92
1	U	451/491 (92%)	447 (99%)	4 (1%)	78	94
1	V	451/491 (92%)	446 (99%)	5 (1%)	73	92
1	W	451/491 (92%)	447 (99%)	4 (1%)	78	94
1	X	451/491 (92%)	447 (99%)	4 (1%)	78	94
2	Y	68/86 (79%)	65 (96%)	3 (4%)	28	61
2	Z	68/86 (79%)	65 (96%)	3 (4%)	28	61
2	a	68/86 (79%)	65 (96%)	3 (4%)	28	61
2	b	68/86 (79%)	65 (96%)	3 (4%)	28	61
2	c	68/86 (79%)	65 (96%)	3 (4%)	28	61
2	d	68/86 (79%)	65 (96%)	3 (4%)	28	61
2	e	68/86 (79%)	65 (96%)	3 (4%)	28	61
2	f	68/86 (79%)	65 (96%)	3 (4%)	28	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	g	68/86 (79%)	65 (96%)	3 (4%)	28	61
2	h	68/86 (79%)	65 (96%)	3 (4%)	28	61
2	i	68/86 (79%)	65 (96%)	3 (4%)	28	61
2	j	68/86 (79%)	67 (98%)	1 (2%)	65	89
All	All	11639/12816 (91%)	11475 (99%)	164 (1%)	67	90

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	78	TYR
1	G	86	TRP
1	G	472	TRP
1	A	78	TYR
1	A	86	TRP
1	A	231	HIS
1	A	427	MET
1	A	472	TRP
1	B	78	TYR
1	B	86	TRP
1	B	231	HIS
1	B	427	MET
1	B	472	TRP
1	C	78	TYR
1	C	86	TRP
1	C	231	HIS
1	C	472	TRP
1	D	71	LYS
1	D	78	TYR
1	D	86	TRP
1	D	106	VAL
1	D	172	THR
1	D	205	SER
1	D	278	THR
1	D	309	VAL
1	D	319	MET
1	D	349	ARG
1	D	427	MET
1	D	446	THR
1	D	472	TRP
1	D	478	GLN
1	D	502	PHE

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Mol	Chain	Res	Type
1	D	513	THR
1	D	528	ASP
1	D	559	THR
1	D	563	HIS
1	E	78	TYR
1	E	86	TRP
1	E	231	HIS
1	E	472	TRP
1	F	78	TYR
1	F	86	TRP
1	F	231	HIS
1	F	472	TRP
1	H	78	TYR
1	H	86	TRP
1	H	231	HIS
1	H	472	TRP
1	I	44	VAL
1	I	78	TYR
1	I	86	TRP
1	I	115	THR
1	I	157	ASN
1	I	205	SER
1	I	231	HIS
1	I	278	THR
1	I	309	VAL
1	I	318	SER
1	I	332	LYS
1	I	349	ARG
1	I	446	THR
1	I	472	TRP
1	I	496	SER
1	I	545	GLU
1	J	78	TYR
1	J	86	TRP
1	J	231	HIS
1	J	472	TRP
1	K	78	TYR
1	K	86	TRP
1	K	231	HIS
1	K	427	MET
1	K	472	TRP
1	L	78	TYR

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Mol	Chain	Res	Type
1	L	86	TRP
1	L	231	HIS
1	L	472	TRP
1	M	78	TYR
1	M	86	TRP
1	M	231	HIS
1	M	472	TRP
1	N	78	TYR
1	N	86	TRP
1	N	231	HIS
1	N	427	MET
1	N	472	TRP
1	O	78	TYR
1	O	86	TRP
1	O	231	HIS
1	O	349	ARG
1	O	472	TRP
1	P	78	TYR
1	P	86	TRP
1	P	231	HIS
1	P	472	TRP
1	Q	78	TYR
1	Q	86	TRP
1	Q	231	HIS
1	Q	427	MET
1	Q	472	TRP
1	R	78	TYR
1	R	86	TRP
1	R	231	HIS
1	R	472	TRP
1	S	78	TYR
1	S	86	TRP
1	S	231	HIS
1	S	472	TRP
1	T	78	TYR
1	T	86	TRP
1	T	231	HIS
1	T	427	MET
1	T	472	TRP
1	U	78	TYR
1	U	86	TRP
1	U	231	HIS

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Mol	Chain	Res	Type
1	U	472	TRP
1	V	78	TYR
1	V	86	TRP
1	V	231	HIS
1	V	427	MET
1	V	472	TRP
1	W	78	TYR
1	W	86	TRP
1	W	231	HIS
1	W	472	TRP
1	X	78	TYR
1	X	86	TRP
1	X	231	HIS
1	X	472	TRP
2	Y	54	GLU
2	Y	79	GLU
2	Y	100	SER
2	Z	54	GLU
2	Z	79	GLU
2	Z	100	SER
2	a	54	GLU
2	a	79	GLU
2	a	100	SER
2	b	54	GLU
2	b	79	GLU
2	b	100	SER
2	c	54	GLU
2	c	79	GLU
2	c	100	SER
2	d	54	GLU
2	d	79	GLU
2	d	100	SER
2	e	54	GLU
2	e	79	GLU
2	e	100	SER
2	f	54	GLU
2	f	79	GLU
2	f	100	SER
2	g	54	GLU
2	g	79	GLU
2	g	100	SER
2	h	54	GLU

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Mol	Chain	Res	Type
2	h	79	GLU
2	h	100	SER
2	i	54	GLU
2	i	79	GLU
2	i	100	SER
2	j	61	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (263) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	102	ASN
1	G	179	GLN
1	G	185	GLN
1	G	199	GLN
1	G	235	GLN
1	G	246	GLN
1	G	410	HIS
1	G	429	ASN
1	G	478	GLN
1	G	479	ASN
1	G	539	HIS
1	A	102	ASN
1	A	179	GLN
1	A	185	GLN
1	A	199	GLN
1	A	235	GLN
1	A	246	GLN
1	A	410	HIS
1	A	429	ASN
1	A	478	GLN
1	A	479	ASN
1	A	539	HIS
1	B	102	ASN
1	B	179	GLN
1	B	185	GLN
1	B	199	GLN
1	B	235	GLN
1	B	246	GLN
1	B	410	HIS
1	B	429	ASN
1	B	478	GLN
1	B	479	ASN

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Mol	Chain	Res	Type
1	B	539	HIS
1	C	102	ASN
1	C	179	GLN
1	C	185	GLN
1	C	199	GLN
1	C	235	GLN
1	C	246	GLN
1	C	410	HIS
1	C	478	GLN
1	C	479	ASN
1	C	539	HIS
1	D	102	ASN
1	D	157	ASN
1	D	179	GLN
1	D	185	GLN
1	D	199	GLN
1	D	235	GLN
1	D	246	GLN
1	D	410	HIS
1	D	429	ASN
1	D	479	ASN
1	D	539	HIS
1	E	102	ASN
1	E	179	GLN
1	E	185	GLN
1	E	199	GLN
1	E	235	GLN
1	E	246	GLN
1	E	410	HIS
1	E	429	ASN
1	E	478	GLN
1	E	479	ASN
1	E	539	HIS
1	F	102	ASN
1	F	179	GLN
1	F	185	GLN
1	F	199	GLN
1	F	235	GLN
1	F	246	GLN
1	F	410	HIS
1	F	478	GLN
1	F	479	ASN

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Mol	Chain	Res	Type
1	F	539	HIS
1	H	42	HIS
1	H	102	ASN
1	H	179	GLN
1	H	185	GLN
1	H	199	GLN
1	H	235	GLN
1	H	246	GLN
1	H	410	HIS
1	H	429	ASN
1	H	478	GLN
1	H	479	ASN
1	H	539	HIS
1	I	102	ASN
1	I	179	GLN
1	I	185	GLN
1	I	199	GLN
1	I	235	GLN
1	I	246	GLN
1	I	399	GLN
1	I	410	HIS
1	I	429	ASN
1	I	478	GLN
1	I	479	ASN
1	I	539	HIS
1	J	102	ASN
1	J	179	GLN
1	J	185	GLN
1	J	199	GLN
1	J	235	GLN
1	J	246	GLN
1	J	410	HIS
1	J	478	GLN
1	J	479	ASN
1	J	539	HIS
1	K	102	ASN
1	K	179	GLN
1	K	185	GLN
1	K	199	GLN
1	K	235	GLN
1	K	246	GLN
1	K	410	HIS

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Mol	Chain	Res	Type
1	K	429	ASN
1	K	478	GLN
1	K	479	ASN
1	K	539	HIS
1	L	42	HIS
1	L	102	ASN
1	L	179	GLN
1	L	185	GLN
1	L	199	GLN
1	L	235	GLN
1	L	246	GLN
1	L	410	HIS
1	L	429	ASN
1	L	478	GLN
1	L	479	ASN
1	L	539	HIS
1	M	102	ASN
1	M	179	GLN
1	M	185	GLN
1	M	199	GLN
1	M	235	GLN
1	M	246	GLN
1	M	410	HIS
1	M	478	GLN
1	M	479	ASN
1	M	539	HIS
1	N	102	ASN
1	N	179	GLN
1	N	185	GLN
1	N	199	GLN
1	N	235	GLN
1	N	246	GLN
1	N	410	HIS
1	N	429	ASN
1	N	478	GLN
1	N	479	ASN
1	N	539	HIS
1	O	102	ASN
1	O	179	GLN
1	O	185	GLN
1	O	199	GLN
1	O	235	GLN

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Mol	Chain	Res	Type
1	O	246	GLN
1	O	410	HIS
1	O	429	ASN
1	O	478	GLN
1	O	479	ASN
1	O	539	HIS
1	P	102	ASN
1	P	179	GLN
1	P	185	GLN
1	P	199	GLN
1	P	235	GLN
1	P	246	GLN
1	P	410	HIS
1	P	429	ASN
1	P	478	GLN
1	P	479	ASN
1	P	539	HIS
1	Q	102	ASN
1	Q	179	GLN
1	Q	185	GLN
1	Q	199	GLN
1	Q	235	GLN
1	Q	246	GLN
1	Q	410	HIS
1	Q	429	ASN
1	Q	478	GLN
1	Q	479	ASN
1	Q	539	HIS
1	R	102	ASN
1	R	179	GLN
1	R	185	GLN
1	R	199	GLN
1	R	235	GLN
1	R	246	GLN
1	R	410	HIS
1	R	429	ASN
1	R	478	GLN
1	R	479	ASN
1	R	539	HIS
1	S	42	HIS
1	S	102	ASN
1	S	179	GLN

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Mol	Chain	Res	Type
1	S	185	GLN
1	S	199	GLN
1	S	235	GLN
1	S	246	GLN
1	S	410	HIS
1	S	429	ASN
1	S	478	GLN
1	S	479	ASN
1	S	539	HIS
1	T	102	ASN
1	T	179	GLN
1	T	185	GLN
1	T	199	GLN
1	T	235	GLN
1	T	246	GLN
1	T	410	HIS
1	T	478	GLN
1	T	479	ASN
1	T	539	HIS
1	U	42	HIS
1	U	102	ASN
1	U	179	GLN
1	U	185	GLN
1	U	199	GLN
1	U	235	GLN
1	U	246	GLN
1	U	410	HIS
1	U	478	GLN
1	U	479	ASN
1	U	539	HIS
1	V	102	ASN
1	V	179	GLN
1	V	185	GLN
1	V	199	GLN
1	V	235	GLN
1	V	246	GLN
1	V	410	HIS
1	V	429	ASN
1	V	478	GLN
1	V	479	ASN
1	V	539	HIS
1	W	102	ASN

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Mol	Chain	Res	Type
1	W	179	GLN
1	W	185	GLN
1	W	199	GLN
1	W	235	GLN
1	W	246	GLN
1	W	410	HIS
1	W	478	GLN
1	W	479	ASN
1	W	539	HIS
1	X	102	ASN
1	X	179	GLN
1	X	185	GLN
1	X	199	GLN
1	X	235	GLN
1	X	246	GLN
1	X	410	HIS
1	X	429	ASN
1	X	478	GLN
1	X	479	ASN
1	X	539	HIS
1	X	540	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 286 ligands modelled in this entry, 4 are monoatomic - leaving 282 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	HEC	W	605	1	26,50,50	1.56	4 (15%)	18,82,82	1.60	4 (22%)
4	SO4	K	610	-	4,4,4	0.34	0	6,6,6	0.10	0
4	SO4	V	610	-	4,4,4	0.35	0	6,6,6	0.12	0
3	HEC	N	600	1	26,50,50	1.59	4 (15%)	18,82,82	1.21	2 (11%)
4	SO4	Y	202	-	4,4,4	0.33	0	6,6,6	0.11	0
3	HEC	I	601	1	26,50,50	1.68	4 (15%)	18,82,82	1.18	1 (5%)
3	HEC	X	603	1,7	26,50,50	2.66	9 (34%)	18,82,82	2.76	6 (33%)
3	HEC	V	602	1	26,50,50	1.58	4 (15%)	18,82,82	1.36	2 (11%)
3	HEC	T	605	1	26,50,50	1.54	4 (15%)	18,82,82	1.69	5 (27%)
3	HEC	X	600	1	26,50,50	1.60	4 (15%)	18,82,82	1.23	2 (11%)
3	HEC	F	605	1	26,50,50	1.58	4 (15%)	18,82,82	1.57	3 (16%)
3	HEC	L	606	1	26,50,50	1.55	4 (15%)	18,82,82	1.39	3 (16%)
3	HEC	D	601	1	26,50,50	1.64	4 (15%)	18,82,82	1.06	1 (5%)
4	SO4	O	609	-	4,4,4	0.36	0	6,6,6	0.08	0
3	HEC	L	602	1	26,50,50	1.62	4 (15%)	18,82,82	1.38	2 (11%)
3	HEC	Q	600	1	26,50,50	1.61	4 (15%)	18,82,82	1.11	2 (11%)
3	HEC	V	600	1	26,50,50	1.61	4 (15%)	18,82,82	1.15	2 (11%)
3	HEC	D	605	1	26,50,50	1.56	4 (15%)	18,82,82	1.80	4 (22%)
3	HEC	Q	601	1	26,50,50	1.64	4 (15%)	18,82,82	1.23	1 (5%)
4	SO4	L	609	-	4,4,4	0.34	0	6,6,6	0.13	0
3	HEC	X	602	1	26,50,50	1.54	4 (15%)	18,82,82	1.40	2 (11%)
4	SO4	I	609	-	4,4,4	0.35	0	6,6,6	0.34	0
3	HEC	C	606	1	26,50,50	1.59	4 (15%)	18,82,82	1.30	2 (11%)
3	HEC	X	607	1	26,50,50	1.57	4 (15%)	18,82,82	1.10	1 (5%)
3	HEC	K	602	1	26,50,50	1.55	4 (15%)	18,82,82	1.37	2 (11%)
5	GOL	J	612	-	5,5,5	0.50	0	5,5,5	0.57	0
3	HEC	X	604	1	26,50,50	1.60	4 (15%)	18,82,82	1.77	2 (11%)
3	HEC	Q	607	1	26,50,50	1.54	4 (15%)	18,82,82	1.26	1 (5%)
3	HEC	G	606	1	26,50,50	1.58	4 (15%)	18,82,82	1.33	3 (16%)
3	HEC	U	606	1	26,50,50	1.56	4 (15%)	18,82,82	1.30	2 (11%)
3	HEC	P	604	1	26,50,50	1.59	4 (15%)	18,82,82	1.87	3 (16%)
3	HEC	R	601	1	26,50,50	1.67	4 (15%)	18,82,82	1.26	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HEC	D	602	1	26,50,50	1.59	4 (15%)	18,82,82	1.43	3 (16%)
4	SO4	Q	610	-	4,4,4	0.33	0	6,6,6	0.11	0
3	HEC	I	602	1	26,50,50	1.59	4 (15%)	18,82,82	1.53	3 (16%)
3	HEC	N	604	1	26,50,50	1.63	4 (15%)	18,82,82	1.79	2 (11%)
3	HEC	Q	605	1	26,50,50	1.56	4 (15%)	18,82,82	1.59	4 (22%)
3	HEC	P	602	1	26,50,50	1.62	4 (15%)	18,82,82	1.33	2 (11%)
3	HEC	U	600	1	26,50,50	1.57	4 (15%)	18,82,82	1.14	2 (11%)
5	GOL	L	613	-	5,5,5	0.25	0	5,5,5	0.35	0
3	HEC	O	606	1	26,50,50	1.51	4 (15%)	18,82,82	1.39	1 (5%)
3	HEC	S	603	1,7	26,50,50	2.71	11 (42%)	18,82,82	2.72	6 (33%)
3	HEC	R	600	1	26,50,50	1.54	4 (15%)	18,82,82	1.21	2 (11%)
5	GOL	I	614	-	5,5,5	0.23	0	5,5,5	0.19	0
3	HEC	G	601	1	26,50,50	1.61	4 (15%)	18,82,82	1.30	2 (11%)
3	HEC	H	603	1,7	26,50,50	2.67	10 (38%)	18,82,82	2.65	8 (44%)
3	HEC	V	604	1	26,50,50	1.61	4 (15%)	18,82,82	1.84	2 (11%)
3	HEC	S	606	1	26,50,50	1.59	4 (15%)	18,82,82	1.30	1 (5%)
3	HEC	T	600	1	26,50,50	1.60	4 (15%)	18,82,82	1.15	2 (11%)
3	HEC	U	602	1	26,50,50	1.57	4 (15%)	18,82,82	1.39	2 (11%)
3	HEC	H	600	1	26,50,50	1.56	4 (15%)	18,82,82	1.21	1 (5%)
3	HEC	M	606	1	26,50,50	1.59	4 (15%)	18,82,82	1.32	2 (11%)
3	HEC	S	601	1	26,50,50	1.67	4 (15%)	18,82,82	1.26	1 (5%)
4	SO4	X	609	-	4,4,4	0.33	0	6,6,6	0.14	0
3	HEC	X	606	1	26,50,50	1.61	4 (15%)	18,82,82	1.32	1 (5%)
4	SO4	N	609	-	4,4,4	0.37	0	6,6,6	0.13	0
3	HEC	W	604	1	26,50,50	1.61	4 (15%)	18,82,82	1.82	3 (16%)
3	HEC	T	606	1	26,50,50	1.58	4 (15%)	18,82,82	1.32	1 (5%)
5	GOL	K	613	-	5,5,5	0.23	0	5,5,5	0.34	0
4	SO4	L	612	-	4,4,4	0.36	0	6,6,6	0.10	0
3	HEC	T	602	1	26,50,50	1.61	4 (15%)	18,82,82	1.39	2 (11%)
4	SO4	F	609	-	4,4,4	0.34	0	6,6,6	0.13	0
3	HEC	V	603	1,7	26,50,50	2.65	10 (38%)	18,82,82	2.68	9 (50%)
3	HEC	S	607	1	26,50,50	1.56	4 (15%)	18,82,82	1.08	0
4	SO4	O	611	-	4,4,4	0.32	0	6,6,6	0.08	0
3	HEC	H	606	1	26,50,50	1.68	4 (15%)	18,82,82	1.27	1 (5%)
5	GOL	K	612	-	5,5,5	0.39	0	5,5,5	0.33	0
3	HEC	L	607	1	26,50,50	1.54	4 (15%)	18,82,82	1.08	0
3	HEC	W	602	1	26,50,50	1.62	4 (15%)	18,82,82	1.27	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HEC	K	607	1	26,50,50	1.58	4 (15%)	18,82,82	1.08	0
4	SO4	U	609	-	4,4,4	0.32	0	6,6,6	0.26	0
5	GOL	D	610	-	5,5,5	0.29	0	5,5,5	0.23	0
3	HEC	H	604	1	26,50,50	1.58	4 (15%)	18,82,82	1.89	3 (16%)
3	HEC	V	601	1	26,50,50	1.60	4 (15%)	18,82,82	1.22	1 (5%)
3	HEC	E	604	1	26,50,50	1.66	4 (15%)	18,82,82	1.83	3 (16%)
4	SO4	C	609	-	4,4,4	0.32	0	6,6,6	0.14	0
4	SO4	P	609	-	4,4,4	0.33	0	6,6,6	0.14	0
3	HEC	K	601	1	26,50,50	1.66	4 (15%)	18,82,82	1.26	1 (5%)
3	HEC	L	601	1	26,50,50	1.59	4 (15%)	18,82,82	1.20	1 (5%)
3	HEC	A	606	1	26,50,50	1.54	4 (15%)	18,82,82	1.36	2 (11%)
4	SO4	Y	201	-	4,4,4	0.32	0	6,6,6	0.11	0
3	HEC	T	607	1	26,50,50	1.56	4 (15%)	18,82,82	1.11	0
4	SO4	M	612	-	4,4,4	0.34	0	6,6,6	0.14	0
3	HEC	A	605	1	26,50,50	1.56	4 (15%)	18,82,82	1.59	3 (16%)
4	SO4	R	611	-	4,4,4	0.31	0	6,6,6	0.06	0
4	SO4	U	611	-	4,4,4	0.32	0	6,6,6	0.08	0
3	HEC	C	600	1	26,50,50	1.56	4 (15%)	18,82,82	1.19	2 (11%)
3	HEC	E	600	1	26,50,50	1.62	4 (15%)	18,82,82	1.22	2 (11%)
3	HEC	L	603	1,7	26,50,50	2.67	9 (34%)	18,82,82	2.78	9 (50%)
3	HEC	D	607	1	26,50,50	1.59	4 (15%)	18,82,82	1.02	0
3	HEC	L	600	1	26,50,50	1.53	4 (15%)	18,82,82	1.15	1 (5%)
5	GOL	A	613	-	5,5,5	0.41	0	5,5,5	0.35	0
3	HEC	N	607	1	26,50,50	1.58	4 (15%)	18,82,82	1.13	0
4	SO4	L	611	-	4,4,4	0.33	0	6,6,6	0.09	0
3	HEC	K	604	1	26,50,50	1.61	4 (15%)	18,82,82	1.87	3 (16%)
3	HEC	O	605	1	26,50,50	1.58	4 (15%)	18,82,82	1.55	3 (16%)
4	SO4	C	610	-	4,4,4	0.34	0	6,6,6	0.12	0
4	SO4	a	201	-	4,4,4	0.34	0	6,6,6	0.08	0
3	HEC	N	606	1	26,50,50	1.57	4 (15%)	18,82,82	1.30	1 (5%)
4	SO4	J	610	-	4,4,4	0.32	0	6,6,6	0.13	0
3	HEC	C	601	1	26,50,50	1.62	4 (15%)	18,82,82	1.21	1 (5%)
3	HEC	J	606	1	26,50,50	1.58	4 (15%)	18,82,82	1.28	1 (5%)
3	HEC	U	604	1	26,50,50	1.57	4 (15%)	18,82,82	1.81	2 (11%)
3	HEC	B	602	1	26,50,50	1.59	4 (15%)	18,82,82	1.43	2 (11%)
3	HEC	M	607	1	26,50,50	1.60	4 (15%)	18,82,82	1.06	0
4	SO4	G	614	-	4,4,4	0.37	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HEC	I	600	1	26,50,50	1.48	4 (15%)	18,82,82	1.38	4 (22%)
3	HEC	F	603	1,7	26,50,50	2.64	10 (38%)	18,82,82	2.90	8 (44%)
3	HEC	X	601	1	26,50,50	1.61	4 (15%)	18,82,82	1.26	1 (5%)
4	SO4	J	609	-	4,4,4	0.36	0	6,6,6	0.09	0
4	SO4	R	609	-	4,4,4	0.32	0	6,6,6	0.25	0
4	SO4	H	611	-	4,4,4	0.32	0	6,6,6	0.21	0
4	SO4	R	610	-	4,4,4	0.35	0	6,6,6	0.10	0
3	HEC	B	604	1	26,50,50	1.57	4 (15%)	18,82,82	1.84	2 (11%)
3	HEC	O	604	1	26,50,50	1.62	4 (15%)	18,82,82	1.82	2 (11%)
4	SO4	K	609	-	4,4,4	0.21	0	6,6,6	0.34	0
3	HEC	R	604	1	26,50,50	1.60	4 (15%)	18,82,82	1.76	3 (16%)
3	HEC	U	603	1,7	26,50,50	2.64	10 (38%)	18,82,82	2.73	8 (44%)
3	HEC	F	606	1	26,50,50	1.57	4 (15%)	18,82,82	1.30	1 (5%)
5	GOL	A	612	-	5,5,5	0.28	0	5,5,5	0.28	0
4	SO4	A	610	-	4,4,4	0.32	0	6,6,6	0.14	0
4	SO4	X	611	-	4,4,4	0.34	0	6,6,6	0.07	0
3	HEC	K	606	1	26,50,50	1.56	4 (15%)	18,82,82	1.39	2 (11%)
3	HEC	G	603	1,7	26,50,50	2.70	9 (34%)	18,82,82	2.56	7 (38%)
3	HEC	R	605	1	26,50,50	1.54	4 (15%)	18,82,82	1.54	3 (16%)
3	HEC	A	600	1	26,50,50	1.57	4 (15%)	18,82,82	1.28	2 (11%)
4	SO4	U	610	-	4,4,4	0.33	0	6,6,6	0.07	0
3	HEC	R	607	1	26,50,50	1.58	4 (15%)	18,82,82	1.13	1 (5%)
3	HEC	H	605	1	26,50,50	1.59	4 (15%)	18,82,82	1.60	4 (22%)
3	HEC	A	601	1	26,50,50	1.66	4 (15%)	18,82,82	1.27	1 (5%)
3	HEC	V	607	1	26,50,50	1.55	4 (15%)	18,82,82	1.07	0
5	GOL	G	615	-	5,5,5	0.45	0	5,5,5	0.34	0
3	HEC	L	605	1	26,50,50	1.53	4 (15%)	18,82,82	1.63	5 (27%)
4	SO4	E	610	-	4,4,4	0.35	0	6,6,6	0.10	0
3	HEC	D	606	1	26,50,50	1.55	4 (15%)	18,82,82	1.24	1 (5%)
3	HEC	M	603	1,7	26,50,50	2.68	10 (38%)	18,82,82	2.74	7 (38%)
3	HEC	J	602	1	26,50,50	1.63	4 (15%)	18,82,82	1.36	2 (11%)
4	SO4	C	611	-	4,4,4	0.34	0	6,6,6	0.16	0
4	SO4	I	610	-	4,4,4	0.35	0	6,6,6	0.05	0
4	SO4	G	611	-	4,4,4	0.34	0	6,6,6	0.10	0
4	SO4	G	613	-	4,4,4	0.29	0	6,6,6	0.37	0
5	GOL	H	614	-	5,5,5	0.41	0	5,5,5	0.77	0
4	SO4	M	611	-	4,4,4	0.35	0	6,6,6	0.11	0
3	HEC	W	600	1	26,50,50	1.62	4 (15%)	18,82,82	1.19	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HEC	W	603	1,7	26,50,50	2.63	9 (34%)	18,82,82	2.63	6 (33%)
3	HEC	O	600	1	26,50,50	1.61	4 (15%)	18,82,82	1.17	2 (11%)
4	SO4	Q	611	-	4,4,4	0.35	0	6,6,6	0.14	0
3	HEC	Q	602	1	26,50,50	1.57	4 (15%)	18,82,82	1.31	2 (11%)
4	SO4	Q	609	-	4,4,4	0.34	0	6,6,6	0.14	0
3	HEC	X	605	1	26,50,50	1.58	4 (15%)	18,82,82	1.62	4 (22%)
4	SO4	W	609	-	4,4,4	0.35	0	6,6,6	0.10	0
4	SO4	N	610	-	4,4,4	0.35	0	6,6,6	0.13	0
5	GOL	I	615	-	5,5,5	0.33	0	5,5,5	0.36	0
4	SO4	X	610	-	4,4,4	0.33	0	6,6,6	0.05	0
3	HEC	B	607	1	26,50,50	1.54	4 (15%)	18,82,82	1.21	0
3	HEC	D	603	1,7	26,50,50	2.66	10 (38%)	18,82,82	2.89	10 (55%)
4	SO4	T	609	-	4,4,4	0.35	0	6,6,6	0.08	0
4	SO4	A	609	-	4,4,4	0.30	0	6,6,6	0.12	0
3	HEC	E	606	1	26,50,50	1.57	4 (15%)	18,82,82	1.31	2 (11%)
3	HEC	M	604	1	26,50,50	1.61	4 (15%)	18,82,82	1.78	2 (11%)
3	HEC	Q	603	1,7	26,50,50	2.69	11 (42%)	18,82,82	2.84	9 (50%)
3	HEC	B	605	1	26,50,50	1.60	4 (15%)	18,82,82	1.51	2 (11%)
3	HEC	P	600	1	26,50,50	1.56	4 (15%)	18,82,82	1.16	1 (5%)
4	SO4	V	611	-	4,4,4	0.34	0	6,6,6	0.05	0
3	HEC	G	607	1	26,50,50	1.62	4 (15%)	18,82,82	1.07	0
5	GOL	K	615	-	5,5,5	0.33	0	5,5,5	0.20	0
3	HEC	T	601	1	26,50,50	1.66	4 (15%)	18,82,82	1.19	1 (5%)
3	HEC	R	603	1	26,50,50	2.68	9 (34%)	18,82,82	2.51	8 (44%)
3	HEC	A	607	1	26,50,50	1.57	4 (15%)	18,82,82	1.08	0
3	HEC	S	602	1	26,50,50	1.57	4 (15%)	18,82,82	1.40	2 (11%)
3	HEC	S	600	1	26,50,50	1.65	4 (15%)	18,82,82	1.13	2 (11%)
4	SO4	J	611	-	4,4,4	0.29	0	6,6,6	0.09	0
3	HEC	I	605	1	26,50,50	1.59	4 (15%)	18,82,82	1.68	4 (22%)
3	HEC	N	601	1	26,50,50	1.65	4 (15%)	18,82,82	1.24	1 (5%)
3	HEC	P	606	1	26,50,50	1.57	4 (15%)	18,82,82	1.30	2 (11%)
4	SO4	c	201	-	4,4,4	0.35	0	6,6,6	0.09	0
3	HEC	G	605	1	26,50,50	1.57	4 (15%)	18,82,82	1.66	4 (22%)
4	SO4	L	610	-	4,4,4	0.30	0	6,6,6	0.16	0
3	HEC	N	602	1	26,50,50	1.64	4 (15%)	18,82,82	1.42	2 (11%)
3	HEC	M	602	1	26,50,50	1.59	4 (15%)	18,82,82	1.39	2 (11%)
5	GOL	K	614	-	5,5,5	0.18	0	5,5,5	0.37	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HEC	H	601	1	26,50,50	1.61	4 (15%)	18,82,82	1.23	1 (5%)
3	HEC	T	604	1	26,50,50	1.59	4 (15%)	18,82,82	1.86	2 (11%)
3	HEC	E	603	1,7	26,50,50	2.71	9 (34%)	18,82,82	2.79	6 (33%)
3	HEC	I	607	1	26,50,50	1.57	4 (15%)	18,82,82	1.12	1 (5%)
4	SO4	A	611	-	4,4,4	0.32	0	6,6,6	0.16	0
3	HEC	U	601	1	26,50,50	1.62	4 (15%)	18,82,82	1.27	1 (5%)
3	HEC	C	604	1	26,50,50	1.62	4 (15%)	18,82,82	1.87	3 (16%)
5	GOL	J	613	-	5,5,5	0.27	0	5,5,5	0.49	0
4	SO4	G	612	-	4,4,4	0.34	0	6,6,6	0.12	0
3	HEC	W	606	1	26,50,50	1.60	4 (15%)	18,82,82	1.27	1 (5%)
3	HEC	R	606	1	26,50,50	1.54	4 (15%)	18,82,82	1.31	1 (5%)
3	HEC	S	604	1	26,50,50	1.60	4 (15%)	18,82,82	1.86	2 (11%)
3	HEC	B	603	1	26,50,50	2.65	10 (38%)	18,82,82	2.65	8 (44%)
3	HEC	W	607	1	26,50,50	1.56	4 (15%)	18,82,82	1.13	0
3	HEC	B	601	1	26,50,50	1.63	4 (15%)	18,82,82	1.32	1 (5%)
3	HEC	H	602	1	26,50,50	1.64	4 (15%)	18,82,82	1.37	2 (11%)
4	SO4	H	613	-	4,4,4	0.33	0	6,6,6	0.23	0
4	SO4	I	612	-	4,4,4	0.36	0	6,6,6	0.06	0
3	HEC	K	603	1,7	26,50,50	2.68	9 (34%)	18,82,82	2.58	8 (44%)
4	SO4	D	609	-	4,4,4	0.35	0	6,6,6	0.11	0
4	SO4	H	612	-	4,4,4	0.35	0	6,6,6	0.07	0
3	HEC	A	603	1,7	26,50,50	2.65	9 (34%)	18,82,82	2.85	8 (44%)
3	HEC	O	602	1	26,50,50	1.53	4 (15%)	18,82,82	1.42	2 (11%)
3	HEC	J	601	1	26,50,50	1.67	4 (15%)	18,82,82	1.19	1 (5%)
4	SO4	K	611	-	4,4,4	0.36	0	6,6,6	0.06	0
5	GOL	A	614	-	5,5,5	0.35	0	5,5,5	0.18	0
4	SO4	H	609	-	4,4,4	0.36	0	6,6,6	0.10	0
3	HEC	K	605	1	26,50,50	1.59	4 (15%)	18,82,82	1.64	4 (22%)
3	HEC	F	607	1	26,50,50	1.52	4 (15%)	18,82,82	1.09	0
3	HEC	E	605	1	26,50,50	1.56	4 (15%)	18,82,82	1.57	3 (16%)
3	HEC	K	600	1	26,50,50	1.55	4 (15%)	18,82,82	1.24	1 (5%)
3	HEC	J	603	1,7	26,50,50	2.61	9 (34%)	18,82,82	2.74	8 (44%)
5	GOL	I	613	-	5,5,5	0.26	0	5,5,5	0.24	0
4	SO4	B	609	-	4,4,4	0.30	0	6,6,6	0.13	0
3	HEC	C	602	1	26,50,50	1.61	4 (15%)	18,82,82	1.40	2 (11%)
3	HEC	O	607	1	26,50,50	1.52	4 (15%)	18,82,82	1.18	1 (5%)
3	HEC	J	607	1	26,50,50	1.63	4 (15%)	18,82,82	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HEC	I	603	1,7	26,50,50	2.64	9 (34%)	18,82,82	4.33	7 (38%)
3	HEC	O	603	1,7	26,50,50	2.68	10 (38%)	18,82,82	2.72	8 (44%)
3	HEC	M	601	1	26,50,50	1.65	4 (15%)	18,82,82	1.20	1 (5%)
3	HEC	C	603	1	26,50,50	2.65	11 (42%)	18,82,82	2.61	8 (44%)
3	HEC	E	607	1	26,50,50	1.60	4 (15%)	18,82,82	1.13	0
3	HEC	P	605	1	26,50,50	1.53	4 (15%)	18,82,82	1.61	4 (22%)
3	HEC	S	605	1	26,50,50	1.58	4 (15%)	18,82,82	1.58	4 (22%)
3	HEC	M	605	1	26,50,50	1.53	4 (15%)	18,82,82	1.58	4 (22%)
3	HEC	N	605	1	26,50,50	1.57	4 (15%)	18,82,82	1.61	4 (22%)
3	HEC	D	600	1	26,50,50	1.59	4 (15%)	18,82,82	1.19	2 (11%)
3	HEC	J	605	1	26,50,50	1.59	4 (15%)	18,82,82	1.62	4 (22%)
3	HEC	O	601	1	26,50,50	1.68	4 (15%)	18,82,82	1.30	1 (5%)
4	SO4	I	611	-	4,4,4	0.34	0	6,6,6	0.07	0
4	SO4	F	610	-	4,4,4	0.33	0	6,6,6	0.08	0
3	HEC	I	604	1	26,50,50	1.68	4 (15%)	18,82,82	1.71	3 (16%)
3	HEC	E	601	1	26,50,50	1.61	4 (15%)	18,82,82	1.29	1 (5%)
3	HEC	P	607	1	26,50,50	1.61	4 (15%)	18,82,82	1.16	0
3	HEC	C	605	1	26,50,50	1.57	4 (15%)	18,82,82	1.57	3 (16%)
3	HEC	G	604	1	26,50,50	1.66	4 (15%)	18,82,82	1.80	3 (16%)
3	HEC	N	603	1,7	26,50,50	2.69	10 (38%)	18,82,82	2.70	7 (38%)
3	HEC	B	606	1	26,50,50	1.54	4 (15%)	18,82,82	1.41	2 (11%)
3	HEC	Q	606	1	26,50,50	1.52	4 (15%)	18,82,82	1.30	1 (5%)
3	HEC	U	605	1	26,50,50	1.52	4 (15%)	18,82,82	1.63	4 (22%)
4	SO4	O	610	-	4,4,4	0.35	0	6,6,6	0.10	0
3	HEC	J	600	1	26,50,50	1.59	4 (15%)	18,82,82	1.15	2 (11%)
3	HEC	C	607	1	26,50,50	1.59	4 (15%)	18,82,82	1.09	0
3	HEC	I	606	1	26,50,50	1.51	4 (15%)	18,82,82	1.38	3 (16%)
3	HEC	W	601	1	26,50,50	1.67	4 (15%)	18,82,82	1.18	1 (5%)
4	SO4	S	609	-	4,4,4	0.34	0	6,6,6	0.05	0
3	HEC	V	606	1	26,50,50	1.63	4 (15%)	18,82,82	1.29	3 (16%)
4	SO4	B	610	-	4,4,4	0.37	0	6,6,6	0.09	0
3	HEC	B	600	1	26,50,50	1.58	4 (15%)	18,82,82	1.24	2 (11%)
3	HEC	G	602	1	26,50,50	1.57	4 (15%)	18,82,82	1.38	2 (11%)
4	SO4	E	609	-	4,4,4	0.38	0	6,6,6	0.36	0
3	HEC	U	607	1	26,50,50	1.59	4 (15%)	18,82,82	1.16	0
3	HEC	M	600	1	26,50,50	1.57	4 (15%)	18,82,82	1.21	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HEC	T	603	1	26,50,50	2.74	10 (38%)	18,82,82	2.77	8 (44%)
4	SO4	H	610	-	4,4,4	0.36	0	6,6,6	0.05	0
3	HEC	A	602	1	26,50,50	1.59	4 (15%)	18,82,82	1.42	2 (11%)
3	HEC	F	602	1	26,50,50	1.60	4 (15%)	18,82,82	1.37	2 (11%)
3	HEC	G	600	1	26,50,50	1.56	4 (15%)	18,82,82	1.26	2 (11%)
3	HEC	E	602	1	26,50,50	1.58	4 (15%)	18,82,82	1.35	2 (11%)
4	SO4	M	609	-	4,4,4	0.35	0	6,6,6	0.09	0
3	HEC	J	604	1	26,50,50	1.57	4 (15%)	18,82,82	1.83	3 (16%)
3	HEC	R	602	1	26,50,50	1.56	4 (15%)	18,82,82	1.28	2 (11%)
3	HEC	D	604	1	26,50,50	1.60	5 (19%)	18,82,82	1.76	3 (16%)
4	SO4	S	610	-	4,4,4	0.35	0	6,6,6	0.08	0
3	HEC	F	604	1	26,50,50	1.57	4 (15%)	18,82,82	1.84	2 (11%)
4	SO4	V	609	-	4,4,4	0.40	0	6,6,6	0.28	0
4	SO4	G	609	-	4,4,4	0.35	0	6,6,6	0.08	0
3	HEC	F	600	1	26,50,50	1.61	4 (15%)	18,82,82	1.09	1 (5%)
3	HEC	P	601	1	26,50,50	1.60	4 (15%)	18,82,82	1.27	1 (5%)
5	GOL	H	615	-	5,5,5	0.46	0	5,5,5	0.57	0
3	HEC	P	603	1,7	26,50,50	2.64	9 (34%)	18,82,82	2.77	8 (44%)
4	SO4	N	611	-	4,4,4	0.33	0	6,6,6	0.09	0
3	HEC	F	601	1	26,50,50	1.66	4 (15%)	18,82,82	1.24	1 (5%)
4	SO4	M	610	-	4,4,4	0.32	0	6,6,6	0.09	0
5	GOL	G	616	-	5,5,5	0.19	0	5,5,5	0.42	0
3	HEC	Q	604	1	26,50,50	1.57	4 (15%)	18,82,82	1.86	2 (11%)
4	SO4	G	610	-	4,4,4	0.29	0	6,6,6	0.09	0
3	HEC	A	604	1	26,50,50	1.62	4 (15%)	18,82,82	1.80	2 (11%)
3	HEC	H	607	1	26,50,50	1.58	4 (15%)	18,82,82	1.17	0
3	HEC	L	604	1	26,50,50	1.61	4 (15%)	18,82,82	1.80	3 (16%)
3	HEC	V	605	1	26,50,50	1.56	4 (15%)	18,82,82	1.60	4 (22%)

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
3	HEC	W	605	1	-	2/6/54/54	-
3	HEC	J	605	1	-	2/6/54/54	-
3	HEC	N	600	1	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	I	601	1	-	2/6/54/54	-
3	HEC	X	603	1,7	-	0/6/54/54	-
3	HEC	V	602	1	-	1/6/54/54	-
3	HEC	T	605	1	-	2/6/54/54	-
3	HEC	X	600	1	-	0/6/54/54	-
3	HEC	F	605	1	-	2/6/54/54	-
3	HEC	L	606	1	-	0/6/54/54	-
3	HEC	D	601	1	-	2/6/54/54	-
3	HEC	L	602	1	-	1/6/54/54	-
3	HEC	Q	600	1	-	0/6/54/54	-
3	HEC	V	600	1	-	0/6/54/54	-
3	HEC	D	605	1	-	2/6/54/54	-
3	HEC	Q	601	1	-	2/6/54/54	-
3	HEC	X	601	1	-	2/6/54/54	-
3	HEC	X	602	1	-	1/6/54/54	-
3	HEC	C	606	1	-	0/6/54/54	-
3	HEC	X	607	1	-	1/6/54/54	-
3	HEC	K	602	1	-	1/6/54/54	-
5	GOL	J	612	-	-	4/4/4/4	-
3	HEC	X	604	1	-	0/6/54/54	-
3	HEC	Q	607	1	-	1/6/54/54	-
3	HEC	G	606	1	-	0/6/54/54	-
3	HEC	U	606	1	-	0/6/54/54	-
3	HEC	P	604	1	-	0/6/54/54	-
3	HEC	R	601	1	-	2/6/54/54	-
3	HEC	D	602	1	-	0/6/54/54	-
3	HEC	I	602	1	-	1/6/54/54	-
3	HEC	N	604	1	-	0/6/54/54	-
3	HEC	Q	605	1	-	2/6/54/54	-
3	HEC	P	602	1	-	1/6/54/54	-
3	HEC	U	600	1	-	0/6/54/54	-
5	GOL	L	613	-	-	2/4/4/4	-
3	HEC	O	606	1	-	0/6/54/54	-
3	HEC	S	603	1,7	-	0/6/54/54	-
3	HEC	M	607	1	-	1/6/54/54	-
5	GOL	I	614	-	-	2/4/4/4	-
3	HEC	G	601	1	-	2/6/54/54	-
3	HEC	H	603	1,7	-	0/6/54/54	-
3	HEC	V	604	1	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	S	606	1	-	0/6/54/54	-
3	HEC	T	600	1	-	0/6/54/54	-
3	HEC	U	602	1	-	1/6/54/54	-
3	HEC	H	600	1	-	0/6/54/54	-
3	HEC	M	606	1	-	0/6/54/54	-
3	HEC	S	601	1	-	2/6/54/54	-
3	HEC	X	606	1	-	0/6/54/54	-
3	HEC	W	604	1	-	0/6/54/54	-
3	HEC	T	606	1	-	0/6/54/54	-
5	GOL	K	613	-	-	2/4/4/4	-
3	HEC	T	602	1	-	1/6/54/54	-
3	HEC	V	603	1,7	-	0/6/54/54	-
3	HEC	S	607	1	-	1/6/54/54	-
3	HEC	H	606	1	-	0/6/54/54	-
5	GOL	K	612	-	-	2/4/4/4	-
3	HEC	L	607	1	-	1/6/54/54	-
3	HEC	W	602	1	-	1/6/54/54	-
3	HEC	K	607	1	-	1/6/54/54	-
5	GOL	D	610	-	-	2/4/4/4	-
3	HEC	H	604	1	-	0/6/54/54	-
3	HEC	V	601	1	-	1/6/54/54	-
3	HEC	E	604	1	-	0/6/54/54	-
3	HEC	J	602	1	-	1/6/54/54	-
3	HEC	K	601	1	-	1/6/54/54	-
3	HEC	L	601	1	-	1/6/54/54	-
3	HEC	A	606	1	-	0/6/54/54	-
3	HEC	T	607	1	-	1/6/54/54	-
3	HEC	A	605	1	-	2/6/54/54	-
3	HEC	T	603	1	-	0/6/54/54	-
3	HEC	C	600	1	-	0/6/54/54	-
3	HEC	E	600	1	-	0/6/54/54	-
3	HEC	L	603	1,7	-	0/6/54/54	-
3	HEC	D	607	1	-	2/6/54/54	-
3	HEC	L	600	1	-	0/6/54/54	-
5	GOL	A	613	-	-	2/4/4/4	-
3	HEC	N	607	1	-	1/6/54/54	-
3	HEC	O	605	1	-	2/6/54/54	-
3	HEC	Q	604	1	-	0/6/54/54	-
3	HEC	N	606	1	-	0/6/54/54	-
3	HEC	C	601	1	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	J	606	1	-	0/6/54/54	-
3	HEC	U	604	1	-	0/6/54/54	-
3	HEC	B	602	1	-	1/6/54/54	-
3	HEC	R	600	1	-	0/6/54/54	-
3	HEC	I	600	1	-	0/6/54/54	-
3	HEC	F	603	1,7	-	0/6/54/54	-
3	HEC	B	604	1	-	0/6/54/54	-
3	HEC	O	604	1	-	0/6/54/54	-
3	HEC	U	603	1,7	-	0/6/54/54	-
3	HEC	F	606	1	-	0/6/54/54	-
5	GOL	A	612	-	-	0/4/4/4	-
3	HEC	M	604	1	-	0/6/54/54	-
3	HEC	K	606	1	-	0/6/54/54	-
3	HEC	G	603	1,7	-	0/6/54/54	-
3	HEC	R	605	1	-	2/6/54/54	-
3	HEC	A	600	1	-	0/6/54/54	-
5	GOL	J	613	-	-	2/4/4/4	-
3	HEC	R	607	1	-	1/6/54/54	-
3	HEC	H	605	1	-	2/6/54/54	-
3	HEC	A	601	1	-	2/6/54/54	-
3	HEC	V	607	1	-	1/6/54/54	-
3	HEC	K	604	1	-	0/6/54/54	-
3	HEC	L	605	1	-	2/6/54/54	-
3	HEC	D	606	1	-	0/6/54/54	-
3	HEC	M	603	1,7	-	0/6/54/54	-
5	GOL	H	614	-	-	4/4/4/4	-
3	HEC	W	600	1	-	0/6/54/54	-
3	HEC	W	603	1,7	-	0/6/54/54	-
3	HEC	O	600	1	-	0/6/54/54	-
3	HEC	Q	602	1	-	1/6/54/54	-
3	HEC	X	605	1	-	2/6/54/54	-
5	GOL	I	615	-	-	2/4/4/4	-
3	HEC	J	603	1,7	-	0/6/54/54	-
3	HEC	B	607	1	-	1/6/54/54	-
3	HEC	D	603	1,7	-	2/6/54/54	-
3	HEC	E	606	1	-	0/6/54/54	-
3	HEC	K	600	1	-	0/6/54/54	-
3	HEC	Q	603	1,7	-	0/6/54/54	-
3	HEC	B	605	1	-	2/6/54/54	-
3	HEC	P	600	1	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	C	604	1	-	0/6/54/54	-
3	HEC	G	607	1	-	1/6/54/54	-
5	GOL	K	615	-	-	4/4/4/4	-
3	HEC	T	601	1	-	1/6/54/54	-
3	HEC	R	603	1	-	0/6/54/54	-
3	HEC	A	607	1	-	1/6/54/54	-
3	HEC	S	602	1	-	1/6/54/54	-
3	HEC	S	600	1	-	0/6/54/54	-
3	HEC	I	605	1	-	2/6/54/54	-
3	HEC	N	601	1	-	1/6/54/54	-
3	HEC	P	606	1	-	0/6/54/54	-
3	HEC	G	605	1	-	2/6/54/54	-
3	HEC	N	602	1	-	1/6/54/54	-
3	HEC	M	602	1	-	1/6/54/54	-
5	GOL	K	614	-	-	4/4/4/4	-
3	HEC	H	601	1	-	1/6/54/54	-
3	HEC	T	604	1	-	0/6/54/54	-
3	HEC	E	603	1,7	-	0/6/54/54	-
3	HEC	I	607	1	-	1/6/54/54	-
3	HEC	U	601	1	-	2/6/54/54	-
3	HEC	W	606	1	-	0/6/54/54	-
3	HEC	R	606	1	-	0/6/54/54	-
3	HEC	S	604	1	-	0/6/54/54	-
3	HEC	B	603	1	-	0/6/54/54	-
3	HEC	W	607	1	-	1/6/54/54	-
3	HEC	B	601	1	-	1/6/54/54	-
3	HEC	H	602	1	-	1/6/54/54	-
3	HEC	K	603	1,7	-	0/6/54/54	-
3	HEC	A	603	1,7	-	0/6/54/54	-
3	HEC	O	602	1	-	1/6/54/54	-
3	HEC	J	601	1	-	2/6/54/54	-
5	GOL	A	614	-	-	4/4/4/4	-
3	HEC	K	605	1	-	2/6/54/54	-
3	HEC	F	607	1	-	1/6/54/54	-
3	HEC	E	605	1	-	2/6/54/54	-
3	HEC	C	602	1	-	1/6/54/54	-
3	HEC	O	607	1	-	1/6/54/54	-
3	HEC	J	607	1	-	1/6/54/54	-
3	HEC	I	603	1,7	-	2/6/54/54	-
3	HEC	O	603	1,7	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	M	601	1	-	1/6/54/54	-
3	HEC	C	603	1	-	0/6/54/54	-
3	HEC	E	607	1	-	1/6/54/54	-
3	HEC	P	605	1	-	2/6/54/54	-
3	HEC	S	605	1	-	2/6/54/54	-
3	HEC	M	605	1	-	2/6/54/54	-
3	HEC	N	605	1	-	2/6/54/54	-
3	HEC	D	600	1	-	0/6/54/54	-
5	GOL	I	613	-	-	4/4/4/4	-
3	HEC	O	601	1	-	2/6/54/54	-
3	HEC	I	604	1	-	0/6/54/54	-
3	HEC	E	601	1	-	2/6/54/54	-
3	HEC	P	607	1	-	1/6/54/54	-
3	HEC	C	605	1	-	2/6/54/54	-
3	HEC	G	604	1	-	0/6/54/54	-
3	HEC	N	603	1,7	-	0/6/54/54	-
3	HEC	B	606	1	-	0/6/54/54	-
3	HEC	Q	606	1	-	0/6/54/54	-
3	HEC	U	605	1	-	2/6/54/54	-
3	HEC	J	600	1	-	0/6/54/54	-
3	HEC	C	607	1	-	1/6/54/54	-
3	HEC	I	606	1	-	0/6/54/54	-
3	HEC	W	601	1	-	2/6/54/54	-
3	HEC	V	606	1	-	0/6/54/54	-
3	HEC	B	600	1	-	0/6/54/54	-
3	HEC	G	602	1	-	1/6/54/54	-
3	HEC	U	607	1	-	1/6/54/54	-
3	HEC	M	600	1	-	0/6/54/54	-
5	GOL	G	615	-	-	2/4/4/4	-
3	HEC	F	602	1	-	1/6/54/54	-
3	HEC	G	600	1	-	0/6/54/54	-
3	HEC	E	602	1	-	1/6/54/54	-
3	HEC	J	604	1	-	0/6/54/54	-
3	HEC	R	602	1	-	1/6/54/54	-
3	HEC	D	604	1	-	1/6/54/54	-
3	HEC	A	602	1	-	1/6/54/54	-
3	HEC	F	604	1	-	0/6/54/54	-
3	HEC	R	604	1	-	0/6/54/54	-
3	HEC	F	600	1	-	0/6/54/54	-
3	HEC	P	601	1	-	1/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	H	615	-	-	2/4/4/4	-
3	HEC	P	603	1,7	-	0/6/54/54	-
3	HEC	F	601	1	-	1/6/54/54	-
5	GOL	G	616	-	-	2/4/4/4	-
3	HEC	A	604	1	-	0/6/54/54	-
3	HEC	H	607	1	-	1/6/54/54	-
3	HEC	L	604	1	-	0/6/54/54	-
3	HEC	V	605	1	-	2/6/54/54	-

All (905) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	603	HEC	C3B-C4B	6.59	1.55	1.43
3	X	603	HEC	C3B-C4B	6.38	1.54	1.43
3	O	603	HEC	C3B-C4B	6.35	1.54	1.43
3	A	603	HEC	C3B-C4B	6.33	1.54	1.43
3	E	603	HEC	C3B-C4B	6.32	1.54	1.43
3	Q	603	HEC	C3B-C4B	6.27	1.54	1.43
3	N	603	HEC	C3B-C4B	6.27	1.54	1.43
3	S	603	HEC	C3B-C4B	6.26	1.54	1.43
3	G	603	HEC	C3B-C4B	6.24	1.54	1.43
3	M	603	HEC	C3B-C4B	6.20	1.54	1.43
3	C	603	HEC	C3B-C4B	6.15	1.54	1.43
3	B	603	HEC	C3B-C4B	6.13	1.54	1.43
3	F	603	HEC	C3B-C4B	6.11	1.54	1.43
3	D	603	HEC	C3B-C4B	6.07	1.54	1.43
3	R	603	HEC	C3B-C4B	6.02	1.54	1.43
3	V	603	HEC	C3B-C4B	5.97	1.53	1.43
3	H	603	HEC	C3B-C4B	5.96	1.53	1.43
3	U	603	HEC	C3B-C4B	5.91	1.53	1.43
3	W	603	HEC	C3B-C4B	5.91	1.53	1.43
3	L	603	HEC	C3B-C4B	5.89	1.53	1.43
3	I	603	HEC	C3B-C4B	5.88	1.53	1.43
3	P	603	HEC	C3B-C4B	5.88	1.53	1.43
3	J	603	HEC	C3B-C4B	5.85	1.53	1.43
3	K	603	HEC	C3B-C4B	5.84	1.53	1.43
3	K	603	HEC	C3C-C4C	5.61	1.53	1.43
3	I	603	HEC	C3C-C4C	5.46	1.53	1.43
3	P	603	HEC	C3C-C4C	5.44	1.52	1.43
3	U	603	HEC	C3C-C4C	5.43	1.52	1.43
3	D	603	HEC	C1A-C2A	5.42	1.54	1.42
3	S	603	HEC	C3C-C4C	5.39	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	603	HEC	C3C-C4C	5.38	1.52	1.43
3	W	603	HEC	C3C-C4C	5.37	1.52	1.43
3	Q	603	HEC	C1A-C2A	5.36	1.54	1.42
3	H	603	HEC	C1A-C2A	5.36	1.54	1.42
3	S	603	HEC	C1A-C2A	5.34	1.54	1.42
3	A	603	HEC	C3C-C4C	5.31	1.52	1.43
3	X	603	HEC	C3C-C4C	5.31	1.52	1.43
3	E	603	HEC	C1A-C2A	5.31	1.54	1.42
3	T	603	HEC	C1A-C2A	5.29	1.54	1.42
3	H	603	HEC	C3C-C4C	5.29	1.52	1.43
3	C	603	HEC	C3C-C4C	5.28	1.52	1.43
3	B	603	HEC	C1A-C2A	5.27	1.54	1.42
3	N	603	HEC	C1A-C2A	5.27	1.54	1.42
3	U	603	HEC	C1A-C2A	5.27	1.54	1.42
3	N	603	HEC	C3C-C4C	5.26	1.52	1.43
3	A	603	HEC	C1A-C2A	5.25	1.54	1.42
3	E	603	HEC	C3C-C4C	5.24	1.52	1.43
3	F	603	HEC	C1A-C2A	5.24	1.54	1.42
3	M	603	HEC	C1A-C2A	5.23	1.54	1.42
3	K	603	HEC	C1A-C2A	5.22	1.54	1.42
3	W	603	HEC	C1A-C2A	5.22	1.54	1.42
3	R	603	HEC	C1A-C2A	5.22	1.54	1.42
3	P	603	HEC	C1A-C2A	5.21	1.54	1.42
3	C	603	HEC	C1A-C2A	5.21	1.54	1.42
3	Q	603	HEC	C3C-C4C	5.19	1.52	1.43
3	J	603	HEC	C1A-C2A	5.17	1.54	1.42
3	X	603	HEC	C1A-C2A	5.15	1.54	1.42
3	R	603	HEC	C3C-C4C	5.15	1.52	1.43
3	B	603	HEC	C3C-C4C	5.15	1.52	1.43
3	I	603	HEC	C1A-C2A	5.14	1.54	1.42
3	V	603	HEC	C3C-C4C	5.14	1.52	1.43
3	M	603	HEC	C3C-C4C	5.13	1.52	1.43
3	T	603	HEC	C3C-C4C	5.13	1.52	1.43
3	V	603	HEC	C1A-C2A	5.12	1.54	1.42
3	G	603	HEC	C3C-C4C	5.12	1.52	1.43
3	D	603	HEC	C3C-C4C	5.11	1.52	1.43
3	O	603	HEC	C1A-C2A	5.11	1.54	1.42
3	J	603	HEC	C3C-C4C	5.09	1.52	1.43
3	G	603	HEC	C1A-C2A	5.08	1.54	1.42
3	L	603	HEC	C1A-C2A	5.07	1.54	1.42
3	O	603	HEC	C3C-C4C	5.01	1.52	1.43
3	F	603	HEC	C3C-C4C	4.92	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	601	HEC	C3B-C2B	-4.78	1.35	1.40
3	L	603	HEC	C3C-C2C	-4.63	1.35	1.40
3	A	601	HEC	C3B-C2B	-4.60	1.35	1.40
3	T	601	HEC	C3B-C2B	-4.60	1.35	1.40
3	K	603	HEC	C3C-C2C	-4.56	1.36	1.40
3	J	601	HEC	C3B-C2B	-4.53	1.36	1.40
3	H	606	HEC	CBC-CAC	-4.50	1.32	1.49
3	R	601	HEC	C3B-C2B	-4.49	1.36	1.40
3	I	603	HEC	C3C-C2C	-4.49	1.36	1.40
3	J	607	HEC	CBB-CAB	-4.46	1.32	1.49
3	E	605	HEC	CBC-CAC	-4.44	1.32	1.49
3	N	606	HEC	CBC-CAC	-4.44	1.32	1.49
3	L	603	HEC	C3B-C2B	-4.44	1.36	1.40
3	K	601	HEC	C3B-C2B	-4.43	1.36	1.40
3	K	605	HEC	CBB-CAB	-4.43	1.32	1.49
3	S	601	HEC	C3B-C2B	-4.43	1.36	1.40
3	I	604	HEC	C3B-C2B	-4.42	1.36	1.40
3	G	603	HEC	C3C-C2C	-4.42	1.36	1.40
3	L	607	HEC	CBB-CAB	-4.41	1.32	1.49
3	K	607	HEC	CBB-CAB	-4.41	1.32	1.49
3	A	606	HEC	CBC-CAC	-4.41	1.32	1.49
3	W	604	HEC	CBB-CAB	-4.41	1.32	1.49
3	H	602	HEC	CBB-CAB	-4.41	1.32	1.49
3	K	602	HEC	CBB-CAB	-4.40	1.33	1.49
3	N	602	HEC	CBC-CAC	-4.40	1.33	1.49
3	I	607	HEC	CBC-CAC	-4.40	1.33	1.49
3	J	600	HEC	CBC-CAC	-4.39	1.33	1.49
3	H	606	HEC	CBB-CAB	-4.39	1.33	1.49
3	F	606	HEC	CBC-CAC	-4.39	1.33	1.49
3	D	605	HEC	CBB-CAB	-4.39	1.33	1.49
3	I	601	HEC	CBB-CAB	-4.38	1.33	1.49
3	E	606	HEC	CBC-CAC	-4.38	1.33	1.49
3	M	603	HEC	C3C-C2C	-4.38	1.36	1.40
3	G	600	HEC	CBC-CAC	-4.38	1.33	1.49
3	W	606	HEC	CBC-CAC	-4.38	1.33	1.49
3	J	607	HEC	CBC-CAC	-4.38	1.33	1.49
3	K	601	HEC	CBC-CAC	-4.38	1.33	1.49
3	B	606	HEC	CBC-CAC	-4.38	1.33	1.49
3	W	602	HEC	CBC-CAC	-4.38	1.33	1.49
3	L	604	HEC	CBB-CAB	-4.38	1.33	1.49
3	S	606	HEC	CBC-CAC	-4.38	1.33	1.49
3	O	603	HEC	C3C-C2C	-4.37	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	605	HEC	CBC-CAC	-4.37	1.33	1.49
3	M	601	HEC	C3B-C2B	-4.37	1.36	1.40
3	F	601	HEC	C3B-C2B	-4.37	1.36	1.40
3	E	602	HEC	CBB-CAB	-4.37	1.33	1.49
3	T	602	HEC	CBC-CAC	-4.37	1.33	1.49
3	R	606	HEC	CBC-CAC	-4.37	1.33	1.49
3	H	607	HEC	CBC-CAC	-4.36	1.33	1.49
3	V	604	HEC	CBC-CAC	-4.36	1.33	1.49
3	T	602	HEC	CBB-CAB	-4.36	1.33	1.49
3	K	604	HEC	CBC-CAC	-4.36	1.33	1.49
3	J	604	HEC	CBC-CAC	-4.36	1.33	1.49
3	H	602	HEC	CBC-CAC	-4.36	1.33	1.49
3	A	602	HEC	CBB-CAB	-4.35	1.33	1.49
3	P	602	HEC	CBC-CAC	-4.35	1.33	1.49
3	R	602	HEC	CBB-CAB	-4.35	1.33	1.49
3	A	602	HEC	CBC-CAC	-4.35	1.33	1.49
3	P	607	HEC	CBC-CAC	-4.35	1.33	1.49
3	L	602	HEC	CBB-CAB	-4.35	1.33	1.49
3	O	602	HEC	CBB-CAB	-4.35	1.33	1.49
3	P	605	HEC	CBC-CAC	-4.35	1.33	1.49
3	E	604	HEC	CBC-CAC	-4.35	1.33	1.49
3	V	606	HEC	CBC-CAC	-4.35	1.33	1.49
3	B	602	HEC	CBC-CAC	-4.35	1.33	1.49
3	M	601	HEC	CBB-CAB	-4.35	1.33	1.49
3	O	607	HEC	CBC-CAC	-4.35	1.33	1.49
3	C	605	HEC	CBC-CAC	-4.34	1.33	1.49
3	I	607	HEC	CBB-CAB	-4.34	1.33	1.49
3	N	601	HEC	C3B-C2B	-4.34	1.36	1.40
3	O	604	HEC	CBB-CAB	-4.34	1.33	1.49
3	G	604	HEC	CBB-CAB	-4.34	1.33	1.49
3	P	607	HEC	CBB-CAB	-4.34	1.33	1.49
3	C	602	HEC	CBC-CAC	-4.34	1.33	1.49
3	S	601	HEC	CBC-CAC	-4.34	1.33	1.49
3	P	604	HEC	CBC-CAC	-4.34	1.33	1.49
3	O	604	HEC	CBC-CAC	-4.34	1.33	1.49
3	U	606	HEC	CBC-CAC	-4.33	1.33	1.49
3	N	604	HEC	CBB-CAB	-4.33	1.33	1.49
3	E	602	HEC	CBC-CAC	-4.33	1.33	1.49
3	N	600	HEC	CBC-CAC	-4.33	1.33	1.49
3	H	605	HEC	CBC-CAC	-4.33	1.33	1.49
3	G	607	HEC	CBB-CAB	-4.33	1.33	1.49
3	G	602	HEC	CBC-CAC	-4.33	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	604	HEC	CBB-CAB	-4.33	1.33	1.49
3	M	606	HEC	CBC-CAC	-4.33	1.33	1.49
3	R	607	HEC	CBB-CAB	-4.33	1.33	1.49
3	S	600	HEC	CBC-CAC	-4.33	1.33	1.49
3	C	601	HEC	C3B-C2B	-4.33	1.36	1.40
3	D	607	HEC	CBC-CAC	-4.33	1.33	1.49
3	M	607	HEC	CBC-CAC	-4.33	1.33	1.49
3	L	601	HEC	CBB-CAB	-4.33	1.33	1.49
3	B	603	HEC	C3C-C2C	-4.32	1.36	1.40
3	U	600	HEC	CBC-CAC	-4.32	1.33	1.49
3	D	601	HEC	CBC-CAC	-4.32	1.33	1.49
3	X	602	HEC	CBC-CAC	-4.32	1.33	1.49
3	C	604	HEC	CBC-CAC	-4.32	1.33	1.49
3	T	606	HEC	CBC-CAC	-4.32	1.33	1.49
3	P	602	HEC	CBB-CAB	-4.32	1.33	1.49
3	W	601	HEC	CBC-CAC	-4.32	1.33	1.49
3	K	607	HEC	CBC-CAC	-4.32	1.33	1.49
3	X	606	HEC	CBC-CAC	-4.32	1.33	1.49
3	E	607	HEC	CBC-CAC	-4.32	1.33	1.49
3	V	602	HEC	CBB-CAB	-4.32	1.33	1.49
3	S	603	HEC	C3C-C2C	-4.32	1.36	1.40
3	I	602	HEC	CBB-CAB	-4.32	1.33	1.49
3	M	600	HEC	CBB-CAB	-4.31	1.33	1.49
3	I	602	HEC	CBC-CAC	-4.31	1.33	1.49
3	Q	607	HEC	CBB-CAB	-4.31	1.33	1.49
3	K	602	HEC	CBC-CAC	-4.31	1.33	1.49
3	G	604	HEC	CBC-CAC	-4.31	1.33	1.49
3	O	607	HEC	CBB-CAB	-4.31	1.33	1.49
3	V	602	HEC	CBC-CAC	-4.31	1.33	1.49
3	C	607	HEC	CBB-CAB	-4.31	1.33	1.49
3	B	602	HEC	CBB-CAB	-4.31	1.33	1.49
3	I	601	HEC	CBC-CAC	-4.31	1.33	1.49
3	Q	601	HEC	CBC-CAC	-4.31	1.33	1.49
3	F	600	HEC	CBB-CAB	-4.31	1.33	1.49
3	D	605	HEC	CBC-CAC	-4.31	1.33	1.49
3	S	605	HEC	CBB-CAB	-4.31	1.33	1.49
3	Q	607	HEC	CBC-CAC	-4.31	1.33	1.49
3	S	602	HEC	CBB-CAB	-4.31	1.33	1.49
3	K	605	HEC	CBC-CAC	-4.31	1.33	1.49
3	A	601	HEC	CBC-CAC	-4.31	1.33	1.49
3	S	604	HEC	CBC-CAC	-4.31	1.33	1.49
3	F	601	HEC	CBC-CAC	-4.31	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	600	HEC	CBC-CAC	-4.31	1.33	1.49
3	H	600	HEC	CBC-CAC	-4.30	1.33	1.49
3	V	601	HEC	CBC-CAC	-4.30	1.33	1.49
3	J	602	HEC	CBC-CAC	-4.30	1.33	1.49
3	X	607	HEC	CBB-CAB	-4.30	1.33	1.49
3	O	605	HEC	CBB-CAB	-4.30	1.33	1.49
3	B	600	HEC	CBC-CAC	-4.30	1.33	1.49
3	C	606	HEC	CBC-CAC	-4.30	1.33	1.49
3	X	605	HEC	CBB-CAB	-4.30	1.33	1.49
3	O	600	HEC	CBC-CAC	-4.30	1.33	1.49
3	U	607	HEC	CBC-CAC	-4.30	1.33	1.49
3	W	604	HEC	CBC-CAC	-4.30	1.33	1.49
3	E	600	HEC	CBC-CAC	-4.30	1.33	1.49
3	U	605	HEC	CBC-CAC	-4.30	1.33	1.49
3	R	601	HEC	CBC-CAC	-4.30	1.33	1.49
3	Q	606	HEC	CBC-CAC	-4.30	1.33	1.49
3	P	606	HEC	CBC-CAC	-4.30	1.33	1.49
3	S	607	HEC	CBC-CAC	-4.30	1.33	1.49
3	H	607	HEC	CBB-CAB	-4.30	1.33	1.49
3	F	602	HEC	CBB-CAB	-4.30	1.33	1.49
3	F	604	HEC	CBC-CAC	-4.30	1.33	1.49
3	V	600	HEC	CBC-CAC	-4.30	1.33	1.49
3	T	603	HEC	C3C-C2C	-4.30	1.36	1.40
3	N	607	HEC	CBB-CAB	-4.30	1.33	1.49
3	P	606	HEC	CBB-CAB	-4.29	1.33	1.49
3	T	605	HEC	CBC-CAC	-4.29	1.33	1.49
3	G	603	HEC	C3B-C2B	-4.29	1.36	1.40
3	P	601	HEC	CBB-CAB	-4.29	1.33	1.49
3	S	607	HEC	CBB-CAB	-4.29	1.33	1.49
3	R	607	HEC	CBC-CAC	-4.29	1.33	1.49
3	M	600	HEC	CBC-CAC	-4.29	1.33	1.49
3	N	603	HEC	C3C-C2C	-4.29	1.36	1.40
3	X	607	HEC	CBC-CAC	-4.29	1.33	1.49
3	Q	602	HEC	CBC-CAC	-4.29	1.33	1.49
3	O	606	HEC	CBC-CAC	-4.29	1.33	1.49
3	R	603	HEC	C3B-C2B	-4.29	1.36	1.40
3	B	605	HEC	CBC-CAC	-4.29	1.33	1.49
3	G	601	HEC	CBC-CAC	-4.29	1.33	1.49
3	S	601	HEC	CBB-CAB	-4.29	1.33	1.49
3	F	606	HEC	CBB-CAB	-4.29	1.33	1.49
3	R	600	HEC	CBC-CAC	-4.29	1.33	1.49
3	N	602	HEC	CBB-CAB	-4.29	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	601	HEC	CBB-CAB	-4.29	1.33	1.49
3	T	600	HEC	CBC-CAC	-4.29	1.33	1.49
3	Q	604	HEC	CBC-CAC	-4.29	1.33	1.49
3	U	602	HEC	CBB-CAB	-4.28	1.33	1.49
3	F	602	HEC	CBC-CAC	-4.28	1.33	1.49
3	H	602	HEC	C3B-C2B	-4.28	1.36	1.40
3	N	607	HEC	CBC-CAC	-4.28	1.33	1.49
3	W	600	HEC	CBB-CAB	-4.28	1.33	1.49
3	L	600	HEC	CBC-CAC	-4.28	1.33	1.49
3	T	601	HEC	CBC-CAC	-4.28	1.33	1.49
3	L	604	HEC	CBC-CAC	-4.28	1.33	1.49
3	X	600	HEC	CBC-CAC	-4.28	1.33	1.49
3	X	606	HEC	CBB-CAB	-4.28	1.33	1.49
3	A	604	HEC	CBC-CAC	-4.28	1.33	1.49
3	I	604	HEC	CBC-CAC	-4.28	1.33	1.49
3	V	606	HEC	CBB-CAB	-4.28	1.33	1.49
3	C	602	HEC	CBB-CAB	-4.28	1.33	1.49
3	D	601	HEC	C3B-C2B	-4.28	1.36	1.40
3	J	602	HEC	CBB-CAB	-4.28	1.33	1.49
3	T	604	HEC	CBC-CAC	-4.28	1.33	1.49
3	D	601	HEC	CBB-CAB	-4.28	1.33	1.49
3	E	601	HEC	CBC-CAC	-4.28	1.33	1.49
3	N	601	HEC	CBC-CAC	-4.28	1.33	1.49
3	N	605	HEC	CBC-CAC	-4.28	1.33	1.49
3	H	603	HEC	C3C-C2C	-4.28	1.36	1.40
3	E	603	HEC	C3C-C2C	-4.28	1.36	1.40
3	Q	605	HEC	CBB-CAB	-4.28	1.33	1.49
3	L	606	HEC	CBC-CAC	-4.28	1.33	1.49
3	L	606	HEC	CBB-CAB	-4.27	1.33	1.49
3	B	607	HEC	CBB-CAB	-4.27	1.33	1.49
3	R	606	HEC	CBB-CAB	-4.27	1.33	1.49
3	M	607	HEC	CBB-CAB	-4.27	1.33	1.49
3	M	604	HEC	CBC-CAC	-4.27	1.33	1.49
3	E	604	HEC	CBB-CAB	-4.27	1.33	1.49
3	X	601	HEC	CBB-CAB	-4.27	1.33	1.49
3	Q	600	HEC	CBB-CAB	-4.27	1.33	1.49
3	B	600	HEC	CBB-CAB	-4.27	1.33	1.49
3	G	601	HEC	CBB-CAB	-4.27	1.33	1.49
3	I	600	HEC	CBC-CAC	-4.27	1.33	1.49
3	P	601	HEC	CBC-CAC	-4.27	1.33	1.49
3	N	604	HEC	CBC-CAC	-4.27	1.33	1.49
3	W	605	HEC	CBC-CAC	-4.27	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	604	HEC	CBC-CAC	-4.27	1.33	1.49
3	V	607	HEC	CBC-CAC	-4.27	1.33	1.49
3	M	604	HEC	CBB-CAB	-4.27	1.33	1.49
3	X	602	HEC	CBB-CAB	-4.27	1.33	1.49
3	J	605	HEC	CBB-CAB	-4.27	1.33	1.49
3	G	606	HEC	CBB-CAB	-4.27	1.33	1.49
3	G	605	HEC	CBB-CAB	-4.27	1.33	1.49
3	J	601	HEC	CBC-CAC	-4.27	1.33	1.49
3	M	602	HEC	CBB-CAB	-4.27	1.33	1.49
3	W	601	HEC	CBB-CAB	-4.27	1.33	1.49
3	P	600	HEC	CBB-CAB	-4.27	1.33	1.49
3	H	606	HEC	C3B-C2B	-4.27	1.36	1.40
3	L	605	HEC	CBB-CAB	-4.27	1.33	1.49
3	W	607	HEC	CBC-CAC	-4.27	1.33	1.49
3	I	606	HEC	CBC-CAC	-4.27	1.33	1.49
3	B	601	HEC	CBC-CAC	-4.27	1.33	1.49
3	D	606	HEC	CBB-CAB	-4.27	1.33	1.49
3	S	604	HEC	CBB-CAB	-4.26	1.33	1.49
3	F	605	HEC	CBB-CAB	-4.26	1.33	1.49
3	B	601	HEC	CBB-CAB	-4.26	1.33	1.49
3	U	604	HEC	CBB-CAB	-4.26	1.33	1.49
3	G	606	HEC	CBC-CAC	-4.26	1.33	1.49
3	J	606	HEC	CBC-CAC	-4.26	1.33	1.49
3	R	602	HEC	CBC-CAC	-4.26	1.33	1.49
3	U	601	HEC	CBC-CAC	-4.26	1.33	1.49
3	D	600	HEC	CBC-CAC	-4.26	1.33	1.49
3	W	602	HEC	CBB-CAB	-4.26	1.33	1.49
3	C	600	HEC	CBC-CAC	-4.26	1.33	1.49
3	W	607	HEC	CBB-CAB	-4.26	1.33	1.49
3	S	600	HEC	CBB-CAB	-4.26	1.33	1.49
3	T	600	HEC	CBB-CAB	-4.26	1.33	1.49
3	C	605	HEC	CBB-CAB	-4.26	1.33	1.49
3	C	601	HEC	CBC-CAC	-4.26	1.33	1.49
3	K	600	HEC	CBC-CAC	-4.26	1.33	1.49
3	D	602	HEC	CBC-CAC	-4.26	1.33	1.49
3	W	601	HEC	C3B-C2B	-4.26	1.36	1.40
3	L	602	HEC	C3B-C2B	-4.26	1.36	1.40
3	B	605	HEC	CBB-CAB	-4.26	1.33	1.49
3	M	601	HEC	CBC-CAC	-4.26	1.33	1.49
3	U	606	HEC	CBB-CAB	-4.26	1.33	1.49
3	F	600	HEC	CBC-CAC	-4.26	1.33	1.49
3	D	606	HEC	CBC-CAC	-4.25	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	607	HEC	CBC-CAC	-4.25	1.33	1.49
3	C	604	HEC	CBB-CAB	-4.25	1.33	1.49
3	L	607	HEC	CBC-CAC	-4.25	1.33	1.49
3	M	605	HEC	CBB-CAB	-4.25	1.33	1.49
3	U	607	HEC	CBB-CAB	-4.25	1.33	1.49
3	X	601	HEC	CBC-CAC	-4.25	1.33	1.49
3	G	604	HEC	C3B-C2B	-4.25	1.36	1.40
3	W	600	HEC	CBC-CAC	-4.25	1.33	1.49
3	V	604	HEC	CBB-CAB	-4.25	1.33	1.49
3	D	604	HEC	CBB-CAB	-4.25	1.33	1.49
3	J	606	HEC	CBB-CAB	-4.25	1.33	1.49
3	U	602	HEC	CBC-CAC	-4.25	1.33	1.49
3	Q	602	HEC	CBB-CAB	-4.25	1.33	1.49
3	Q	604	HEC	CBB-CAB	-4.25	1.33	1.49
3	A	601	HEC	CBB-CAB	-4.25	1.33	1.49
3	A	607	HEC	CBC-CAC	-4.25	1.33	1.49
3	A	605	HEC	CBB-CAB	-4.25	1.33	1.49
3	T	607	HEC	CBB-CAB	-4.24	1.33	1.49
3	K	606	HEC	CBC-CAC	-4.24	1.33	1.49
3	A	600	HEC	CBB-CAB	-4.24	1.33	1.49
3	R	605	HEC	CBC-CAC	-4.24	1.33	1.49
3	V	607	HEC	CBB-CAB	-4.24	1.33	1.49
3	R	604	HEC	CBC-CAC	-4.24	1.33	1.49
3	T	606	HEC	CBB-CAB	-4.24	1.33	1.49
3	E	605	HEC	CBB-CAB	-4.24	1.33	1.49
3	R	600	HEC	CBB-CAB	-4.24	1.33	1.49
3	G	607	HEC	CBC-CAC	-4.24	1.33	1.49
3	M	602	HEC	CBC-CAC	-4.24	1.33	1.49
3	T	607	HEC	CBC-CAC	-4.24	1.33	1.49
3	B	604	HEC	CBB-CAB	-4.24	1.33	1.49
3	T	604	HEC	CBB-CAB	-4.24	1.33	1.49
3	J	601	HEC	CBB-CAB	-4.24	1.33	1.49
3	O	601	HEC	CBC-CAC	-4.24	1.33	1.49
3	V	601	HEC	CBB-CAB	-4.24	1.33	1.49
3	C	600	HEC	CBB-CAB	-4.24	1.33	1.49
3	H	601	HEC	C3B-C2B	-4.23	1.36	1.40
3	W	606	HEC	CBB-CAB	-4.23	1.33	1.49
3	T	605	HEC	CBB-CAB	-4.23	1.33	1.49
3	O	602	HEC	CBC-CAC	-4.23	1.33	1.49
3	J	603	HEC	C3C-C2C	-4.23	1.36	1.40
3	Q	601	HEC	CBB-CAB	-4.23	1.33	1.49
3	F	605	HEC	CBC-CAC	-4.23	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	604	HEC	CBB-CAB	-4.23	1.33	1.49
3	O	600	HEC	CBB-CAB	-4.23	1.33	1.49
3	D	604	HEC	CBC-CAC	-4.23	1.33	1.49
3	U	600	HEC	CBB-CAB	-4.23	1.33	1.49
3	C	601	HEC	CBB-CAB	-4.23	1.33	1.49
3	E	606	HEC	CBB-CAB	-4.22	1.33	1.49
3	V	605	HEC	CBC-CAC	-4.22	1.33	1.49
3	Q	600	HEC	CBC-CAC	-4.22	1.33	1.49
3	R	605	HEC	CBB-CAB	-4.22	1.33	1.49
3	H	600	HEC	CBB-CAB	-4.22	1.33	1.49
3	E	601	HEC	CBB-CAB	-4.22	1.33	1.49
3	W	605	HEC	CBB-CAB	-4.22	1.33	1.49
3	V	605	HEC	CBB-CAB	-4.22	1.33	1.49
3	A	605	HEC	CBC-CAC	-4.22	1.33	1.49
3	I	604	HEC	CBB-CAB	-4.22	1.33	1.49
3	B	607	HEC	CBC-CAC	-4.22	1.33	1.49
3	U	601	HEC	CBB-CAB	-4.21	1.33	1.49
3	X	605	HEC	CBC-CAC	-4.21	1.33	1.49
3	H	604	HEC	CBC-CAC	-4.21	1.33	1.49
3	A	604	HEC	CBB-CAB	-4.21	1.33	1.49
3	X	604	HEC	CBB-CAB	-4.21	1.33	1.49
3	X	600	HEC	CBB-CAB	-4.21	1.33	1.49
3	J	604	HEC	CBB-CAB	-4.21	1.33	1.49
3	N	601	HEC	CBB-CAB	-4.21	1.33	1.49
3	I	600	HEC	CBB-CAB	-4.21	1.33	1.49
3	G	605	HEC	CBC-CAC	-4.21	1.33	1.49
3	U	604	HEC	CBC-CAC	-4.21	1.33	1.49
3	B	606	HEC	CBB-CAB	-4.21	1.33	1.49
3	Q	606	HEC	CBB-CAB	-4.20	1.33	1.49
3	O	601	HEC	CBB-CAB	-4.20	1.33	1.49
3	M	606	HEC	CBB-CAB	-4.20	1.33	1.49
3	H	601	HEC	CBC-CAC	-4.20	1.33	1.49
3	K	604	HEC	CBB-CAB	-4.20	1.33	1.49
3	D	607	HEC	CBB-CAB	-4.20	1.33	1.49
3	B	604	HEC	CBC-CAC	-4.20	1.33	1.49
3	T	601	HEC	CBB-CAB	-4.20	1.33	1.49
3	R	604	HEC	CBB-CAB	-4.20	1.33	1.49
3	L	605	HEC	CBC-CAC	-4.20	1.33	1.49
3	S	605	HEC	CBC-CAC	-4.20	1.33	1.49
3	C	607	HEC	CBC-CAC	-4.20	1.33	1.49
3	F	601	HEC	CBB-CAB	-4.20	1.33	1.49
3	D	602	HEC	CBB-CAB	-4.20	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	600	HEC	CBB-CAB	-4.20	1.33	1.49
3	J	605	HEC	CBC-CAC	-4.20	1.33	1.49
3	A	600	HEC	CBC-CAC	-4.20	1.33	1.49
3	P	603	HEC	C3B-C2B	-4.19	1.36	1.40
3	I	605	HEC	CBB-CAB	-4.19	1.33	1.49
3	D	600	HEC	CBB-CAB	-4.19	1.33	1.49
3	S	606	HEC	CBB-CAB	-4.19	1.33	1.49
3	E	607	HEC	CBB-CAB	-4.19	1.33	1.49
3	V	600	HEC	CBB-CAB	-4.19	1.33	1.49
3	O	606	HEC	CBB-CAB	-4.18	1.33	1.49
3	N	605	HEC	CBB-CAB	-4.18	1.33	1.49
3	G	602	HEC	CBB-CAB	-4.18	1.33	1.49
3	S	602	HEC	CBC-CAC	-4.18	1.33	1.49
3	F	607	HEC	CBB-CAB	-4.18	1.33	1.49
3	Q	605	HEC	CBC-CAC	-4.18	1.33	1.49
3	P	605	HEC	CBB-CAB	-4.18	1.33	1.49
3	K	606	HEC	CBB-CAB	-4.17	1.33	1.49
3	M	605	HEC	CBC-CAC	-4.17	1.33	1.49
3	H	604	HEC	CBB-CAB	-4.17	1.33	1.49
3	L	601	HEC	CBC-CAC	-4.17	1.33	1.49
3	N	606	HEC	CBB-CAB	-4.17	1.33	1.49
3	C	603	HEC	C3C-C2C	-4.17	1.36	1.40
3	E	600	HEC	CBB-CAB	-4.17	1.33	1.49
3	O	605	HEC	CBC-CAC	-4.16	1.33	1.49
3	L	602	HEC	CBC-CAC	-4.16	1.33	1.49
3	G	600	HEC	CBB-CAB	-4.16	1.33	1.49
3	Q	601	HEC	C3B-C2B	-4.16	1.36	1.40
3	J	600	HEC	CBB-CAB	-4.16	1.33	1.49
3	H	605	HEC	CBB-CAB	-4.16	1.33	1.49
3	U	605	HEC	CBB-CAB	-4.15	1.33	1.49
3	U	603	HEC	C3C-C2C	-4.15	1.36	1.40
3	I	606	HEC	CBB-CAB	-4.14	1.33	1.49
3	C	606	HEC	CBB-CAB	-4.14	1.33	1.49
3	C	604	HEC	C3B-C2B	-4.14	1.36	1.40
3	K	601	HEC	CBB-CAB	-4.14	1.34	1.49
3	N	602	HEC	C3B-C2B	-4.13	1.36	1.40
3	A	607	HEC	CBB-CAB	-4.13	1.34	1.49
3	J	602	HEC	C3B-C2B	-4.13	1.36	1.40
3	F	603	HEC	C3C-C2C	-4.13	1.36	1.40
3	L	600	HEC	CBB-CAB	-4.13	1.34	1.49
3	H	601	HEC	CBB-CAB	-4.13	1.34	1.49
3	P	602	HEC	C3B-C2B	-4.12	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	603	HEC	C3B-C2B	-4.12	1.36	1.40
3	E	604	HEC	C3B-C2B	-4.11	1.36	1.40
3	R	603	HEC	C3C-C2C	-4.10	1.36	1.40
3	N	600	HEC	CBB-CAB	-4.10	1.34	1.49
3	D	603	HEC	C3C-C2C	-4.10	1.36	1.40
3	A	606	HEC	CBB-CAB	-4.09	1.34	1.49
3	U	601	HEC	C3B-C2B	-4.09	1.36	1.40
3	C	602	HEC	C3B-C2B	-4.09	1.36	1.40
3	X	603	HEC	C3C-C2C	-4.09	1.36	1.40
3	V	603	HEC	C3B-C2B	-4.09	1.36	1.40
3	V	603	HEC	C3C-C2C	-4.08	1.36	1.40
3	B	601	HEC	C3B-C2B	-4.07	1.36	1.40
3	F	602	HEC	C3B-C2B	-4.07	1.36	1.40
3	X	601	HEC	C3B-C2B	-4.06	1.36	1.40
3	F	600	HEC	C3B-C2B	-4.05	1.36	1.40
3	Q	603	HEC	C3C-C2C	-4.02	1.36	1.40
3	X	600	HEC	C3B-C2B	-4.01	1.36	1.40
3	V	606	HEC	C3B-C2B	-4.00	1.36	1.40
3	X	606	HEC	C3B-C2B	-3.99	1.36	1.40
3	W	602	HEC	C3B-C2B	-3.98	1.36	1.40
3	V	601	HEC	C3B-C2B	-3.98	1.36	1.40
3	I	601	HEC	C3B-C2B	-3.97	1.36	1.40
3	D	603	HEC	C3B-C2B	-3.95	1.36	1.40
3	W	603	HEC	C3C-C2C	-3.95	1.36	1.40
3	P	603	HEC	C3C-C2C	-3.94	1.36	1.40
3	C	606	HEC	C3B-C2B	-3.94	1.36	1.40
3	W	603	HEC	C3B-C2B	-3.94	1.36	1.40
3	M	604	HEC	C3B-C2B	-3.93	1.36	1.40
3	E	600	HEC	C3B-C2B	-3.92	1.36	1.40
3	E	601	HEC	C3B-C2B	-3.91	1.36	1.40
3	O	604	HEC	C3B-C2B	-3.91	1.36	1.40
3	G	601	HEC	C3B-C2B	-3.91	1.36	1.40
3	N	604	HEC	C3B-C2B	-3.90	1.36	1.40
3	L	601	HEC	C3B-C2B	-3.90	1.36	1.40
3	C	603	HEC	C3B-C2B	-3.89	1.36	1.40
3	M	603	HEC	C3B-C2B	-3.89	1.36	1.40
3	W	600	HEC	C3B-C2B	-3.87	1.36	1.40
3	P	601	HEC	C3B-C2B	-3.87	1.36	1.40
3	G	607	HEC	C3B-C2B	-3.86	1.36	1.40
3	S	600	HEC	C3B-C2B	-3.86	1.36	1.40
3	B	602	HEC	C3B-C2B	-3.86	1.36	1.40
3	H	604	HEC	C3B-C2B	-3.85	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	602	HEC	C3B-C2B	-3.84	1.36	1.40
3	S	605	HEC	C3B-C2B	-3.84	1.36	1.40
3	E	602	HEC	C3B-C2B	-3.82	1.36	1.40
3	V	600	HEC	C3B-C2B	-3.82	1.36	1.40
3	V	604	HEC	C3B-C2B	-3.82	1.36	1.40
3	A	603	HEC	C3C-C2C	-3.82	1.36	1.40
3	B	605	HEC	C3B-C2B	-3.81	1.36	1.40
3	J	603	HEC	C3B-C2B	-3.81	1.36	1.40
3	H	603	HEC	C3B-C2B	-3.80	1.36	1.40
3	J	606	HEC	C3B-C2B	-3.80	1.36	1.40
3	Q	600	HEC	C3B-C2B	-3.80	1.36	1.40
3	D	602	HEC	C3B-C2B	-3.80	1.36	1.40
3	M	606	HEC	C3B-C2B	-3.80	1.36	1.40
3	G	602	HEC	C3B-C2B	-3.79	1.36	1.40
3	Q	602	HEC	C3B-C2B	-3.79	1.36	1.40
3	O	600	HEC	C3B-C2B	-3.79	1.36	1.40
3	R	604	HEC	C3B-C2B	-3.79	1.36	1.40
3	W	606	HEC	C3B-C2B	-3.78	1.36	1.40
3	T	602	HEC	C3B-C2B	-3.78	1.36	1.40
3	P	604	HEC	C3B-C2B	-3.78	1.36	1.40
3	W	604	HEC	C3B-C2B	-3.77	1.36	1.40
3	K	604	HEC	C3B-C2B	-3.77	1.36	1.40
3	S	602	HEC	C3B-C2B	-3.77	1.36	1.40
3	E	607	HEC	C3B-C2B	-3.76	1.36	1.40
3	S	606	HEC	C3B-C2B	-3.76	1.36	1.40
3	D	606	HEC	C3B-C2B	-3.75	1.36	1.40
3	V	602	HEC	C3B-C2B	-3.75	1.36	1.40
3	T	606	HEC	C3B-C2B	-3.75	1.36	1.40
3	A	604	HEC	C3B-C2B	-3.74	1.36	1.40
3	K	606	HEC	C3B-C2B	-3.74	1.36	1.40
3	J	607	HEC	C3B-C2B	-3.73	1.36	1.40
3	J	605	HEC	C3B-C2B	-3.73	1.36	1.40
3	T	600	HEC	C3B-C2B	-3.73	1.36	1.40
3	X	604	HEC	C3B-C2B	-3.73	1.36	1.40
3	K	603	HEC	C3B-C2B	-3.72	1.36	1.40
3	M	602	HEC	C3B-C2B	-3.71	1.36	1.40
3	H	605	HEC	C3B-C2B	-3.71	1.36	1.40
3	S	603	HEC	C3B-C2B	-3.70	1.36	1.40
3	Q	603	HEC	C3B-C2B	-3.70	1.36	1.40
3	N	603	HEC	C3B-C2B	-3.69	1.36	1.40
3	R	607	HEC	C3B-C2B	-3.68	1.36	1.40
3	B	604	HEC	C3B-C2B	-3.67	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	603	HEC	C3B-C2B	-3.65	1.36	1.40
3	L	604	HEC	C3B-C2B	-3.65	1.36	1.40
3	U	602	HEC	C3B-C2B	-3.64	1.36	1.40
3	N	600	HEC	C3B-C2B	-3.62	1.37	1.40
3	G	605	HEC	C3B-C2B	-3.62	1.37	1.40
3	T	604	HEC	C3B-C2B	-3.62	1.37	1.40
3	R	602	HEC	C3B-C2B	-3.62	1.37	1.40
3	G	606	HEC	C3B-C2B	-3.61	1.37	1.40
3	X	603	HEC	C3B-C2B	-3.61	1.37	1.40
3	X	605	HEC	C3B-C2B	-3.60	1.37	1.40
3	F	606	HEC	C3B-C2B	-3.60	1.37	1.40
3	T	603	HEC	C3B-C2B	-3.60	1.37	1.40
3	C	600	HEC	C3B-C2B	-3.59	1.37	1.40
3	A	602	HEC	C3B-C2B	-3.59	1.37	1.40
3	A	603	HEC	C3B-C2B	-3.58	1.37	1.40
3	O	605	HEC	C3B-C2B	-3.57	1.37	1.40
3	F	603	HEC	C3B-C2B	-3.57	1.37	1.40
3	H	600	HEC	C3B-C2B	-3.57	1.37	1.40
3	A	600	HEC	C3B-C2B	-3.57	1.37	1.40
3	D	605	HEC	C3B-C2B	-3.57	1.37	1.40
3	J	600	HEC	C3B-C2B	-3.56	1.37	1.40
3	I	605	HEC	C3B-C4B	3.56	1.49	1.43
3	P	606	HEC	C3B-C2B	-3.56	1.37	1.40
3	E	606	HEC	C3B-C2B	-3.55	1.37	1.40
3	P	607	HEC	C3B-C4B	3.53	1.49	1.43
3	K	600	HEC	C3B-C2B	-3.53	1.37	1.40
3	S	604	HEC	C3B-C2B	-3.53	1.37	1.40
3	X	607	HEC	C3B-C4B	3.52	1.49	1.43
3	D	607	HEC	C3B-C4B	3.52	1.49	1.43
3	N	606	HEC	C3B-C2B	-3.51	1.37	1.40
3	C	607	HEC	C3B-C2B	-3.51	1.37	1.40
3	D	604	HEC	C3B-C2B	-3.51	1.37	1.40
3	U	604	HEC	C3B-C2B	-3.51	1.37	1.40
3	U	607	HEC	C3B-C2B	-3.51	1.37	1.40
3	D	600	HEC	C3B-C4B	3.50	1.49	1.43
3	A	606	HEC	C3B-C2B	-3.50	1.37	1.40
3	O	602	HEC	C3B-C2B	-3.50	1.37	1.40
3	Q	605	HEC	C3B-C2B	-3.50	1.37	1.40
3	M	600	HEC	C3B-C2B	-3.50	1.37	1.40
3	T	607	HEC	C3B-C2B	-3.50	1.37	1.40
3	U	603	HEC	C3B-C2B	-3.49	1.37	1.40
3	U	600	HEC	C3B-C2B	-3.49	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	604	HEC	C3B-C2B	-3.49	1.37	1.40
3	V	605	HEC	C3B-C2B	-3.48	1.37	1.40
3	M	607	HEC	C3B-C4B	3.48	1.49	1.43
3	A	607	HEC	C3B-C2B	-3.48	1.37	1.40
3	M	607	HEC	C3B-C2B	-3.47	1.37	1.40
3	N	607	HEC	C3B-C2B	-3.47	1.37	1.40
3	K	607	HEC	C3B-C2B	-3.46	1.37	1.40
3	O	603	HEC	C4D-ND	3.45	1.43	1.36
3	F	604	HEC	C3B-C2B	-3.45	1.37	1.40
3	R	600	HEC	C3B-C2B	-3.44	1.37	1.40
3	U	607	HEC	C3B-C4B	3.43	1.49	1.43
3	E	605	HEC	C3B-C2B	-3.43	1.37	1.40
3	L	606	HEC	C3B-C2B	-3.43	1.37	1.40
3	R	605	HEC	C3B-C2B	-3.43	1.37	1.40
3	X	602	HEC	C3B-C2B	-3.42	1.37	1.40
3	S	607	HEC	C3B-C4B	3.42	1.49	1.43
3	N	605	HEC	C3B-C2B	-3.42	1.37	1.40
3	C	605	HEC	C3B-C4B	3.41	1.49	1.43
3	B	600	HEC	C3B-C2B	-3.41	1.37	1.40
3	B	606	HEC	C3B-C2B	-3.40	1.37	1.40
3	H	607	HEC	C3B-C2B	-3.39	1.37	1.40
3	A	605	HEC	C3B-C4B	3.38	1.49	1.43
3	F	607	HEC	C3B-C4B	3.38	1.49	1.43
3	D	607	HEC	C3B-C2B	-3.38	1.37	1.40
3	G	600	HEC	C3B-C2B	-3.37	1.37	1.40
3	O	606	HEC	C3B-C2B	-3.37	1.37	1.40
3	F	605	HEC	C3B-C4B	3.37	1.49	1.43
3	P	607	HEC	C3B-C2B	-3.37	1.37	1.40
3	W	605	HEC	C3B-C2B	-3.37	1.37	1.40
3	B	603	HEC	C3B-C2B	-3.37	1.37	1.40
3	Q	603	HEC	C4D-ND	3.36	1.43	1.36
3	Q	604	HEC	C3B-C2B	-3.36	1.37	1.40
3	F	605	HEC	C3B-C2B	-3.36	1.37	1.40
3	J	607	HEC	C3B-C4B	3.35	1.49	1.43
3	C	607	HEC	C3B-C4B	3.35	1.49	1.43
3	K	605	HEC	C3B-C2B	-3.35	1.37	1.40
3	P	600	HEC	C3B-C2B	-3.35	1.37	1.40
3	M	605	HEC	C3B-C4B	3.34	1.49	1.43
3	N	607	HEC	C3B-C4B	3.34	1.49	1.43
3	K	602	HEC	C3B-C2B	-3.34	1.37	1.40
3	W	607	HEC	C3B-C2B	-3.34	1.37	1.40
3	W	607	HEC	C3B-C4B	3.32	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	605	HEC	C3B-C2B	-3.32	1.37	1.40
3	H	607	HEC	C3B-C4B	3.32	1.49	1.43
3	A	607	HEC	C3B-C4B	3.31	1.49	1.43
3	E	607	HEC	C3B-C4B	3.31	1.49	1.43
3	D	600	HEC	C3B-C2B	-3.31	1.37	1.40
3	S	607	HEC	C3B-C2B	-3.31	1.37	1.40
3	P	605	HEC	C3B-C4B	3.31	1.49	1.43
3	V	605	HEC	C3B-C4B	3.31	1.49	1.43
3	Q	605	HEC	C3B-C4B	3.30	1.49	1.43
3	I	601	HEC	C3B-C4B	3.30	1.49	1.43
3	L	605	HEC	C3B-C2B	-3.29	1.37	1.40
3	G	603	HEC	C4D-ND	3.29	1.42	1.36
3	B	607	HEC	C3B-C2B	-3.29	1.37	1.40
3	O	607	HEC	C3B-C2B	-3.29	1.37	1.40
3	A	605	HEC	C3B-C2B	-3.28	1.37	1.40
3	Q	607	HEC	C3B-C4B	3.28	1.49	1.43
3	V	607	HEC	C3B-C4B	3.28	1.49	1.43
3	S	603	HEC	C4D-ND	3.28	1.42	1.36
3	U	606	HEC	C3B-C2B	-3.27	1.37	1.40
3	G	607	HEC	C3B-C4B	3.27	1.49	1.43
3	L	607	HEC	C3B-C2B	-3.26	1.37	1.40
3	X	605	HEC	C3B-C4B	3.26	1.49	1.43
3	I	606	HEC	C3B-C2B	-3.26	1.37	1.40
3	W	605	HEC	C3B-C4B	3.26	1.49	1.43
3	Q	607	HEC	C3B-C2B	-3.26	1.37	1.40
3	O	605	HEC	C3B-C4B	3.25	1.49	1.43
3	X	607	HEC	C3B-C2B	-3.24	1.37	1.40
3	V	607	HEC	C3B-C2B	-3.24	1.37	1.40
3	T	607	HEC	C3B-C4B	3.24	1.48	1.43
3	T	603	HEC	C4D-ND	3.23	1.42	1.36
3	T	603	HEC	C1C-CHC	3.23	1.50	1.41
3	C	605	HEC	C3B-C2B	-3.23	1.37	1.40
3	I	605	HEC	C3B-C2B	-3.22	1.37	1.40
3	V	603	HEC	C4D-ND	3.22	1.42	1.36
3	K	607	HEC	C3B-C4B	3.22	1.48	1.43
3	M	603	HEC	C4D-ND	3.21	1.42	1.36
3	B	605	HEC	C3B-C4B	3.21	1.48	1.43
3	A	604	HEC	C3B-C4B	3.21	1.48	1.43
3	Q	606	HEC	C3B-C2B	-3.21	1.37	1.40
3	R	603	HEC	C4D-ND	3.21	1.42	1.36
3	F	603	HEC	C4D-ND	3.21	1.42	1.36
3	M	603	HEC	C1D-ND	3.20	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	600	HEC	C3B-C2B	-3.20	1.37	1.40
3	E	603	HEC	C4D-ND	3.20	1.42	1.36
3	R	605	HEC	C3B-C4B	3.20	1.48	1.43
3	S	600	HEC	C3B-C4B	3.19	1.48	1.43
3	K	605	HEC	C3B-C4B	3.19	1.48	1.43
3	J	605	HEC	C3B-C4B	3.18	1.48	1.43
3	T	605	HEC	C3B-C4B	3.18	1.48	1.43
3	U	605	HEC	C3B-C2B	-3.17	1.37	1.40
3	U	603	HEC	C4D-ND	3.17	1.42	1.36
3	S	605	HEC	C3B-C4B	3.17	1.48	1.43
3	Q	600	HEC	C3B-C4B	3.16	1.48	1.43
3	N	604	HEC	C3B-C4B	3.16	1.48	1.43
3	J	603	HEC	C4D-ND	3.16	1.42	1.36
3	N	603	HEC	C4D-ND	3.15	1.42	1.36
3	W	601	HEC	C3B-C4B	3.15	1.48	1.43
3	D	602	HEC	C3B-C4B	3.15	1.48	1.43
3	W	600	HEC	C3B-C4B	3.15	1.48	1.43
3	J	600	HEC	C3B-C4B	3.14	1.48	1.43
3	E	604	HEC	C3B-C4B	3.14	1.48	1.43
3	G	605	HEC	C3B-C4B	3.13	1.48	1.43
3	I	607	HEC	C3B-C4B	3.13	1.48	1.43
3	U	605	HEC	C3B-C4B	3.13	1.48	1.43
3	K	604	HEC	C3B-C4B	3.12	1.48	1.43
3	B	607	HEC	C3B-C4B	3.12	1.48	1.43
3	M	602	HEC	C3B-C4B	3.12	1.48	1.43
3	O	603	HEC	C1D-ND	3.12	1.42	1.36
3	O	600	HEC	C3B-C4B	3.12	1.48	1.43
3	T	604	HEC	C3B-C4B	3.12	1.48	1.43
3	A	603	HEC	C1D-ND	3.11	1.42	1.36
3	V	603	HEC	C1D-ND	3.10	1.42	1.36
3	W	602	HEC	C3B-C4B	3.10	1.48	1.43
3	H	603	HEC	C4D-ND	3.10	1.42	1.36
3	F	603	HEC	C1D-ND	3.10	1.42	1.36
3	V	604	HEC	C3B-C4B	3.10	1.48	1.43
3	H	605	HEC	C3B-C4B	3.10	1.48	1.43
3	K	603	HEC	C4D-ND	3.10	1.42	1.36
3	I	603	HEC	C4D-ND	3.09	1.42	1.36
3	B	604	HEC	C3B-C4B	3.09	1.48	1.43
3	A	603	HEC	C4D-ND	3.09	1.42	1.36
3	S	604	HEC	C3B-C4B	3.09	1.48	1.43
3	U	600	HEC	C3B-C4B	3.09	1.48	1.43
3	R	606	HEC	C3B-C2B	-3.09	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	605	HEC	C3B-C4B	3.08	1.48	1.43
3	P	603	HEC	C4D-ND	3.08	1.42	1.36
3	X	604	HEC	C3B-C4B	3.08	1.48	1.43
3	T	600	HEC	C3B-C4B	3.07	1.48	1.43
3	P	602	HEC	C3B-C4B	3.07	1.48	1.43
3	K	601	HEC	C3B-C4B	3.07	1.48	1.43
3	D	603	HEC	C1D-ND	3.07	1.42	1.36
3	B	603	HEC	C4D-ND	3.07	1.42	1.36
3	I	607	HEC	C3B-C2B	-3.06	1.37	1.40
3	D	603	HEC	C4D-ND	3.06	1.42	1.36
3	G	603	HEC	C1C-CHC	3.05	1.49	1.41
3	A	602	HEC	C3B-C4B	3.05	1.48	1.43
3	R	603	HEC	C1D-ND	3.05	1.42	1.36
3	R	607	HEC	C3B-C4B	3.05	1.48	1.43
3	U	604	HEC	C3B-C4B	3.04	1.48	1.43
3	N	606	HEC	C3B-C4B	3.04	1.48	1.43
3	E	605	HEC	C3B-C4B	3.04	1.48	1.43
3	X	603	HEC	C4D-ND	3.03	1.42	1.36
3	G	602	HEC	C3B-C4B	3.03	1.48	1.43
3	E	603	HEC	C1D-ND	3.03	1.42	1.36
3	H	603	HEC	C1D-ND	3.03	1.42	1.36
3	B	600	HEC	C3B-C4B	3.03	1.48	1.43
3	L	607	HEC	C3B-C4B	3.02	1.48	1.43
3	N	600	HEC	C3B-C4B	3.02	1.48	1.43
3	I	600	HEC	C3B-C4B	3.02	1.48	1.43
3	R	604	HEC	C3B-C4B	3.02	1.48	1.43
3	M	605	HEC	C3B-C2B	-3.02	1.37	1.40
3	Q	606	HEC	C3B-C4B	3.02	1.48	1.43
3	Q	603	HEC	C1D-ND	3.01	1.42	1.36
3	H	604	HEC	C3B-C4B	3.00	1.48	1.43
3	S	603	HEC	C1D-ND	3.00	1.42	1.36
3	T	603	HEC	C1D-ND	3.00	1.42	1.36
3	O	604	HEC	C3B-C4B	3.00	1.48	1.43
3	U	602	HEC	C3B-C4B	3.00	1.48	1.43
3	D	603	HEC	C1C-CHC	2.99	1.49	1.41
3	E	601	HEC	C3B-C4B	2.99	1.48	1.43
3	U	601	HEC	C3B-C4B	2.99	1.48	1.43
3	H	606	HEC	C3B-C4B	2.98	1.48	1.43
3	I	603	HEC	C3B-C2B	-2.98	1.37	1.40
3	G	601	HEC	C3B-C4B	2.98	1.48	1.43
3	V	600	HEC	C3B-C4B	2.98	1.48	1.43
3	N	603	HEC	C1D-ND	2.97	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	606	HEC	C3B-C4B	2.97	1.48	1.43
3	P	606	HEC	C3B-C4B	2.97	1.48	1.43
3	F	607	HEC	C3B-C2B	-2.97	1.37	1.40
3	F	603	HEC	C1C-CHC	2.97	1.49	1.41
3	J	603	HEC	C1C-CHC	2.97	1.49	1.41
3	G	604	HEC	C3B-C4B	2.97	1.48	1.43
3	L	604	HEC	C3B-C4B	2.97	1.48	1.43
3	T	602	HEC	C3B-C4B	2.96	1.48	1.43
3	I	604	HEC	C3B-C4B	2.96	1.48	1.43
3	M	606	HEC	C3B-C4B	2.96	1.48	1.43
3	W	604	HEC	C3B-C4B	2.96	1.48	1.43
3	W	603	HEC	C1D-ND	2.96	1.42	1.36
3	Q	604	HEC	C3B-C4B	2.96	1.48	1.43
3	U	606	HEC	C3B-C4B	2.96	1.48	1.43
3	P	600	HEC	C3B-C4B	2.96	1.48	1.43
3	E	600	HEC	C3B-C4B	2.95	1.48	1.43
3	L	602	HEC	C3B-C4B	2.95	1.48	1.43
3	T	606	HEC	C3B-C4B	2.95	1.48	1.43
3	K	603	HEC	C1D-ND	2.95	1.42	1.36
3	A	600	HEC	C3B-C4B	2.95	1.48	1.43
3	H	601	HEC	C3B-C4B	2.95	1.48	1.43
3	W	606	HEC	C3B-C4B	2.95	1.48	1.43
3	R	603	HEC	C1C-CHC	2.95	1.49	1.41
3	G	603	HEC	C1D-ND	2.94	1.42	1.36
3	V	602	HEC	C3B-C4B	2.94	1.48	1.43
3	W	603	HEC	C4D-ND	2.94	1.42	1.36
3	G	600	HEC	C3B-C4B	2.94	1.48	1.43
3	L	601	HEC	C3B-C4B	2.94	1.48	1.43
3	S	603	HEC	C1C-CHC	2.94	1.49	1.41
3	J	603	HEC	C1D-ND	2.93	1.42	1.36
3	Q	603	HEC	C1C-CHC	2.93	1.49	1.41
3	V	601	HEC	C3B-C4B	2.93	1.48	1.43
3	X	603	HEC	C1C-CHC	2.92	1.49	1.41
3	M	604	HEC	C3B-C4B	2.92	1.48	1.43
3	K	602	HEC	C3B-C4B	2.92	1.48	1.43
3	X	600	HEC	C3B-C4B	2.92	1.48	1.43
3	C	604	HEC	C3B-C4B	2.92	1.48	1.43
3	C	602	HEC	C3B-C4B	2.91	1.48	1.43
3	U	603	HEC	C1D-ND	2.91	1.42	1.36
3	F	600	HEC	C3B-C4B	2.91	1.48	1.43
3	H	600	HEC	C3B-C4B	2.91	1.48	1.43
3	J	601	HEC	C3B-C4B	2.91	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	603	HEC	C1C-CHC	2.90	1.49	1.41
3	S	602	HEC	C3B-C4B	2.90	1.48	1.43
3	X	601	HEC	C3B-C4B	2.90	1.48	1.43
3	Q	601	HEC	C3B-C4B	2.89	1.48	1.43
3	B	602	HEC	C3B-C4B	2.89	1.48	1.43
3	X	603	HEC	C1D-ND	2.89	1.42	1.36
3	O	607	HEC	C3B-C4B	2.89	1.48	1.43
3	V	606	HEC	C3B-C4B	2.89	1.48	1.43
3	F	604	HEC	C3B-C4B	2.89	1.48	1.43
3	L	605	HEC	C3B-C4B	2.89	1.48	1.43
3	R	602	HEC	C3B-C4B	2.88	1.48	1.43
3	H	602	HEC	C3B-C4B	2.88	1.48	1.43
3	D	605	HEC	C3B-C4B	2.88	1.48	1.43
3	W	603	HEC	C1C-CHC	2.87	1.49	1.41
3	A	606	HEC	C3B-C4B	2.87	1.48	1.43
3	B	603	HEC	C1D-ND	2.87	1.42	1.36
3	S	601	HEC	C3B-C4B	2.86	1.48	1.43
3	C	606	HEC	C3B-C4B	2.86	1.48	1.43
3	F	602	HEC	C3B-C4B	2.85	1.48	1.43
3	D	604	HEC	C3B-C4B	2.85	1.48	1.43
3	Q	602	HEC	C3B-C4B	2.85	1.48	1.43
3	J	602	HEC	C3B-C4B	2.85	1.48	1.43
3	O	601	HEC	C3B-C4B	2.84	1.48	1.43
3	N	602	HEC	C3B-C4B	2.84	1.48	1.43
3	K	606	HEC	C3B-C4B	2.84	1.48	1.43
3	C	603	HEC	C4D-ND	2.84	1.42	1.36
3	N	601	HEC	C3B-C4B	2.83	1.48	1.43
3	R	606	HEC	C3B-C4B	2.83	1.48	1.43
3	P	604	HEC	C3B-C4B	2.83	1.48	1.43
3	X	602	HEC	C3B-C4B	2.82	1.48	1.43
3	P	605	HEC	C3B-C2B	-2.82	1.37	1.40
3	A	601	HEC	C3B-C4B	2.82	1.48	1.43
3	M	600	HEC	C3B-C4B	2.82	1.48	1.43
3	O	606	HEC	C3B-C4B	2.81	1.48	1.43
3	P	603	HEC	C1D-ND	2.81	1.42	1.36
3	I	602	HEC	C3B-C4B	2.81	1.48	1.43
3	X	606	HEC	C3B-C4B	2.81	1.48	1.43
3	E	603	HEC	C1C-CHC	2.80	1.48	1.41
3	L	600	HEC	C3B-C4B	2.80	1.48	1.43
3	L	603	HEC	C4D-ND	2.80	1.41	1.36
3	B	603	HEC	C1C-CHC	2.80	1.48	1.41
3	J	606	HEC	C3B-C4B	2.80	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	601	HEC	C3B-C4B	2.79	1.48	1.43
3	R	601	HEC	C3B-C4B	2.79	1.48	1.43
3	S	606	HEC	C3B-C4B	2.79	1.48	1.43
3	R	600	HEC	C3B-C4B	2.79	1.48	1.43
3	C	600	HEC	C3B-C4B	2.78	1.48	1.43
3	K	603	HEC	C1C-CHC	2.77	1.48	1.41
3	D	601	HEC	C3B-C4B	2.77	1.48	1.43
3	B	601	HEC	C3B-C4B	2.77	1.48	1.43
3	I	603	HEC	C1C-CHC	2.76	1.48	1.41
3	E	606	HEC	C3B-C4B	2.76	1.48	1.43
3	V	603	HEC	C1C-CHC	2.76	1.48	1.41
3	N	603	HEC	C1C-CHC	2.76	1.48	1.41
3	O	602	HEC	C3B-C4B	2.75	1.48	1.43
3	B	606	HEC	C3B-C4B	2.75	1.48	1.43
3	I	603	HEC	C1D-ND	2.74	1.41	1.36
3	I	606	HEC	C3B-C4B	2.74	1.48	1.43
3	O	603	HEC	C1C-CHC	2.74	1.48	1.41
3	L	606	HEC	C3B-C4B	2.73	1.48	1.43
3	P	601	HEC	C3B-C4B	2.73	1.48	1.43
3	L	603	HEC	C1C-CHC	2.72	1.48	1.41
3	U	603	HEC	C1C-CHC	2.71	1.48	1.41
3	E	602	HEC	C3B-C4B	2.71	1.48	1.43
3	M	601	HEC	C3B-C4B	2.71	1.48	1.43
3	A	603	HEC	C1C-CHC	2.69	1.48	1.41
3	C	603	HEC	C1D-ND	2.67	1.41	1.36
3	H	603	HEC	C1C-CHC	2.66	1.48	1.41
3	J	604	HEC	C3B-C4B	2.66	1.47	1.43
3	P	603	HEC	C1C-CHC	2.66	1.48	1.41
3	T	601	HEC	C3B-C4B	2.65	1.47	1.43
3	C	603	HEC	C1C-CHC	2.65	1.48	1.41
3	I	603	HEC	C4A-C3A	2.64	1.48	1.42
3	K	600	HEC	C3B-C4B	2.62	1.47	1.43
3	T	603	HEC	C4A-C3A	2.60	1.48	1.42
3	I	600	HEC	C3B-C2B	-2.59	1.38	1.40
3	C	601	HEC	C3B-C4B	2.58	1.47	1.43
3	L	603	HEC	C1D-ND	2.57	1.41	1.36
3	Q	603	HEC	C4A-C3A	2.50	1.48	1.42
3	B	603	HEC	C4A-C3A	2.50	1.48	1.42
3	L	603	HEC	C4A-C3A	2.50	1.48	1.42
3	E	603	HEC	C4A-C3A	2.49	1.48	1.42
3	A	603	HEC	C4A-C3A	2.47	1.48	1.42
3	P	603	HEC	C4A-C3A	2.47	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	606	HEC	C3B-C4B	2.47	1.47	1.43
3	N	603	HEC	C4A-C3A	2.46	1.48	1.42
3	W	603	HEC	C4A-C3A	2.45	1.48	1.42
3	U	603	HEC	C4A-C3A	2.45	1.48	1.42
3	R	603	HEC	C4A-C3A	2.43	1.48	1.42
3	F	603	HEC	C4A-C3A	2.42	1.48	1.42
3	S	603	HEC	C4A-C3A	2.42	1.48	1.42
3	F	606	HEC	C3B-C4B	2.41	1.47	1.43
3	V	603	HEC	C4A-C3A	2.41	1.48	1.42
3	J	603	HEC	C4A-C3A	2.40	1.48	1.42
3	C	603	HEC	C4A-C3A	2.39	1.48	1.42
3	H	603	HEC	C4A-C3A	2.38	1.48	1.42
3	X	603	HEC	C4A-C3A	2.36	1.47	1.42
3	K	603	HEC	C4A-C3A	2.34	1.47	1.42
3	D	603	HEC	C4A-C3A	2.33	1.47	1.42
3	H	603	HEC	CAD-C3D	-2.32	1.48	1.52
3	O	603	HEC	C4A-C3A	2.32	1.47	1.42
3	M	603	HEC	C4A-C3A	2.25	1.47	1.42
3	C	603	HEC	CAD-C3D	-2.22	1.48	1.52
3	T	603	HEC	C1B-NB	2.21	1.40	1.36
3	G	603	HEC	C4A-C3A	2.17	1.47	1.42
3	M	603	HEC	CAD-C3D	-2.15	1.48	1.52
3	C	603	HEC	C1B-NB	2.12	1.40	1.36
3	U	603	HEC	CAD-C3D	-2.12	1.48	1.52
3	D	604	HEC	C3C-C2C	-2.11	1.38	1.40
3	N	603	HEC	CAD-C3D	-2.09	1.49	1.52
3	F	603	HEC	CAD-C3D	-2.07	1.49	1.52
3	B	603	HEC	C1B-NB	2.06	1.40	1.36
3	S	603	HEC	CAD-C3D	-2.06	1.49	1.52
3	D	603	HEC	CAD-C3D	-2.04	1.49	1.52
3	Q	603	HEC	CAD-C3D	-2.03	1.49	1.52
3	O	603	HEC	CAD-C3D	-2.02	1.49	1.52
3	S	603	HEC	C1B-NB	2.02	1.40	1.36
3	Q	603	HEC	C1B-NB	2.01	1.40	1.36
3	V	603	HEC	CAD-C3D	-2.00	1.49	1.52

All (501) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	603	HEC	CBA-CAA-C2A	16.22	142.36	112.48
3	F	603	HEC	CAA-CBA-CGA	8.64	127.17	112.67
3	A	603	HEC	CAA-CBA-CGA	8.59	127.09	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	603	HEC	CAA-CBA-CGA	8.56	127.03	112.67
3	L	603	HEC	CAA-CBA-CGA	8.44	126.82	112.67
3	M	603	HEC	CAA-CBA-CGA	8.39	126.75	112.67
3	Q	603	HEC	CAA-CBA-CGA	8.21	126.45	112.67
3	X	603	HEC	CAA-CBA-CGA	8.16	126.36	112.67
3	P	603	HEC	CAA-CBA-CGA	8.14	126.33	112.67
3	U	603	HEC	CAA-CBA-CGA	8.02	126.13	112.67
3	J	603	HEC	CAA-CBA-CGA	7.95	126.02	112.67
3	T	603	HEC	CAA-CBA-CGA	7.88	125.90	112.67
3	S	603	HEC	CAA-CBA-CGA	7.87	125.87	112.67
3	O	603	HEC	CAA-CBA-CGA	7.74	125.66	112.67
3	D	603	HEC	CAA-CBA-CGA	7.69	125.57	112.67
3	N	603	HEC	CAA-CBA-CGA	7.67	125.54	112.67
3	V	603	HEC	CAA-CBA-CGA	7.67	125.53	112.67
3	W	603	HEC	CAA-CBA-CGA	7.63	125.47	112.67
3	B	603	HEC	CAA-CBA-CGA	7.57	125.37	112.67
3	C	603	HEC	CAA-CBA-CGA	7.39	125.07	112.67
3	H	603	HEC	CAA-CBA-CGA	7.34	124.98	112.67
3	G	603	HEC	CAA-CBA-CGA	7.16	124.68	112.67
3	K	603	HEC	CAA-CBA-CGA	7.03	124.46	112.67
3	R	603	HEC	CAA-CBA-CGA	6.78	124.05	112.67
3	D	604	HEC	CBD-CAD-C3D	-5.35	102.61	112.49
3	I	604	HEC	CBD-CAD-C3D	-5.10	103.08	112.49
3	H	604	HEC	CBD-CAD-C3D	-4.93	103.39	112.49
3	K	604	HEC	CBD-CAD-C3D	-4.93	103.39	112.49
3	W	604	HEC	CBD-CAD-C3D	-4.87	103.51	112.49
3	N	604	HEC	CBD-CAD-C3D	-4.82	103.60	112.49
3	V	604	HEC	CBD-CAD-C3D	-4.81	103.61	112.49
3	T	604	HEC	CBD-CAD-C3D	-4.80	103.63	112.49
3	O	604	HEC	CBD-CAD-C3D	-4.79	103.65	112.49
3	A	604	HEC	CBD-CAD-C3D	-4.78	103.68	112.49
3	B	604	HEC	CBD-CAD-C3D	-4.77	103.69	112.49
3	L	604	HEC	CBD-CAD-C3D	-4.77	103.69	112.49
3	M	604	HEC	CBD-CAD-C3D	-4.75	103.72	112.49
3	E	604	HEC	CBD-CAD-C3D	-4.75	103.73	112.49
3	S	604	HEC	CBD-CAD-C3D	-4.74	103.74	112.49
3	P	604	HEC	CBD-CAD-C3D	-4.72	103.78	112.49
3	F	604	HEC	CBD-CAD-C3D	-4.70	103.81	112.49
3	J	604	HEC	CBD-CAD-C3D	-4.67	103.87	112.49
3	U	604	HEC	CBD-CAD-C3D	-4.67	103.87	112.49
3	Q	604	HEC	CBD-CAD-C3D	-4.58	104.05	112.49
3	G	604	HEC	CBD-CAD-C3D	-4.56	104.08	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	604	HEC	CBD-CAD-C3D	-4.56	104.08	112.49
3	X	604	HEC	CBD-CAD-C3D	-4.55	104.10	112.49
3	D	603	HEC	CMC-C2C-C1C	-4.54	121.49	128.46
3	R	604	HEC	CBD-CAD-C3D	-4.49	104.20	112.49
3	T	603	HEC	C3B-C4B-NB	-4.31	102.80	110.94
3	G	603	HEC	C3B-C4B-NB	-4.20	103.01	110.94
3	N	603	HEC	C3B-C4B-NB	-4.14	103.13	110.94
3	X	603	HEC	C3B-C4B-NB	-4.13	103.15	110.94
3	S	603	HEC	C3B-C4B-NB	-4.07	103.25	110.94
3	Q	603	HEC	C3B-C4B-NB	-4.06	103.27	110.94
3	J	603	HEC	C3B-C4B-NB	-4.06	103.28	110.94
3	H	603	HEC	C3B-C4B-NB	-4.06	103.29	110.94
3	D	603	HEC	C3B-C4B-NB	-4.00	103.39	110.94
3	A	603	HEC	C3B-C4B-NB	-3.99	103.40	110.94
3	E	603	HEC	C3B-C4B-NB	-3.98	103.42	110.94
3	F	603	HEC	C3B-C4B-NB	-3.96	103.46	110.94
3	K	603	HEC	C3B-C4B-NB	-3.96	103.47	110.94
3	I	603	HEC	CMC-C2C-C1C	-3.95	122.39	128.46
3	W	603	HEC	C3B-C4B-NB	-3.95	103.48	110.94
3	O	603	HEC	C3B-C4B-NB	-3.94	103.50	110.94
3	V	603	HEC	C3B-C4B-NB	-3.91	103.56	110.94
3	M	603	HEC	C3B-C4B-NB	-3.89	103.61	110.94
3	R	603	HEC	C3B-C4B-NB	-3.88	103.61	110.94
3	P	603	HEC	C3B-C4B-NB	-3.87	103.64	110.94
3	G	604	HEC	CBA-CAA-C2A	-3.85	105.39	112.48
3	D	605	HEC	CBD-CAD-C3D	3.84	119.57	112.49
3	B	603	HEC	C3B-C4B-NB	-3.82	103.73	110.94
3	K	604	HEC	CBA-CAA-C2A	-3.78	105.52	112.48
3	E	604	HEC	CBA-CAA-C2A	-3.77	105.53	112.48
3	J	604	HEC	CBA-CAA-C2A	-3.76	105.55	112.48
3	O	604	HEC	CBA-CAA-C2A	-3.75	105.56	112.48
3	U	603	HEC	C3B-C4B-NB	-3.75	103.86	110.94
3	F	603	HEC	CMC-C2C-C1C	-3.75	122.71	128.46
3	Q	603	HEC	CMC-C2C-C1C	-3.74	122.71	128.46
3	C	603	HEC	C3B-C4B-NB	-3.67	104.01	110.94
3	U	604	HEC	CBA-CAA-C2A	-3.66	105.73	112.48
3	K	603	HEC	CMC-C2C-C1C	-3.65	122.85	128.46
3	F	604	HEC	CBA-CAA-C2A	-3.64	105.77	112.48
3	A	603	HEC	CMC-C2C-C1C	-3.64	122.87	128.46
3	V	604	HEC	CBA-CAA-C2A	-3.63	105.78	112.48
3	O	603	HEC	CMC-C2C-C1C	-3.62	122.89	128.46
3	L	604	HEC	CBA-CAA-C2A	-3.62	105.81	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	604	HEC	CBA-CAA-C2A	-3.61	105.83	112.48
3	L	603	HEC	C3B-C4B-NB	-3.60	104.14	110.94
3	N	604	HEC	CBA-CAA-C2A	-3.60	105.85	112.48
3	U	603	HEC	CMC-C2C-C1C	-3.59	122.95	128.46
3	P	603	HEC	CMC-C2C-C1C	-3.58	122.97	128.46
3	X	603	HEC	CMC-C2C-C1C	-3.56	123.00	128.46
3	K	601	HEC	CBD-CAD-C3D	-3.56	105.93	112.49
3	T	603	HEC	CMC-C2C-C1C	-3.55	123.00	128.46
3	T	604	HEC	CBA-CAA-C2A	-3.55	105.93	112.48
3	J	605	HEC	CBD-CAD-C3D	3.55	119.04	112.49
3	H	603	HEC	CMC-C2C-C1C	-3.55	123.01	128.46
3	S	604	HEC	CBA-CAA-C2A	-3.55	105.94	112.48
3	M	604	HEC	CBA-CAA-C2A	-3.54	105.95	112.48
3	M	603	HEC	CMC-C2C-C1C	-3.54	123.03	128.46
3	H	604	HEC	CBA-CAA-C2A	-3.53	105.97	112.48
3	I	603	HEC	C3B-C4B-NB	-3.53	104.28	110.94
3	U	601	HEC	CBD-CAD-C3D	-3.52	106.00	112.49
3	A	601	HEC	CBD-CAD-C3D	-3.51	106.01	112.49
3	W	603	HEC	CMC-C2C-C1C	-3.50	123.08	128.46
3	C	604	HEC	CBA-CAA-C2A	-3.49	106.04	112.48
3	B	601	HEC	CBD-CAD-C3D	-3.49	106.05	112.49
3	P	601	HEC	CBD-CAD-C3D	-3.48	106.07	112.49
3	O	601	HEC	CBD-CAD-C3D	-3.47	106.08	112.49
3	J	603	HEC	CMC-C2C-C1C	-3.47	123.13	128.46
3	V	603	HEC	CMC-C2C-C1C	-3.46	123.14	128.46
3	R	601	HEC	CBD-CAD-C3D	-3.45	106.11	112.49
3	C	601	HEC	CBD-CAD-C3D	-3.45	106.12	112.49
3	S	603	HEC	CMC-C2C-C1C	-3.45	123.17	128.46
3	S	601	HEC	CBD-CAD-C3D	-3.44	106.13	112.49
3	E	603	HEC	CMC-C2C-C1C	-3.43	123.19	128.46
3	I	602	HEC	CAD-CBD-CGD	-3.43	106.91	112.67
3	B	603	HEC	CMC-C2C-C1C	-3.43	123.19	128.46
3	T	601	HEC	CBD-CAD-C3D	-3.43	106.16	112.49
3	W	601	HEC	CBD-CAD-C3D	-3.43	106.16	112.49
3	H	601	HEC	CBD-CAD-C3D	-3.42	106.18	112.49
3	L	603	HEC	CMC-C2C-C1C	-3.41	123.22	128.46
3	W	604	HEC	CBA-CAA-C2A	-3.41	106.19	112.48
3	R	604	HEC	CBA-CAA-C2A	-3.40	106.20	112.48
3	L	601	HEC	CBD-CAD-C3D	-3.40	106.21	112.49
3	X	604	HEC	CBA-CAA-C2A	-3.40	106.22	112.48
3	C	603	HEC	CMC-C2C-C1C	-3.39	123.25	128.46
3	N	603	HEC	CMC-C2C-C1C	-3.39	123.25	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	HEC	CAD-CBD-CGD	-3.39	106.99	112.67
3	G	601	HEC	CBD-CAD-C3D	-3.37	106.27	112.49
3	R	603	HEC	CMC-C2C-C1C	-3.36	123.30	128.46
3	B	604	HEC	CBA-CAA-C2A	-3.35	106.31	112.48
3	A	604	HEC	CBA-CAA-C2A	-3.33	106.34	112.48
3	D	603	HEC	C3C-C4C-NC	-3.33	104.66	110.94
3	E	601	HEC	CBD-CAD-C3D	-3.32	106.36	112.49
3	J	601	HEC	CBD-CAD-C3D	-3.32	106.37	112.49
3	N	602	HEC	CAD-CBD-CGD	-3.30	107.13	112.67
3	A	605	HEC	CBD-CAD-C3D	3.30	118.57	112.49
3	T	605	HEC	CBD-CAD-C3D	3.30	118.56	112.49
3	K	605	HEC	CBD-CAD-C3D	3.29	118.55	112.49
3	P	604	HEC	CBA-CAA-C2A	-3.28	106.43	112.48
3	A	606	HEC	CBA-CAA-C2A	-3.27	106.45	112.48
3	G	605	HEC	CBD-CAD-C3D	3.27	118.51	112.49
3	G	603	HEC	CMC-C2C-C1C	-3.27	123.44	128.46
3	A	602	HEC	CAD-CBD-CGD	-3.27	107.19	112.67
3	Q	601	HEC	CBD-CAD-C3D	-3.26	106.47	112.49
3	F	605	HEC	CBD-CAD-C3D	3.26	118.50	112.49
3	U	602	HEC	CAD-CBD-CGD	-3.25	107.21	112.67
3	S	605	HEC	CBD-CAD-C3D	3.25	118.48	112.49
3	F	601	HEC	CBD-CAD-C3D	-3.24	106.50	112.49
3	N	601	HEC	CBD-CAD-C3D	-3.24	106.51	112.49
3	V	601	HEC	CBD-CAD-C3D	-3.23	106.52	112.49
3	X	601	HEC	CBD-CAD-C3D	-3.23	106.53	112.49
3	W	605	HEC	CBD-CAD-C3D	3.22	118.42	112.49
3	K	606	HEC	CBA-CAA-C2A	-3.20	106.58	112.48
3	N	605	HEC	CBD-CAD-C3D	3.20	118.39	112.49
3	J	602	HEC	CAD-CBD-CGD	-3.20	107.31	112.67
3	D	605	HEC	CAD-CBD-CGD	-3.20	107.31	112.67
3	X	603	HEC	C4B-C3B-C2B	3.18	109.79	106.35
3	O	602	HEC	CAD-CBD-CGD	-3.18	107.34	112.67
3	T	603	HEC	C3C-C4C-NC	-3.16	104.97	110.94
3	C	605	HEC	CBD-CAD-C3D	3.16	118.31	112.49
3	T	603	HEC	C4B-C3B-C2B	3.13	109.73	106.35
3	M	602	HEC	CAD-CBD-CGD	-3.13	107.42	112.67
3	L	602	HEC	CAD-CBD-CGD	-3.12	107.43	112.67
3	L	606	HEC	CBA-CAA-C2A	-3.12	106.73	112.48
3	M	601	HEC	CBD-CAD-C3D	-3.12	106.73	112.49
3	U	605	HEC	CBD-CAD-C3D	3.12	118.23	112.49
3	O	605	HEC	CBD-CAD-C3D	3.12	118.23	112.49
3	V	603	HEC	C4B-C3B-C2B	3.11	109.71	106.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	603	HEC	C4B-C3B-C2B	3.10	109.70	106.35
3	H	605	HEC	CBD-CAD-C3D	3.10	118.20	112.49
3	S	603	HEC	C3C-C4C-NC	-3.09	105.11	110.94
3	J	603	HEC	C3C-C4C-NC	-3.07	105.15	110.94
3	B	603	HEC	C3C-C4C-NC	-3.06	105.16	110.94
3	H	603	HEC	C4B-C3B-C2B	3.06	109.66	106.35
3	B	606	HEC	CBA-CAA-C2A	-3.06	106.84	112.48
3	C	603	HEC	C3C-C4C-NC	-3.05	105.19	110.94
3	G	603	HEC	C4B-C3B-C2B	3.05	109.64	106.35
3	P	605	HEC	CBD-CAD-C3D	3.05	118.11	112.49
3	E	602	HEC	CAD-CBD-CGD	-3.04	107.56	112.67
3	P	602	HEC	CAD-CBD-CGD	-3.04	107.57	112.67
3	F	602	HEC	CAD-CBD-CGD	-3.03	107.58	112.67
3	A	603	HEC	CMB-C2B-C1B	-3.03	123.81	128.46
3	A	600	HEC	CAD-CBD-CGD	-3.03	107.59	112.67
3	R	606	HEC	CBA-CAA-C2A	-3.02	106.91	112.48
3	N	603	HEC	CMB-C2B-C1B	-3.02	123.82	128.46
3	H	606	HEC	CBA-CAA-C2A	-3.02	106.92	112.48
3	E	605	HEC	CBD-CAD-C3D	3.02	118.05	112.49
3	X	602	HEC	CAD-CBD-CGD	-3.02	107.61	112.67
3	P	606	HEC	CBA-CAA-C2A	-3.01	106.92	112.48
3	Q	603	HEC	C3C-C4C-NC	-3.01	105.26	110.94
3	R	603	HEC	C3C-C4C-NC	-3.01	105.26	110.94
3	K	602	HEC	CAD-CBD-CGD	-3.00	107.63	112.67
3	M	605	HEC	CBD-CAD-C3D	3.00	118.02	112.49
3	C	602	HEC	CAD-CBD-CGD	-3.00	107.64	112.67
3	X	606	HEC	CBA-CAA-C2A	-2.99	106.96	112.48
3	I	602	HEC	CAA-CBA-CGA	-2.99	107.65	112.67
3	S	603	HEC	C4B-C3B-C2B	2.99	109.58	106.35
3	V	603	HEC	C3C-C4C-NC	-2.99	105.30	110.94
3	P	603	HEC	CMB-C2B-C1B	-2.99	123.87	128.46
3	I	601	HEC	CBD-CAD-C3D	-2.98	107.00	112.49
3	X	605	HEC	CBD-CAD-C3D	2.98	117.97	112.49
3	V	605	HEC	CBD-CAD-C3D	2.98	117.97	112.49
3	I	603	HEC	CMB-C2B-C1B	-2.97	123.89	128.46
3	O	603	HEC	C3C-C4C-NC	-2.97	105.33	110.94
3	G	606	HEC	CBA-CAA-C2A	-2.96	107.02	112.48
3	Q	602	HEC	CAD-CBD-CGD	-2.96	107.71	112.67
3	P	603	HEC	C3C-C4C-NC	-2.96	105.36	110.94
3	Q	605	HEC	CBD-CAD-C3D	2.96	117.94	112.49
3	G	602	HEC	CAD-CBD-CGD	-2.95	107.71	112.67
3	N	603	HEC	C3C-C4C-NC	-2.95	105.37	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	602	HEC	CAD-CBD-CGD	-2.95	107.72	112.67
3	O	606	HEC	CBA-CAA-C2A	-2.95	107.04	112.48
3	B	603	HEC	CMB-C2B-C1B	-2.95	123.94	128.46
3	U	603	HEC	C3C-C4C-NC	-2.94	105.39	110.94
3	E	603	HEC	C4B-C3B-C2B	2.94	109.53	106.35
3	V	602	HEC	CAD-CBD-CGD	-2.93	107.76	112.67
3	F	603	HEC	CBA-CAA-C2A	-2.93	107.09	112.48
3	R	602	HEC	CAD-CBD-CGD	-2.93	107.76	112.67
3	J	606	HEC	CBA-CAA-C2A	-2.92	107.09	112.48
3	H	603	HEC	C3C-C4C-NC	-2.92	105.42	110.94
3	L	603	HEC	C3C-C4C-NC	-2.92	105.42	110.94
3	E	603	HEC	C3C-C4C-NC	-2.92	105.44	110.94
3	I	606	HEC	CBA-CAA-C2A	-2.91	107.11	112.48
3	T	606	HEC	CBA-CAA-C2A	-2.91	107.11	112.48
3	Q	603	HEC	C4B-C3B-C2B	2.91	109.49	106.35
3	K	603	HEC	C3C-C4C-NC	-2.90	105.46	110.94
3	T	603	HEC	CMB-C2B-C1B	-2.90	124.01	128.46
3	I	605	HEC	CBD-CAD-C3D	2.90	117.83	112.49
3	W	603	HEC	CMB-C2B-C1B	-2.89	124.02	128.46
3	F	603	HEC	C3C-C4C-NC	-2.88	105.50	110.94
3	S	602	HEC	CAD-CBD-CGD	-2.88	107.83	112.67
3	L	605	HEC	CBD-CAD-C3D	2.88	117.80	112.49
3	A	603	HEC	C3C-C4C-NC	-2.88	105.51	110.94
3	B	603	HEC	C4B-C3B-C2B	2.88	109.46	106.35
3	N	606	HEC	CBA-CAA-C2A	-2.87	107.18	112.48
3	O	603	HEC	CMB-C2B-C1B	-2.87	124.05	128.46
3	V	606	HEC	CBA-CAA-C2A	-2.87	107.19	112.48
3	F	603	HEC	C4B-C3B-C2B	2.87	109.45	106.35
3	U	603	HEC	CMB-C2B-C1B	-2.87	124.06	128.46
3	J	603	HEC	CMB-C2B-C1B	-2.87	124.06	128.46
3	C	603	HEC	C4B-C3B-C2B	2.86	109.44	106.35
3	G	603	HEC	C3C-C4C-NC	-2.86	105.54	110.94
3	F	603	HEC	CMB-C2B-C1B	-2.86	124.07	128.46
3	S	606	HEC	CBA-CAA-C2A	-2.86	107.21	112.48
3	X	603	HEC	C3C-C4C-NC	-2.86	105.55	110.94
3	E	606	HEC	CBA-CAA-C2A	-2.85	107.22	112.48
3	R	605	HEC	CBD-CAD-C3D	2.85	117.74	112.49
3	C	606	HEC	CBA-CAA-C2A	-2.85	107.23	112.48
3	M	606	HEC	CBA-CAA-C2A	-2.84	107.24	112.48
3	Q	606	HEC	CBA-CAA-C2A	-2.83	107.27	112.48
3	M	603	HEC	C3C-C4C-NC	-2.82	105.61	110.94
3	N	602	HEC	CBA-CAA-C2A	-2.82	107.28	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	603	HEC	CMB-C2B-C1B	-2.82	124.13	128.46
3	D	603	HEC	CMB-C2B-C1B	-2.82	124.13	128.46
3	S	603	HEC	CMB-C2B-C1B	-2.81	124.14	128.46
3	B	605	HEC	CBD-CAD-C3D	2.81	117.67	112.49
3	K	603	HEC	C4B-C3B-C2B	2.81	109.39	106.35
3	I	603	HEC	C3C-C4C-NC	-2.80	105.65	110.94
3	H	602	HEC	CAD-CBD-CGD	-2.80	107.97	112.67
3	L	603	HEC	CMB-C2B-C1B	-2.80	124.16	128.46
3	K	603	HEC	CMB-C2B-C1B	-2.77	124.20	128.46
3	Q	603	HEC	CMB-C2B-C1B	-2.77	124.20	128.46
3	W	606	HEC	CBA-CAA-C2A	-2.77	107.38	112.48
3	I	605	HEC	CAD-CBD-CGD	-2.77	108.03	112.67
3	U	606	HEC	CBA-CAA-C2A	-2.76	107.39	112.48
3	H	605	HEC	CMD-C2D-C1D	-2.76	124.22	128.46
3	E	603	HEC	CMB-C2B-C1B	-2.76	124.22	128.46
3	F	606	HEC	CBA-CAA-C2A	-2.76	107.40	112.48
3	D	606	HEC	CBA-CAA-C2A	-2.75	107.40	112.48
3	I	603	HEC	CAA-CBA-CGA	2.75	117.28	112.67
3	R	603	HEC	C4B-C3B-C2B	2.74	109.31	106.35
3	C	603	HEC	CMB-C2B-C1B	-2.74	124.25	128.46
3	W	603	HEC	C4B-C3B-C2B	2.73	109.30	106.35
3	D	603	HEC	CAA-C2A-C3A	-2.72	119.43	127.25
3	W	603	HEC	C3C-C4C-NC	-2.72	105.81	110.94
3	X	603	HEC	CMB-C2B-C1B	-2.71	124.30	128.46
3	A	603	HEC	C4B-C3B-C2B	2.71	109.27	106.35
3	J	603	HEC	C4B-C3B-C2B	2.67	109.23	106.35
3	D	603	HEC	C4B-C3B-C2B	2.66	109.23	106.35
3	P	603	HEC	C4B-C3B-C2B	2.65	109.21	106.35
3	D	601	HEC	CBD-CAD-C3D	-2.65	107.60	112.49
3	V	603	HEC	CMB-C2B-C1B	-2.64	124.40	128.46
3	G	605	HEC	CAD-CBD-CGD	-2.63	108.26	112.67
3	L	603	HEC	C4B-C3B-C2B	2.62	109.18	106.35
3	U	603	HEC	C4B-C3B-C2B	2.62	109.18	106.35
3	M	603	HEC	C4B-C3B-C2B	2.62	109.18	106.35
3	G	603	HEC	CMB-C2B-C1B	-2.61	124.44	128.46
3	R	603	HEC	CMB-C2B-C1B	-2.61	124.45	128.46
3	D	603	HEC	CBA-CAA-C2A	-2.61	107.68	112.48
3	O	603	HEC	C4B-C3B-C2B	2.58	109.13	106.35
3	W	602	HEC	CAD-CBD-CGD	-2.57	108.36	112.67
3	M	603	HEC	CMB-C2B-C1B	-2.57	124.51	128.46
3	O	603	HEC	CMC-C2C-C3C	2.55	128.82	125.82
3	X	605	HEC	CAD-CBD-CGD	-2.55	108.39	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	600	HEC	CAD-CBD-CGD	-2.54	108.41	112.67
3	H	600	HEC	CAD-CBD-CGD	-2.54	108.42	112.67
3	B	600	HEC	CAA-CBA-CGA	-2.53	108.43	112.67
3	V	605	HEC	CMD-C2D-C1D	-2.52	124.59	128.46
3	P	602	HEC	CBA-CAA-C2A	-2.51	107.86	112.48
3	B	602	HEC	CBA-CAA-C2A	-2.51	107.86	112.48
3	T	605	HEC	CAD-CBD-CGD	-2.50	108.47	112.67
3	P	605	HEC	CMD-C2D-C1D	-2.50	124.63	128.46
3	O	605	HEC	CMD-C2D-C1D	-2.49	124.63	128.46
3	L	605	HEC	CMD-C2D-C1D	-2.48	124.66	128.46
3	J	605	HEC	CAD-CBD-CGD	-2.47	108.52	112.67
3	H	605	HEC	CAD-CBD-CGD	-2.47	108.53	112.67
3	I	604	HEC	CBA-CAA-C2A	-2.47	107.93	112.48
3	O	603	HEC	CBA-CAA-C2A	-2.47	107.94	112.48
3	T	600	HEC	CAD-CBD-CGD	-2.46	108.54	112.67
3	I	600	HEC	CAD-CBD-CGD	-2.46	108.55	112.67
3	U	603	HEC	CBA-CAA-C2A	-2.46	107.95	112.48
3	A	605	HEC	CMD-C2D-C1D	-2.46	124.69	128.46
3	S	602	HEC	CBA-CAA-C2A	-2.45	107.97	112.48
3	W	602	HEC	CBA-CAA-C2A	-2.45	107.97	112.48
3	E	605	HEC	CAD-CBD-CGD	-2.44	108.58	112.67
3	R	604	HEC	CAD-CBD-CGD	2.44	116.76	112.67
3	X	602	HEC	CBA-CAA-C2A	-2.44	107.99	112.48
3	V	605	HEC	CAD-CBD-CGD	-2.43	108.59	112.67
3	H	602	HEC	CBA-CAA-C2A	-2.43	108.00	112.48
3	X	605	HEC	CMD-C2D-C1D	-2.42	124.74	128.46
3	T	602	HEC	CBA-CAA-C2A	-2.42	108.02	112.48
3	K	602	HEC	CBA-CAA-C2A	-2.42	108.02	112.48
3	E	600	HEC	CAD-CBD-CGD	-2.42	108.61	112.67
3	N	600	HEC	CAD-CBD-CGD	-2.41	108.62	112.67
3	I	606	HEC	CAD-CBD-CGD	-2.41	108.62	112.67
3	Q	605	HEC	CAD-CBD-CGD	-2.41	108.63	112.67
3	J	602	HEC	CBA-CAA-C2A	-2.41	108.04	112.48
3	M	605	HEC	CAD-CBD-CGD	-2.41	108.63	112.67
3	K	605	HEC	CMD-C2D-C1D	-2.40	124.77	128.46
3	K	606	HEC	CAD-CBD-CGD	-2.40	108.65	112.67
3	U	605	HEC	CAD-CBD-CGD	-2.39	108.65	112.67
3	Q	603	HEC	CMC-C2C-C3C	2.39	128.63	125.82
3	O	602	HEC	CBA-CAA-C2A	-2.39	108.08	112.48
3	G	600	HEC	CAA-CBA-CGA	-2.39	108.67	112.67
3	X	600	HEC	CAA-CBA-CGA	-2.38	108.67	112.67
3	D	605	HEC	CMD-C2D-C1D	-2.37	124.82	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	603	HEC	CBA-CAA-C2A	-2.37	108.11	112.48
3	W	600	HEC	CAD-CBD-CGD	-2.37	108.70	112.67
3	H	604	HEC	CAD-CBD-CGD	2.36	116.63	112.67
3	L	602	HEC	CBA-CAA-C2A	-2.36	108.13	112.48
3	D	604	HEC	CAD-CBD-CGD	2.36	116.63	112.67
3	C	604	HEC	CAD-CBD-CGD	2.36	116.63	112.67
3	I	605	HEC	CMD-C2D-C1D	-2.36	124.84	128.46
3	I	604	HEC	CAD-CBD-CGD	2.35	116.62	112.67
3	A	602	HEC	CBA-CAA-C2A	-2.35	108.15	112.48
3	Q	605	HEC	CMD-C2D-C1D	-2.35	124.85	128.46
3	A	600	HEC	CAA-CBA-CGA	-2.35	108.73	112.67
3	C	605	HEC	CMD-C2D-C1D	-2.34	124.86	128.46
3	M	600	HEC	CAD-CBD-CGD	-2.34	108.75	112.67
3	K	605	HEC	CAD-CBD-CGD	-2.33	108.76	112.67
3	I	605	HEC	CMD-C2D-C3D	2.33	129.34	124.94
3	K	604	HEC	CAD-CBD-CGD	2.33	116.58	112.67
3	L	603	HEC	CBA-CAA-C2A	-2.33	108.19	112.48
3	R	600	HEC	CAA-CBA-CGA	-2.32	108.77	112.67
3	S	600	HEC	CAD-CBD-CGD	-2.32	108.78	112.67
3	G	603	HEC	CMA-C3A-C2A	2.32	129.31	124.94
3	N	600	HEC	CAA-CBA-CGA	-2.31	108.80	112.67
3	G	606	HEC	CAD-CBD-CGD	-2.31	108.80	112.67
3	L	603	HEC	CMA-C3A-C2A	2.30	129.28	124.94
3	O	600	HEC	CAD-CBD-CGD	-2.30	108.81	112.67
3	U	605	HEC	CMD-C2D-C1D	-2.30	124.93	128.46
3	N	605	HEC	CAD-CBD-CGD	-2.29	108.83	112.67
3	T	605	HEC	CMD-C2D-C1D	-2.28	124.96	128.46
3	I	607	HEC	CAA-CBA-CGA	-2.28	108.85	112.67
3	D	602	HEC	CMC-C2C-C1C	-2.27	124.97	128.46
3	C	602	HEC	CBA-CAA-C2A	-2.27	108.29	112.48
3	V	602	HEC	CBA-CAA-C2A	-2.27	108.29	112.48
3	K	600	HEC	CAD-CBD-CGD	-2.27	108.86	112.67
3	B	600	HEC	CAD-CBD-CGD	-2.27	108.87	112.67
3	G	600	HEC	CAD-CBD-CGD	-2.26	108.87	112.67
3	U	602	HEC	CBA-CAA-C2A	-2.26	108.31	112.48
3	E	602	HEC	CBA-CAA-C2A	-2.26	108.31	112.48
3	F	605	HEC	CMD-C2D-C1D	-2.26	125.00	128.46
3	Q	602	HEC	CBA-CAA-C2A	-2.26	108.32	112.48
3	W	605	HEC	CMD-C2D-C1D	-2.25	125.00	128.46
3	D	605	HEC	CMD-C2D-C3D	2.25	129.19	124.94
3	D	603	HEC	CMA-C3A-C2A	2.25	129.18	124.94
3	H	603	HEC	CMA-C3A-C2A	2.25	129.18	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	602	HEC	CBA-CAA-C2A	-2.25	108.34	112.48
3	L	605	HEC	CAD-CBD-CGD	-2.24	108.91	112.67
3	L	603	HEC	CMC-C2C-C3C	2.24	128.45	125.82
3	I	600	HEC	CMB-C2B-C3B	2.24	128.45	125.82
3	W	604	HEC	CAD-CBD-CGD	2.24	116.42	112.67
3	W	605	HEC	CAD-CBD-CGD	-2.23	108.92	112.67
3	C	603	HEC	CMC-C2C-C3C	2.23	128.44	125.82
3	D	600	HEC	CAD-CBD-CGD	-2.23	108.94	112.67
3	P	603	HEC	CMA-C3A-C2A	2.22	129.13	124.94
3	P	605	HEC	CAD-CBD-CGD	-2.22	108.95	112.67
3	R	600	HEC	CAD-CBD-CGD	-2.22	108.95	112.67
3	O	605	HEC	CMD-C2D-C3D	2.22	129.12	124.94
3	F	605	HEC	CAD-CBD-CGD	-2.21	108.96	112.67
3	P	605	HEC	CMD-C2D-C3D	2.21	129.11	124.94
3	M	600	HEC	CAA-CBA-CGA	-2.21	108.96	112.67
3	V	600	HEC	CAD-CBD-CGD	-2.21	108.96	112.67
3	J	604	HEC	CAD-CBD-CGD	2.21	116.38	112.67
3	A	603	HEC	CBA-CAA-C2A	-2.21	108.41	112.48
3	V	603	HEC	CBA-CAA-C2A	-2.21	108.41	112.48
3	S	605	HEC	CMD-C2D-C1D	-2.20	125.08	128.46
3	G	602	HEC	CBA-CAA-C2A	-2.20	108.42	112.48
3	E	600	HEC	CAA-CBA-CGA	-2.20	108.98	112.67
3	B	605	HEC	CAD-CBD-CGD	-2.20	108.99	112.67
3	I	602	HEC	CMB-C2B-C1B	-2.19	125.09	128.46
3	D	602	HEC	CAD-CBD-CGD	-2.19	108.99	112.67
3	T	600	HEC	CAA-CBA-CGA	-2.19	108.99	112.67
3	I	600	HEC	CMB-C2B-C1B	-2.19	125.10	128.46
3	F	602	HEC	CBA-CAA-C2A	-2.19	108.45	112.48
3	H	605	HEC	CMD-C2D-C3D	2.19	129.06	124.94
3	L	606	HEC	CAD-CBD-CGD	-2.18	109.01	112.67
3	N	605	HEC	CMD-C2D-C1D	-2.18	125.11	128.46
3	U	600	HEC	CAA-CBA-CGA	-2.18	109.02	112.67
3	U	603	HEC	CMC-C2C-C3C	2.18	128.38	125.82
3	O	600	HEC	CAA-CBA-CGA	-2.17	109.02	112.67
3	B	603	HEC	CMA-C3A-C2A	2.17	129.04	124.94
3	P	606	HEC	C3B-C4B-NB	-2.17	106.84	110.94
3	L	604	HEC	CAD-CBD-CGD	2.17	116.31	112.67
3	C	606	HEC	C3B-C4B-NB	-2.17	106.85	110.94
3	J	600	HEC	CAD-CBD-CGD	-2.17	109.03	112.67
3	Q	603	HEC	CMA-C3A-C2A	2.17	129.03	124.94
3	X	605	HEC	CMD-C2D-C3D	2.17	129.03	124.94
3	O	607	HEC	CAA-CBA-CGA	-2.17	109.04	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	603	HEC	CMC-C2C-C3C	2.16	128.36	125.82
3	R	605	HEC	CMD-C2D-C1D	-2.16	125.15	128.46
3	V	600	HEC	CAA-CBA-CGA	-2.16	109.05	112.67
3	V	603	HEC	CMC-C2C-C3C	2.15	128.35	125.82
3	C	600	HEC	CAA-CBA-CGA	-2.14	109.07	112.67
3	S	600	HEC	CAA-CBA-CGA	-2.14	109.08	112.67
3	C	605	HEC	CMD-C2D-C3D	2.14	128.98	124.94
3	K	605	HEC	CMD-C2D-C3D	2.14	128.97	124.94
3	J	603	HEC	CMA-C3A-C2A	2.13	128.97	124.94
3	T	605	HEC	CMC-C2C-C1C	-2.13	125.19	128.46
3	L	605	HEC	CMB-C2B-C1B	-2.13	125.19	128.46
3	V	606	HEC	CAD-CBD-CGD	-2.13	109.10	112.67
3	L	600	HEC	CAD-CBD-CGD	-2.12	109.11	112.67
3	W	600	HEC	CAA-CBA-CGA	-2.12	109.11	112.67
3	G	604	HEC	CAD-CBD-CGD	2.12	116.23	112.67
3	U	605	HEC	CMD-C2D-C3D	2.12	128.94	124.94
3	P	603	HEC	CMC-C2C-C3C	2.12	128.31	125.82
3	P	600	HEC	CAA-CBA-CGA	-2.12	109.12	112.67
3	C	603	HEC	CBA-CAA-C2A	-2.12	108.58	112.48
3	V	605	HEC	CMD-C2D-C3D	2.11	128.93	124.94
3	V	603	HEC	CMA-C3A-C2A	2.10	128.91	124.94
3	J	603	HEC	CMC-C2C-C3C	2.10	128.29	125.82
3	D	602	HEC	CMB-C2B-C1B	-2.10	125.24	128.46
3	E	605	HEC	CMC-C2C-C1C	-2.09	125.24	128.46
3	Q	600	HEC	CAA-CBA-CGA	-2.09	109.16	112.67
3	L	606	HEC	C3B-C4B-NB	-2.09	107.00	110.94
3	S	605	HEC	CAD-CBD-CGD	-2.09	109.17	112.67
3	J	605	HEC	CMD-C2D-C1D	-2.09	125.25	128.46
3	G	606	HEC	C3B-C4B-NB	-2.09	107.01	110.94
3	C	600	HEC	CAD-CBD-CGD	-2.08	109.17	112.67
3	U	606	HEC	C3B-C4B-NB	-2.08	107.01	110.94
3	L	605	HEC	CMD-C2D-C3D	2.08	128.86	124.94
3	U	600	HEC	CAD-CBD-CGD	-2.07	109.19	112.67
3	M	605	HEC	CMD-C2D-C1D	-2.07	125.28	128.46
3	M	602	HEC	CBA-CAA-C2A	-2.07	108.66	112.48
3	A	605	HEC	CMD-C2D-C3D	2.07	128.84	124.94
3	D	604	HEC	CBA-CAA-C2A	-2.07	108.67	112.48
3	H	603	HEC	CMC-C2C-C3C	2.06	128.25	125.82
3	J	600	HEC	CAA-CBA-CGA	-2.06	109.21	112.67
3	M	606	HEC	C3B-C4B-NB	-2.06	107.05	110.94
3	T	605	HEC	CMD-C2D-C3D	2.06	128.83	124.94
3	G	605	HEC	CMD-C2D-C1D	-2.06	125.30	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	607	HEC	CMC-C2C-C1C	-2.06	125.30	128.46
3	I	606	HEC	C3B-C4B-NB	-2.06	107.06	110.94
3	I	600	HEC	CMC-C2C-C1C	-2.06	125.30	128.46
3	B	606	HEC	C3B-C4B-NB	-2.05	107.06	110.94
3	W	605	HEC	CMD-C2D-C3D	2.05	128.81	124.94
3	N	603	HEC	CMA-C3A-C2A	2.05	128.80	124.94
3	F	603	HEC	CMC-C2C-C3C	2.05	128.23	125.82
3	R	605	HEC	CAD-CBD-CGD	-2.05	109.24	112.67
3	M	603	HEC	CMA-C3A-C2A	2.05	128.80	124.94
3	P	604	HEC	CAD-CBD-CGD	2.04	116.10	112.67
3	N	605	HEC	CMD-C2D-C3D	2.04	128.80	124.94
3	I	603	HEC	CMD-C2D-C1D	-2.04	125.32	128.46
3	E	604	HEC	CAD-CBD-CGD	2.04	116.10	112.67
3	Q	600	HEC	CAD-CBD-CGD	-2.04	109.25	112.67
3	D	600	HEC	CBD-CAD-C3D	2.04	116.25	112.49
3	R	603	HEC	CMA-C3A-C2A	2.04	128.79	124.94
3	Q	605	HEC	CMC-C2C-C1C	-2.04	125.33	128.46
3	R	607	HEC	CAA-CBA-CGA	-2.04	109.25	112.67
3	D	603	HEC	CMC-C2C-C3C	2.04	128.22	125.82
3	K	603	HEC	CMC-C2C-C3C	2.04	128.22	125.82
3	G	605	HEC	CMD-C2D-C3D	2.04	128.78	124.94
3	R	603	HEC	CMC-C2C-C3C	2.04	128.22	125.82
3	X	607	HEC	CBD-CAD-C3D	-2.03	108.74	112.49
3	T	603	HEC	CBA-CAA-C2A	-2.03	108.74	112.48
3	M	605	HEC	CMD-C2D-C3D	2.03	128.76	124.94
3	K	603	HEC	CMA-C3A-C2A	2.02	128.75	124.94
3	F	600	HEC	CAA-CBA-CGA	-2.02	109.29	112.67
3	B	603	HEC	CMC-C2C-C3C	2.01	128.19	125.82
3	E	606	HEC	C3B-C4B-NB	-2.01	107.14	110.94
3	S	605	HEC	CMD-C2D-C3D	2.01	128.73	124.94
3	A	606	HEC	CAD-CBD-CGD	-2.01	109.30	112.67
3	G	601	HEC	CAA-CBA-CGA	-2.01	109.30	112.67
3	W	602	HEC	C3B-C4B-NB	-2.00	107.16	110.94
3	J	605	HEC	CMD-C2D-C3D	2.00	128.72	124.94
3	T	603	HEC	CMC-C2C-C3C	2.00	128.18	125.82
3	V	606	HEC	C3B-C4B-NB	-2.00	107.17	110.94

There are no chirality outliers.

