



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 7, 2024 – 05:07 am GMT

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 wwPDB X-ray Structure Validation Summary 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

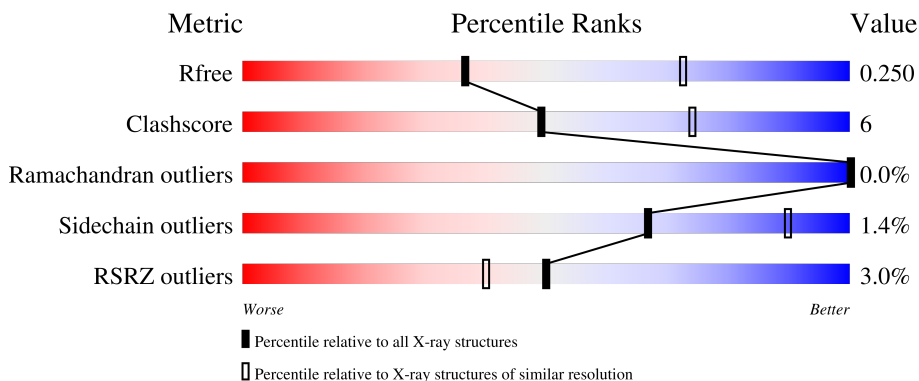
# 1 Overall quality at a glance

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 of 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	
1	B	582	
1	C	582	
1	D	582	

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Mol	Chain	Length	Quality of chain
1	E	582	2% 81% 10% 9%
1	F	582	2% 80% 11% 9%
1	G	582	80% 11% 9%
1	H	582	80% 11% 9%
1	I	582	71% 19% 9%
1	J	582	80% 11% 9%
1	K	582	79% 12% 9%
1	L	582	81% 10% 9%
1	M	582	82% 9% 9%
1	N	582	2% 81% 10% 9%
1	O	582	81% 10% 9%
1	P	582	81% 10% 9%
1	Q	582	80% 11% 9%
1	R	582	80% 11% 9%
1	S	582	8% 81% 10% 9%
1	T	582	4% 81% 10% 9%
1	U	582	6% 82% 9% 9%
1	V	582	8% 82% 9% 9%
1	W	582	5% 81% 10% 9%
1	X	582	6% 81% 10% 9%
2	Y	114	3% 68% 6% 25%
2	Z	114	19% 69% 5% 25%
2	a	114	7% 73% 25%
2	b	114	4% 73% 25%
2	c	114	4% 73% 25%

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Mol	Chain	Length	Quality of chain
2	d	114	
2	e	114	
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
			Total	C	N	O	S			
1	G	531	4226	2647	745	798	36	0	0	0
1	A	531	4226	2647	745	798	36	0	0	0
1	B	531	4226	2647	745	798	36	0	0	0
1	C	531	4226	2647	745	798	36	0	0	0
1	D	531	4226	2647	745	798	36	0	0	0
1	E	531	4226	2647	745	798	36	0	0	0
1	F	531	4226	2647	745	798	36	0	0	0
1	H	531	4226	2647	745	798	36	0	0	0
1	I	527	4201	2633	739	793	36	0	0	0
1	J	531	4226	2647	745	798	36	0	0	0
1	K	531	4226	2647	745	798	36	0	0	0
1	L	531	4226	2647	745	798	36	0	0	0
1	M	531	4226	2647	745	798	36	0	0	0
1	N	531	4226	2647	745	798	36	0	0	0
1	O	531	4226	2647	745	798	36	0	0	0
1	P	531	4226	2647	745	798	36	0	0	0

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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.

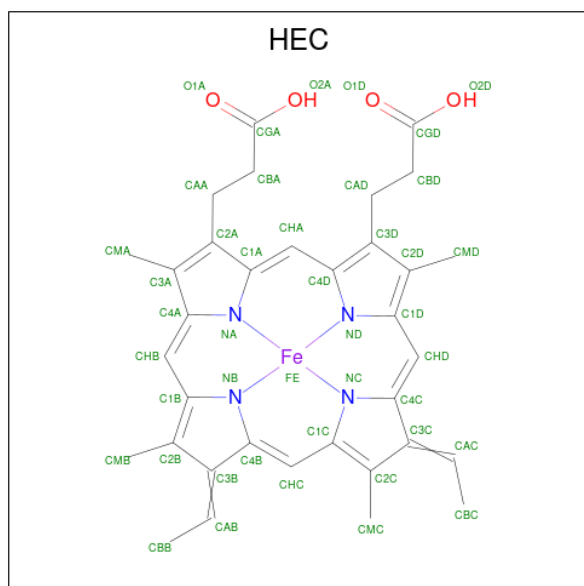
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	Z	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	a	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	b	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	c	86	Total	C	N	O	S	0	0	0
			640	403	110	125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

- Molecule 3 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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

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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	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	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	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	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	C	Fe	N	O	0	0
			43	34	1	4	4		
3	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	L	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	L	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	L	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	L	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	L	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

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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	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

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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	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 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0

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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
			Total	O	S		
4	L	1	5	4	1	0	0
4	L	1	5	4	1	0	0
4	L	1	5	4	1	0	0
4	M	1	5	4	1	0	0
4	M	1	5	4	1	0	0
4	M	1	5	4	1	0	0
4	M	1	5	4	1	0	0
4	N	1	5	4	1	0	0
4	N	1	5	4	1	0	0
4	N	1	5	4	1	0	0
4	O	1	5	4	1	0	0
4	O	1	5	4	1	0	0
4	O	1	5	4	1	0	0
4	P	1	5	4	1	0	0
4	Q	1	5	4	1	0	0
4	Q	1	5	4	1	0	0
4	Q	1	5	4	1	0	0
4	R	1	5	4	1	0	0
4	R	1	5	4	1	0	0
4	R	1	5	4	1	0	0
4	S	1	5	4	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 6 3 3	0	0
5	G	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	H	1	Total C O 6 3 3	0	0
5	H	1	Total C O 6 3 3	0	0
5	I	1	Total C O 6 3 3	0	0
5	I	1	Total C O 6 3 3	0	0
5	I	1	Total C O 6 3 3	0	0
5	J	1	Total C O 6 3 3	0	0
5	J	1	Total C O 6 3 3	0	0
5	K	1	Total C O 6 3 3	0	0

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

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

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

- Molecule 7 is water.

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

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

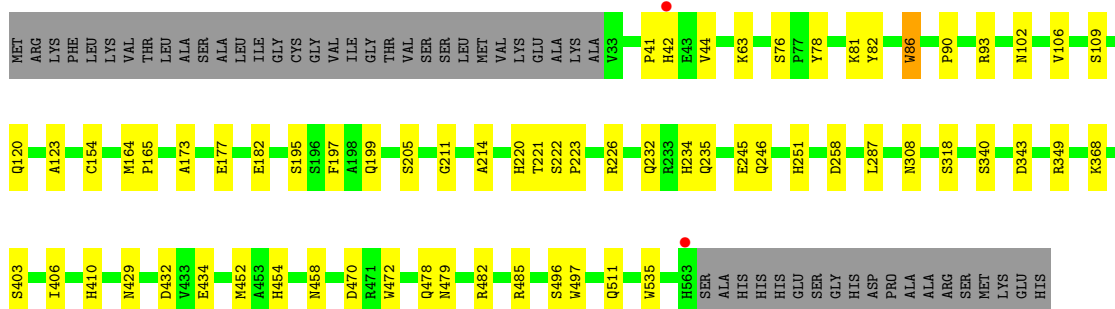


### 3 Residue-property plots [i](#)


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

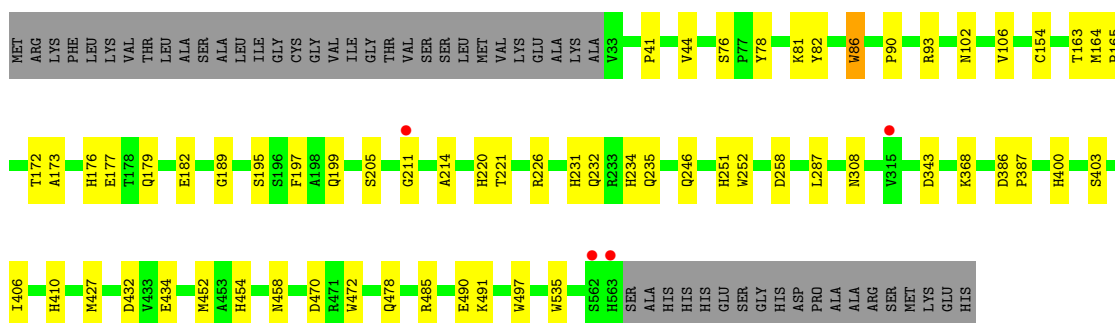
- Molecule 1: Hydrazine dehydrogenase

Chain G: 




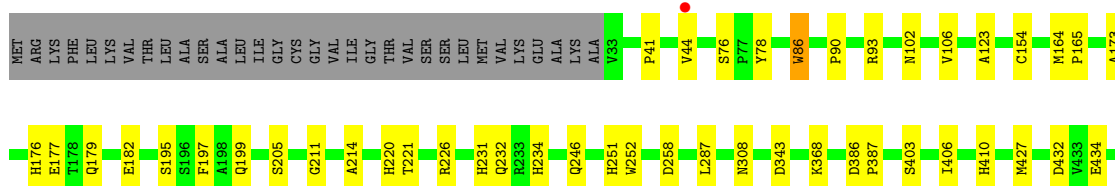
- Molecule 1: Hydrazine dehydrogenase

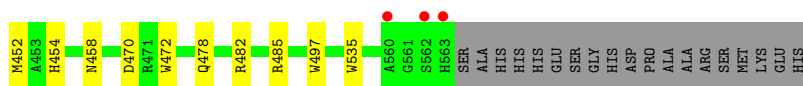
Chain A: 



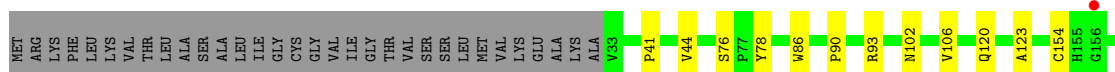
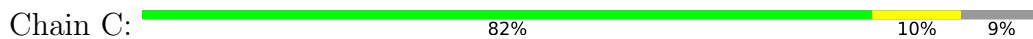
- Molecule 1: Hydrazine dehydrogenase

Chain B: 

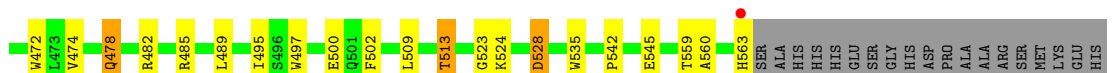
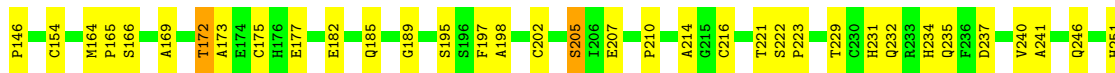
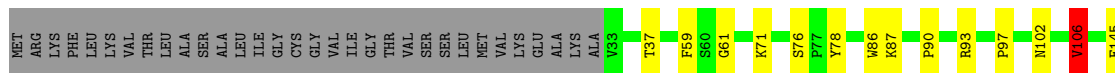




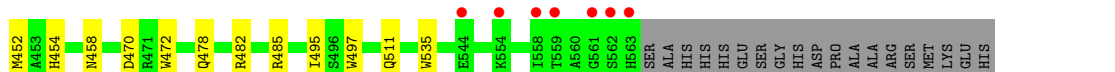
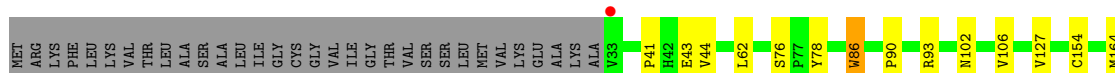
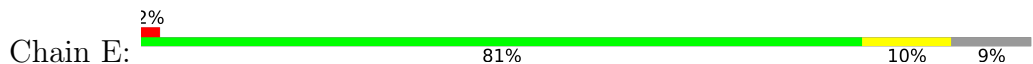
• Molecule 1: Hydrazine dehydrogenase



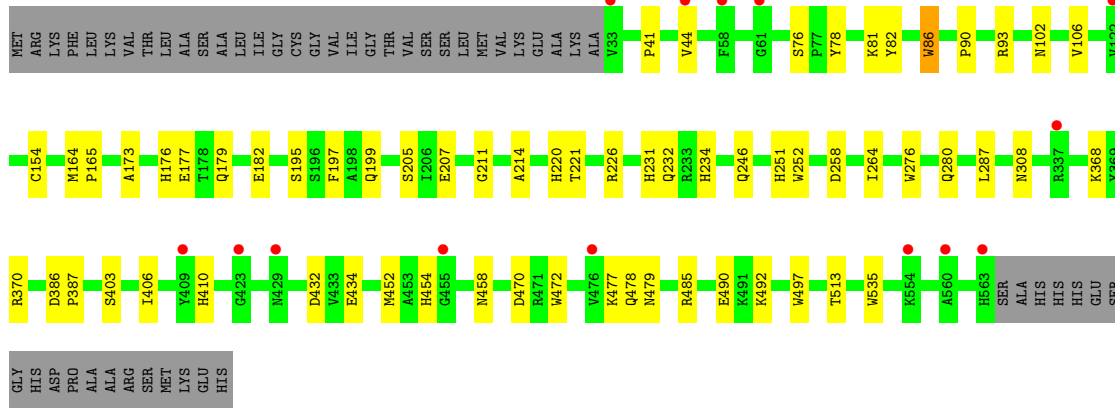
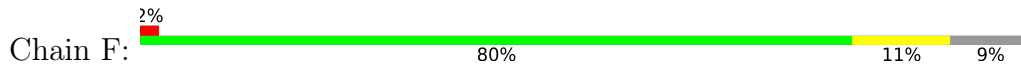
• Molecule 1: Hydrazine dehydrogenase



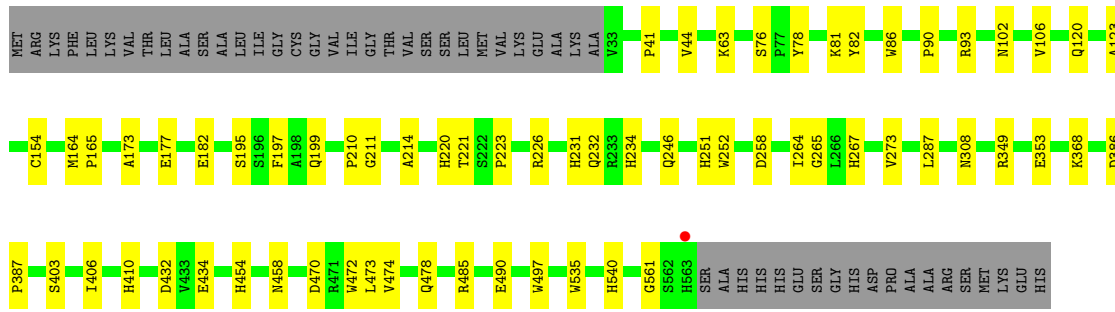
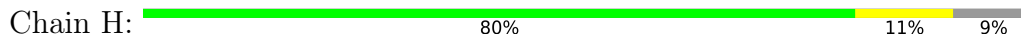
• Molecule 1: Hydrazine dehydrogenase



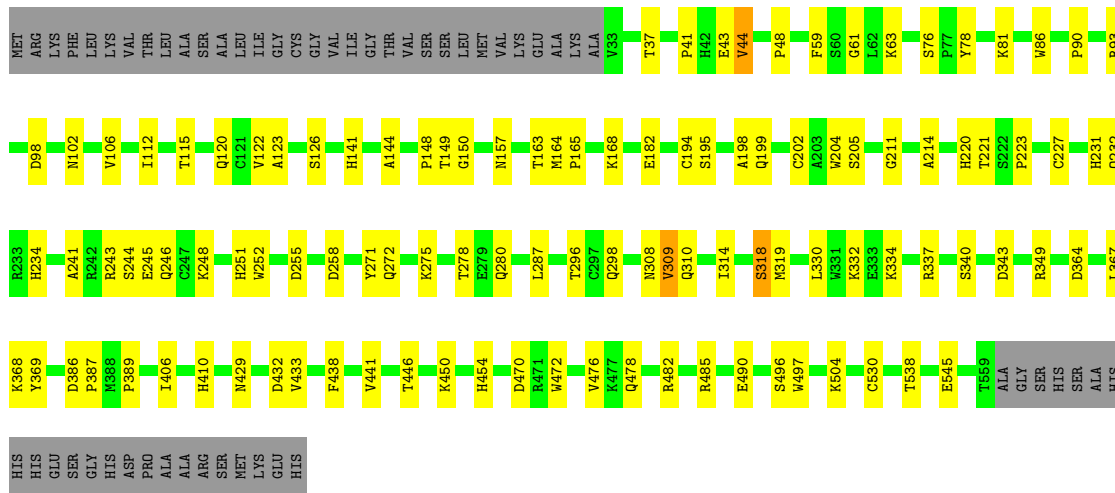
• Molecule 1: Hydrazine dehydrogenase




• Molecule 1: Hydrazine dehydrogenase

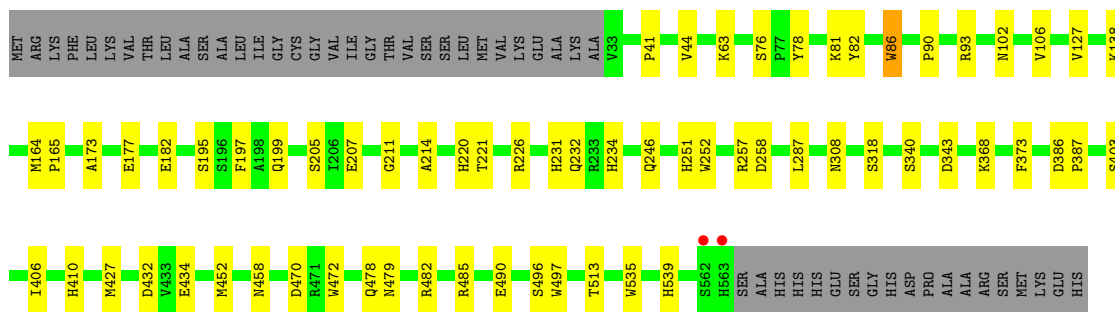


• Molecule 1: Hydrazine dehydrogenase




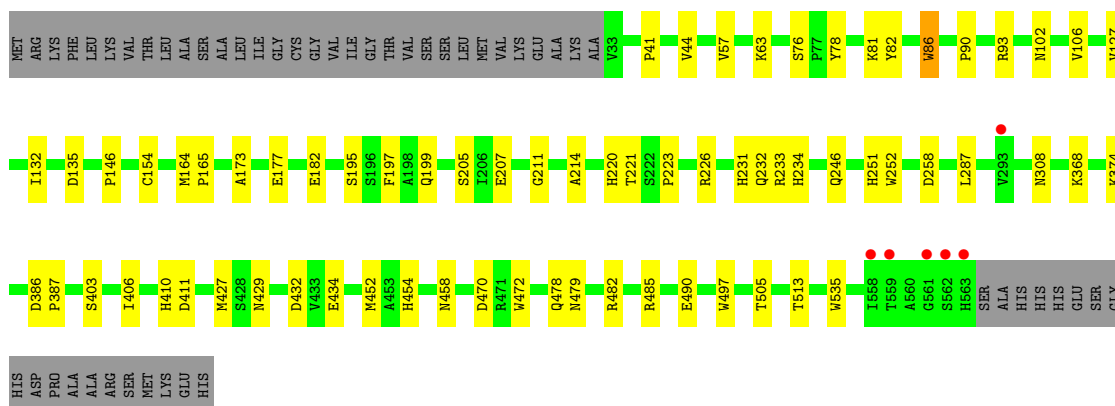
• Molecule 1: Hydrazine dehydrogenase

Chain J:  80% 11% 9%




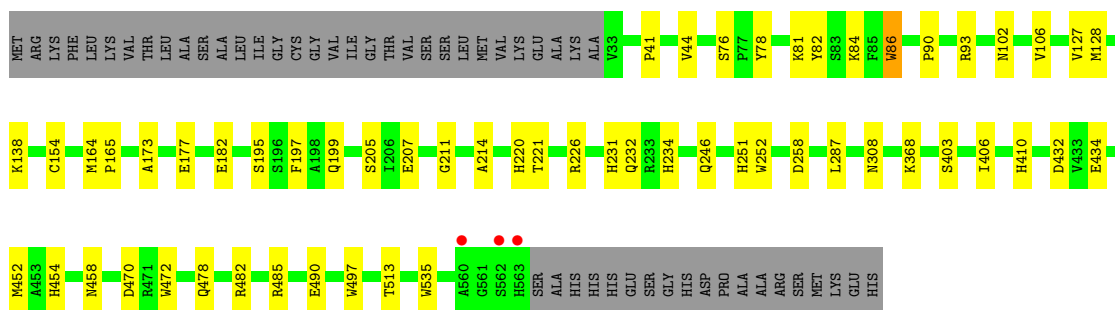
• Molecule 1: Hydrazine dehydrogenase

Chain K:  79% 12% 9%




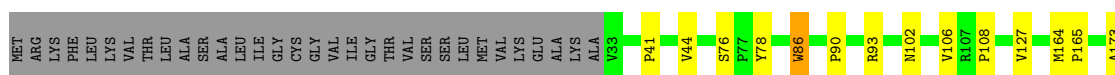
• Molecule 1: Hydrazine dehydrogenase

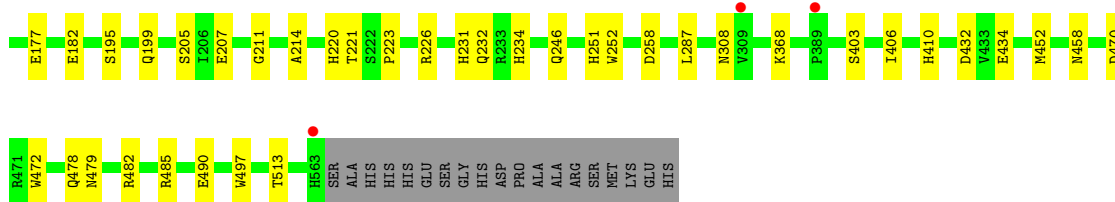
Chain L:  81% 10% 9%



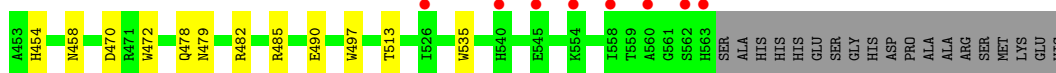
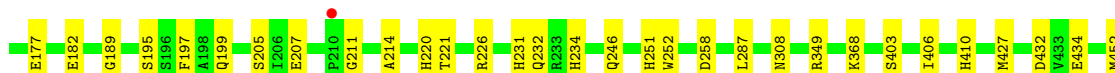
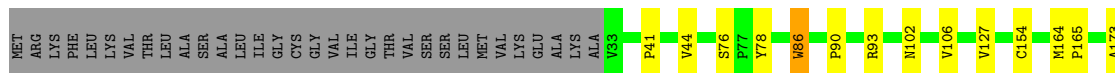
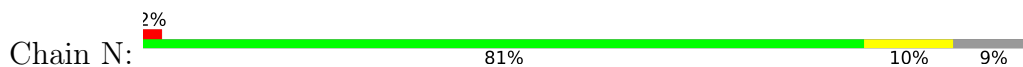
• Molecule 1: Hydrazine dehydrogenase

Chain M:  82% 9% 9%

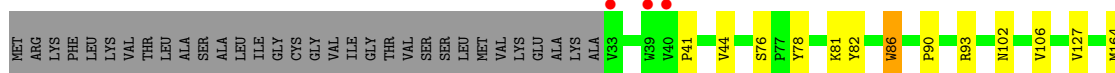
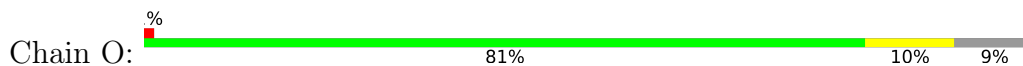




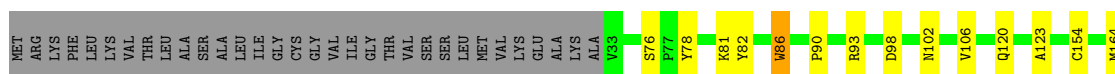
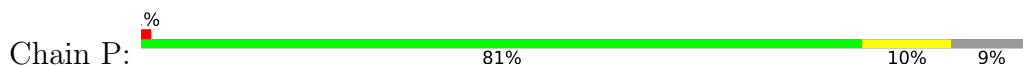
- Molecule 1: Hydrazine dehydrogenase



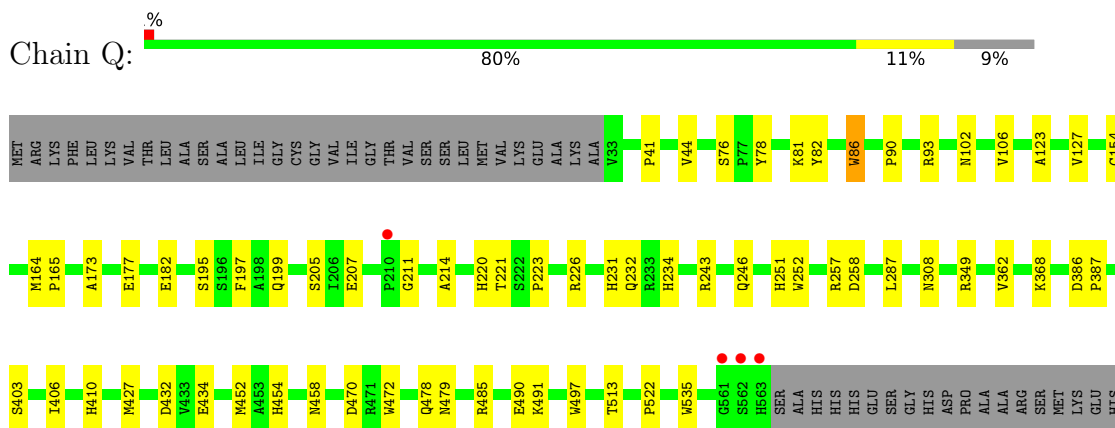
- Molecule 1: Hydrazine dehydrogenase



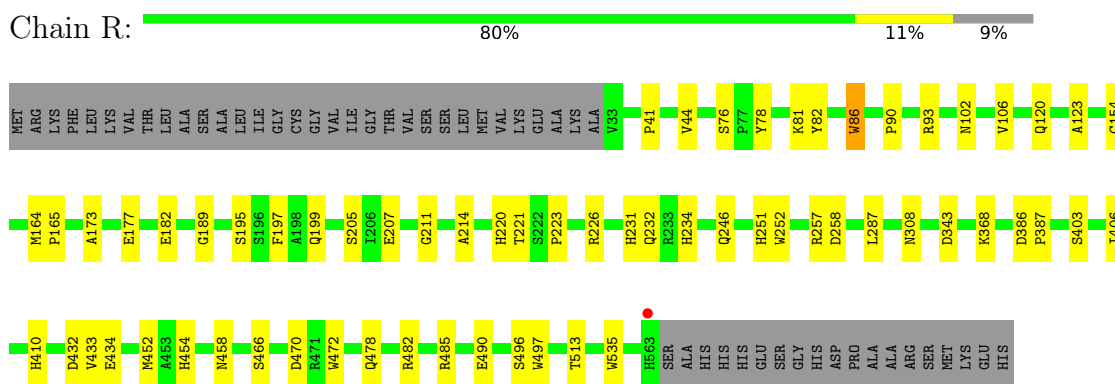
- Molecule 1: Hydrazine dehydrogenase



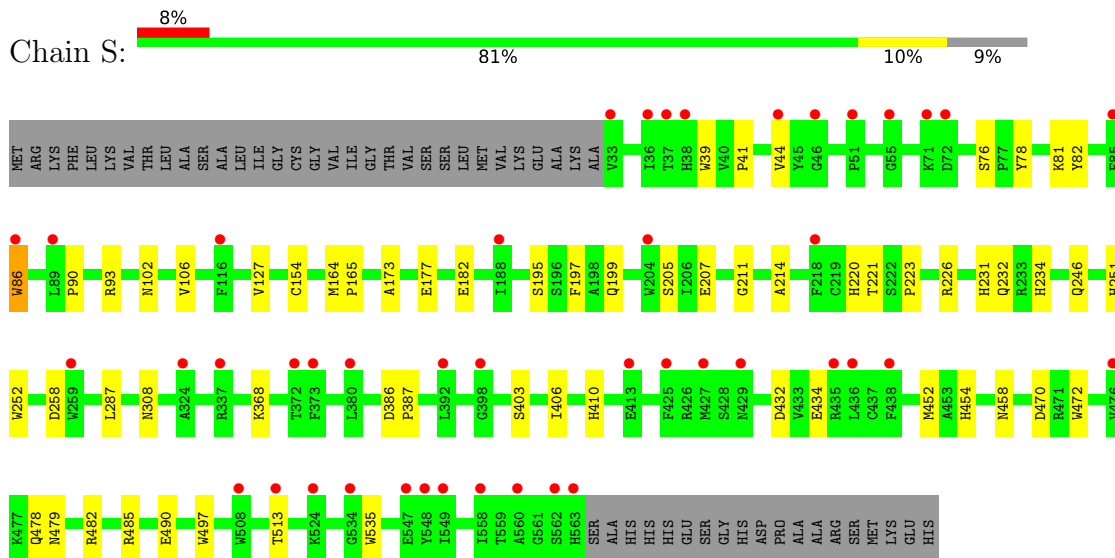
- Molecule 1: Hydrazine dehydrogenase



● Molecule 1: Hydrazine dehydrogenase

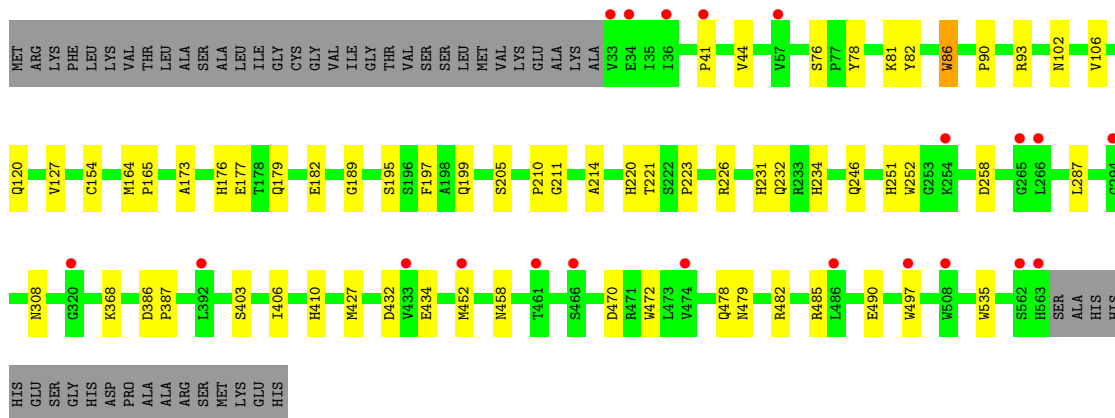


● Molecule 1: Hydrazine dehydrogenase

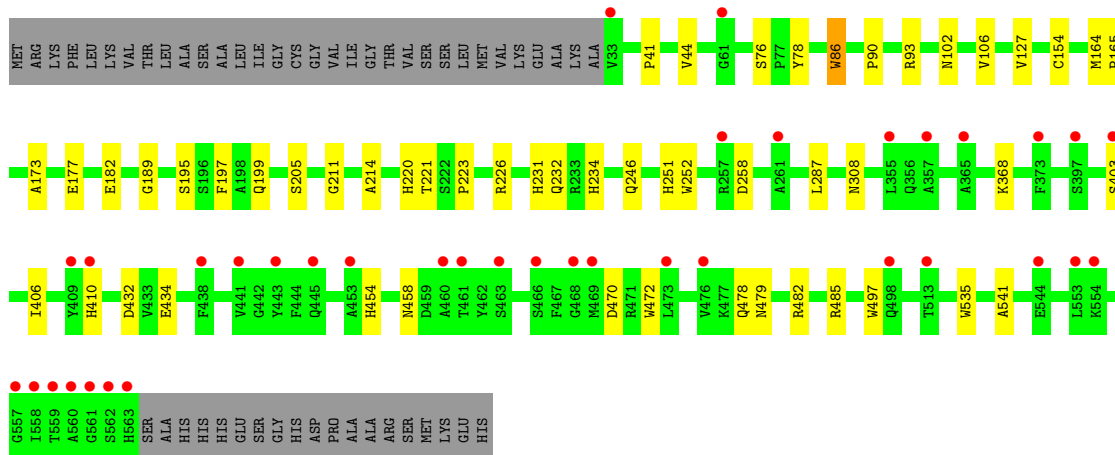
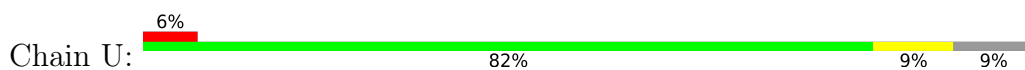


● Molecule 1: Hydrazine dehydrogenase

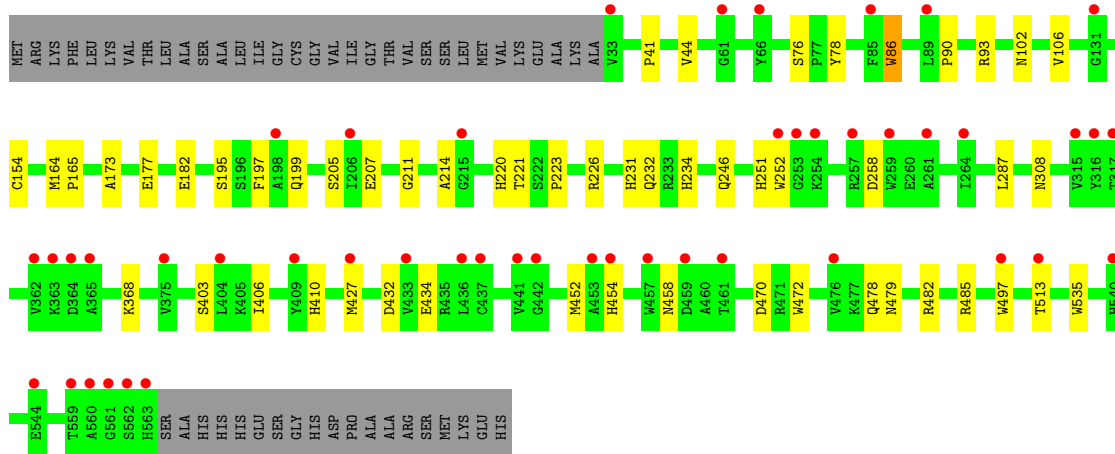
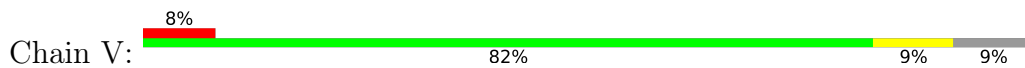




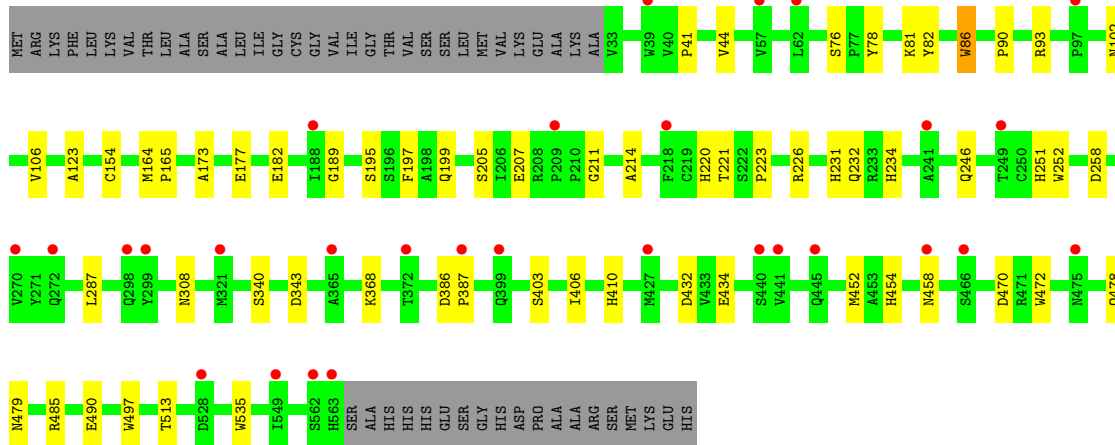
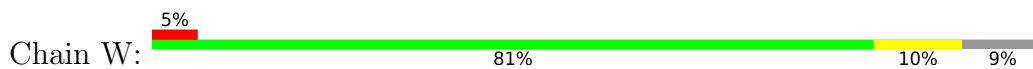
● Molecule 1: Hydrazine dehydrogenase



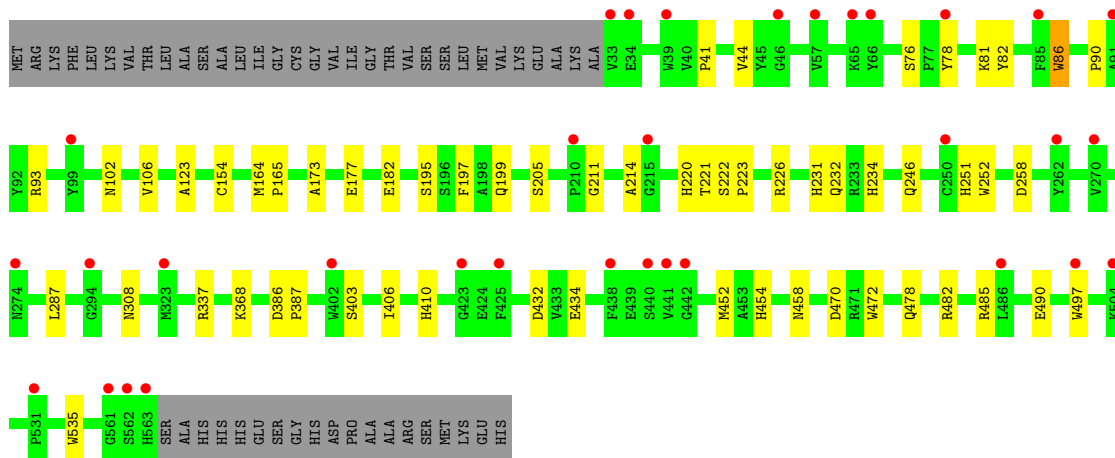
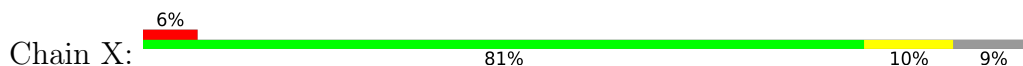
● Molecule 1: Hydrazine dehydrogenase



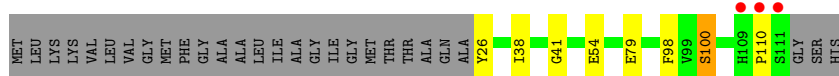
● Molecule 1: Hydrazine dehydrogenase



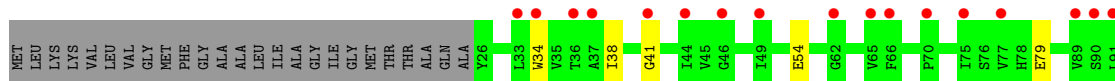
- Molecule 1: Hydrazine dehydrogenase



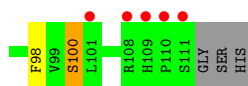
- Molecule 2: hdh assembly factor Kustc1130



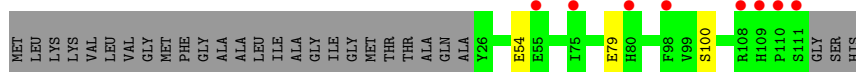
- Molecule 2: hdh assembly factor Kustc1130



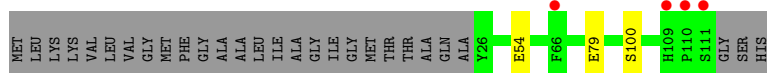




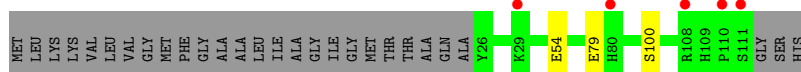
- Molecule 2: hdh assembly factor Kustc1130



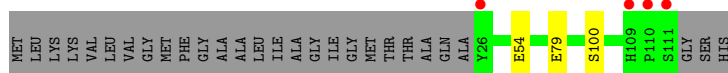
- Molecule 2: hdh assembly factor Kustc1130



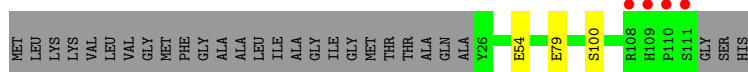
- Molecule 2: hdh assembly factor Kustc1130



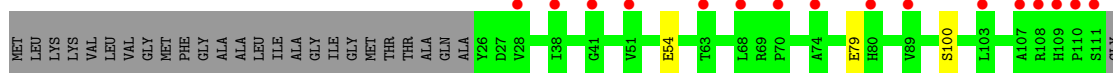
- Molecule 2: hdh assembly factor Kustc1130



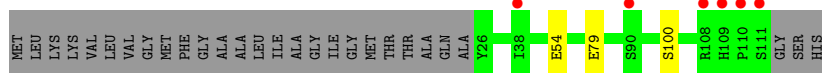
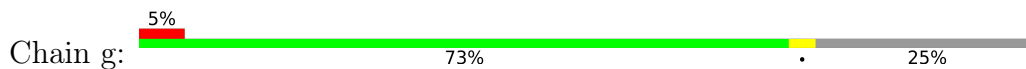
- Molecule 2: hdh assembly factor Kustc1130



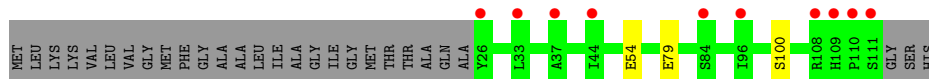
- Molecule 2: hdh assembly factor Kustc1130



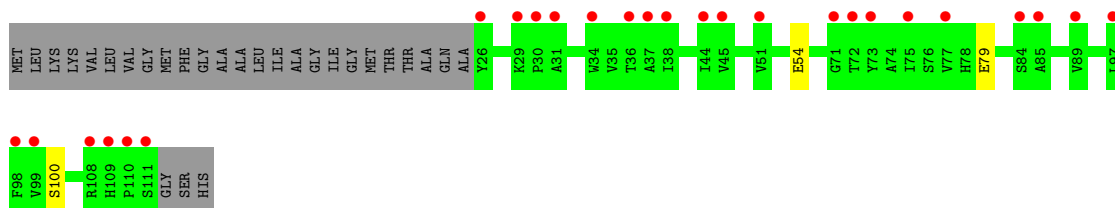
• Molecule 2: hdh assembly factor Kustc1130



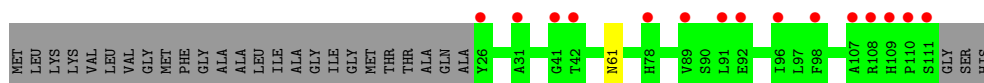
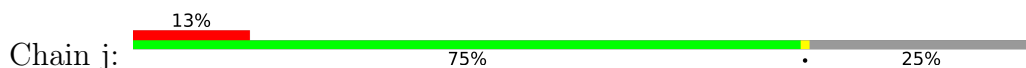
• Molecule 2: hdh assembly factor Kustc1130



• 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)	Xtrriage
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	Xtrriage
Anisotropy	0.123	Xtrriage
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>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.000 for -h,-k,l 0.000 for h,-h-k,-l 0.000 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	118753	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage'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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, SO4, K, GOL

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.

The worst 5 of 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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	451/491 (92%)	446 (99%)	5 (1%)	73	92
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

5 of 164 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	231	HIS
2	c	79	GLU
1	V	231	HIS
2	Y	54	GLU
2	e	100	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 263 such sidechains are listed below:

Mol	Chain	Res	Type
1	V	179	GLN
1	V	478	GLN
1	X	479	ASN
1	I	479	ASN
1	I	410	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 monosaccharides 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	A	607	1	32,50,50	1.51	4 (12%)	24,82,82	1.15	0
3	HEC	U	603	1,7	32,50,50	2.50	11 (34%)	24,82,82	2.10	9 (37%)
3	HEC	W	604	1	32,50,50	1.52	4 (12%)	24,82,82	1.75	2 (8%)
4	SO4	V	609	-	4,4,4	0.40	0	6,6,6	0.28	0
3	HEC	I	601	1	32,50,50	1.58	4 (12%)	24,82,82	1.38	3 (12%)
3	HEC	A	603	1,7	32,50,50	2.51	10 (31%)	24,82,82	2.16	10 (41%)
3	HEC	X	606	1	32,50,50	1.52	4 (12%)	24,82,82	1.40	2 (8%)
4	SO4	G	611	-	4,4,4	0.34	0	6,6,6	0.10	0
4	SO4	K	610	-	4,4,4	0.34	0	6,6,6	0.10	0
4	SO4	X	610	-	4,4,4	0.33	0	6,6,6	0.05	0
3	HEC	K	601	1	32,50,50	1.56	4 (12%)	24,82,82	1.44	3 (12%)
3	HEC	X	600	1	32,50,50	1.52	4 (12%)	24,82,82	1.23	1 (4%)
4	SO4	H	611	-	4,4,4	0.32	0	6,6,6	0.21	0
3	HEC	F	606	1	32,50,50	1.48	4 (12%)	24,82,82	1.39	2 (8%)
4	SO4	J	610	-	4,4,4	0.32	0	6,6,6	0.13	0
3	HEC	F	602	1	32,50,50	1.51	4 (12%)	24,82,82	1.37	3 (12%)
3	HEC	D	602	1	32,50,50	1.51	4 (12%)	24,82,82	1.40	4 (16%)
3	HEC	E	600	1	32,50,50	1.53	4 (12%)	24,82,82	1.18	0
3	HEC	H	603	1,7	32,50,50	2.52	11 (34%)	24,82,82	2.07	9 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HEC	M	602	1	32,50,50	1.50	4 (12%)	24,82,82	1.38	3 (12%)
3	HEC	O	601	1	32,50,50	1.59	4 (12%)	24,82,82	1.38	2 (8%)
3	HEC	G	607	1	32,50,50	1.53	4 (12%)	24,82,82	1.18	1 (4%)
3	HEC	A	605	1	32,50,50	1.49	4 (12%)	24,82,82	1.61	5 (20%)
3	HEC	W	600	1	32,50,50	1.53	4 (12%)	24,82,82	1.24	1 (4%)
3	HEC	H	606	1	32,50,50	1.58	4 (12%)	24,82,82	1.34	1 (4%)
3	HEC	L	600	1	32,50,50	1.45	4 (12%)	24,82,82	1.19	1 (4%)
4	SO4	c	201	-	4,4,4	0.35	0	6,6,6	0.09	0
4	SO4	Y	201	-	4,4,4	0.32	0	6,6,6	0.11	0
3	HEC	I	603	1,7	32,50,50	2.48	10 (31%)	24,82,82	4.07	8 (33%)
3	HEC	N	601	1	32,50,50	1.55	4 (12%)	24,82,82	1.37	2 (8%)
3	HEC	J	604	1	32,50,50	1.49	4 (12%)	24,82,82	1.76	2 (8%)
3	HEC	V	600	1	32,50,50	1.52	4 (12%)	24,82,82	1.20	1 (4%)
4	SO4	M	612	-	4,4,4	0.34	0	6,6,6	0.14	0
4	SO4	C	609	-	4,4,4	0.32	0	6,6,6	0.14	0
4	SO4	I	612	-	4,4,4	0.36	0	6,6,6	0.06	0
3	HEC	P	606	1	32,50,50	1.49	4 (12%)	24,82,82	1.37	3 (12%)
4	SO4	K	611	-	4,4,4	0.36	0	6,6,6	0.06	0
3	HEC	M	601	1	32,50,50	1.56	4 (12%)	24,82,82	1.37	2 (8%)
3	HEC	D	601	1	32,50,50	1.55	4 (12%)	24,82,82	1.32	3 (12%)
4	SO4	C	610	-	4,4,4	0.34	0	6,6,6	0.12	0
3	HEC	W	601	1	32,50,50	1.57	4 (12%)	24,82,82	1.34	3 (12%)
3	HEC	X	604	1	32,50,50	1.52	4 (12%)	24,82,82	1.71	2 (8%)
3	HEC	B	603	1	32,50,50	2.49	11 (34%)	24,82,82	2.03	9 (37%)
3	HEC	I	607	1	32,50,50	1.50	4 (12%)	24,82,82	1.13	0
3	HEC	O	603	1,7	32,50,50	2.53	11 (34%)	24,82,82	2.11	9 (37%)
3	HEC	M	607	1	32,50,50	1.52	4 (12%)	24,82,82	1.13	0
3	HEC	X	602	1	32,50,50	1.46	4 (12%)	24,82,82	1.40	3 (12%)
3	HEC	T	604	1	32,50,50	1.51	4 (12%)	24,82,82	1.78	2 (8%)
3	HEC	S	603	1,7	32,50,50	2.56	12 (37%)	24,82,82	2.12	10 (41%)
3	HEC	V	601	1	32,50,50	1.51	4 (12%)	24,82,82	1.42	3 (12%)
3	HEC	T	600	1	32,50,50	1.52	4 (12%)	24,82,82	1.19	1 (4%)
4	SO4	F	610	-	4,4,4	0.33	0	6,6,6	0.08	0
4	SO4	W	609	-	4,4,4	0.35	0	6,6,6	0.10	0
3	HEC	O	607	1	32,50,50	1.46	4 (12%)	24,82,82	1.21	1 (4%)
4	SO4	H	613	-	4,4,4	0.33	0	6,6,6	0.23	0
3	HEC	V	602	1	32,50,50	1.49	4 (12%)	24,82,82	1.38	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	K	614	-	5,5,5	0.18	0	5,5,5	0.37	0
3	HEC	X	601	1	32,50,50	1.52	4 (12%)	24,82,82	1.40	3 (12%)
4	SO4	H	610	-	4,4,4	0.36	0	6,6,6	0.05	0
4	SO4	I	609	-	4,4,4	0.35	0	6,6,6	0.34	0
4	SO4	S	609	-	4,4,4	0.34	0	6,6,6	0.05	0
5	GOL	K	613	-	5,5,5	0.23	0	5,5,5	0.34	0
3	HEC	A	600	1	32,50,50	1.49	4 (12%)	24,82,82	1.26	2 (8%)
3	HEC	A	604	1	32,50,50	1.54	4 (12%)	24,82,82	1.73	2 (8%)
3	HEC	P	602	1	32,50,50	1.54	4 (12%)	24,82,82	1.33	2 (8%)
4	SO4	L	612	-	4,4,4	0.36	0	6,6,6	0.10	0
4	SO4	N	611	-	4,4,4	0.33	0	6,6,6	0.09	0
3	HEC	L	601	1	32,50,50	1.51	4 (12%)	24,82,82	1.36	3 (12%)
3	HEC	S	607	1	32,50,50	1.50	4 (12%)	24,82,82	1.18	2 (8%)
3	HEC	W	606	1	32,50,50	1.51	4 (12%)	24,82,82	1.38	2 (8%)
3	HEC	D	604	1	32,50,50	1.52	5 (15%)	24,82,82	1.68	2 (8%)
4	SO4	G	610	-	4,4,4	0.29	0	6,6,6	0.09	0
3	HEC	T	602	1	32,50,50	1.52	4 (12%)	24,82,82	1.39	3 (12%)
3	HEC	T	601	1	32,50,50	1.57	4 (12%)	24,82,82	1.36	3 (12%)
4	SO4	H	609	-	4,4,4	0.36	0	6,6,6	0.10	0
3	HEC	Q	601	1	32,50,50	1.54	4 (12%)	24,82,82	1.39	3 (12%)
3	HEC	F	607	1	32,50,50	1.46	4 (12%)	24,82,82	1.19	0
4	SO4	M	610	-	4,4,4	0.32	0	6,6,6	0.09	0
3	HEC	K	607	1	32,50,50	1.51	4 (12%)	24,82,82	1.19	2 (8%)
3	HEC	R	604	1	32,50,50	1.52	4 (12%)	24,82,82	1.66	2 (8%)
3	HEC	F	604	1	32,50,50	1.49	4 (12%)	24,82,82	1.76	2 (8%)
3	HEC	X	603	1,7	32,50,50	2.51	10 (31%)	24,82,82	2.10	8 (33%)
4	SO4	V	610	-	4,4,4	0.35	0	6,6,6	0.12	0
3	HEC	R	600	1	32,50,50	1.46	4 (12%)	24,82,82	1.23	1 (4%)
3	HEC	G	604	1	32,50,50	1.57	4 (12%)	24,82,82	1.72	2 (8%)
3	HEC	E	606	1	32,50,50	1.48	4 (12%)	24,82,82	1.41	4 (16%)
3	HEC	E	603	1,7	32,50,50	2.55	10 (31%)	24,82,82	2.10	7 (29%)
4	SO4	G	614	-	4,4,4	0.37	0	6,6,6	0.15	0
4	SO4	K	609	-	4,4,4	0.21	0	6,6,6	0.34	0
4	SO4	Q	609	-	4,4,4	0.34	0	6,6,6	0.14	0
4	SO4	Q	611	-	4,4,4	0.35	0	6,6,6	0.14	0
3	HEC	I	602	1	32,50,50	1.50	4 (12%)	24,82,82	1.35	4 (16%)
3	HEC	L	606	1	32,50,50	1.46	4 (12%)	24,82,82	1.44	3 (12%)
3	HEC	M	605	1	32,50,50	1.46	4 (12%)	24,82,82	1.56	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HEC	I	605	1	32,50,50	1.51	4 (12%)	24,82,82	1.65	6 (25%)
4	SO4	R	611	-	4,4,4	0.31	0	6,6,6	0.06	0
4	SO4	L	609	-	4,4,4	0.34	0	6,6,6	0.13	0
3	HEC	J	606	1	32,50,50	1.48	4 (12%)	24,82,82	1.38	2 (8%)
4	SO4	O	609	-	4,4,4	0.36	0	6,6,6	0.08	0
3	HEC	H	607	1	32,50,50	1.51	4 (12%)	24,82,82	1.20	1 (4%)
3	HEC	J	600	1	32,50,50	1.51	4 (12%)	24,82,82	1.20	1 (4%)
4	SO4	N	609	-	4,4,4	0.37	0	6,6,6	0.13	0
4	SO4	Q	610	-	4,4,4	0.33	0	6,6,6	0.11	0
3	HEC	B	605	1	32,50,50	1.52	4 (12%)	24,82,82	1.54	3 (12%)
5	GOL	D	610	-	5,5,5	0.29	0	5,5,5	0.23	0
3	HEC	P	603	1,7	32,50,50	2.49	10 (31%)	24,82,82	2.14	11 (45%)
3	HEC	M	603	1,7	32,50,50	2.54	12 (37%)	24,82,82	2.05	7 (29%)
4	SO4	O	611	-	4,4,4	0.32	0	6,6,6	0.08	0
3	HEC	C	603	1	32,50,50	2.50	13 (40%)	24,82,82	2.03	9 (37%)
3	HEC	K	606	1	32,50,50	1.47	4 (12%)	24,82,82	1.46	3 (12%)
3	HEC	Q	602	1	32,50,50	1.49	4 (12%)	24,82,82	1.35	3 (12%)
3	HEC	K	604	1	32,50,50	1.52	4 (12%)	24,82,82	1.76	2 (8%)
3	HEC	V	606	1	32,50,50	1.53	4 (12%)	24,82,82	1.38	4 (16%)
3	HEC	Q	604	1	32,50,50	1.49	4 (12%)	24,82,82	1.77	2 (8%)
3	HEC	Q	607	1	32,50,50	1.47	4 (12%)	24,82,82	1.28	2 (8%)
4	SO4	L	610	-	4,4,4	0.30	0	6,6,6	0.16	0
3	HEC	J	601	1	32,50,50	1.57	4 (12%)	24,82,82	1.32	2 (8%)
3	HEC	K	600	1	32,50,50	1.47	4 (12%)	24,82,82	1.28	1 (4%)
3	HEC	R	605	1	32,50,50	1.47	4 (12%)	24,82,82	1.62	5 (20%)
4	SO4	A	609	-	4,4,4	0.30	0	6,6,6	0.12	0
4	SO4	M	609	-	4,4,4	0.35	0	6,6,6	0.09	0
5	GOL	I	615	-	5,5,5	0.33	0	5,5,5	0.36	0
3	HEC	U	604	1	32,50,50	1.50	4 (12%)	24,82,82	1.73	2 (8%)
3	HEC	E	602	1	32,50,50	1.50	4 (12%)	24,82,82	1.35	2 (8%)
3	HEC	U	600	1	32,50,50	1.49	4 (12%)	24,82,82	1.22	2 (8%)
3	HEC	G	600	1	32,50,50	1.48	4 (12%)	24,82,82	1.26	1 (4%)
3	HEC	F	603	1,7	32,50,50	2.49	11 (34%)	24,82,82	2.20	8 (33%)
3	HEC	B	607	1	32,50,50	1.47	4 (12%)	24,82,82	1.27	2 (8%)
3	HEC	E	605	1	32,50,50	1.48	4 (12%)	24,82,82	1.57	4 (16%)
3	HEC	C	605	1	32,50,50	1.49	4 (12%)	24,82,82	1.59	5 (20%)
3	HEC	J	605	1	32,50,50	1.50	4 (12%)	24,82,82	1.62	5 (20%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HEC	L	604	1	32,50,50	1.53	4 (12%)	24,82,82	1.74	2 (8%)
3	HEC	D	607	1	32,50,50	1.51	4 (12%)	24,82,82	1.19	1 (4%)
3	HEC	J	602	1	32,50,50	1.54	4 (12%)	24,82,82	1.35	3 (12%)
4	SO4	U	611	-	4,4,4	0.32	0	6,6,6	0.08	0
3	HEC	P	600	1	32,50,50	1.49	4 (12%)	24,82,82	1.22	2 (8%)
3	HEC	E	601	1	32,50,50	1.52	4 (12%)	24,82,82	1.39	3 (12%)
4	SO4	J	611	-	4,4,4	0.29	0	6,6,6	0.09	0
3	HEC	F	605	1	32,50,50	1.50	4 (12%)	24,82,82	1.60	4 (16%)
3	HEC	I	606	1	32,50,50	1.42	4 (12%)	24,82,82	1.42	3 (12%)
3	HEC	B	600	1	32,50,50	1.49	4 (12%)	24,82,82	1.23	1 (4%)
3	HEC	M	606	1	32,50,50	1.50	4 (12%)	24,82,82	1.42	3 (12%)
3	HEC	W	607	1	32,50,50	1.49	4 (12%)	24,82,82	1.22	1 (4%)
3	HEC	C	604	1	32,50,50	1.53	4 (12%)	24,82,82	1.77	2 (8%)
3	HEC	S	601	1	32,50,50	1.57	4 (12%)	24,82,82	1.40	3 (12%)
3	HEC	W	603	1,7	32,50,50	2.48	10 (31%)	24,82,82	2.03	7 (29%)
3	HEC	I	600	1	32,50,50	1.41	4 (12%)	24,82,82	1.41	5 (20%)
4	SO4	E	609	-	4,4,4	0.38	0	6,6,6	0.36	0
3	HEC	C	602	1	32,50,50	1.52	4 (12%)	24,82,82	1.39	3 (12%)
3	HEC	S	606	1	32,50,50	1.50	4 (12%)	24,82,82	1.39	2 (8%)
4	SO4	R	610	-	4,4,4	0.35	0	6,6,6	0.10	0
4	SO4	M	611	-	4,4,4	0.35	0	6,6,6	0.11	0
3	HEC	S	604	1	32,50,50	1.51	4 (12%)	24,82,82	1.77	2 (8%)
3	HEC	N	607	1	32,50,50	1.50	4 (12%)	24,82,82	1.15	0
4	SO4	B	609	-	4,4,4	0.30	0	6,6,6	0.13	0
3	HEC	F	601	1	32,50,50	1.56	4 (12%)	24,82,82	1.39	3 (12%)
3	HEC	R	606	1	32,50,50	1.45	4 (12%)	24,82,82	1.45	3 (12%)
3	HEC	G	603	1,7	32,50,50	2.55	10 (31%)	24,82,82	2.02	8 (33%)
5	GOL	A	612	-	5,5,5	0.28	0	5,5,5	0.28	0
3	HEC	H	605	1	32,50,50	1.51	4 (12%)	24,82,82	1.64	6 (25%)
3	HEC	V	603	1,7	32,50,50	2.50	11 (34%)	24,82,82	2.09	10 (41%)
5	GOL	I	614	-	5,5,5	0.23	0	5,5,5	0.19	0
3	HEC	T	605	1	32,50,50	1.47	4 (12%)	24,82,82	1.64	5 (20%)
3	HEC	U	602	1	32,50,50	1.49	4 (12%)	24,82,82	1.38	3 (12%)
3	HEC	V	605	1	32,50,50	1.48	4 (12%)	24,82,82	1.60	4 (16%)
3	HEC	U	605	1	32,50,50	1.45	4 (12%)	24,82,82	1.64	4 (16%)
3	HEC	W	605	1	32,50,50	1.49	4 (12%)	24,82,82	1.60	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	F	609	-	4,4,4	0.34	0	6,6,6	0.13	0
5	GOL	K	615	-	5,5,5	0.33	0	5,5,5	0.20	0
3	HEC	N	602	1	32,50,50	1.54	4 (12%)	24,82,82	1.37	2 (8%)
3	HEC	X	607	1	32,50,50	1.49	4 (12%)	24,82,82	1.21	1 (4%)
4	SO4	H	612	-	4,4,4	0.35	0	6,6,6	0.07	0
3	HEC	Q	605	1	32,50,50	1.48	4 (12%)	24,82,82	1.59	4 (16%)
3	HEC	Q	606	1	32,50,50	1.45	4 (12%)	24,82,82	1.41	2 (8%)
3	HEC	A	602	1	32,50,50	1.51	4 (12%)	24,82,82	1.38	3 (12%)
3	HEC	B	604	1	32,50,50	1.50	4 (12%)	24,82,82	1.75	2 (8%)
3	HEC	E	604	1	32,50,50	1.57	4 (12%)	24,82,82	1.76	2 (8%)
4	SO4	G	612	-	4,4,4	0.34	0	6,6,6	0.12	0
4	SO4	O	610	-	4,4,4	0.35	0	6,6,6	0.10	0
3	HEC	E	607	1	32,50,50	1.53	4 (12%)	24,82,82	1.21	1 (4%)
3	HEC	B	602	1	32,50,50	1.50	4 (12%)	24,82,82	1.40	3 (12%)
3	HEC	T	603	1	32,50,50	2.58	11 (34%)	24,82,82	2.14	9 (37%)
3	HEC	I	604	1	32,50,50	1.59	4 (12%)	24,82,82	1.61	2 (8%)
3	HEC	H	604	1	32,50,50	1.50	4 (12%)	24,82,82	1.77	2 (8%)
3	HEC	G	601	1	32,50,50	1.53	4 (12%)	24,82,82	1.39	2 (8%)
4	SO4	T	609	-	4,4,4	0.35	0	6,6,6	0.08	0
3	HEC	D	600	1	32,50,50	1.52	4 (12%)	24,82,82	1.28	3 (12%)
3	HEC	L	607	1	32,50,50	1.47	4 (12%)	24,82,82	1.15	0
3	HEC	S	600	1	32,50,50	1.55	4 (12%)	24,82,82	1.20	2 (8%)
4	SO4	N	610	-	4,4,4	0.35	0	6,6,6	0.13	0
3	HEC	S	602	1	32,50,50	1.49	4 (12%)	24,82,82	1.39	3 (12%)
4	SO4	X	609	-	4,4,4	0.33	0	6,6,6	0.14	0
3	HEC	W	602	1	32,50,50	1.53	4 (12%)	24,82,82	1.35	3 (12%)
4	SO4	a	201	-	4,4,4	0.34	0	6,6,6	0.08	0
5	GOL	H	614	-	5,5,5	0.41	0	5,5,5	0.77	0
3	HEC	Q	603	1,7	32,50,50	2.53	12 (37%)	24,82,82	2.18	9 (37%)
3	HEC	K	603	1,7	32,50,50	2.53	10 (31%)	24,82,82	2.03	9 (37%)
3	HEC	N	606	1	32,50,50	1.49	4 (12%)	24,82,82	1.38	2 (8%)
4	SO4	L	611	-	4,4,4	0.33	0	6,6,6	0.09	0
3	HEC	V	604	1	32,50,50	1.53	4 (12%)	24,82,82	1.78	2 (8%)
5	GOL	J	612	-	5,5,5	0.50	0	5,5,5	0.57	0
4	SO4	U	610	-	4,4,4	0.33	0	6,6,6	0.07	0
3	HEC	G	602	1	32,50,50	1.49	4 (12%)	24,82,82	1.38	3 (12%)
3	HEC	O	606	1	32,50,50	1.44	4 (12%)	24,82,82	1.46	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HEC	R	602	1	32,50,50	1.48	4 (12%)	24,82,82	1.31	3 (12%)
3	HEC	O	604	1	32,50,50	1.54	4 (12%)	24,82,82	1.76	2 (8%)
4	SO4	A	610	-	4,4,4	0.32	0	6,6,6	0.14	0
5	GOL	G	615	-	5,5,5	0.45	0	5,5,5	0.34	0
3	HEC	L	603	1,7	32,50,50	2.51	10 (31%)	24,82,82	2.11	10 (41%)
3	HEC	U	606	1	32,50,50	1.48	4 (12%)	24,82,82	1.40	3 (12%)
4	SO4	B	610	-	4,4,4	0.37	0	6,6,6	0.09	0
3	HEC	P	607	1	32,50,50	1.53	4 (12%)	24,82,82	1.19	1 (4%)
4	SO4	G	613	-	4,4,4	0.29	0	6,6,6	0.37	0
3	HEC	N	604	1	32,50,50	1.54	4 (12%)	24,82,82	1.74	2 (8%)
3	HEC	A	606	1	32,50,50	1.46	4 (12%)	24,82,82	1.41	2 (8%)
3	HEC	C	607	1	32,50,50	1.51	4 (12%)	24,82,82	1.16	1 (4%)
3	HEC	O	605	1	32,50,50	1.50	4 (12%)	24,82,82	1.59	5 (20%)
5	GOL	K	612	-	5,5,5	0.39	0	5,5,5	0.33	0
3	HEC	B	606	1	32,50,50	1.47	4 (12%)	24,82,82	1.48	3 (12%)
3	HEC	N	605	1	32,50,50	1.49	4 (12%)	24,82,82	1.60	5 (20%)
3	HEC	R	601	1	32,50,50	1.57	4 (12%)	24,82,82	1.38	3 (12%)
3	HEC	T	606	1	32,50,50	1.49	4 (12%)	24,82,82	1.41	2 (8%)
3	HEC	T	607	1	32,50,50	1.49	4 (12%)	24,82,82	1.20	1 (4%)
3	HEC	O	602	1	32,50,50	1.46	4 (12%)	24,82,82	1.39	2 (8%)
3	HEC	H	600	1	32,50,50	1.49	4 (12%)	24,82,82	1.22	0
4	SO4	X	611	-	4,4,4	0.34	0	6,6,6	0.07	0
4	SO4	I	610	-	4,4,4	0.35	0	6,6,6	0.05	0
3	HEC	M	600	1	32,50,50	1.50	4 (12%)	24,82,82	1.23	1 (4%)
4	SO4	Y	202	-	4,4,4	0.33	0	6,6,6	0.11	0
3	HEC	G	606	1	32,50,50	1.49	4 (12%)	24,82,82	1.43	4 (16%)
3	HEC	C	601	1	32,50,50	1.53	4 (12%)	24,82,82	1.39	3 (12%)
4	SO4	P	609	-	4,4,4	0.33	0	6,6,6	0.14	0
3	HEC	Q	600	1	32,50,50	1.53	4 (12%)	24,82,82	1.15	0
3	HEC	R	603	1	32,50,50	2.54	11 (34%)	24,82,82	2.01	11 (45%)
4	SO4	V	611	-	4,4,4	0.34	0	6,6,6	0.05	0
3	HEC	A	601	1	32,50,50	1.56	4 (12%)	24,82,82	1.39	3 (12%)
3	HEC	G	605	1	32,50,50	1.49	4 (12%)	24,82,82	1.66	5 (20%)
4	SO4	D	609	-	4,4,4	0.35	0	6,6,6	0.11	0
3	HEC	H	602	1	32,50,50	1.54	4 (12%)	24,82,82	1.38	3 (12%)
4	SO4	C	611	-	4,4,4	0.34	0	6,6,6	0.16	0
4	SO4	S	610	-	4,4,4	0.35	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	H	615	-	5,5,5	0.46	0	5,5,5	0.57	0
3	HEC	J	603	1,7	32,50,50	2.46	10 (31%)	24,82,82	2.11	10 (41%)
5	GOL	A	613	-	5,5,5	0.41	0	5,5,5	0.35	0
3	HEC	O	600	1	32,50,50	1.52	4 (12%)	24,82,82	1.25	1 (4%)
4	SO4	J	609	-	4,4,4	0.36	0	6,6,6	0.09	0
5	GOL	A	614	-	5,5,5	0.35	0	5,5,5	0.18	0
5	GOL	L	613	-	5,5,5	0.25	0	5,5,5	0.35	0
3	HEC	S	605	1	32,50,50	1.50	4 (12%)	24,82,82	1.59	4 (16%)
4	SO4	G	609	-	4,4,4	0.35	0	6,6,6	0.08	0
3	HEC	N	600	1	32,50,50	1.51	4 (12%)	24,82,82	1.23	1 (4%)
3	HEC	X	605	1	32,50,50	1.50	4 (12%)	24,82,82	1.60	4 (16%)
4	SO4	A	611	-	4,4,4	0.32	0	6,6,6	0.16	0
3	HEC	R	607	1	32,50,50	1.51	4 (12%)	24,82,82	1.17	1 (4%)
3	HEC	H	601	1	32,50,50	1.52	4 (12%)	24,82,82	1.39	3 (12%)
3	HEC	P	604	1	32,50,50	1.51	4 (12%)	24,82,82	1.76	2 (8%)
3	HEC	M	604	1	32,50,50	1.53	4 (12%)	24,82,82	1.72	2 (8%)
3	HEC	C	606	1	32,50,50	1.50	4 (12%)	24,82,82	1.38	3 (12%)
3	HEC	J	607	1	32,50,50	1.55	4 (12%)	24,82,82	1.17	2 (8%)
3	HEC	V	607	1	32,50,50	1.49	4 (12%)	24,82,82	1.15	1 (4%)
4	SO4	E	610	-	4,4,4	0.35	0	6,6,6	0.10	0
3	HEC	D	603	1,7	32,50,50	2.51	11 (34%)	24,82,82	2.25	10 (41%)
3	HEC	U	601	1	32,50,50	1.53	4 (12%)	24,82,82	1.41	3 (12%)
3	HEC	P	605	1	32,50,50	1.46	4 (12%)	24,82,82	1.63	5 (20%)
3	HEC	C	600	1	32,50,50	1.49	4 (12%)	24,82,82	1.24	1 (4%)
5	GOL	G	616	-	5,5,5	0.19	0	5,5,5	0.42	0
3	HEC	D	605	1	32,50,50	1.49	4 (12%)	24,82,82	1.70	5 (20%)
3	HEC	D	606	1	32,50,50	1.47	4 (12%)	24,82,82	1.31	2 (8%)
3	HEC	U	607	1	32,50,50	1.51	4 (12%)	24,82,82	1.22	1 (4%)
5	GOL	I	613	-	5,5,5	0.26	0	5,5,5	0.24	0
3	HEC	K	602	1	32,50,50	1.47	4 (12%)	24,82,82	1.36	2 (8%)
3	HEC	N	603	1,7	32,50,50	2.53	11 (34%)	24,82,82	2.11	9 (37%)
4	SO4	U	609	-	4,4,4	0.32	0	6,6,6	0.26	0
3	HEC	K	605	1	32,50,50	1.51	4 (12%)	24,82,82	1.66	5 (20%)
3	HEC	P	601	1	32,50,50	1.51	4 (12%)	24,82,82	1.40	2 (8%)
4	SO4	I	611	-	4,4,4	0.34	0	6,6,6	0.07	0
3	HEC	F	600	1	32,50,50	1.53	4 (12%)	24,82,82	1.17	0
3	HEC	L	602	1	32,50,50	1.53	4 (12%)	24,82,82	1.37	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	R	609	-	4,4,4	0.32	0	6,6,6	0.25	0
3	HEC	L	605	1	32,50,50	1.45	4 (12%)	24,82,82	1.61	6 (25%)
3	HEC	B	601	1	32,50,50	1.54	4 (12%)	24,82,82	1.42	2 (8%)
5	GOL	J	613	-	5,5,5	0.27	0	5,5,5	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	A	607	1	-	3/10/54/54	-
3	HEC	U	603	1,7	-	0/10/54/54	-
3	HEC	W	604	1	-	4/10/54/54	-
3	HEC	I	601	1	-	6/10/54/54	-
3	HEC	A	603	1,7	-	1/10/54/54	-
3	HEC	X	606	1	-	2/10/54/54	-
3	HEC	K	601	1	-	4/10/54/54	-
3	HEC	X	600	1	-	4/10/54/54	-
3	HEC	F	606	1	-	2/10/54/54	-
3	HEC	F	602	1	-	5/10/54/54	-
3	HEC	D	602	1	-	2/10/54/54	-
3	HEC	E	600	1	-	4/10/54/54	-
3	HEC	H	603	1,7	-	2/10/54/54	-
3	HEC	M	602	1	-	5/10/54/54	-
3	HEC	O	601	1	-	5/10/54/54	-
3	HEC	G	607	1	-	3/10/54/54	-
3	HEC	A	605	1	-	4/10/54/54	-
3	HEC	W	600	1	-	4/10/54/54	-
3	HEC	H	606	1	-	2/10/54/54	-
3	HEC	L	600	1	-	4/10/54/54	-
3	HEC	I	603	1,7	-	2/10/54/54	-
3	HEC	N	601	1	-	3/10/54/54	-
3	HEC	J	604	1	-	4/10/54/54	-
3	HEC	V	600	1	-	4/10/54/54	-
3	HEC	P	606	1	-	2/10/54/54	-
3	HEC	M	601	1	-	4/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	D	601	1	-	3/10/54/54	-
3	HEC	W	601	1	-	5/10/54/54	-
3	HEC	X	604	1	-	4/10/54/54	-
3	HEC	B	603	1	-	0/10/54/54	-
3	HEC	I	607	1	-	4/10/54/54	-
3	HEC	O	603	1,7	-	1/10/54/54	-
3	HEC	M	607	1	-	3/10/54/54	-
3	HEC	X	602	1	-	5/10/54/54	-
3	HEC	T	604	1	-	4/10/54/54	-
3	HEC	S	603	1,7	-	2/10/54/54	-
3	HEC	V	601	1	-	4/10/54/54	-
3	HEC	T	600	1	-	4/10/54/54	-
3	HEC	O	607	1	-	3/10/54/54	-
3	HEC	V	602	1	-	5/10/54/54	-
5	GOL	K	614	-	-	4/4/4/4	-
3	HEC	X	601	1	-	5/10/54/54	-
5	GOL	K	613	-	-	2/4/4/4	-
3	HEC	A	600	1	-	4/10/54/54	-
3	HEC	A	604	1	-	4/10/54/54	-
3	HEC	P	602	1	-	5/10/54/54	-
3	HEC	L	601	1	-	3/10/54/54	-
3	HEC	S	607	1	-	3/10/54/54	-
3	HEC	W	606	1	-	2/10/54/54	-
3	HEC	D	604	1	-	3/10/54/54	-
3	HEC	T	602	1	-	5/10/54/54	-
3	HEC	T	601	1	-	4/10/54/54	-
3	HEC	Q	601	1	-	5/10/54/54	-
3	HEC	F	607	1	-	3/10/54/54	-
3	HEC	K	607	1	-	3/10/54/54	-
3	HEC	R	604	1	-	4/10/54/54	-
3	HEC	F	604	1	-	4/10/54/54	-
3	HEC	X	603	1,7	-	2/10/54/54	-
3	HEC	R	600	1	-	4/10/54/54	-
3	HEC	G	604	1	-	4/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	E	606	1	-	2/10/54/54	-
3	HEC	E	603	1,7	-	2/10/54/54	-
3	HEC	I	602	1	-	5/10/54/54	-
3	HEC	L	606	1	-	2/10/54/54	-
3	HEC	M	605	1	-	4/10/54/54	-
3	HEC	I	605	1	-	5/10/54/54	-
3	HEC	J	606	1	-	2/10/54/54	-
3	HEC	H	607	1	-	3/10/54/54	-
3	HEC	J	600	1	-	4/10/54/54	-
3	HEC	B	605	1	-	4/10/54/54	-
5	GOL	D	610	-	-	2/4/4/4	-
3	HEC	P	603	1,7	-	0/10/54/54	-
3	HEC	M	603	1,7	-	2/10/54/54	-
3	HEC	C	603	1	-	0/10/54/54	-
3	HEC	K	606	1	-	3/10/54/54	-
3	HEC	Q	602	1	-	5/10/54/54	-
3	HEC	K	604	1	-	4/10/54/54	-
3	HEC	V	606	1	-	2/10/54/54	-
3	HEC	Q	604	1	-	4/10/54/54	-
3	HEC	Q	607	1	-	3/10/54/54	-
3	HEC	J	601	1	-	6/10/54/54	-
3	HEC	K	600	1	-	4/10/54/54	-
3	HEC	R	605	1	-	4/10/54/54	-
5	GOL	I	615	-	-	2/4/4/4	-
3	HEC	U	604	1	-	4/10/54/54	-
3	HEC	E	602	1	-	5/10/54/54	-
3	HEC	U	600	1	-	4/10/54/54	-
3	HEC	G	600	1	-	4/10/54/54	-
3	HEC	F	603	1,7	-	0/10/54/54	-
3	HEC	B	607	1	-	3/10/54/54	-
3	HEC	E	605	1	-	4/10/54/54	-
3	HEC	C	605	1	-	4/10/54/54	-
3	HEC	J	605	1	-	4/10/54/54	-
3	HEC	L	604	1	-	4/10/54/54	-
3	HEC	D	607	1	-	5/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	J	602	1	-	5/10/54/54	-
3	HEC	P	600	1	-	4/10/54/54	-
3	HEC	E	601	1	-	5/10/54/54	-
3	HEC	F	605	1	-	4/10/54/54	-
3	HEC	I	606	1	-	3/10/54/54	-
3	HEC	B	600	1	-	4/10/54/54	-
3	HEC	M	606	1	-	2/10/54/54	-
3	HEC	W	607	1	-	3/10/54/54	-
3	HEC	C	604	1	-	4/10/54/54	-
3	HEC	S	601	1	-	4/10/54/54	-
3	HEC	W	603	1,7	-	2/10/54/54	-
3	HEC	I	600	1	-	2/10/54/54	-
3	HEC	C	602	1	-	5/10/54/54	-
3	HEC	S	606	1	-	2/10/54/54	-
3	HEC	S	604	1	-	4/10/54/54	-
3	HEC	N	607	1	-	3/10/54/54	-
5	GOL	I	614	-	-	2/4/4/4	-
3	HEC	F	601	1	-	3/10/54/54	-
3	HEC	R	606	1	-	2/10/54/54	-
3	HEC	G	603	1,7	-	2/10/54/54	-
5	GOL	A	612	-	-	0/4/4/4	-
3	HEC	H	605	1	-	4/10/54/54	-
3	HEC	V	603	1,7	-	0/10/54/54	-
3	HEC	T	605	1	-	4/10/54/54	-
3	HEC	U	602	1	-	5/10/54/54	-
3	HEC	V	605	1	-	4/10/54/54	-
3	HEC	U	605	1	-	4/10/54/54	-
3	HEC	W	605	1	-	4/10/54/54	-
5	GOL	K	615	-	-	4/4/4/4	-
3	HEC	N	602	1	-	5/10/54/54	-
3	HEC	X	607	1	-	3/10/54/54	-
3	HEC	Q	605	1	-	4/10/54/54	-
3	HEC	Q	606	1	-	2/10/54/54	-
3	HEC	A	602	1	-	5/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	B	604	1	-	4/10/54/54	-
3	HEC	E	604	1	-	4/10/54/54	-
3	HEC	E	607	1	-	3/10/54/54	-
3	HEC	B	602	1	-	5/10/54/54	-
3	HEC	T	603	1	-	0/10/54/54	-
3	HEC	I	604	1	-	5/10/54/54	-
3	HEC	H	604	1	-	4/10/54/54	-
3	HEC	G	601	1	-	4/10/54/54	-
3	HEC	D	600	1	-	2/10/54/54	-
3	HEC	L	607	1	-	3/10/54/54	-
3	HEC	S	600	1	-	4/10/54/54	-
5	GOL	H	614	-	-	4/4/4/4	-
3	HEC	S	602	1	-	5/10/54/54	-
3	HEC	W	602	1	-	5/10/54/54	-
3	HEC	Q	603	1,7	-	1/10/54/54	-
3	HEC	K	603	1,7	-	1/10/54/54	-
3	HEC	N	606	1	-	3/10/54/54	-
3	HEC	V	604	1	-	4/10/54/54	-
5	GOL	J	612	-	-	4/4/4/4	-
3	HEC	G	602	1	-	5/10/54/54	-
3	HEC	O	606	1	-	2/10/54/54	-
3	HEC	R	602	1	-	5/10/54/54	-
3	HEC	O	604	1	-	4/10/54/54	-
5	GOL	G	615	-	-	2/4/4/4	-
3	HEC	L	603	1,7	-	0/10/54/54	-
3	HEC	U	606	1	-	2/10/54/54	-
3	HEC	P	607	1	-	3/10/54/54	-
3	HEC	N	604	1	-	4/10/54/54	-
3	HEC	A	606	1	-	2/10/54/54	-
3	HEC	C	607	1	-	3/10/54/54	-
3	HEC	O	605	1	-	4/10/54/54	-
5	GOL	K	612	-	-	2/4/4/4	-
3	HEC	B	606	1	-	3/10/54/54	-
3	HEC	N	605	1	-	4/10/54/54	-
3	HEC	R	601	1	-	4/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	T	606	1	-	2/10/54/54	-
3	HEC	T	607	1	-	3/10/54/54	-
3	HEC	O	602	1	-	5/10/54/54	-
3	HEC	H	600	1	-	4/10/54/54	-
3	HEC	M	600	1	-	4/10/54/54	-
3	HEC	G	606	1	-	2/10/54/54	-
3	HEC	C	601	1	-	4/10/54/54	-
3	HEC	Q	600	1	-	4/10/54/54	-
3	HEC	R	603	1	-	0/10/54/54	-
3	HEC	A	601	1	-	5/10/54/54	-
3	HEC	G	605	1	-	4/10/54/54	-
3	HEC	H	602	1	-	5/10/54/54	-
5	GOL	H	615	-	-	2/4/4/4	-
3	HEC	J	603	1,7	-	1/10/54/54	-
5	GOL	A	613	-	-	2/4/4/4	-
3	HEC	O	600	1	-	4/10/54/54	-
5	GOL	A	614	-	-	4/4/4/4	-
5	GOL	L	613	-	-	2/4/4/4	-
3	HEC	S	605	1	-	4/10/54/54	-
3	HEC	N	600	1	-	4/10/54/54	-
3	HEC	X	605	1	-	4/10/54/54	-
3	HEC	R	607	1	-	3/10/54/54	-
3	HEC	H	601	1	-	5/10/54/54	-
3	HEC	P	604	1	-	4/10/54/54	-
3	HEC	M	604	1	-	4/10/54/54	-
3	HEC	C	606	1	-	2/10/54/54	-
3	HEC	J	607	1	-	3/10/54/54	-
3	HEC	V	607	1	-	3/10/54/54	-
3	HEC	D	603	1,7	-	3/10/54/54	-
3	HEC	U	601	1	-	5/10/54/54	-
3	HEC	P	605	1	-	4/10/54/54	-
3	HEC	C	600	1	-	4/10/54/54	-
5	GOL	G	616	-	-	2/4/4/4	-
3	HEC	D	605	1	-	4/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	D	606	1	-	2/10/54/54	-
3	HEC	U	607	1	-	3/10/54/54	-
5	GOL	I	613	-	-	4/4/4/4	-
3	HEC	K	602	1	-	5/10/54/54	-
3	HEC	N	603	1,7	-	2/10/54/54	-
3	HEC	K	605	1	-	4/10/54/54	-
3	HEC	P	601	1	-	5/10/54/54	-
3	HEC	F	600	1	-	4/10/54/54	-
3	HEC	L	602	1	-	5/10/54/54	-
3	HEC	L	605	1	-	4/10/54/54	-
3	HEC	B	601	1	-	4/10/54/54	-
5	GOL	J	613	-	-	2/4/4/4	-

The worst 5 of 932 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	603	HEC	C4B-C3B	6.59	1.55	1.43
3	X	603	HEC	C4B-C3B	6.38	1.54	1.43
3	O	603	HEC	C4B-C3B	6.35	1.54	1.43
3	A	603	HEC	C4B-C3B	6.33	1.54	1.43
3	E	603	HEC	C4B-C3B	6.32	1.54	1.43

The worst 5 of 625 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	603	HEC	CBA-CAA-C2A	17.66	142.36	112.60
3	D	604	HEC	CBD-CAD-C3D	-5.86	102.61	112.62
3	I	604	HEC	CBD-CAD-C3D	-5.59	103.08	112.62
3	H	604	HEC	CBD-CAD-C3D	-5.41	103.39	112.62
3	K	604	HEC	CBD-CAD-C3D	-5.41	103.39	112.62

There are no chirality outliers.

5 of 706 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	605	HEC	C2D-C3D-CAD-CBD
3	G	605	HEC	C4D-C3D-CAD-CBD
3	A	605	HEC	C2D-C3D-CAD-CBD
3	A	605	HEC	C4D-C3D-CAD-CBD

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

There are no ring outliers.

171 monomers are involved in 453 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	607	HEC	3	0
3	W	604	HEC	3	0
3	I	601	HEC	6	0
3	X	606	HEC	3	0
4	X	610	SO4	1	0
3	K	601	HEC	7	0
3	X	600	HEC	3	0
3	F	606	HEC	3	0
3	D	602	HEC	1	0
3	E	600	HEC	3	0
3	O	601	HEC	5	0
3	G	607	HEC	3	0
3	A	605	HEC	5	0
3	W	600	HEC	3	0
3	H	606	HEC	4	0
3	L	600	HEC	3	0
3	I	603	HEC	3	0
3	N	601	HEC	4	0
3	J	604	HEC	3	0
3	V	600	HEC	3	0
3	P	606	HEC	3	0
3	M	601	HEC	4	0
3	D	601	HEC	5	0
3	W	601	HEC	5	0
3	X	604	HEC	3	0
3	I	607	HEC	2	0
3	M	607	HEC	3	0
3	T	604	HEC	3	0
3	V	601	HEC	4	0
3	T	600	HEC	3	0
3	O	607	HEC	2	0
5	K	614	GOL	10	0
3	X	601	HEC	5	0
5	K	613	GOL	1	0
3	A	600	HEC	3	0
3	A	604	HEC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	601	HEC	4	0
3	S	607	HEC	1	0
3	W	606	HEC	3	0
3	D	604	HEC	3	0
4	G	610	SO4	2	0
3	T	601	HEC	4	0
4	H	609	SO4	1	0
3	Q	601	HEC	5	0
3	F	607	HEC	1	0
3	K	607	HEC	3	0
3	R	604	HEC	3	0
3	F	604	HEC	3	0
3	R	600	HEC	3	0
3	G	604	HEC	2	0
3	E	606	HEC	2	0
4	Q	609	SO4	1	0
3	I	602	HEC	1	0
3	L	606	HEC	3	0
3	M	605	HEC	5	0
3	I	605	HEC	8	0
3	J	606	HEC	2	0
3	H	607	HEC	1	0
3	J	600	HEC	3	0
3	B	605	HEC	6	0
3	K	606	HEC	3	0
3	K	604	HEC	3	0
3	V	606	HEC	3	0
3	Q	604	HEC	3	0
3	Q	607	HEC	3	0
4	L	610	SO4	1	0
3	J	601	HEC	4	0
3	K	600	HEC	3	0
3	R	605	HEC	7	0
5	I	615	GOL	1	0
3	U	604	HEC	3	0
3	U	600	HEC	3	0
3	G	600	HEC	3	0
3	B	607	HEC	2	0
3	E	605	HEC	6	0
3	C	605	HEC	7	0
3	J	605	HEC	5	0
3	L	604	HEC	3	0

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	606	HEC	3	0
3	O	604	HEC	2	0
5	G	615	GOL	1	0
3	U	606	HEC	3	0
3	P	607	HEC	2	0
3	N	604	HEC	3	0
3	A	606	HEC	3	0
3	C	607	HEC	3	0
3	O	605	HEC	6	0
3	B	606	HEC	3	0
3	N	605	HEC	6	0
3	R	601	HEC	4	0
3	T	606	HEC	2	0
3	T	607	HEC	2	0
3	H	600	HEC	3	0
3	M	600	HEC	3	0
3	G	606	HEC	3	0
3	C	601	HEC	4	0
3	Q	600	HEC	3	0
3	A	601	HEC	4	0
3	G	605	HEC	5	0
5	H	615	GOL	9	0
5	A	613	GOL	1	0
3	O	600	HEC	4	0
5	L	613	GOL	1	0
3	S	605	HEC	6	0
4	G	609	SO4	1	0
3	N	600	HEC	3	0
3	X	605	HEC	6	0
3	R	607	HEC	3	0
3	H	601	HEC	4	0
3	P	604	HEC	3	0
3	M	604	HEC	2	0
3	C	606	HEC	3	0
3	J	607	HEC	3	0
3	V	607	HEC	3	0
3	D	603	HEC	2	0
3	U	601	HEC	5	0
3	P	605	HEC	7	0
3	C	600	HEC	4	0
5	G	616	GOL	1	0
3	D	605	HEC	7	0

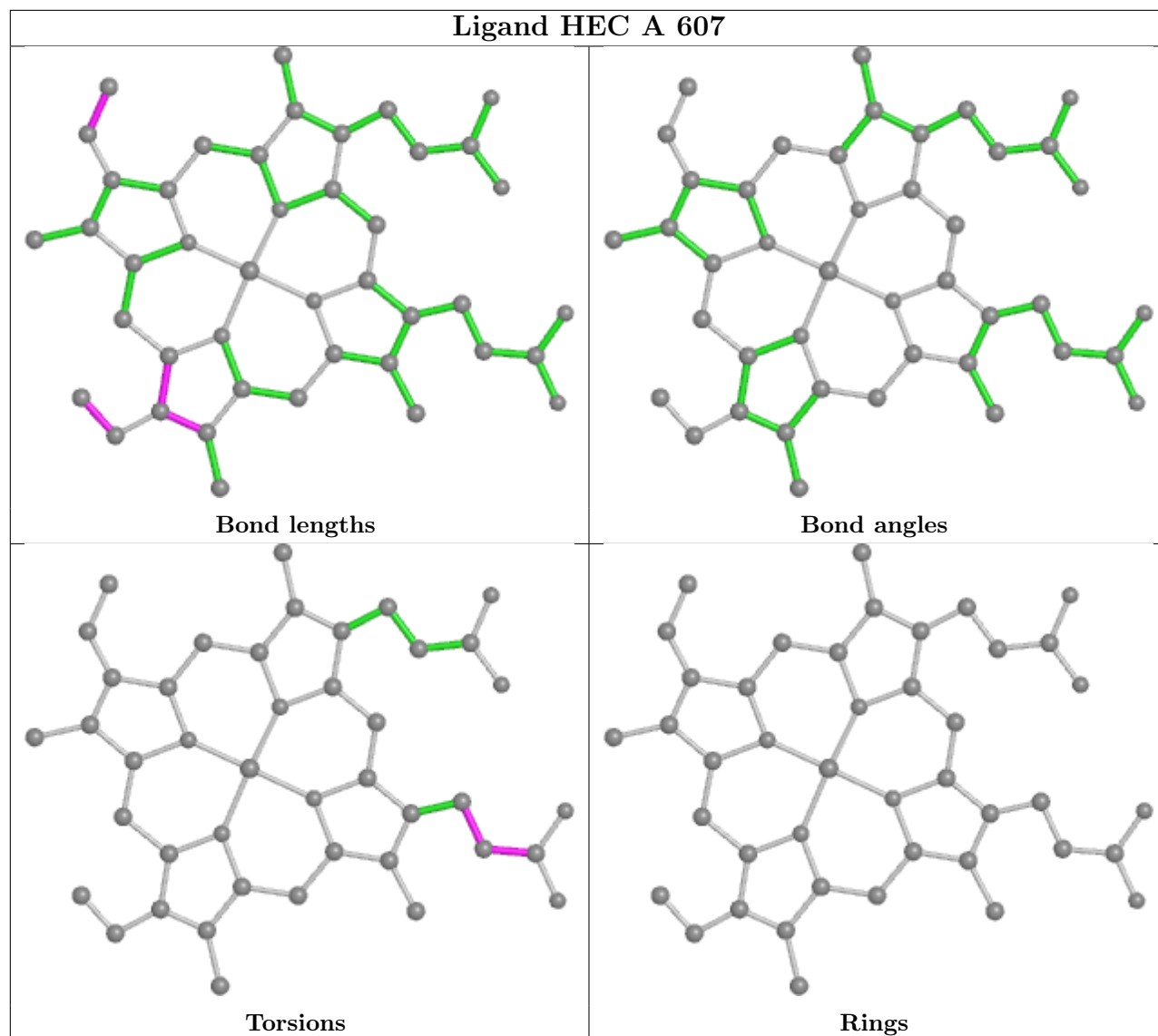
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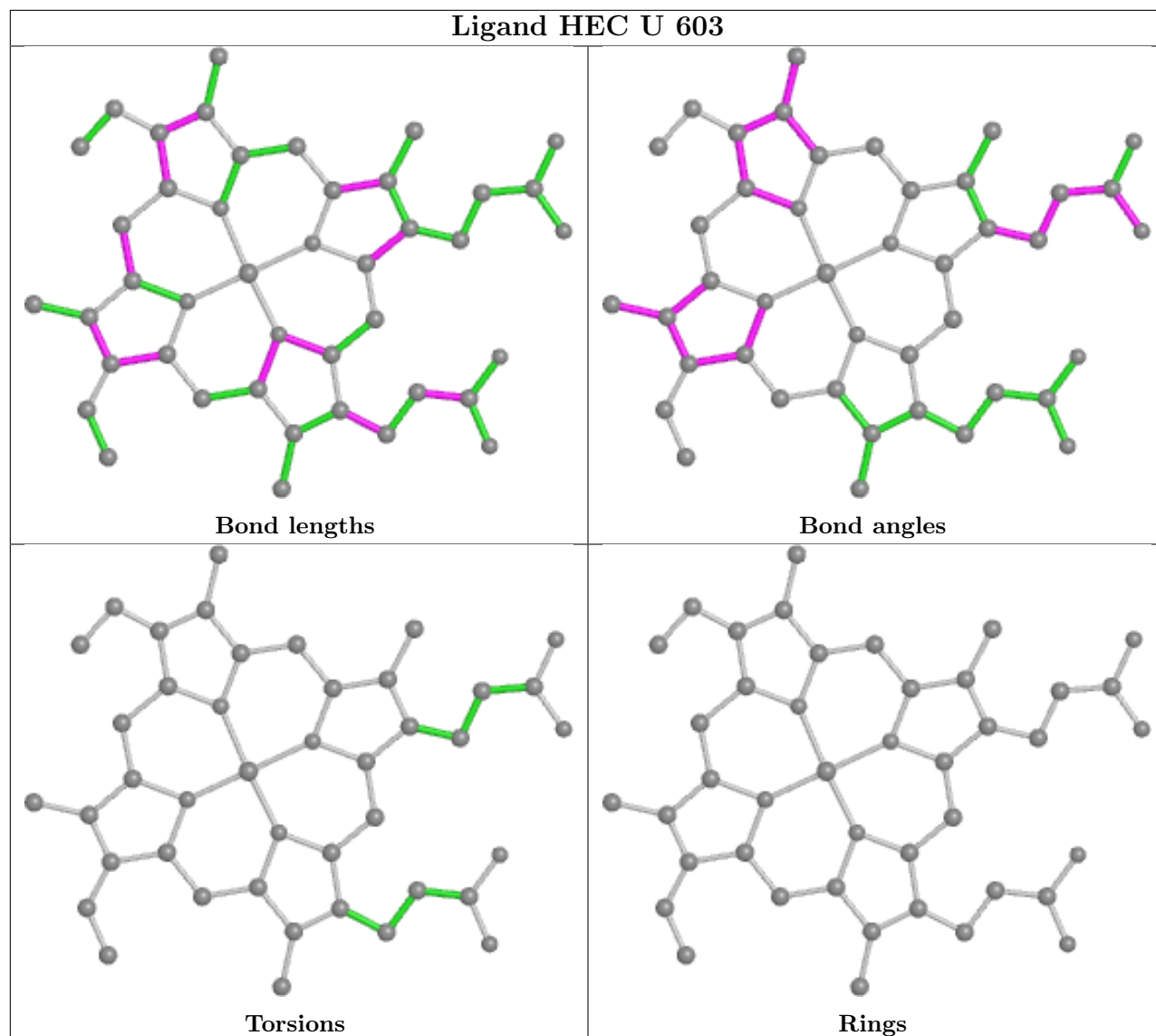
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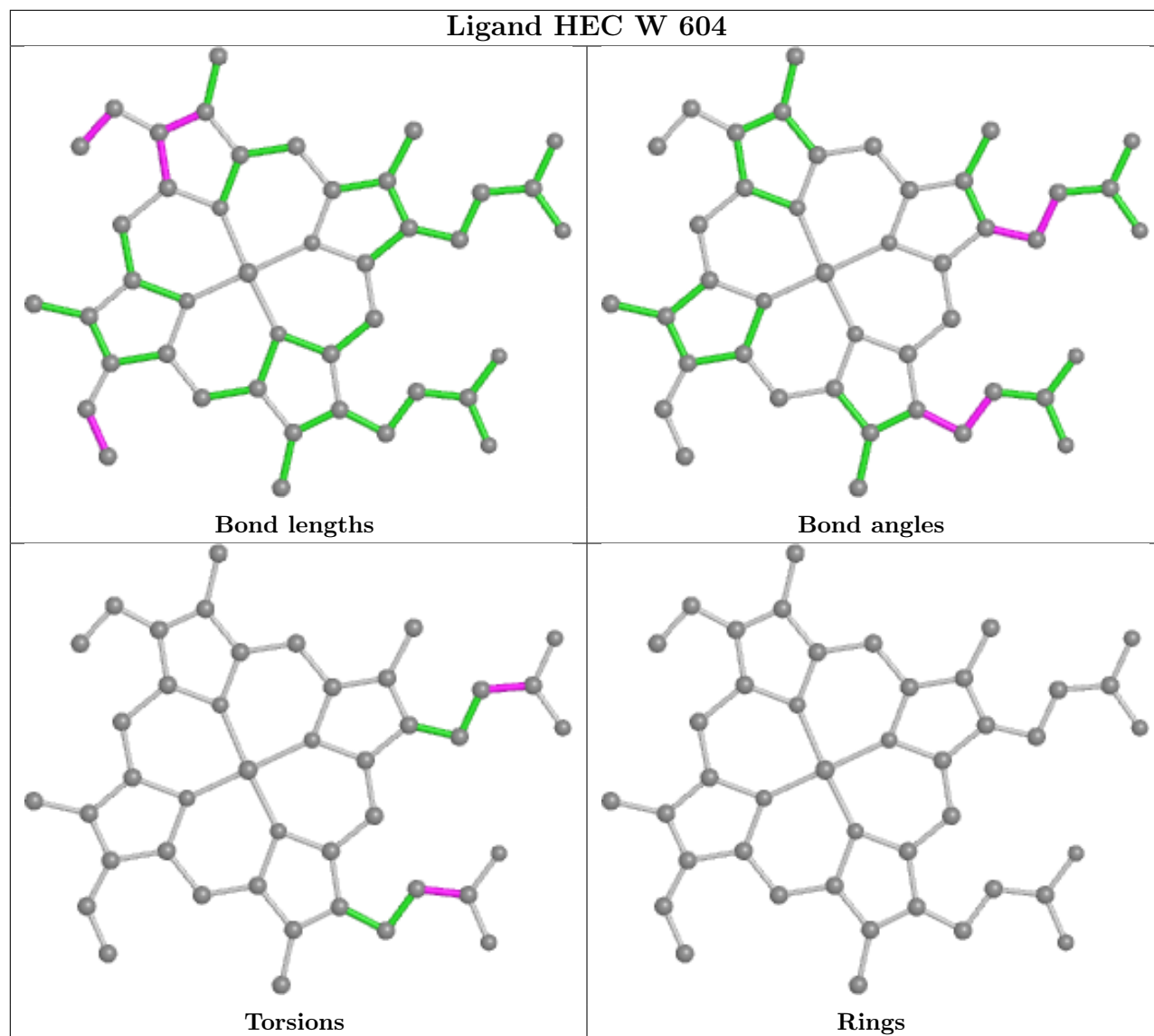
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	606	HEC	3	0
3	U	607	HEC	2	0
3	K	602	HEC	1	0
3	K	605	HEC	6	0
3	P	601	HEC	4	0
3	F	600	HEC	4	0
3	L	605	HEC	5	0
3	B	601	HEC	4	0
5	J	613	GOL	3	0

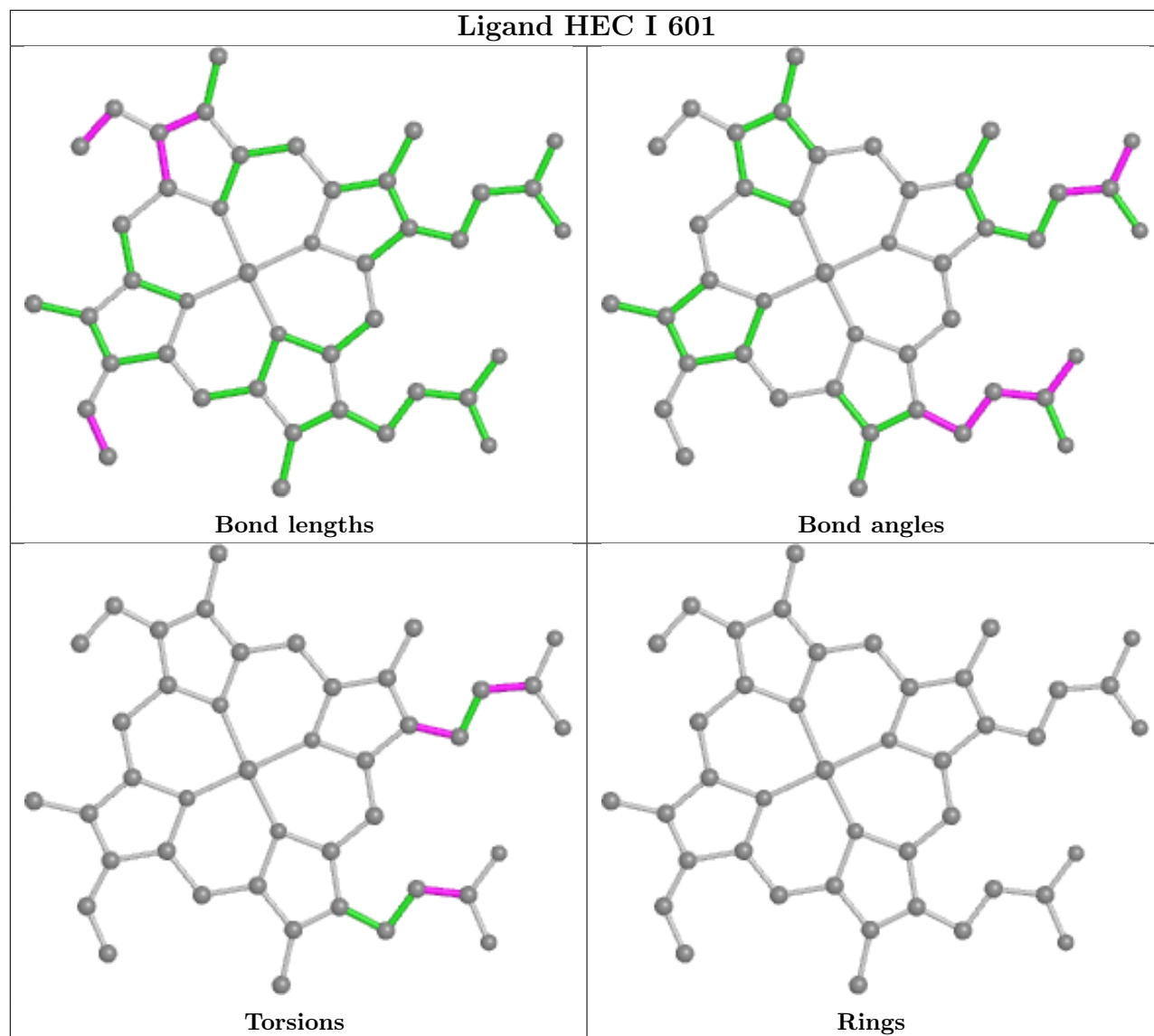
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