All (183) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	W	605	HEC	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
3	W	605	HEC	C4D-C3D-CAD-CBD
3	I	601	HEC	C1A-C2A-CAA-CBA
3	I	601	HEC	C3A-C2A-CAA-CBA
3	T	605	HEC	C2D-C3D-CAD-CBD
3	T	605	HEC	C4D-C3D-CAD-CBD
3	F	605	HEC	C2D-C3D-CAD-CBD
3	F	605	HEC	C4D-C3D-CAD-CBD
3	D	601	HEC	C1A-C2A-CAA-CBA
3	D	601	HEC	C3A-C2A-CAA-CBA
3	D	605	HEC	C2D-C3D-CAD-CBD
3	D	605	HEC	C4D-C3D-CAD-CBD
5	J	612	GOL	O1-C1-C2-C3
5	L	613	GOL	C1-C2-C3-O3
3	Q	605	HEC	C2D-C3D-CAD-CBD
3	Q	605	HEC	C4D-C3D-CAD-CBD
5	D	610	GOL	O1-C1-C2-C3
5	I	614	GOL	C1-C2-C3-O3
5	K	613	GOL	O1-C1-C2-C3
3	A	605	HEC	C2D-C3D-CAD-CBD
3	A	605	HEC	C4D-C3D-CAD-CBD
5	A	613	GOL	C1-C2-C3-O3
3	R	605	HEC	C2D-C3D-CAD-CBD
3	R	605	HEC	C4D-C3D-CAD-CBD
3	O	605	HEC	C2D-C3D-CAD-CBD
3	O	605	HEC	C4D-C3D-CAD-CBD
3	H	605	HEC	C2D-C3D-CAD-CBD
3	H	605	HEC	C4D-C3D-CAD-CBD
3	L	605	HEC	C2D-C3D-CAD-CBD
3	L	605	HEC	C4D-C3D-CAD-CBD
5	J	613	GOL	C1-C2-C3-O3
5	J	613	GOL	O2-C2-C3-O3
3	X	605	HEC	C2D-C3D-CAD-CBD
3	X	605	HEC	C4D-C3D-CAD-CBD
5	I	615	GOL	C1-C2-C3-O3
3	B	605	HEC	C2D-C3D-CAD-CBD
3	B	605	HEC	C4D-C3D-CAD-CBD
5	K	615	GOL	O1-C1-C2-O2
5	K	615	GOL	O1-C1-C2-C3
3	I	605	HEC	C2D-C3D-CAD-CBD
3	I	605	HEC	C4D-C3D-CAD-CBD
3	G	605	HEC	C2D-C3D-CAD-CBD
3	G	605	HEC	C4D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
5	H	614	GOL	O1-C1-C2-C3
3	I	607	HEC	C2A-CAA-CBA-CGA
5	A	614	GOL	O1-C1-C2-C3
5	A	614	GOL	C1-C2-C3-O3
5	A	614	GOL	O2-C2-C3-O3
3	K	605	HEC	C2D-C3D-CAD-CBD
3	K	605	HEC	C4D-C3D-CAD-CBD
3	E	605	HEC	C2D-C3D-CAD-CBD
3	E	605	HEC	C4D-C3D-CAD-CBD
5	I	613	GOL	O1-C1-C2-C3
5	I	613	GOL	C1-C2-C3-O3
3	I	603	HEC	C1A-C2A-CAA-CBA
3	I	603	HEC	C4D-C3D-CAD-CBD
5	H	615	GOL	C1-C2-C3-O3
3	P	605	HEC	C2D-C3D-CAD-CBD
3	P	605	HEC	C4D-C3D-CAD-CBD
3	S	605	HEC	C2D-C3D-CAD-CBD
3	S	605	HEC	C4D-C3D-CAD-CBD
3	M	605	HEC	C2D-C3D-CAD-CBD
3	M	605	HEC	C4D-C3D-CAD-CBD
3	N	605	HEC	C2D-C3D-CAD-CBD
3	N	605	HEC	C4D-C3D-CAD-CBD
3	J	605	HEC	C2D-C3D-CAD-CBD
3	J	605	HEC	C4D-C3D-CAD-CBD
3	C	605	HEC	C2D-C3D-CAD-CBD
3	C	605	HEC	C4D-C3D-CAD-CBD
3	U	605	HEC	C2D-C3D-CAD-CBD
3	U	605	HEC	C4D-C3D-CAD-CBD
3	D	604	HEC	C2A-CAA-CBA-CGA
5	G	615	GOL	C1-C2-C3-O3
5	G	616	GOL	O1-C1-C2-C3
3	V	605	HEC	C2D-C3D-CAD-CBD
3	V	605	HEC	C4D-C3D-CAD-CBD
5	J	612	GOL	O1-C1-C2-O2
5	L	613	GOL	O2-C2-C3-O3
5	K	614	GOL	O2-C2-C3-O3
5	A	614	GOL	O1-C1-C2-O2
5	G	615	GOL	O2-C2-C3-O3
5	J	612	GOL	C1-C2-C3-O3
5	K	612	GOL	O1-C1-C2-C3
5	K	614	GOL	C1-C2-C3-O3
5	K	615	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	H	614	GOL	C1-C2-C3-O3
5	D	610	GOL	O1-C1-C2-O2
5	I	614	GOL	O2-C2-C3-O3
5	A	613	GOL	O2-C2-C3-O3
5	I	615	GOL	O2-C2-C3-O3
5	H	614	GOL	O1-C1-C2-O2
5	H	614	GOL	O2-C2-C3-O3
5	I	613	GOL	O1-C1-C2-O2
5	I	613	GOL	O2-C2-C3-O3
5	G	616	GOL	O1-C1-C2-O2
5	J	612	GOL	O2-C2-C3-O3
5	H	615	GOL	O2-C2-C3-O3
3	Q	607	HEC	C2A-CAA-CBA-CGA
3	N	607	HEC	C2A-CAA-CBA-CGA
3	D	603	HEC	C2A-CAA-CBA-CGA
5	K	615	GOL	O2-C2-C3-O3
3	O	607	HEC	C2A-CAA-CBA-CGA
3	P	607	HEC	C2A-CAA-CBA-CGA
3	C	607	HEC	C2A-CAA-CBA-CGA
3	Q	601	HEC	C1A-C2A-CAA-CBA
3	Q	601	HEC	C3A-C2A-CAA-CBA
3	E	601	HEC	C1A-C2A-CAA-CBA
3	E	601	HEC	C3A-C2A-CAA-CBA
3	R	601	HEC	C1A-C2A-CAA-CBA
3	R	601	HEC	C3A-C2A-CAA-CBA
3	G	601	HEC	C1A-C2A-CAA-CBA
3	G	601	HEC	C3A-C2A-CAA-CBA
3	S	601	HEC	C1A-C2A-CAA-CBA
3	S	601	HEC	C3A-C2A-CAA-CBA
3	V	601	HEC	C3A-C2A-CAA-CBA
3	K	601	HEC	C3A-C2A-CAA-CBA
3	L	601	HEC	C3A-C2A-CAA-CBA
3	D	607	HEC	C3A-C2A-CAA-CBA
3	A	601	HEC	C1A-C2A-CAA-CBA
3	A	601	HEC	C3A-C2A-CAA-CBA
3	X	601	HEC	C1A-C2A-CAA-CBA
3	X	601	HEC	C3A-C2A-CAA-CBA
3	D	603	HEC	C1A-C2A-CAA-CBA
3	T	601	HEC	C3A-C2A-CAA-CBA
3	N	601	HEC	C3A-C2A-CAA-CBA
3	F	601	HEC	C3A-C2A-CAA-CBA
3	H	601	HEC	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
3	U	601	HEC	C1A-C2A-CAA-CBA
3	U	601	HEC	C3A-C2A-CAA-CBA
3	M	601	HEC	C3A-C2A-CAA-CBA
3	B	601	HEC	C3A-C2A-CAA-CBA
3	J	601	HEC	C1A-C2A-CAA-CBA
3	J	601	HEC	C3A-C2A-CAA-CBA
3	O	601	HEC	C1A-C2A-CAA-CBA
3	O	601	HEC	C3A-C2A-CAA-CBA
3	W	601	HEC	C1A-C2A-CAA-CBA
3	W	601	HEC	C3A-C2A-CAA-CBA
3	P	601	HEC	C3A-C2A-CAA-CBA
5	K	613	GOL	O1-C1-C2-O2
5	K	614	GOL	O1-C1-C2-O2
3	E	602	HEC	C3D-CAD-CBD-CGD
3	V	602	HEC	C3D-CAD-CBD-CGD
3	L	602	HEC	C3D-CAD-CBD-CGD
3	X	602	HEC	C3D-CAD-CBD-CGD
3	X	607	HEC	C2A-CAA-CBA-CGA
3	P	602	HEC	C3D-CAD-CBD-CGD
3	U	602	HEC	C3D-CAD-CBD-CGD
3	T	602	HEC	C3D-CAD-CBD-CGD
3	S	607	HEC	C2A-CAA-CBA-CGA
3	L	607	HEC	C2A-CAA-CBA-CGA
3	W	602	HEC	C3D-CAD-CBD-CGD
3	K	607	HEC	C2A-CAA-CBA-CGA
3	J	602	HEC	C3D-CAD-CBD-CGD
3	T	607	HEC	C2A-CAA-CBA-CGA
3	B	602	HEC	C3D-CAD-CBD-CGD
3	M	607	HEC	C2A-CAA-CBA-CGA
3	M	602	HEC	C3D-CAD-CBD-CGD
3	R	607	HEC	C2A-CAA-CBA-CGA
3	V	607	HEC	C2A-CAA-CBA-CGA
3	K	602	HEC	C3D-CAD-CBD-CGD
3	Q	602	HEC	C3D-CAD-CBD-CGD
3	B	607	HEC	C2A-CAA-CBA-CGA
3	G	607	HEC	C2A-CAA-CBA-CGA
3	A	607	HEC	C2A-CAA-CBA-CGA
3	S	602	HEC	C3D-CAD-CBD-CGD
3	N	602	HEC	C3D-CAD-CBD-CGD
3	W	607	HEC	C2A-CAA-CBA-CGA
3	H	602	HEC	C3D-CAD-CBD-CGD
3	O	602	HEC	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
3	F	607	HEC	C2A-CAA-CBA-CGA
3	C	602	HEC	C3D-CAD-CBD-CGD
3	E	607	HEC	C2A-CAA-CBA-CGA
3	G	602	HEC	C3D-CAD-CBD-CGD
3	U	607	HEC	C2A-CAA-CBA-CGA
3	F	602	HEC	C3D-CAD-CBD-CGD
3	R	602	HEC	C3D-CAD-CBD-CGD
3	A	602	HEC	C3D-CAD-CBD-CGD
3	H	607	HEC	C2A-CAA-CBA-CGA
5	K	614	GOL	O1-C1-C2-C3
3	I	602	HEC	C3D-CAD-CBD-CGD
3	D	607	HEC	C2A-CAA-CBA-CGA
3	J	607	HEC	C2A-CAA-CBA-CGA
5	K	612	GOL	O1-C1-C2-O2

There are no ring outliers.

171 monomers are involved in 453 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	W	605	HEC	7	0
3	N	600	HEC	3	0
3	I	601	HEC	6	0
3	T	605	HEC	7	0
3	X	600	HEC	3	0
3	F	605	HEC	5	0
3	L	606	HEC	3	0
3	D	601	HEC	5	0
3	Q	600	HEC	3	0
3	V	600	HEC	3	0
3	D	605	HEC	7	0
3	Q	601	HEC	5	0
3	C	606	HEC	3	0
3	X	607	HEC	2	0
3	K	602	HEC	1	0
3	X	604	HEC	3	0
3	Q	607	HEC	3	0
3	G	606	HEC	3	0
3	U	606	HEC	3	0
3	P	604	HEC	3	0
3	R	601	HEC	4	0
3	D	602	HEC	1	0
3	I	602	HEC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	604	HEC	3	0
3	Q	605	HEC	6	0
3	U	600	HEC	3	0
5	L	613	GOL	1	0
3	O	606	HEC	3	0
3	R	600	HEC	3	0
5	I	614	GOL	4	0
3	G	601	HEC	4	0
3	V	604	HEC	3	0
3	S	606	HEC	2	0
3	T	600	HEC	3	0
3	H	600	HEC	3	0
3	M	606	HEC	2	0
3	S	601	HEC	5	0
3	X	606	HEC	3	0
3	W	604	HEC	3	0
3	T	606	HEC	2	0
5	K	613	GOL	1	0
3	S	607	HEC	1	0
3	H	606	HEC	4	0
3	L	607	HEC	3	0
3	K	607	HEC	3	0
3	H	604	HEC	3	0
3	V	601	HEC	4	0
3	E	604	HEC	3	0
3	K	601	HEC	7	0
3	L	601	HEC	4	0
3	A	606	HEC	3	0
3	T	607	HEC	2	0
3	A	605	HEC	5	0
3	C	600	HEC	4	0
3	E	600	HEC	3	0
3	D	607	HEC	1	0
3	L	600	HEC	3	0
5	A	613	GOL	1	0
3	N	607	HEC	3	0
3	K	604	HEC	3	0
3	O	605	HEC	6	0
3	N	606	HEC	3	0
3	C	601	HEC	4	0
3	J	606	HEC	2	0
3	U	604	HEC	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	607	HEC	3	0
3	I	600	HEC	5	0
3	X	601	HEC	5	0
3	B	604	HEC	3	0
3	O	604	HEC	2	0
3	R	604	HEC	3	0
3	F	606	HEC	3	0
5	A	612	GOL	1	0
3	K	606	HEC	3	0
3	R	605	HEC	7	0
3	A	600	HEC	3	0
3	R	607	HEC	3	0
3	H	605	HEC	7	0
3	A	601	HEC	4	0
3	V	607	HEC	3	0
5	G	615	GOL	1	0
3	L	605	HEC	5	0
3	D	606	HEC	3	0
5	H	614	GOL	11	0
3	W	600	HEC	3	0
3	O	600	HEC	4	0
4	Q	609	SO4	1	0
3	X	605	HEC	6	0
4	N	610	SO4	1	0
5	I	615	GOL	1	0
4	X	610	SO4	1	0
3	B	607	HEC	2	0
3	D	603	HEC	2	0
3	E	606	HEC	2	0
3	M	604	HEC	2	0
3	B	605	HEC	6	0
3	P	600	HEC	3	0
3	G	607	HEC	3	0
5	K	615	GOL	3	0
3	T	601	HEC	4	0
3	A	607	HEC	3	0
3	S	600	HEC	3	0
4	J	611	SO4	2	0
3	I	605	HEC	8	0
3	N	601	HEC	4	0
3	P	606	HEC	3	0
3	G	605	HEC	5	0

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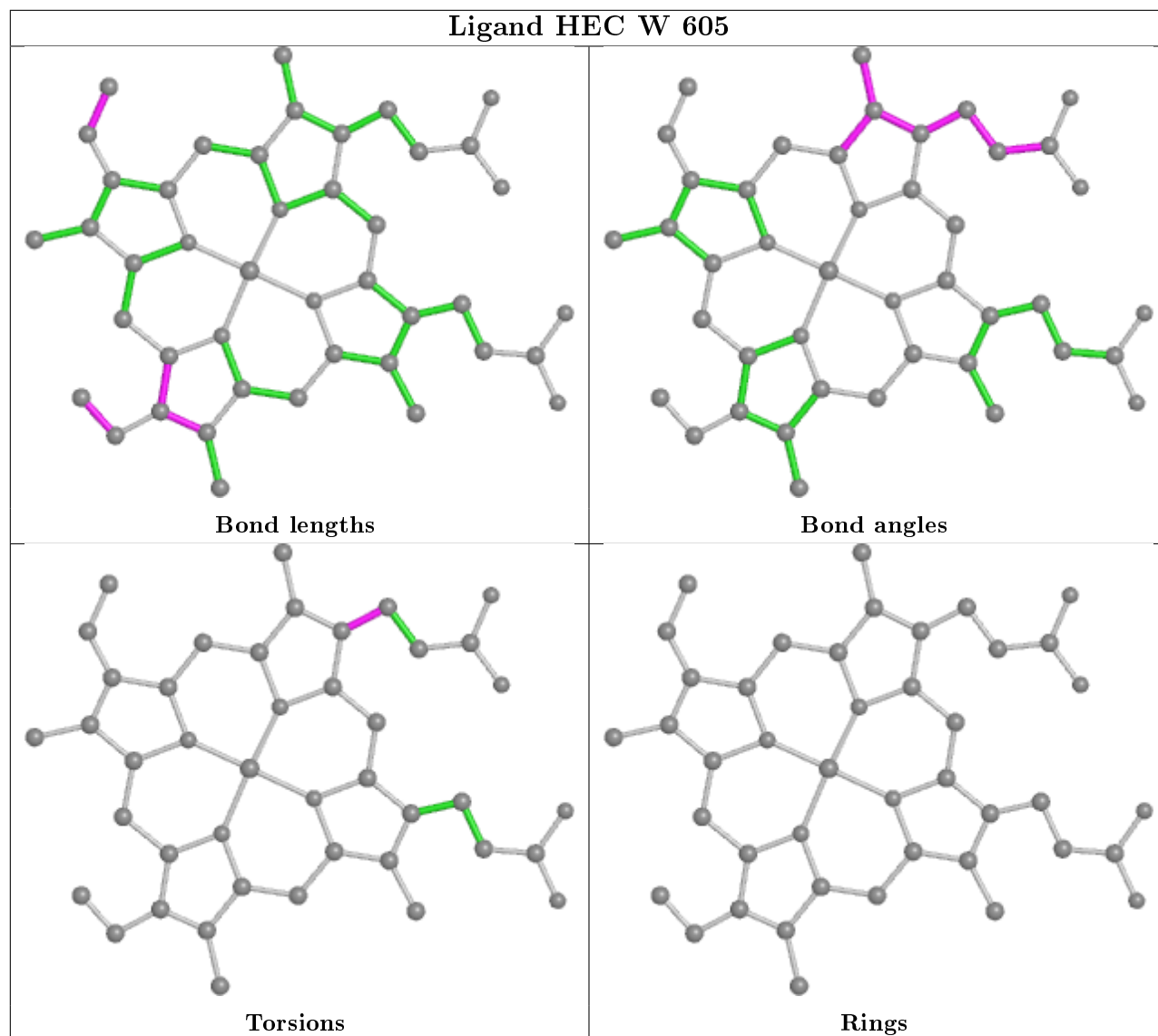
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	610	SO4	1	0
5	K	614	GOL	10	0
3	H	601	HEC	4	0
3	T	604	HEC	3	0
3	I	607	HEC	2	0
3	U	601	HEC	5	0
3	C	604	HEC	3	0
5	J	613	GOL	3	0
3	W	606	HEC	3	0
3	R	606	HEC	3	0
3	S	604	HEC	3	0
3	W	607	HEC	3	0
3	B	601	HEC	4	0
3	J	601	HEC	4	0
4	H	609	SO4	1	0
3	K	605	HEC	6	0
3	F	607	HEC	1	0
3	E	605	HEC	6	0
3	K	600	HEC	3	0
4	B	609	SO4	1	0
3	O	607	HEC	2	0
3	J	607	HEC	3	0
3	I	603	HEC	3	0
3	M	601	HEC	4	0
3	E	607	HEC	1	0
3	P	605	HEC	7	0
3	S	605	HEC	6	0
3	M	605	HEC	5	0
3	N	605	HEC	6	0
3	D	600	HEC	3	0
3	J	605	HEC	5	0
3	O	601	HEC	5	0
3	I	604	HEC	3	0
3	E	601	HEC	5	0
3	P	607	HEC	2	0
3	C	605	HEC	7	0
3	G	604	HEC	2	0
3	B	606	HEC	3	0
3	Q	606	HEC	3	0
3	U	605	HEC	7	0
3	J	600	HEC	3	0
3	C	607	HEC	3	0

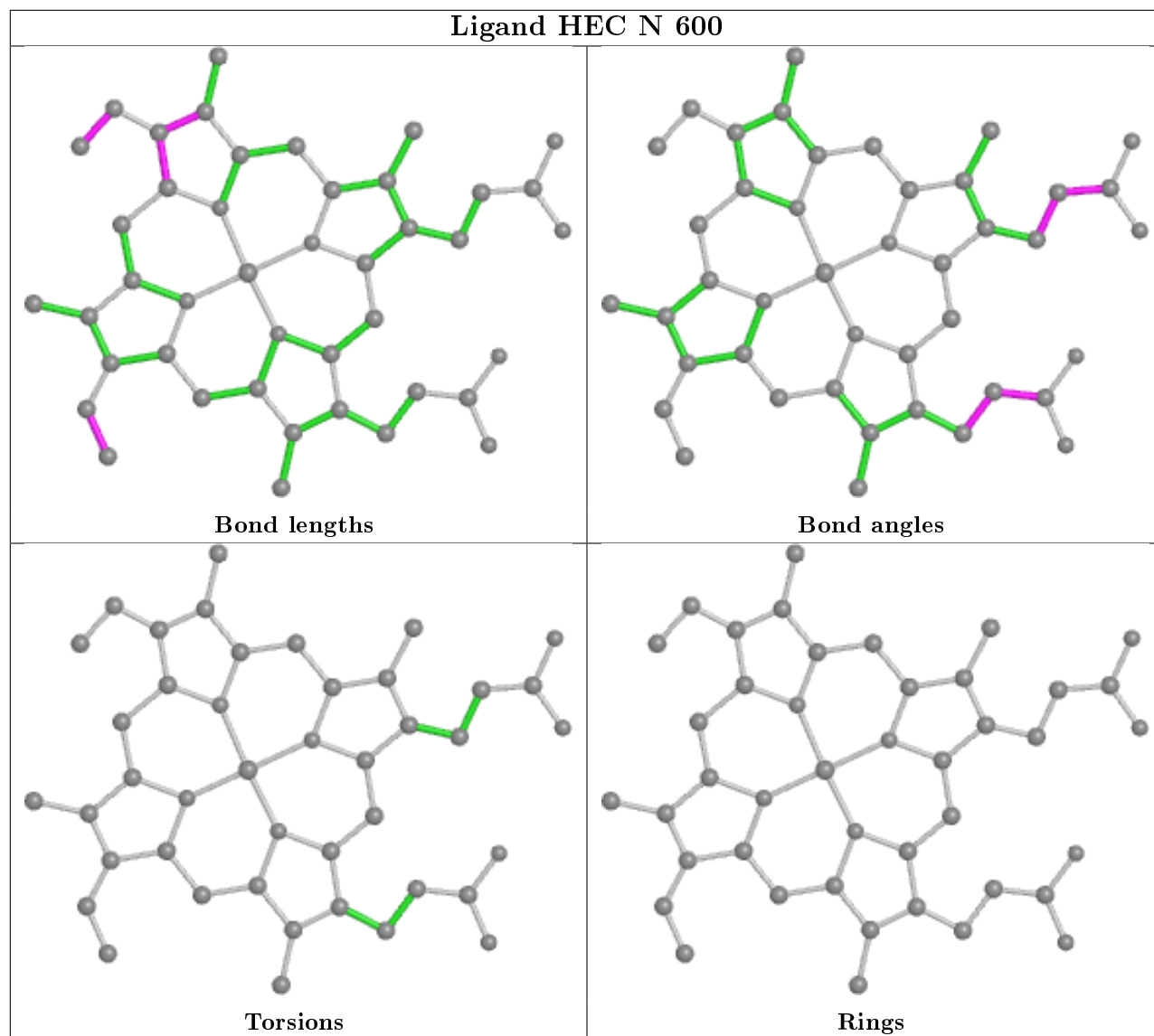
*Continued on next page...*

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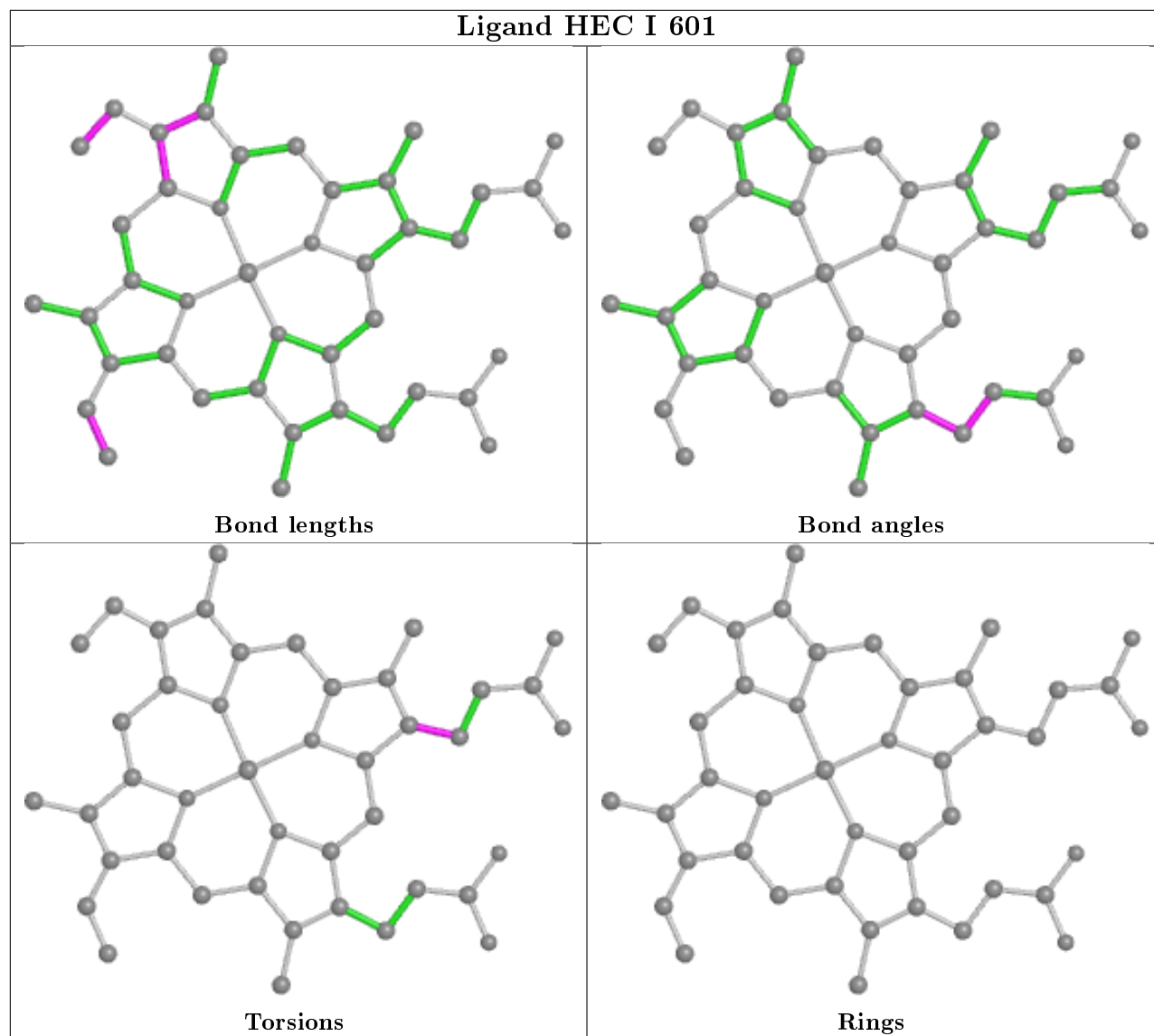
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	606	HEC	4	0
3	W	601	HEC	5	0
3	V	606	HEC	3	0
3	B	600	HEC	3	0
3	U	607	HEC	2	0
3	M	600	HEC	3	0
3	G	600	HEC	3	0
3	J	604	HEC	3	0
3	D	604	HEC	3	0
3	F	604	HEC	3	0
4	G	609	SO4	1	0
3	F	600	HEC	4	0
3	P	601	HEC	4	0
5	H	615	GOL	9	0
3	F	601	HEC	4	0
5	G	616	GOL	1	0
3	Q	604	HEC	3	0
4	G	610	SO4	2	0
3	A	604	HEC	2	0
3	H	607	HEC	1	0
3	L	604	HEC	3	0
3	V	605	HEC	6	0

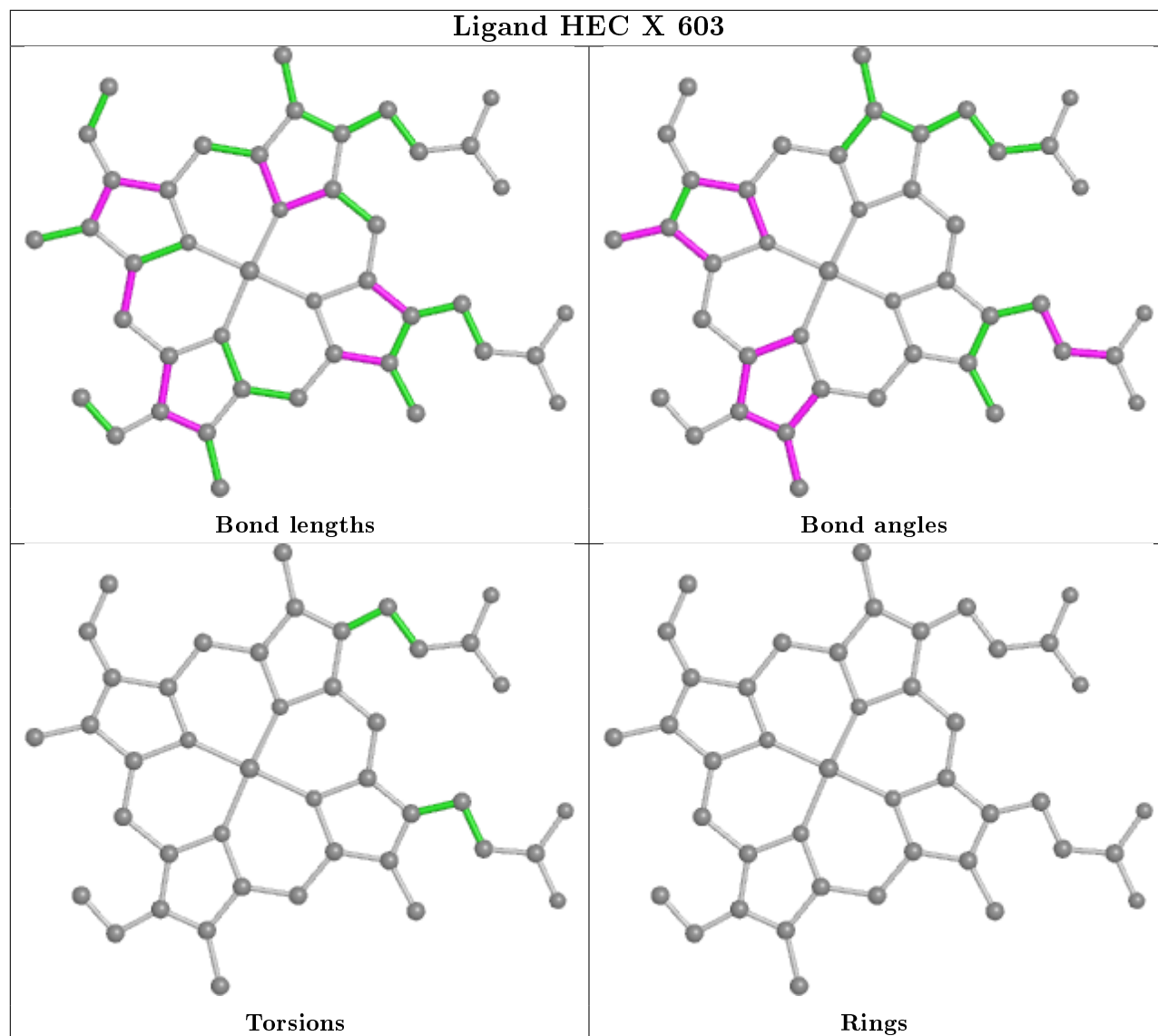
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

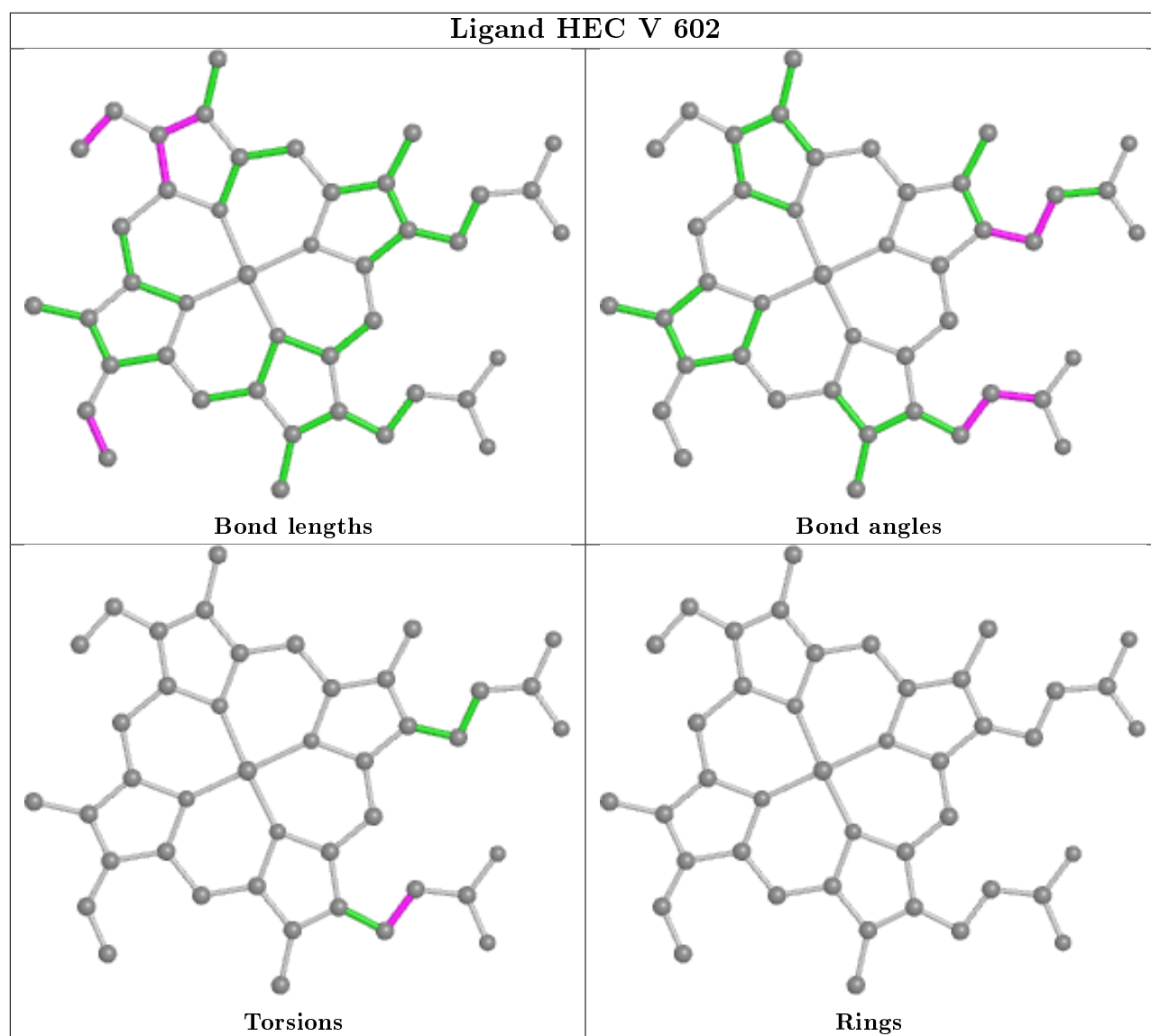




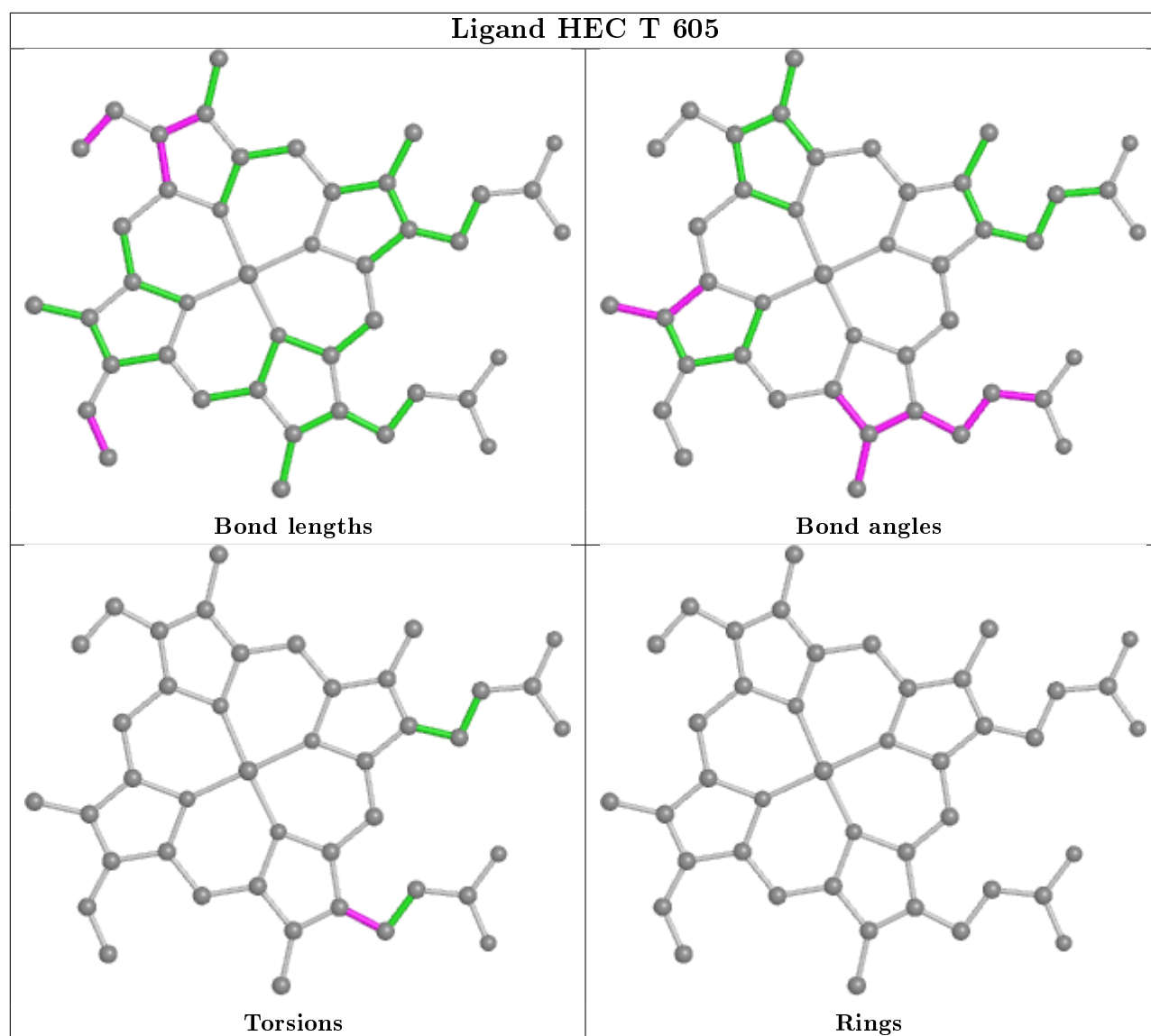
## Ligand HEC I 601

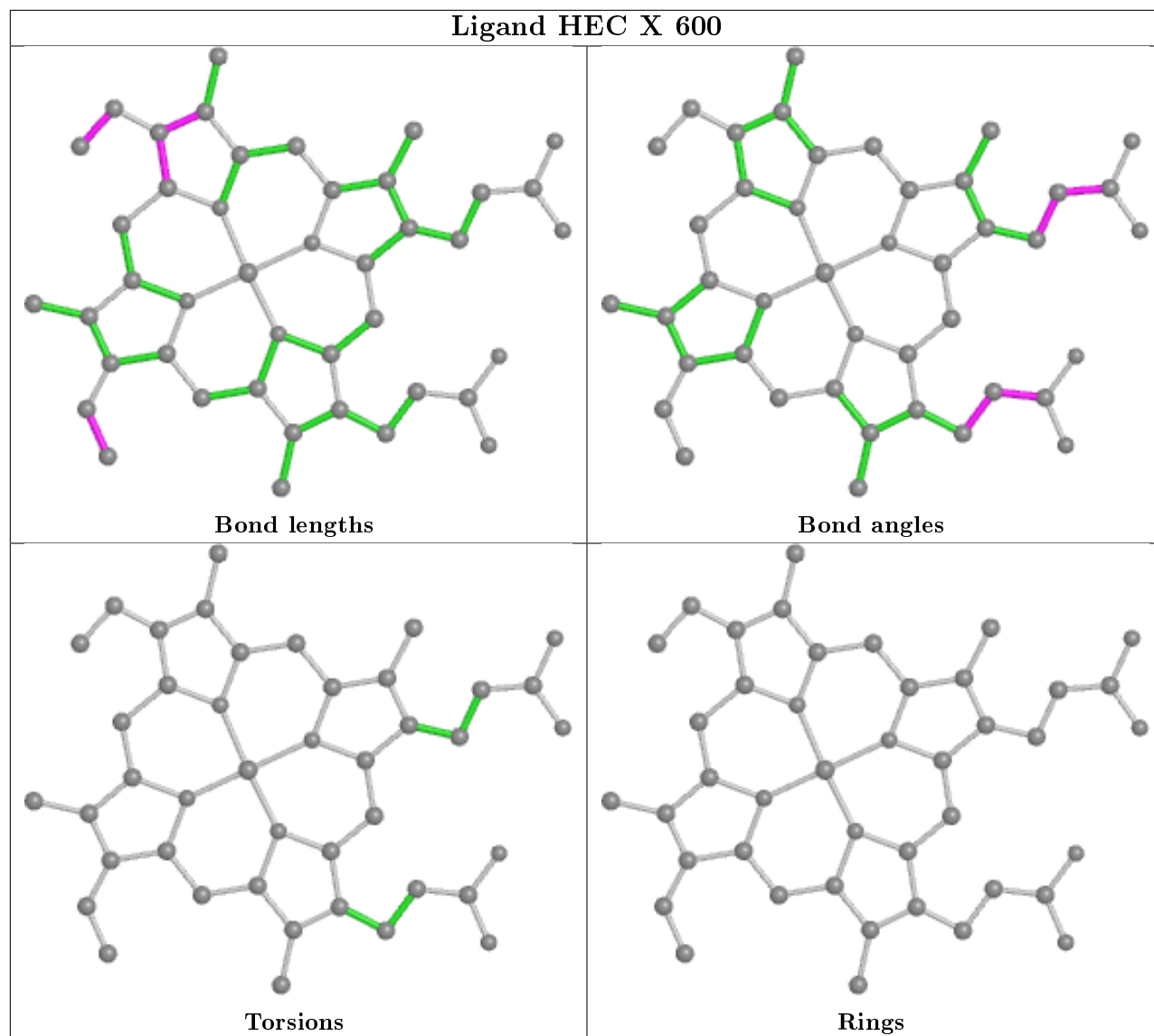




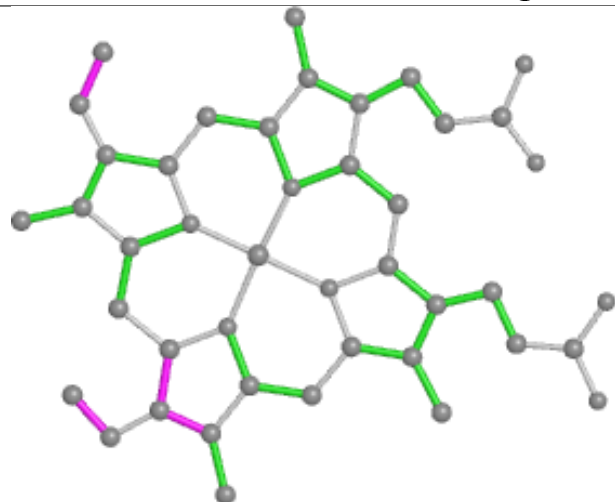




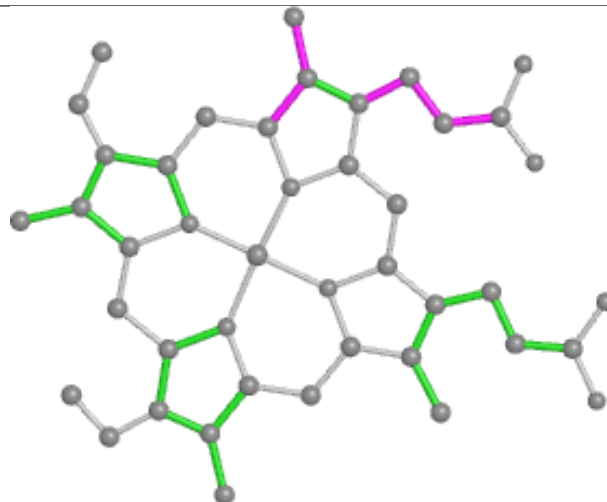




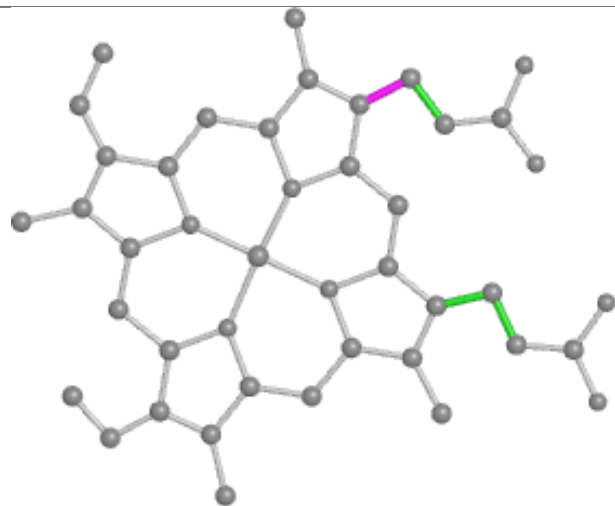
## Ligand HEC F 605



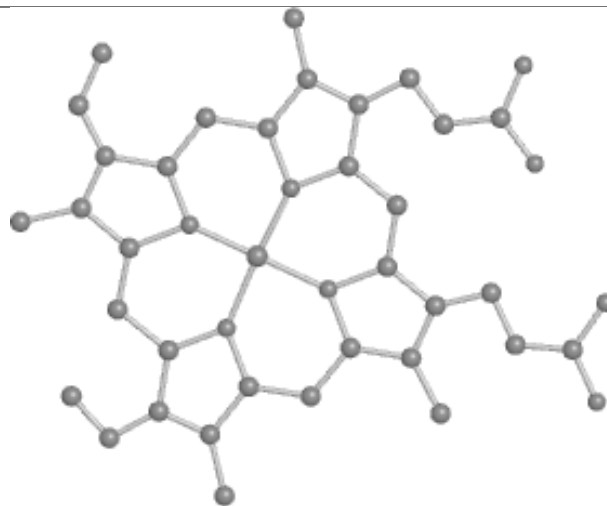
Bond lengths



Bond angles

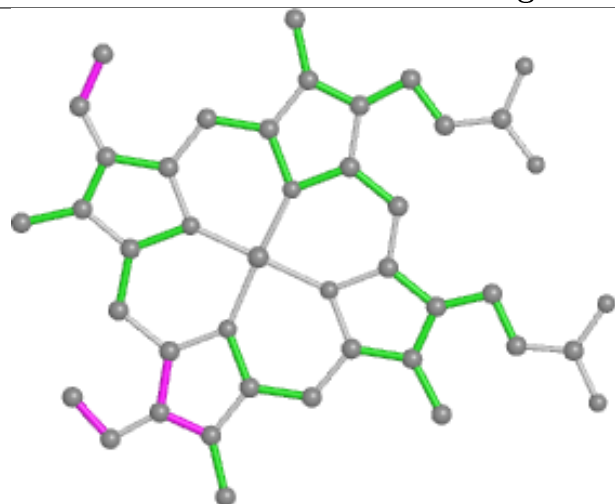


Torsions

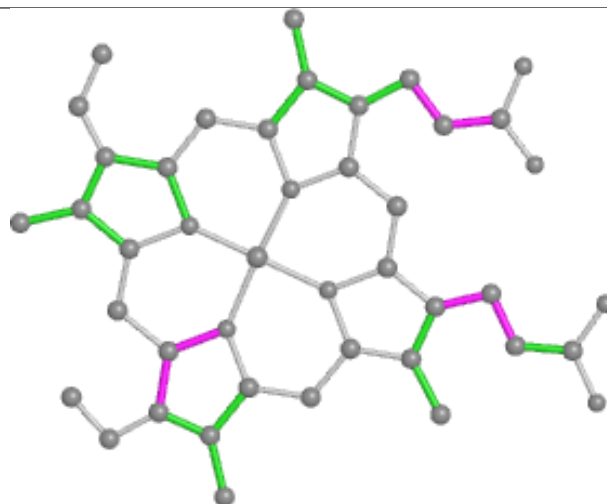


Rings

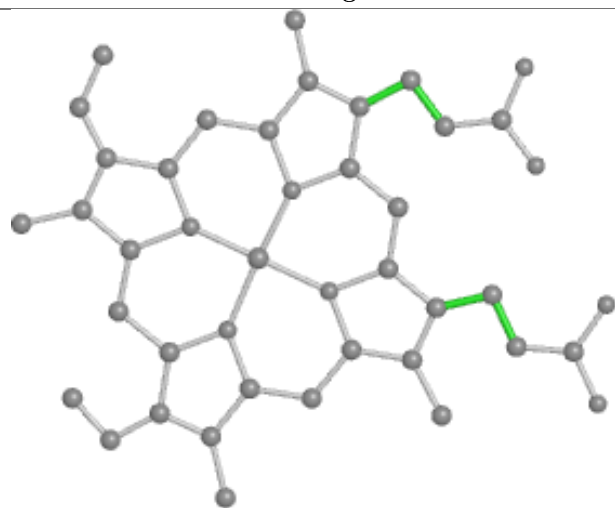
## Ligand HEC L 606



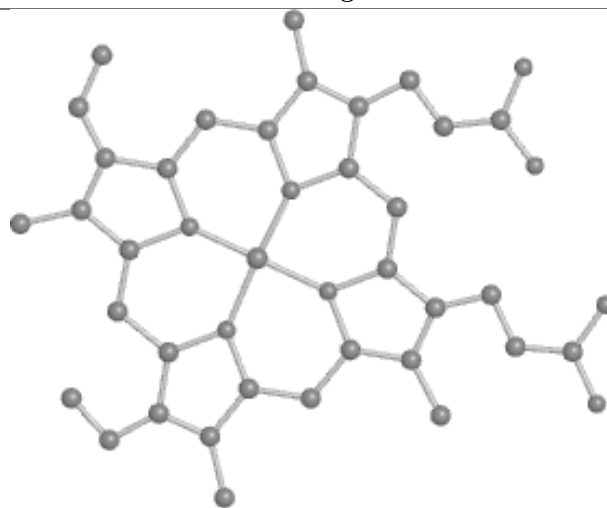
Bond lengths



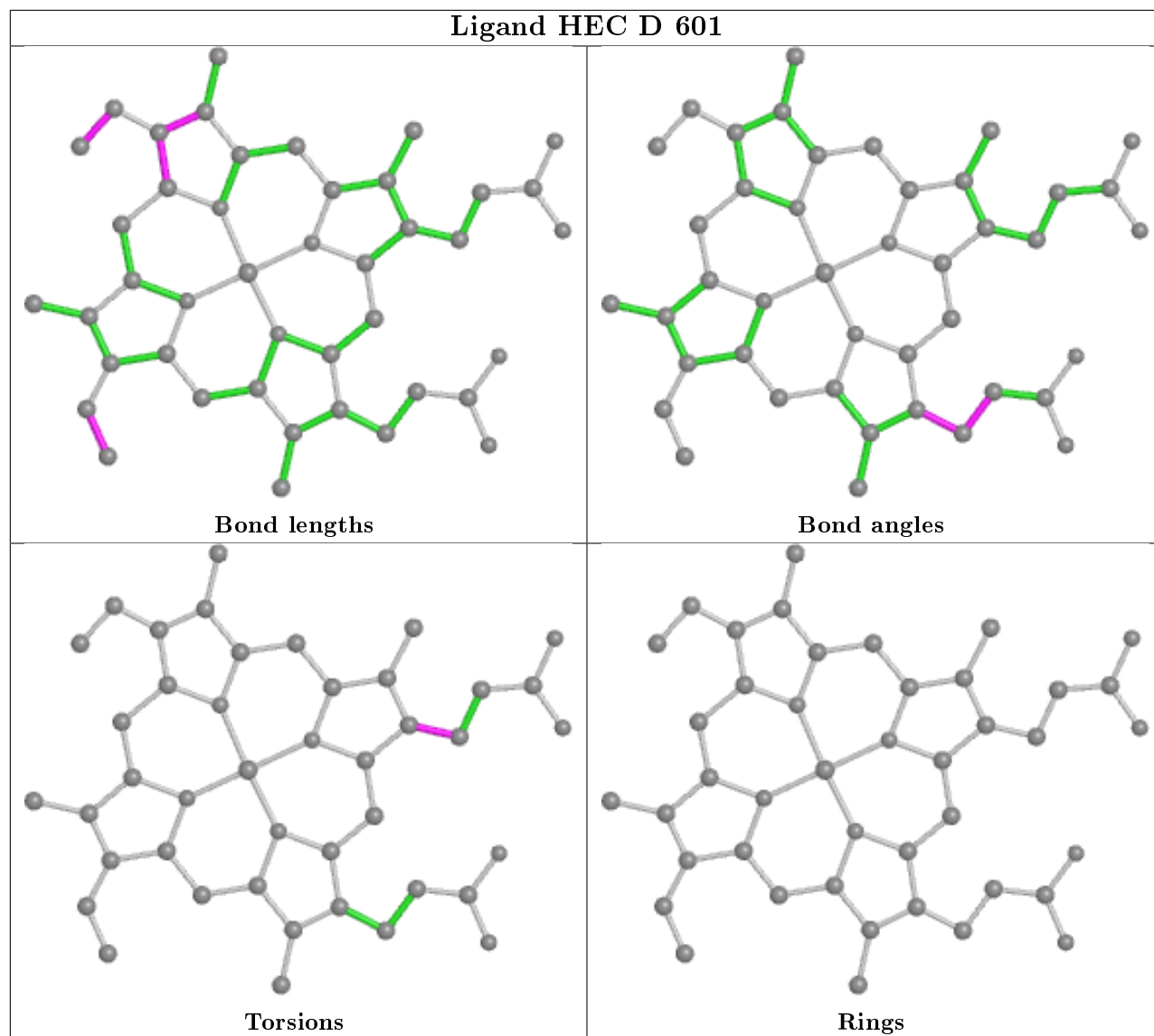
Bond angles

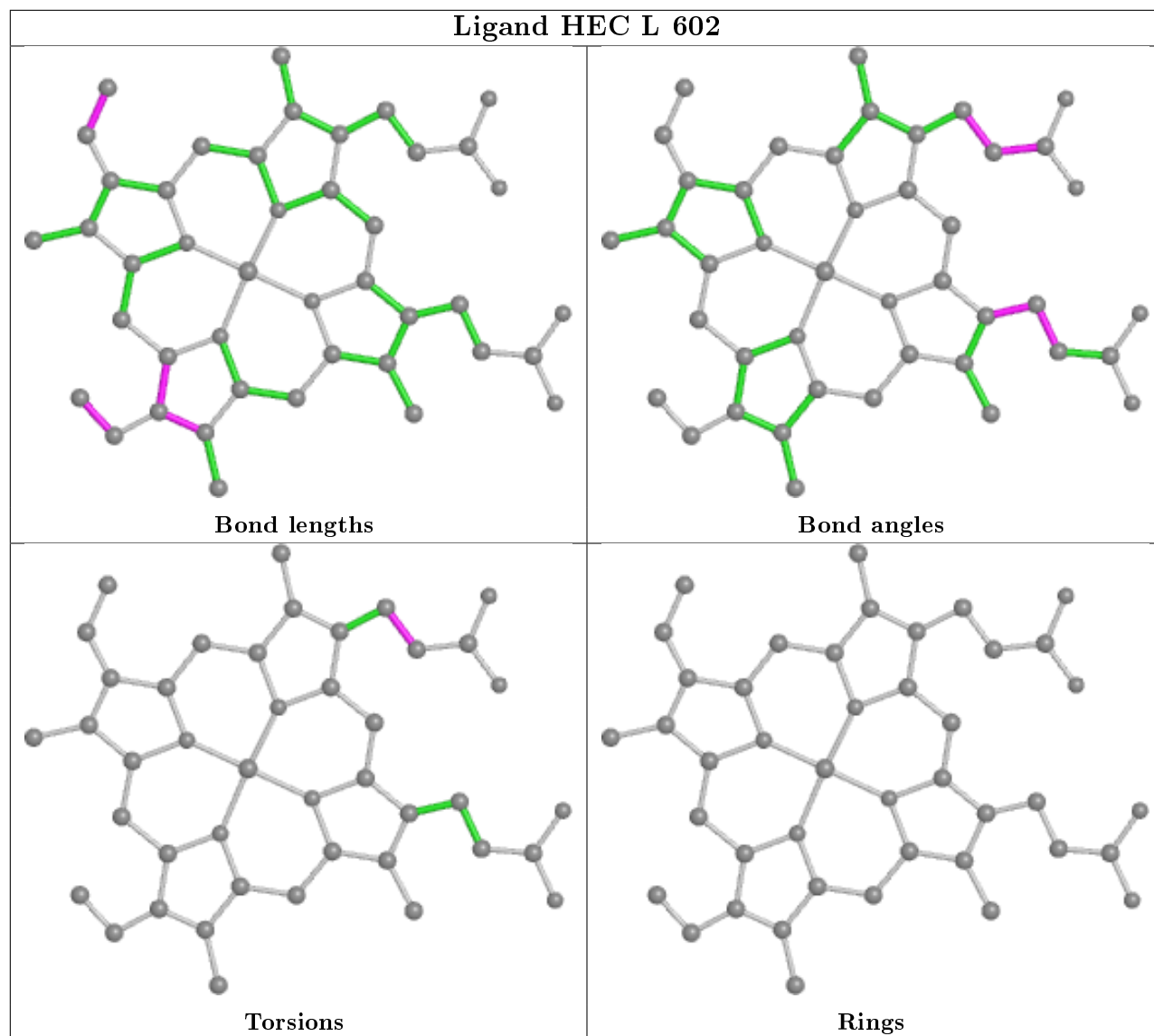


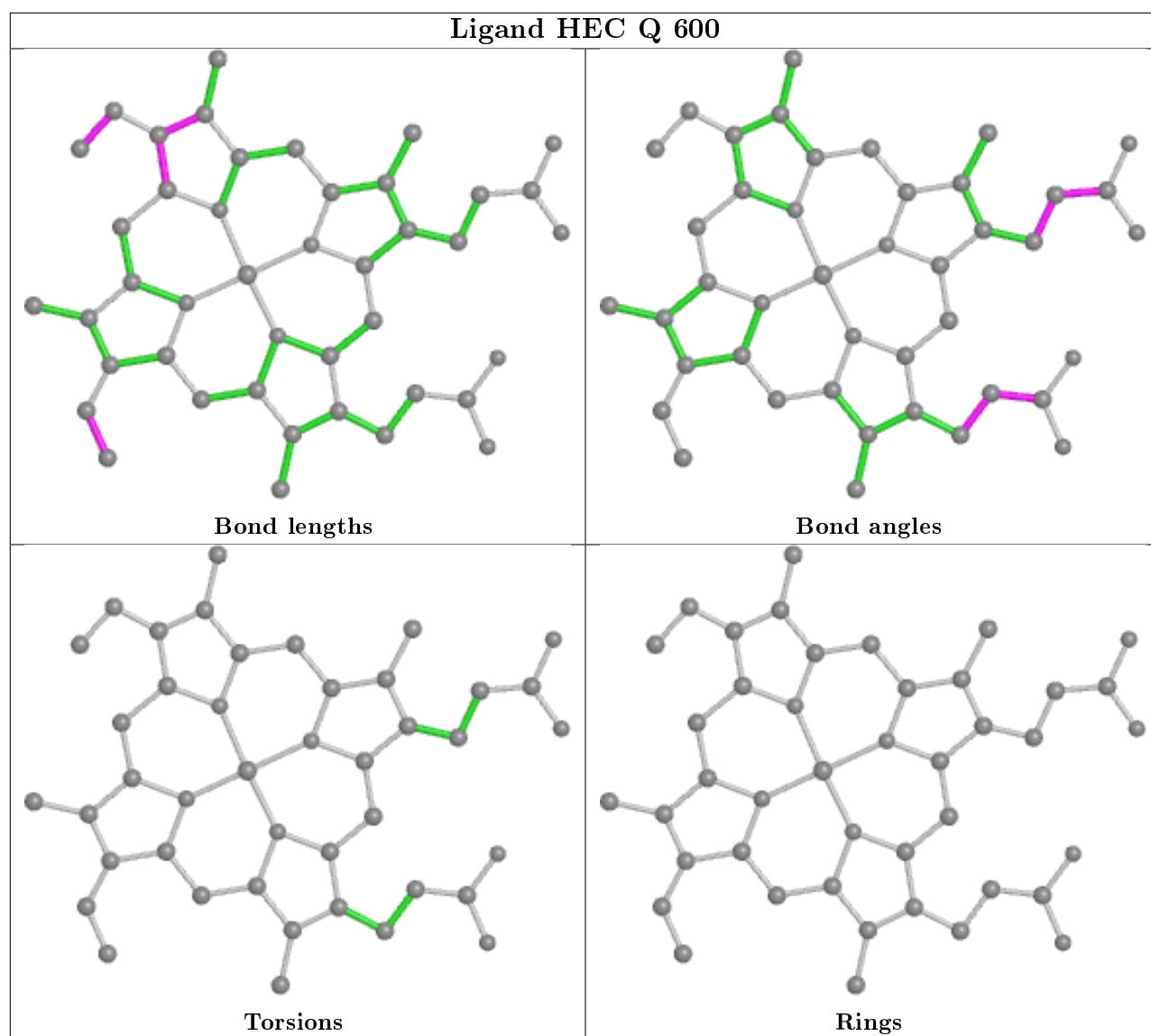
Torsions

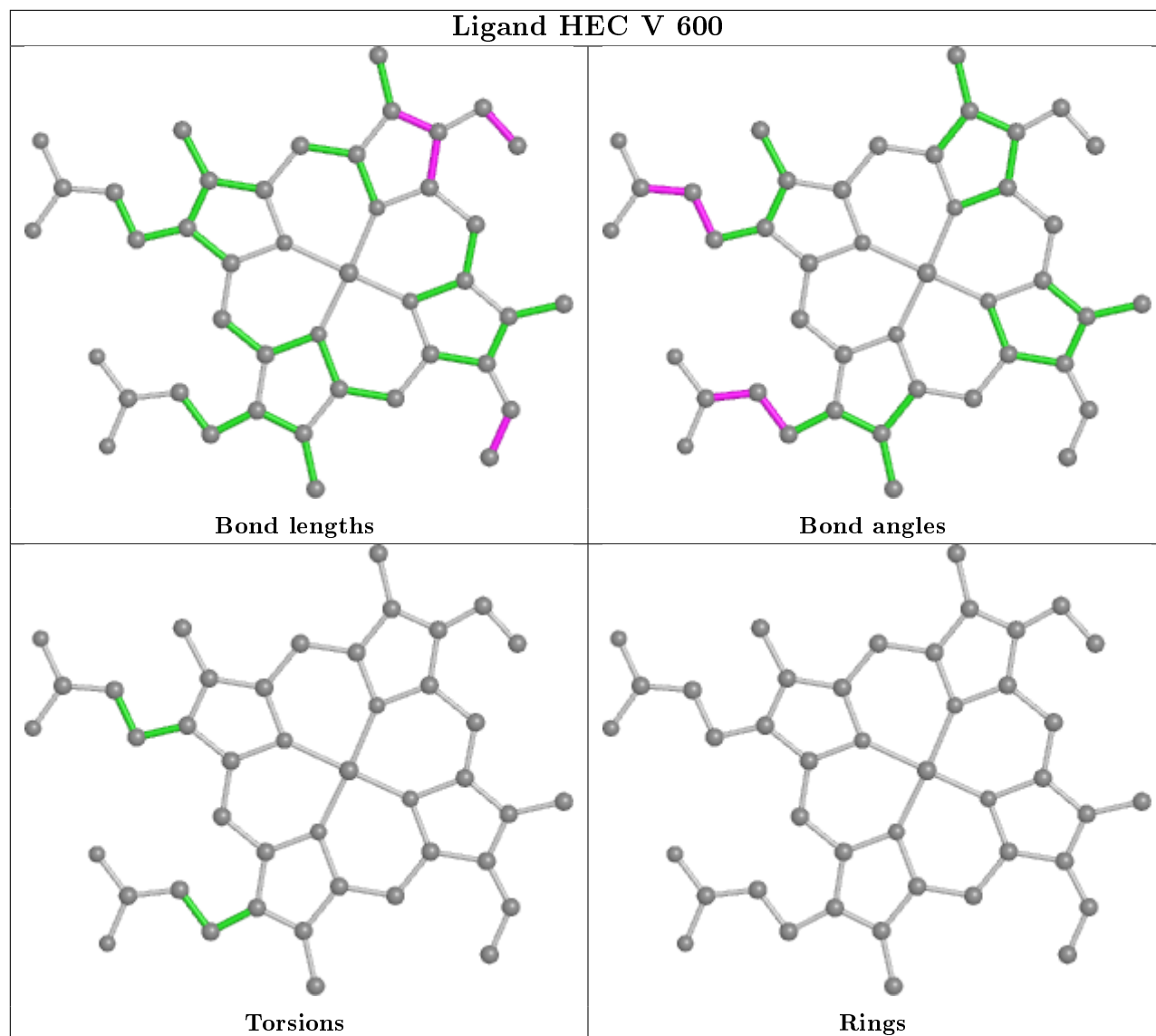


Rings

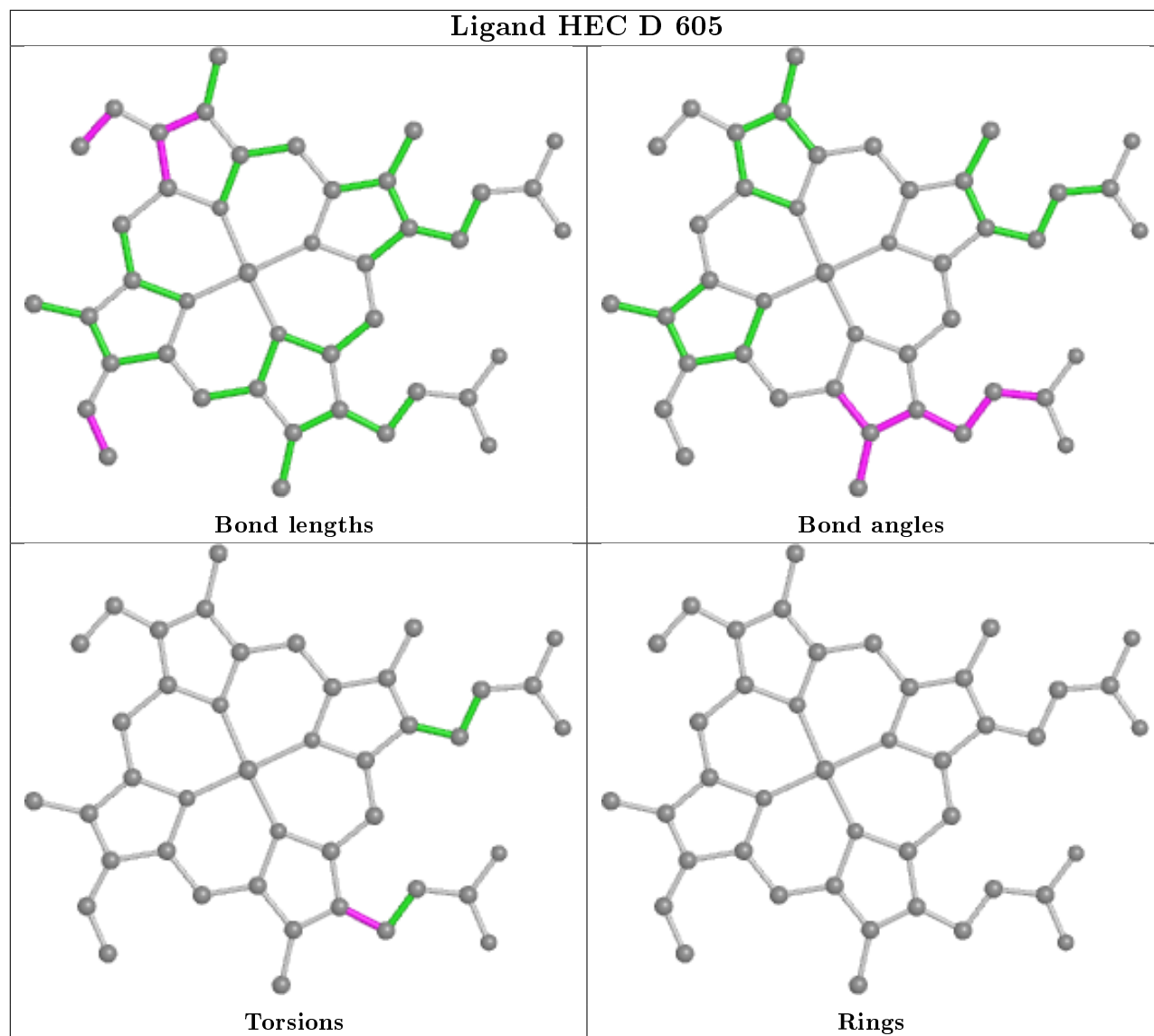


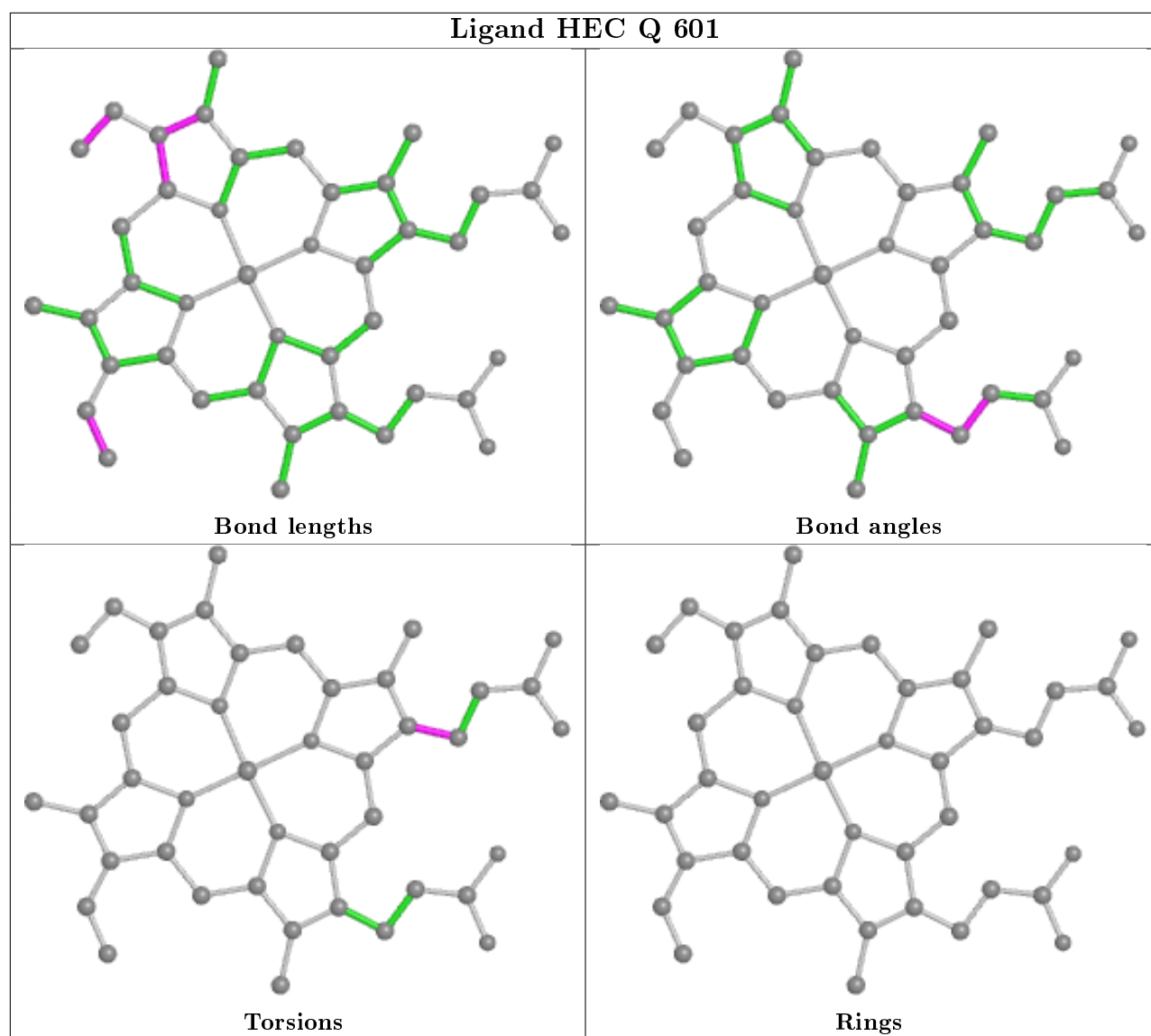


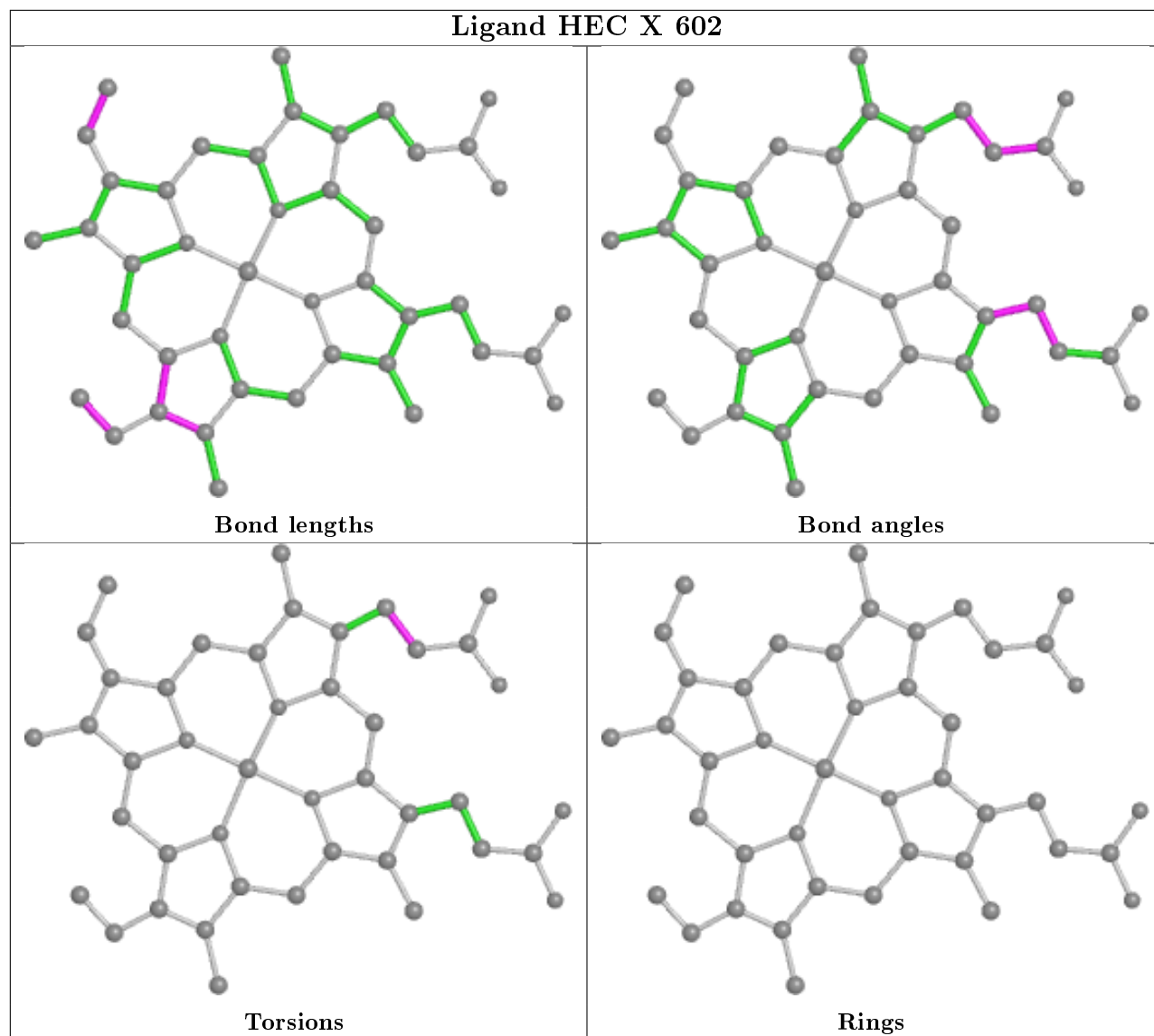


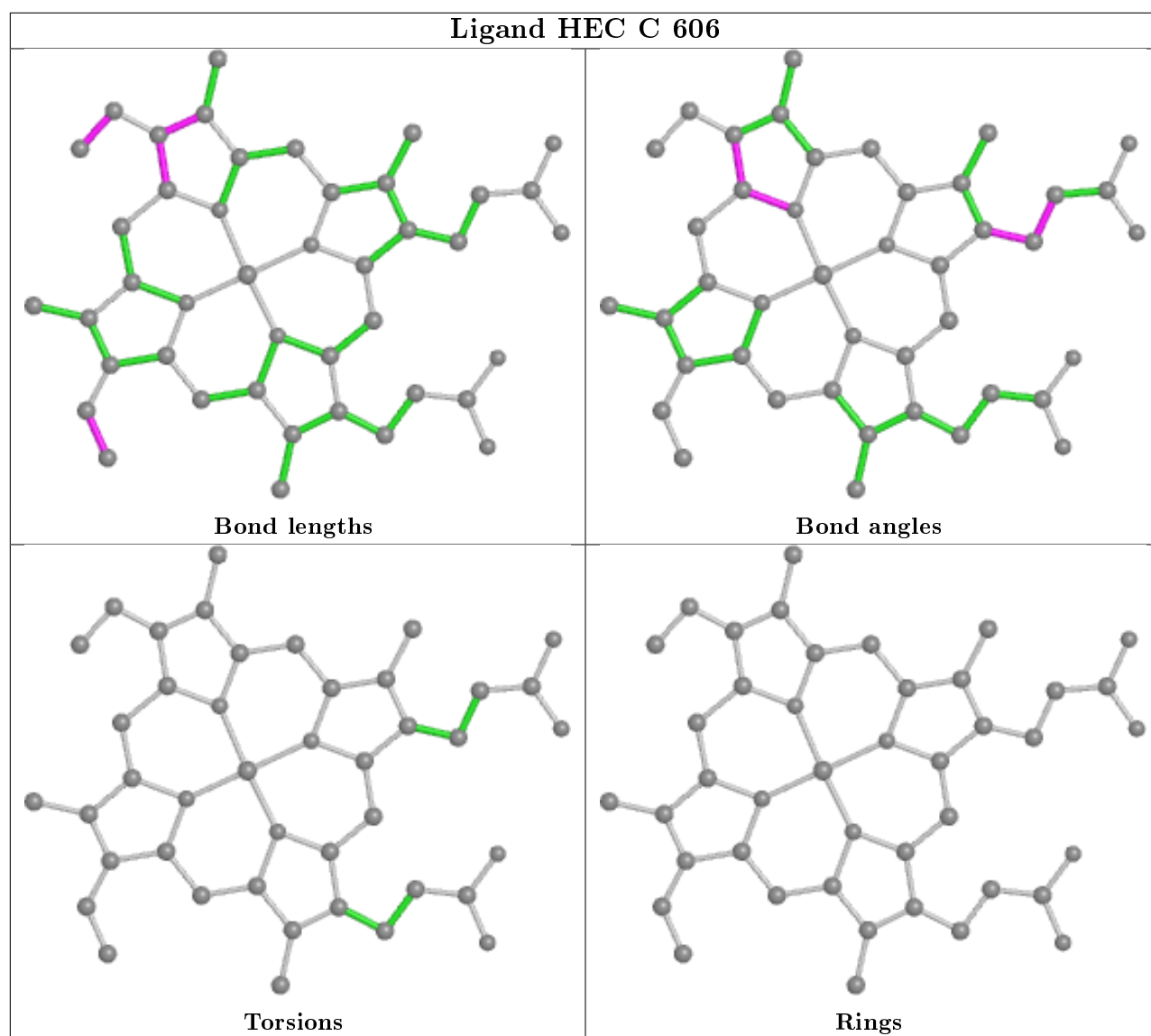


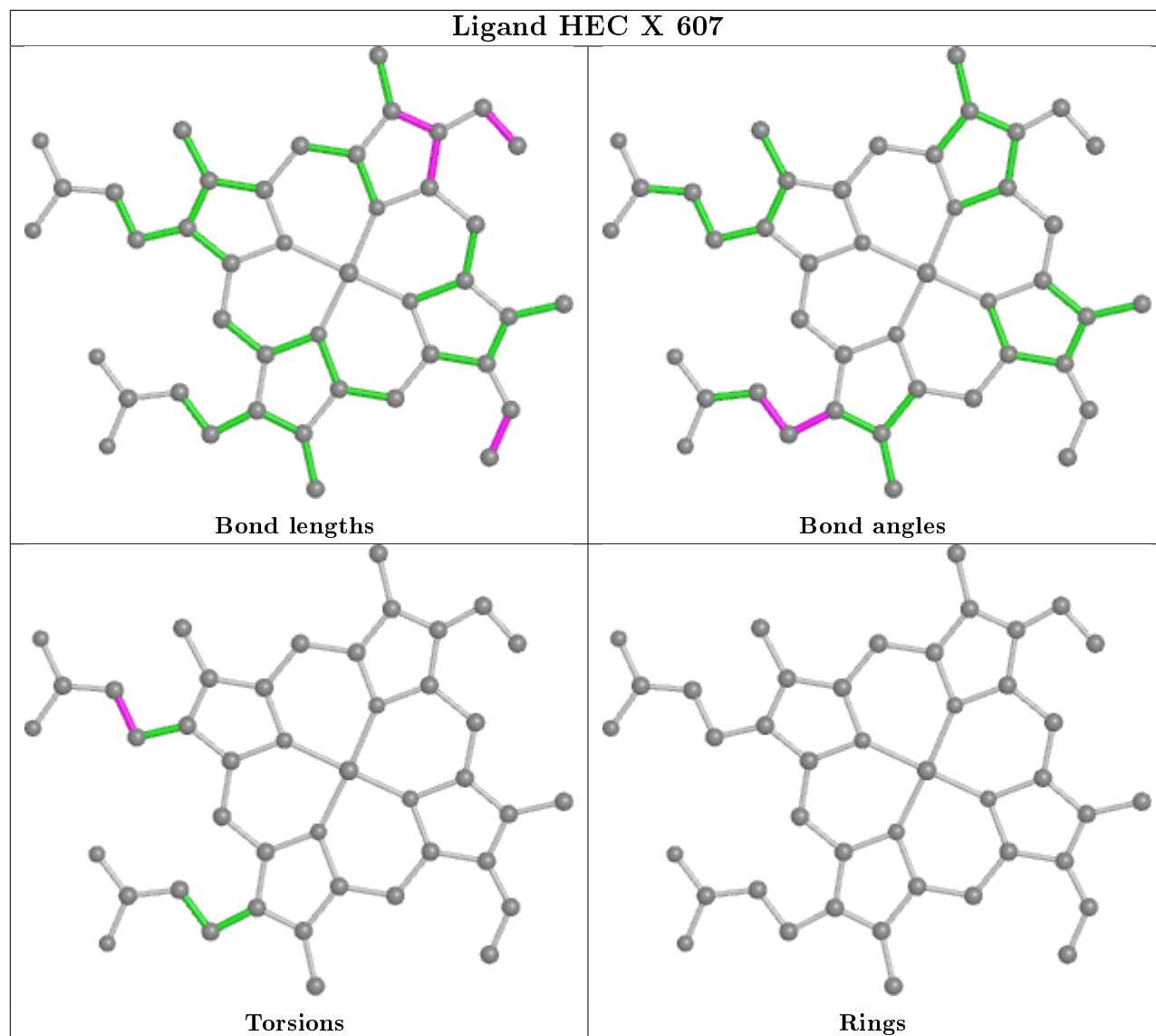


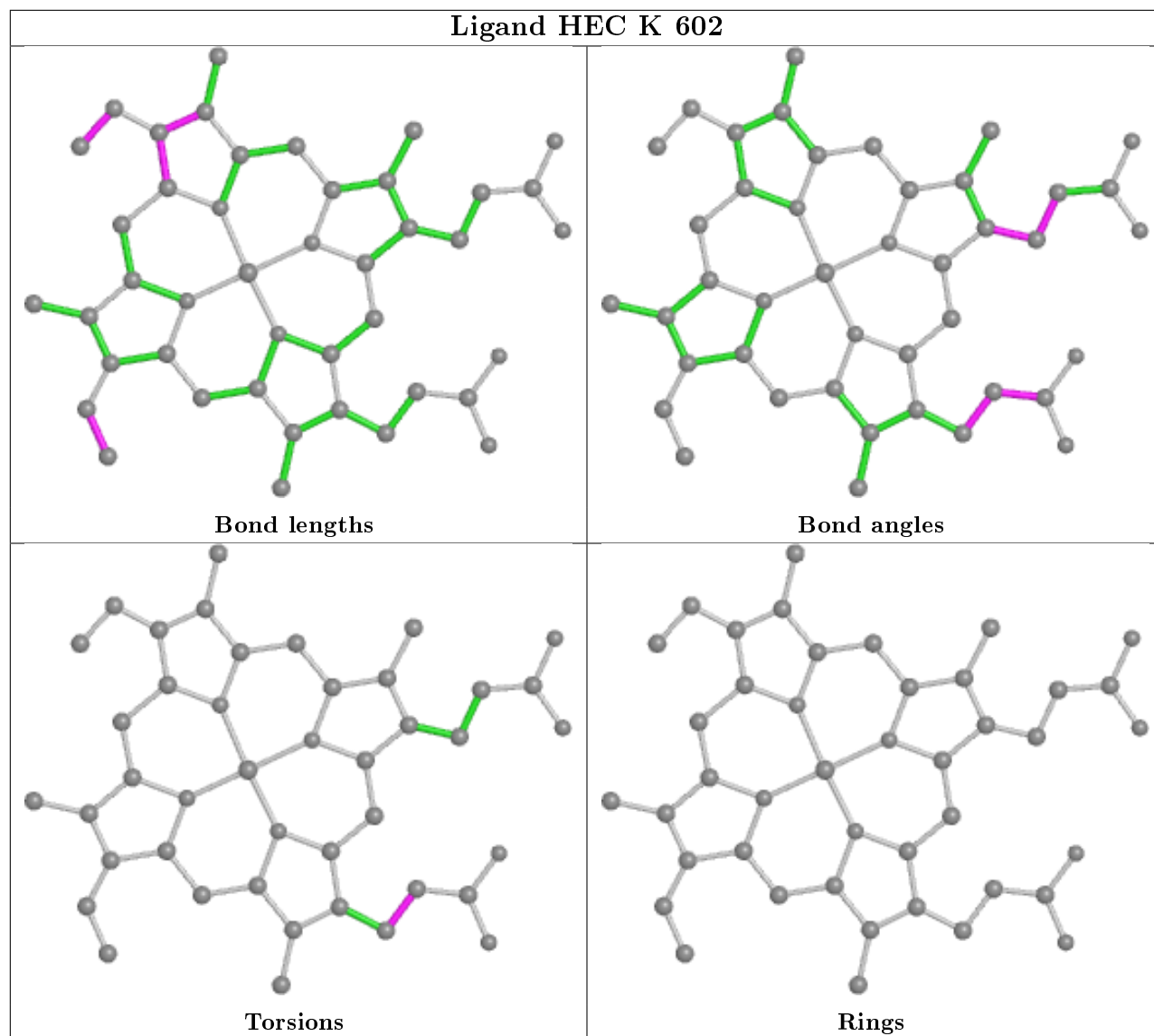


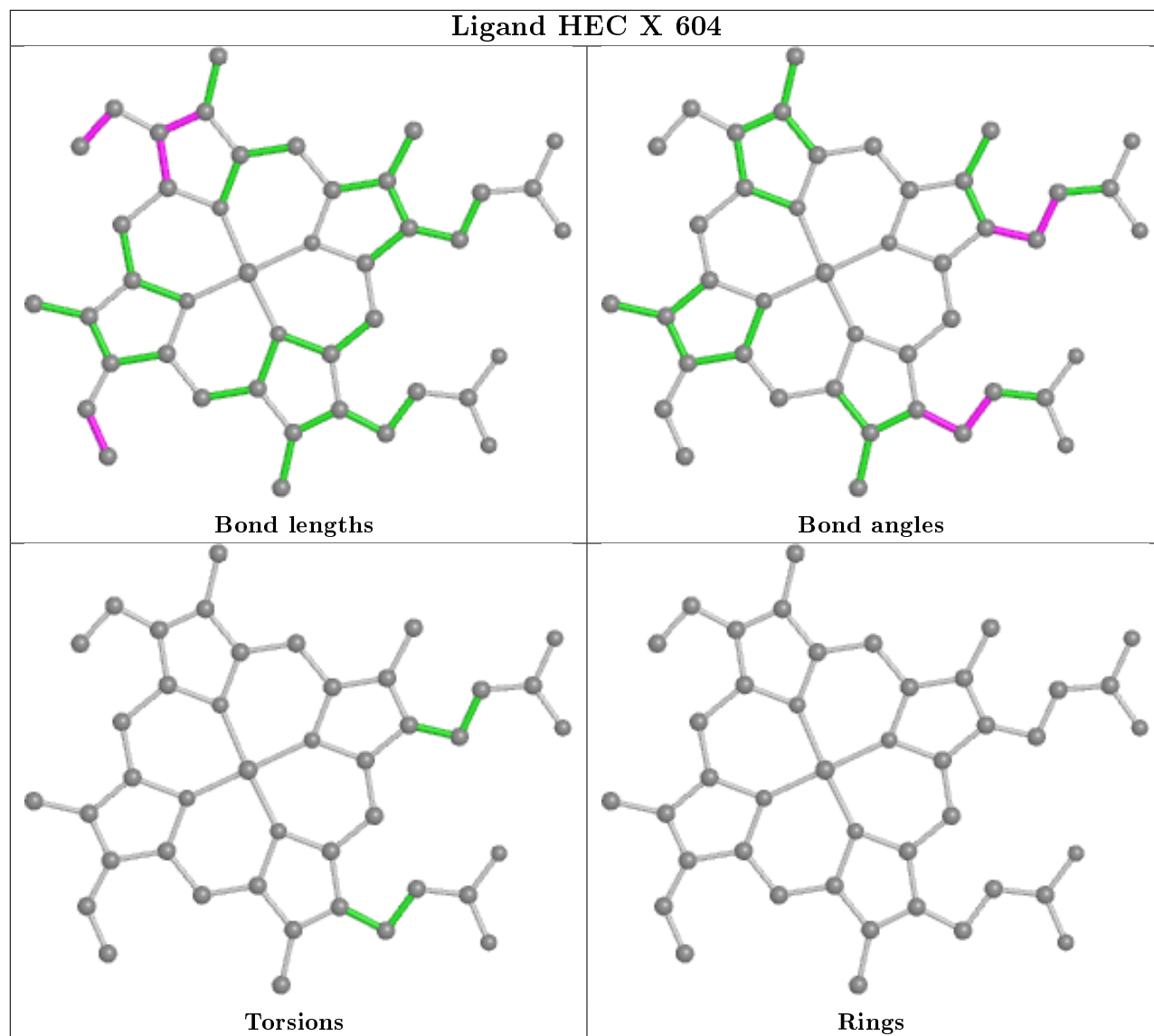


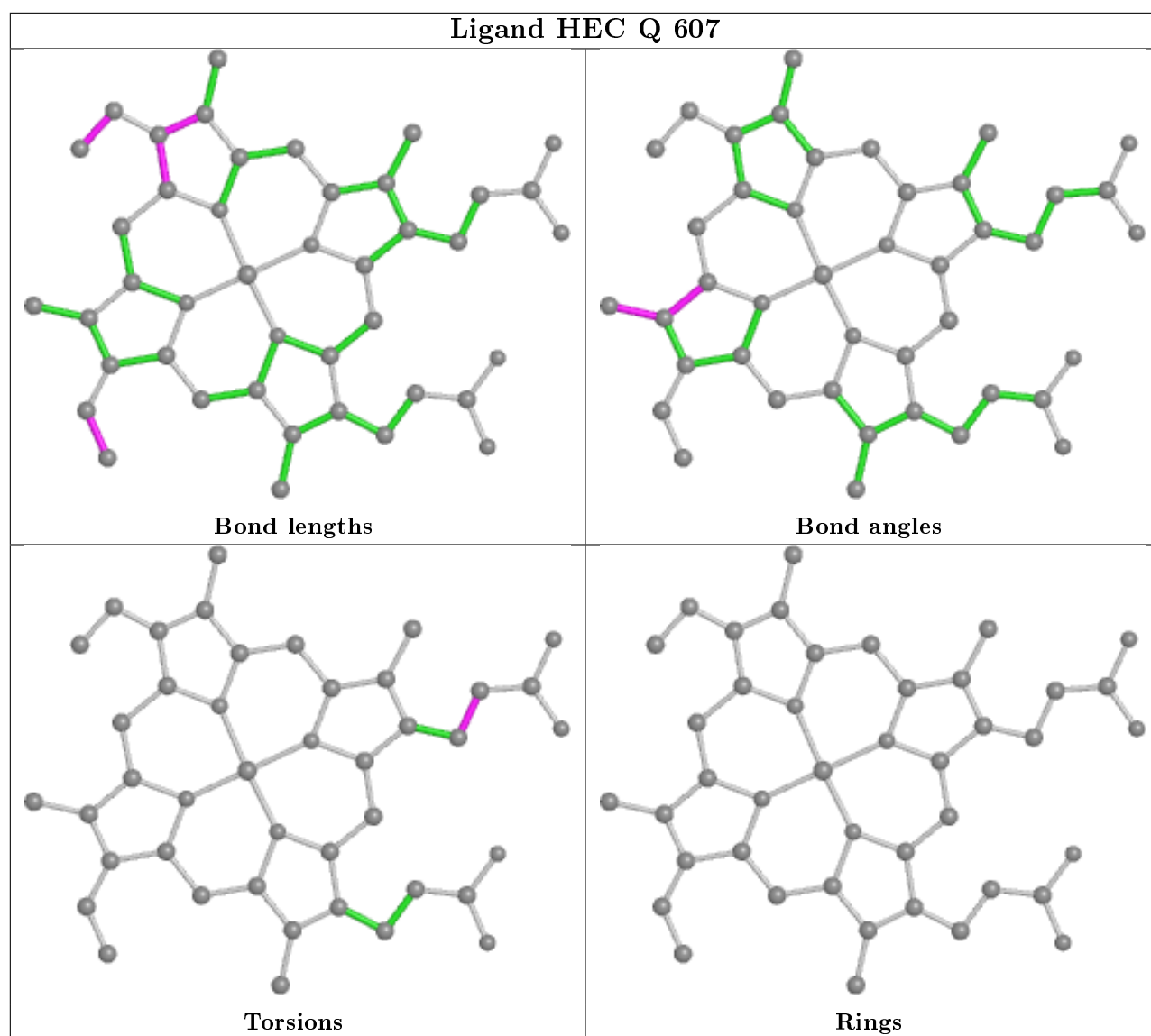




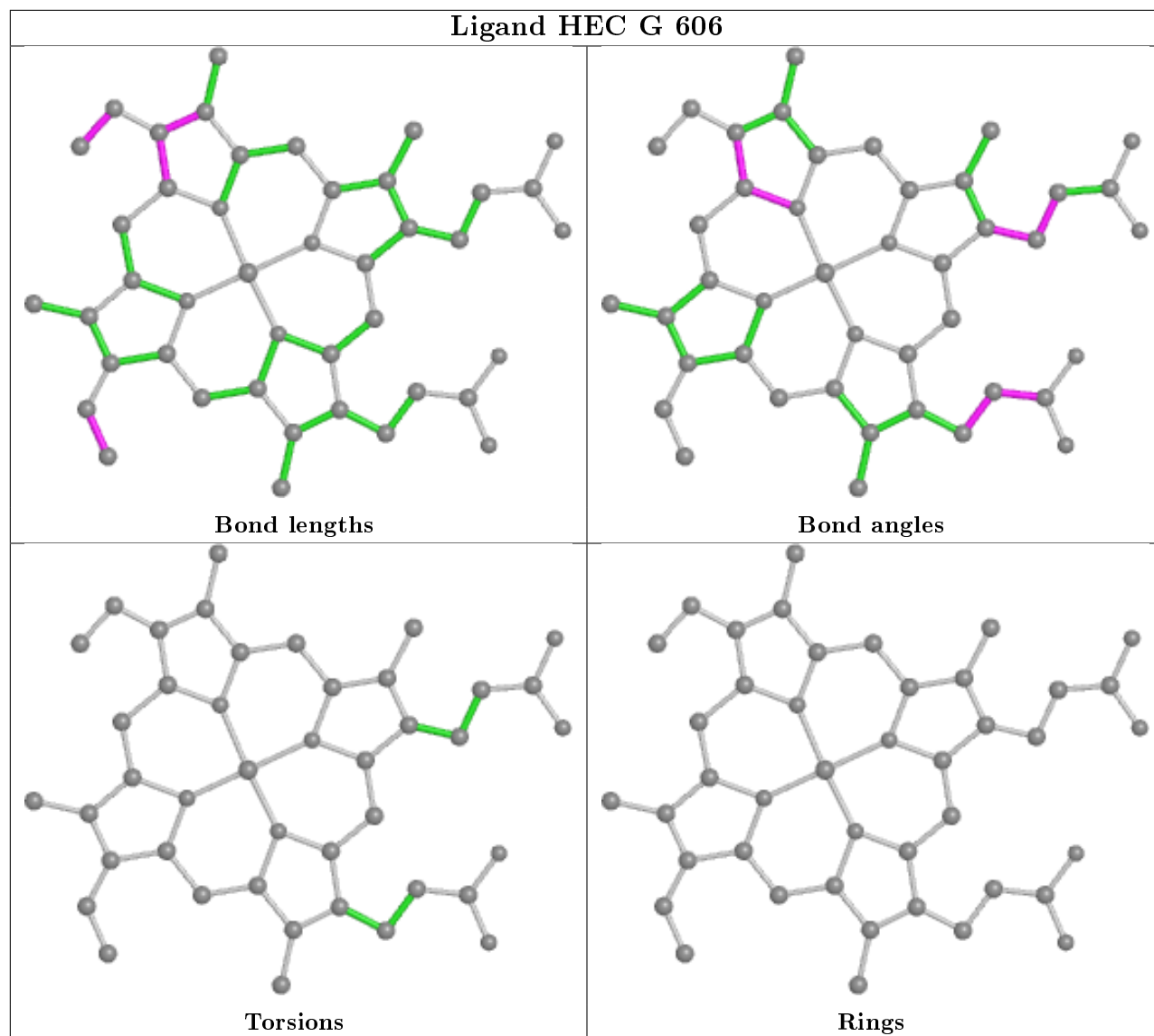


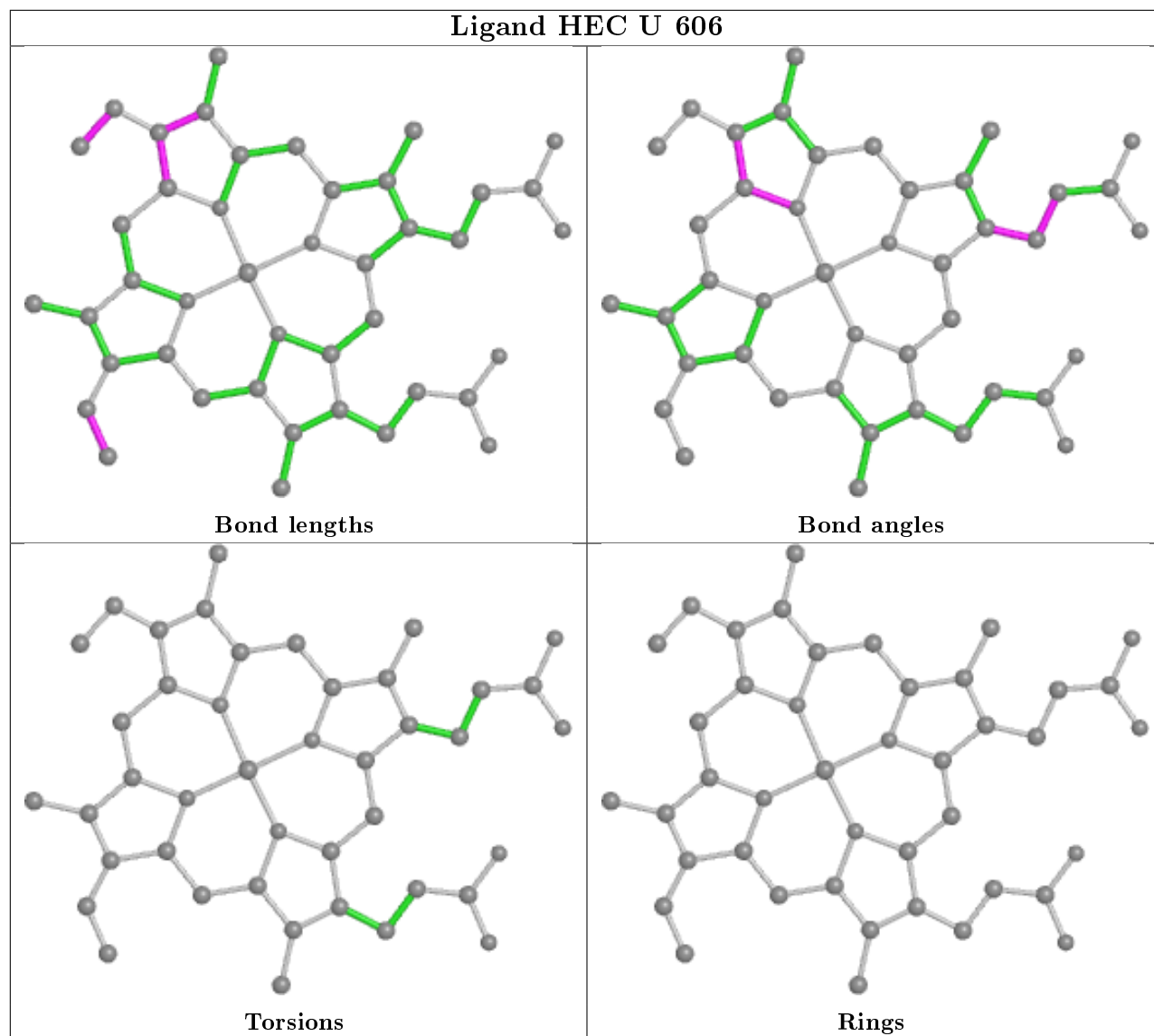




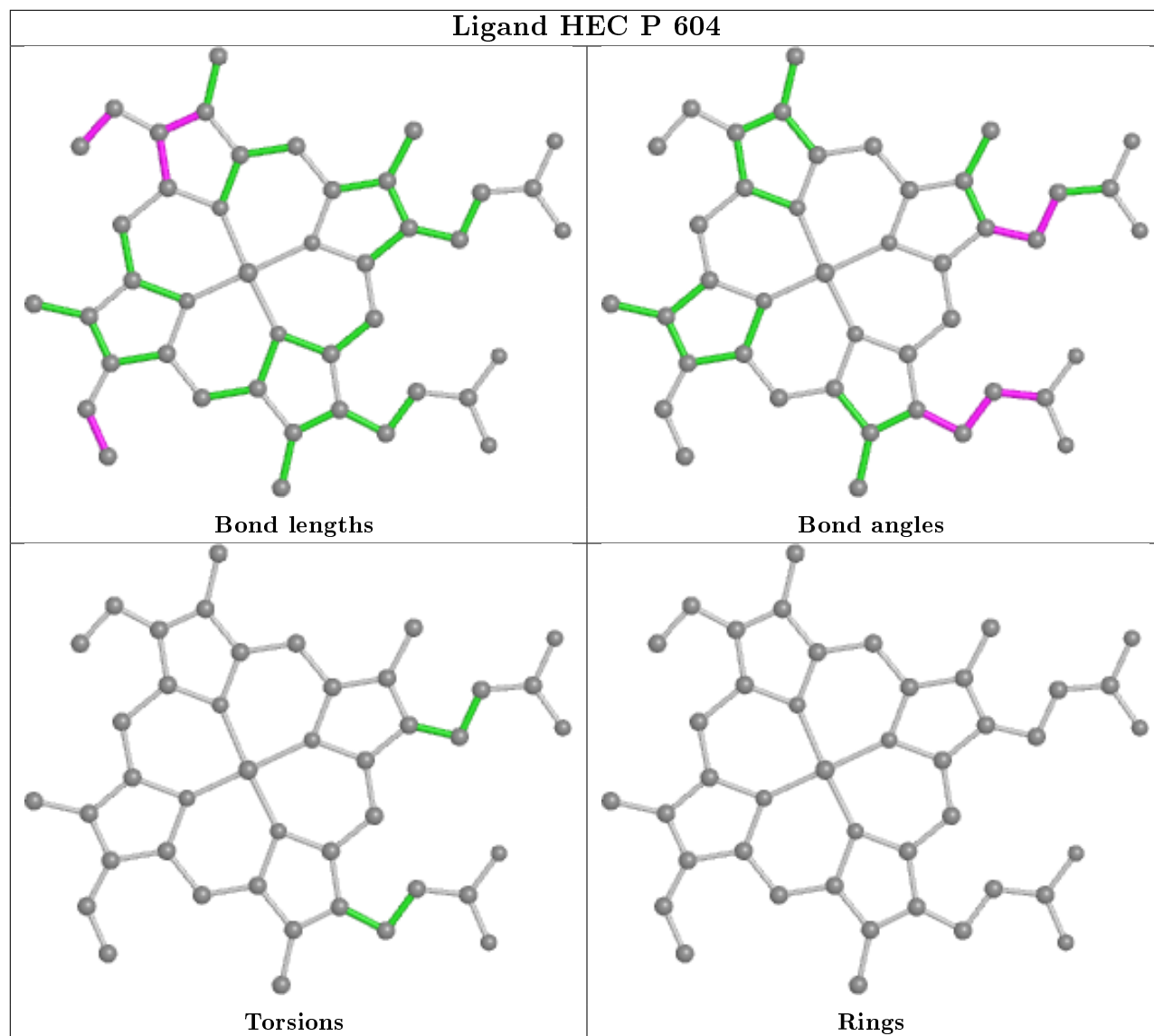


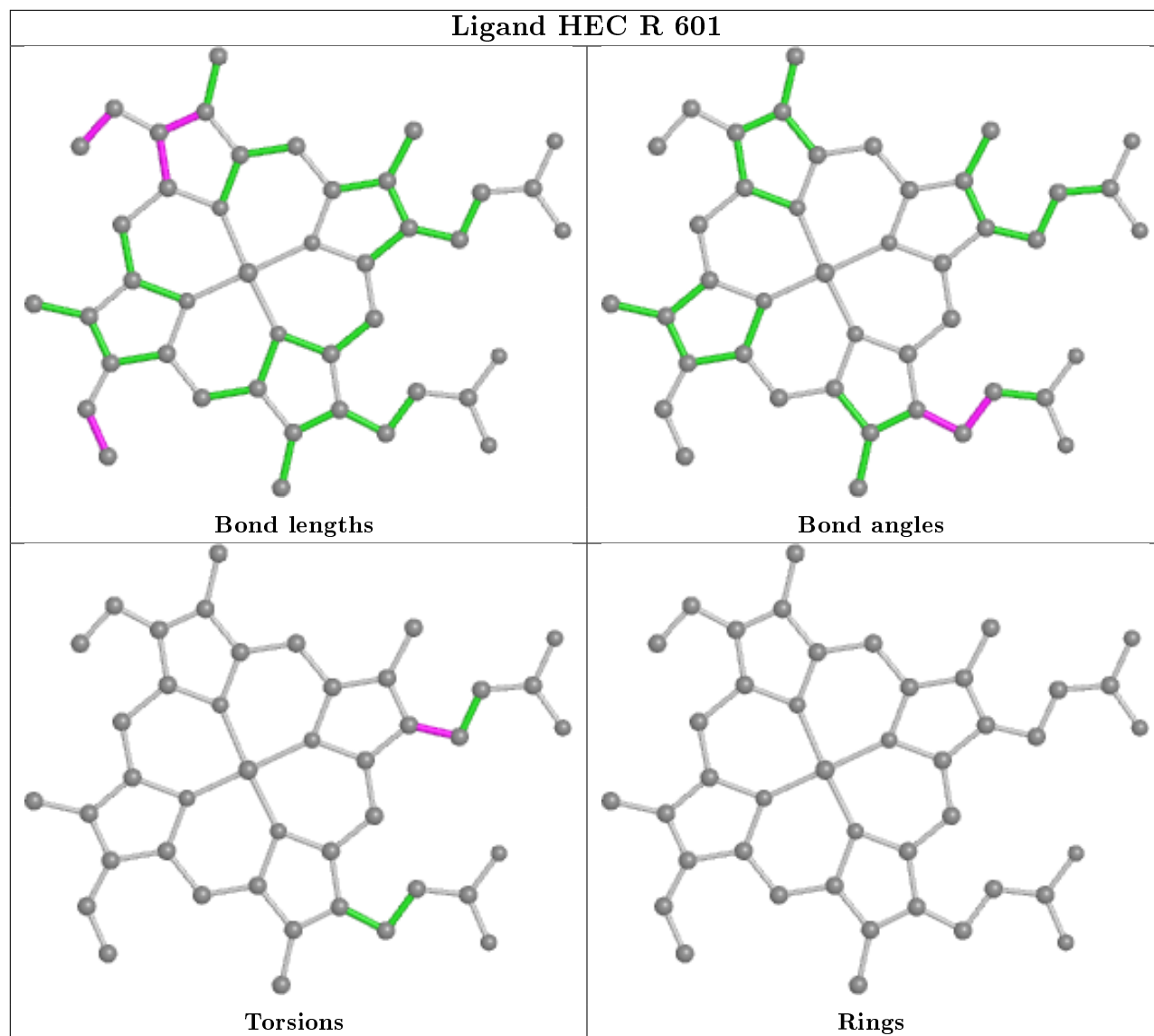


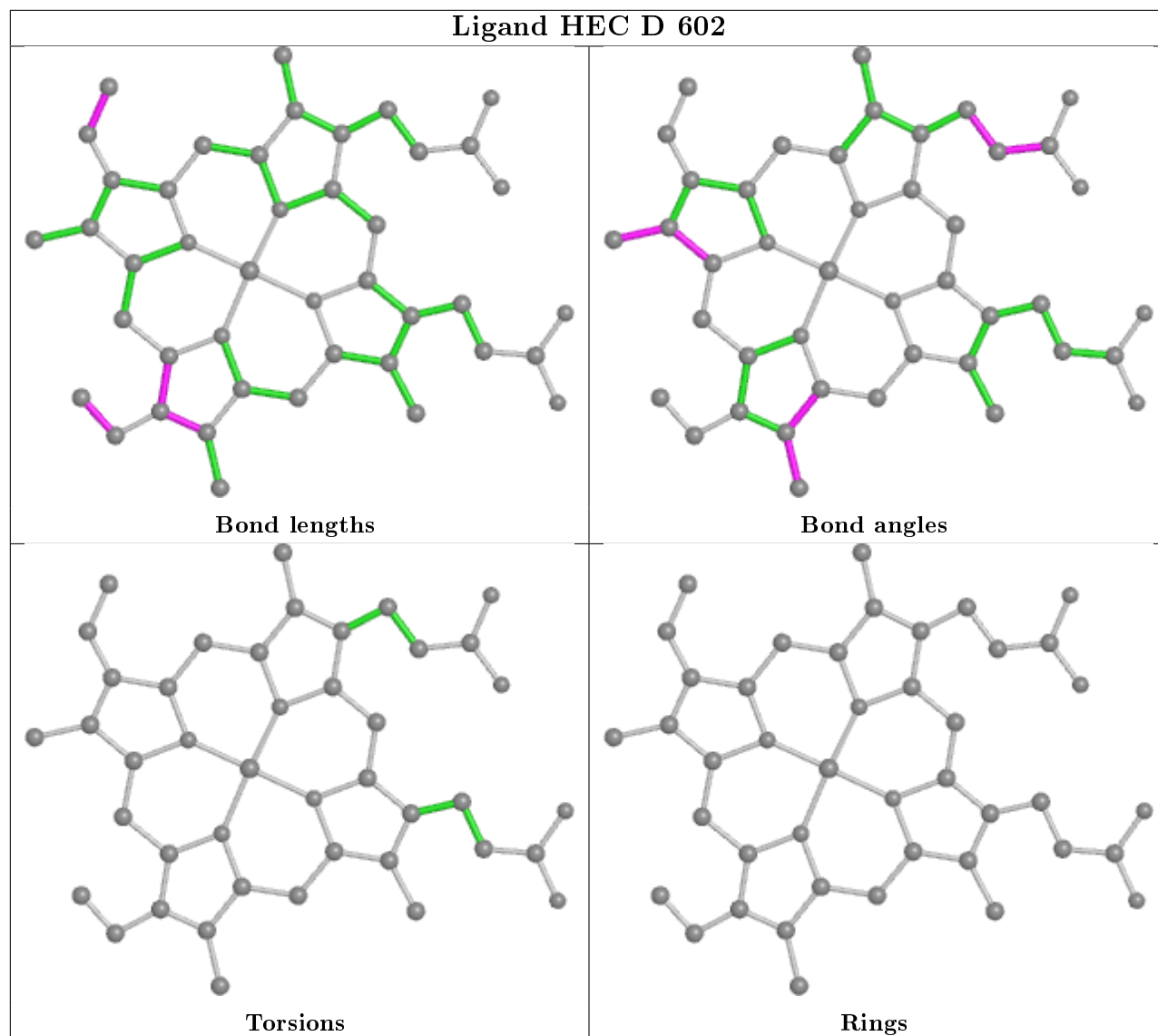




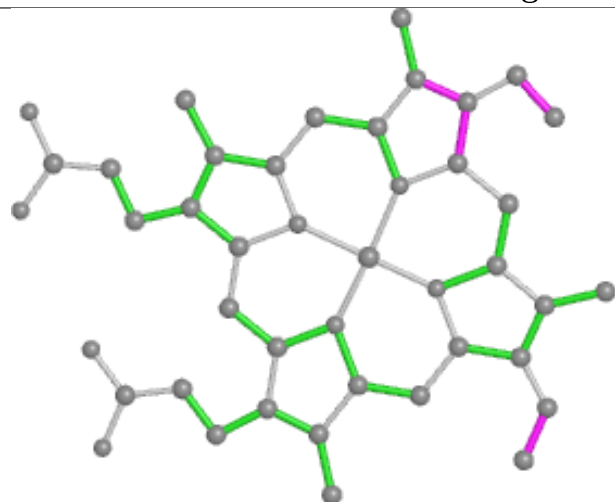
## Ligand HEC P 604



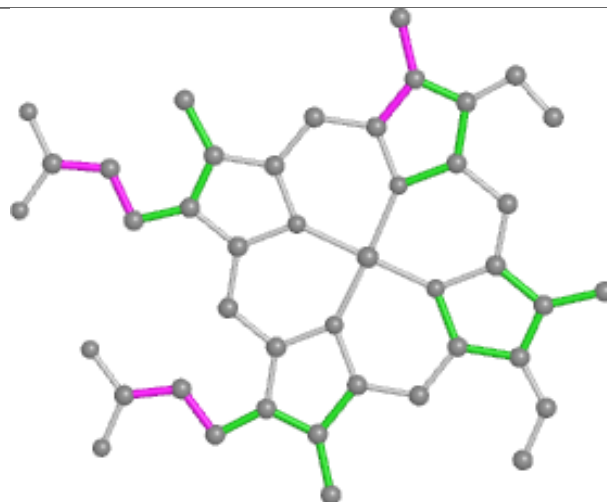




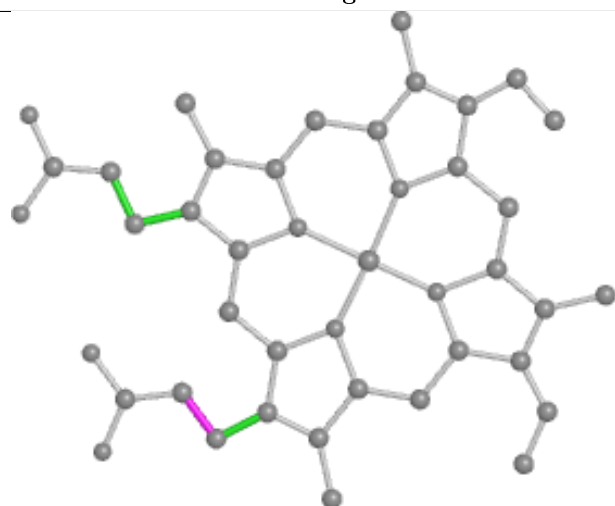
## Ligand HEC I 602



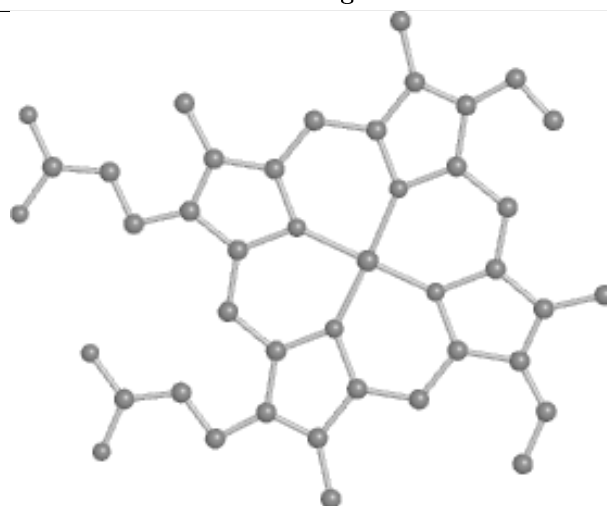
Bond lengths



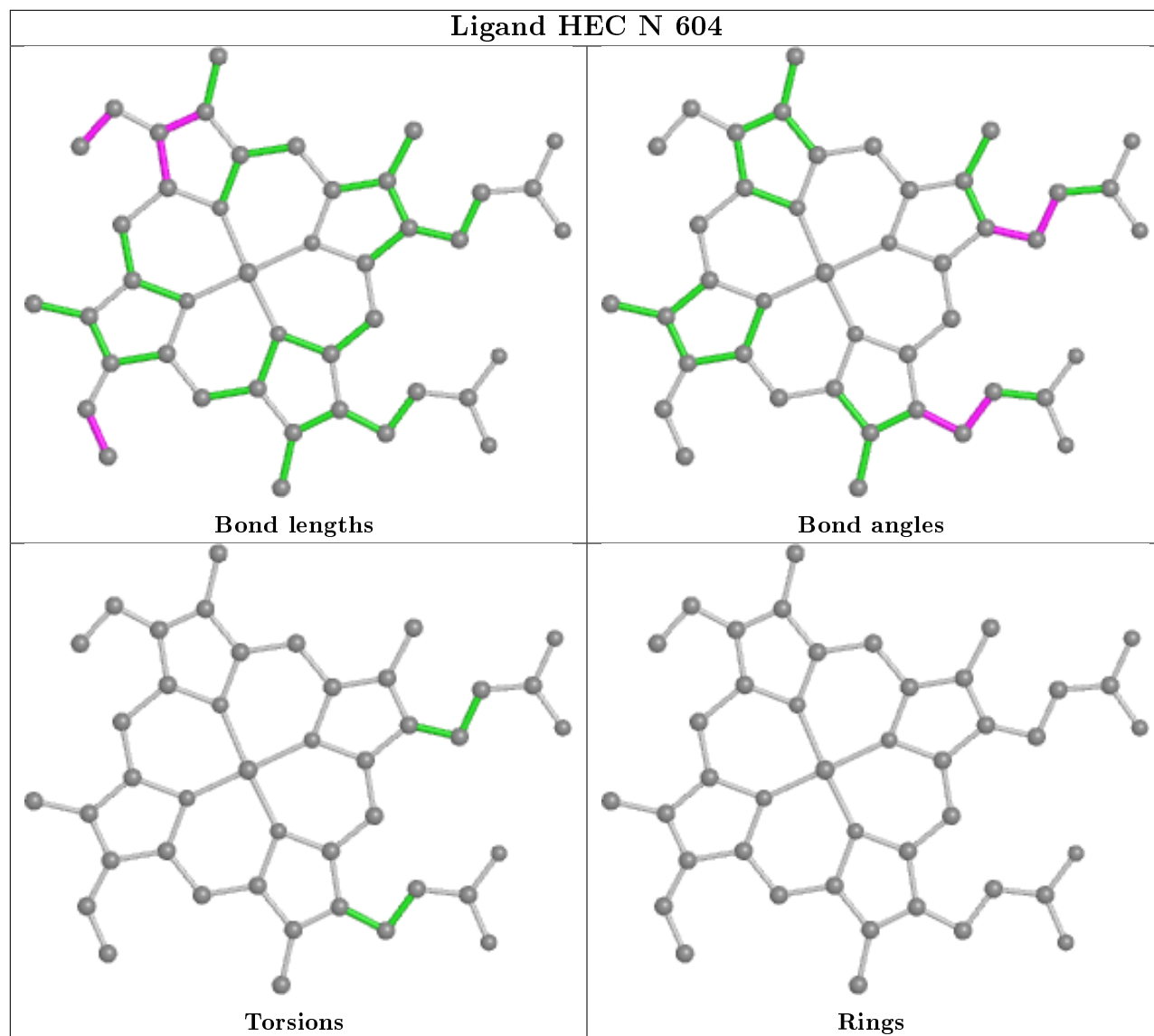
Bond angles

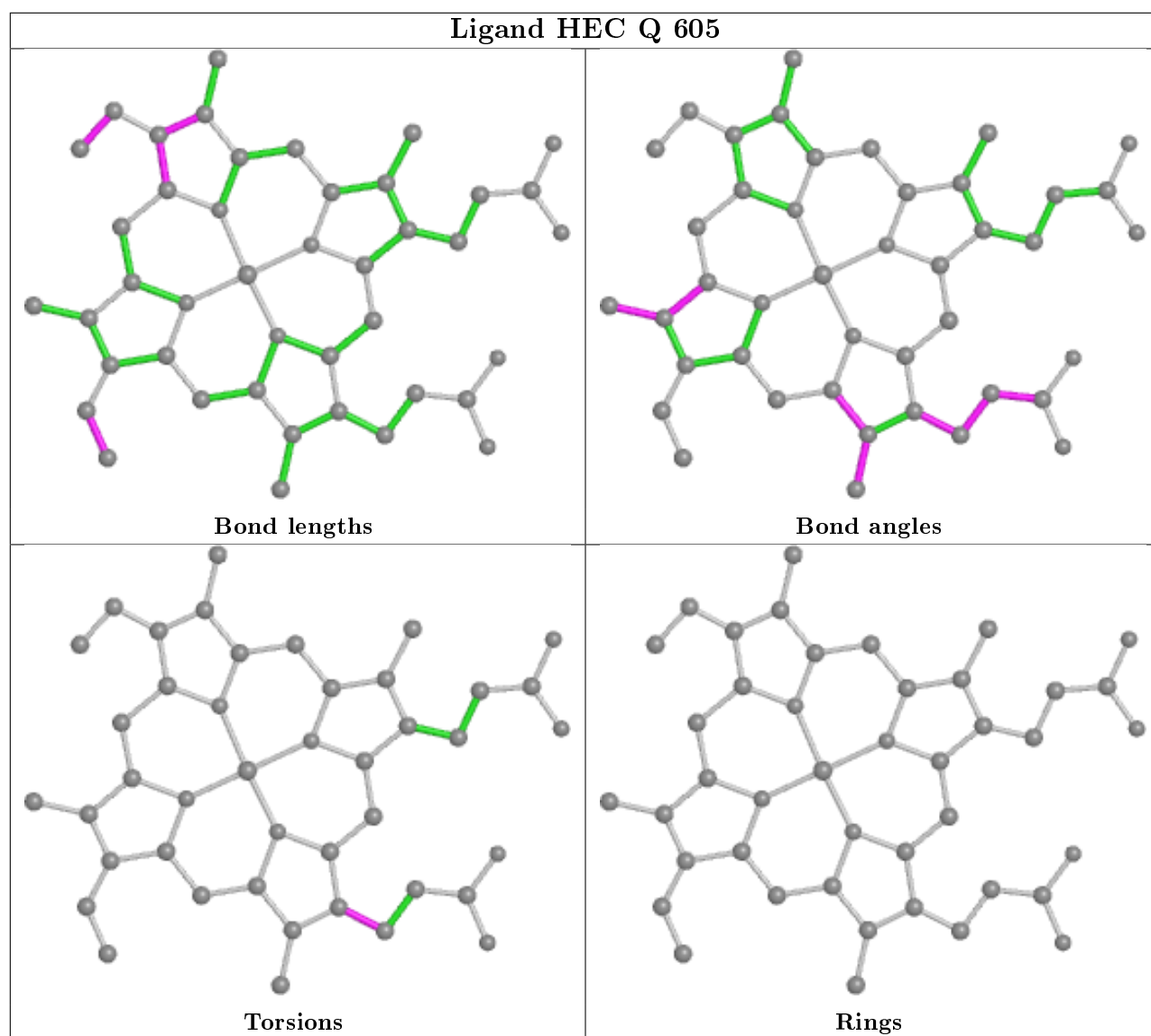


Torsions



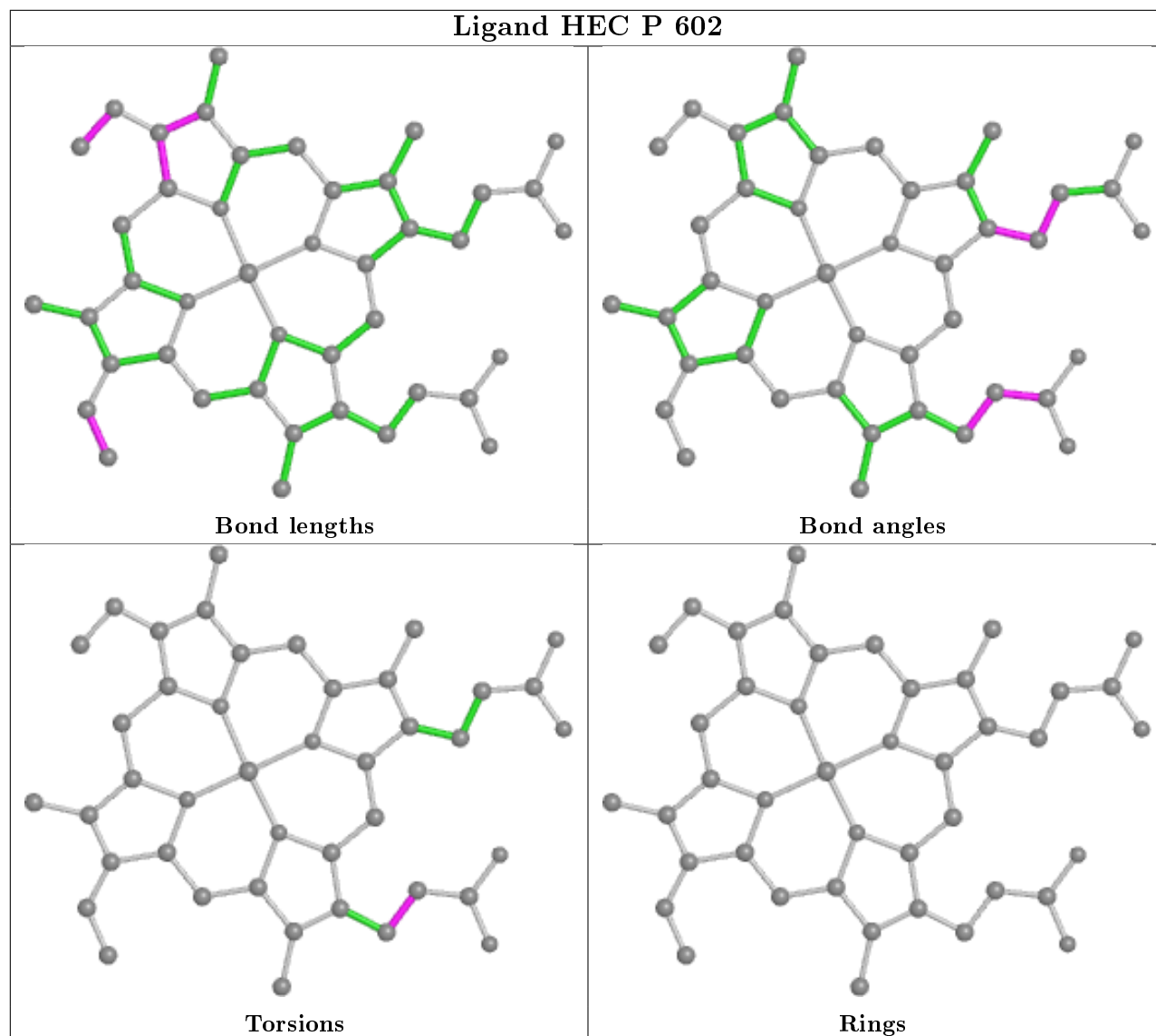
Rings

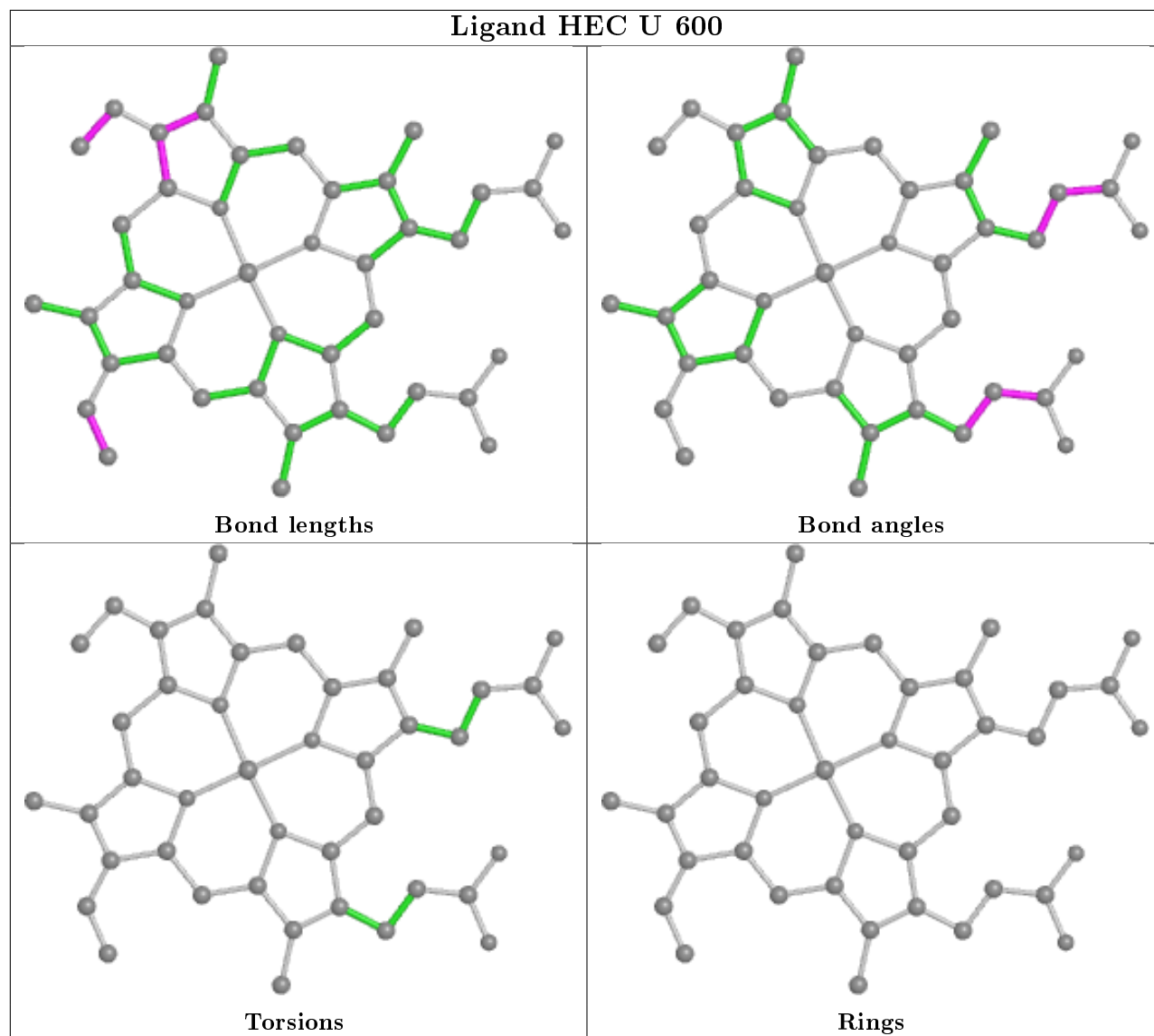


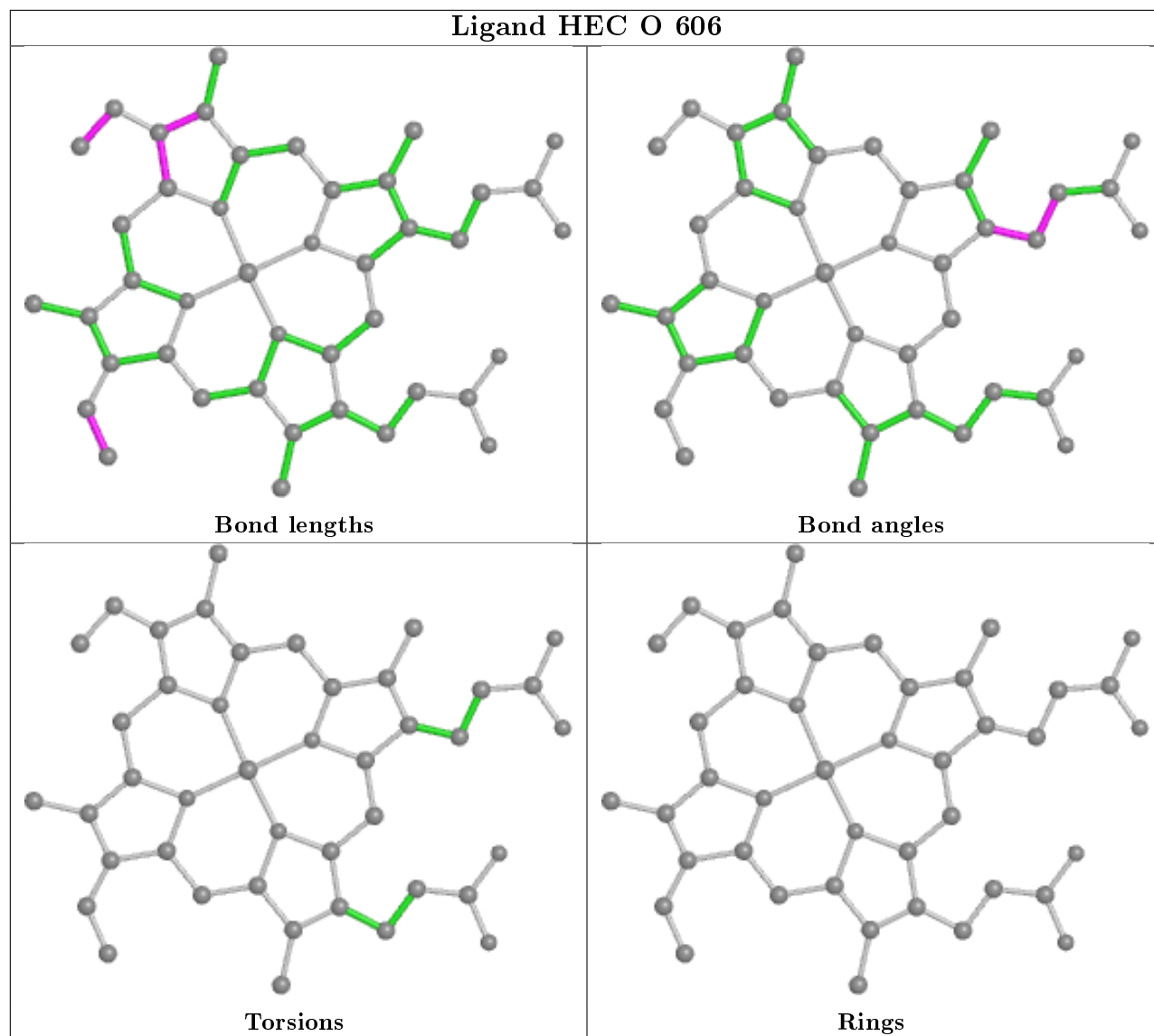




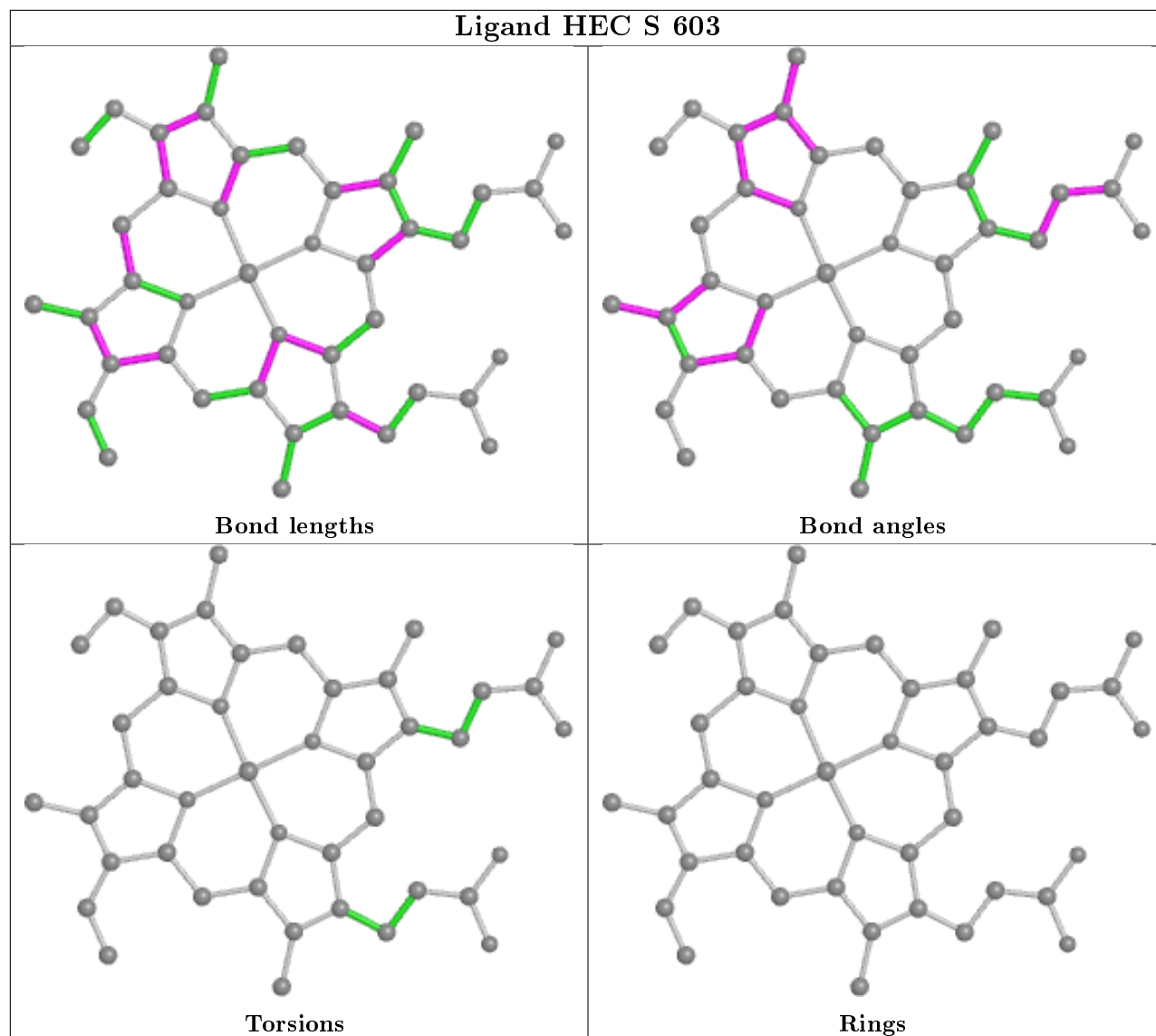
## Ligand HEC P 602

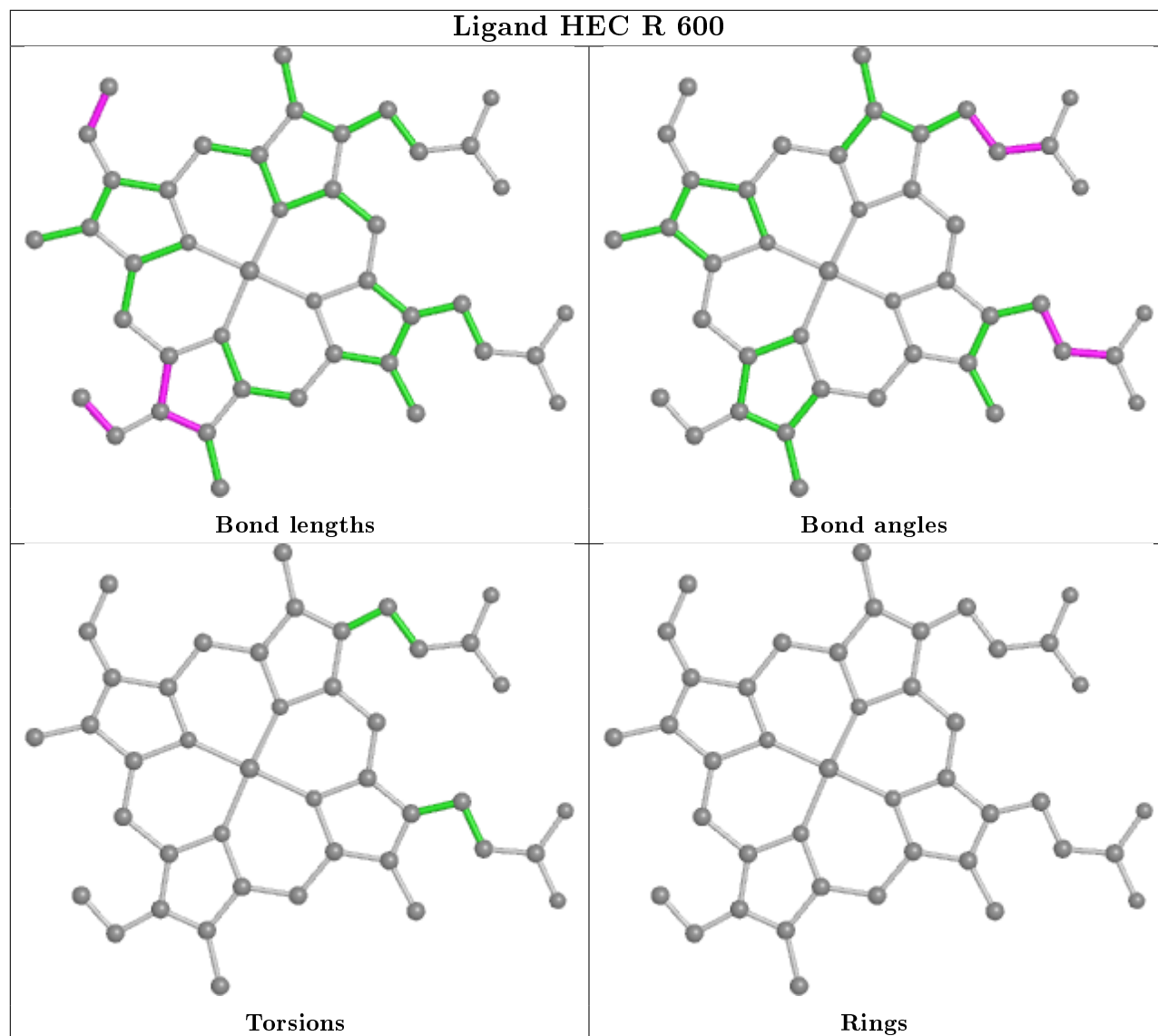


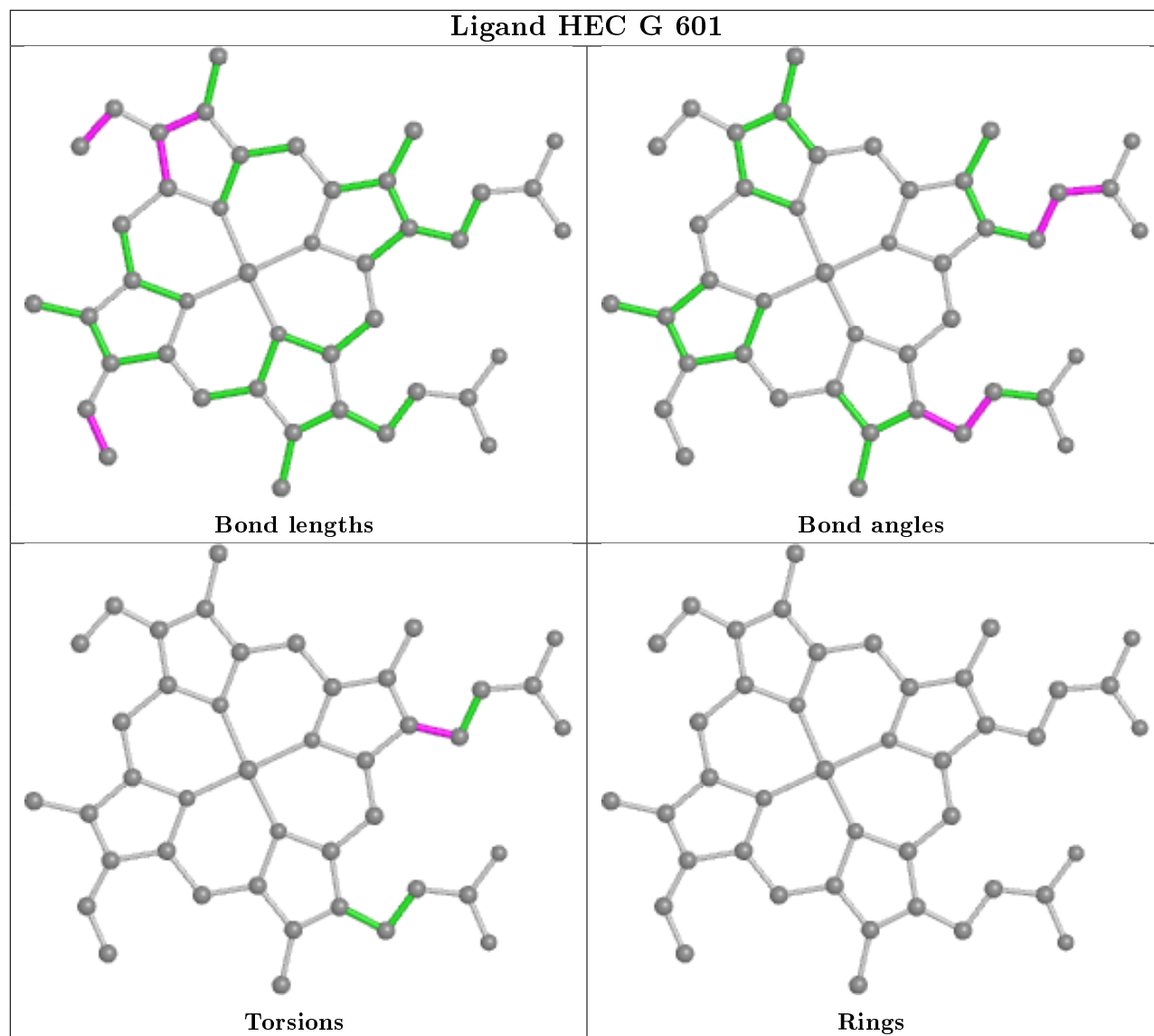


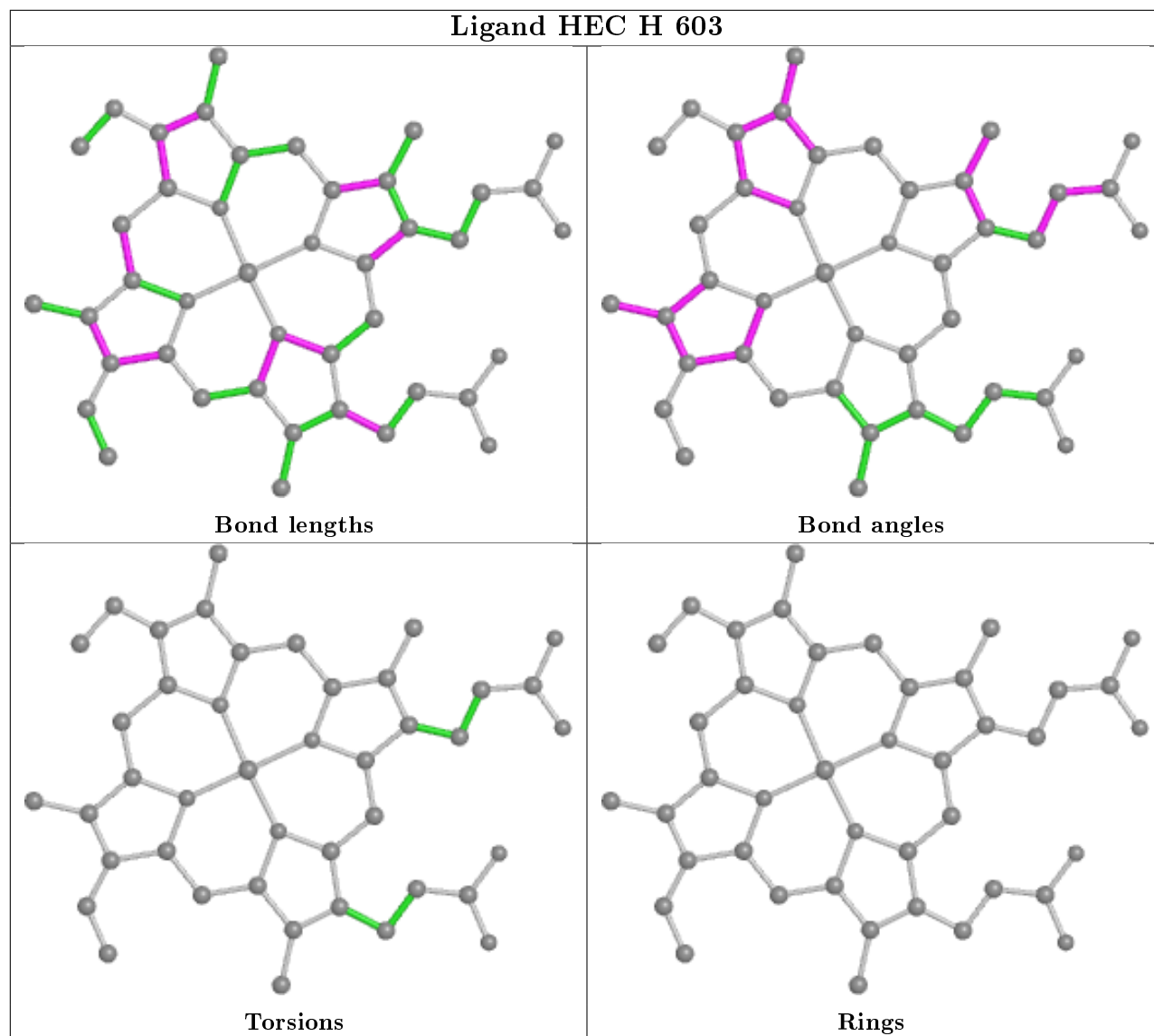


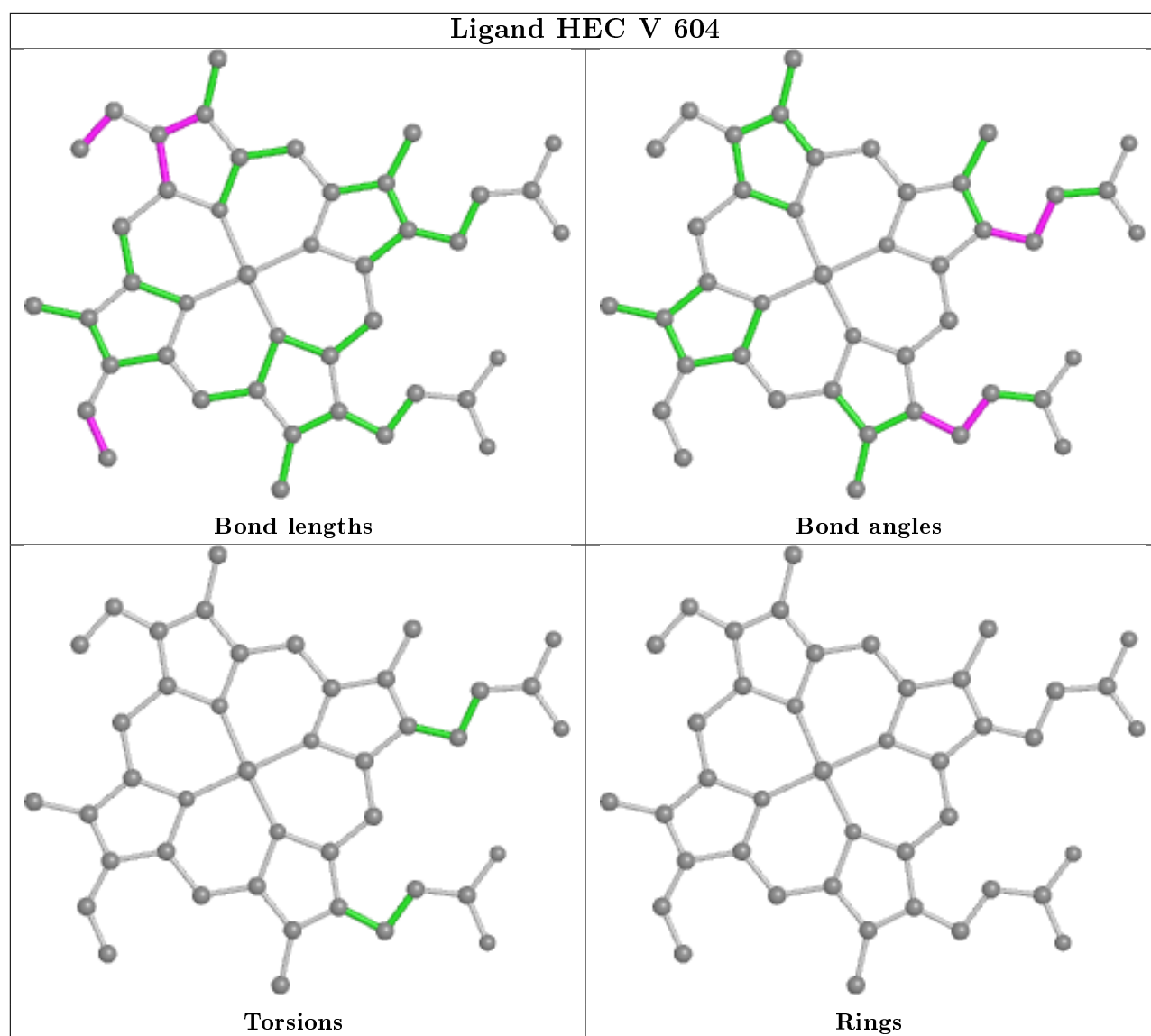
## Ligand HEC S 603





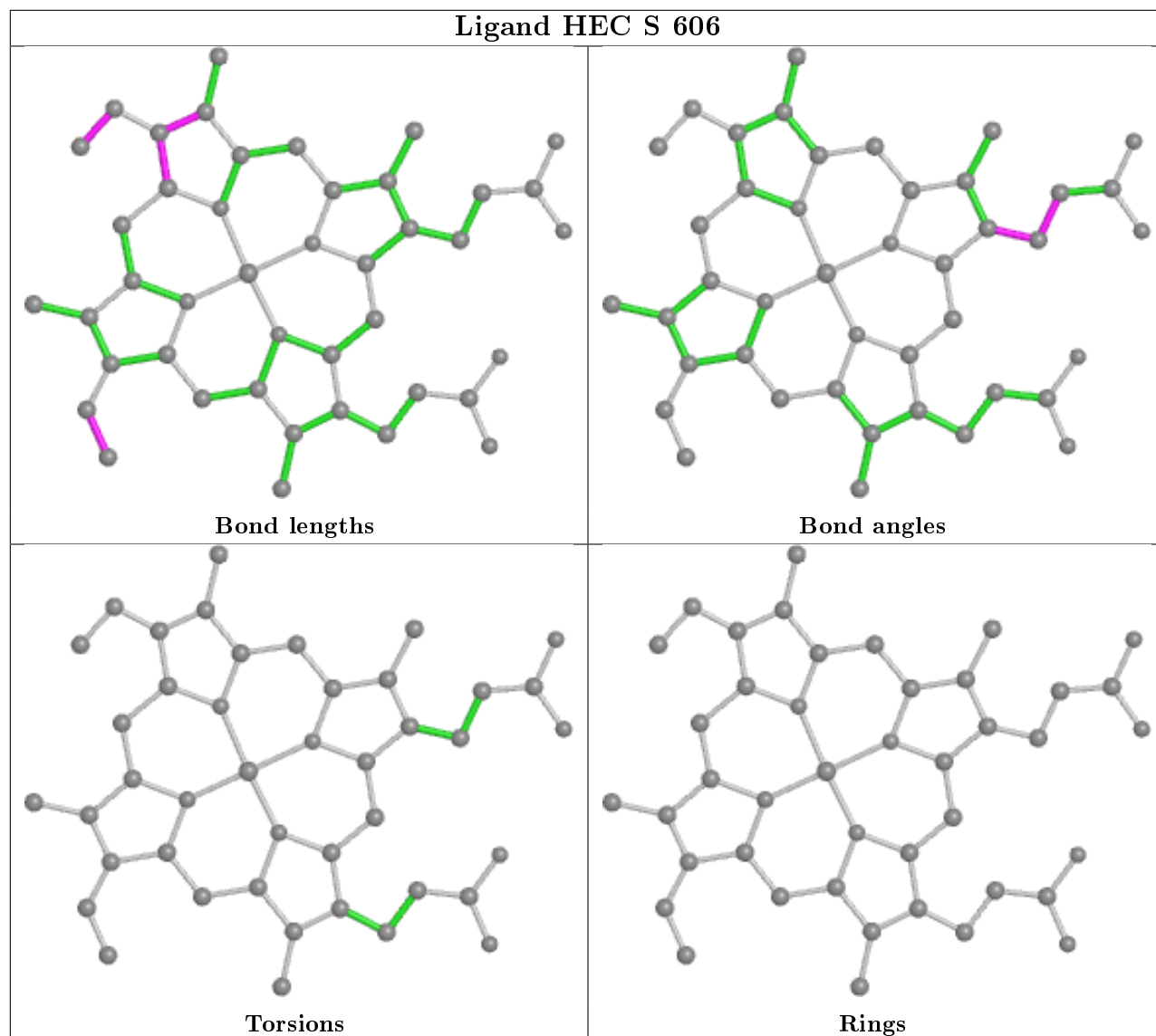




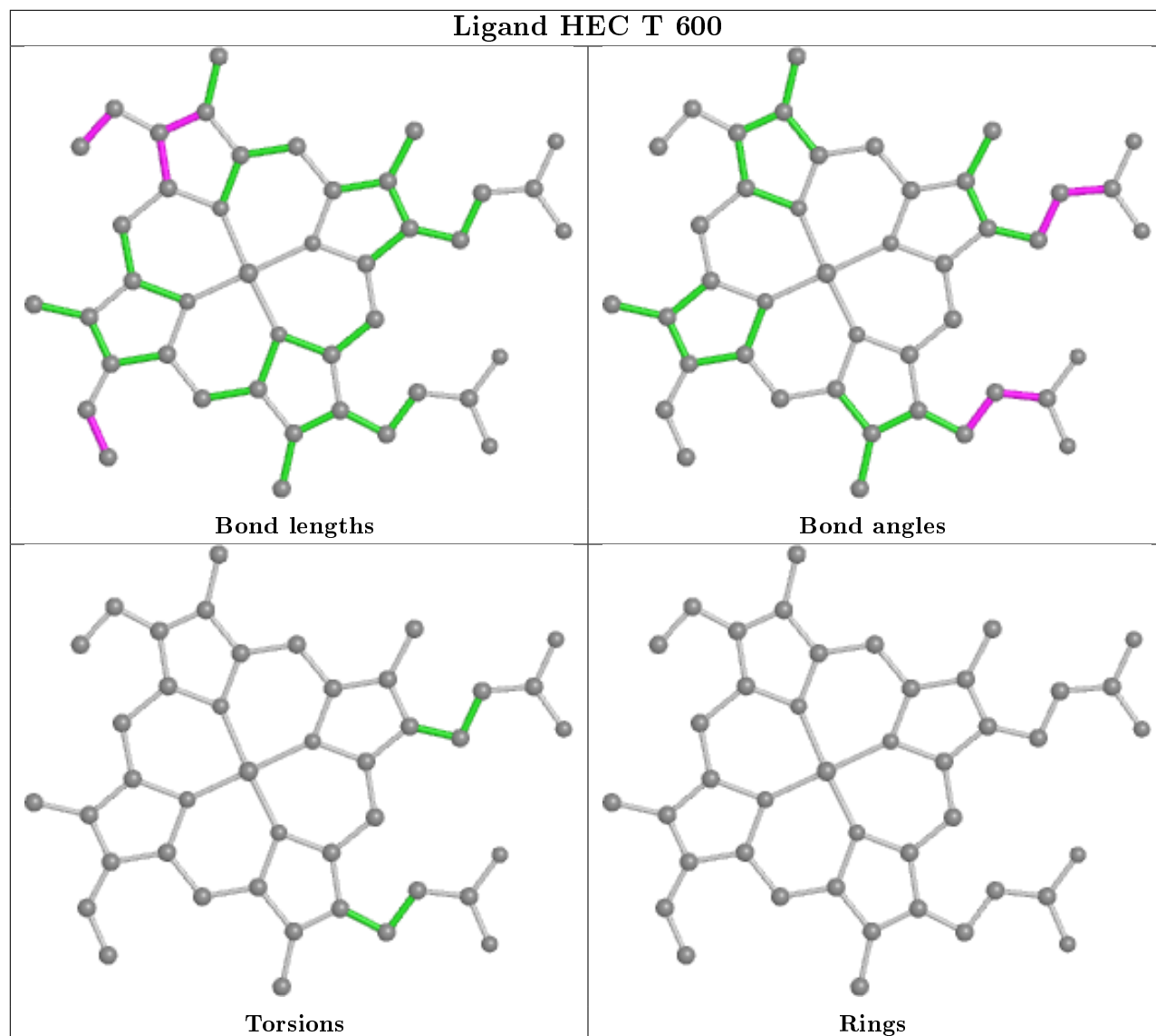


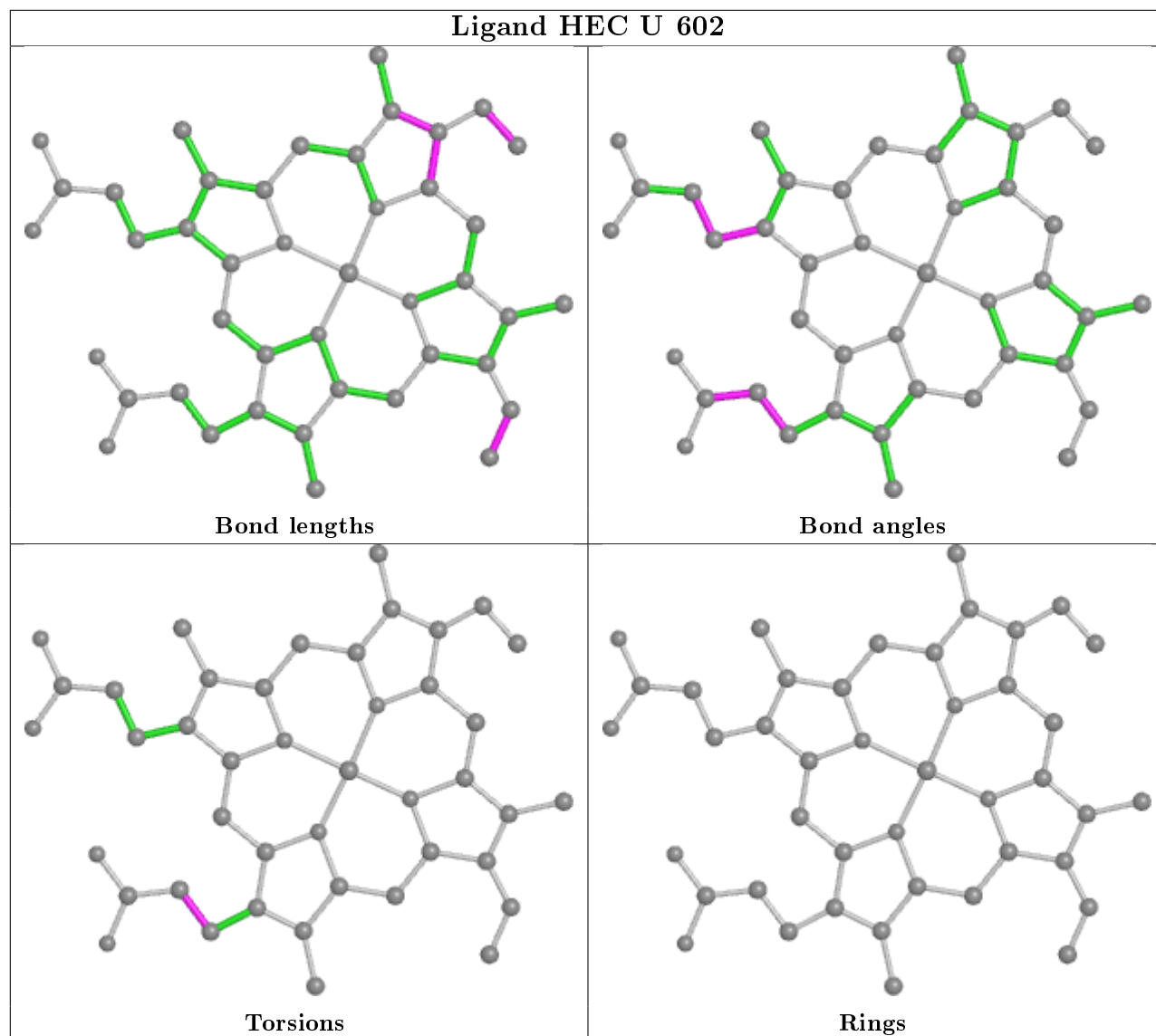


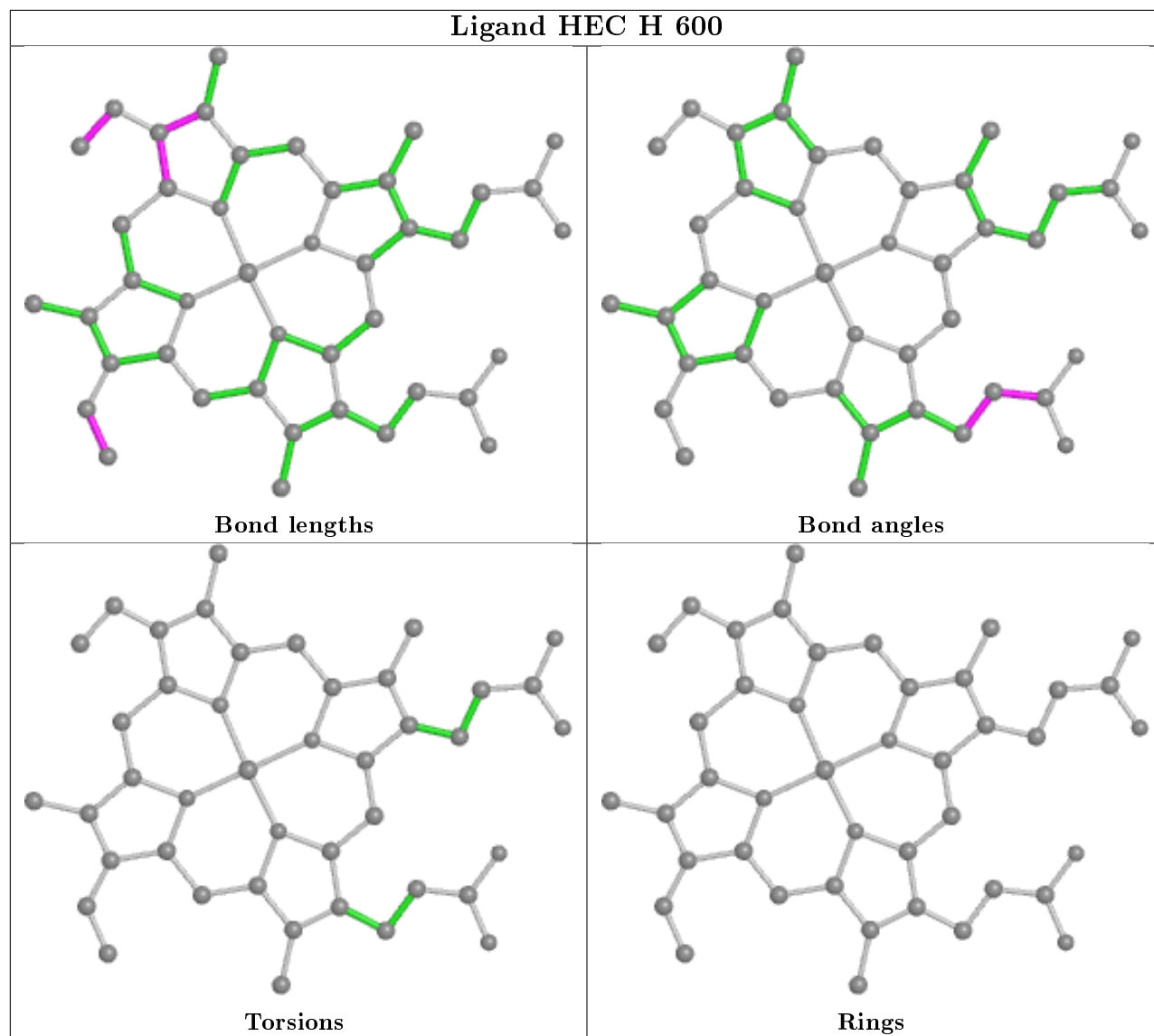
## Ligand HEC S 606

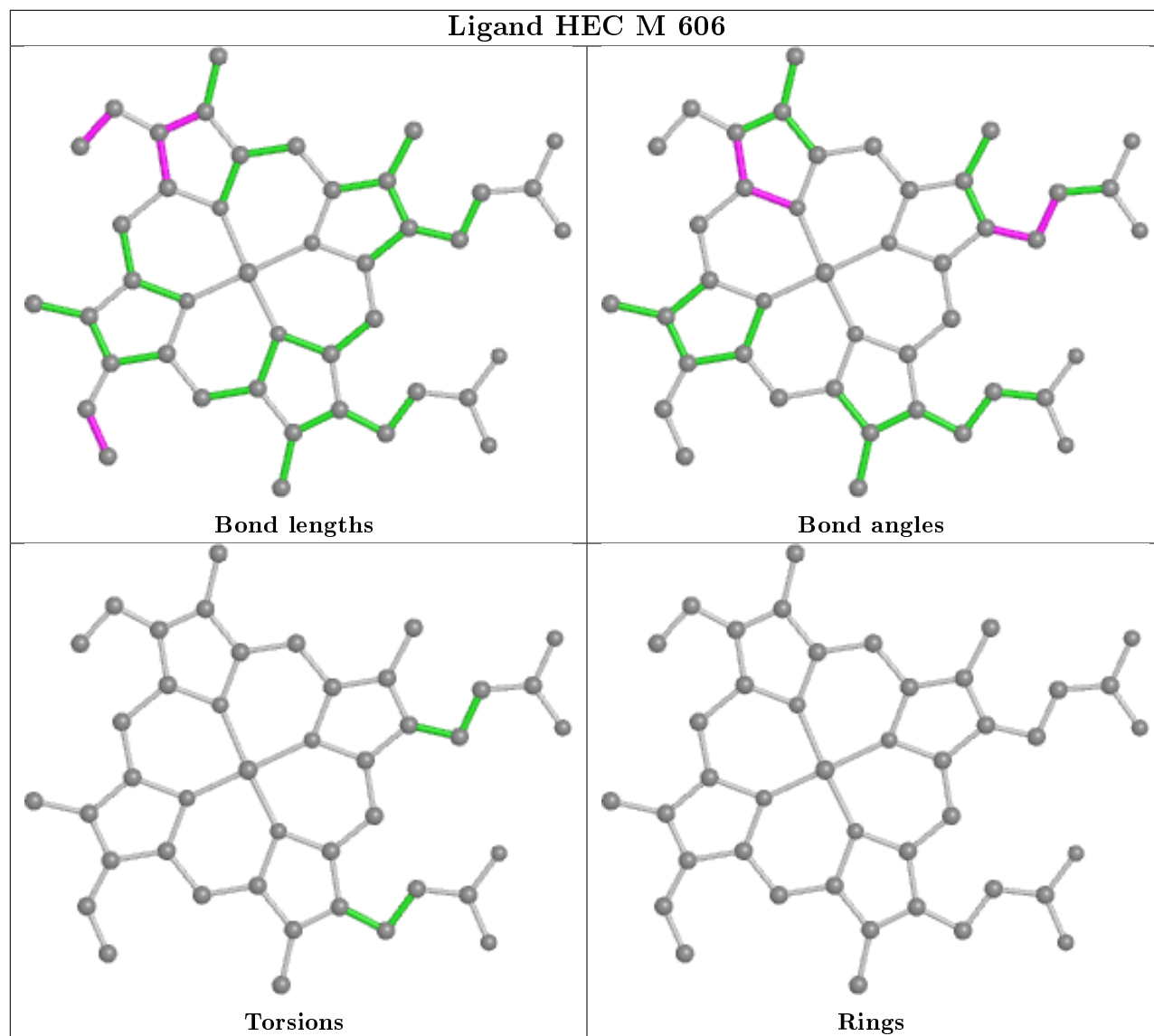


## Ligand HEC T 600

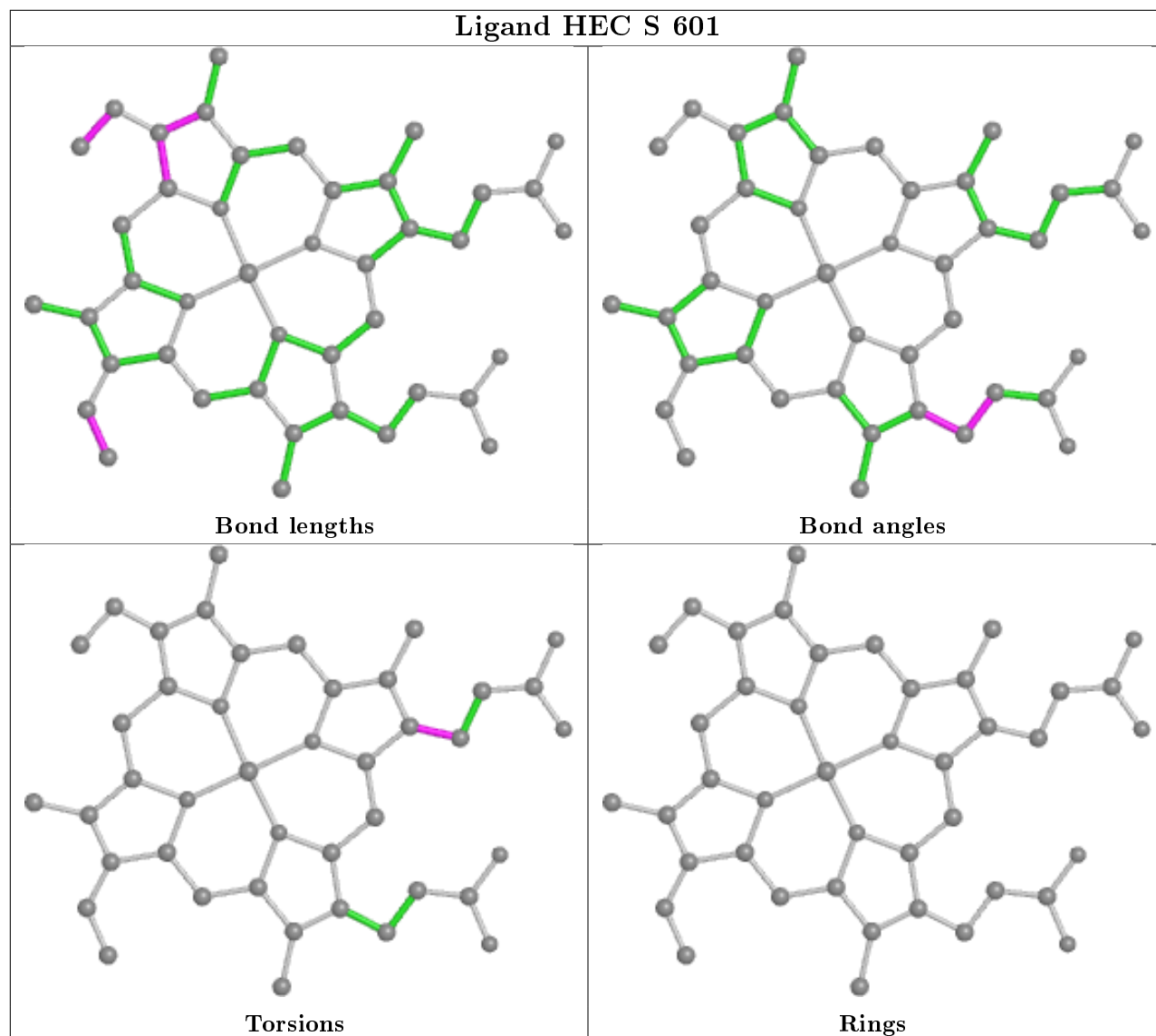


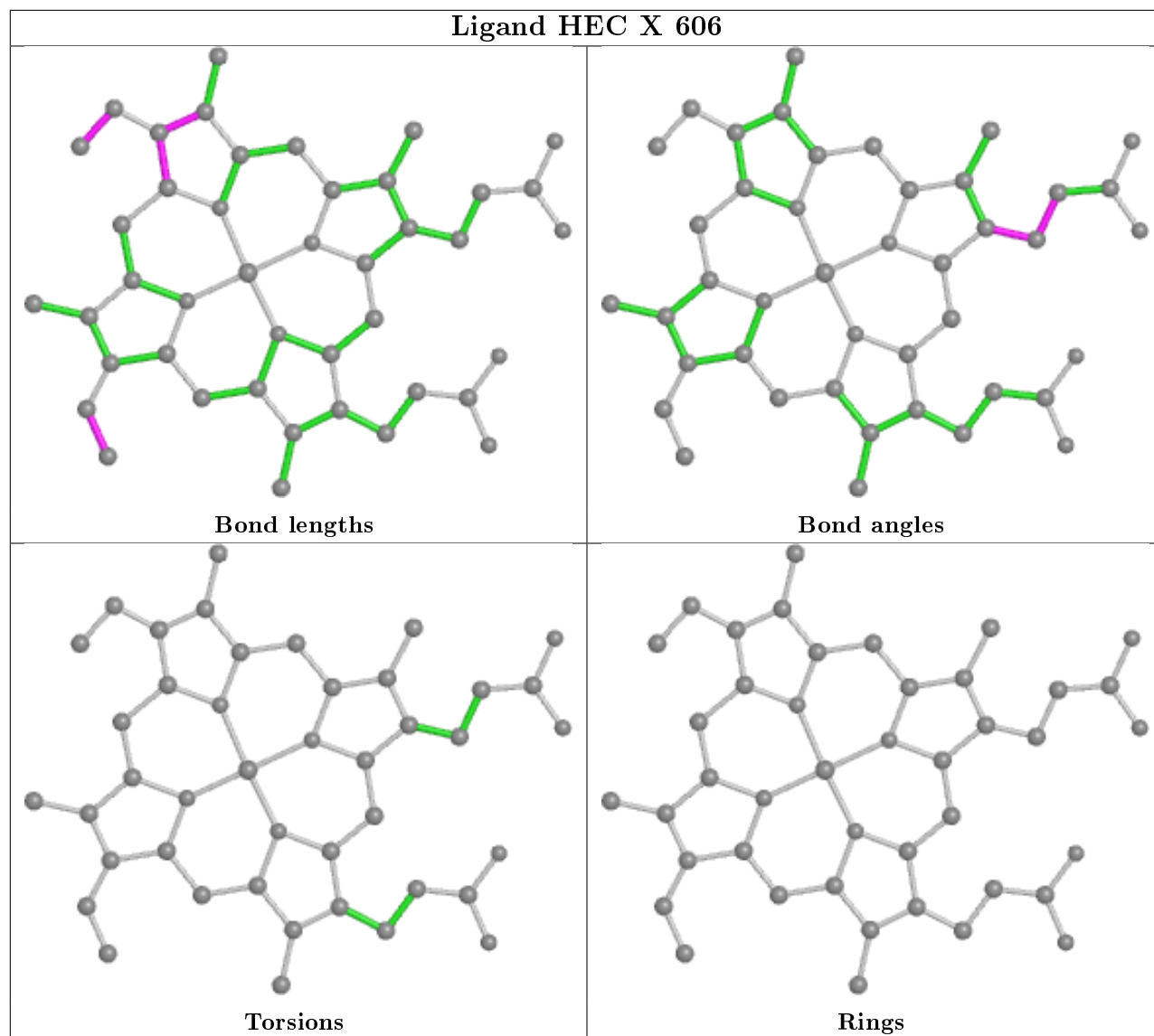


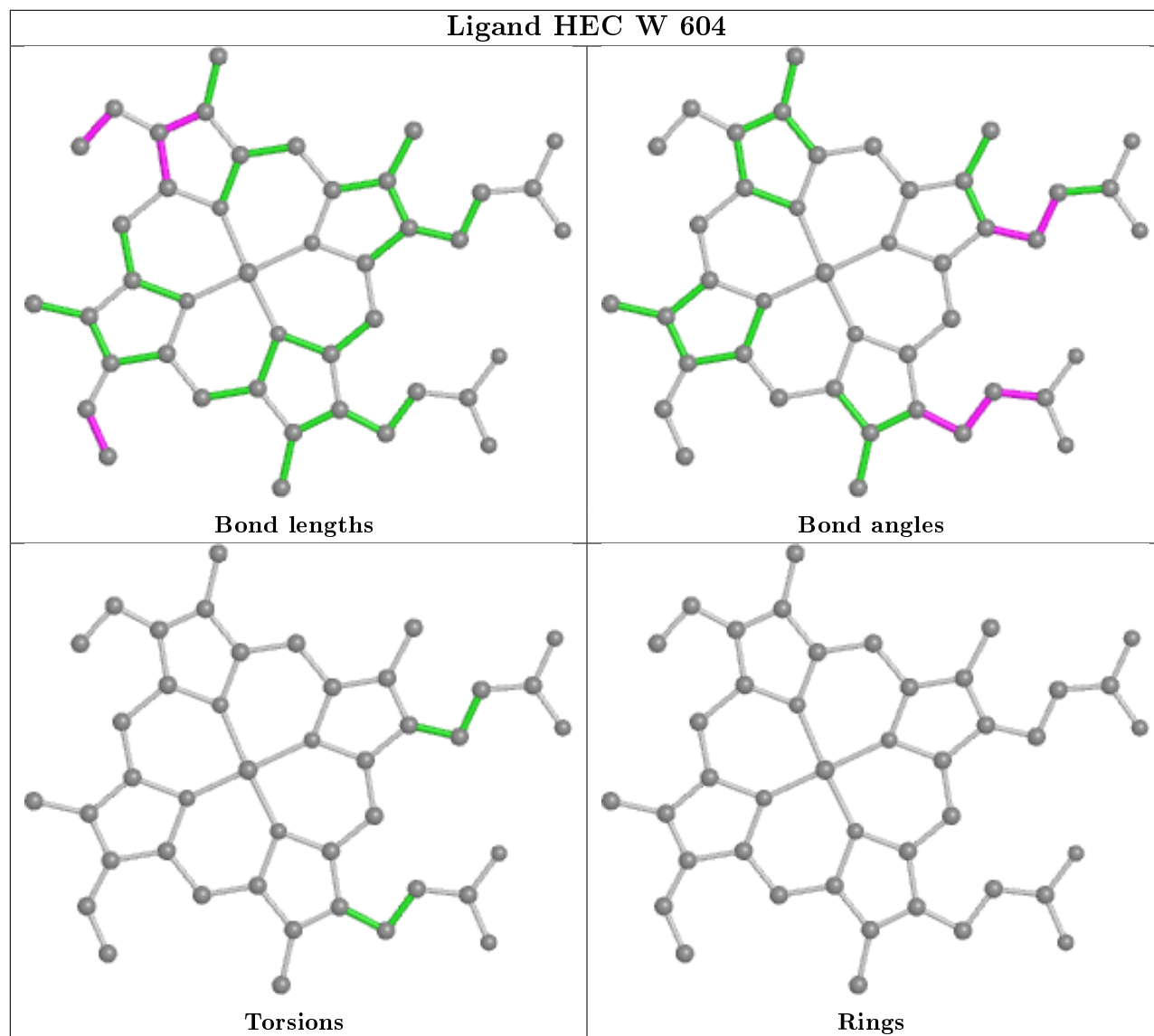




## Ligand HEC S 601

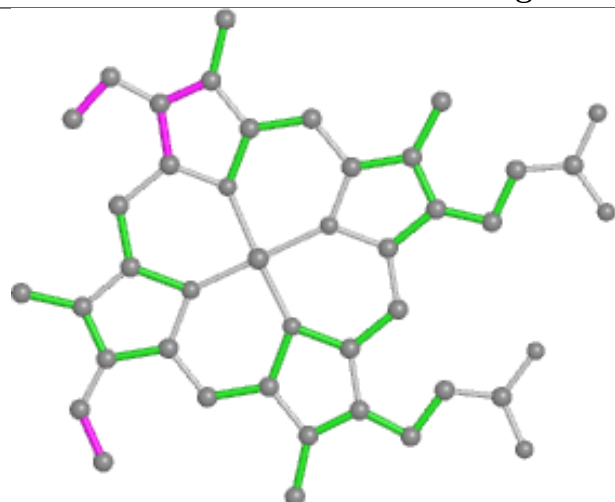




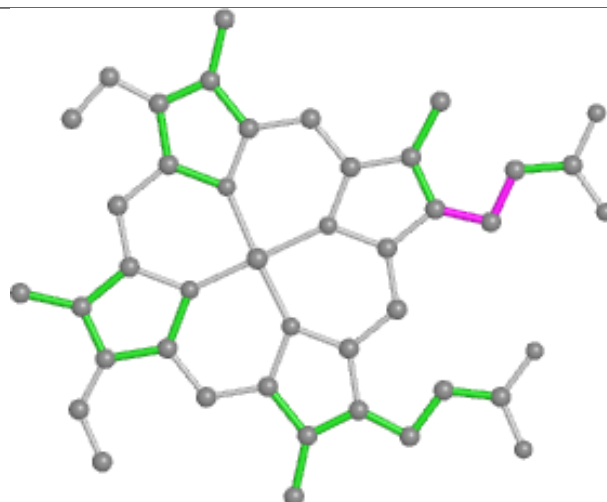




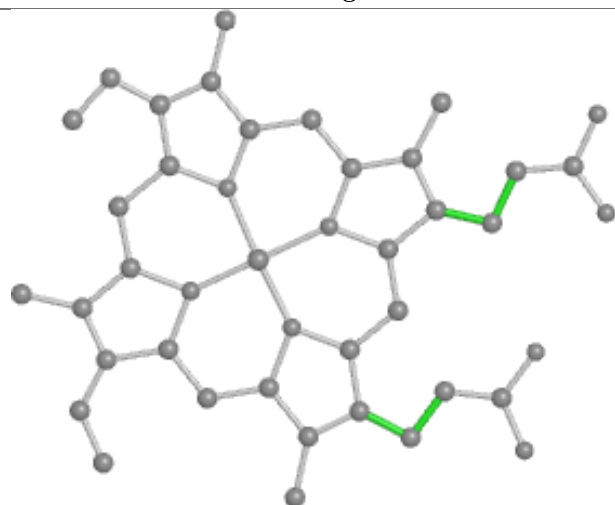
## Ligand HEC T 606



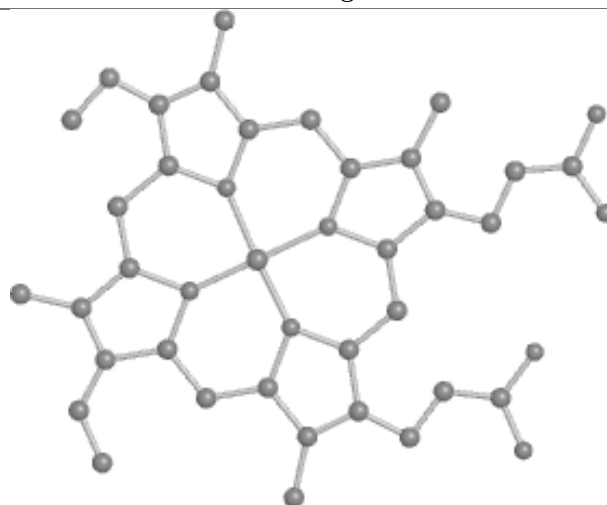
Bond lengths



Bond angles

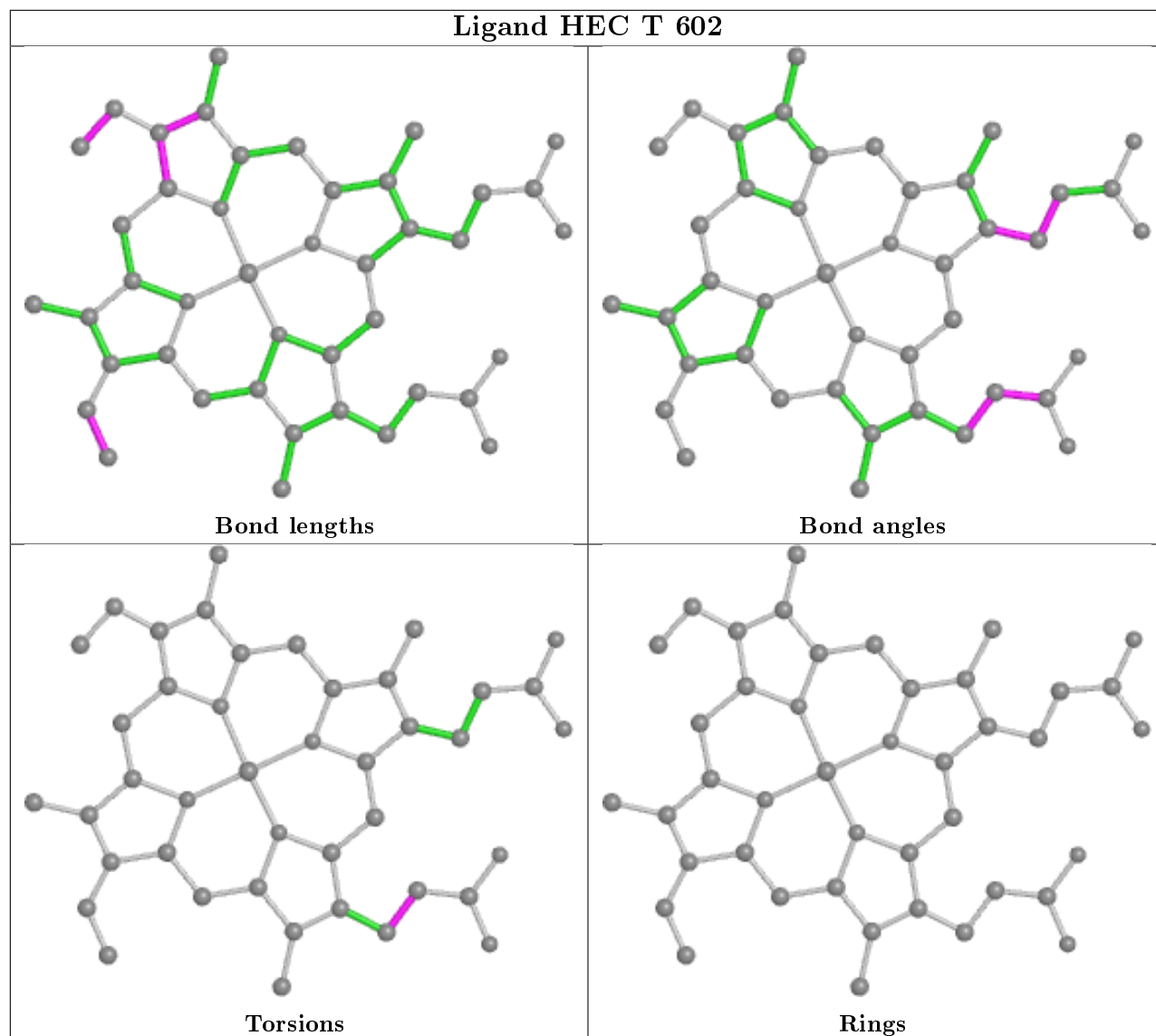


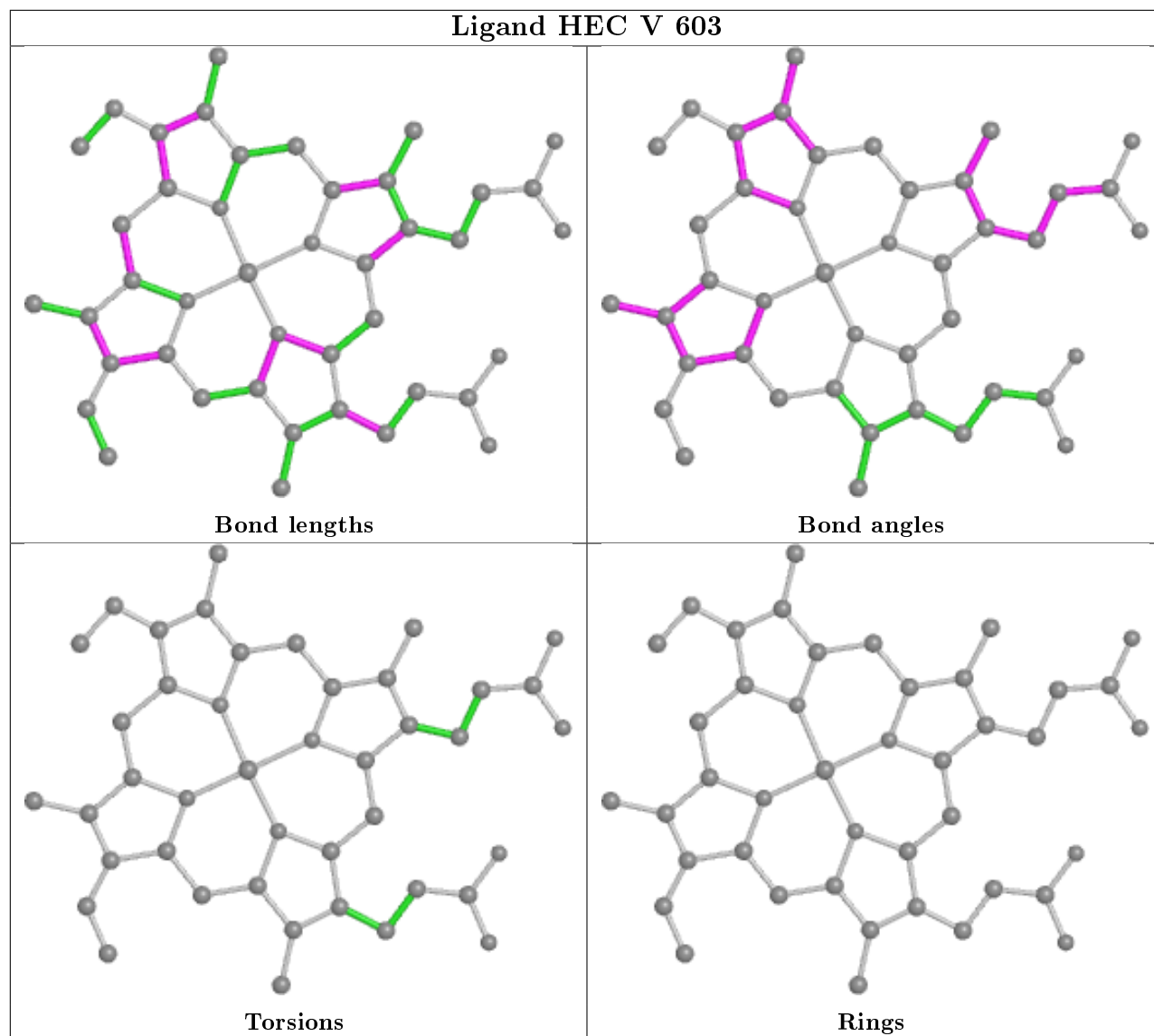
Torsions



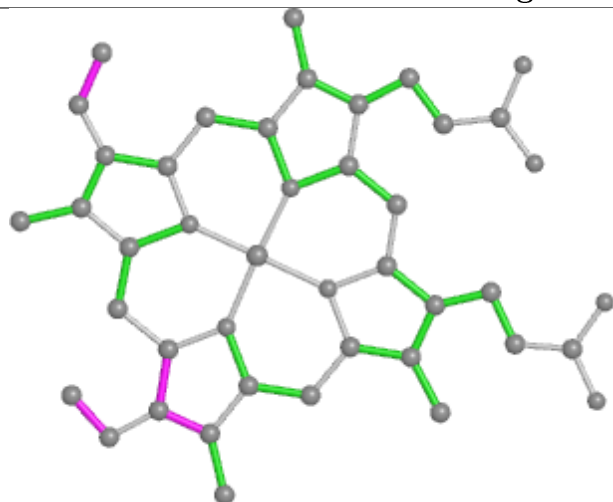
Rings

## Ligand HEC T 602

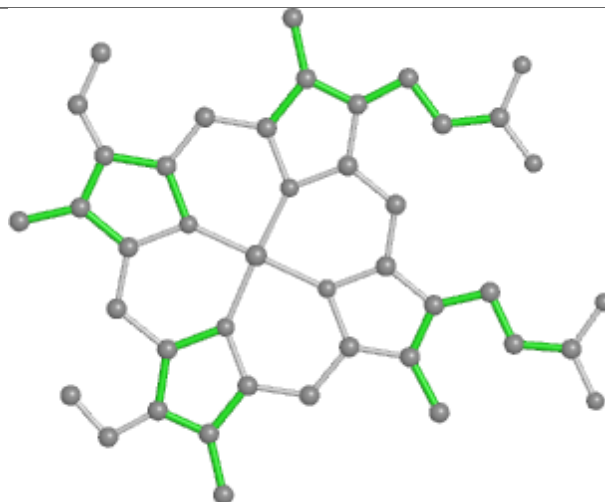




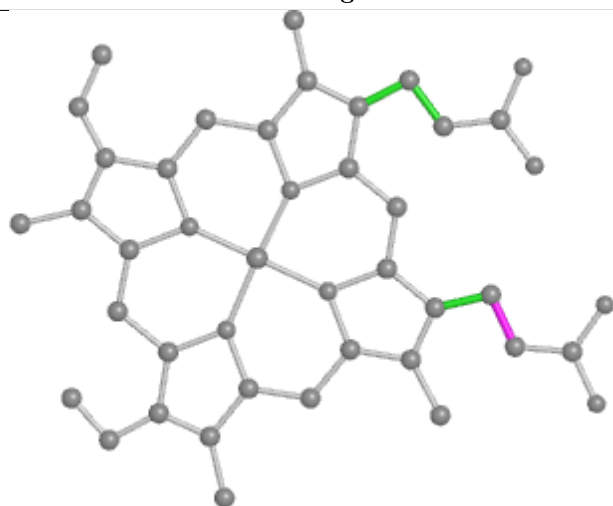
## Ligand HEC S 607



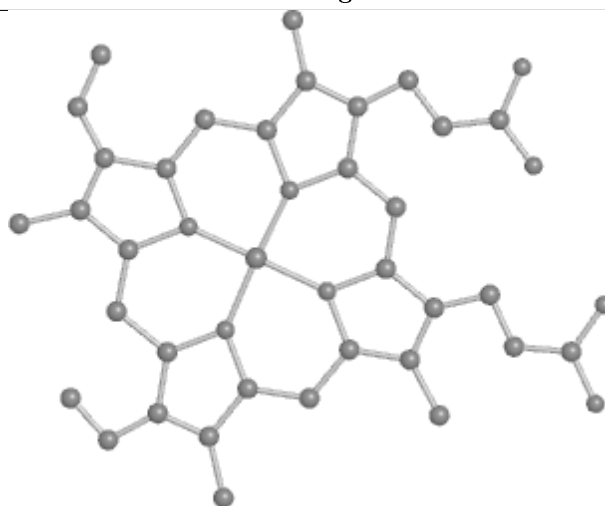
Bond lengths



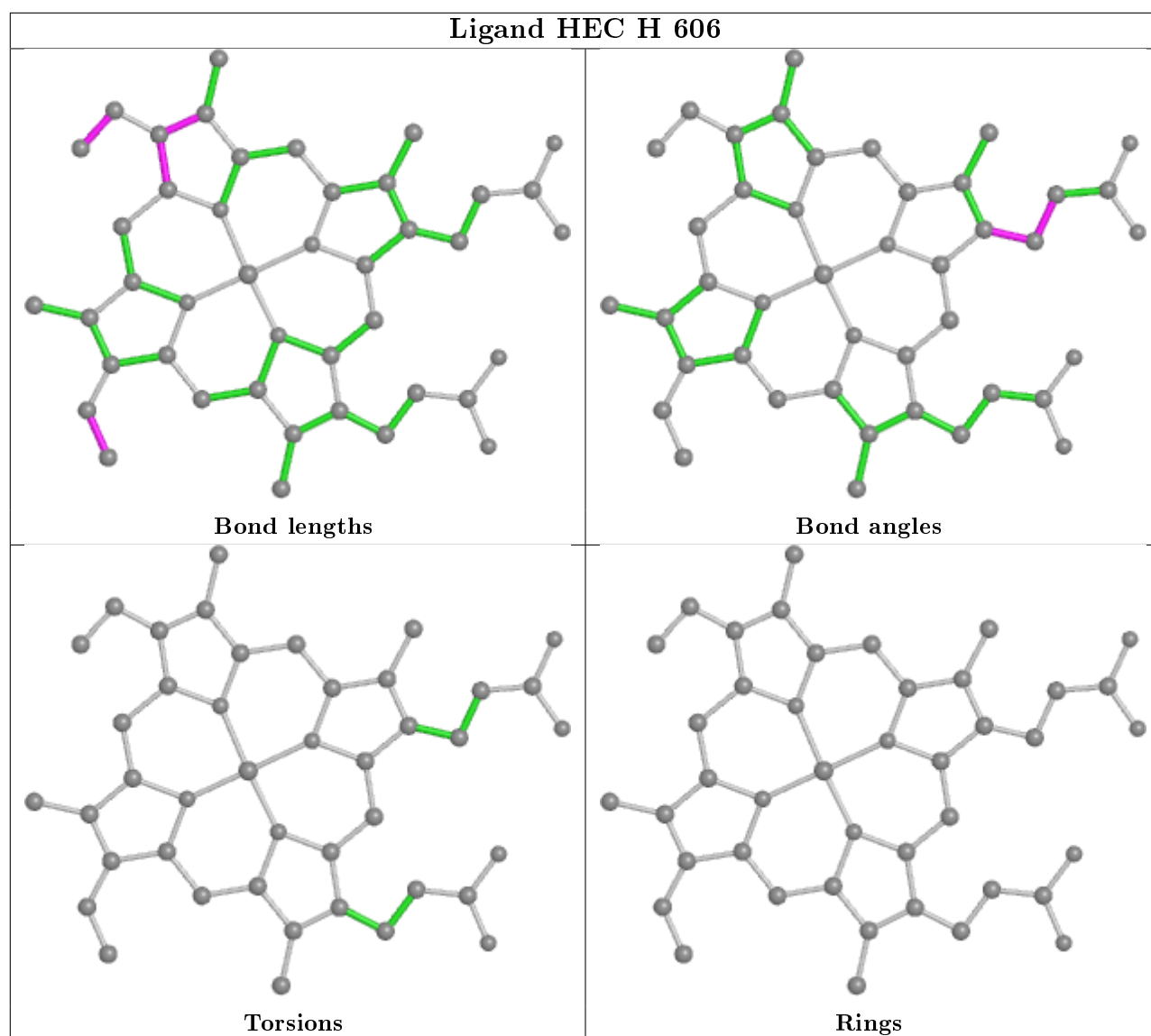
Bond angles



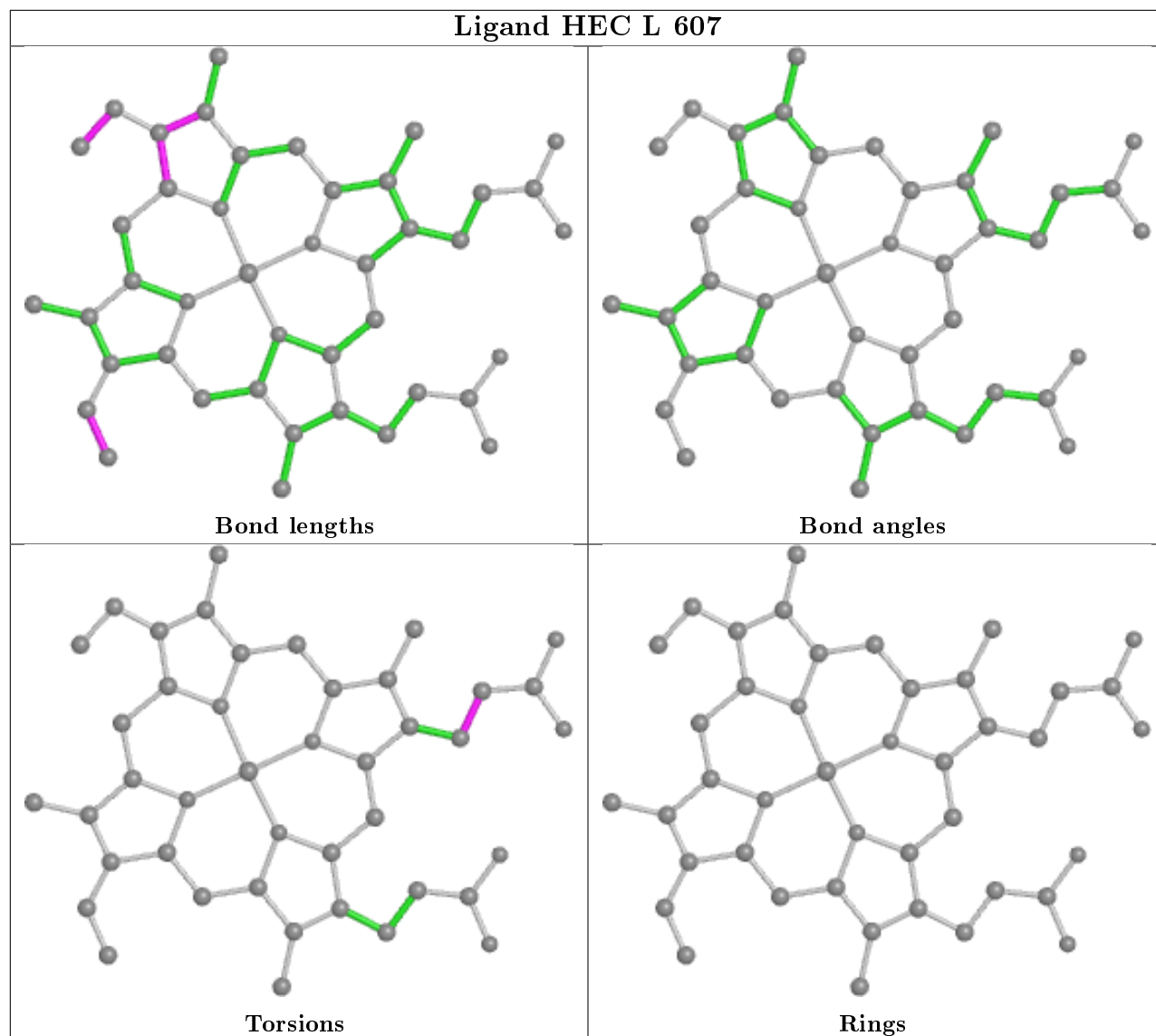
Torsions

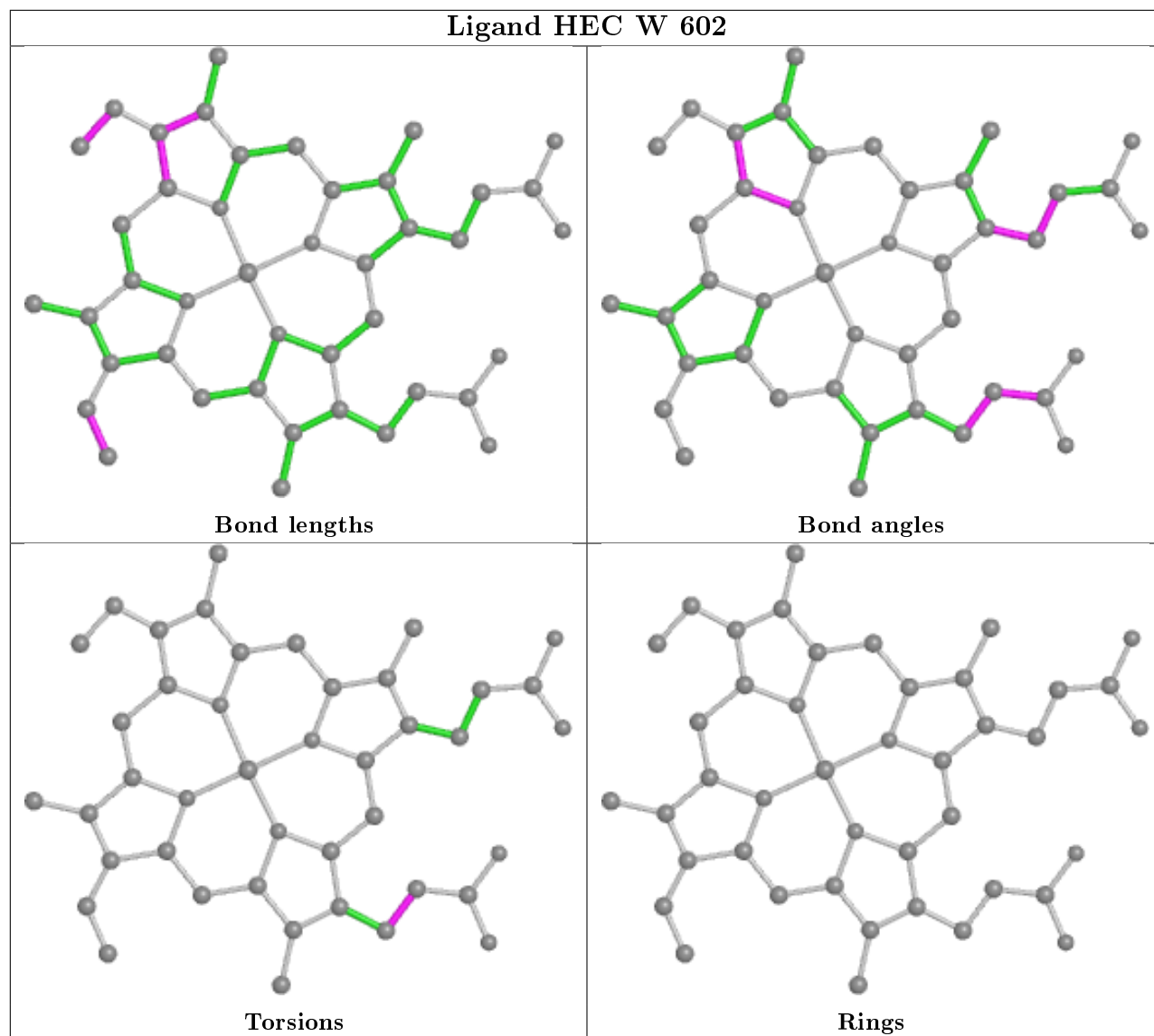


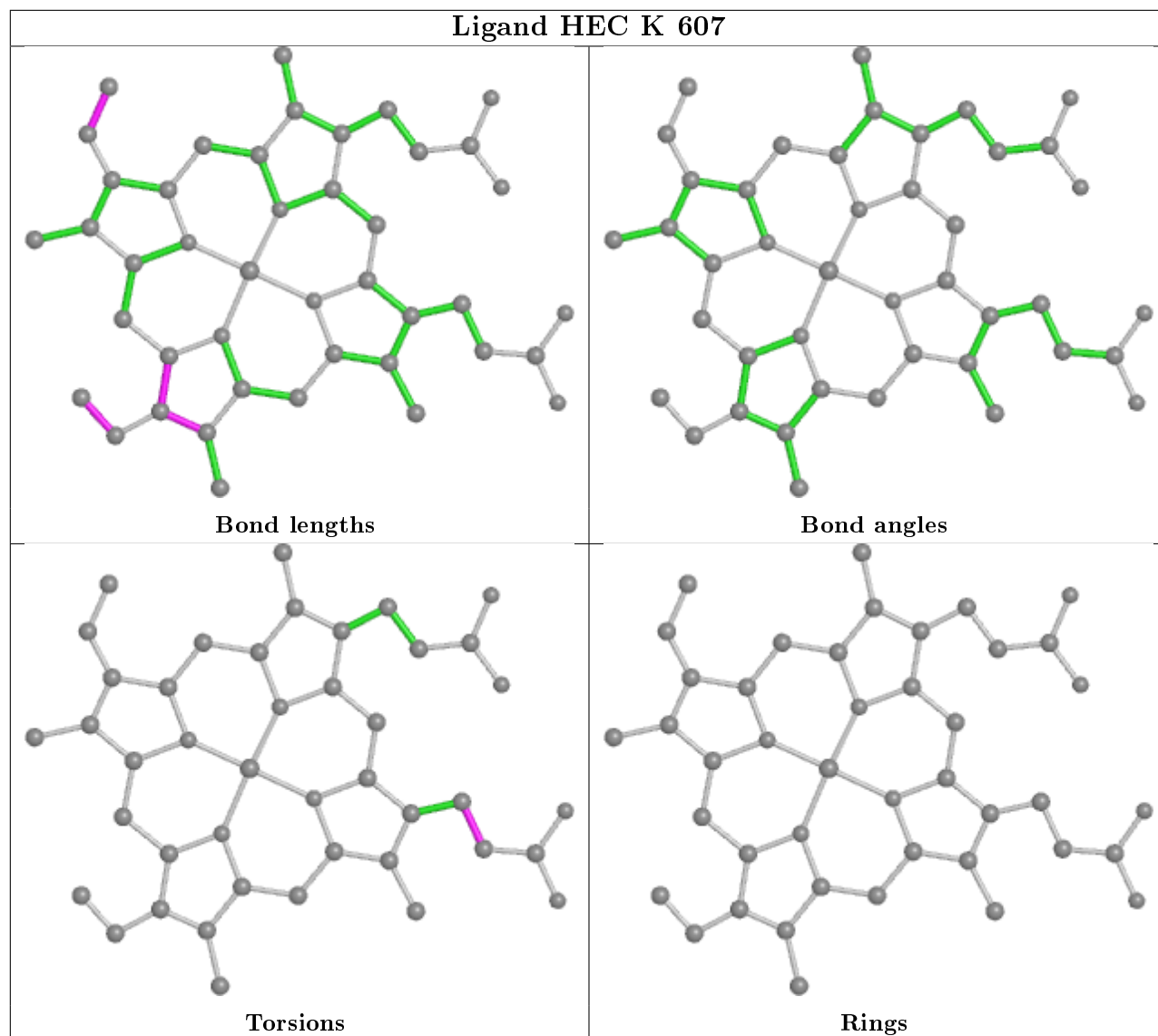
Rings



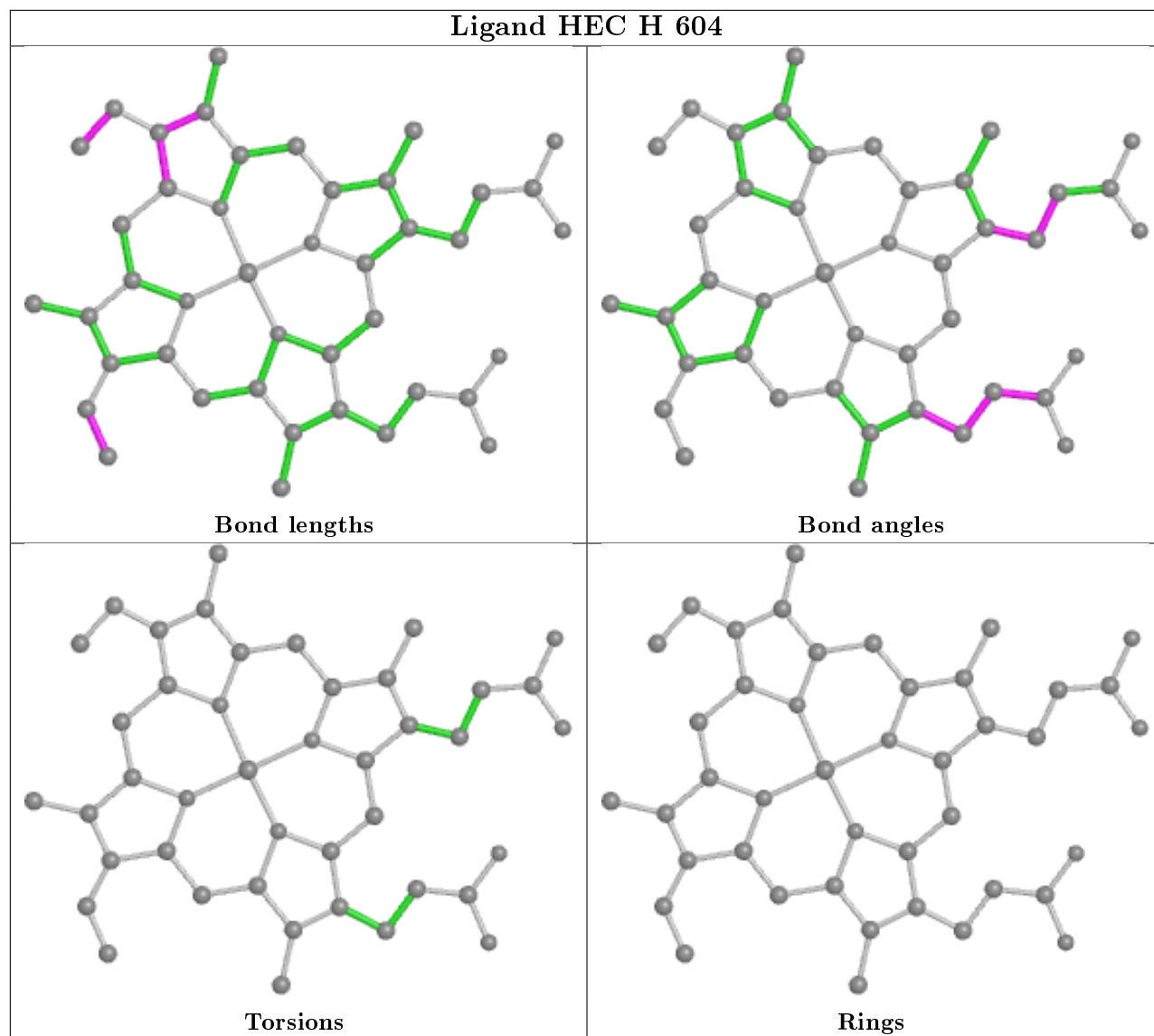
## Ligand HEC L 607

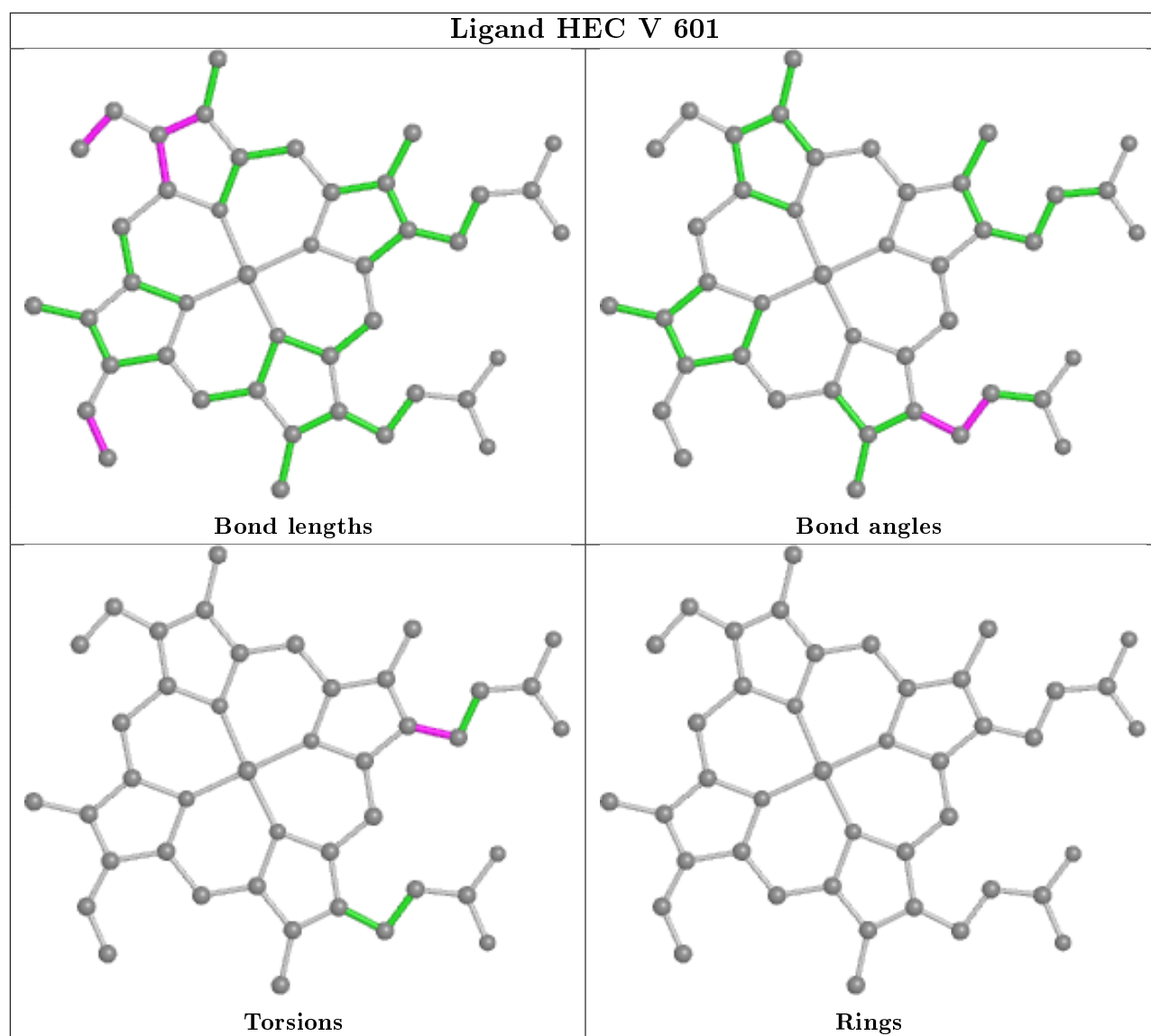




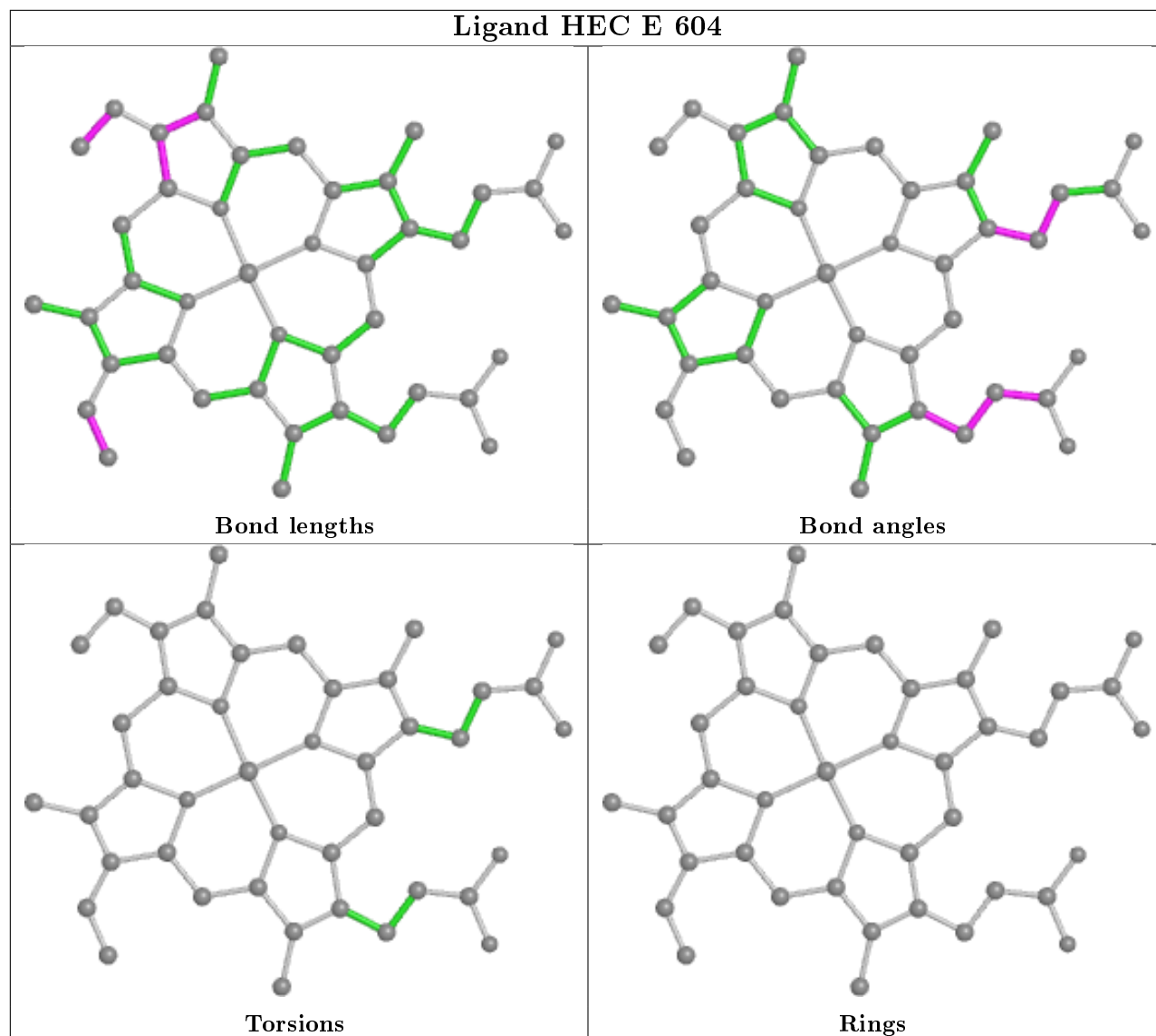


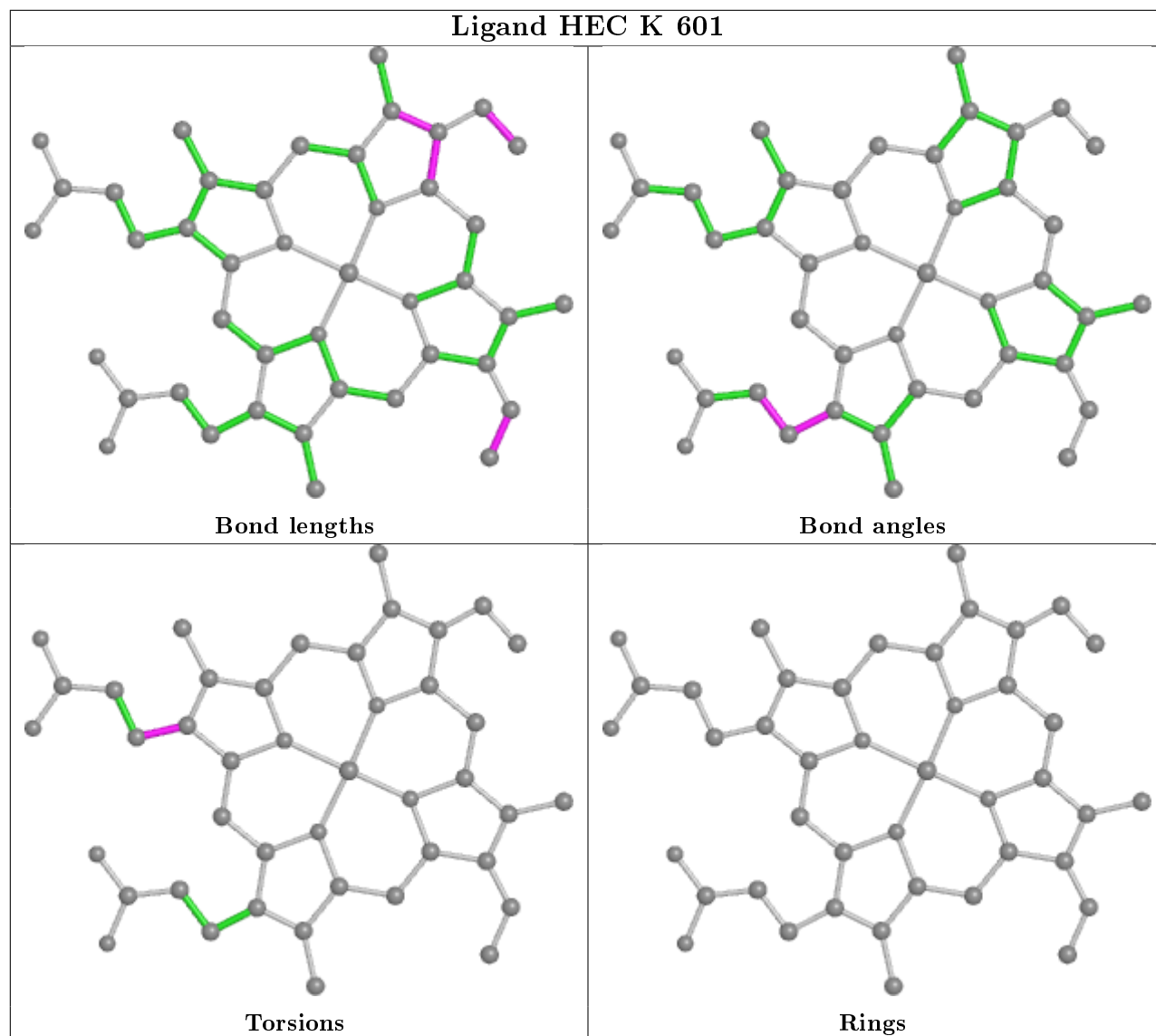




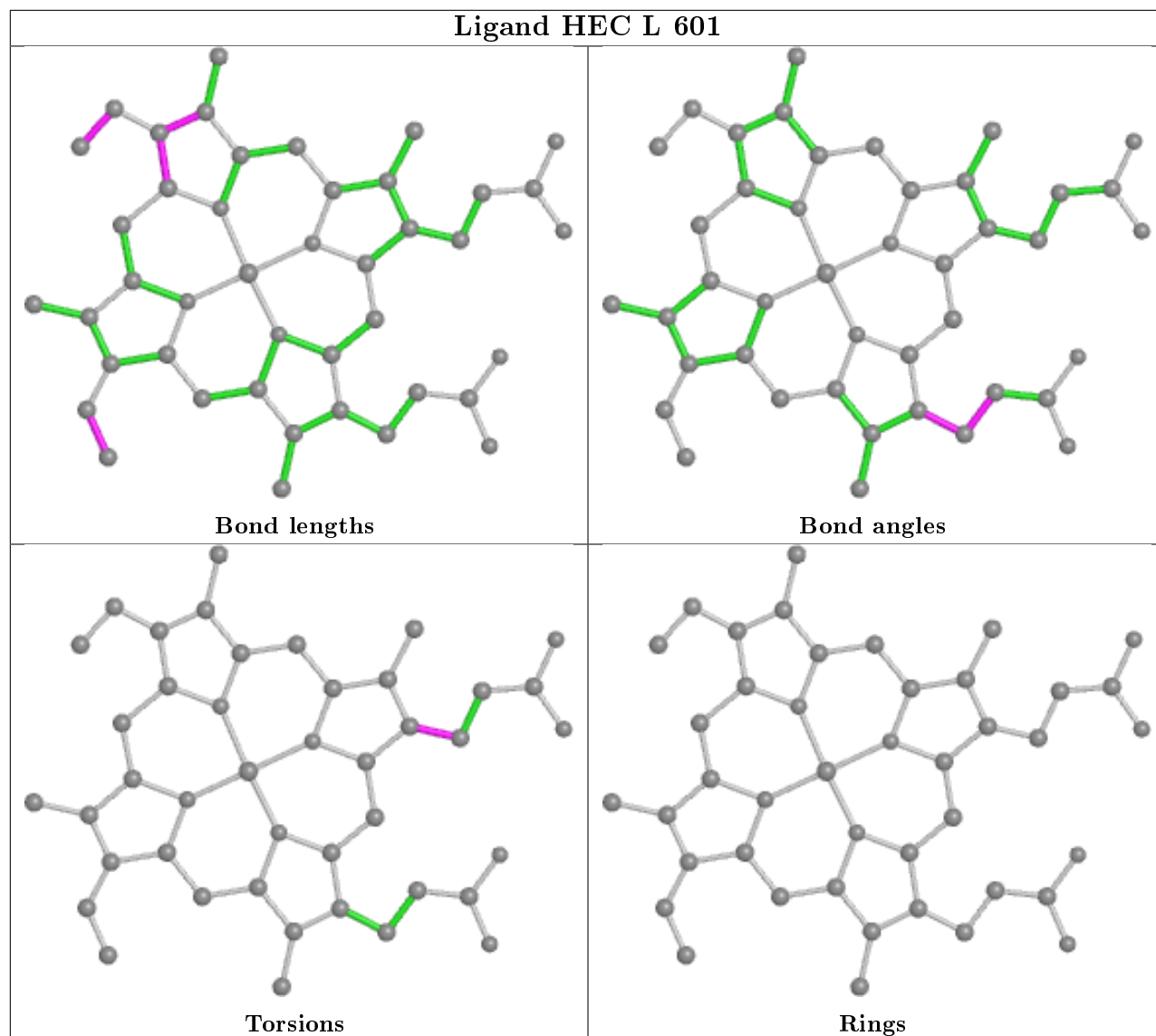


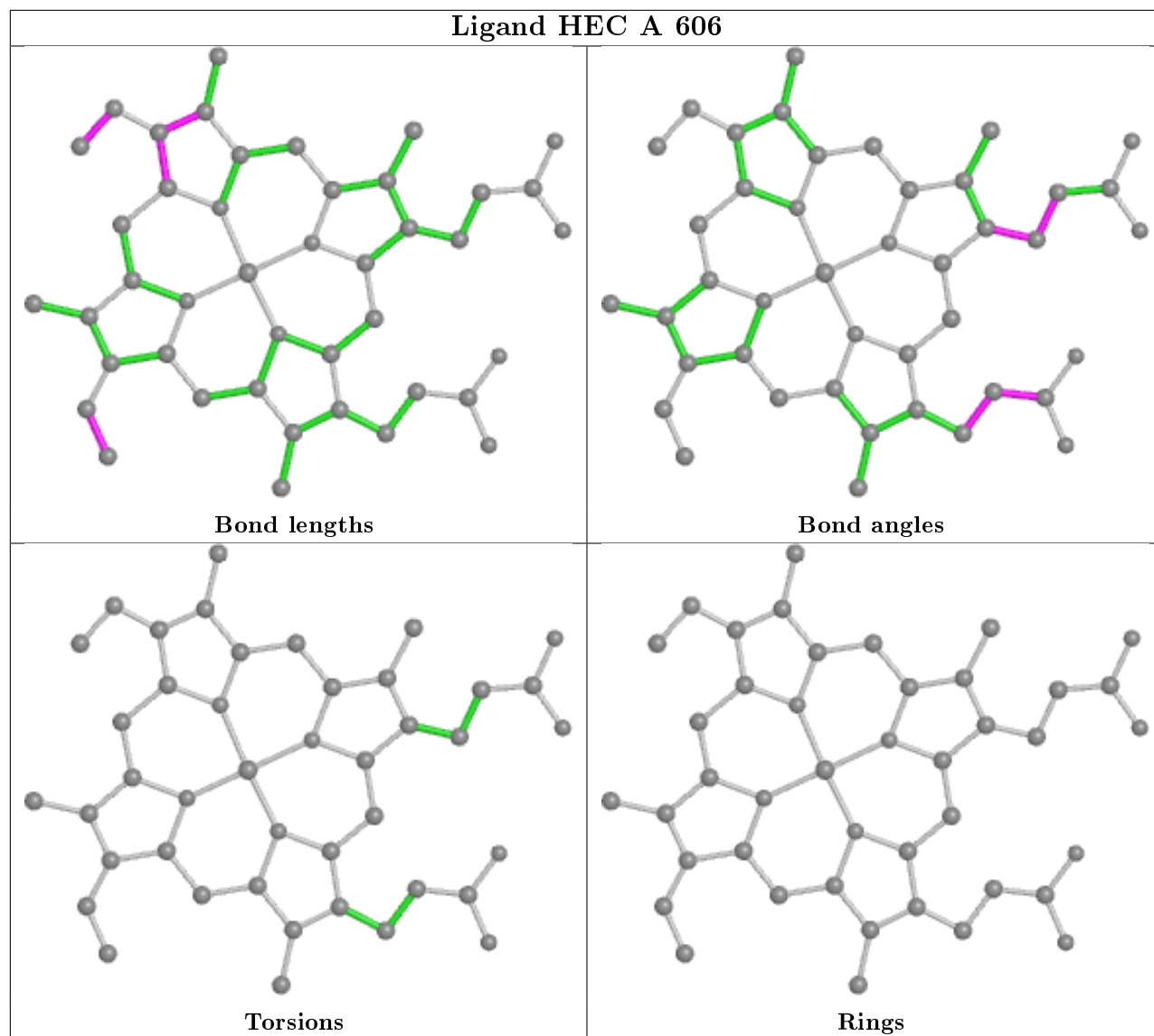
## Ligand HEC E 604

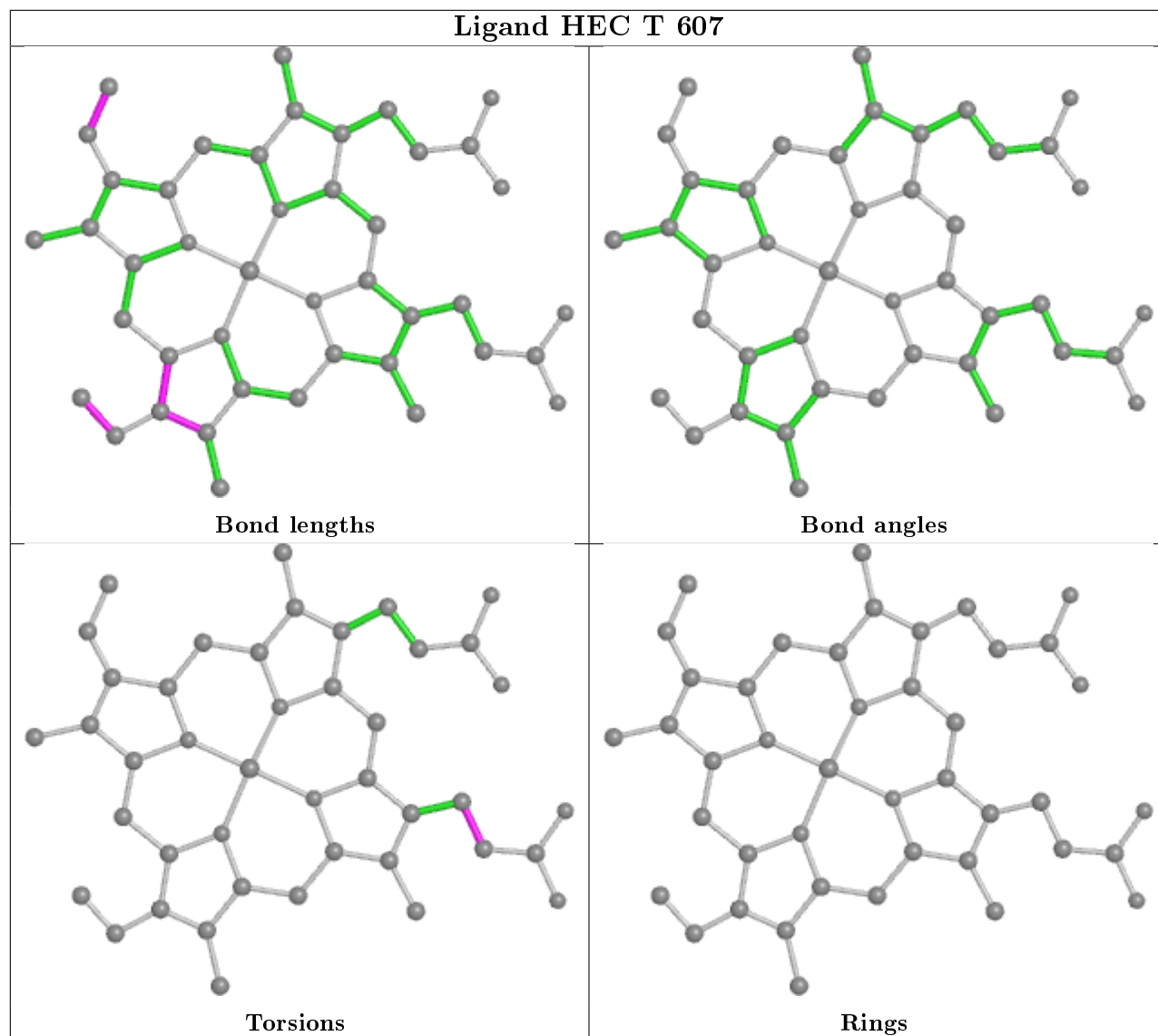


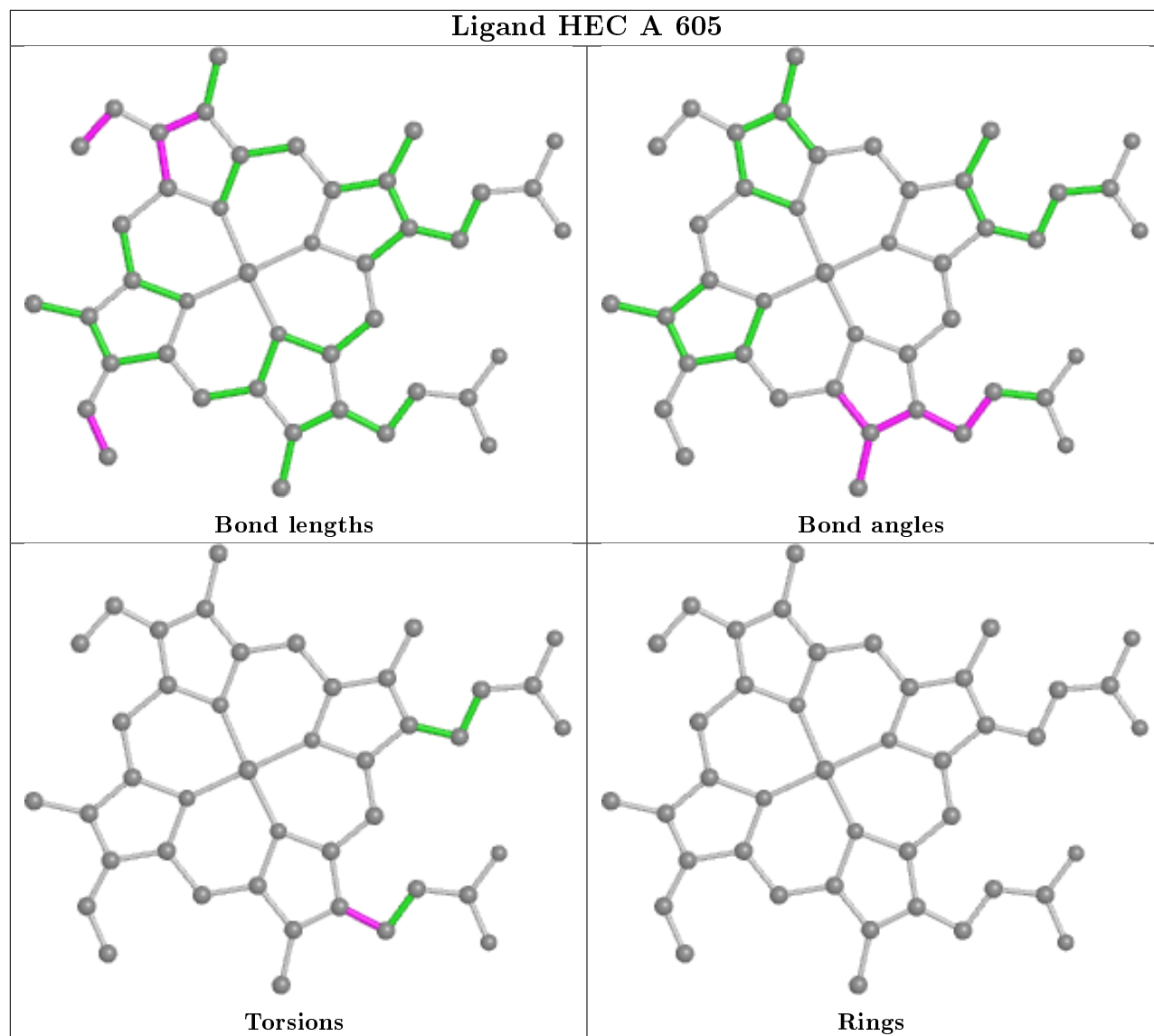


## Ligand HEC L 601

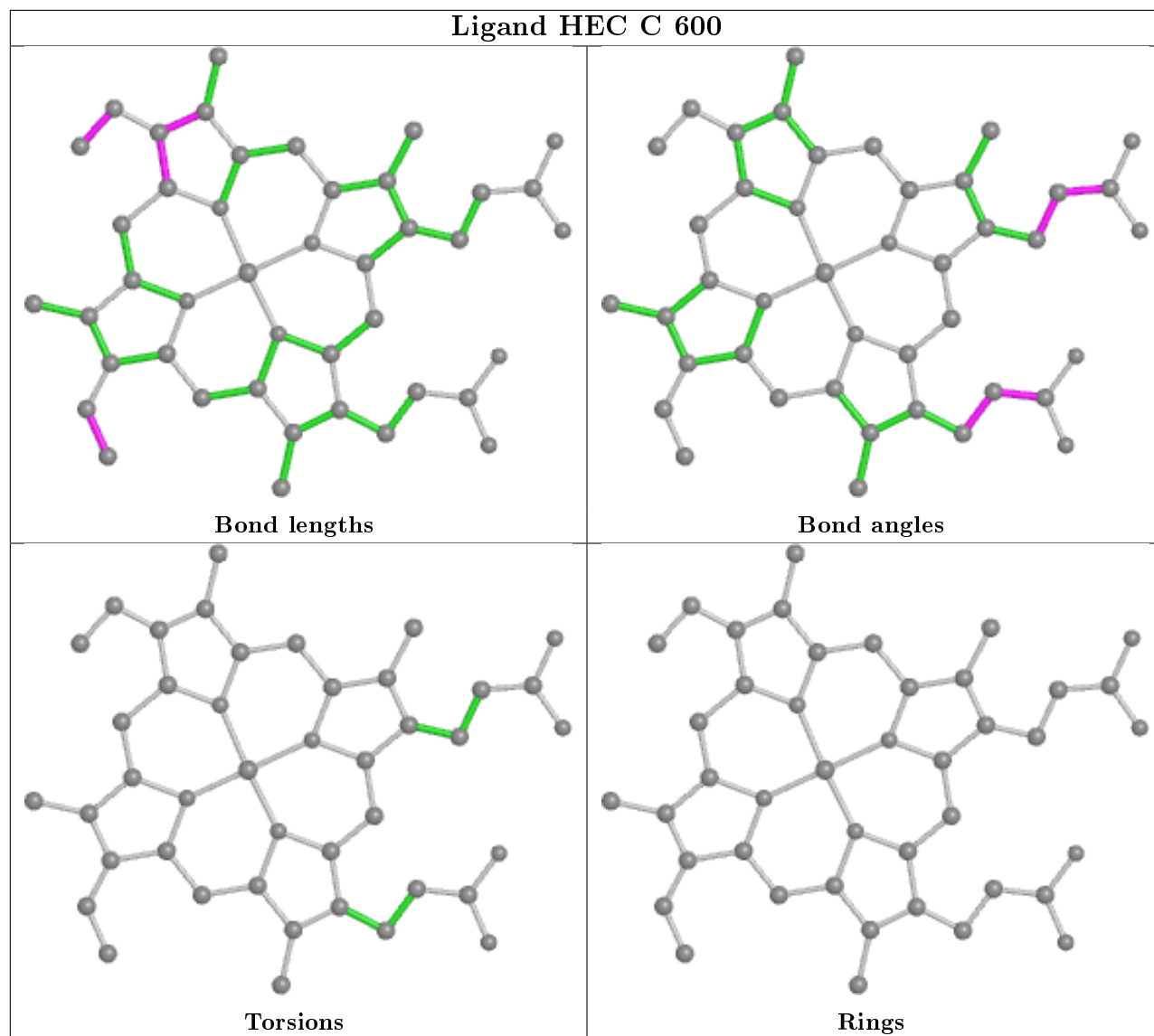


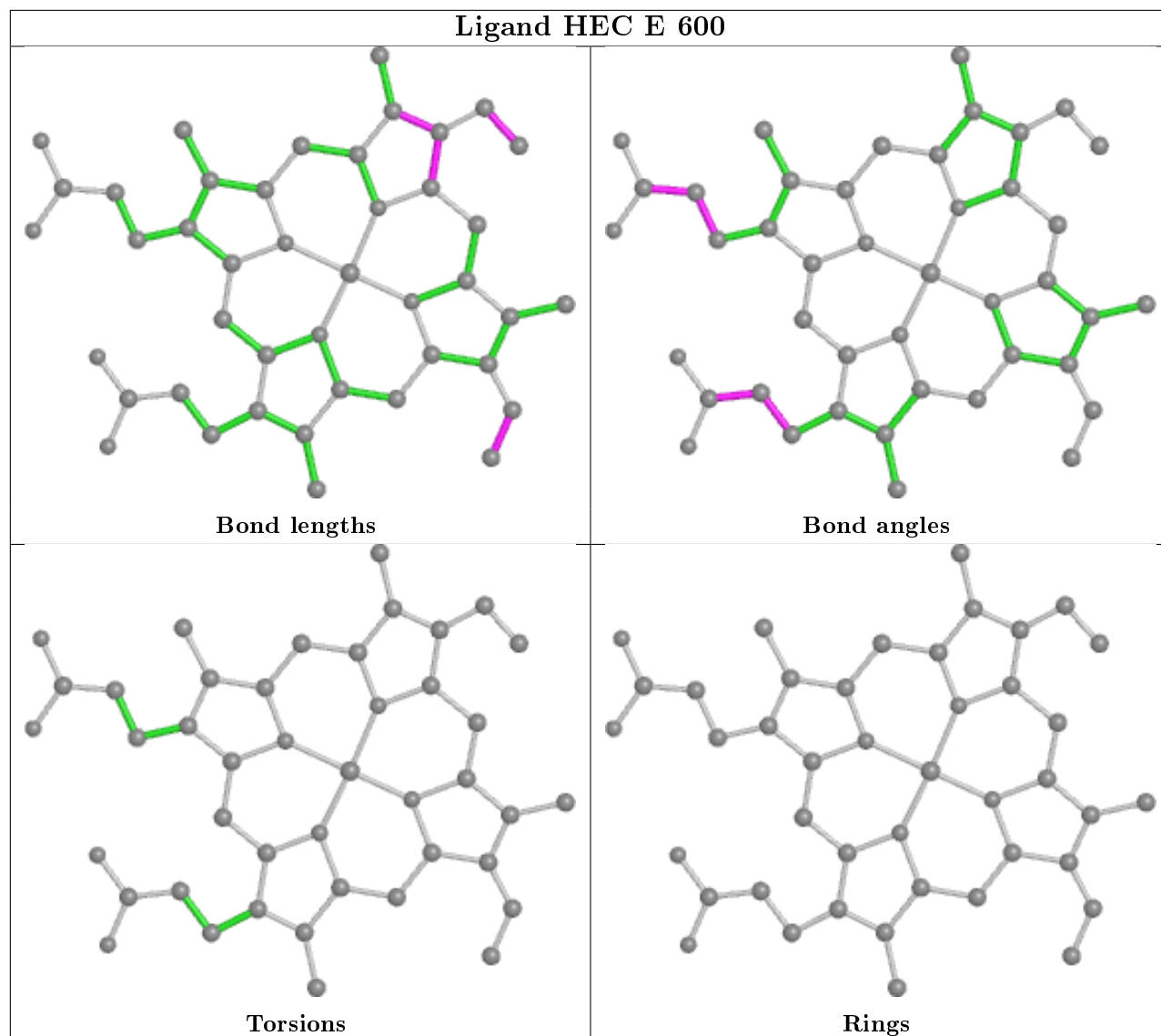




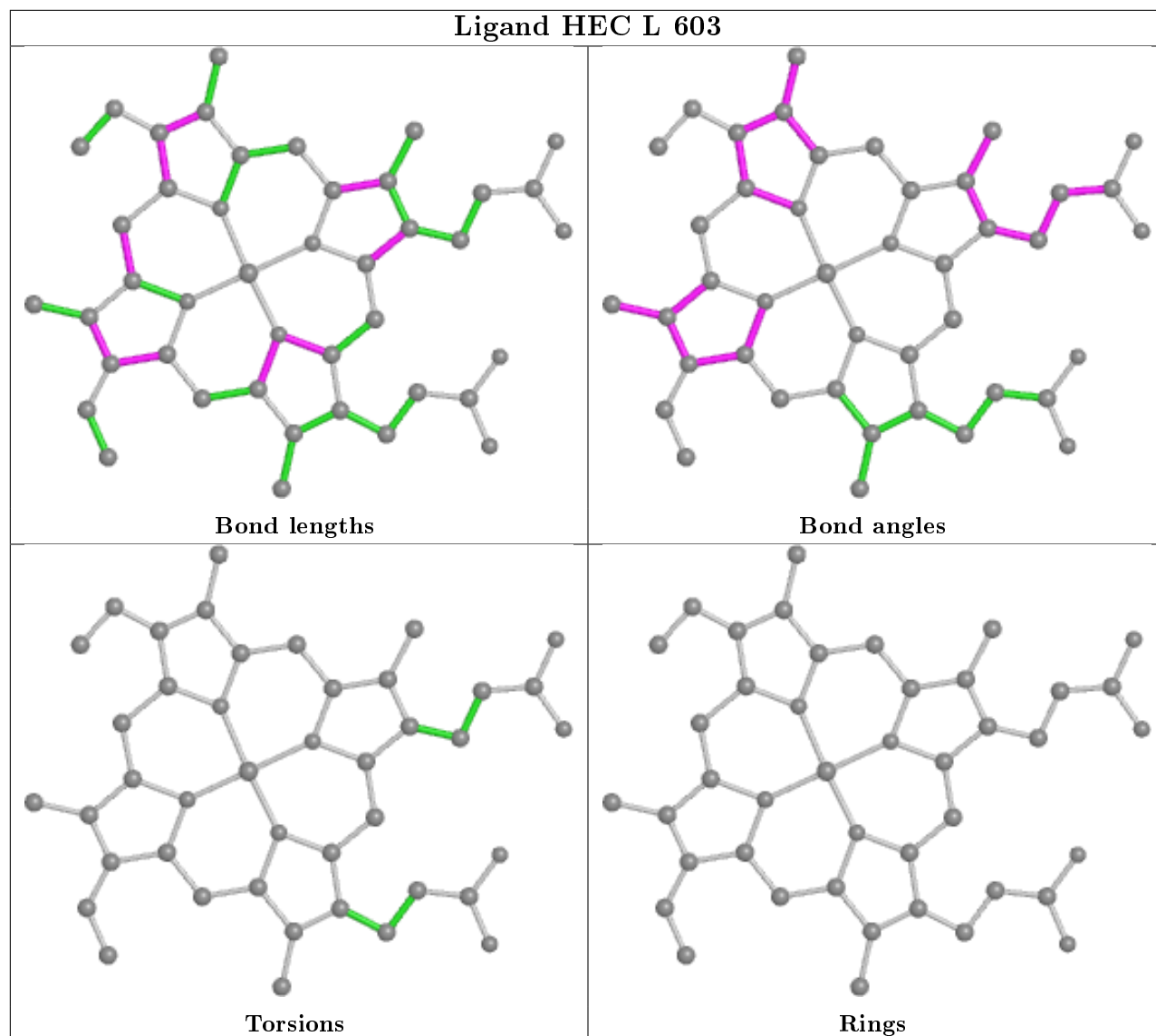


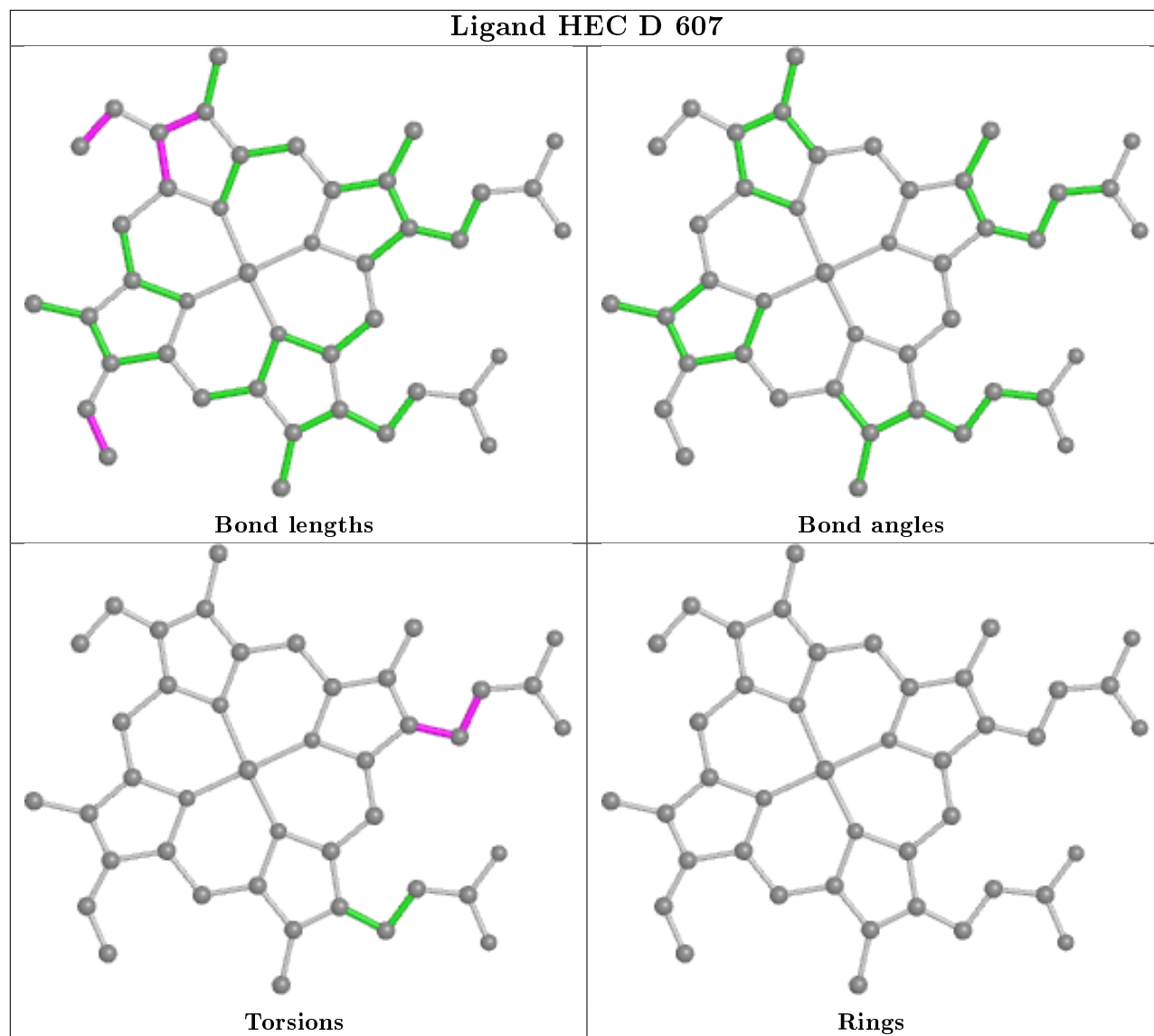




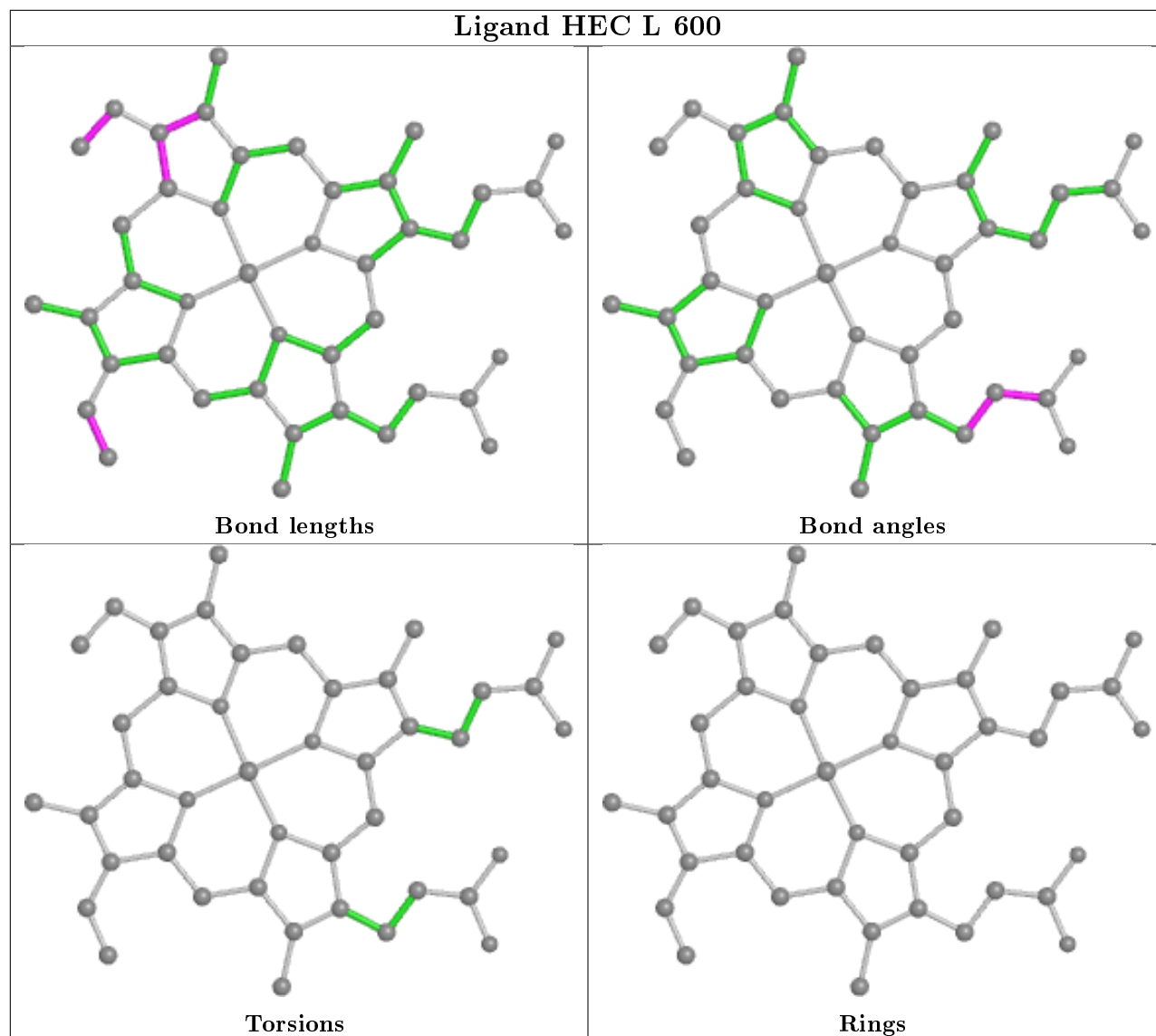


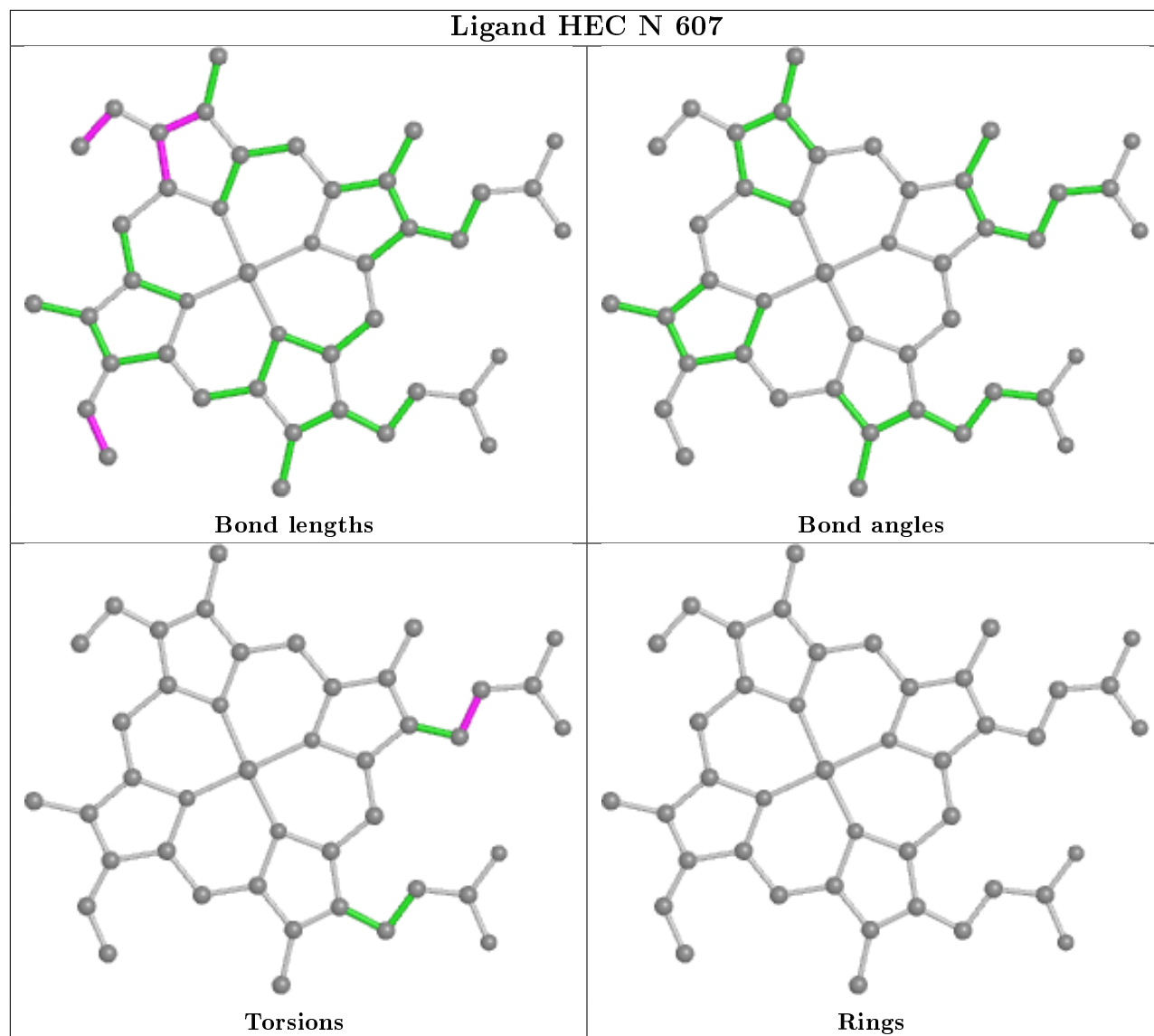
## Ligand HEC L 603

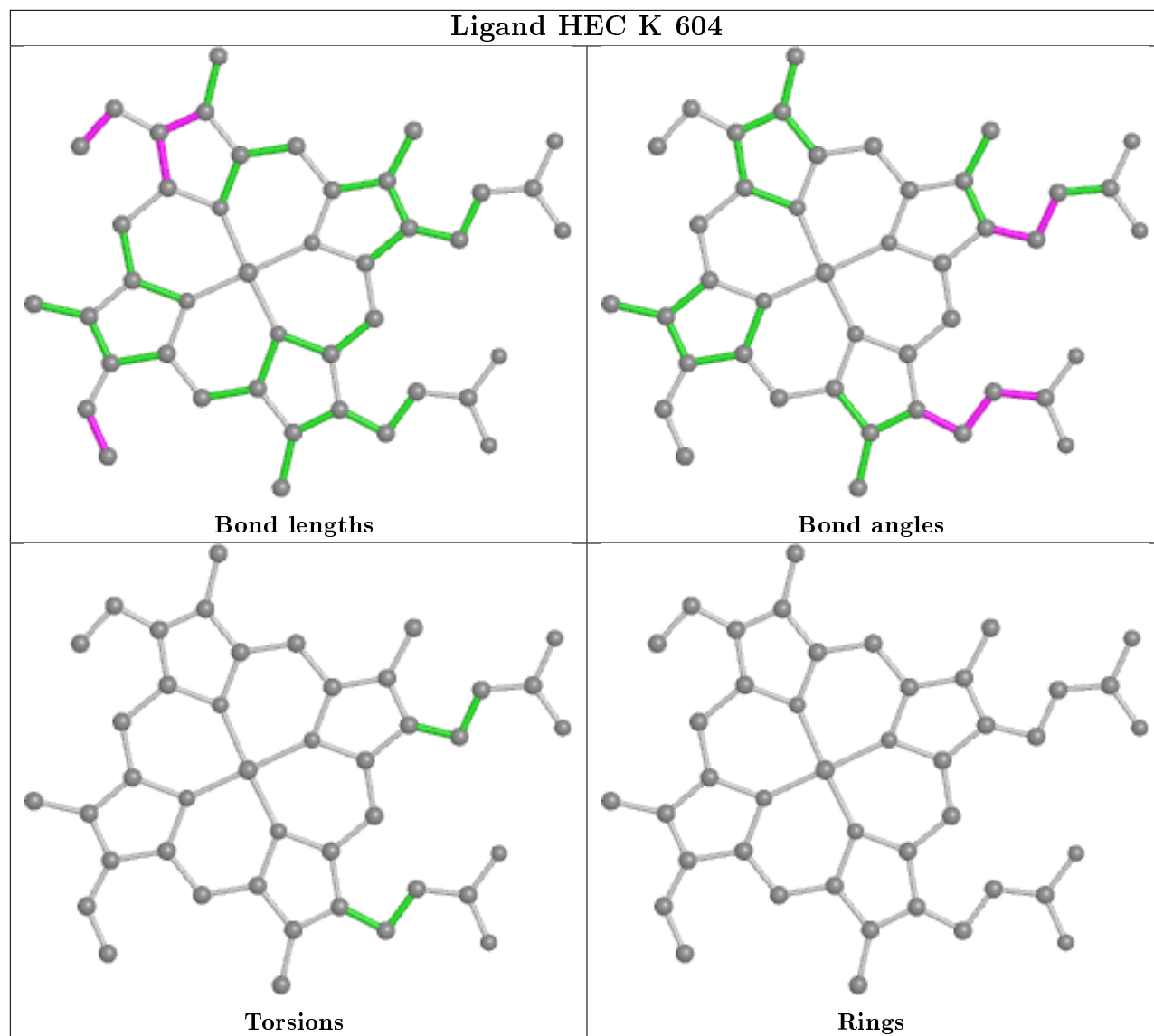


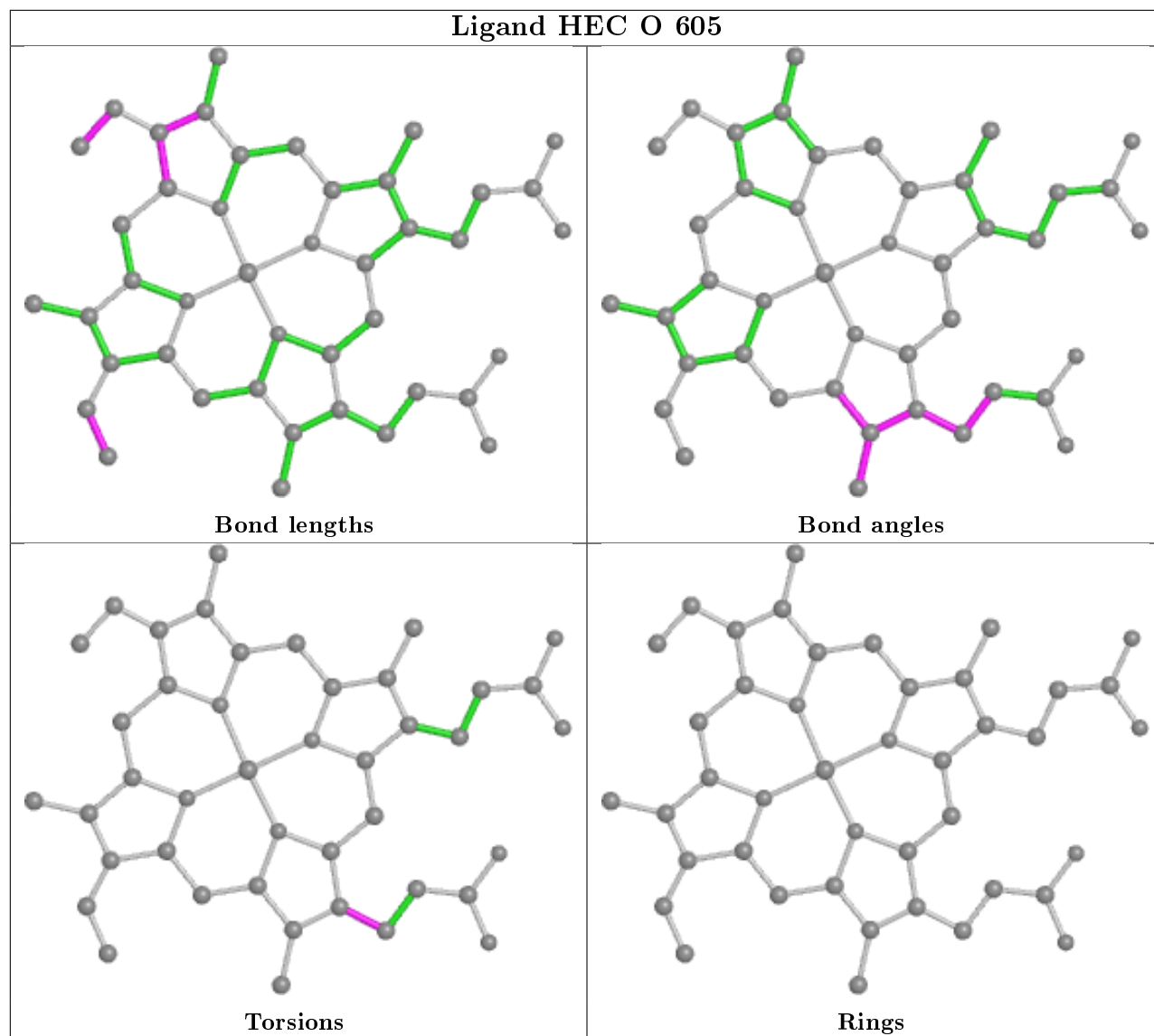


## Ligand HEC L 600

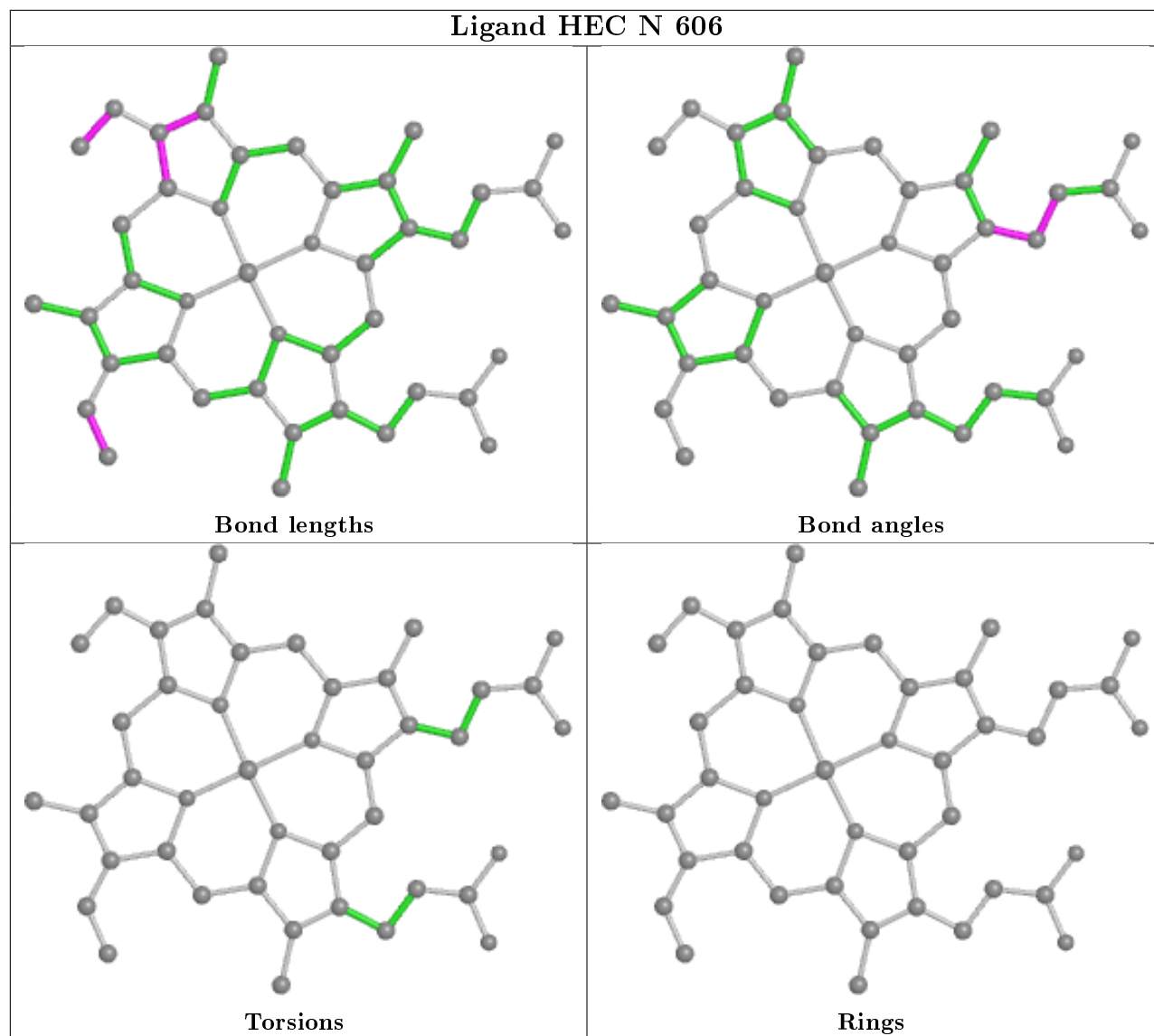


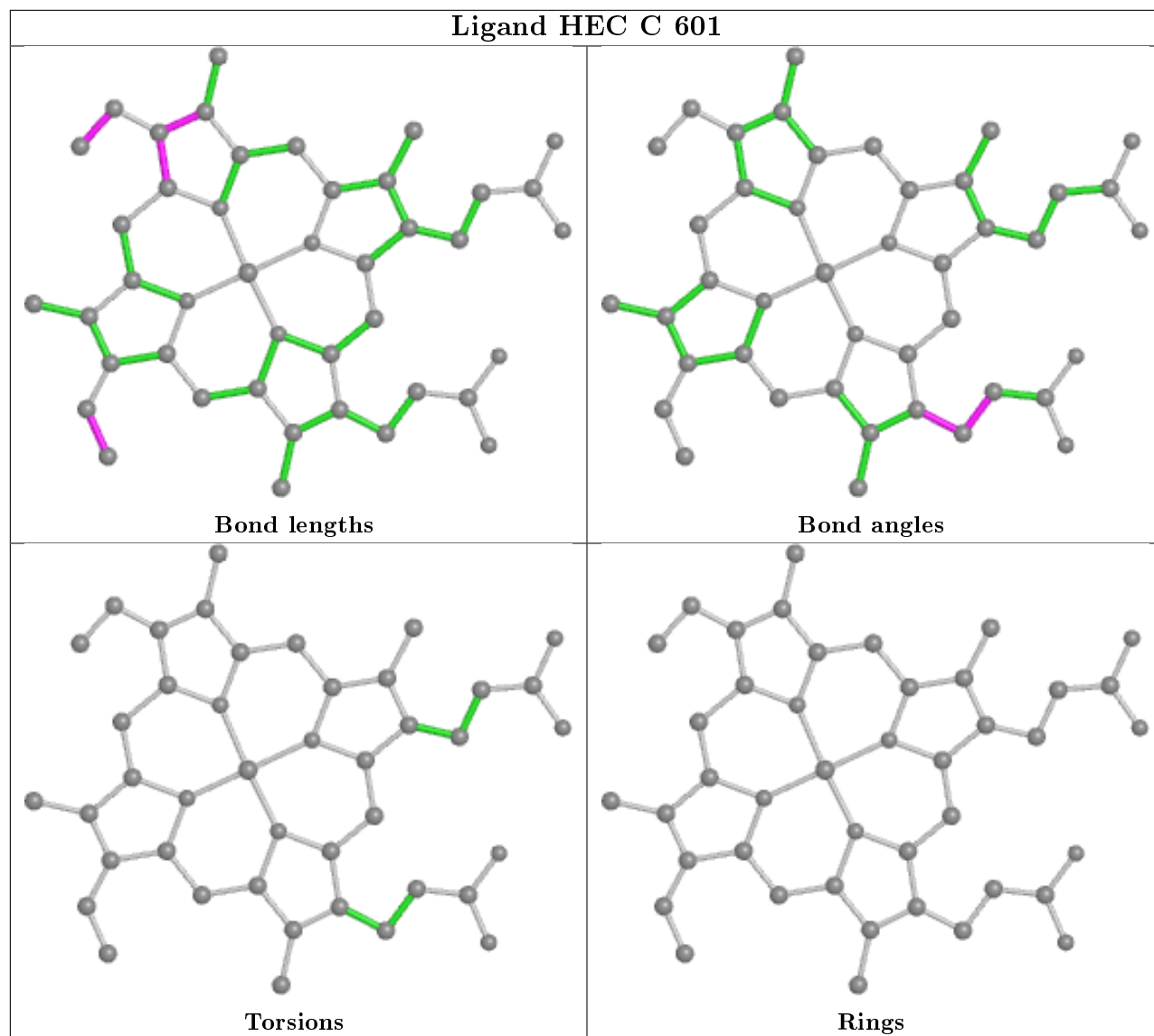




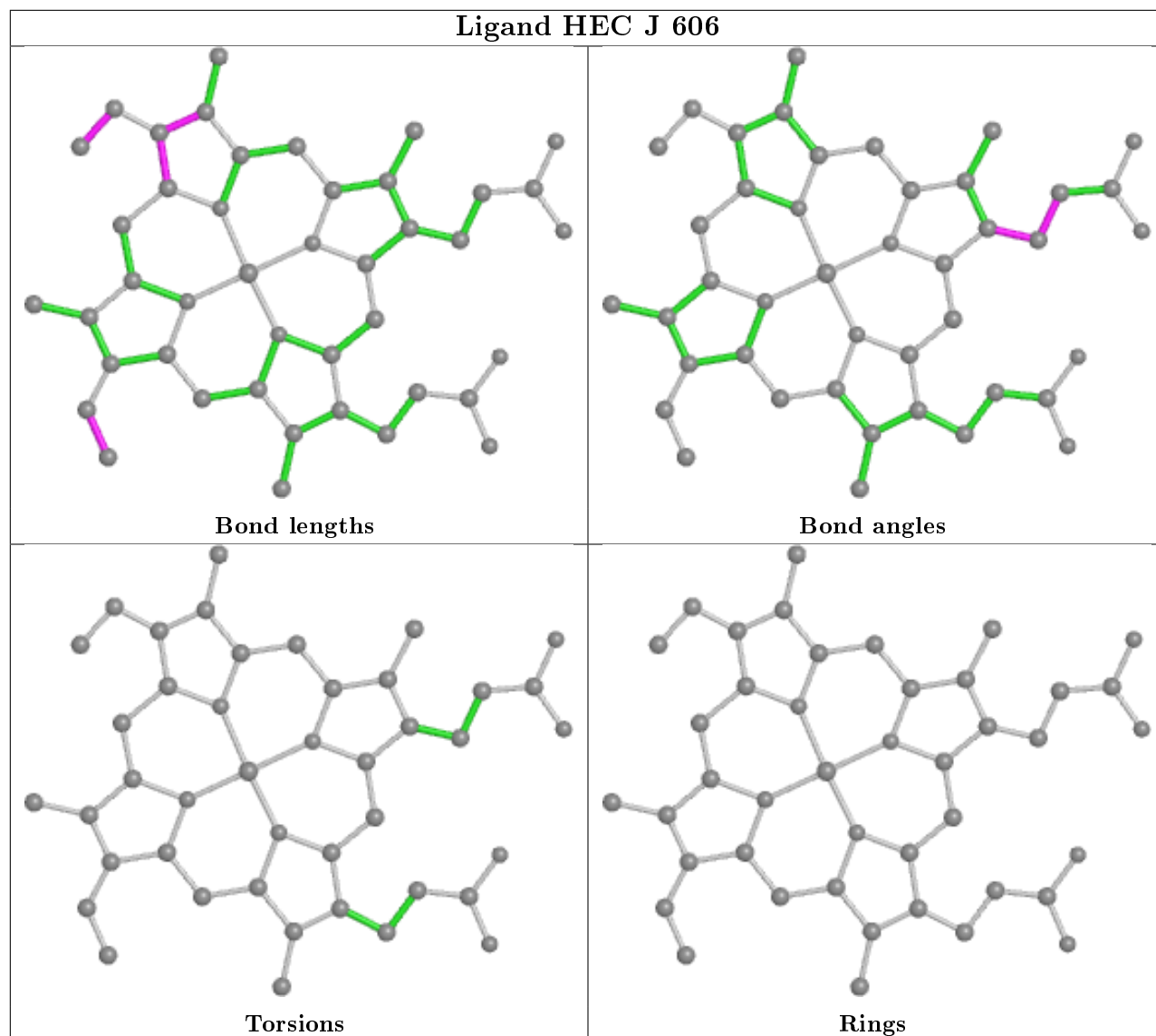


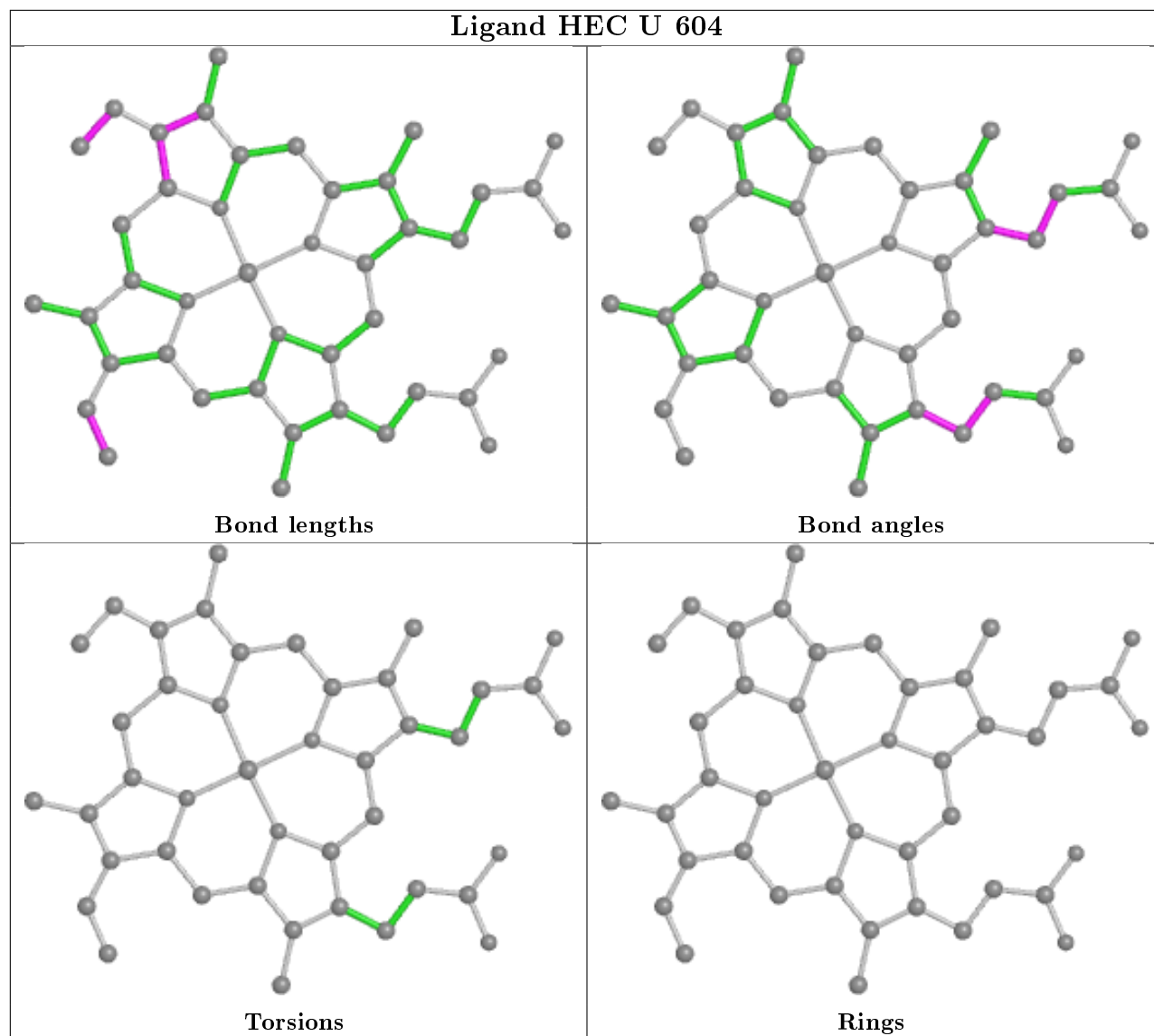




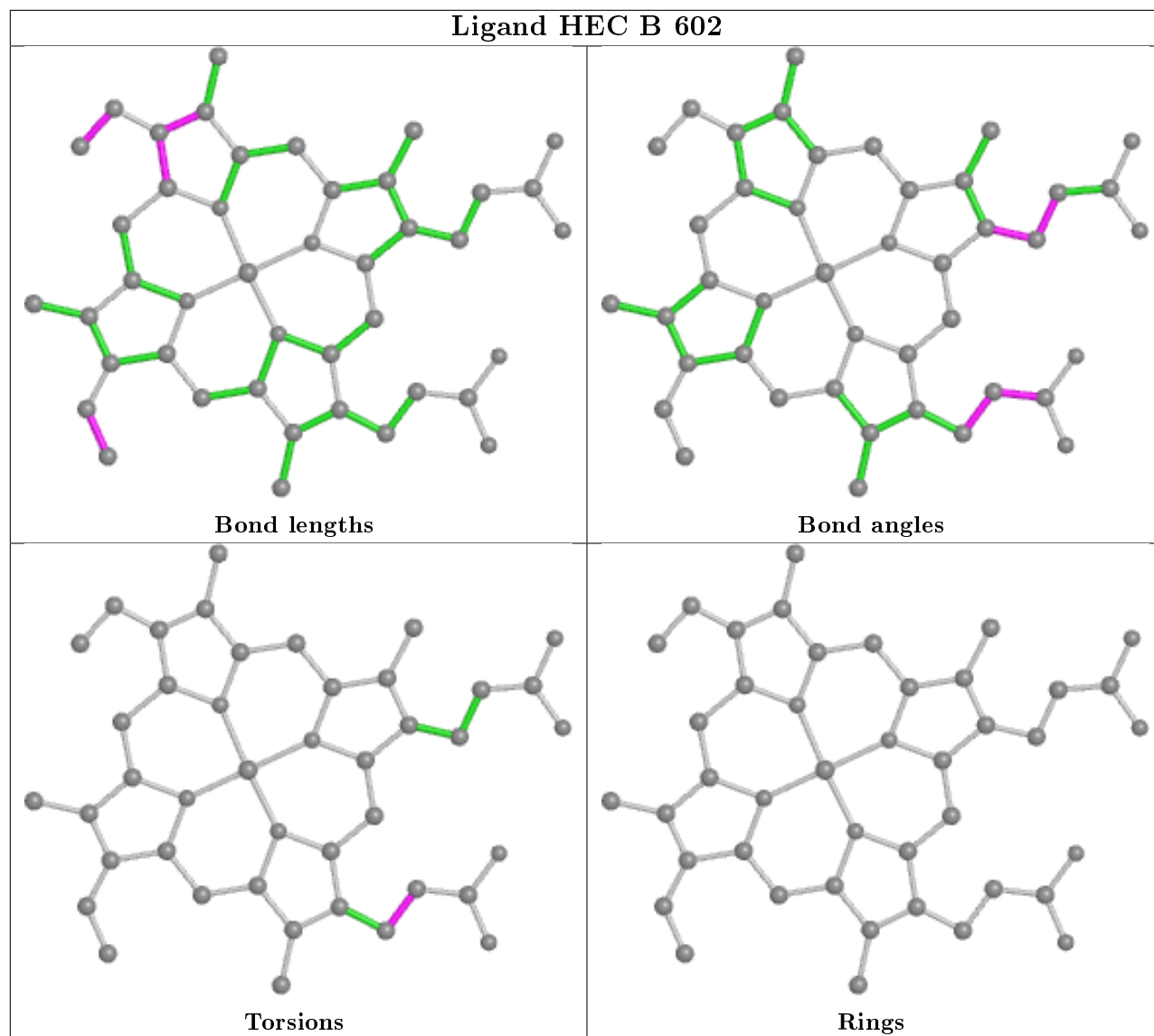


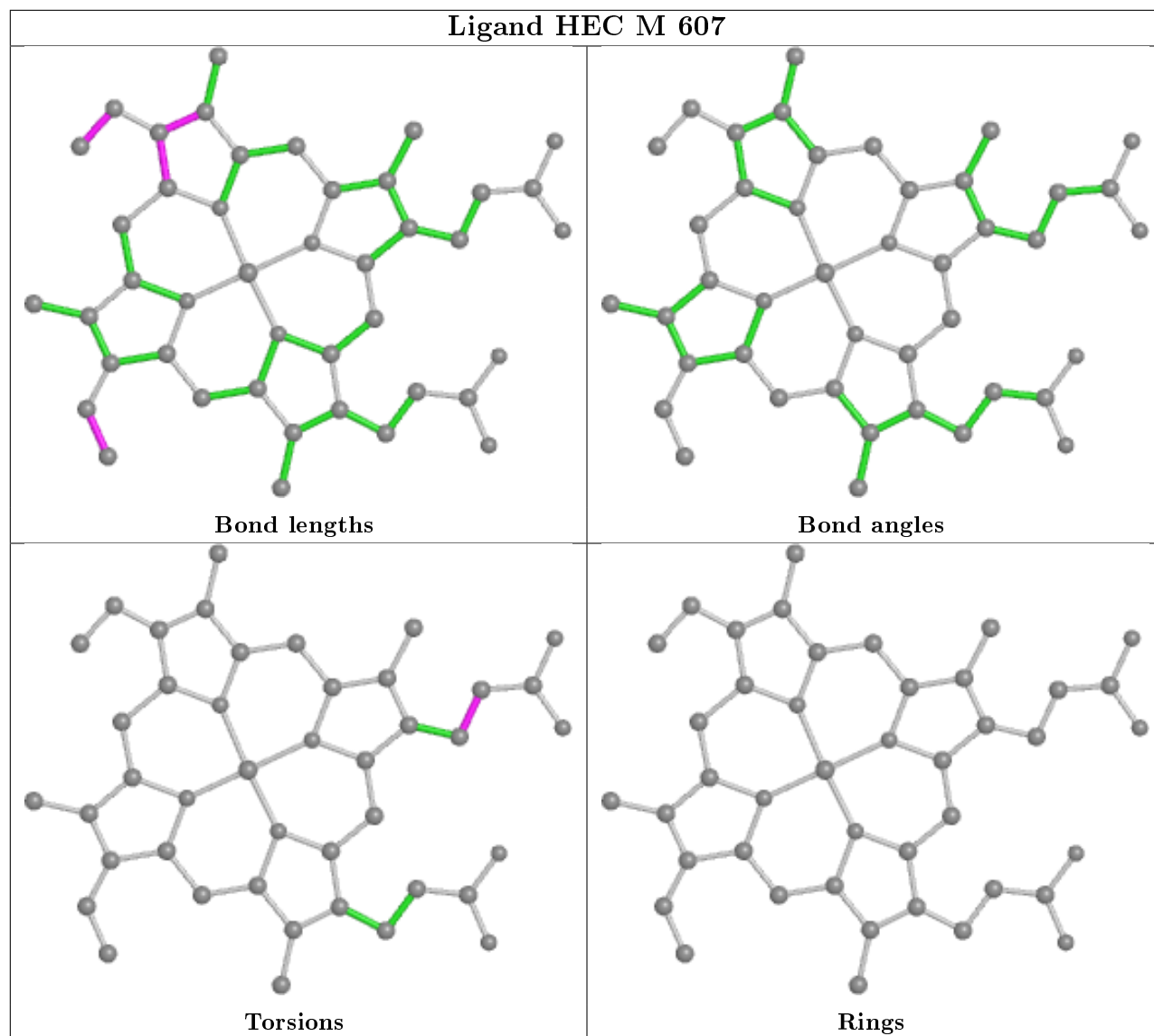
## Ligand HEC J 606



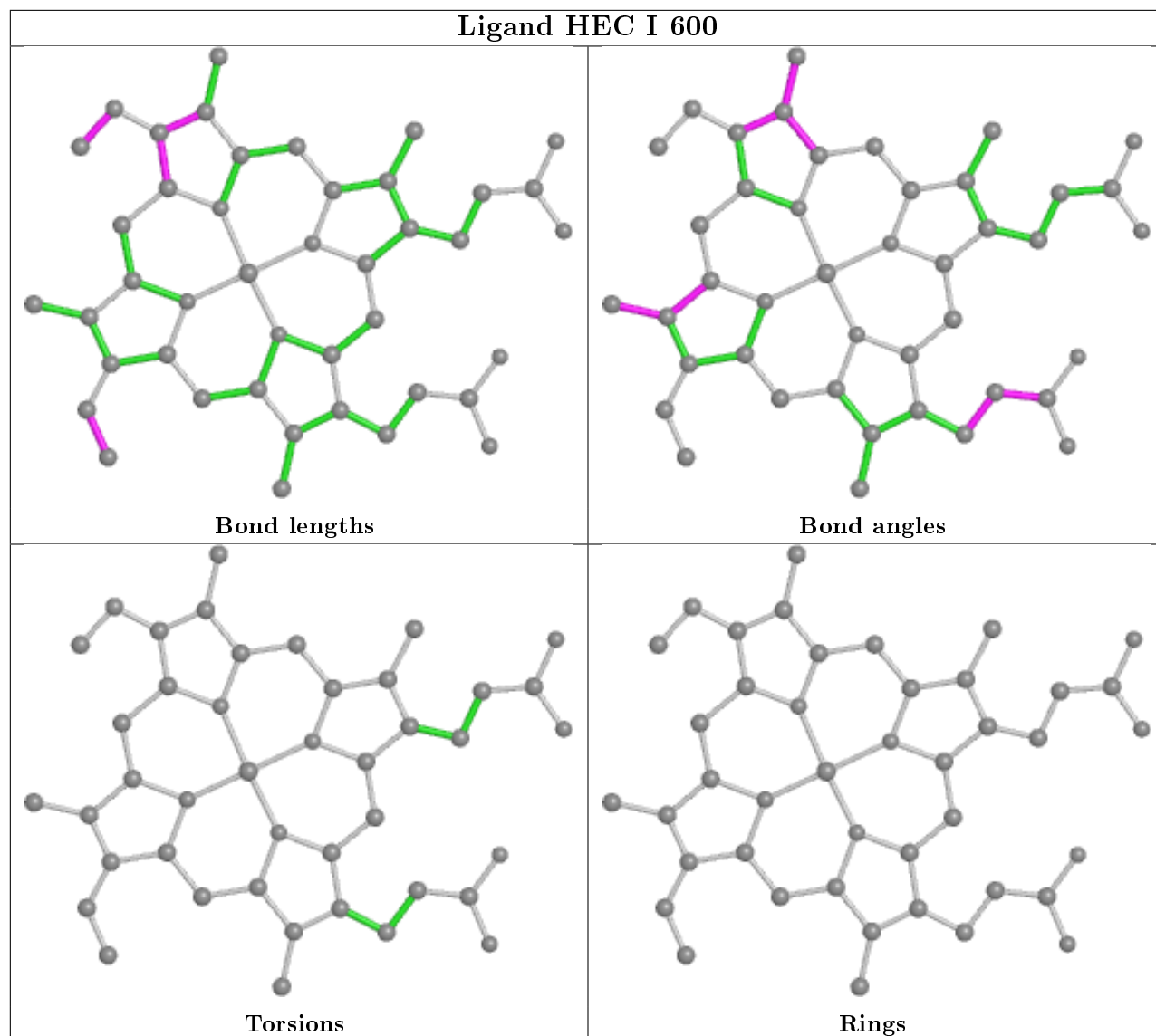


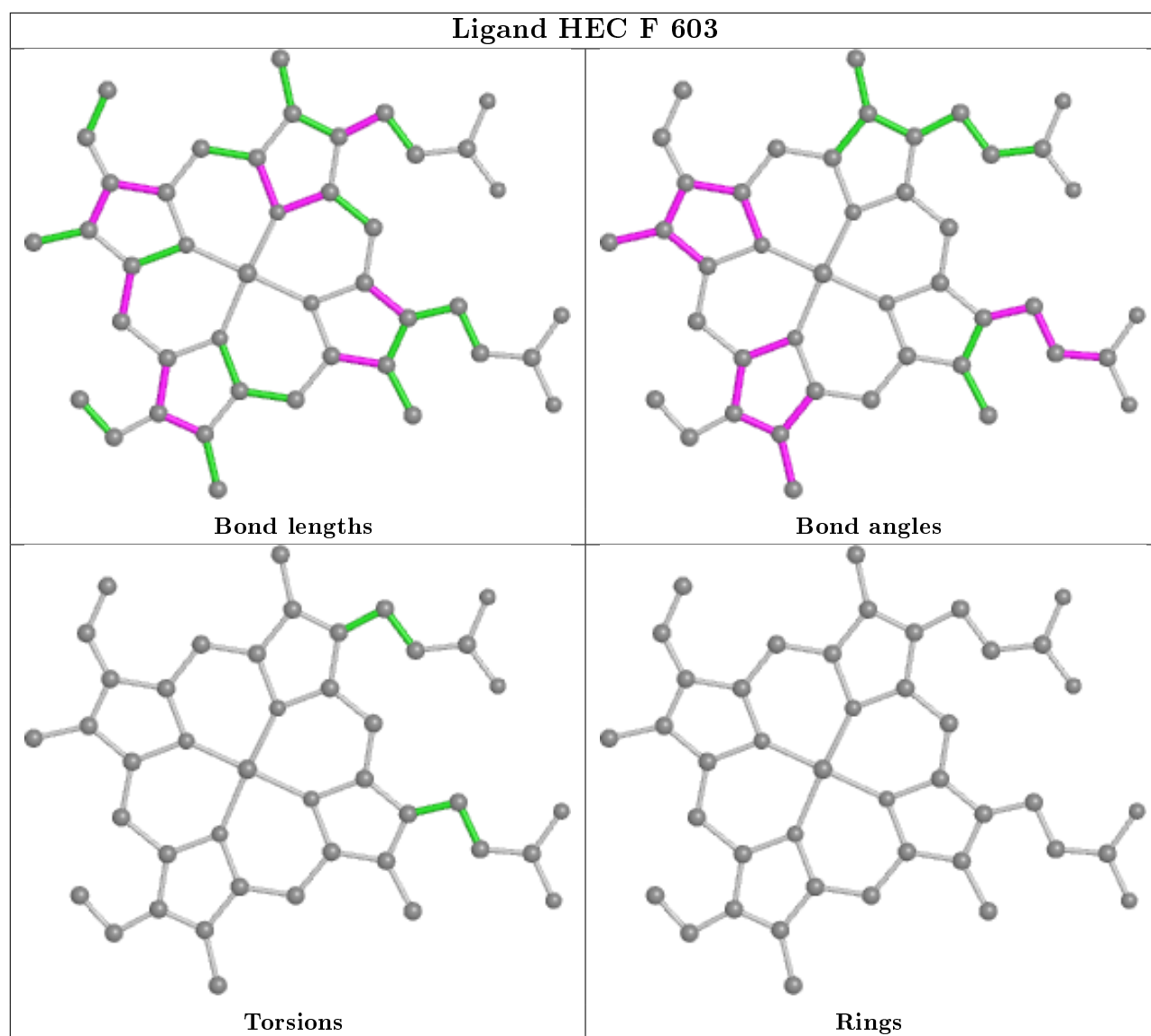
## Ligand HEC B 602



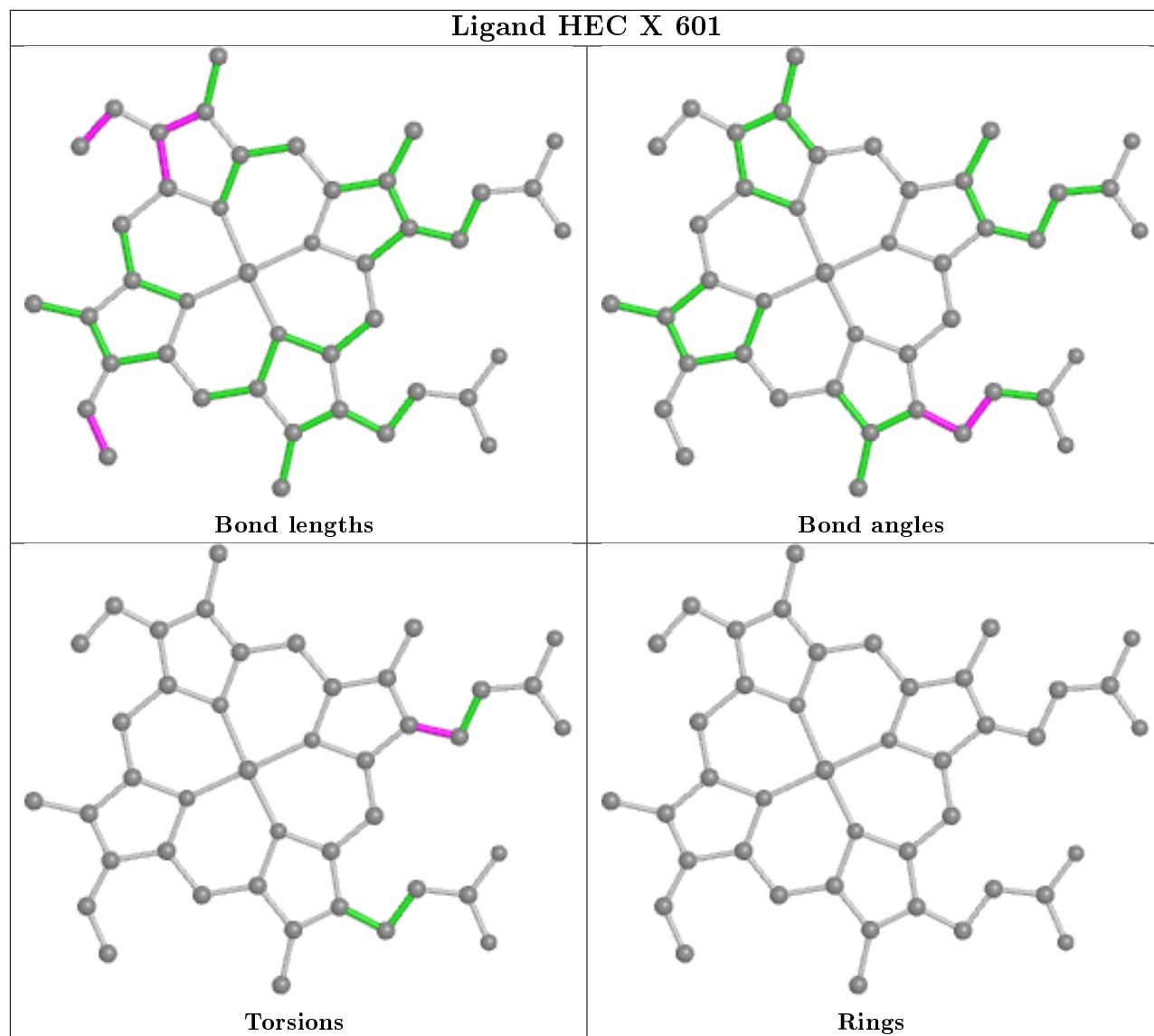


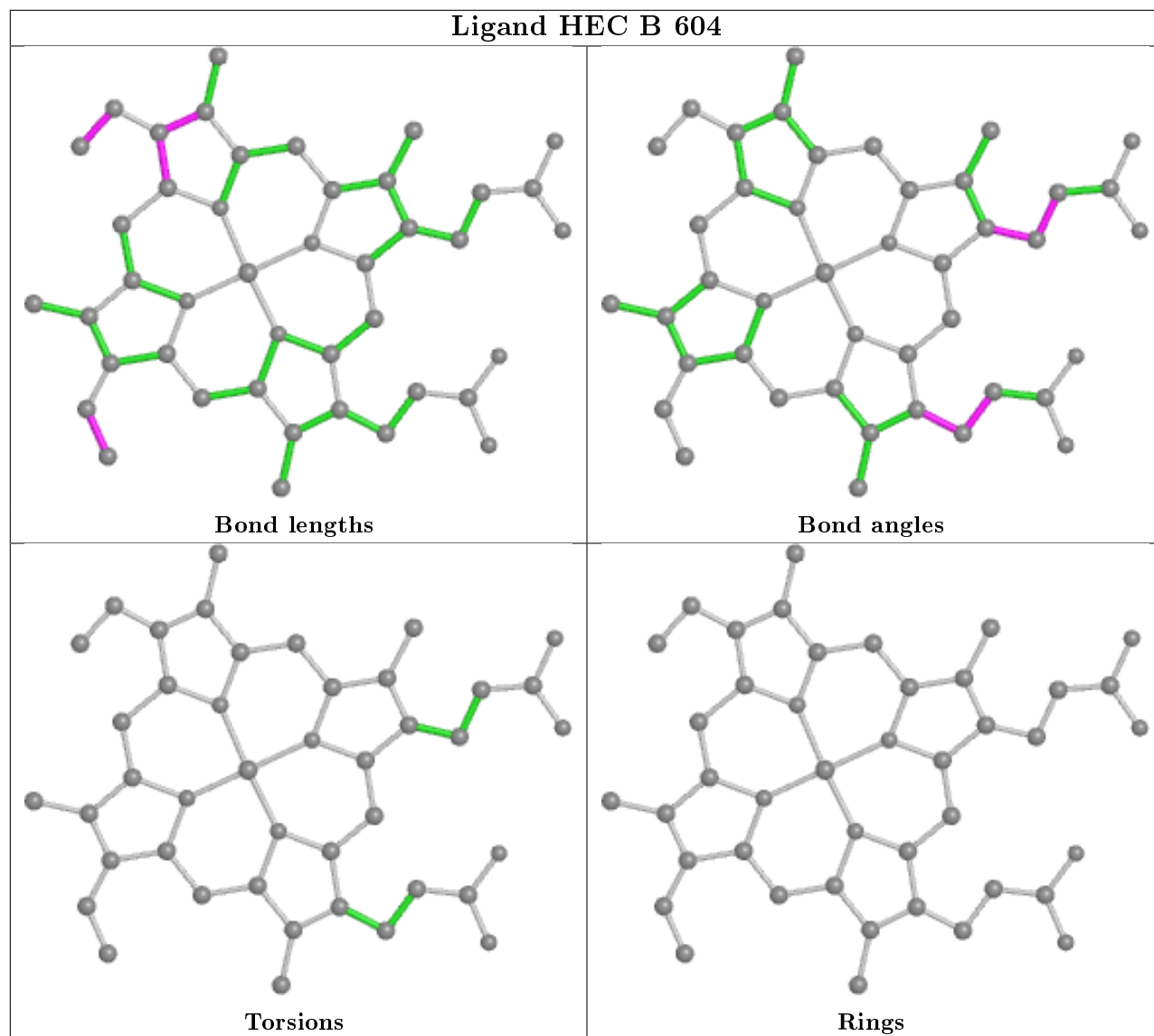
## Ligand HEC I 600

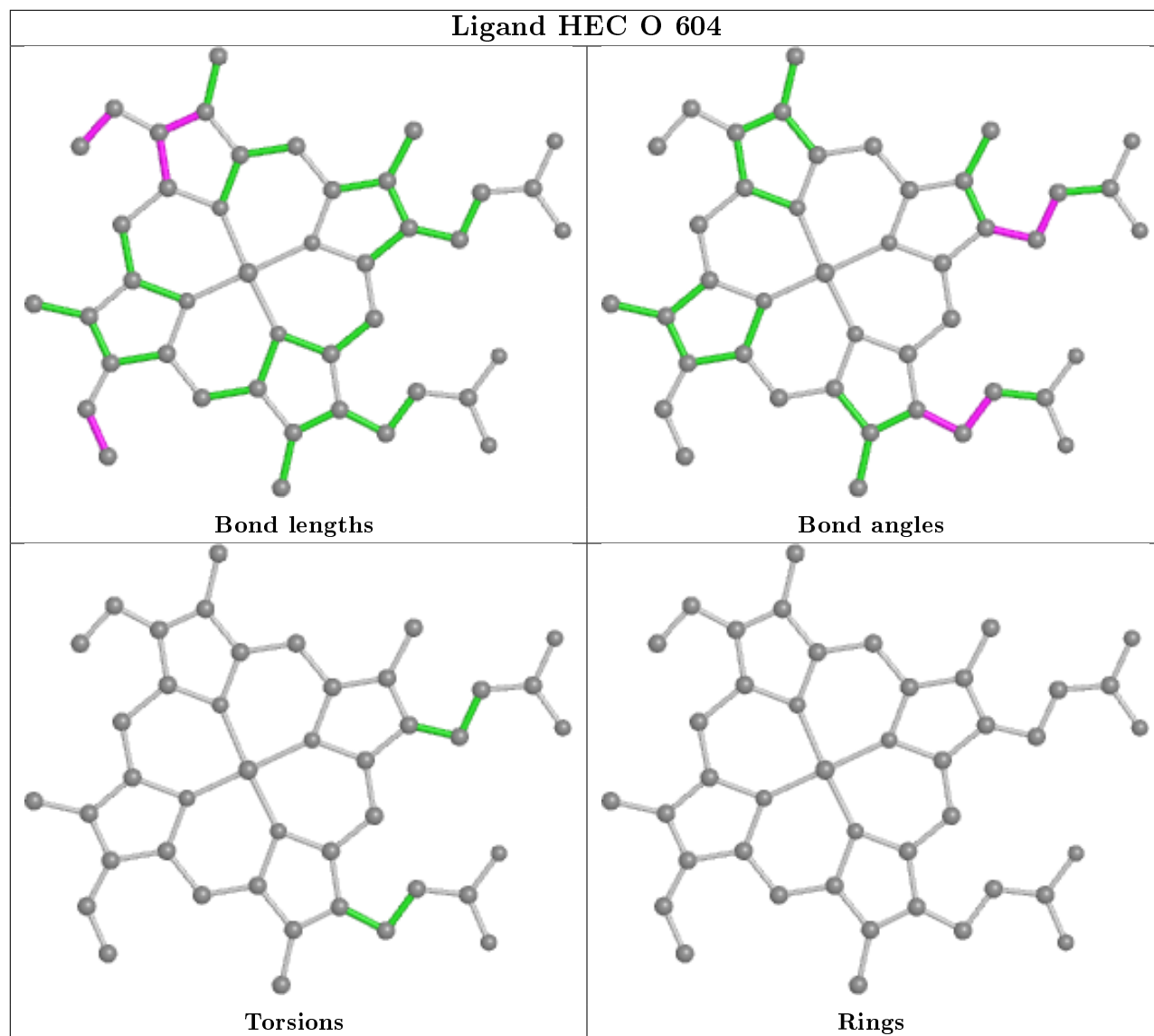


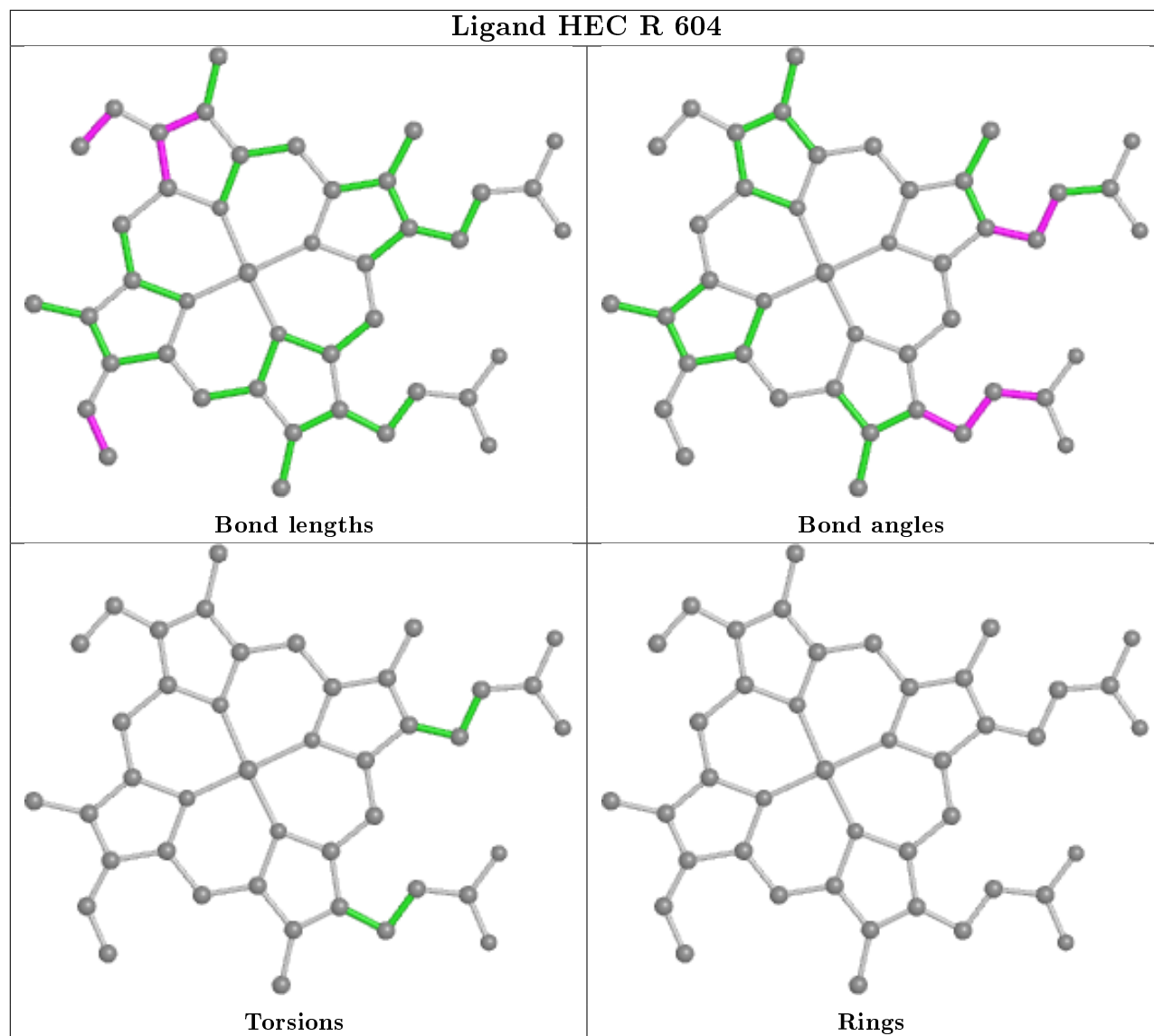


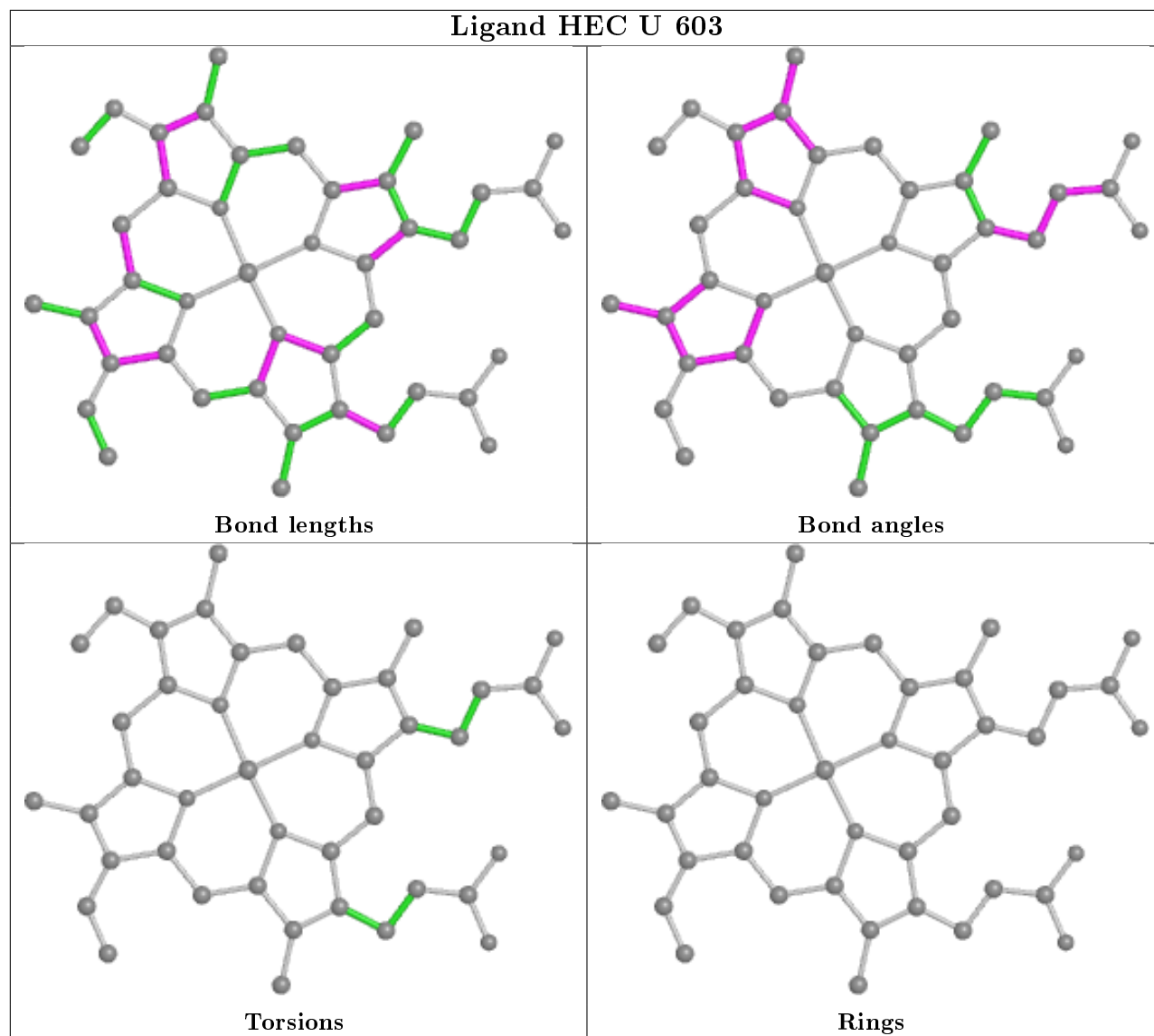




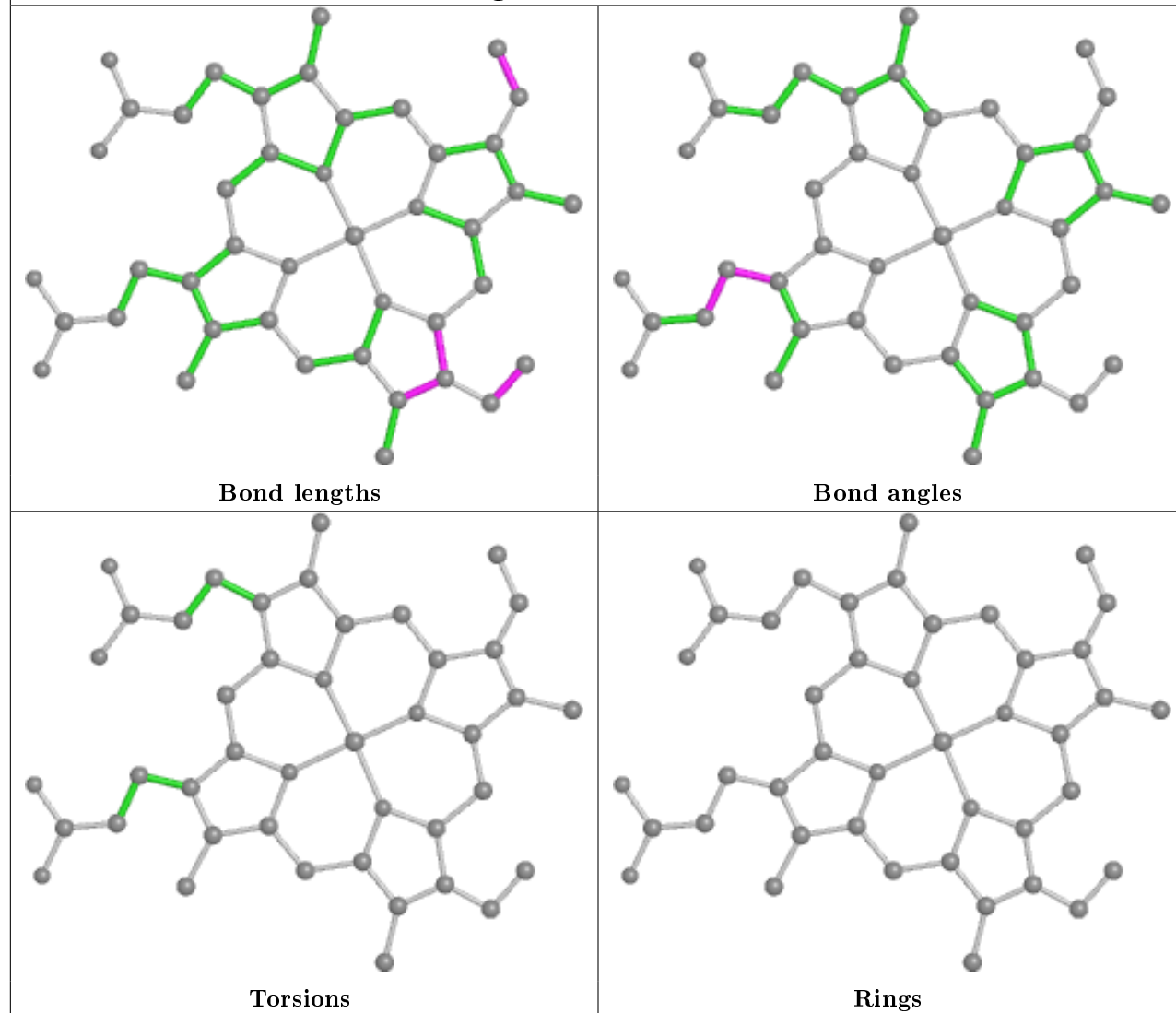


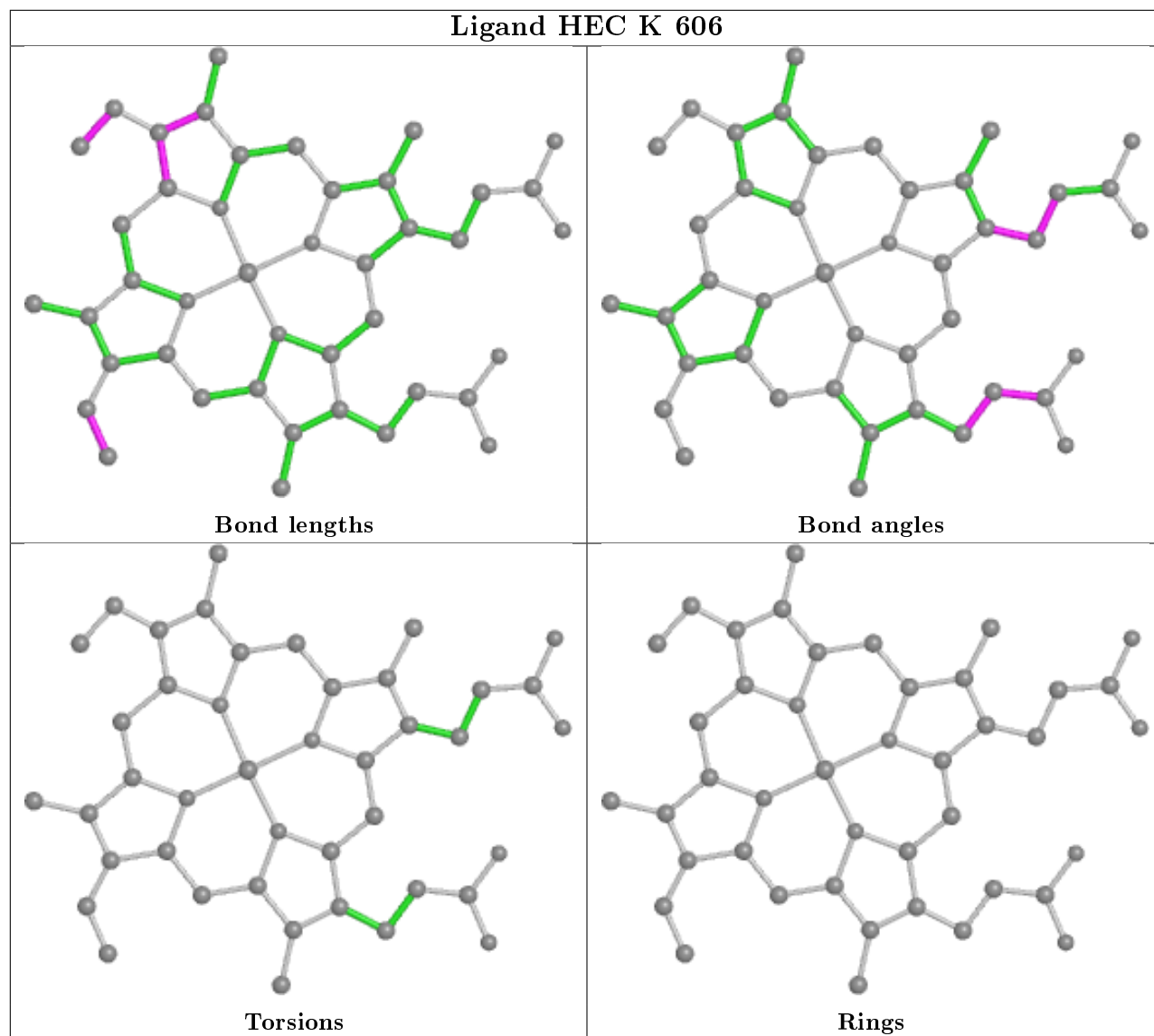


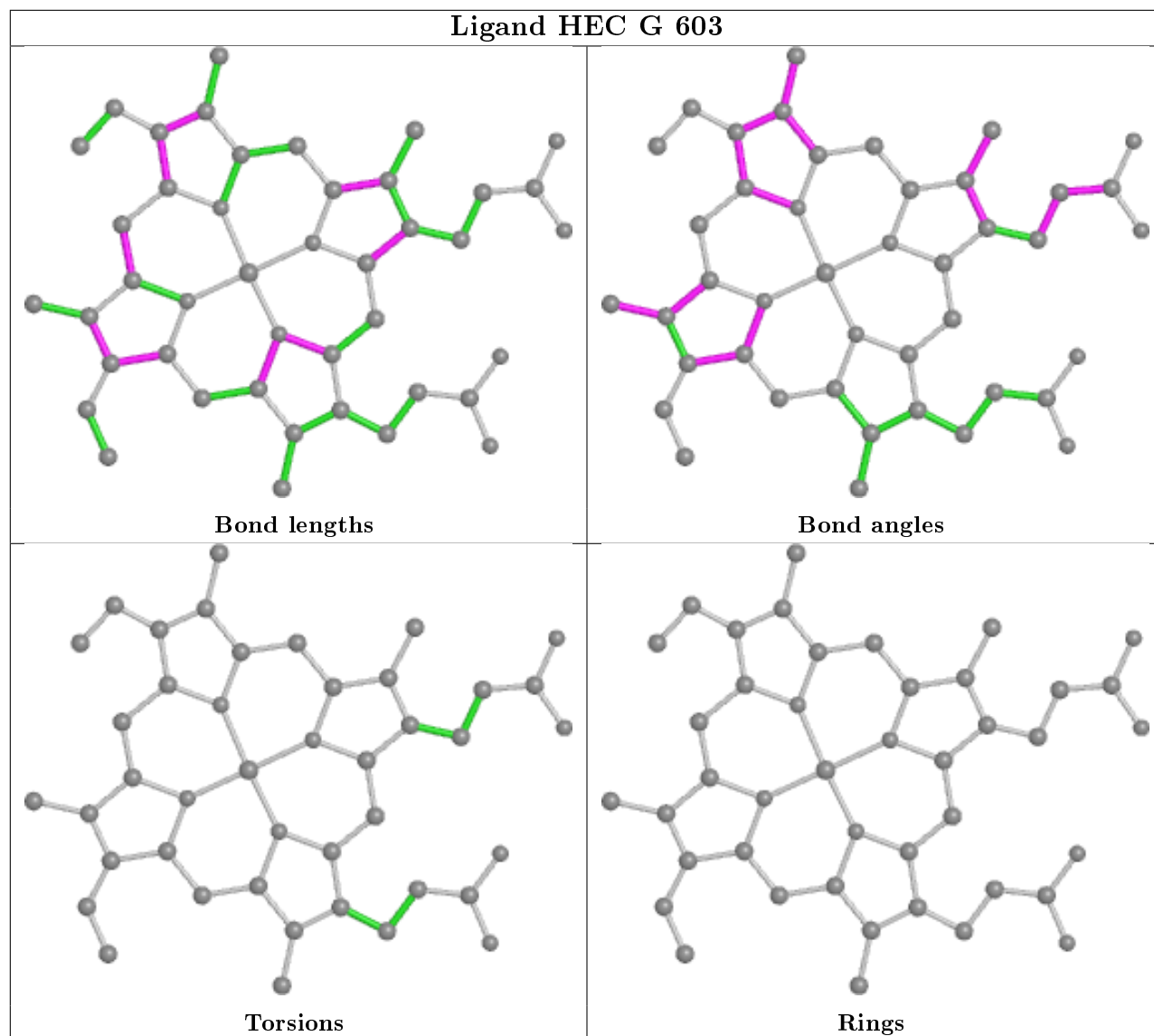




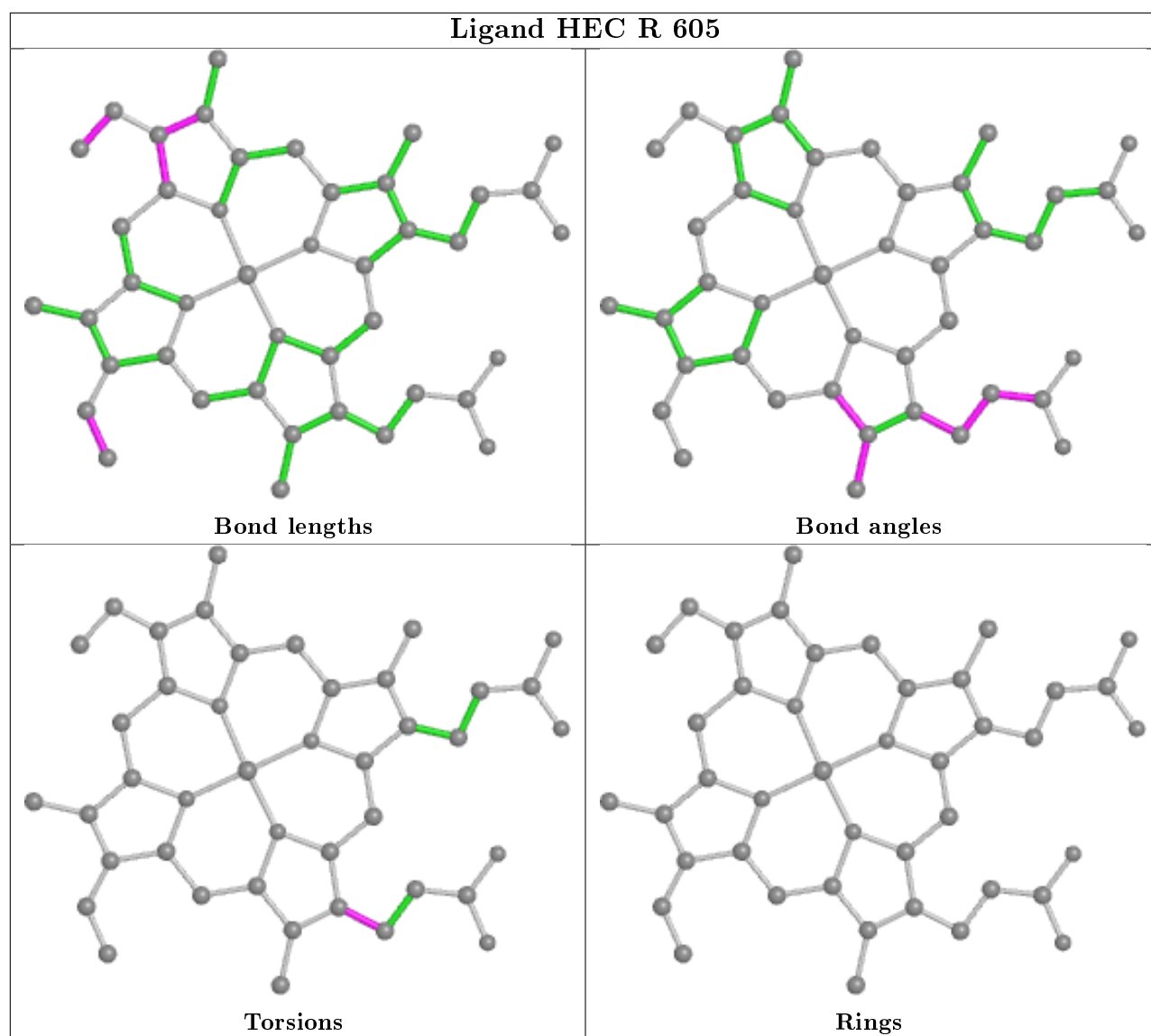
## Ligand HEC F 606

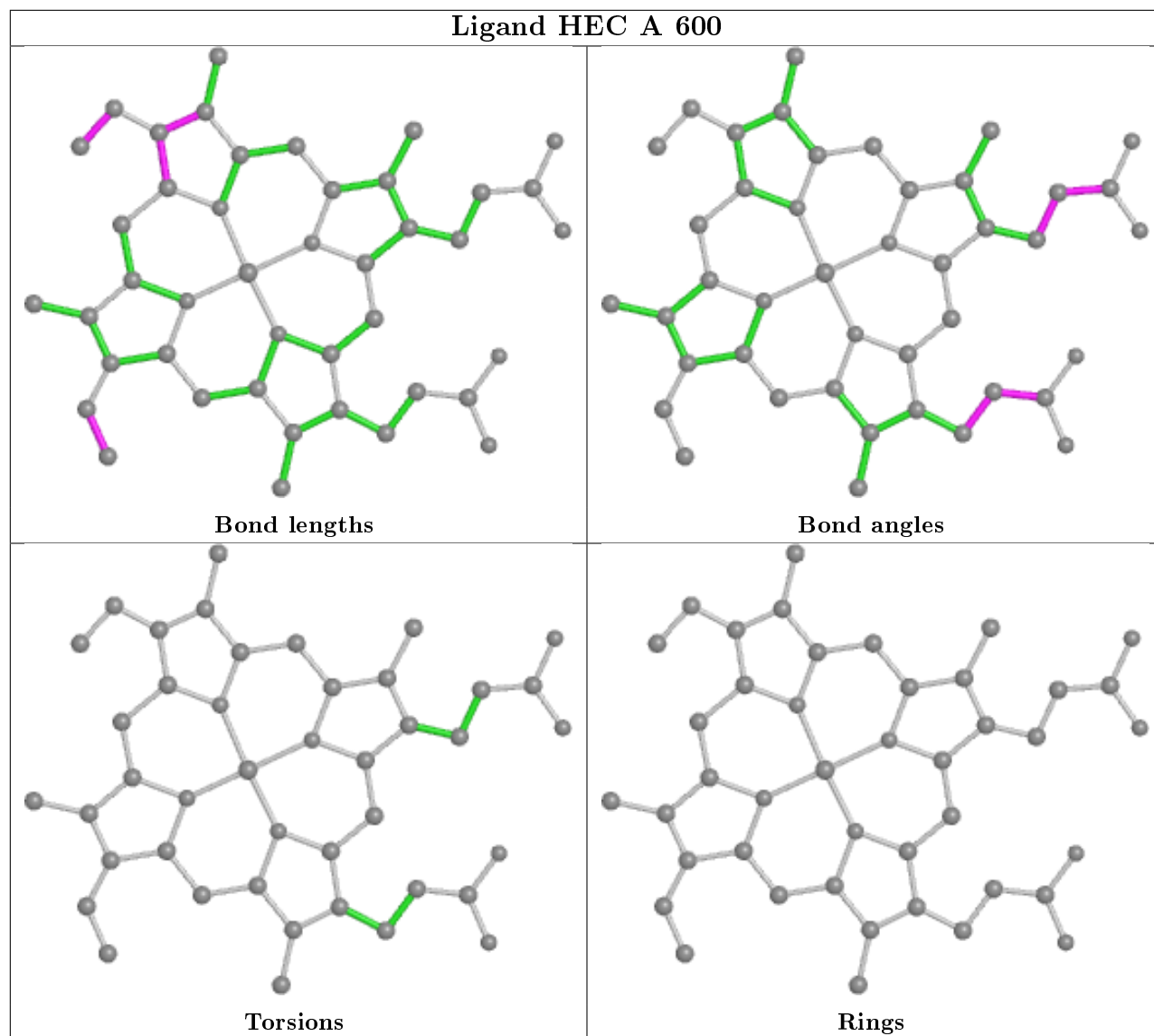


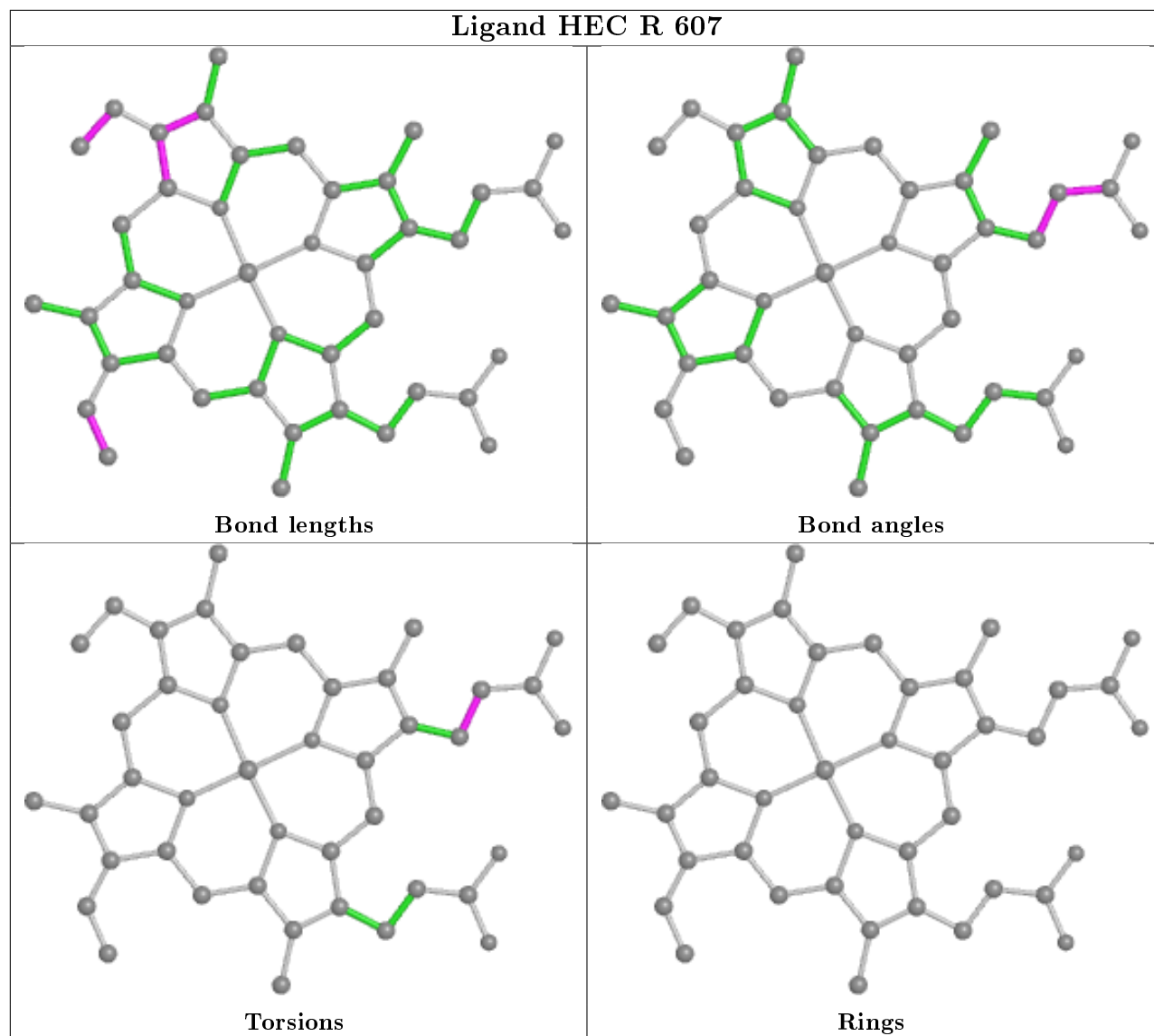


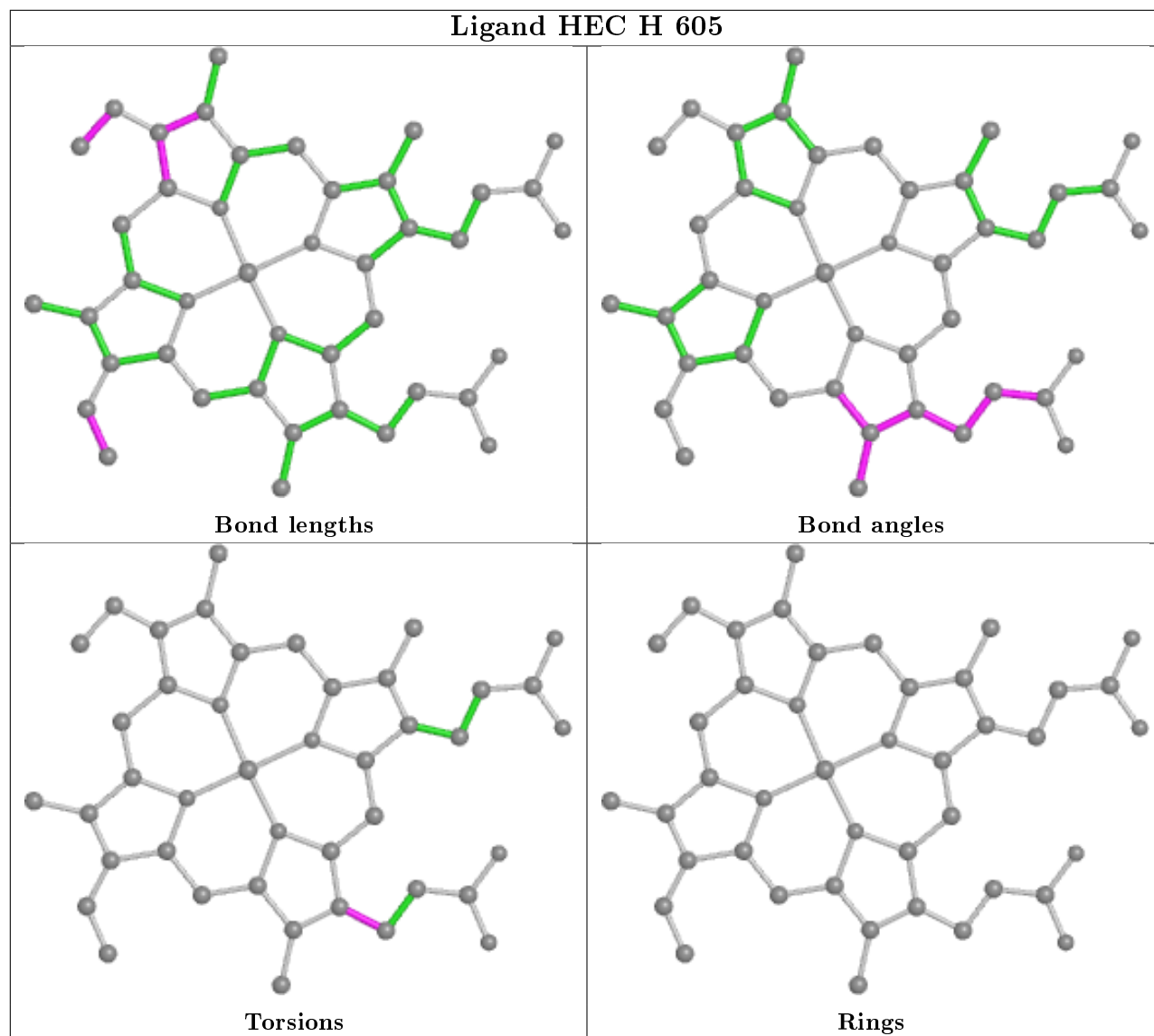


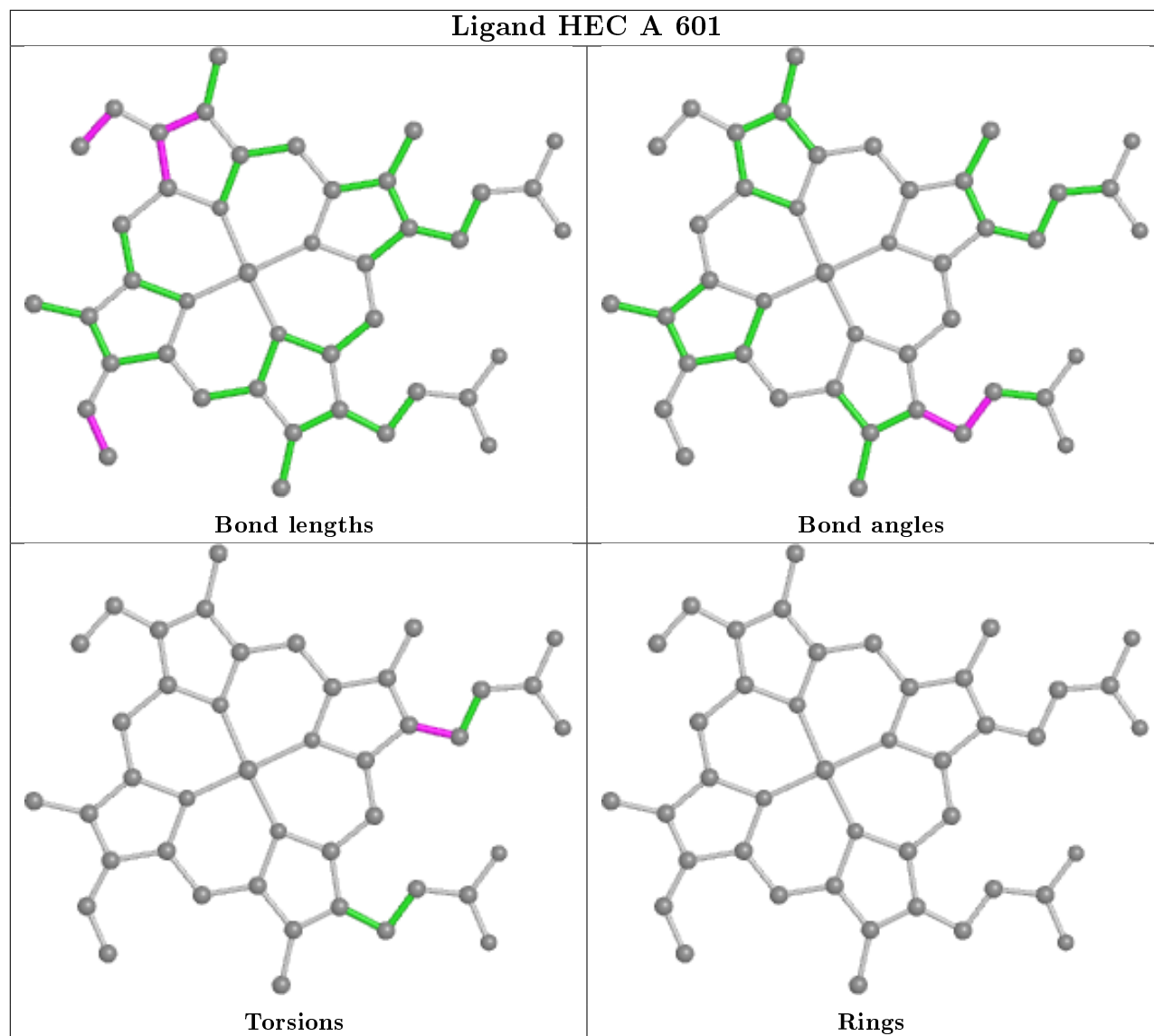


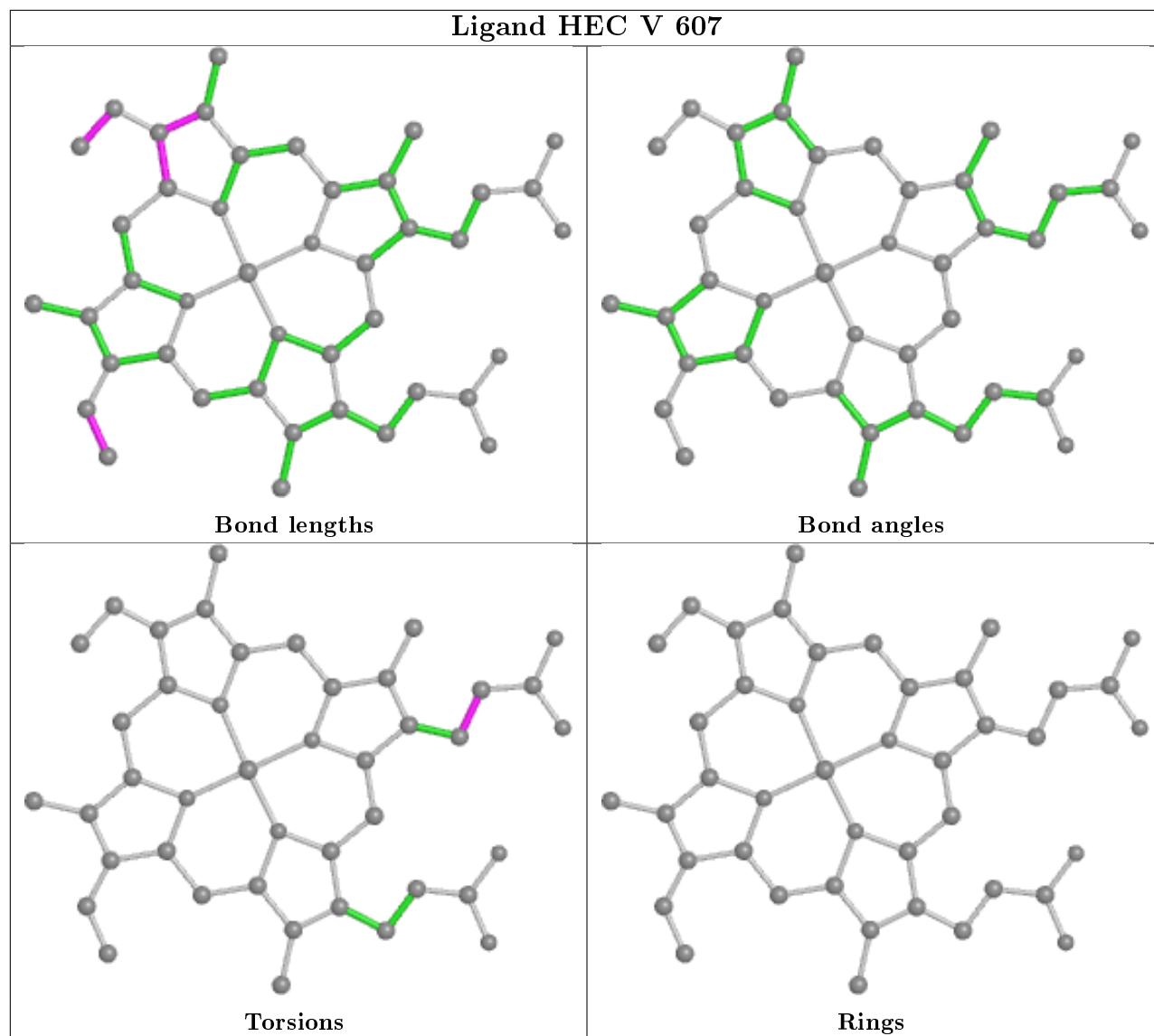




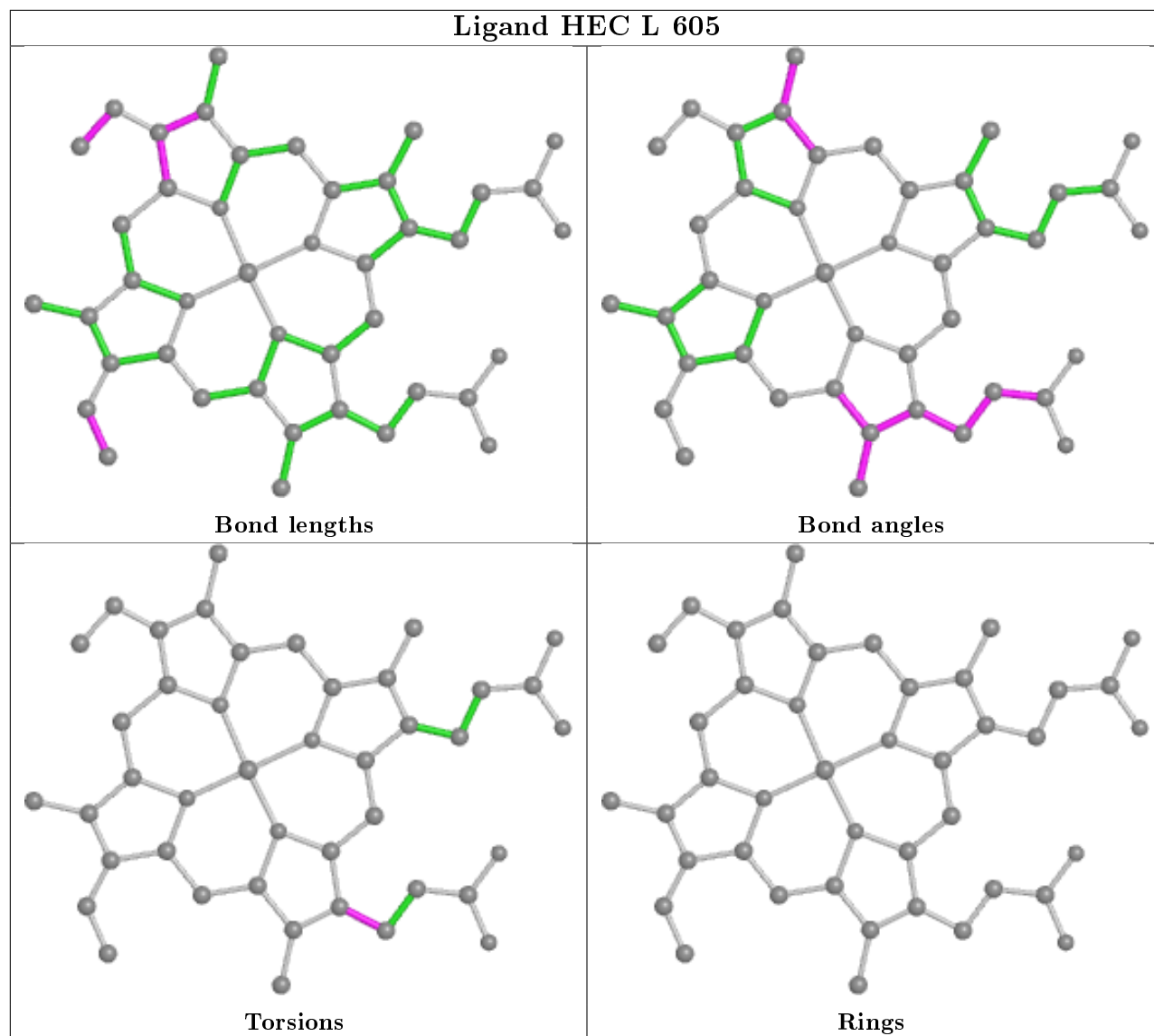


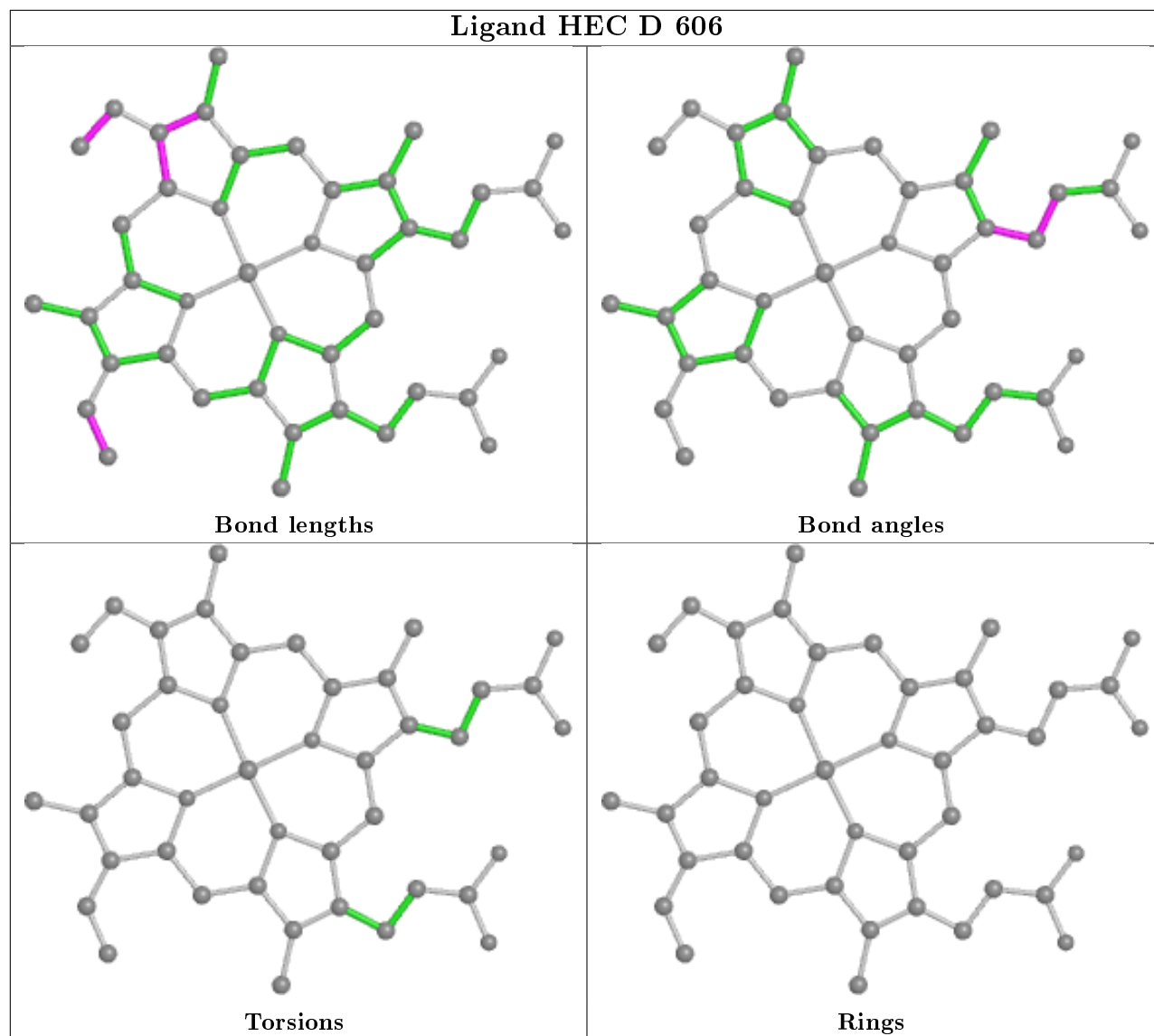




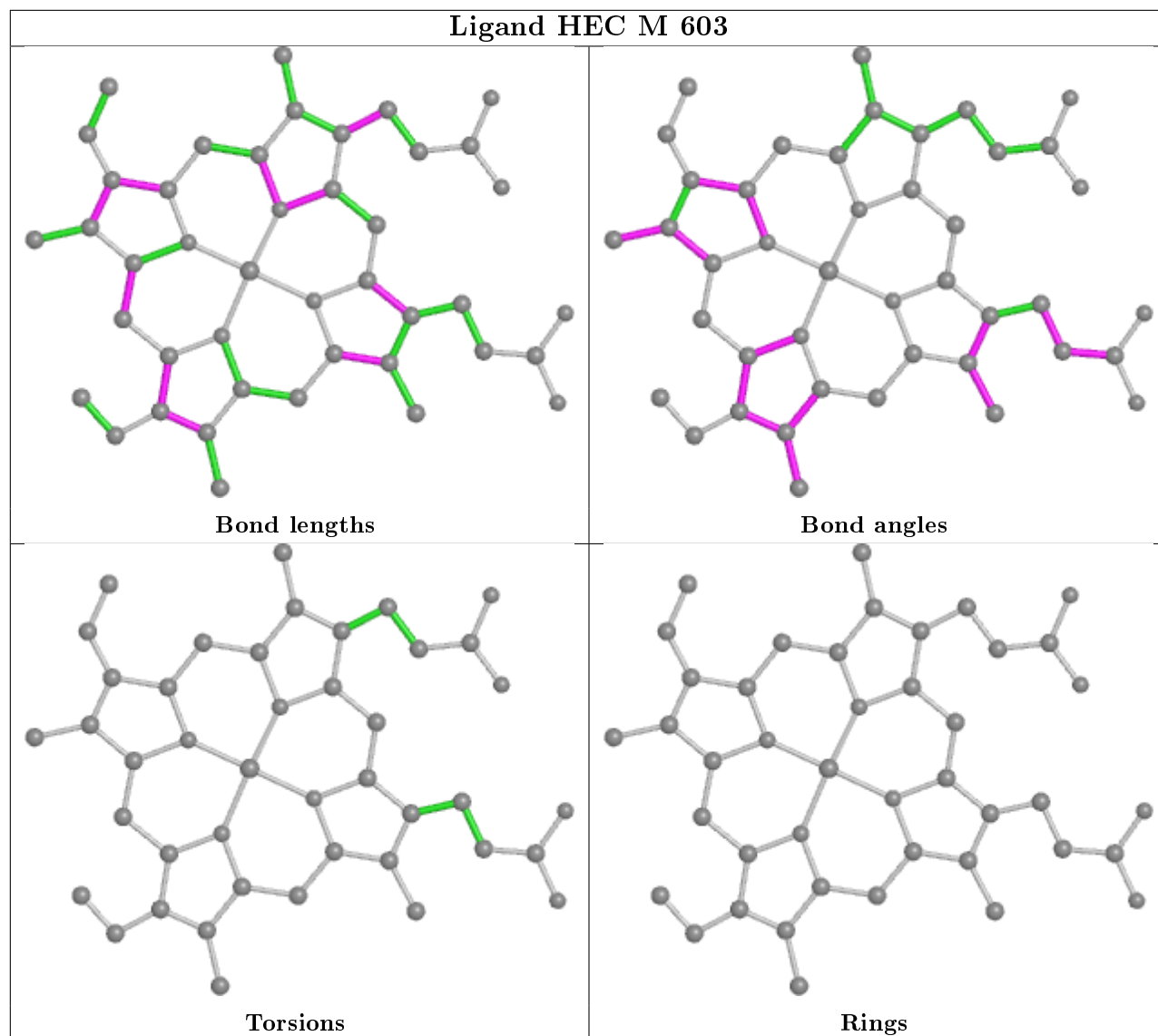


## Ligand HEC L 605

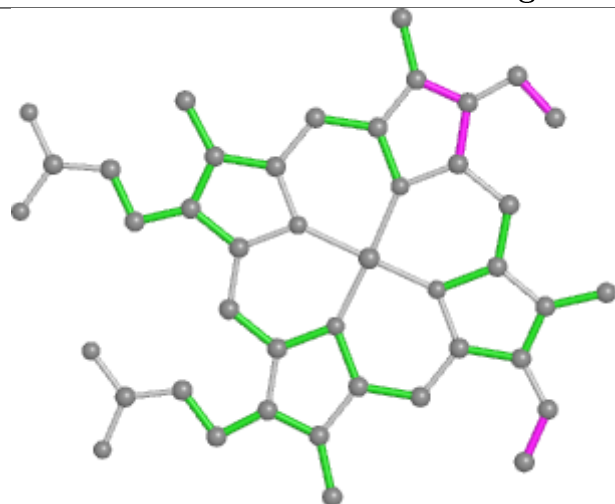




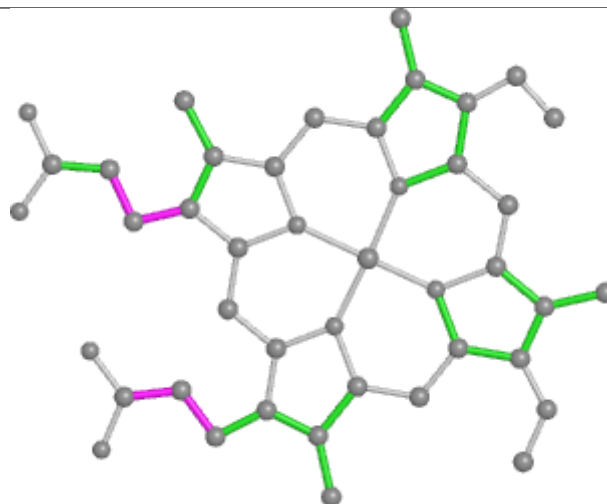




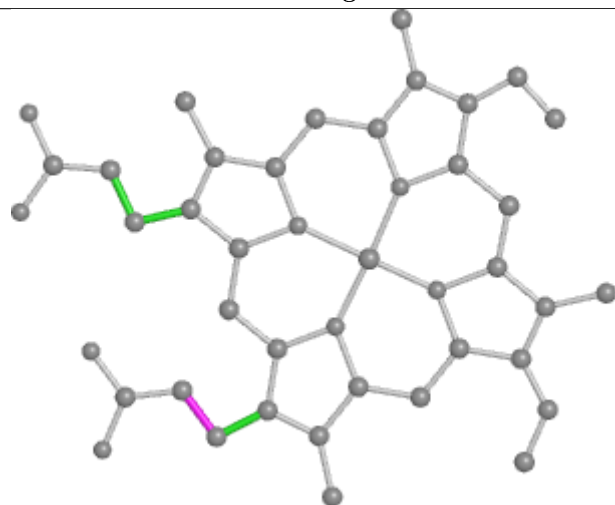
## Ligand HEC J 602



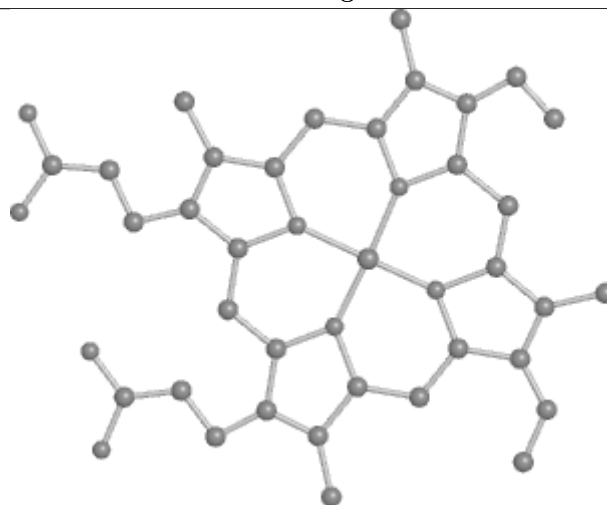
Bond lengths



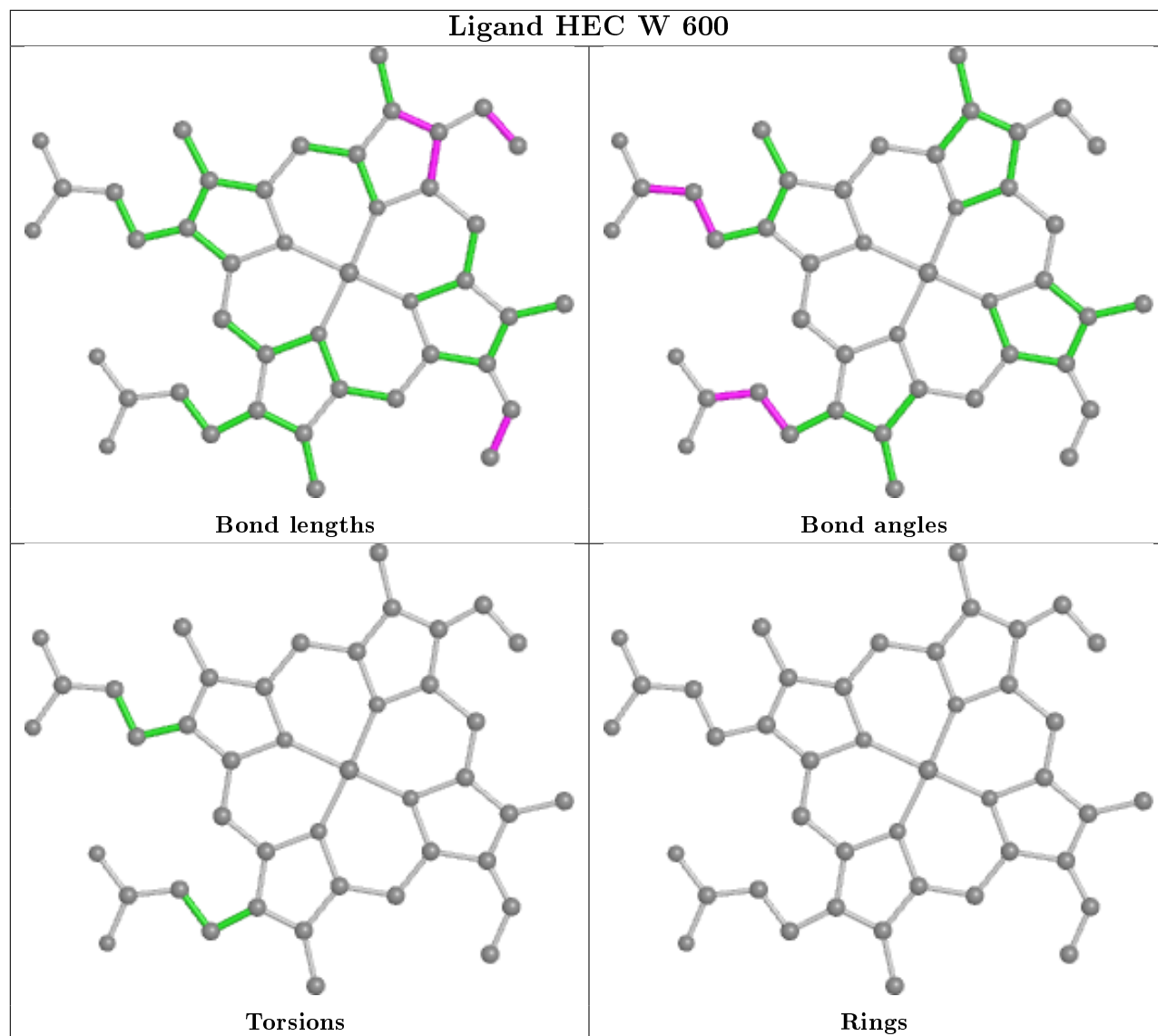
Bond angles

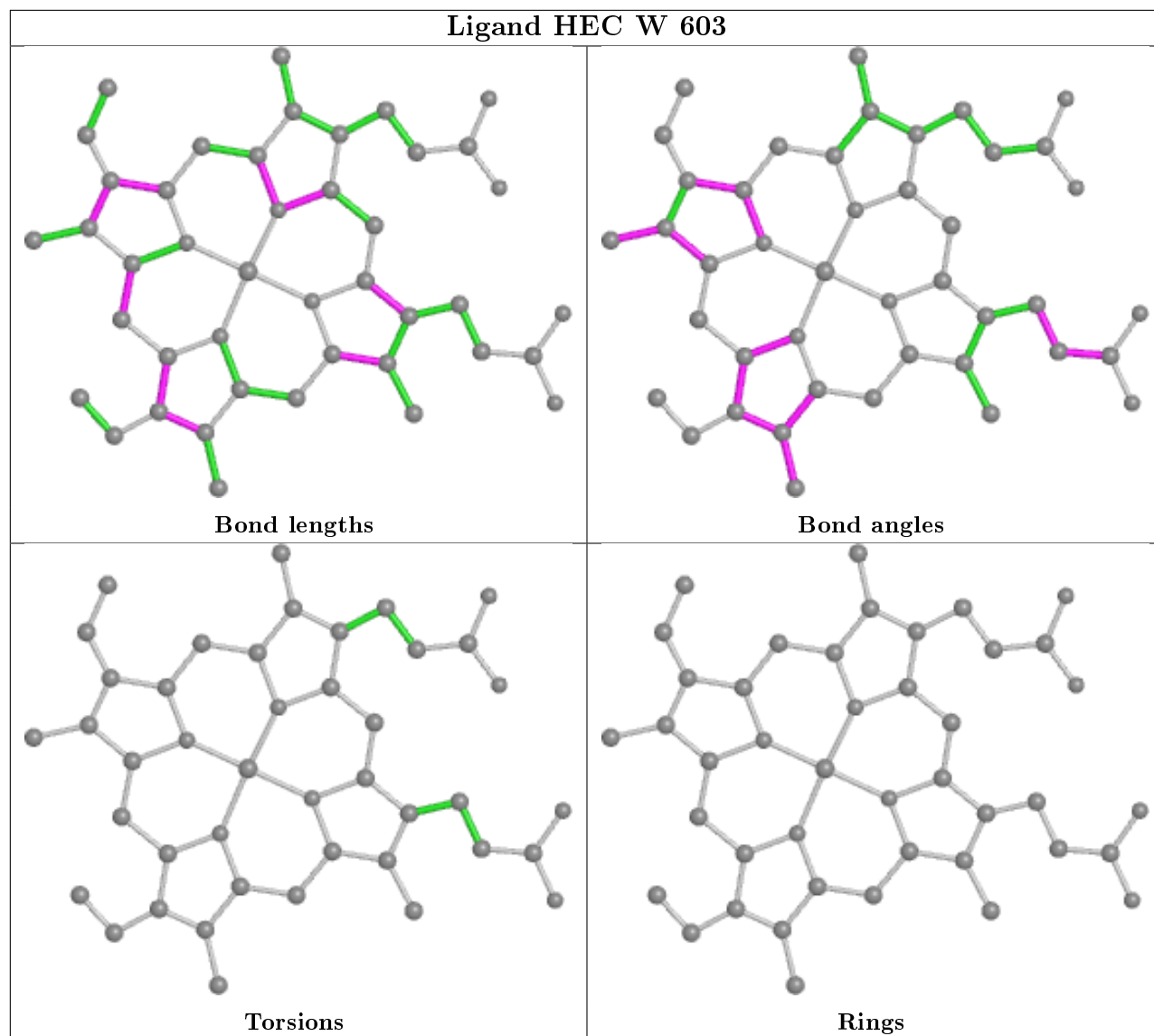


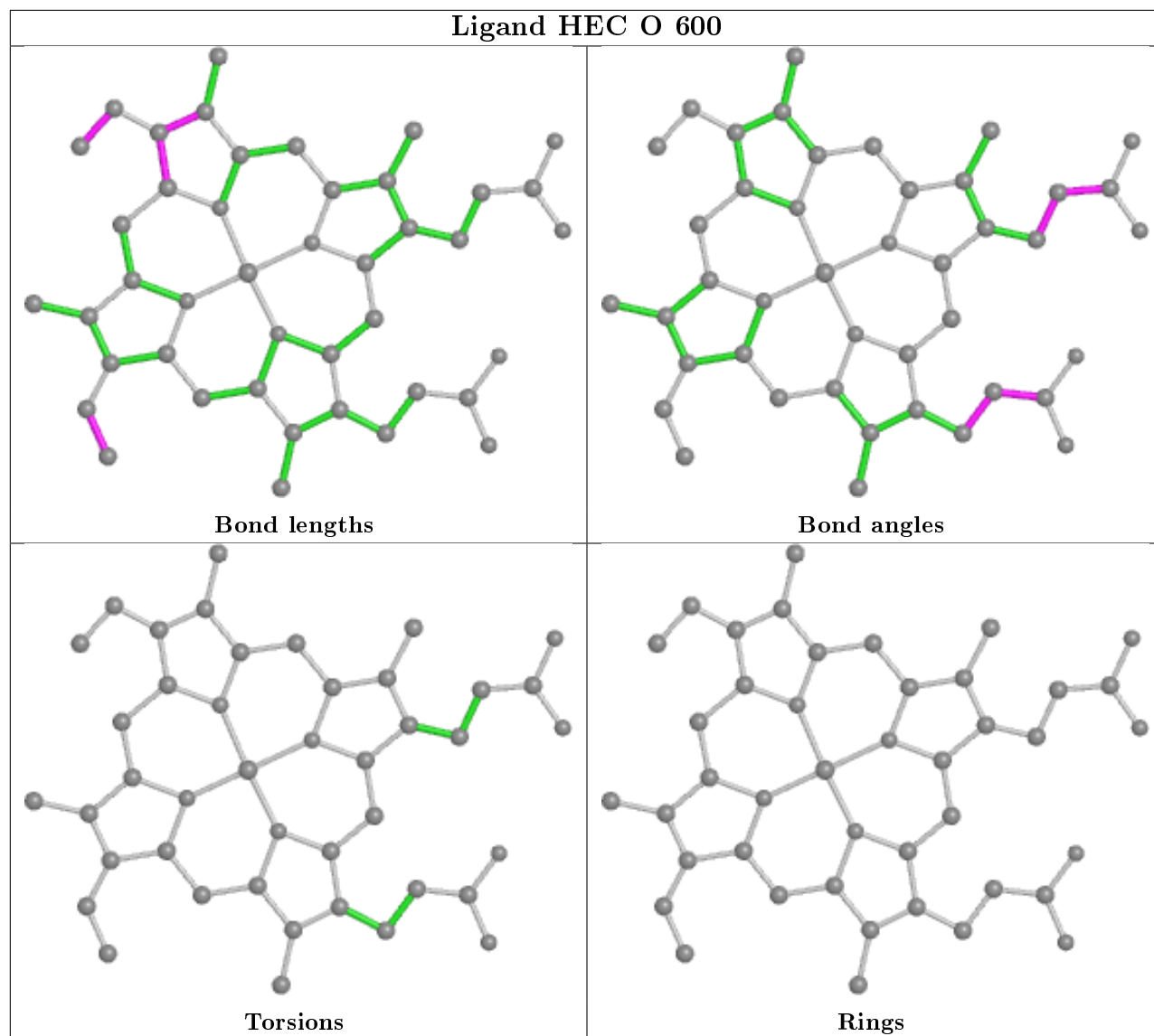
Torsions

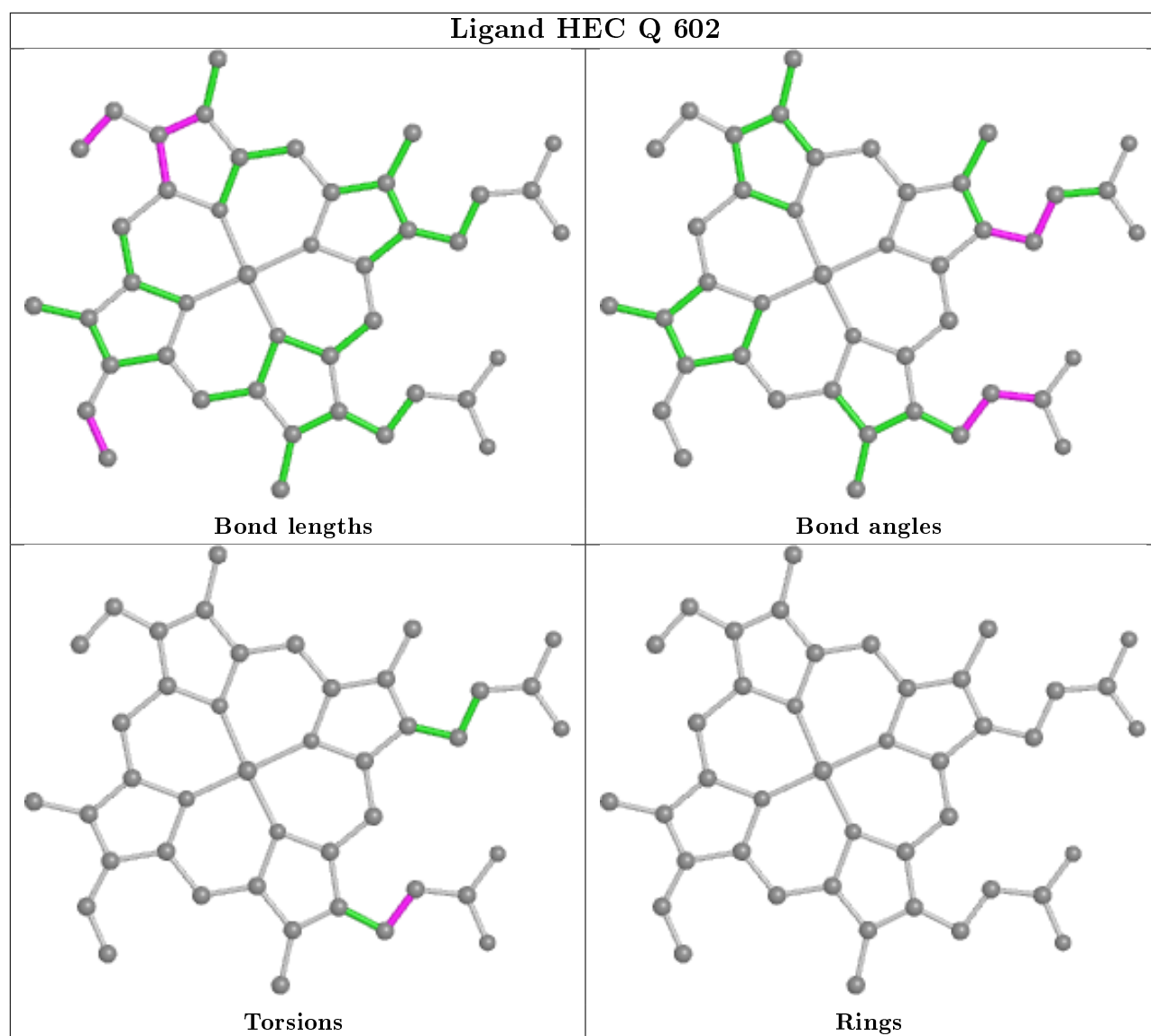


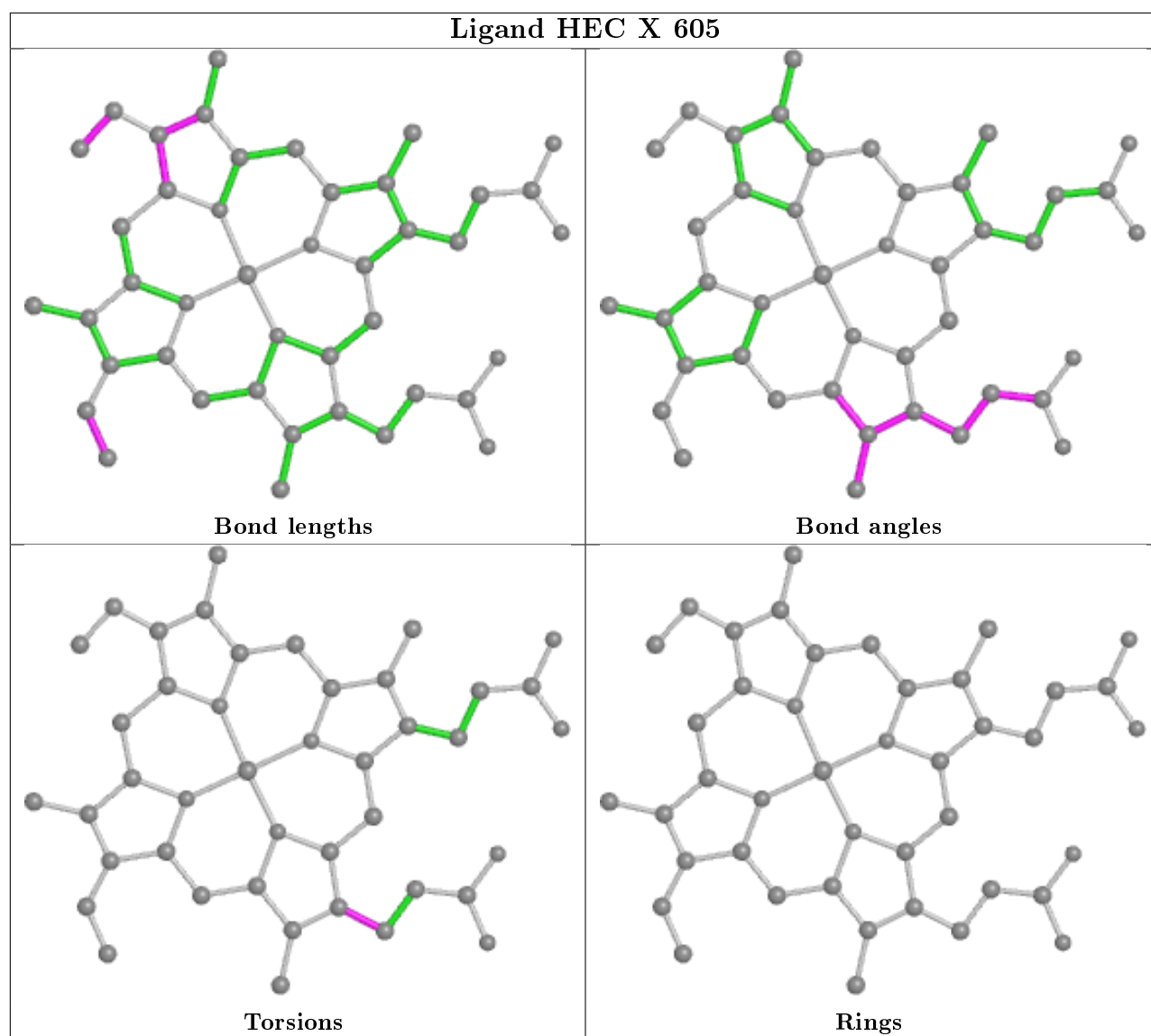
Rings

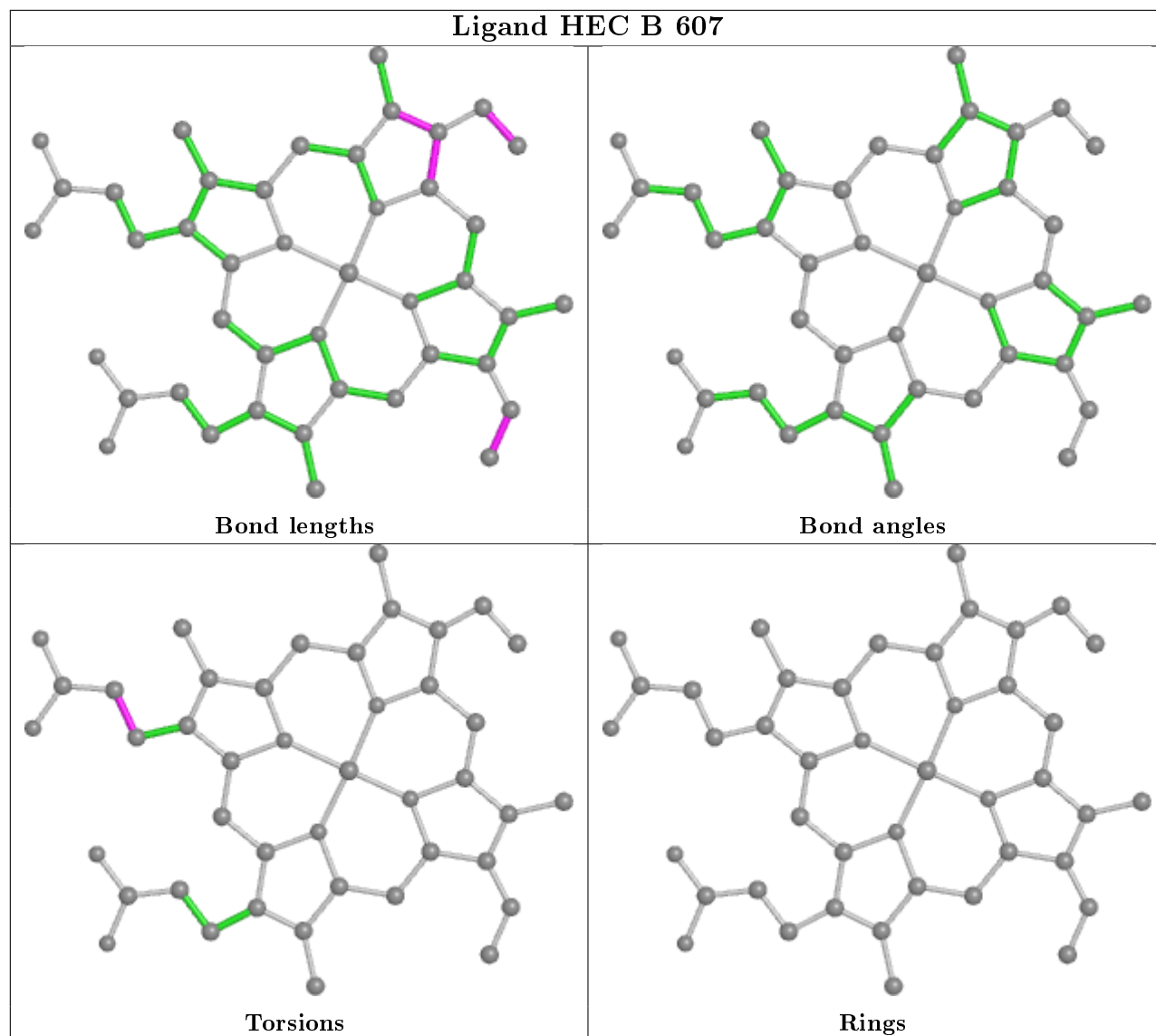




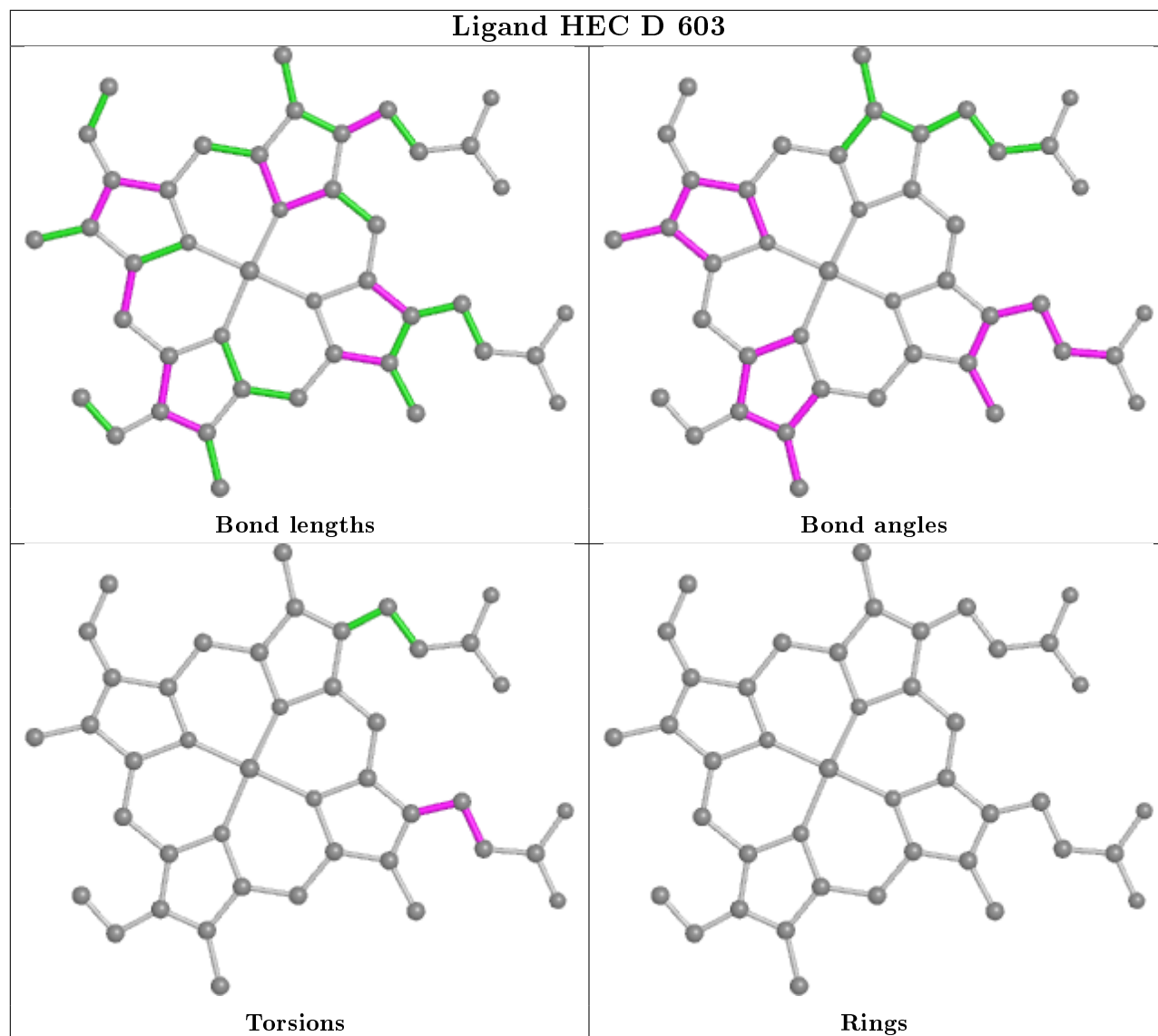




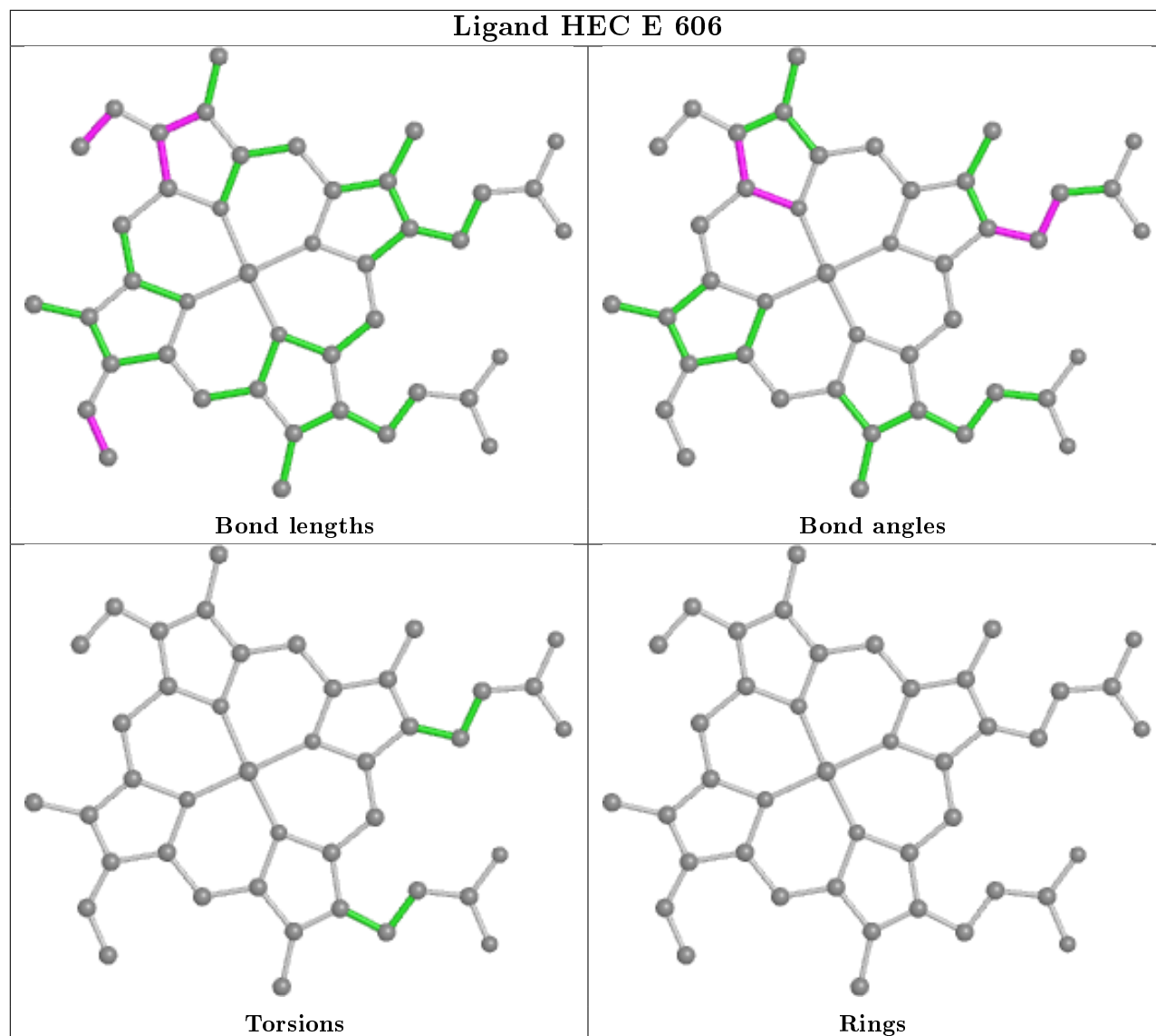


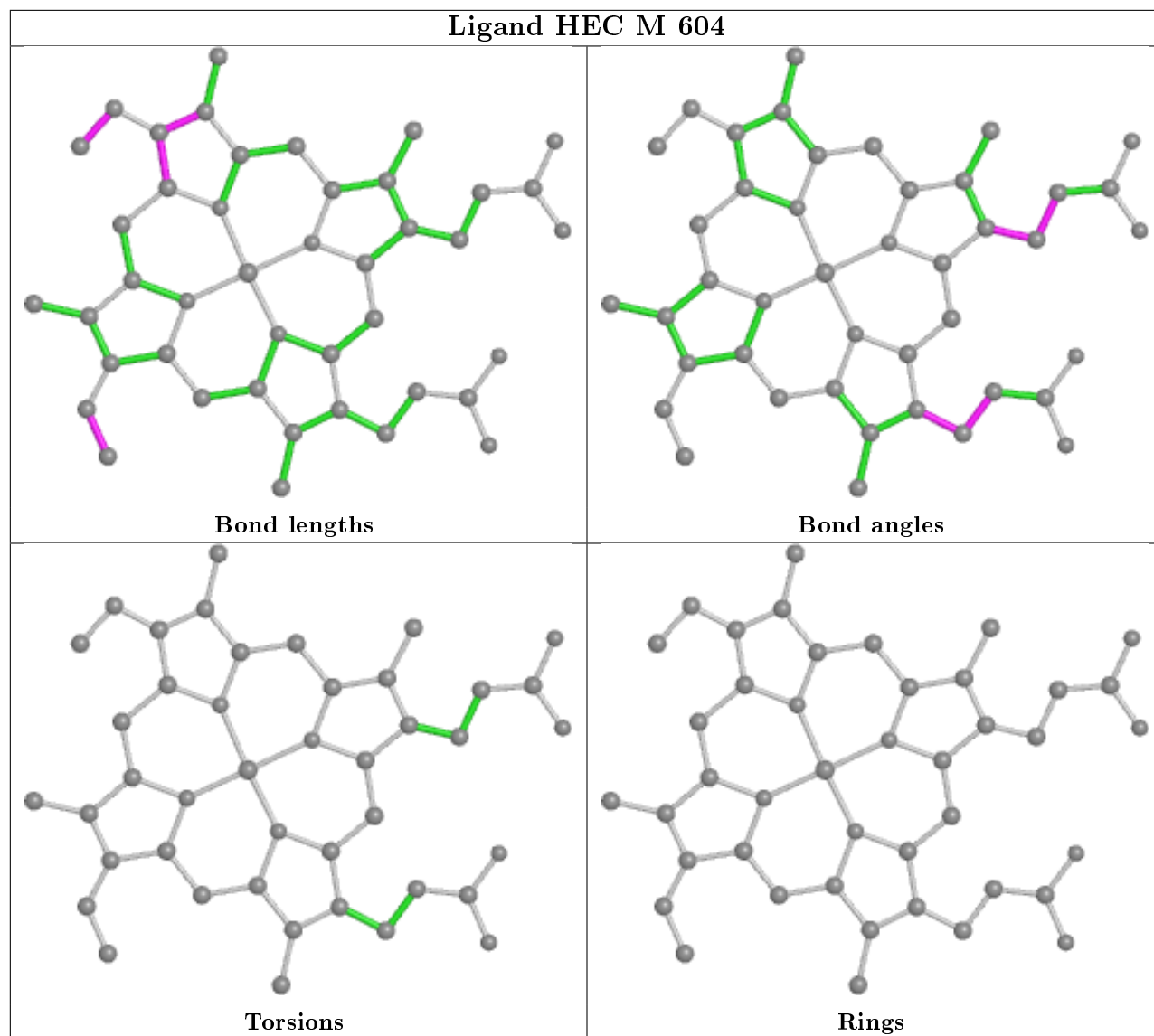


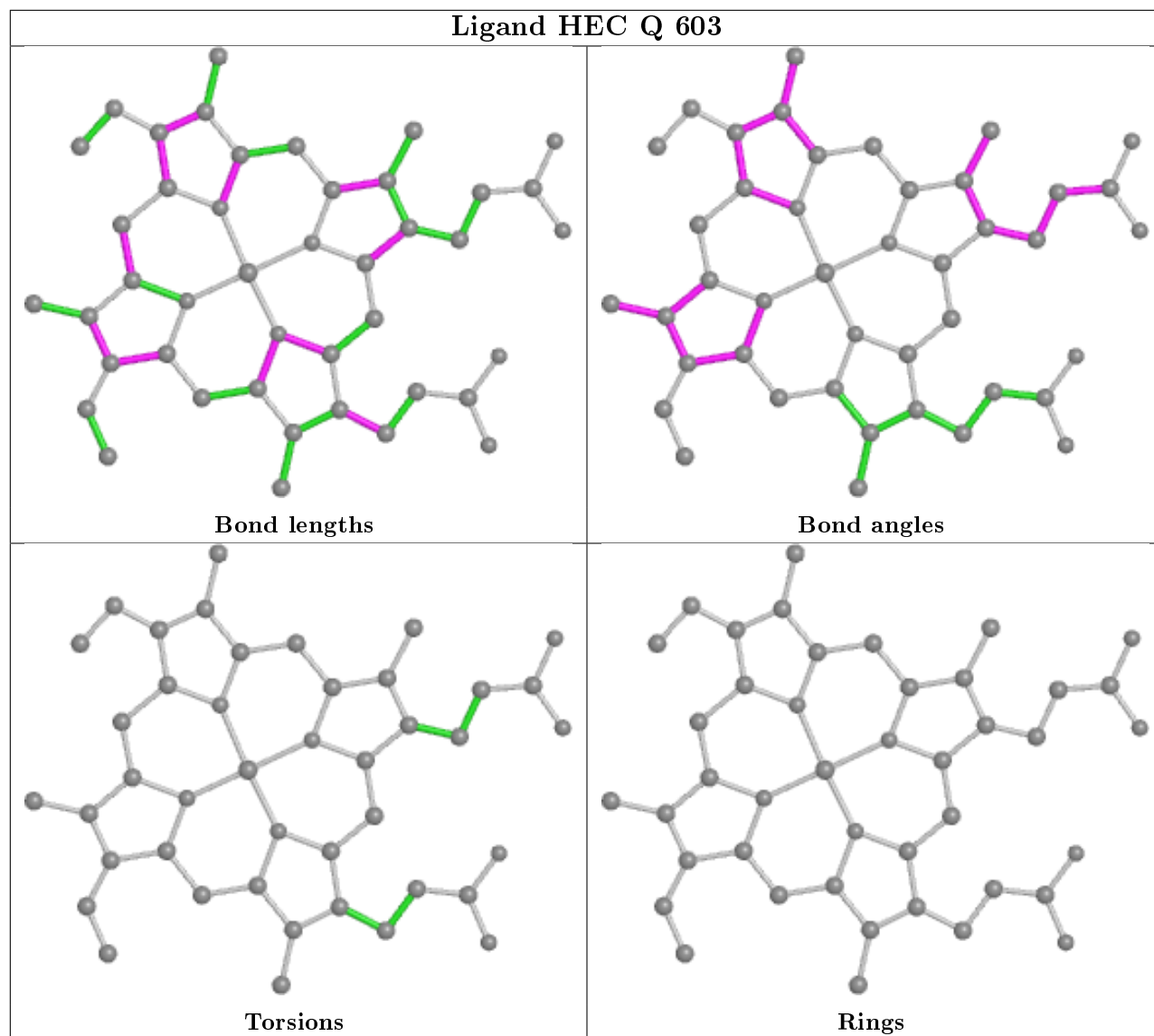


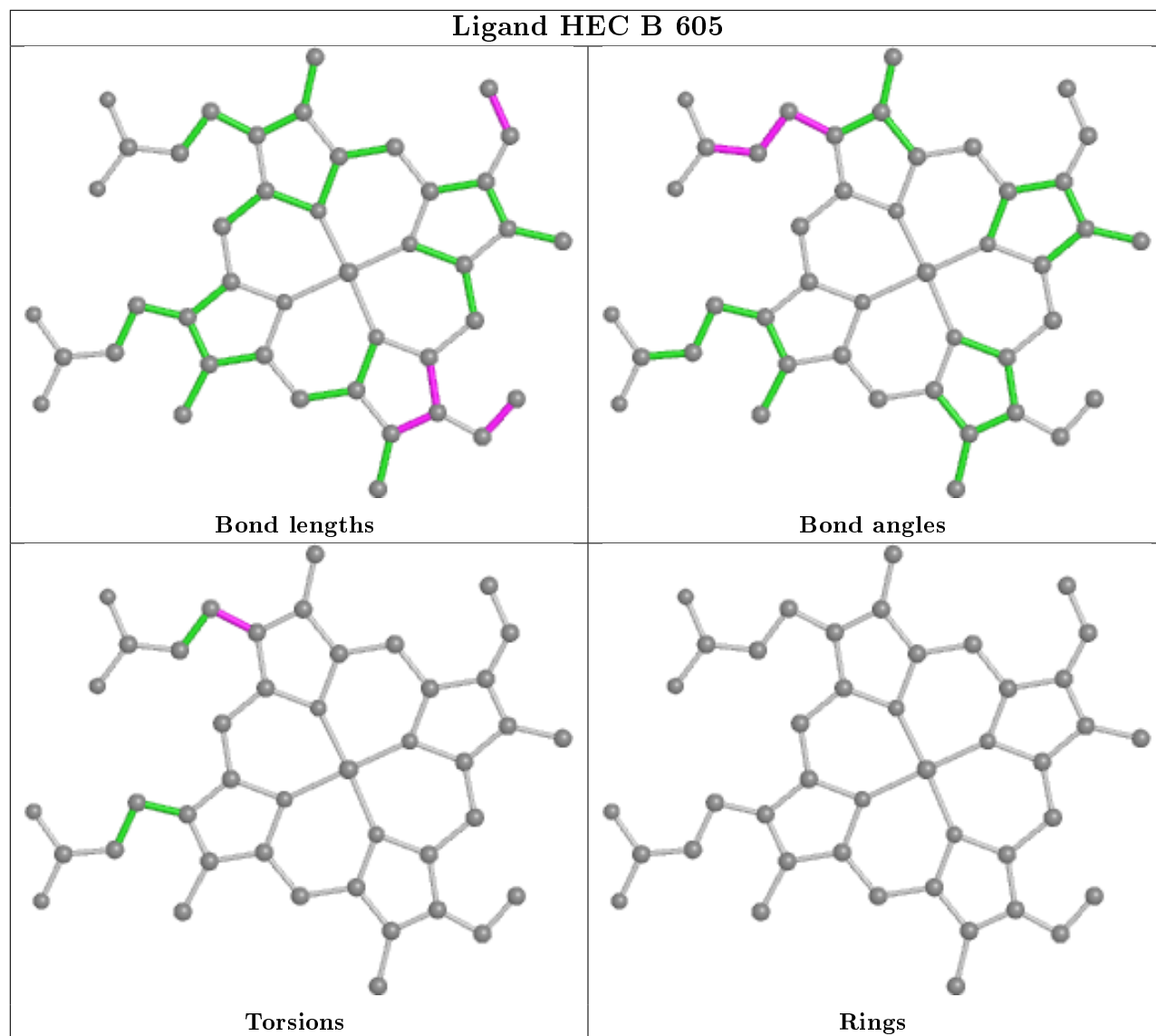


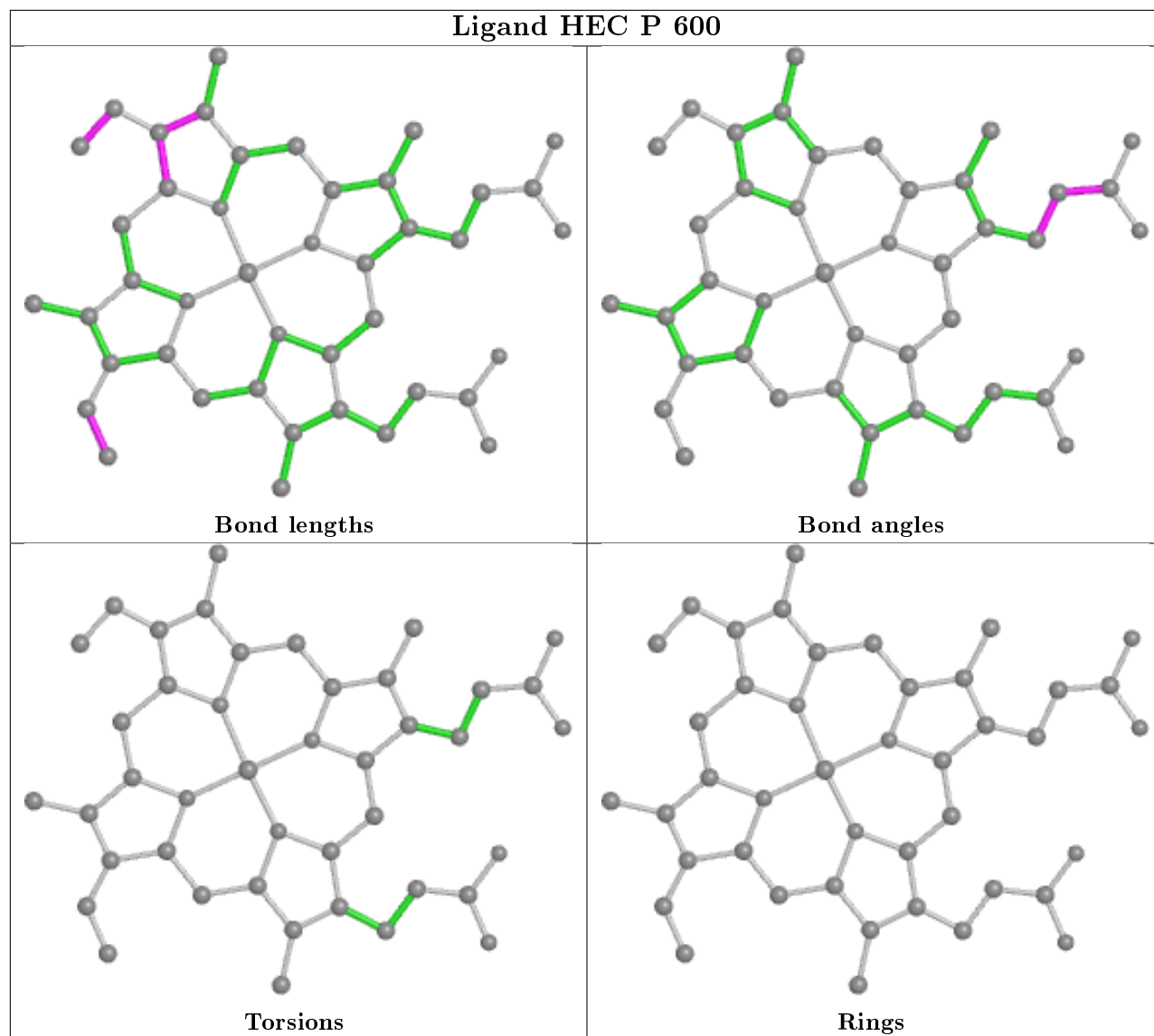
## Ligand HEC E 606

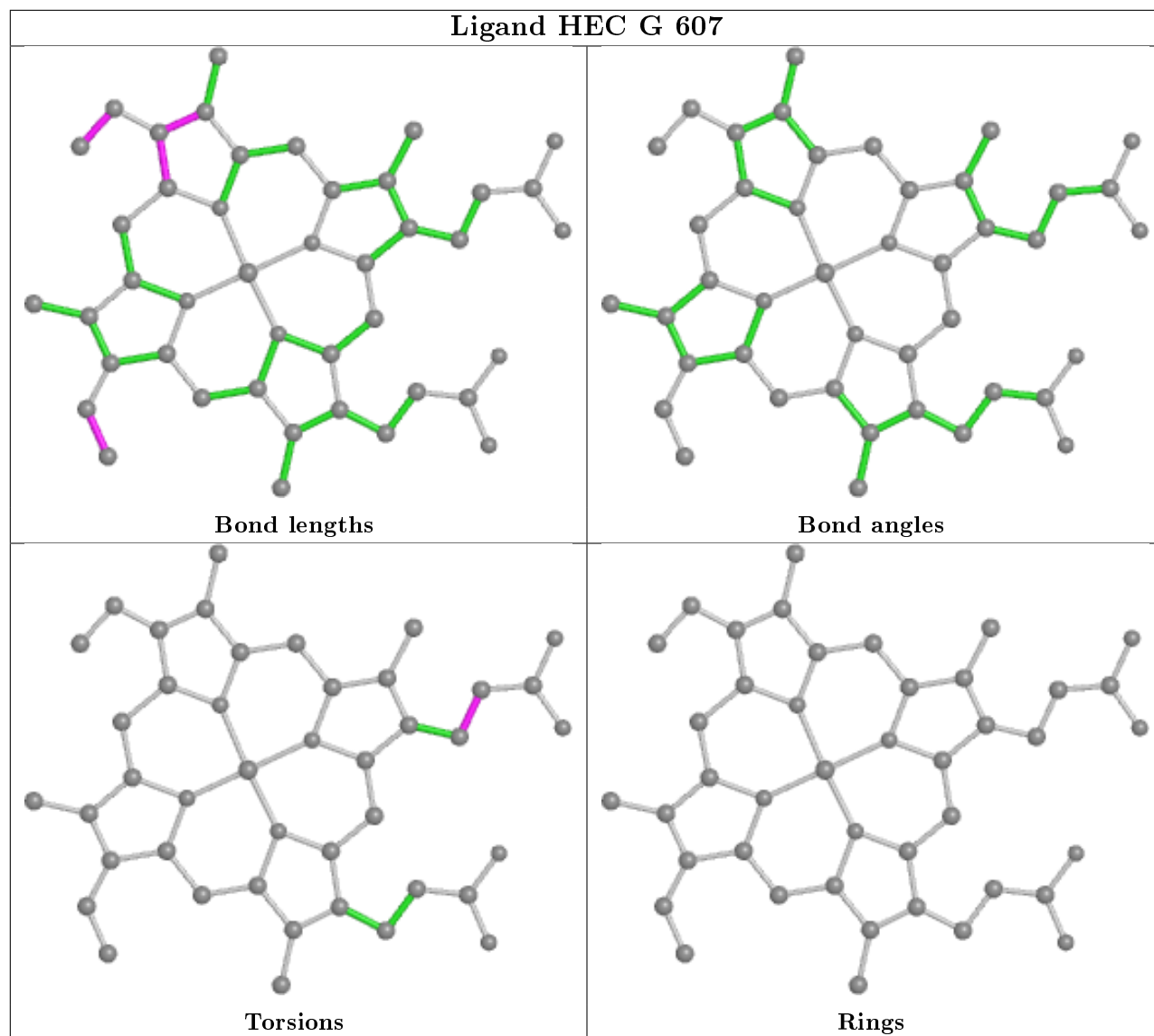




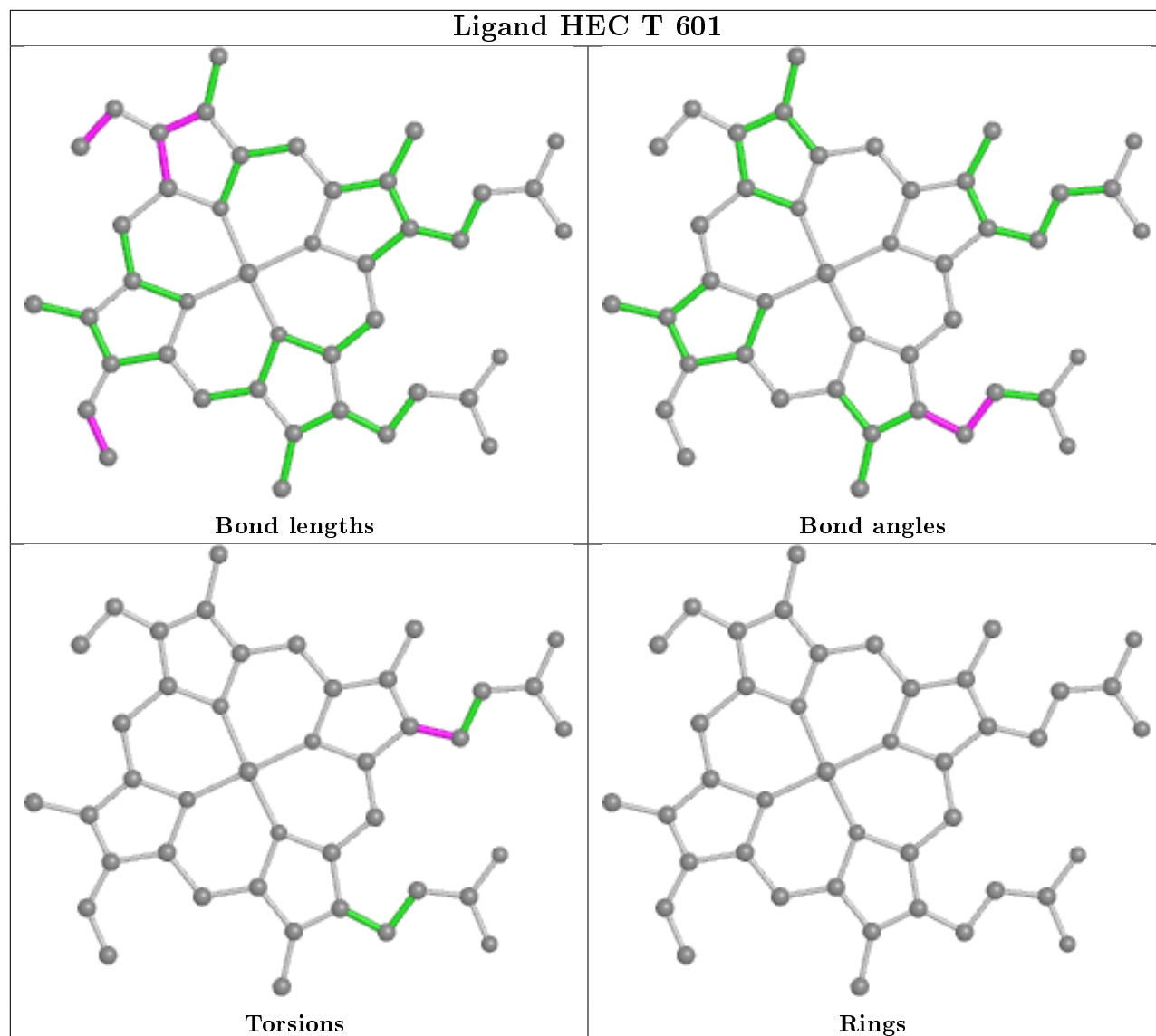




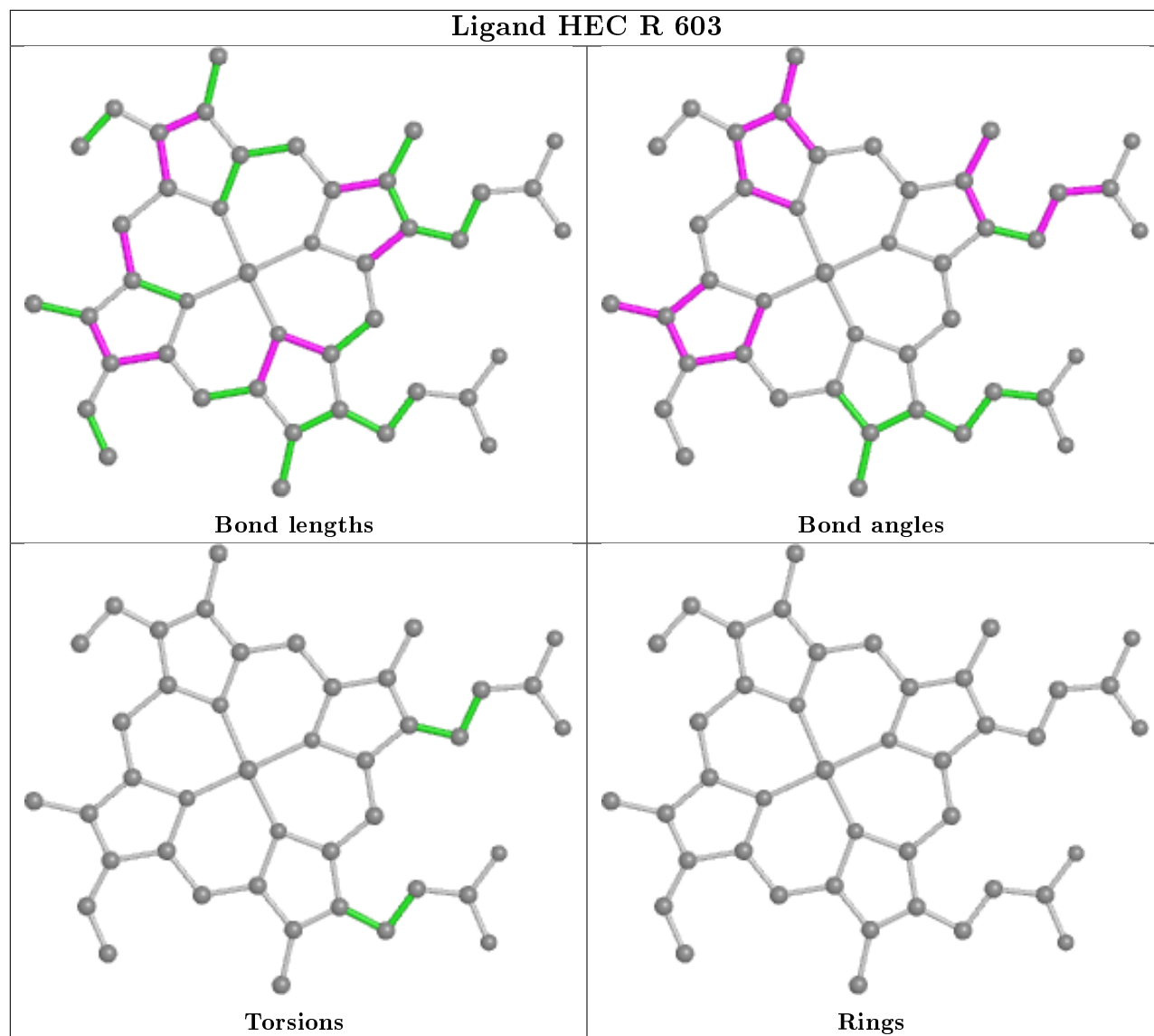


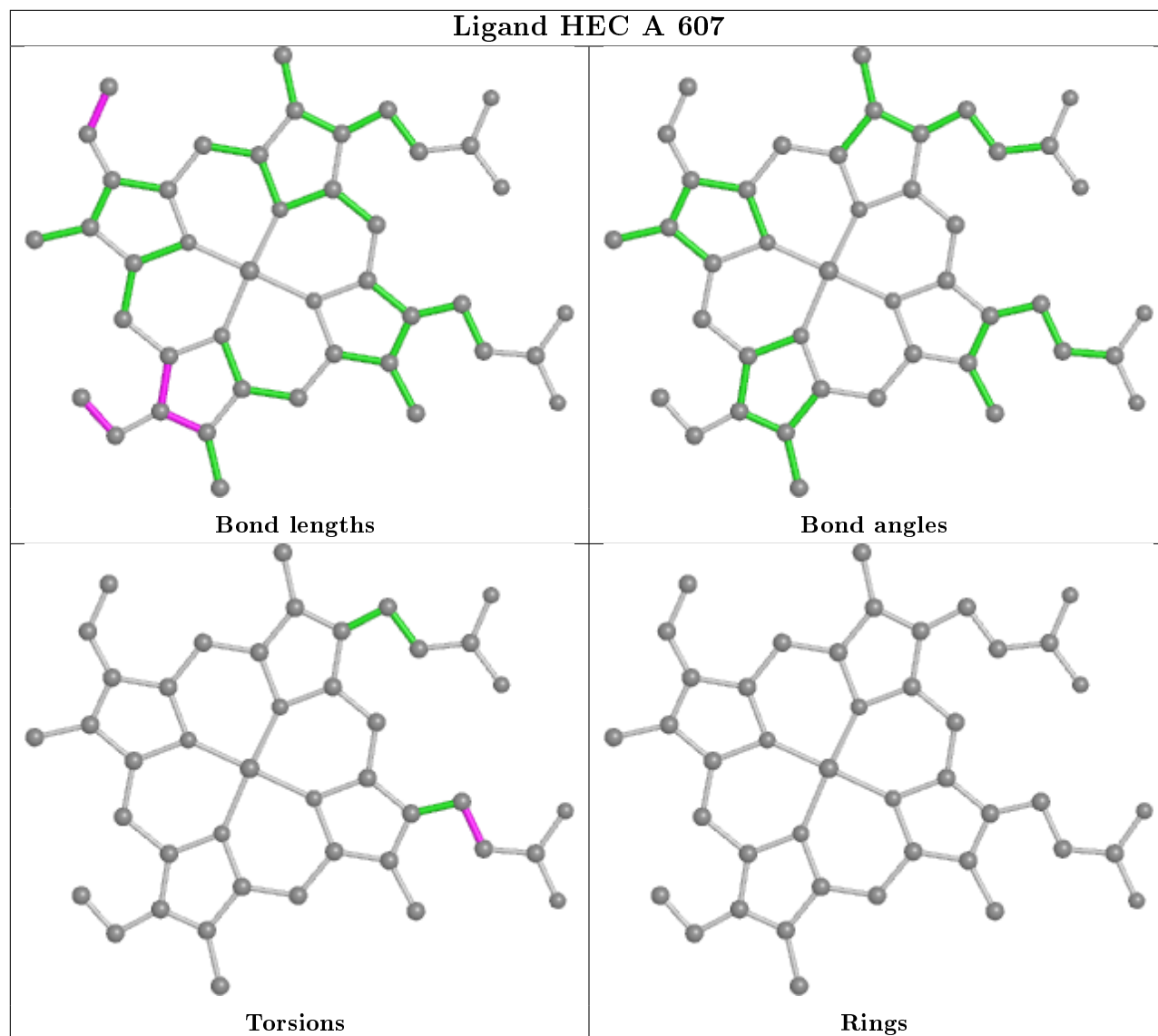


## Ligand HEC T 601

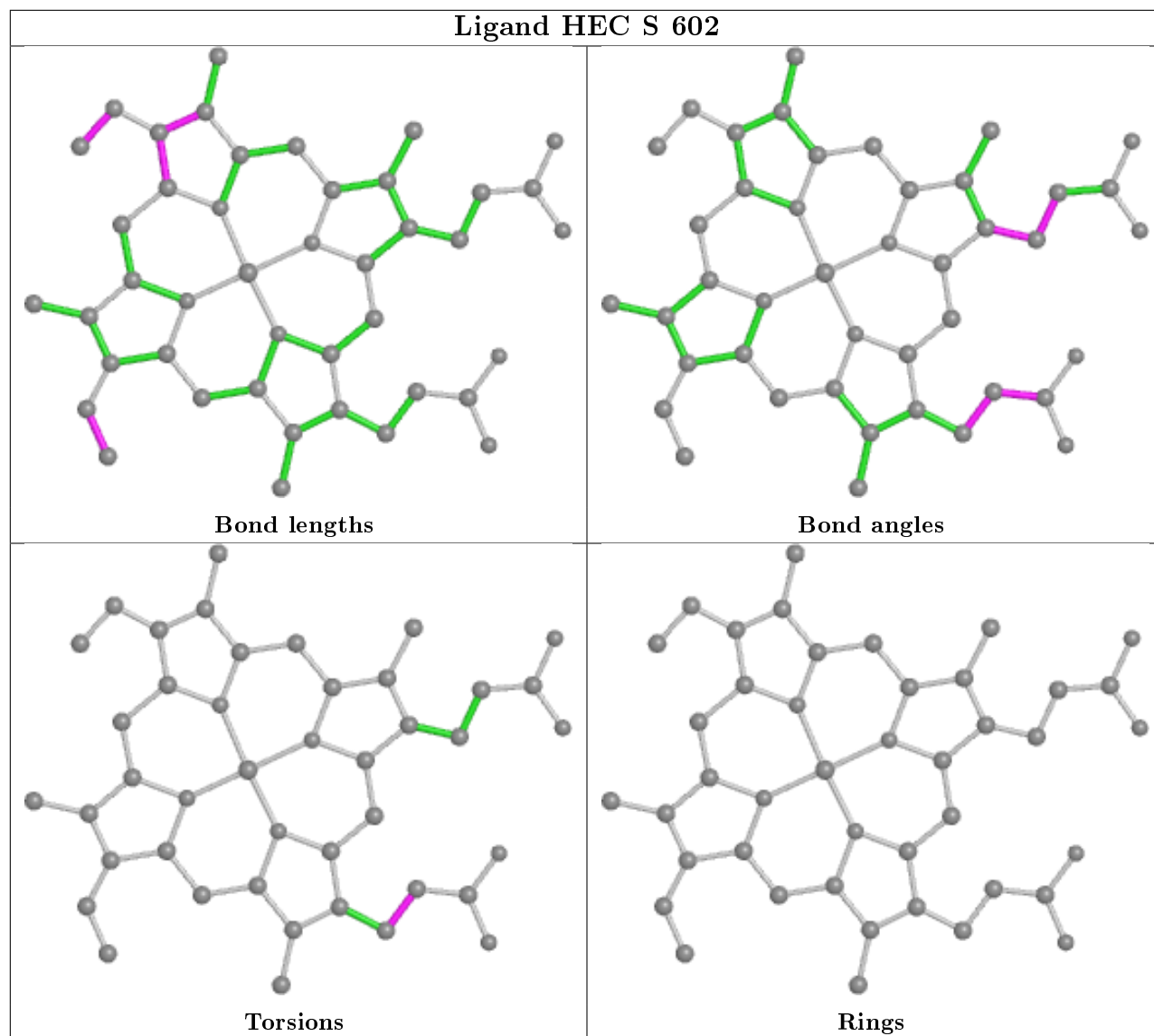




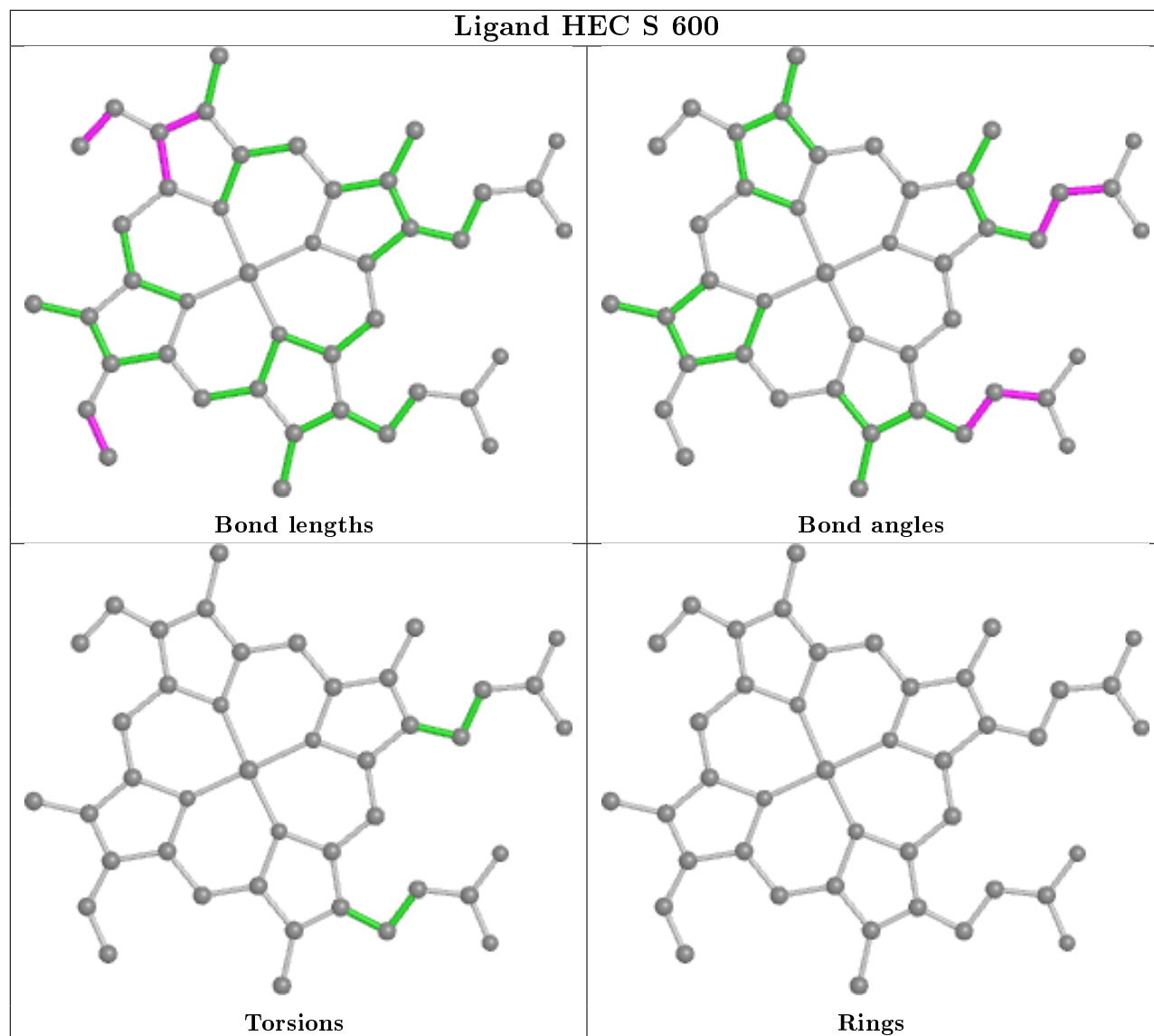




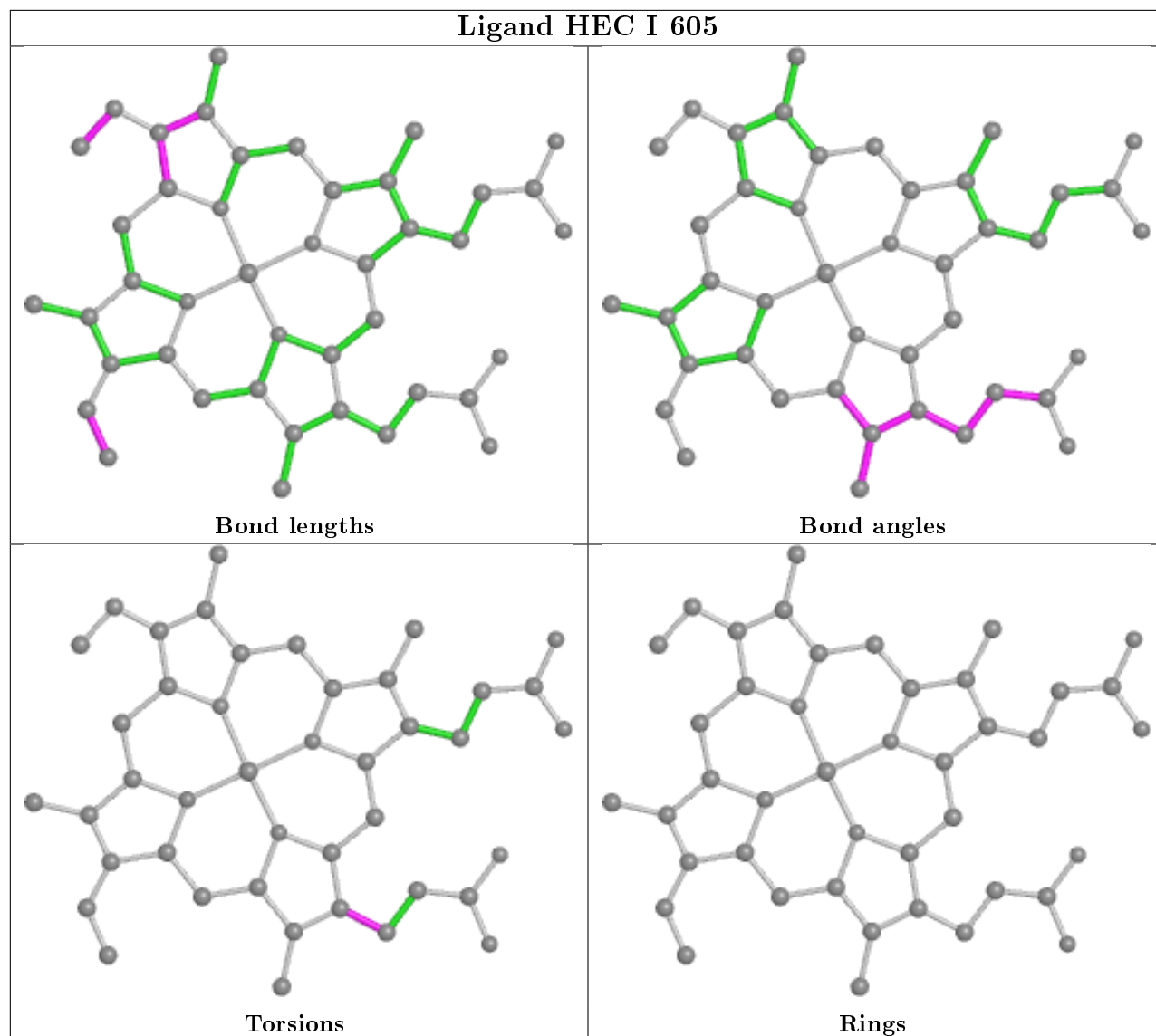
## Ligand HEC S 602

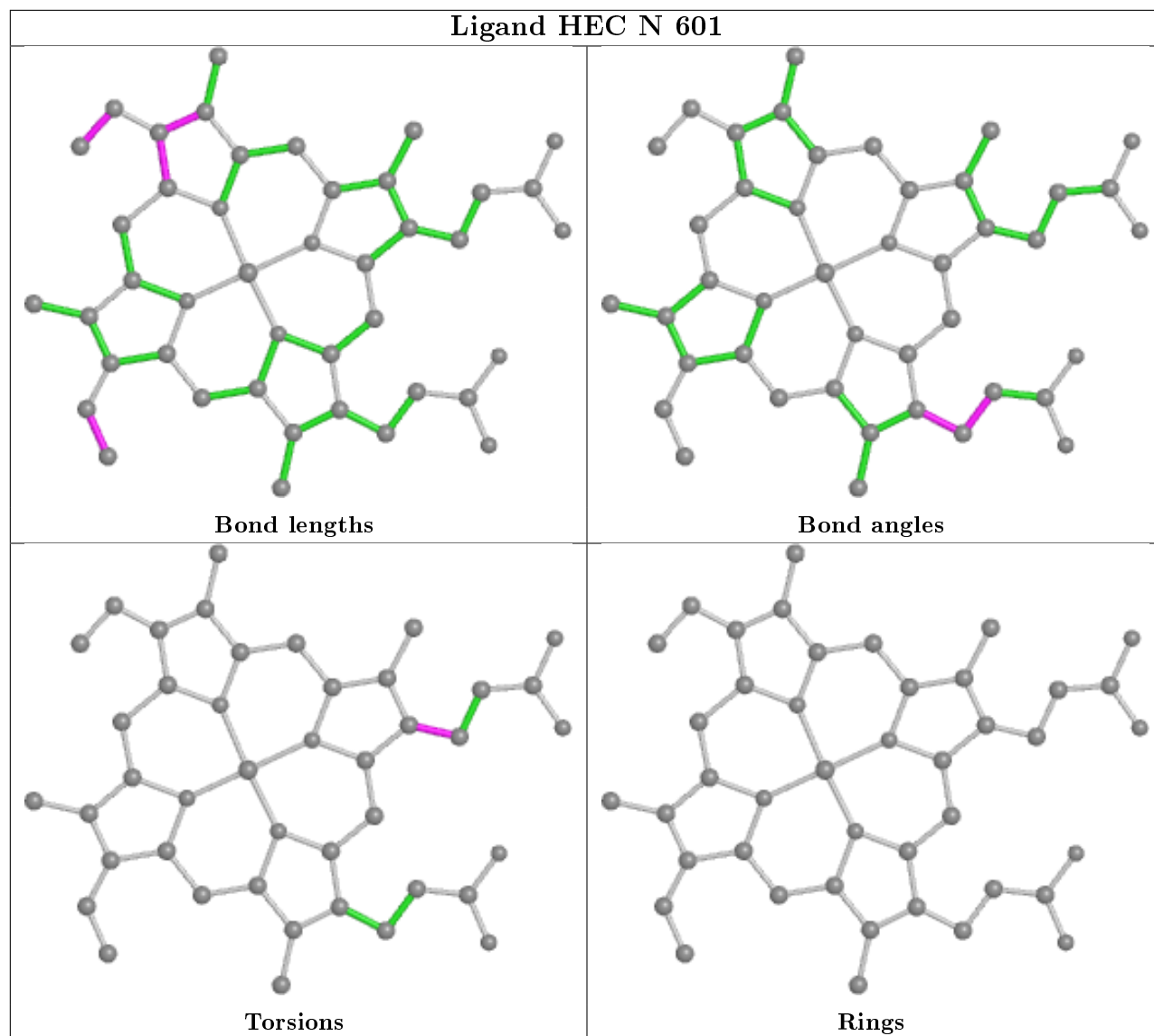


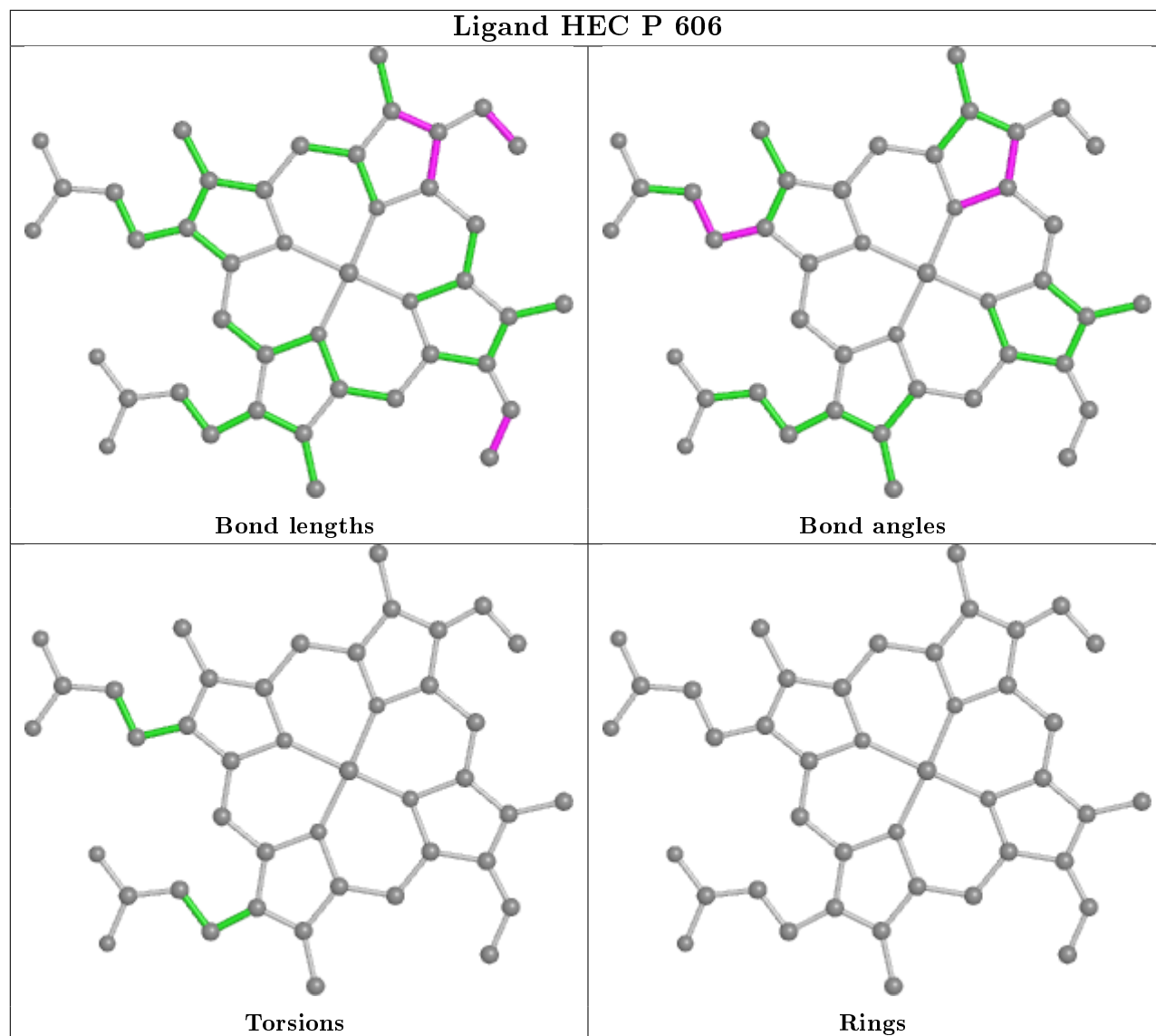
## Ligand HEC S 600

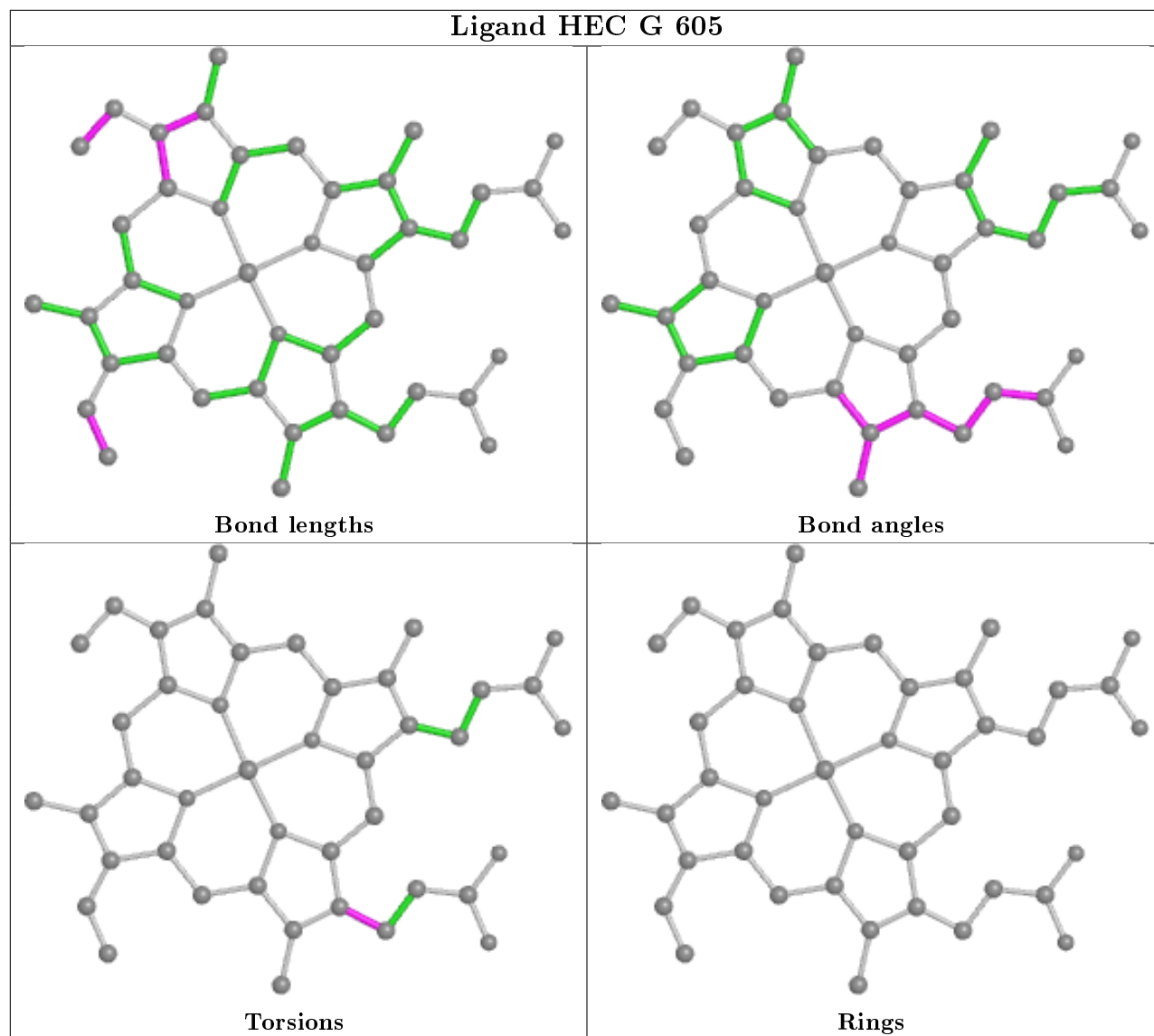


## Ligand HEC I 605

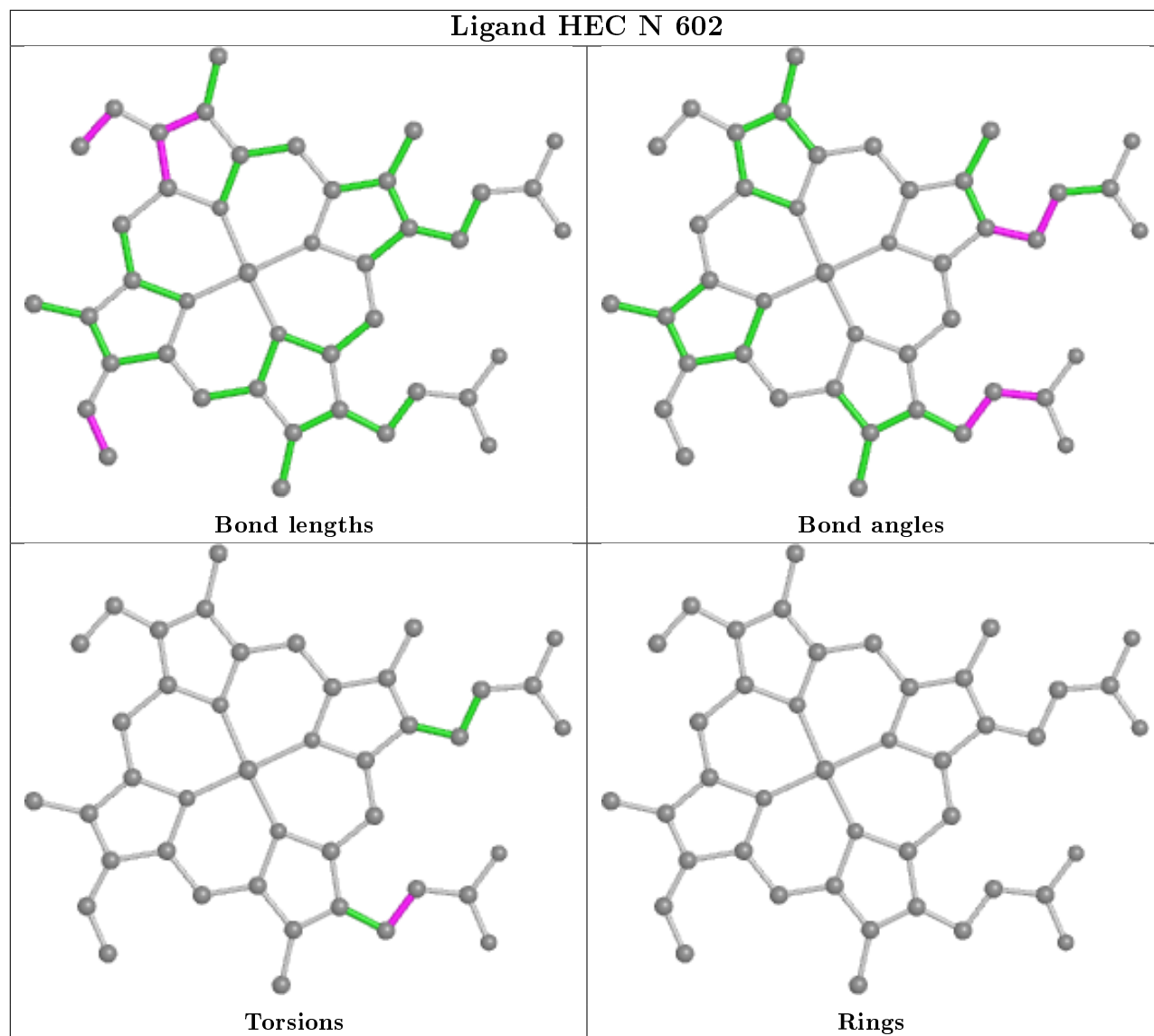


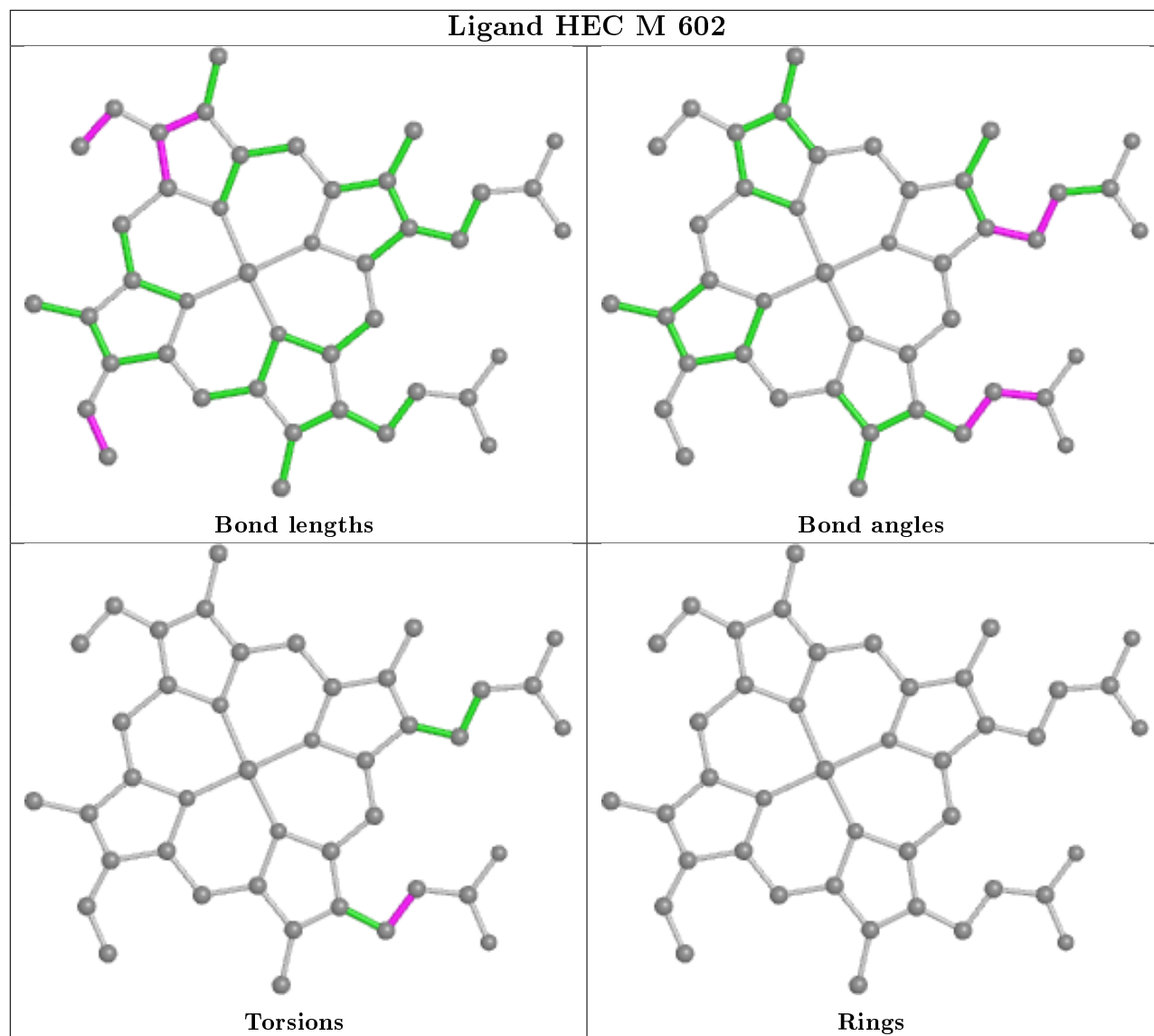


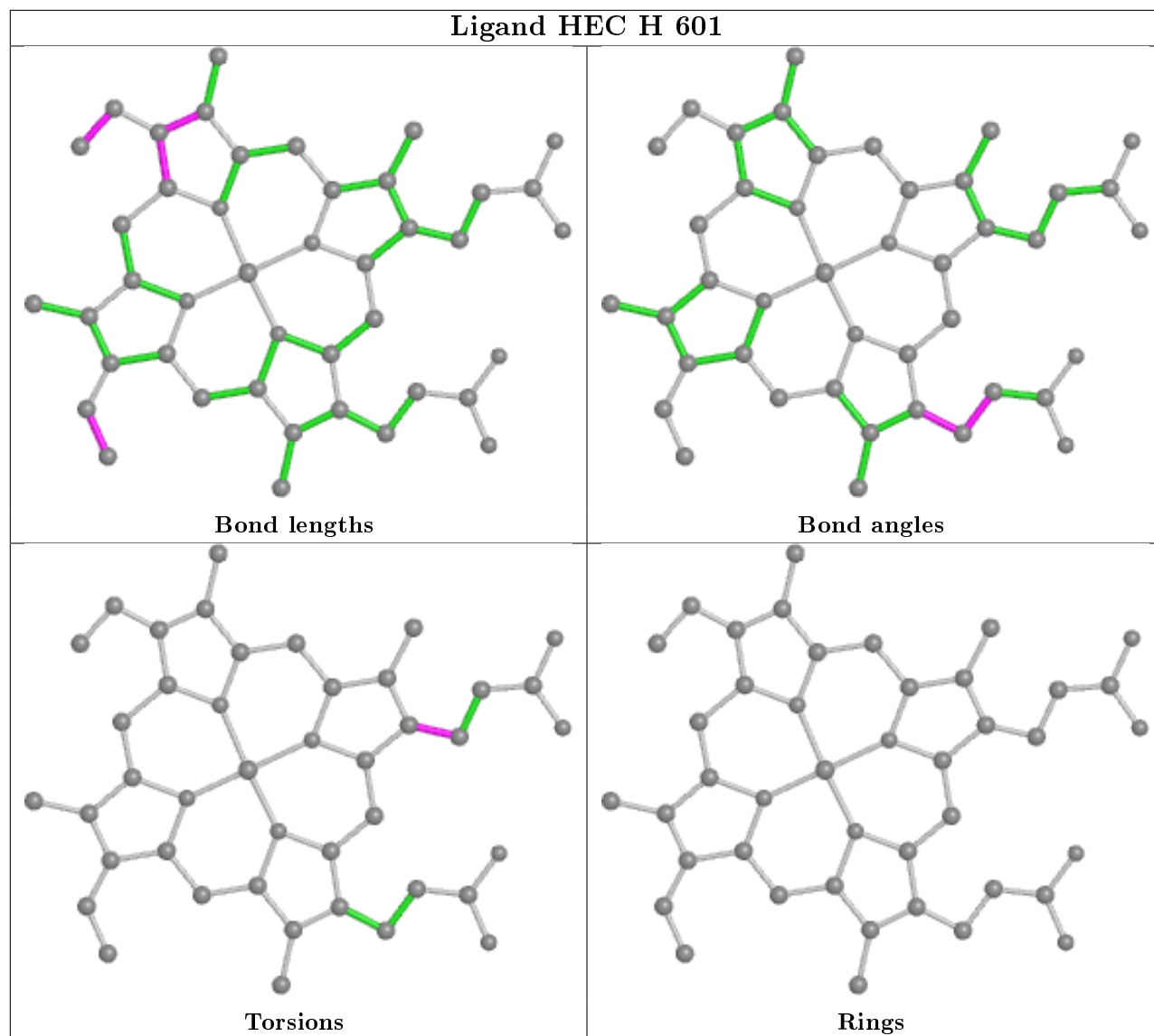


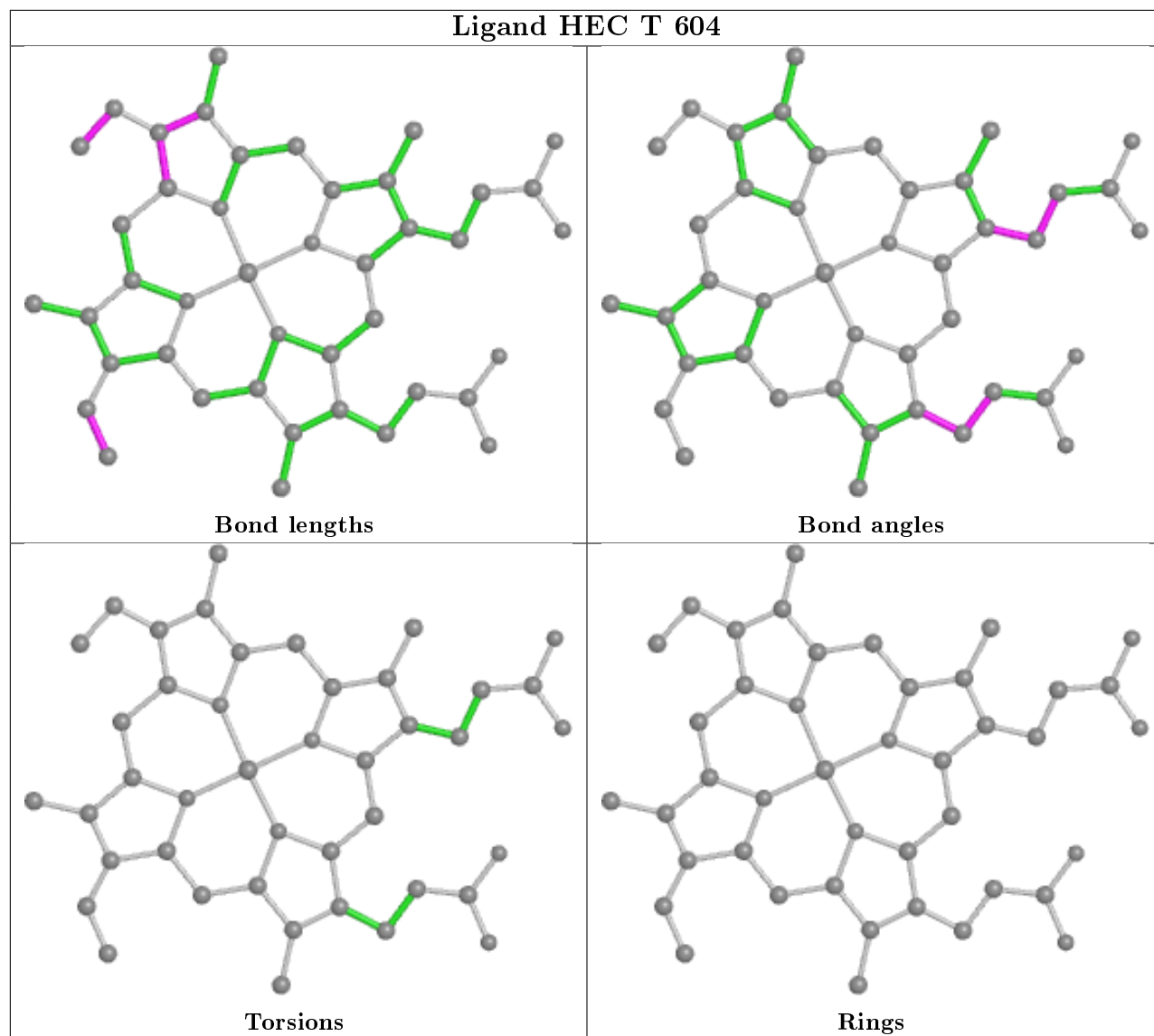




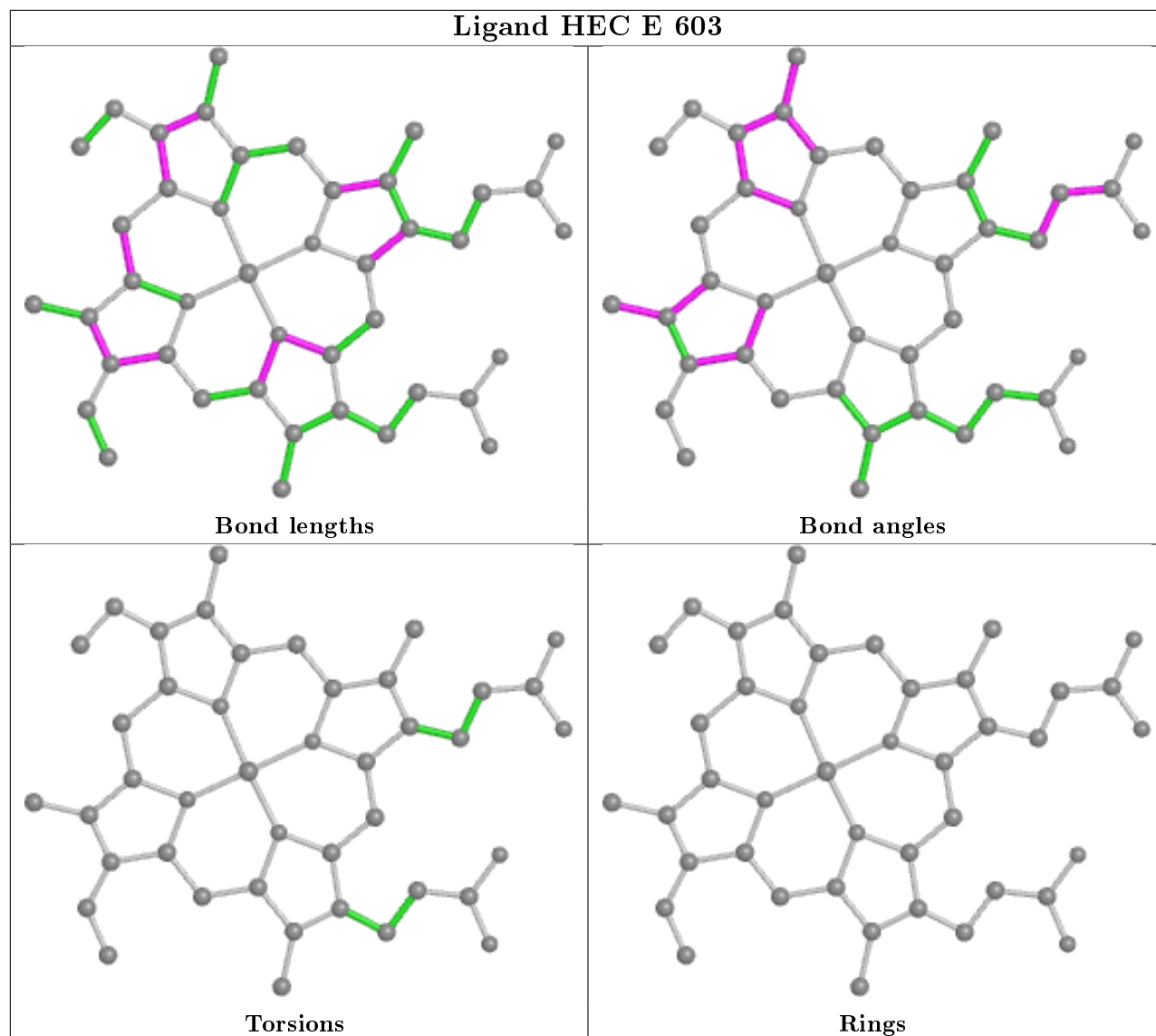




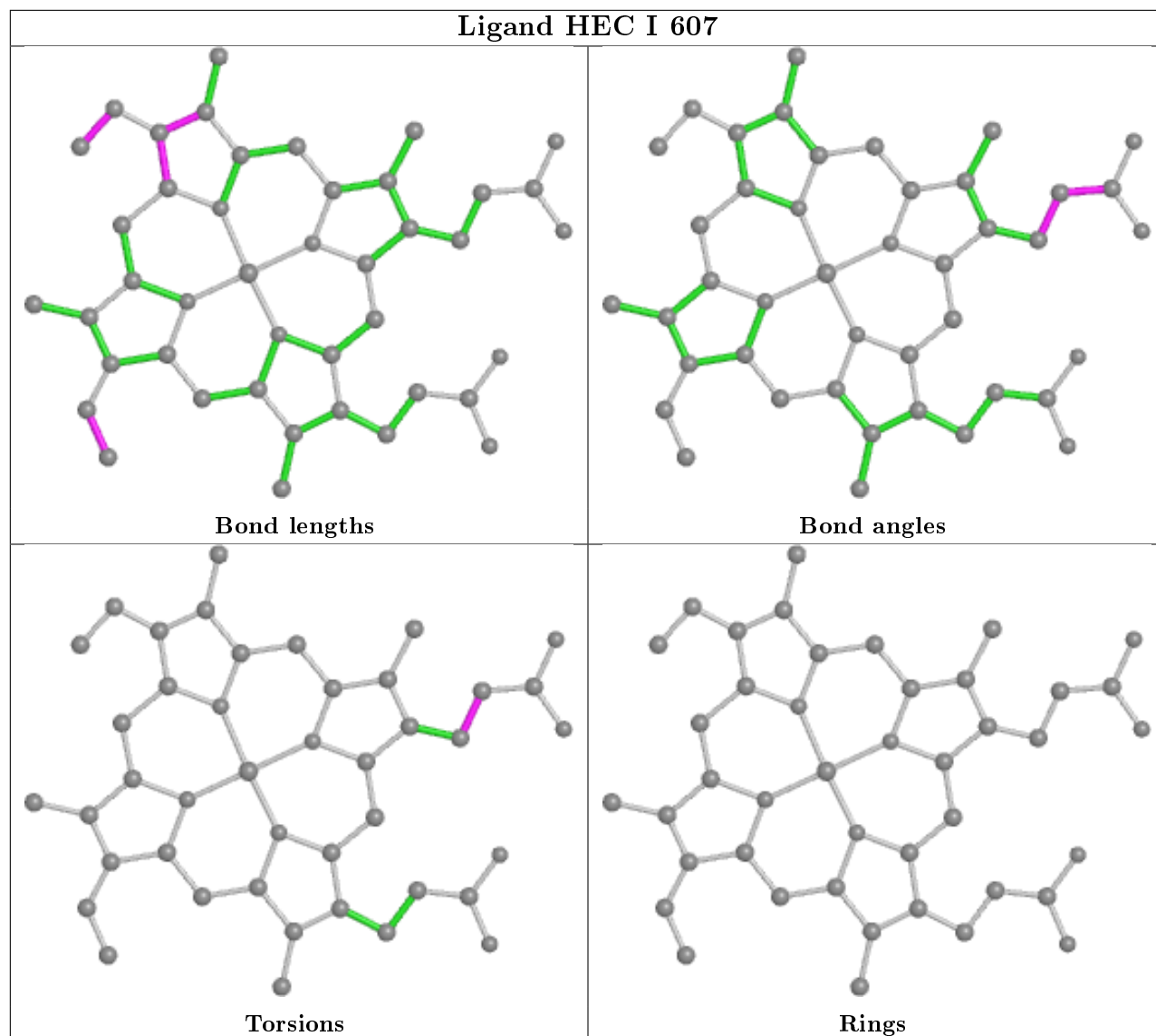


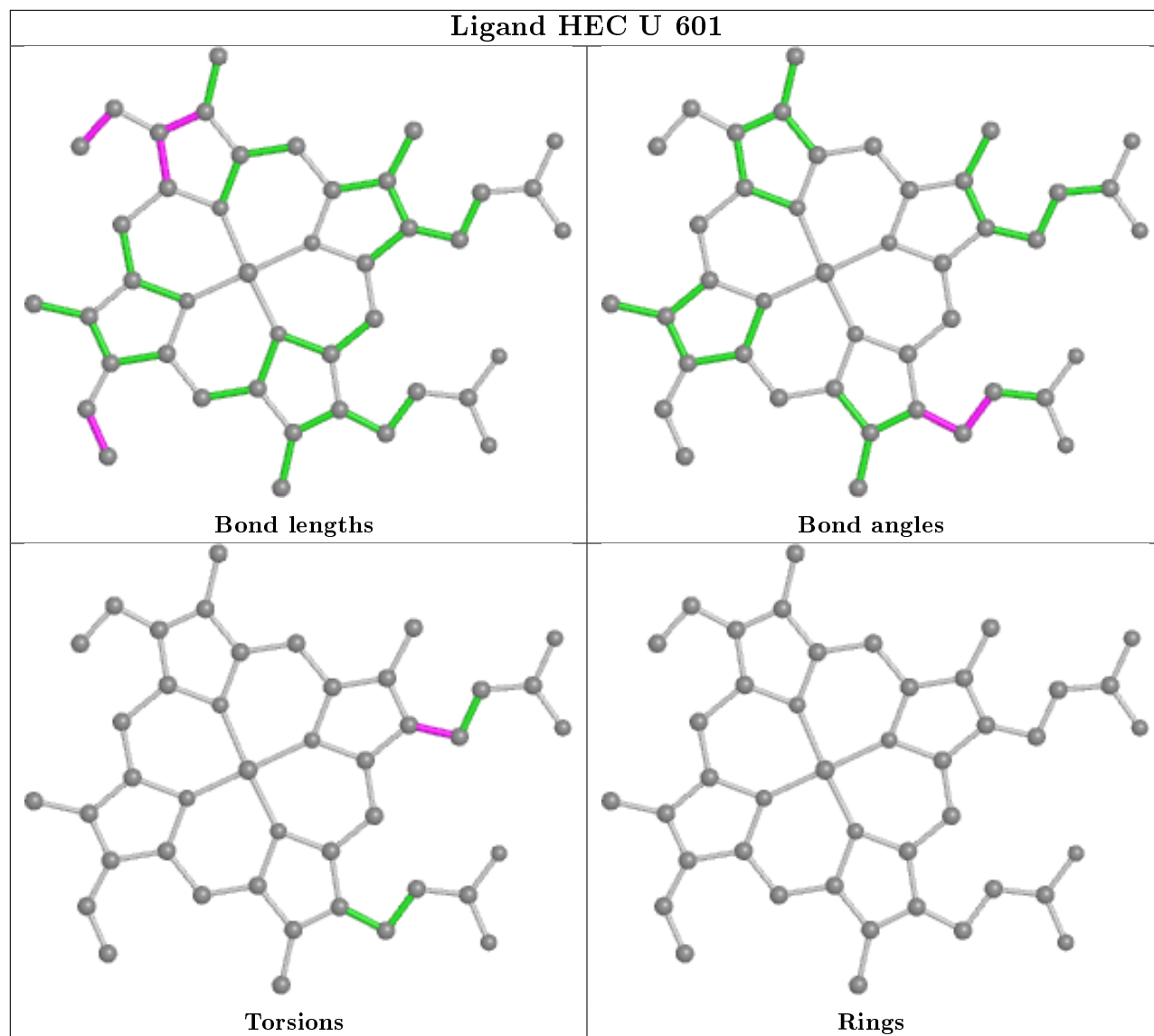


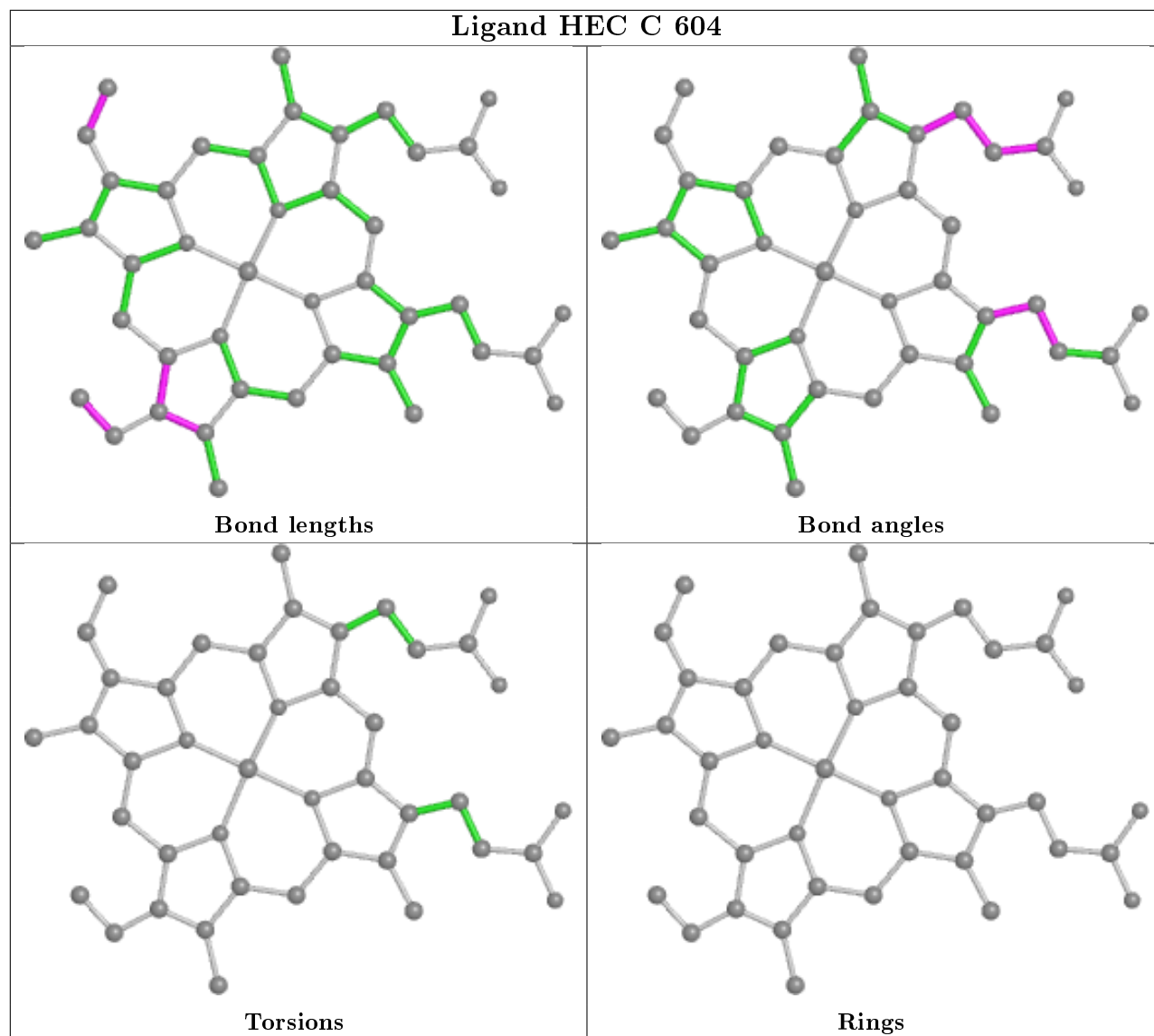
## Ligand HEC E 603



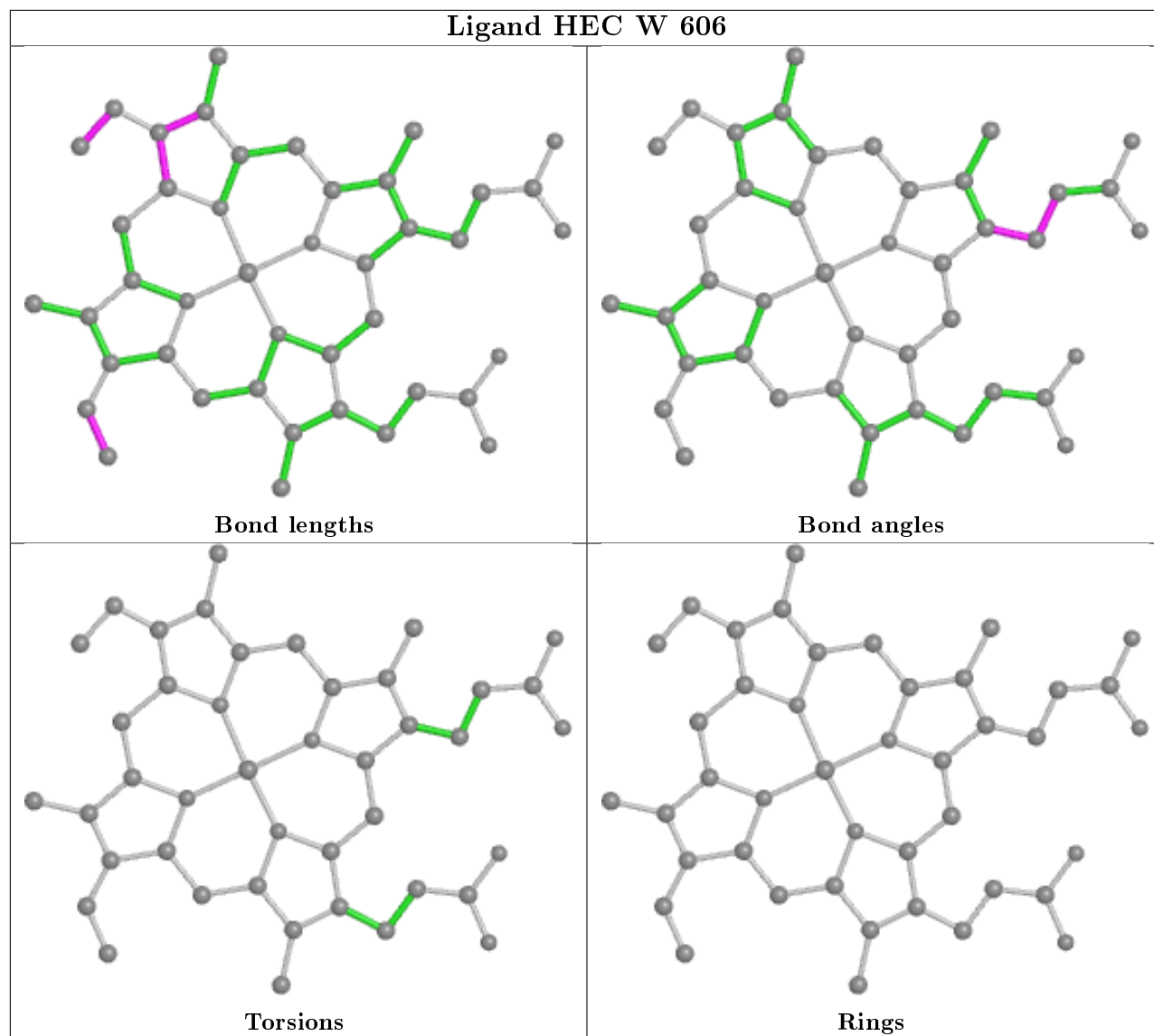
## Ligand HEC I 607

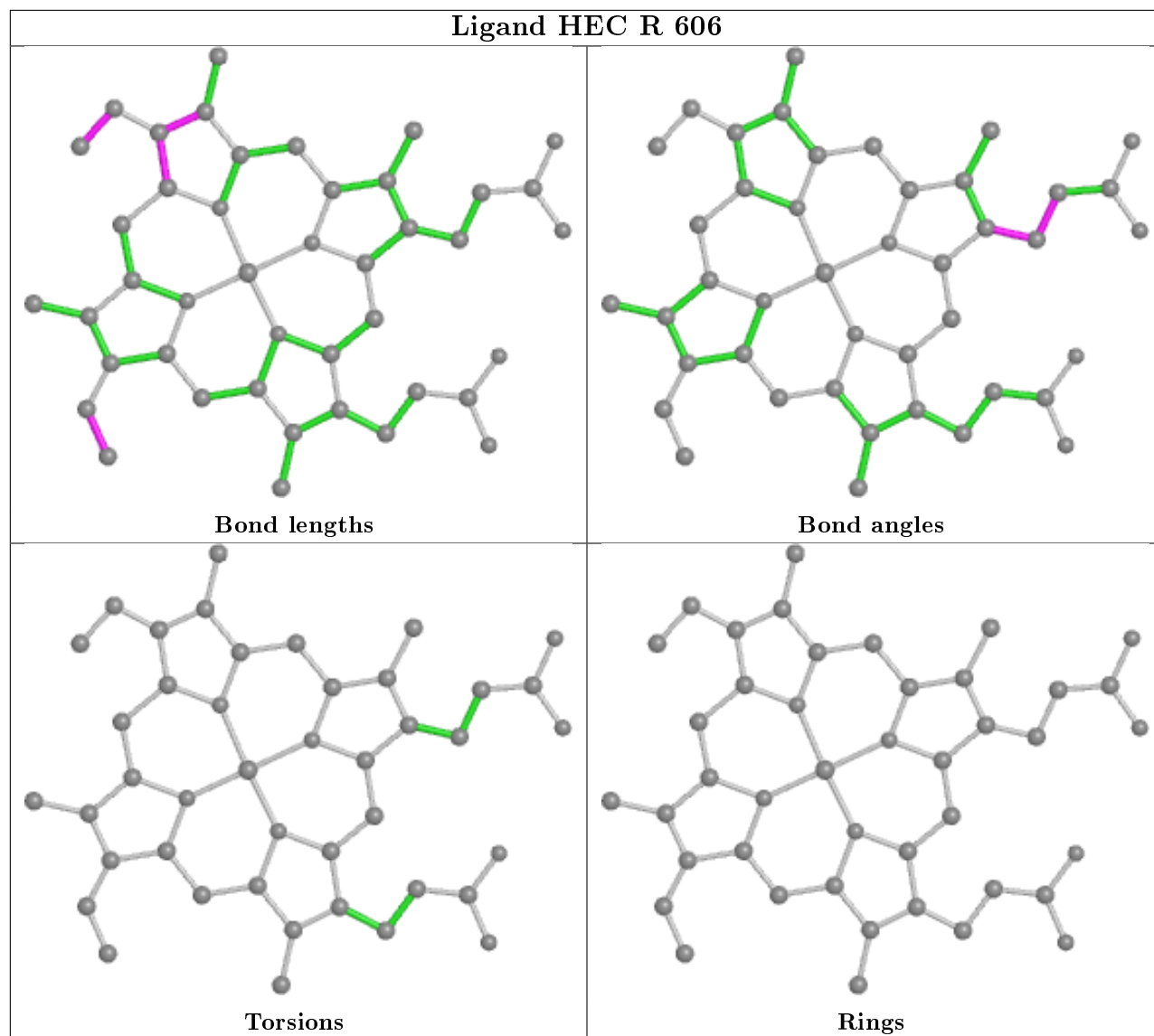




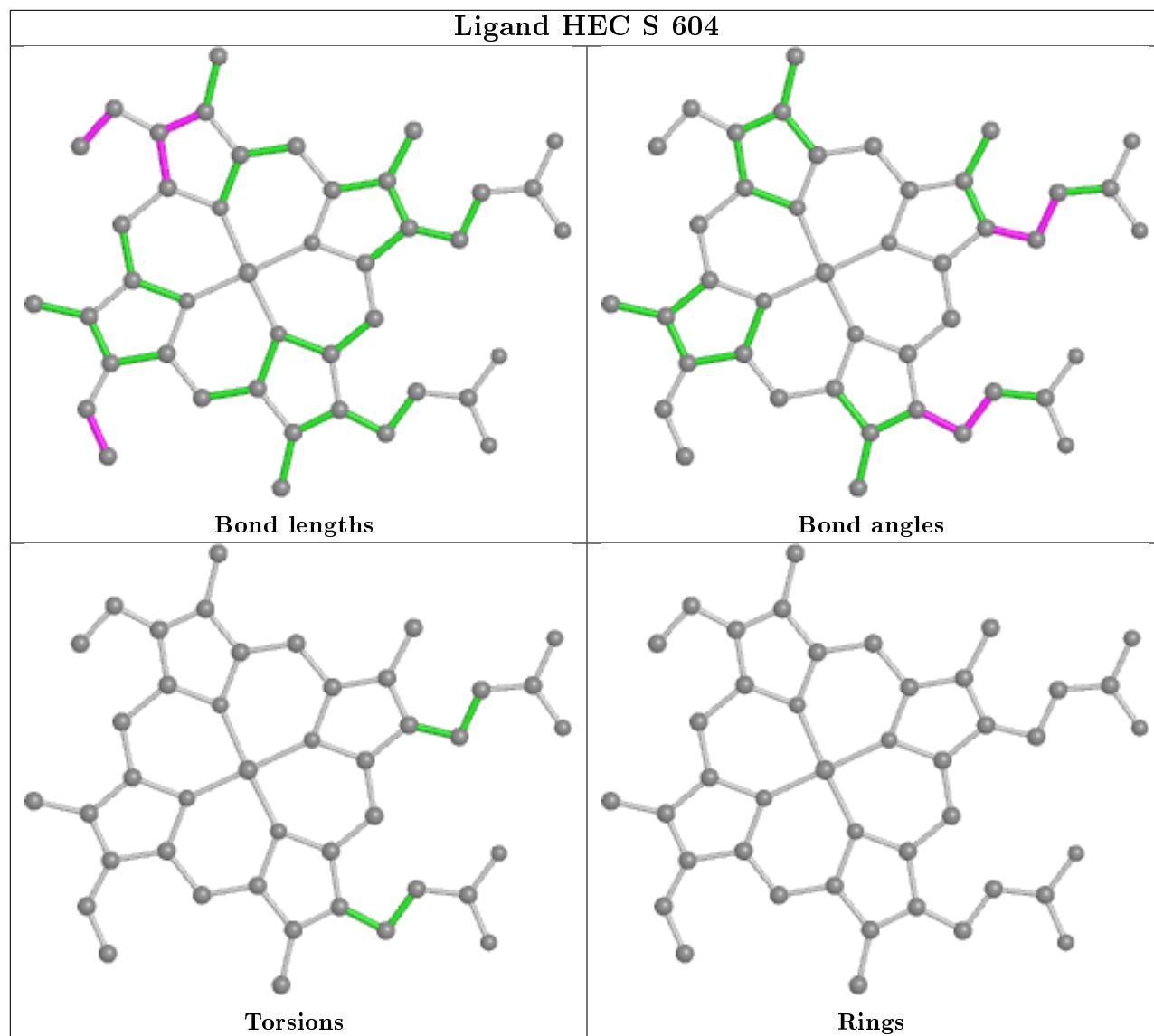


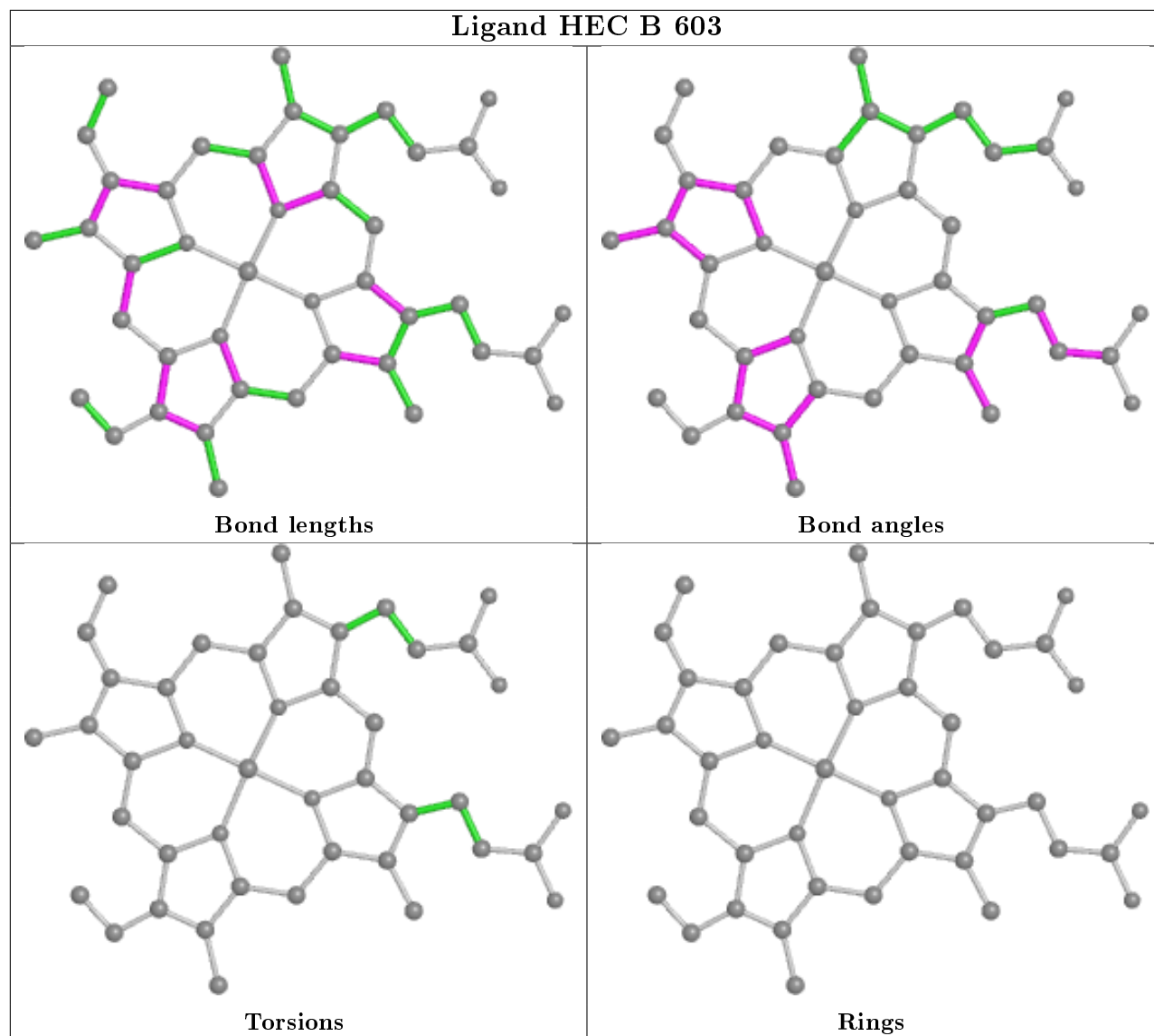


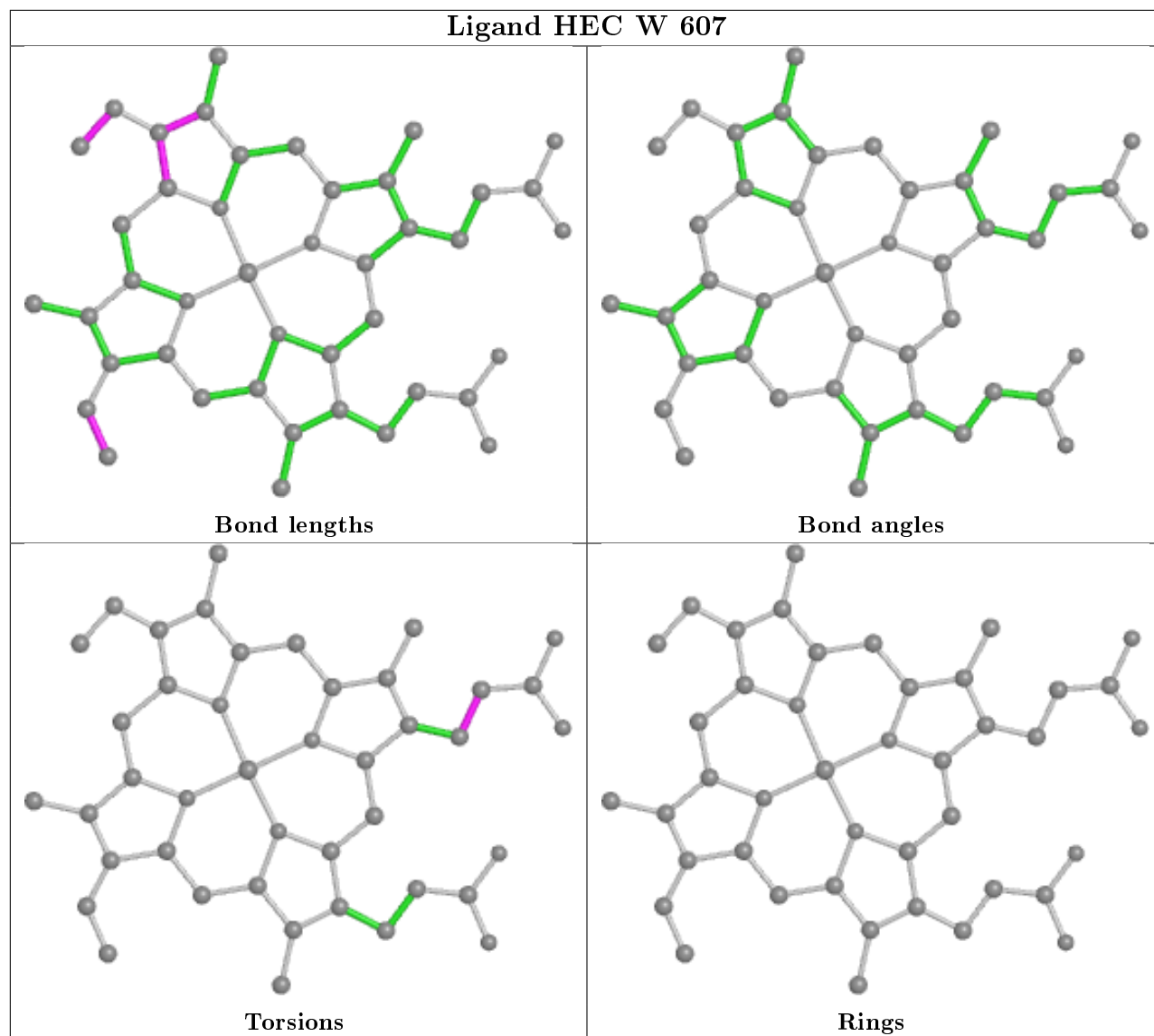


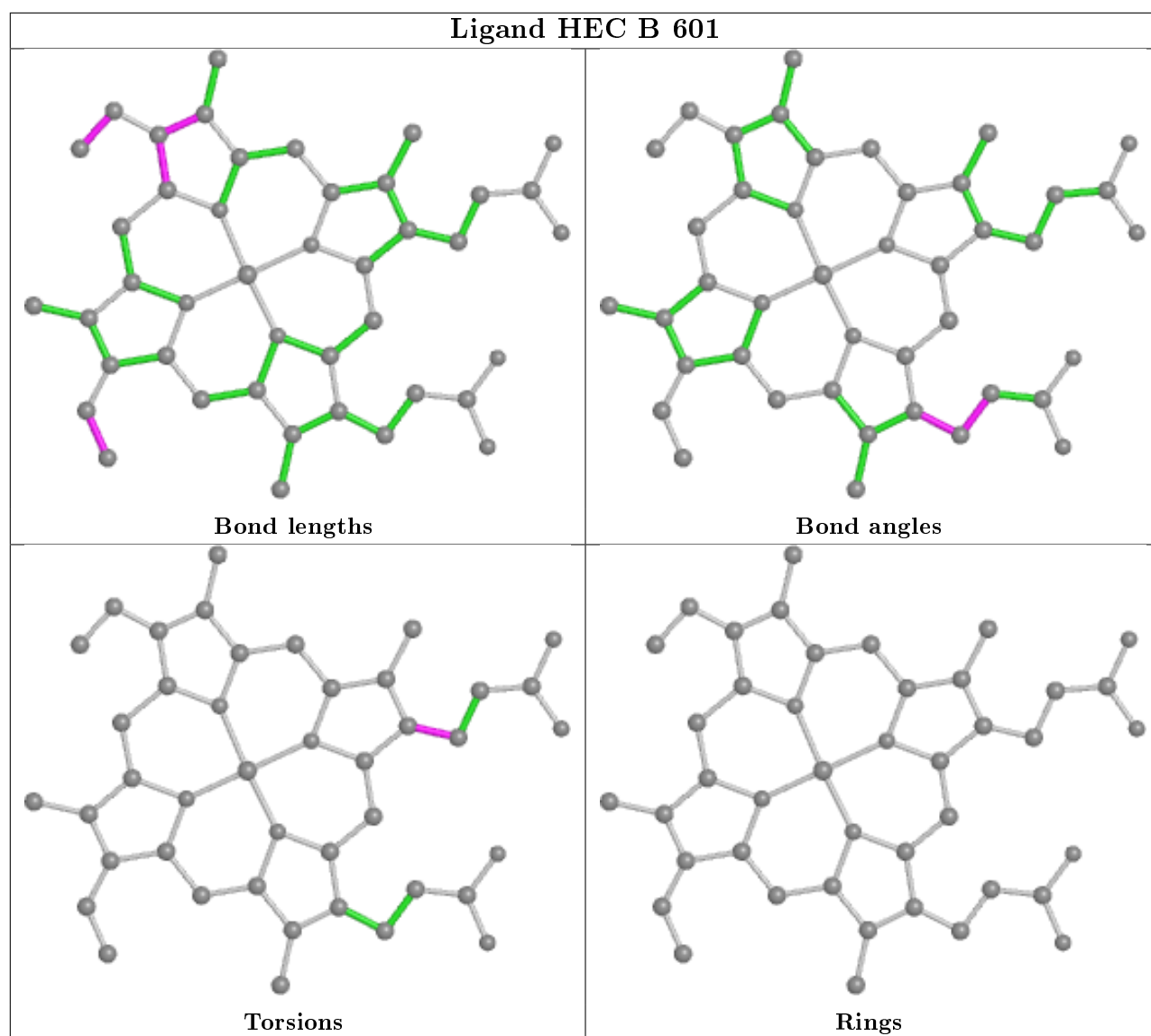


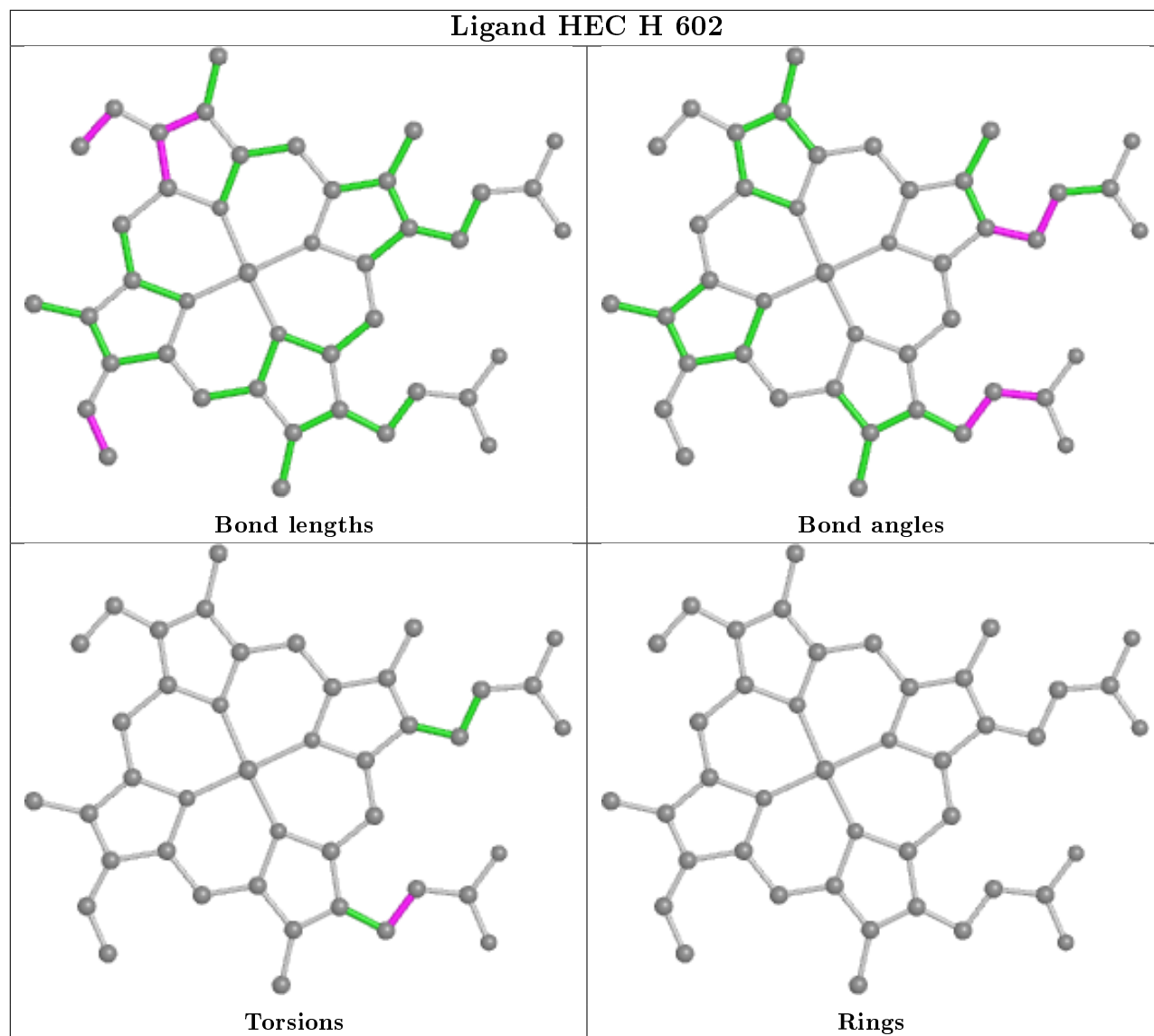
## Ligand HEC S 604

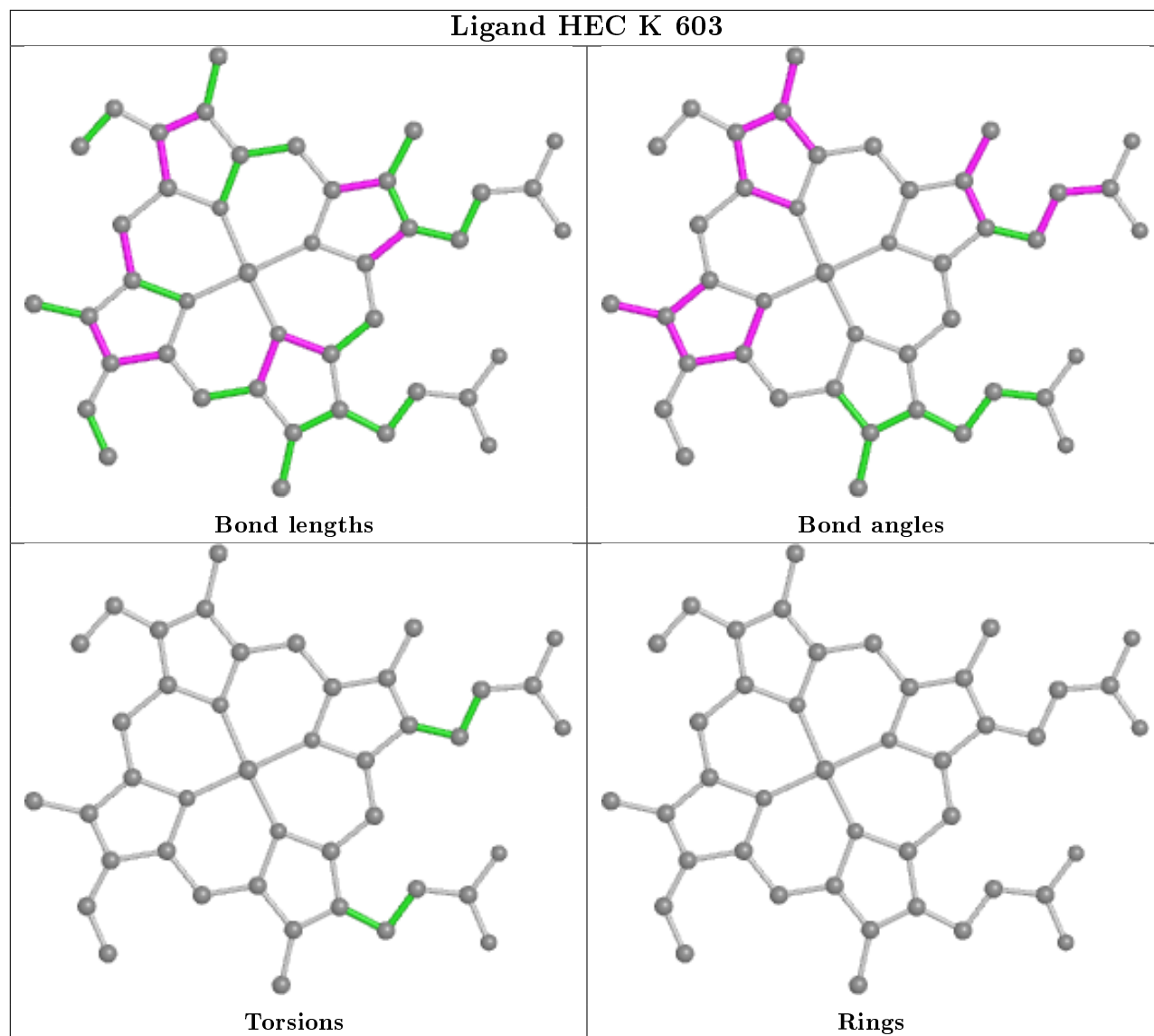




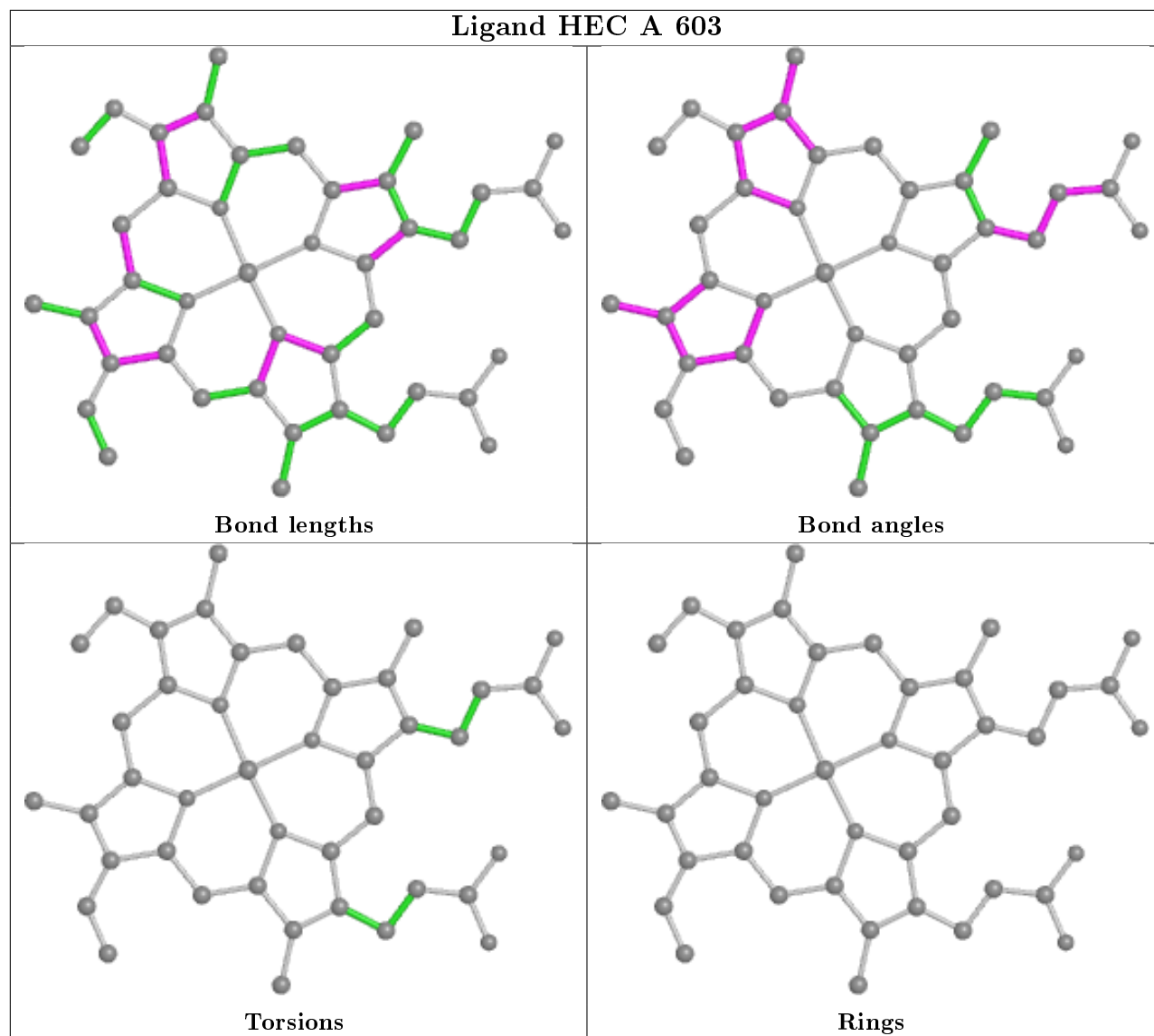


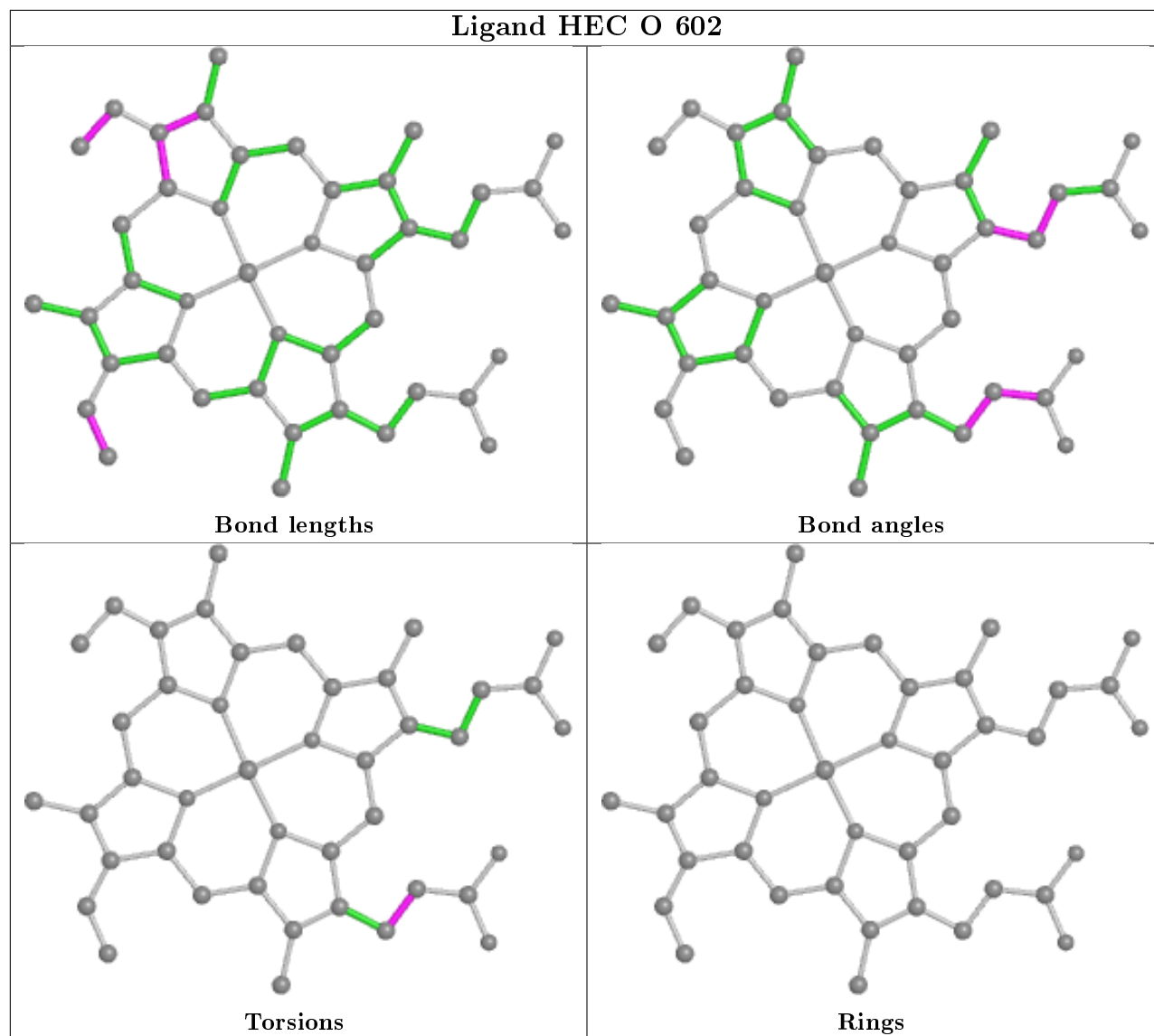




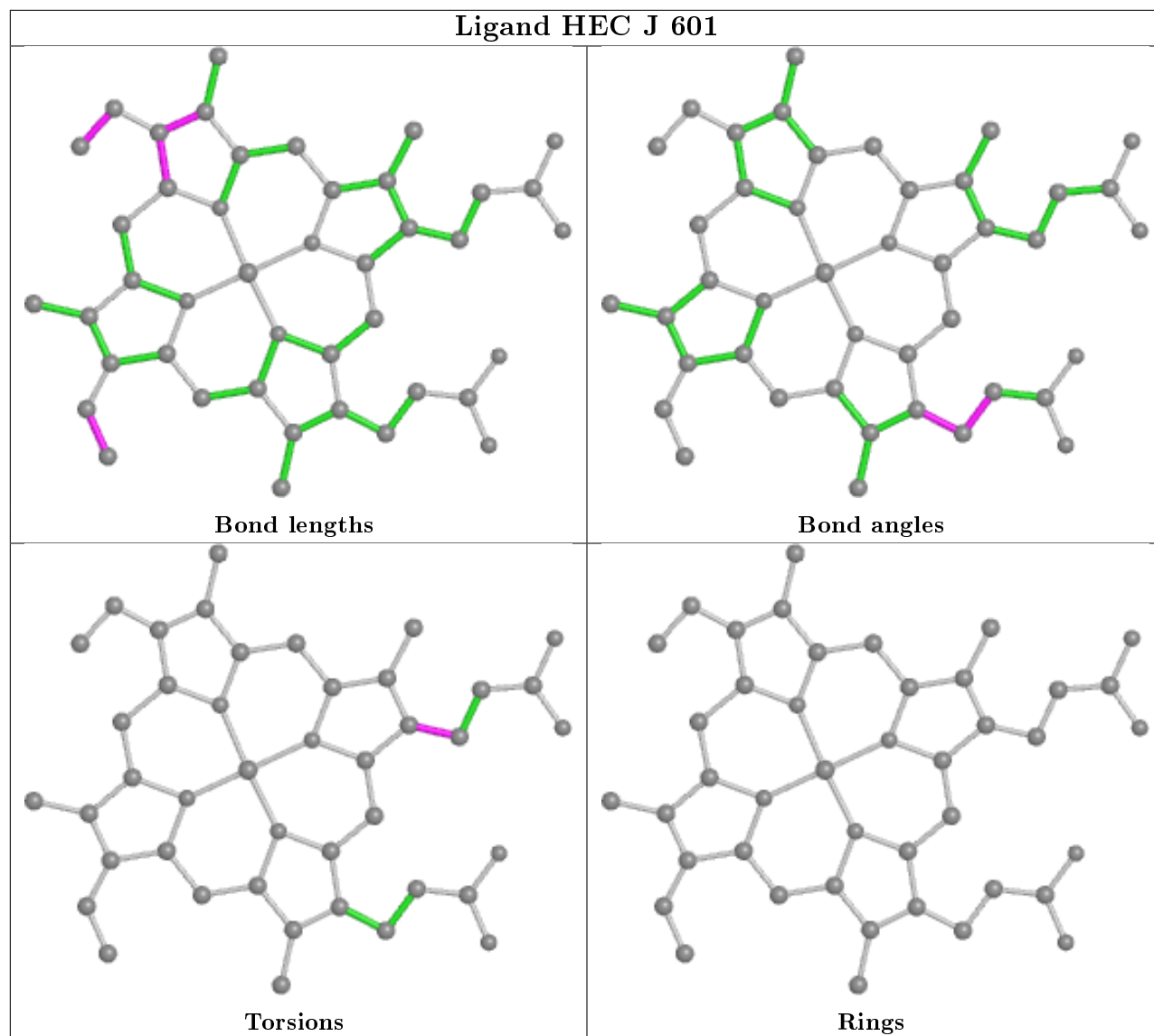


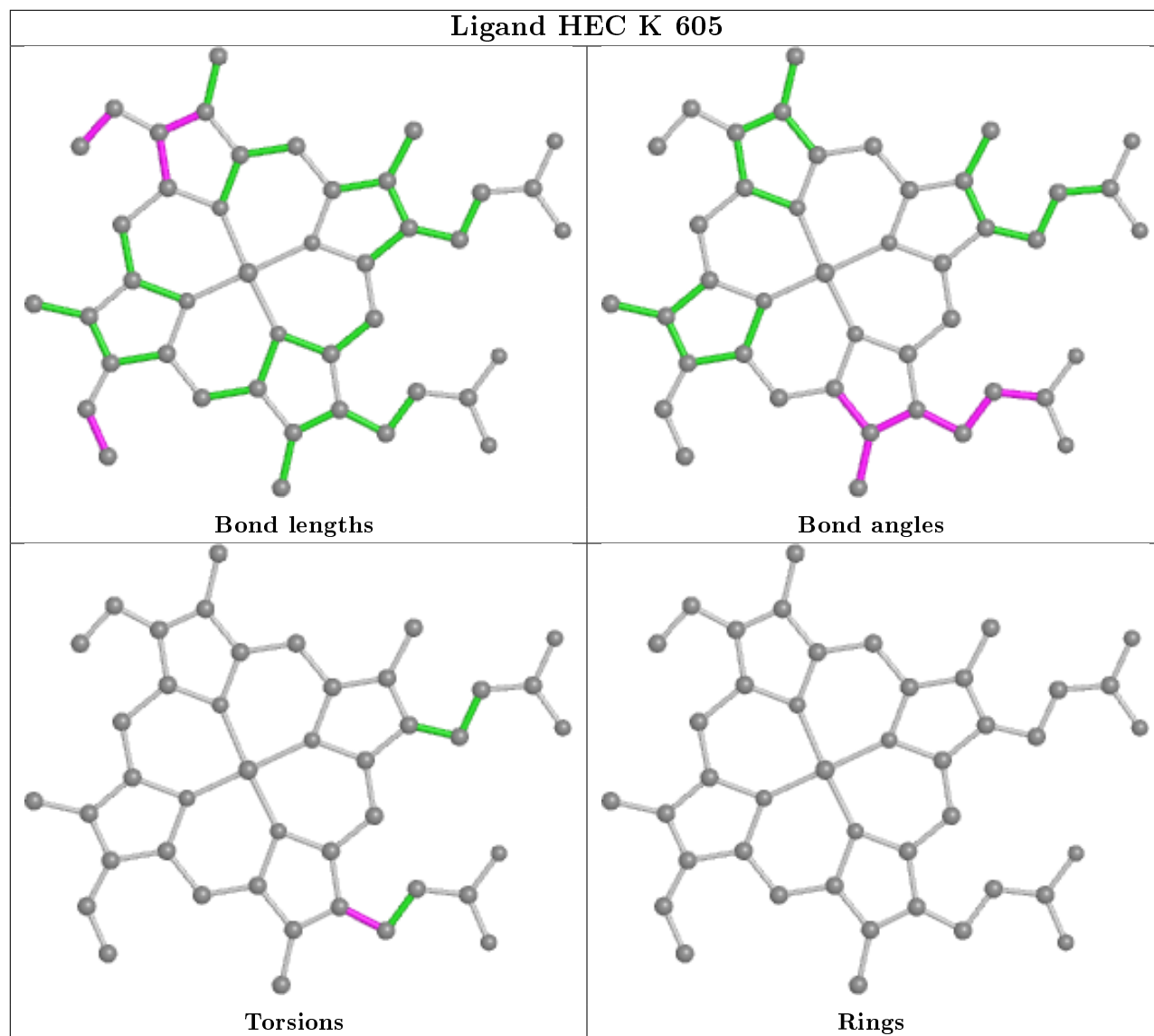




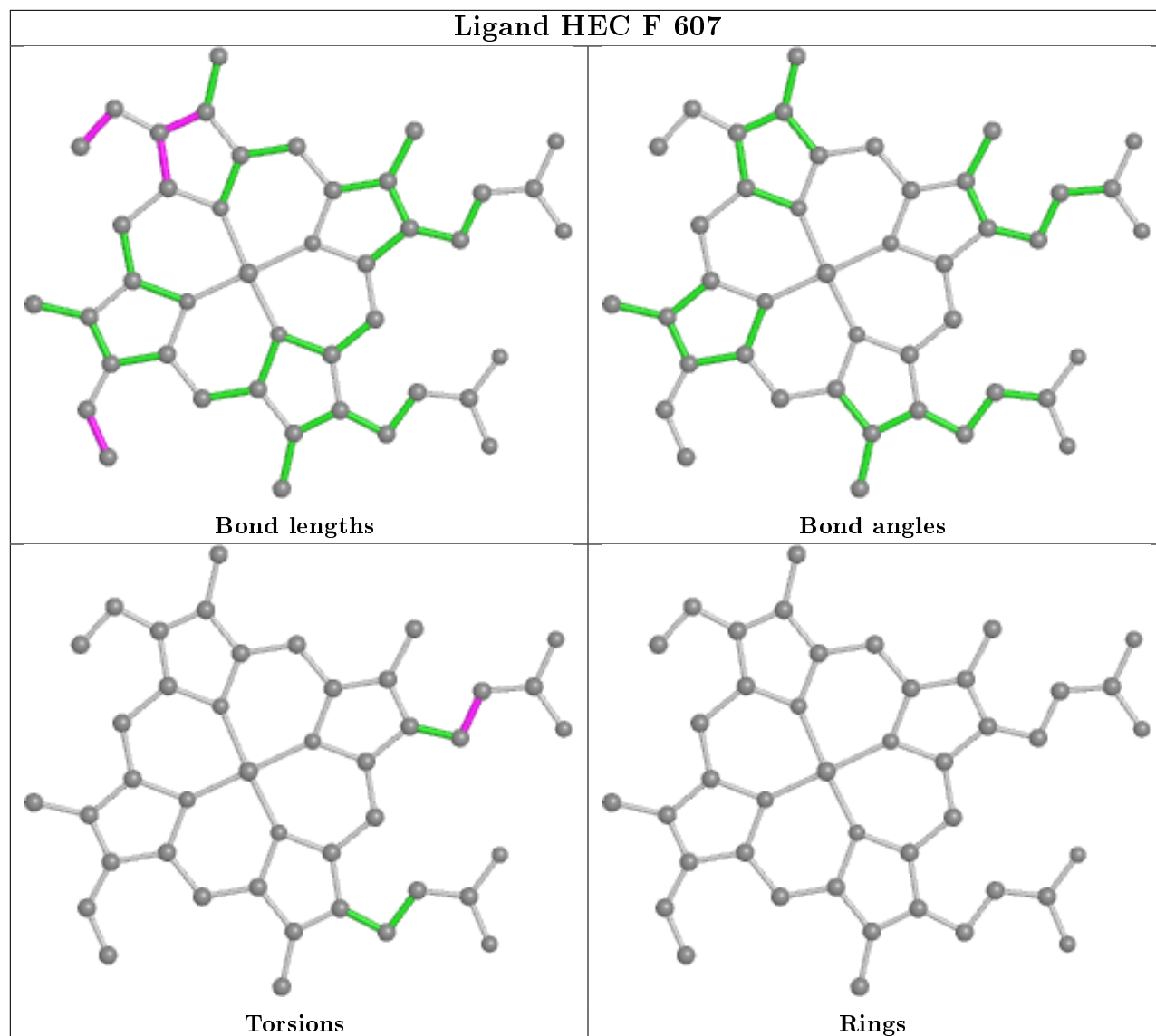


## Ligand HEC J 601

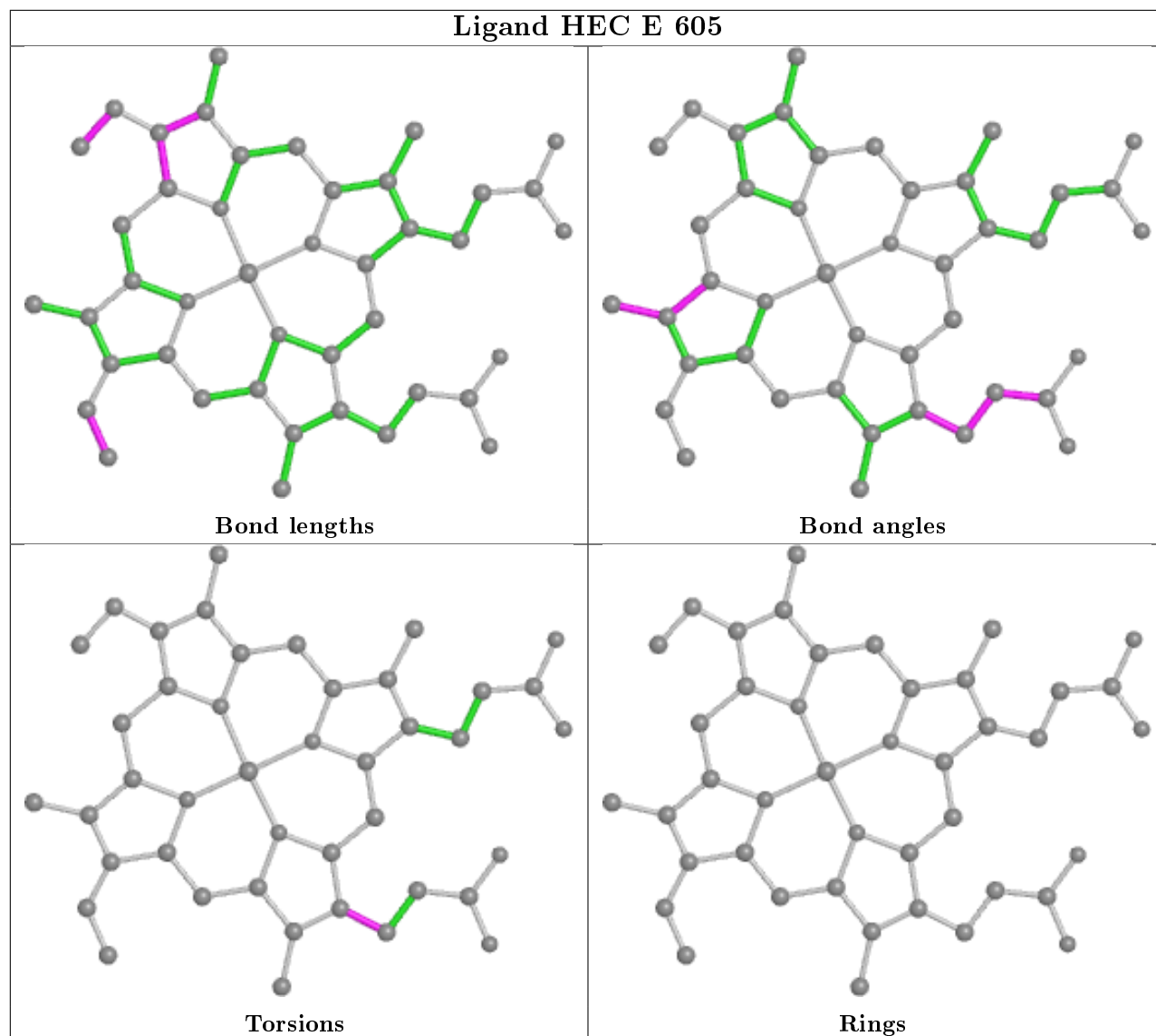


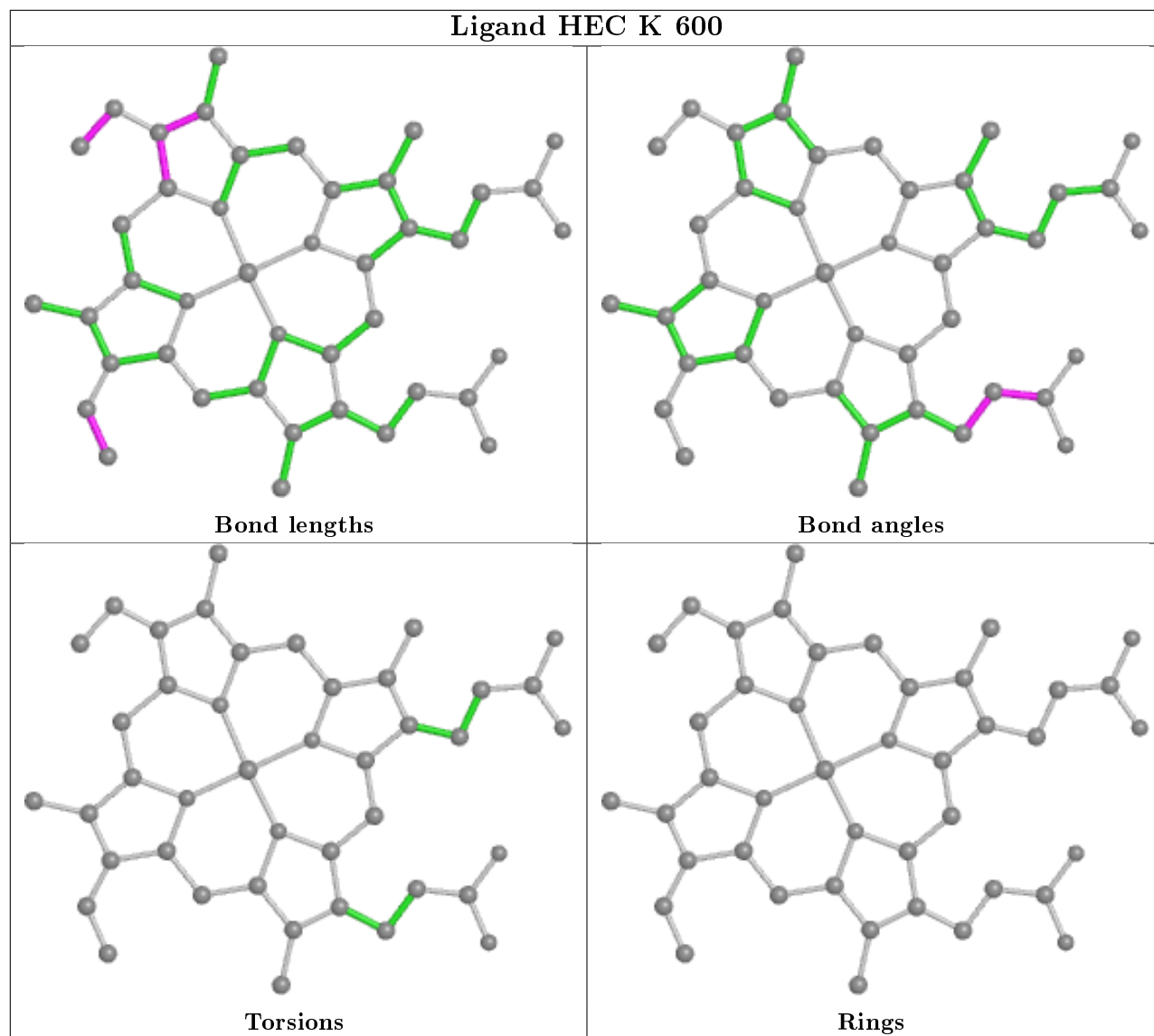


## Ligand HEC F 607

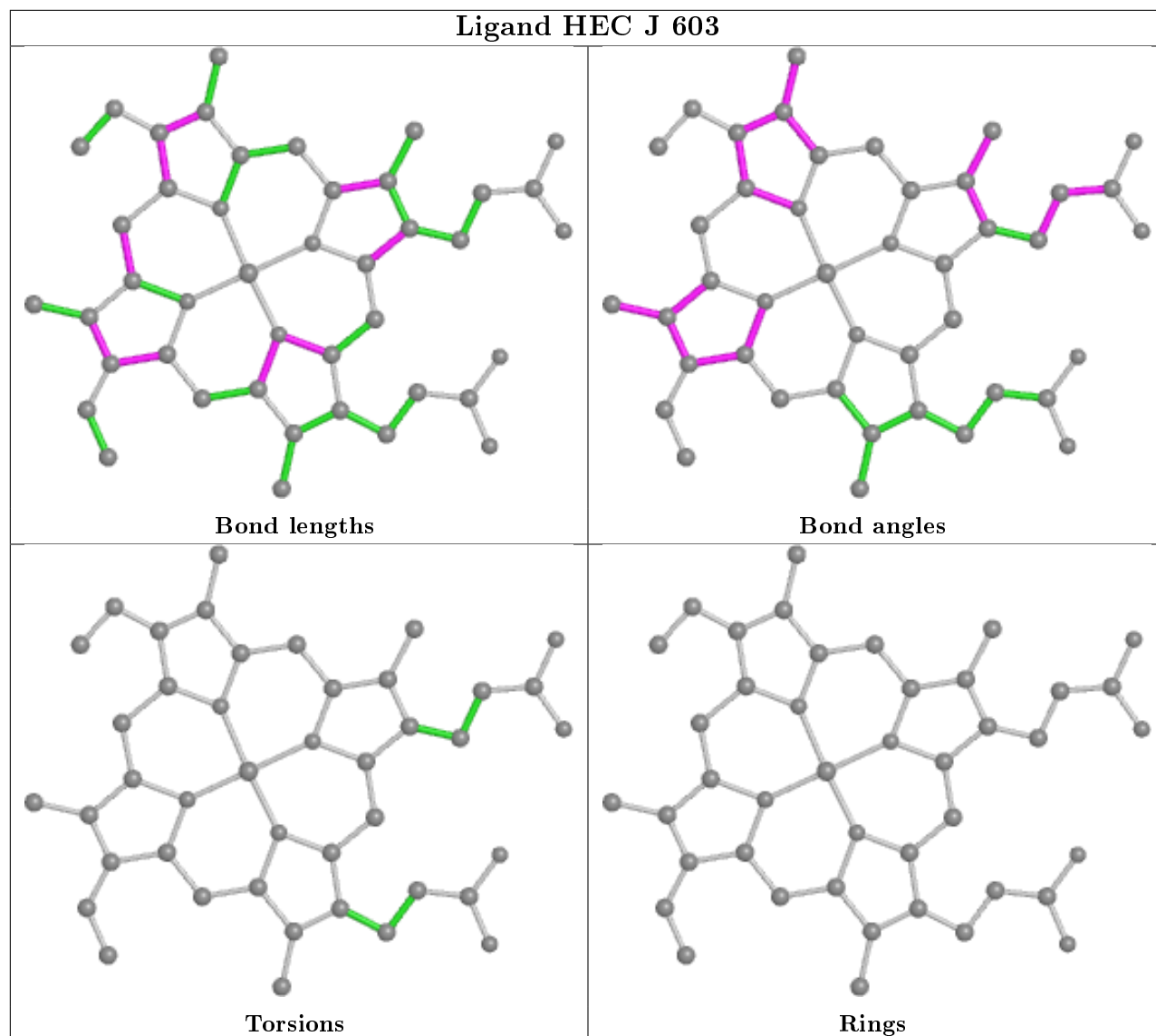


## Ligand HEC E 605

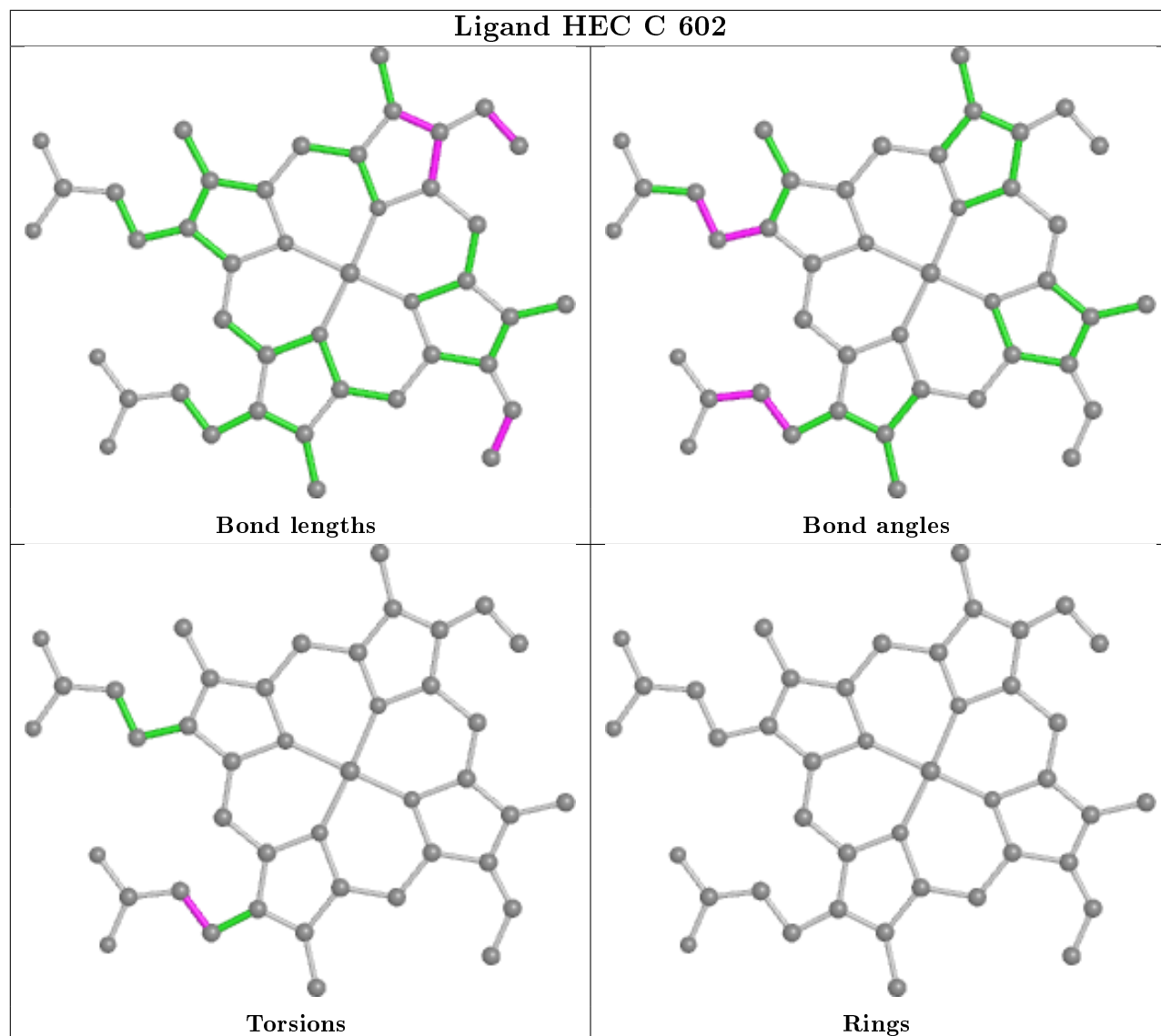


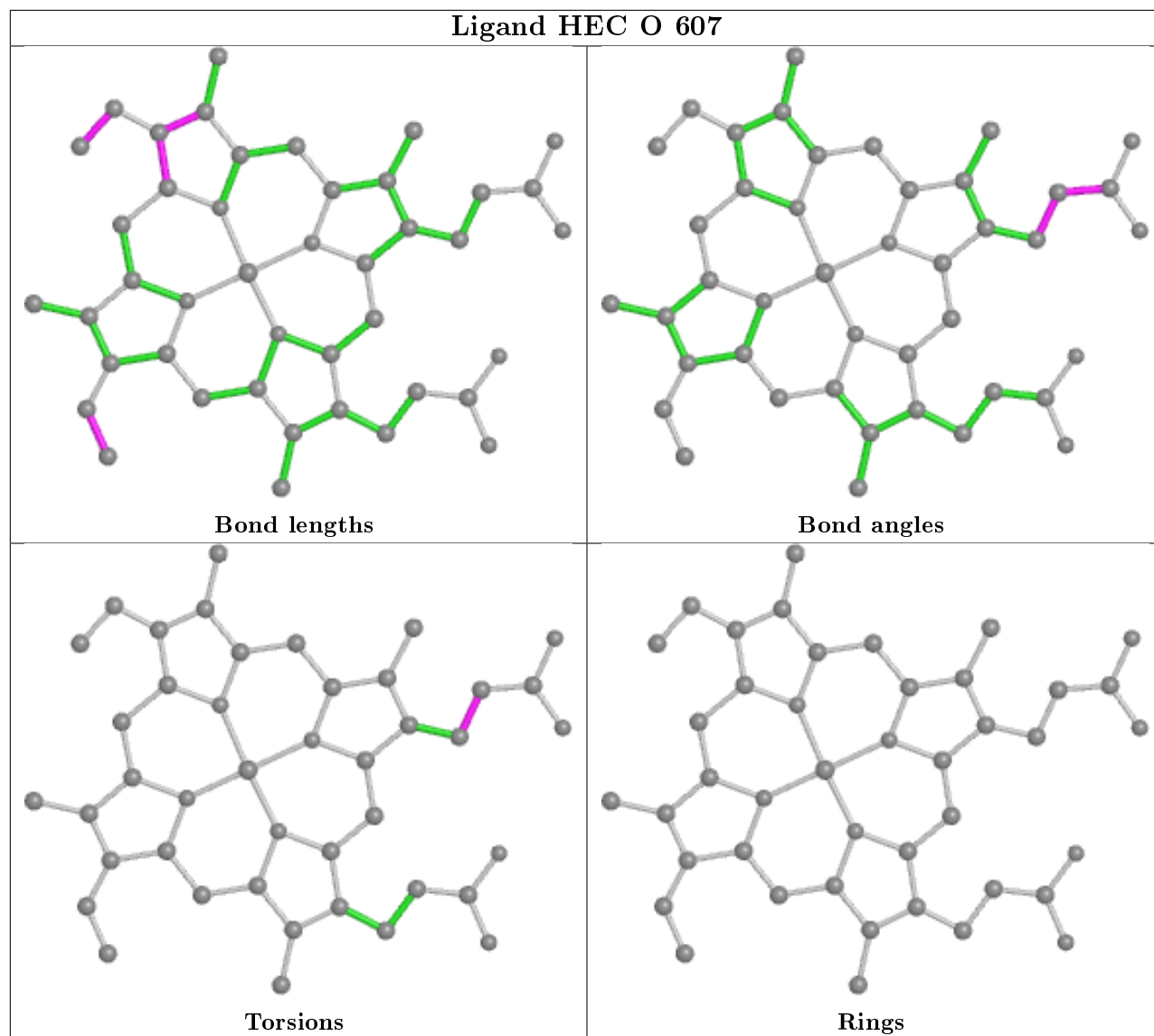


## Ligand HEC J 603

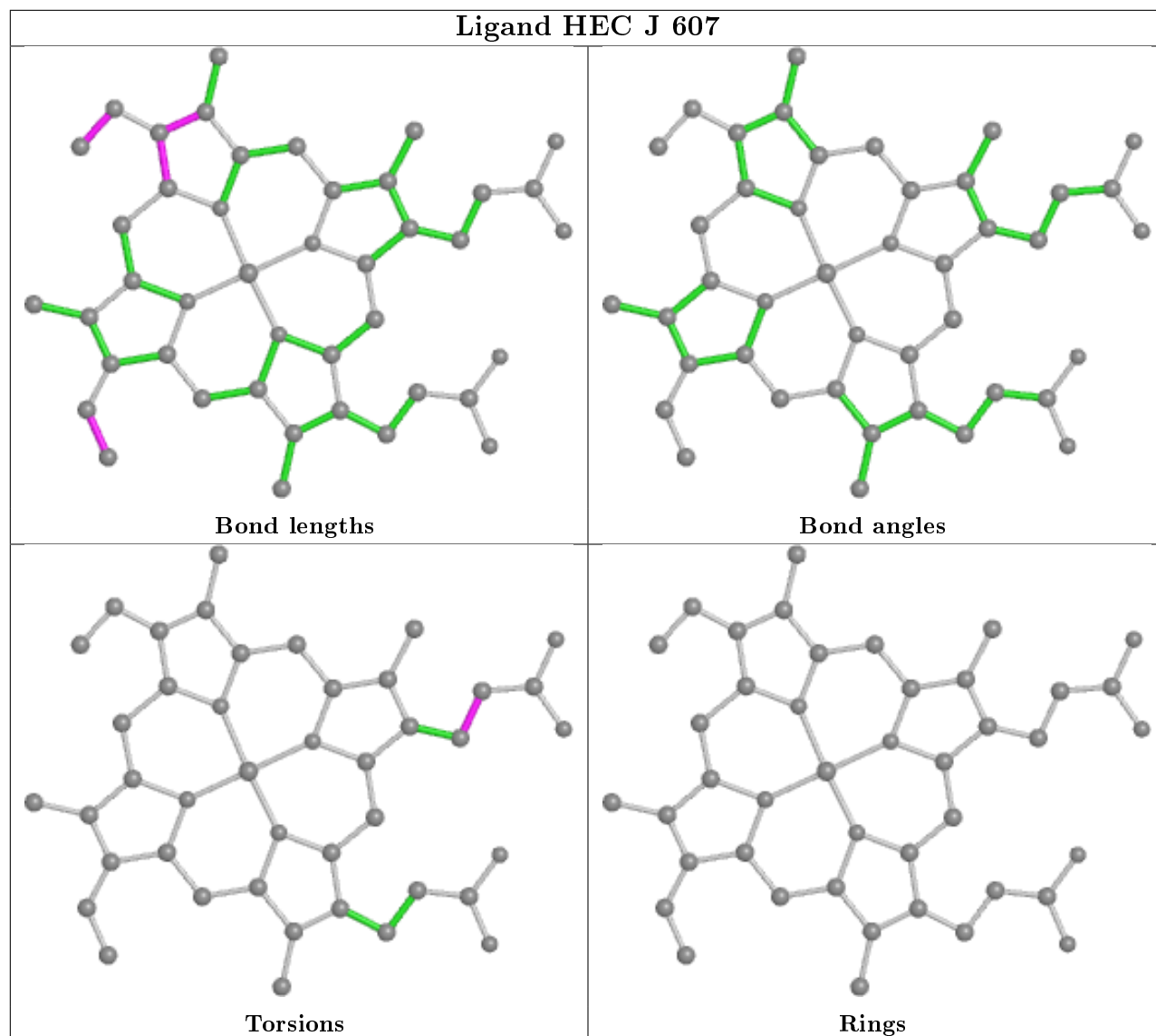




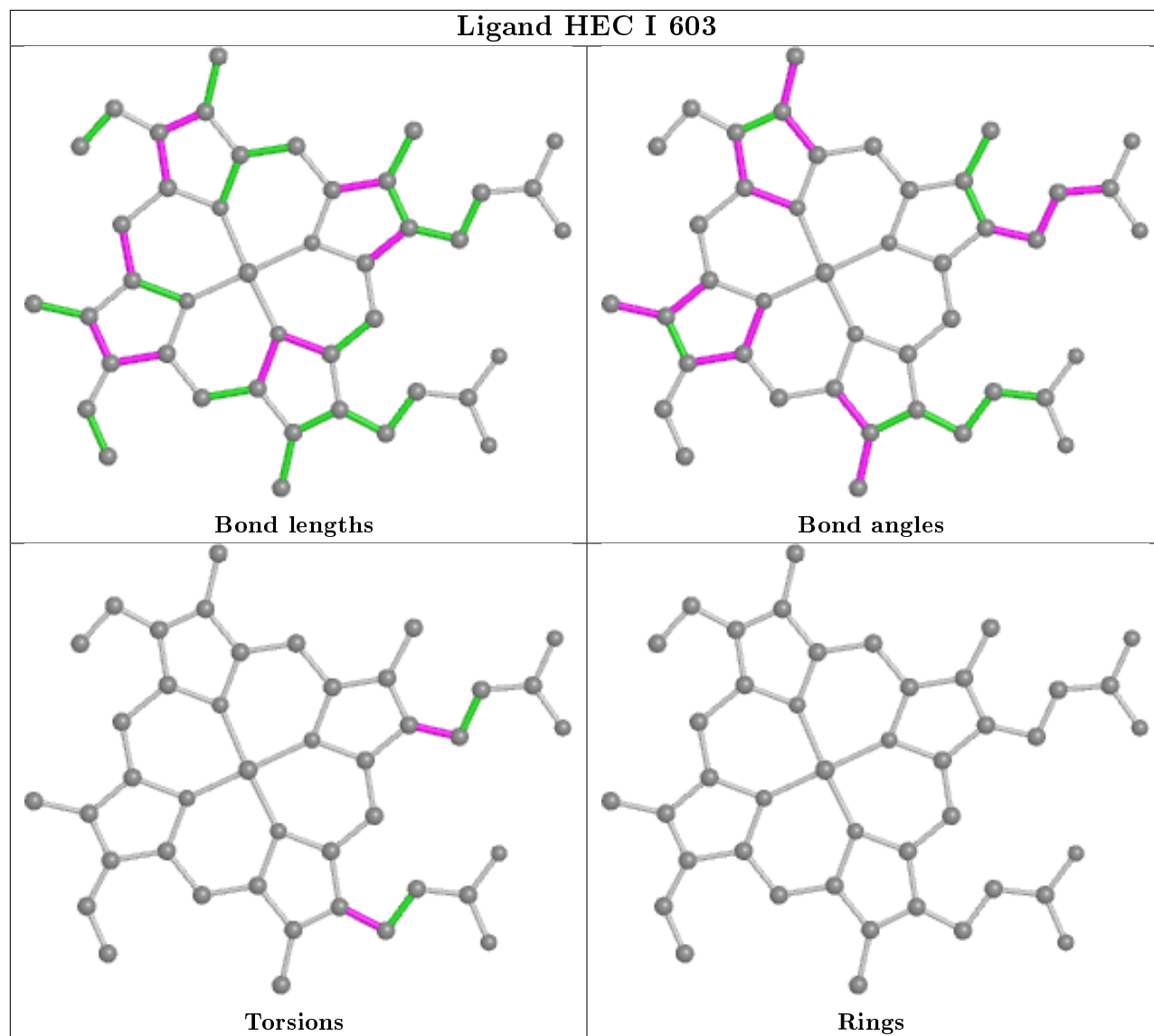


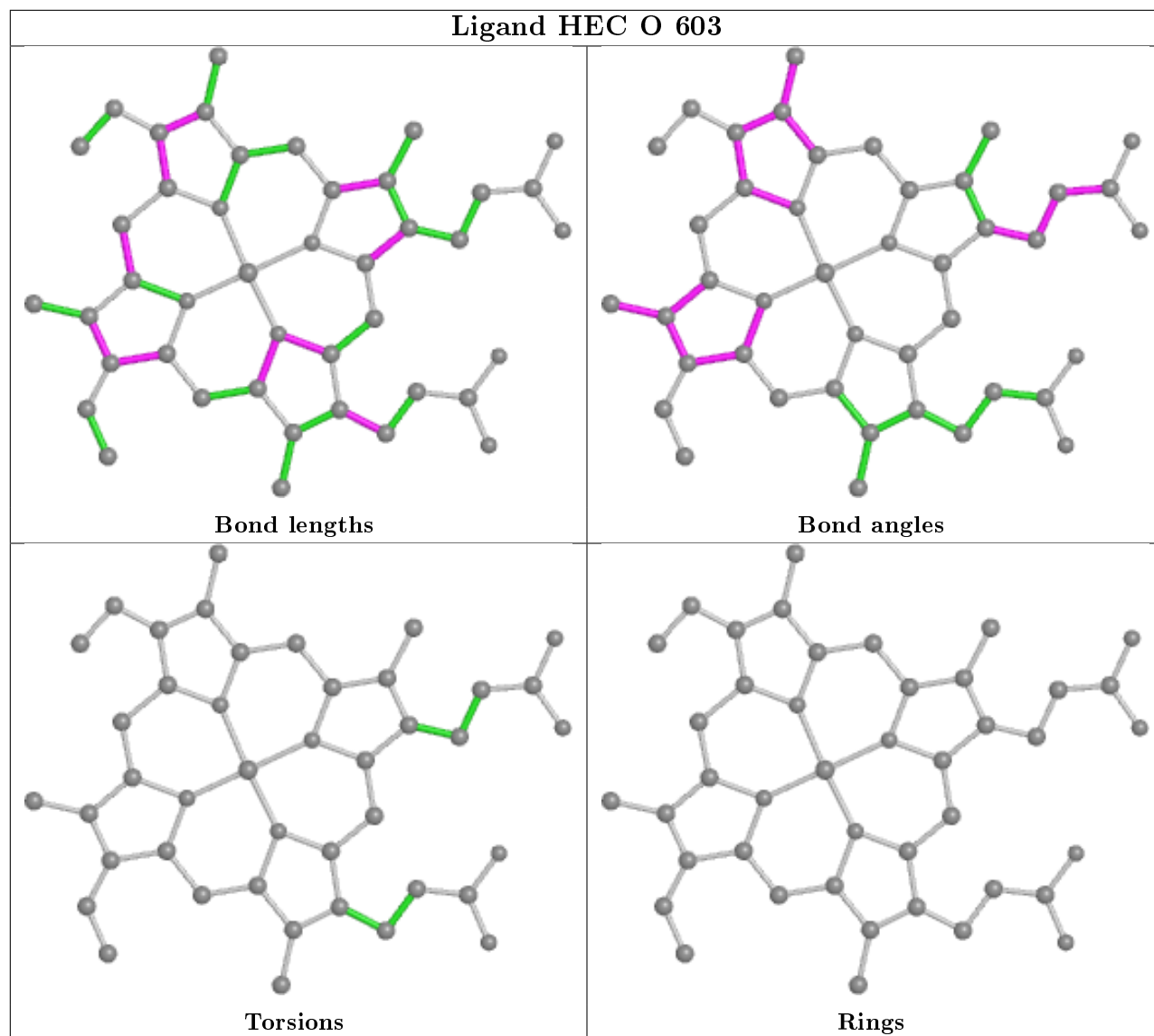


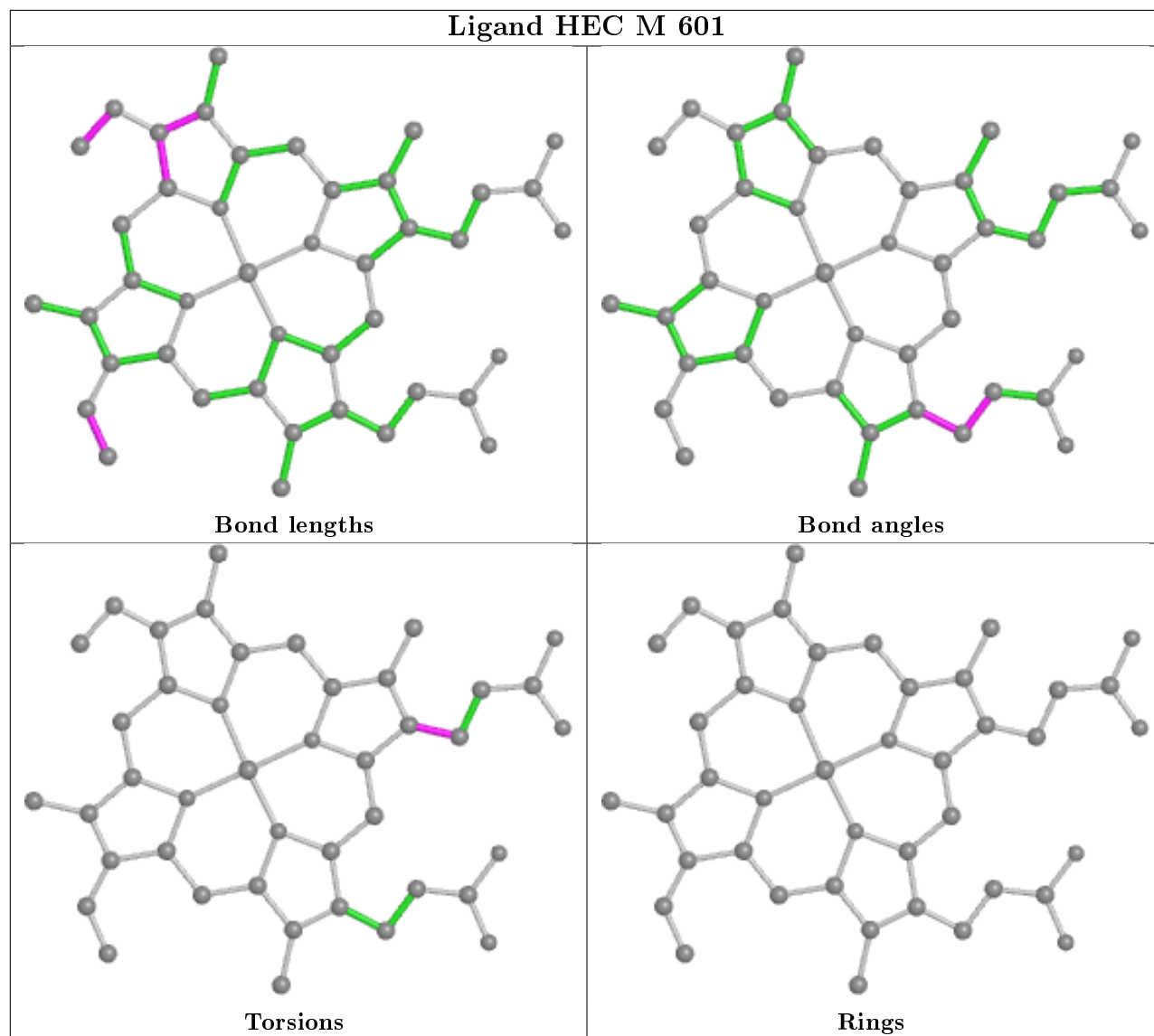
## Ligand HEC J 607

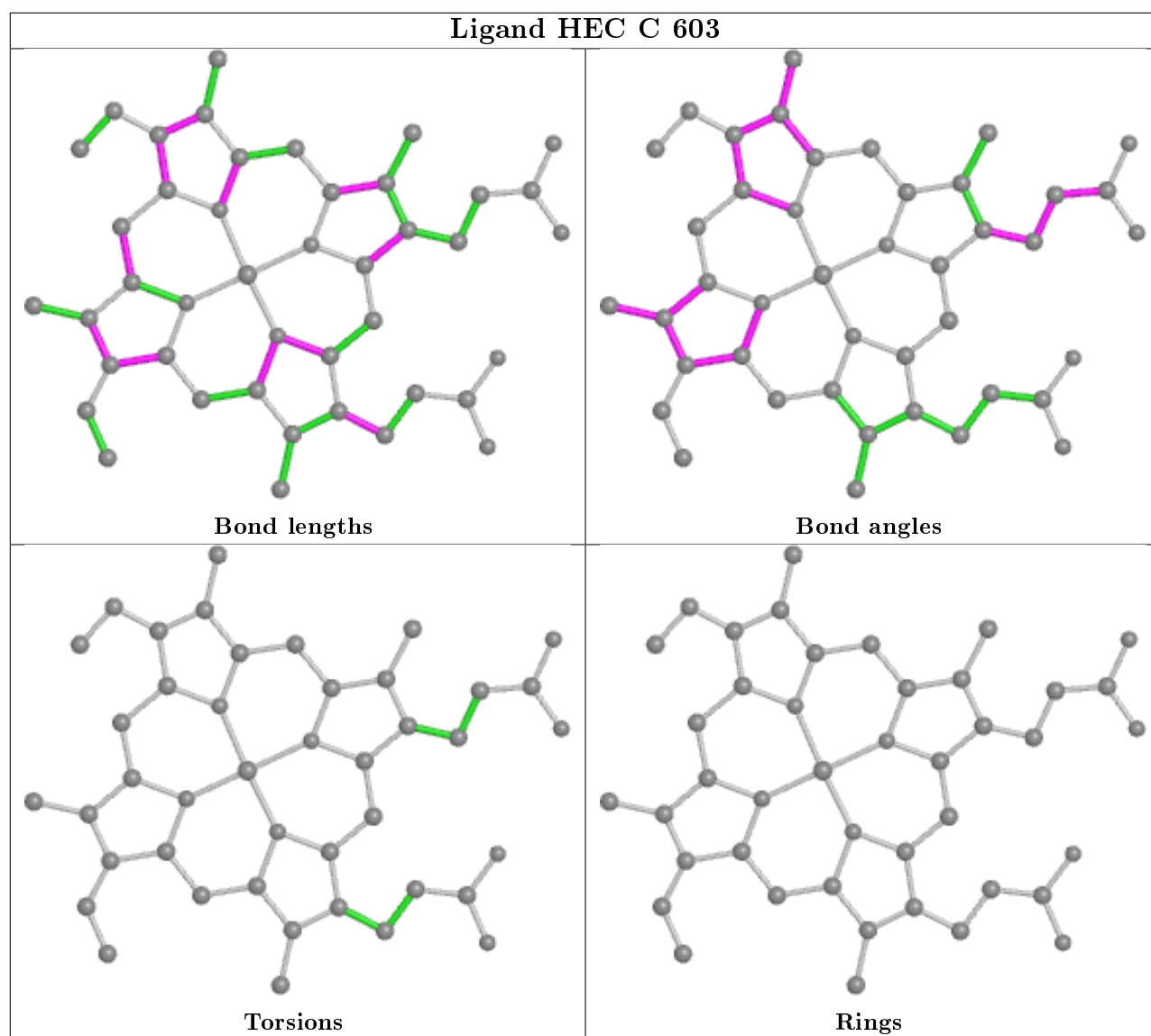