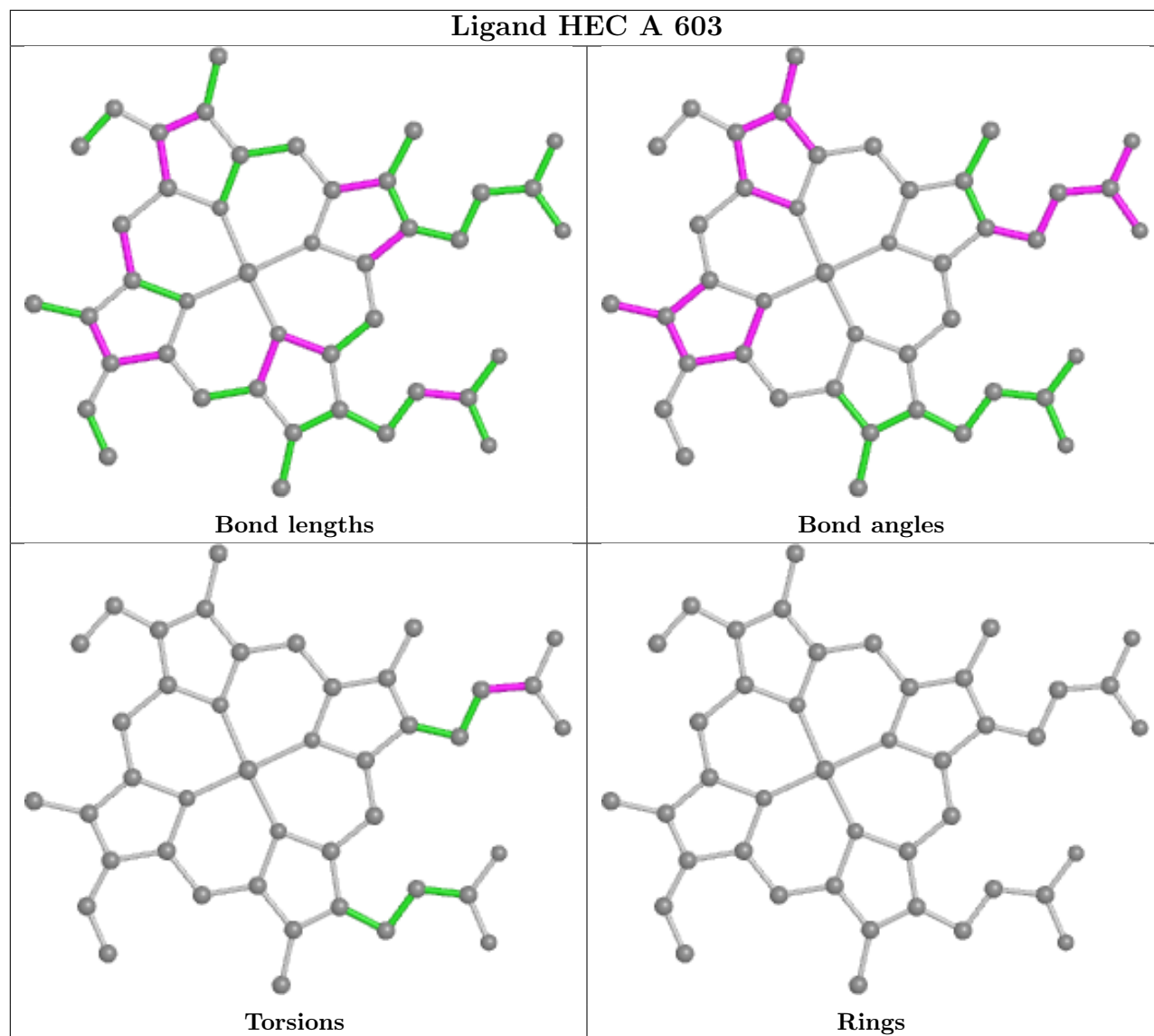


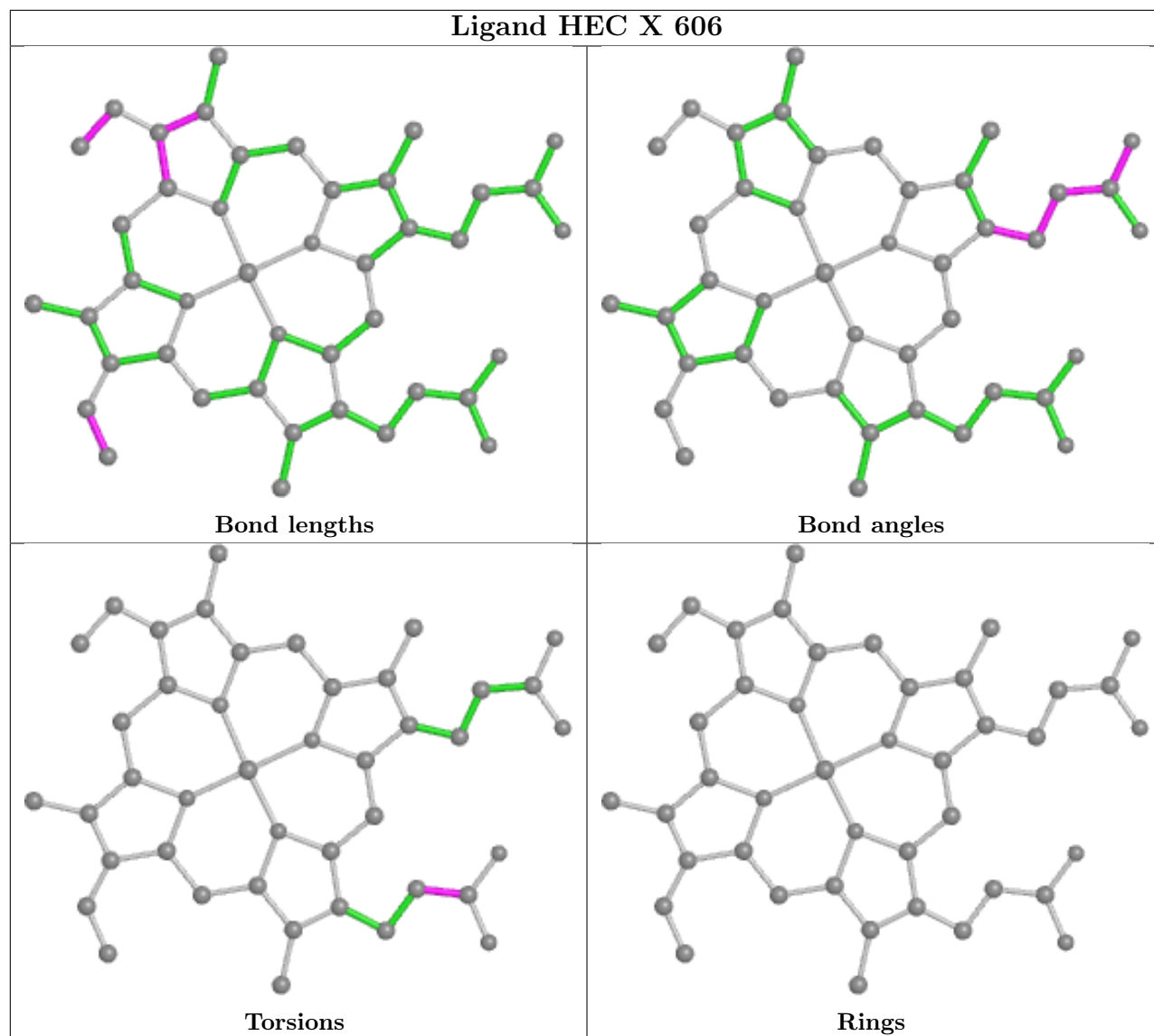


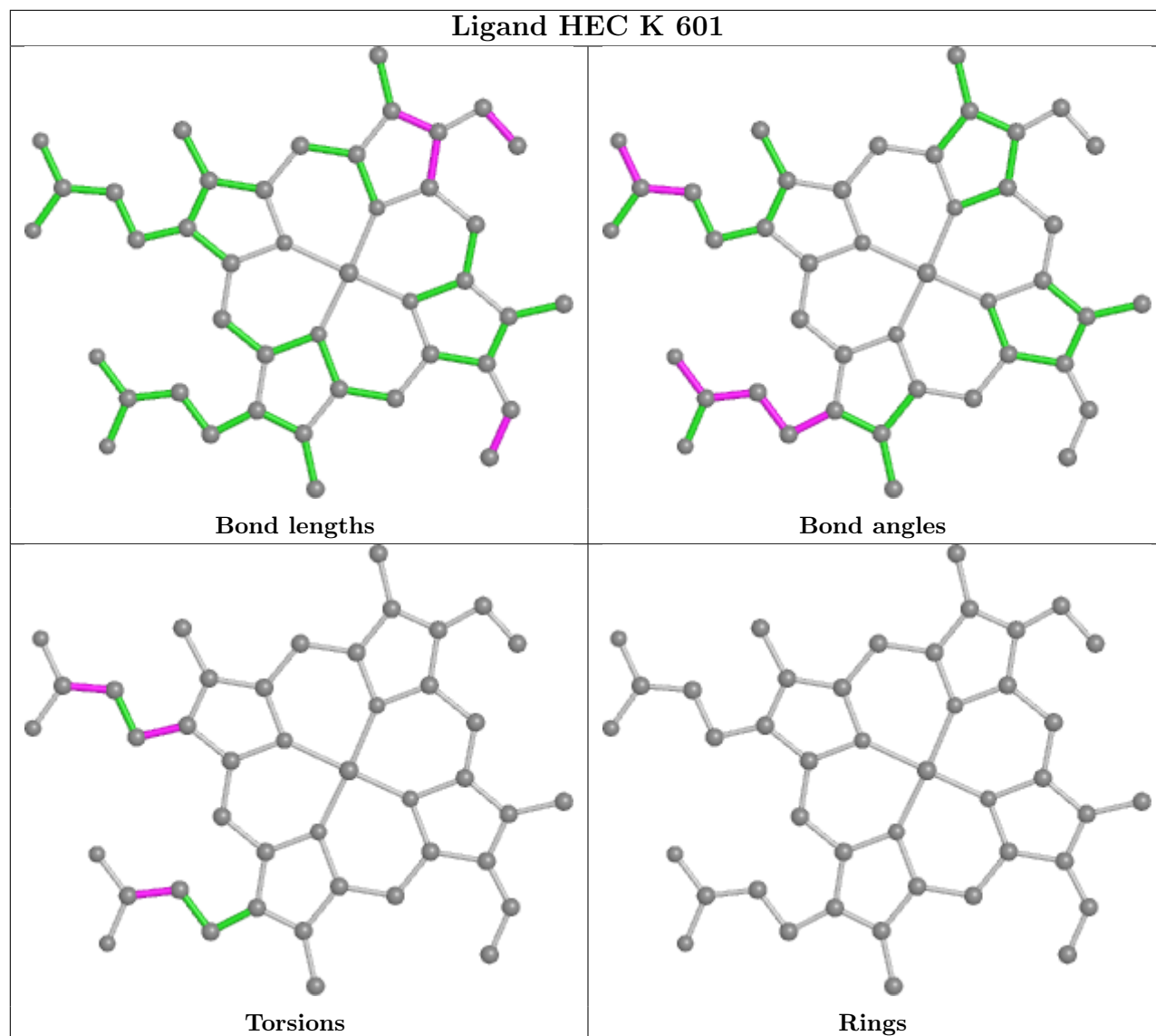


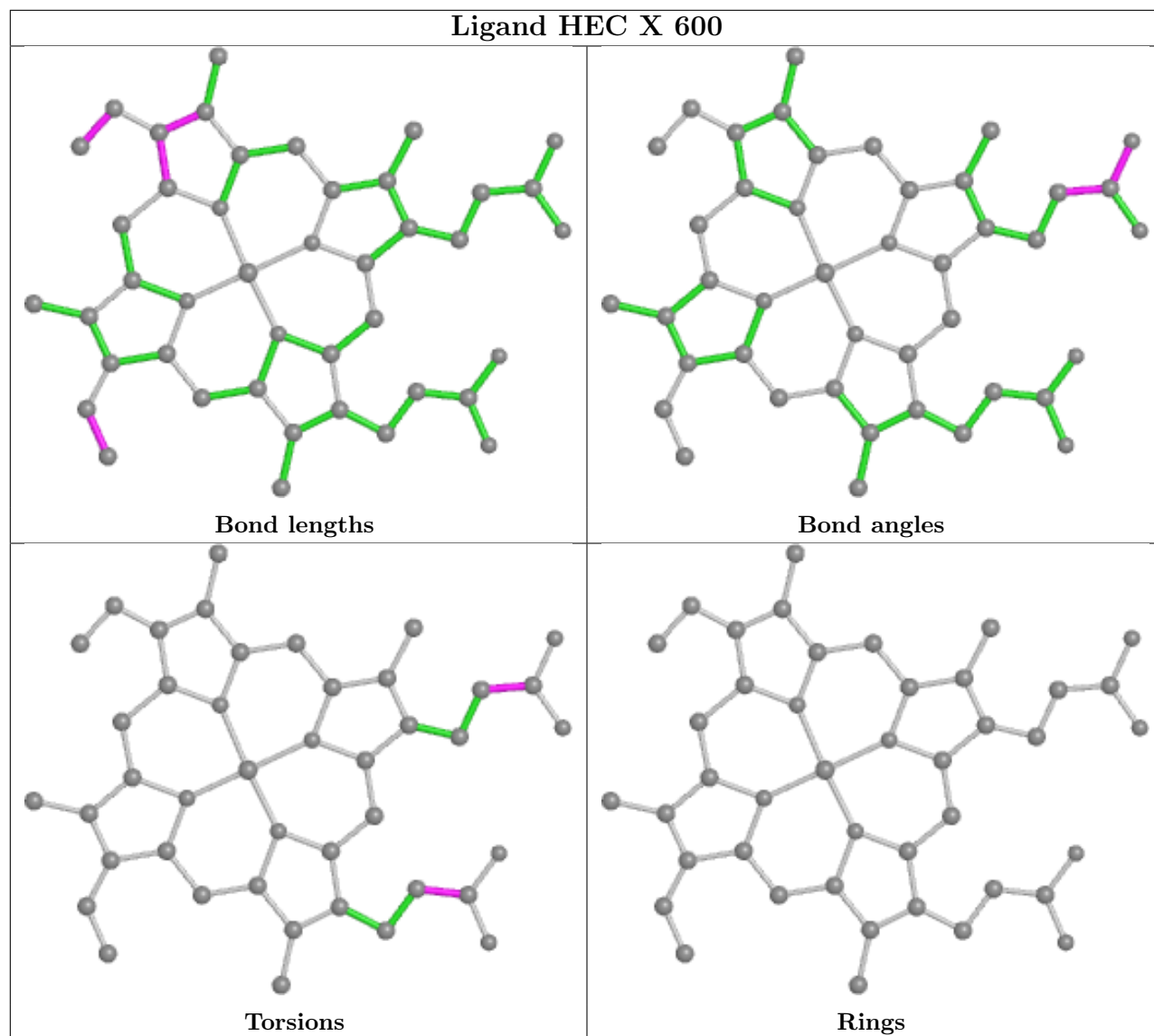




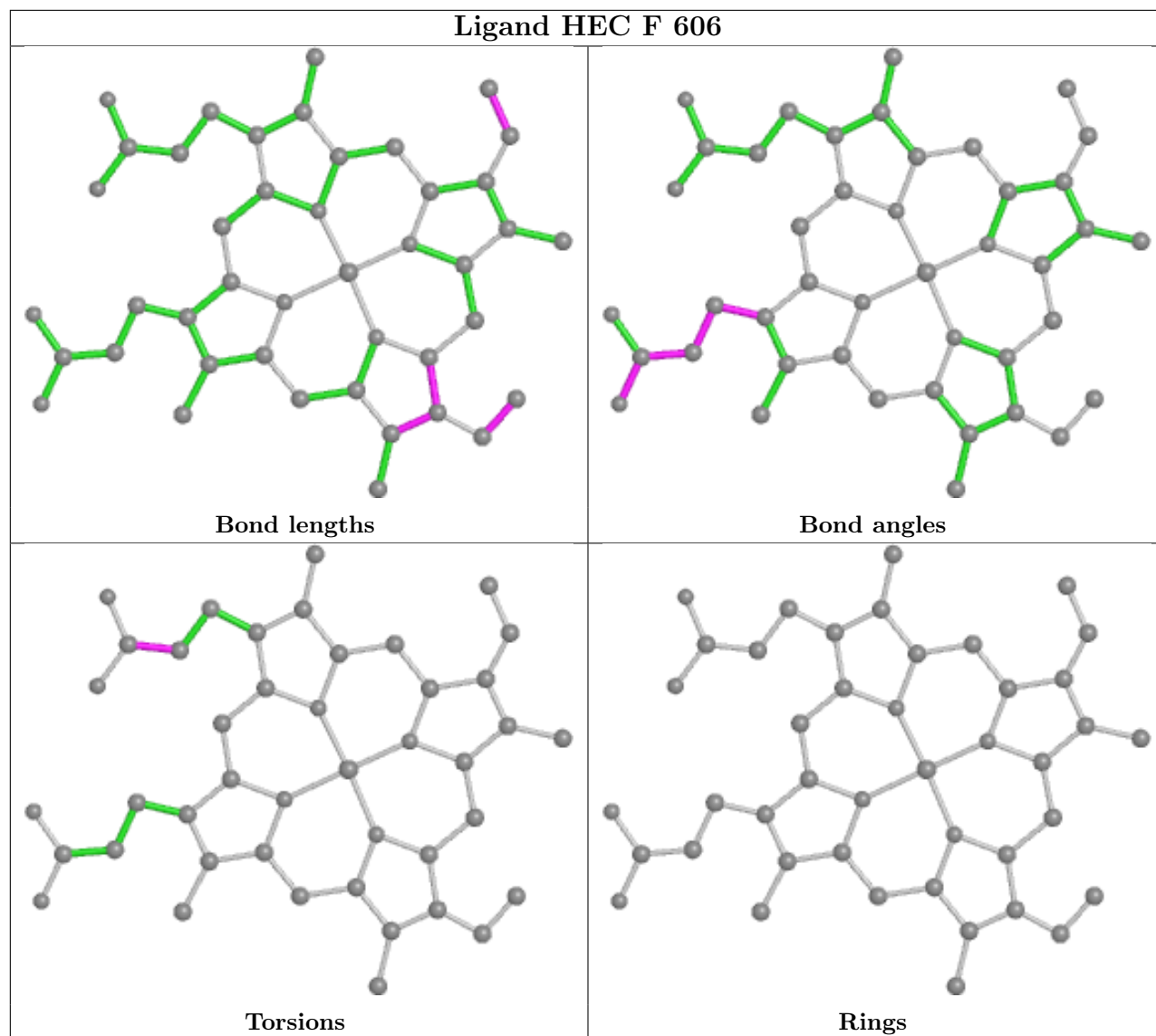


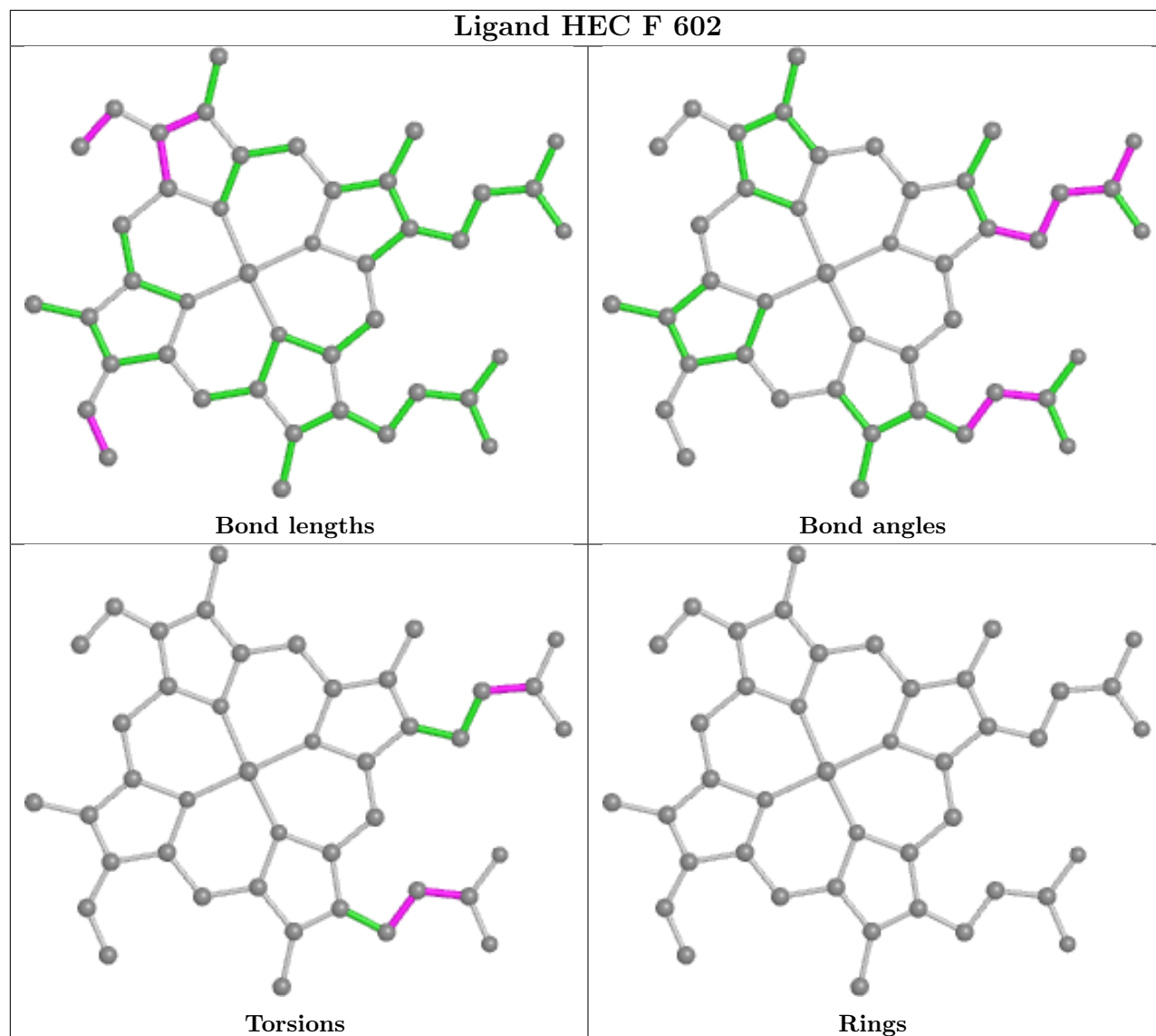


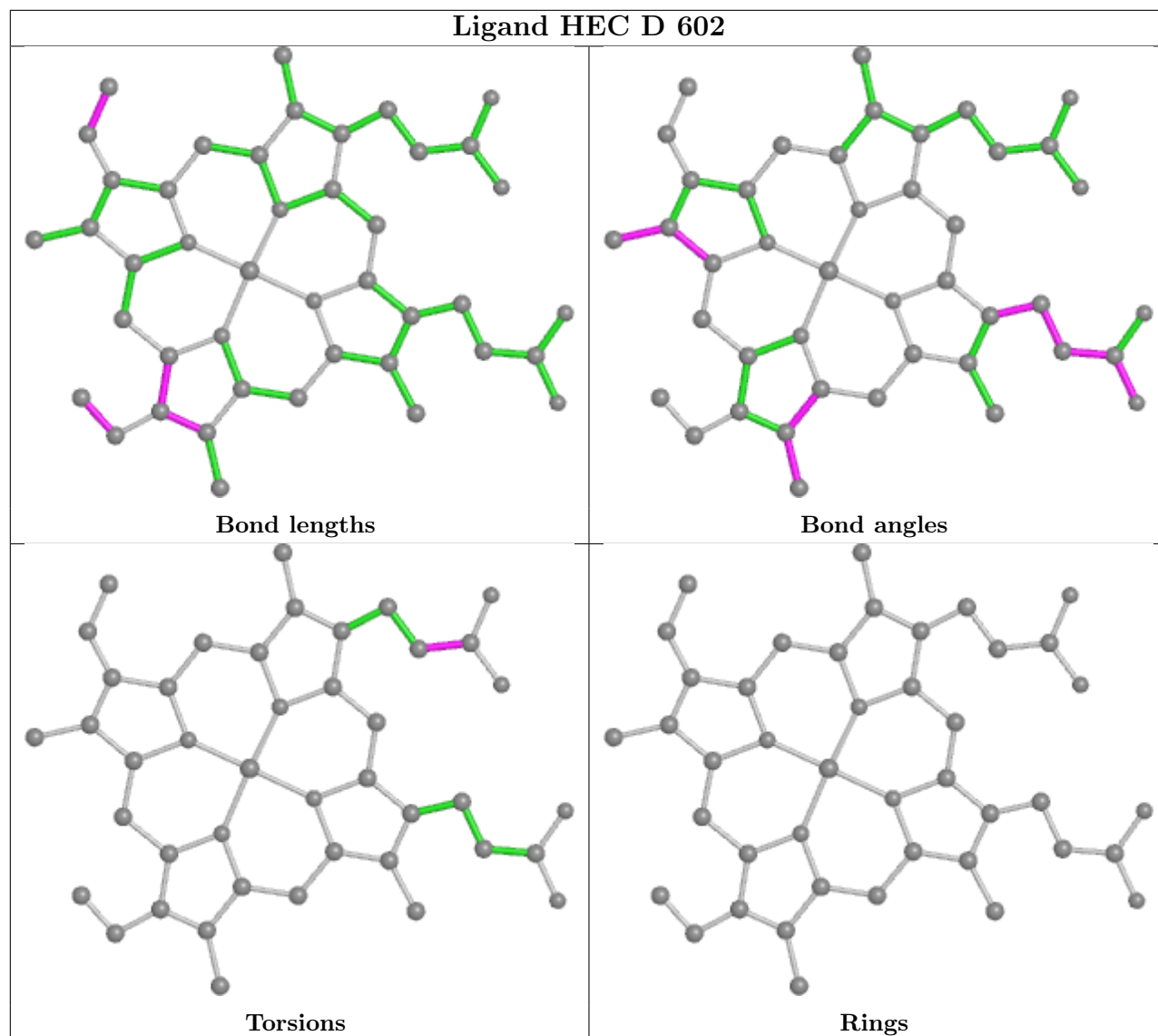


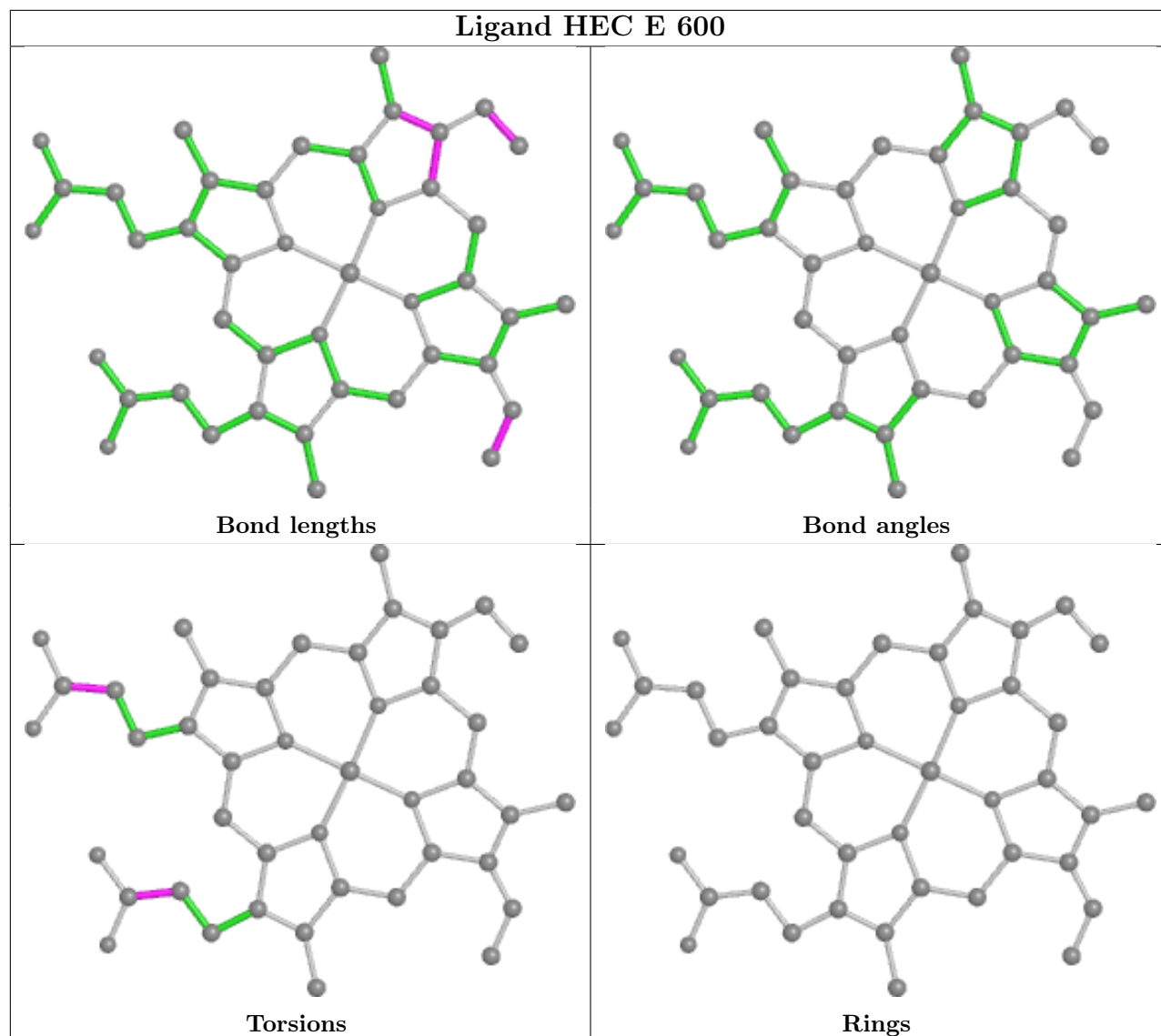


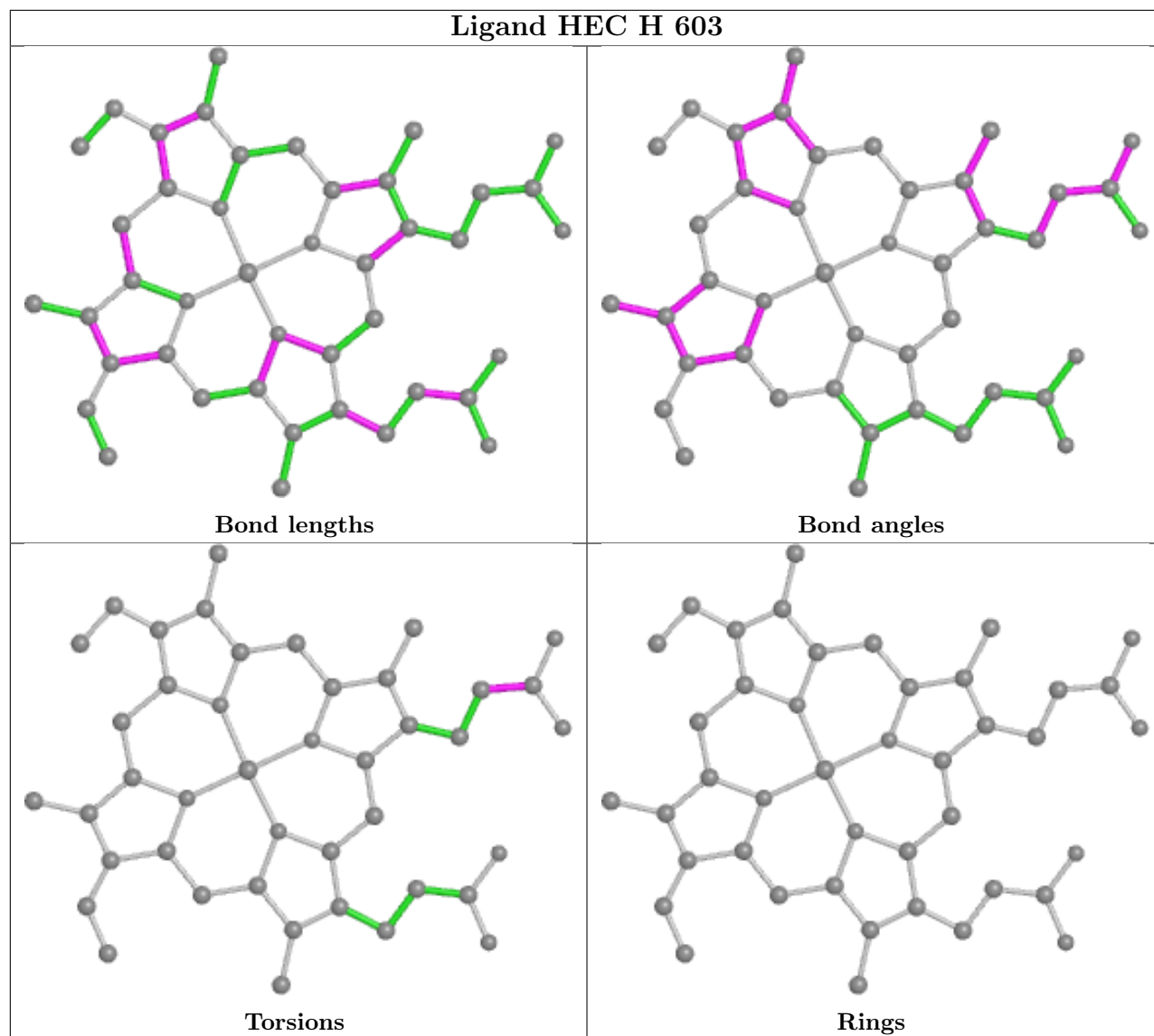


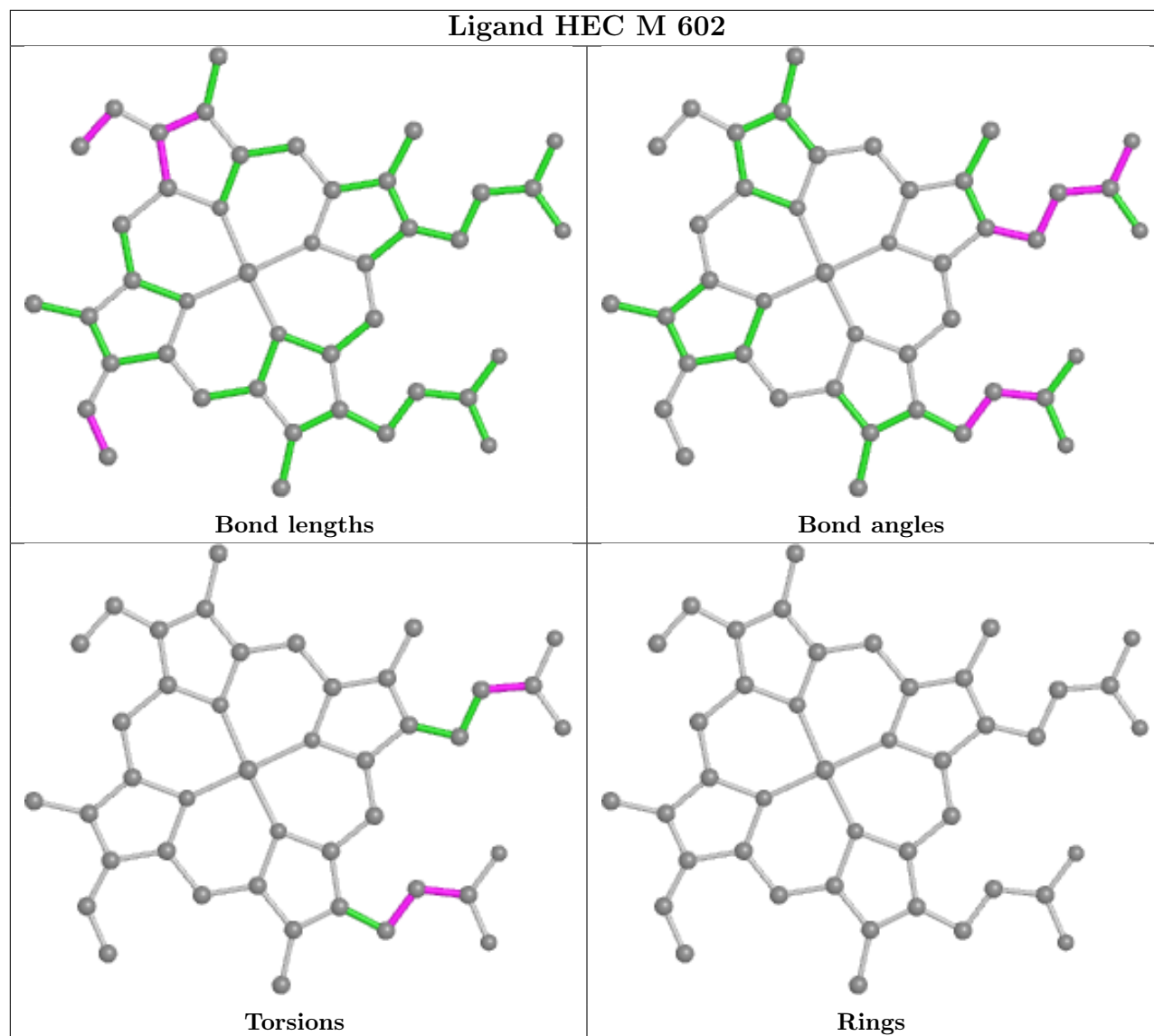


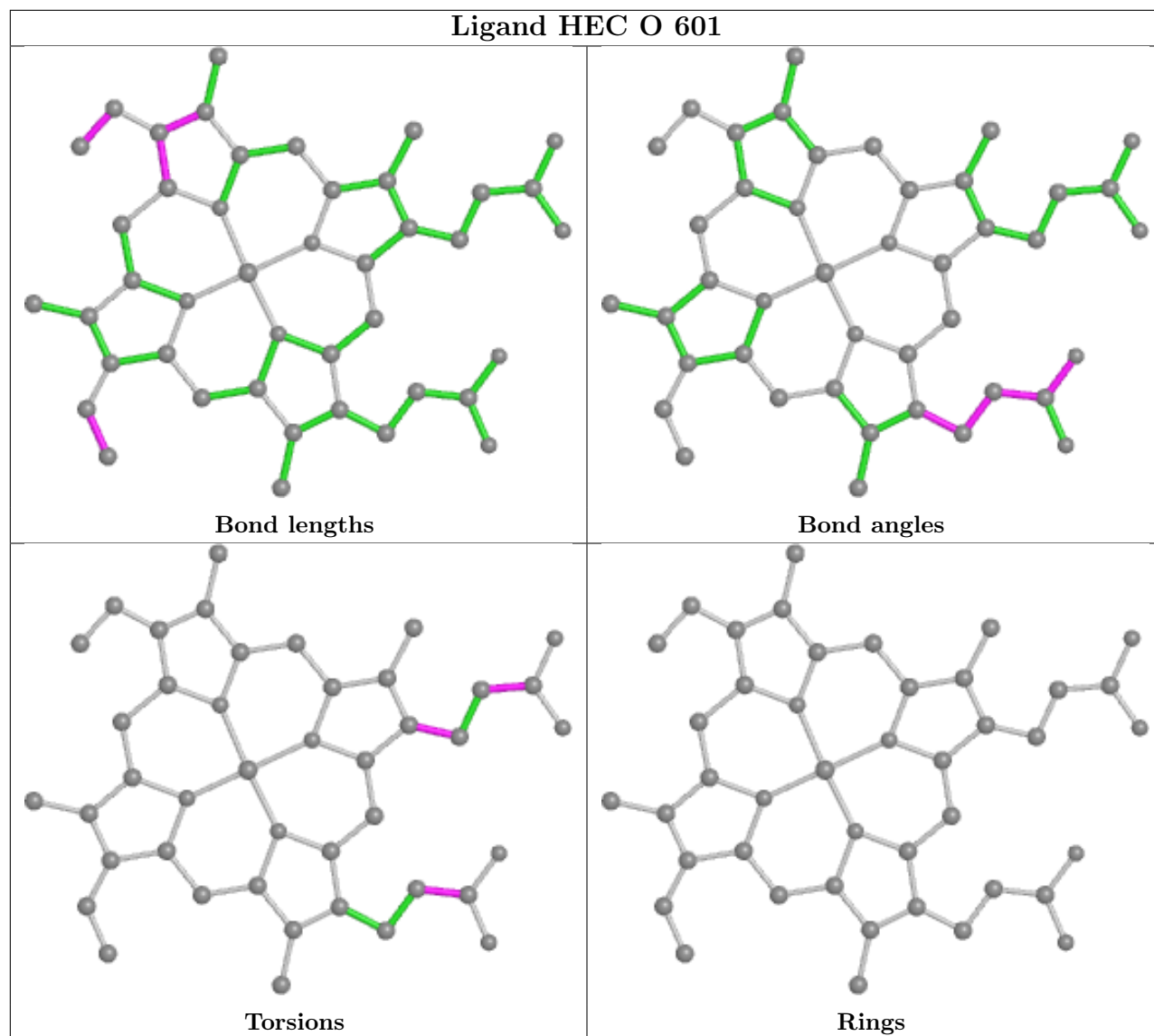


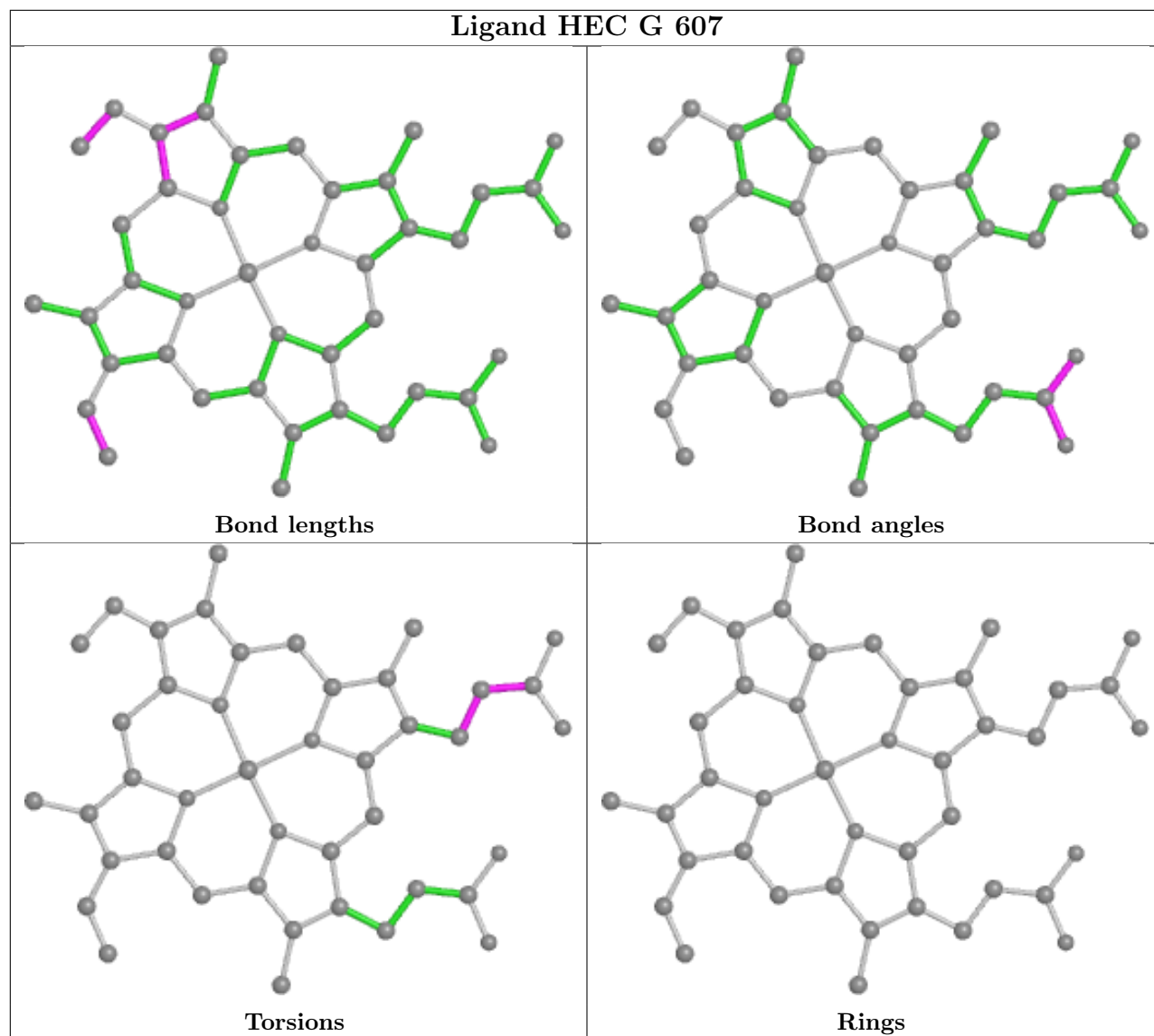




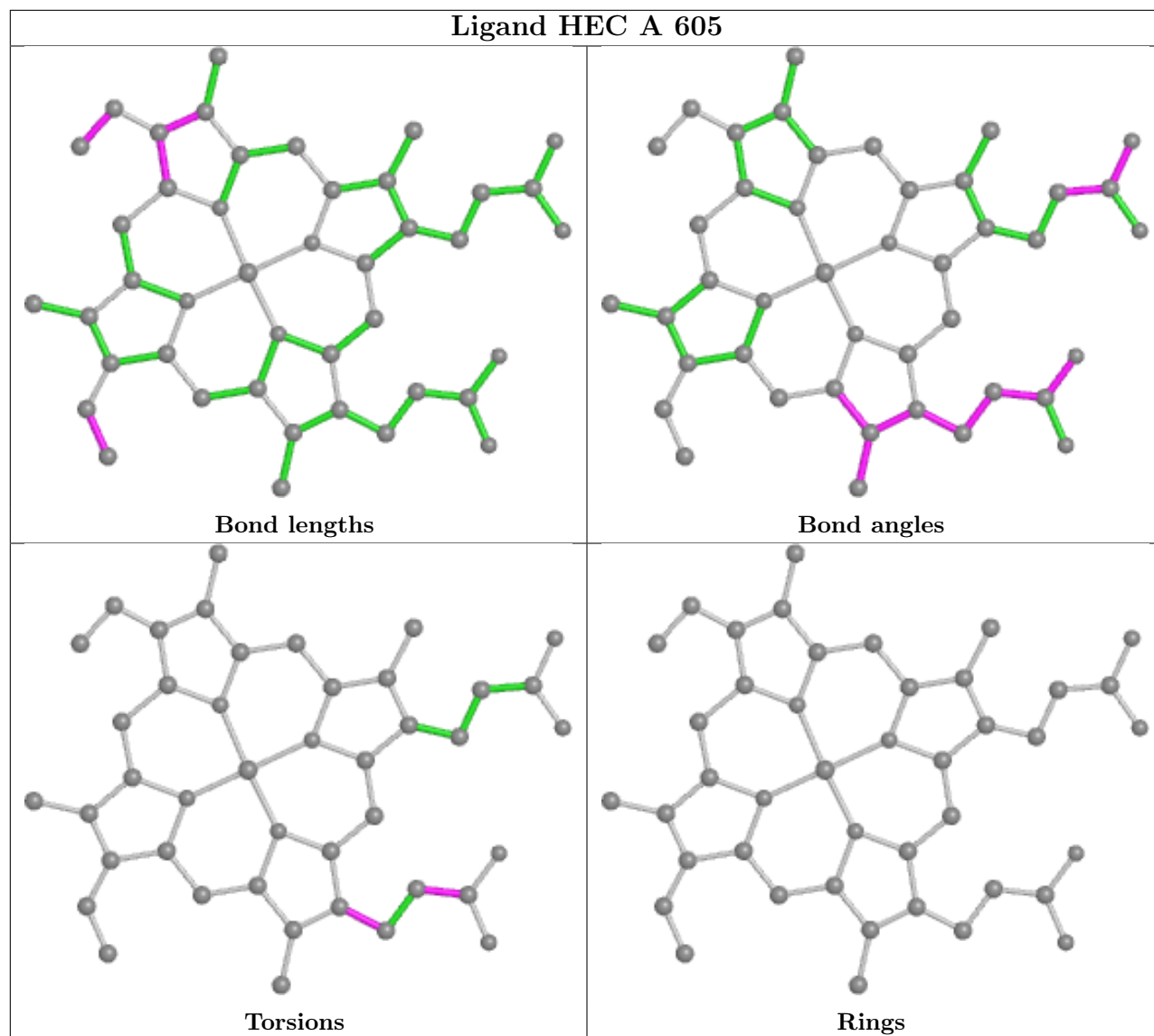


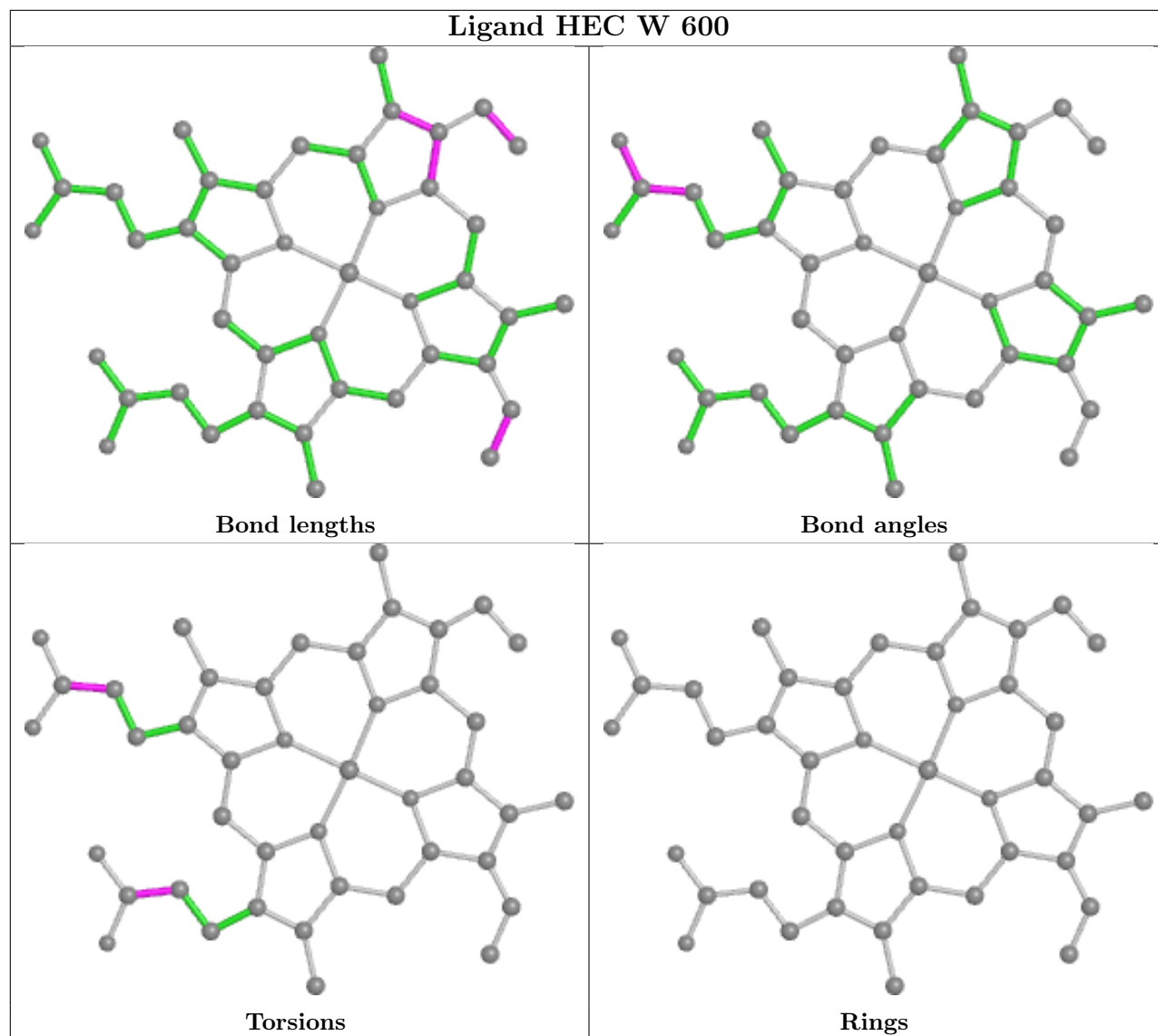


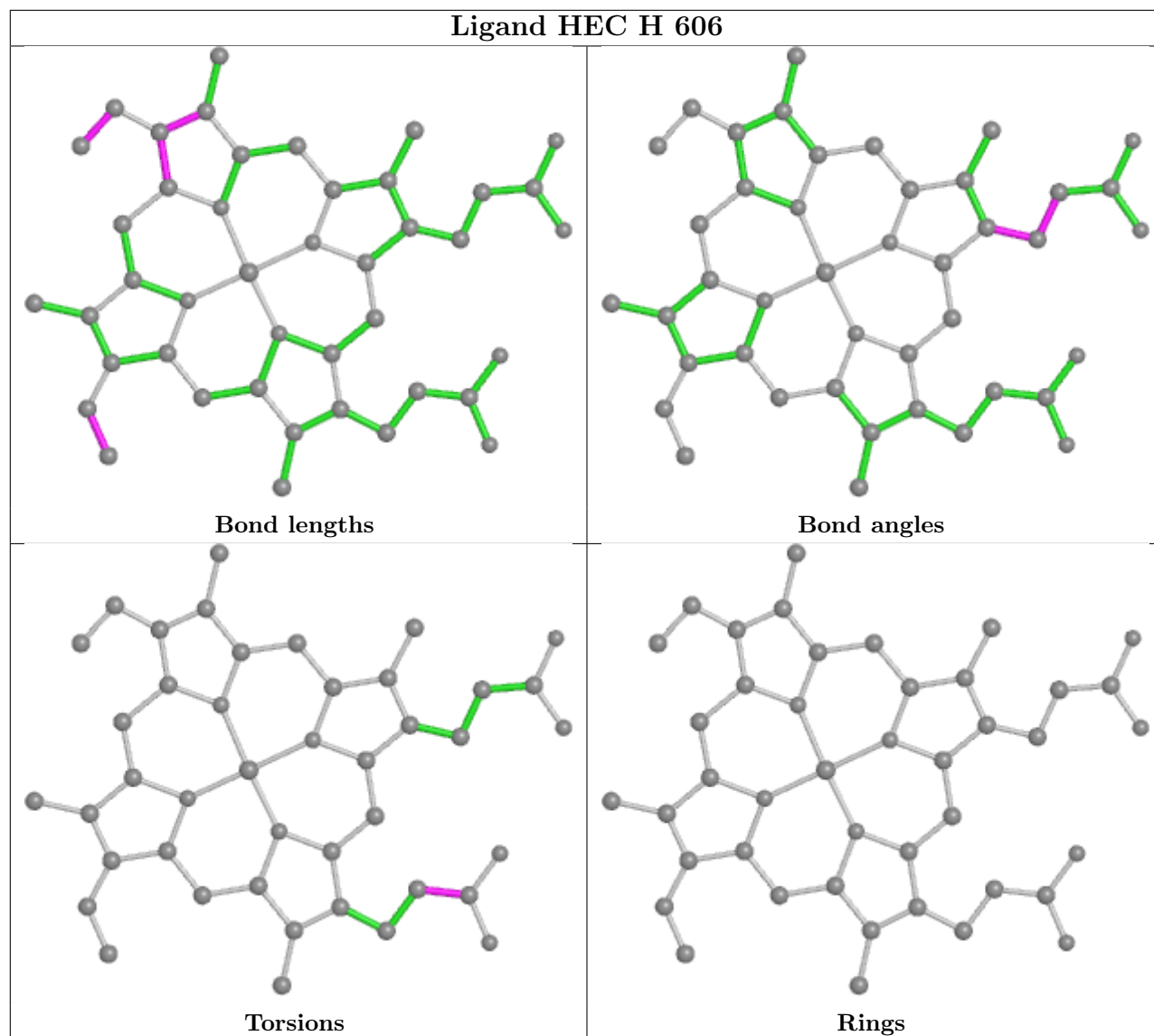


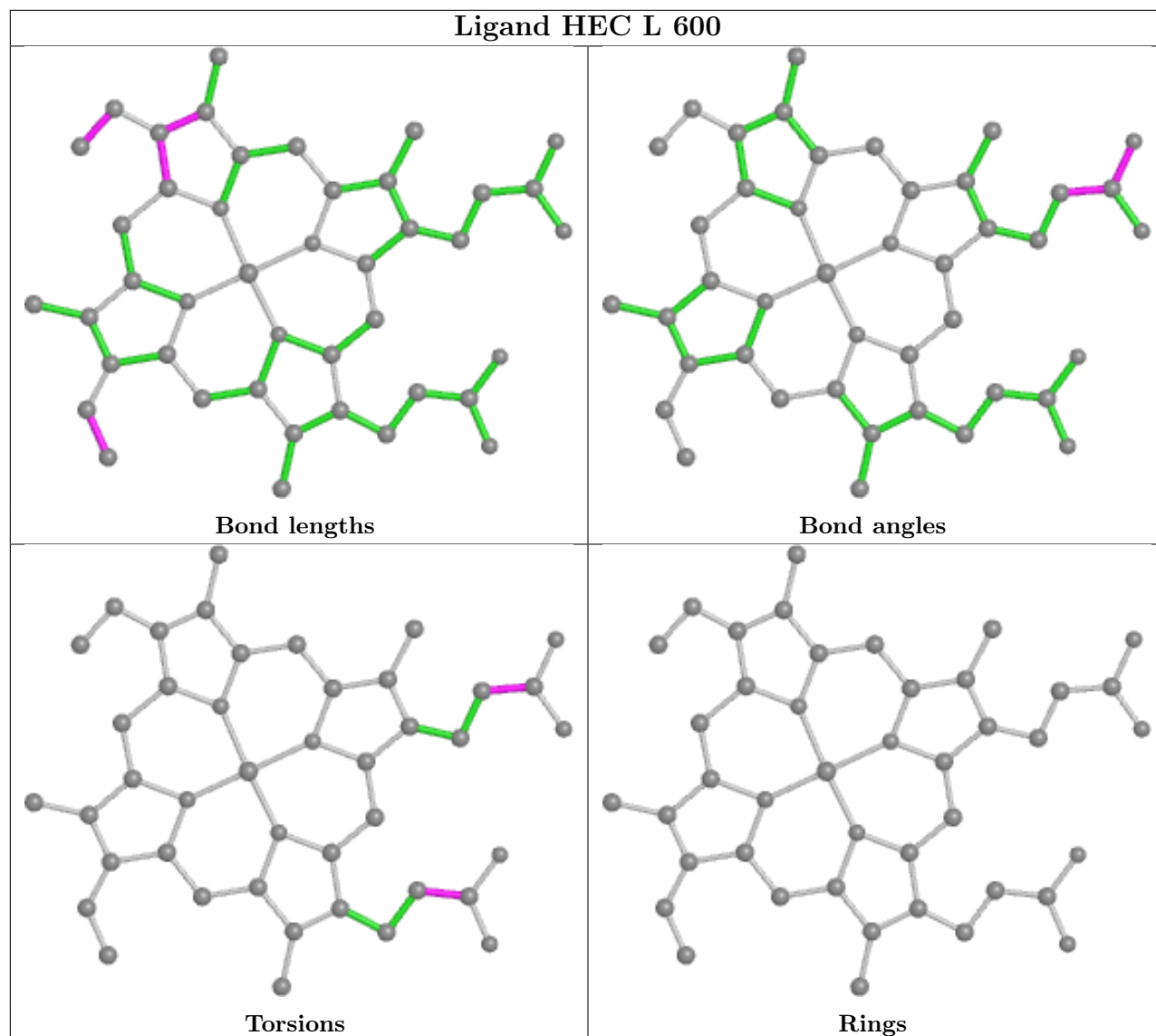


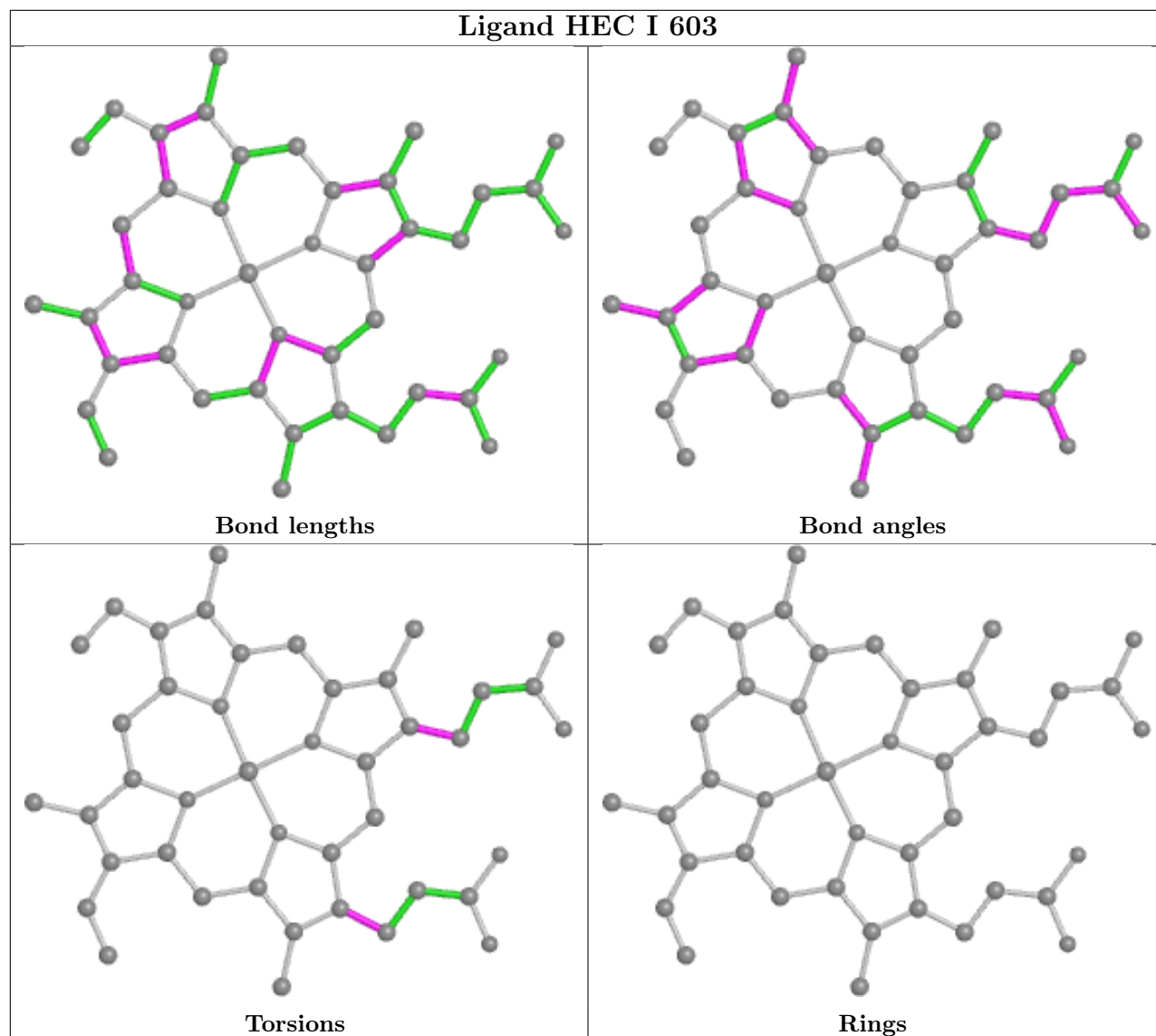


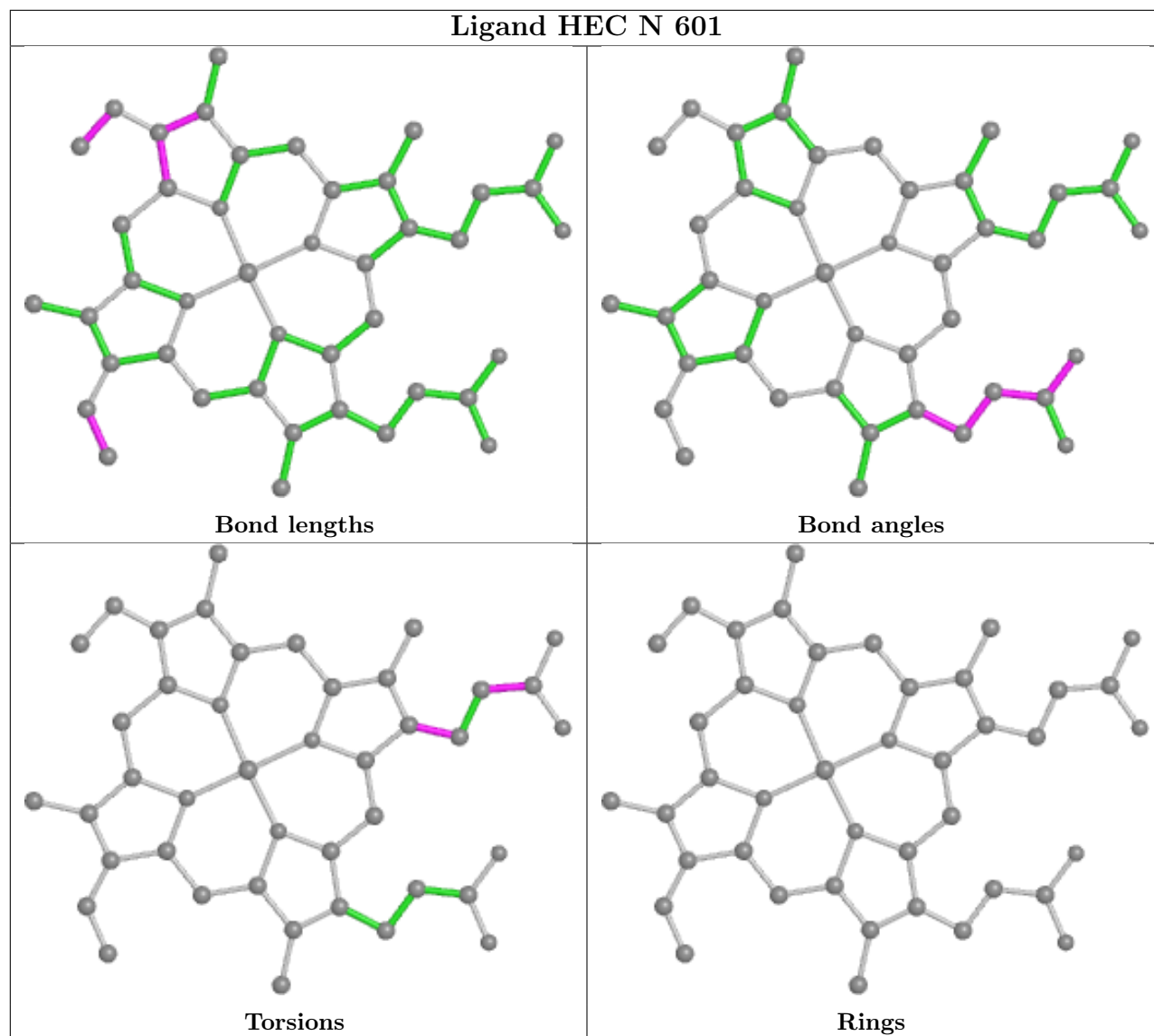


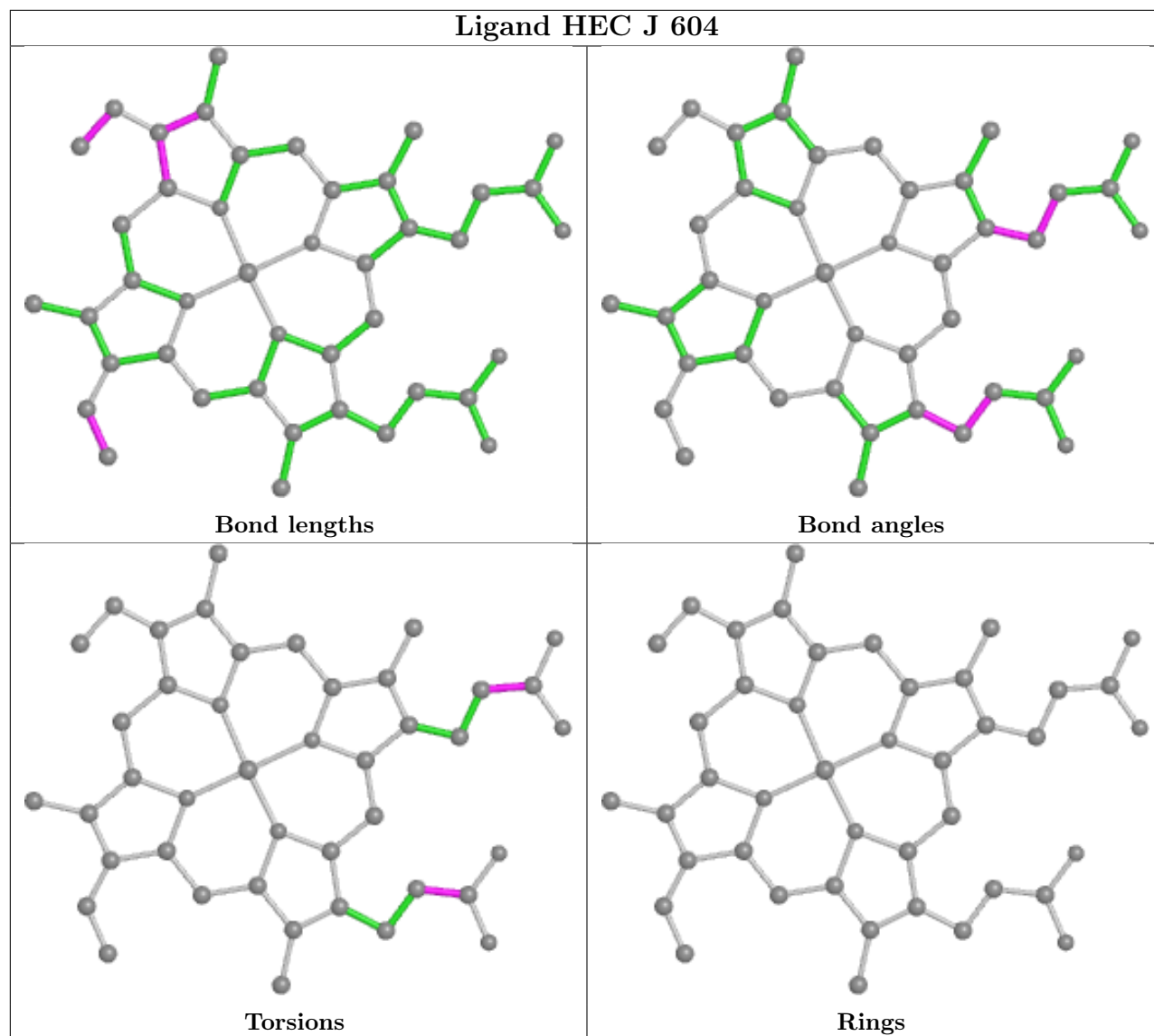


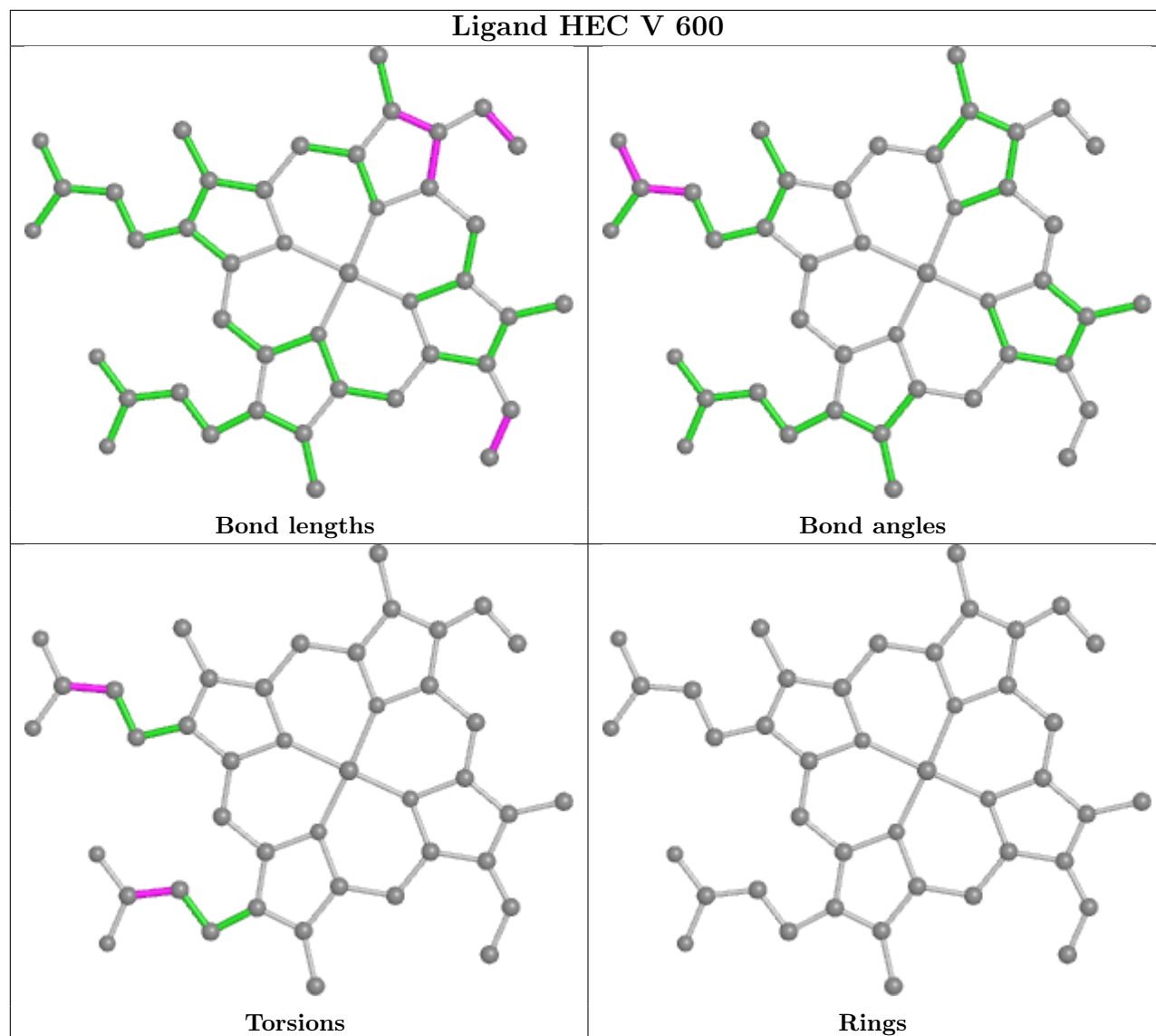




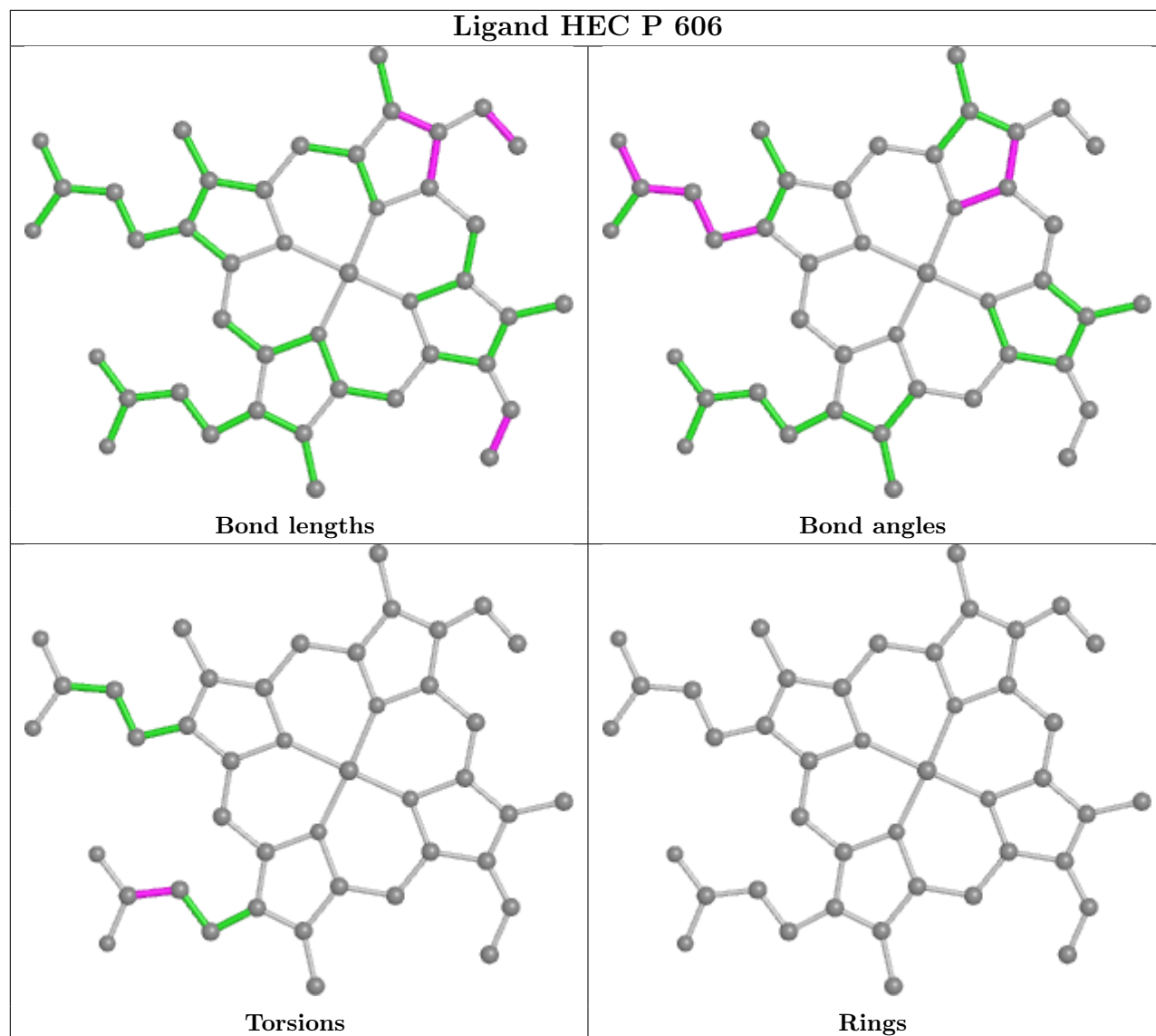


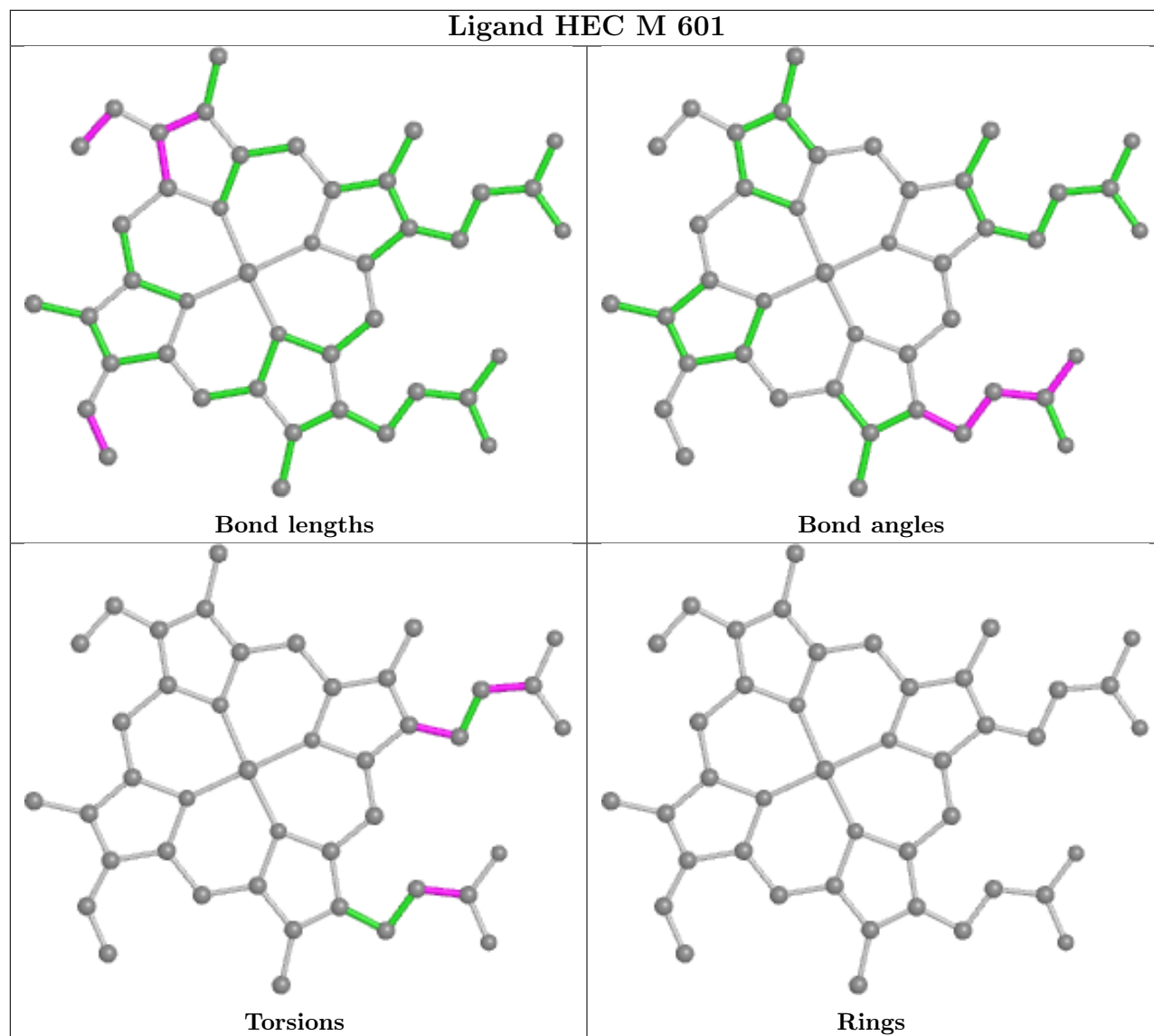


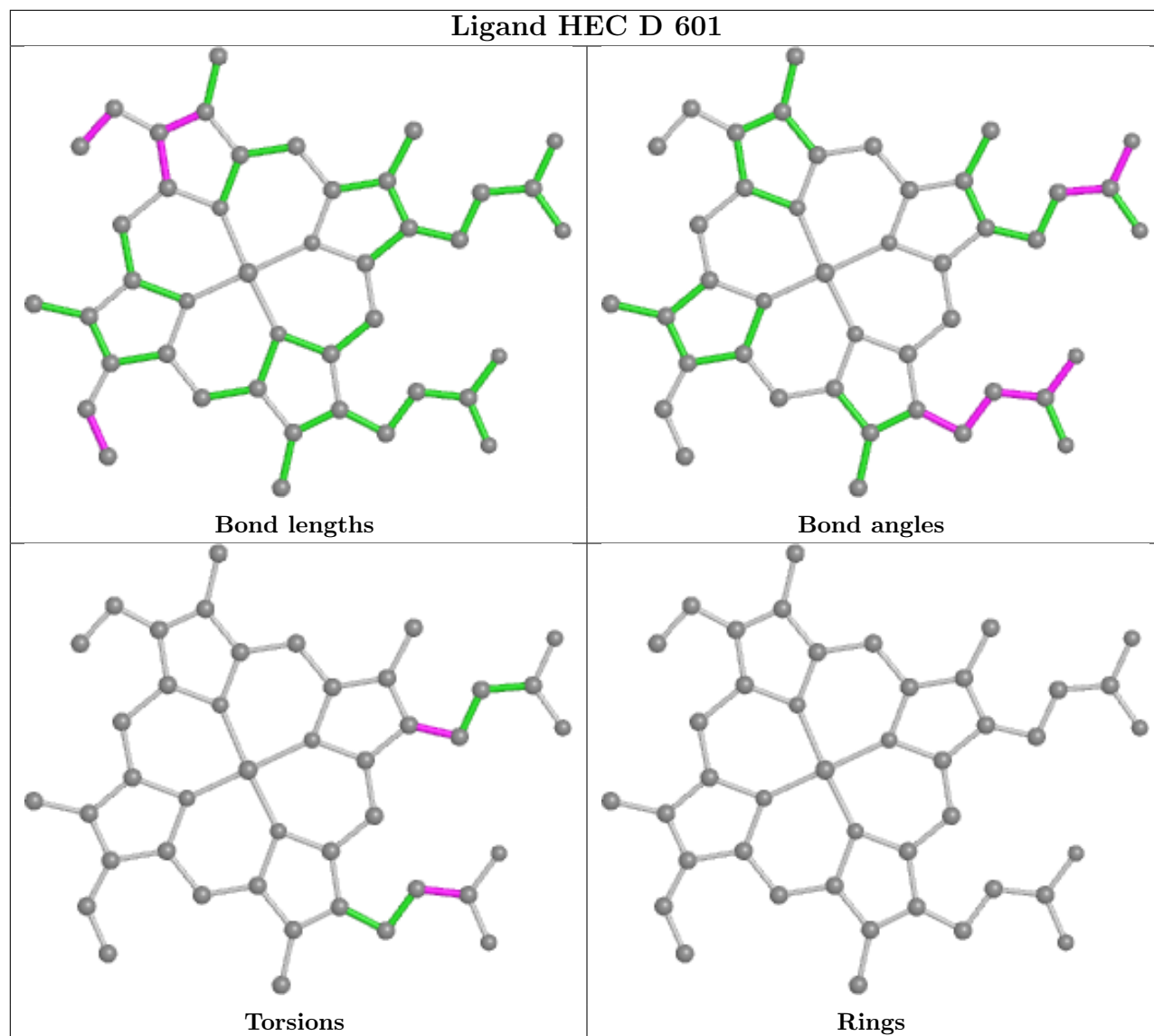


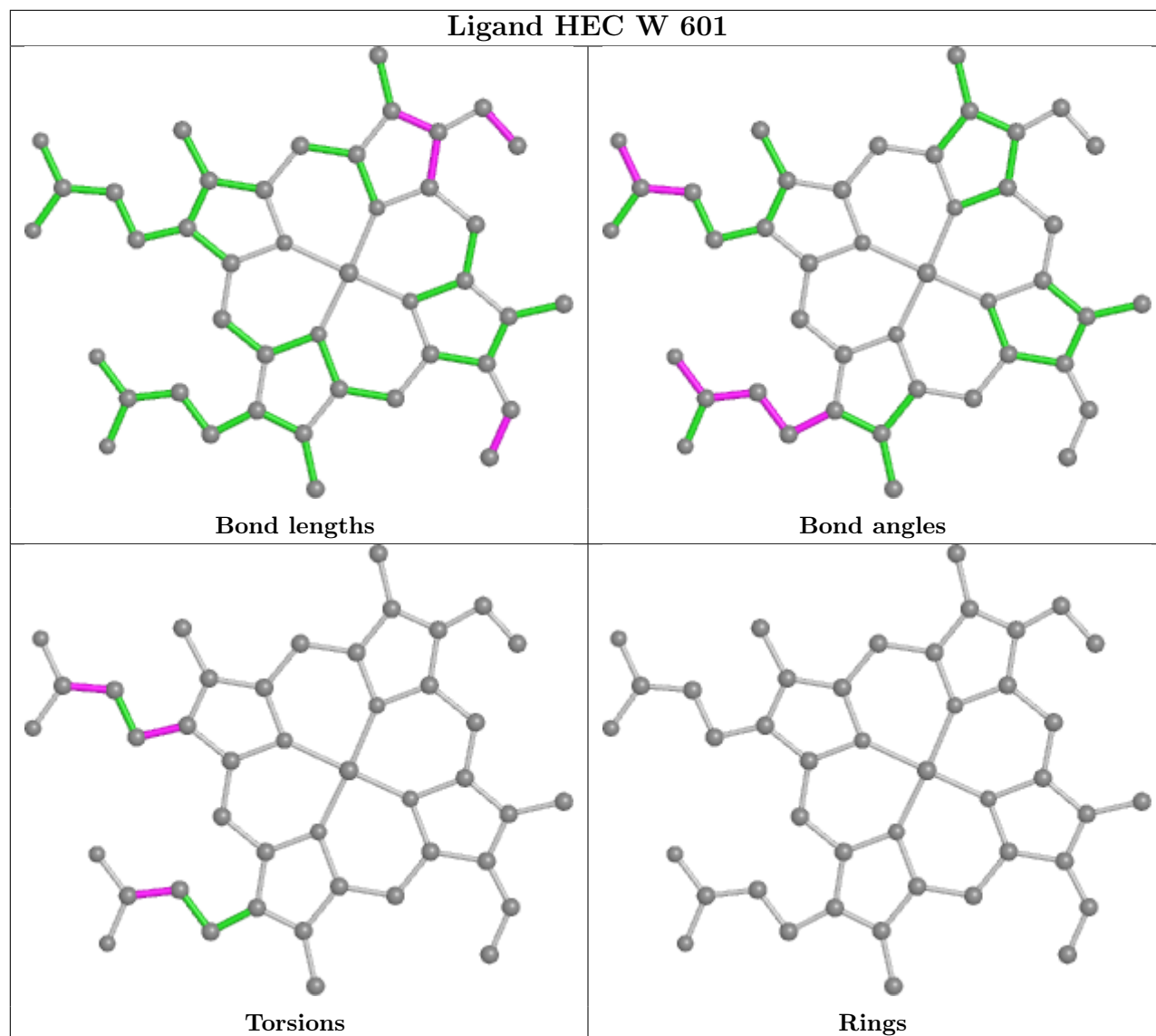


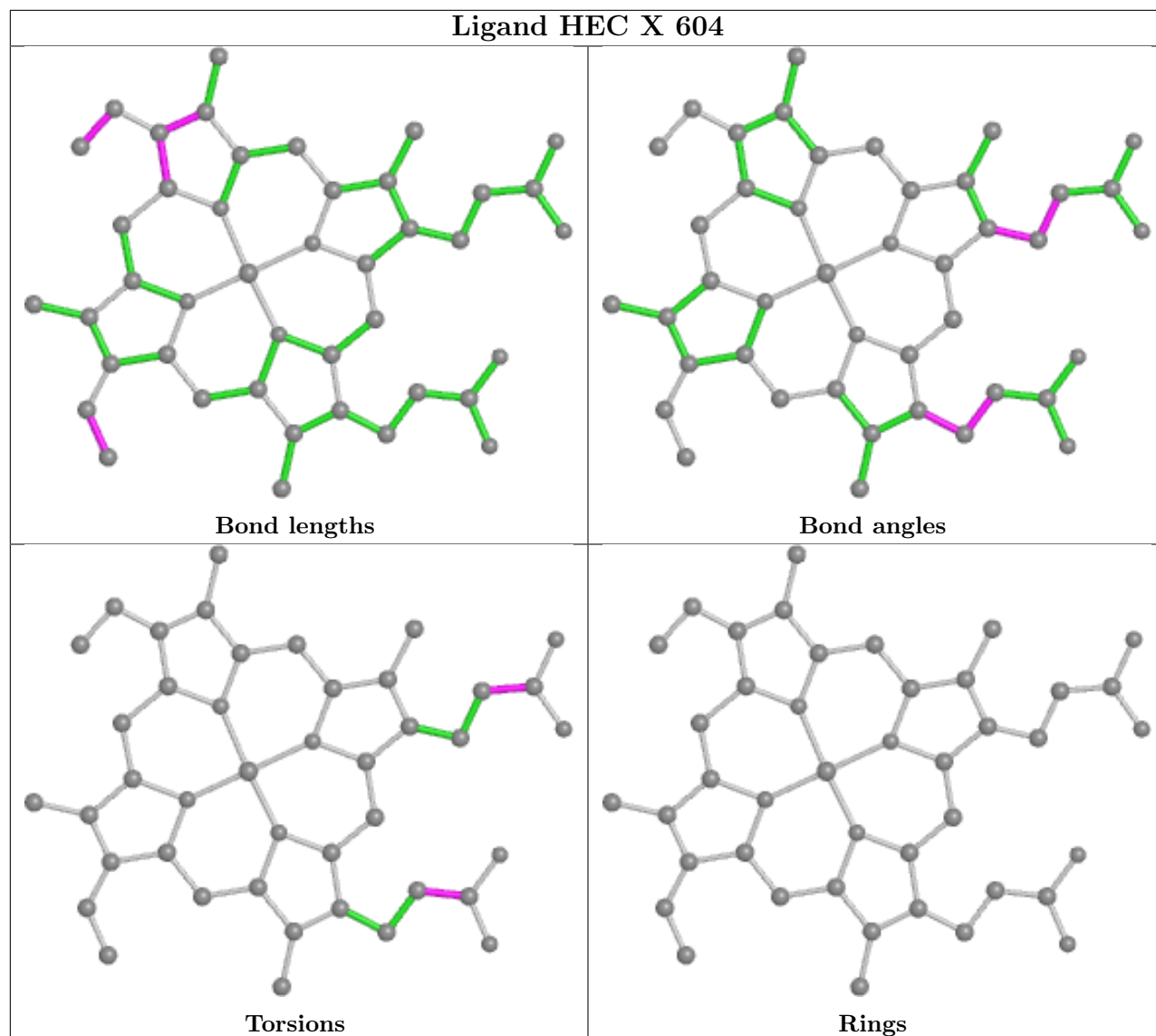


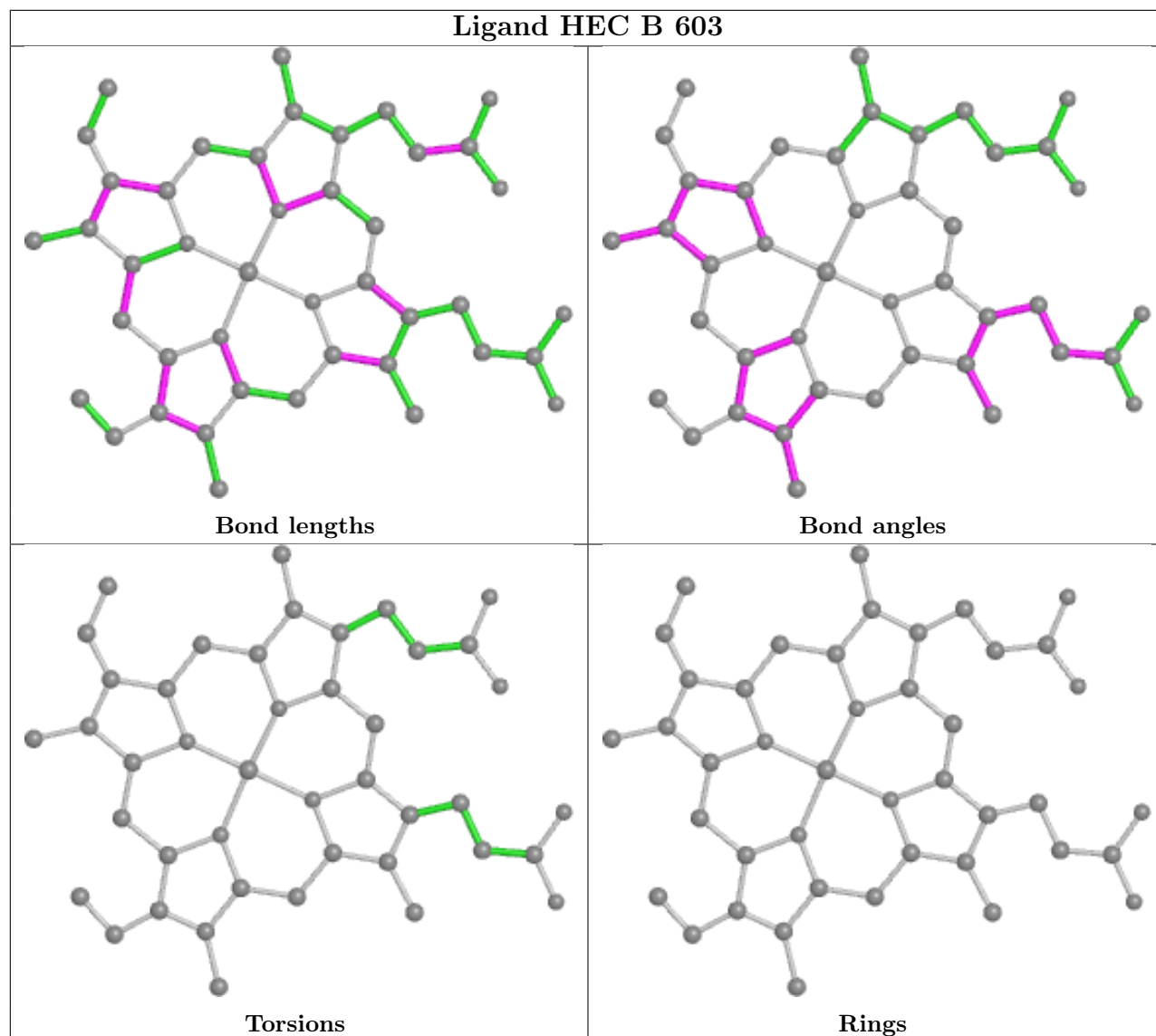


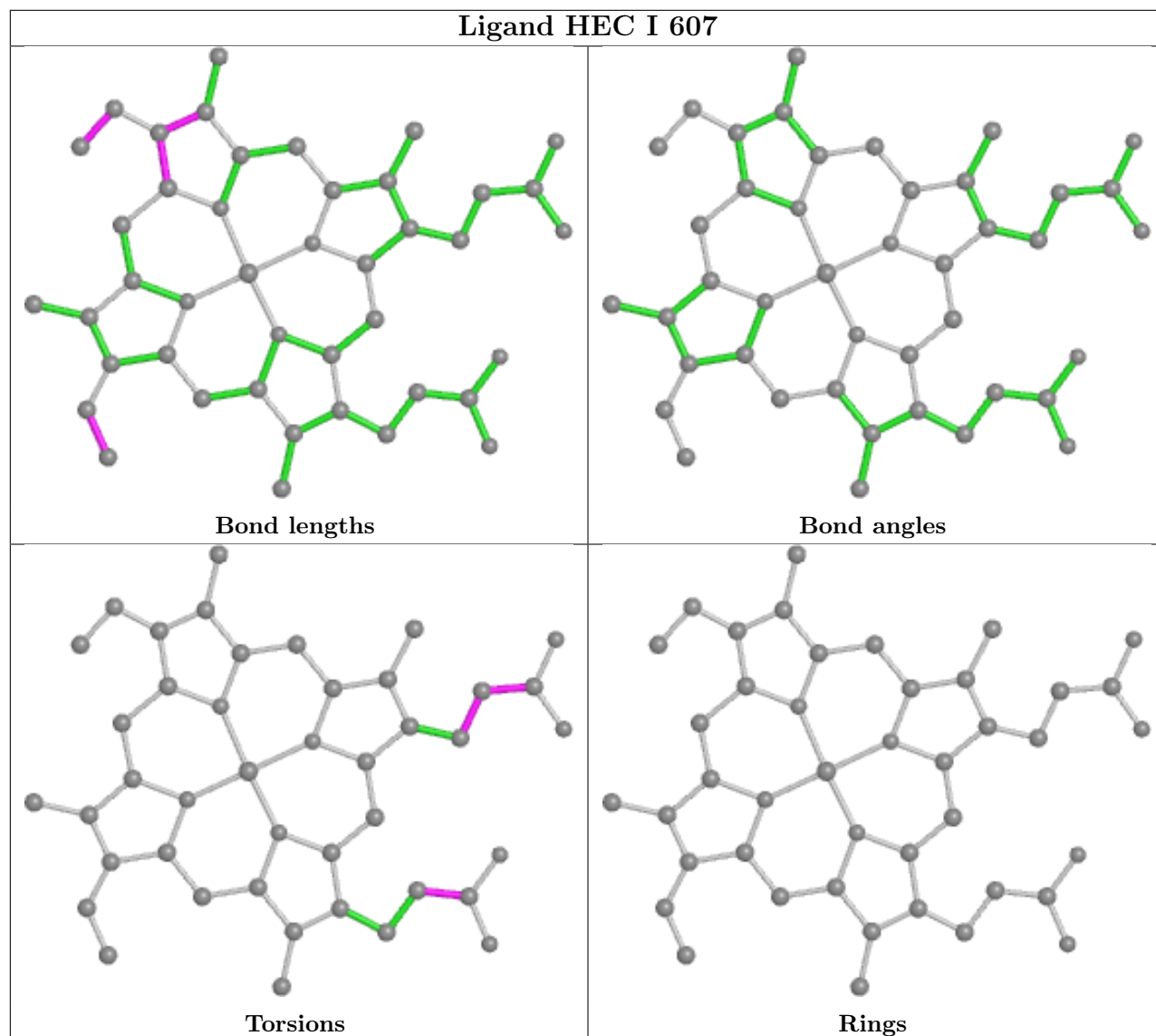


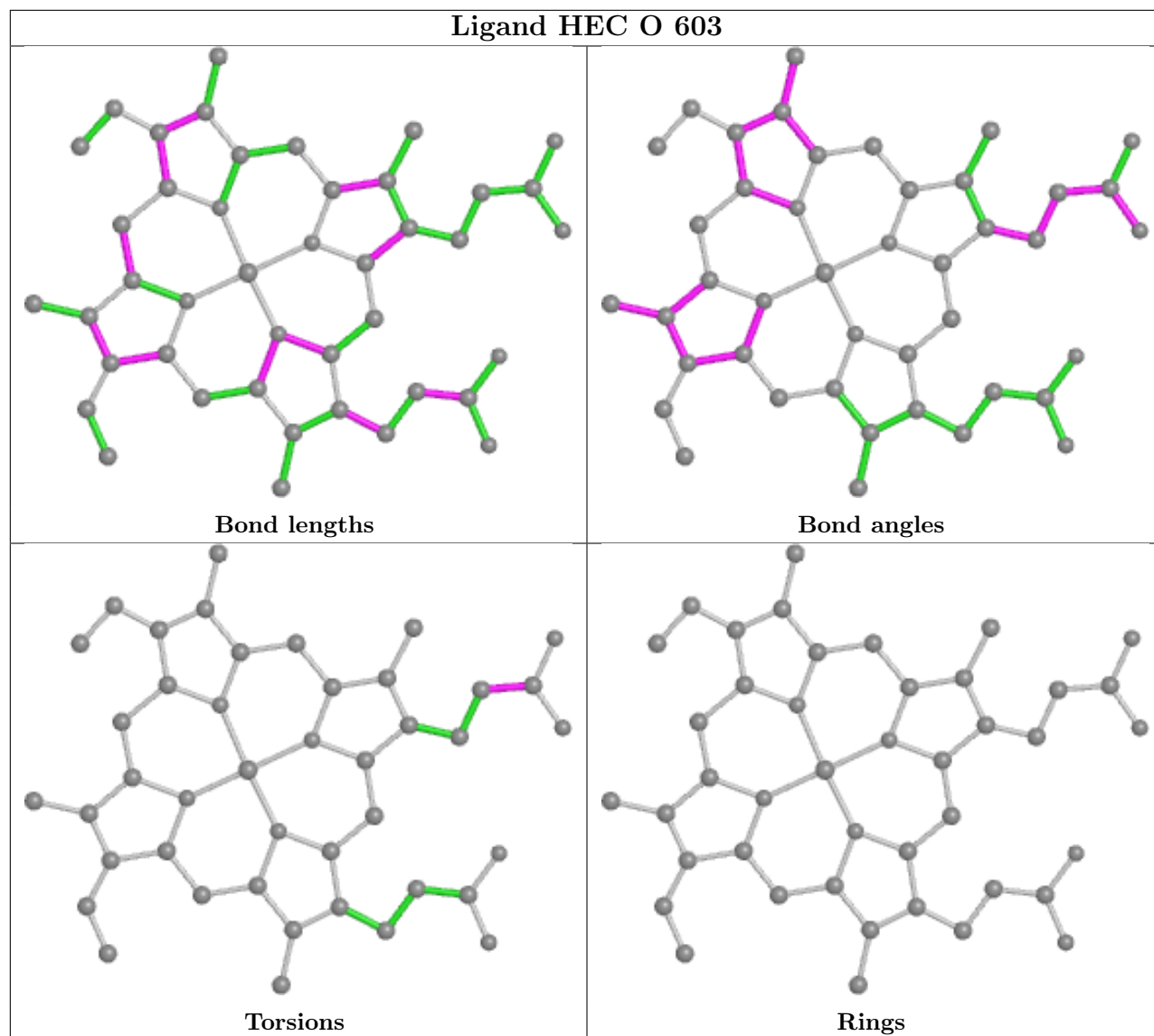




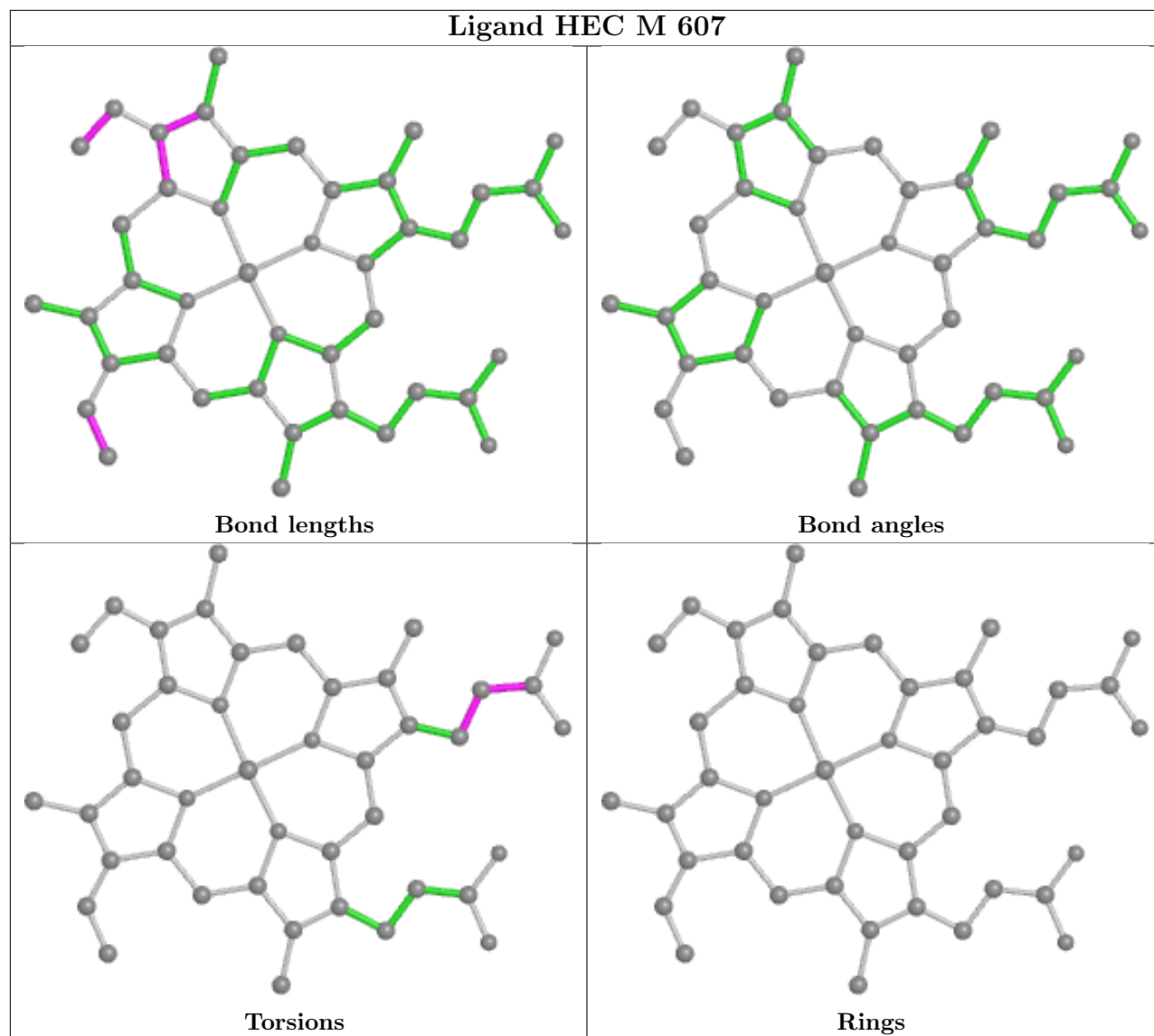


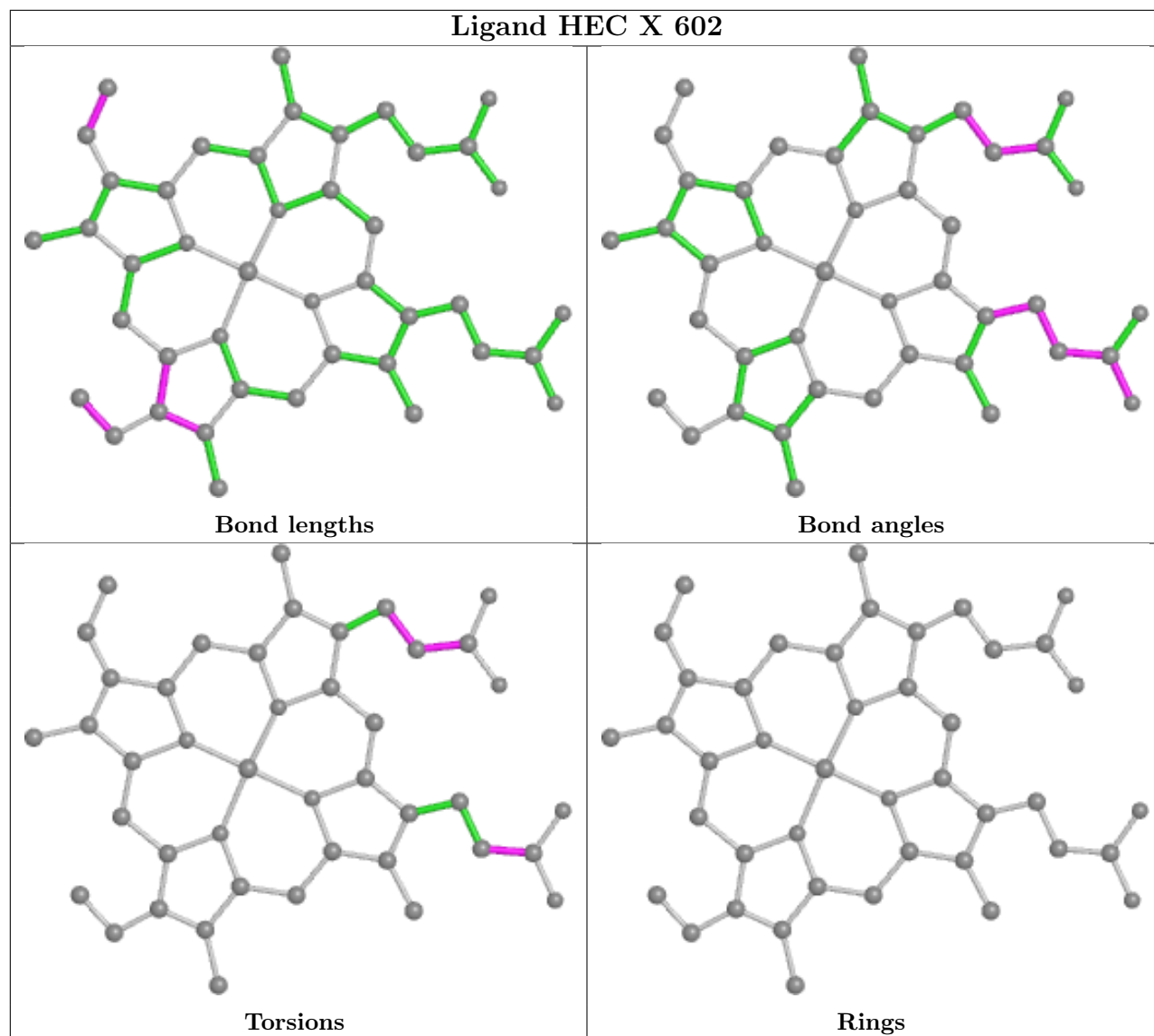


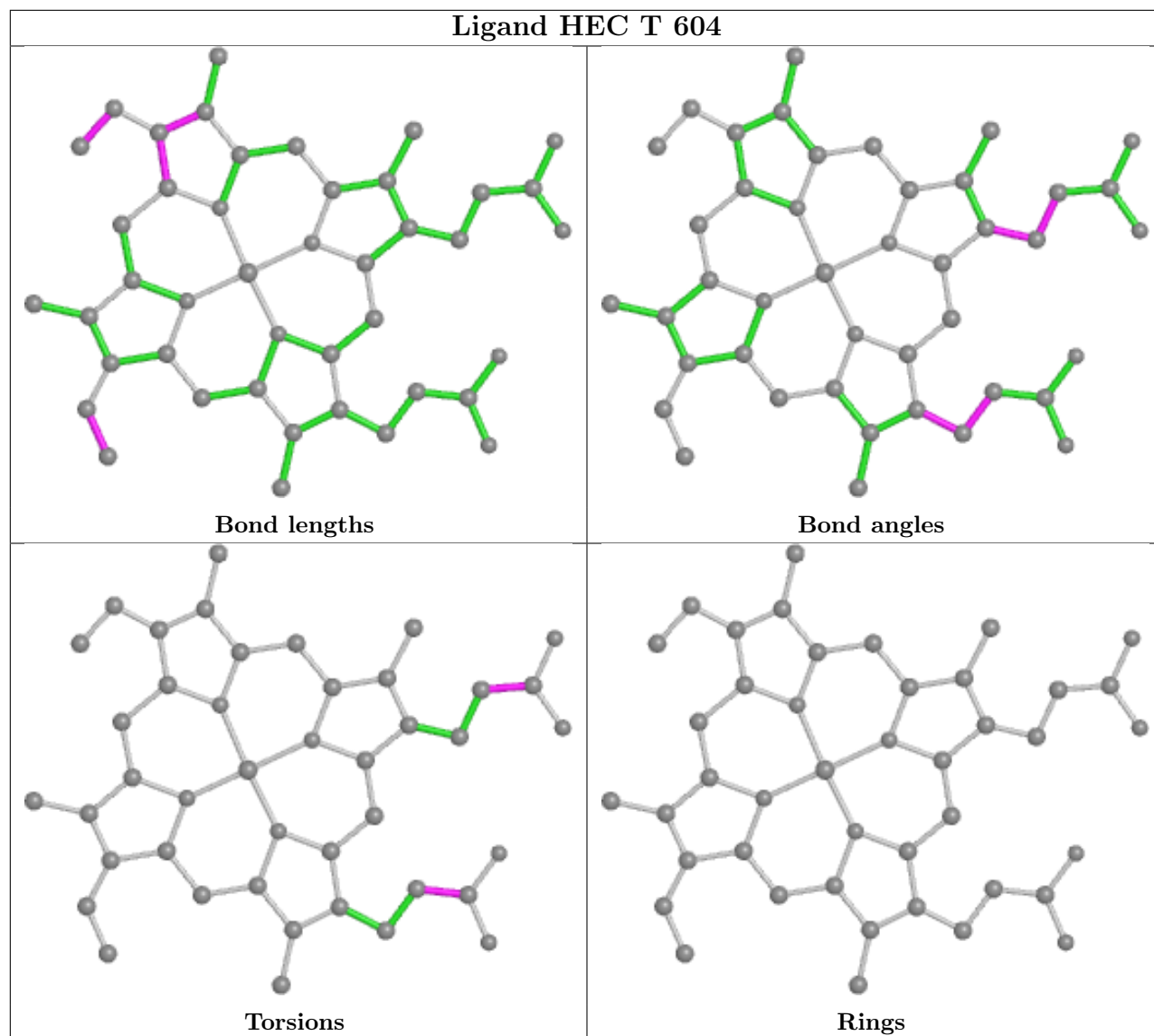


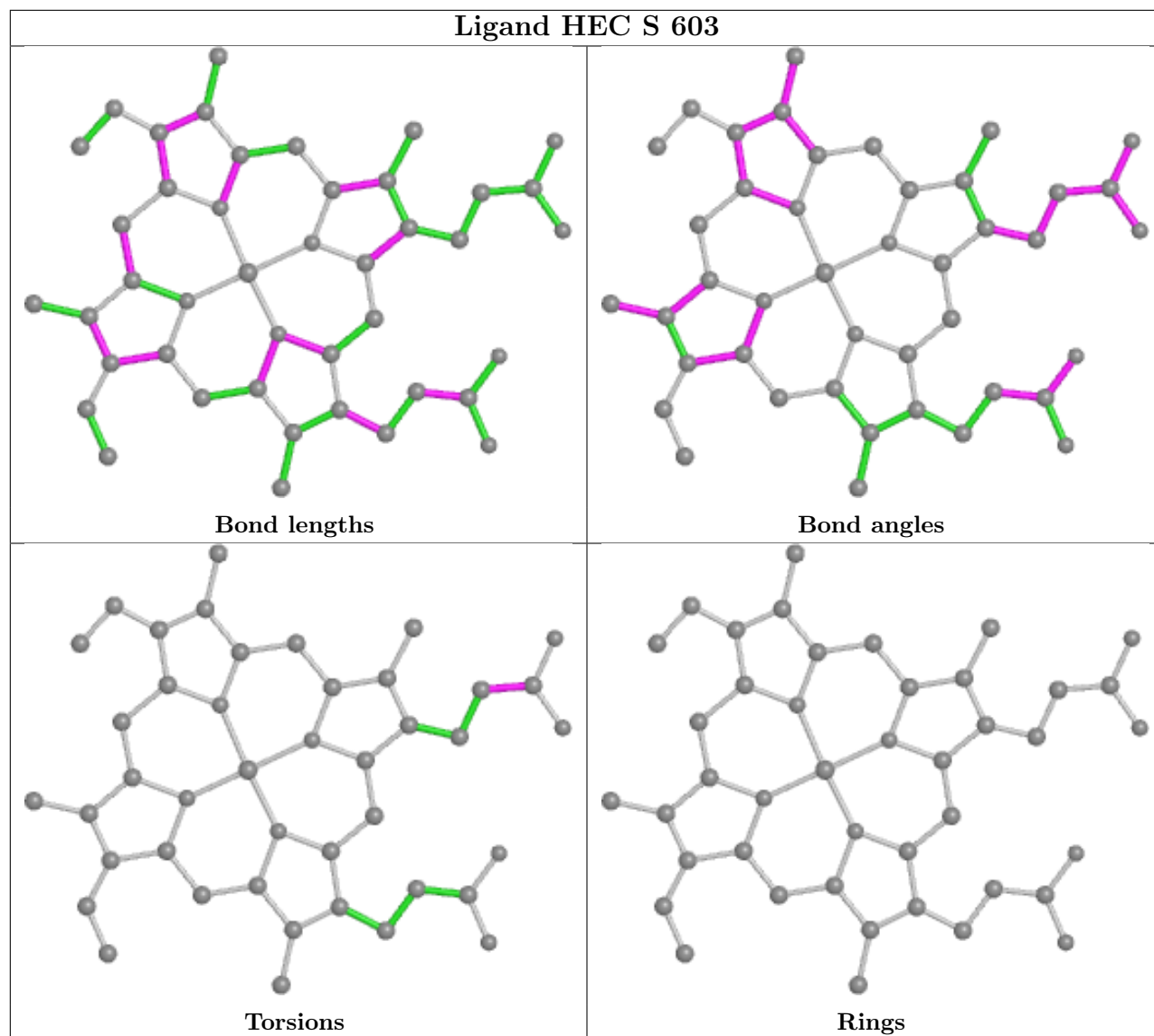


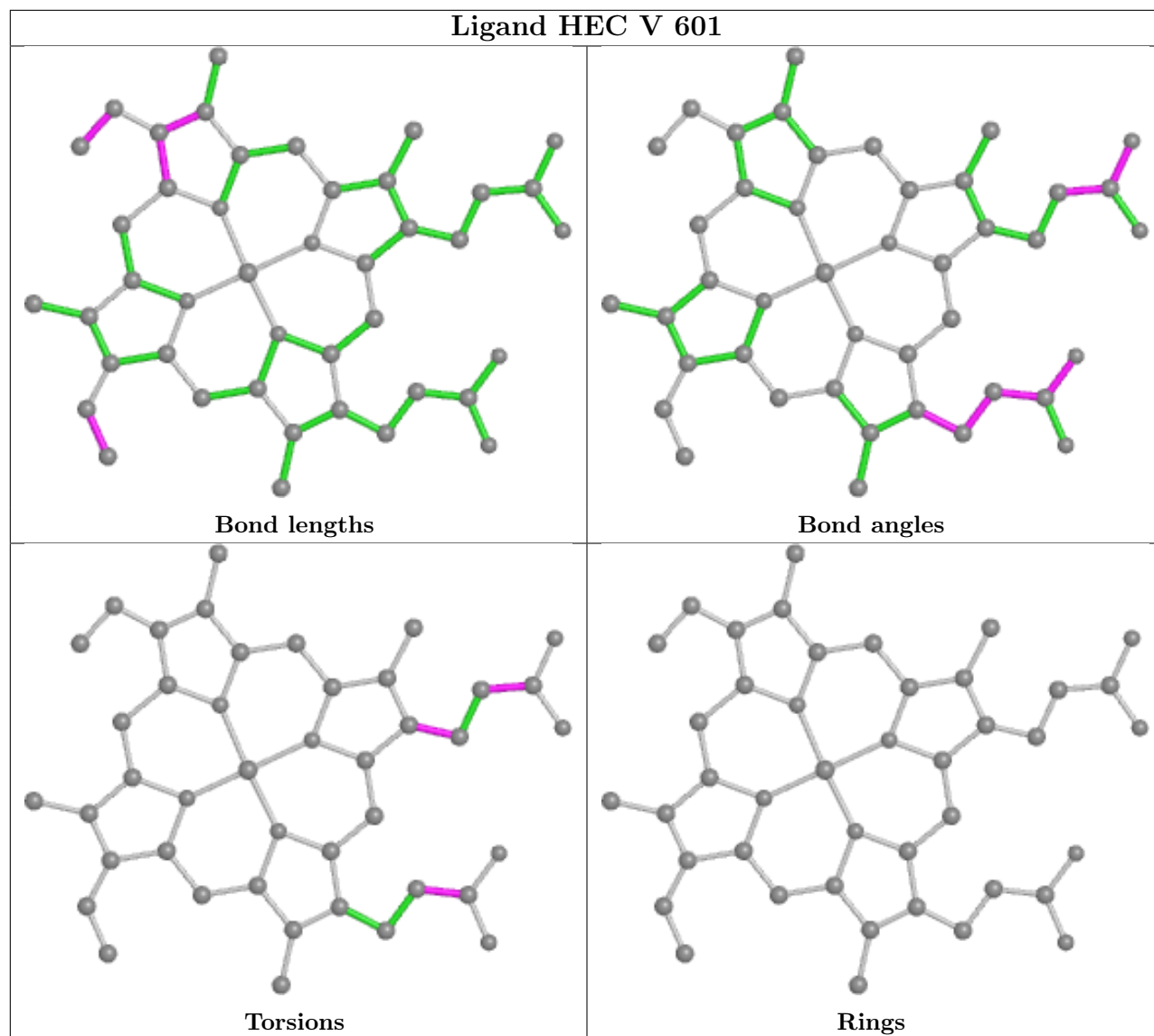


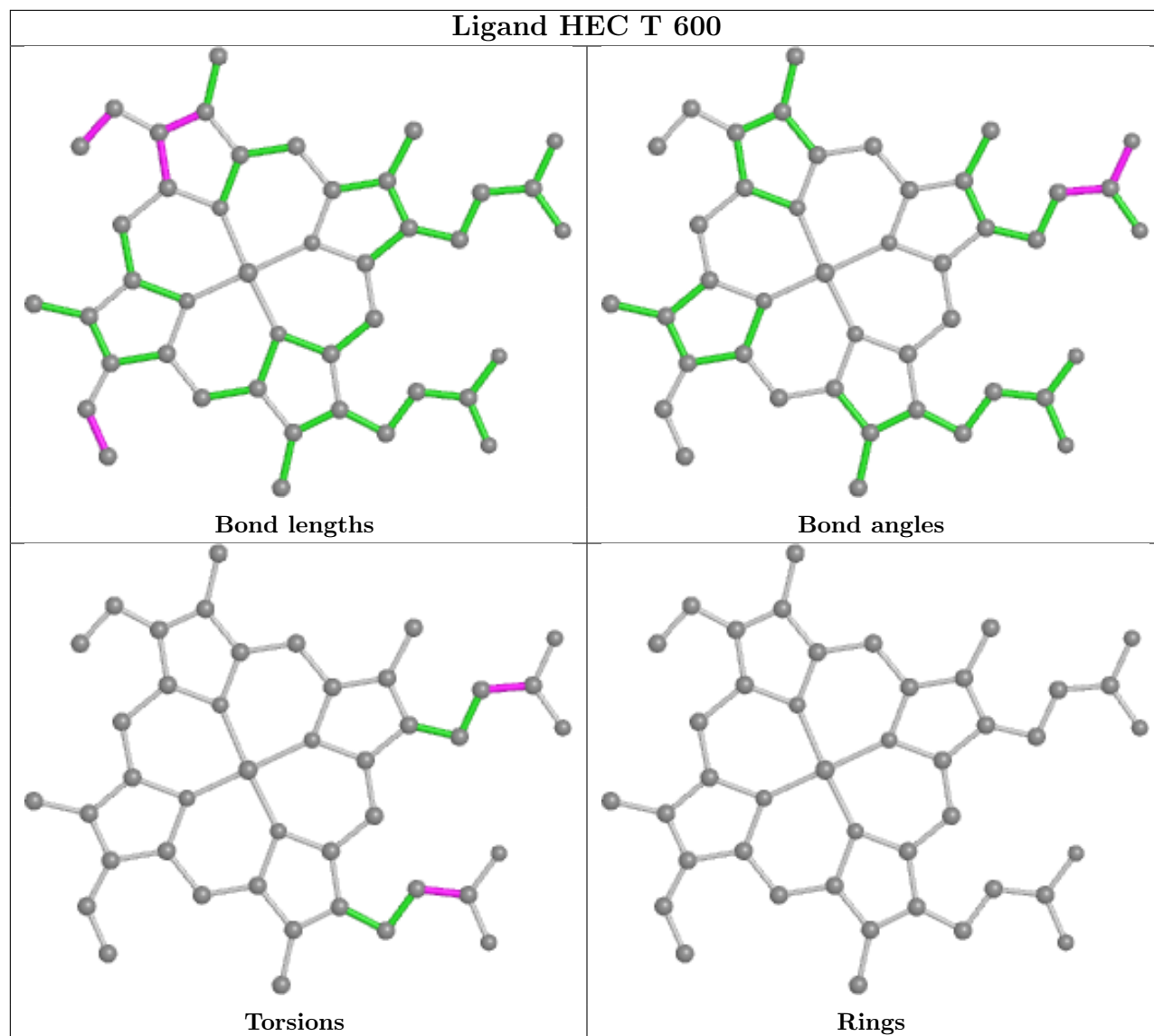