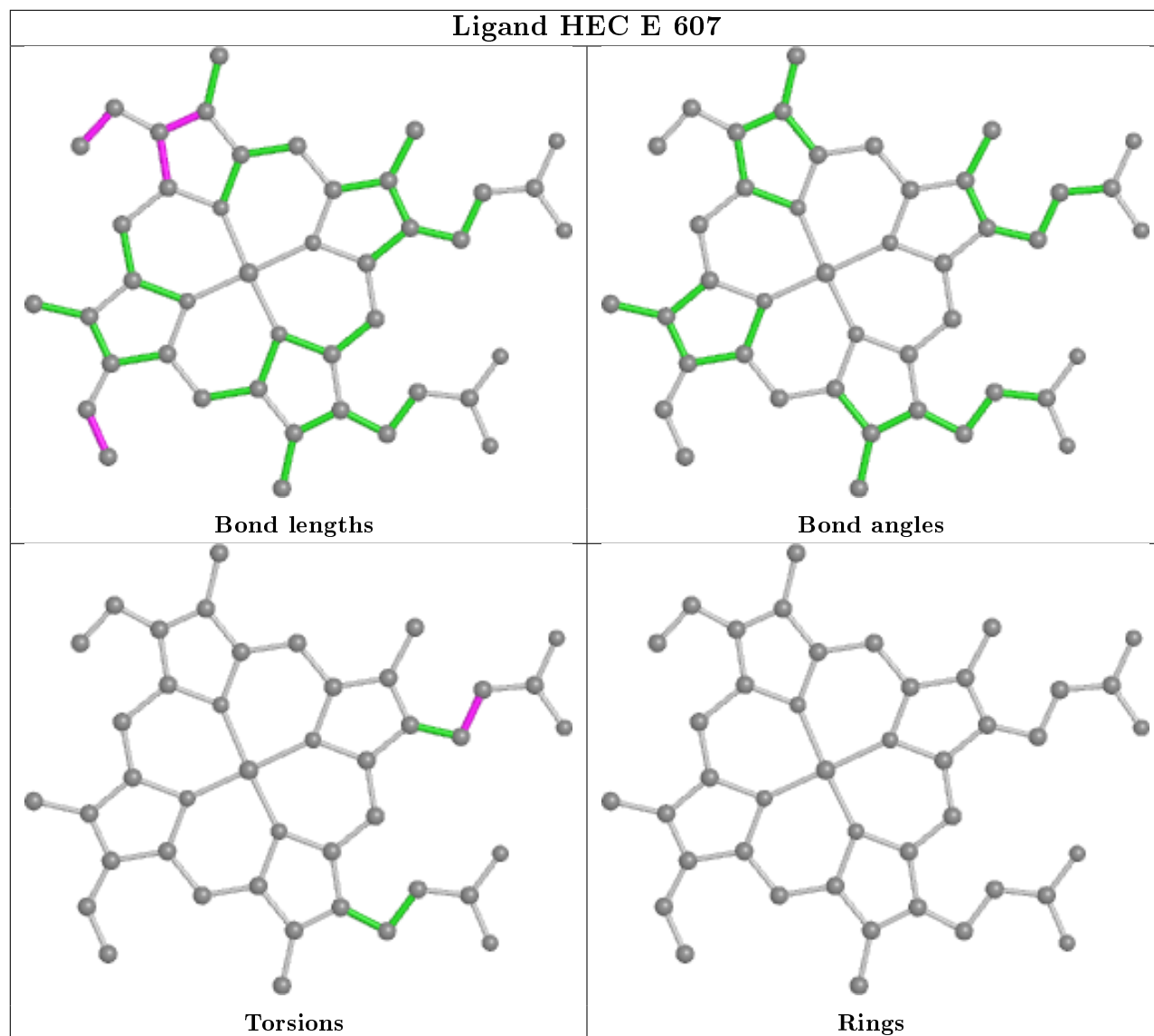
## Ligand HEC I 603



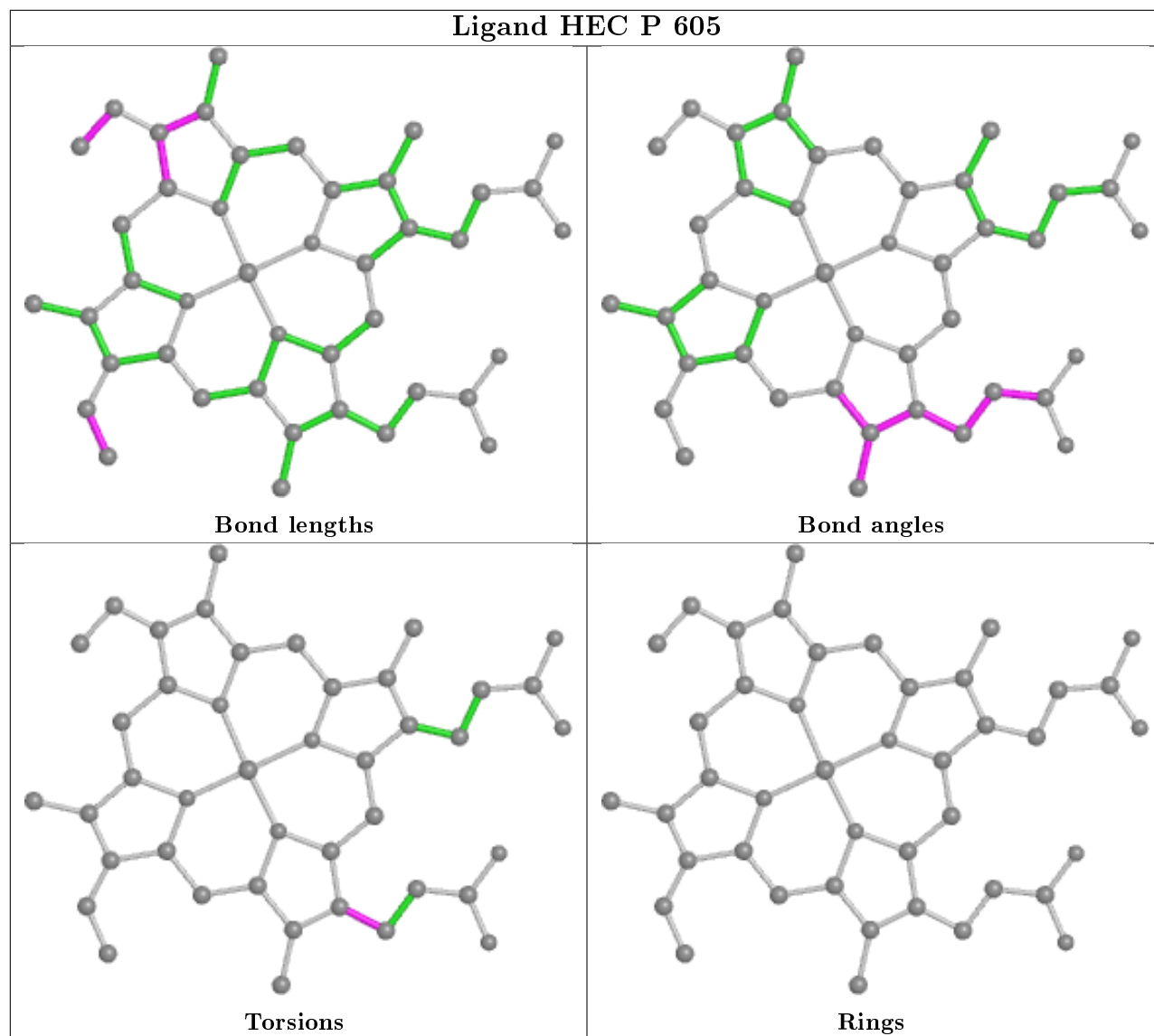




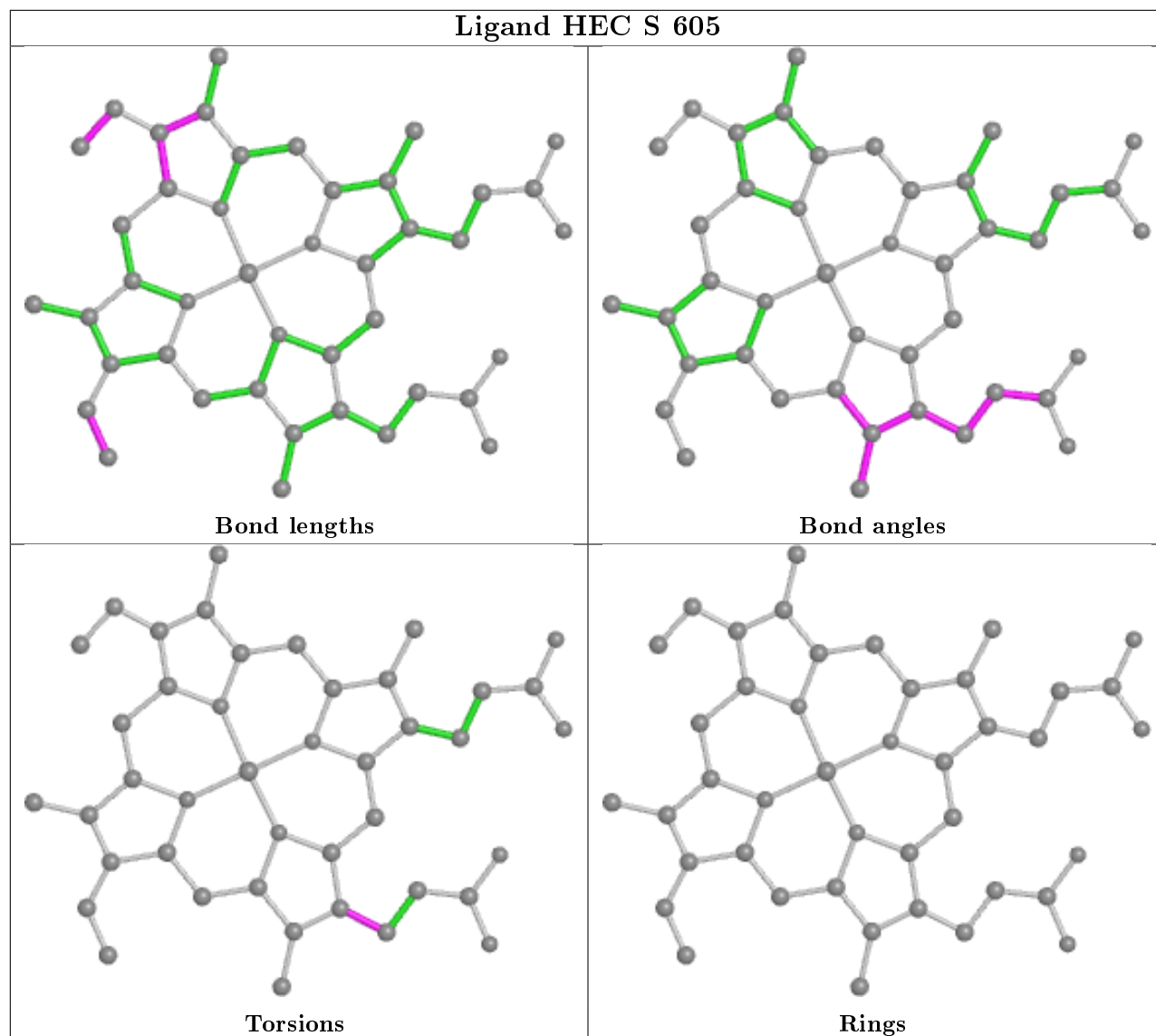


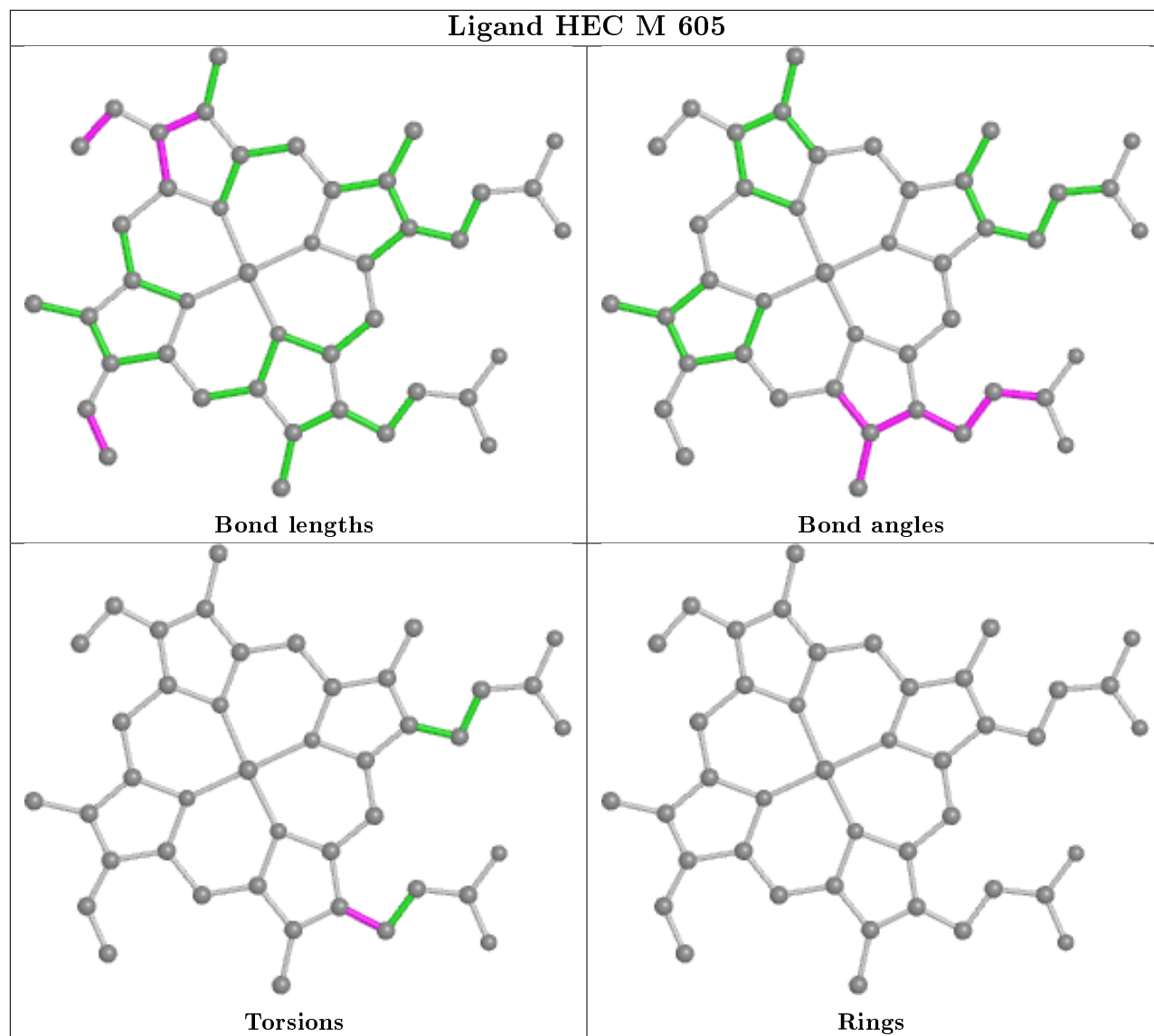


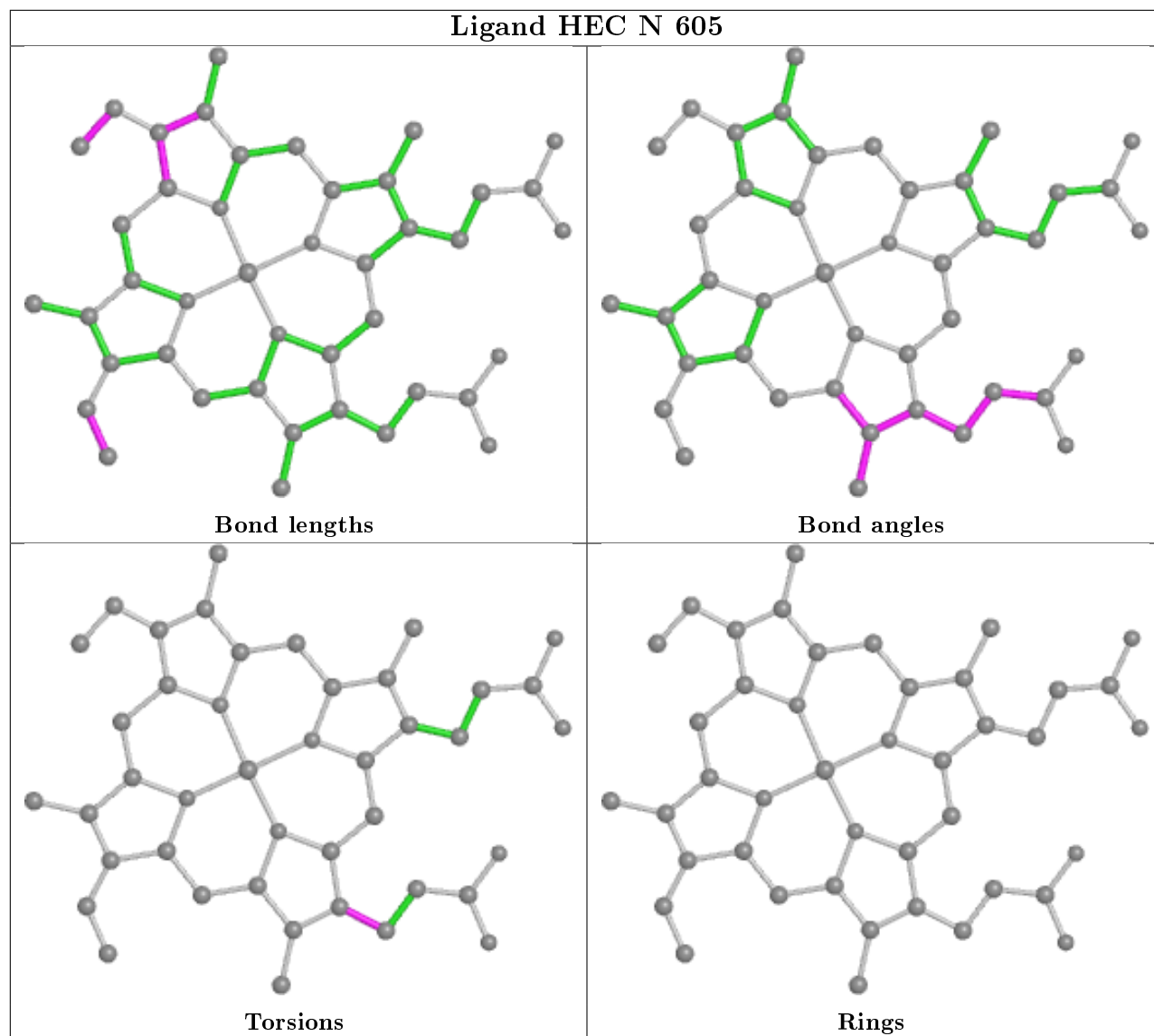


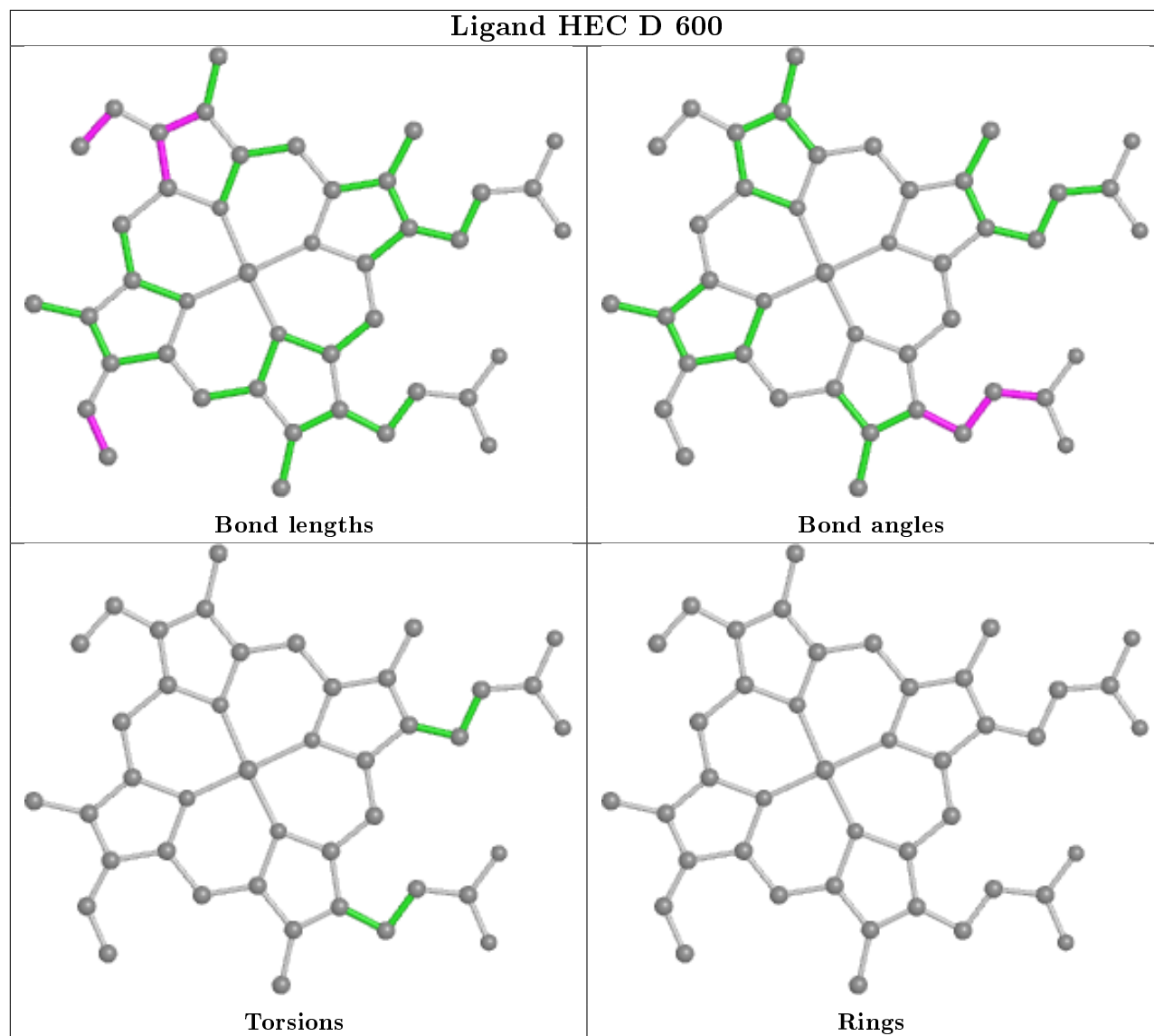


## Ligand HEC S 605

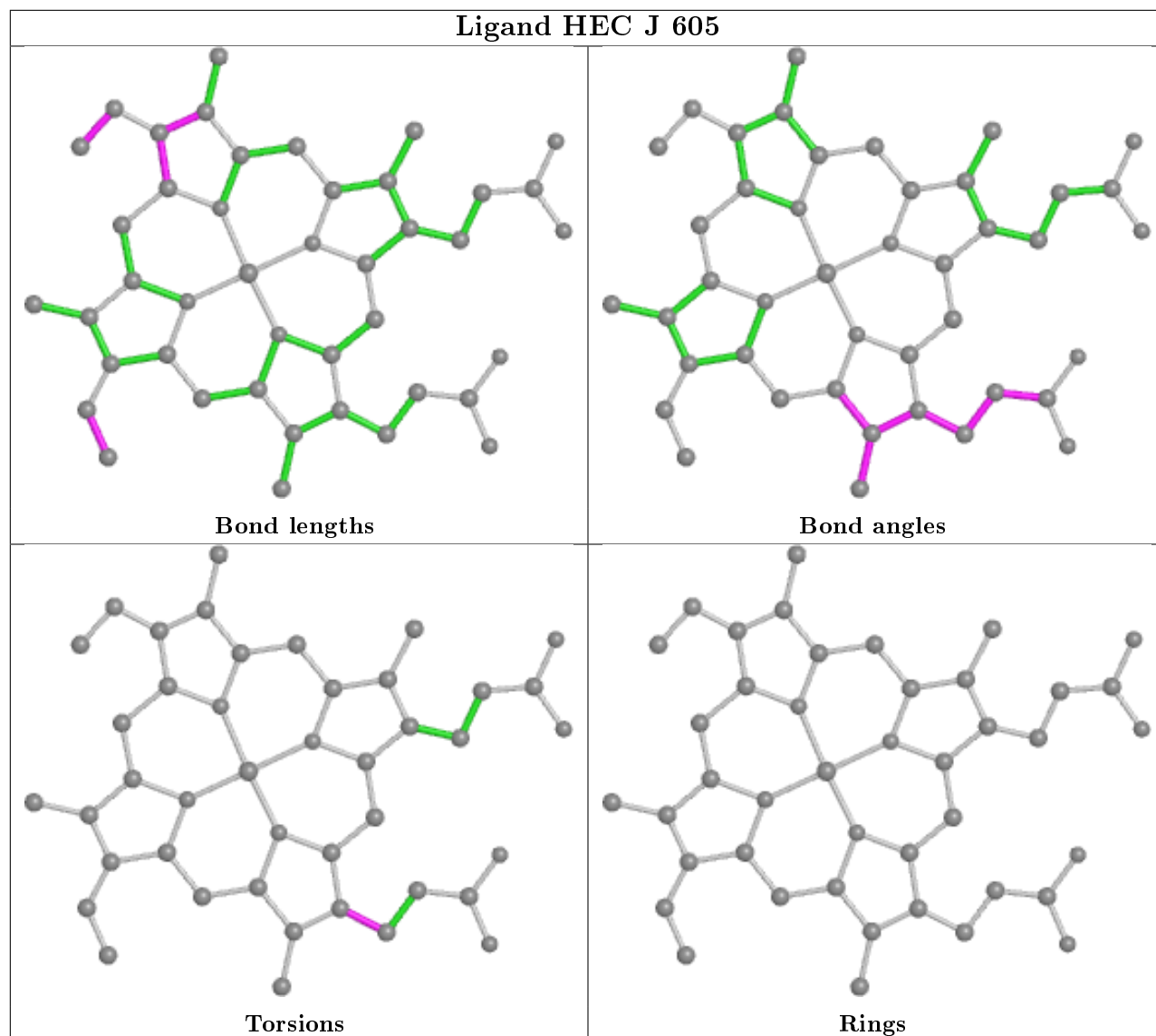


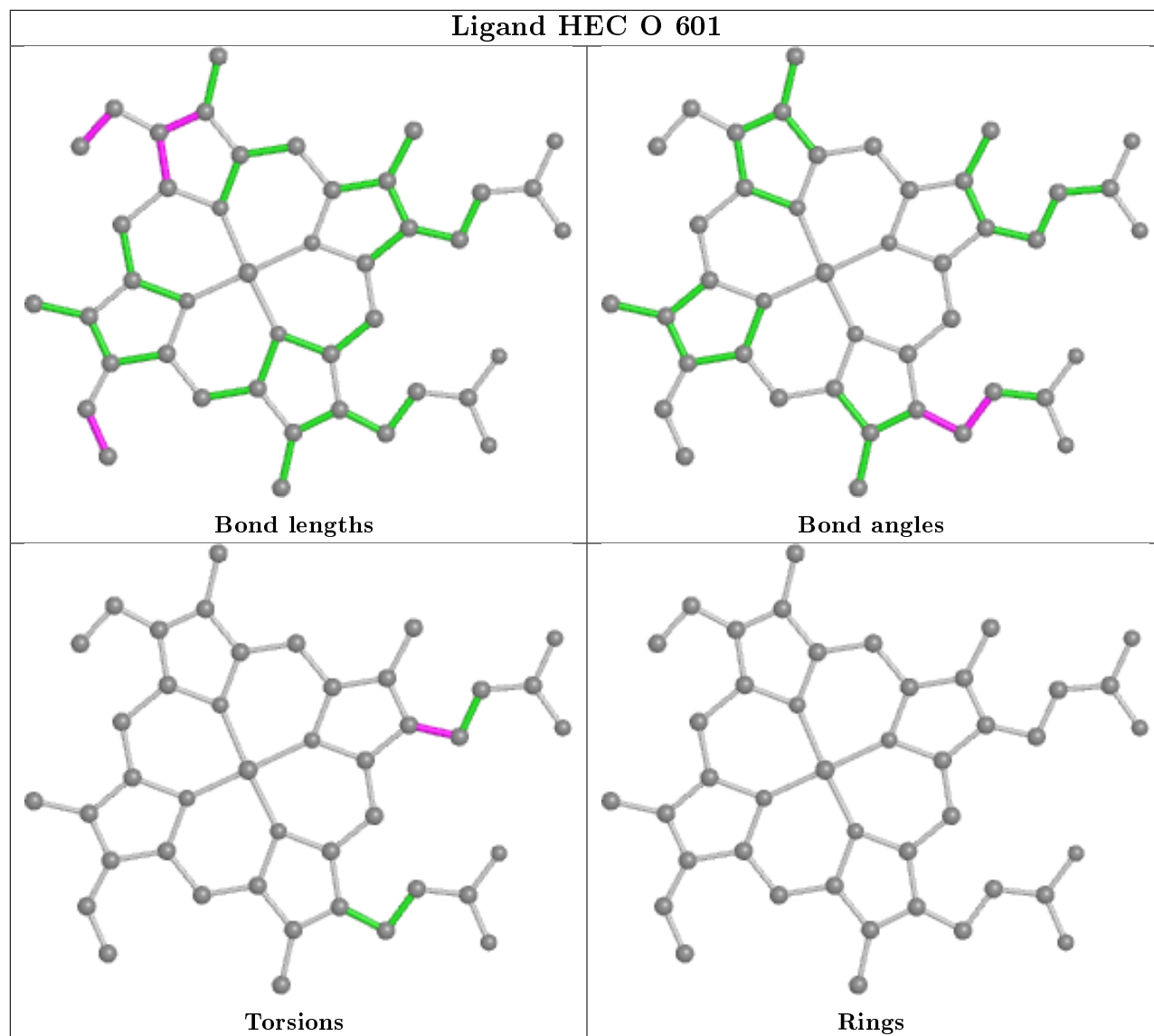




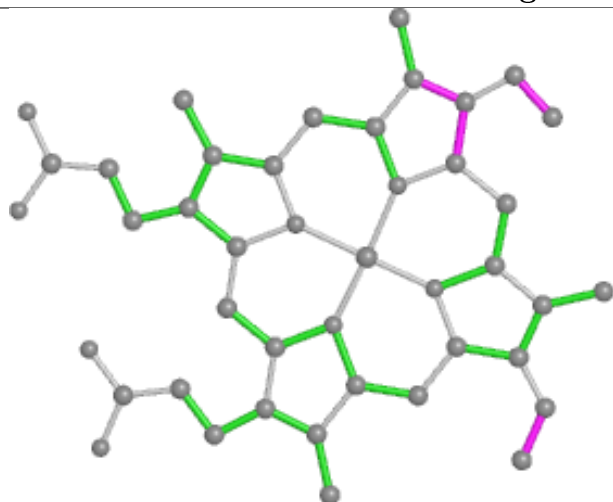


## Ligand HEC J 605

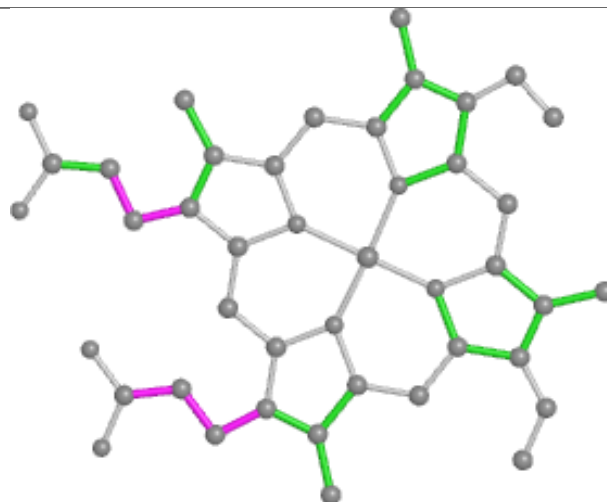




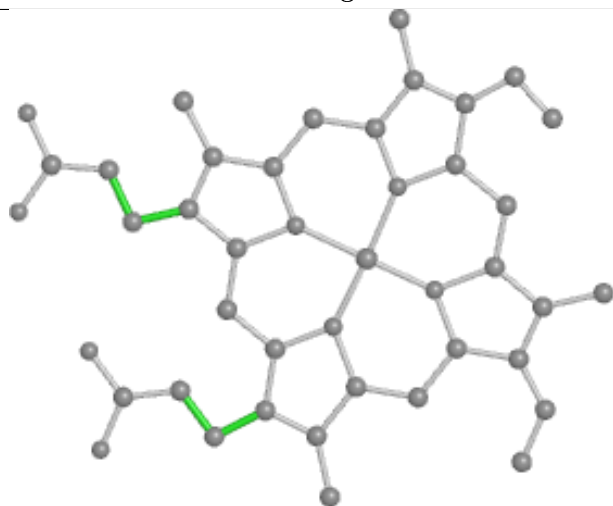
## Ligand HEC I 604



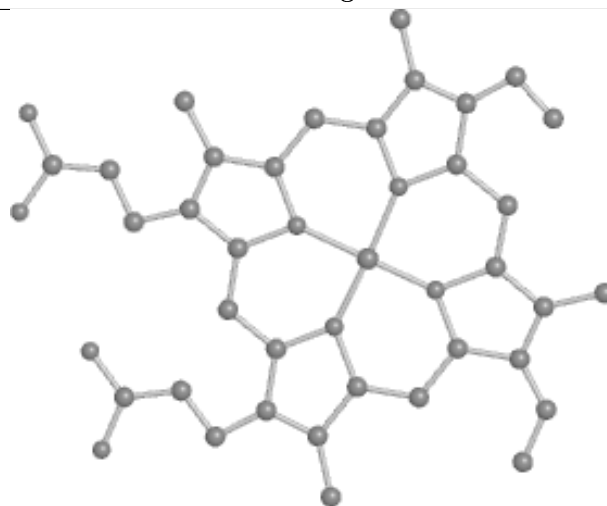
Bond lengths



Bond angles



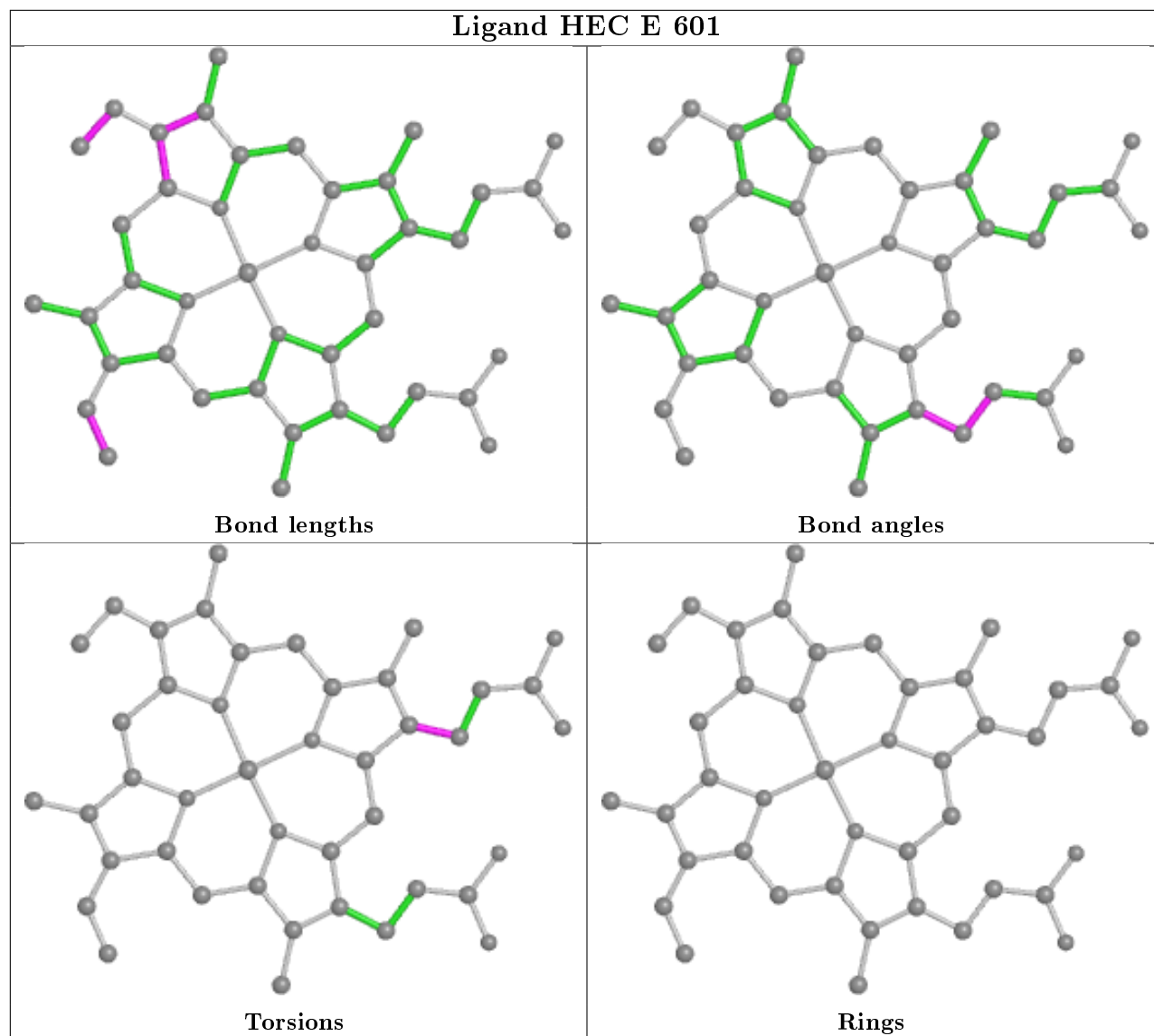
Torsions



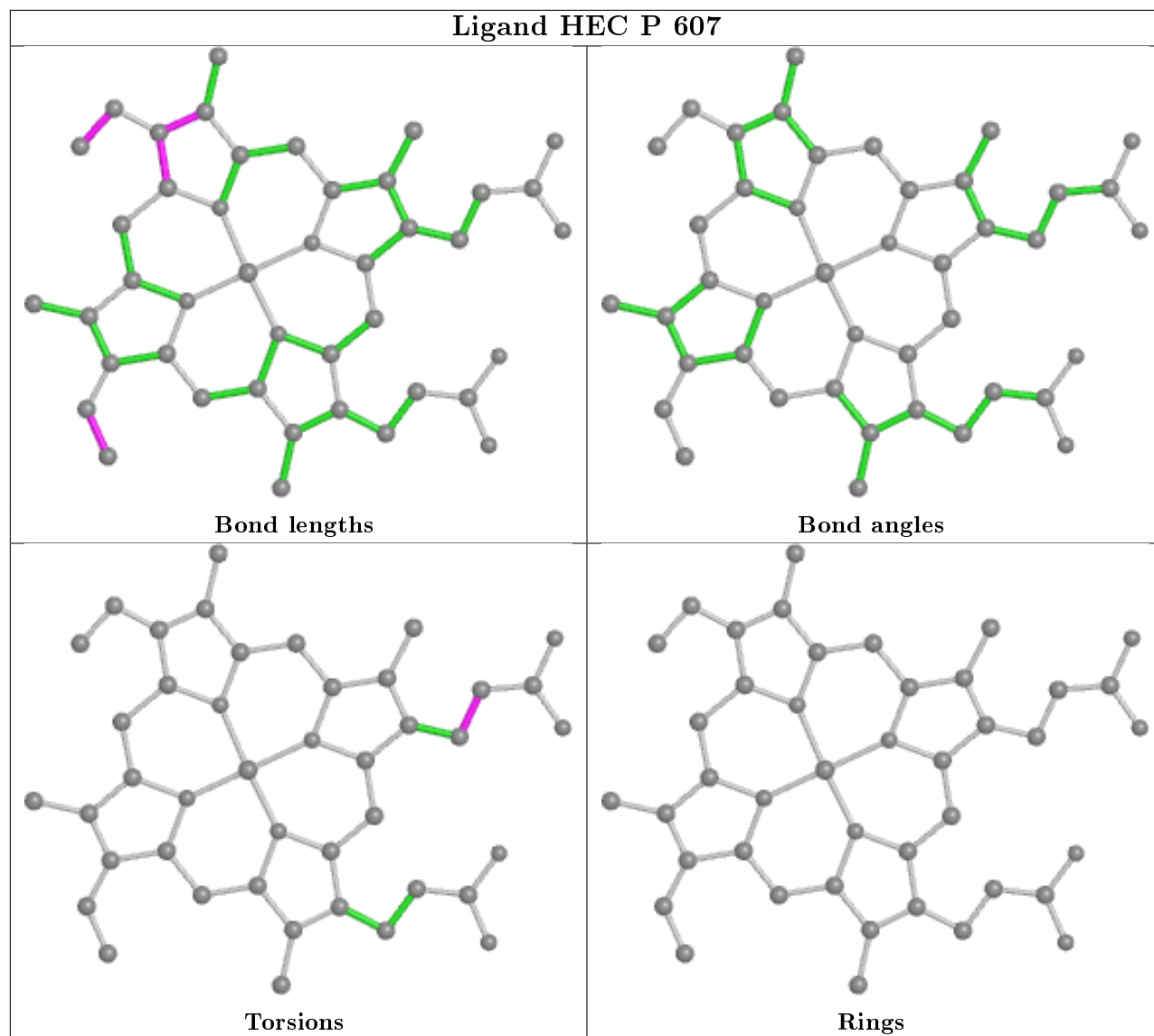
Rings

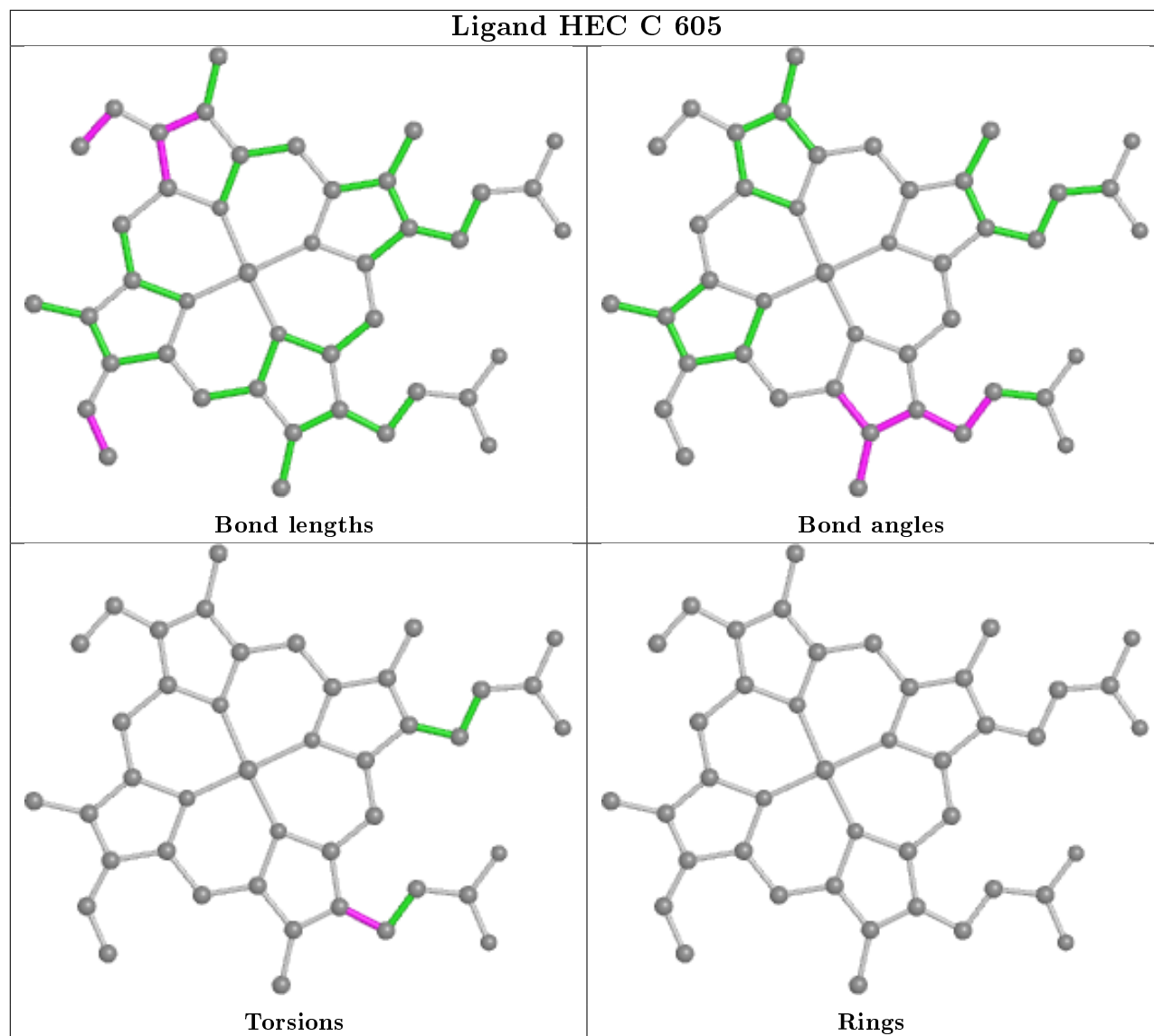


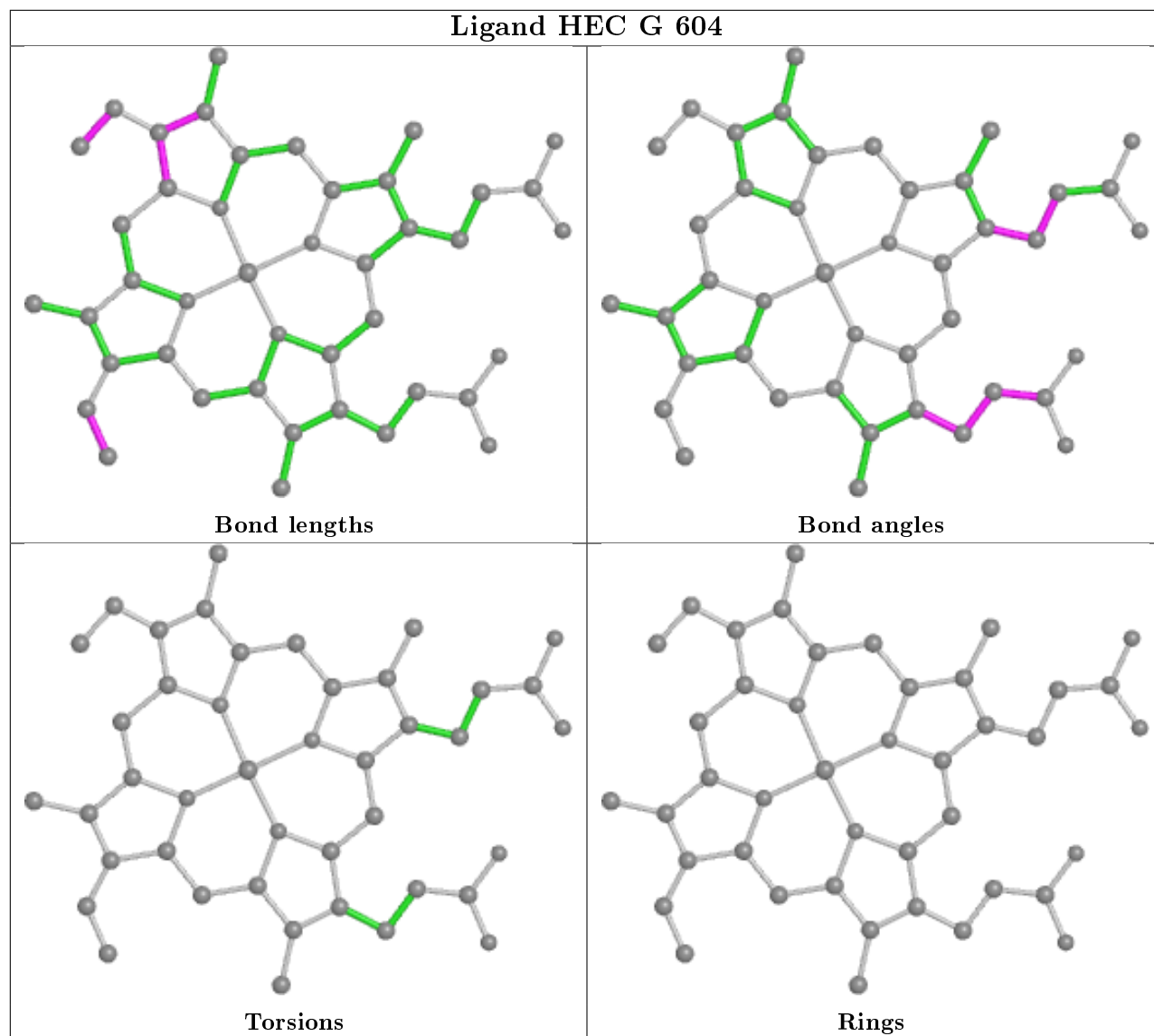
## Ligand HEC E 601

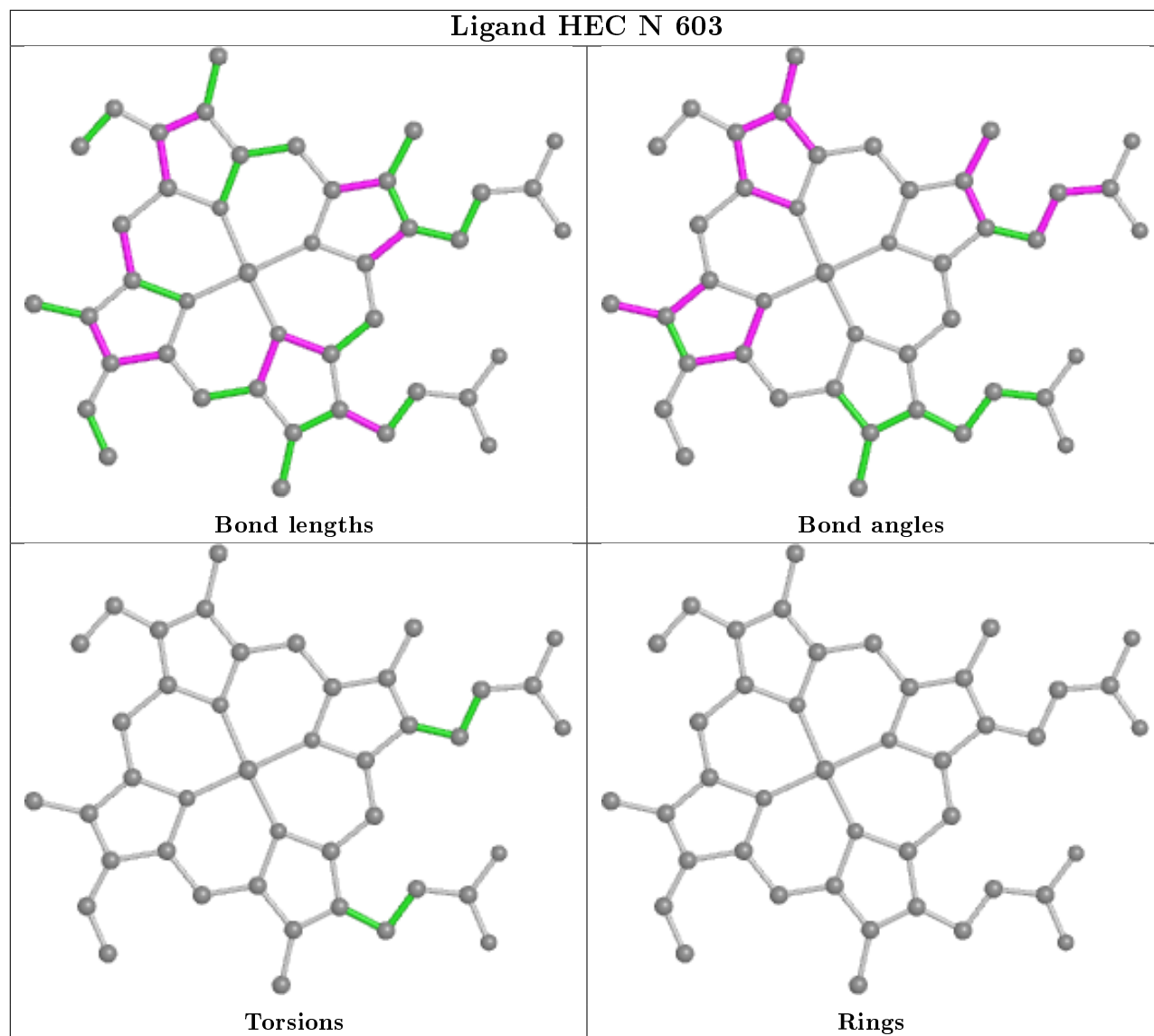


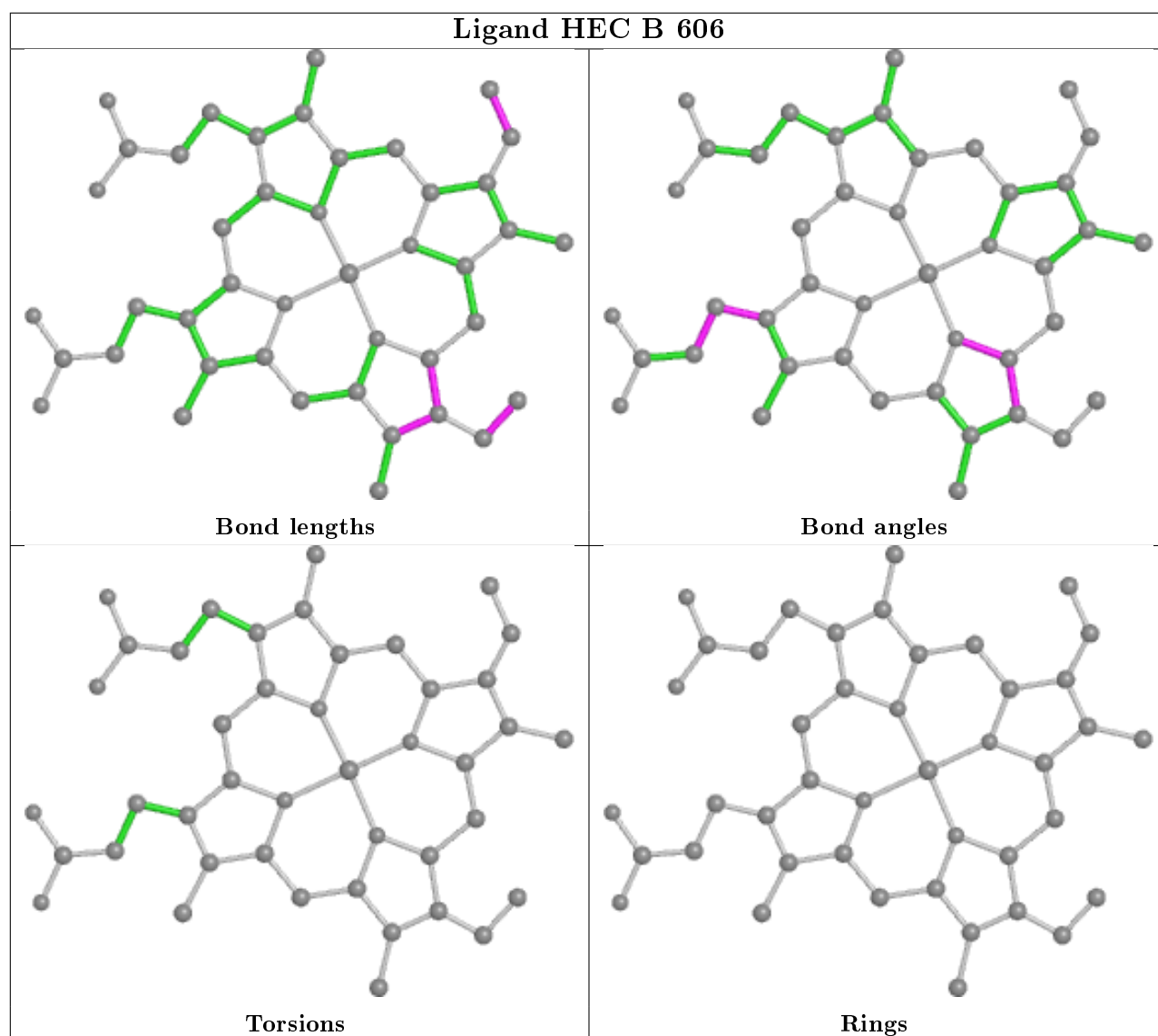
## Ligand HEC P 607

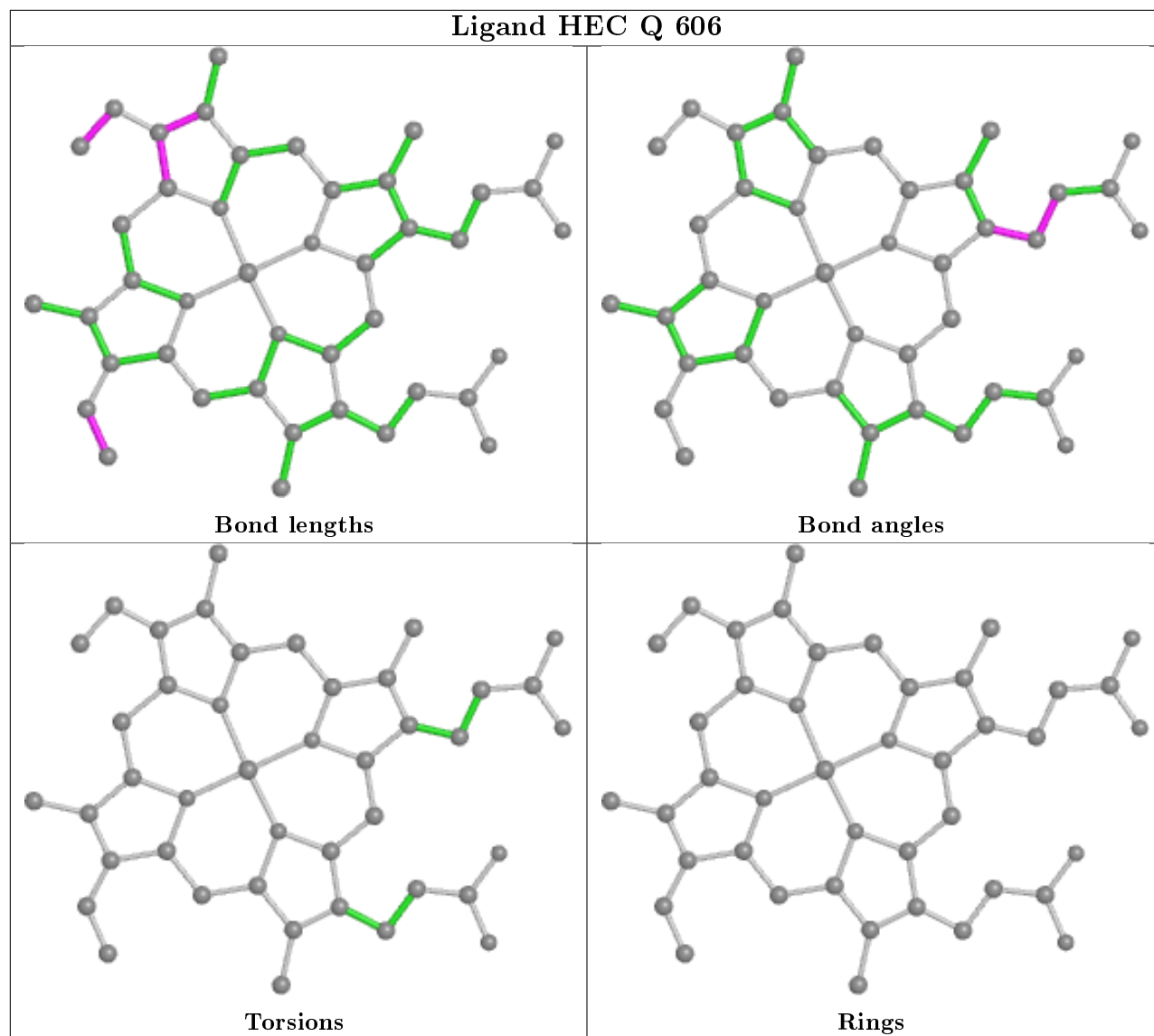


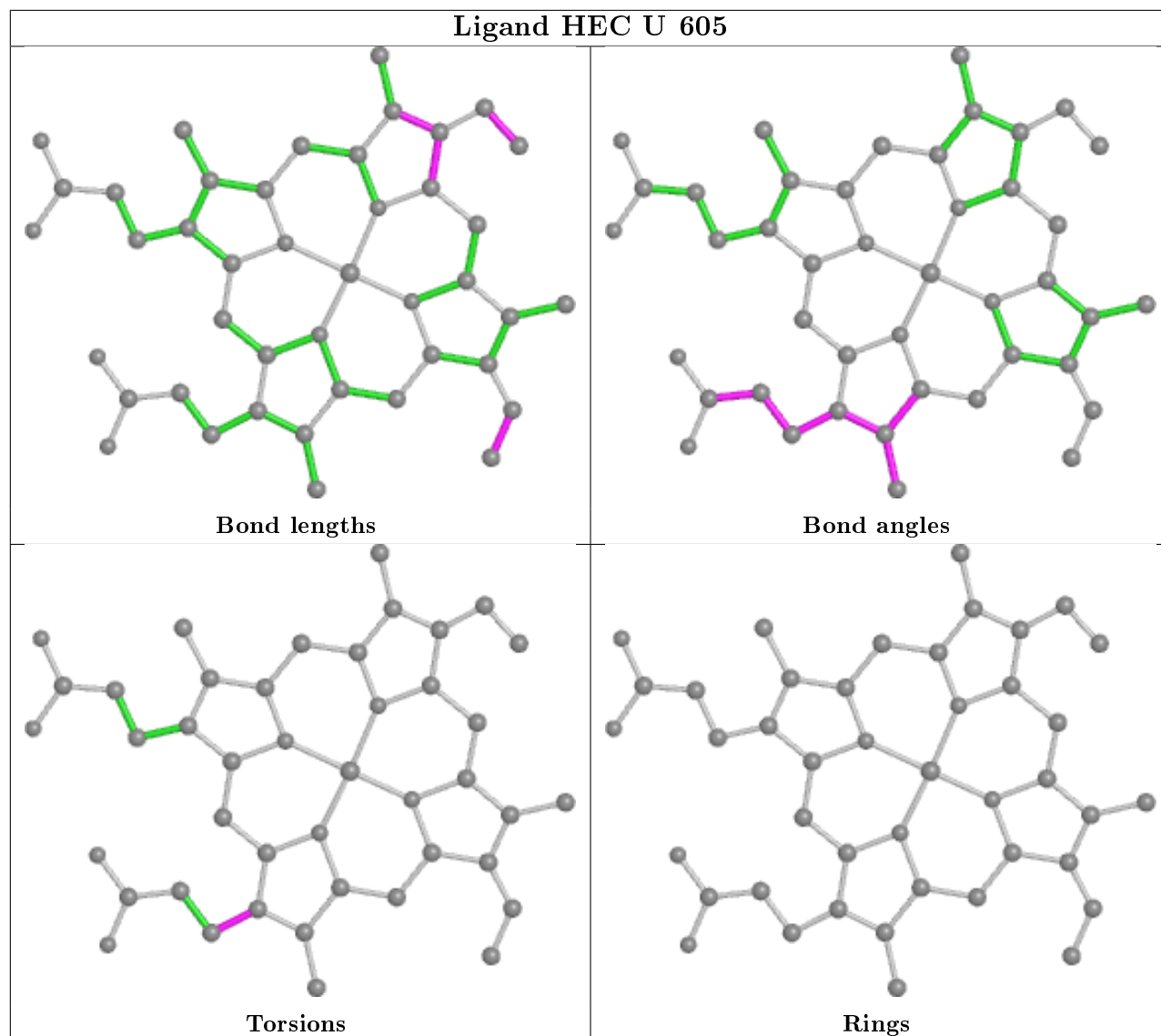






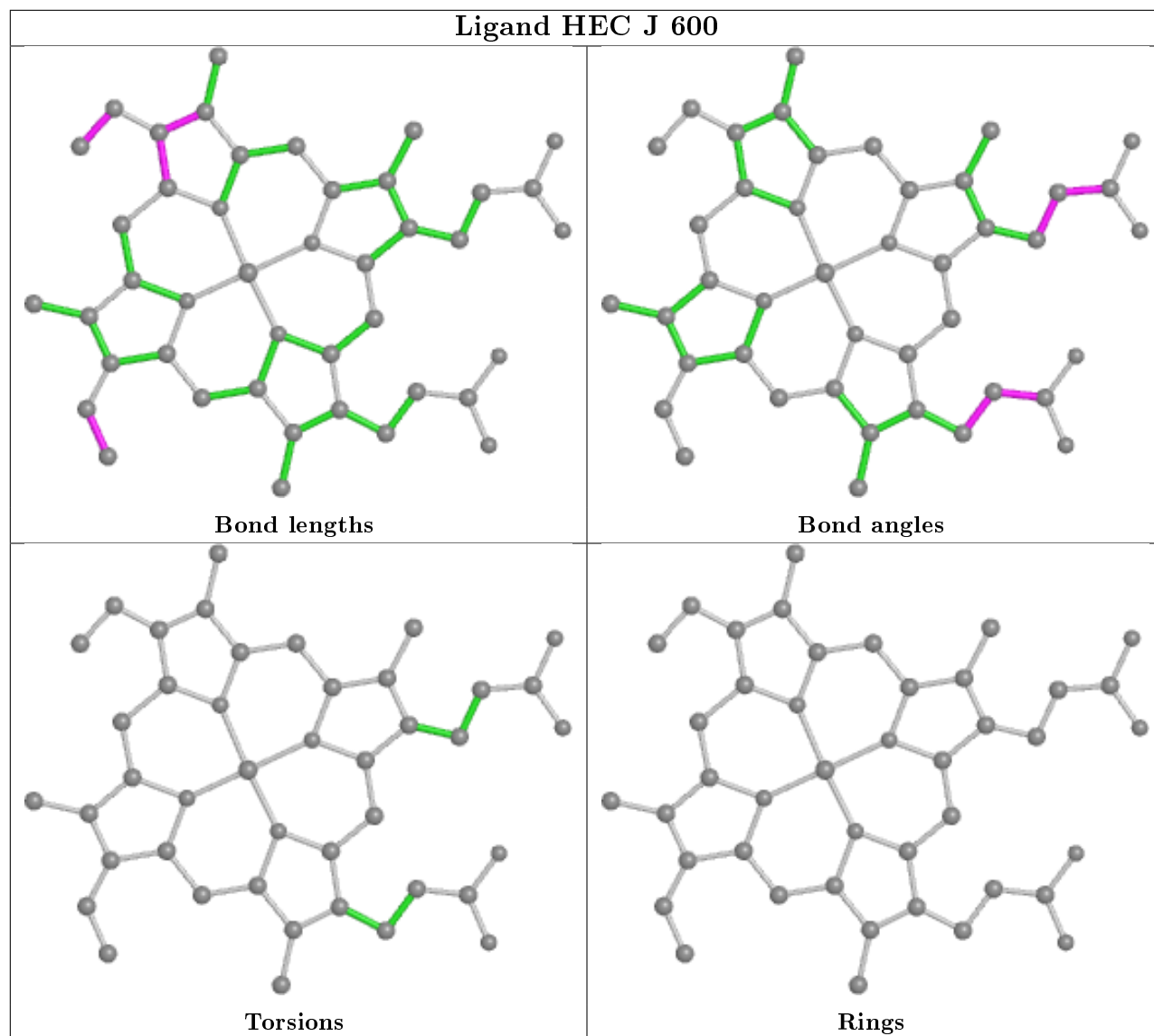


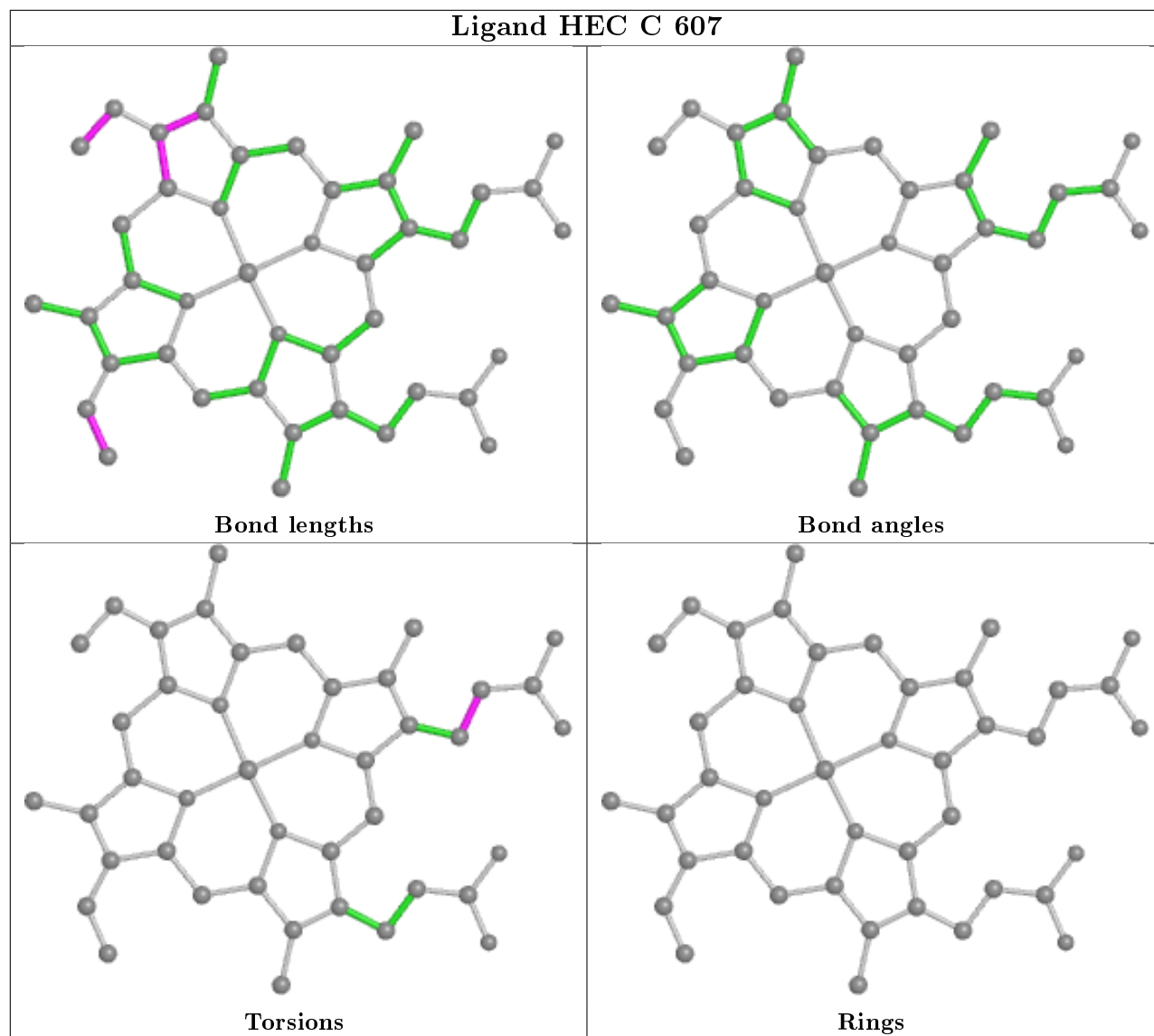




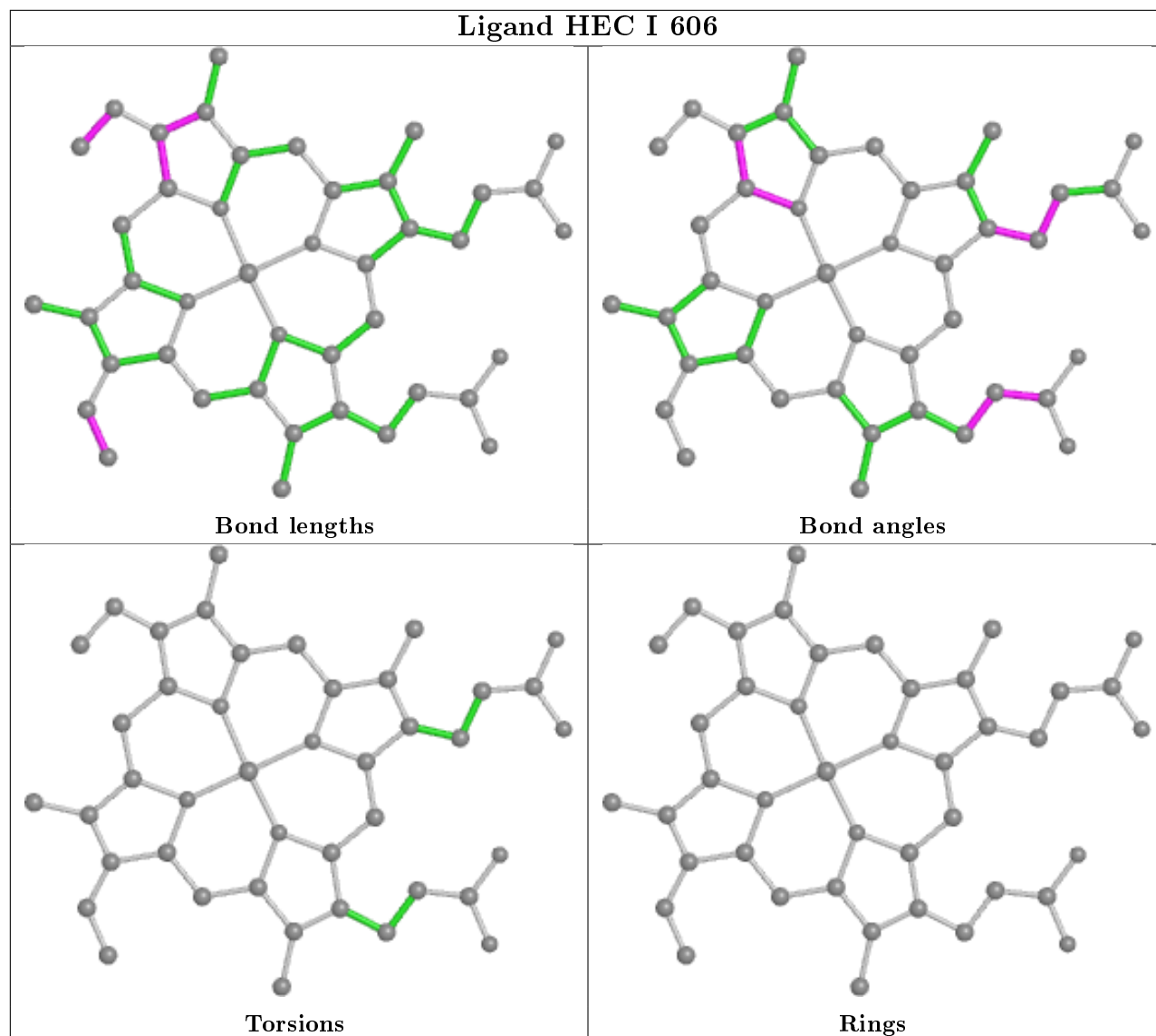


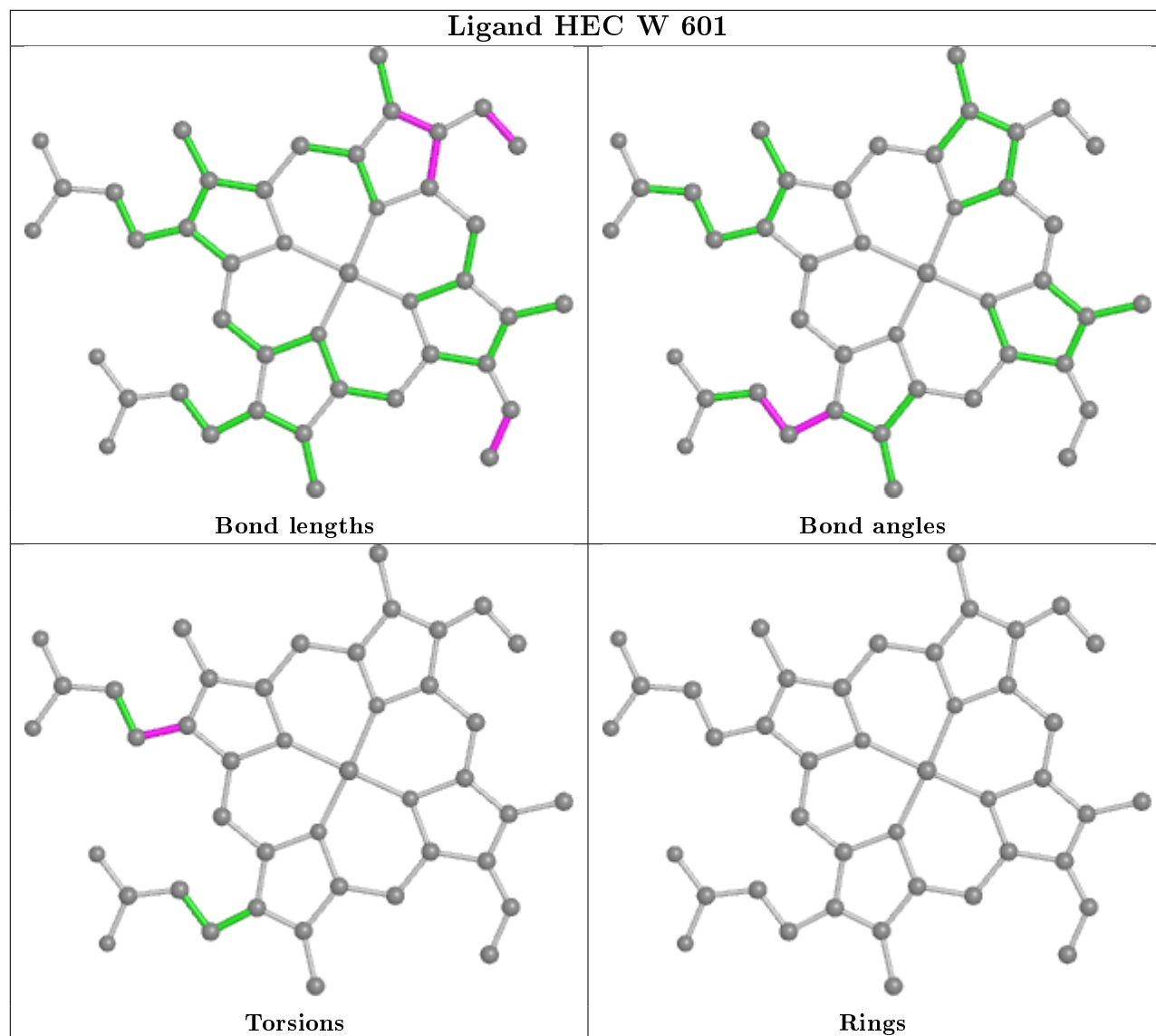
## Ligand HEC J 600

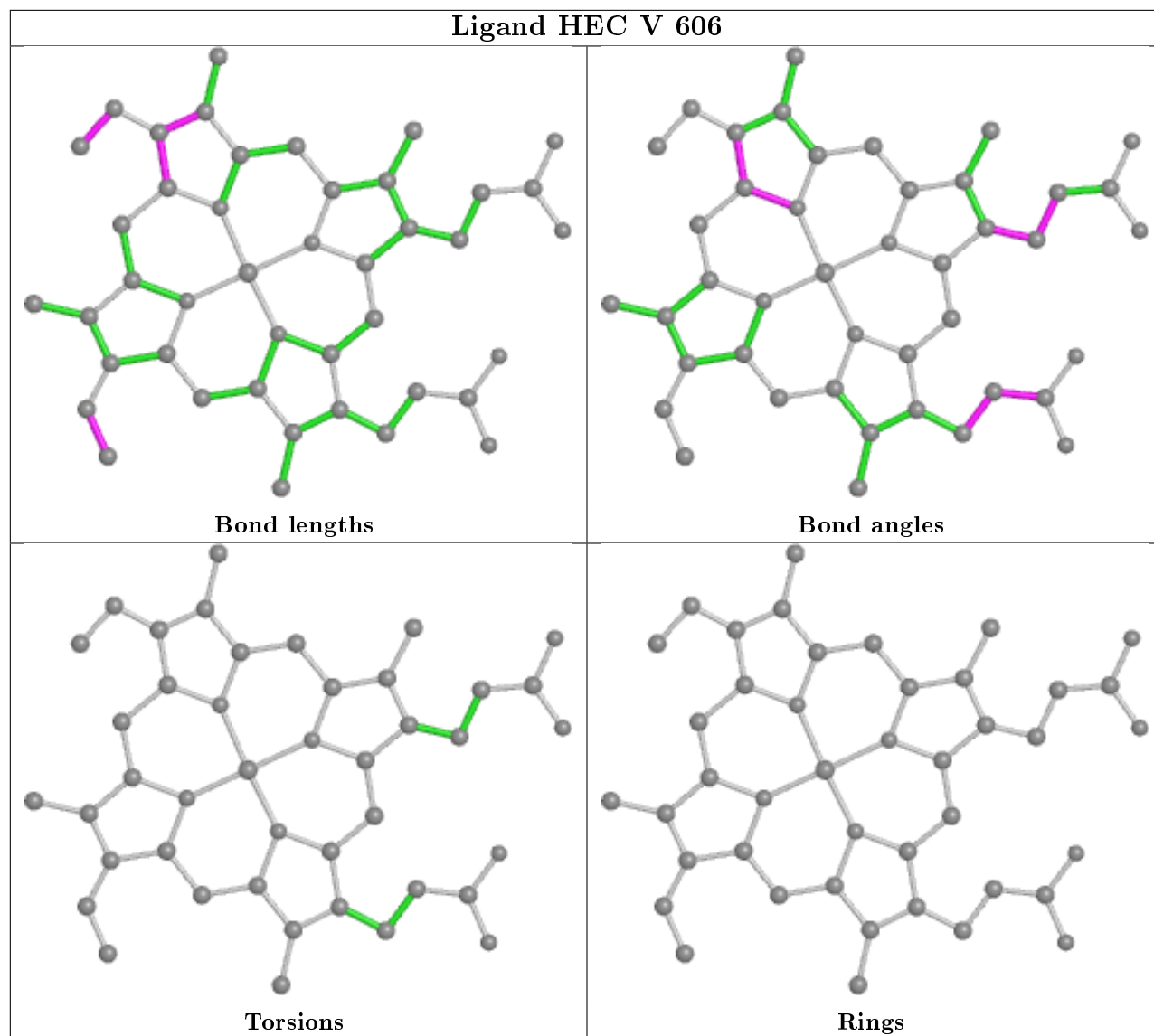


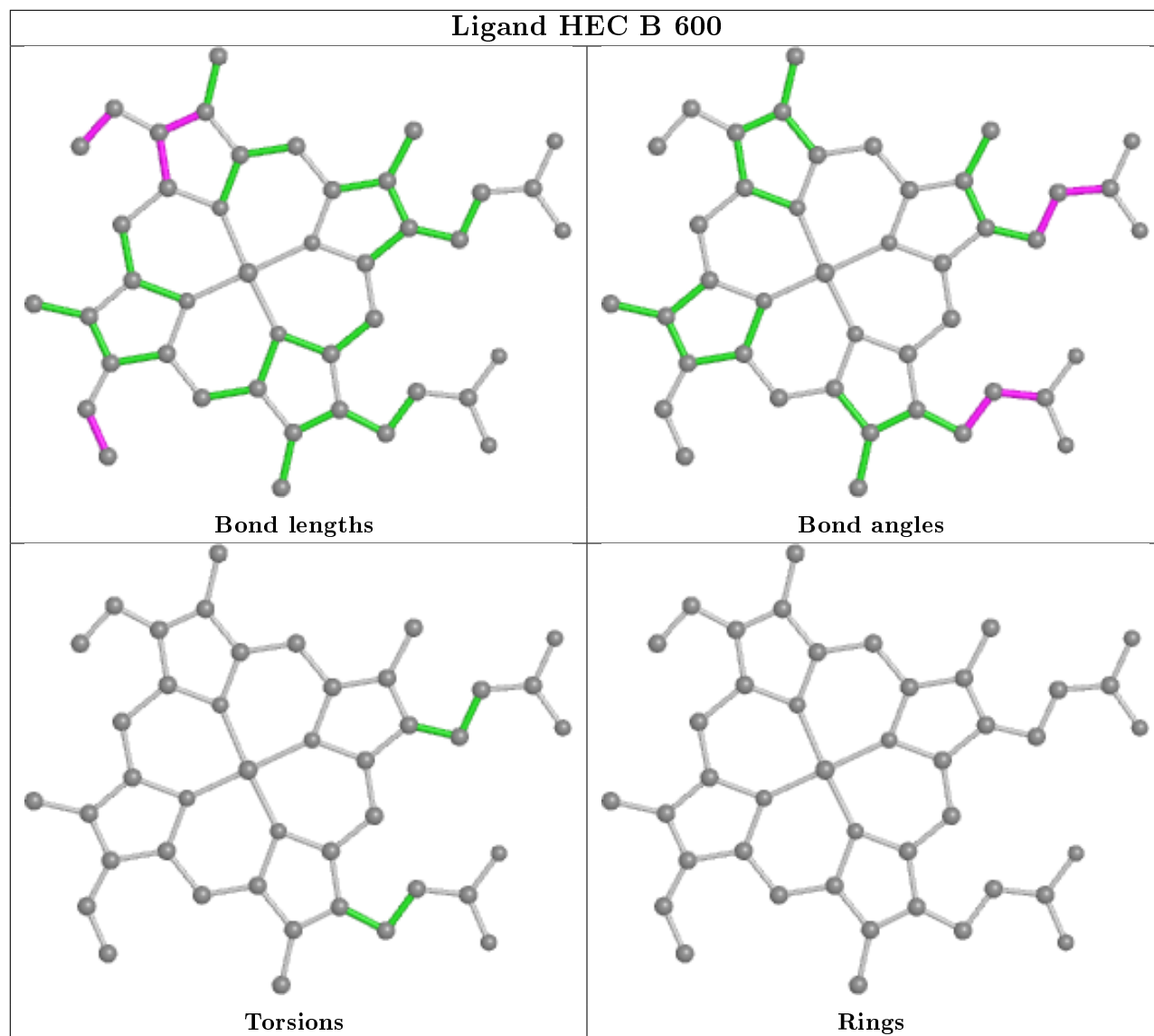


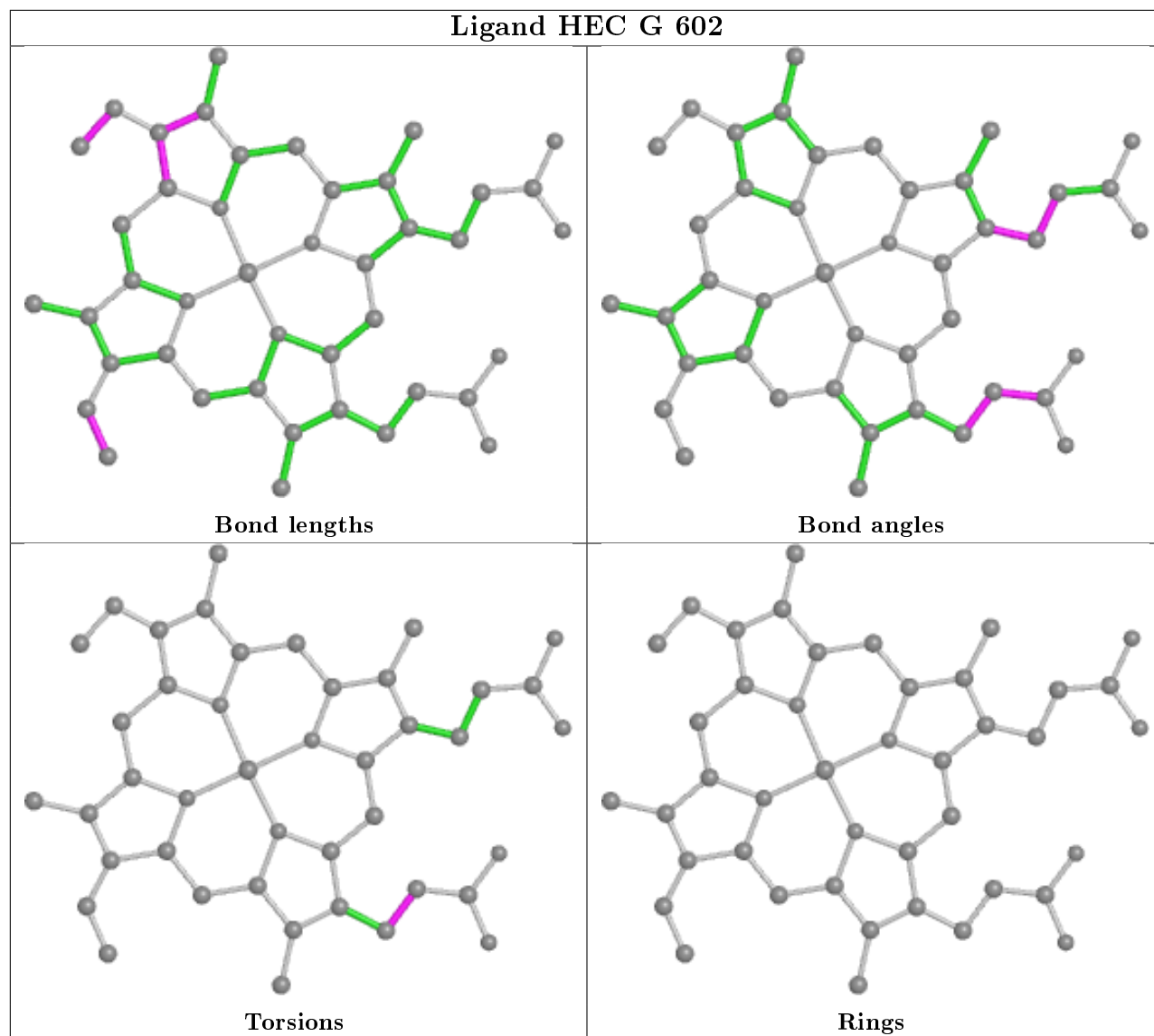
## Ligand HEC I 606

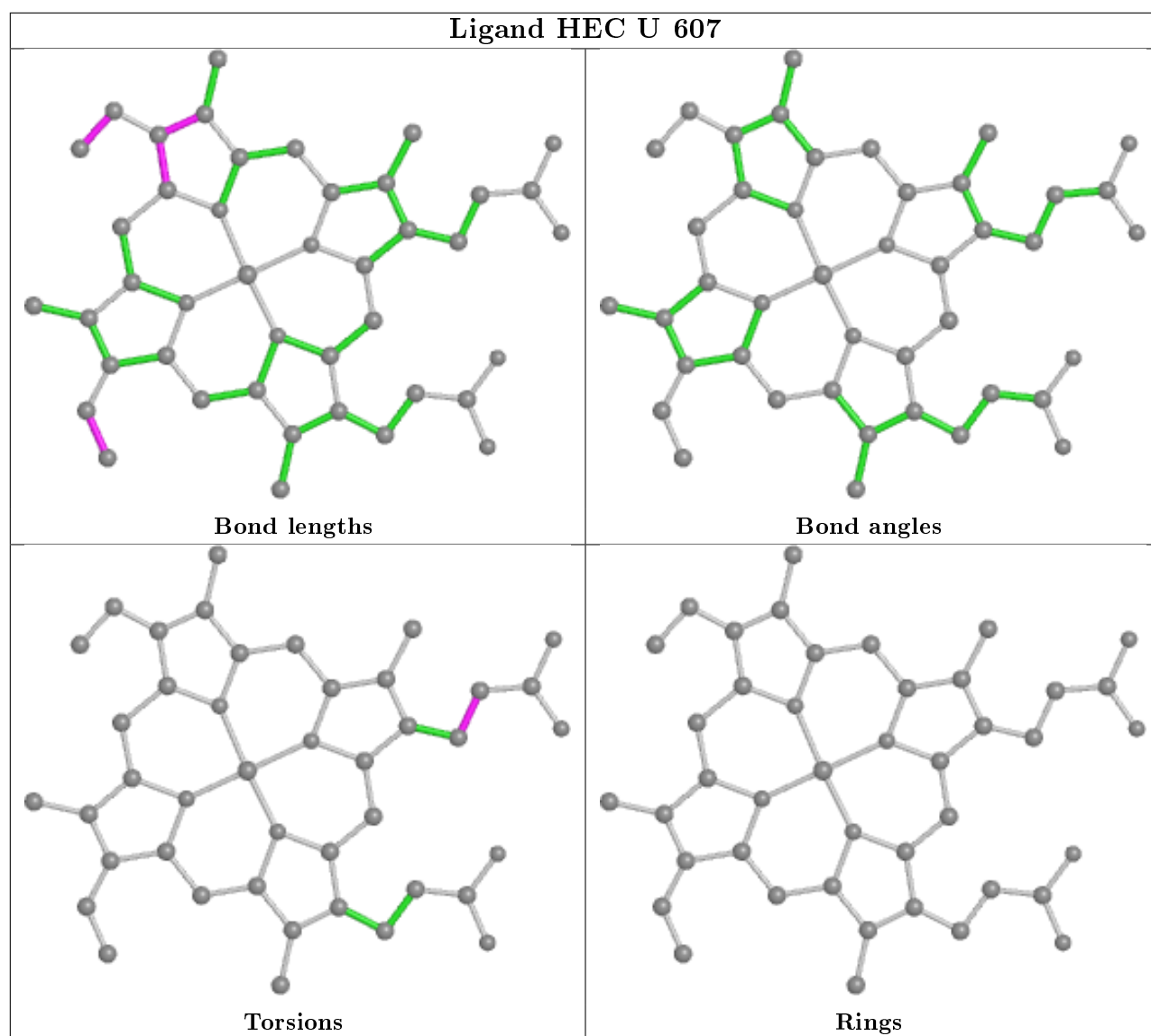




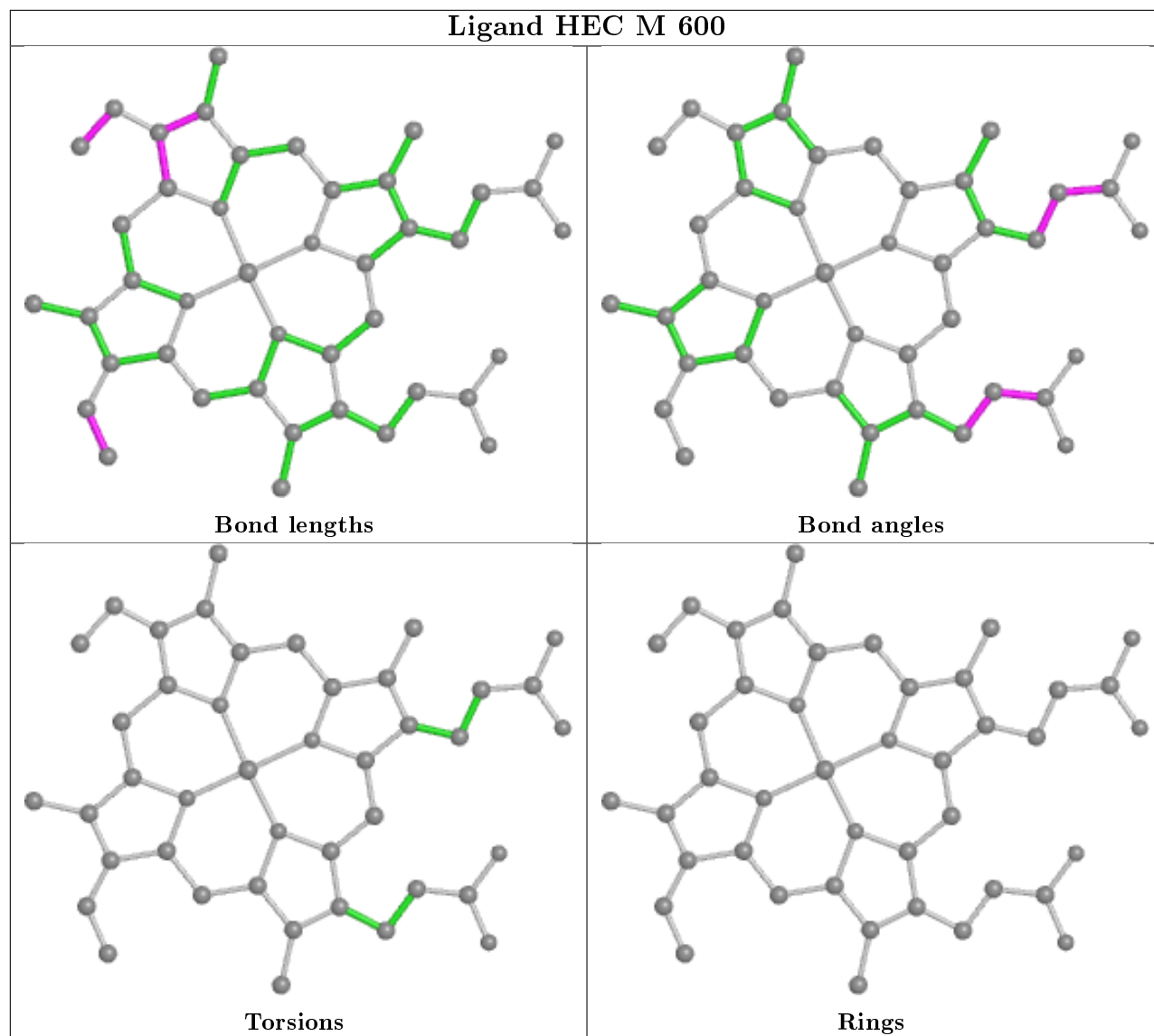


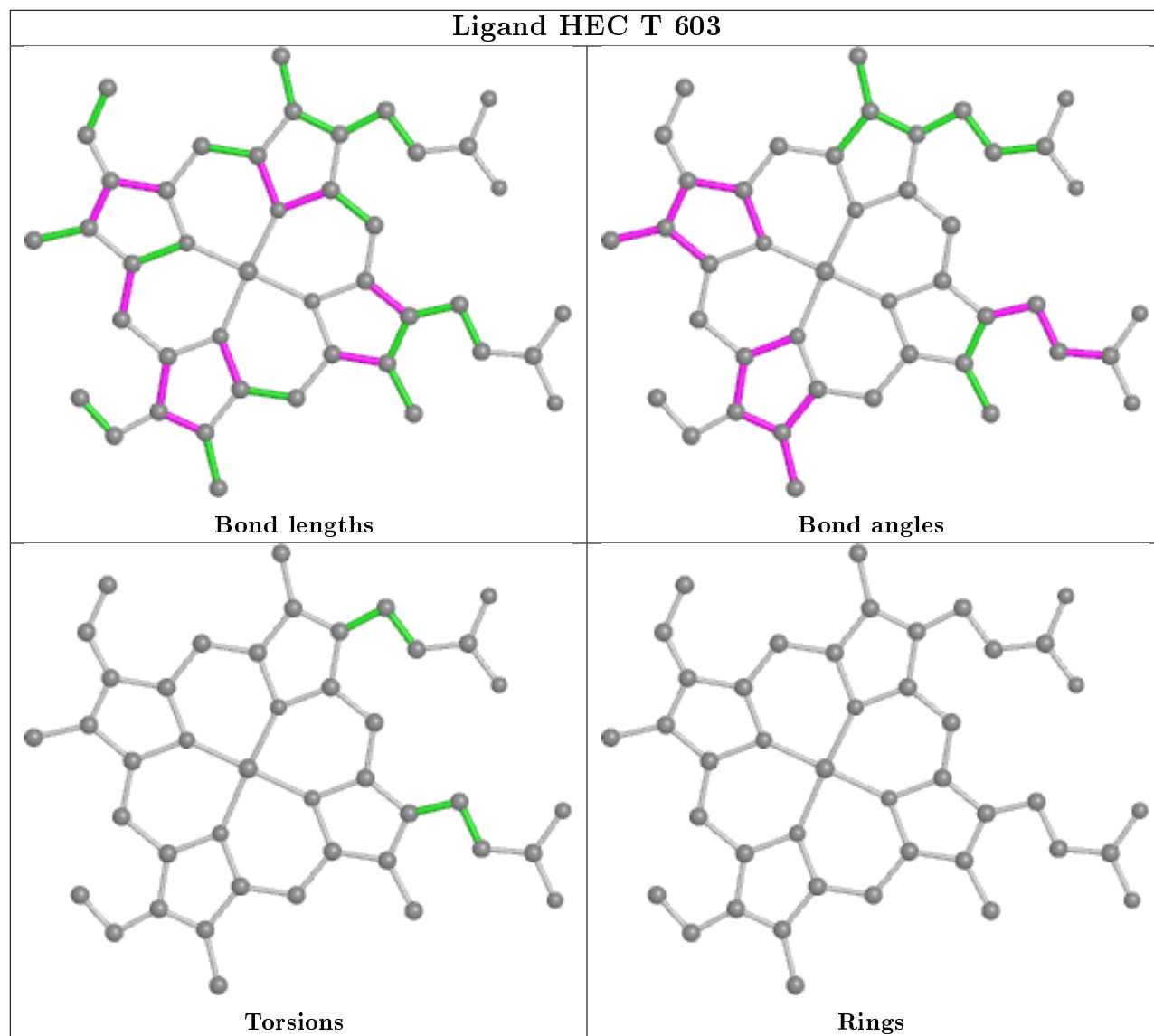


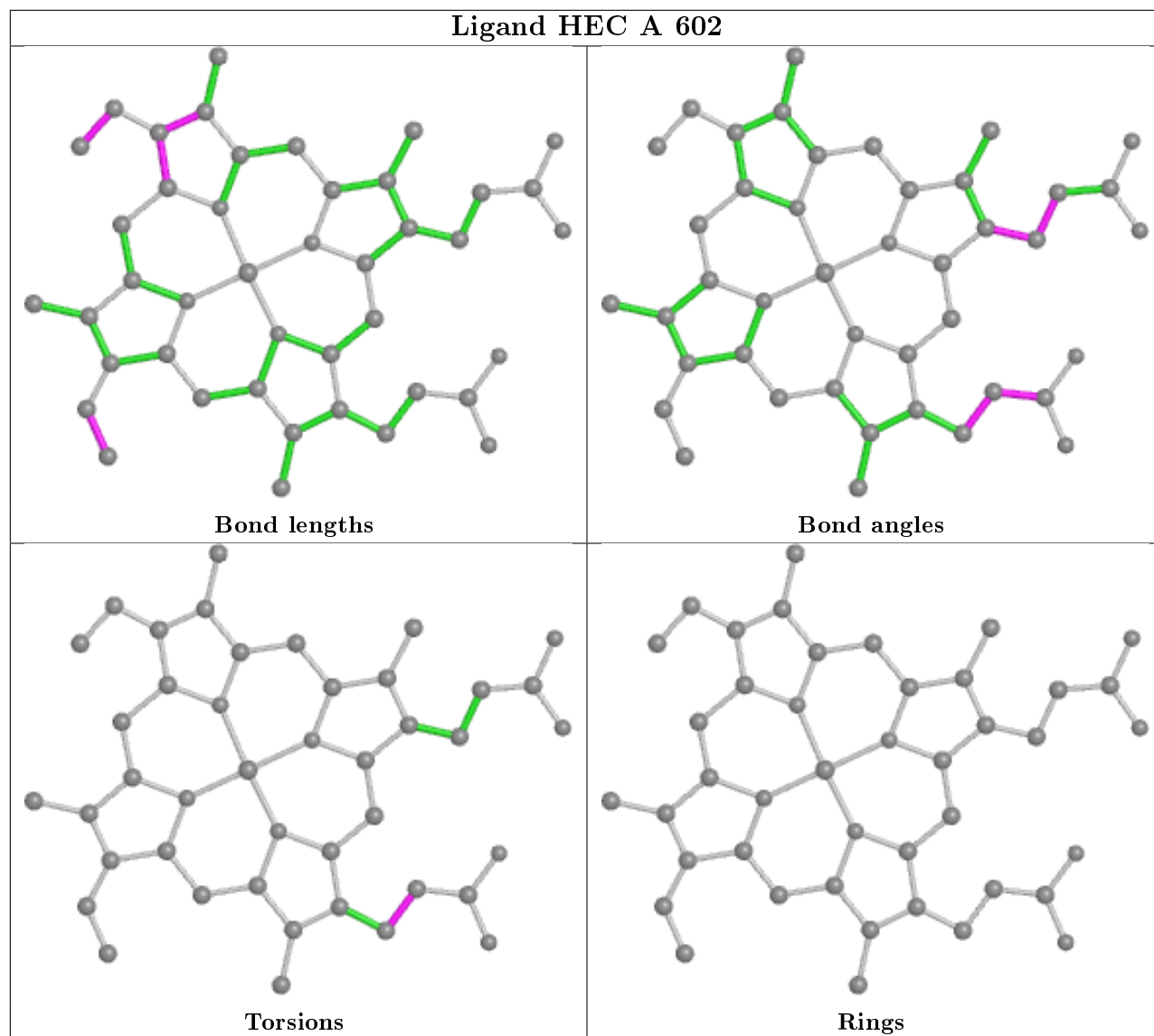




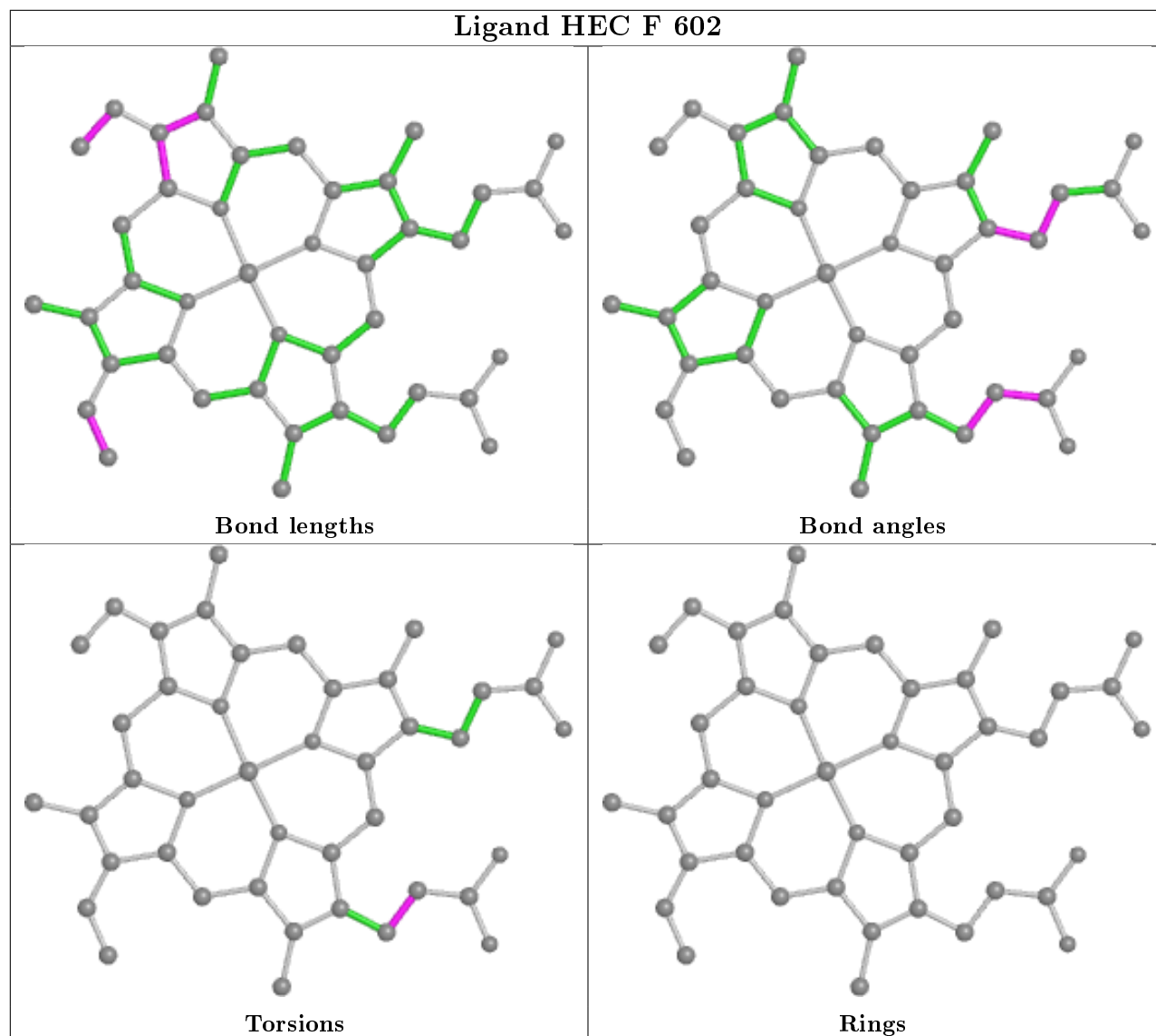


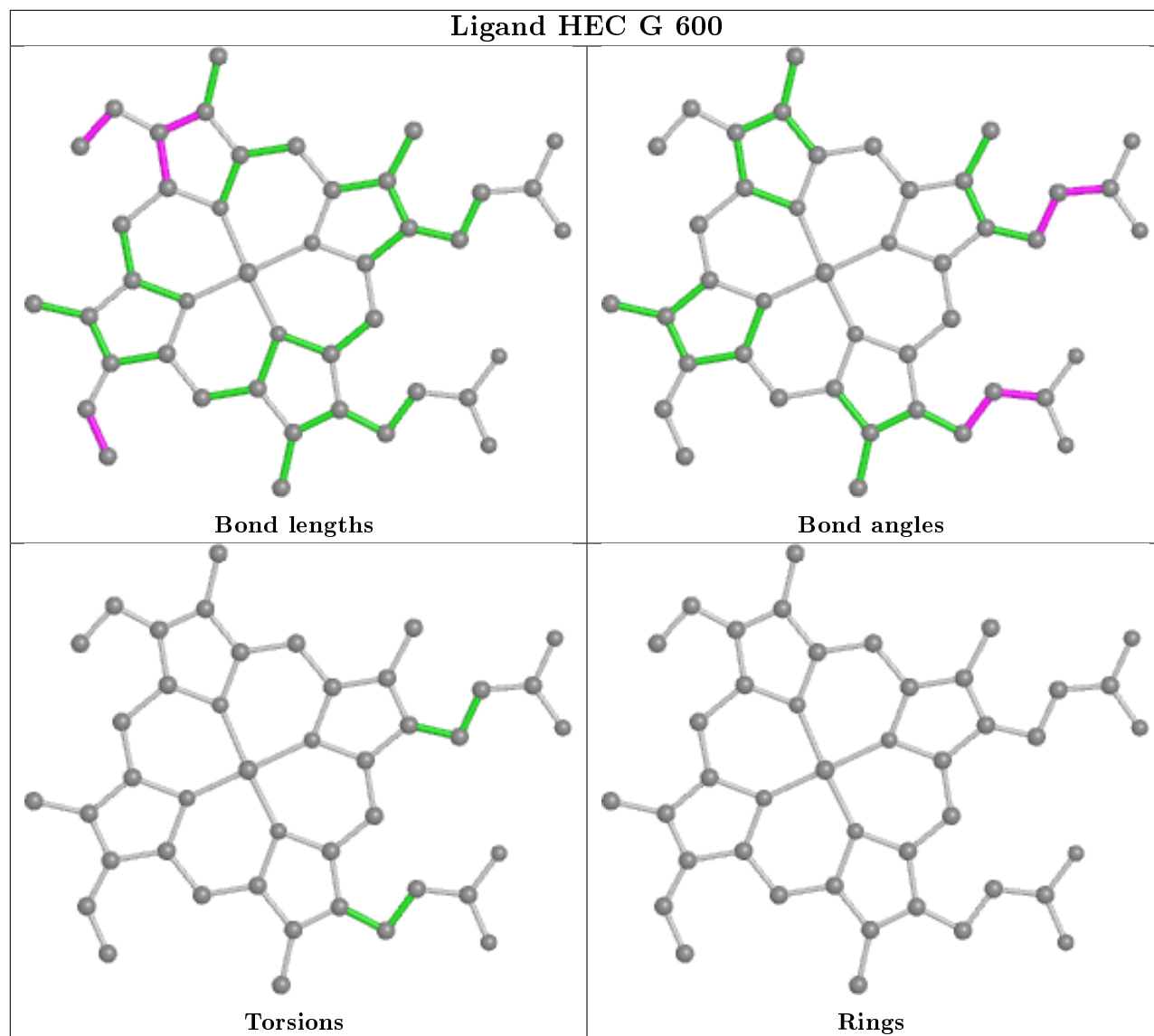




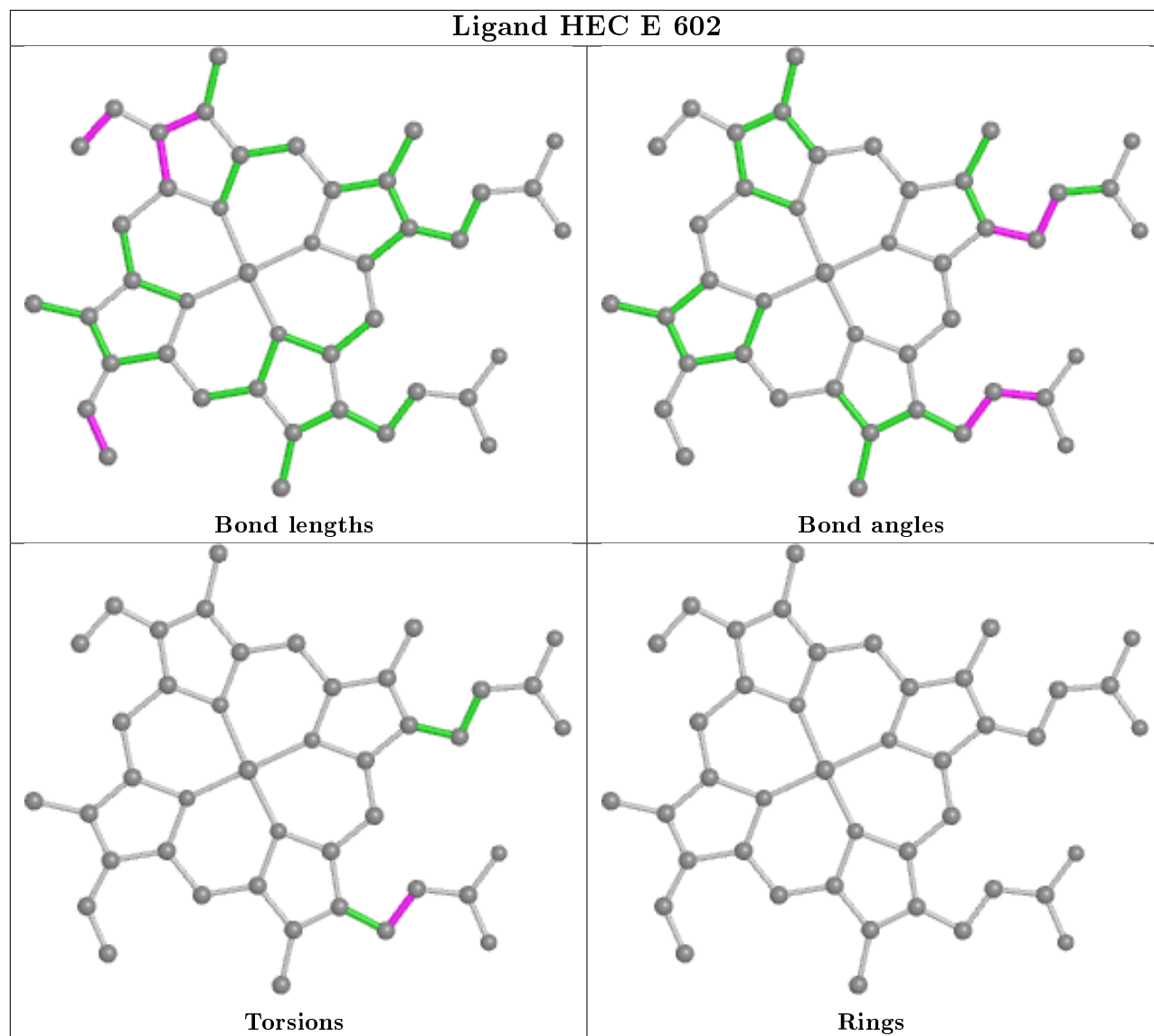


## Ligand HEC F 602

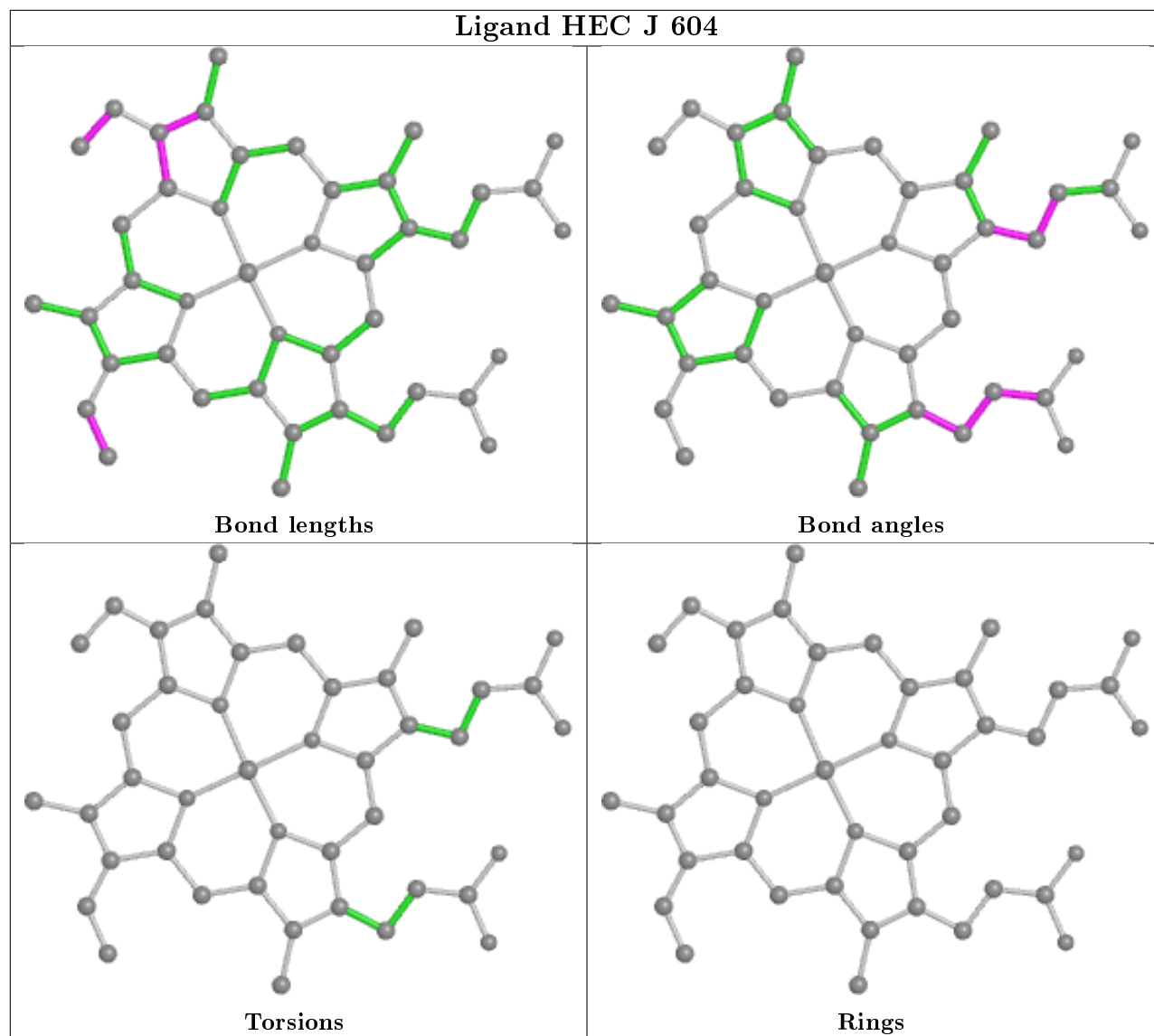


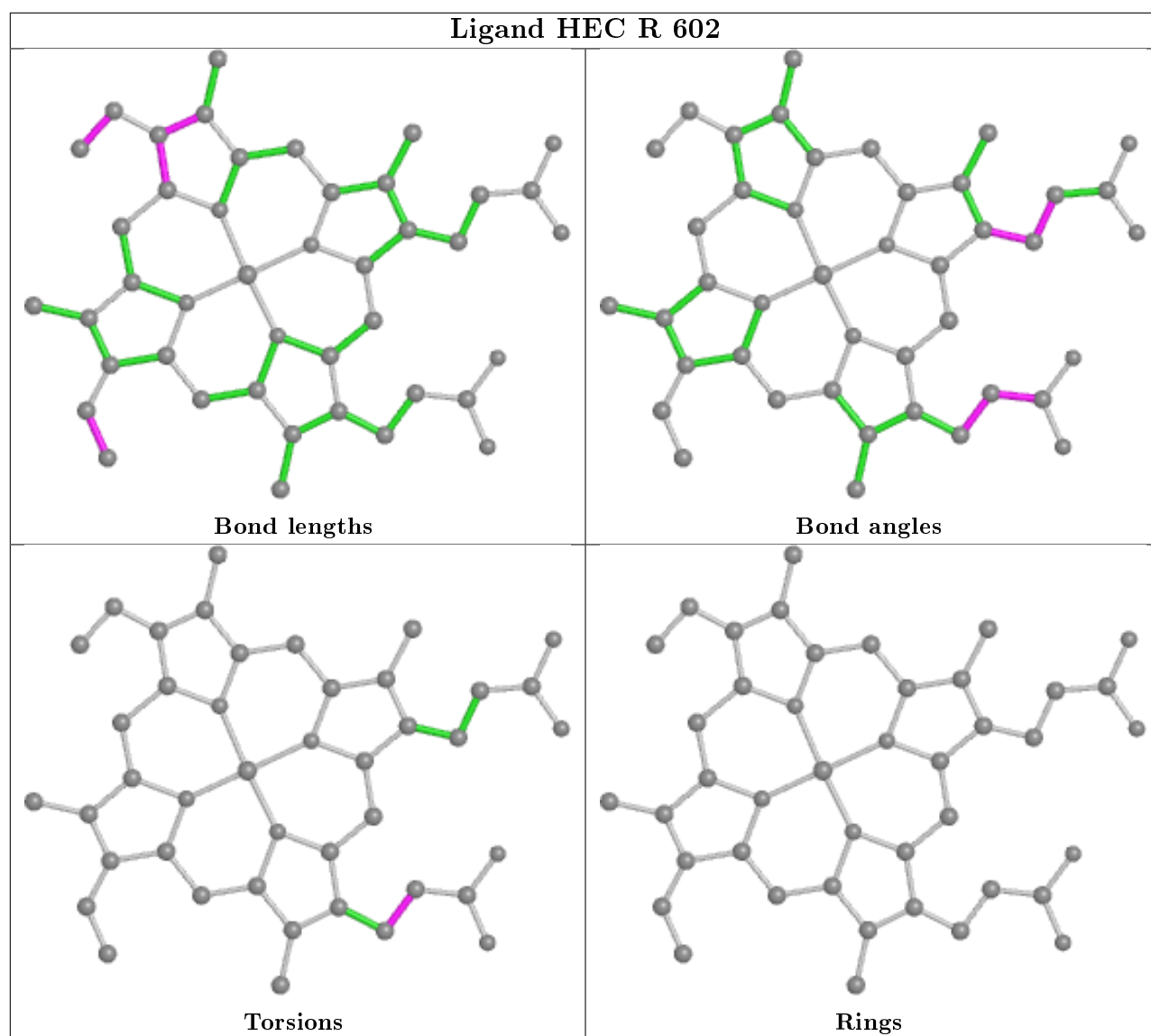


## Ligand HEC E 602

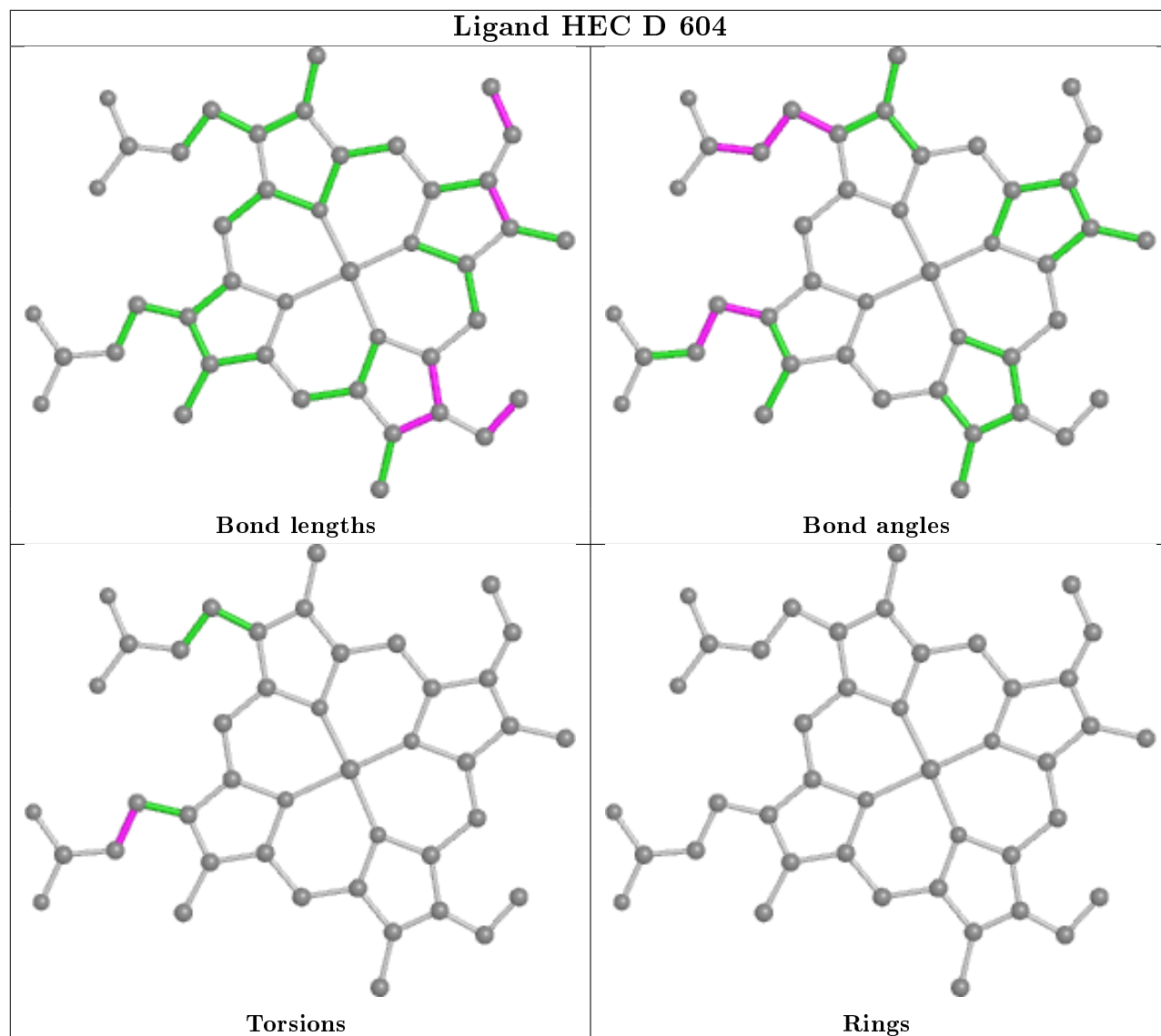


## Ligand HEC J 604

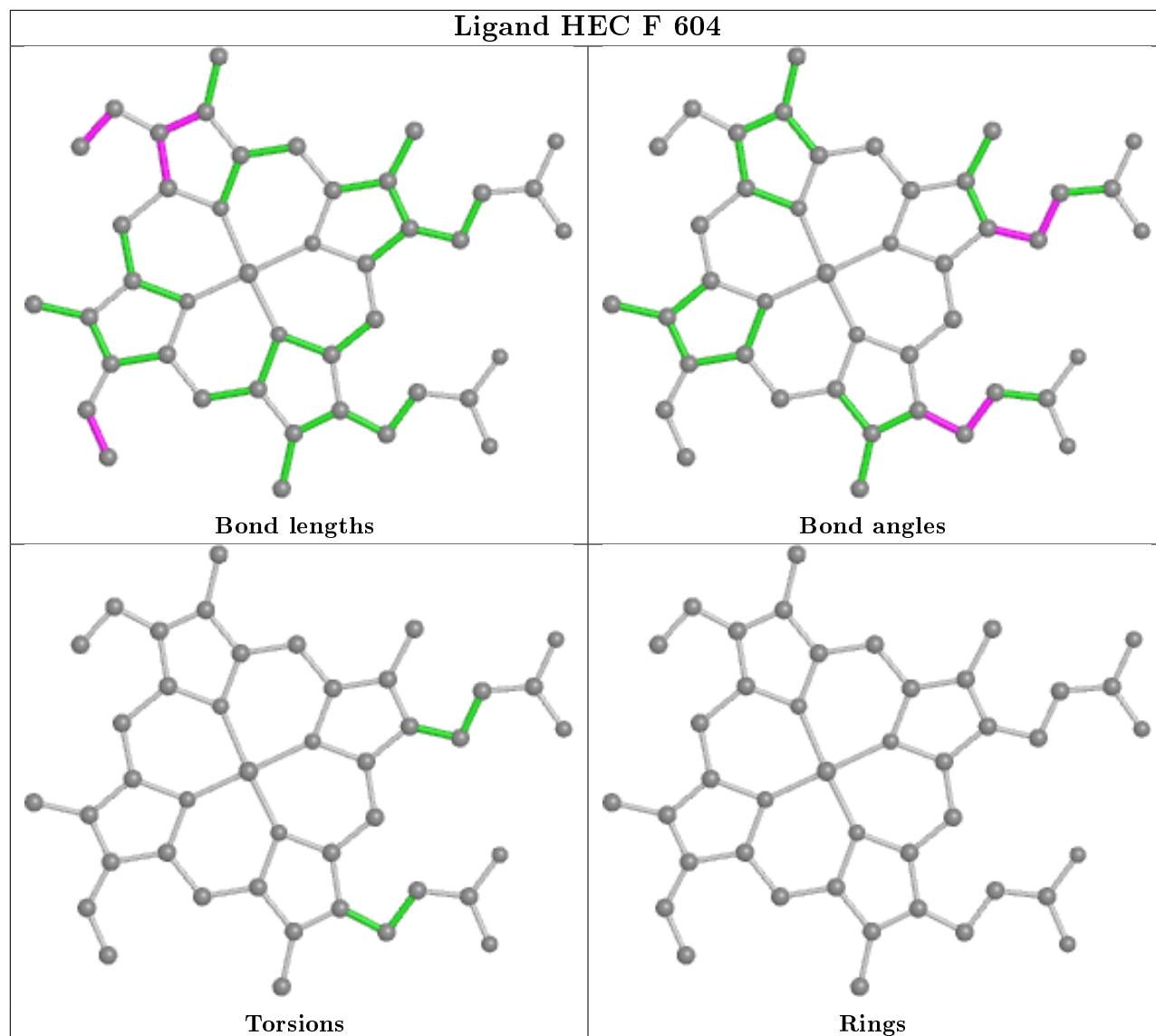




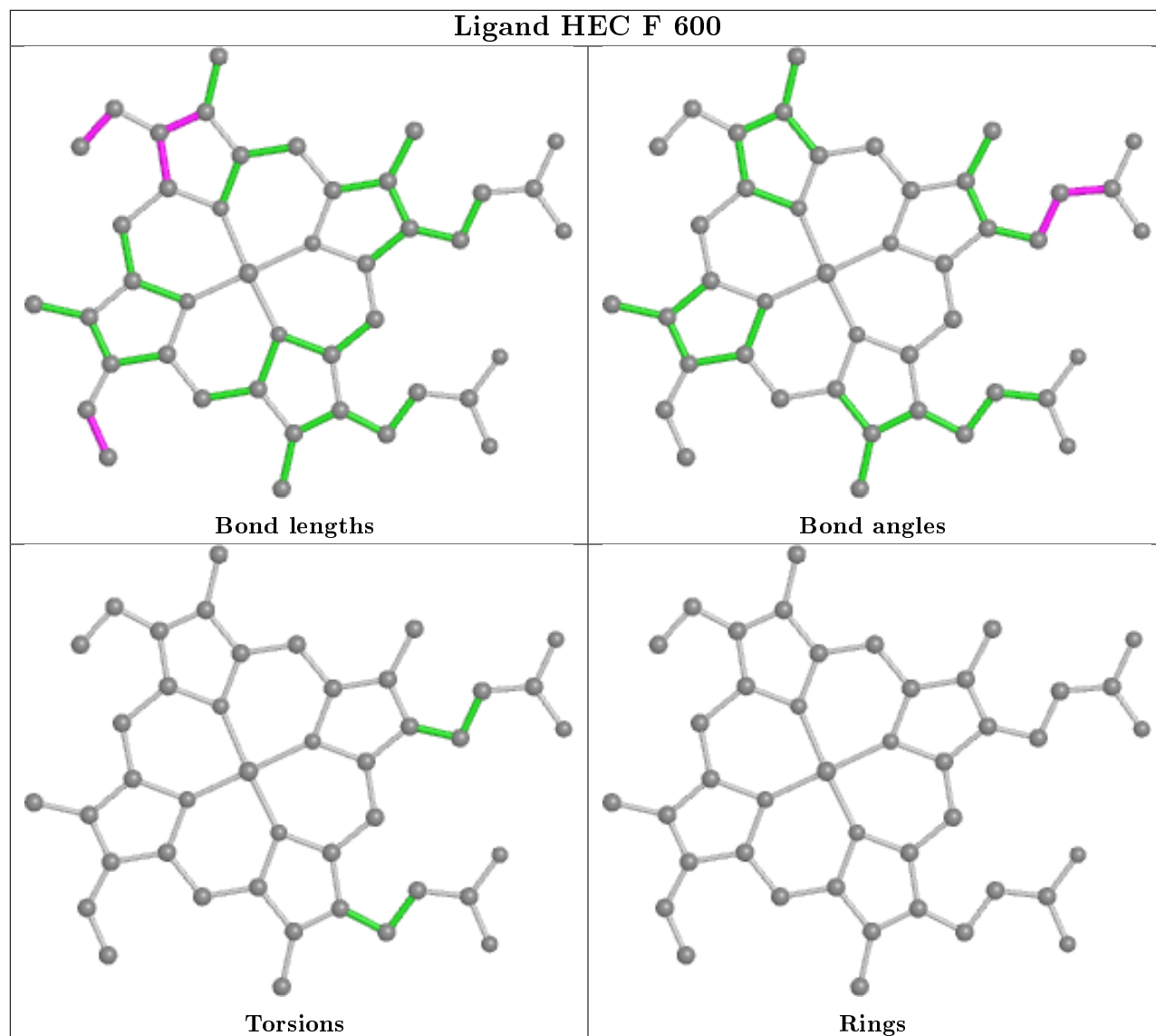




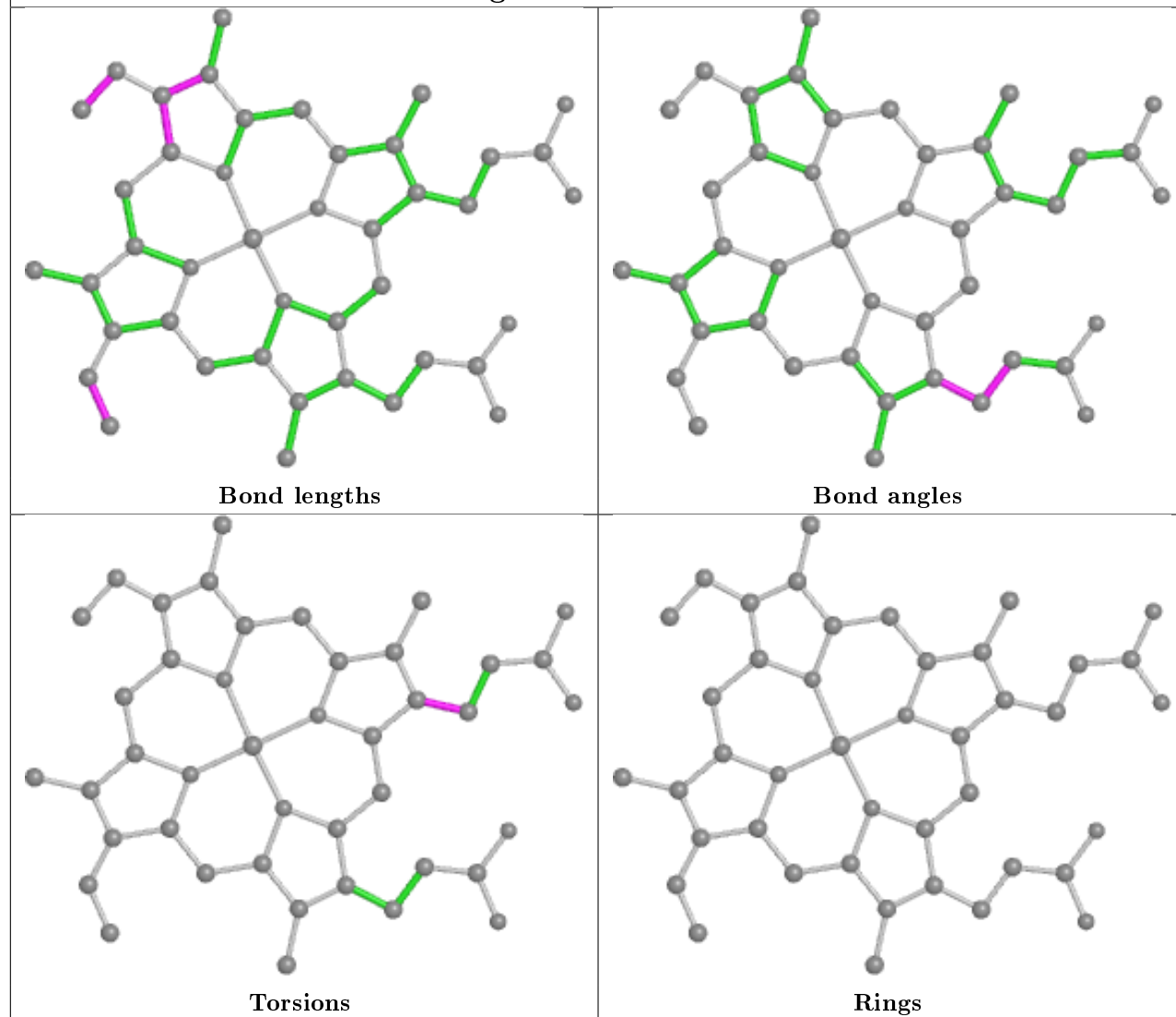
## Ligand HEC F 604

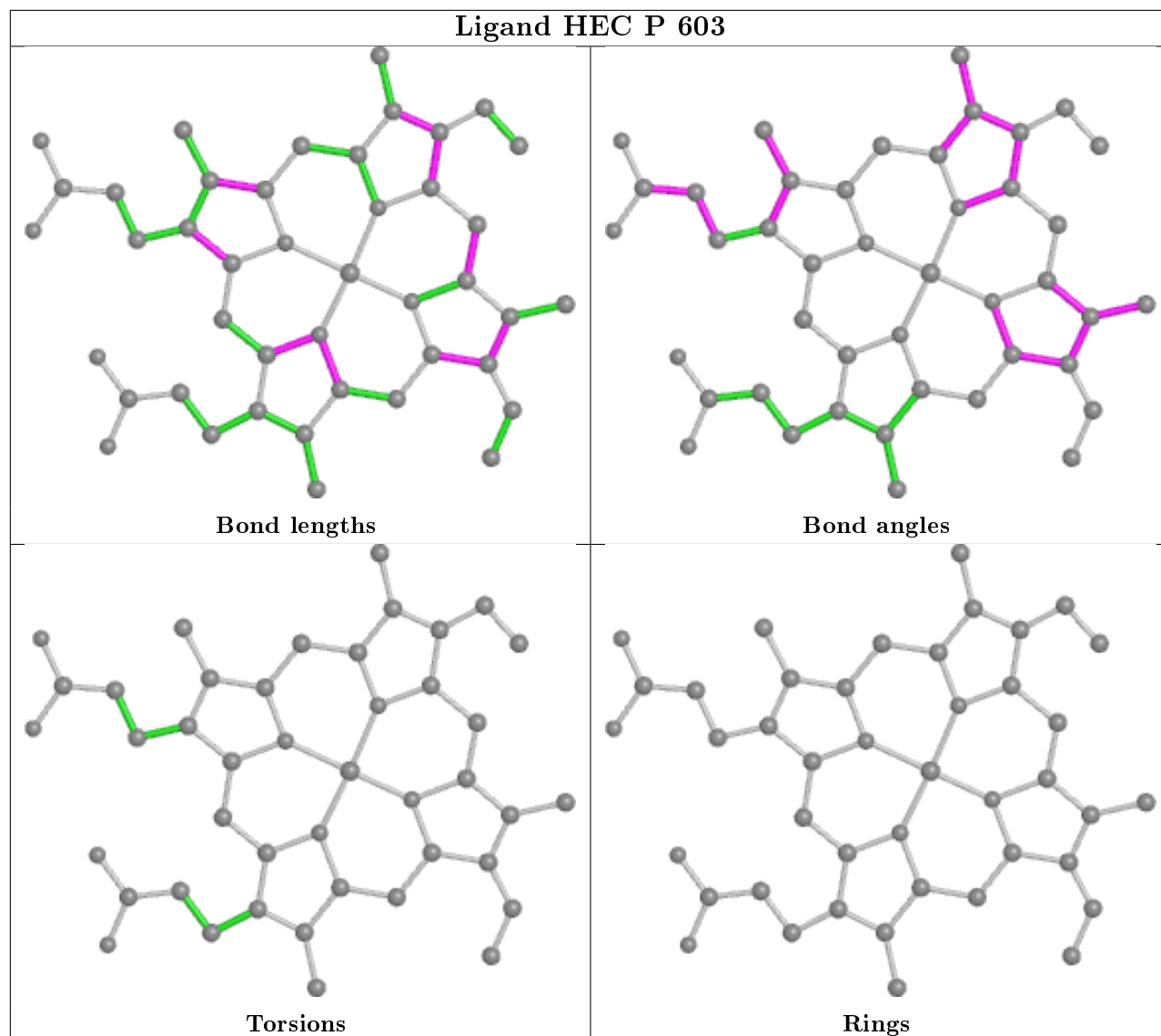


## Ligand HEC F 600

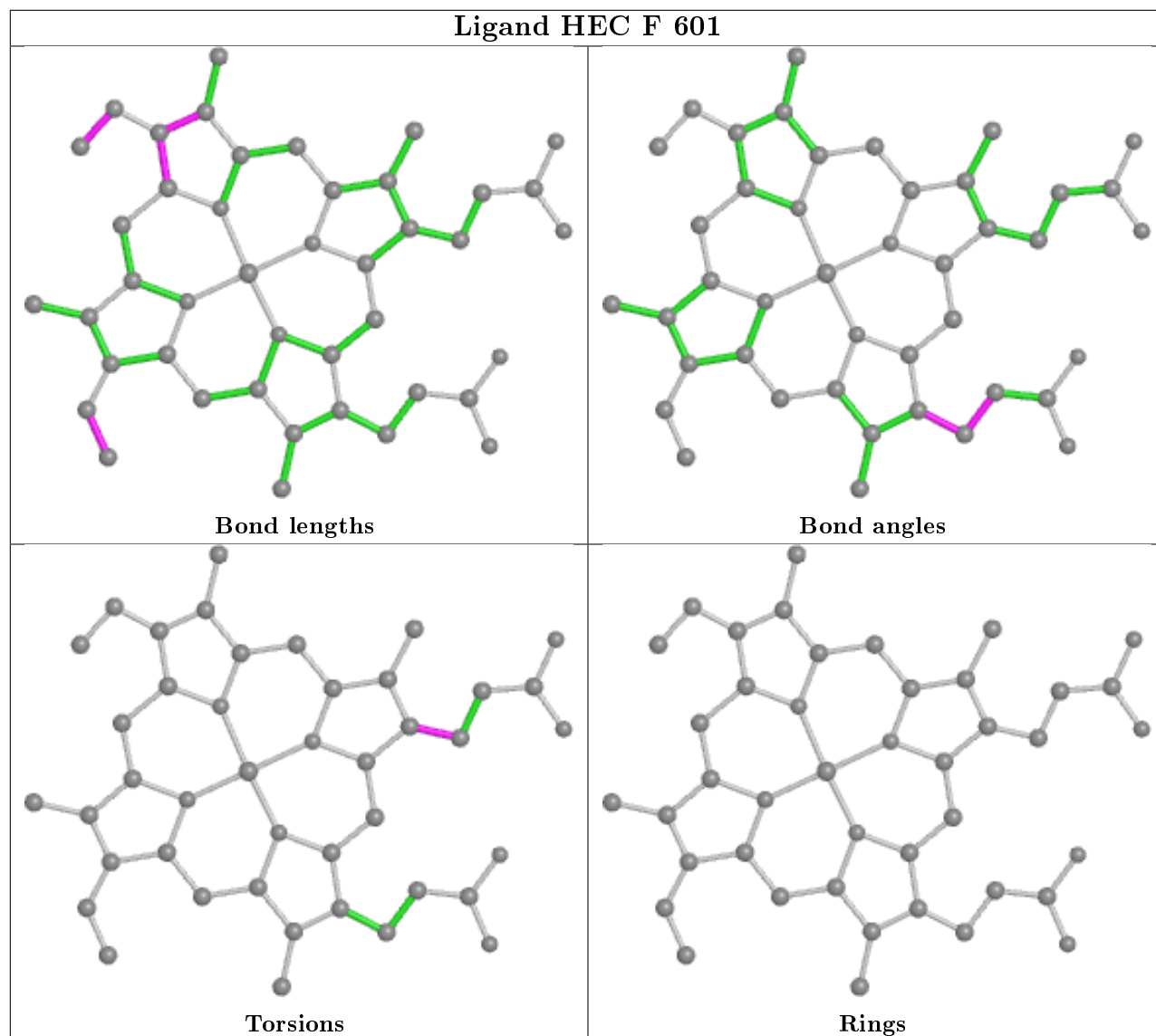


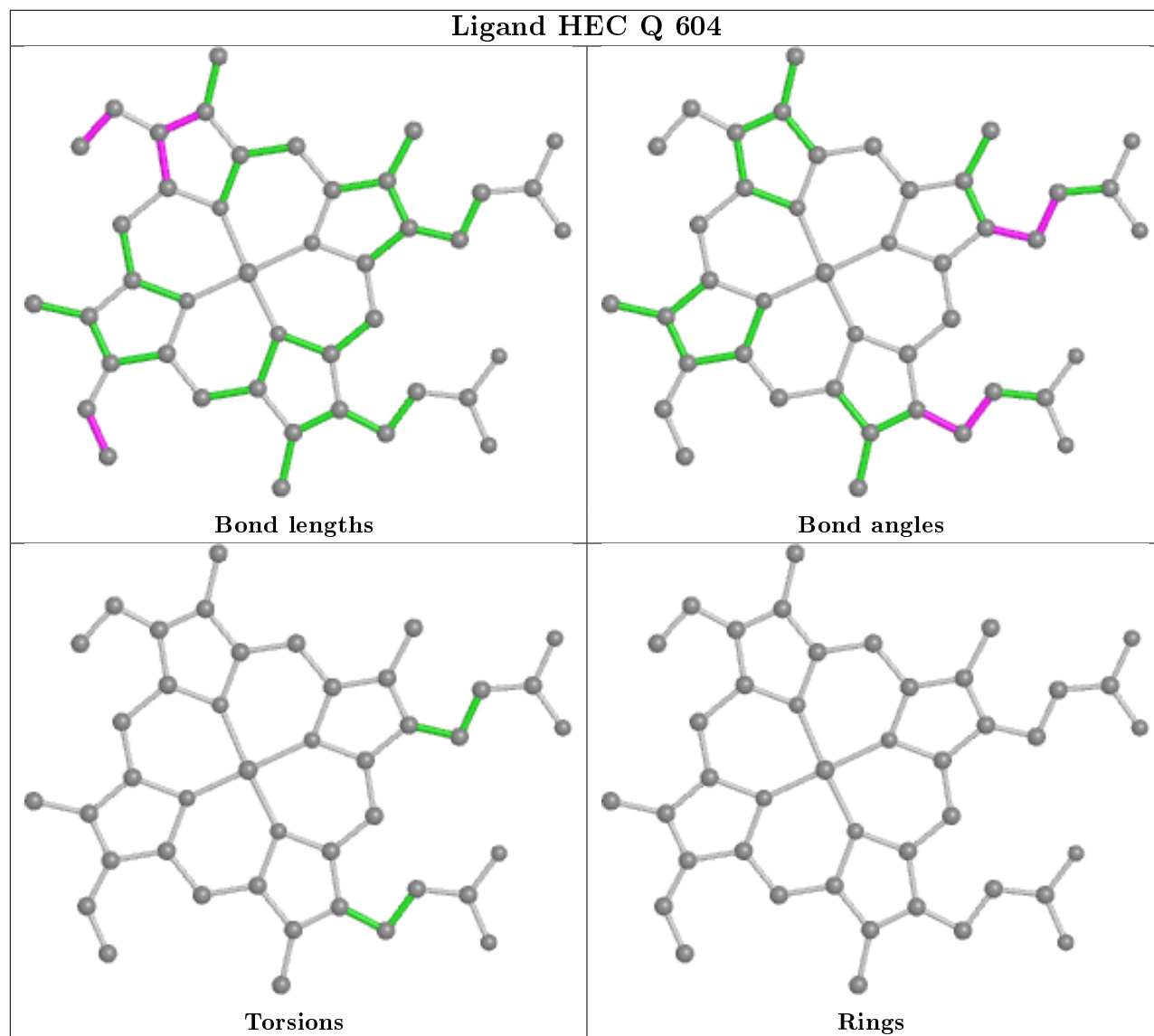
## Ligand HEC P 601

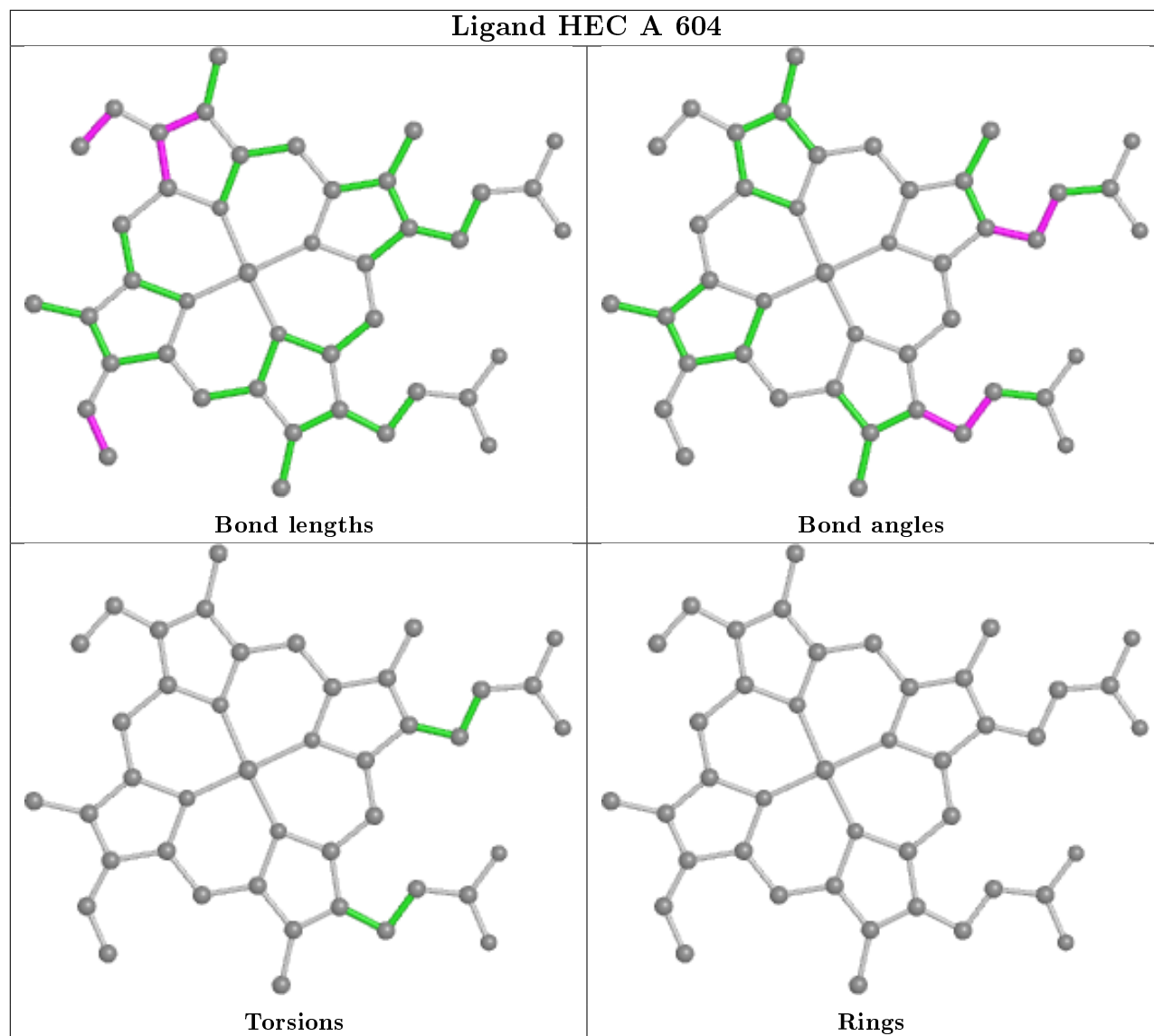




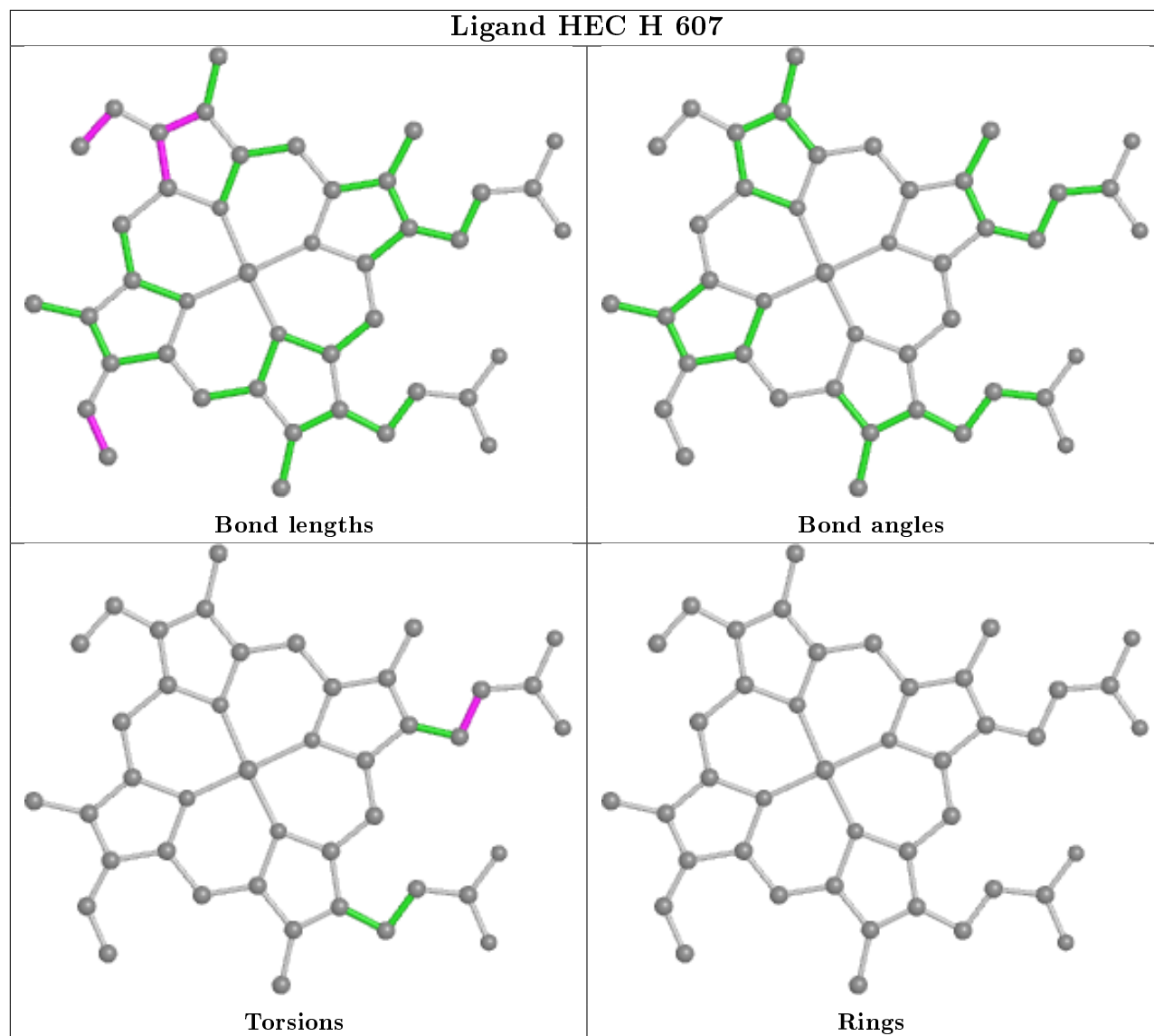
## Ligand HEC F 601



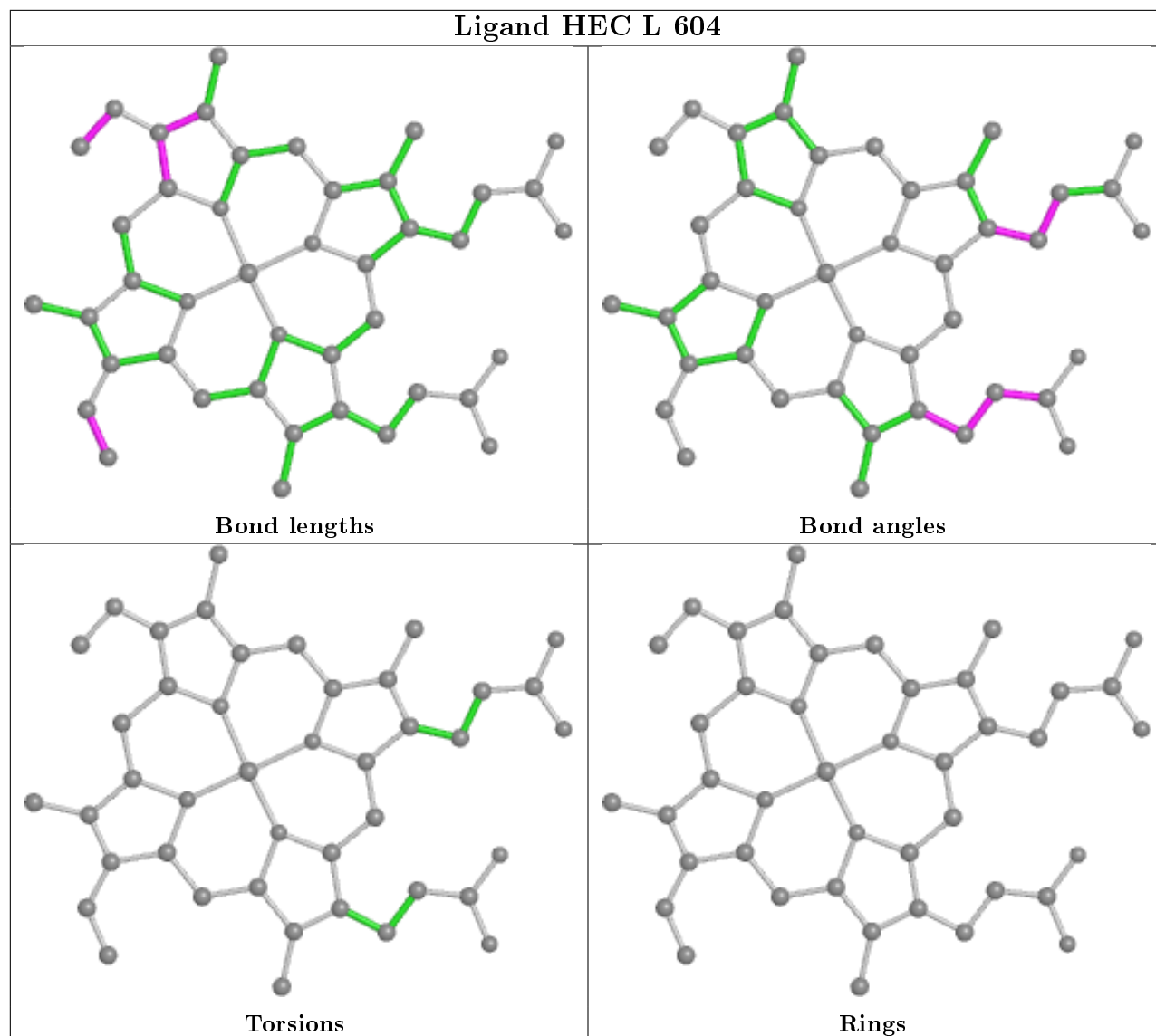


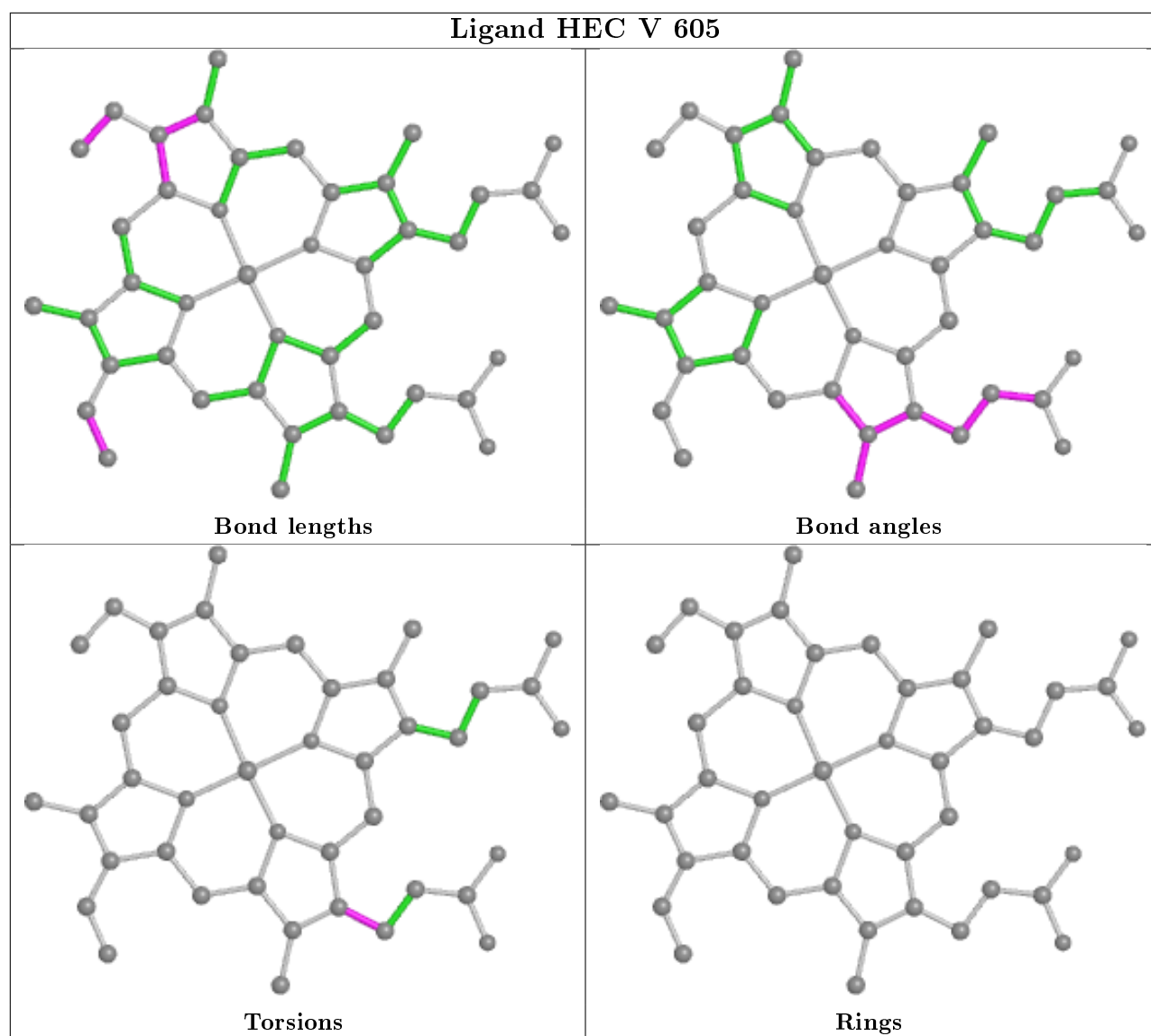






## Ligand HEC L 604





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	531/582 (91%)	0.30	4 (0%) 86 81	39, 59, 87, 153	0
1	B	531/582 (91%)	0.31	4 (0%) 86 81	39, 57, 81, 173	0
1	C	531/582 (91%)	0.23	1 (0%) 95 94	40, 54, 84, 123	0
1	D	531/582 (91%)	0.30	1 (0%) 95 94	42, 68, 100, 140	0
1	E	531/582 (91%)	0.51	9 (1%) 70 63	39, 69, 104, 165	0
1	F	531/582 (91%)	0.58	14 (2%) 56 46	43, 76, 108, 158	0
1	G	531/582 (91%)	0.19	2 (0%) 92 91	29, 41, 64, 139	0
1	H	531/582 (91%)	0.22	1 (0%) 95 94	29, 39, 63, 156	0
1	I	527/582 (90%)	0.11	0 100 100	27, 38, 57, 104	0
1	J	531/582 (91%)	0.20	2 (0%) 92 91	29, 42, 66, 166	0
1	K	531/582 (91%)	0.28	6 (1%) 80 75	32, 44, 70, 159	0
1	L	531/582 (91%)	0.28	3 (0%) 89 86	32, 45, 73, 157	0
1	M	531/582 (91%)	0.34	3 (0%) 89 86	37, 54, 84, 150	0
1	N	531/582 (91%)	0.39	9 (1%) 70 63	37, 58, 85, 157	0
1	O	531/582 (91%)	0.24	5 (0%) 84 80	37, 51, 77, 133	0
1	P	531/582 (91%)	0.21	4 (0%) 86 81	37, 51, 72, 124	0
1	Q	531/582 (91%)	0.30	4 (0%) 86 81	34, 57, 82, 124	0
1	R	531/582 (91%)	0.23	1 (0%) 95 94	34, 52, 78, 142	0
1	S	531/582 (91%)	0.80	44 (8%) 11 6	51, 80, 111, 158	0
1	T	531/582 (91%)	0.60	21 (3%) 38 28	50, 74, 107, 184	0
1	U	531/582 (91%)	0.73	37 (6%) 16 9	50, 80, 111, 150	0
1	V	531/582 (91%)	0.83	47 (8%) 9 5	52, 79, 108, 161	0
1	W	531/582 (91%)	0.78	29 (5%) 25 16	50, 80, 105, 163	0
1	X	531/582 (91%)	0.76	33 (6%) 20 13	56, 83, 111, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
2	Y	86/114 (75%)	0.41	3 (3%) 44 34	38, 54, 76, 105	0
2	Z	86/114 (75%)	1.63	22 (25%) 0 0	76, 96, 128, 192	0
2	a	86/114 (75%)	0.82	8 (9%) 8 4	64, 87, 116, 166	0
2	b	86/114 (75%)	0.82	4 (4%) 31 22	61, 83, 118, 167	0
2	c	86/114 (75%)	0.63	5 (5%) 23 15	58, 76, 101, 166	0
2	d	86/114 (75%)	0.55	4 (4%) 31 22	54, 68, 107, 152	0
2	e	86/114 (75%)	0.88	4 (4%) 31 22	57, 76, 109, 155	0
2	f	86/114 (75%)	1.24	16 (18%) 1 1	71, 96, 131, 168	0
2	g	86/114 (75%)	0.78	6 (6%) 16 9	68, 82, 114, 179	0
2	h	86/114 (75%)	0.99	10 (11%) 4 2	82, 96, 130, 166	0
2	i	86/114 (75%)	1.60	26 (30%) 0 0	85, 107, 137, 185	0
2	j	86/114 (75%)	1.10	15 (17%) 1 1	96, 109, 147, 178	0
All	All	13772/15336 (89%)	0.45	407 (2%) 50 40	27, 60, 104, 192	0

All (407) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Z	111	SER	18.0
1	T	563	HIS	12.2
1	B	563	HIS	9.7
2	a	111	SER	9.5
1	W	563	HIS	9.4
2	i	111	SER	9.0
2	e	111	SER	9.0
1	T	562	SER	8.0
1	L	563	HIS	7.9
2	g	111	SER	7.7
1	V	561	GLY	7.5
2	f	111	SER	7.3
1	E	562	SER	7.1
2	e	109	HIS	7.1
1	V	563	HIS	7.1
1	K	563	HIS	6.9
1	J	563	HIS	6.8
2	d	111	SER	6.7
2	h	111	SER	6.6
1	L	562	SER	6.5
1	S	563	HIS	6.3

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Mol	Chain	Res	Type	RSRZ
2	b	109	HIS	6.3
1	N	563	HIS	6.0
1	A	563	HIS	5.8
2	j	111	SER	5.7
2	Z	110	PRO	5.7
2	h	110	PRO	5.7
2	f	109	HIS	5.5
1	N	562	SER	5.5
1	V	562	SER	5.5
2	c	111	SER	5.5
1	U	563	HIS	5.2
2	f	107	ALA	5.2
1	M	563	HIS	5.1
1	N	560	ALA	5.1
1	X	33	VAL	5.0
2	a	109	HIS	5.0
2	b	110	PRO	4.9
1	T	36	ILE	4.9
1	X	563	HIS	4.8
2	a	110	PRO	4.8
1	E	563	HIS	4.7
2	Y	111	SER	4.6
2	c	110	PRO	4.6
1	F	563	HIS	4.6
1	U	560	ALA	4.5
1	W	441	VAL	4.4
1	S	562	SER	4.4
1	X	34	GLU	4.3
2	b	111	SER	4.3
2	j	108	ARG	4.3
1	D	563	HIS	4.3
1	J	562	SER	4.2
1	E	561	GLY	4.2
2	i	108	ARG	4.2
2	f	110	PRO	4.1
1	U	558	ILE	4.1
1	U	562	SER	4.1
1	S	37	THR	4.1
1	N	558	ILE	4.0
2	h	109	HIS	3.9
1	T	433	VAL	3.9
2	Y	110	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
2	i	97	LEU	3.9
1	T	33	VAL	3.8
1	H	563	HIS	3.8
2	d	110	PRO	3.8
1	S	46	GLY	3.8
1	W	562	SER	3.8
1	X	57	VAL	3.8
1	A	562	SER	3.8
1	S	508	TRP	3.8
2	f	38	ILE	3.7
2	f	80	HIS	3.7
1	X	294	GLY	3.7
2	Z	37	ALA	3.7
2	g	108	ARG	3.7
1	V	362	VAL	3.7
2	a	108	ARG	3.6
2	i	36	THR	3.6
2	i	89	VAL	3.5
1	U	441	VAL	3.5
1	F	58	PHE	3.4
2	i	73	TYR	3.4
2	e	108	ARG	3.4
2	j	110	PRO	3.4
1	V	441	VAL	3.4
2	Z	89	VAL	3.4
2	h	84	SER	3.4
1	O	33	VAL	3.3
1	U	476	VAL	3.3
1	E	558	ILE	3.3
2	h	108	ARG	3.3
1	B	562	SER	3.3
1	E	559	THR	3.3
1	U	561	GLY	3.3
1	U	373	PHE	3.3
1	V	560	ALA	3.2
2	f	108	ARG	3.2
1	V	437	CYS	3.2
1	F	33	VAL	3.2
1	S	524	LYS	3.2
1	P	563	HIS	3.2
2	f	70	PRO	3.2
1	U	410	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
2	i	77	VAL	3.2
1	K	562	SER	3.2
2	Z	90	SER	3.2
2	f	89	VAL	3.1
2	c	108	ARG	3.1
2	i	75	ILE	3.1
1	X	46	GLY	3.1
1	X	91	ALA	3.1
1	E	33	VAL	3.1
1	V	33	VAL	3.1
2	f	68	LEU	3.1
2	j	98	PHE	3.1
1	U	445	GLN	3.1
2	g	110	PRO	3.1
1	F	455	GLY	3.1
1	X	562	SER	3.0
2	a	80	HIS	3.0
1	X	99	TYR	3.0
2	Z	33	LEU	3.0
1	T	34	GLU	3.0
2	j	42	THR	3.0
1	V	253	GLY	3.0
1	V	436	LEU	3.0
2	Z	101	LEU	3.0
2	c	80	HIS	3.0
1	V	89	LEU	3.0
1	F	560	ALA	3.0
1	S	324	ALA	3.0
1	U	453	ALA	3.0
2	e	110	PRO	3.0
1	X	402	TRP	3.0
1	P	562	SER	3.0
1	W	475	ASN	2.9
1	W	188	ILE	2.9
1	R	563	HIS	2.9
1	S	549	ILE	2.9
1	S	372	THR	2.9
1	U	357	ALA	2.9
1	X	531	PRO	2.9
2	d	109	HIS	2.9
2	i	45	VAL	2.9
1	W	218	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	W	372	THR	2.8
1	W	458	ASN	2.8
1	S	85	PHE	2.8
1	S	89	LEU	2.8
2	g	109	HIS	2.8
1	S	55	GLY	2.8
1	S	72	ASP	2.8
1	S	425	PHE	2.8
1	S	413	GLU	2.8
2	f	74	ALA	2.8
1	V	215	GLY	2.7
1	V	559	THR	2.7
1	K	558	ILE	2.7
1	F	122	VAL	2.7
1	K	559	THR	2.7
2	Z	109	HIS	2.7
1	V	85	PHE	2.7
1	V	404	LEU	2.7
1	T	497	TRP	2.7
1	V	442	GLY	2.7
2	Z	62	GLY	2.7
2	i	31	ALA	2.7
1	V	257	ARG	2.7
1	X	78	TYR	2.7
1	X	323	MET	2.7
2	Z	108	ARG	2.7
1	G	563	HIS	2.6
2	h	26	TYR	2.6
1	W	249	THR	2.6
1	S	558	ILE	2.6
1	X	270	VAL	2.6
2	i	85	ALA	2.6
1	W	549	ILE	2.6
2	h	44	ILE	2.6
1	T	466	SER	2.6
1	V	457	TRP	2.6
1	S	513	THR	2.6
1	O	563	HIS	2.6
2	Z	75	ILE	2.6
1	T	486	LEU	2.6
2	j	31	ALA	2.6
1	V	454	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	U	33	VAL	2.6
2	j	92	GLU	2.6
1	W	39	TRP	2.6
1	E	544	GLU	2.5
2	j	109	HIS	2.5
1	W	387	PRO	2.5
1	S	392	LEU	2.5
1	U	257	ARG	2.5
2	f	63	THR	2.5
2	i	109	HIS	2.5
2	Z	36	THR	2.5
1	N	210	PRO	2.5