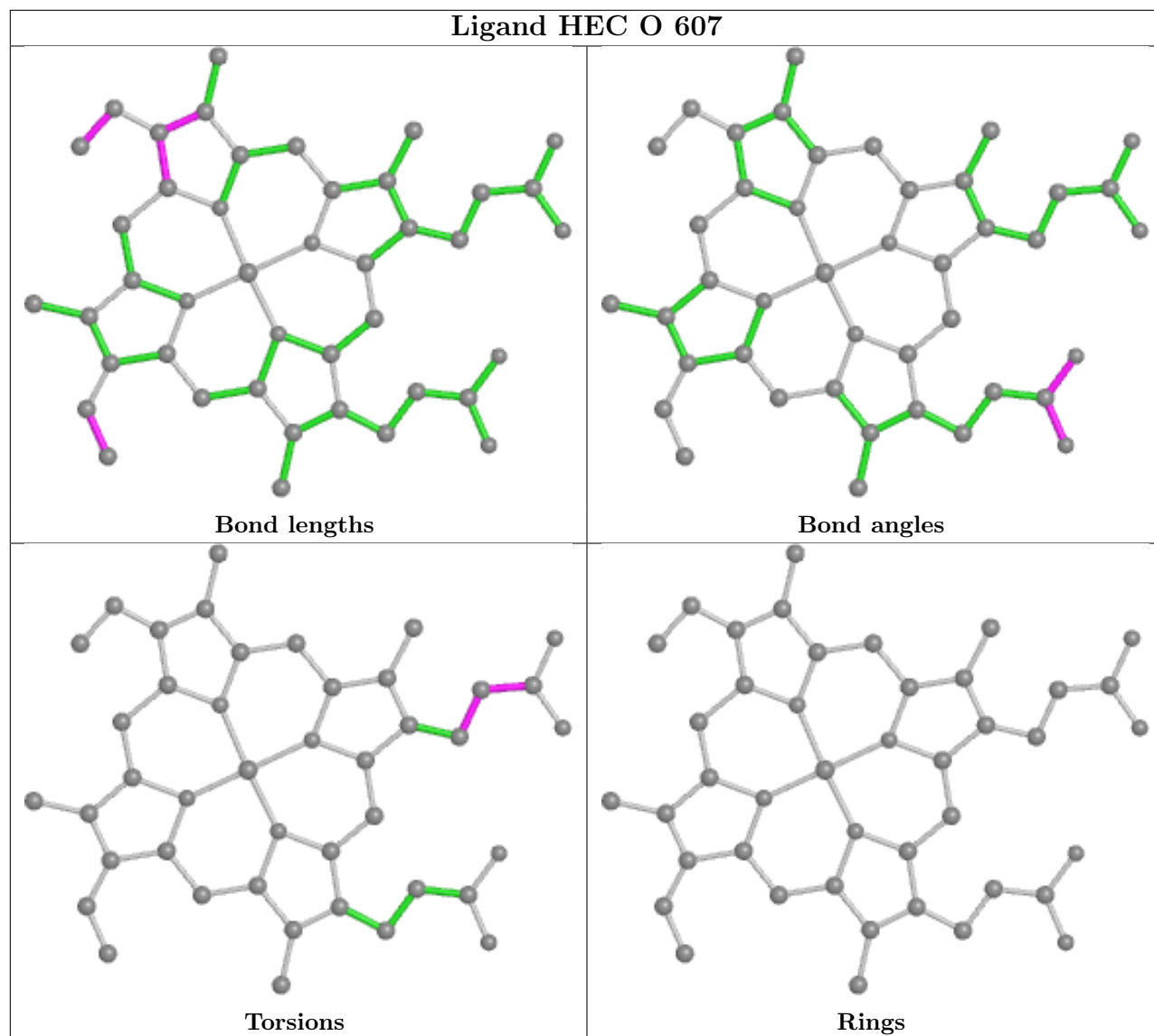


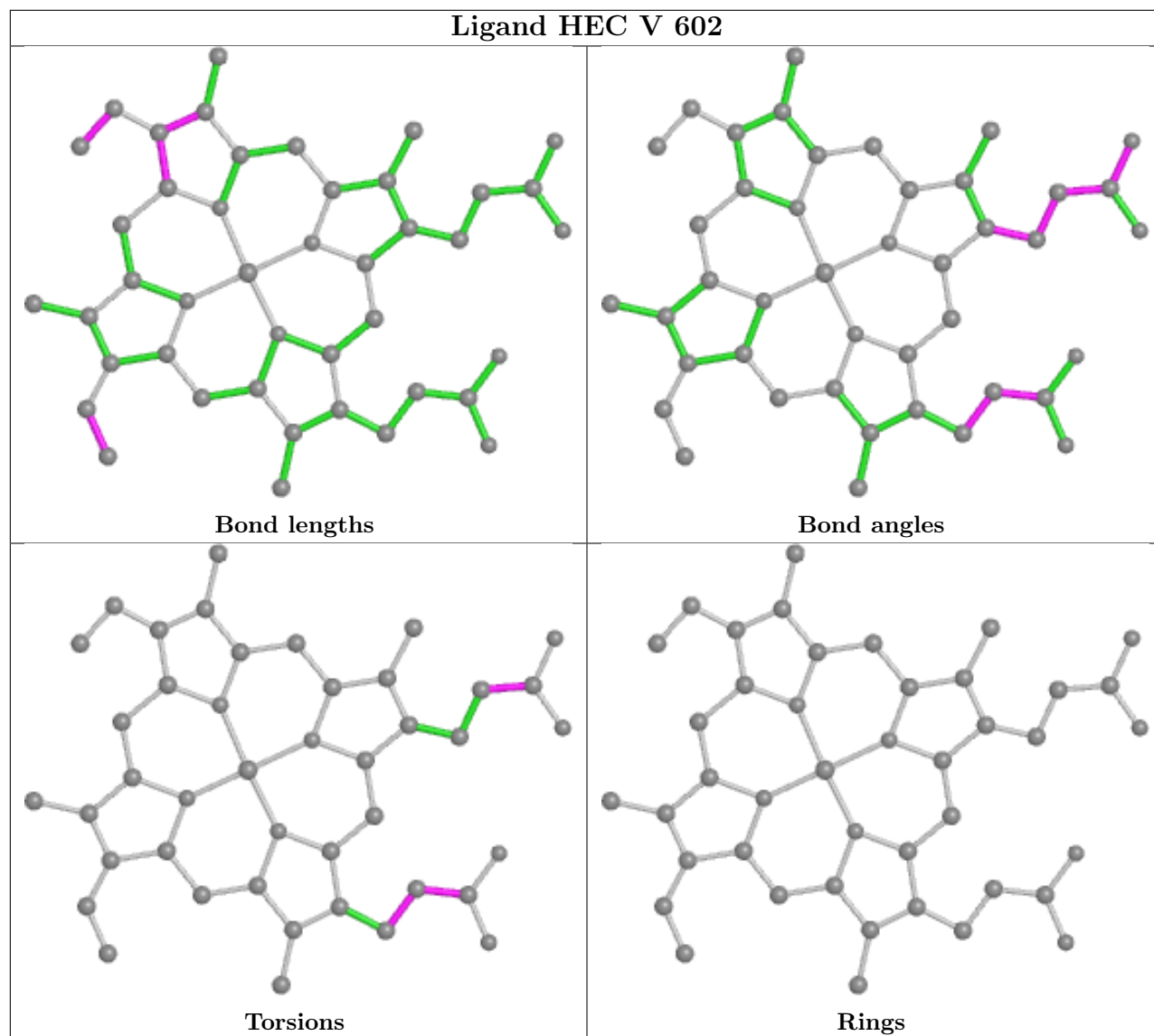




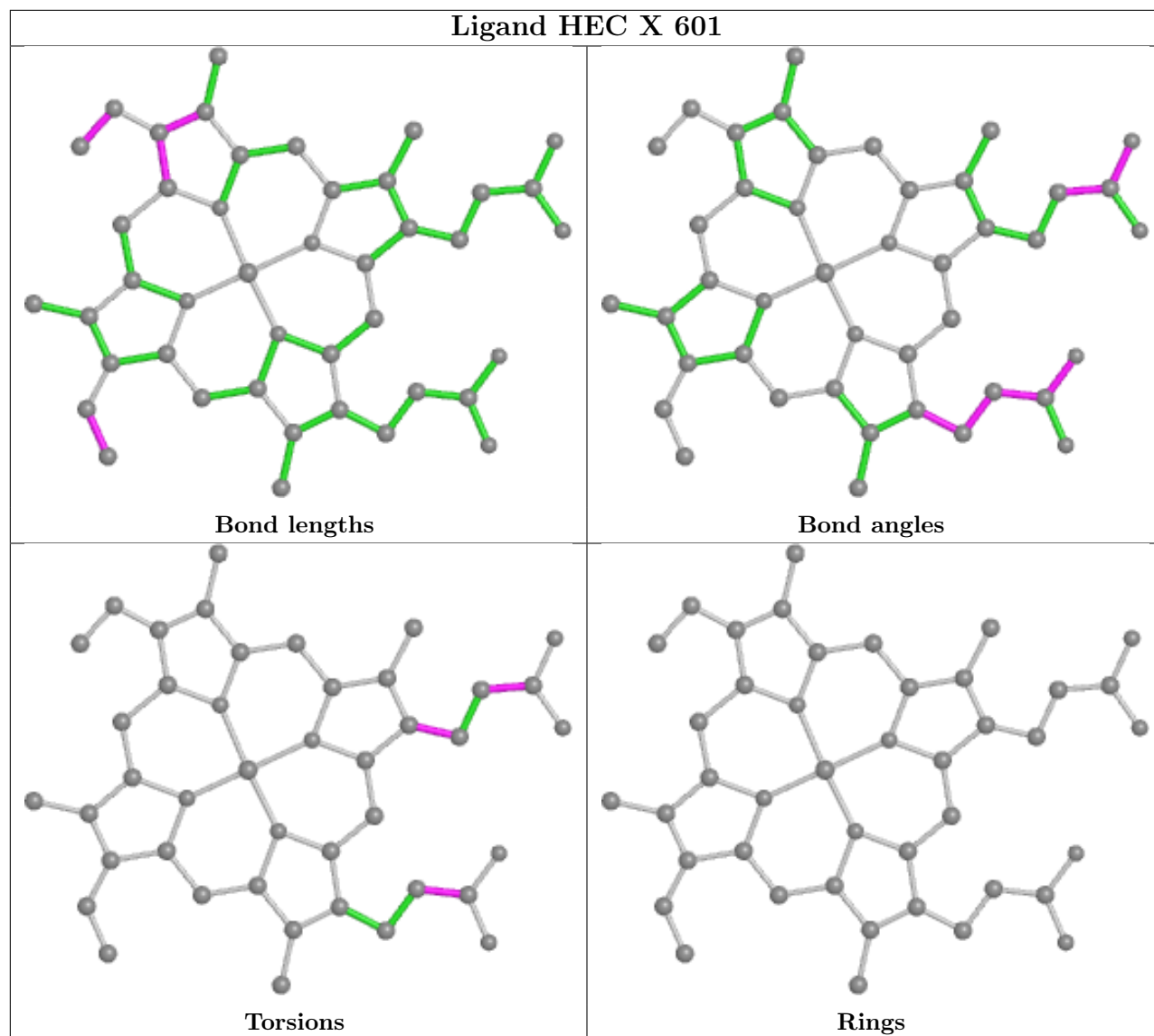


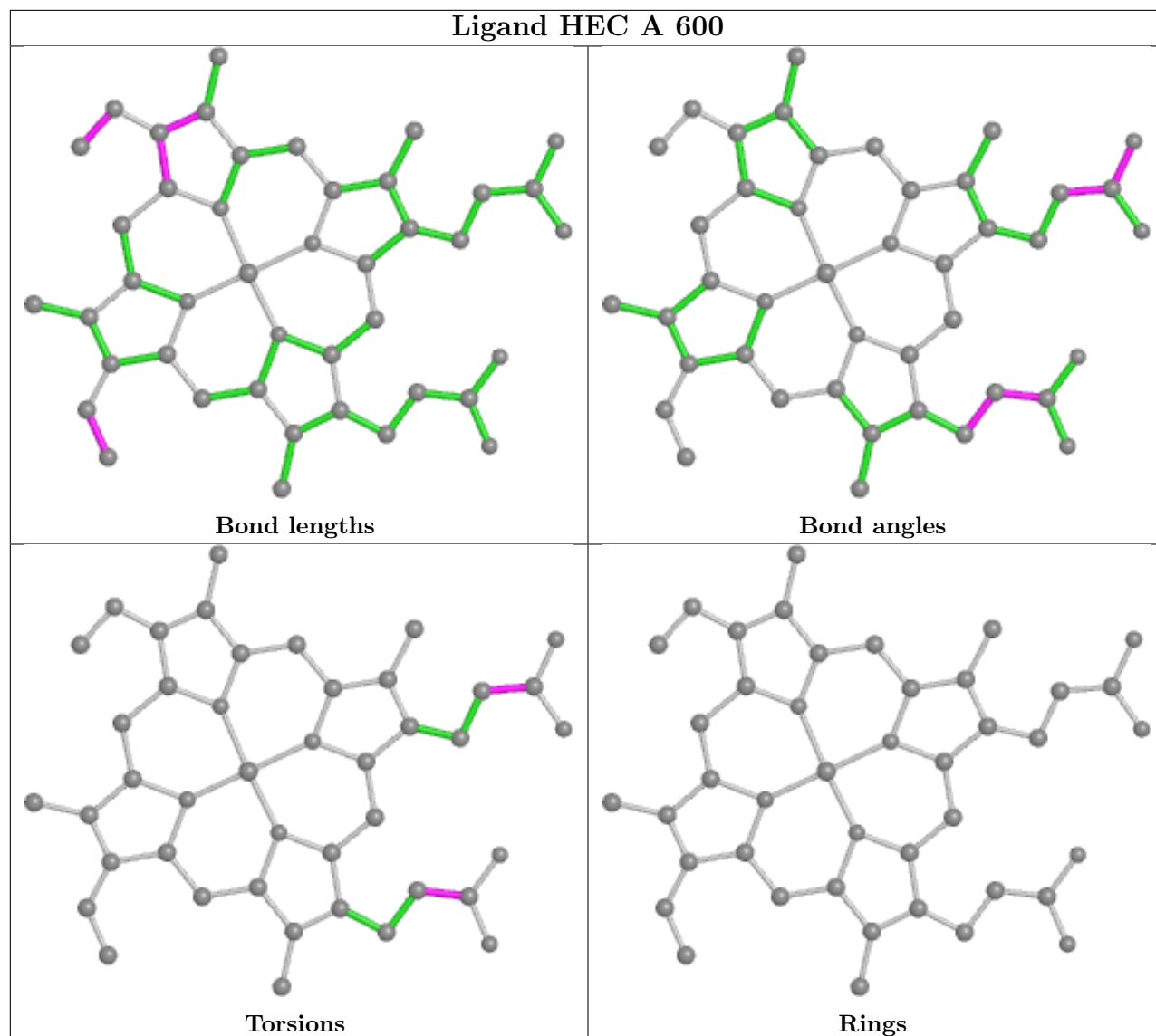


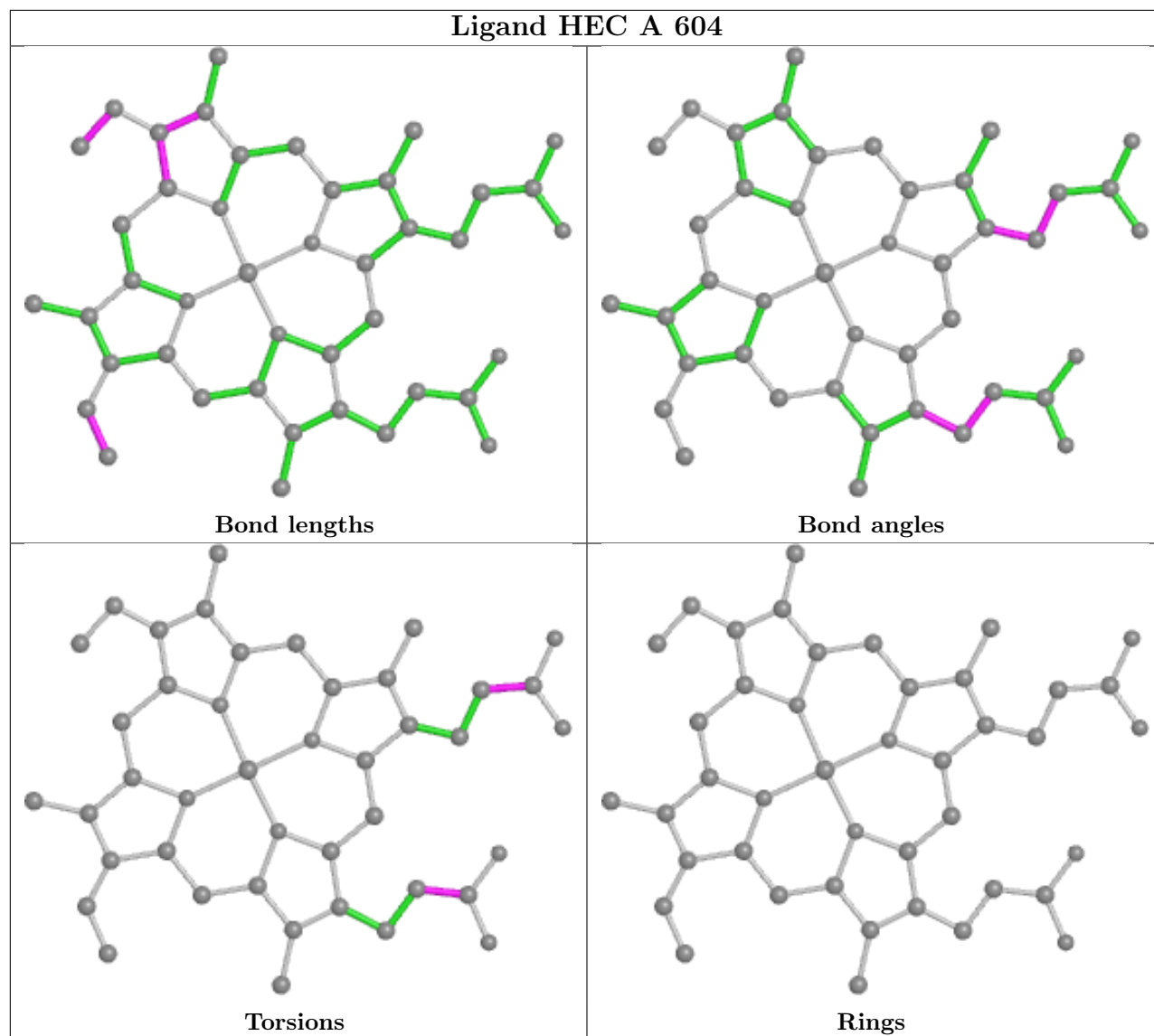


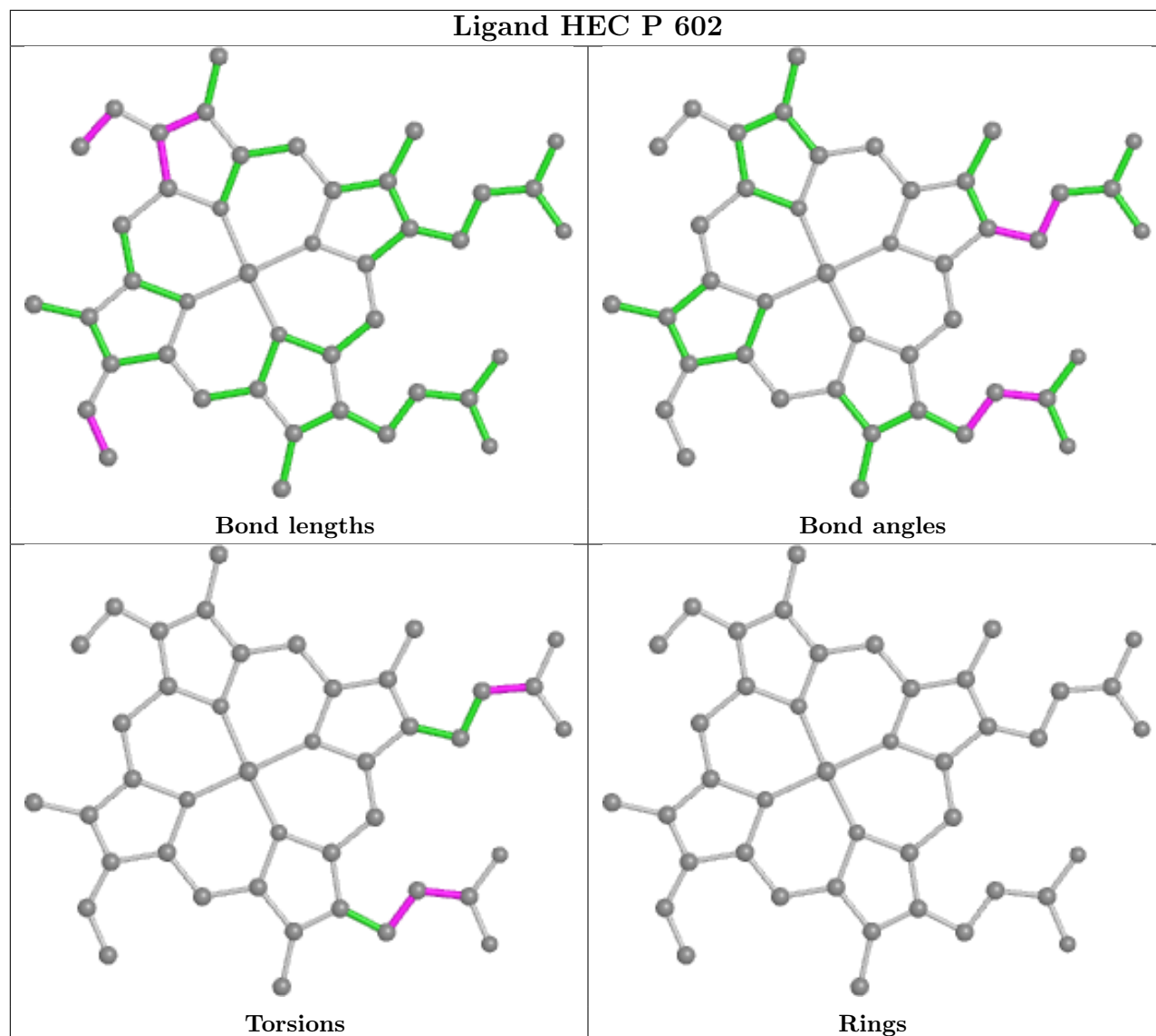


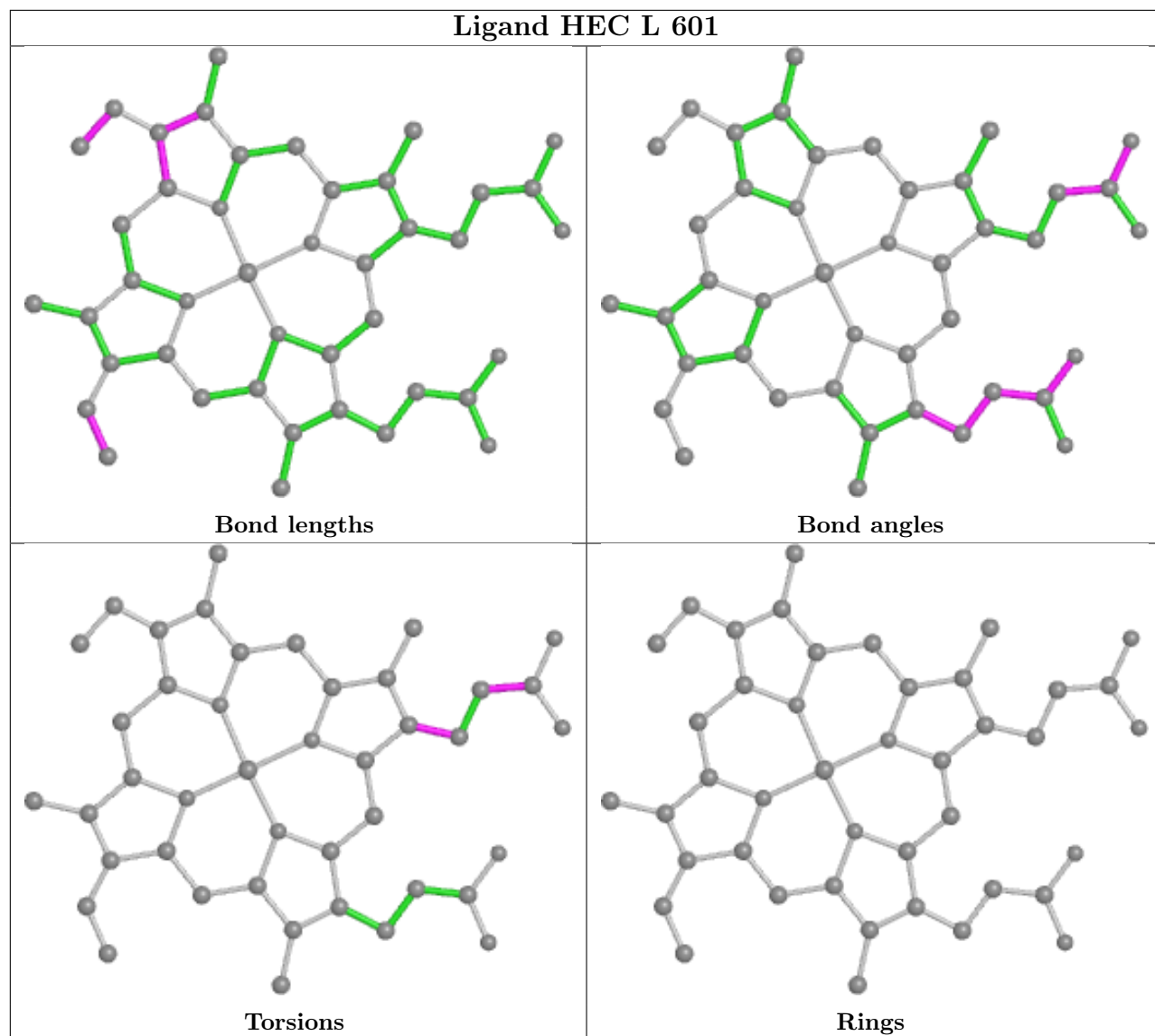


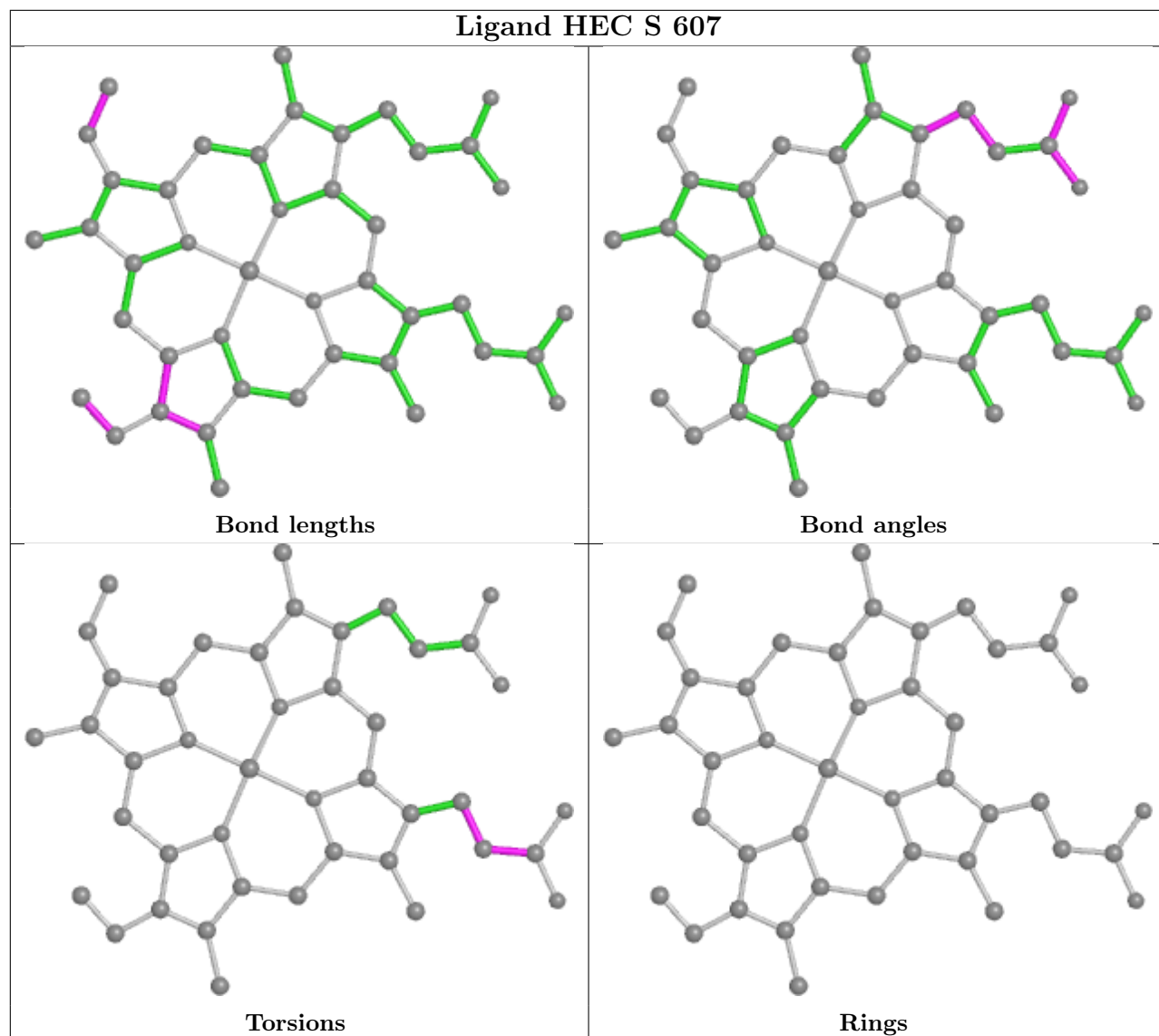


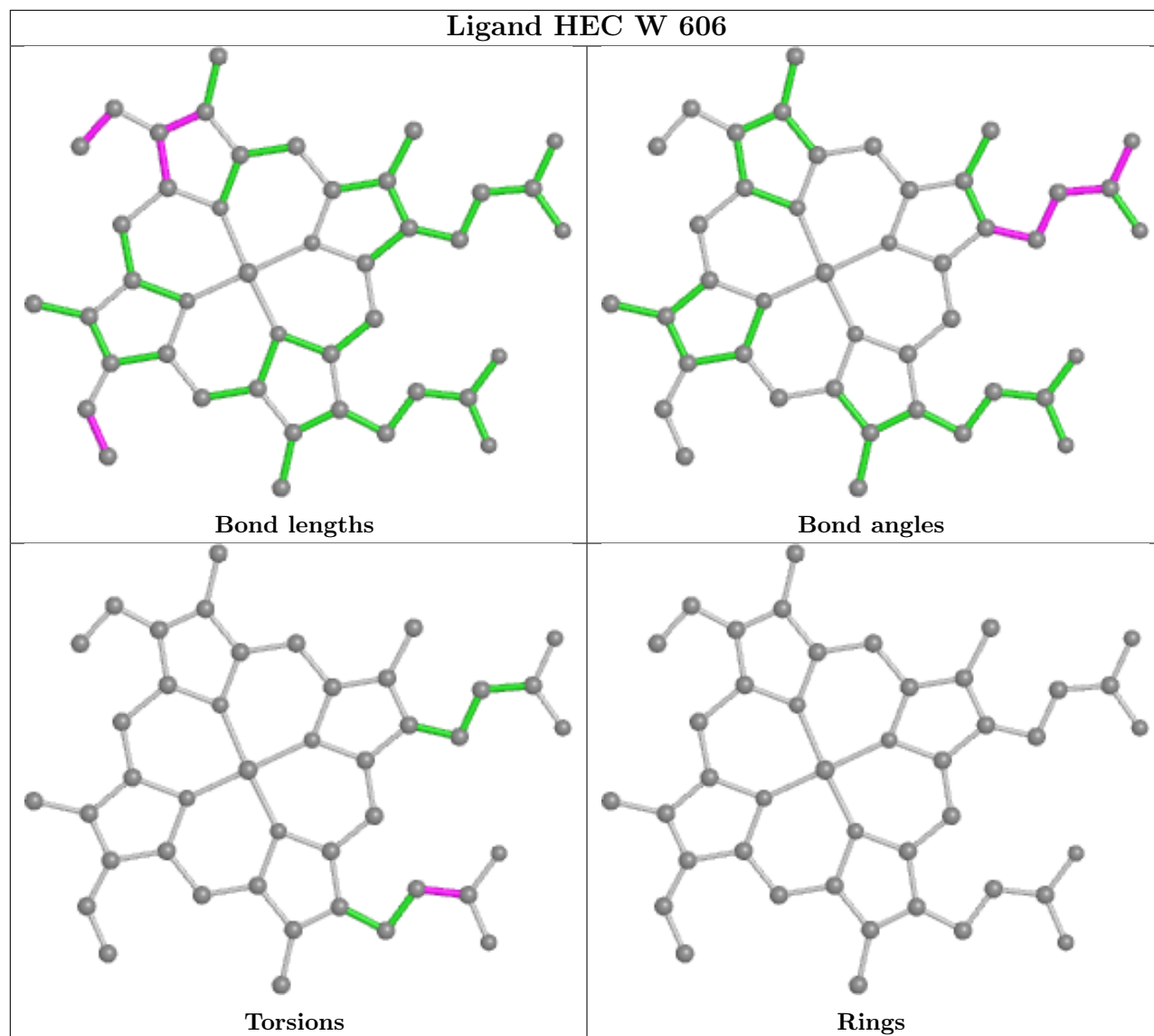


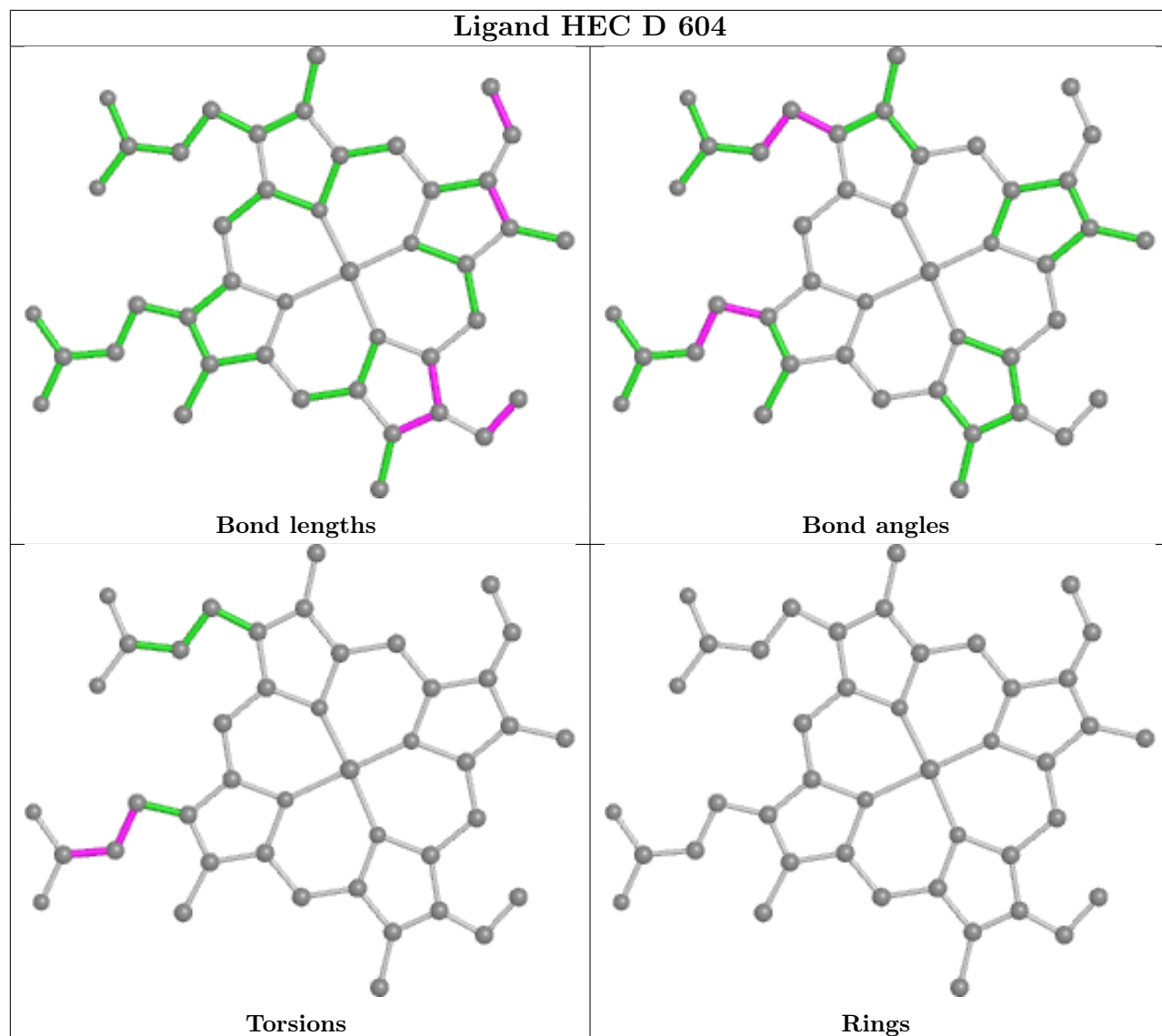




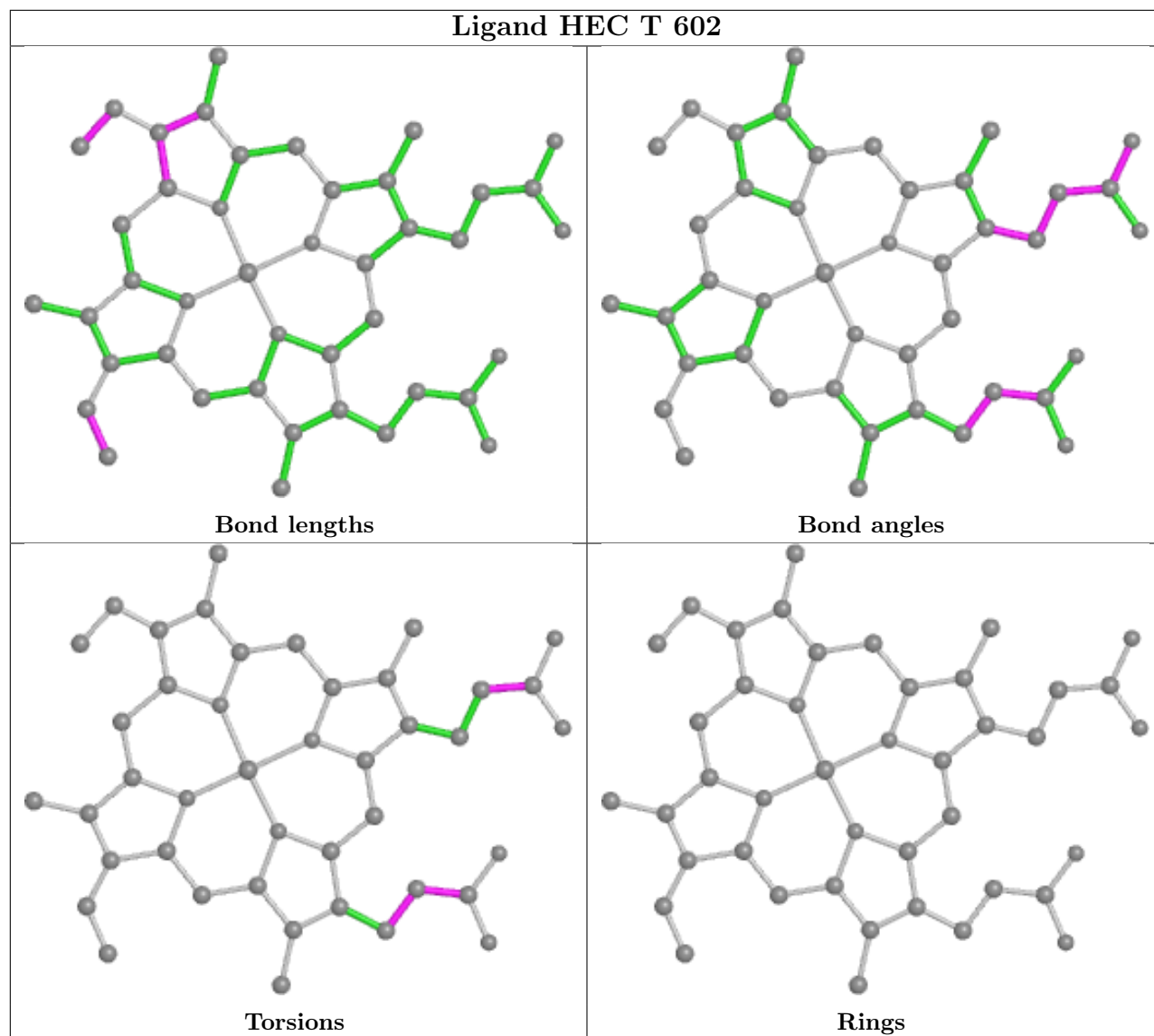


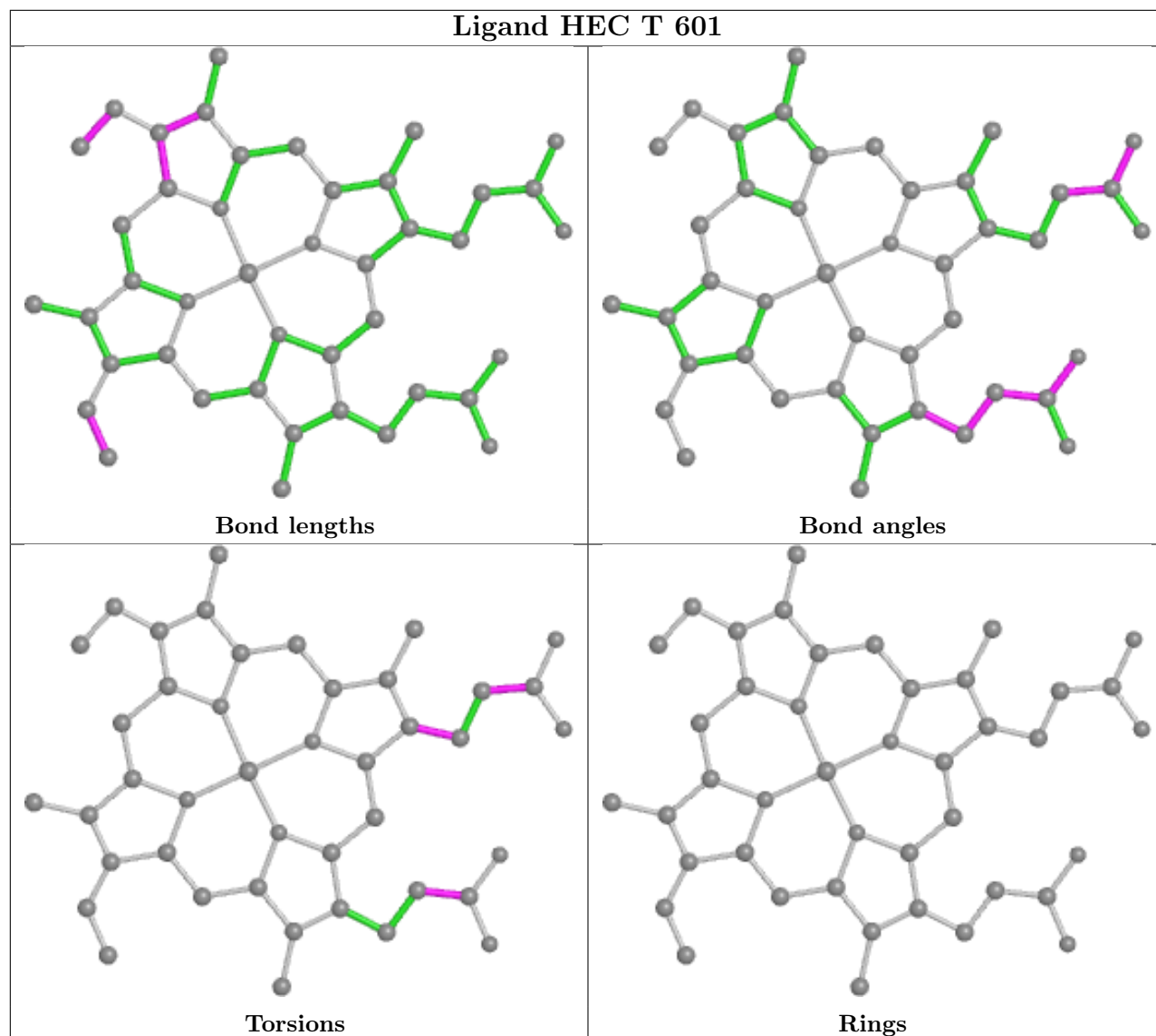


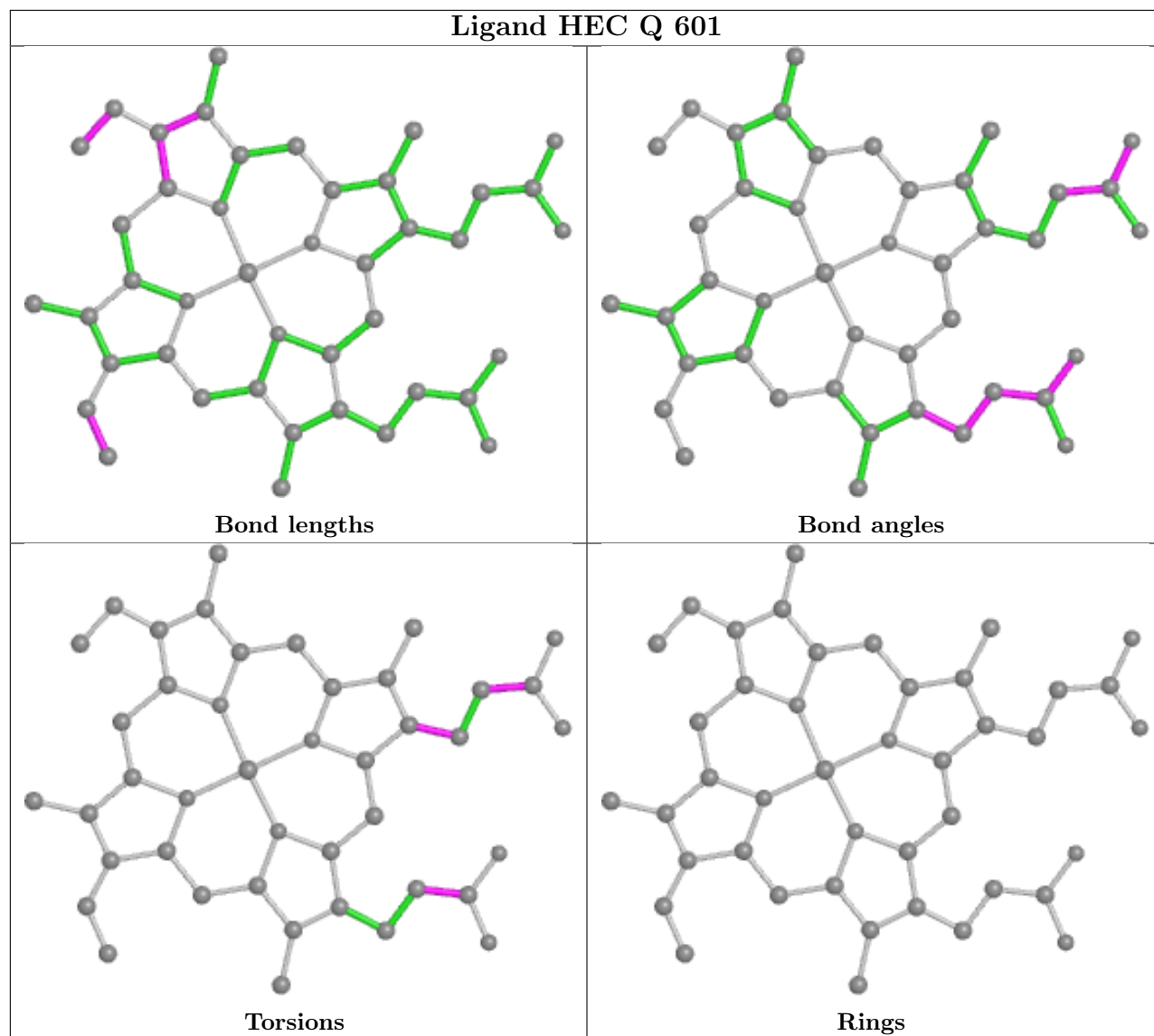


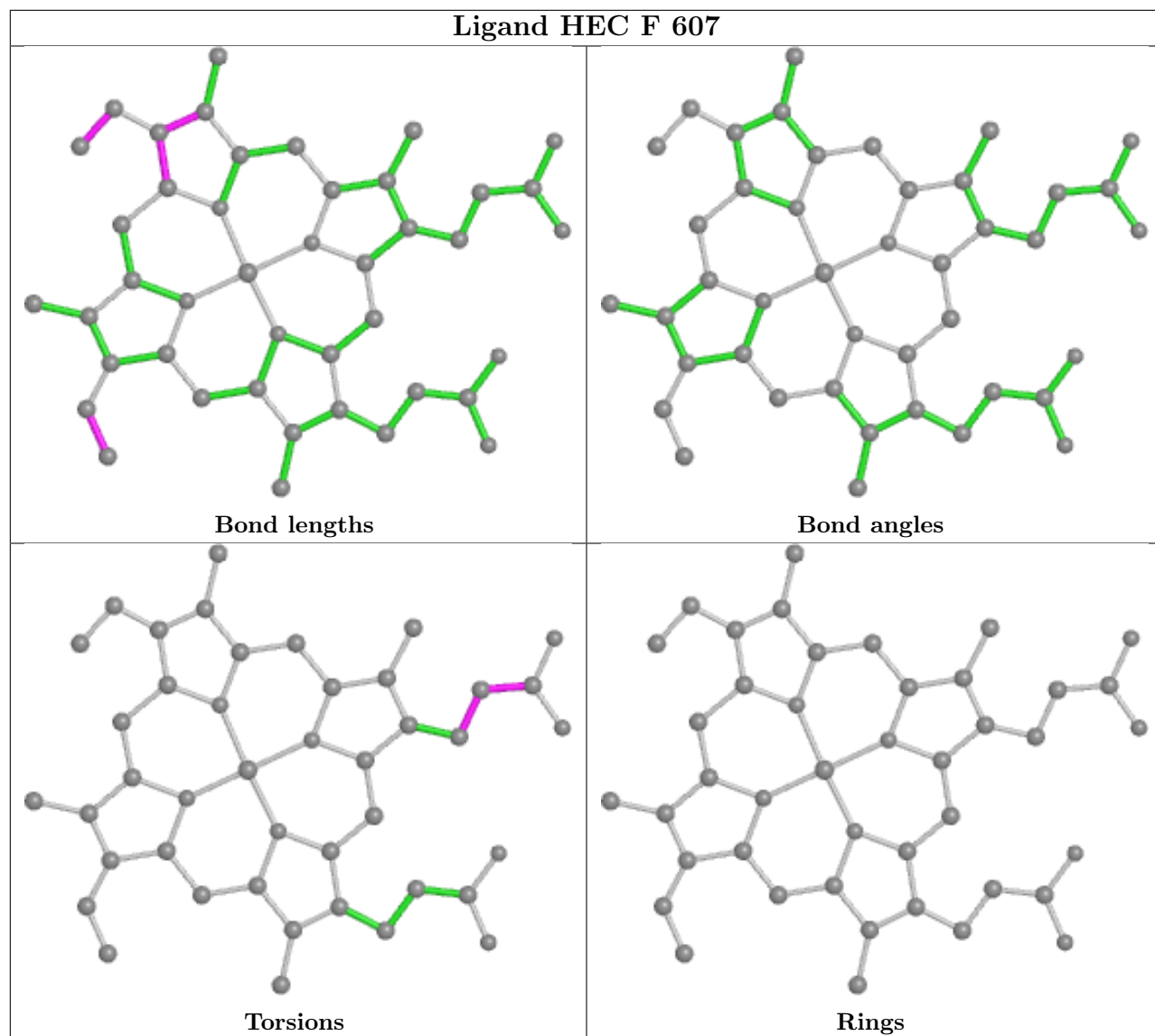


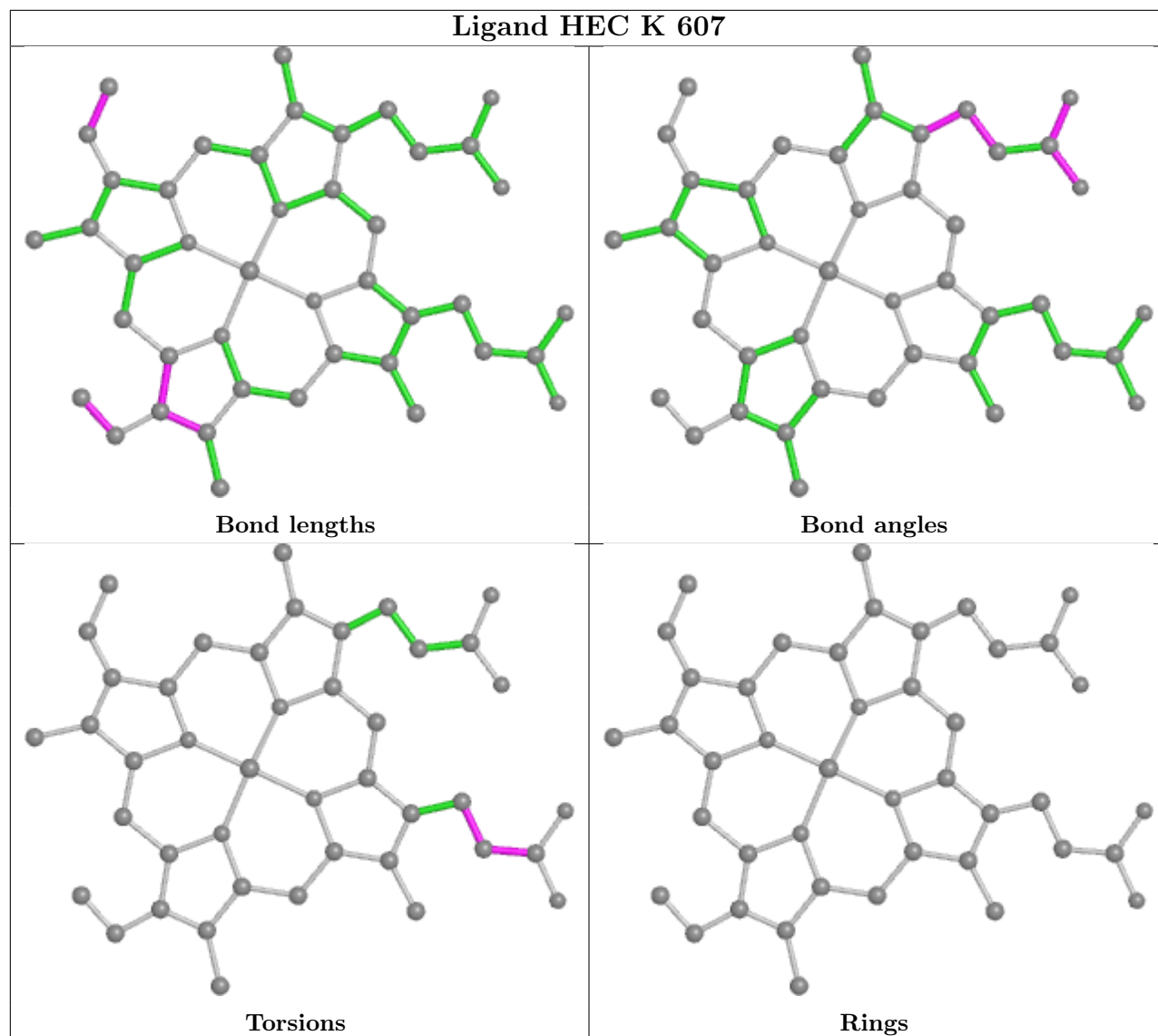


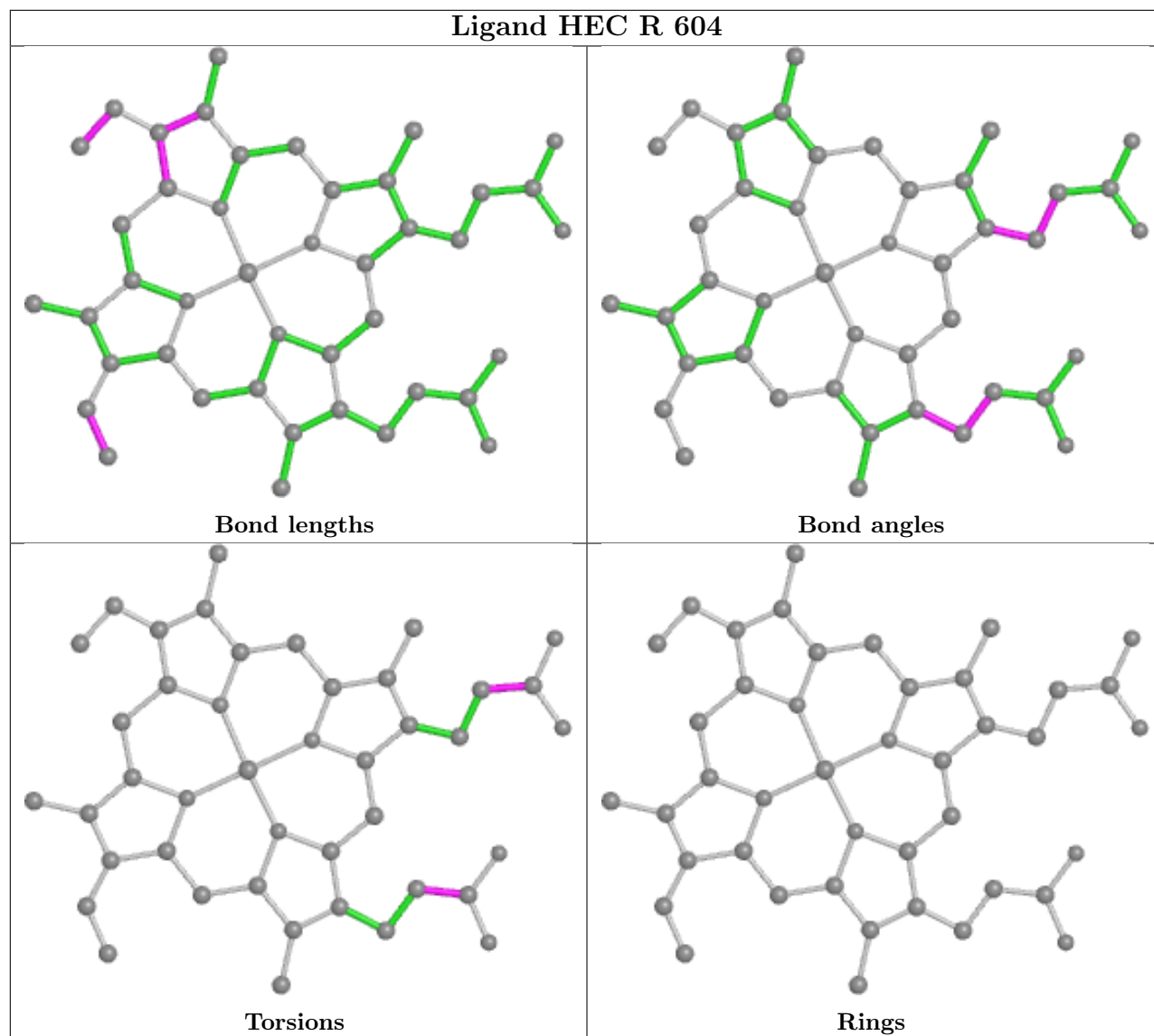


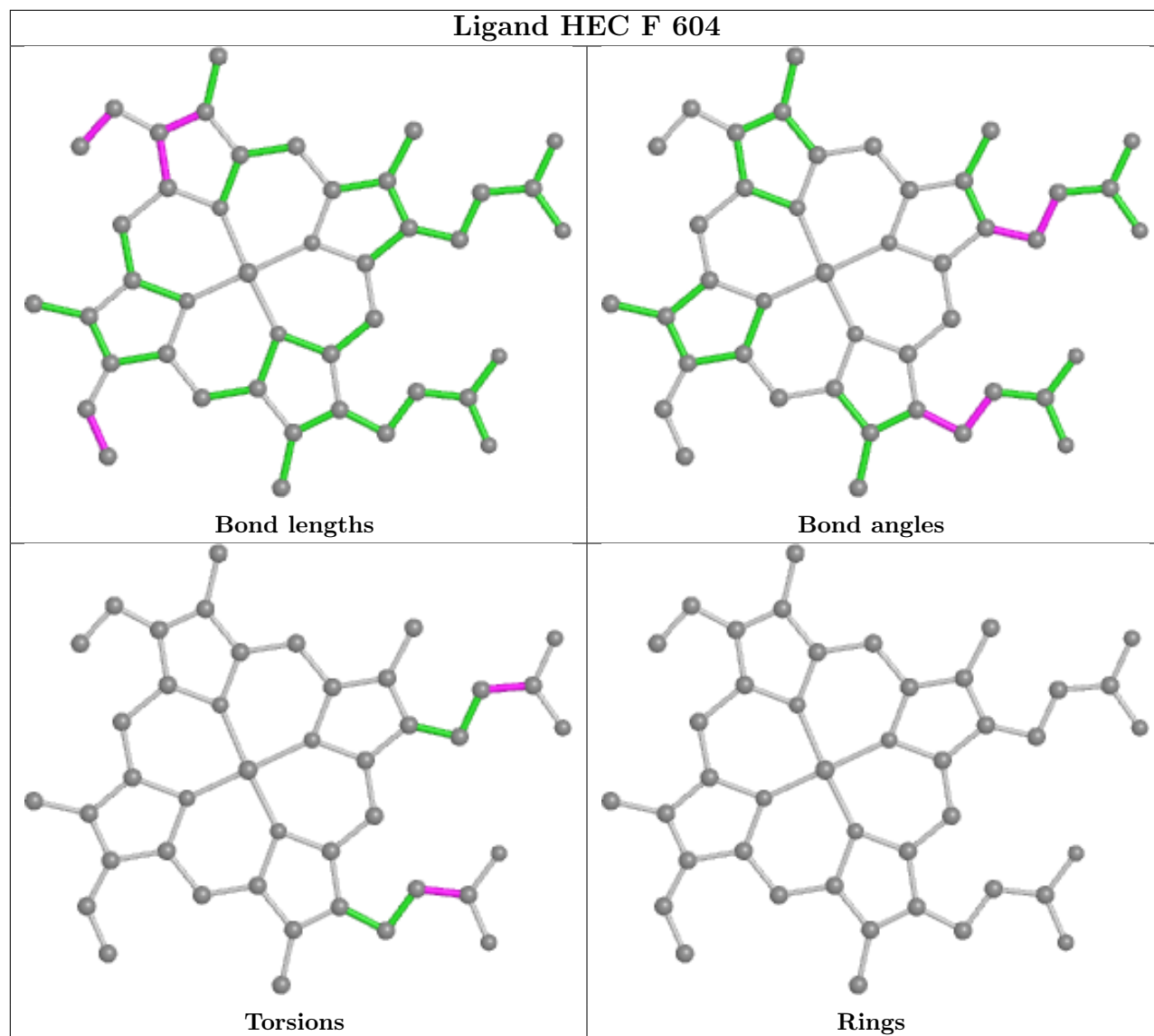