1	W	57	VAL	2.5
1	X	440	SER	2.5
1	V	427	MET	2.5
1	V	259	TRP	2.5
2	i	26	TYR	2.5
1	E	554	LYS	2.5
2	j	91	LEU	2.5
1	S	33	VAL	2.5
1	W	427	MET	2.5
1	T	320	GLY	2.5
2	Z	46	GLY	2.5
1	V	316	TYR	2.5
2	i	38	ILE	2.5
2	i	110	PRO	2.4
2	Z	65	VAL	2.4
2	f	28	VAL	2.4
1	S	38	HIS	2.4
1	Q	210	PRO	2.4
1	Q	561	GLY	2.4
1	U	553	LEU	2.4
1	V	513	THR	2.4
2	i	30	PRO	2.4
1	X	85	PHE	2.4
1	X	441	VAL	2.4
1	F	61	GLY	2.4
1	S	560	ALA	2.4
1	T	266	LEU	2.4
2	h	33	LEU	2.4
1	V	476	VAL	2.4
2	f	51	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	S	398	GLY	2.4
1	U	557	GLY	2.4
1	V	497	TRP	2.4
1	W	62	LEU	2.4
1	S	51	PRO	2.4
1	U	443	TYR	2.4
1	U	61	GLY	2.4
2	i	51	VAL	2.4
1	V	252	TRP	2.4
1	X	504	LYS	2.4
1	W	365	ALA	2.4
1	N	526	ILE	2.4
1	X	215	GLY	2.4
1	S	429	ASN	2.4
2	i	84	SER	2.4
2	g	38	ILE	2.4
1	X	39	TRP	2.4
1	G	42	HIS	2.3
1	U	468	GLY	2.3
1	O	39	TRP	2.3
1	X	497	TRP	2.3
2	Z	44	ILE	2.3
1	N	540	HIS	2.3
1	S	438	PHE	2.3
1	V	61	GLY	2.3
2	a	98	PHE	2.3
2	j	41	GLY	2.3
1	B	44	VAL	2.3
1	S	435	ARG	2.3
2	j	107	ALA	2.3
1	S	36	ILE	2.3
1	S	373	PHE	2.3
1	U	438	PHE	2.3
2	Z	66	PHE	2.3
1	F	44	VAL	2.3
1	U	554	LYS	2.3
1	F	337	ARG	2.3
1	N	545	GLU	2.3
1	S	534	GLY	2.3
1	X	250	CYS	2.3
1	T	452	MET	2.3
2	h	37	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	U	559	THR	2.3
1	U	403	SER	2.3
1	S	337	ARG	2.3
2	f	41	GLY	2.3
1	P	441	VAL	2.3
1	U	397	SER	2.3
1	W	298	GLN	2.3
1	X	210	PRO	2.3
2	i	71	GLY	2.3
1	F	554	LYS	2.3
1	A	315	VAL	2.3
1	O	40	VAL	2.3
1	N	554	LYS	2.3
1	X	274	ASN	2.2
2	j	96	ILE	2.2
1	F	429	ASN	2.2
1	F	423	GLY	2.2
1	V	365	ALA	2.2
1	X	442	GLY	2.2
1	V	264	ILE	2.2
1	P	262	TYR	2.2
2	j	26	TYR	2.2
1	T	461	THR	2.2
2	g	90	SER	2.2
1	S	116	PHE	2.2
1	X	438	PHE	2.2
1	W	445	GLN	2.2
1	X	66	TYR	2.2
2	d	26	TYR	2.2
1	E	323	MET	2.2
1	W	270	VAL	2.2
1	X	561	GLY	2.2
1	Q	563	HIS	2.2
1	S	188	ILE	2.2
1	V	254	LYS	2.2
2	j	78	HIS	2.2
1	O	451	GLY	2.2
1	V	544	GLU	2.2
1	U	513	THR	2.2
1	V	317	THR	2.2
1	W	440	SER	2.2
2	Z	49	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	i	99	VAL	2.2
1	V	206	ILE	2.2
1	W	466	SER	2.2
2	Z	41	GLY	2.2
1	S	204	TRP	2.2
1	X	423	GLY	2.1
1	U	498	GLN	2.1
1	V	198	ALA	2.1
1	S	427	MET	2.1
1	T	254	LYS	2.1
1	V	540	HIS	2.1
1	V	131	GLY	2.1
2	i	98	PHE	2.1
1	B	560	ALA	2.1
1	W	241	ALA	2.1
1	X	65	LYS	2.1
1	U	466	SER	2.1
1	V	461	THR	2.1
1	S	548	TYR	2.1
1	X	425	PHE	2.1
2	Z	91	LEU	2.1
1	U	460	ALA	2.1
2	Z	70	PRO	2.1
2	c	29	LYS	2.1
1	U	409	TYR	2.1
1	S	547	GLU	2.1
1	W	399	GLN	2.1
1	S	476	VAL	2.1
1	T	294	GLY	2.1
1	V	315	VAL	2.1
1	V	433	VAL	2.1
2	i	29	LYS	2.1
2	j	89	VAL	2.1
1	F	409	TYR	2.1
1	S	218	PHE	2.1
1	S	436	LEU	2.1
2	a	55	GLU	2.1
1	V	363	LYS	2.1
1	F	476	VAL	2.1
2	i	34	TRP	2.1
1	U	461	THR	2.1
1	V	66	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	V	459	ASP	2.1
1	W	299	TYR	2.1
2	i	72	THR	2.1
1	V	364	ASP	2.1
2	i	37	ALA	2.1
1	T	474	VAL	2.1
1	W	209	PRO	2.1
1	U	355	LEU	2.1
1	V	453	ALA	2.1
2	i	44	ILE	2.1
1	M	389	PRO	2.1
1	W	97	PRO	2.1
1	Q	562	SER	2.1
1	X	486	LEU	2.1
1	U	261	ALA	2.1
1	V	409	TYR	2.1
1	W	528	ASP	2.1
1	K	561	GLY	2.1
1	K	293	VAL	2.1
1	S	44	VAL	2.1
1	T	57	VAL	2.1
1	W	272	GLN	2.0
1	S	86	TRP	2.0
1	T	508	TRP	2.0
2	Z	34	TRP	2.0
1	X	262	TYR	2.0
1	A	211	GLY	2.0
1	U	469	MET	2.0
1	V	375	VAL	2.0
1	U	473	LEU	2.0
1	C	156	GLY	2.0
1	L	560	ALA	2.0
2	h	96	ILE	2.0
1	T	265	GLY	2.0
1	W	321	MET	2.0
1	S	380	LEU	2.0
1	T	392	LEU	2.0
2	f	103	LEU	2.0
2	Y	109	HIS	2.0
1	S	71	LYS	2.0
1	U	463	SER	2.0
2	a	75	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	U	544	GLU	2.0
1	V	261	ALA	2.0
1	M	309	VAL	2.0
2	b	66	PHE	2.0
1	U	365	ALA	2.0
1	S	259	TRP	2.0
2	Z	77	VAL	2.0
1	T	41	PRO	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	K	X	612	1/1	0.33	0.16	93,93,93,93	0
4	SO4	H	613	5/5	0.55	0.26	116,120,125,127	0
5	GOL	A	614	6/6	0.56	0.29	82,89,90,91	0
4	SO4	X	610	5/5	0.61	0.23	158,161,161,162	0
6	K	H	616	1/1	0.62	0.14	82,82,82,82	0
4	SO4	M	611	5/5	0.64	0.27	129,131,136,137	0
6	K	Q	612	1/1	0.67	0.15	96,96,96,96	0
4	SO4	S	609	5/5	0.69	0.18	129,133,135,135	0
5	GOL	J	612	6/6	0.69	0.28	58,64,67,67	0
6	K	K	616	1/1	0.69	0.11	85,85,85,85	0
4	SO4	V	611	5/5	0.70	0.18	131,133,134,135	0
4	SO4	G	612	5/5	0.71	0.28	120,124,126,126	0
5	GOL	A	612	6/6	0.71	0.25	76,78,79,81	0
4	SO4	L	610	5/5	0.71	0.24	142,143,145,150	0
5	GOL	H	615	6/6	0.76	0.68	78,86,90,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	G	611	5/5	0.76	0.41	139,139,143,149	0
4	SO4	H	612	5/5	0.77	0.23	110,113,116,118	0
5	GOL	A	613	6/6	0.78	0.27	74,77,78,79	0
4	SO4	H	610	5/5	0.79	0.17	106,111,113,114	0
4	SO4	U	611	5/5	0.80	0.19	127,130,131,133	0
4	SO4	X	611	5/5	0.80	0.33	139,139,141,144	0
4	SO4	Q	611	5/5	0.80	0.16	112,118,119,119	0
4	SO4	c	201	5/5	0.81	0.15	132,133,135,135	0
4	SO4	F	610	5/5	0.81	0.21	135,136,139,139	0
5	GOL	G	615	6/6	0.81	0.23	61,67,68,68	0
4	SO4	Y	201	5/5	0.82	0.22	136,136,137,141	0
4	SO4	C	610	5/5	0.82	0.40	143,145,147,149	0
4	SO4	I	611	5/5	0.82	0.17	115,115,116,117	0
4	SO4	a	201	5/5	0.83	0.23	139,139,140,140	0
5	GOL	I	614	6/6	0.83	0.71	67,78,80,83	0
4	SO4	M	612	5/5	0.83	0.18	121,122,123,125	0
5	GOL	K	612	6/6	0.83	0.36	76,80,86,90	0
4	SO4	N	611	5/5	0.83	0.18	123,126,127,129	0
4	SO4	L	611	5/5	0.84	0.14	116,119,121,122	0
4	SO4	Y	202	5/5	0.84	0.17	130,130,132,136	0
4	SO4	O	610	5/5	0.84	0.21	109,111,112,112	0
4	SO4	M	610	5/5	0.84	0.49	134,135,138,139	0
4	SO4	I	612	5/5	0.85	0.20	120,121,124,125	0
4	SO4	C	611	5/5	0.85	0.31	111,111,114,116	0
4	SO4	L	612	5/5	0.85	0.18	110,112,115,115	0
4	SO4	A	611	5/5	0.86	0.15	117,118,119,120	0
5	GOL	D	610	6/6	0.86	0.25	86,88,88,89	0
4	SO4	Q	610	5/5	0.87	0.34	133,136,137,137	0
4	SO4	O	611	5/5	0.87	0.13	114,114,119,120	0
4	SO4	G	614	5/5	0.87	0.17	91,94,95,95	0
4	SO4	J	611	5/5	0.87	0.49	118,118,120,123	0
4	SO4	J	610	5/5	0.88	0.20	99,100,101,103	0
5	GOL	I	615	6/6	0.88	0.20	51,55,56,57	0
4	SO4	W	609	5/5	0.88	0.16	114,118,119,124	0
4	SO4	X	609	5/5	0.88	0.17	107,108,110,112	0
4	SO4	R	611	5/5	0.89	0.52	142,143,145,147	0
4	SO4	E	610	5/5	0.90	0.14	103,105,106,109	0
5	GOL	I	613	6/6	0.91	0.23	59,64,66,73	0
5	GOL	H	614	6/6	0.91	0.74	56,63,64,68	0
4	SO4	F	609	5/5	0.91	0.12	95,99,102,104	0
4	SO4	K	611	5/5	0.91	0.22	102,104,105,105	0
4	SO4	U	610	5/5	0.91	0.19	99,101,103,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	J	613	6/6	0.91	0.27	58,61,62,63	0
4	SO4	B	609	5/5	0.92	0.46	116,117,119,124	0
4	SO4	B	610	5/5	0.93	0.15	88,89,91,91	0
4	SO4	C	609	5/5	0.93	0.16	96,102,106,108	0
4	SO4	V	610	5/5	0.93	0.16	94,97,98,99	0
5	GOL	K	613	6/6	0.93	0.23	45,51,52,53	0
4	SO4	H	609	5/5	0.93	0.15	78,81,82,83	0
4	SO4	N	610	5/5	0.93	0.16	101,105,107,109	0
4	SO4	P	609	5/5	0.93	0.17	95,95,96,98	0
5	GOL	L	613	6/6	0.94	0.31	56,59,60,61	0
4	SO4	H	611	5/5	0.94	0.15	97,100,101,105	0
4	SO4	T	609	5/5	0.94	0.10	98,100,102,102	0
5	GOL	K	615	6/6	0.94	0.65	53,55,58,59	0
4	SO4	L	609	5/5	0.94	0.13	91,94,94,97	0
4	SO4	O	609	5/5	0.94	0.13	77,78,80,82	0
4	SO4	Q	609	5/5	0.94	0.09	84,87,88,89	0
4	SO4	A	610	5/5	0.94	0.14	73,77,79,80	0
4	SO4	G	610	5/5	0.94	0.42	104,106,107,108	0
4	SO4	D	609	5/5	0.95	0.11	82,82,84,87	0
4	SO4	K	610	5/5	0.95	0.16	84,84,86,88	0
3	HEC	X	606	43/43	0.95	0.25	69,83,87,90	0
4	SO4	R	610	5/5	0.95	0.12	75,77,79,79	0
3	HEC	X	605	43/43	0.95	0.31	79,86,97,100	0
3	HEC	V	602	43/43	0.95	0.24	68,73,87,100	0
5	GOL	G	616	6/6	0.95	0.19	37,40,41,41	0
5	GOL	K	614	6/6	0.95	0.65	49,56,57,59	0
3	HEC	A	606	43/43	0.96	0.26	45,60,73,78	0
3	HEC	U	602	43/43	0.96	0.27	60,69,94,116	0
3	HEC	S	604	43/43	0.96	0.23	59,66,75,86	0
3	HEC	H	602	43/43	0.96	0.23	35,44,64,77	0
3	HEC	T	607	43/43	0.96	0.26	49,57,60,62	0
3	HEC	U	606	43/43	0.96	0.29	65,72,88,96	0
3	HEC	W	605	43/43	0.96	0.28	74,81,87,89	0
3	HEC	X	602	43/43	0.96	0.24	69,75,91,106	0
3	HEC	P	602	43/43	0.96	0.20	41,45,63,76	0
3	HEC	T	602	43/43	0.96	0.23	59,68,83,97	0
3	HEC	Q	604	43/43	0.96	0.25	54,60,68,76	0
3	HEC	E	605	43/43	0.96	0.23	53,63,75,82	0
3	HEC	W	603	43/43	0.96	0.27	67,77,85,89	0
3	HEC	U	600	43/43	0.96	0.18	58,64,71,72	0
3	HEC	Q	602	43/43	0.96	0.23	64,68,88,97	0
3	HEC	N	606	43/43	0.96	0.22	47,51,60,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	HEC	S	605	43/43	0.96	0.30	63,72,82,83	0
3	HEC	V	603	43/43	0.96	0.25	51,65,82,86	0
3	HEC	U	604	43/43	0.96	0.23	52,60,72,81	0
3	HEC	B	602	43/43	0.96	0.22	49,56,80,99	0
4	SO4	S	610	5/5	0.96	0.09	92,93,94,95	0