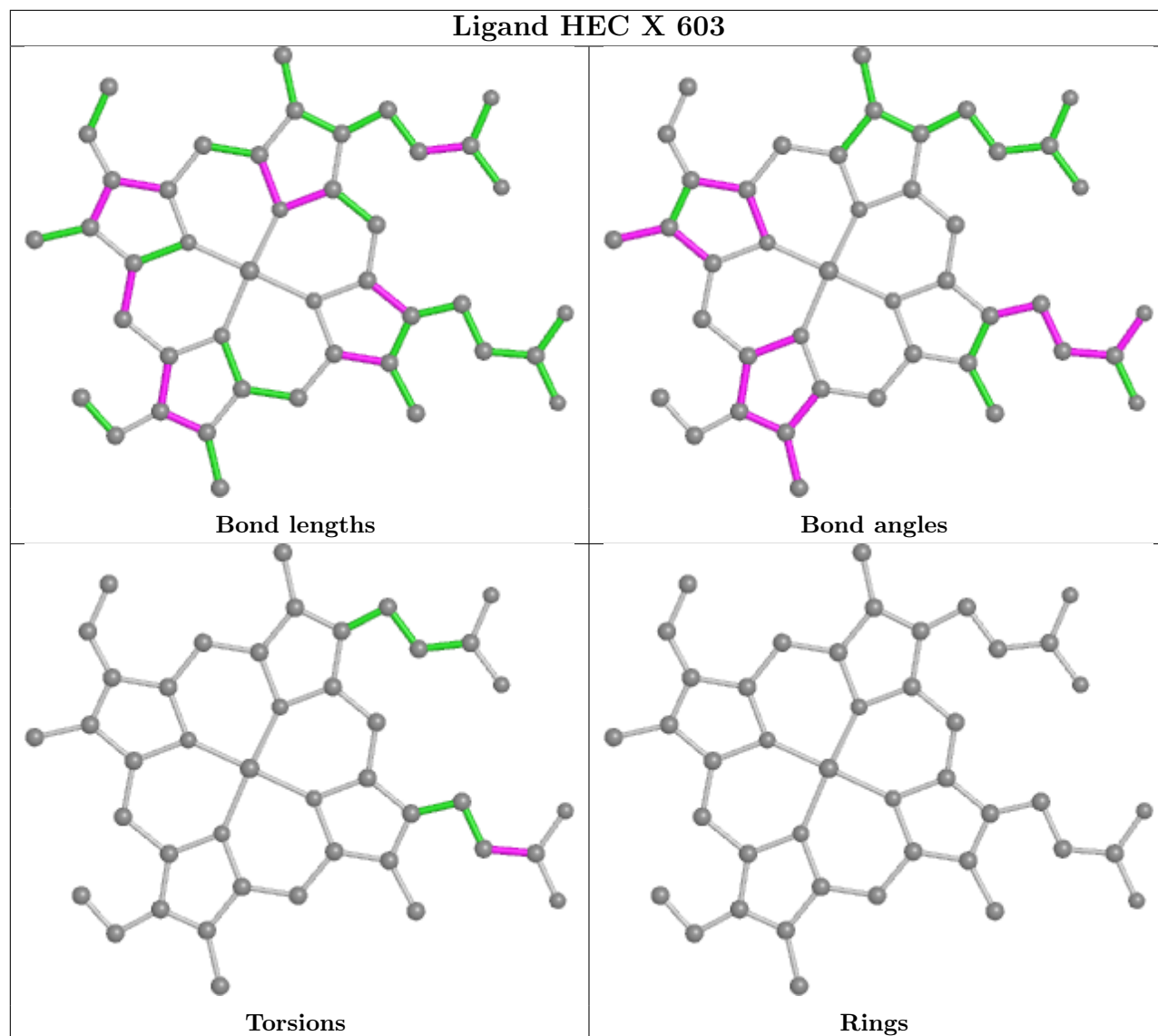




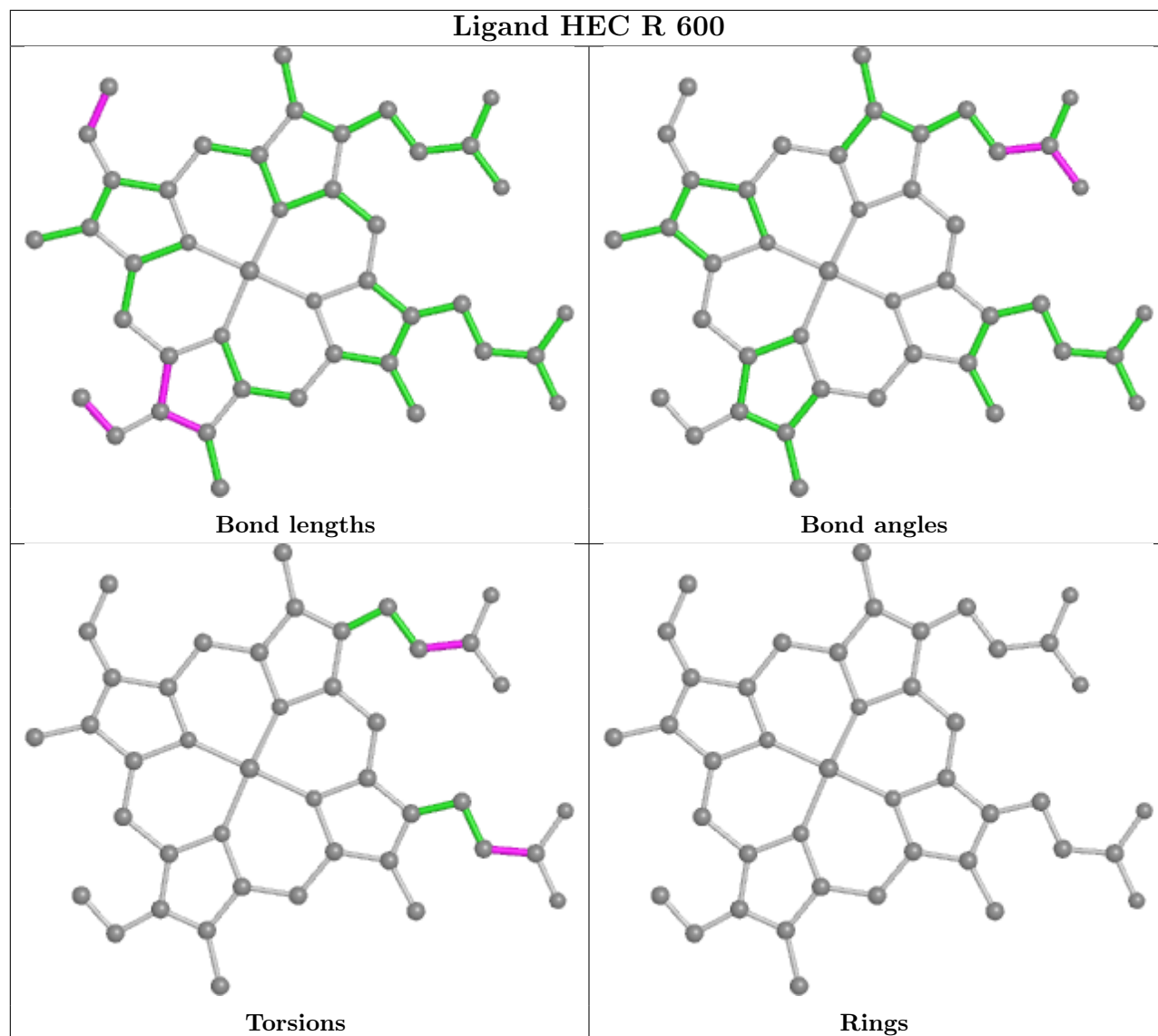


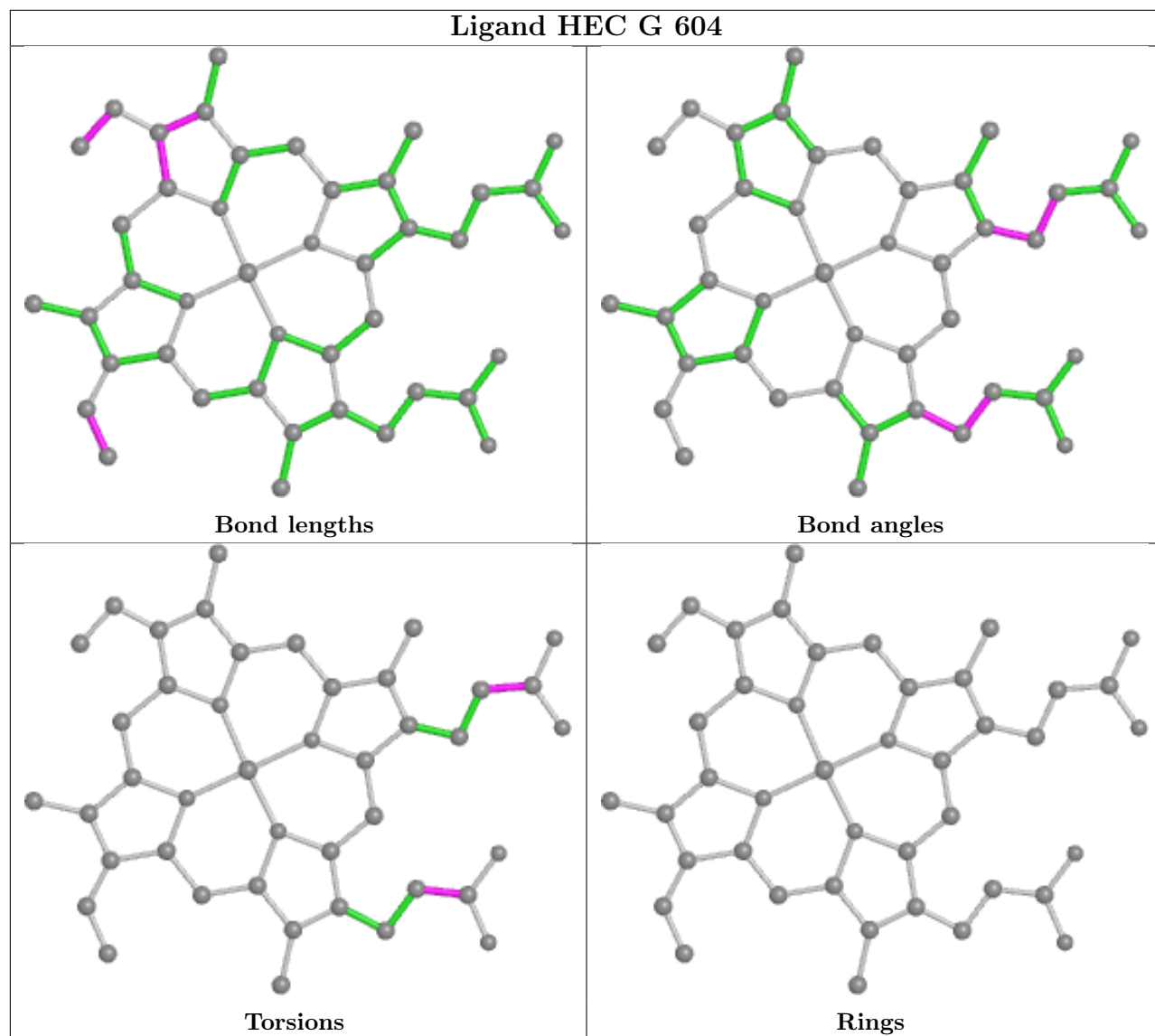


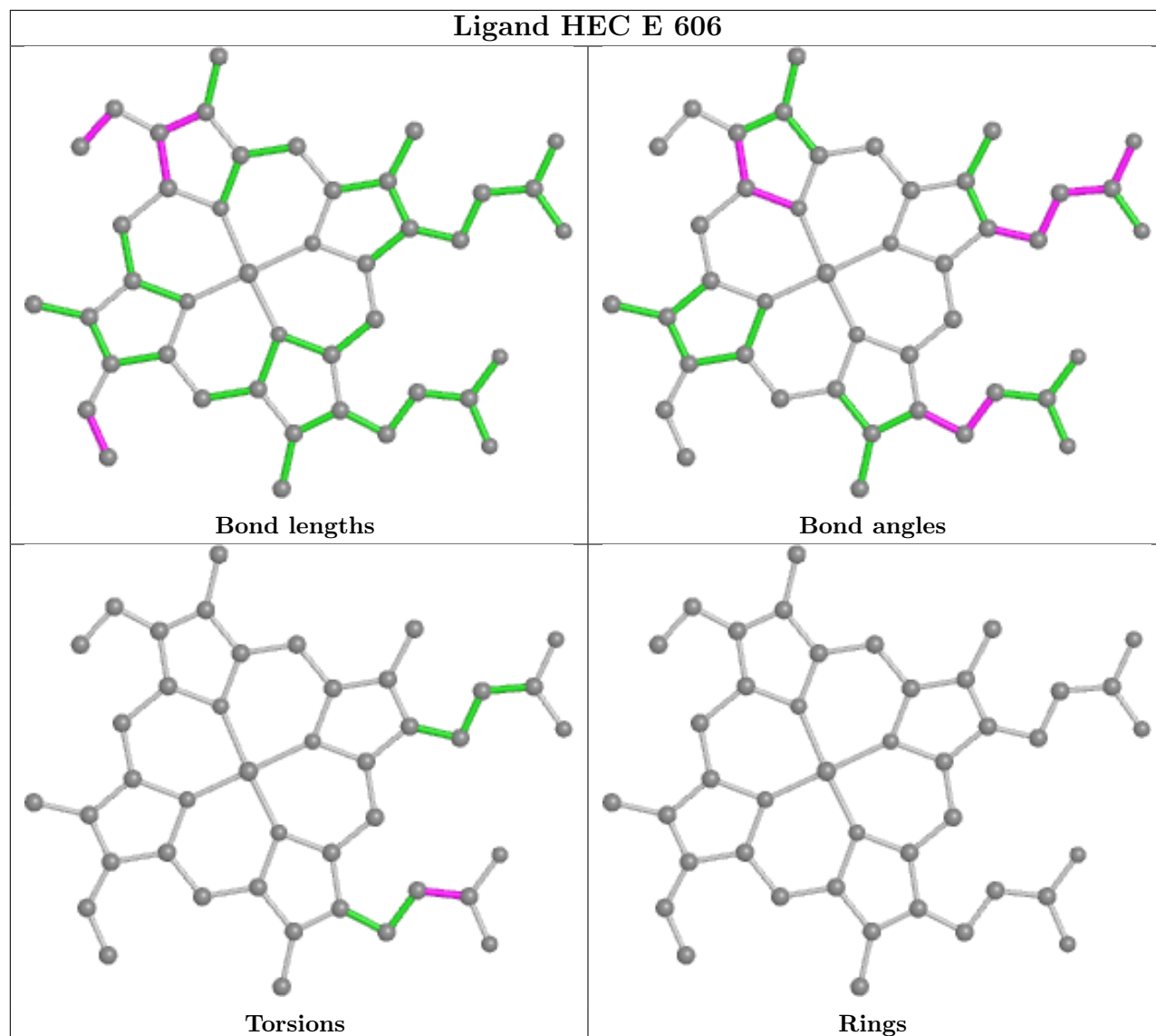


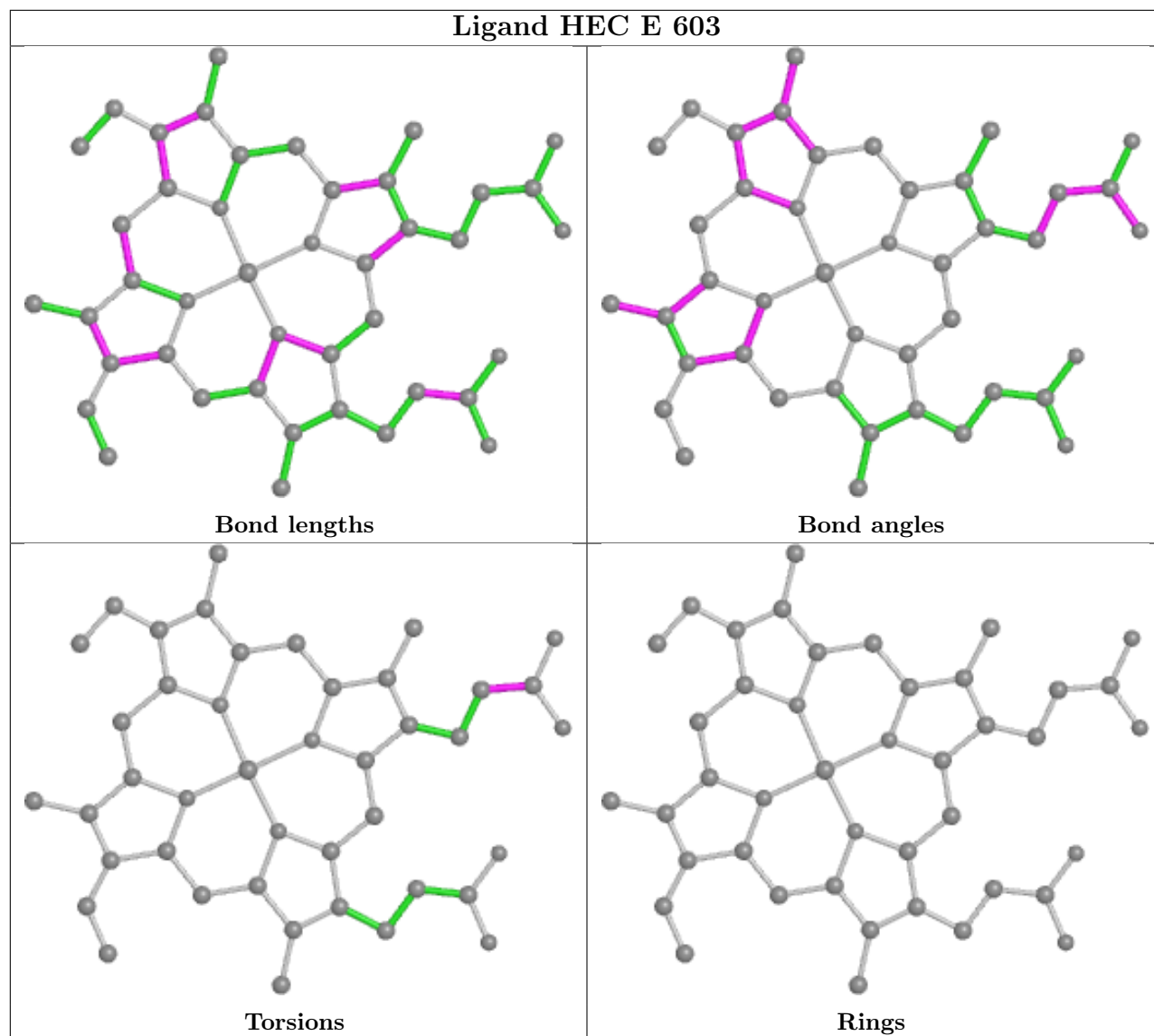


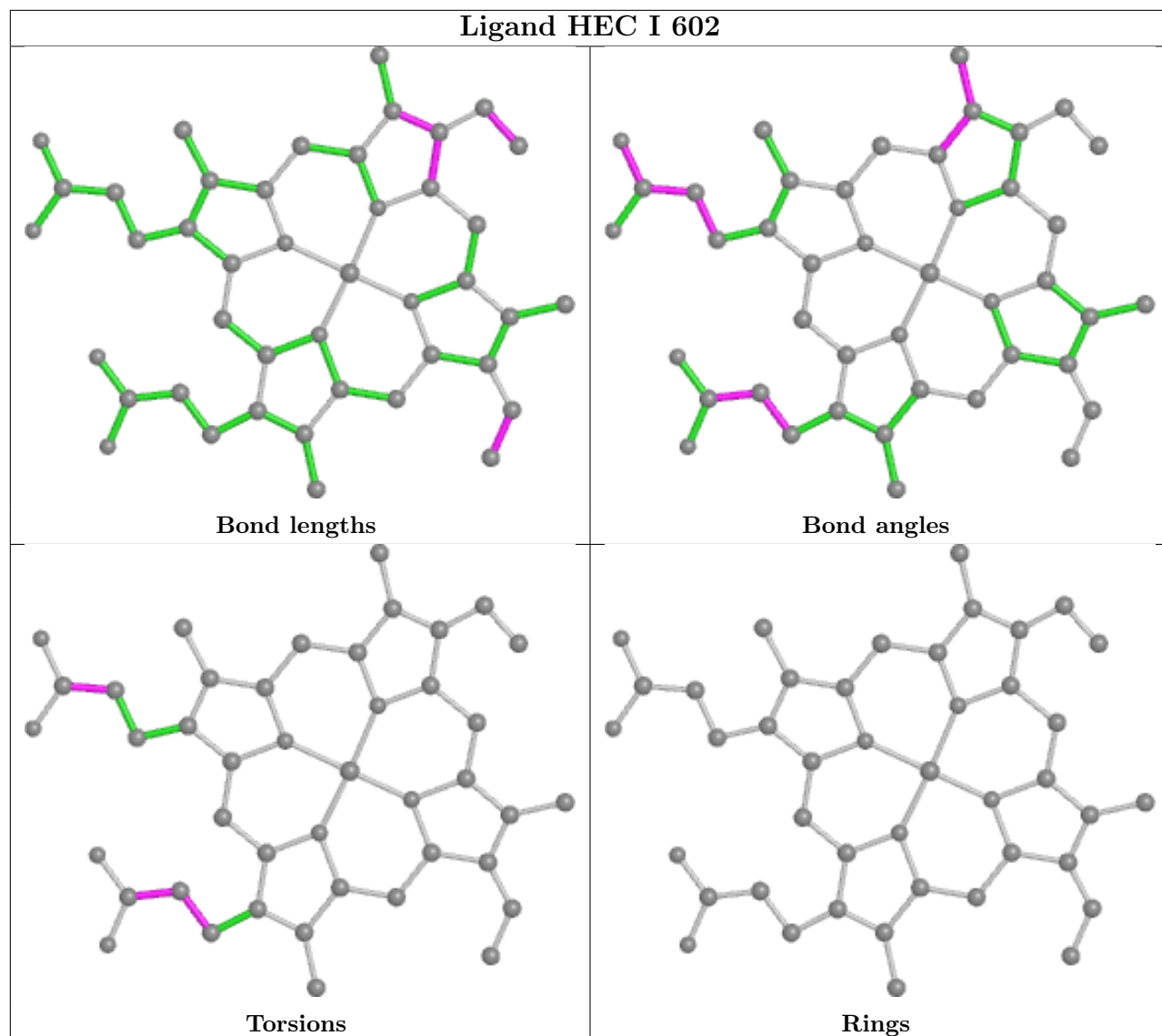


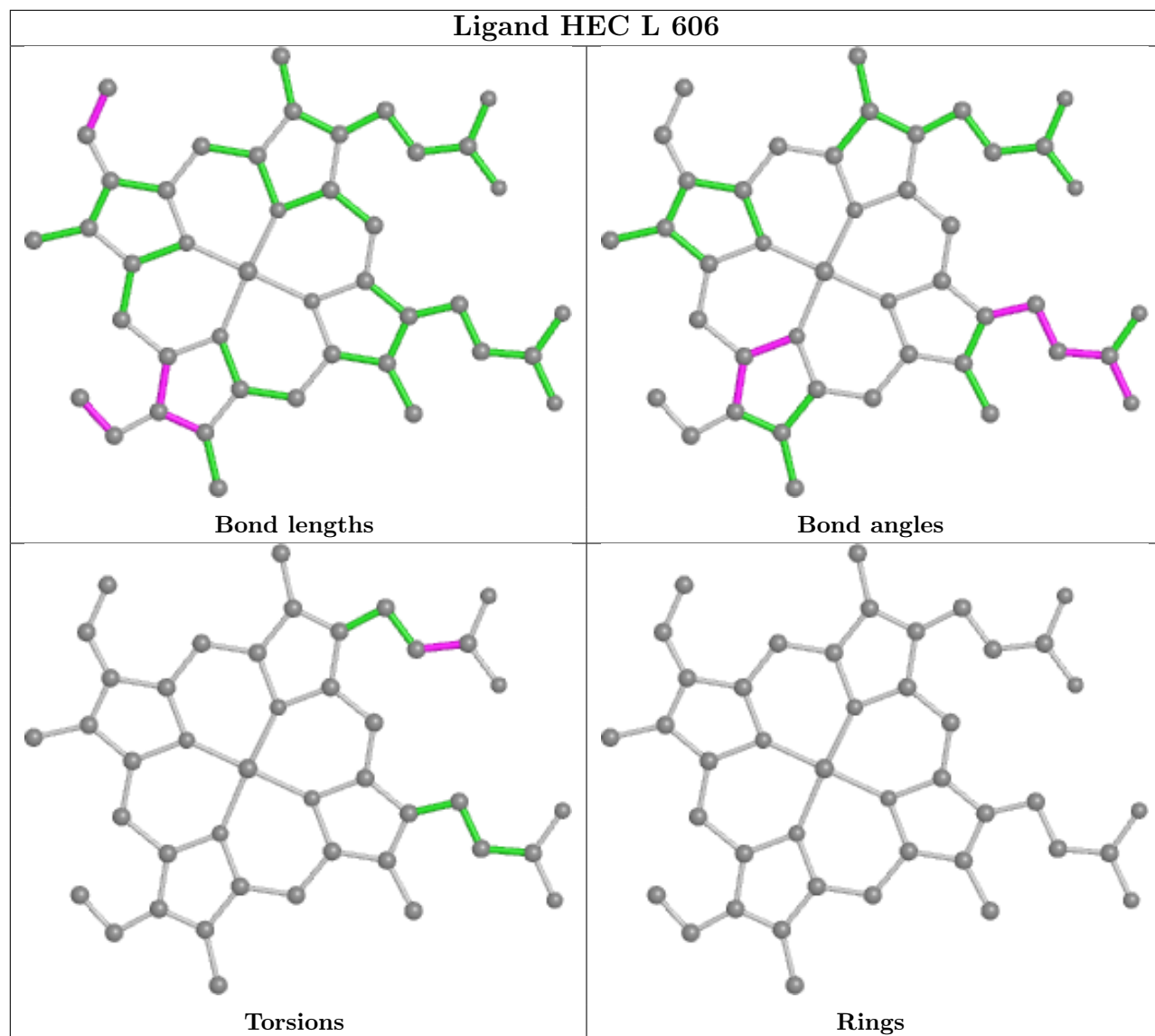


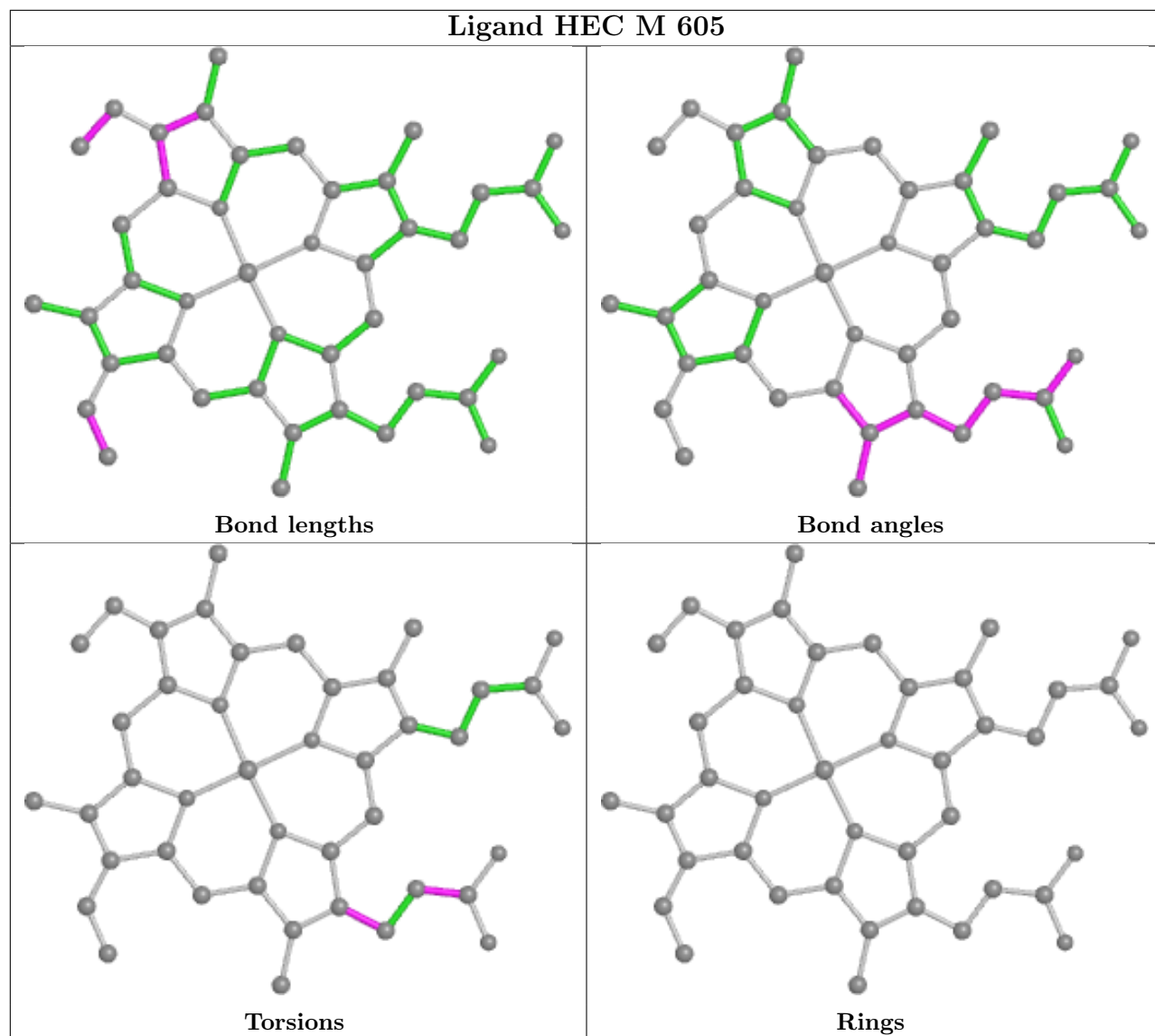


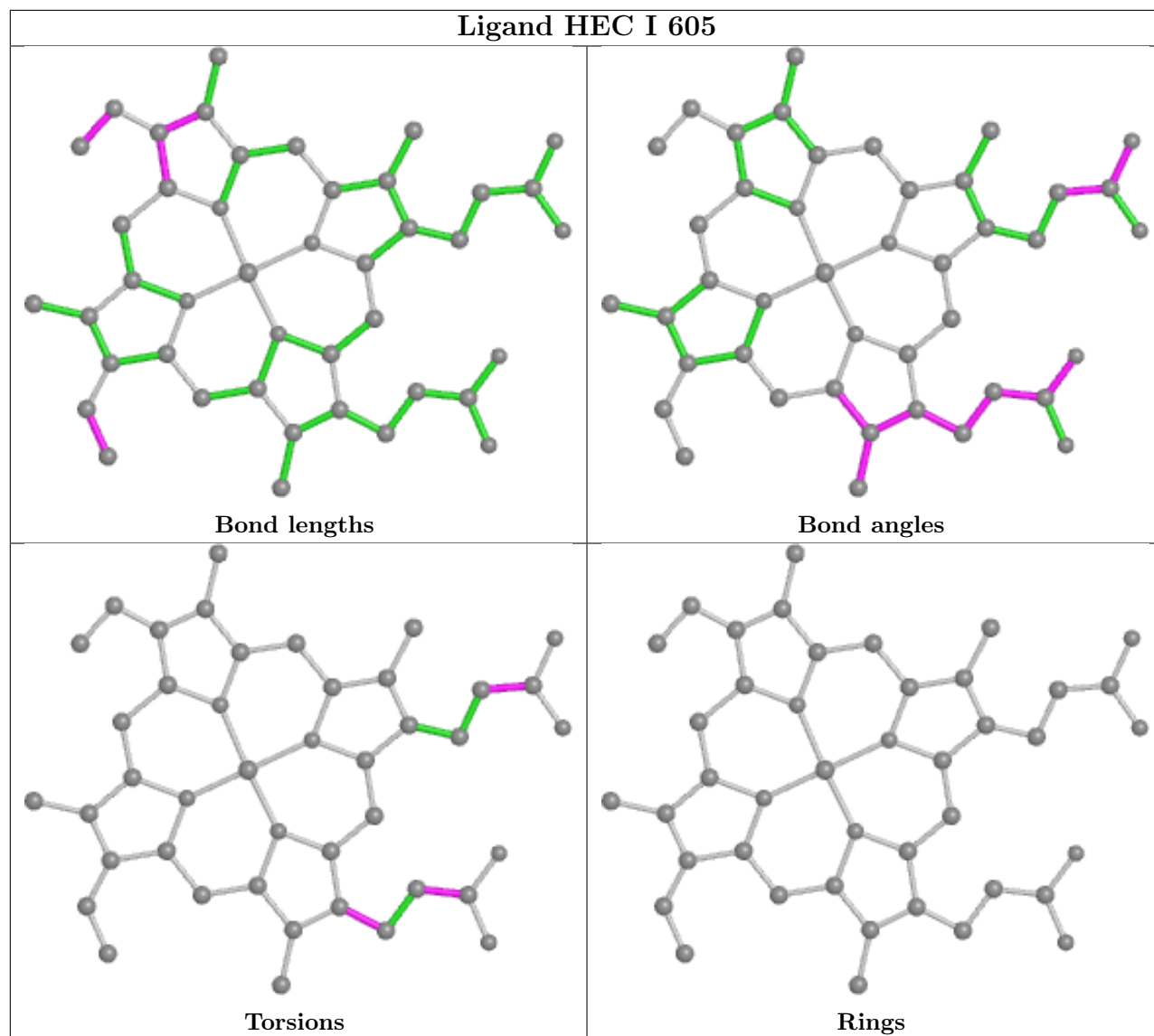




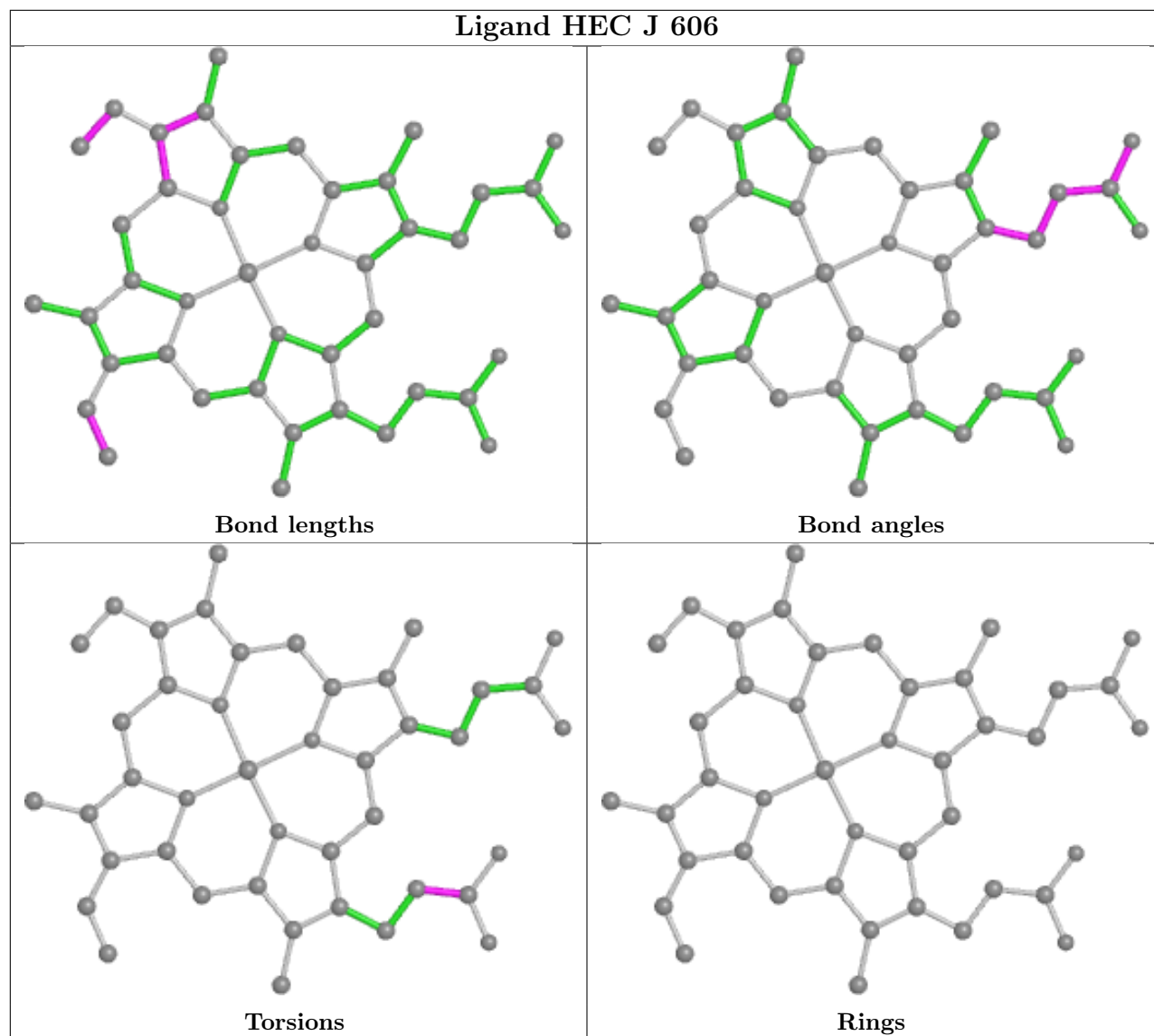


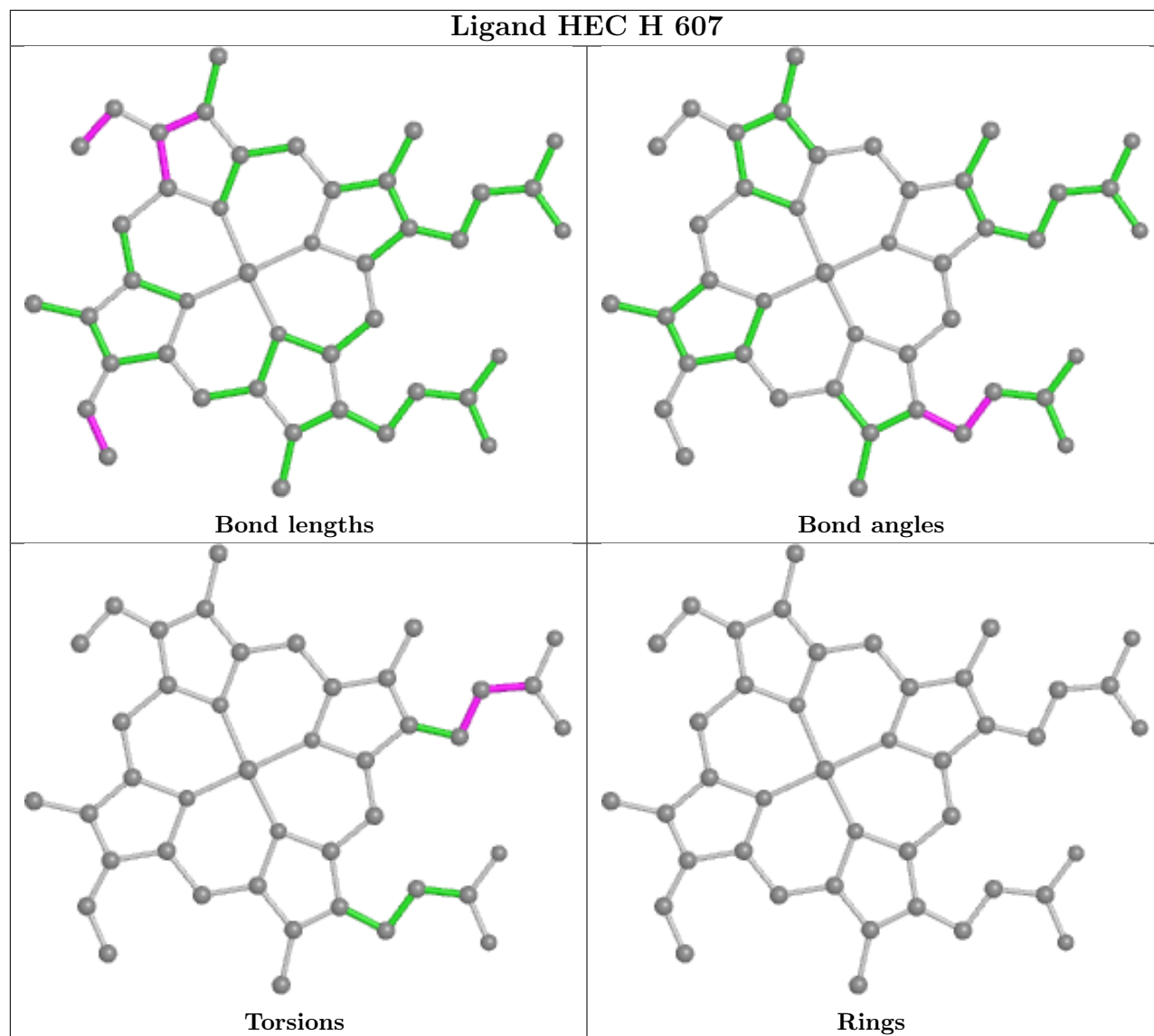


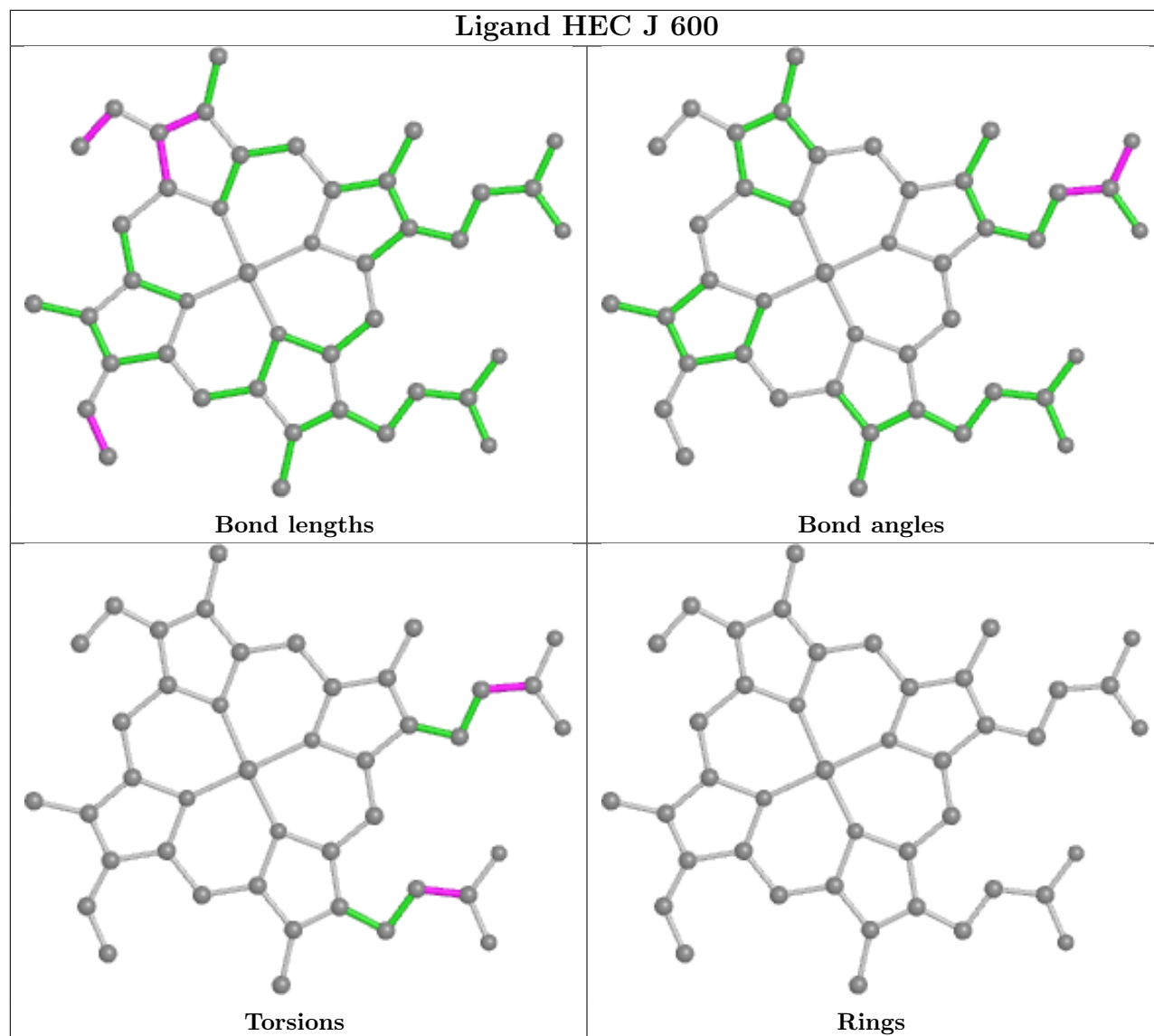


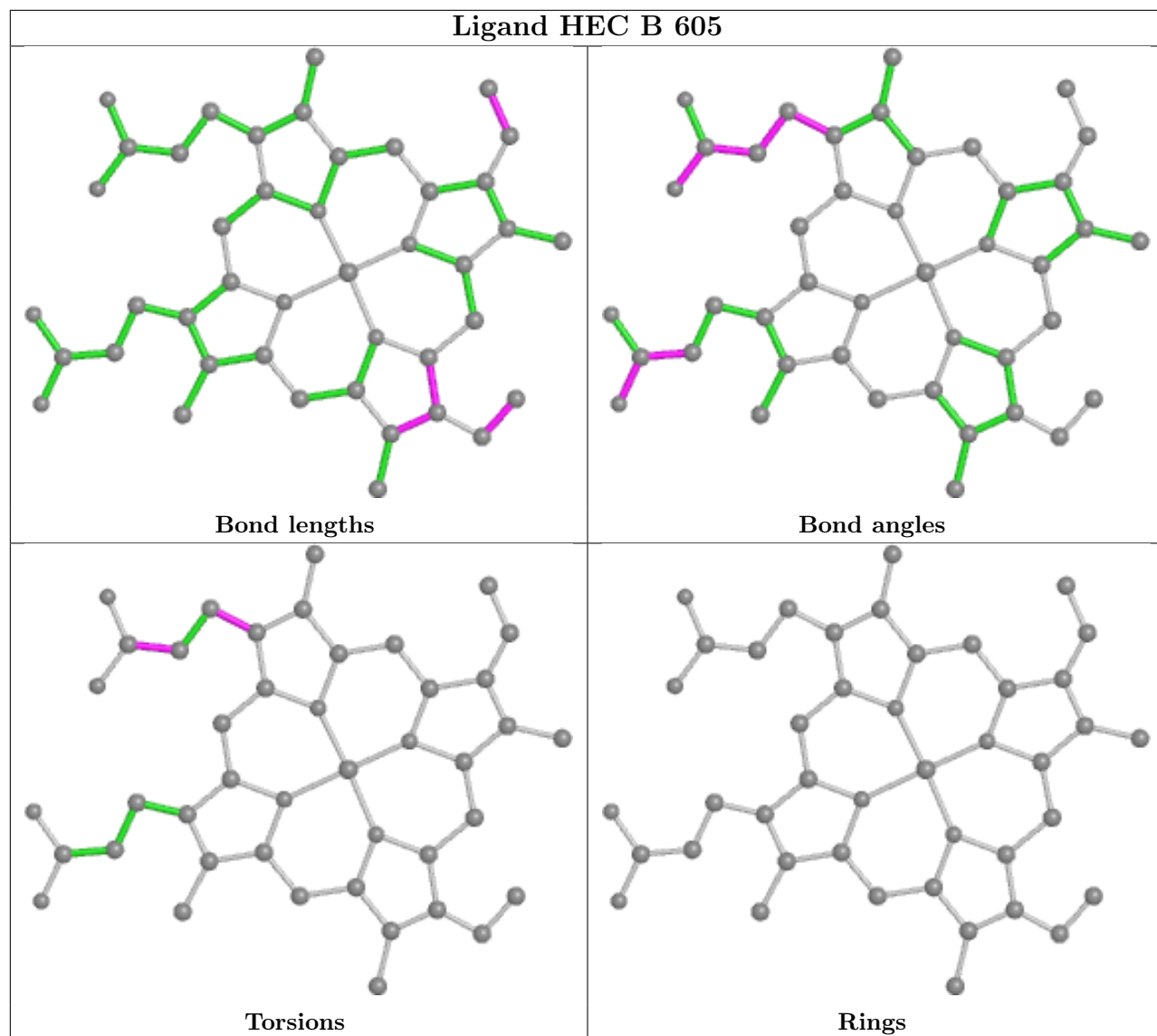


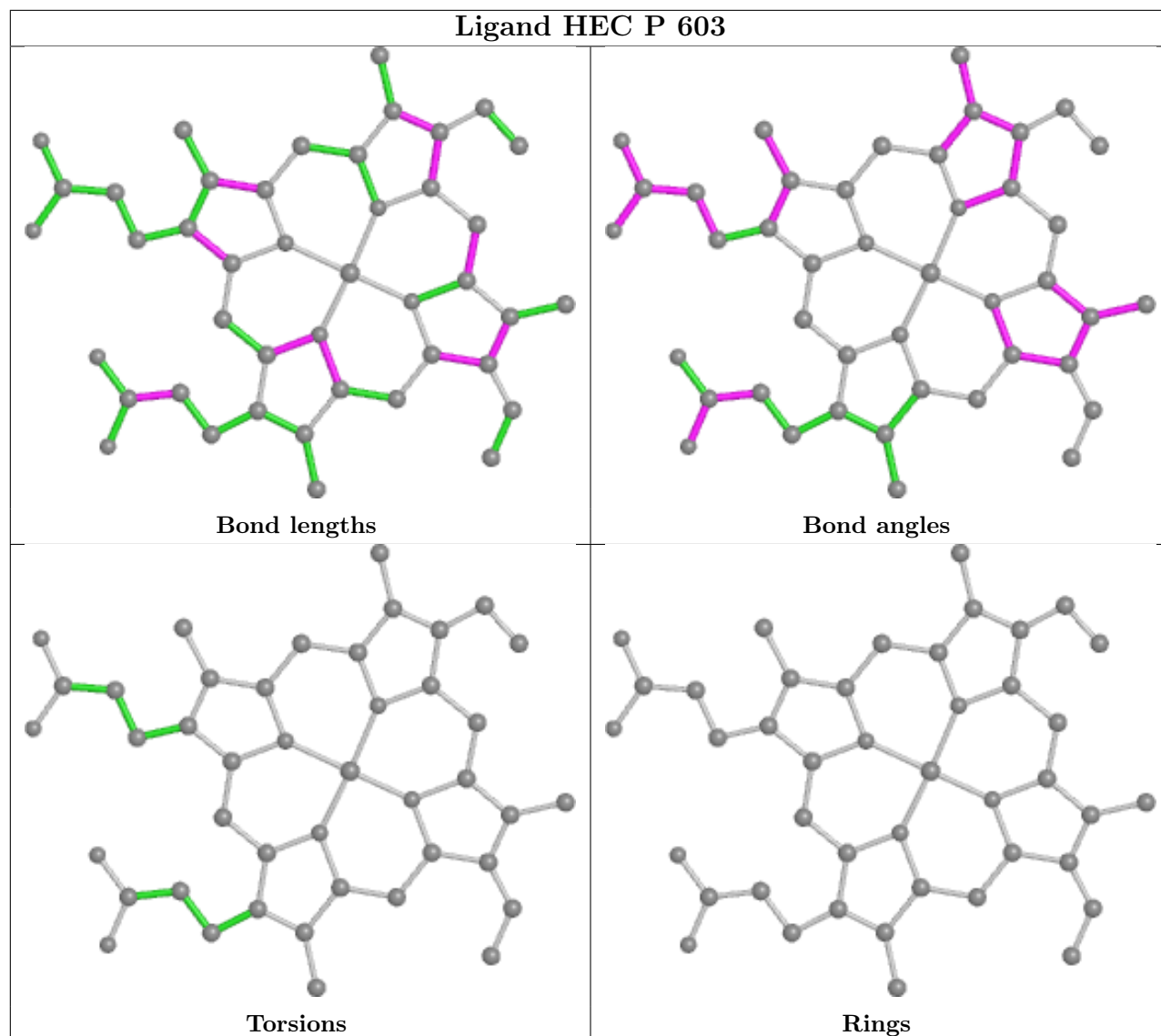


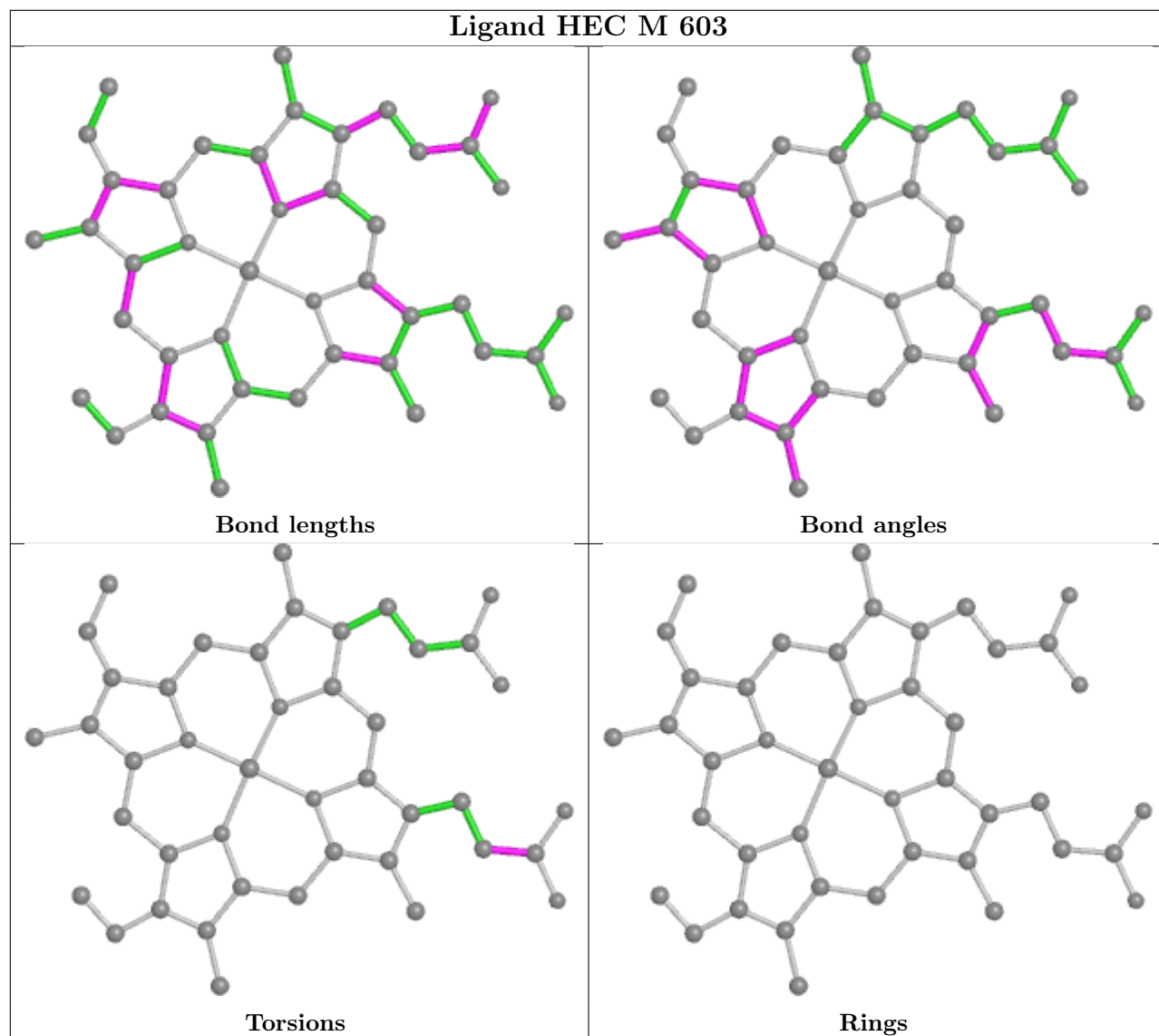


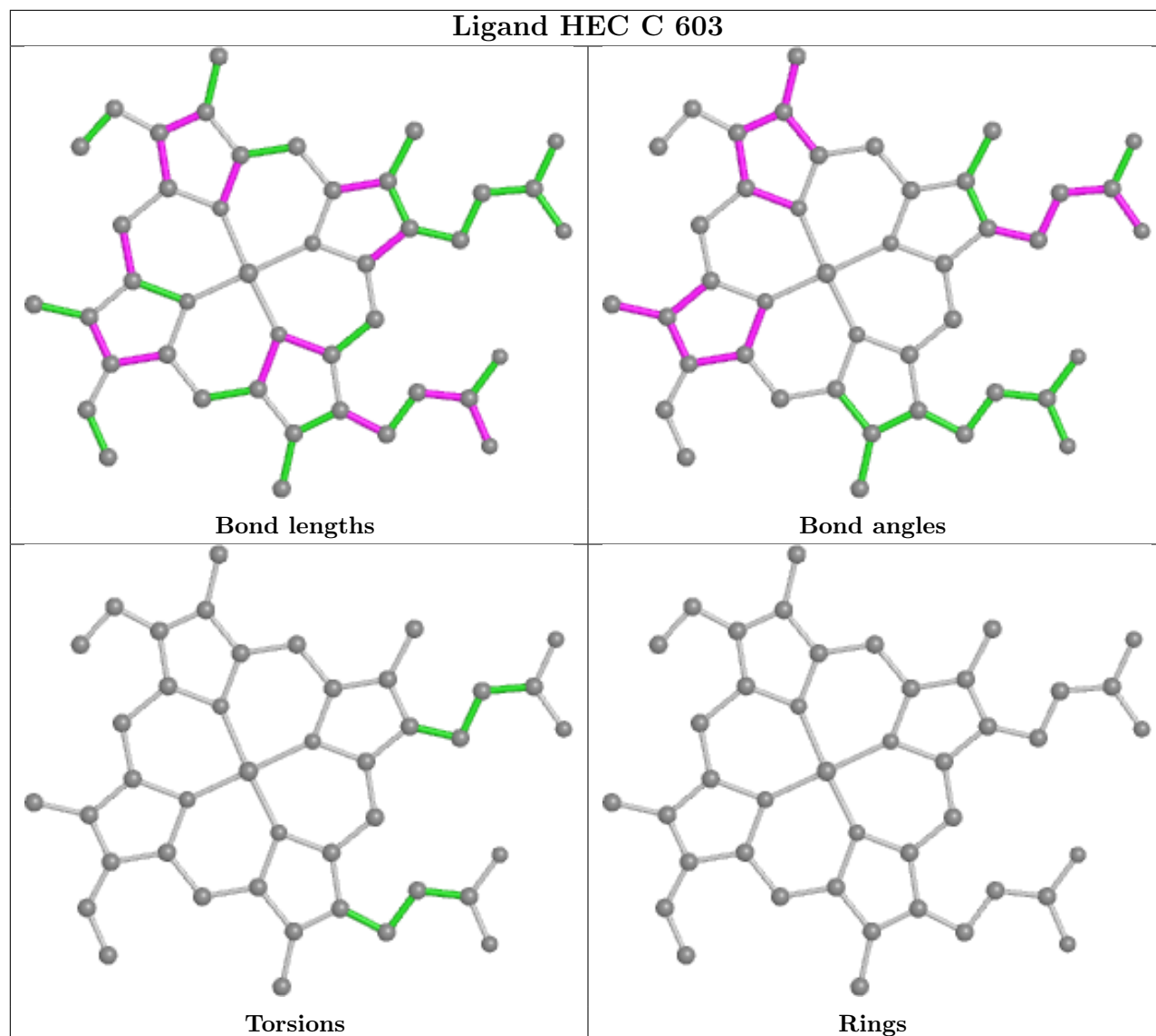


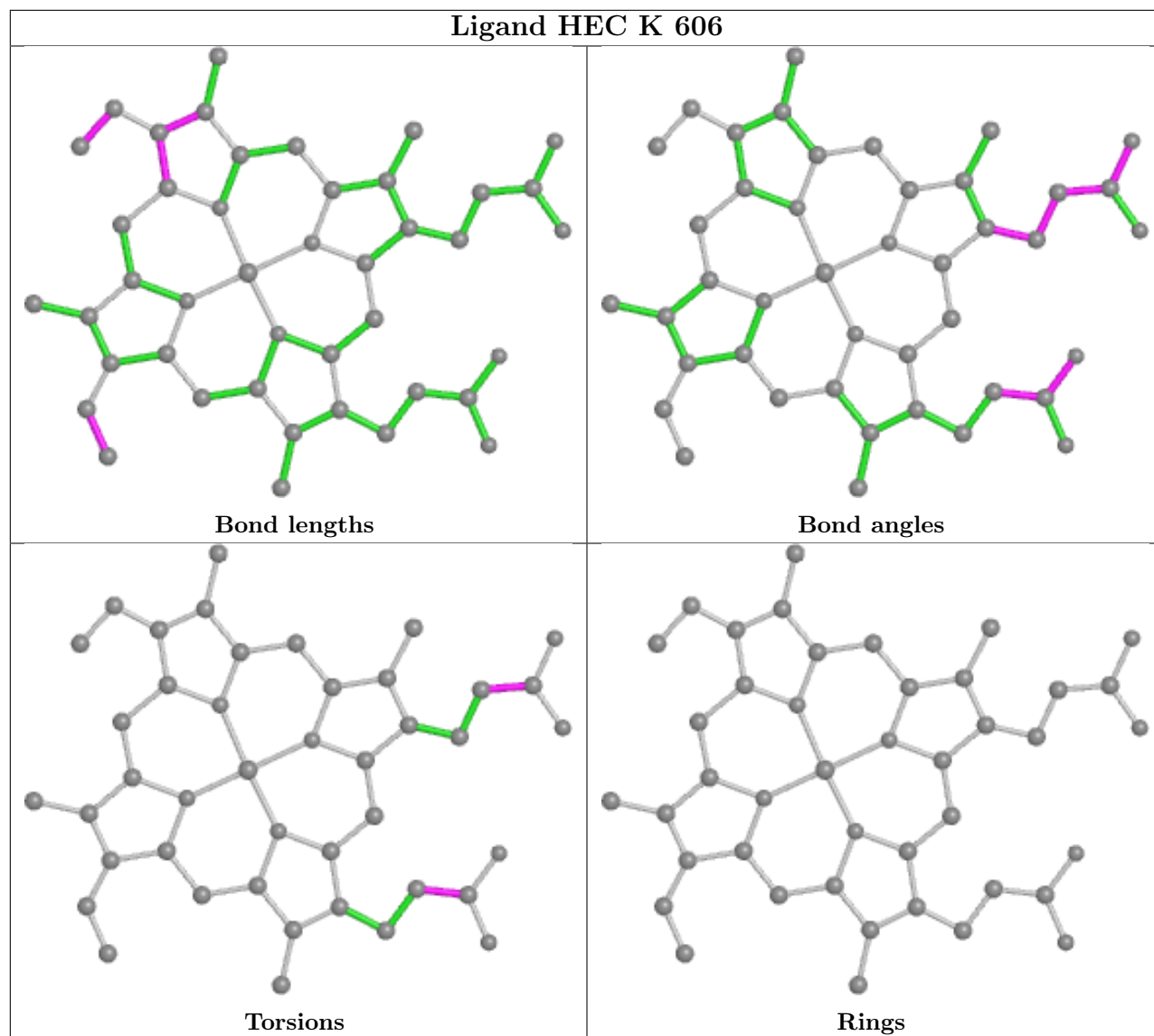




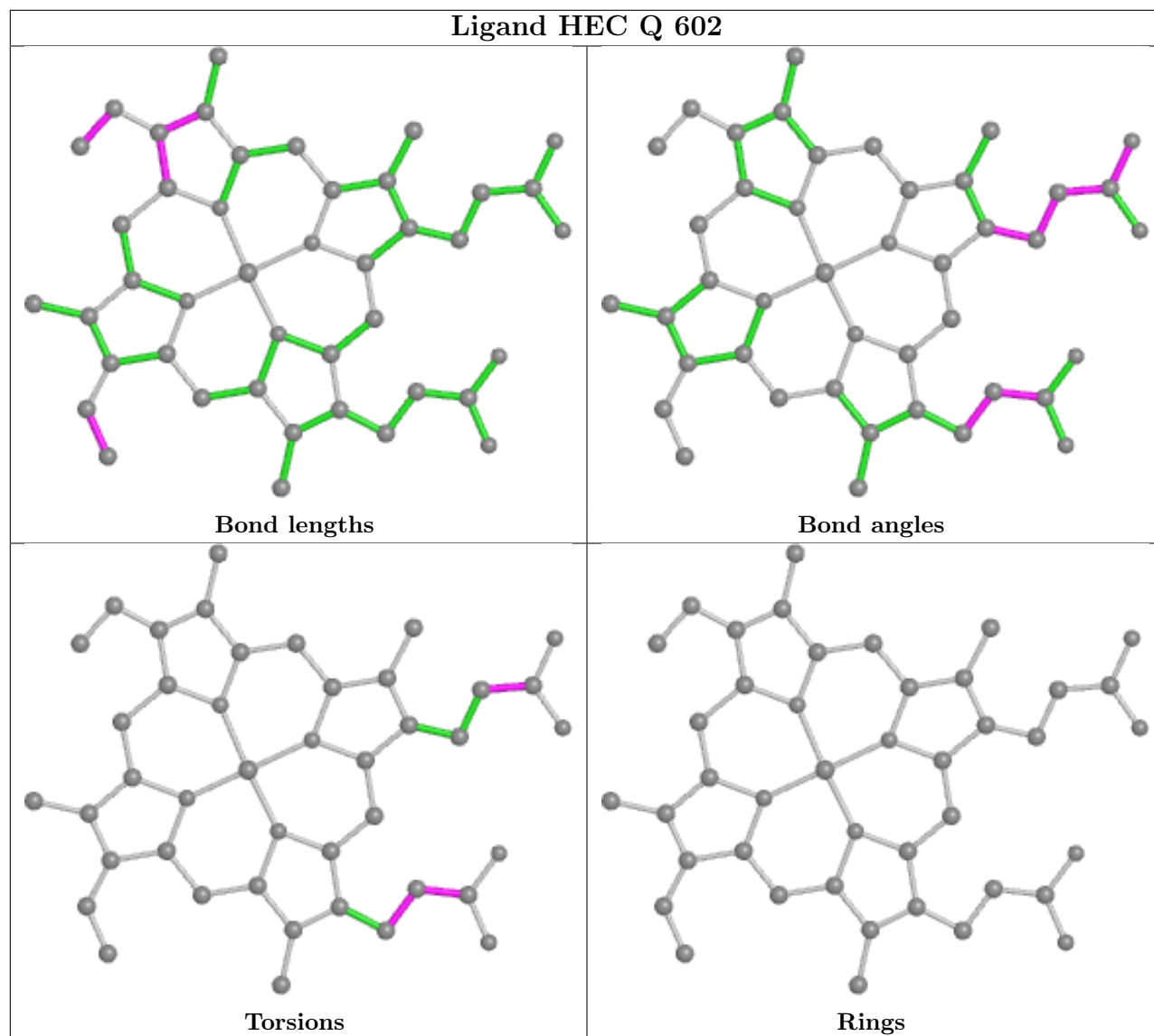