3	HEC	F	603	43/43	0.96	0.22	62,70,74,79	0
3	HEC	E	606	43/43	0.96	0.26	55,60,68,75	0
4	SO4	J	609	5/5	0.96	0.19	77,79,80,80	0
3	HEC	S	603	43/43	0.96	0.25	72,77,88,94	0
3	HEC	F	602	43/43	0.96	0.23	64,75,85,96	0
4	SO4	M	609	5/5	0.96	0.11	89,90,91,92	0
4	SO4	G	609	5/5	0.96	0.12	72,72,74,74	0
3	HEC	S	602	43/43	0.96	0.23	63,71,86,104	0
3	HEC	W	602	43/43	0.96	0.23	54,58,83,99	0
3	HEC	E	602	43/43	0.96	0.24	48,53,73,94	0
3	HEC	X	604	43/43	0.96	0.21	63,73,78,80	0
3	HEC	V	604	43/43	0.96	0.28	59,71,81,85	0
3	HEC	A	604	43/43	0.96	0.22	47,50,61,73	0
3	HEC	C	600	43/43	0.97	0.22	49,52,56,58	0
3	HEC	E	600	43/43	0.97	0.21	39,41,53,55	0
3	HEC	T	600	43/43	0.97	0.20	53,60,68,69	0
3	HEC	L	600	43/43	0.97	0.22	41,44,50,51	0
3	HEC	F	605	43/43	0.97	0.25	54,60,69,78	0
3	HEC	S	601	43/43	0.97	0.25	67,70,81,85	0
3	HEC	X	603	43/43	0.97	0.24	70,80,103,109	0
3	HEC	K	600	43/43	0.97	0.22	38,40,46,55	0
3	HEC	C	604	43/43	0.97	0.22	42,47,53,60	0
3	HEC	Q	607	43/43	0.97	0.20	36,40,44,46	0
3	HEC	R	603	43/43	0.97	0.19	37,43,48,52	0
3	HEC	W	604	43/43	0.97	0.21	50,57,67,74	0
3	HEC	A	607	43/43	0.97	0.21	41,45,50,53	0
3	HEC	T	606	43/43	0.97	0.27	52,56,65,74	0
3	HEC	S	600	43/43	0.97	0.22	60,65,73,75	0
3	HEC	N	600	43/43	0.97	0.25	46,49,57,63	0
3	HEC	N	601	43/43	0.97	0.23	41,44,55,65	0
3	HEC	P	606	43/43	0.97	0.23	43,47,48,49	0
3	HEC	L	602	43/43	0.97	0.22	42,45,57,72	0
3	HEC	M	607	43/43	0.97	0.23	36,39,52,62	0
3	HEC	N	602	43/43	0.97	0.23	48,52,75,92	0
3	HEC	F	601	43/43	0.97	0.25	51,55,68,70	0
3	HEC	P	604	43/43	0.97	0.22	36,40,52,63	0
3	HEC	T	604	43/43	0.97	0.23	59,65,70,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	HEC	E	603	43/43	0.97	0.23	56,66,92,96	0
3	HEC	D	602	43/43	0.97	0.19	45,48,65,79	0
3	HEC	U	601	43/43	0.97	0.23	54,57,67,73	0
3	HEC	W	606	43/43	0.97	0.31	64,76,88,96	0
3	HEC	Q	600	43/43	0.97	0.23	47,52,59,65	0
3	HEC	S	607	43/43	0.97	0.24	51,57,59,60	0
3	HEC	W	607	43/43	0.97	0.25	63,68,71,71	0
3	HEC	I	602	43/43	0.97	0.21	37,42,59,70	0
3	HEC	B	604	43/43	0.97	0.21	44,51,62,67	0
3	HEC	O	604	43/43	0.97	0.21	34,41,50,60	0
3	HEC	U	603	43/43	0.97	0.24	61,72,83,85	0
3	HEC	V	600	43/43	0.97	0.23	67,70,84,91	0
3	HEC	A	603	43/43	0.97	0.22	54,66,71,73	0
3	HEC	O	602	43/43	0.97	0.22	47,51,72,91	0
3	HEC	F	606	43/43	0.97	0.24	50,56,67,76	0
3	HEC	D	605	43/43	0.97	0.26	48,53,61,66	0
3	HEC	Q	601	43/43	0.97	0.22	46,50,54,56	0
3	HEC	F	607	43/43	0.97	0.27	49,56,57,60	0
3	HEC	V	601	43/43	0.97	0.20	52,63,65,67	0
3	HEC	M	604	43/43	0.97	0.24	40,43,51,62	0
3	HEC	M	602	43/43	0.97	0.23	44,48,72,89	0
3	HEC	A	600	43/43	0.97	0.22	47,49,56,59	0
3	HEC	C	602	43/43	0.97	0.21	45,48,66,80	0
3	HEC	O	603	43/43	0.97	0.20	40,44,49,51	0
3	HEC	T	605	43/43	0.97	0.24	54,60,74,76	0
3	HEC	C	603	43/43	0.97	0.22	44,48,58,63	0
3	HEC	E	607	43/43	0.97	0.27	47,54,60,62	0
3	HEC	E	604	43/43	0.97	0.21	40,45,53,63	0
3	HEC	M	605	43/43	0.97	0.27	36,38,46,51	0
3	HEC	D	600	43/43	0.97	0.22	54,60,68,74	0
3	HEC	O	601	43/43	0.97	0.23	40,44,49,56	0
3	HEC	V	607	43/43	0.97	0.29	54,66,69,70	0
3	HEC	K	604	43/43	0.97	0.20	36,41,49,57	0
3	HEC	P	607	43/43	0.97	0.22	38,48,52,54	0
3	HEC	C	605	43/43	0.97	0.22	38,43,53,57	0
3	HEC	G	604	43/43	0.97	0.23	31,34,49,57	0
3	HEC	Q	606	43/43	0.97	0.23	44,55,65,69	0
3	HEC	U	605	43/43	0.97	0.27	62,68,80,87	0
3	HEC	J	602	43/43	0.97	0.22	38,41,67,86	0
3	HEC	J	600	43/43	0.97	0.22	37,41,52,60	0
3	HEC	C	607	43/43	0.97	0.22	44,48,49,52	0
3	HEC	W	601	43/43	0.97	0.27	61,70,77,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	HEC	M	603	43/43	0.97	0.24	42,46,49,50	0
3	HEC	V	606	43/43	0.97	0.26	57,60,76,81	0
3	HEC	X	600	43/43	0.97	0.19	57,63,75,81	0
3	HEC	B	600	43/43	0.97	0.19	48,52,59,61	0
3	HEC	G	602	43/43	0.97	0.22	34,38,59,77	0
3	HEC	L	601	43/43	0.97	0.22	36,40,45,46	0
4	SO4	E	609	5/5	0.97	0.15	50,51,53,53	0
3	HEC	U	607	43/43	0.97	0.29	53,70,73,74	0
3	HEC	M	600	43/43	0.97	0.21	44,48,56,62	0
3	HEC	T	603	43/43	0.97	0.23	60,66,71,73	0
4	SO4	I	610	5/5	0.97	0.11	67,67,69,69	0
3	HEC	R	600	43/43	0.97	0.21	49,54,62,64	0
4	SO4	G	613	5/5	0.97	0.18	63,63,64,66	0
3	HEC	G	600	43/43	0.97	0.21	40,42,45,49	0
3	HEC	X	601	43/43	0.97	0.23	62,69,78,82	0
3	HEC	R	602	43/43	0.97	0.24	45,48,74,89	0
3	HEC	A	602	43/43	0.97	0.23	51,56,79,99	0
3	HEC	F	604	43/43	0.97	0.23	58,65,74,84	0
3	HEC	R	604	43/43	0.97	0.21	38,43,53,61	0
3	HEC	X	607	43/43	0.97	0.23	57,61,65,67	0
3	HEC	F	600	43/43	0.97	0.21	46,52,62,68	0
3	HEC	P	601	43/43	0.97	0.22	39,44,46,47	0
3	HEC	G	601	43/43	0.97	0.21	37,41,43,48	0
3	HEC	P	603	43/43	0.97	0.23	40,49,56,62	0
3	HEC	W	600	43/43	0.97	0.23	61,68,74,77	0
3	HEC	K	602	43/43	0.97	0.22	44,47,65,81	0
3	HEC	E	601	43/43	0.97	0.22	39,43,47,55	0
3	HEC	A	605	43/43	0.97	0.26	50,59,63,64	0
3	HEC	S	606	43/43	0.97	0.26	61,69,74,79	0
3	HEC	L	604	43/43	0.97	0.22	35,41,48,58	0
3	HEC	V	605	43/43	0.97	0.26	56,65,73,76	0
3	HEC	G	603	43/43	0.98	0.20	34,36,39,42	0
3	HEC	H	604	43/43	0.98	0.21	38,43,53,64	0
3	HEC	Q	603	43/43	0.98	0.23	52,55,58,59	0
3	HEC	O	607	43/43	0.98	0.23	34,37,38,39	0
3	HEC	J	607	43/43	0.98	0.22	28,30,33,37	0
3	HEC	I	603	43/43	0.98	0.21	30,33,37,39	0
3	HEC	B	605	43/43	0.98	0.22	42,45,53,59	0
3	HEC	P	600	43/43	0.98	0.20	44,46,51,53	0
3	HEC	R	605	43/43	0.98	0.19	35,40,45,46	0
3	HEC	G	607	43/43	0.98	0.21	30,31,34,34	0
3	HEC	P	605	43/43	0.98	0.23	43,46,49,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	HEC	O	605	43/43	0.98	0.21	36,41,49,52	0
3	HEC	T	601	43/43	0.98	0.22	55,58,61,63	0
3	HEC	N	605	43/43	0.98	0.24	48,52,66,73	0
3	HEC	R	607	43/43	0.98	0.22	37,38,43,48	0
3	HEC	J	605	43/43	0.98	0.23	32,38,43,47	0
3	HEC	N	604	43/43	0.98	0.23	42,47,56,59	0
3	HEC	H	605	43/43	0.98	0.23	28,32,34,35	0
3	HEC	A	601	43/43	0.98	0.23	44,47,53,54	0
3	HEC	I	604	43/43	0.98	0.22	36,38,51,58	0
3	HEC	J	606	43/43	0.98	0.23	33,39,41,46	0
3	HEC	Q	605	43/43	0.98	0.24	45,51,57,60	0
3	HEC	H	603	43/43	0.98	0.22	31,34,42,48	0
3	HEC	I	605	43/43	0.98	0.23	29,33,38,40	0
3	HEC	N	603	43/43	0.98	0.20	47,56,60,62	0
3	HEC	B	606	43/43	0.98	0.23	39,42,50,57	0
3	HEC	L	605	43/43	0.98	0.23	35,37,41,45	0
3	HEC	D	601	43/43	0.98	0.23	51,59,61,62	0
3	HEC	D	606	43/43	0.98	0.27	46,51,62,66	0
3	HEC	G	605	43/43	0.98	0.22	33,36,41,43	0
3	HEC	C	601	43/43	0.98	0.23	41,45,50,51	0
3	HEC	I	606	43/43	0.98	0.22	34,35,44,47	0
3	HEC	C	606	43/43	0.98	0.22	41,43,59,65	0
3	HEC	K	601	43/43	0.98	0.20	33,34,38,43	0
3	HEC	R	601	43/43	0.98	0.23	43,48,50,50	0
3	HEC	H	601	43/43	0.98	0.21	34,36,41,47	0
3	HEC	O	606	43/43	0.98	0.21	37,41,49,52	0
3	HEC	I	600	43/43	0.98	0.21	39,43,50,52	0
3	HEC	I	607	43/43	0.98	0.21	32,34,36,38	0
3	HEC	H	600	43/43	0.98	0.20	32,37,42,44	0
3	HEC	M	606	43/43	0.98	0.25	37,40,50,55	0
3	HEC	H	606	43/43	0.98	0.22	32,34,39,44	0
3	HEC	I	601	43/43	0.98	0.21	35,37,41,44	0
3	HEC	M	601	43/43	0.98	0.23	41,44,47,51	0
3	HEC	L	607	43/43	0.98	0.23	32,34,35,36	0
3	HEC	B	603	43/43	0.98	0.20	45,49,53,54	0
3	HEC	G	606	43/43	0.98	0.21	35,37,42,46	0
3	HEC	B	601	43/43	0.98	0.21	43,47,56,68	0
3	HEC	J	604	43/43	0.98	0.20	32,35,44,55	0
3	HEC	O	600	43/43	0.98	0.21	44,48,58,60	0
3	HEC	D	604	43/43	0.98	0.21	44,47,54,60	0
3	HEC	K	607	43/43	0.98	0.21	30,32,34,36	0
3	HEC	L	603	43/43	0.98	0.24	35,41,50,52	0

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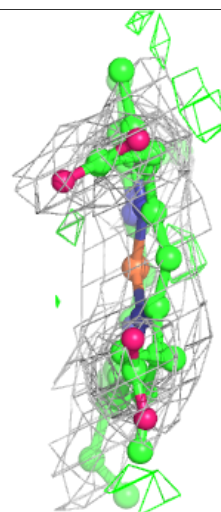
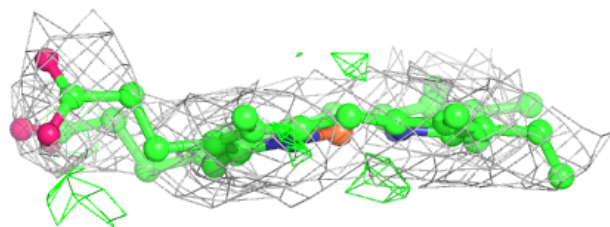
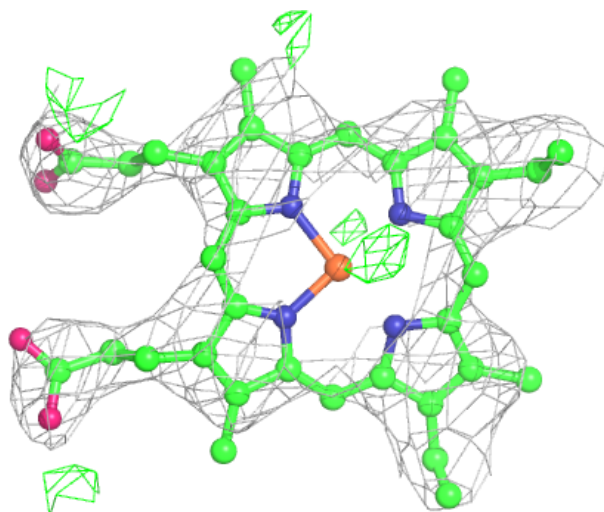
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	HEC	K	603	43/43	0.98	0.20	37,39,42,44	0
4	SO4	U	609	5/5	0.98	0.18	57,58,60,64	0
3	HEC	D	607	43/43	0.98	0.23	40,45,55,61	0
4	SO4	V	609	5/5	0.98	0.20	56,59,60,62	0
3	HEC	R	606	43/43	0.98	0.22	37,43,59,63	0
3	HEC	J	601	43/43	0.98	0.21	34,37,41,47	0
3	HEC	L	606	43/43	0.98	0.21	35,37,43,47	0
3	HEC	J	603	43/43	0.98	0.20	37,39,44,46	0
3	HEC	B	607	43/43	0.98	0.23	37,40,45,47	0
3	HEC	K	605	43/43	0.98	0.23	35,38,43,48	0
3	HEC	D	603	43/43	0.98	0.22	54,66,69,72	0
3	HEC	H	607	43/43	0.98	0.21	28,30,32,35	0
3	HEC	N	607	43/43	0.98	0.20	37,41,44,46	0
3	HEC	K	606	43/43	0.98	0.23	33,39,42,46	0
4	SO4	I	609	5/5	0.99	0.22	28,28,29,30	0
4	SO4	K	609	5/5	0.99	0.23	28,28,29,30	0
4	SO4	N	609	5/5	0.99	0.20	40,40,41,42	0
4	SO4	R	609	5/5	0.99	0.20	36,39,40,40	0
4	SO4	A	609	5/5	0.99	0.21	47,49,49,52	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.