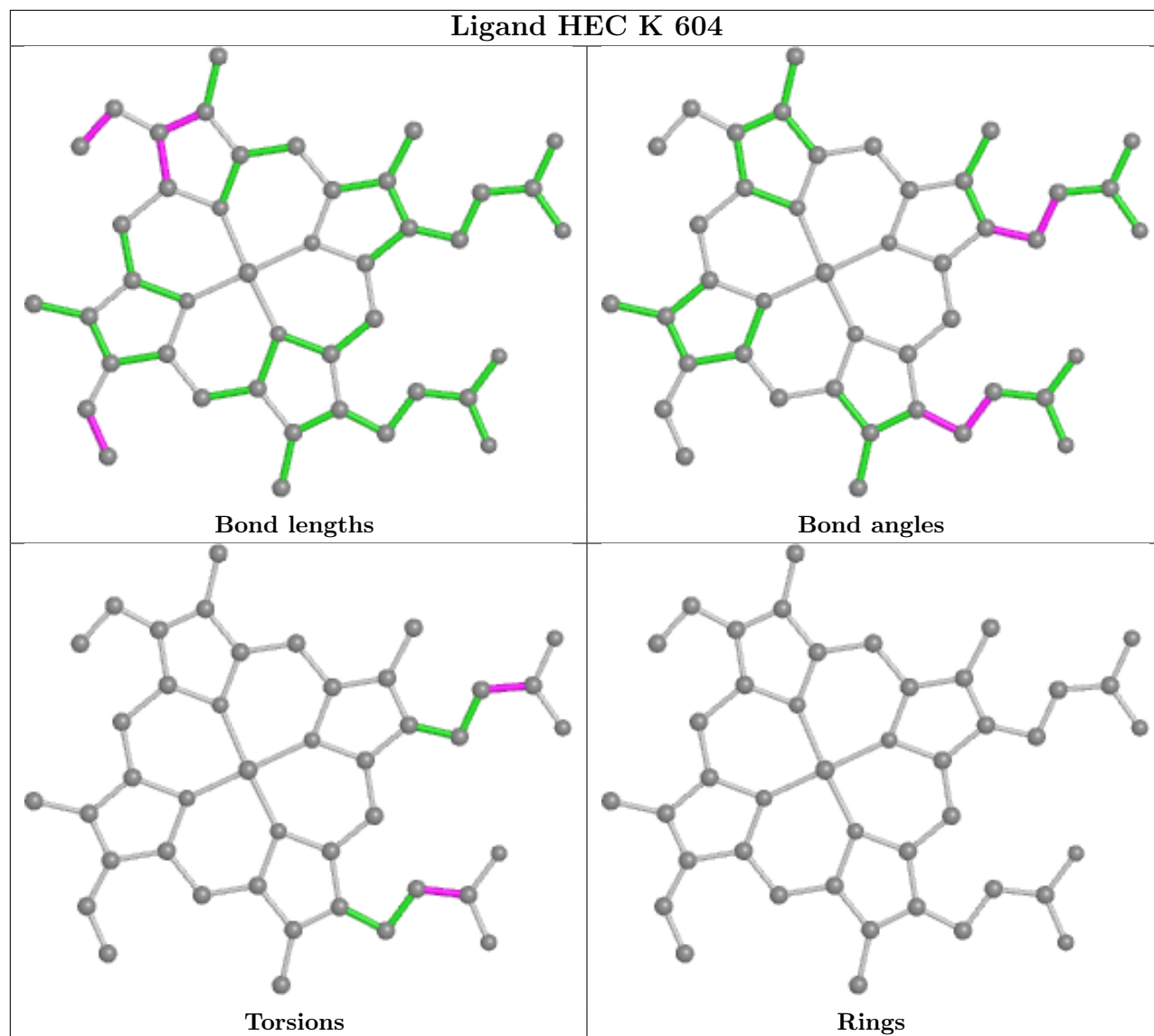


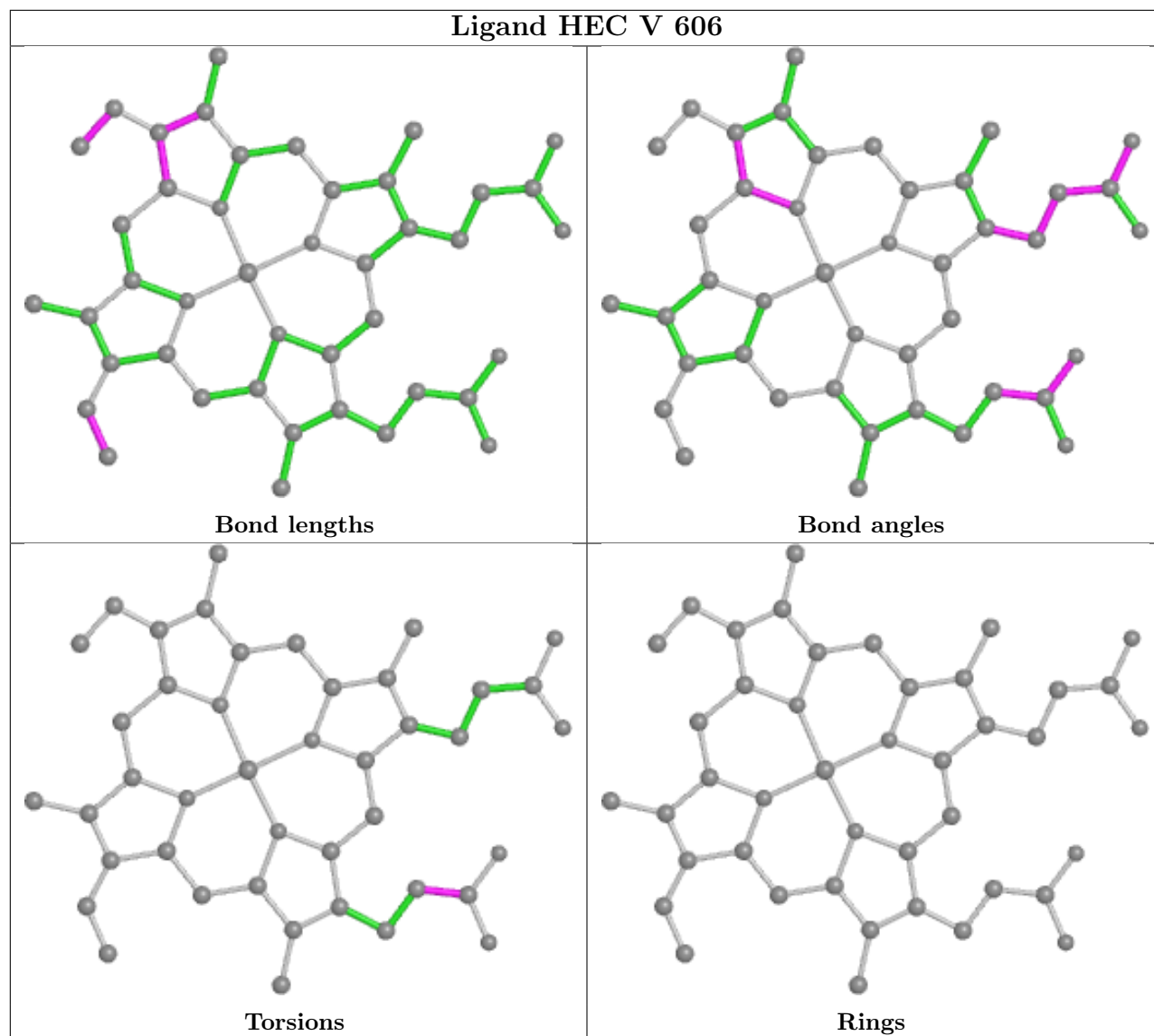


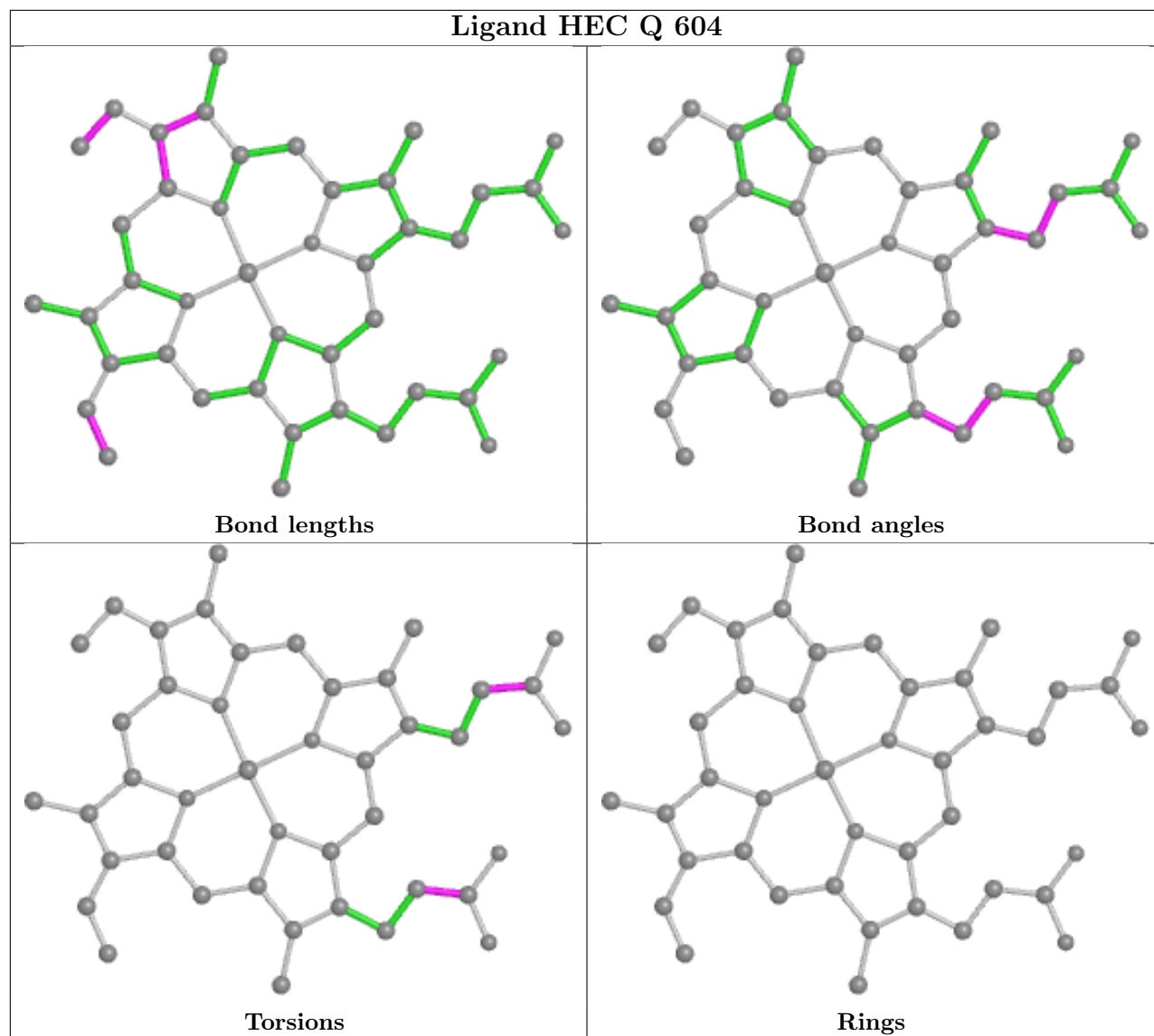


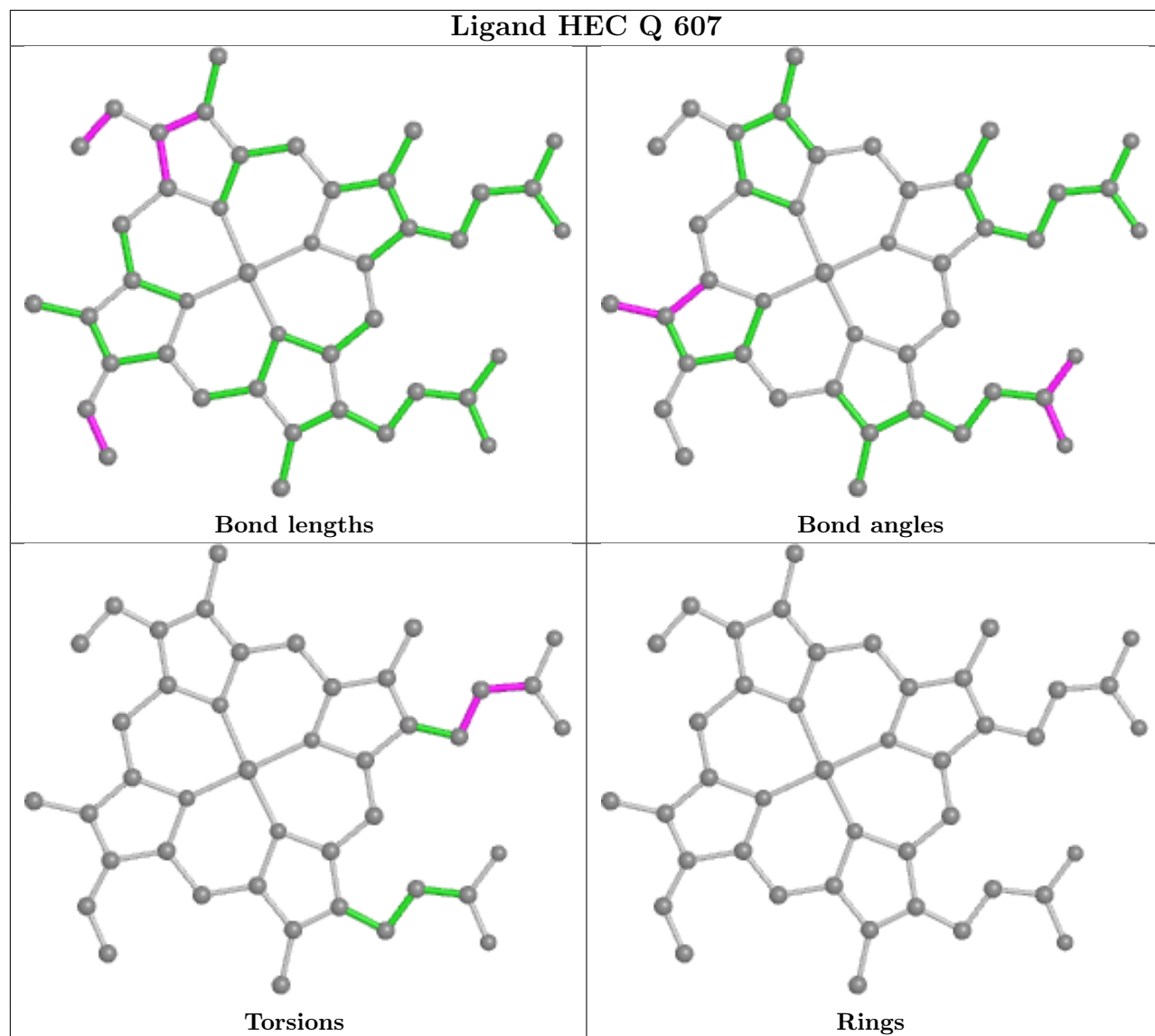


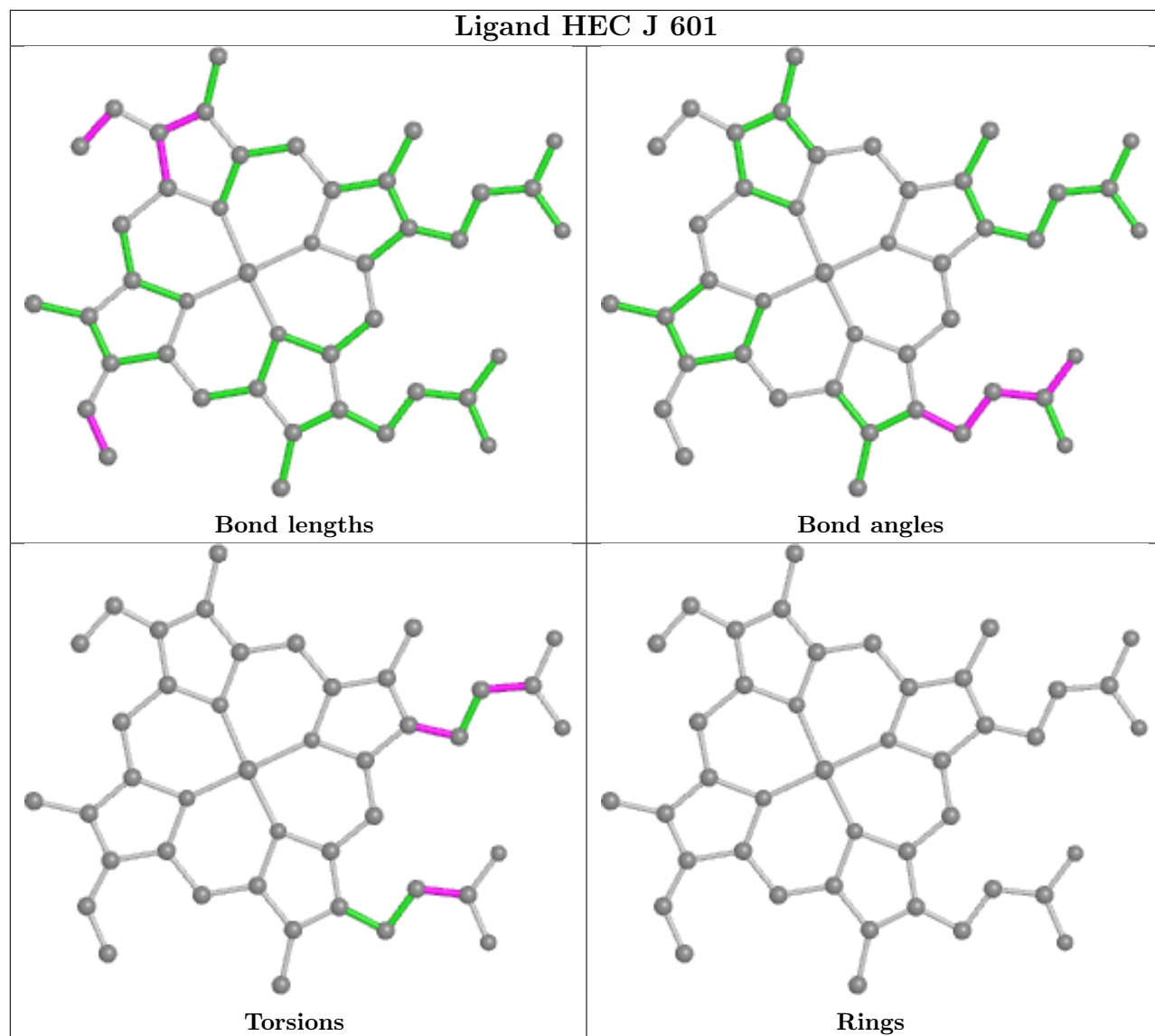


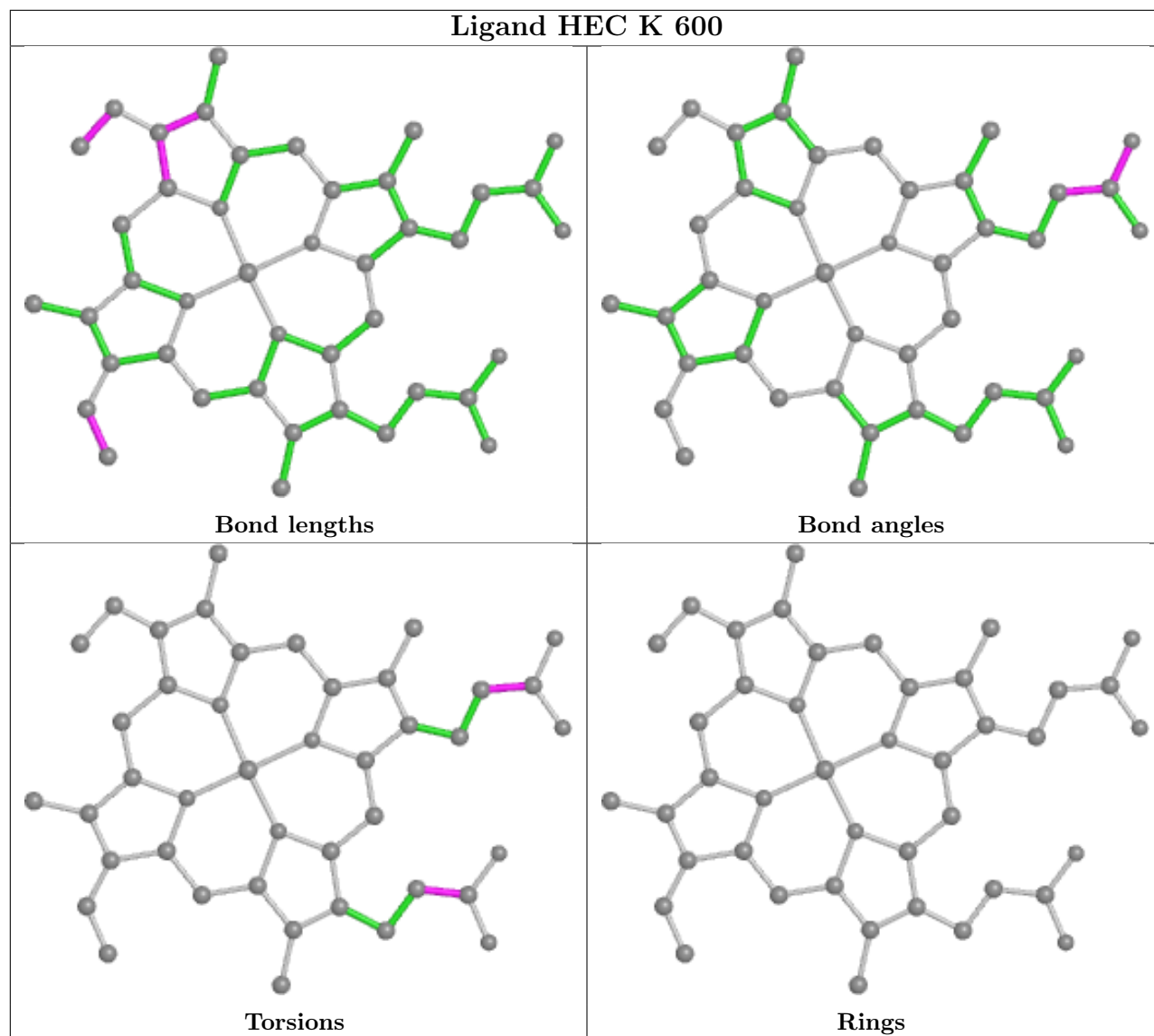


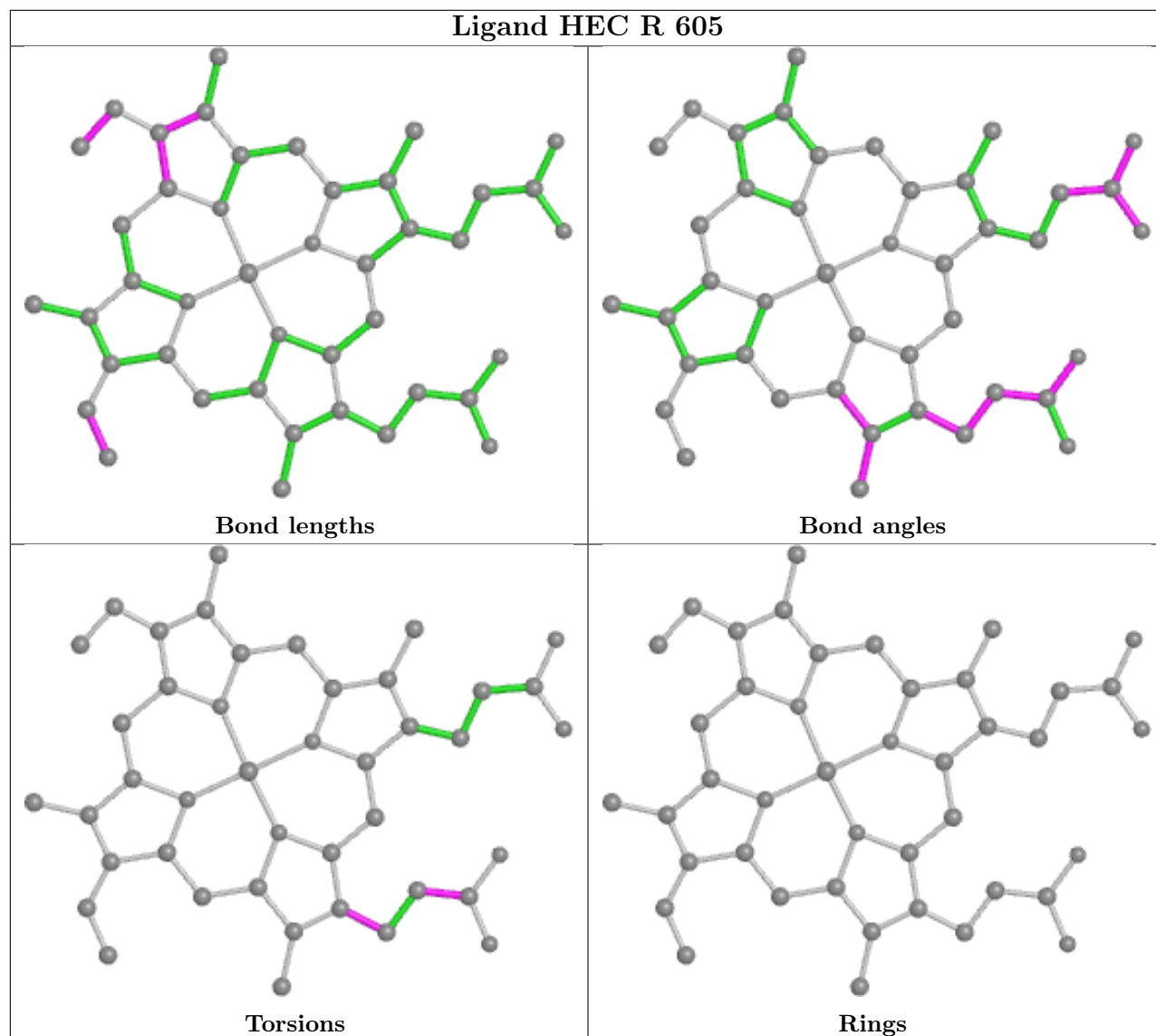




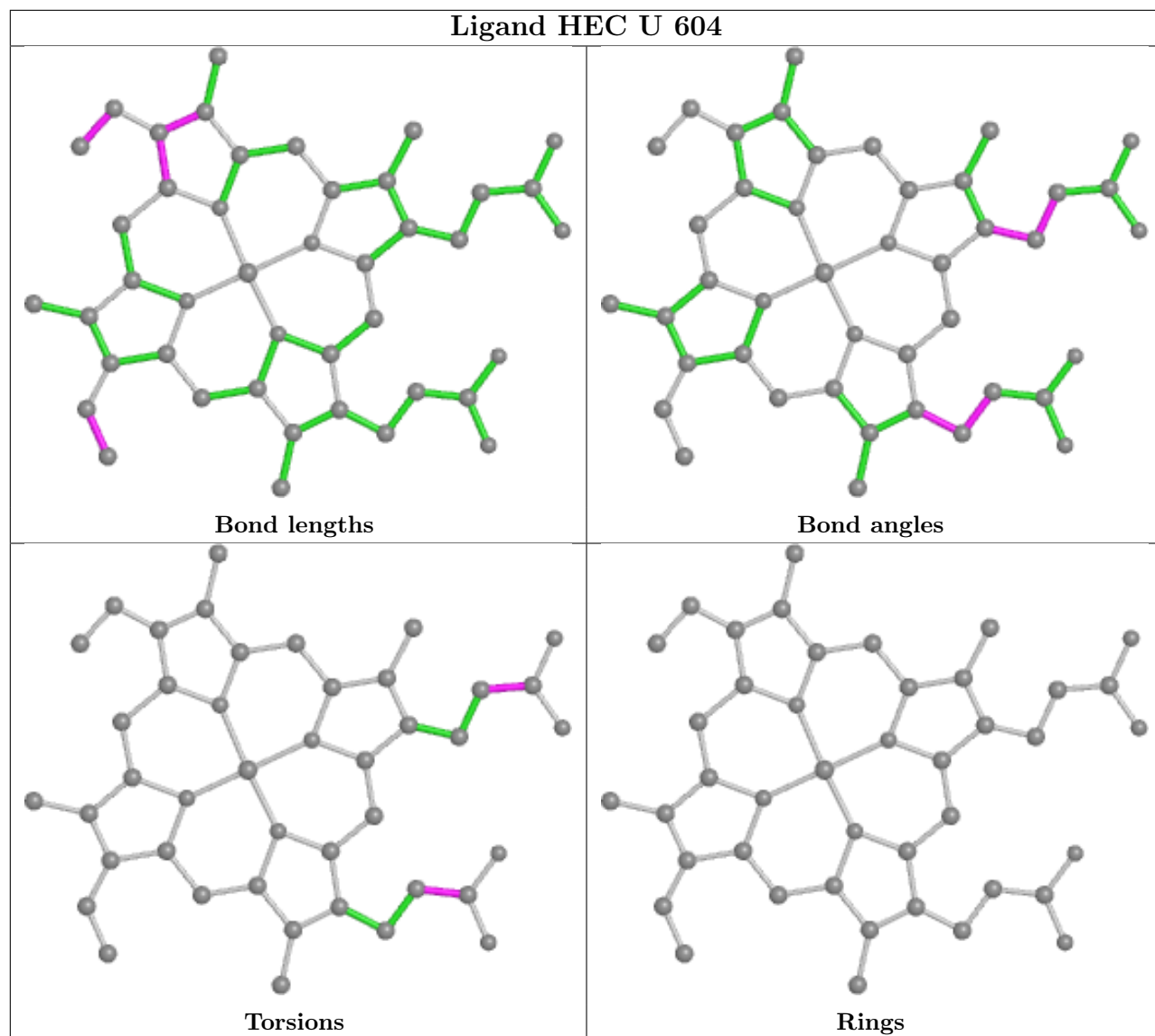


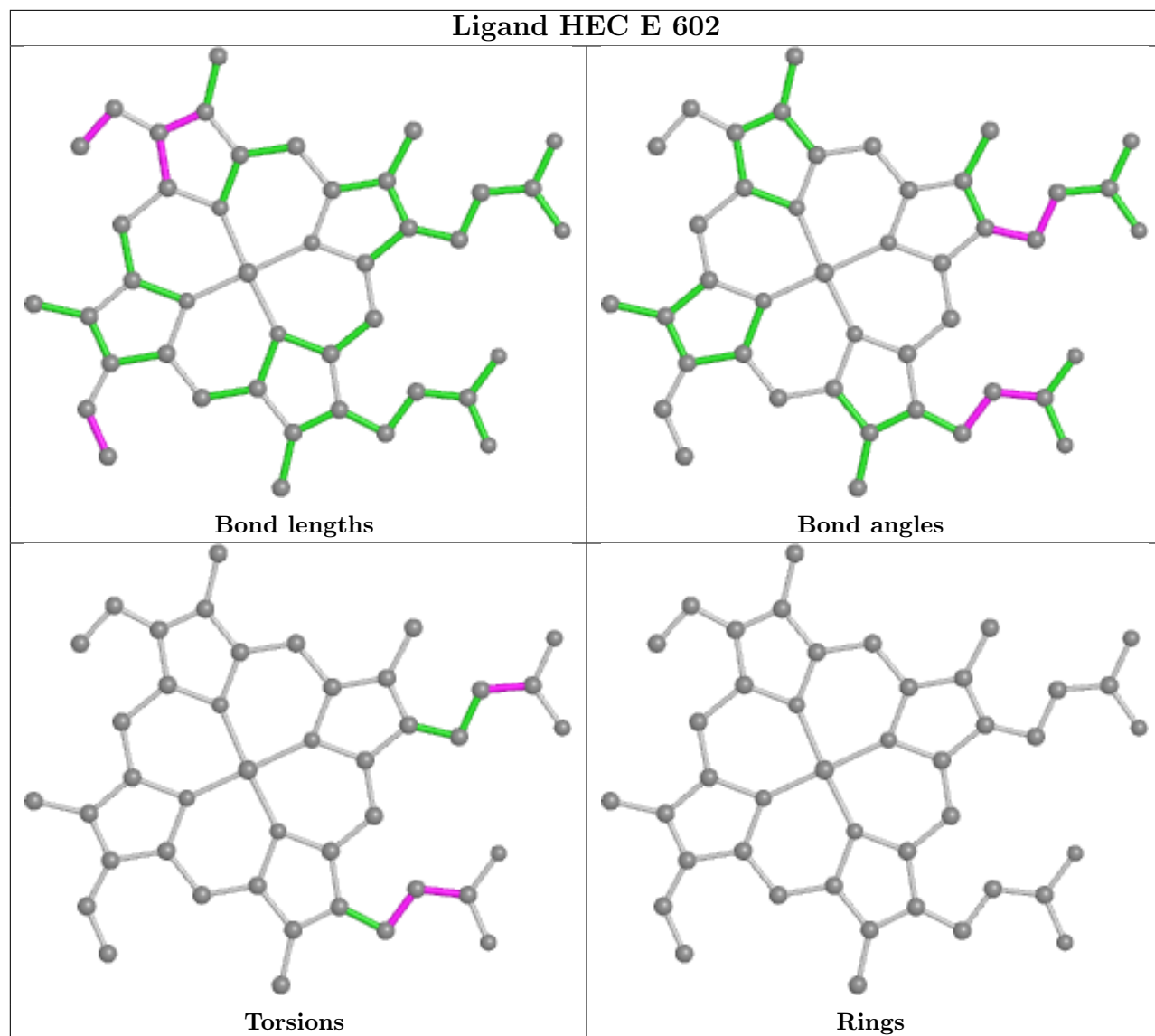


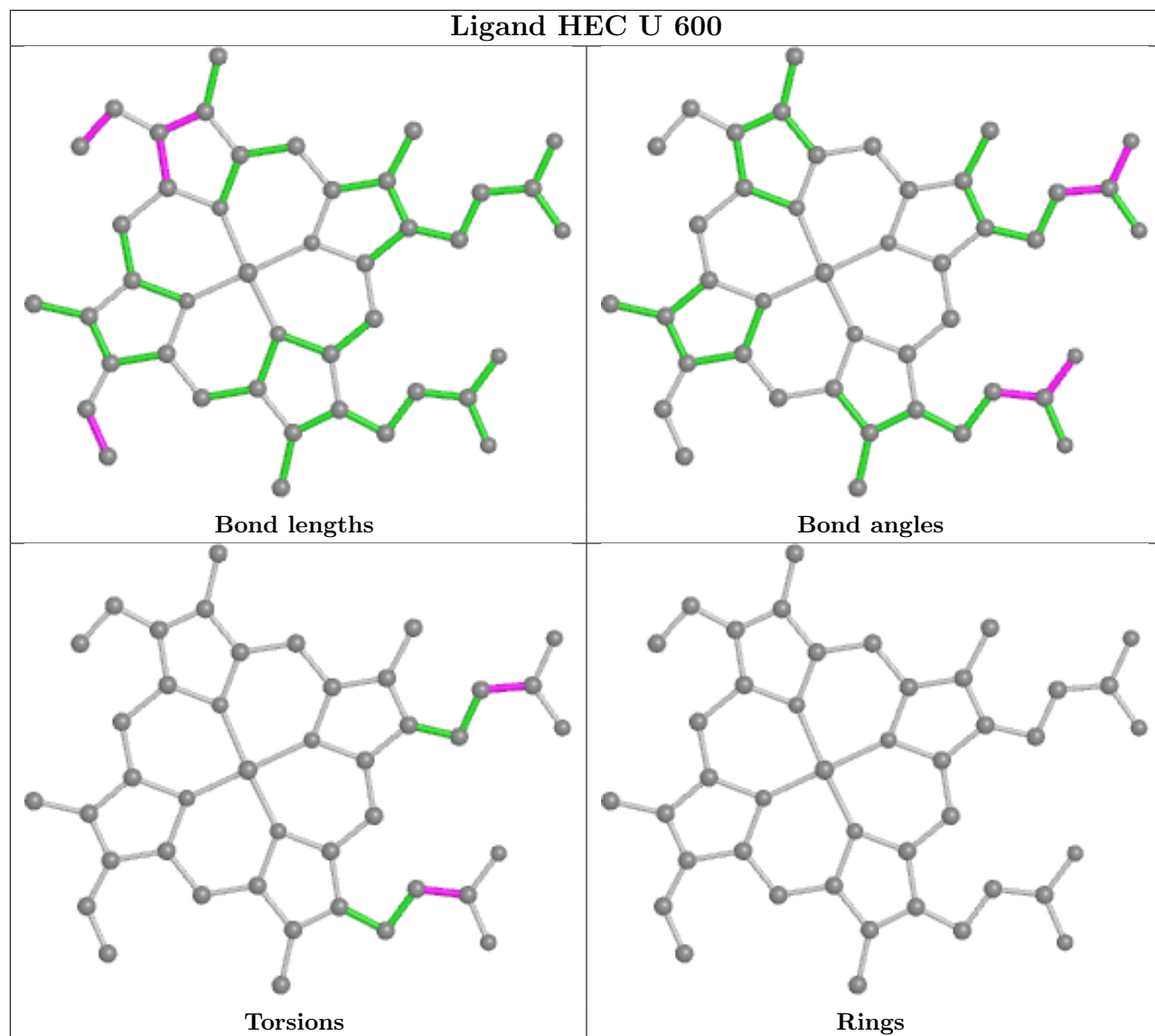


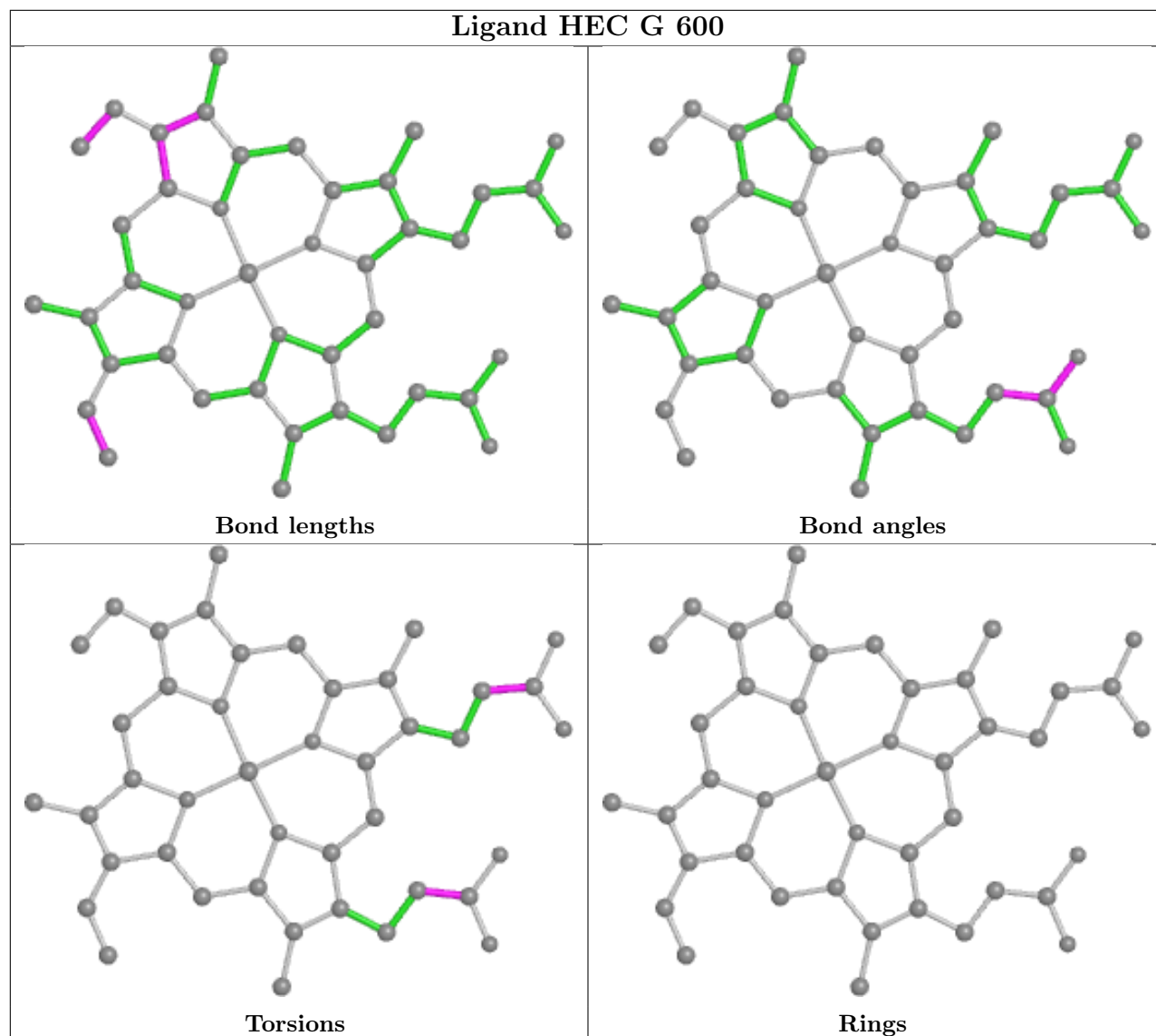


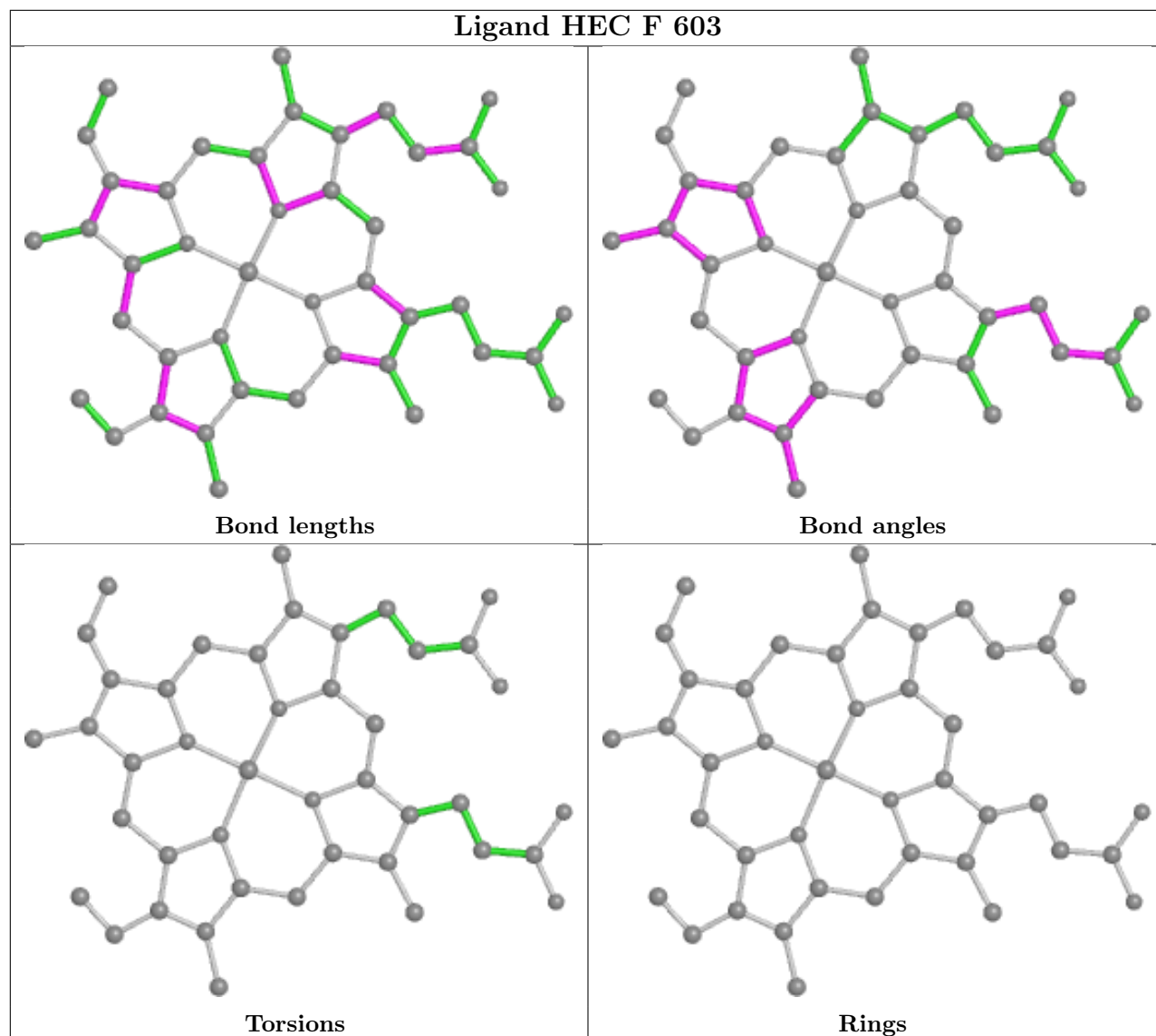


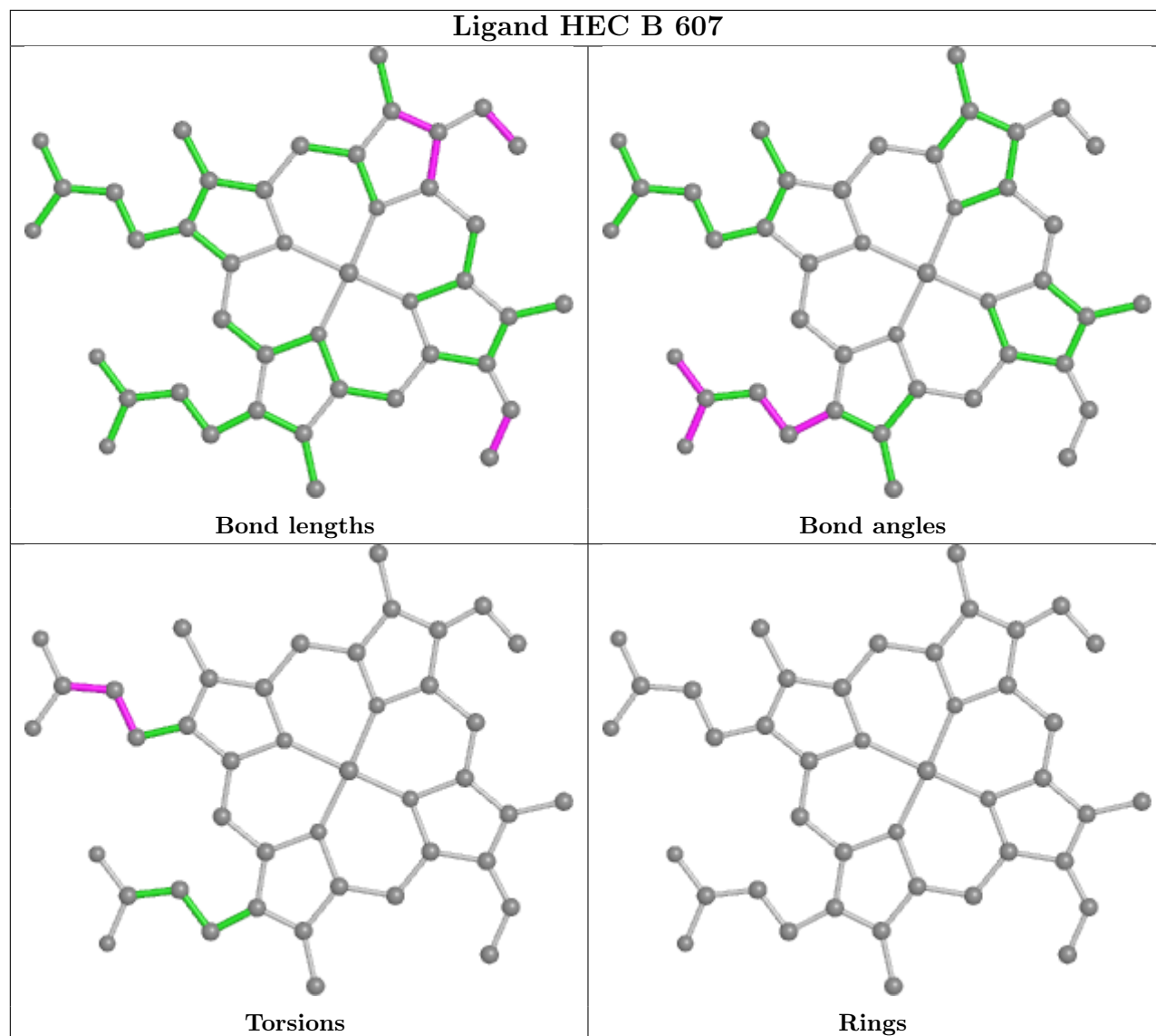


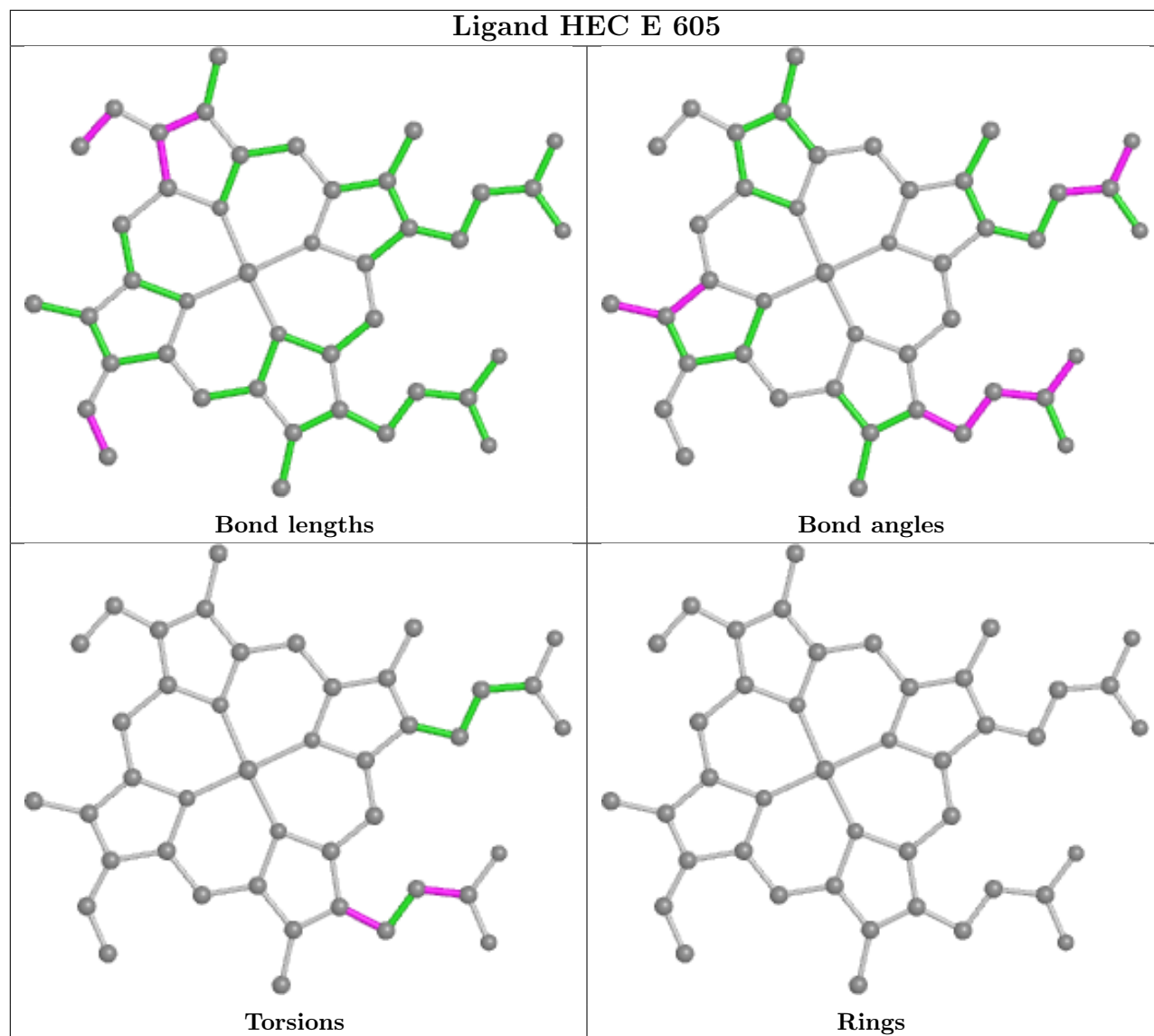


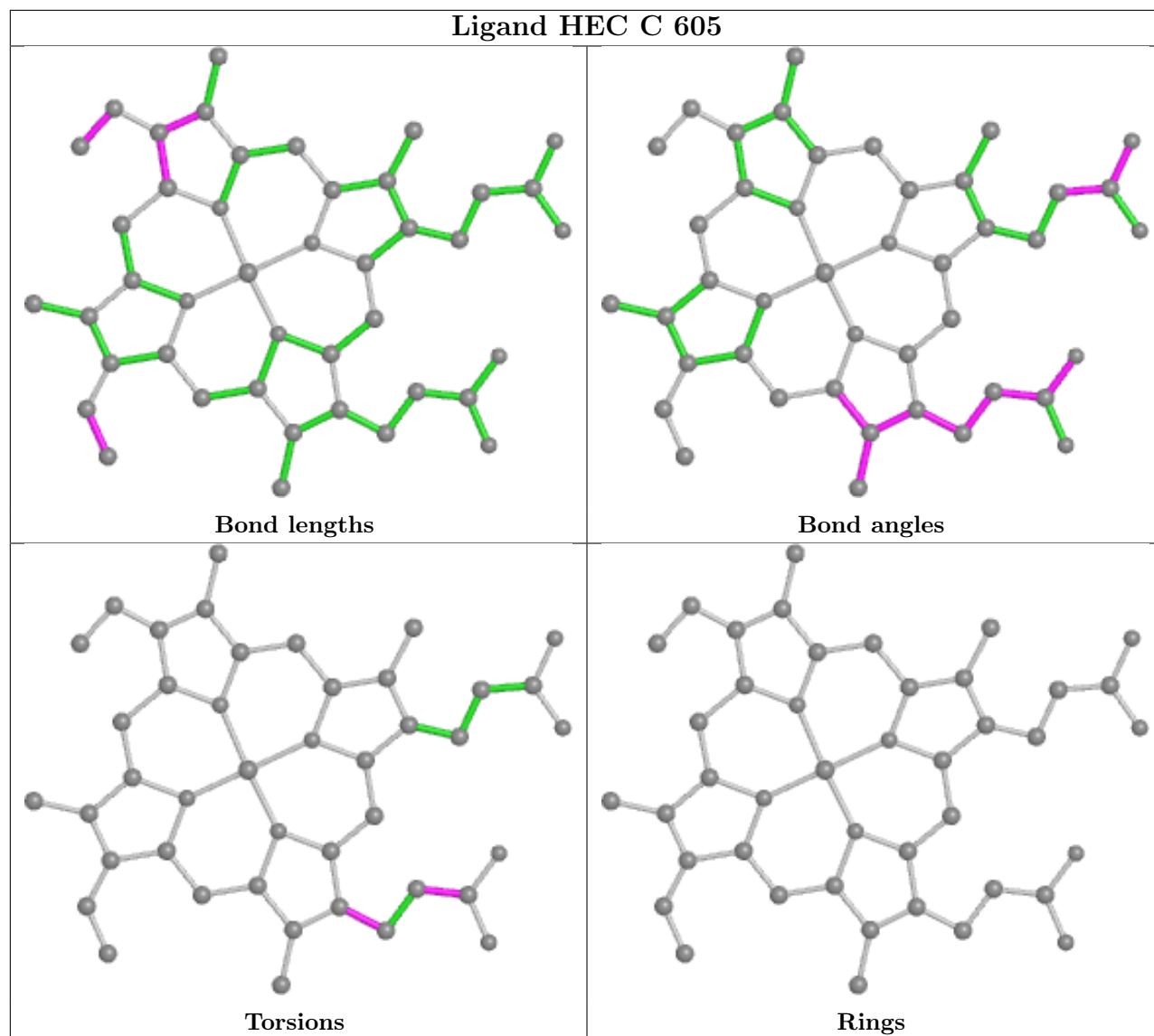




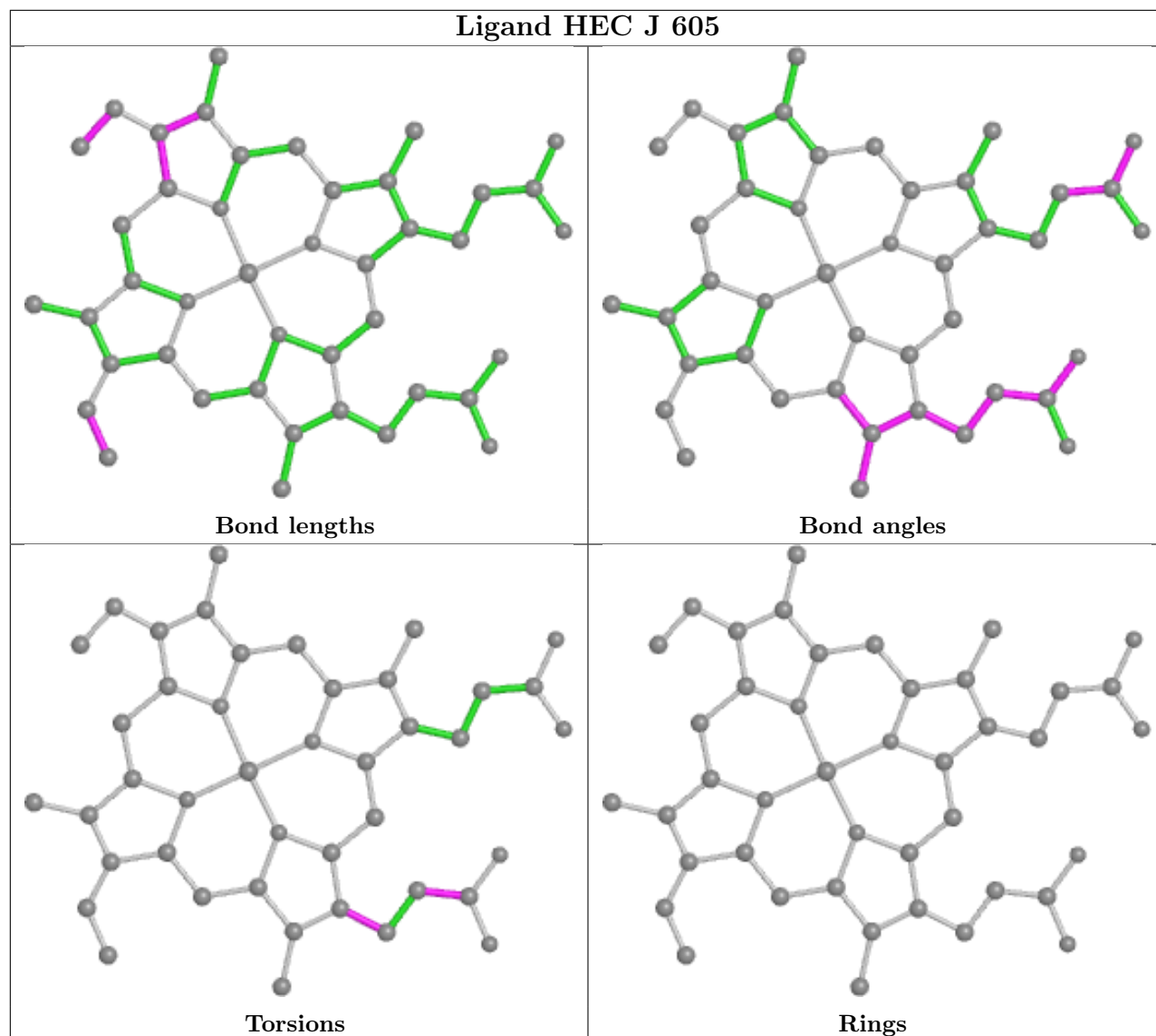


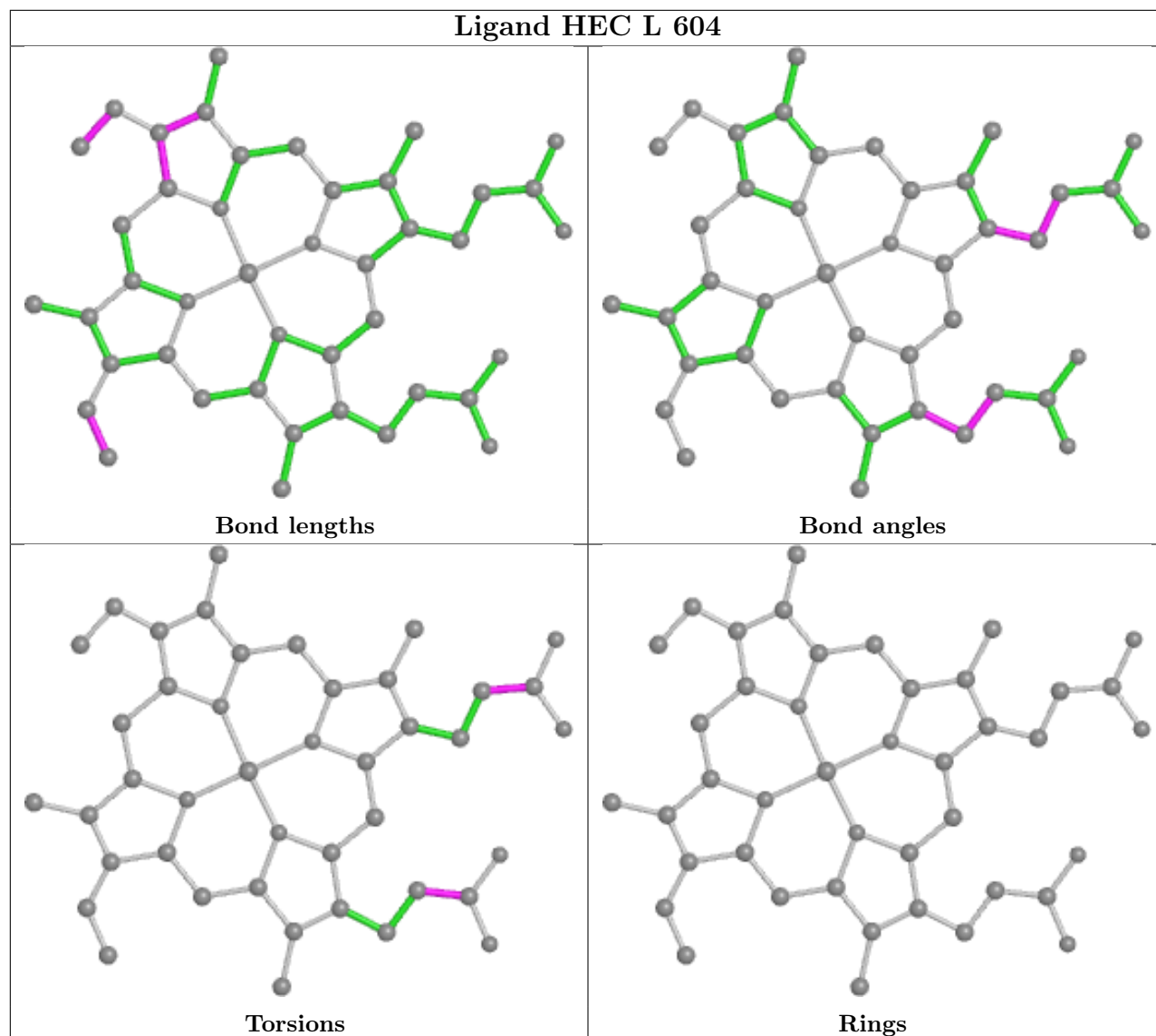