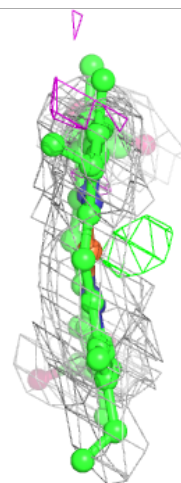
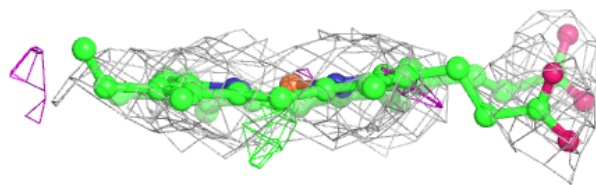
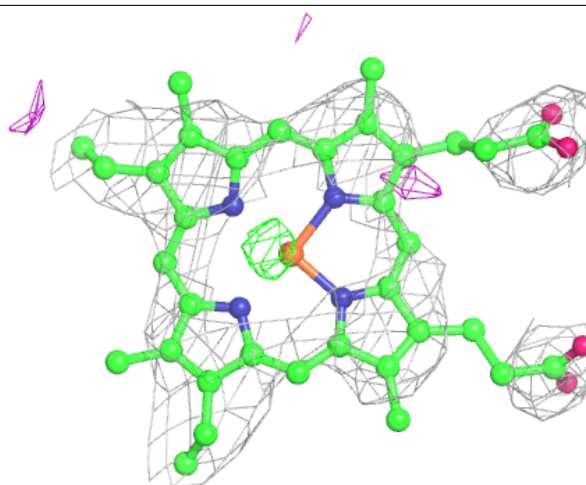
**Electron density around HEC X 606:**

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



**Electron density around HEC X 605:**

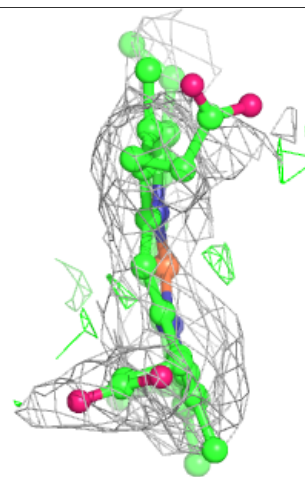
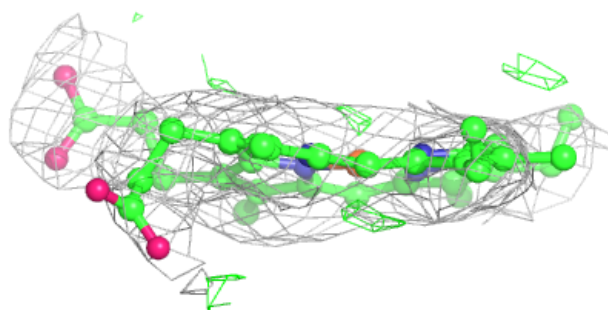
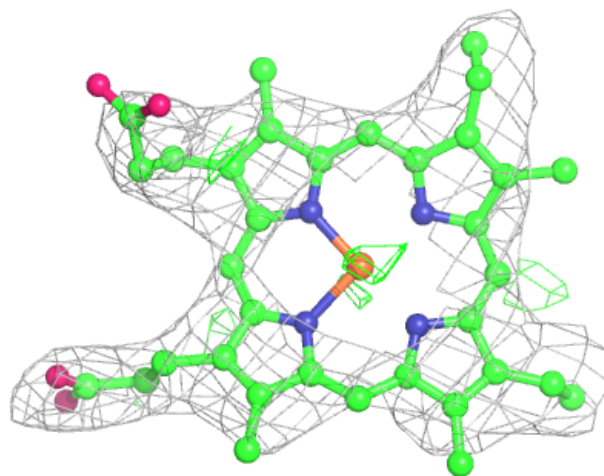
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





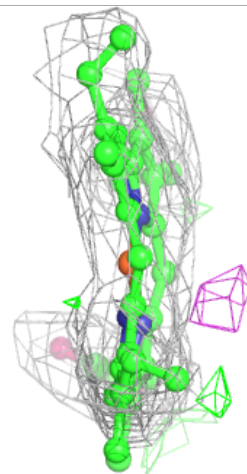
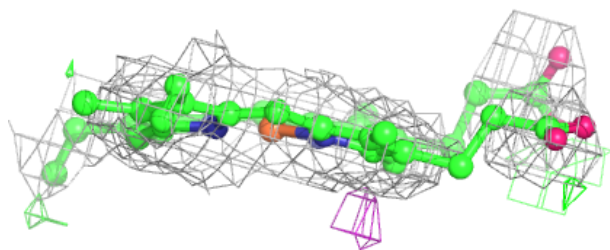
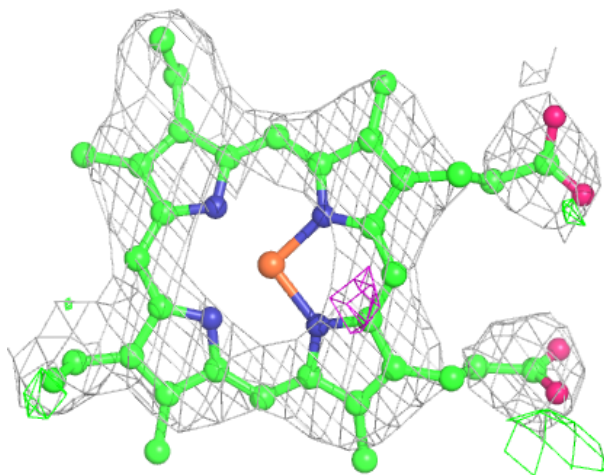
**Electron density around HEC V 602:**

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



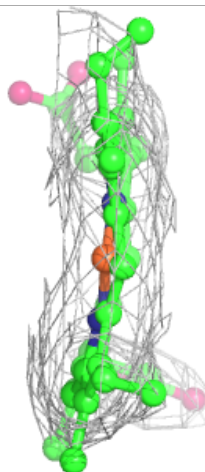
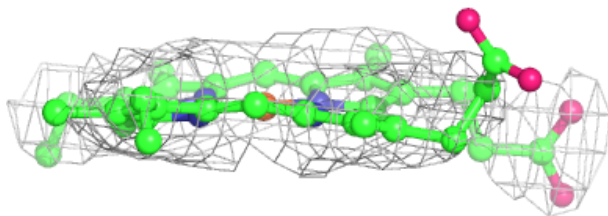
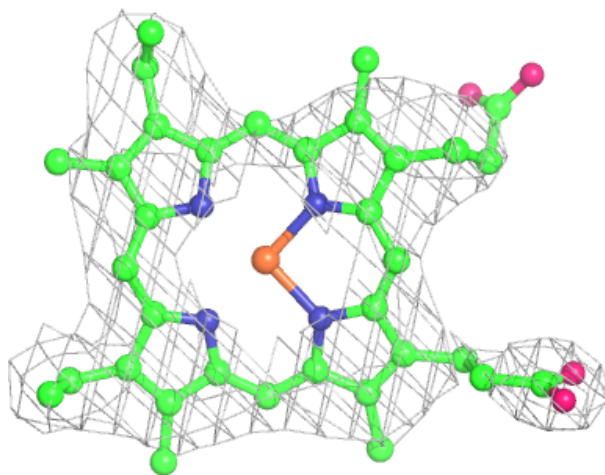
**Electron density around HEC A 606:**

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



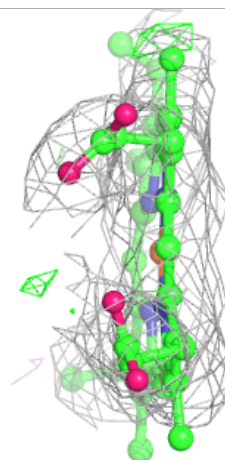
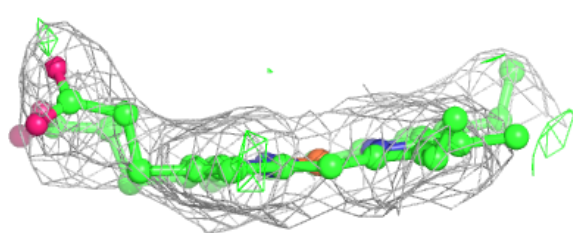
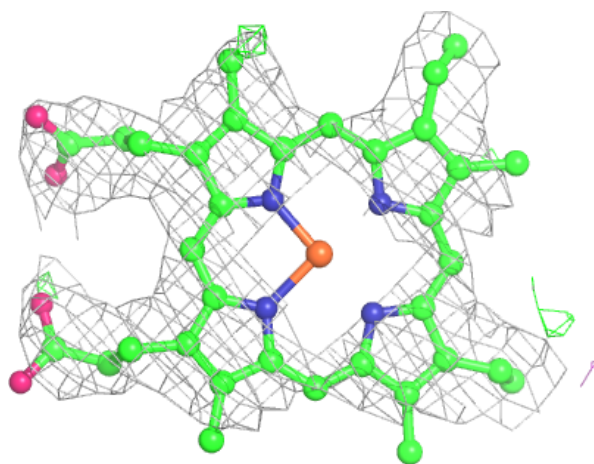
**Electron density around HEC U 602:**

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



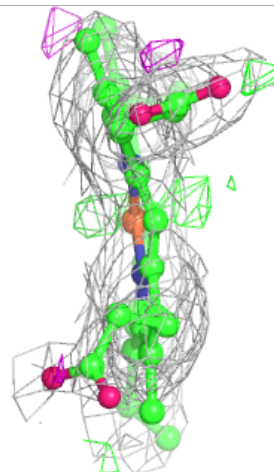
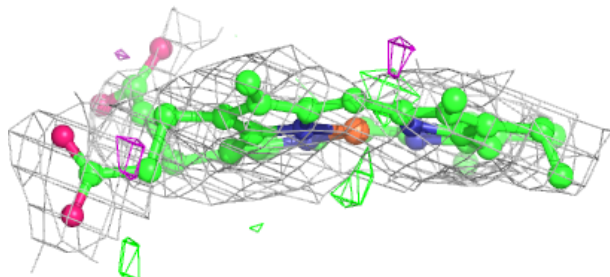
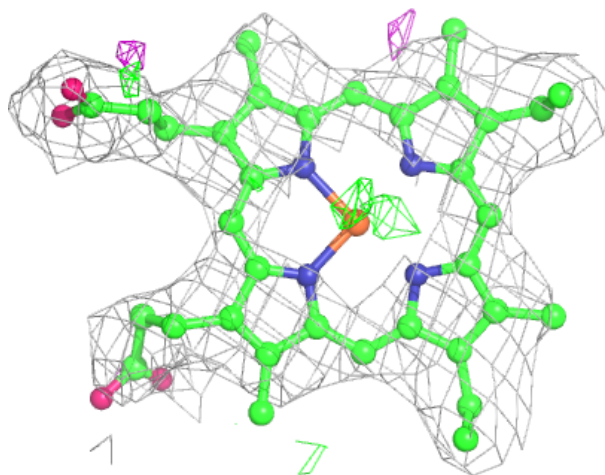
**Electron density around HEC S 604:**

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



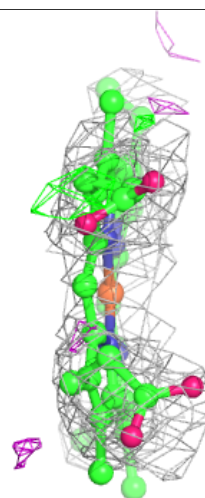
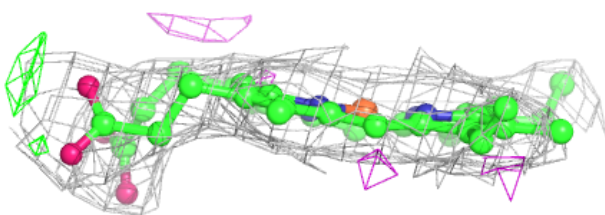
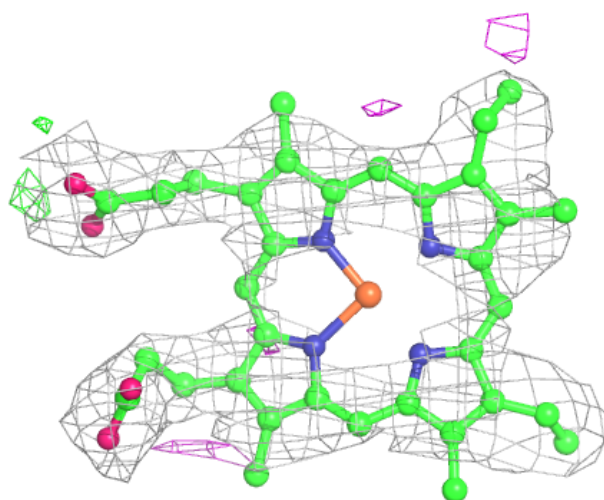
**Electron density around HEC H 602:**

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



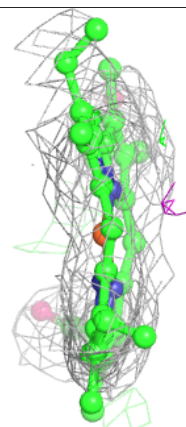
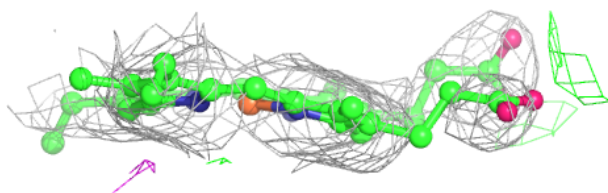
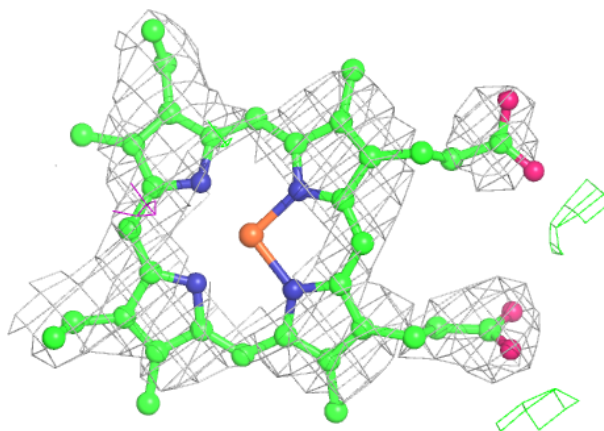
**Electron density around HEC T 607:**

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



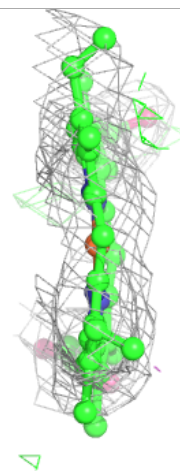
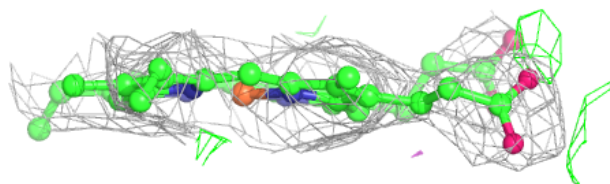
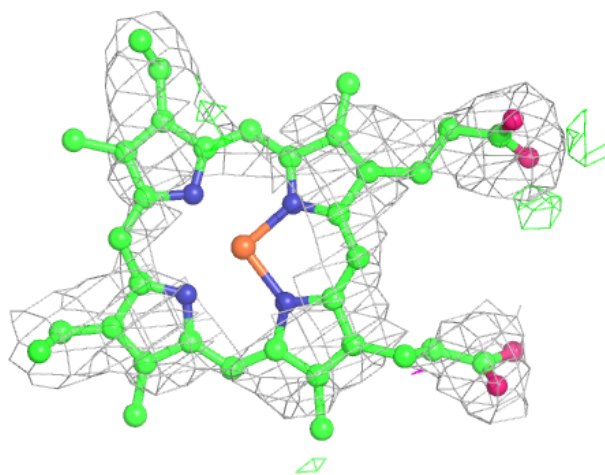
**Electron density around HEC U 606:**

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



**Electron density around HEC W 605:**

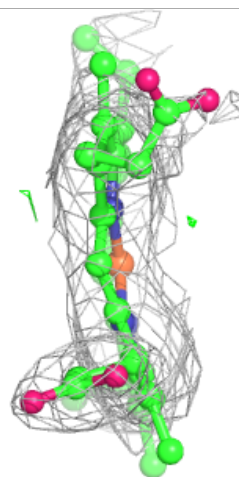
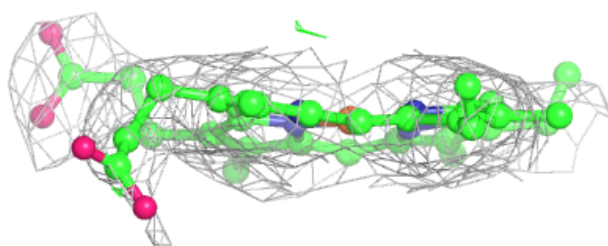
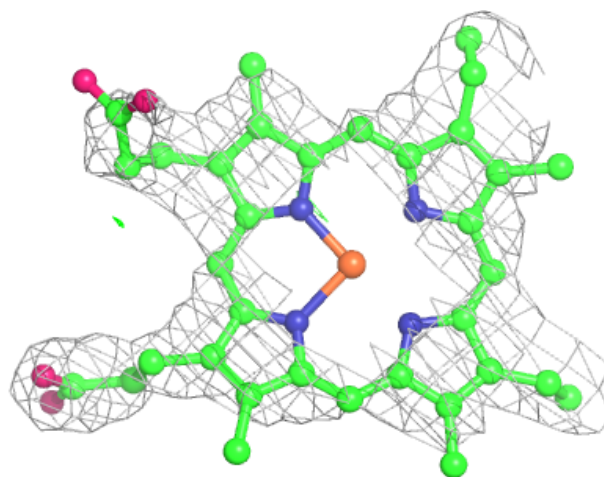
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





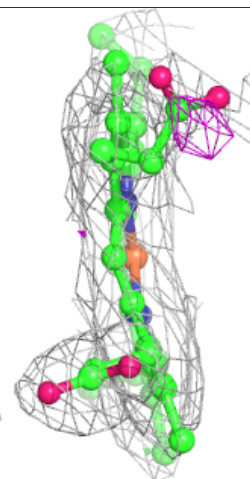
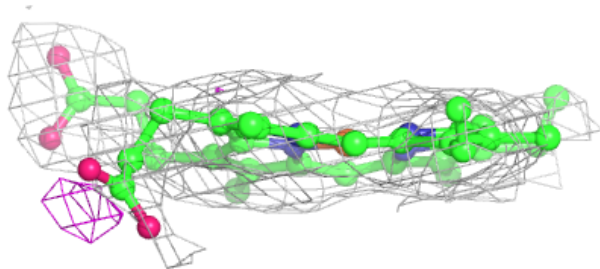
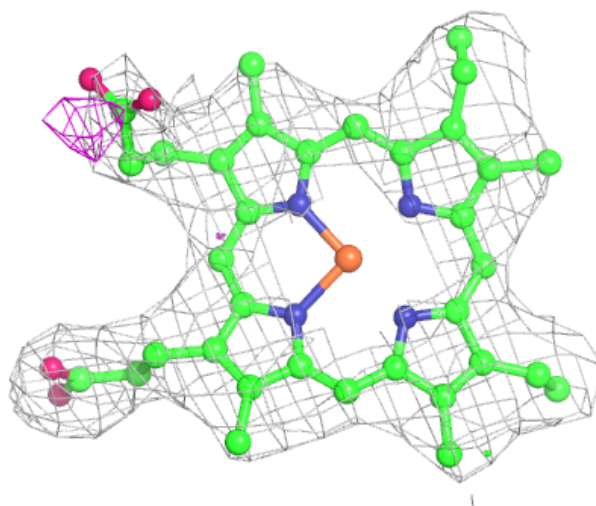
**Electron density around HEC X 602:**

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



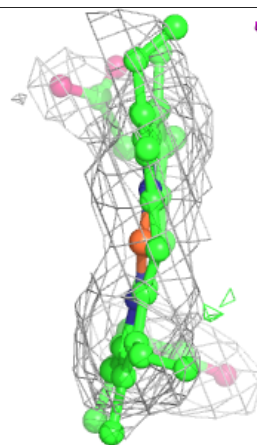
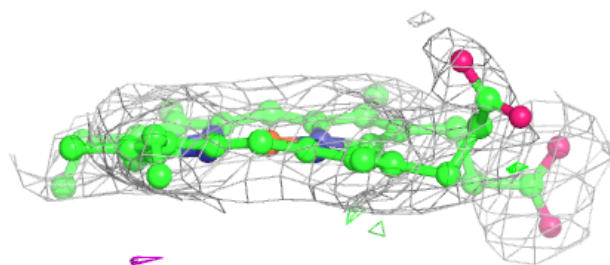
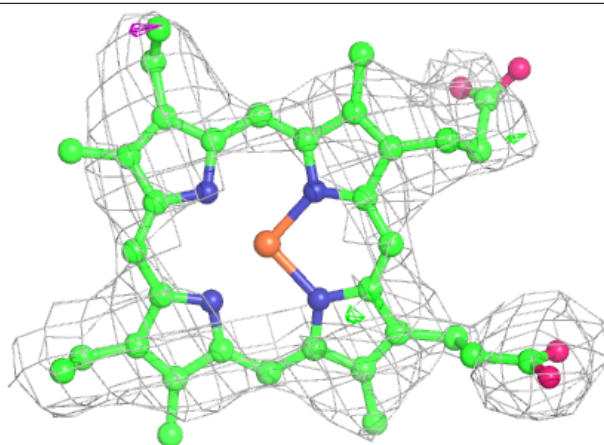
**Electron density around HEC P 602:**

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



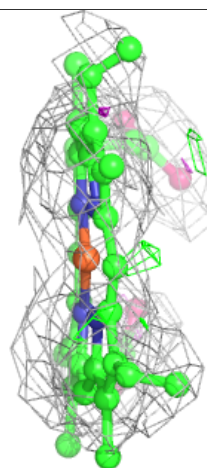
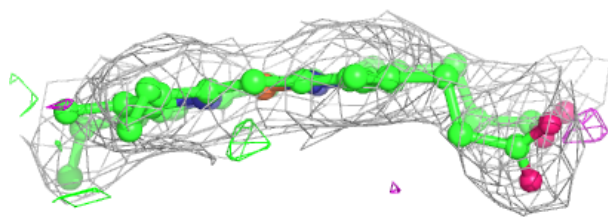
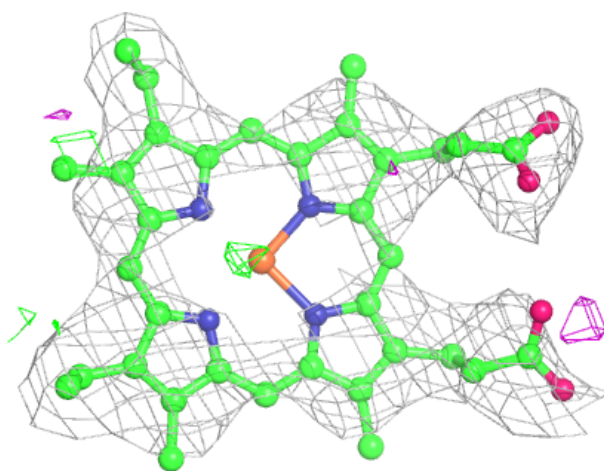
**Electron density around HEC T 602:**

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



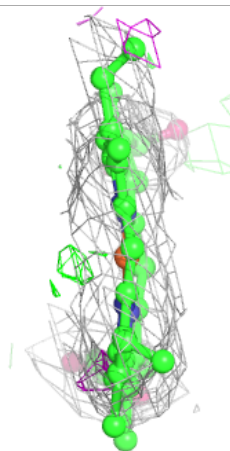
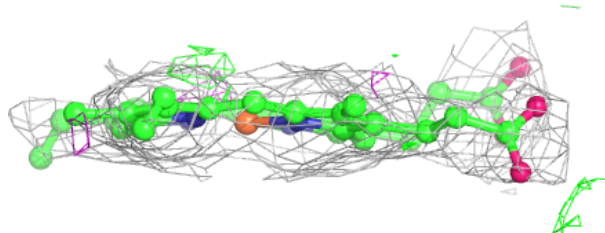
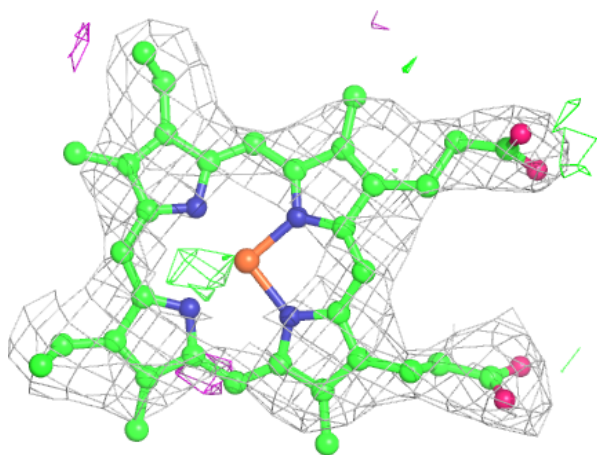
**Electron density around HEC Q 604:**

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



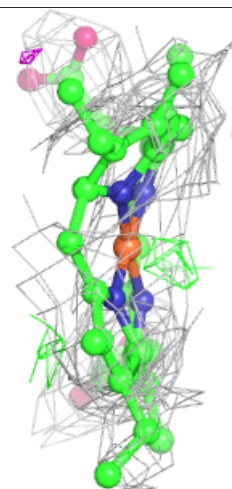
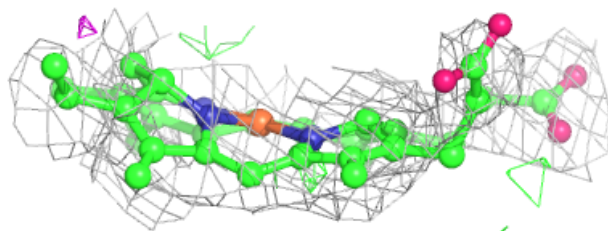
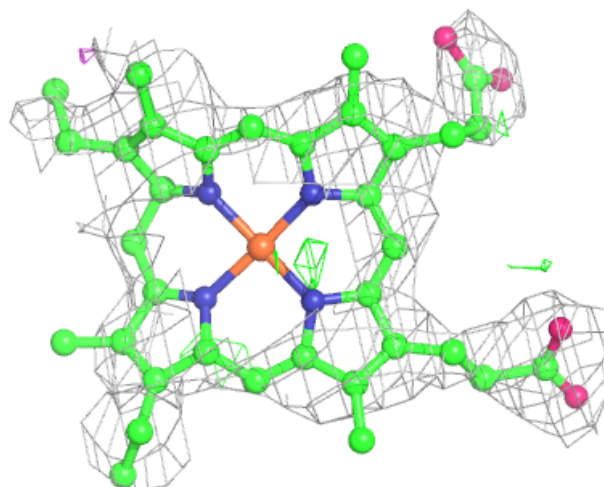
**Electron density around HEC E 605:**

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



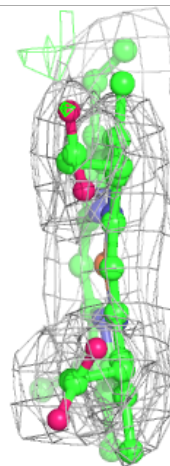
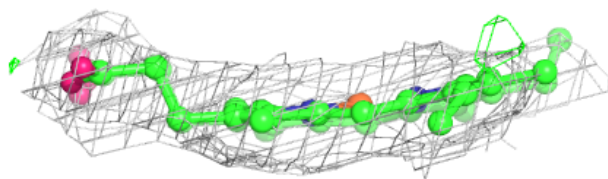
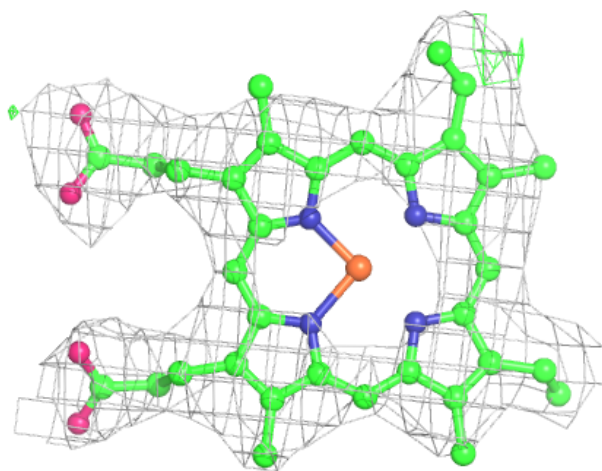
**Electron density around HEC W 603:**

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



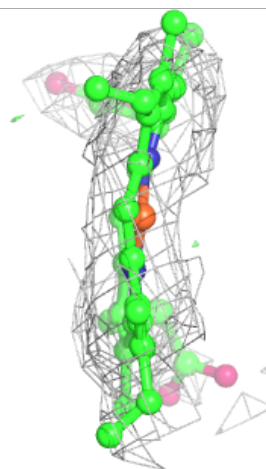
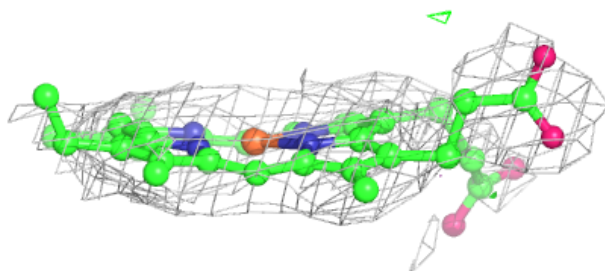
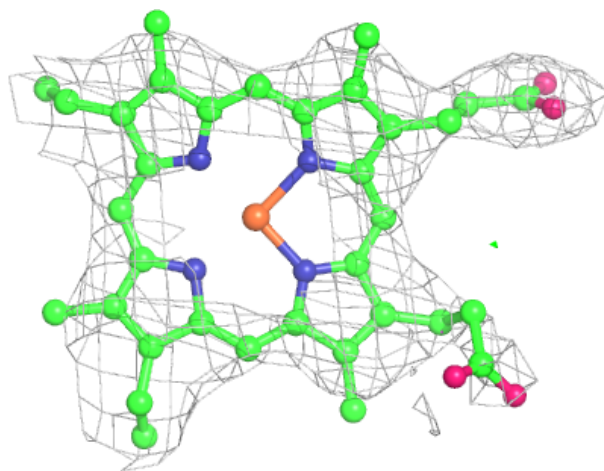
**Electron density around HEC U 600:**

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



**Electron density around HEC Q 602:**

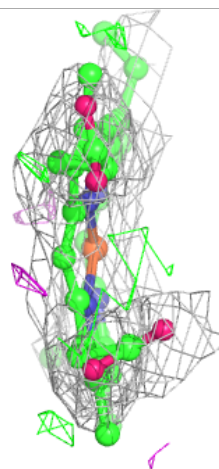
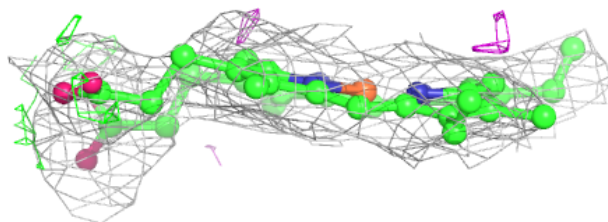
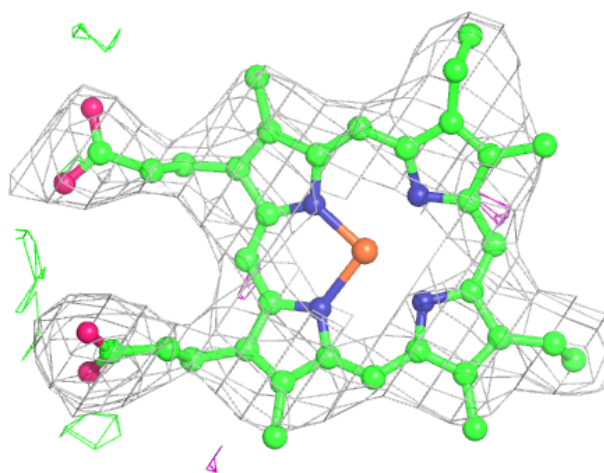
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





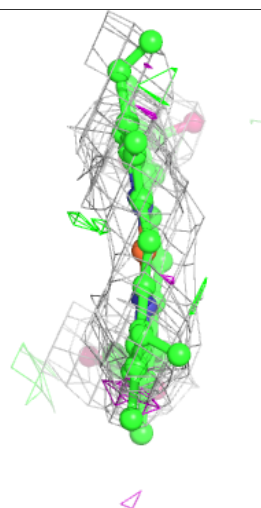
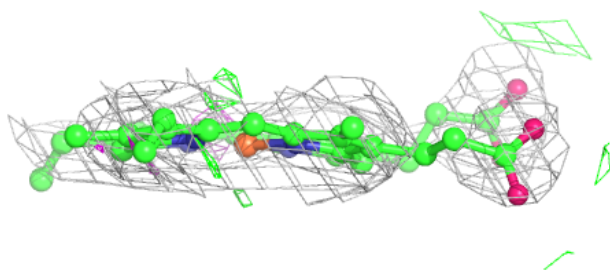
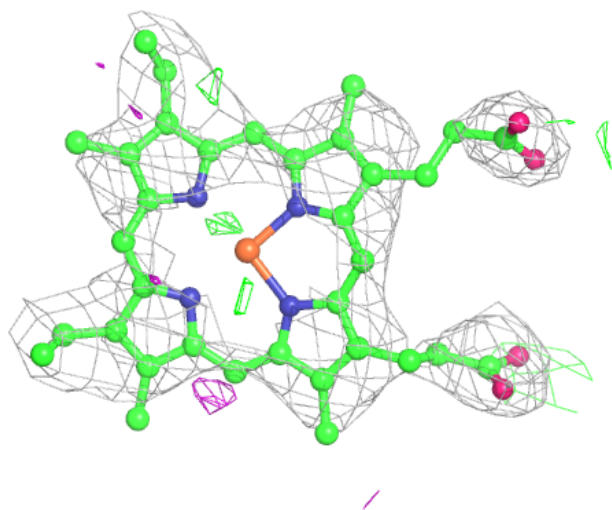
**Electron density around HEC N 606:**

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



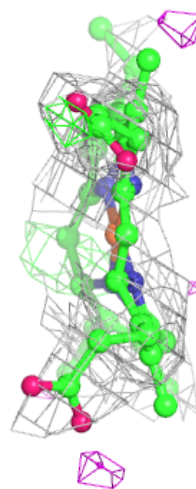
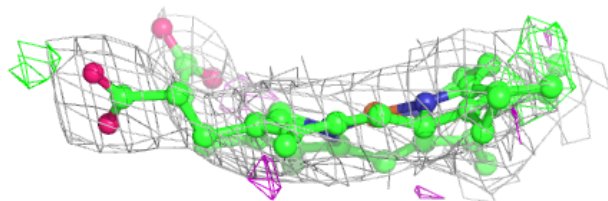
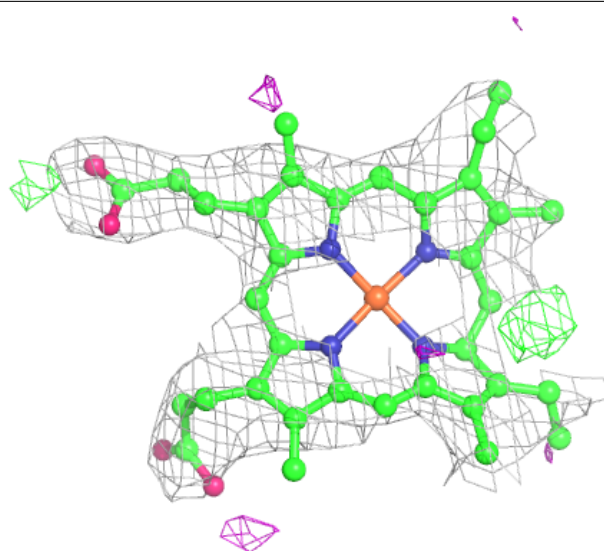
**Electron density around HEC S 605:**

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



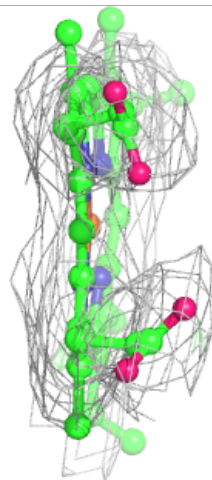
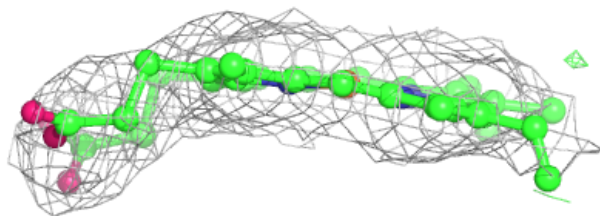
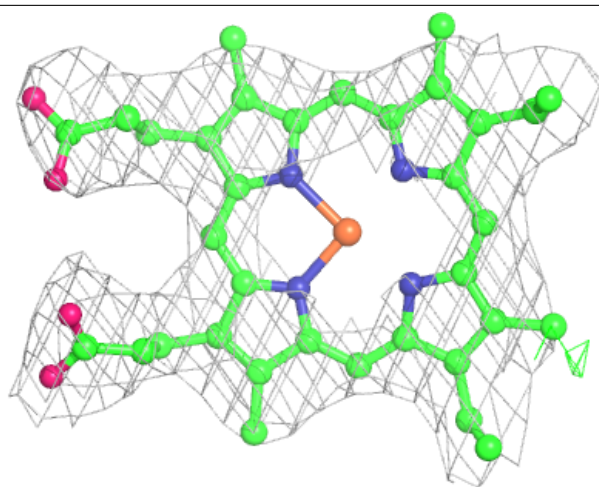
**Electron density around HEC V 603:**

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



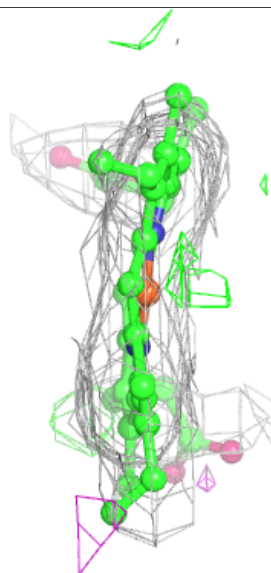
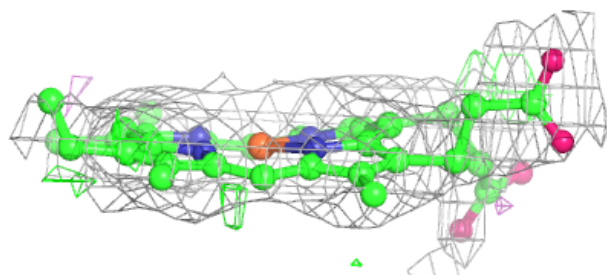
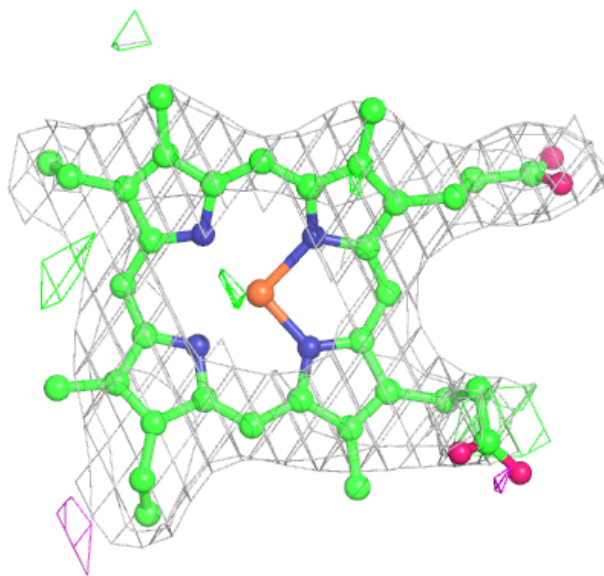
**Electron density around HEC U 604:**

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



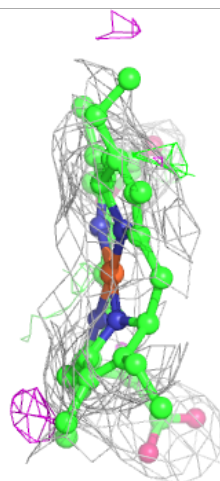
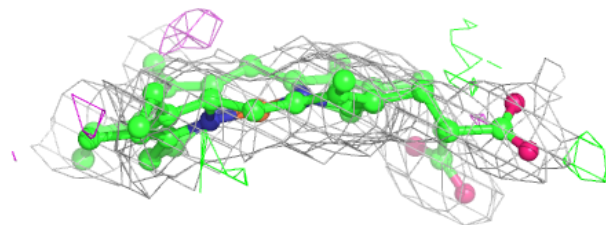
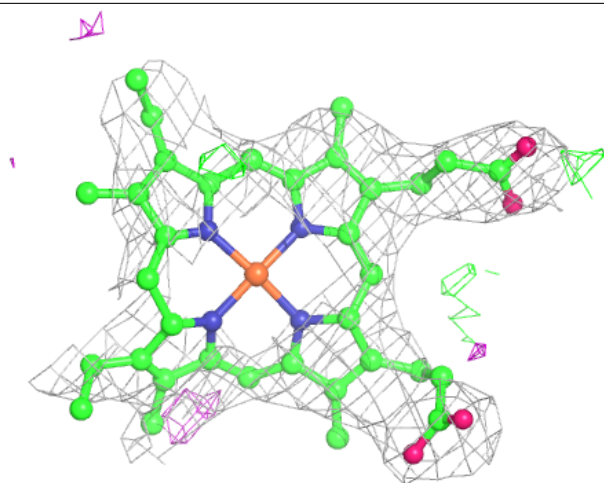
**Electron density around HEC B 602:**

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



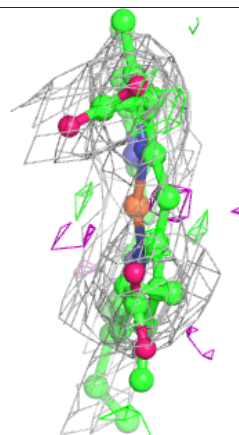
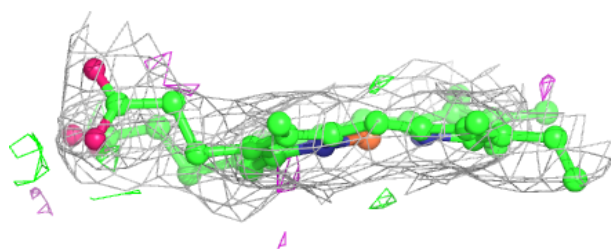
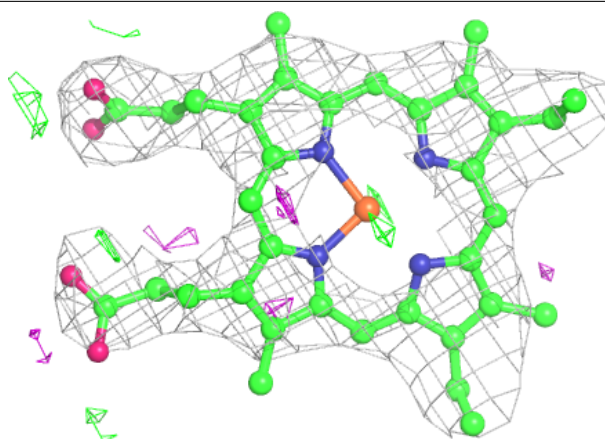
**Electron density around HEC F 603:**

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



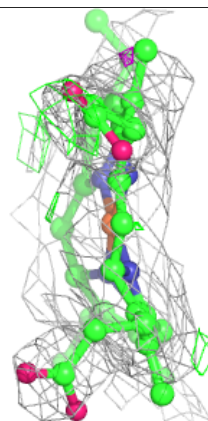
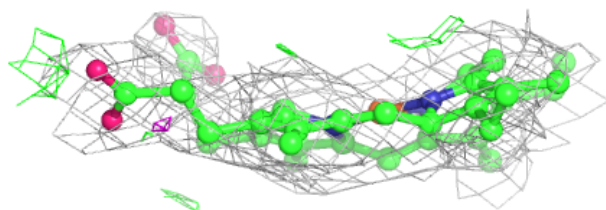
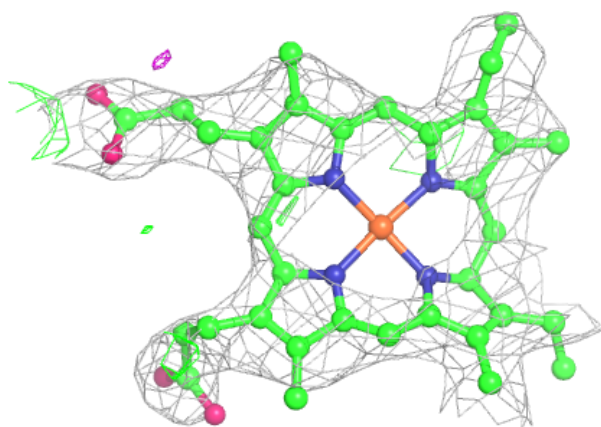
**Electron density around HEC E 606:**

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



**Electron density around HEC S 603:**

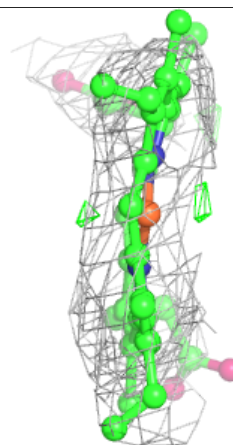
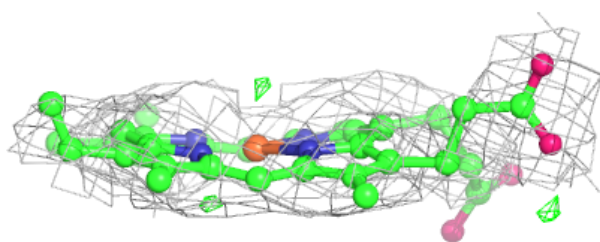
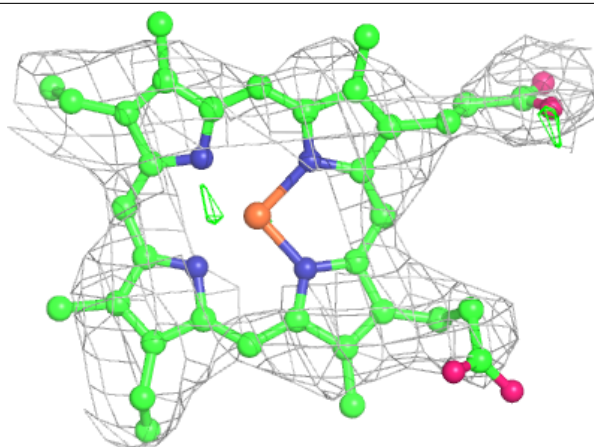
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





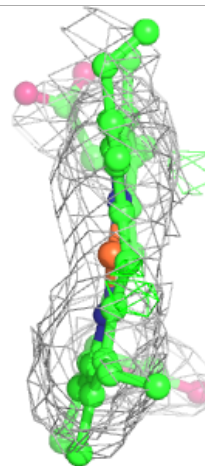
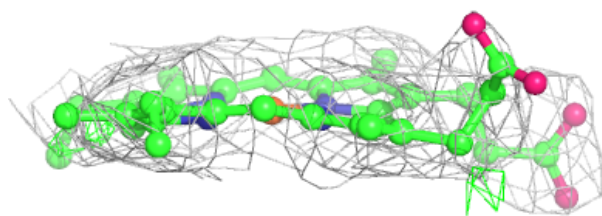
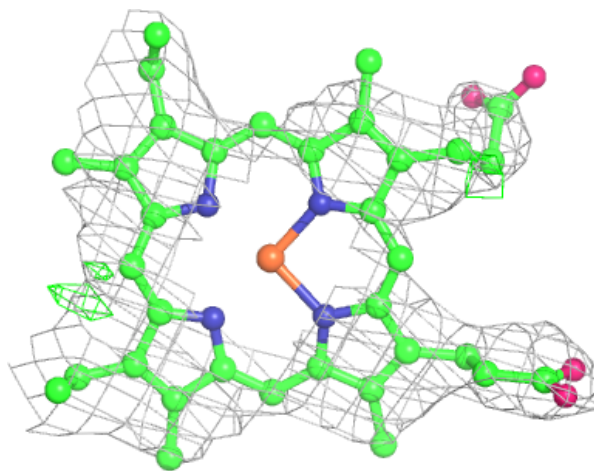
**Electron density around HEC F 602:**

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



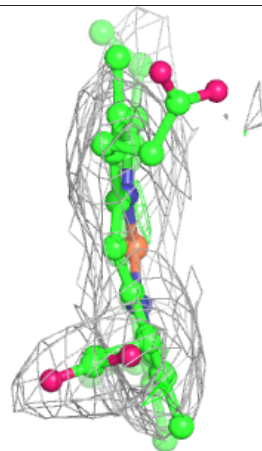
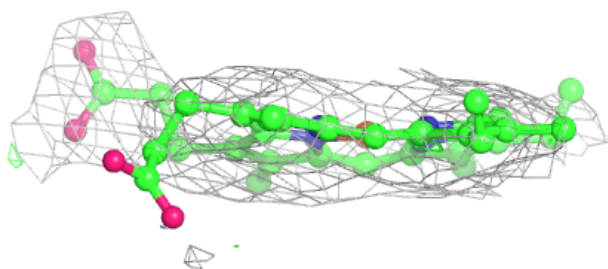
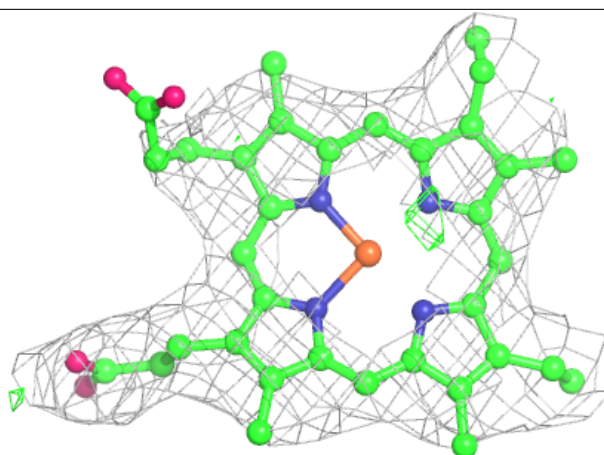
**Electron density around HEC S 602:**

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



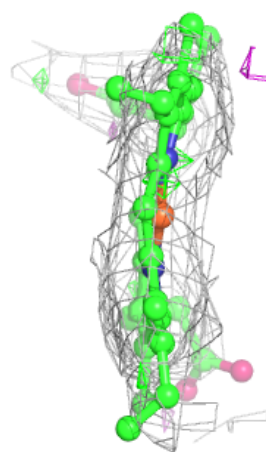
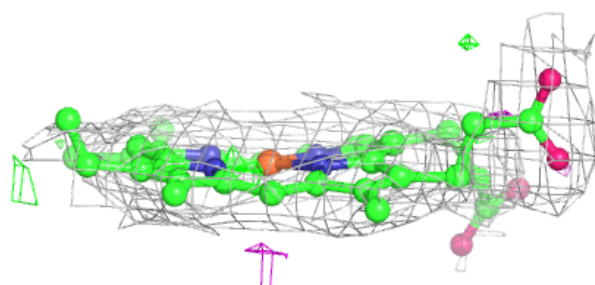
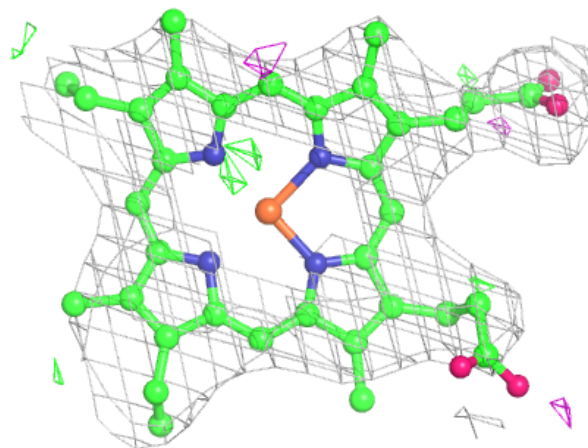
**Electron density around HEC W 602:**

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



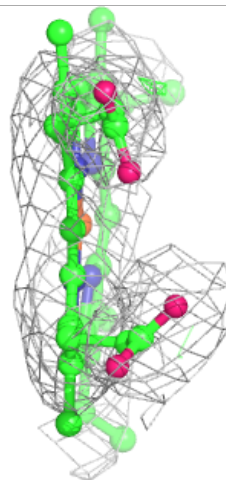
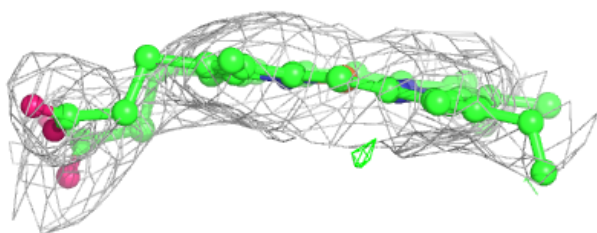
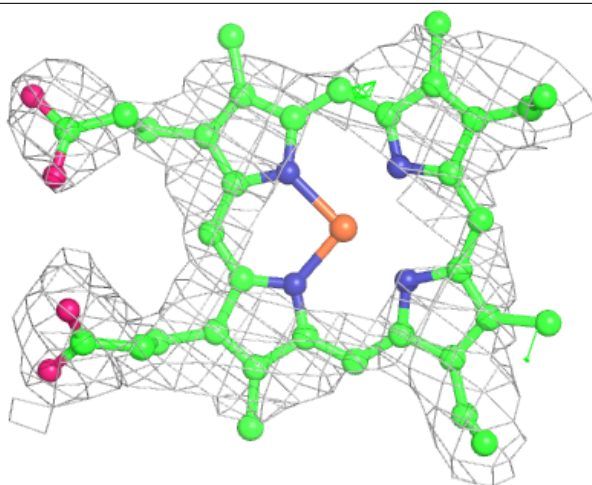
**Electron density around HEC E 602:**

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



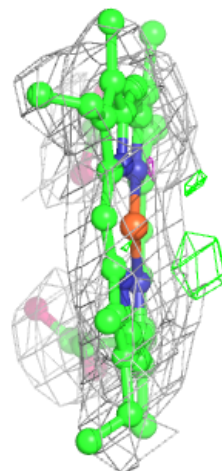
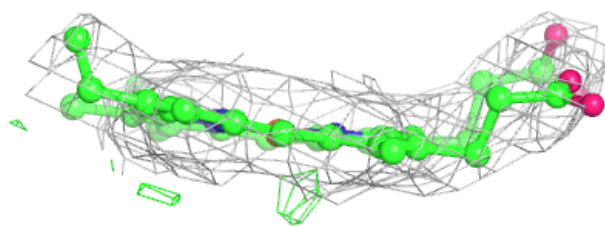
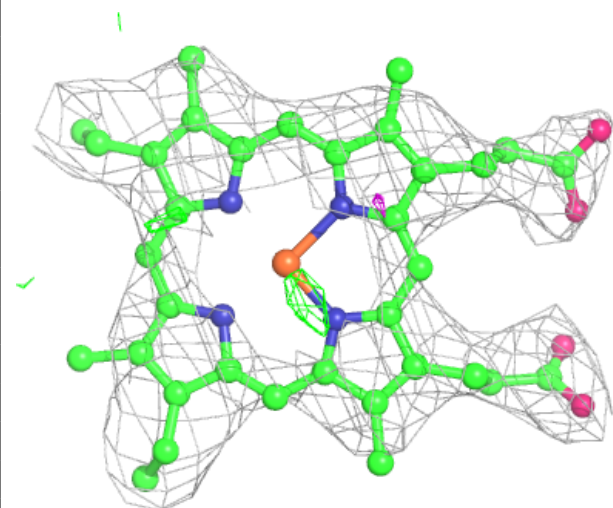
**Electron density around HEC X 604:**

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



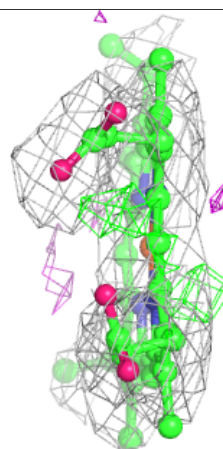
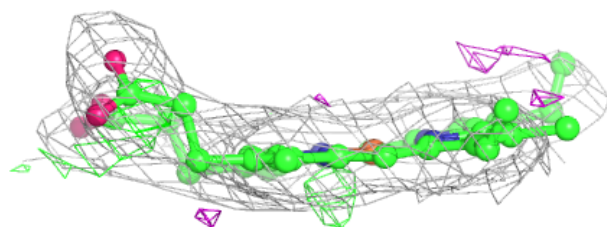
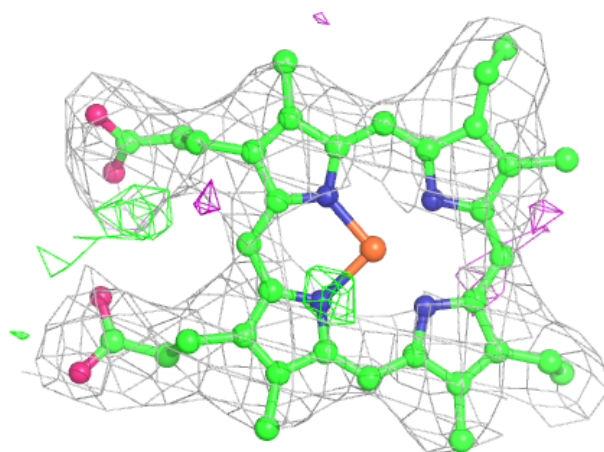
**Electron density around HEC V 604:**

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



**Electron density around HEC A 604:**

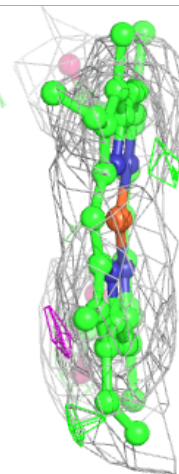
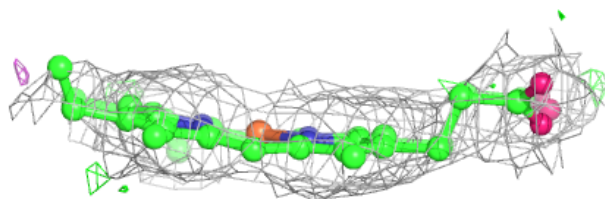
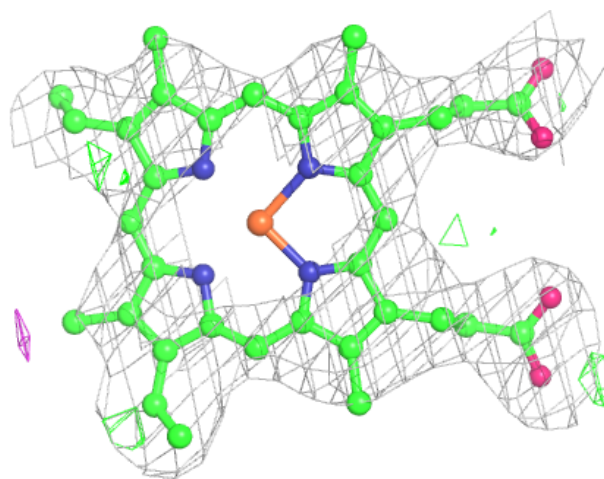
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC C 600:**

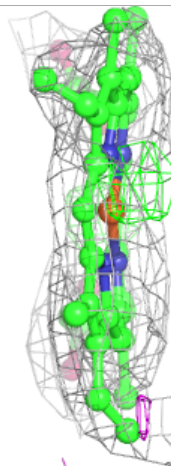
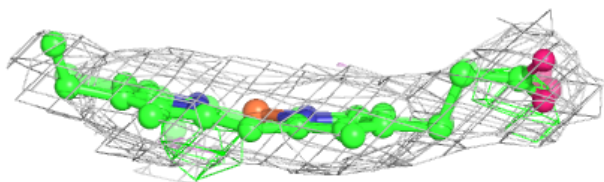
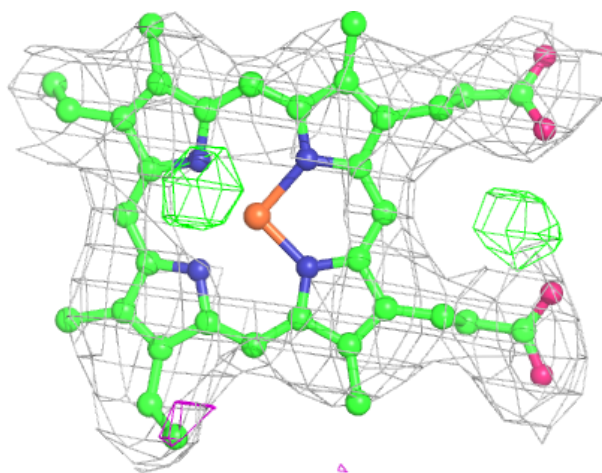
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





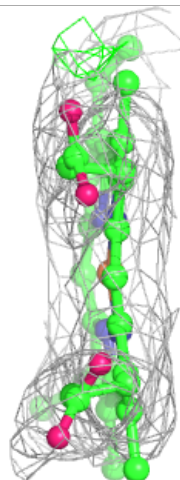
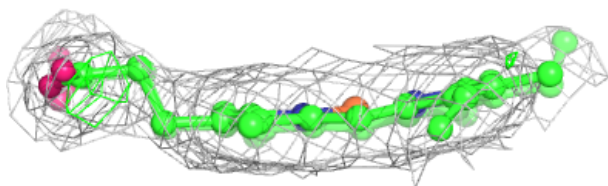
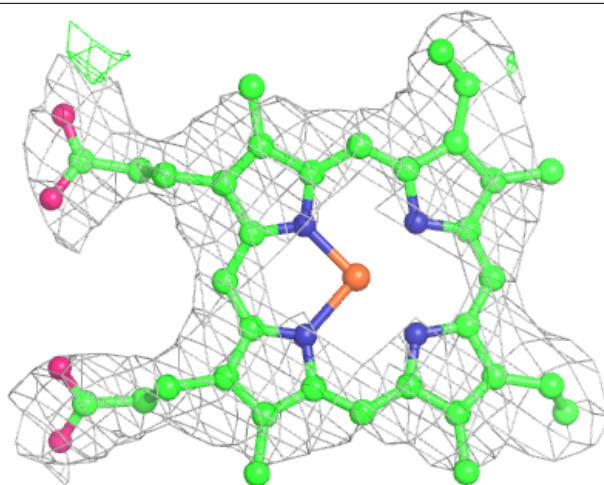
**Electron density around HEC E 600:**

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



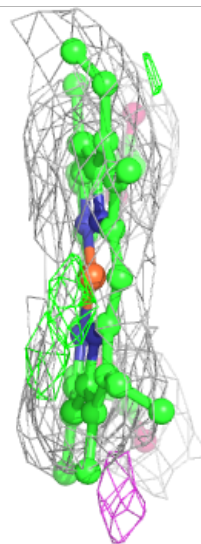
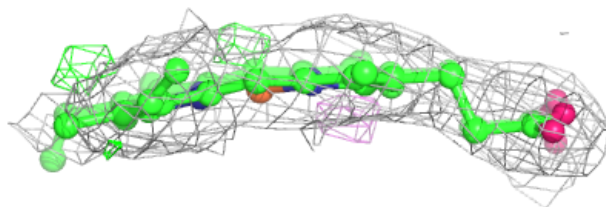
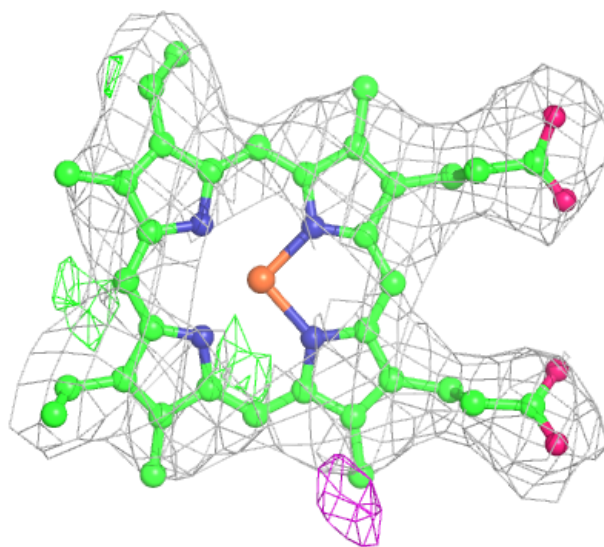
**Electron density around HEC T 600:**

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



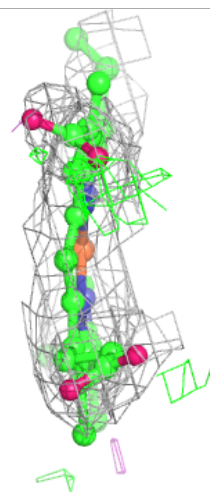
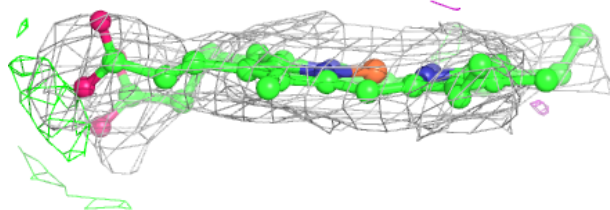
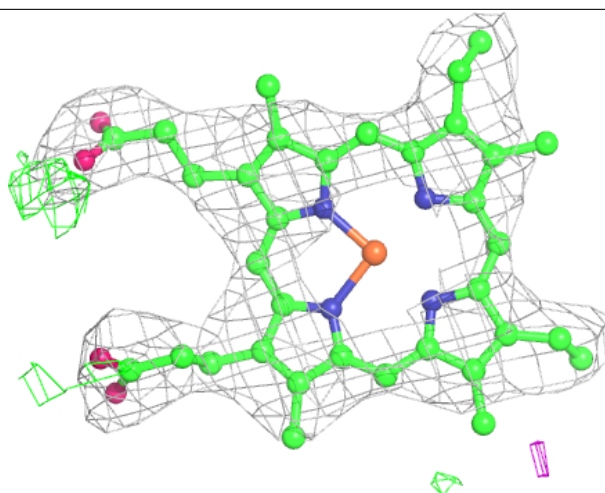
**Electron density around HEC L 600:**

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



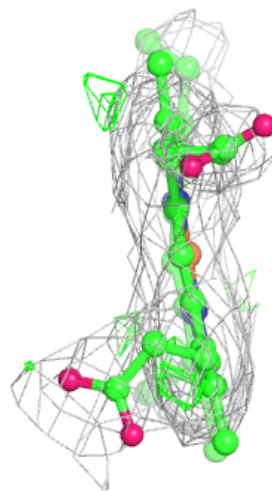
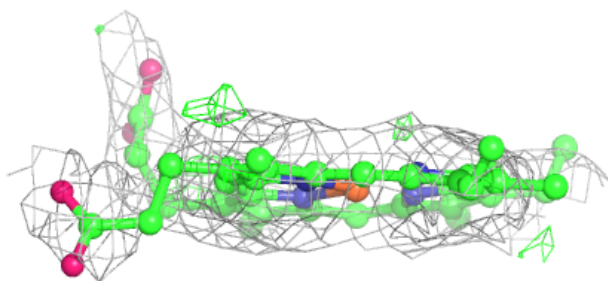
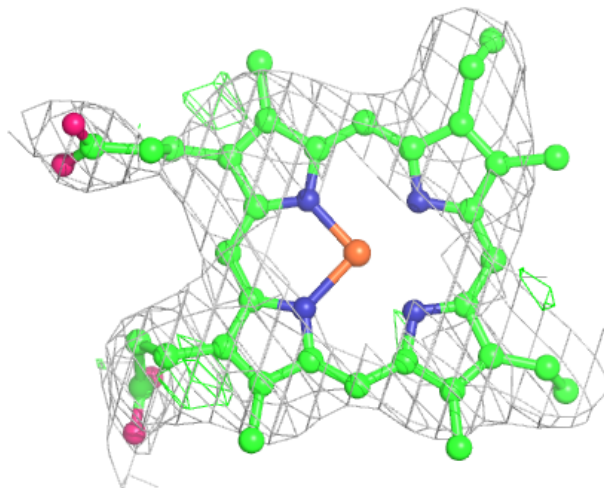
**Electron density around HEC F 605:**

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



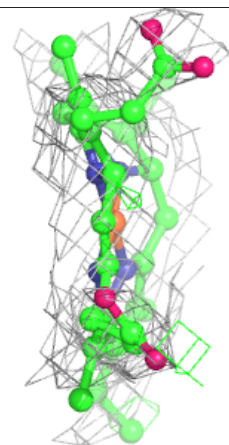
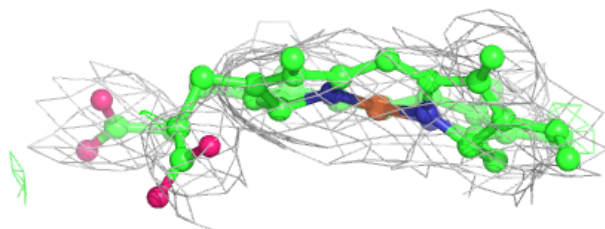
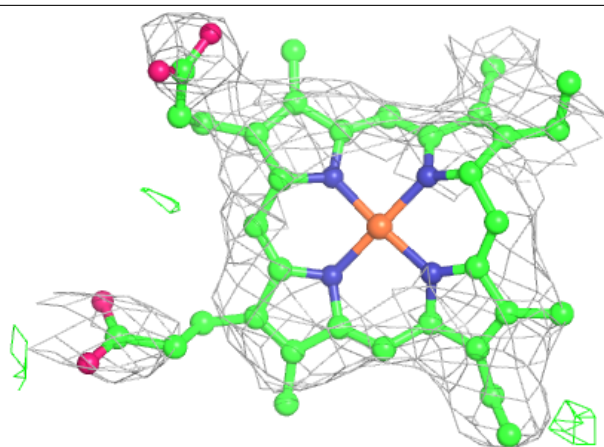
**Electron density around HEC S 601:**

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



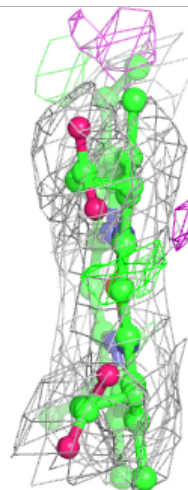
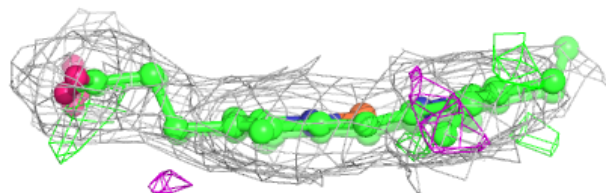
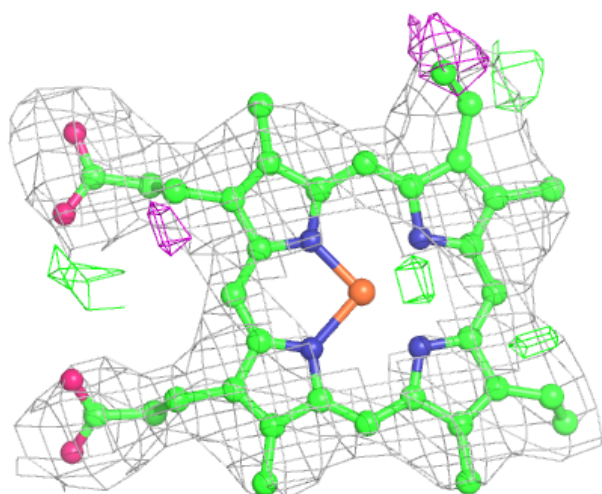
**Electron density around HEC X 603:**

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



**Electron density around HEC K 600:**

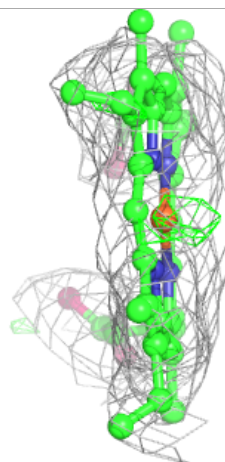
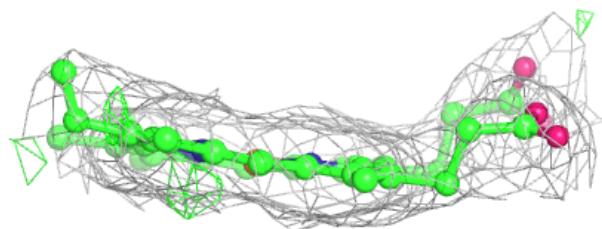
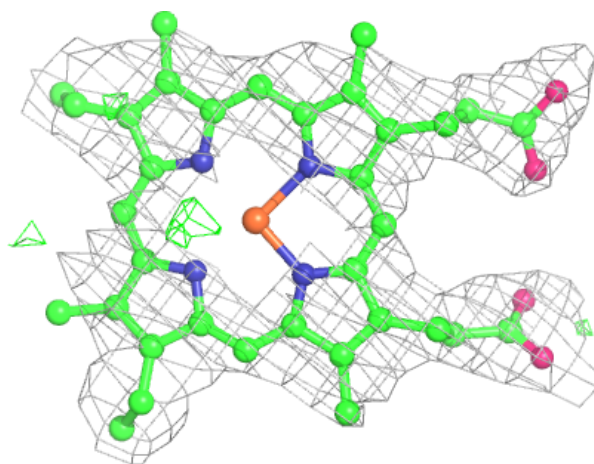
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC C 604:**

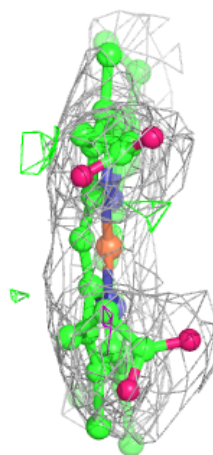
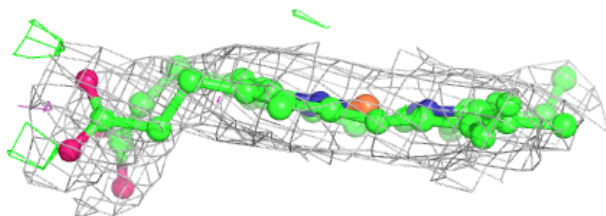
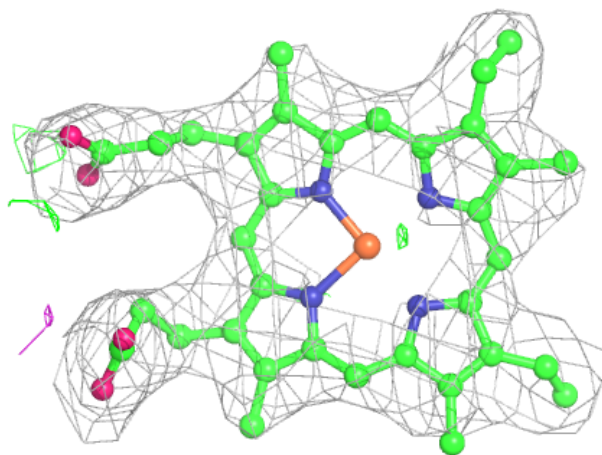
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





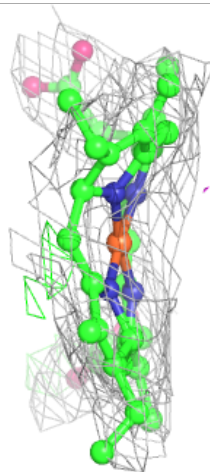
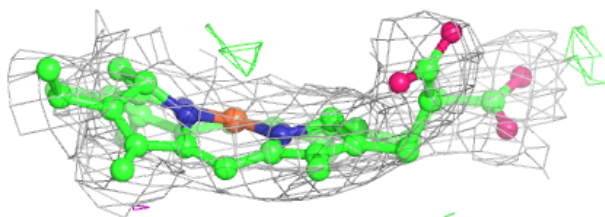
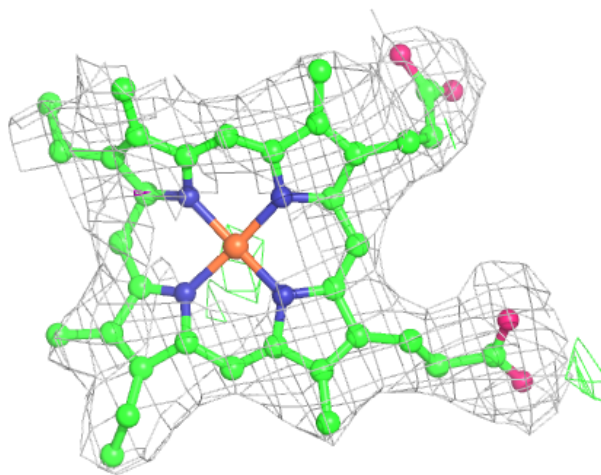
**Electron density around HEC Q 607:**

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



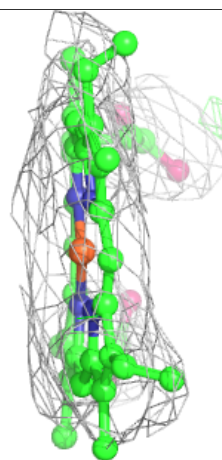
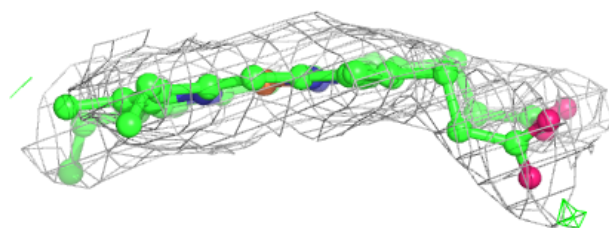
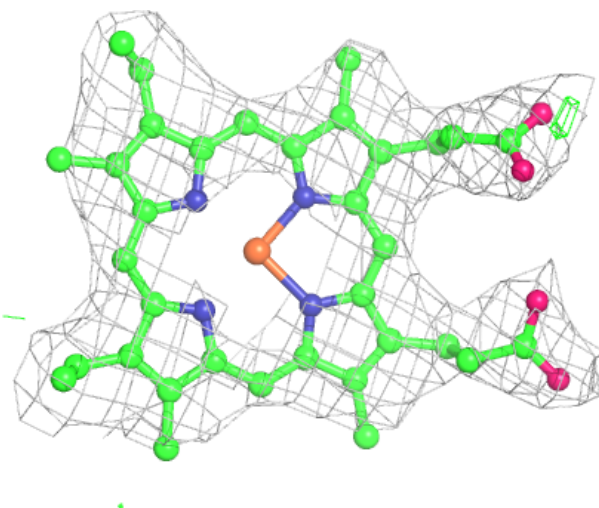
**Electron density around HEC R 603:**

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



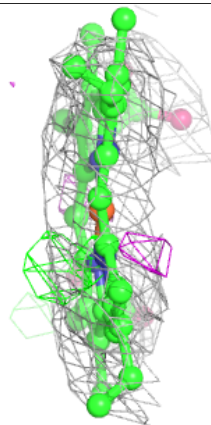
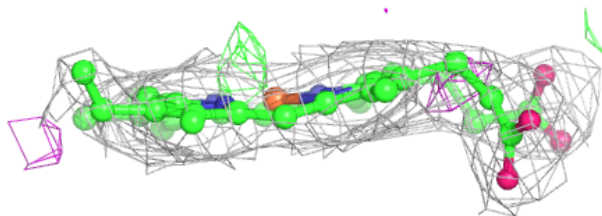
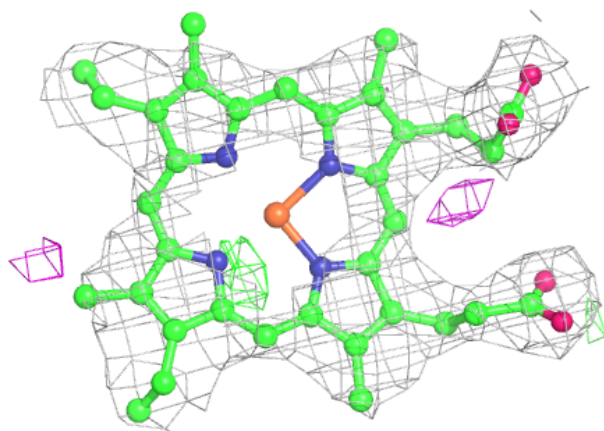
**Electron density around HEC W 604:**

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



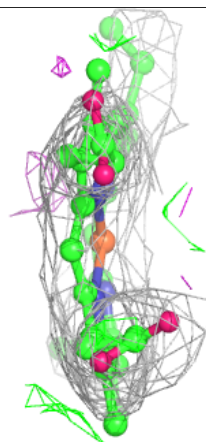
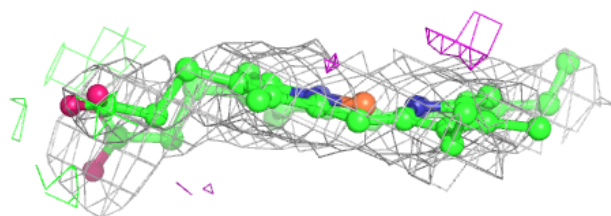
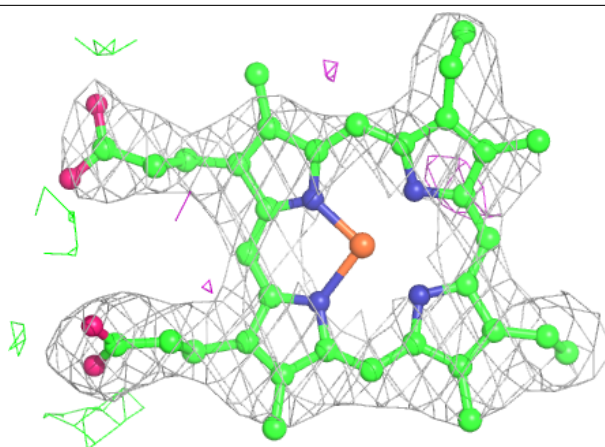
**Electron density around HEC A 607:**

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



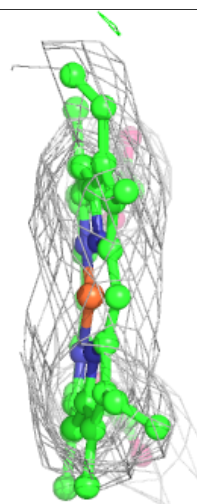
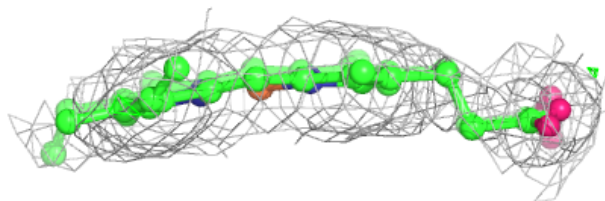
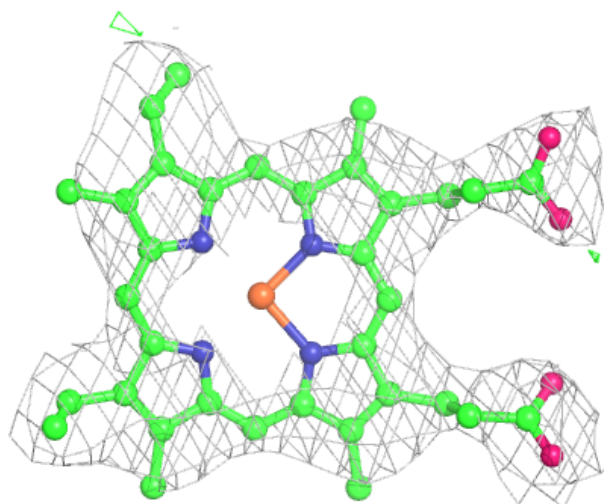
**Electron density around HEC T 606:**

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



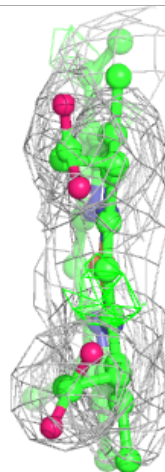
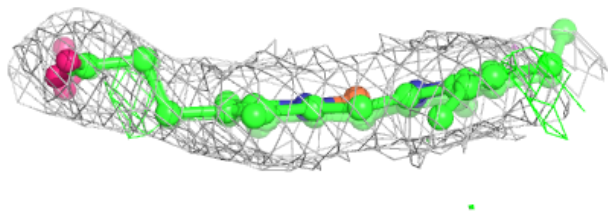
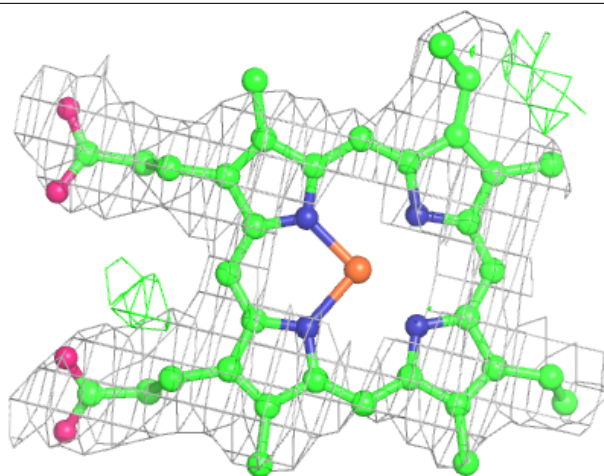
**Electron density around HEC S 600:**

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



**Electron density around HEC N 600:**

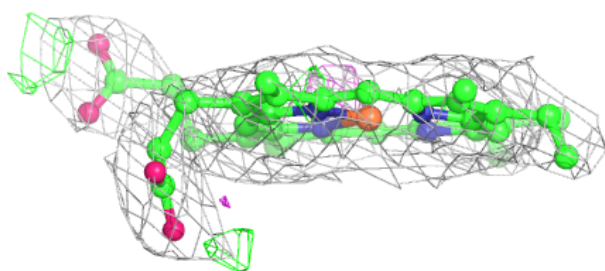
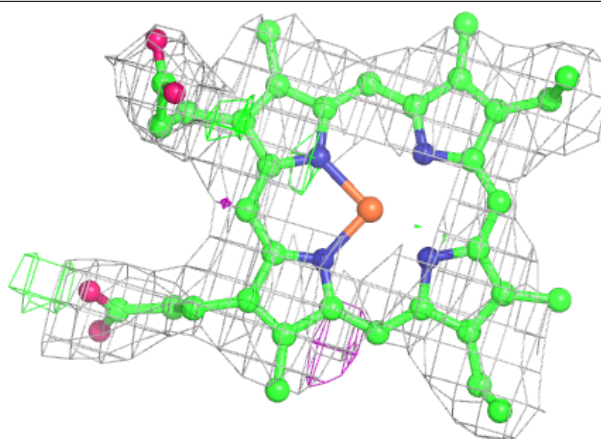
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC N 601:**

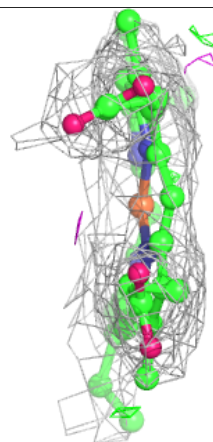
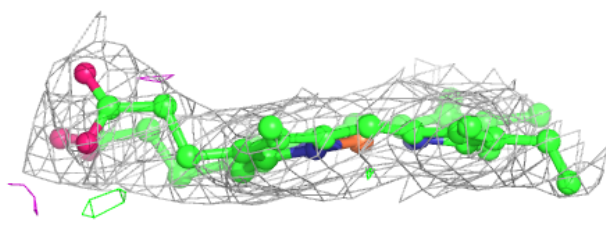
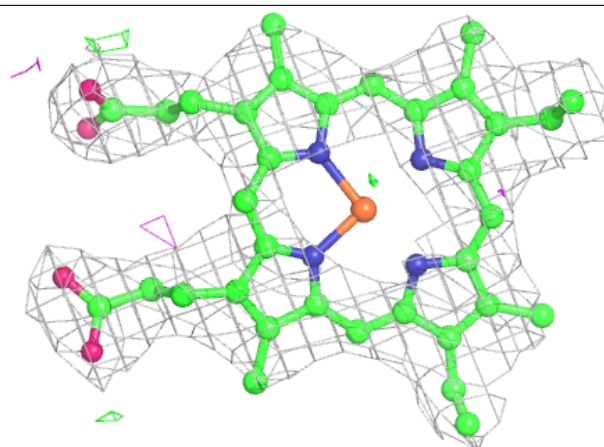
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





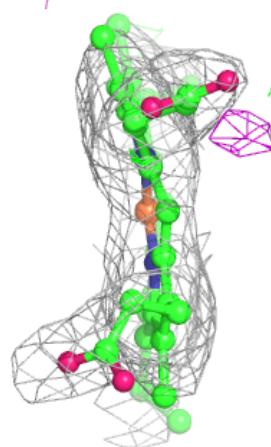
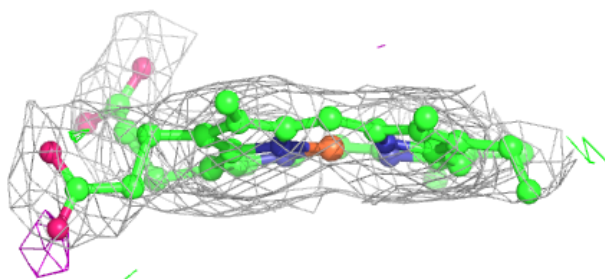
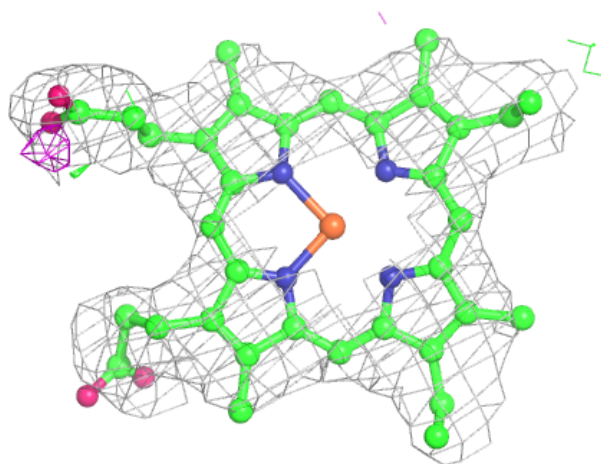
**Electron density around HEC P 606:**

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



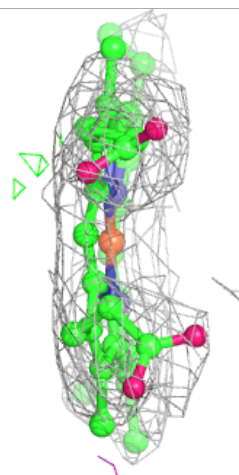
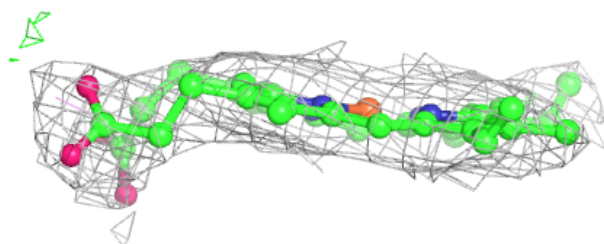
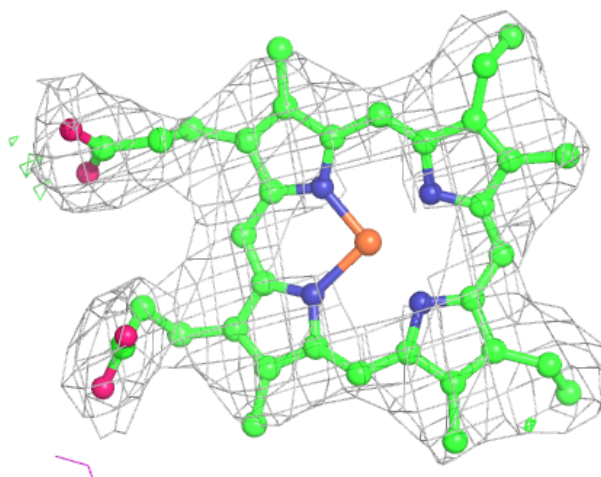
**Electron density around HEC L 602:**

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



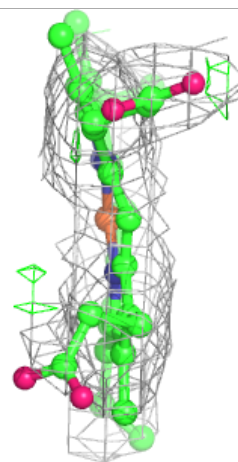
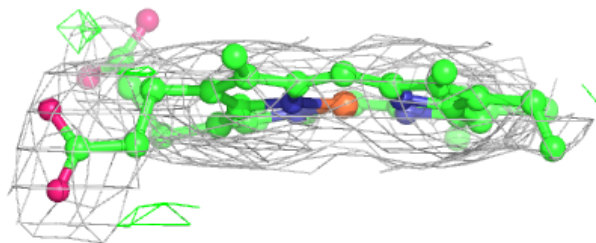
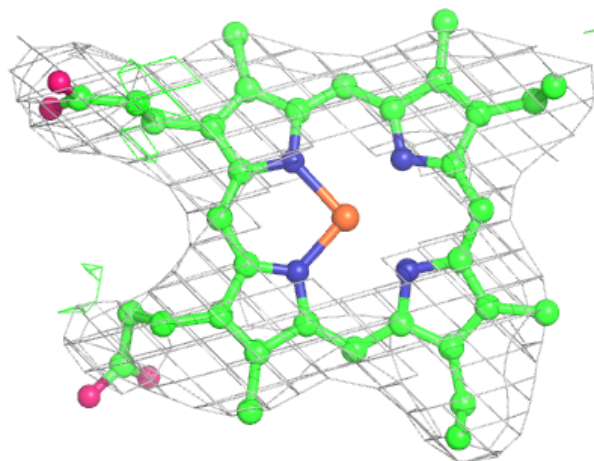
**Electron density around HEC M 607:**

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



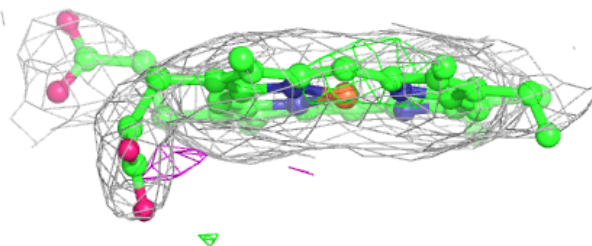
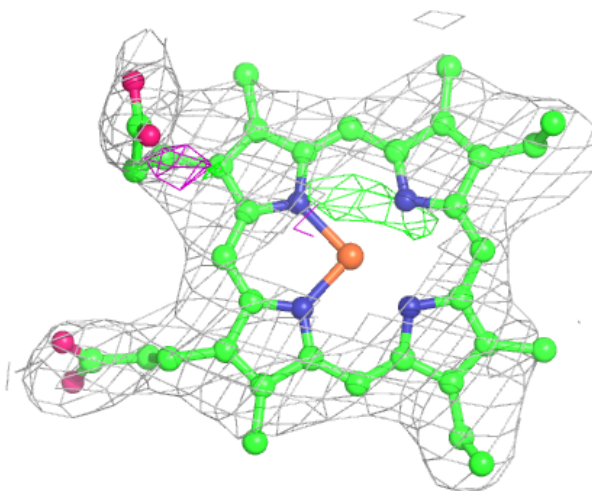
**Electron density around HEC N 602:**

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



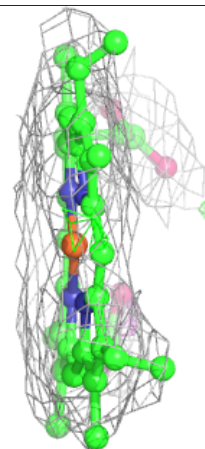
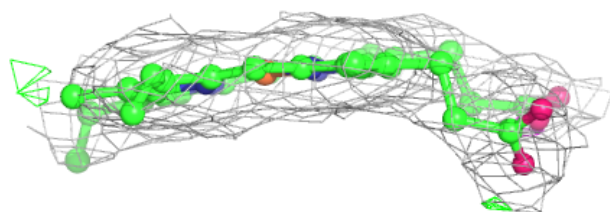
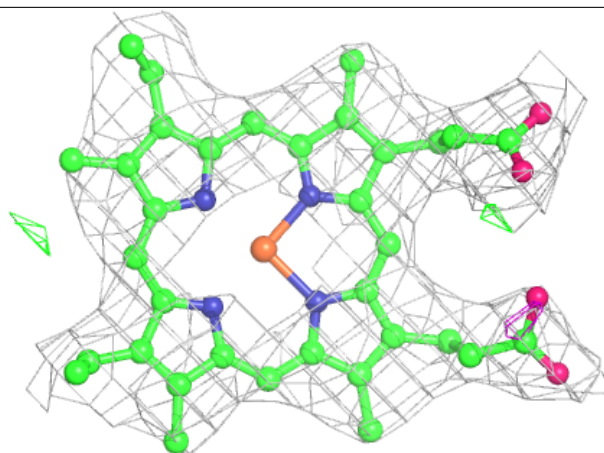
**Electron density around HEC F 601:**

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



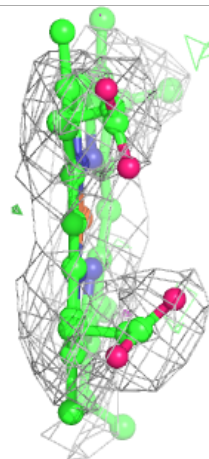
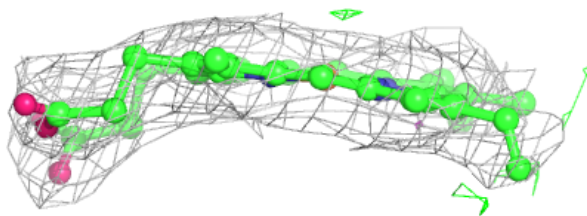
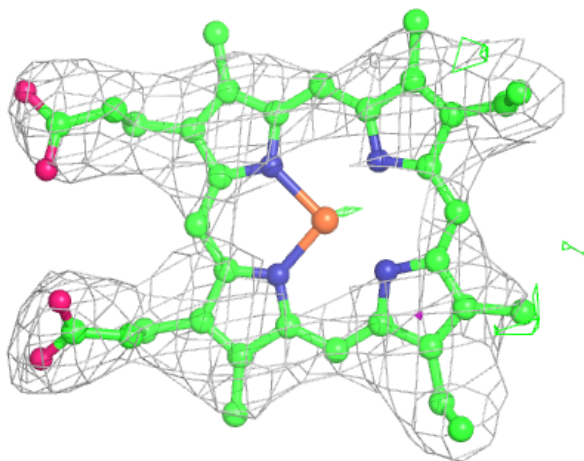
**Electron density around HEC P 604:**

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



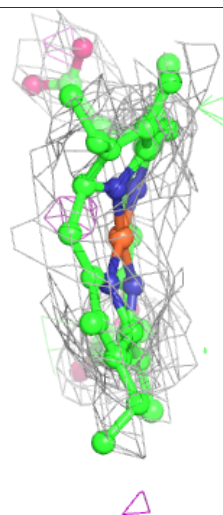
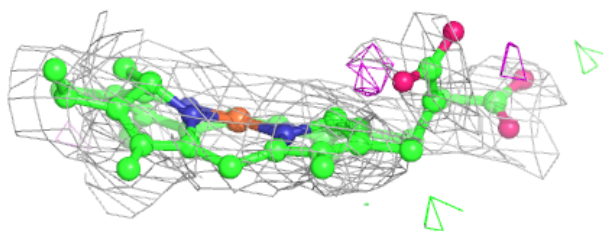
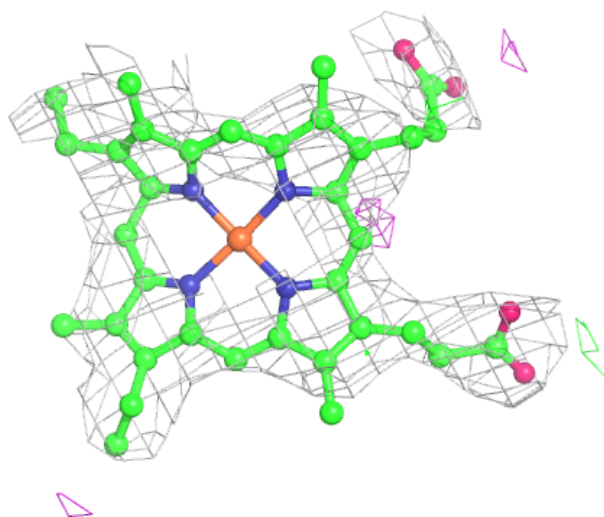
**Electron density around HEC T 604:**

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



**Electron density around HEC E 603:**

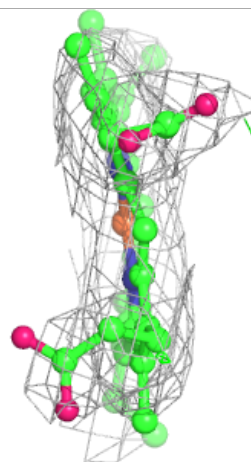
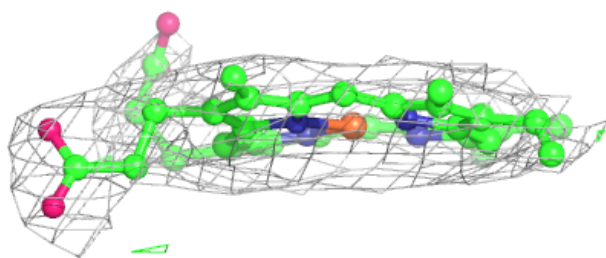
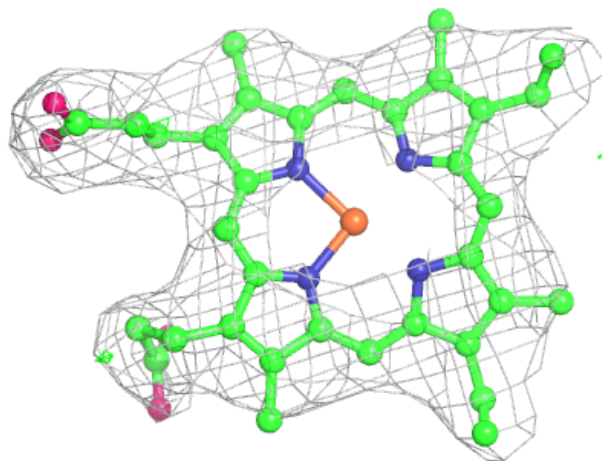
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





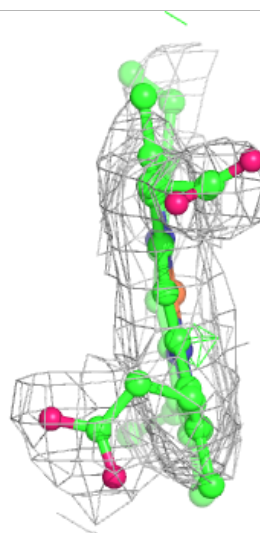
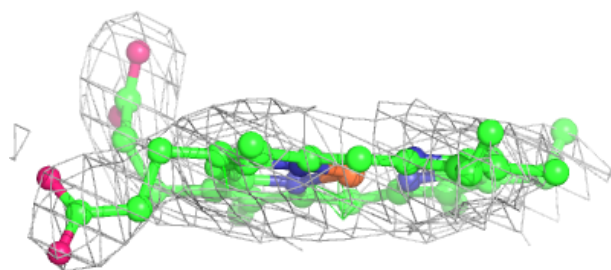
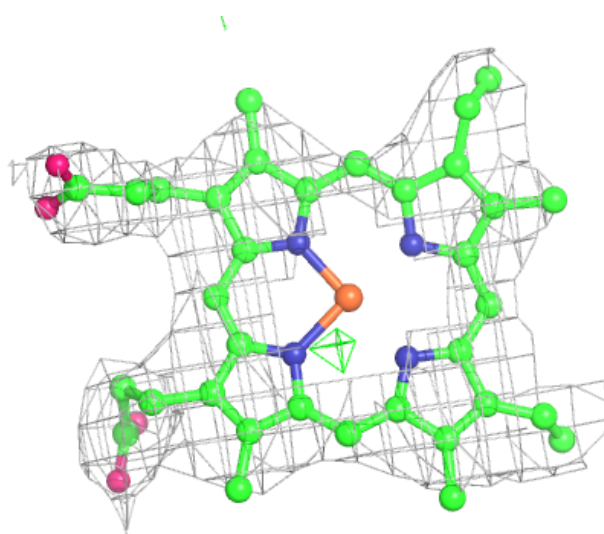
**Electron density around HEC D 602:**

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



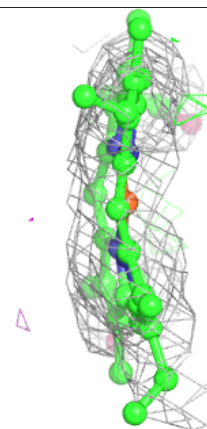
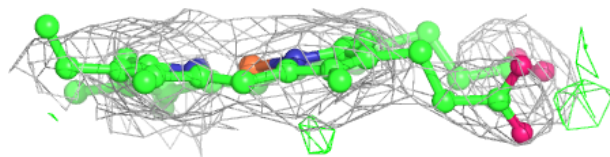
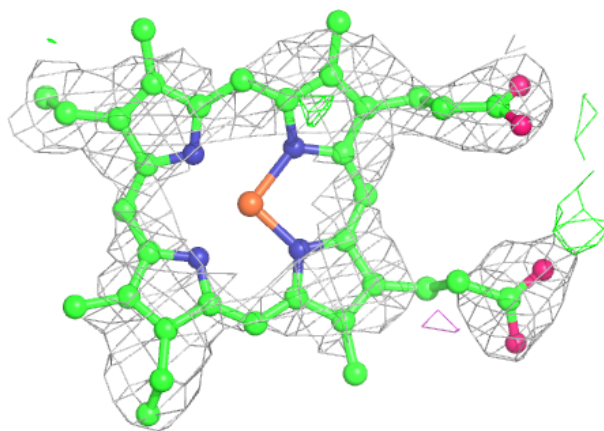
**Electron density around HEC U 601:**

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



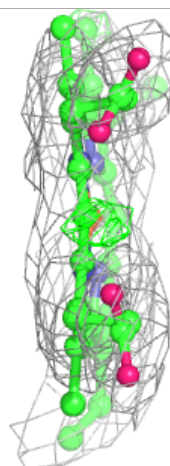
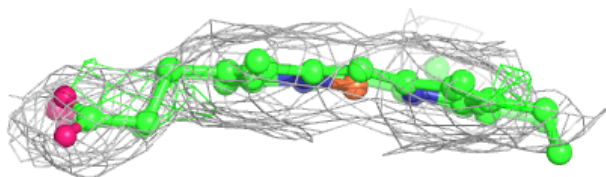
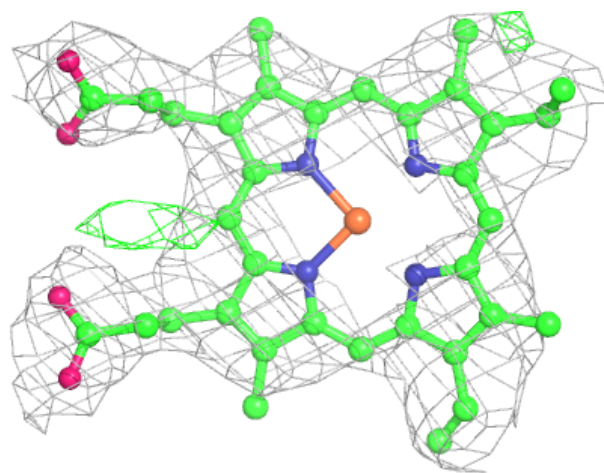
**Electron density around HEC W 606:**

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



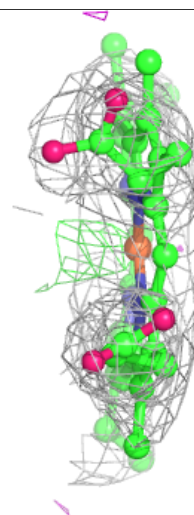
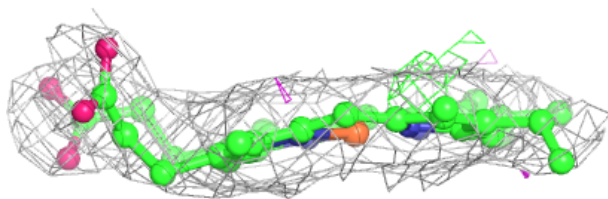
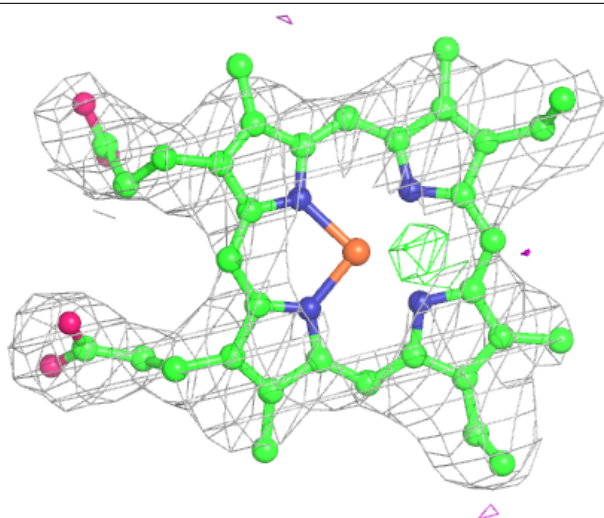
**Electron density around HEC Q 600:**

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



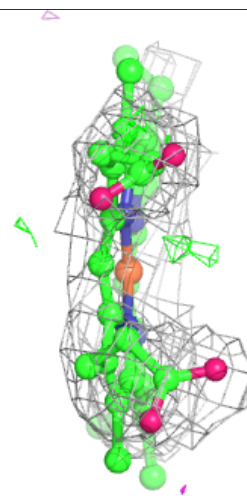
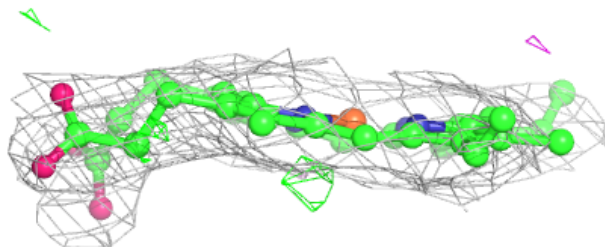
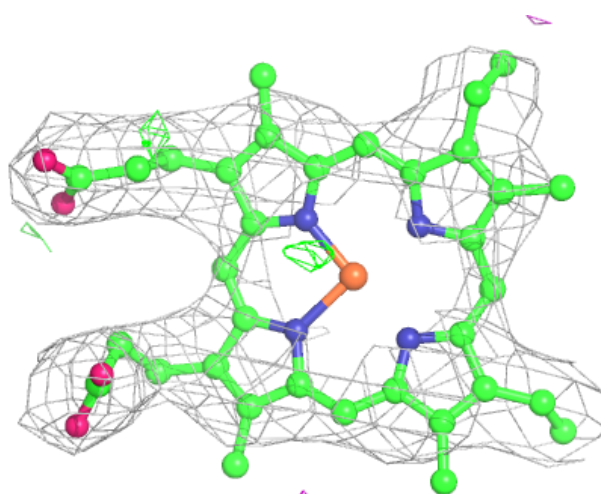
**Electron density around HEC S 607:**

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



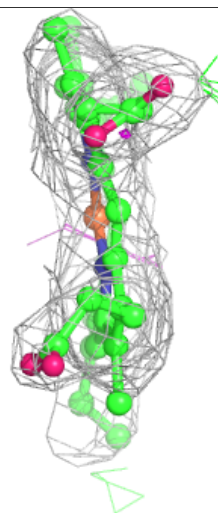
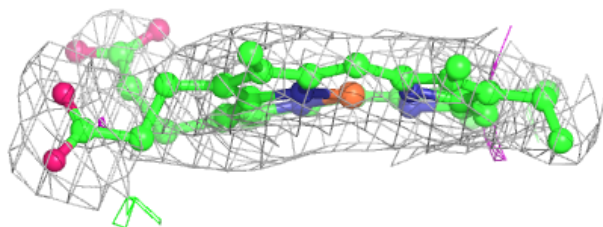
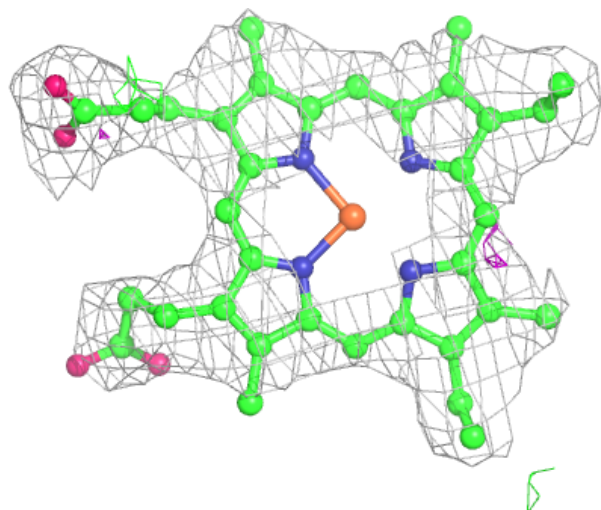
**Electron density around HEC W 607:**

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



**Electron density around HEC I 602:**

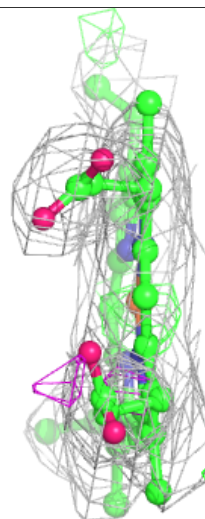
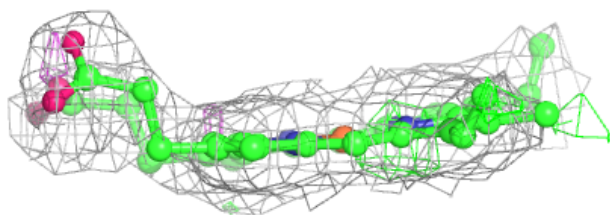
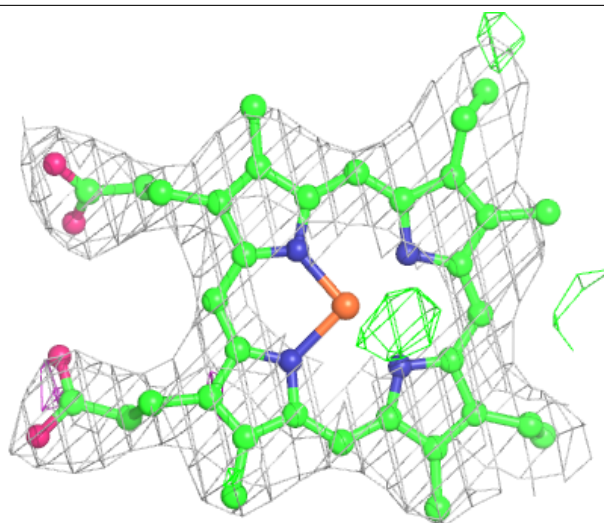
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC B 604:**

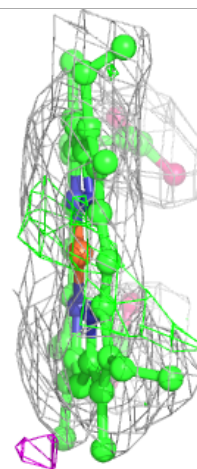
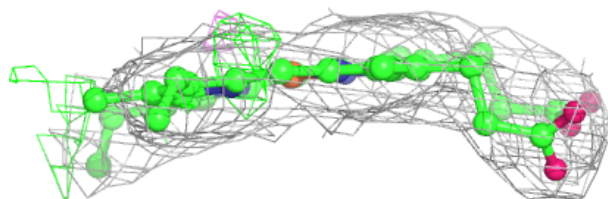
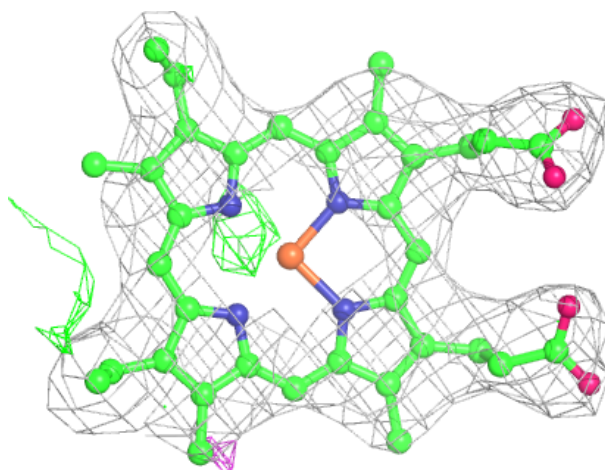
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





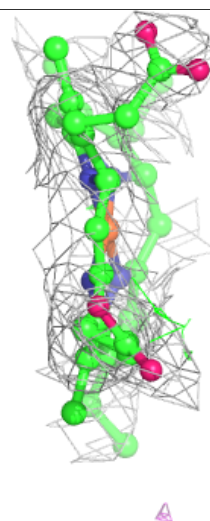
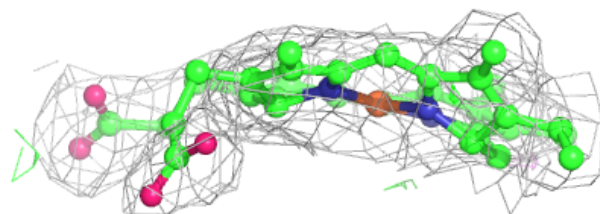
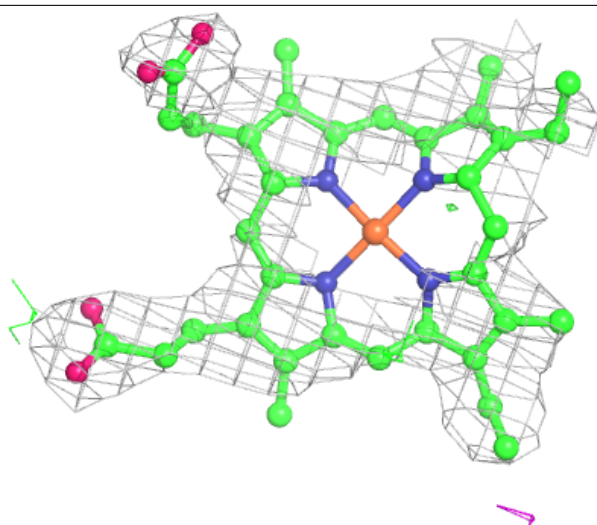
**Electron density around HEC O 604:**

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



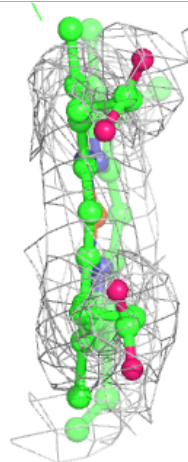
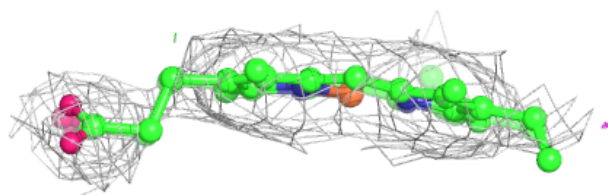
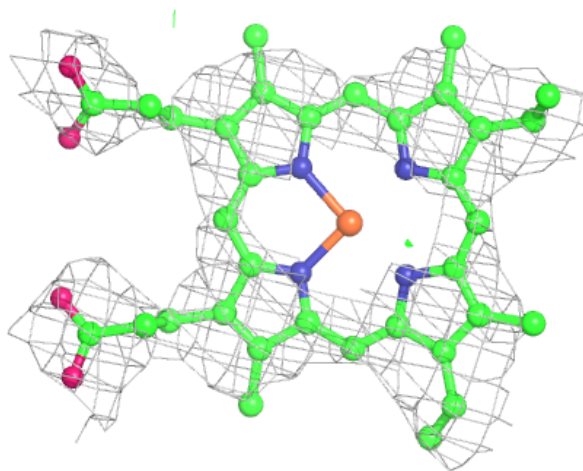
**Electron density around HEC U 603:**

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



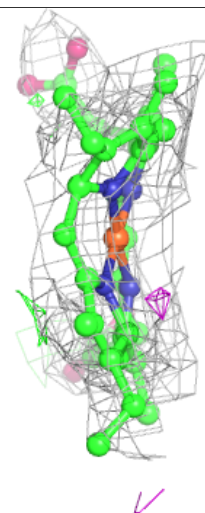
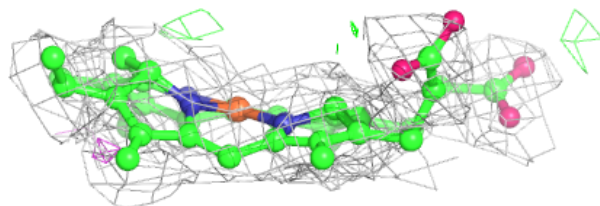
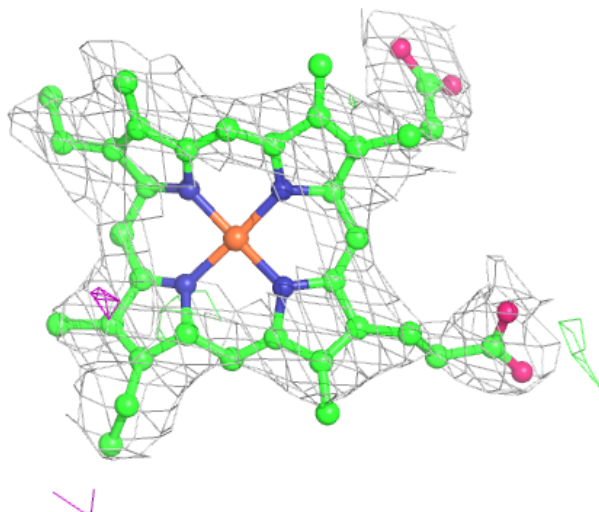
**Electron density around HEC V 600:**

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



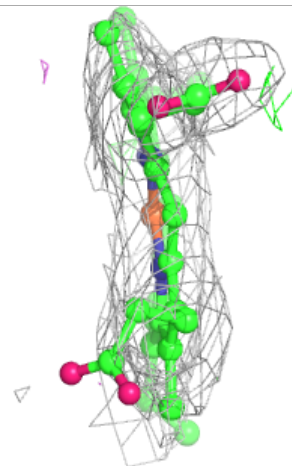
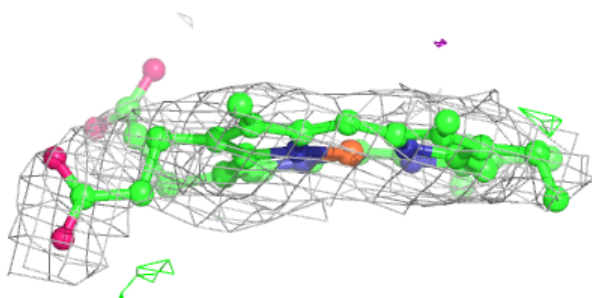
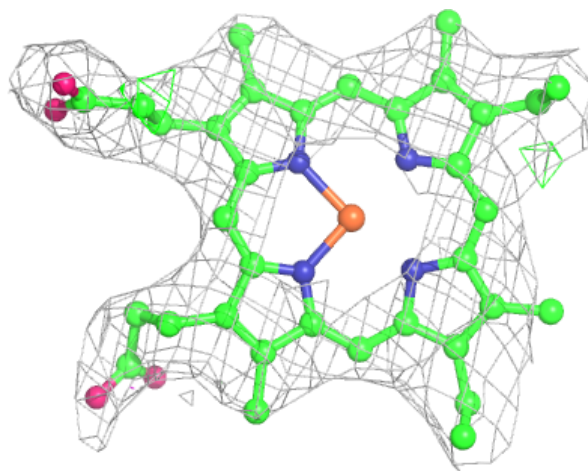
**Electron density around HEC A 603:**

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



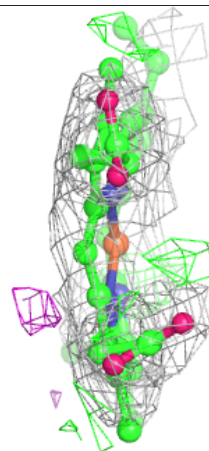
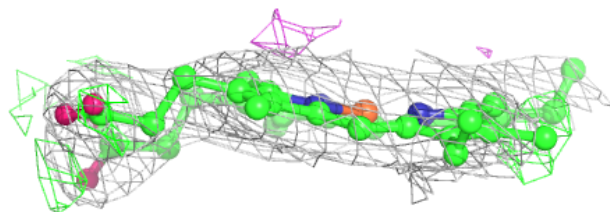
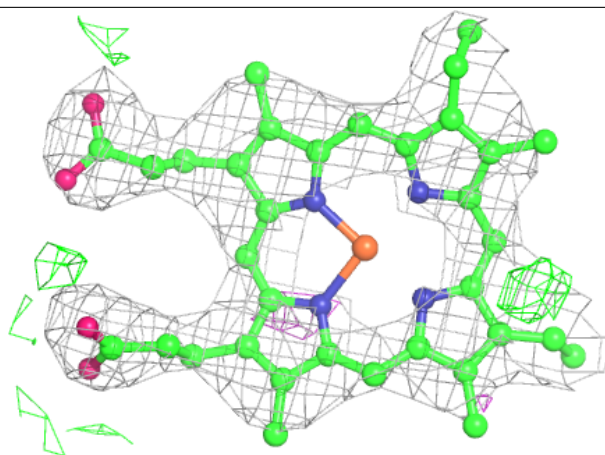
**Electron density around HEC O 602:**

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



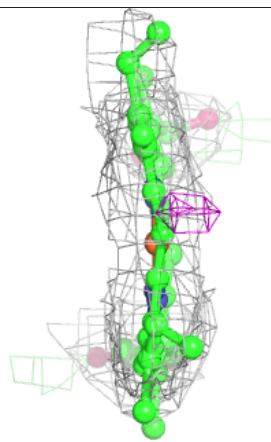
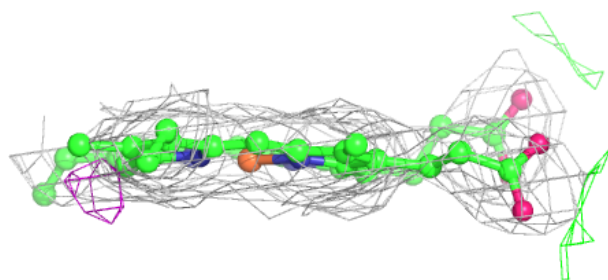
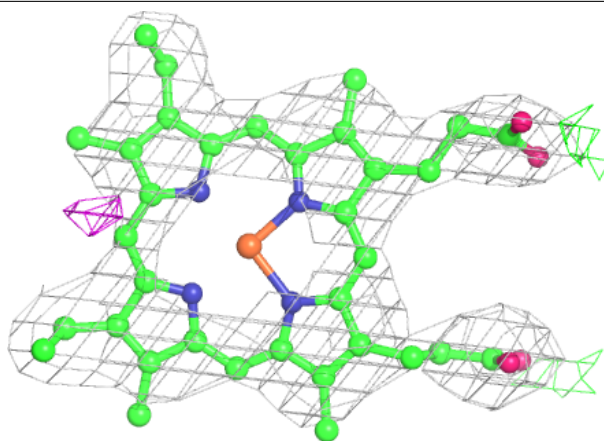
**Electron density around HEC F 606:**

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



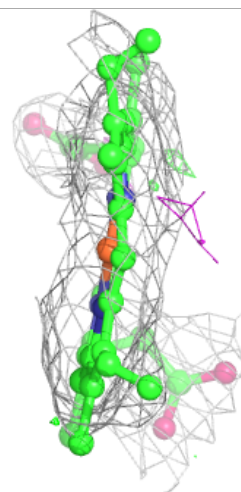
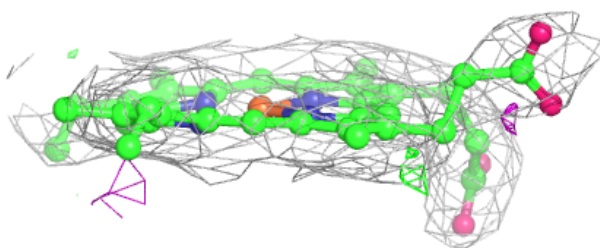
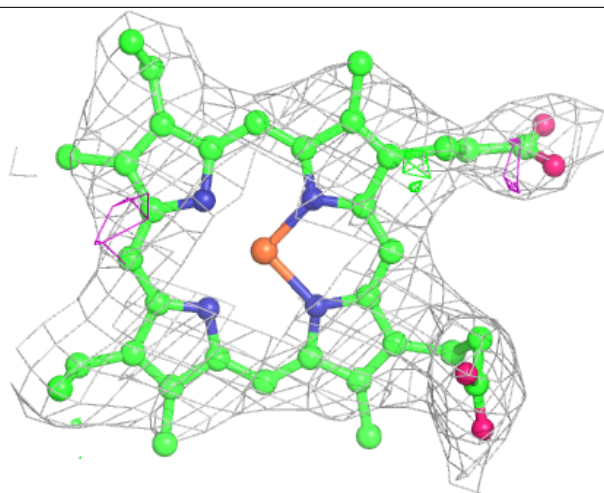
**Electron density around HEC D 605:**

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



**Electron density around HEC Q 601:**

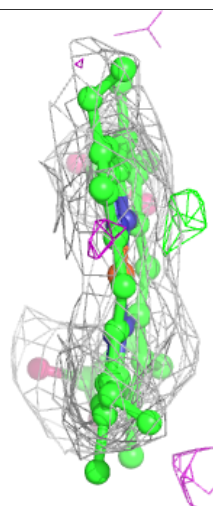
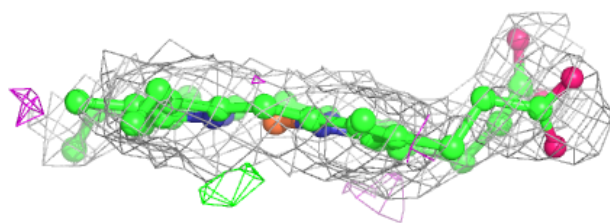
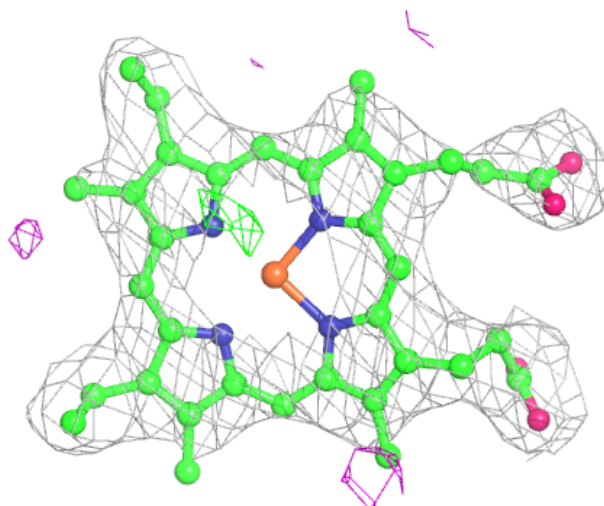
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





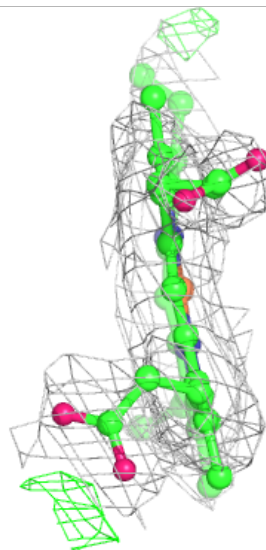
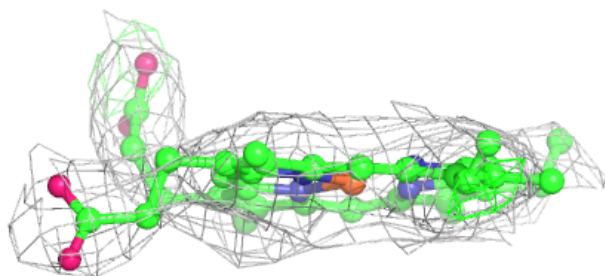
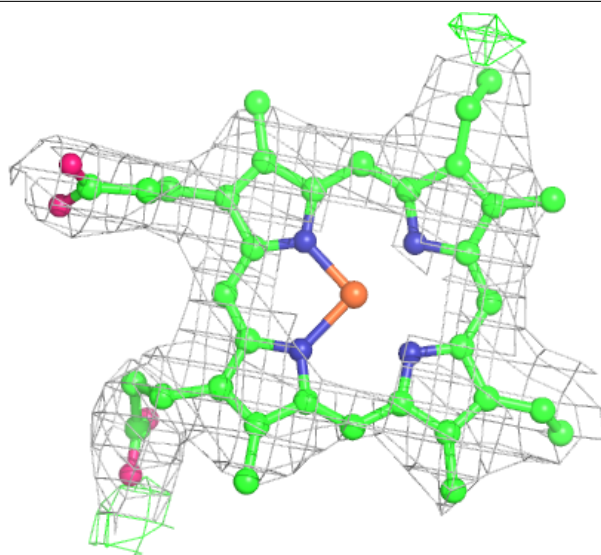
**Electron density around HEC F 607:**

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



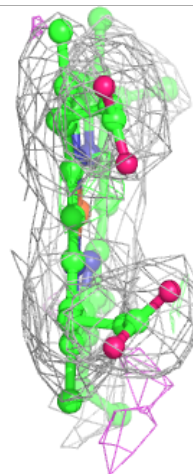
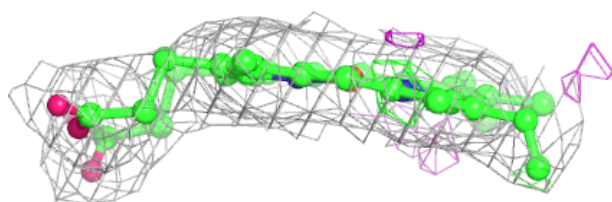
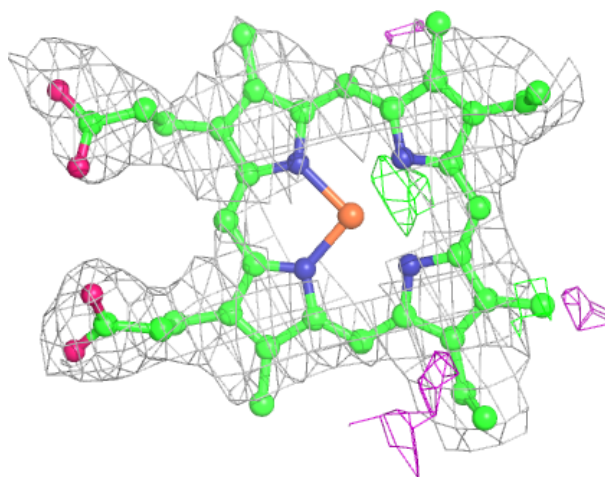
**Electron density around HEC V 601:**

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



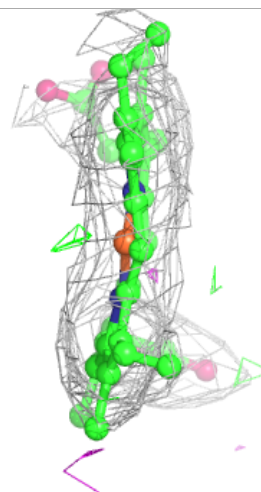
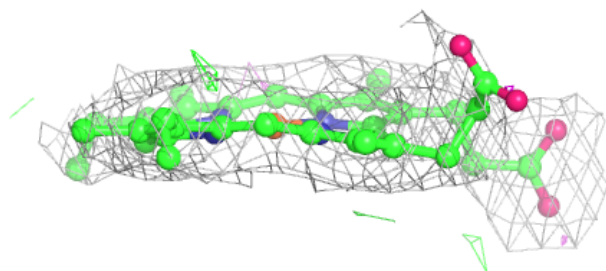
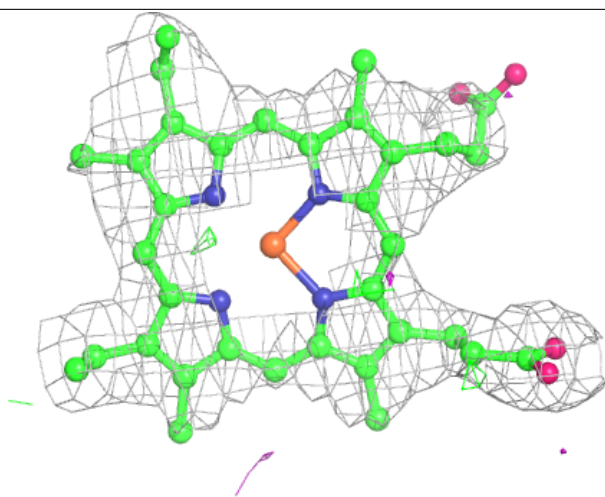
**Electron density around HEC M 604:**

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



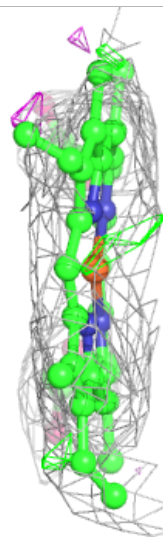
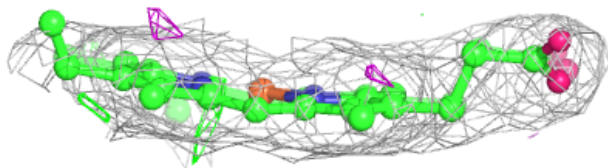
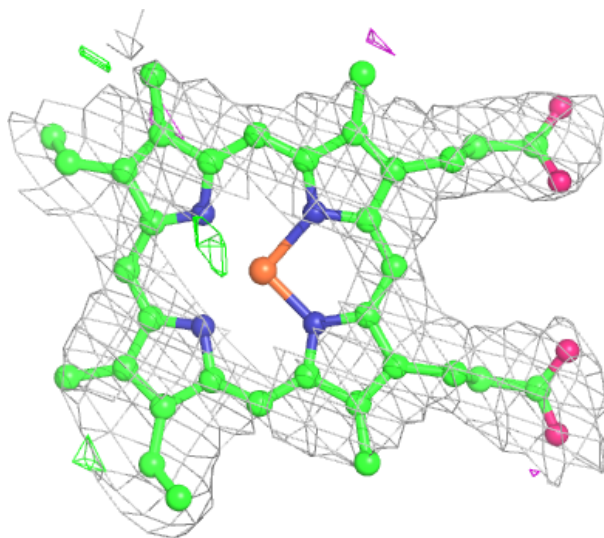
**Electron density around HEC M 602:**

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



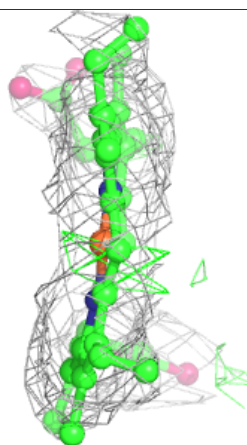
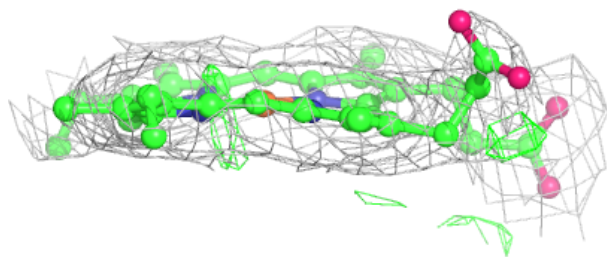
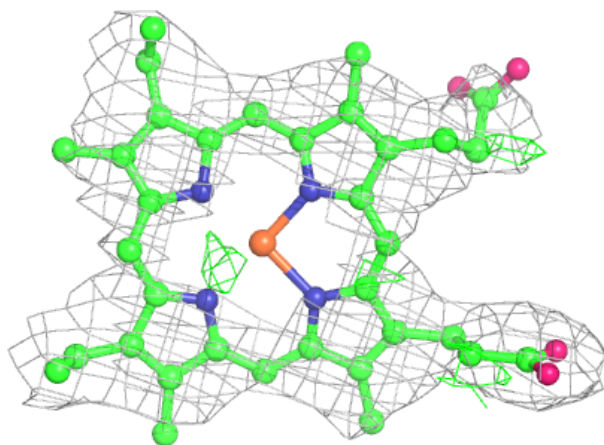
**Electron density around HEC A 600:**

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



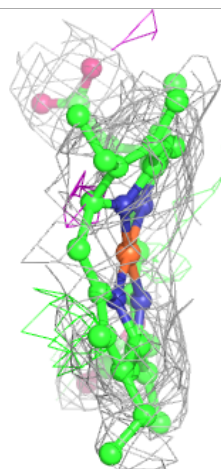
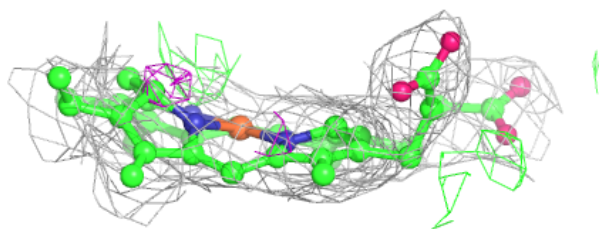
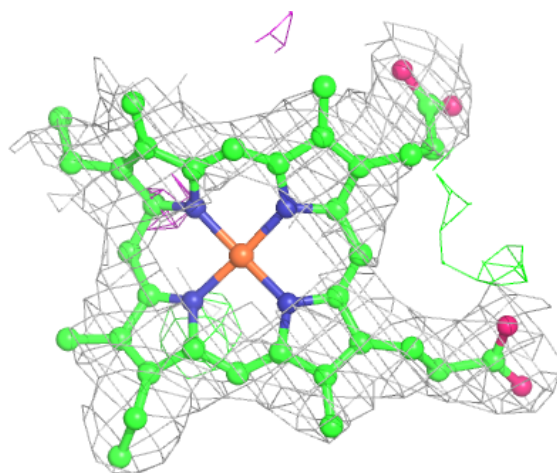
**Electron density around HEC C 602:**

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



**Electron density around HEC O 603:**

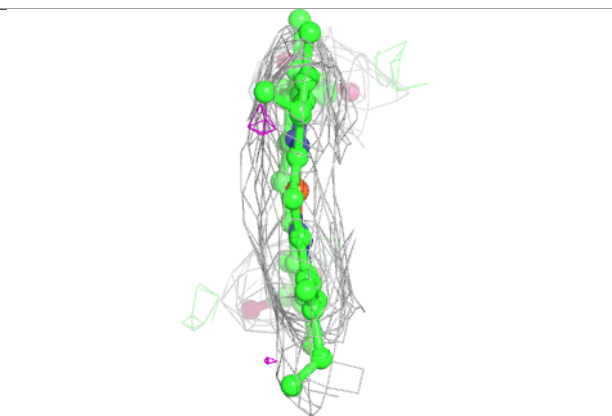
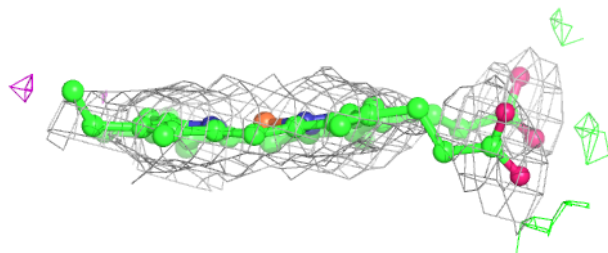
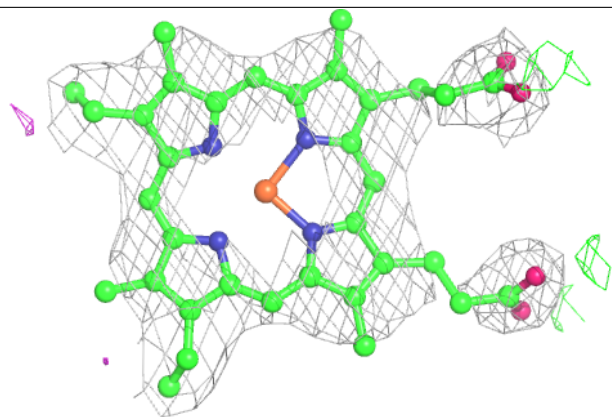
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



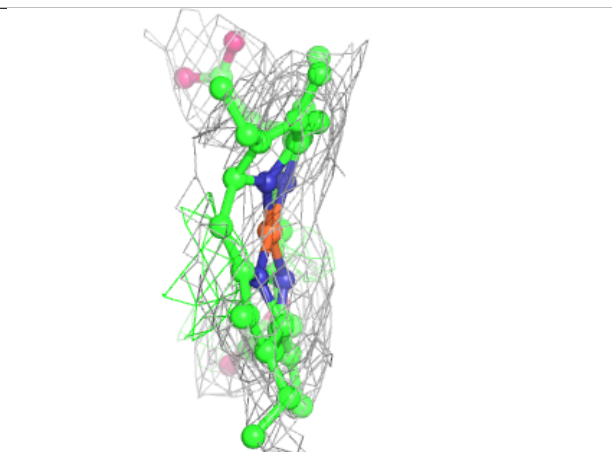
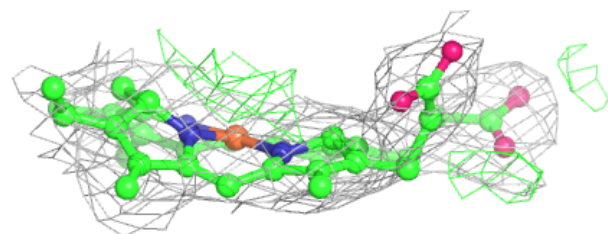
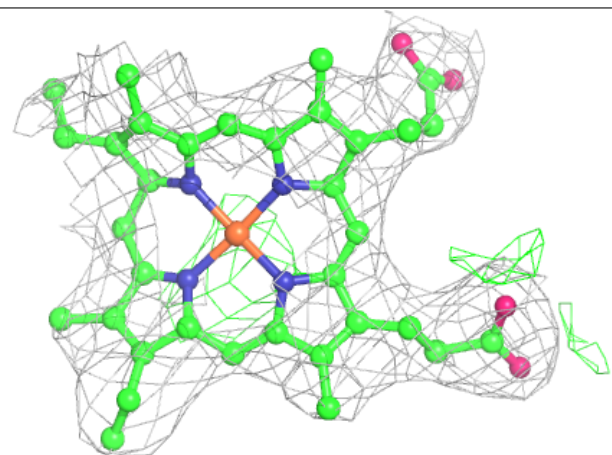


**Electron density around HEC T 605:**

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

**Electron density around HEC C 603:**

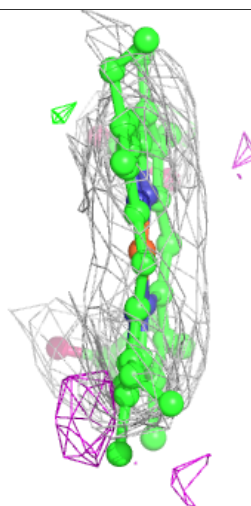
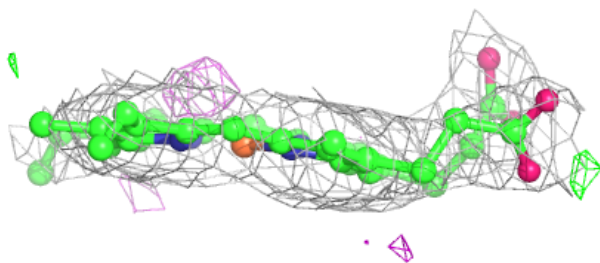
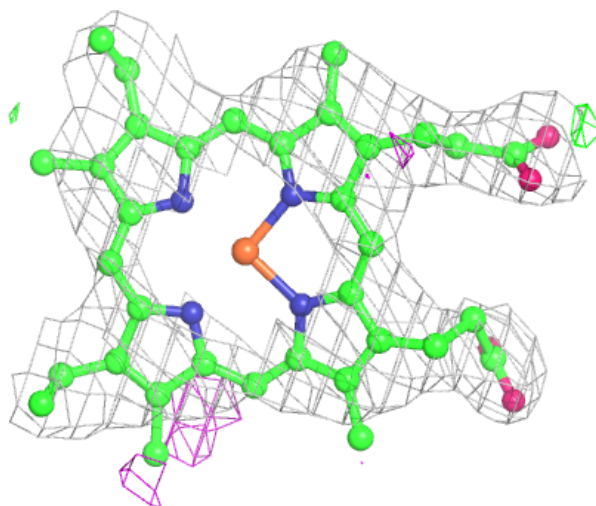
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





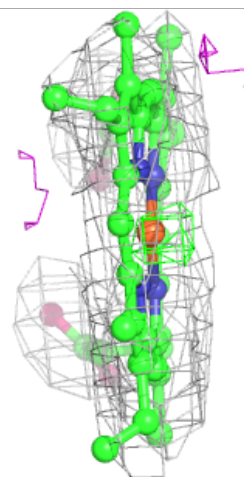
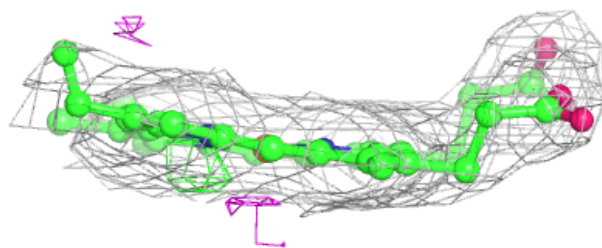
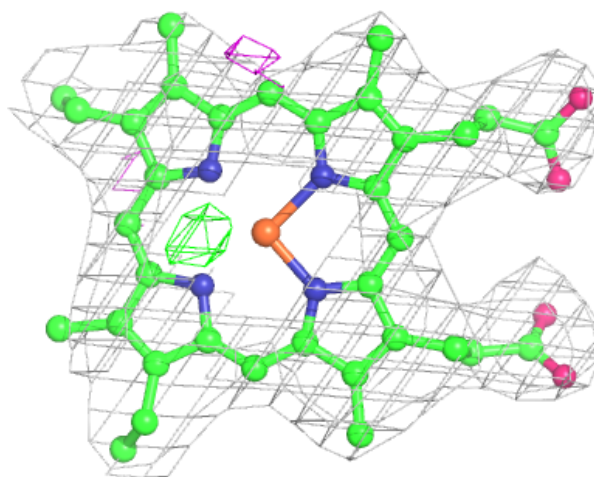
**Electron density around HEC E 607:**

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



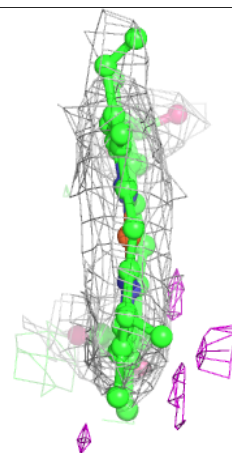
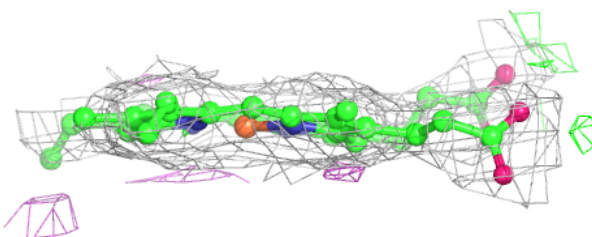
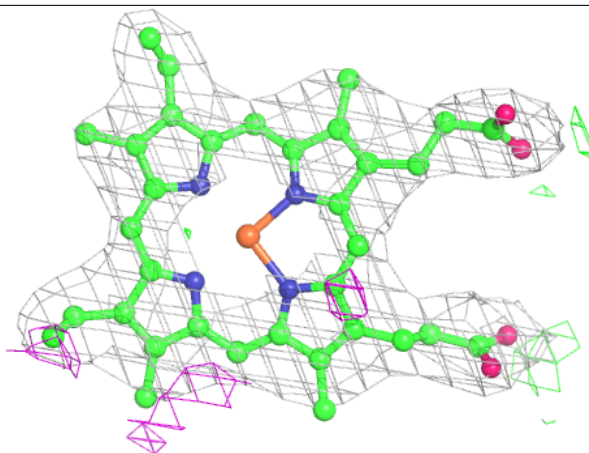
**Electron density around HEC E 604:**

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



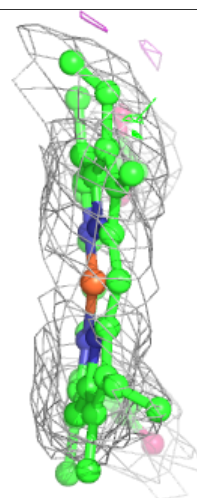
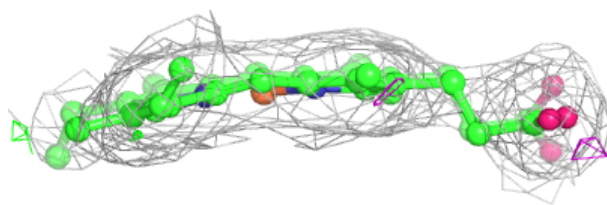
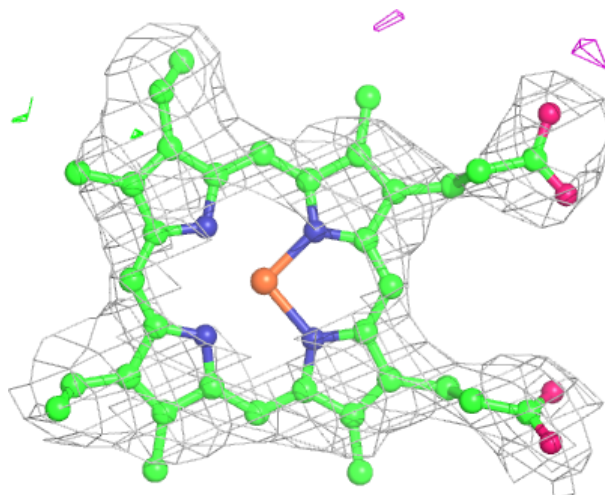
**Electron density around HEC M 605:**

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



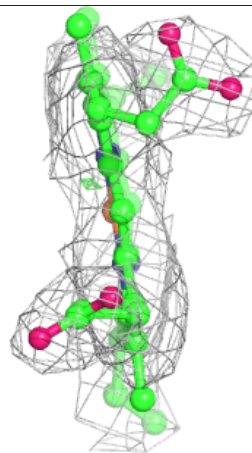
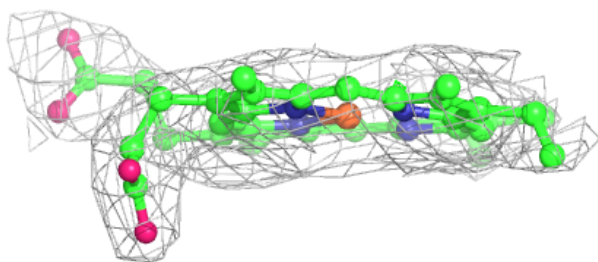
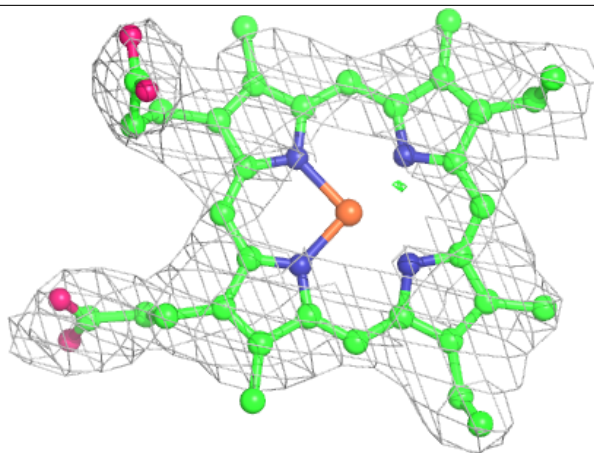
**Electron density around HEC D 600:**

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



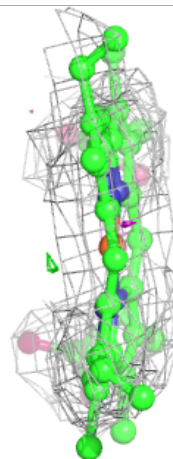
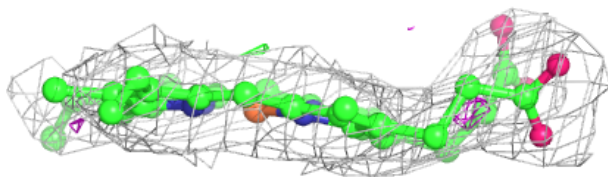
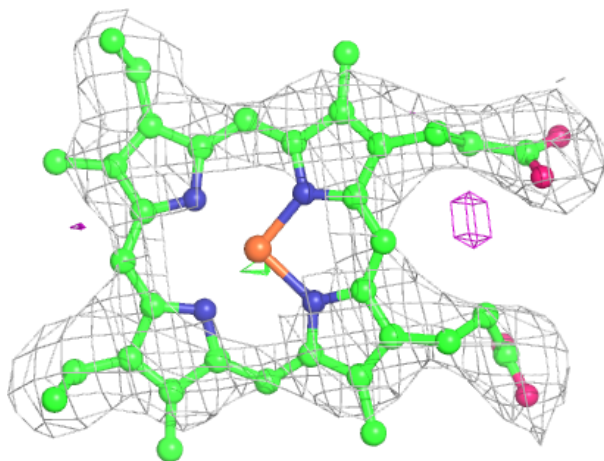
**Electron density around HEC O 601:**

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



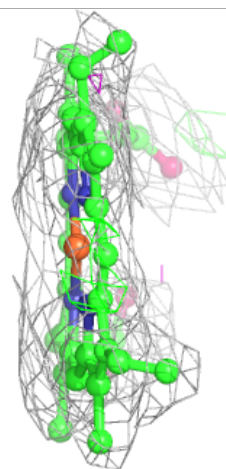
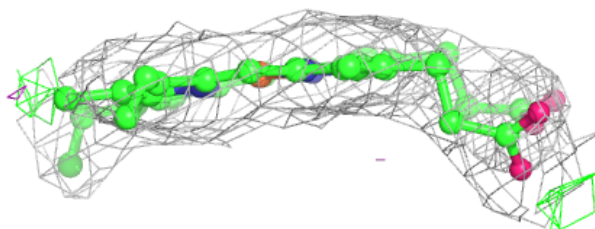
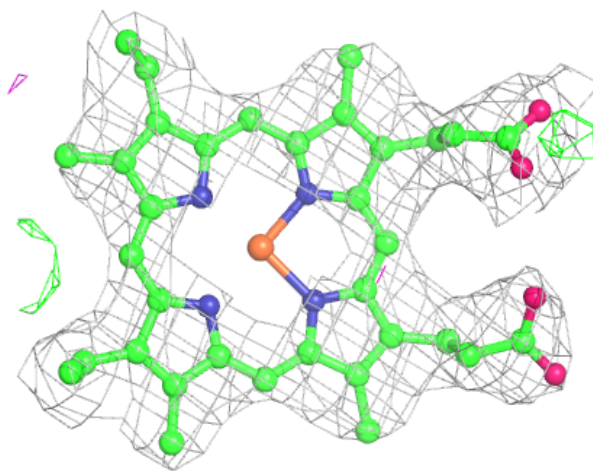
**Electron density around HEC V 607:**

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



**Electron density around HEC K 604:**

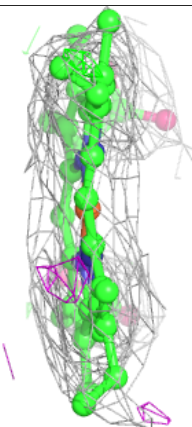
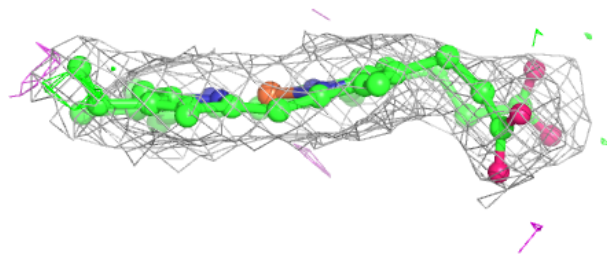
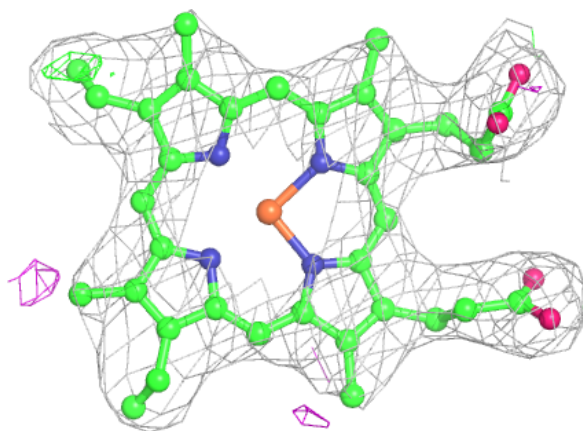
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC P 607:**

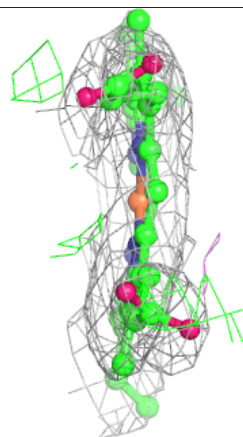
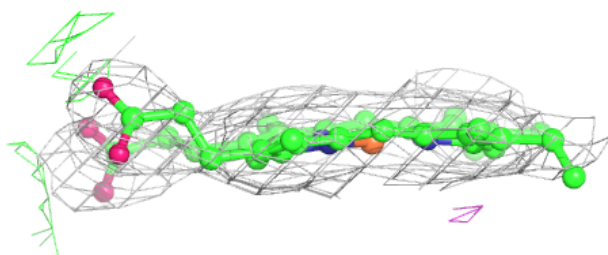
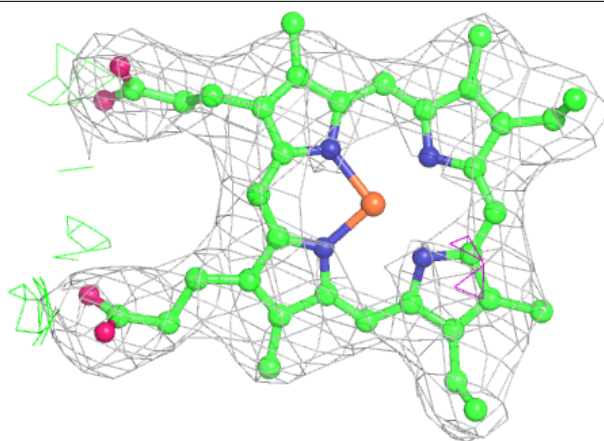
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





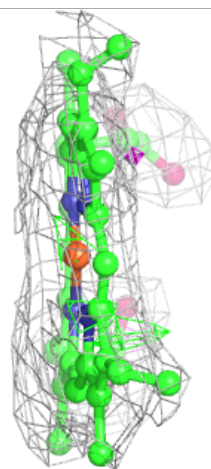
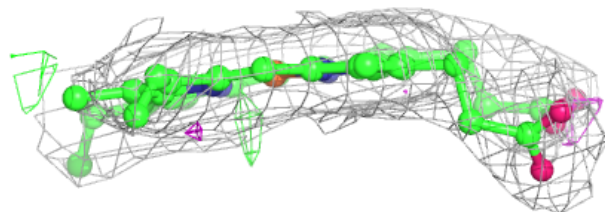
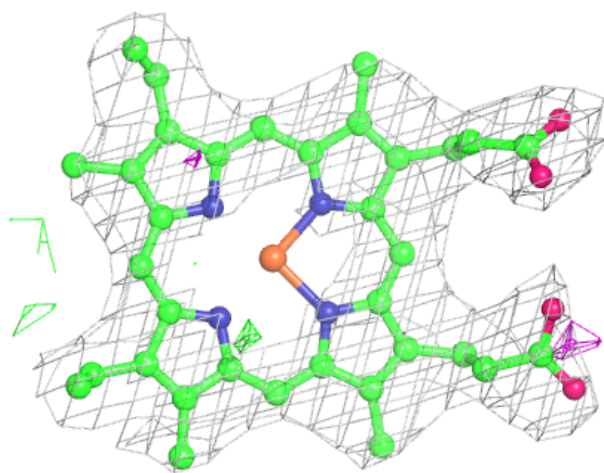
**Electron density around HEC C 605:**

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



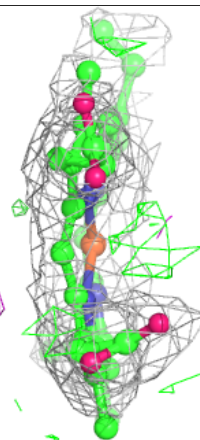
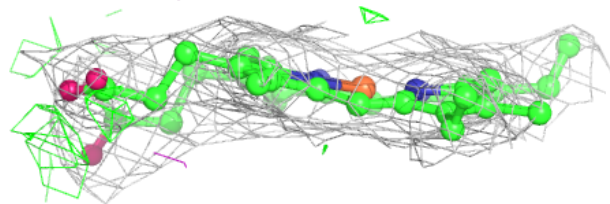
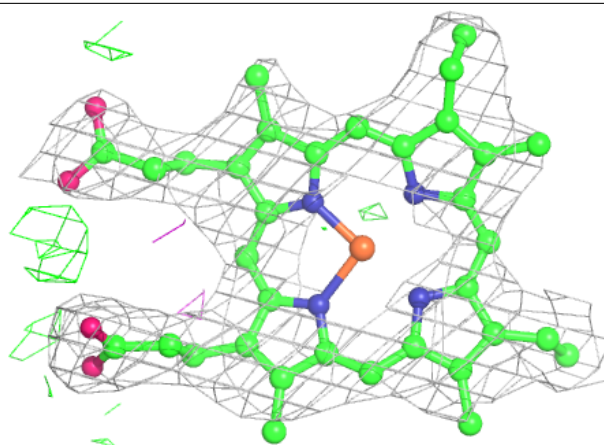
**Electron density around HEC G 604:**

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



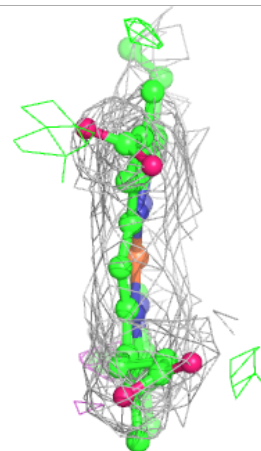
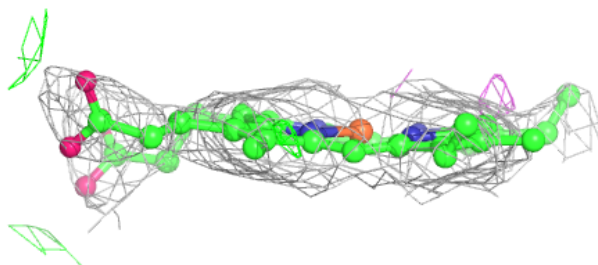
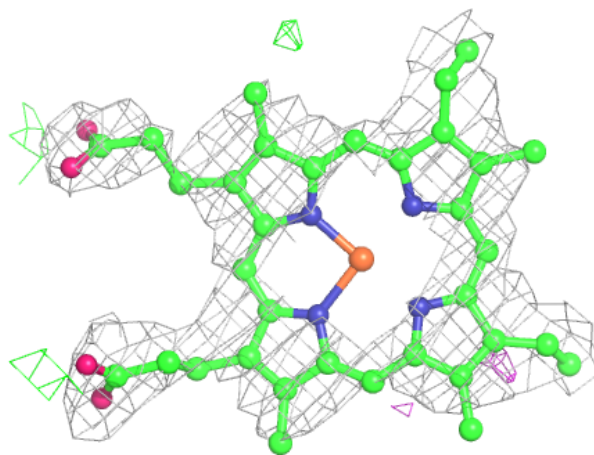
**Electron density around HEC Q 606:**

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



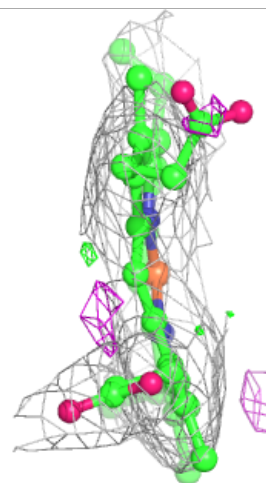
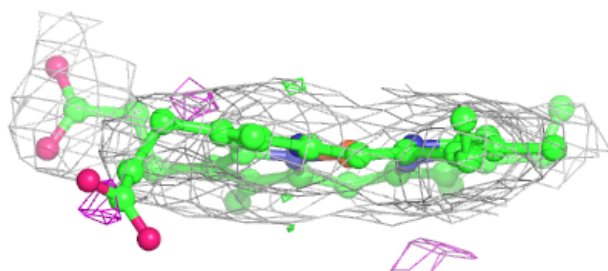
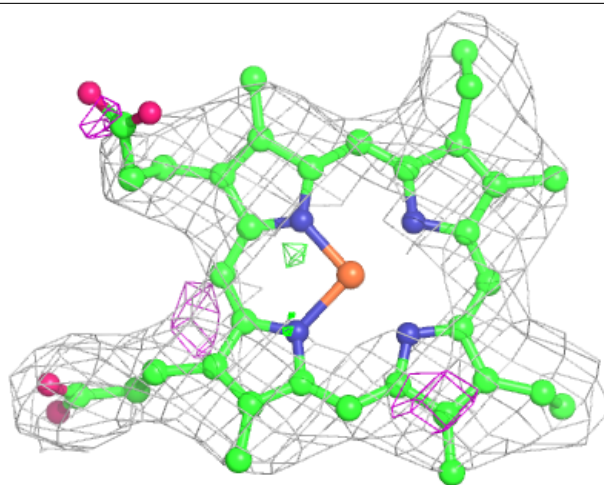
**Electron density around HEC U 605:**

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



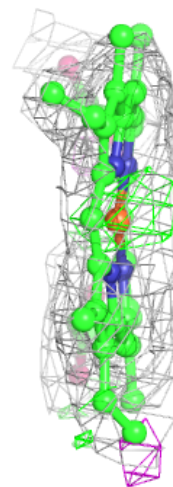
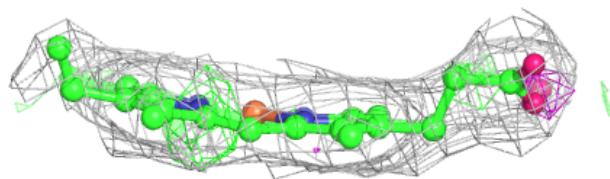
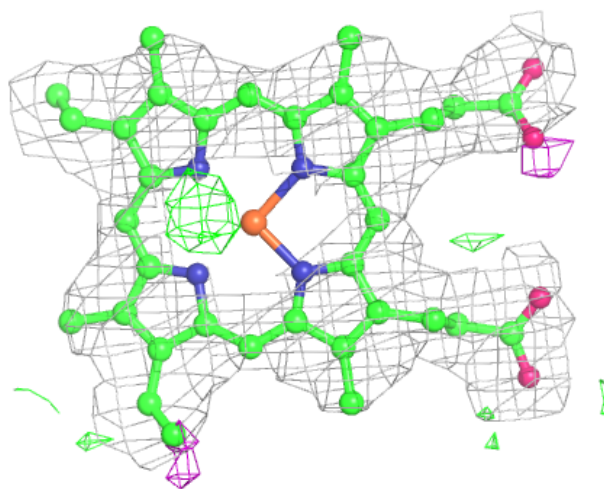
**Electron density around HEC J 602:**

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



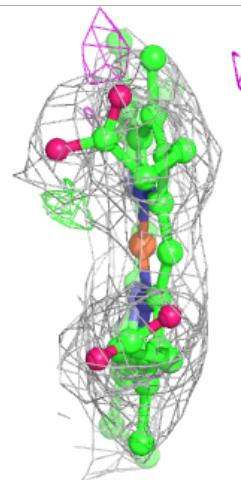
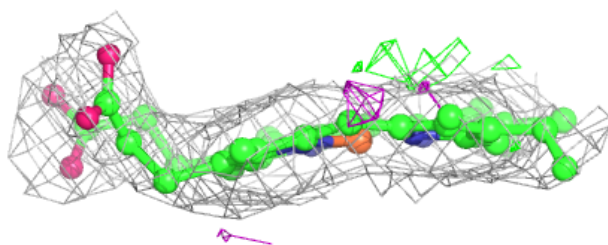
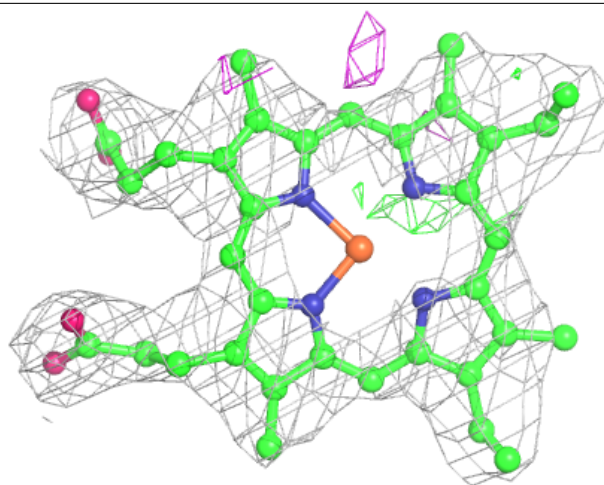
**Electron density around HEC J 600:**

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



**Electron density around HEC C 607:**

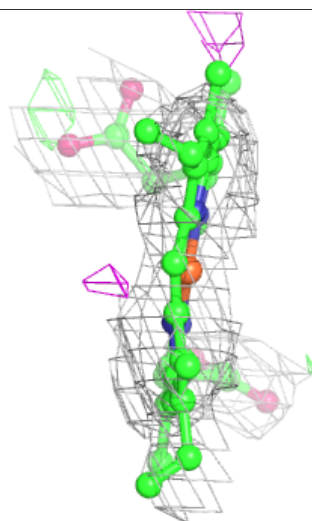
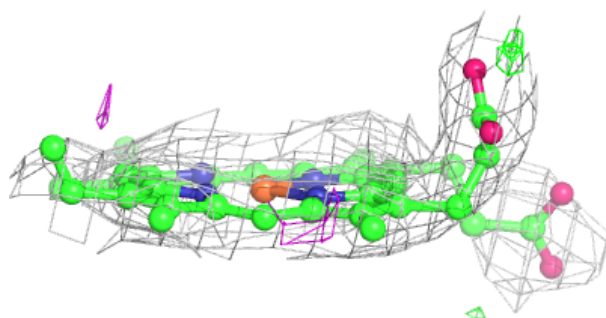
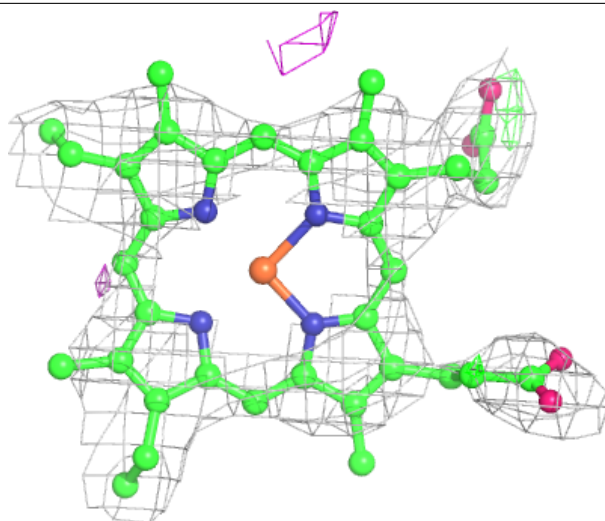
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC W 601:**

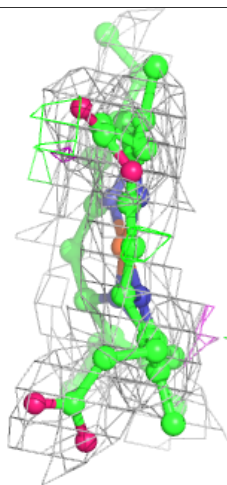
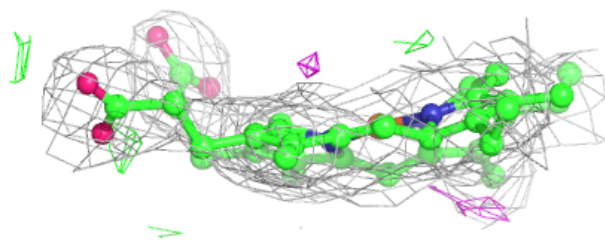
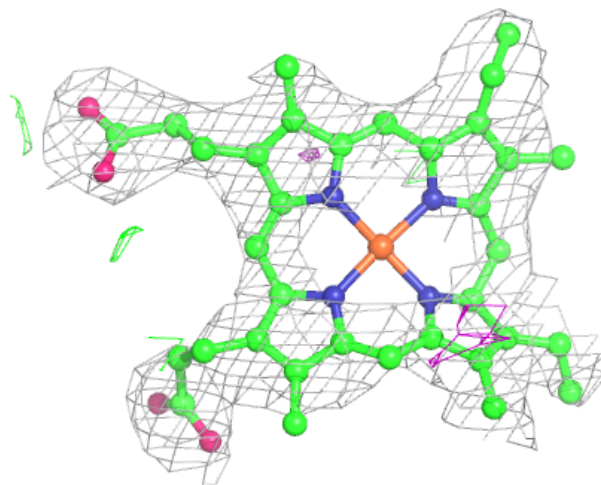
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





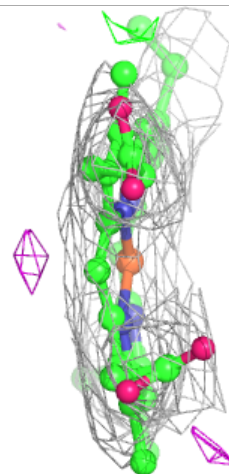
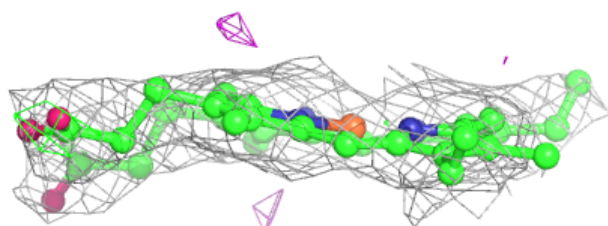
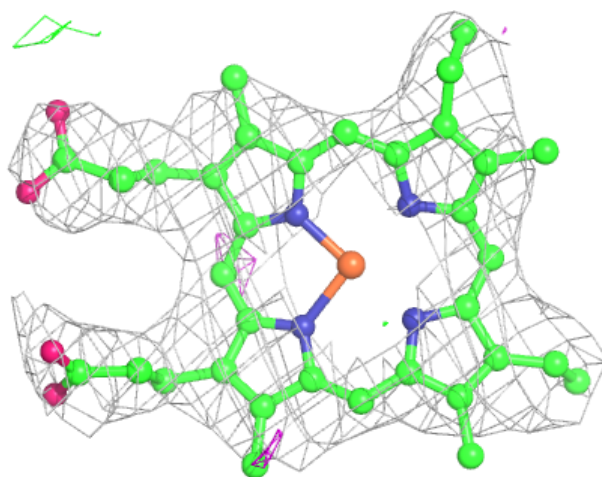
**Electron density around HEC M 603:**

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



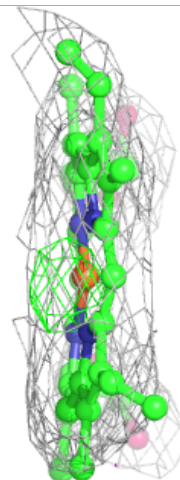
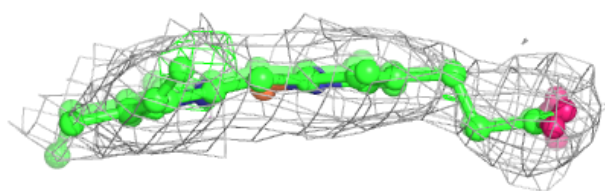
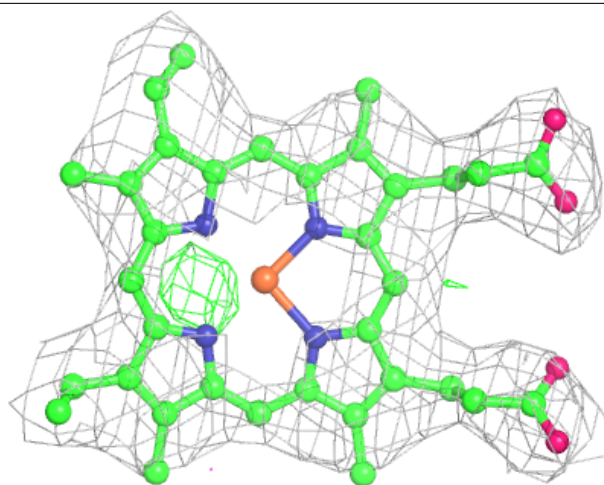
**Electron density around HEC V 606:**

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



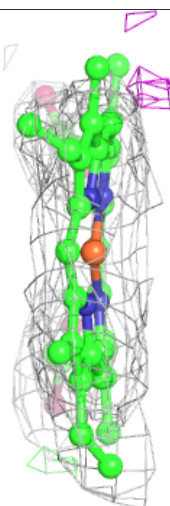
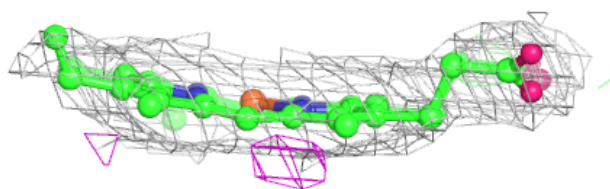
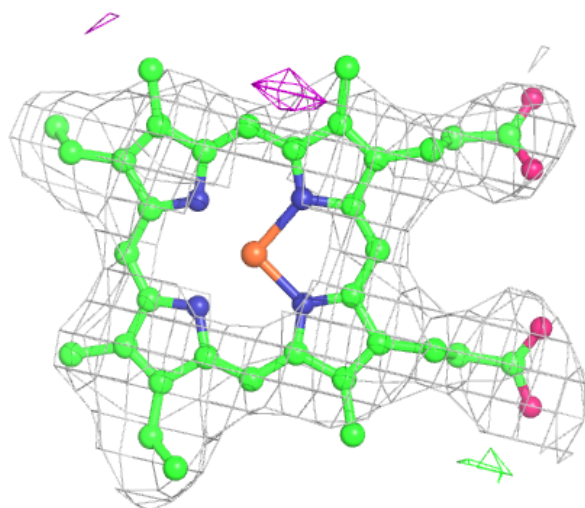
**Electron density around HEC X 600:**

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



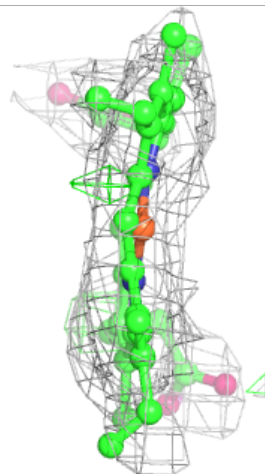
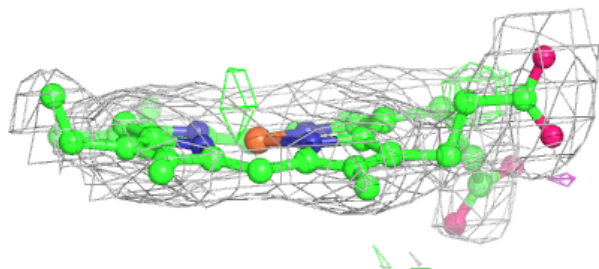
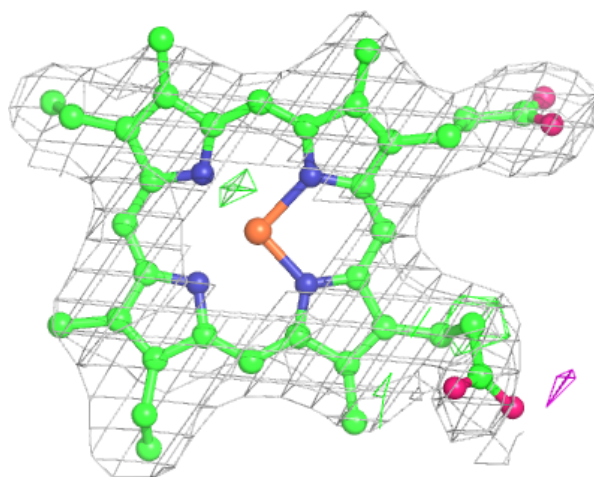
**Electron density around HEC B 600:**

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



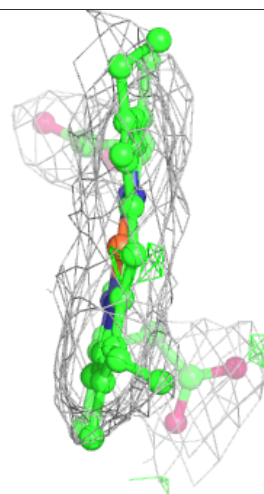
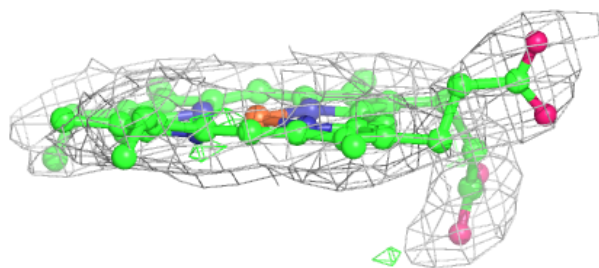
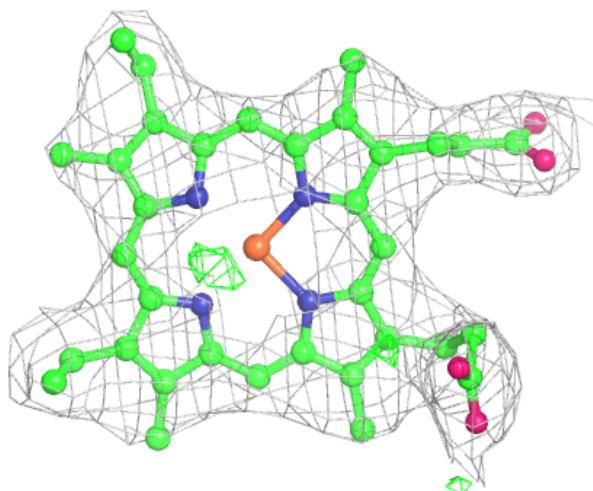
**Electron density around HEC G 602:**

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



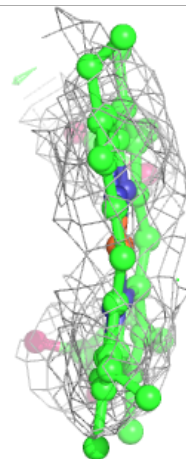
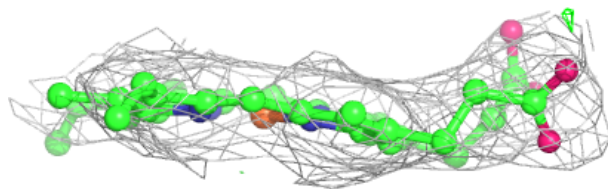
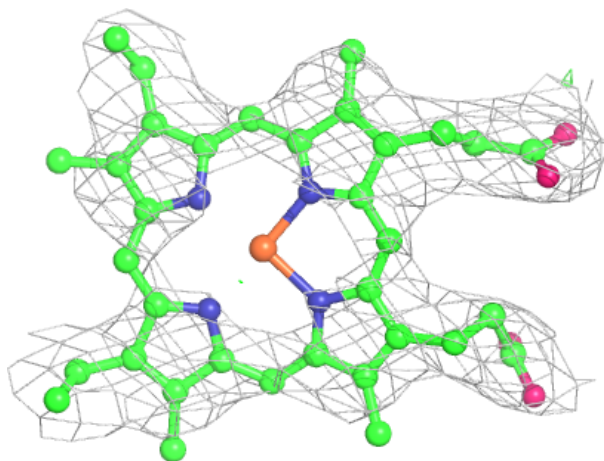
**Electron density around HEC L 601:**

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



**Electron density around HEC U 607:**

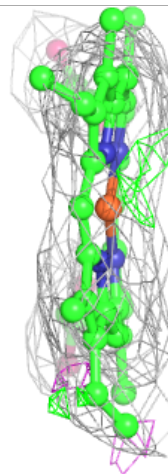
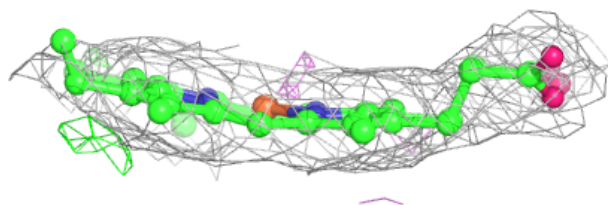
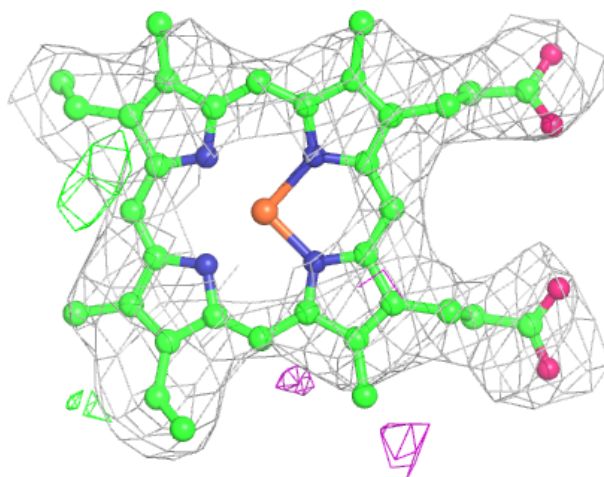
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC M 600:**

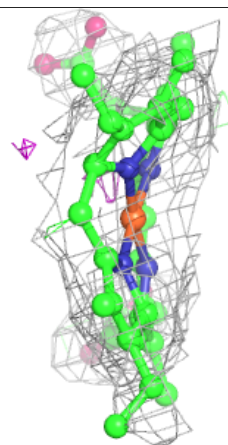
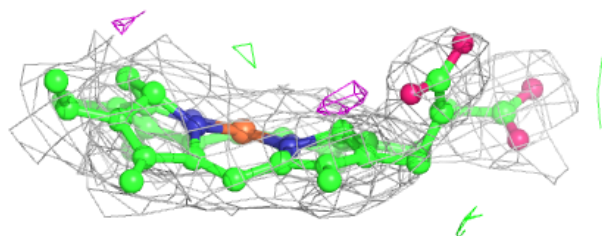
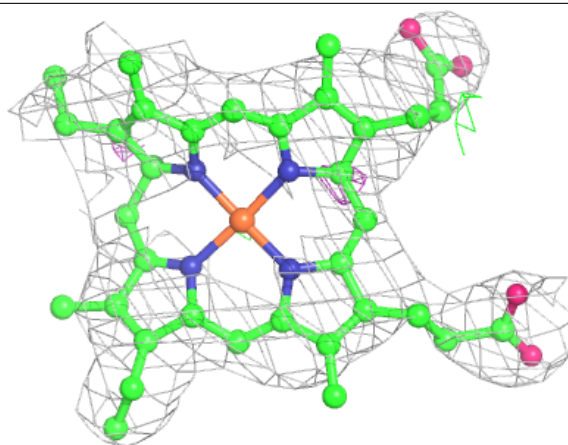
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





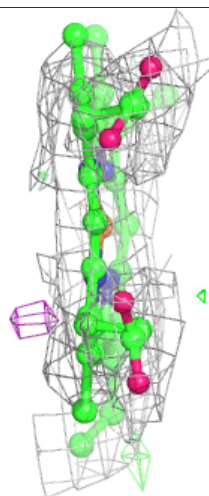
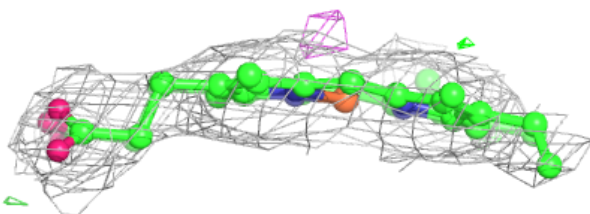
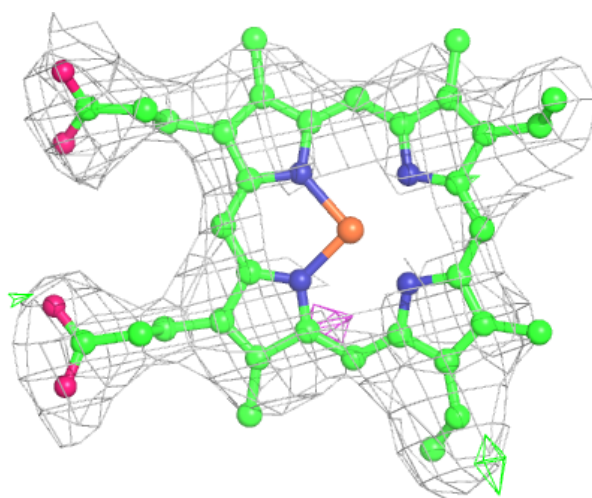
**Electron density around HEC T 603:**

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



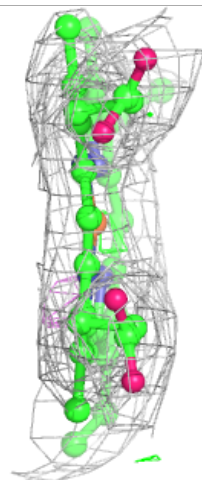
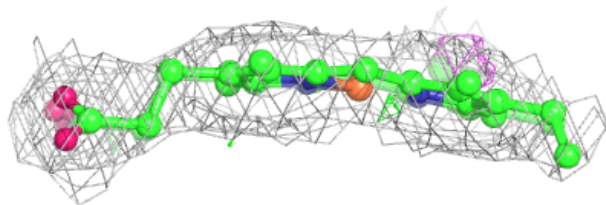
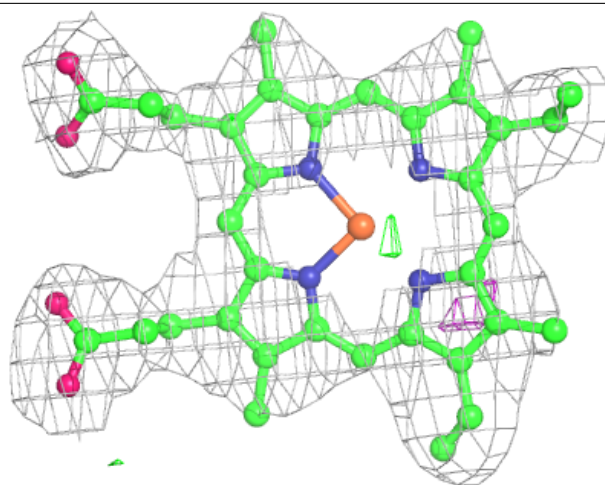
**Electron density around HEC R 600:**

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



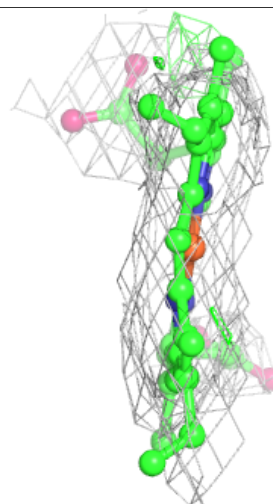
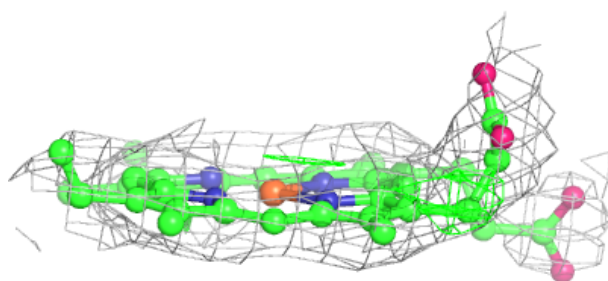
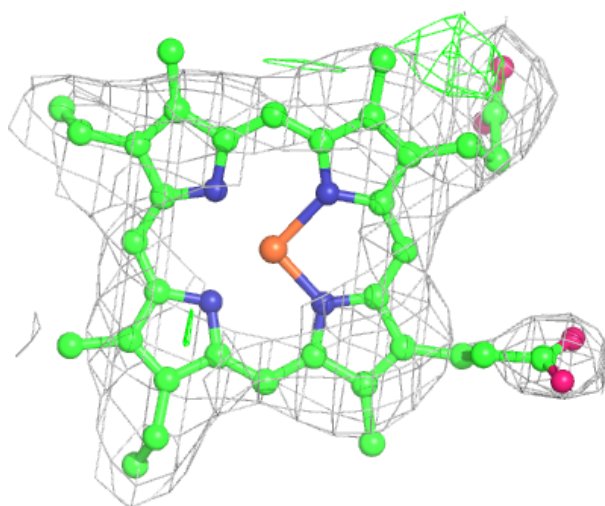
**Electron density around HEC G 600:**

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



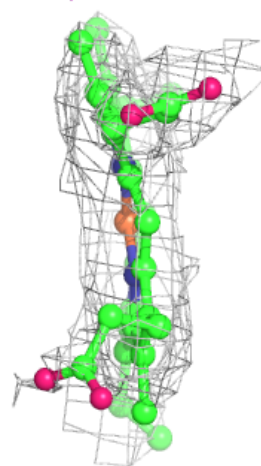
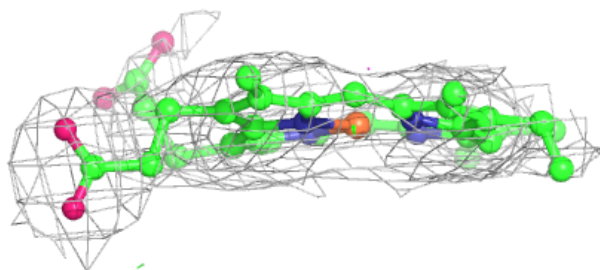
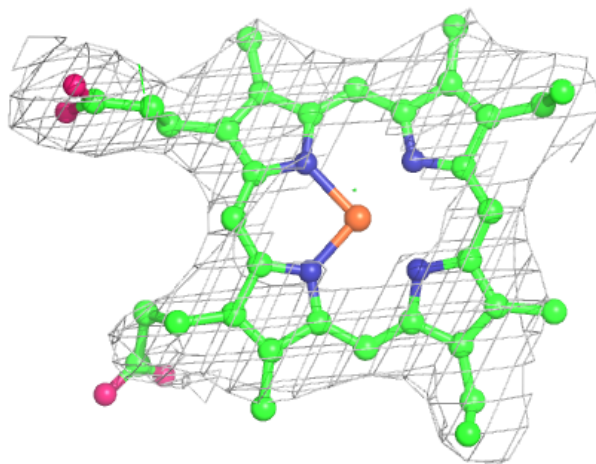
**Electron density around HEC X 601:**

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



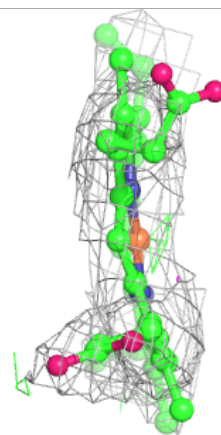
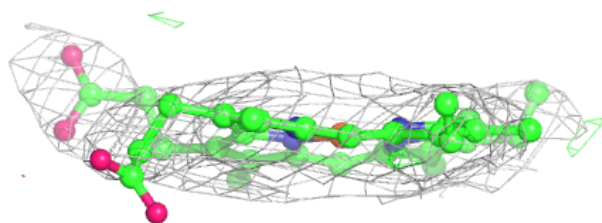
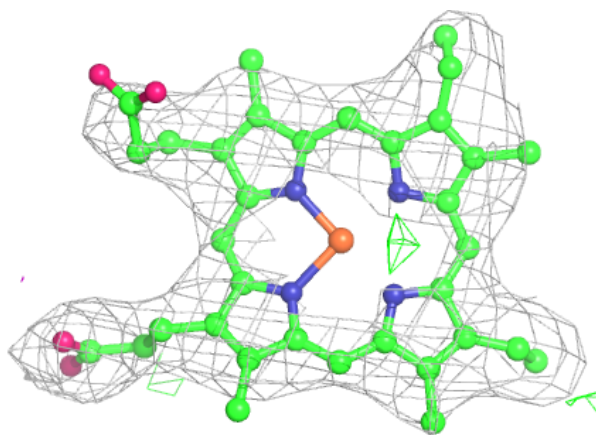
**Electron density around HEC R 602:**

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



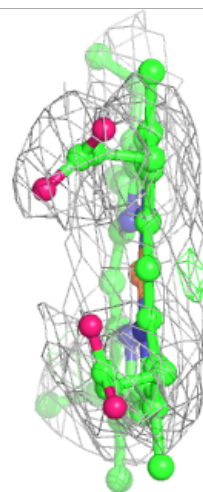
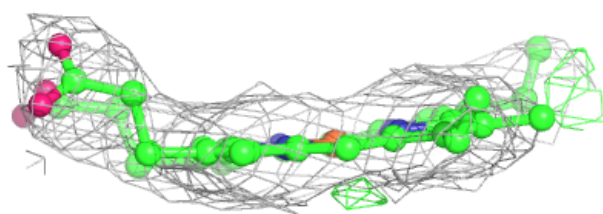
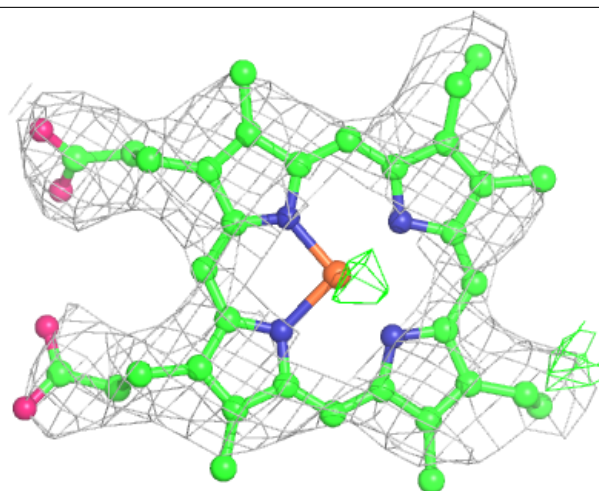
**Electron density around HEC A 602:**

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



**Electron density around HEC F 604:**

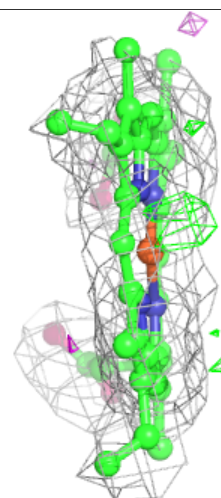
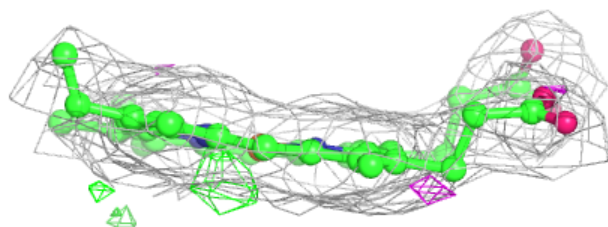
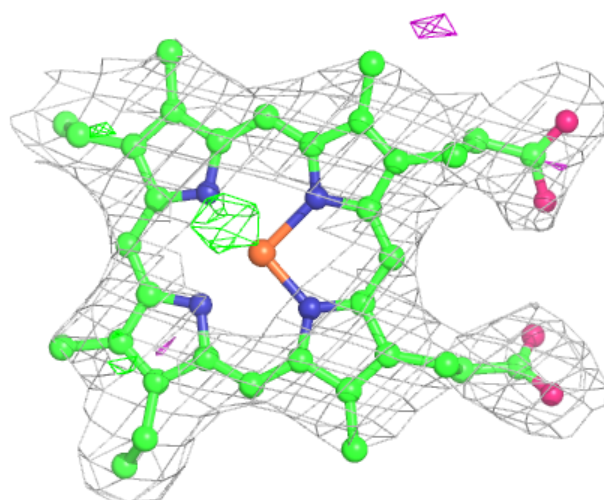
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC R 604:**

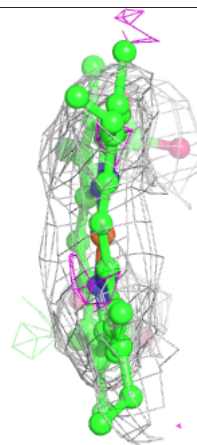
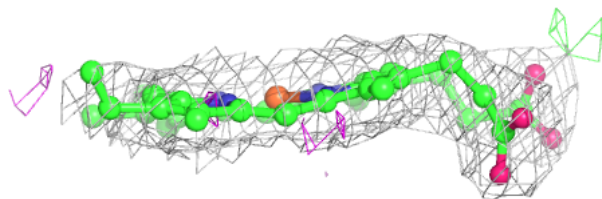
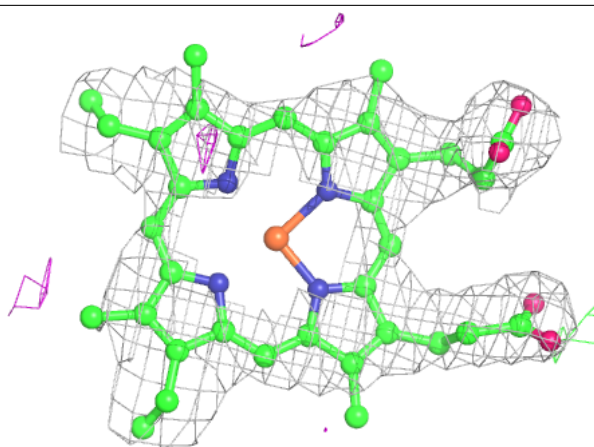
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





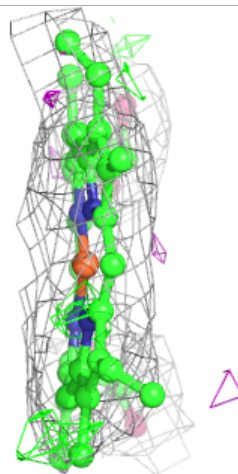
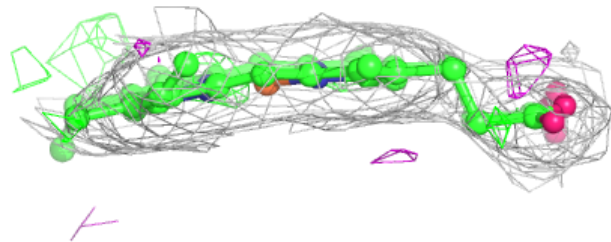
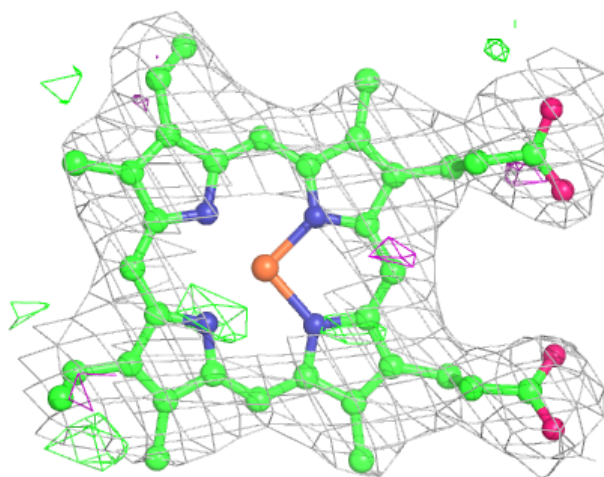
**Electron density around HEC X 607:**

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



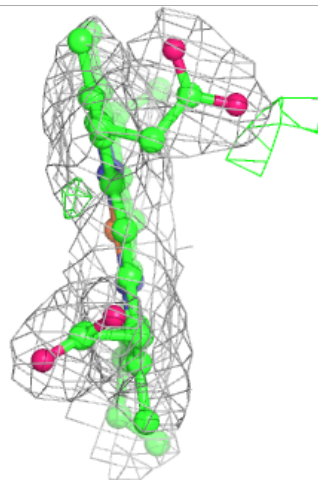
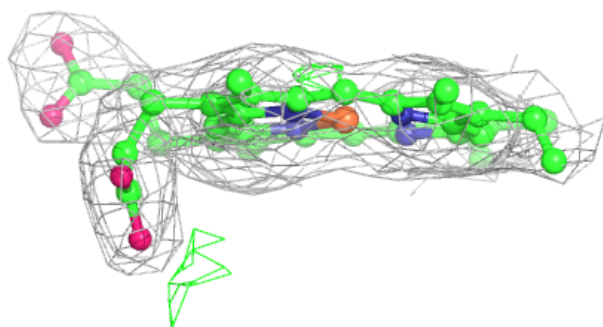
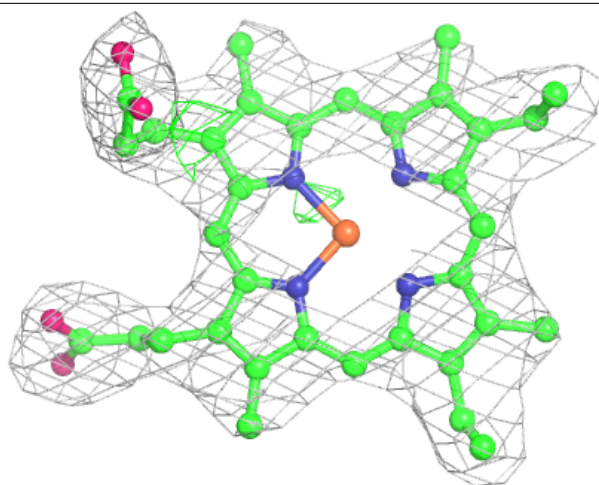
**Electron density around HEC F 600:**

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



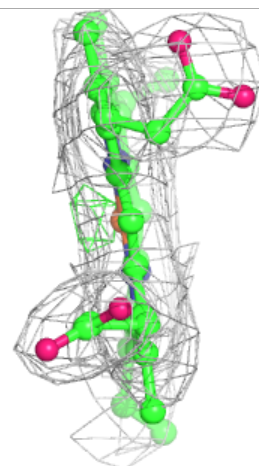
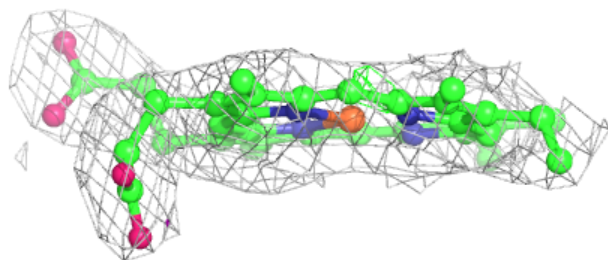
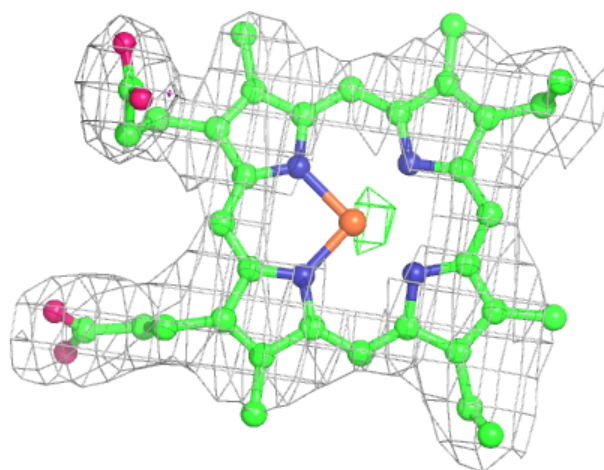
**Electron density around HEC P 601:**

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



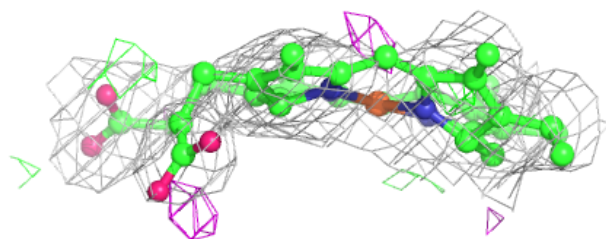
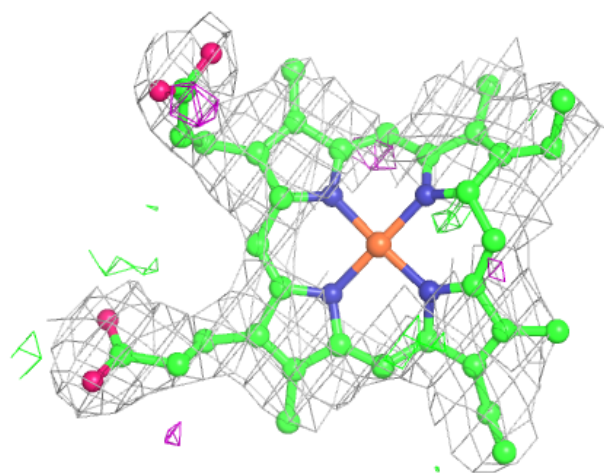
**Electron density around HEC G 601:**

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



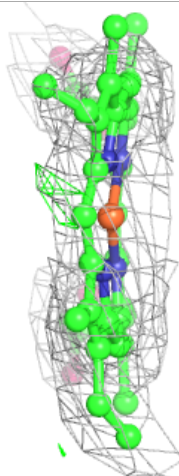
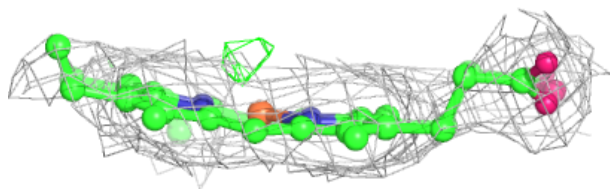
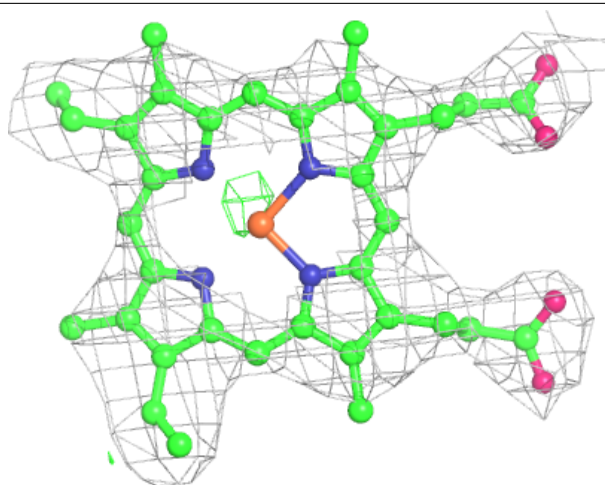
**Electron density around HEC P 603:**

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



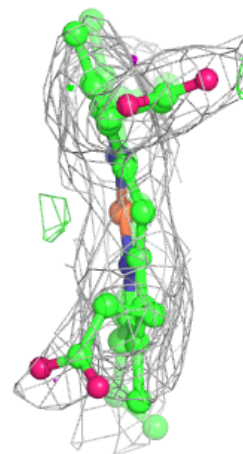
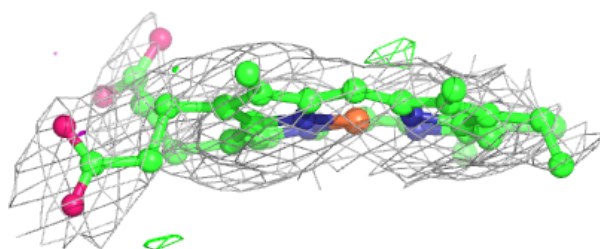
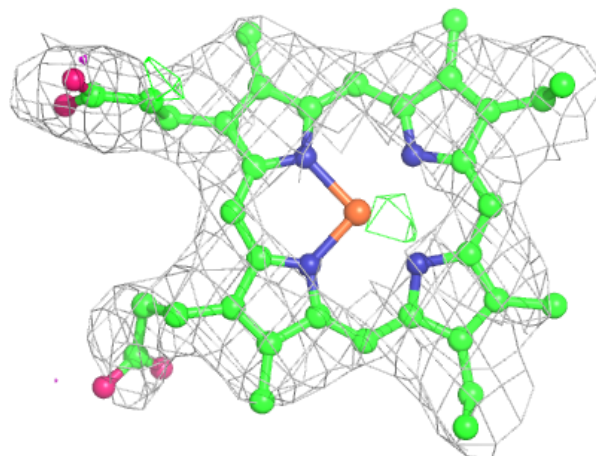
**Electron density around HEC W 600:**

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



**Electron density around HEC K 602:**

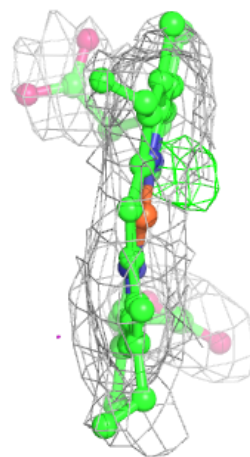
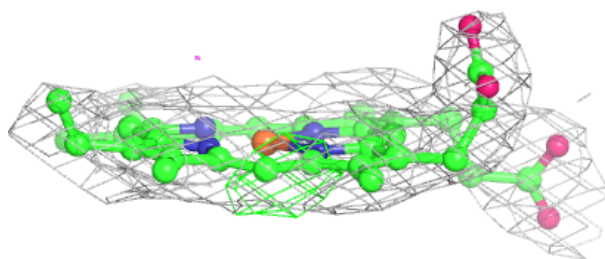
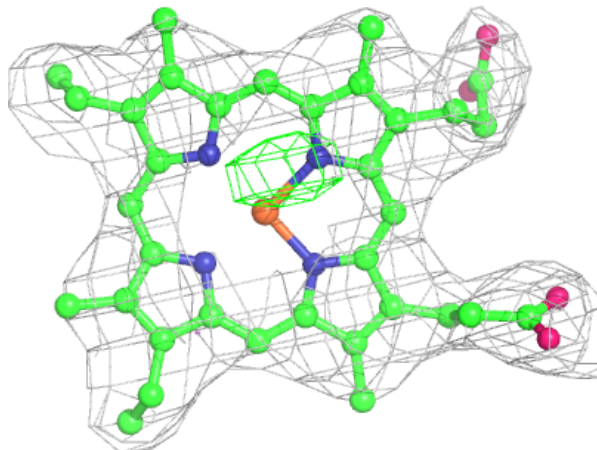
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC E 601:**

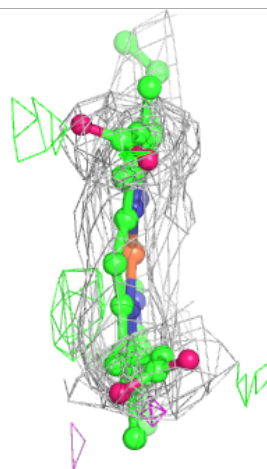
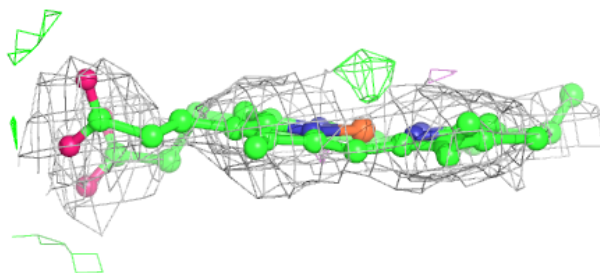
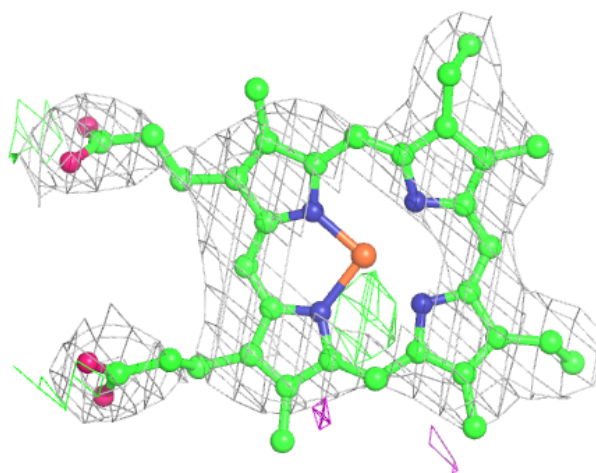
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





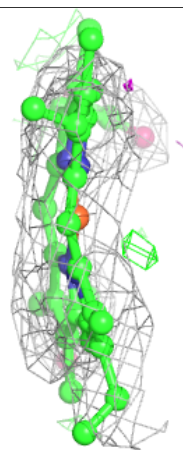
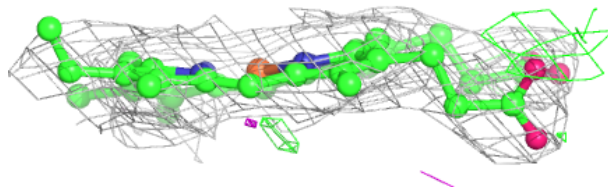
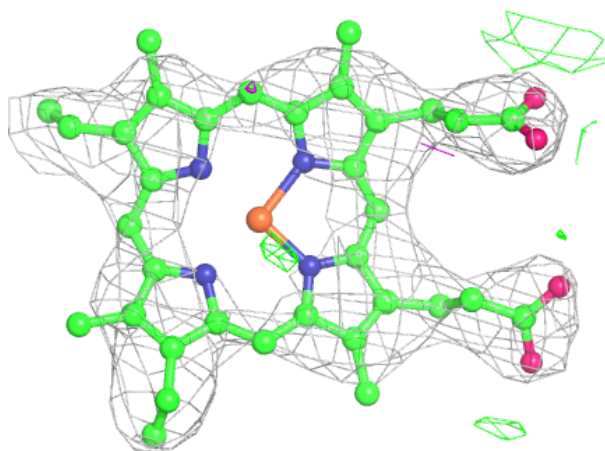
**Electron density around HEC A 605:**

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



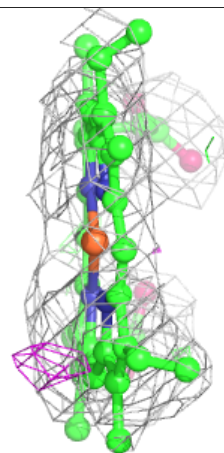
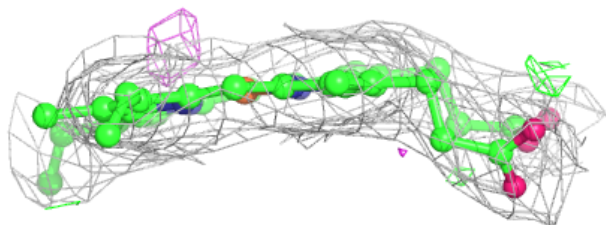
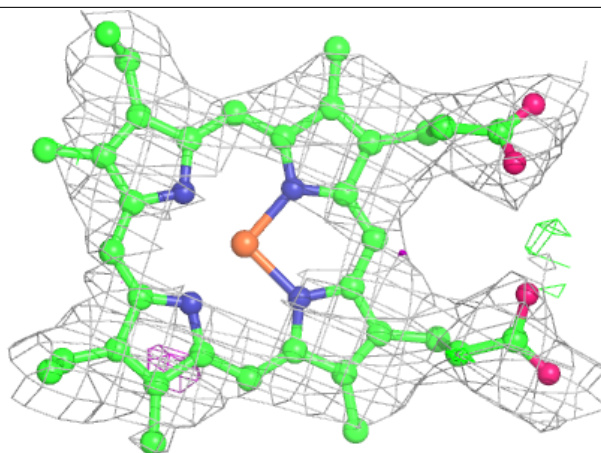
**Electron density around HEC S 606:**

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



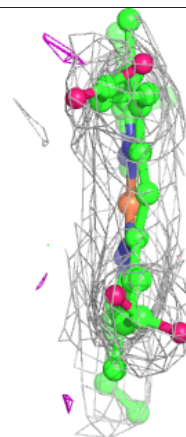
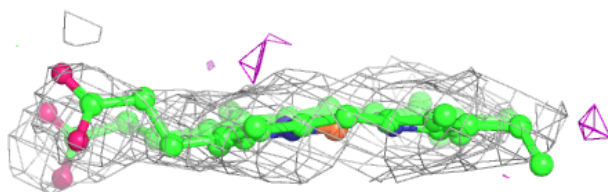
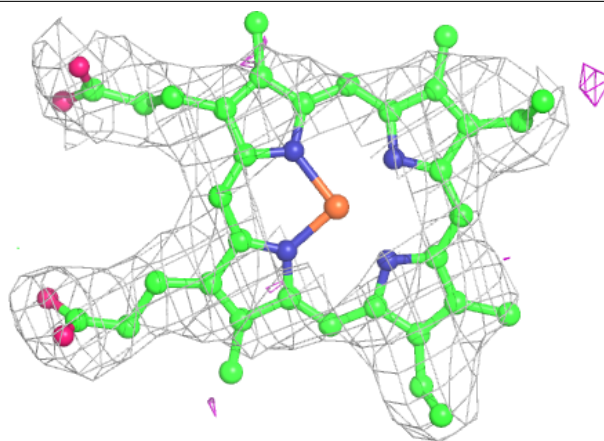
**Electron density around HEC L 604:**

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



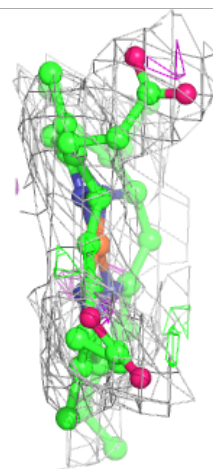
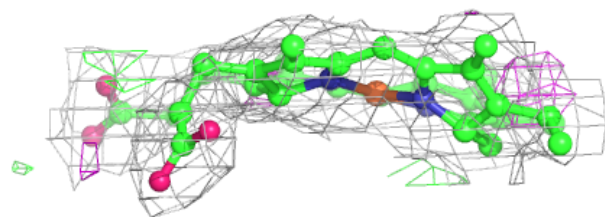
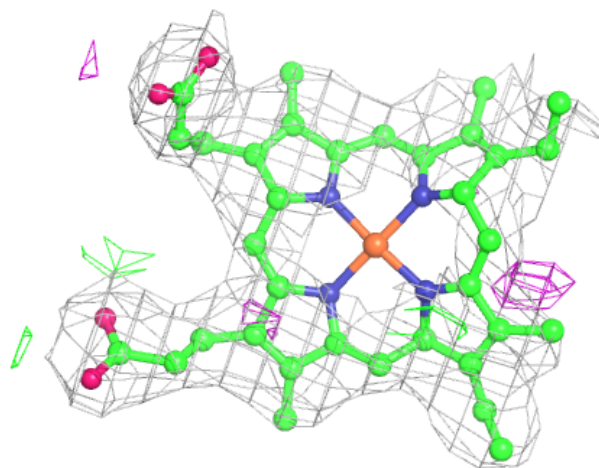
**Electron density around HEC V 605:**

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



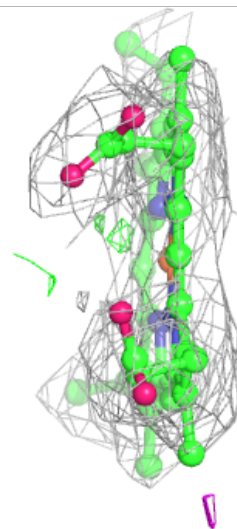
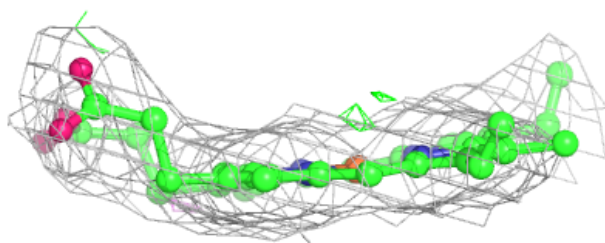
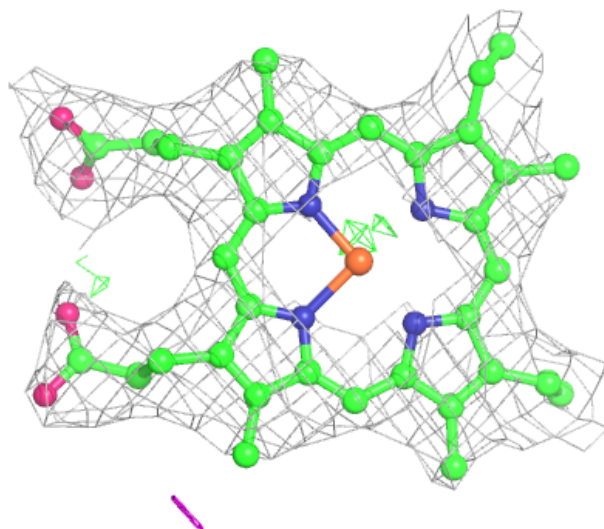
**Electron density around HEC G 603:**

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



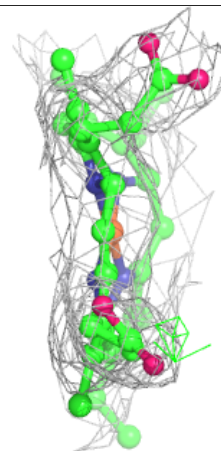
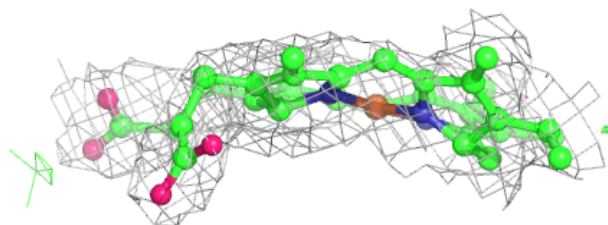
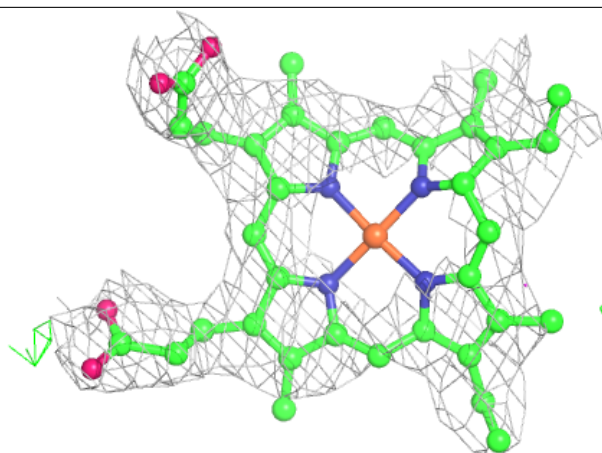
**Electron density around HEC H 604:**

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



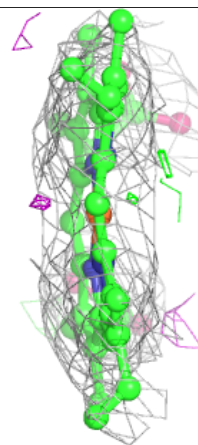
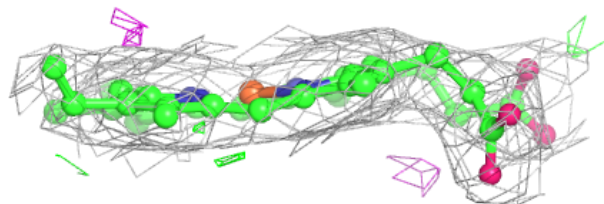
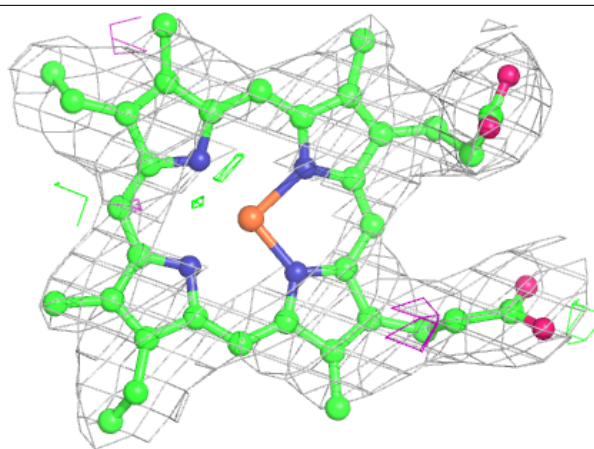
**Electron density around HEC Q 603:**

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



**Electron density around HEC O 607:**

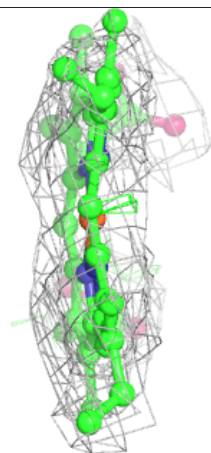
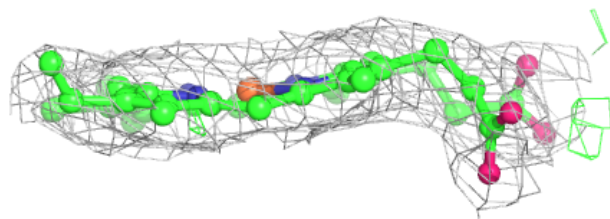
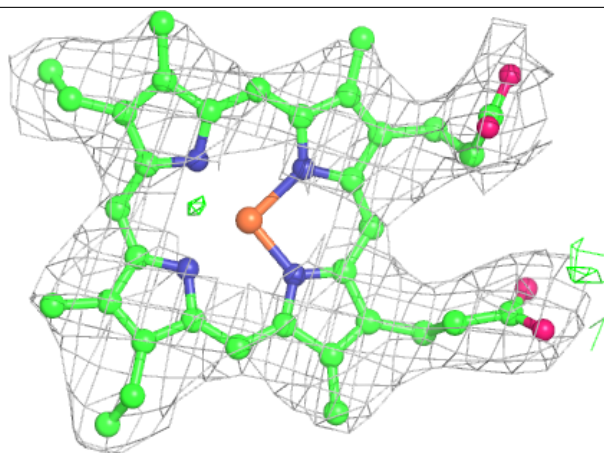
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





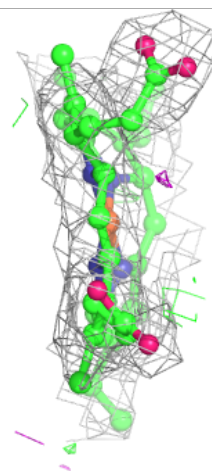
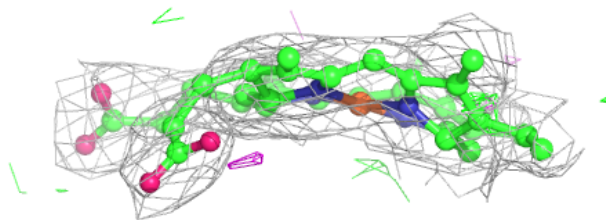
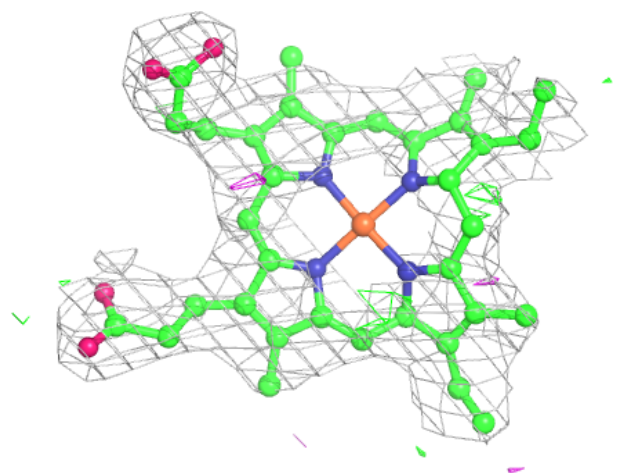
**Electron density around HEC J 607:**

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



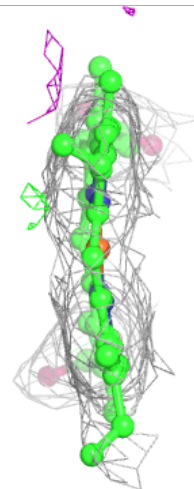
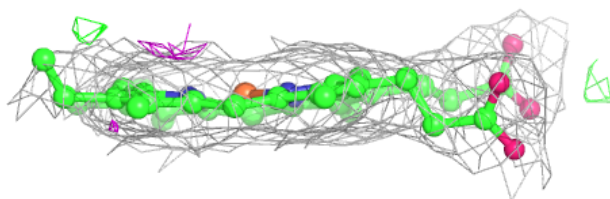
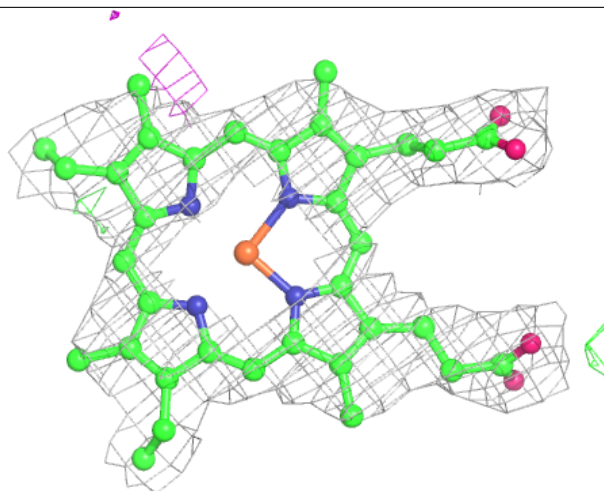
**Electron density around HEC I 603:**

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



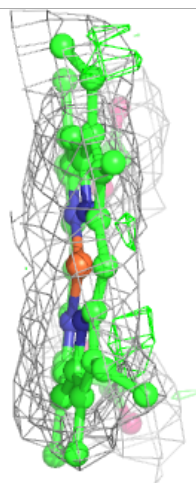
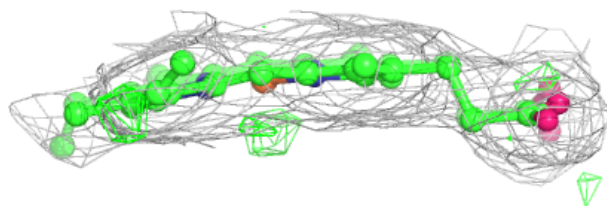
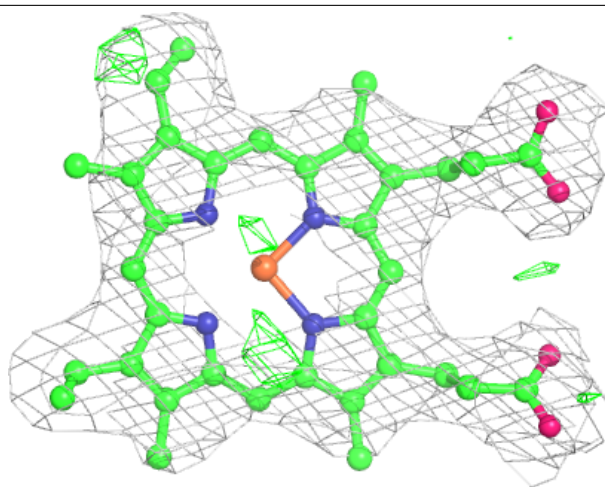
**Electron density around HEC B 605:**

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



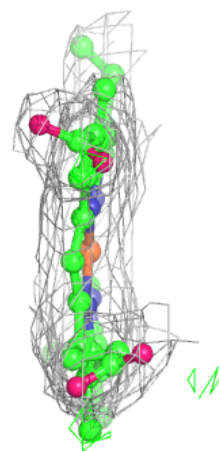
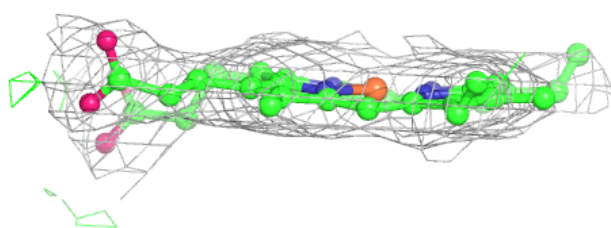
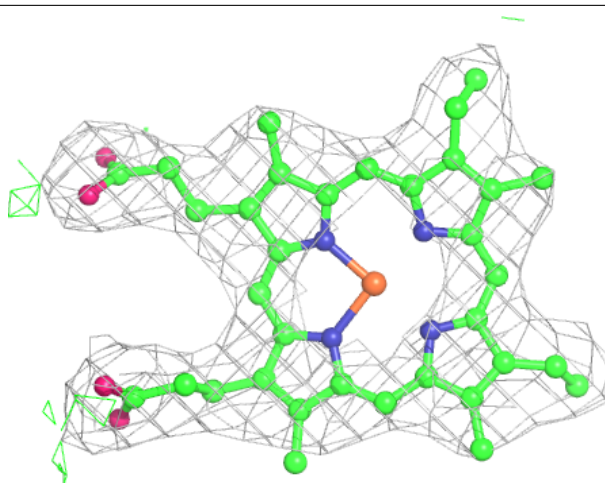
**Electron density around HEC P 600:**

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



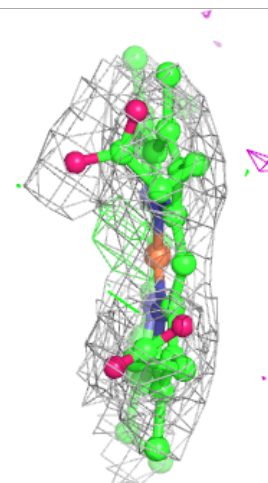
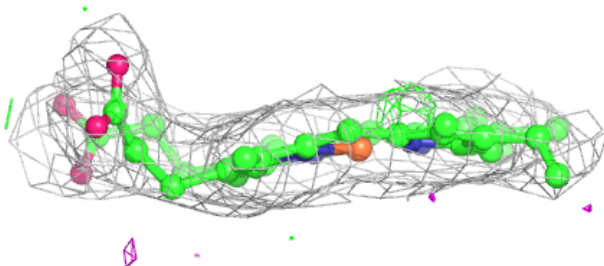
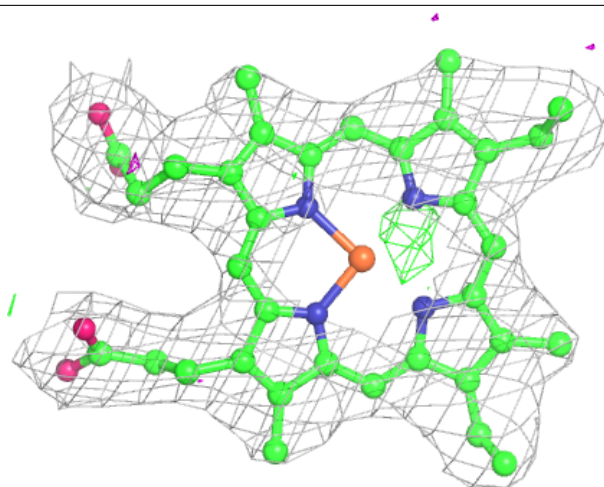
**Electron density around HEC R 605:**

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



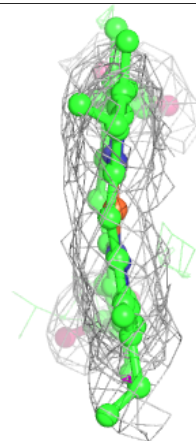
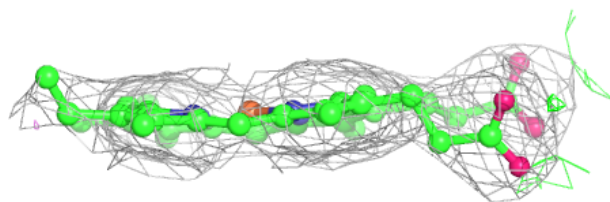
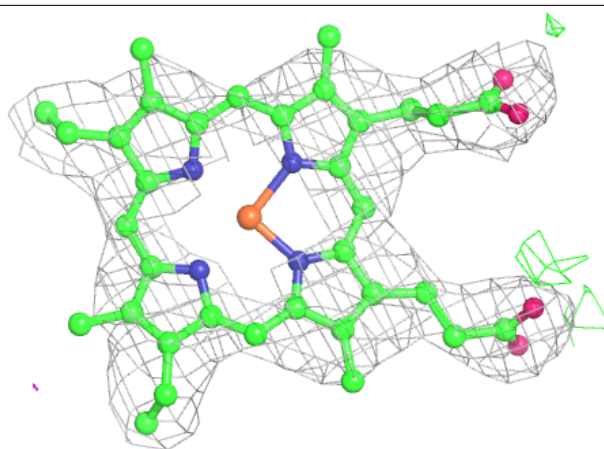
**Electron density around HEC G 607:**

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



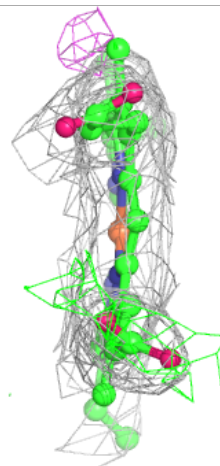
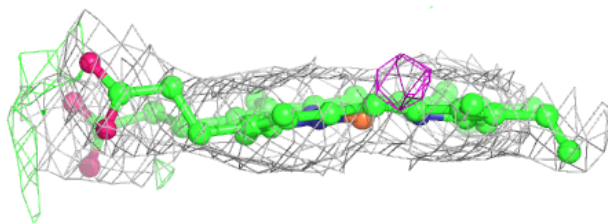
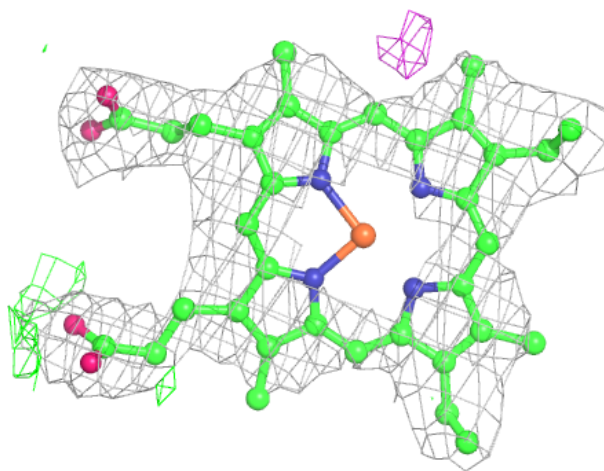
**Electron density around HEC P 605:**

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



**Electron density around HEC O 605:**

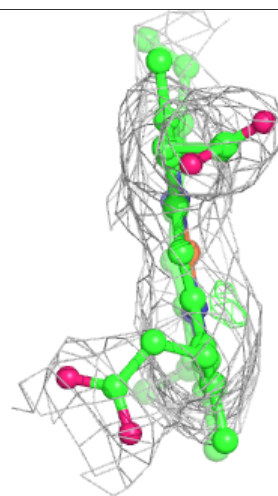
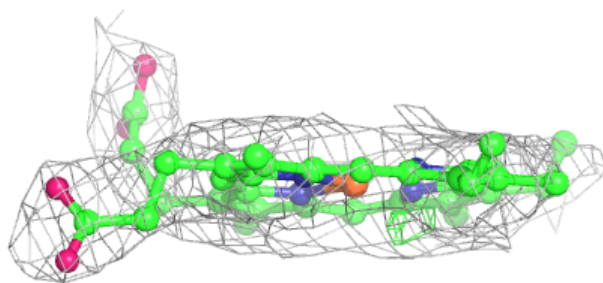
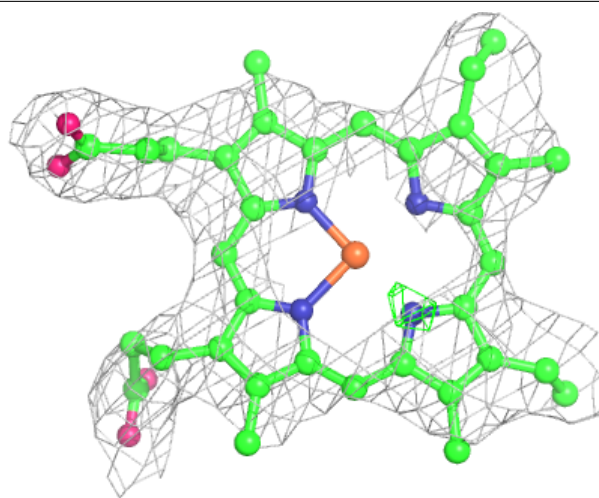
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





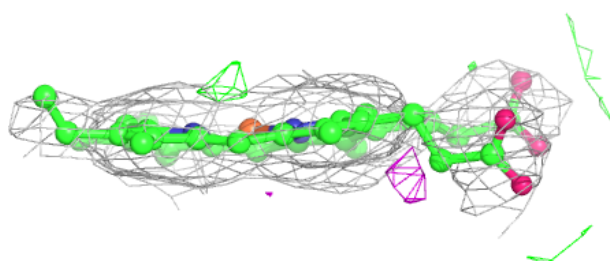
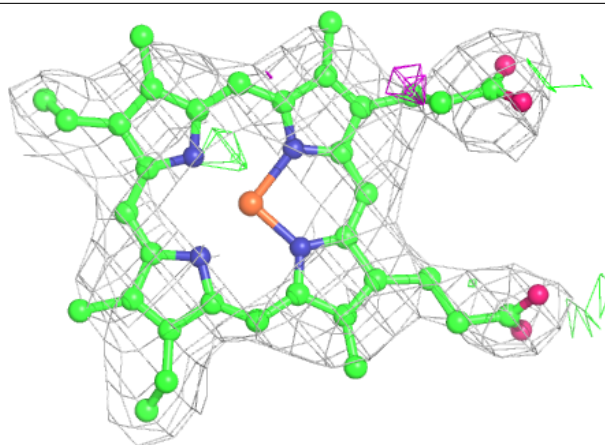
**Electron density around HEC T 601:**

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

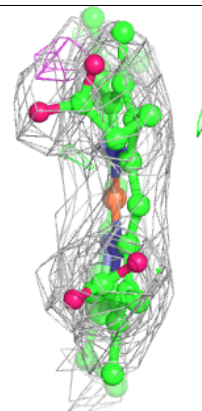
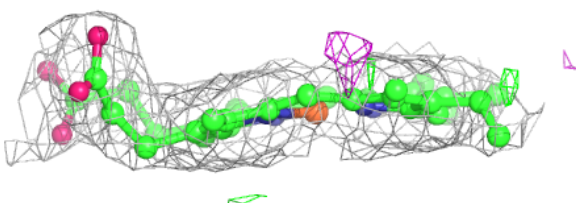
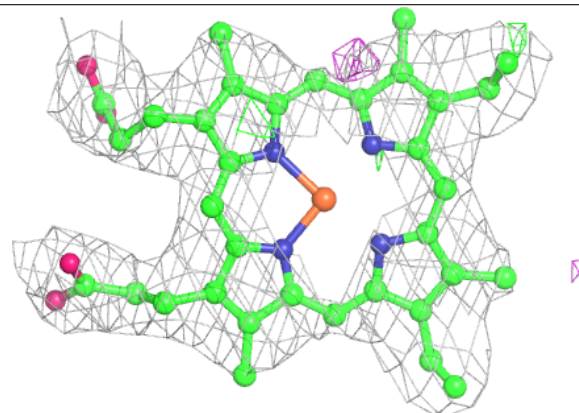


**Electron density around HEC N 605:**

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

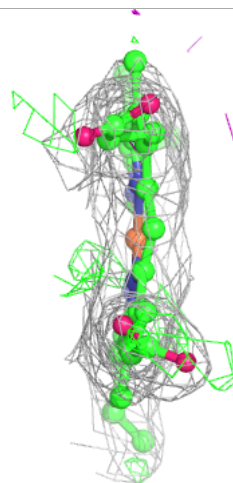
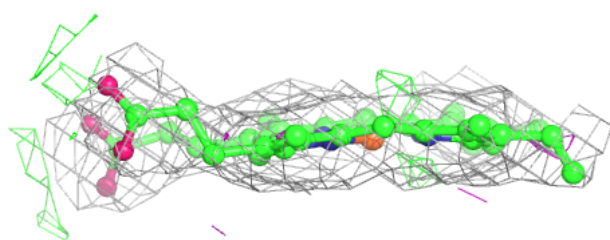
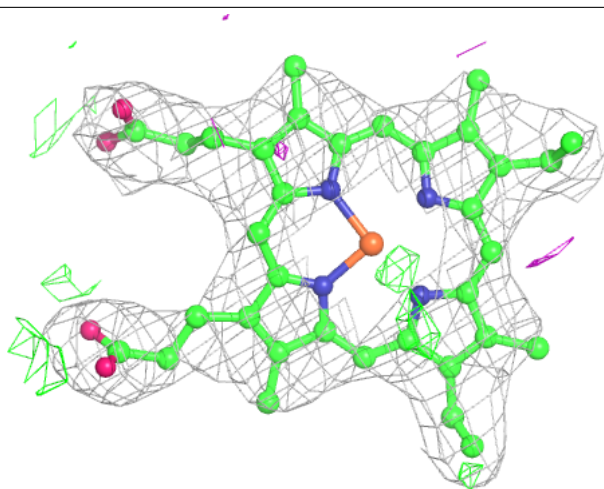
**Electron density around HEC R 607:**

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



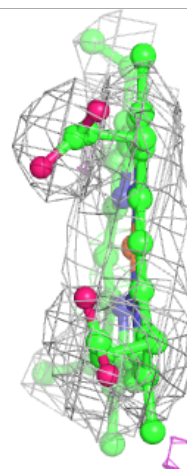
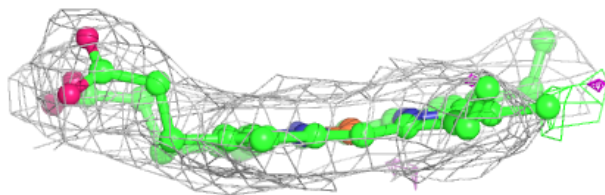
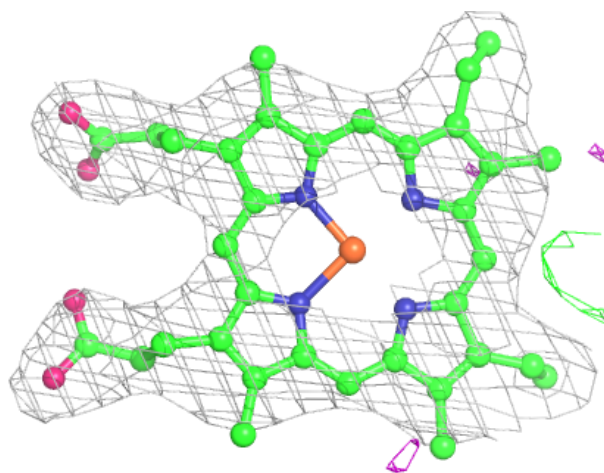
**Electron density around HEC J 605:**

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



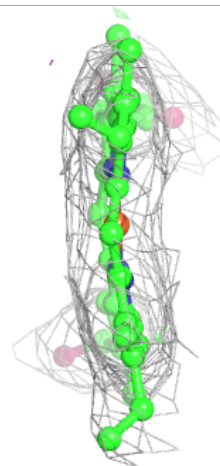
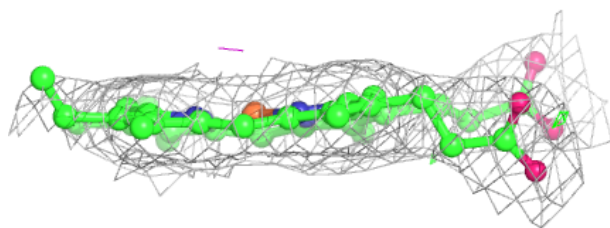
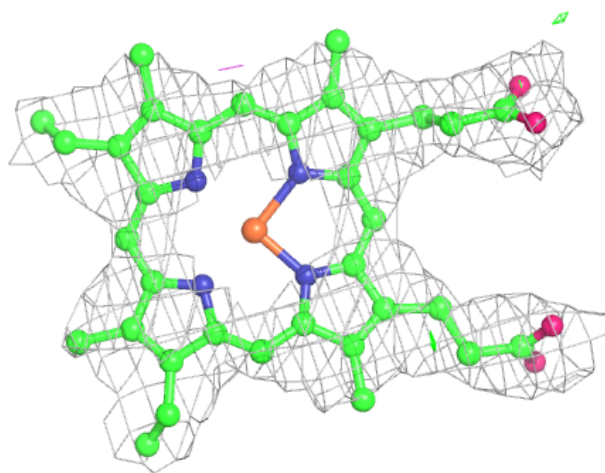
**Electron density around HEC N 604:**

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



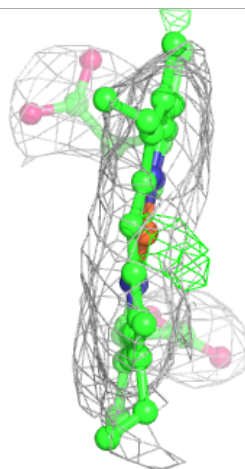
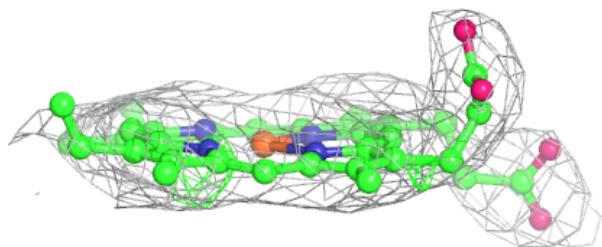
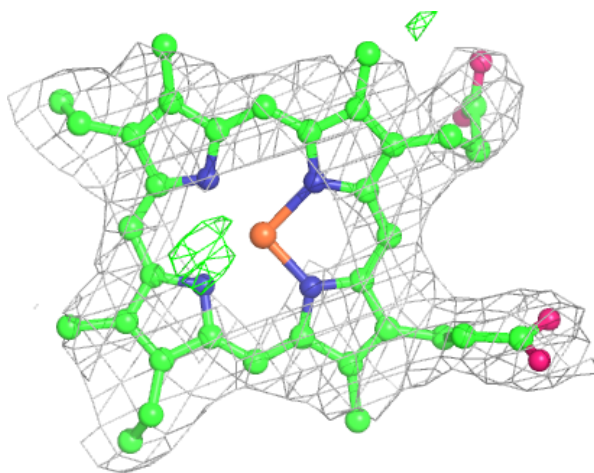
**Electron density around HEC H 605:**

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



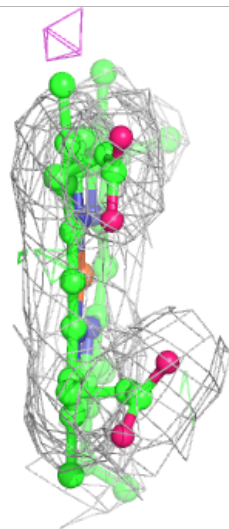
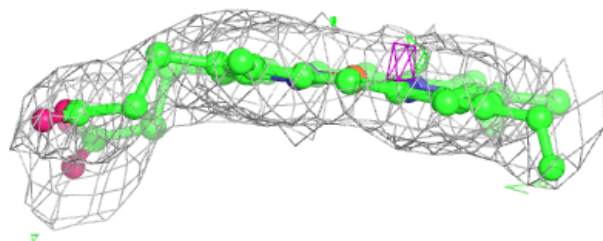
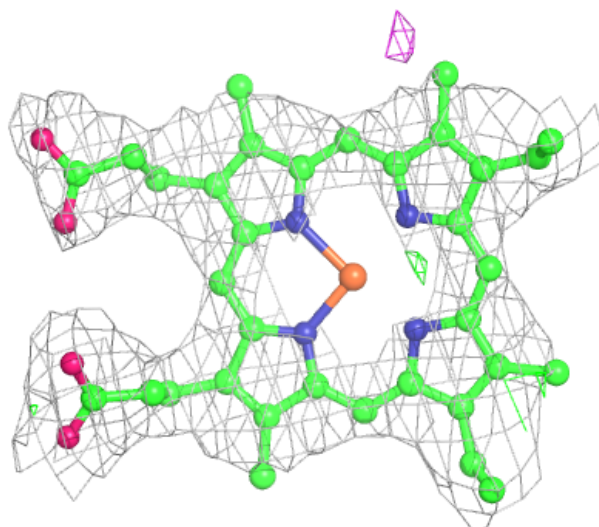
**Electron density around HEC A 601:**

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



**Electron density around HEC I 604:**

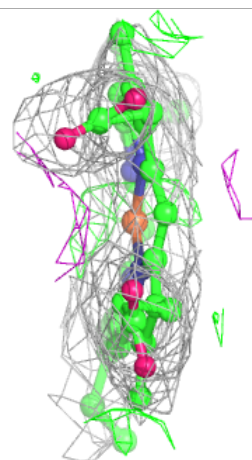
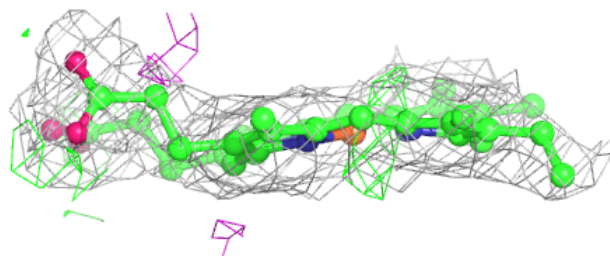
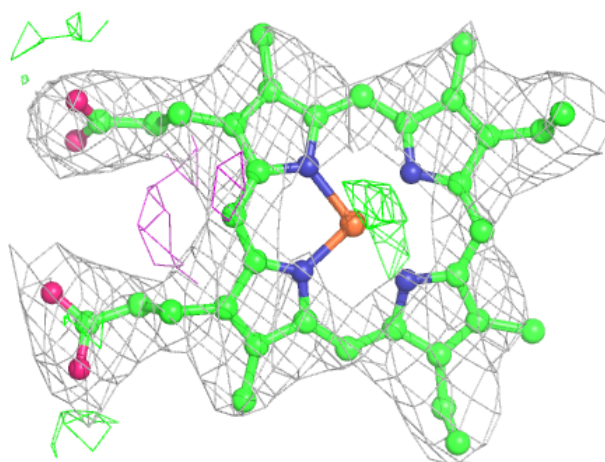
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC J 606:**

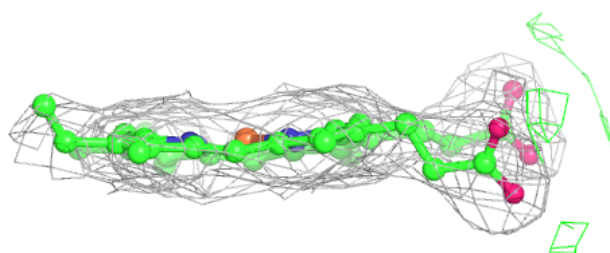
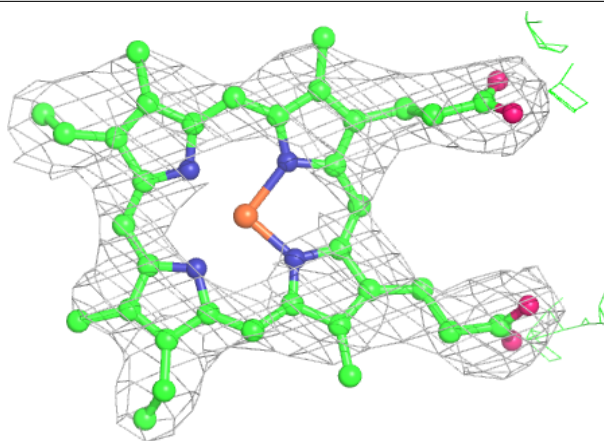
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





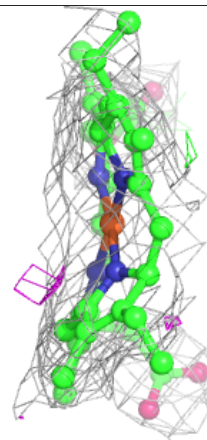
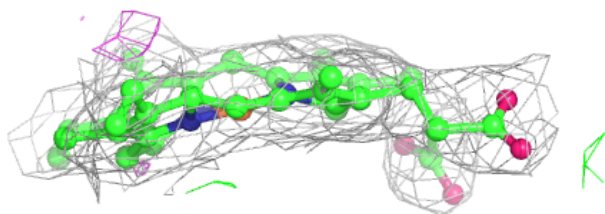
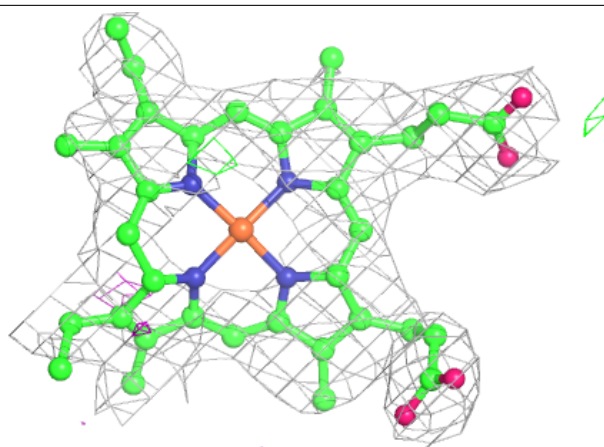
**Electron density around HEC Q 605:**

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



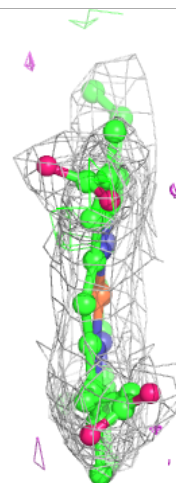
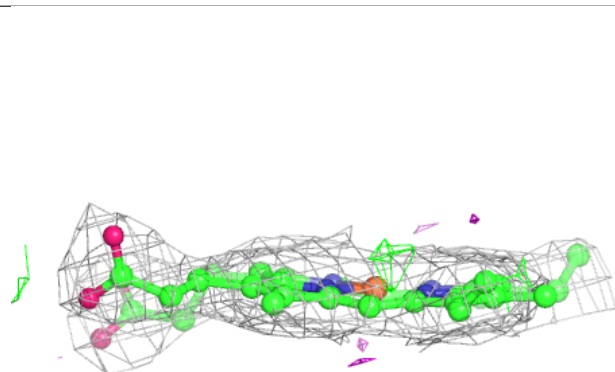
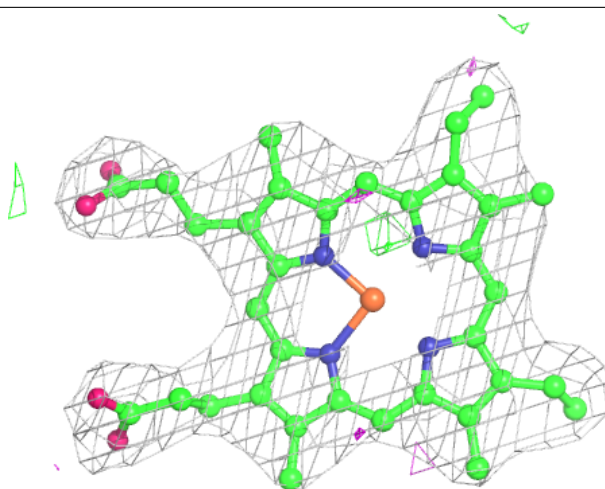
**Electron density around HEC H 603:**

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



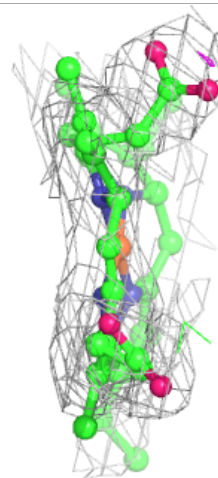
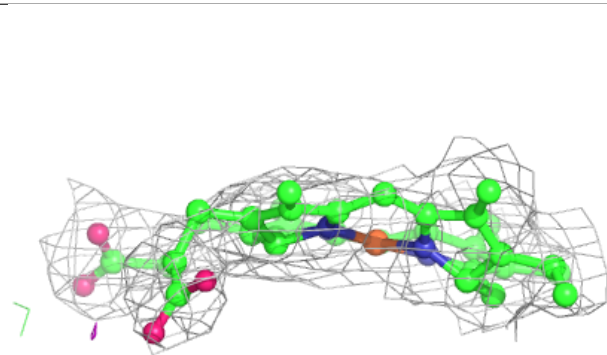
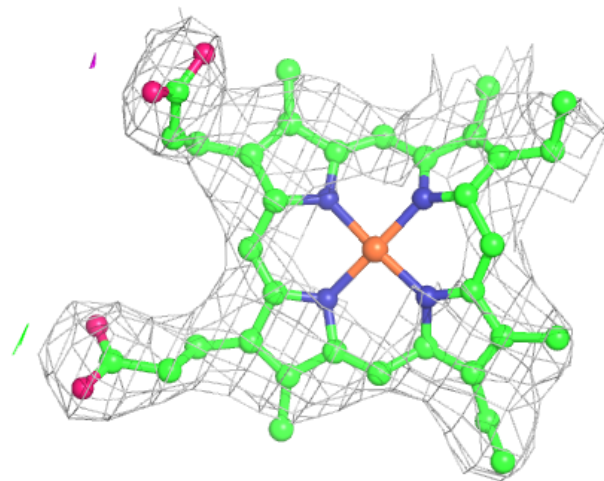
**Electron density around HEC I 605:**

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



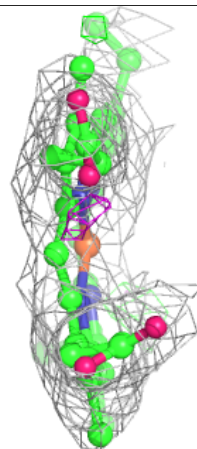
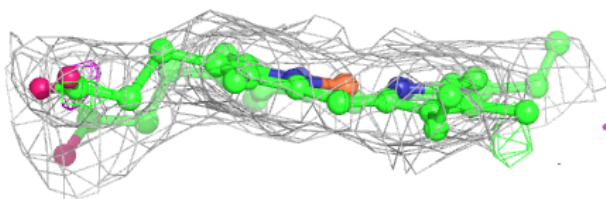
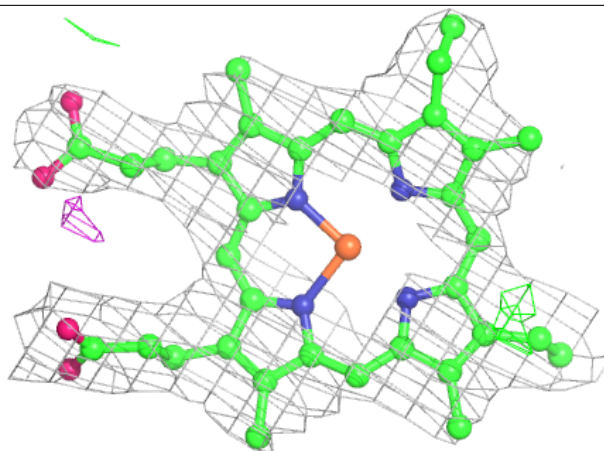
**Electron density around HEC N 603:**

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



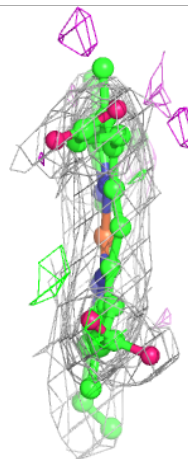
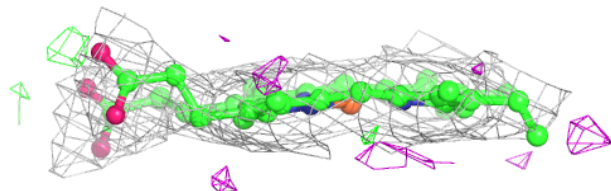
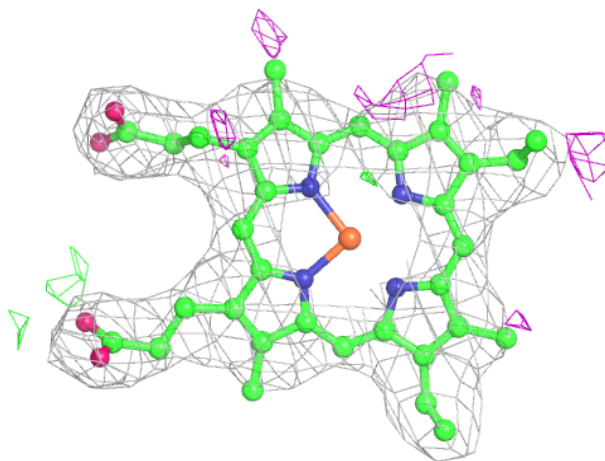
**Electron density around HEC B 606:**

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



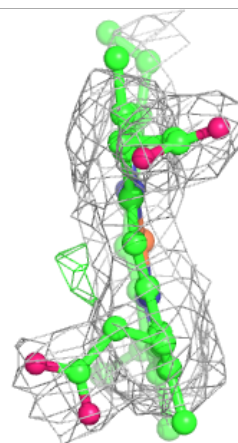
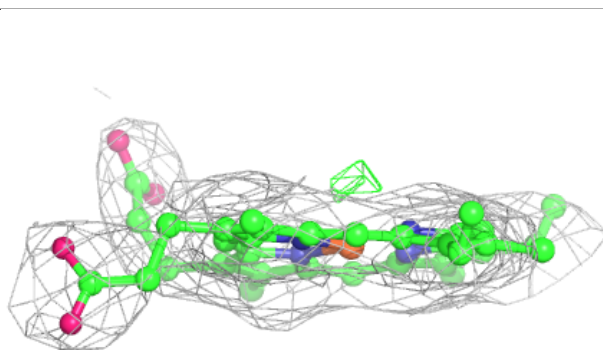
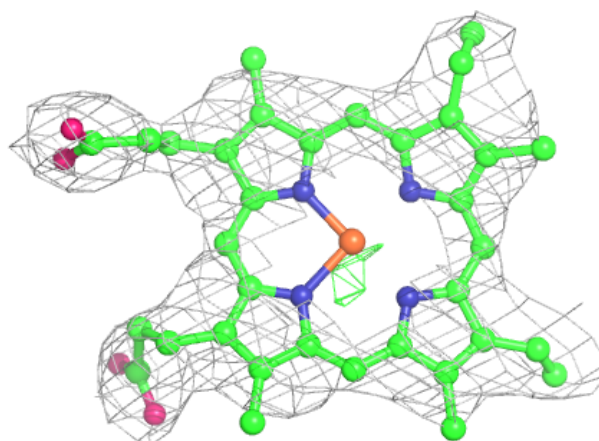
**Electron density around HEC L 605:**

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



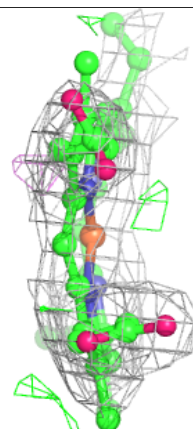
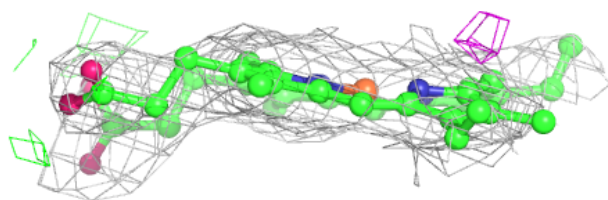
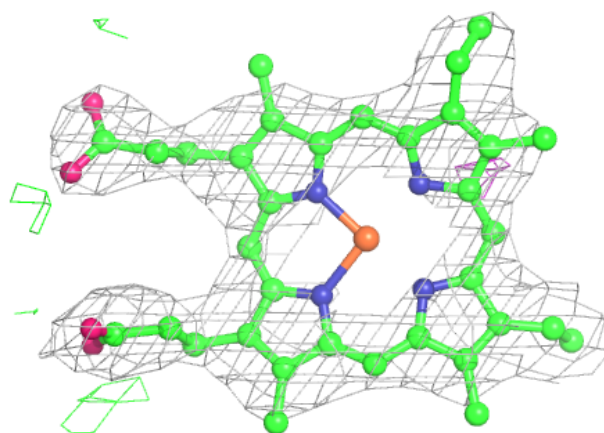
**Electron density around HEC D 601:**

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



**Electron density around HEC D 606:**

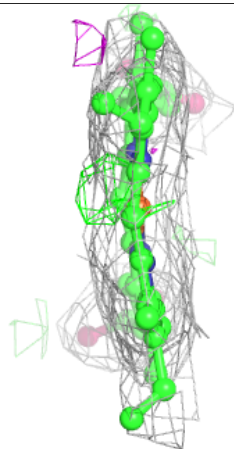
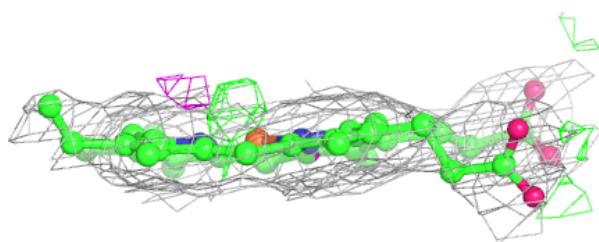
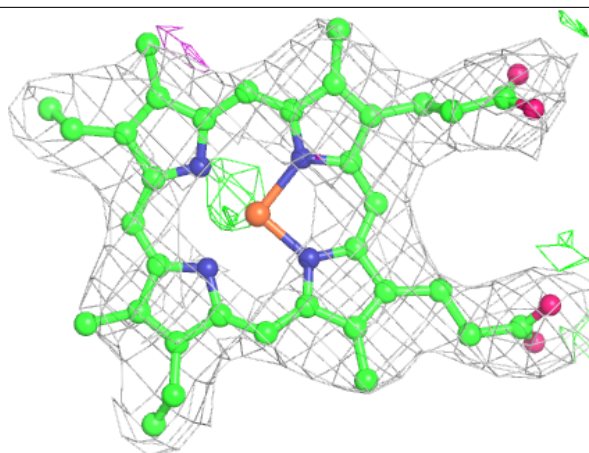
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





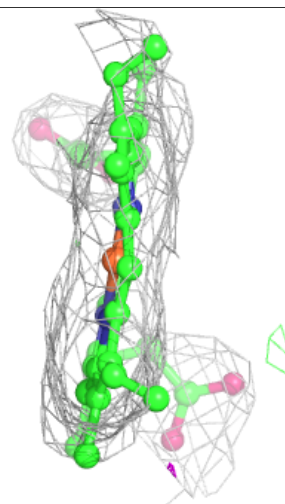
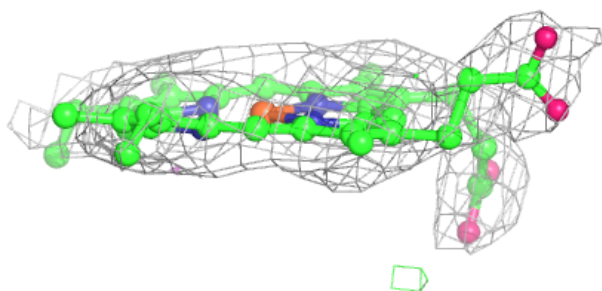
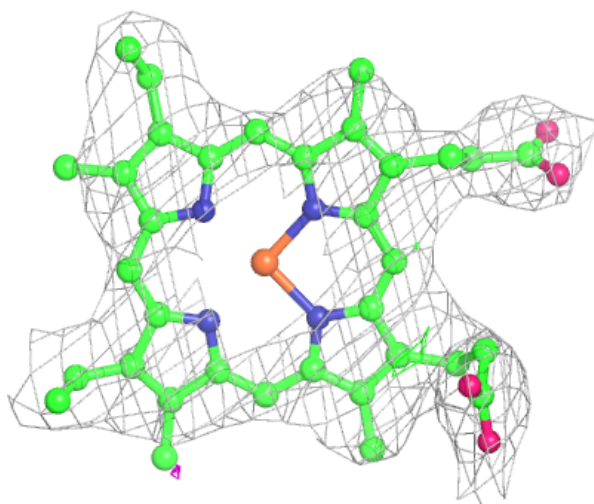
**Electron density around HEC G 605:**

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



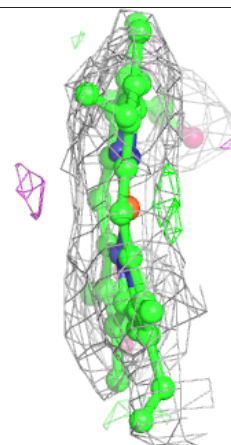
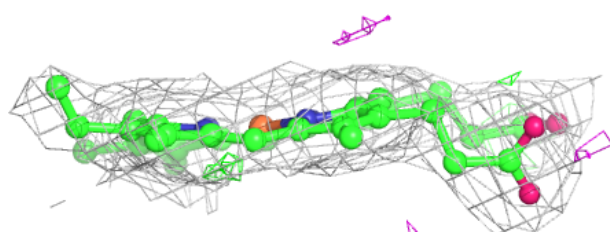
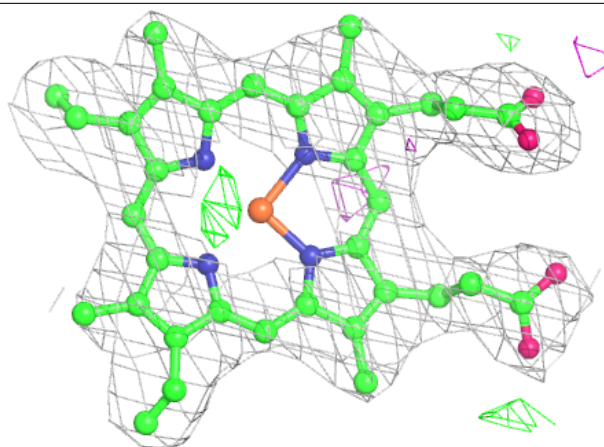
**Electron density around HEC C 601:**

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



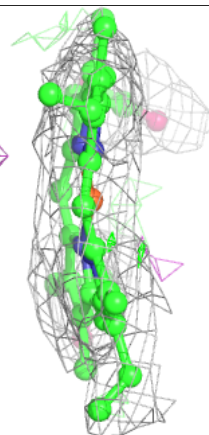
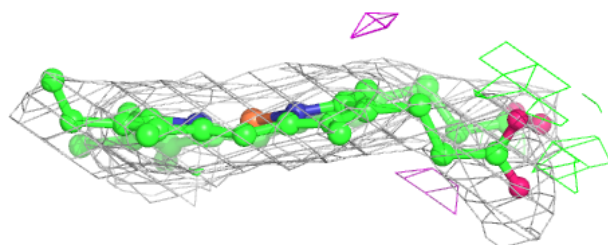
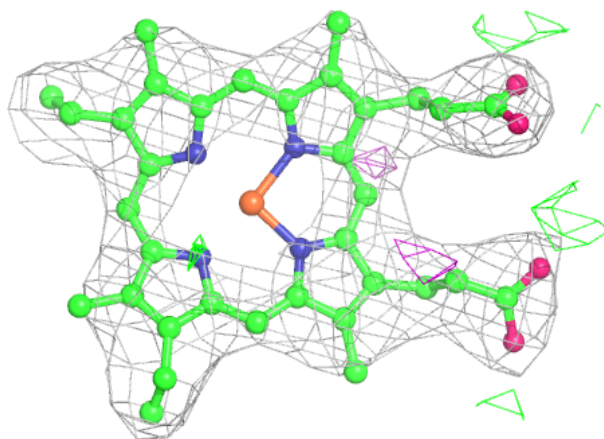
**Electron density around HEC I 606:**

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



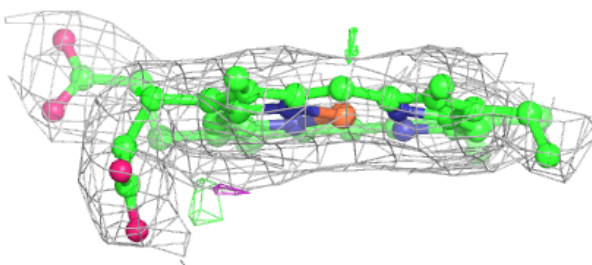
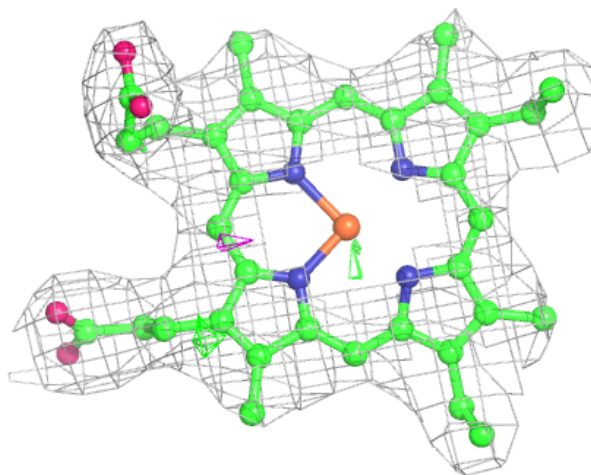
**Electron density around HEC C 606:**

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



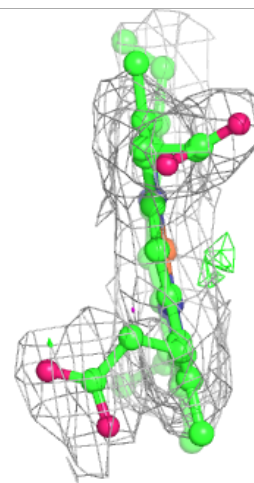
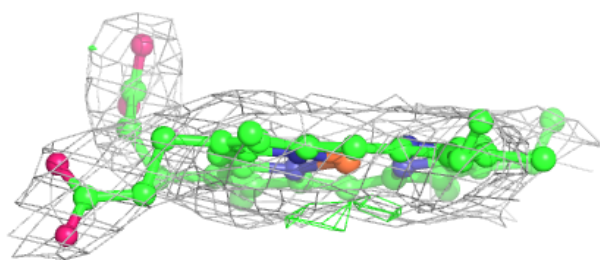
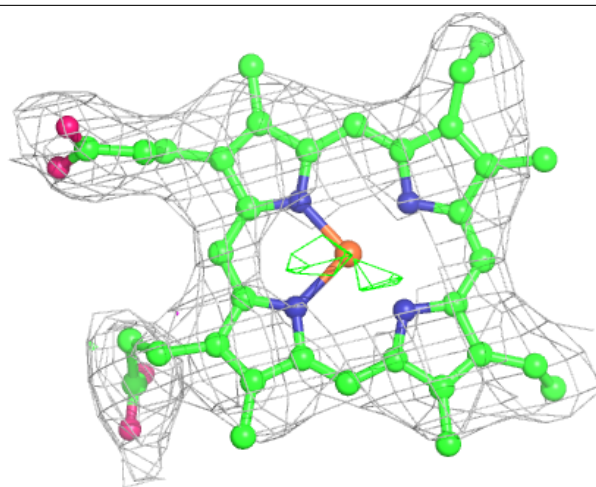
**Electron density around HEC K 601:**

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



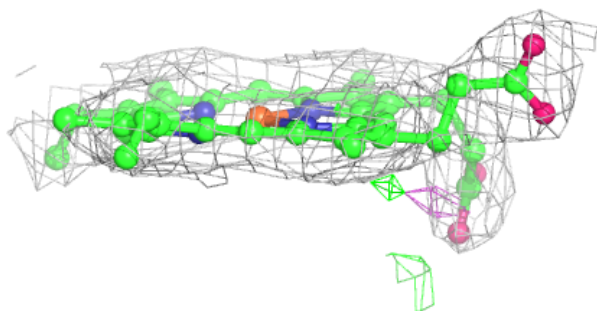
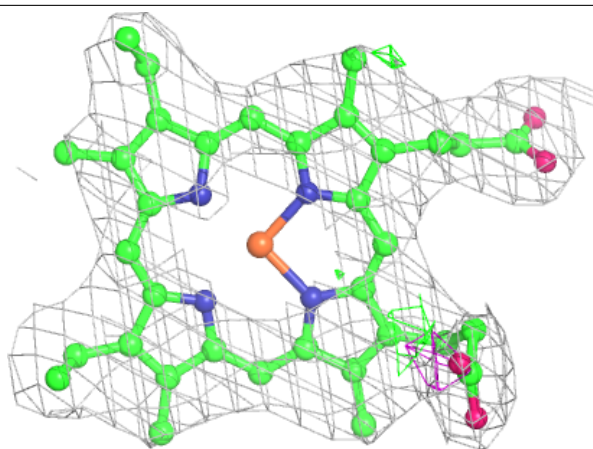
**Electron density around HEC R 601:**

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



**Electron density around HEC H 601:**

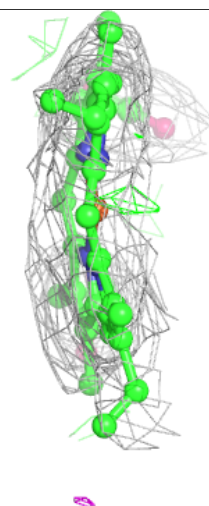
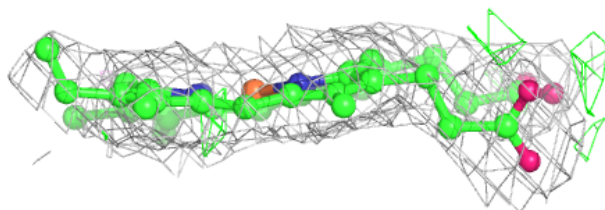
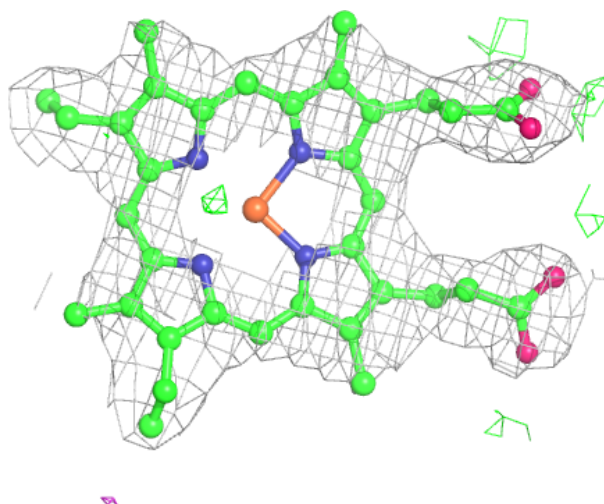
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC O 606:**

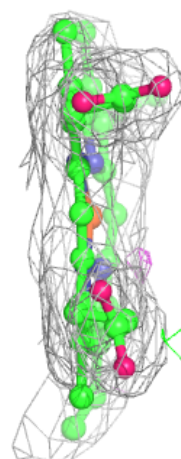
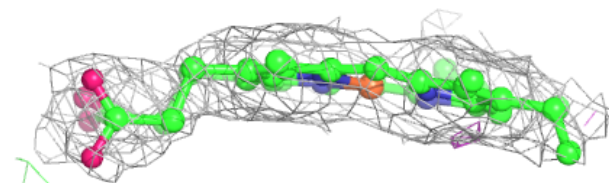
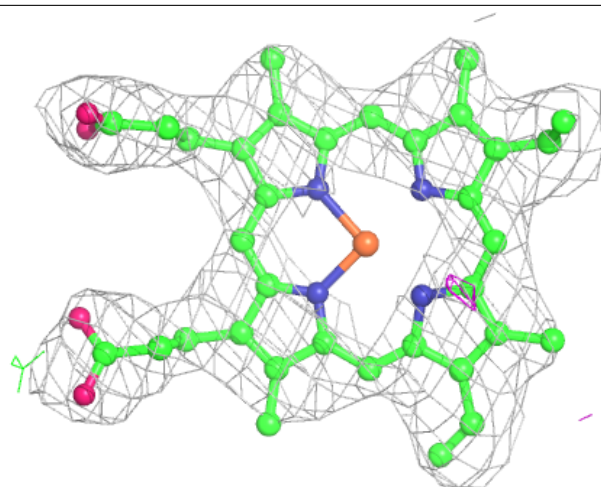
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





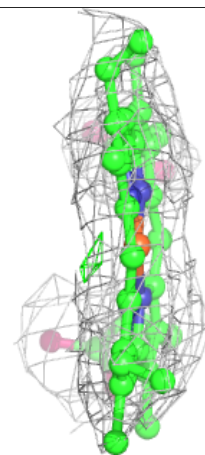
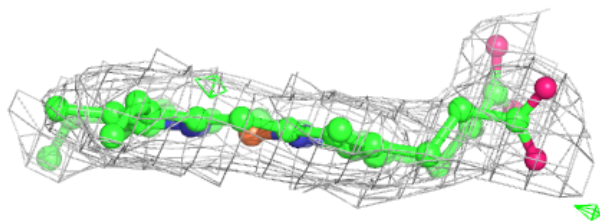
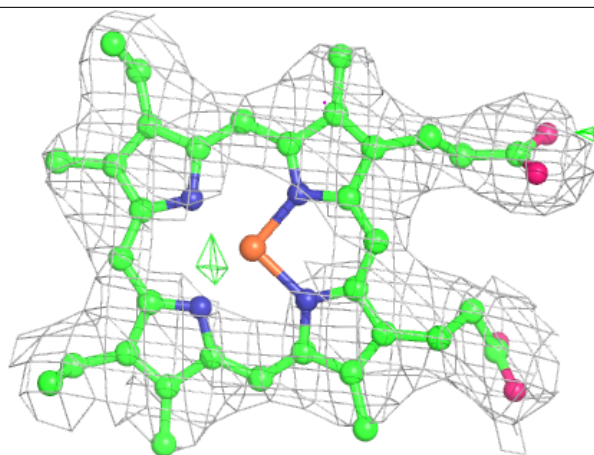
**Electron density around HEC I 600:**

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



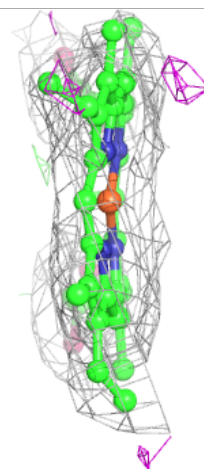
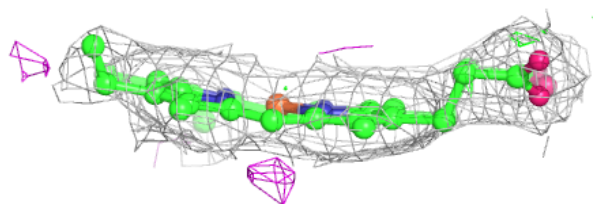
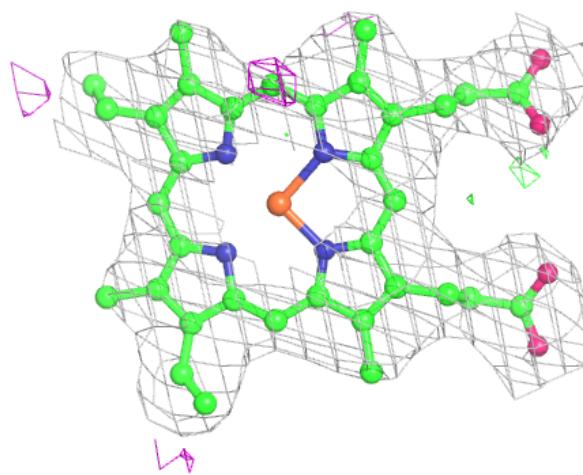
**Electron density around HEC I 607:**

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



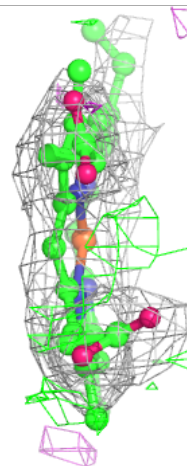
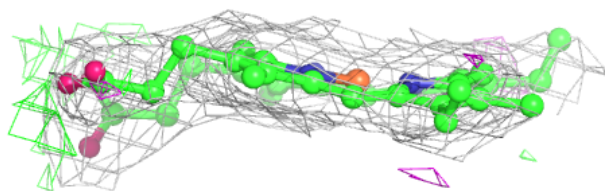
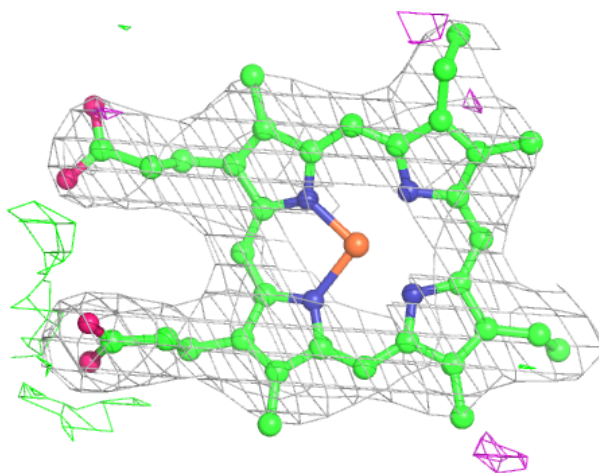
**Electron density around HEC H 600:**

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



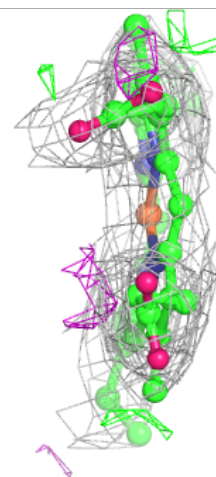
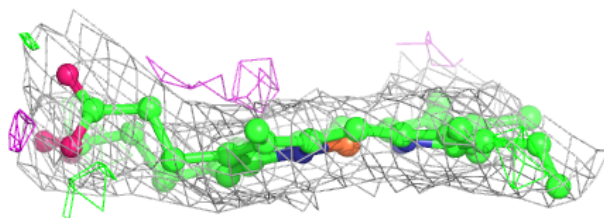
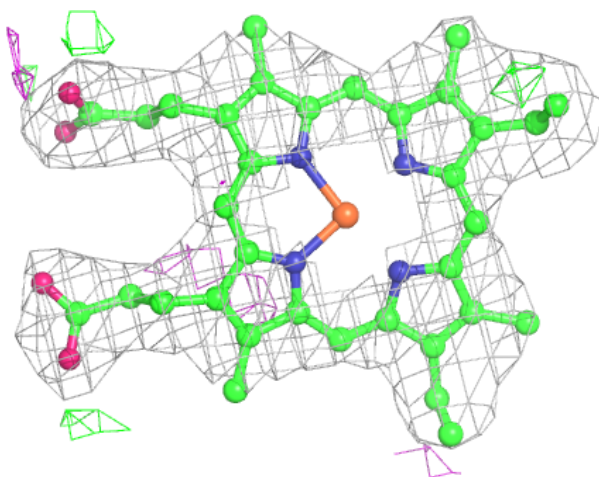
**Electron density around HEC M 606:**

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



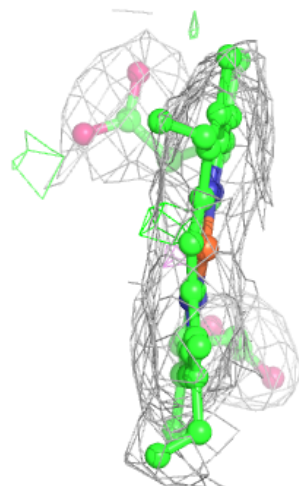
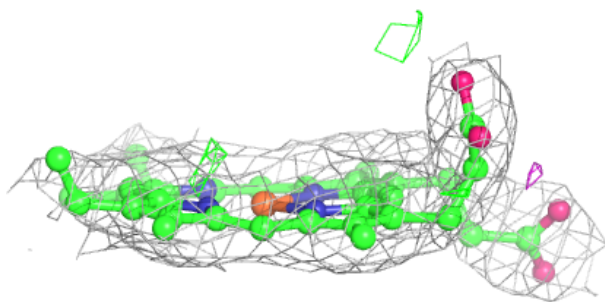
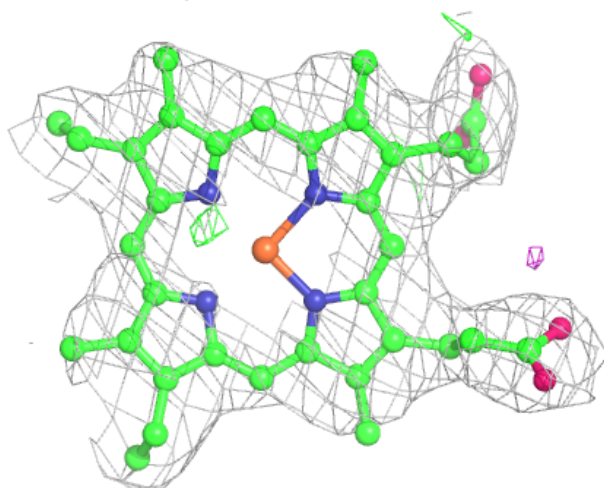
**Electron density around HEC H 606:**

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



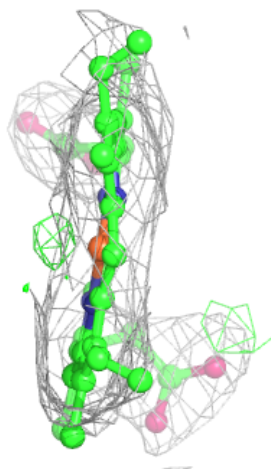
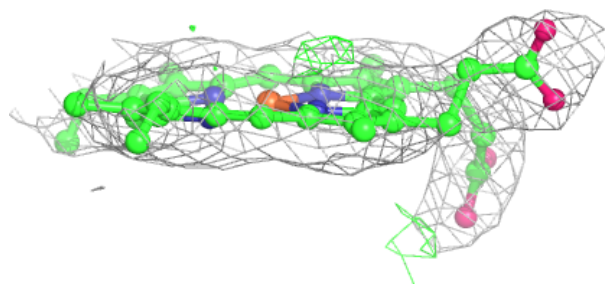
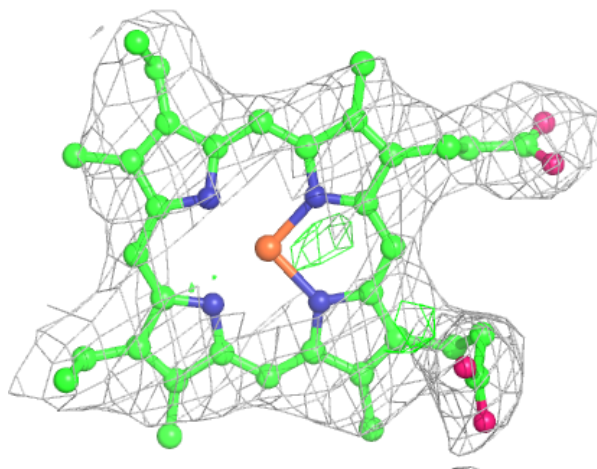
**Electron density around HEC I 601:**

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



**Electron density around HEC M 601:**

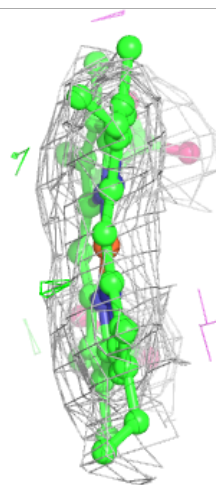
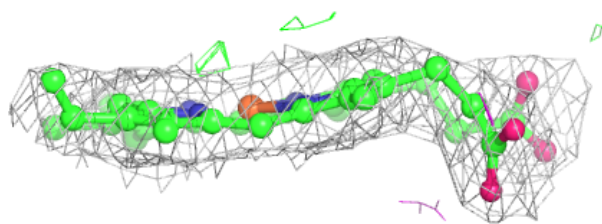
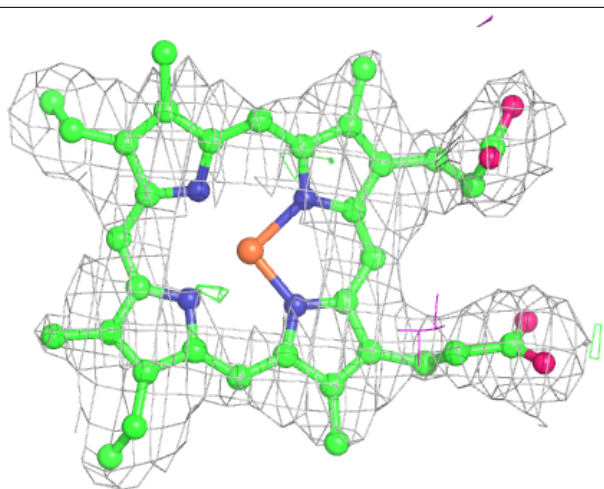
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC L 607:**

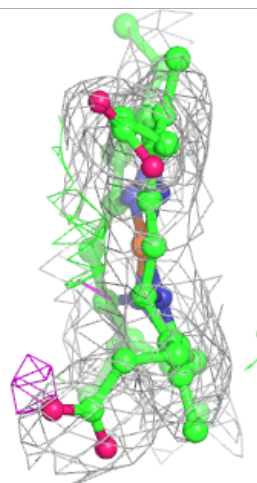
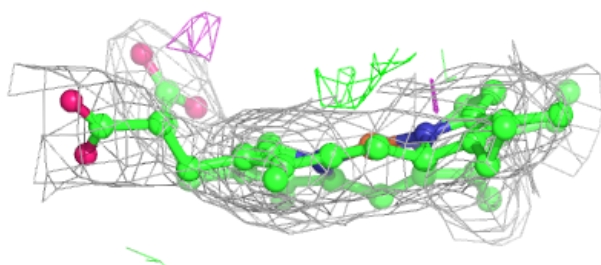
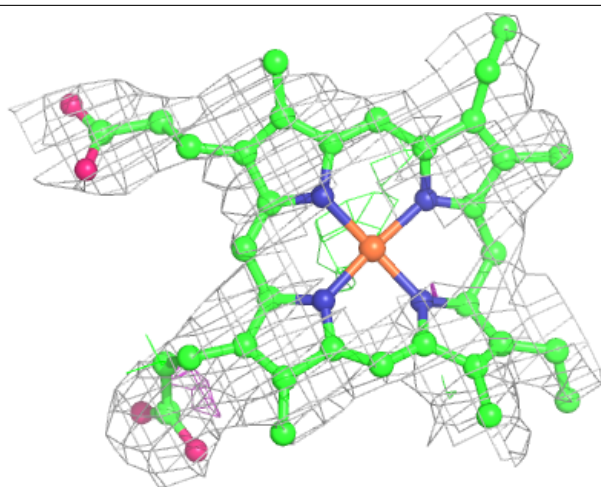
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





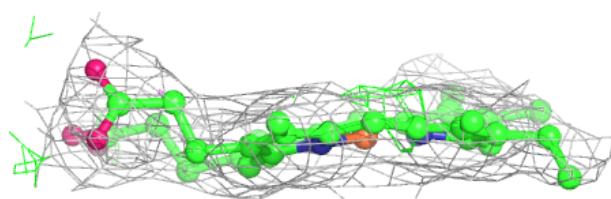
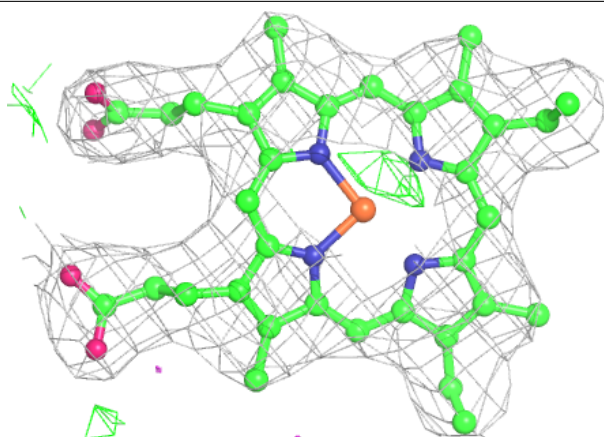
**Electron density around HEC B 603:**

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



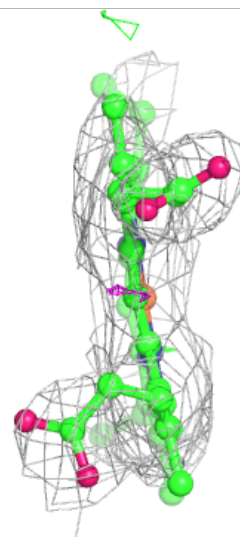
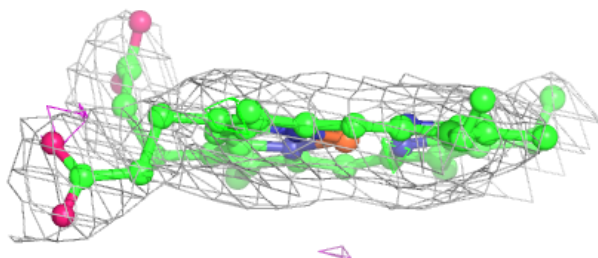
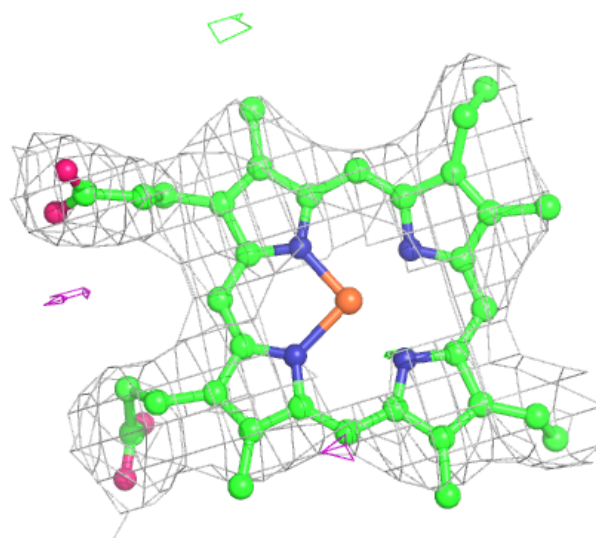
**Electron density around HEC G 606:**

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



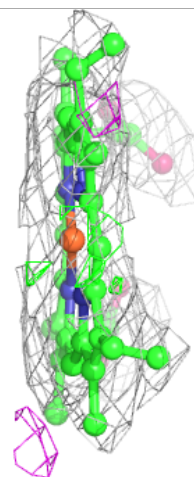
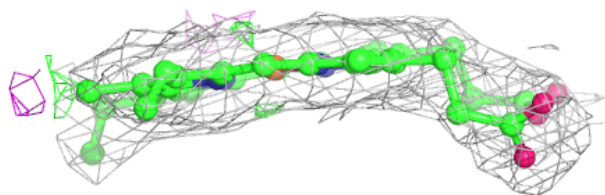
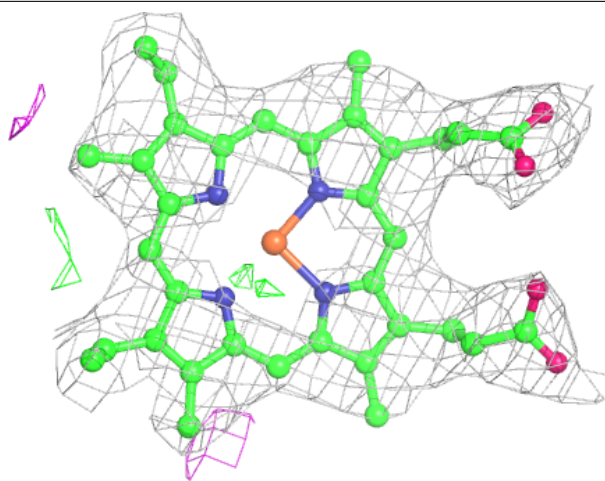
**Electron density around HEC B 601:**

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



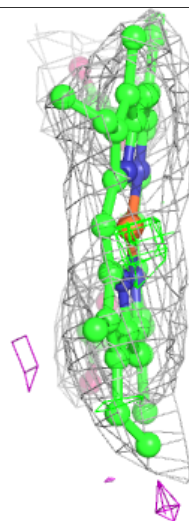
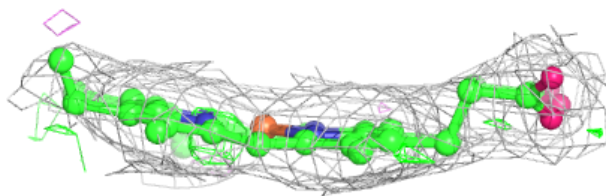
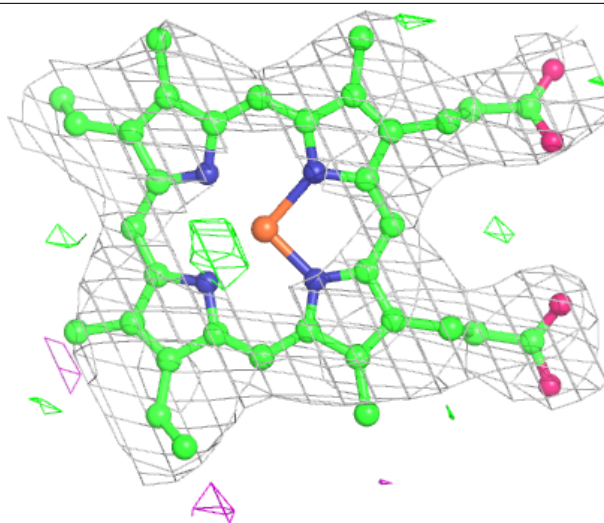
**Electron density around HEC J 604:**

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



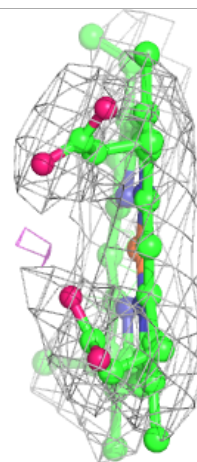
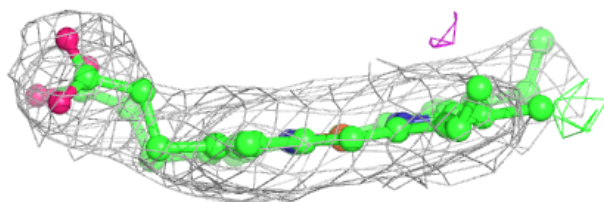
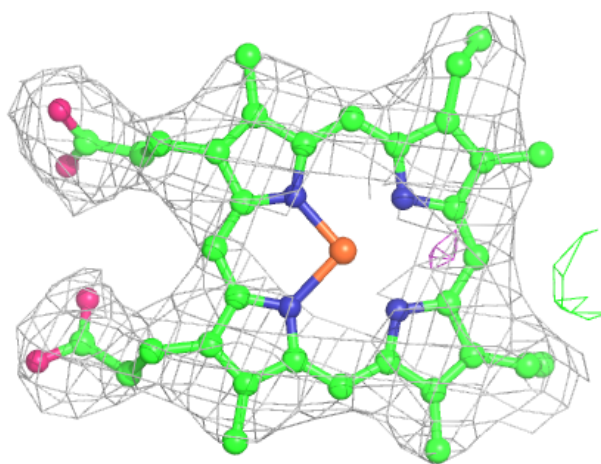
**Electron density around HEC O 600:**

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



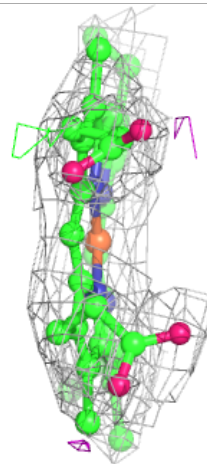
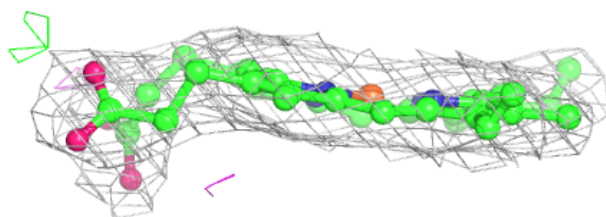
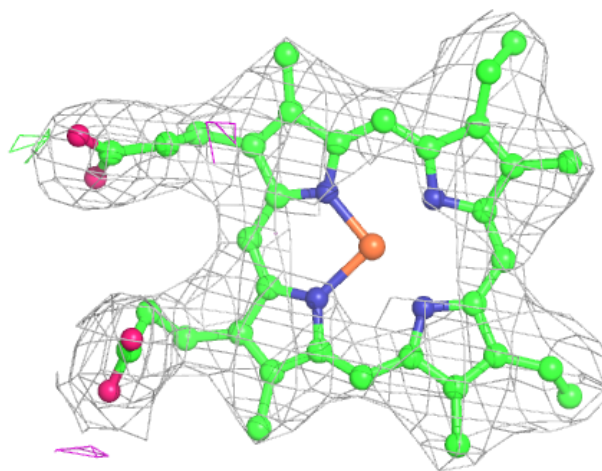
**Electron density around HEC D 604:**

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



**Electron density around HEC K 607:**

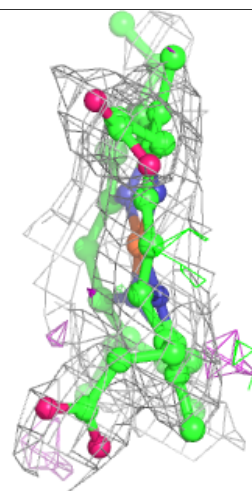
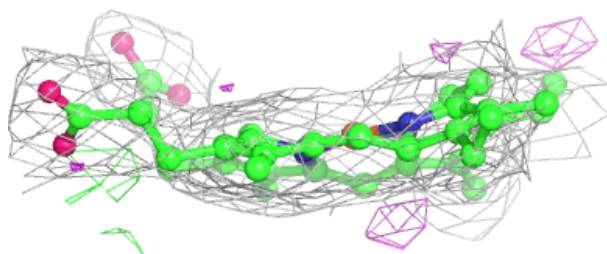
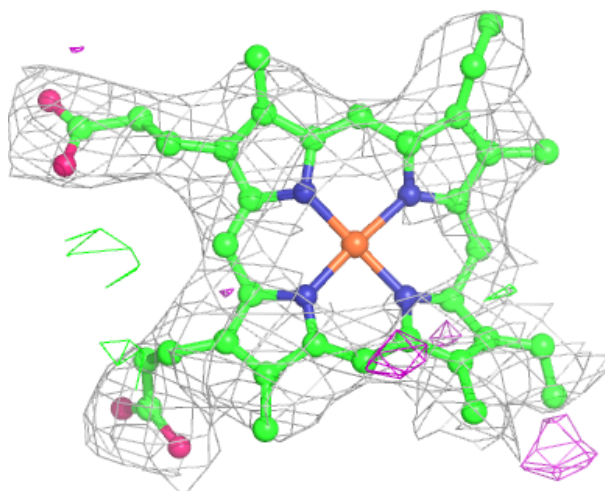
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC L 603:**

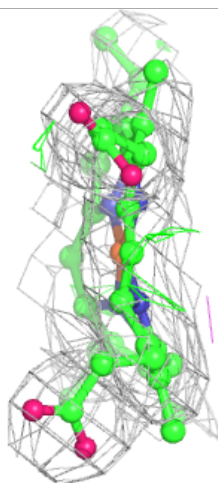
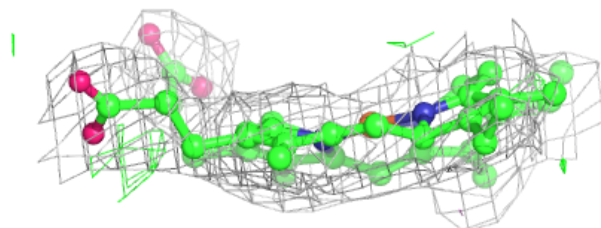
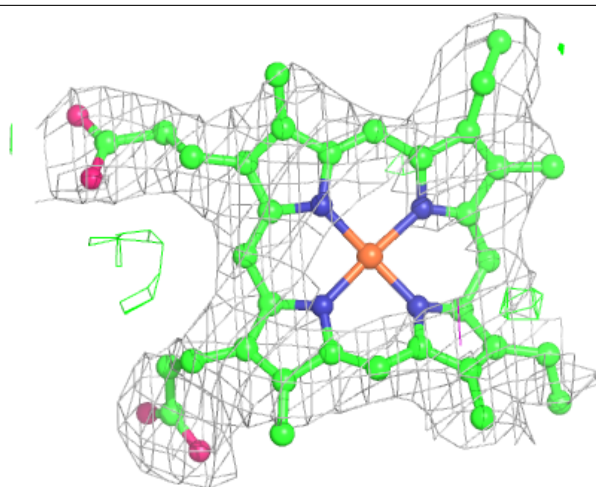
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





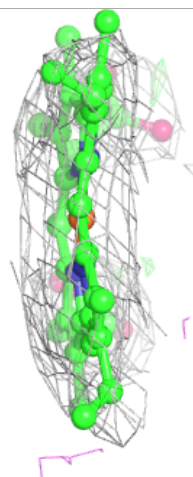
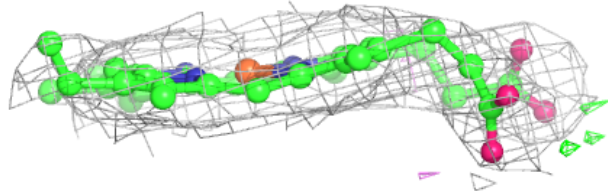
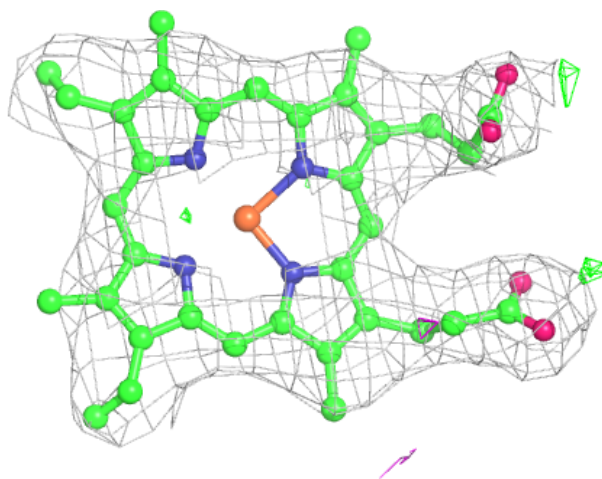
**Electron density around HEC K 603:**

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



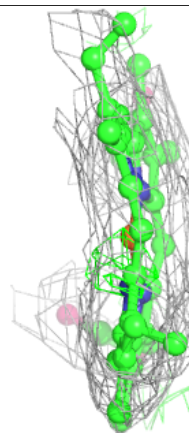
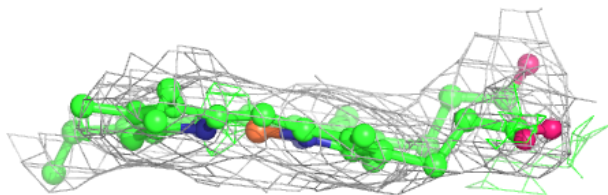
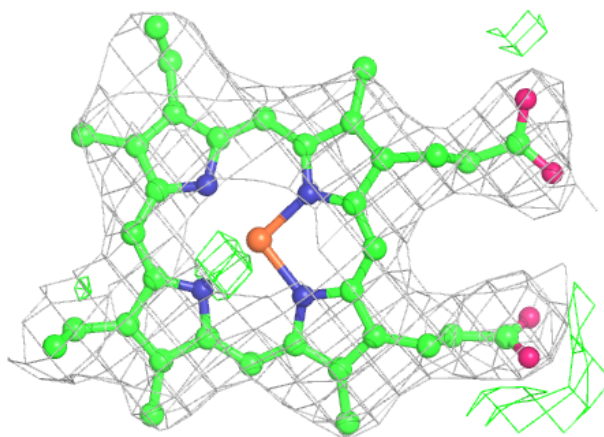
**Electron density around HEC D 607:**

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



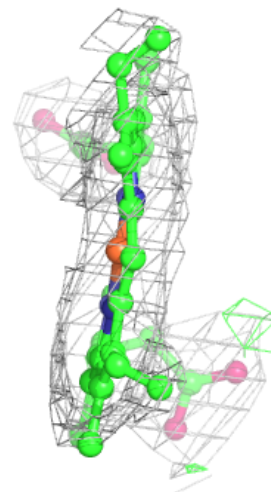
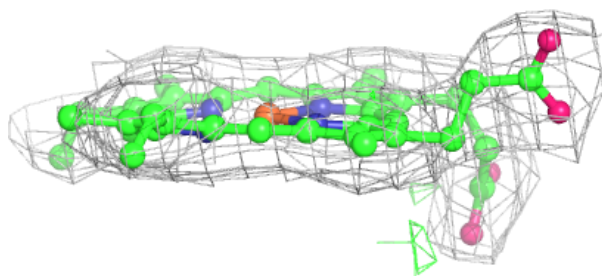
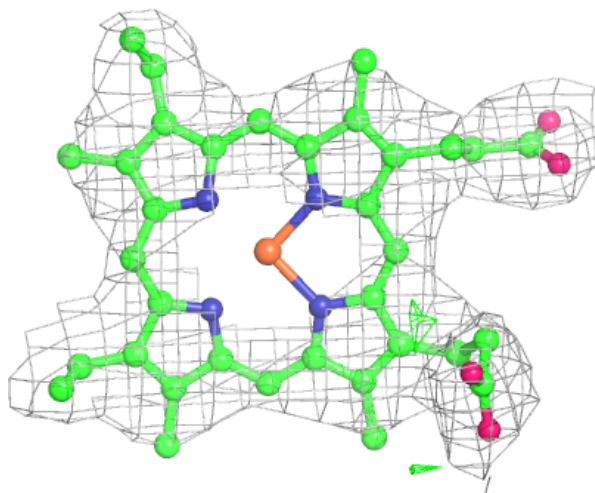
**Electron density around HEC R 606:**

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



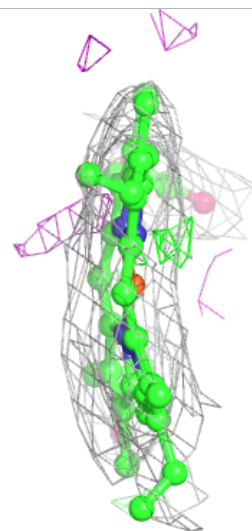
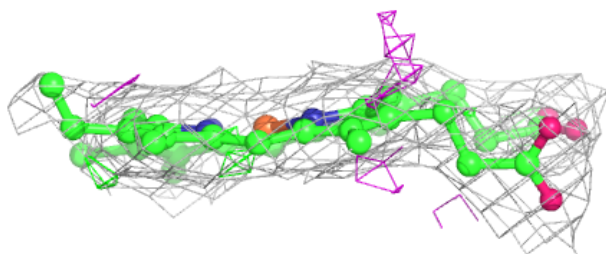
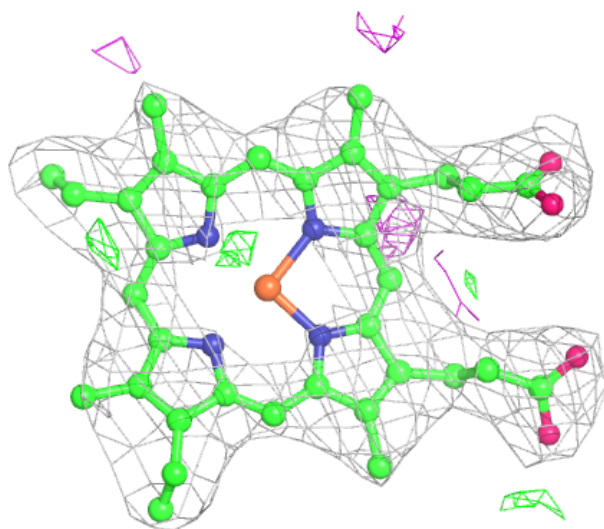
**Electron density around HEC J 601:**

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



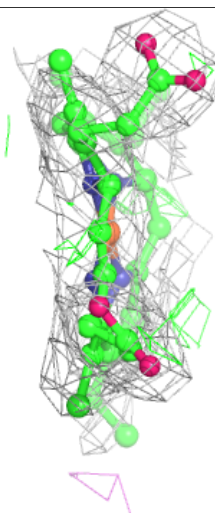
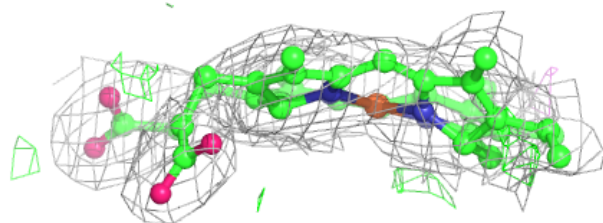
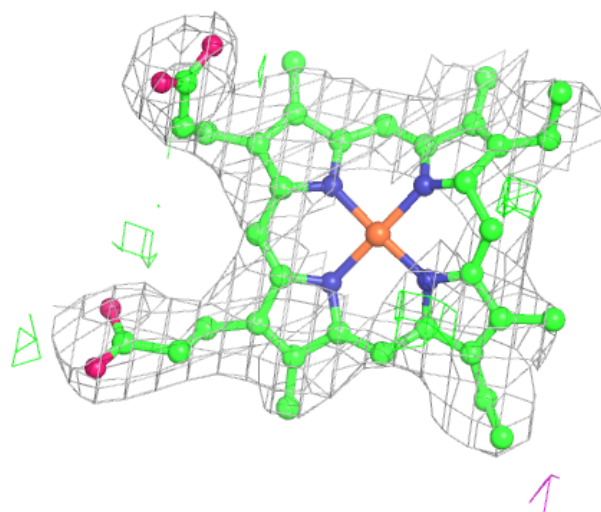
**Electron density around HEC L 606:**

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



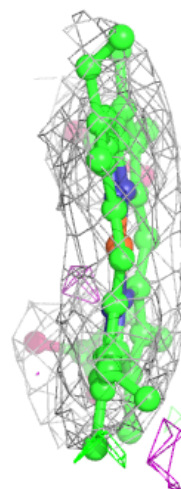
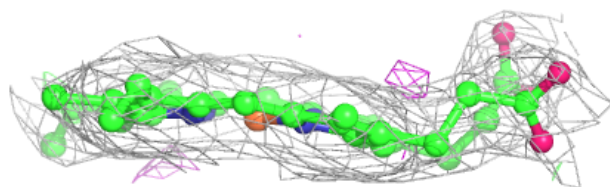
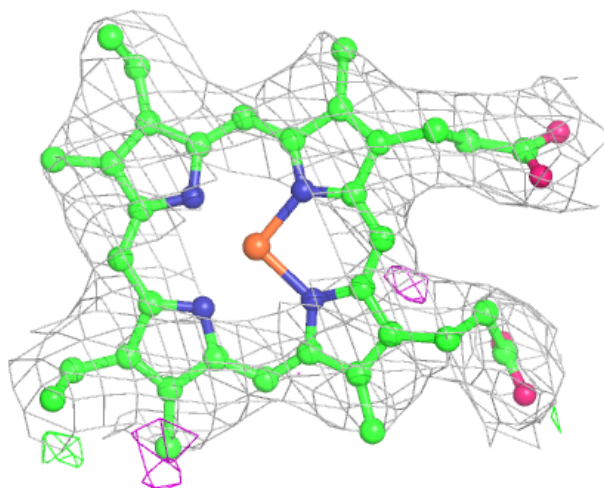
**Electron density around HEC J 603:**

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



**Electron density around HEC B 607:**

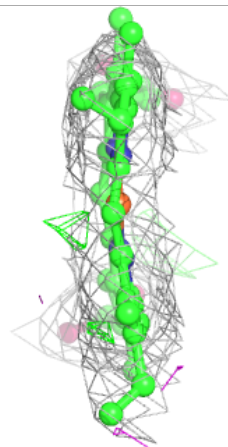
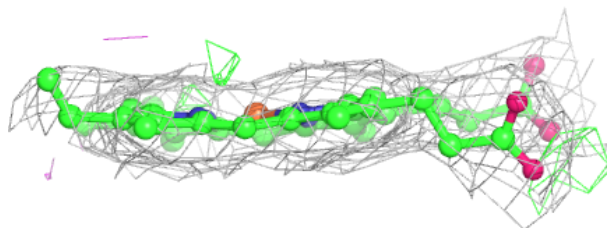
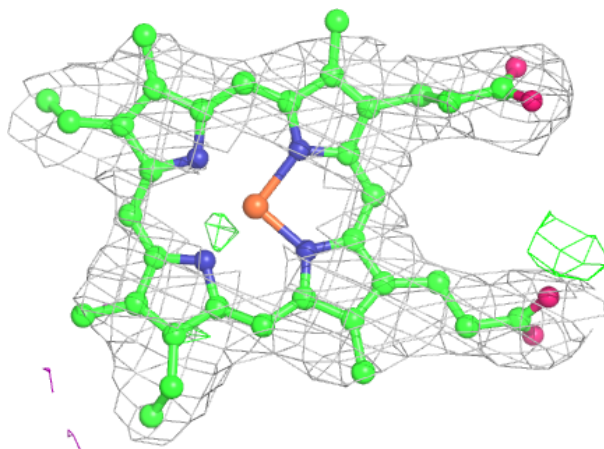
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC K 605:**

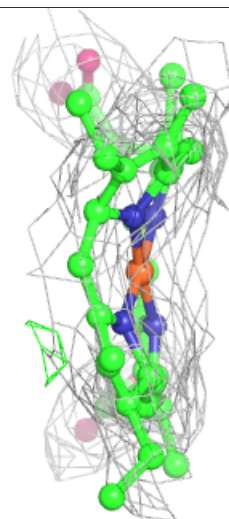
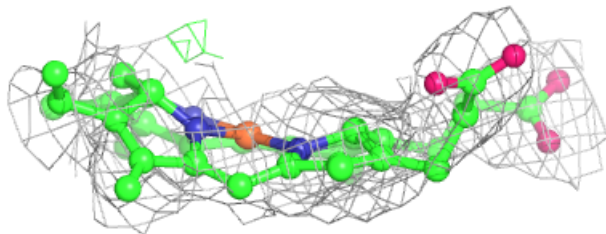
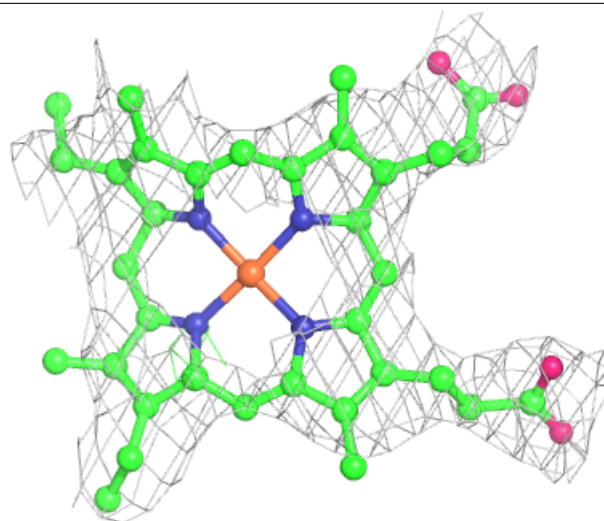
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





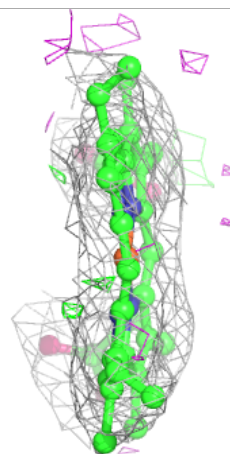
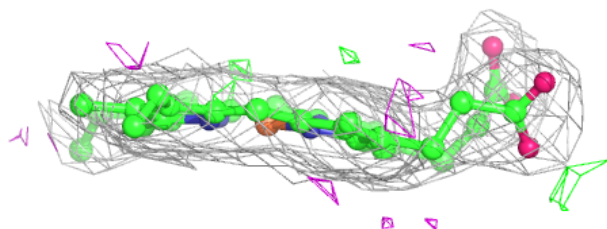
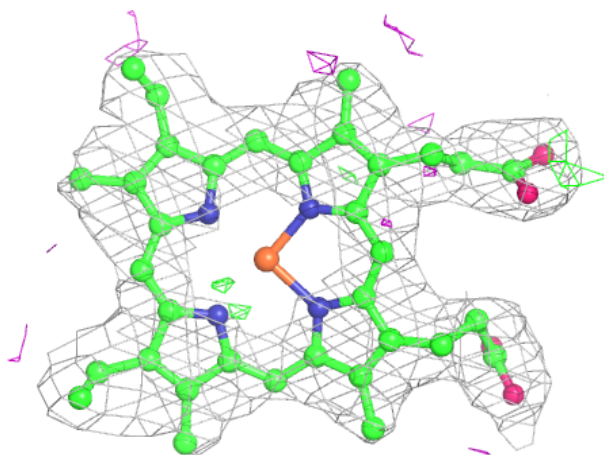
**Electron density around HEC D 603:**

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



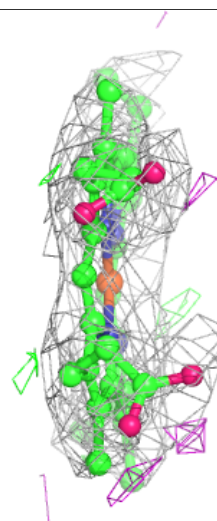
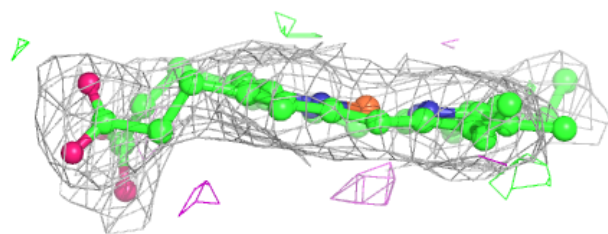
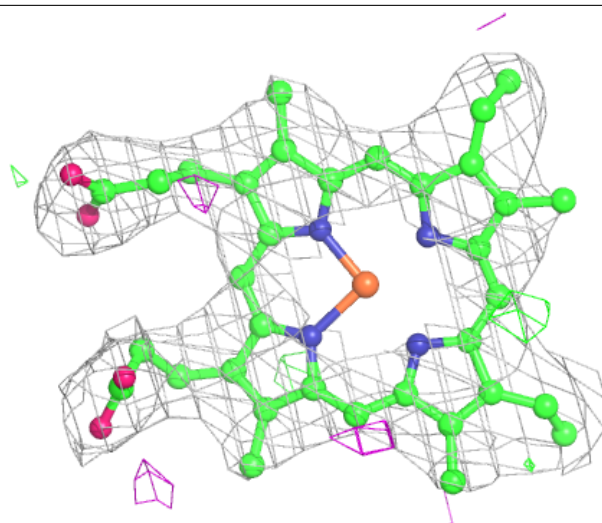
**Electron density around HEC H 607:**

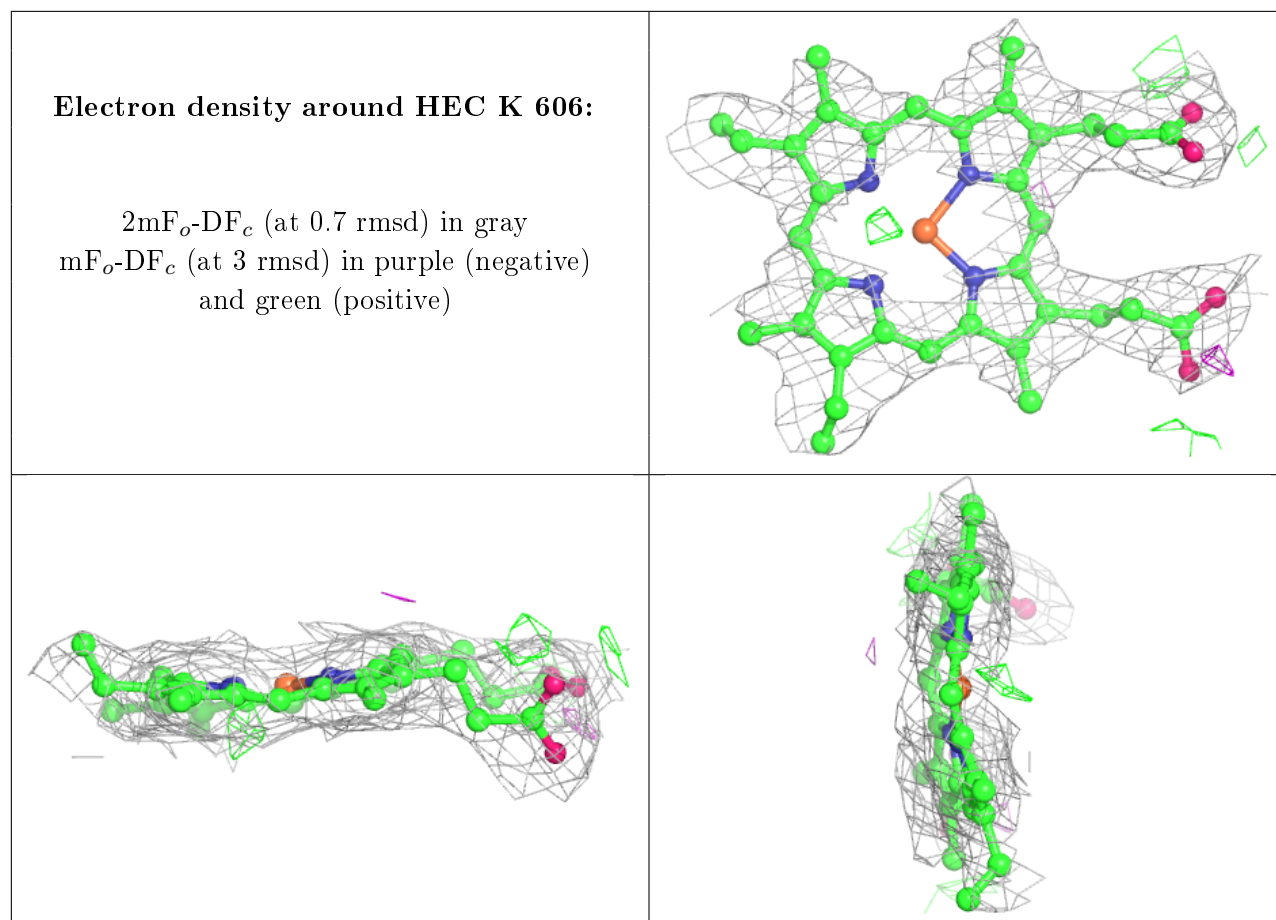
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC N 607:**

$2mF_o-DF_c$  (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.