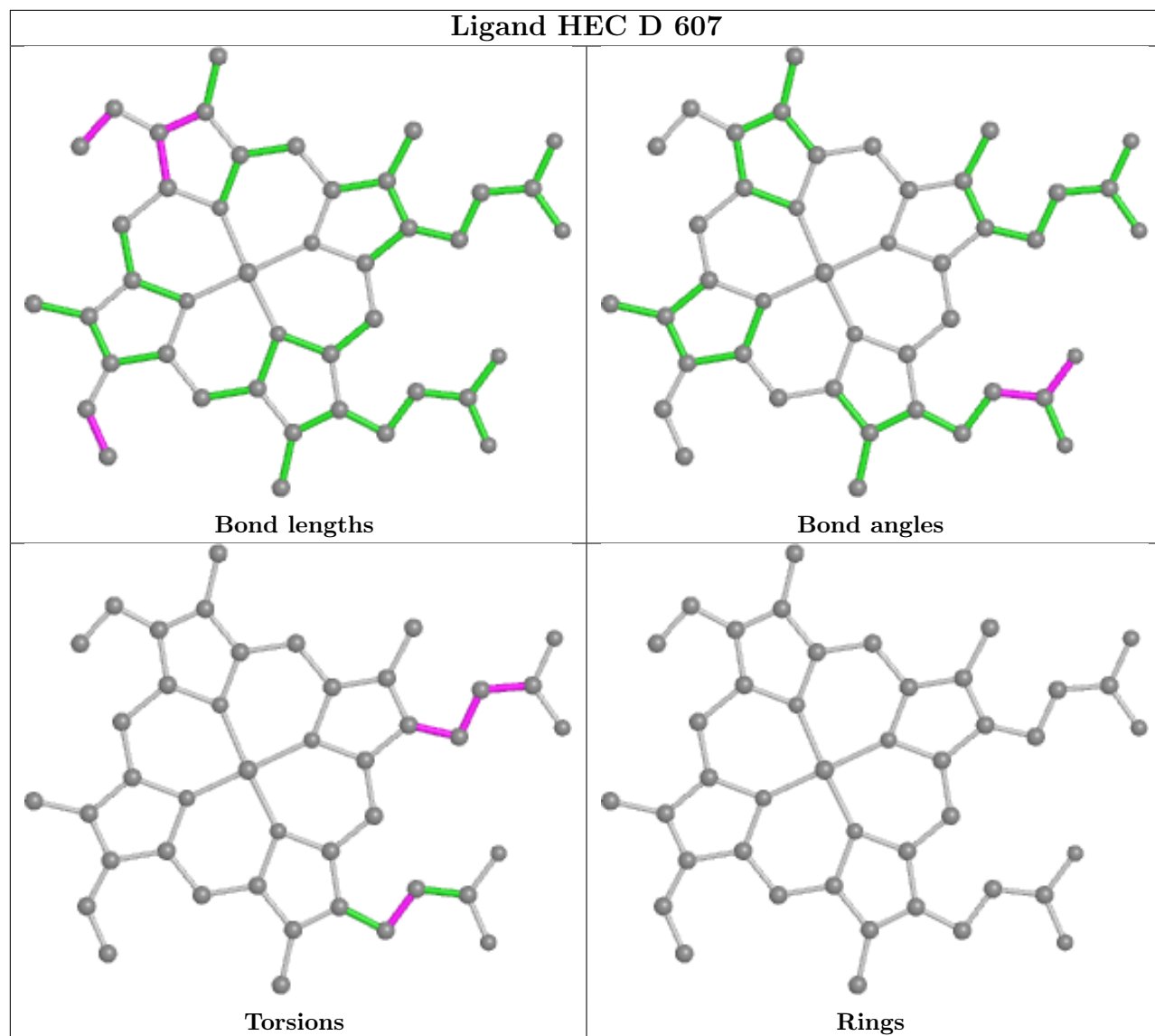


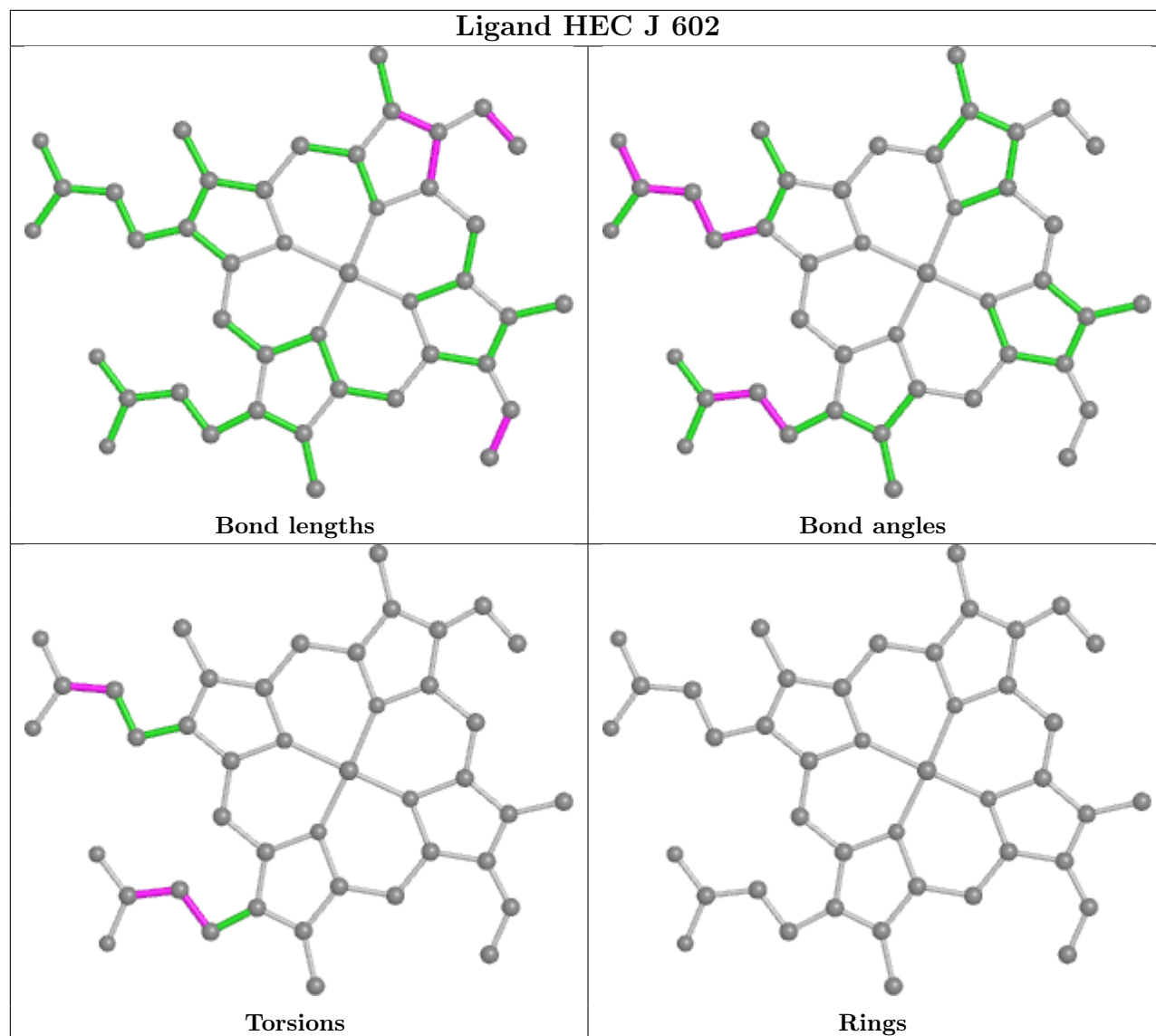


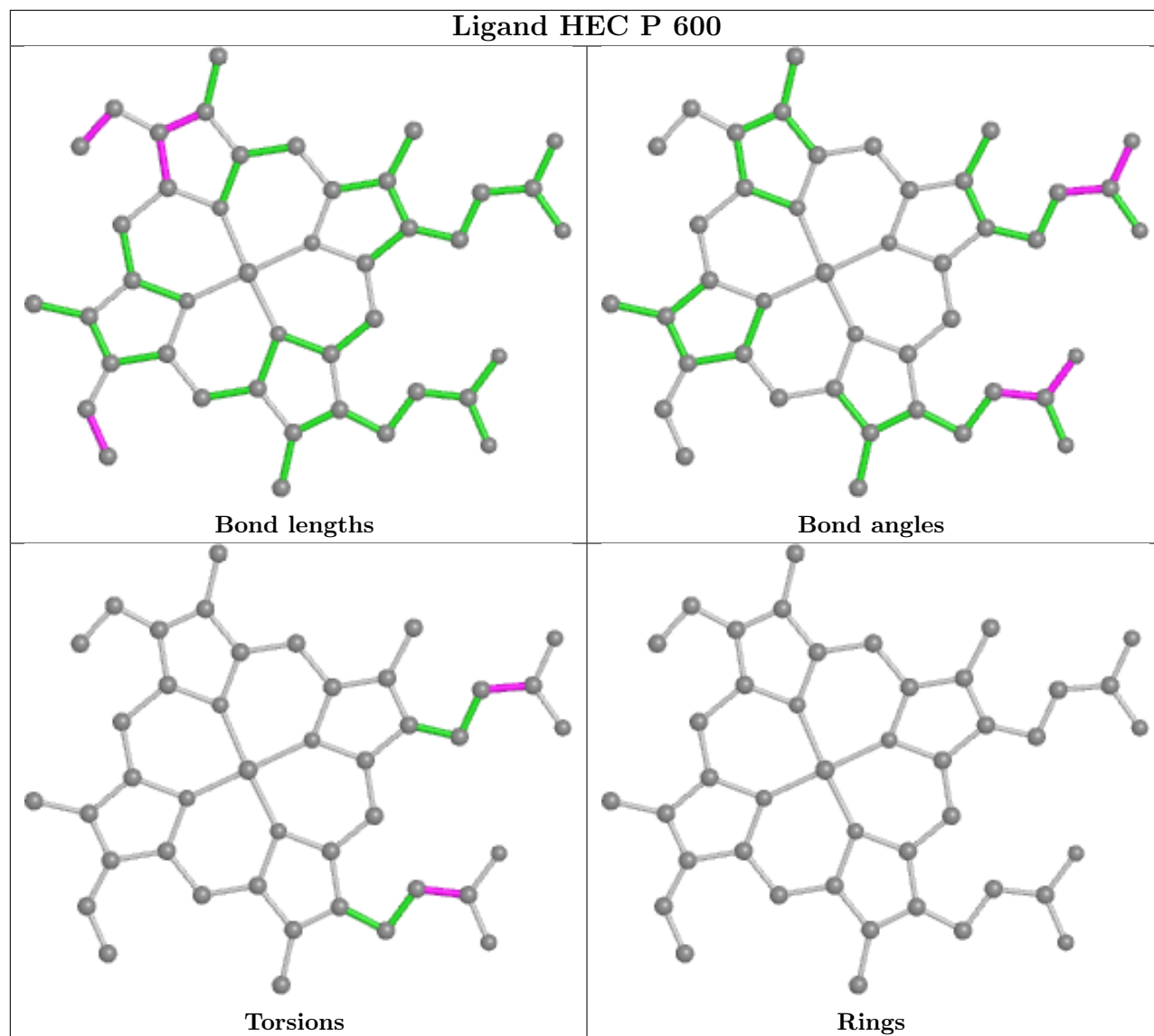


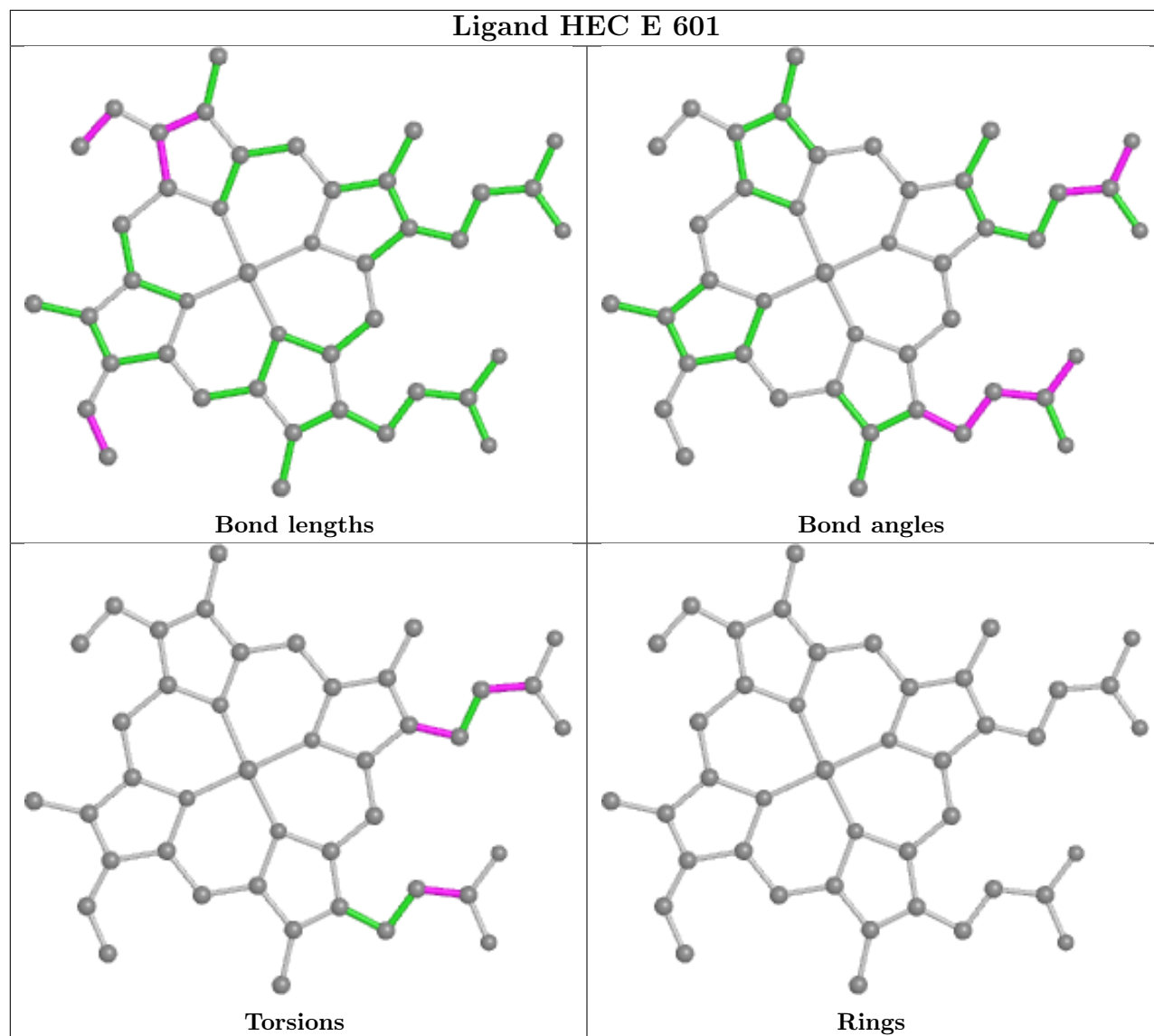


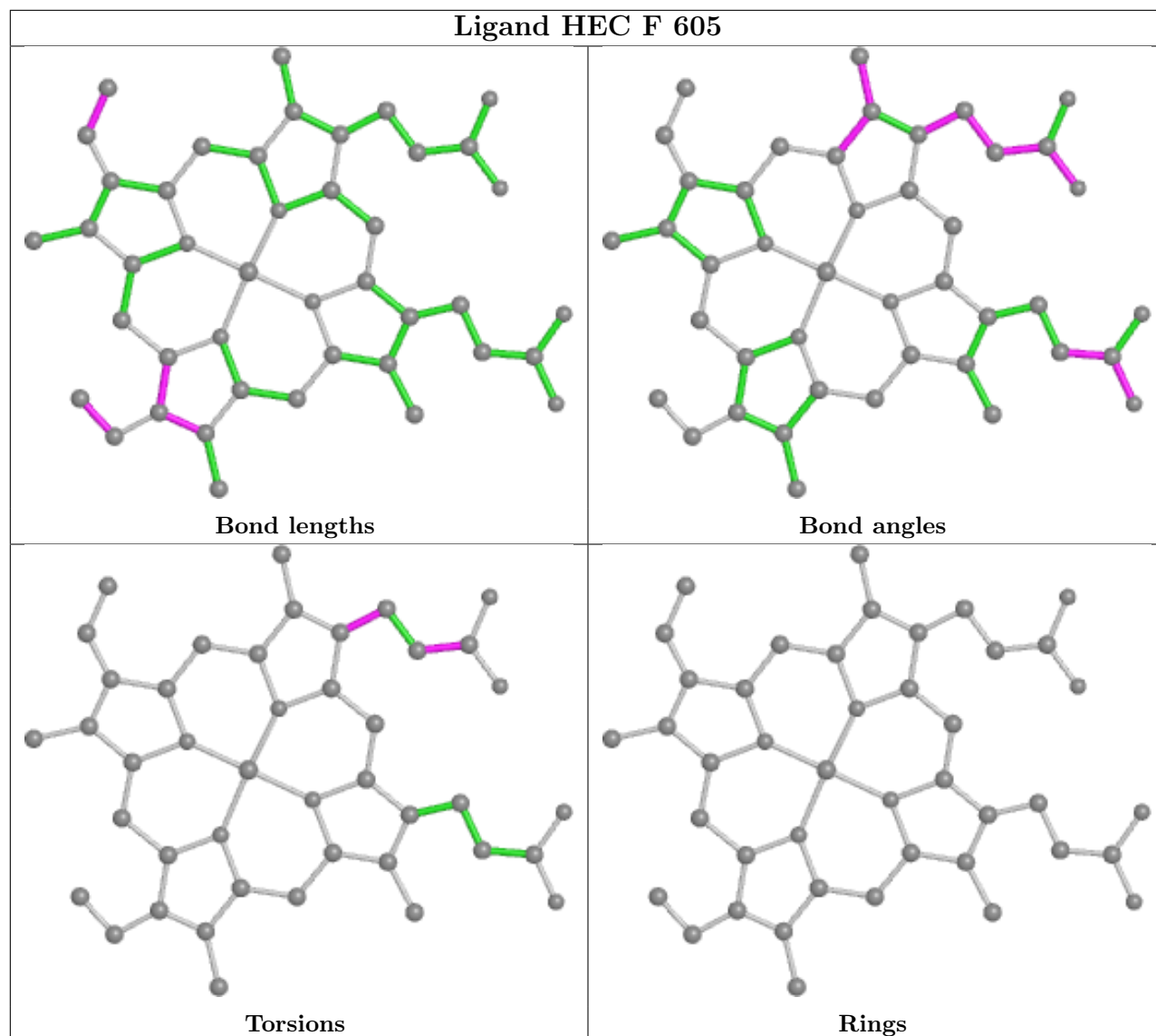


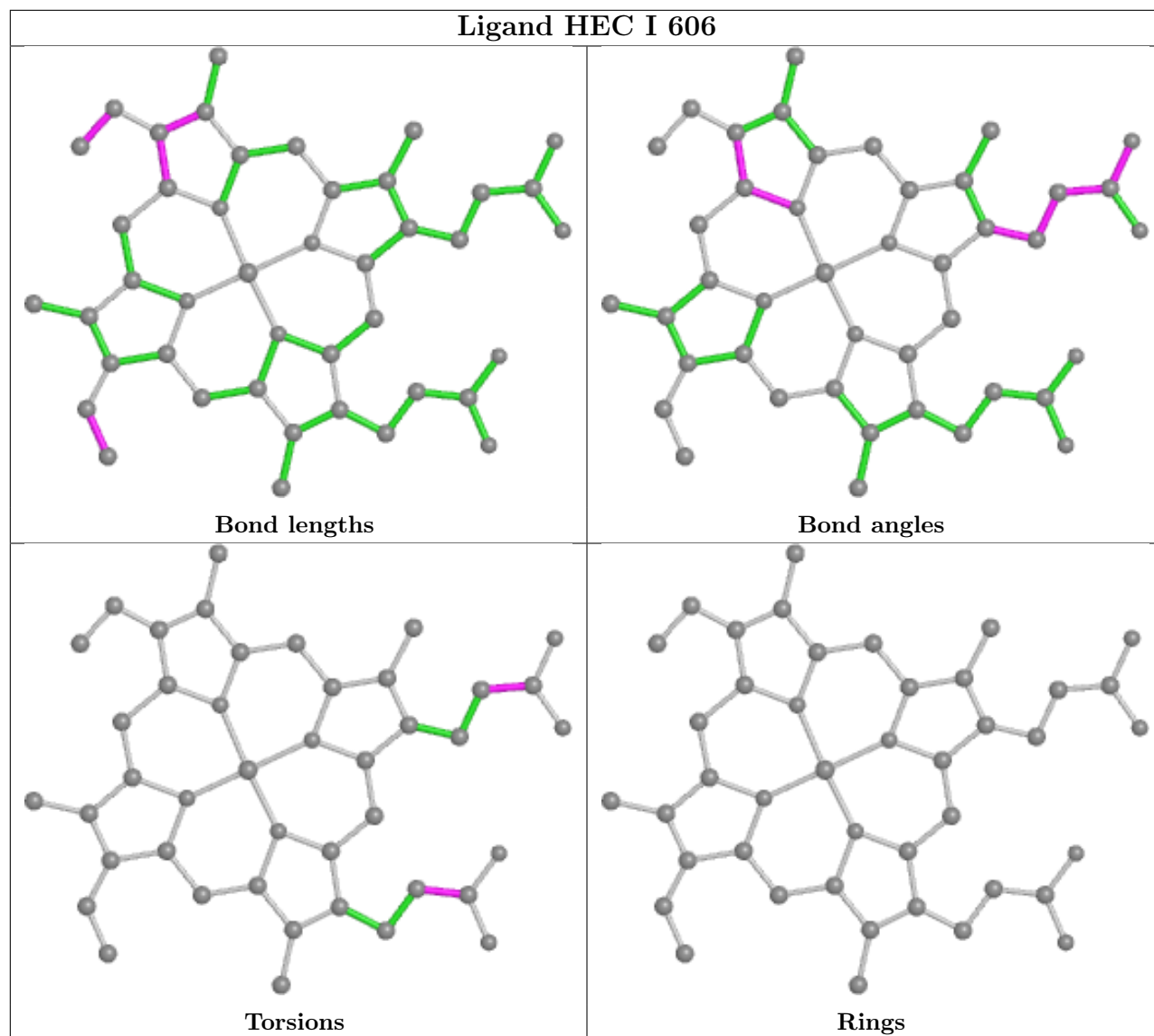




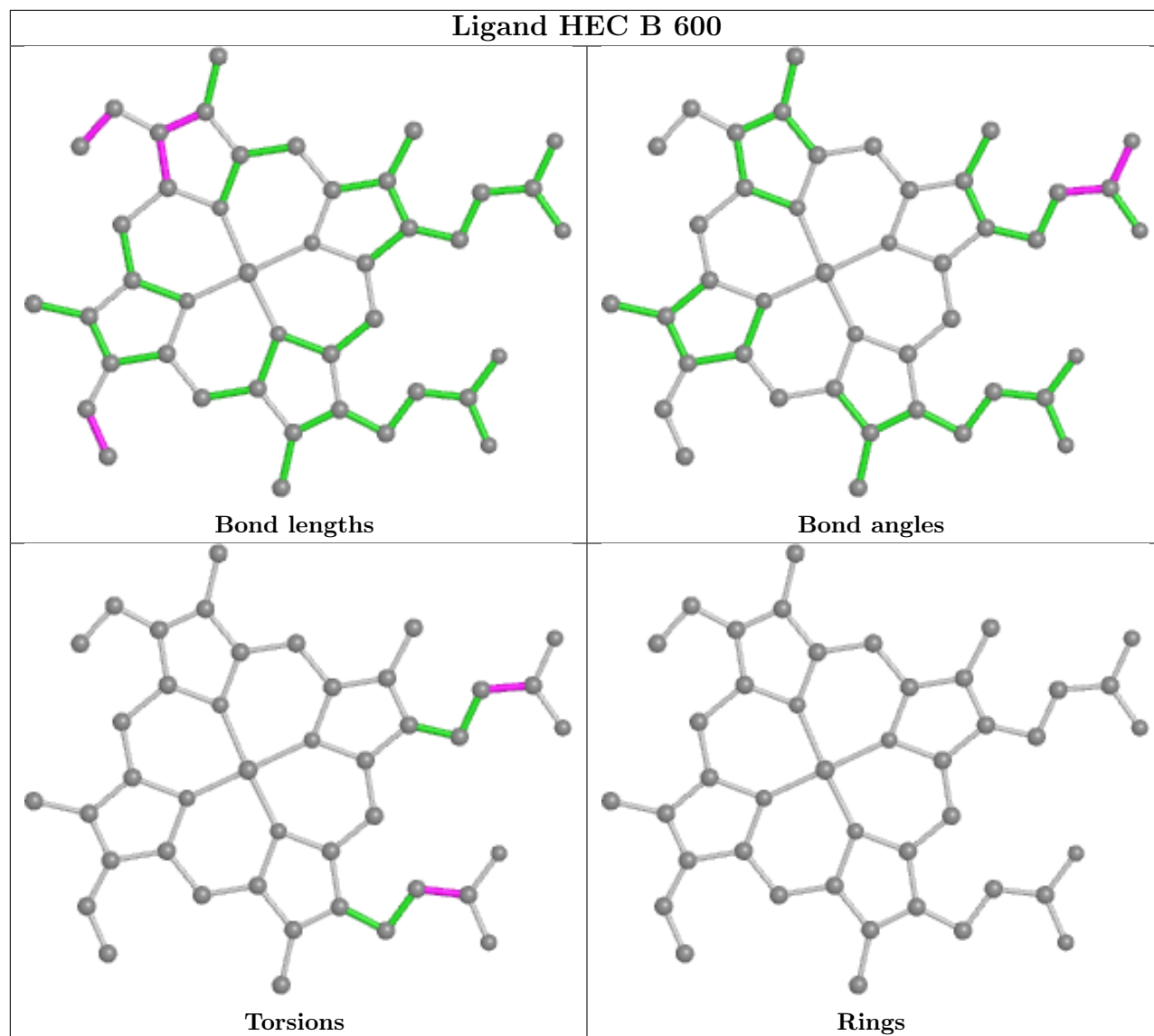


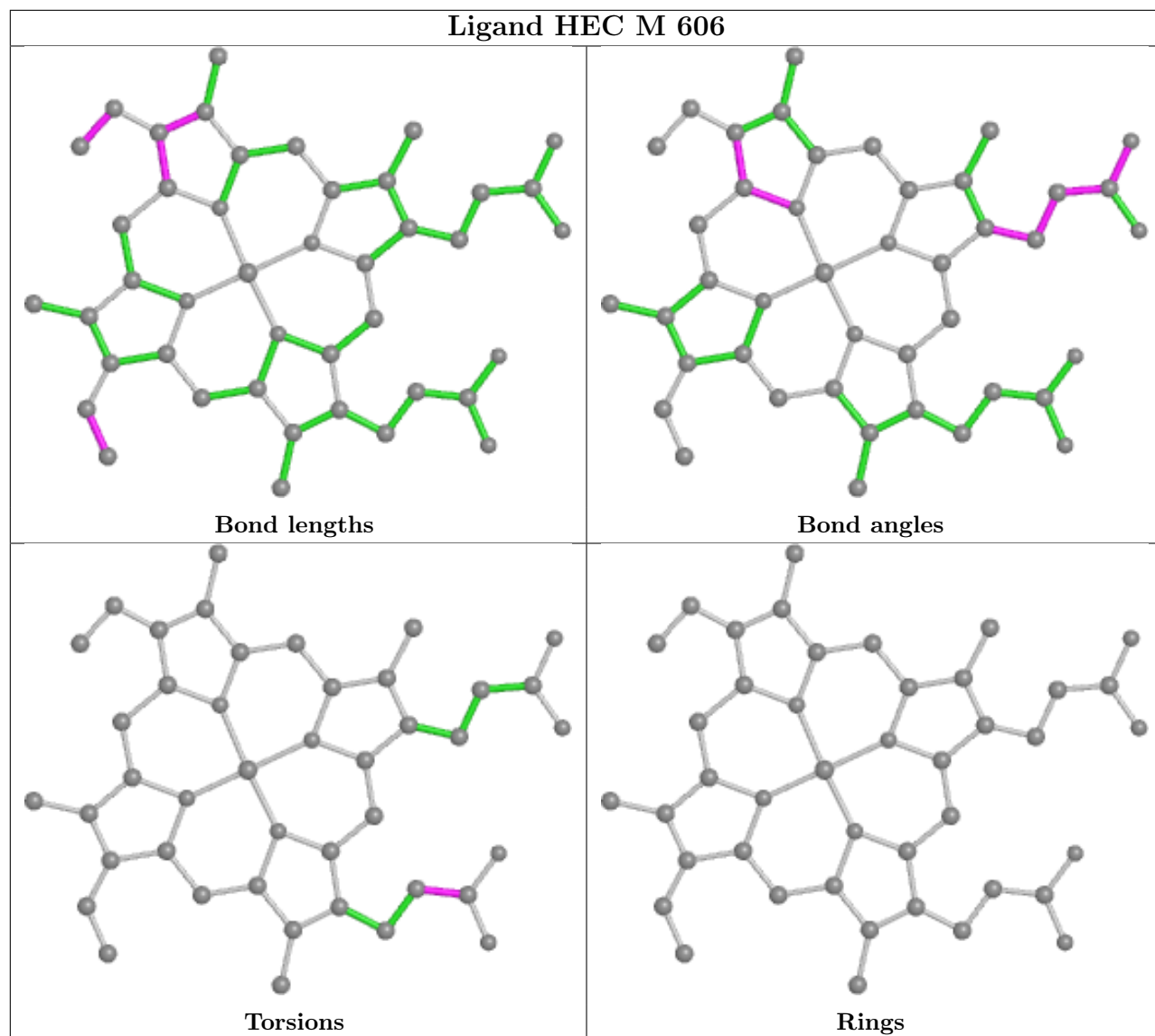


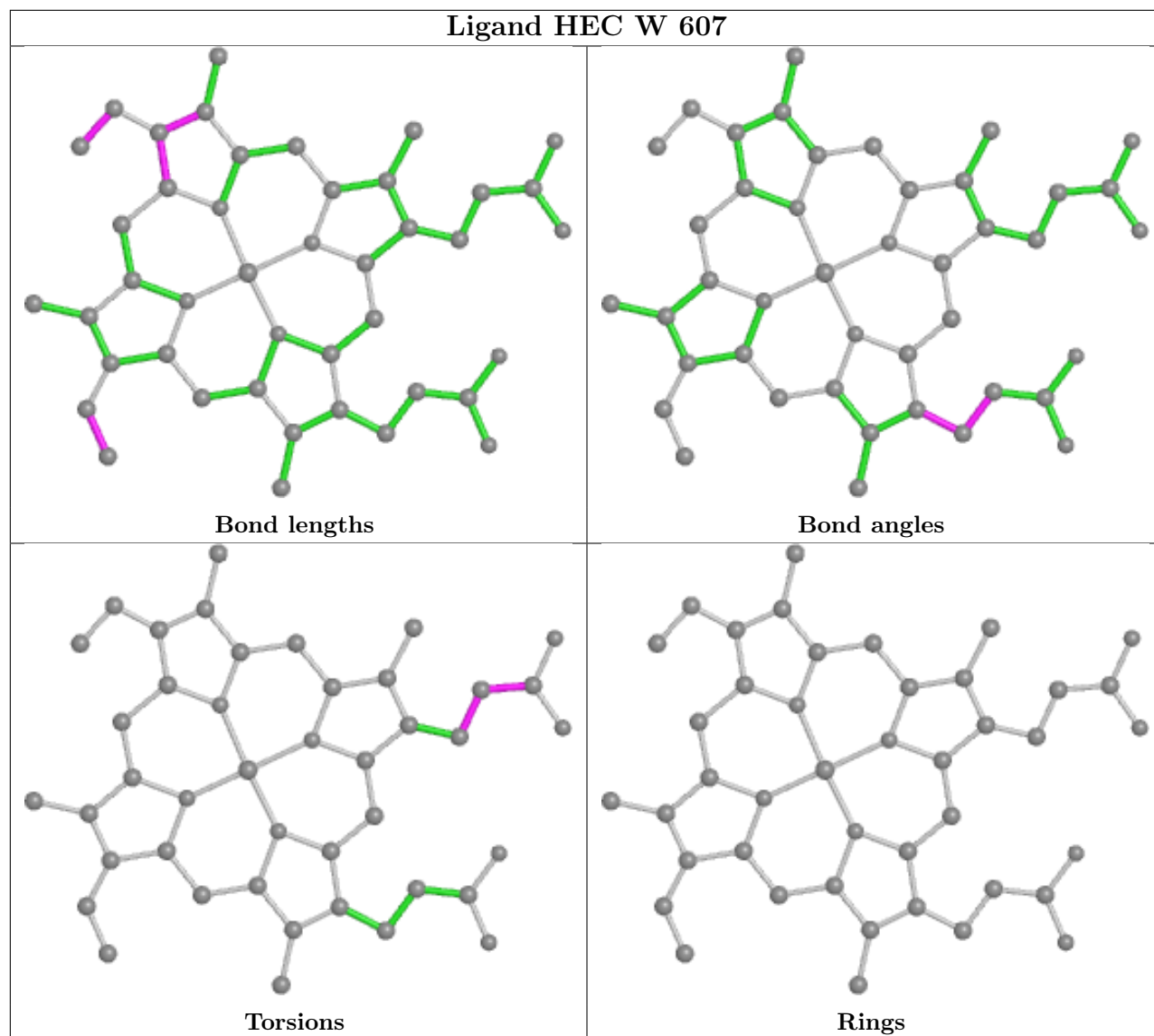


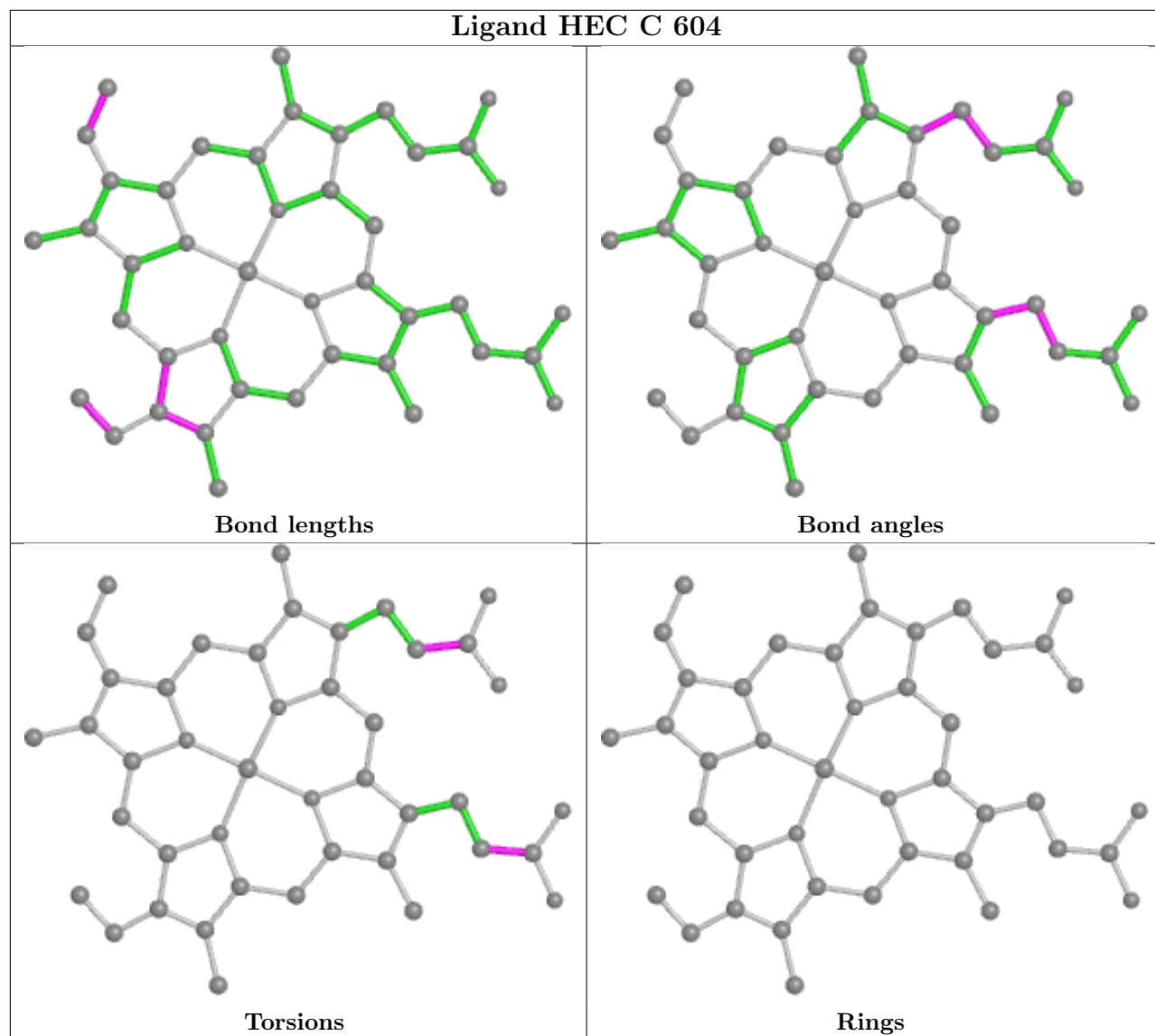


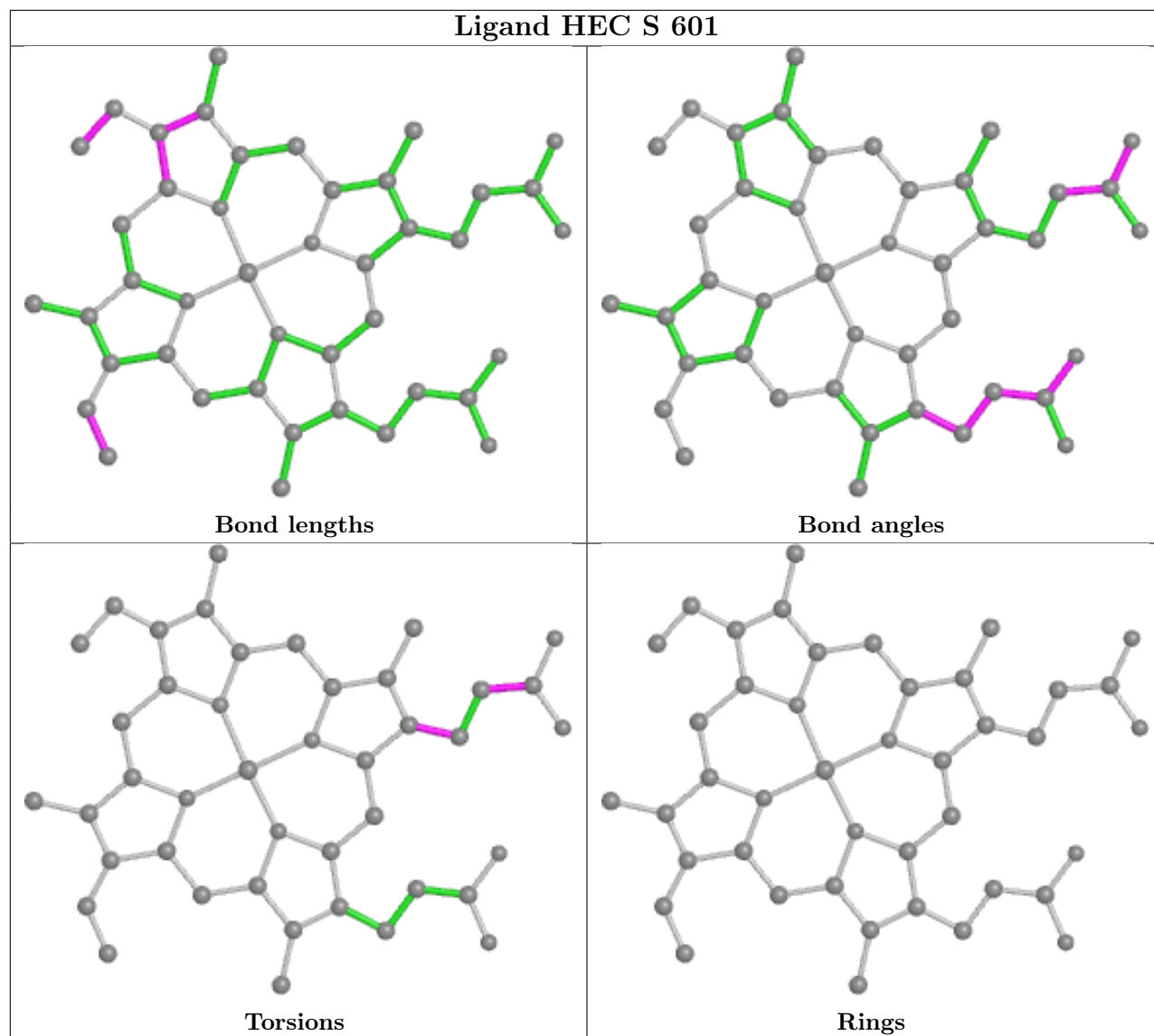


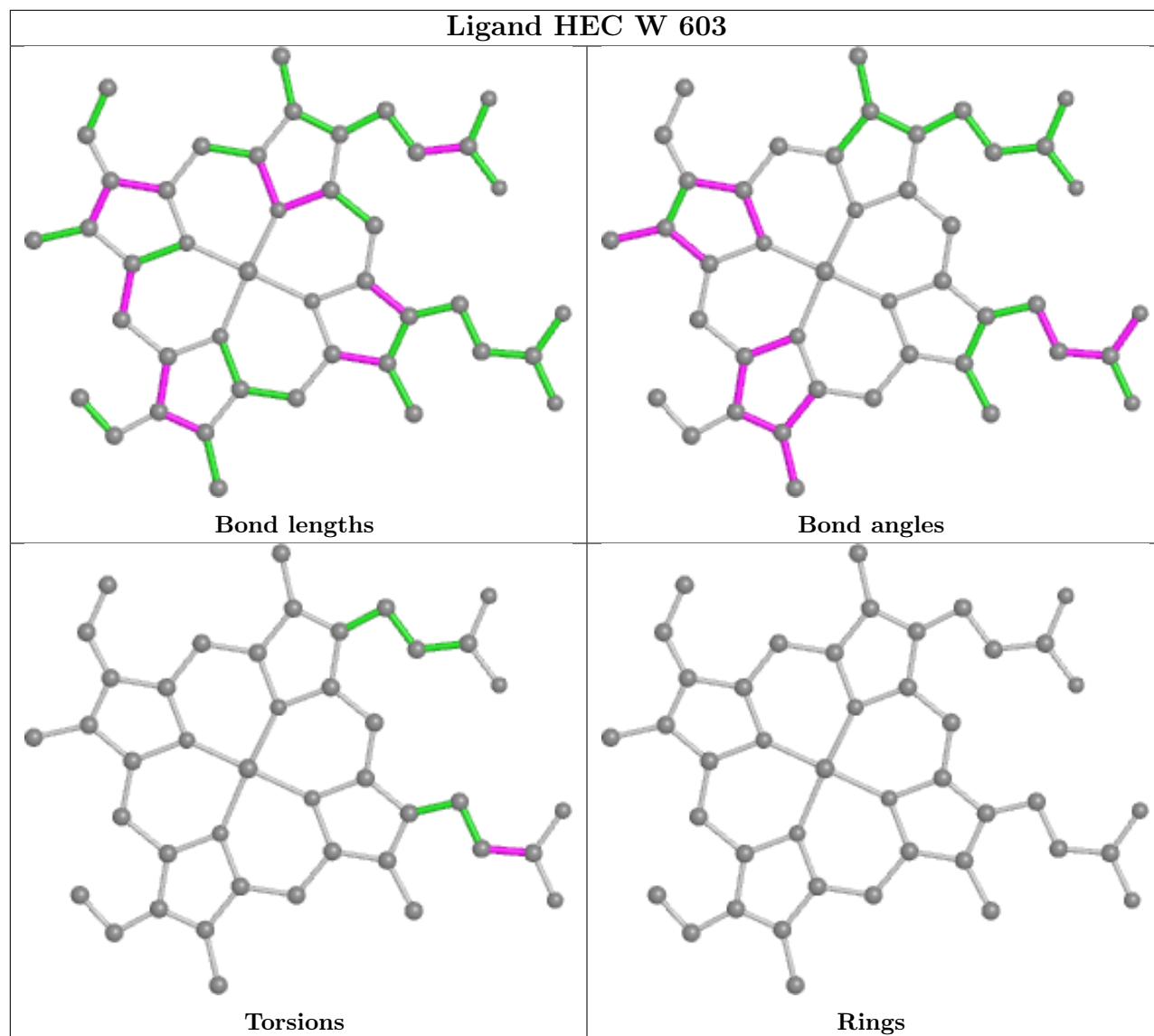


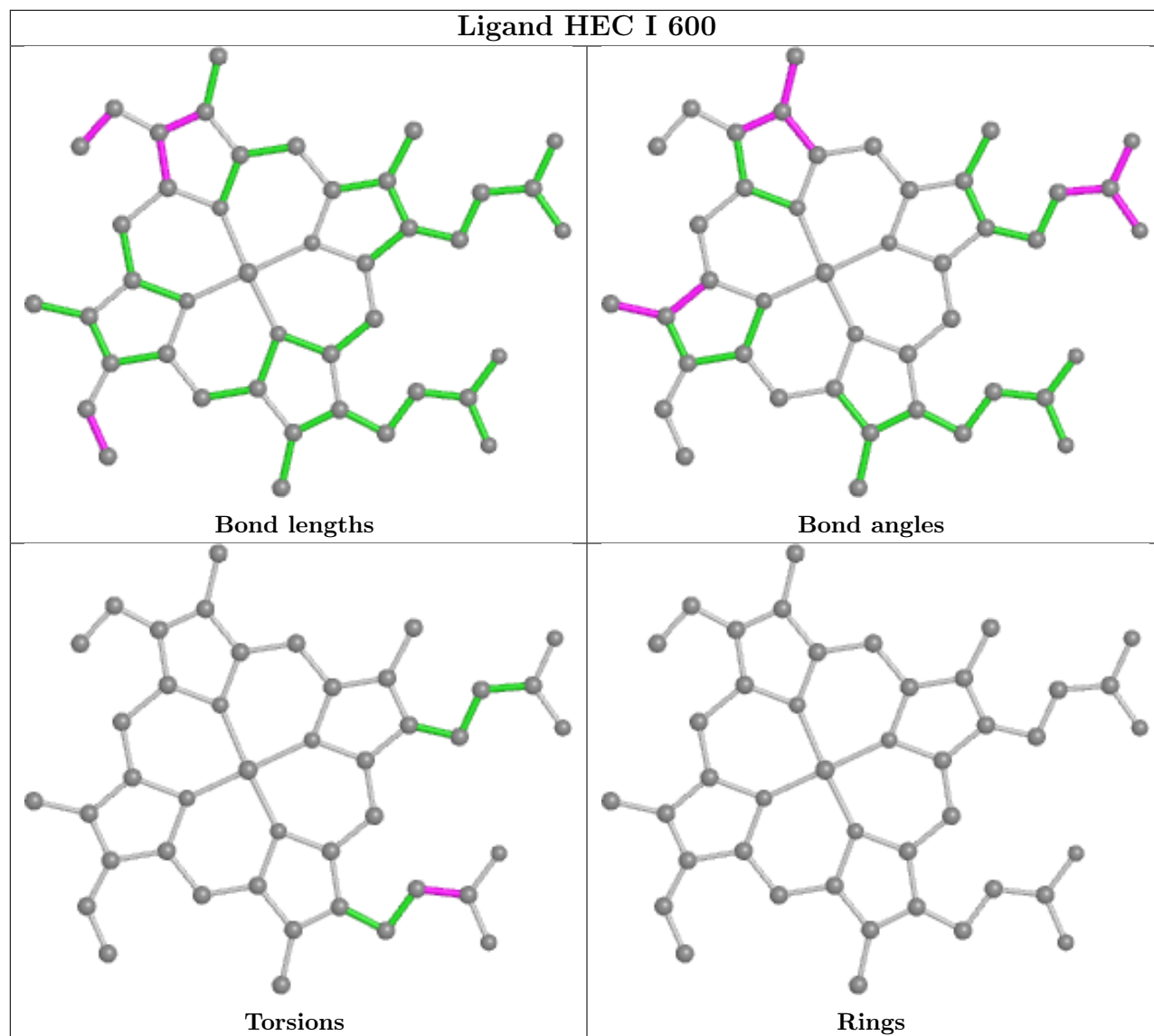


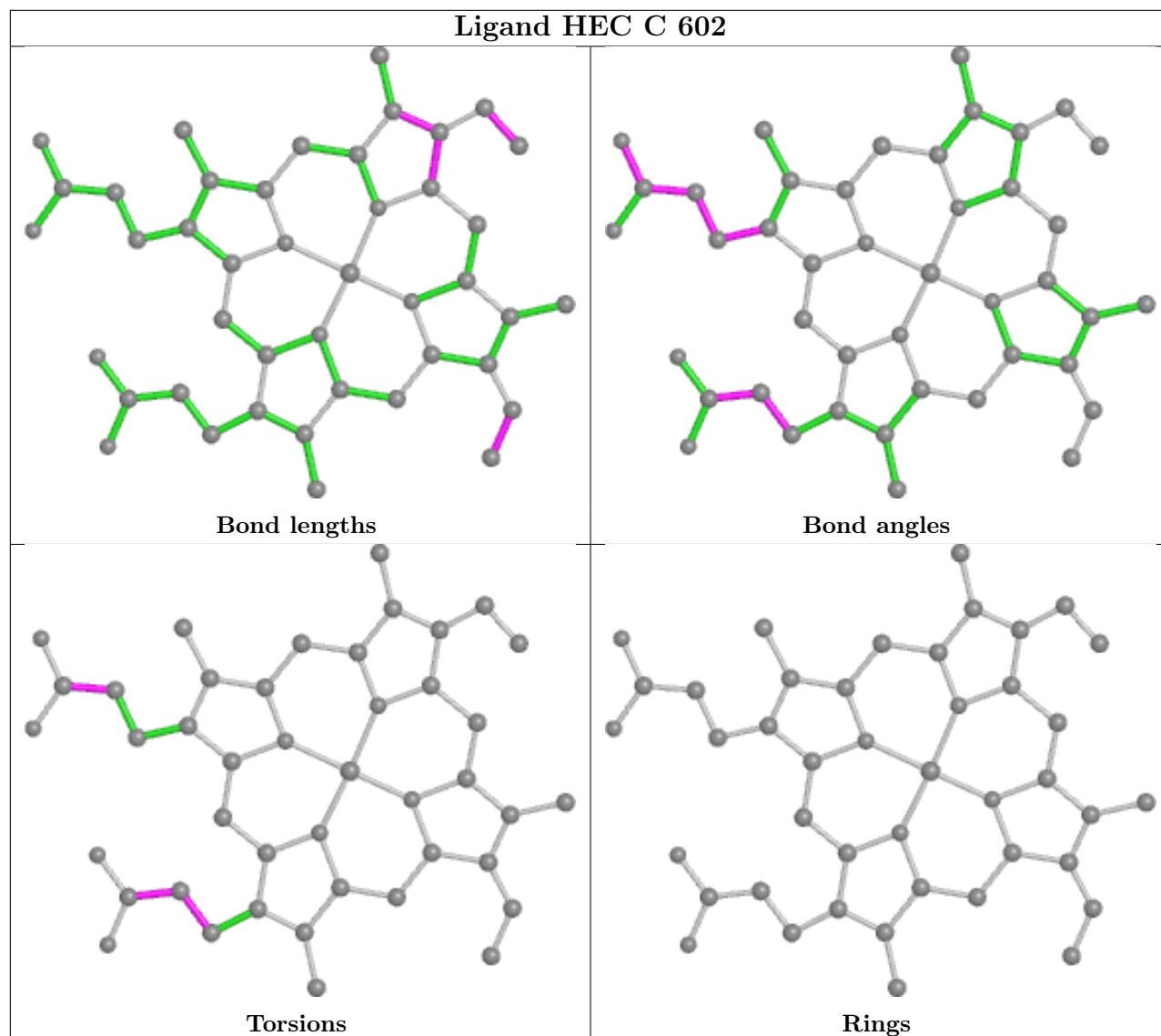




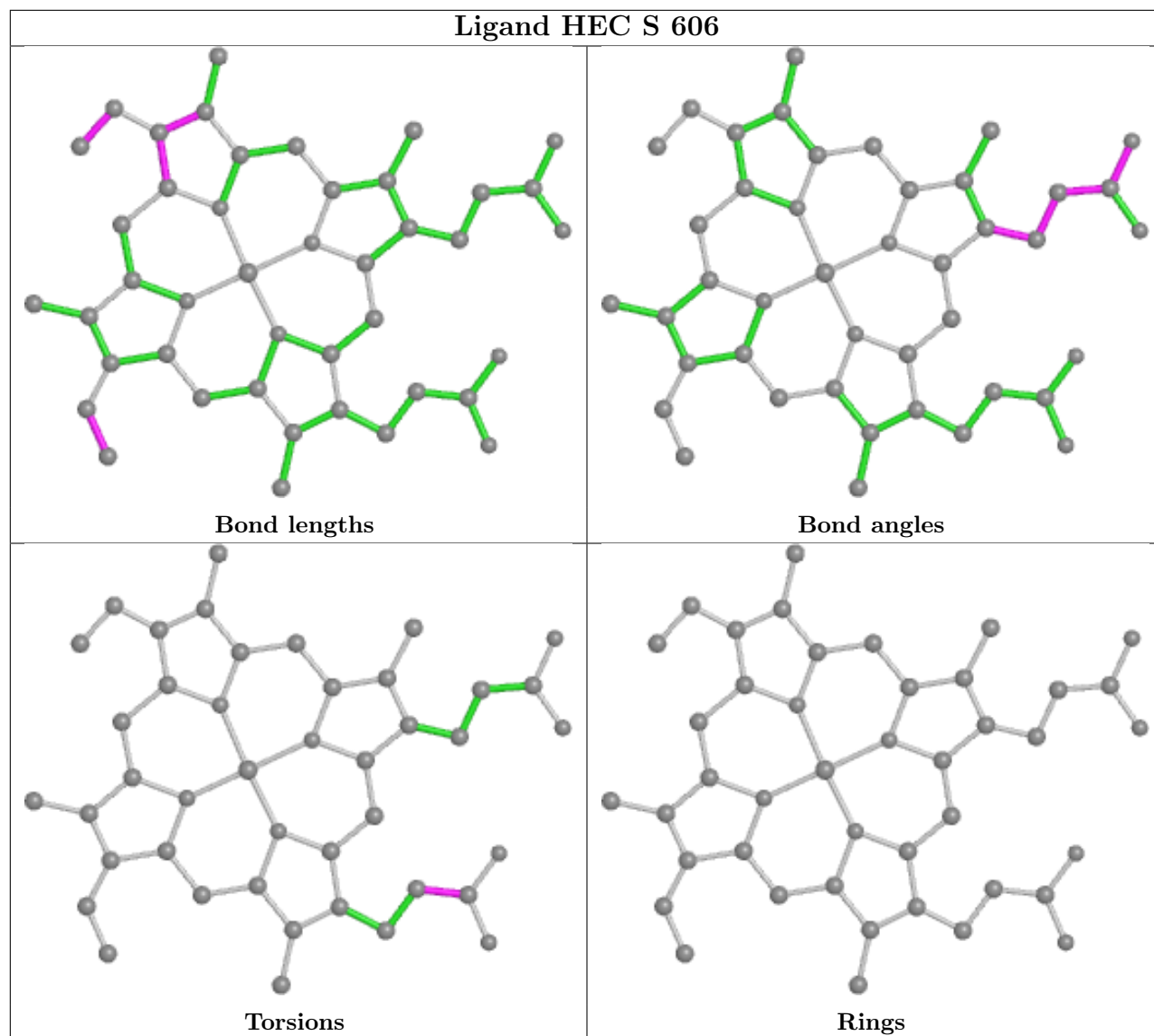


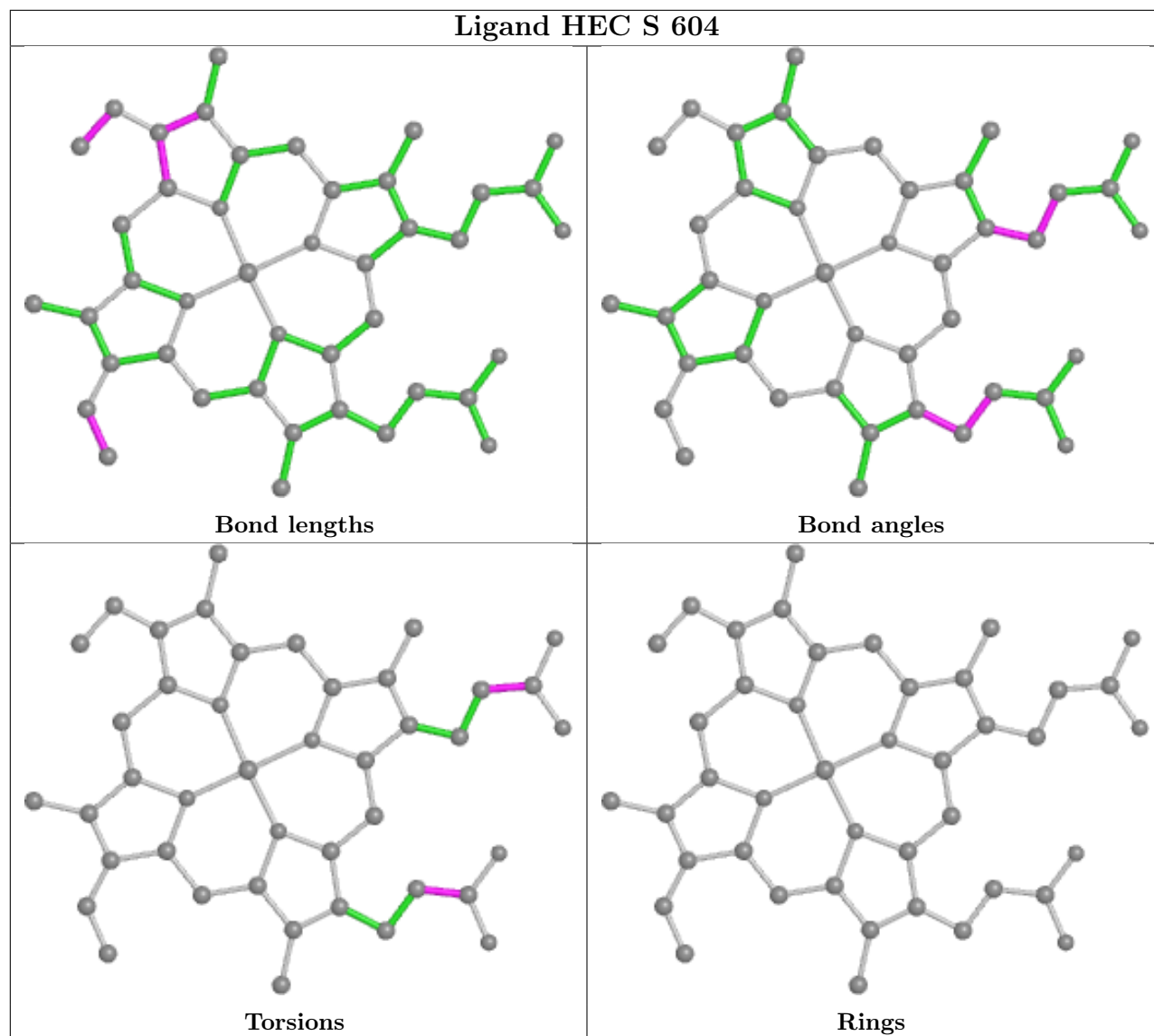


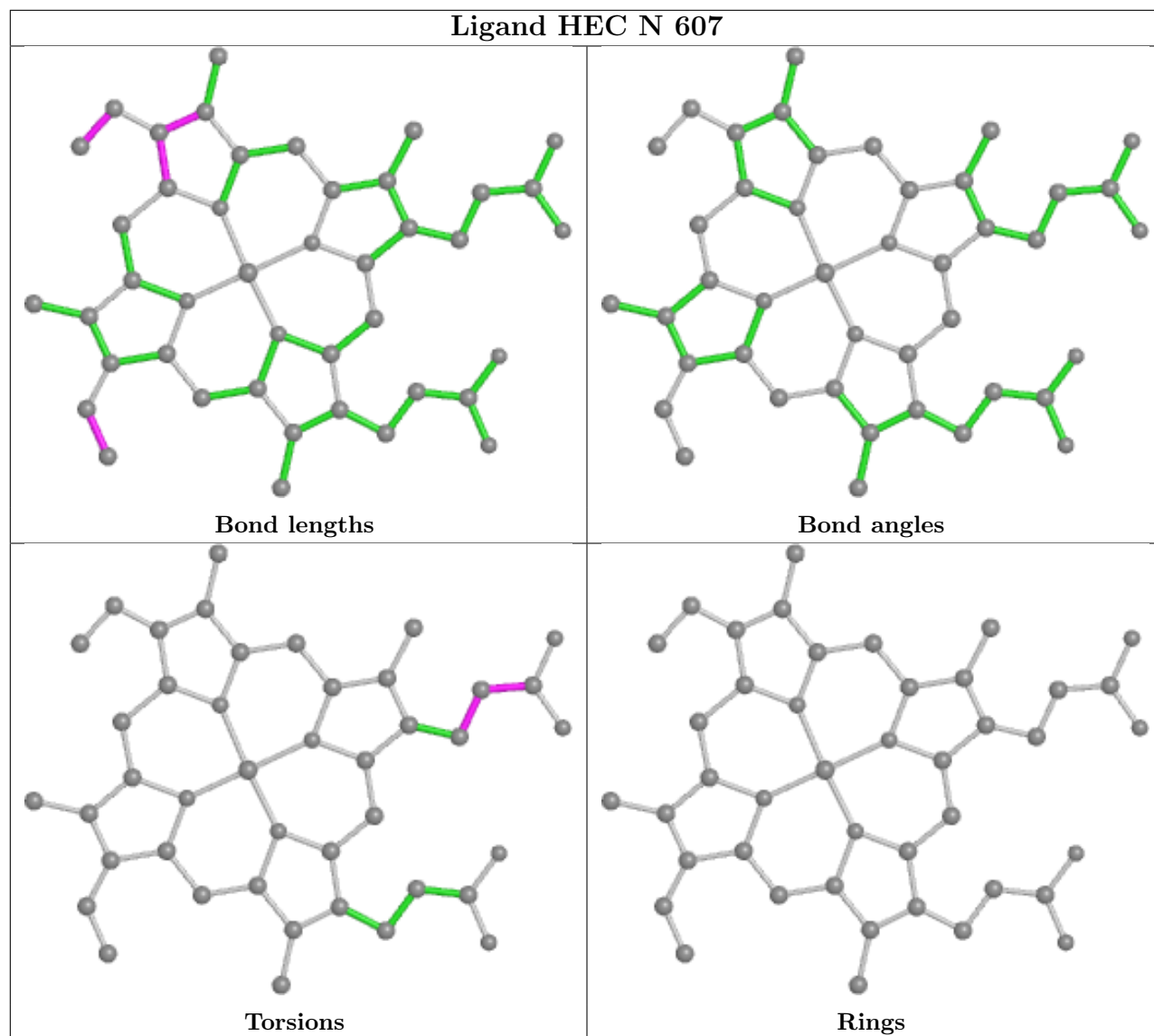


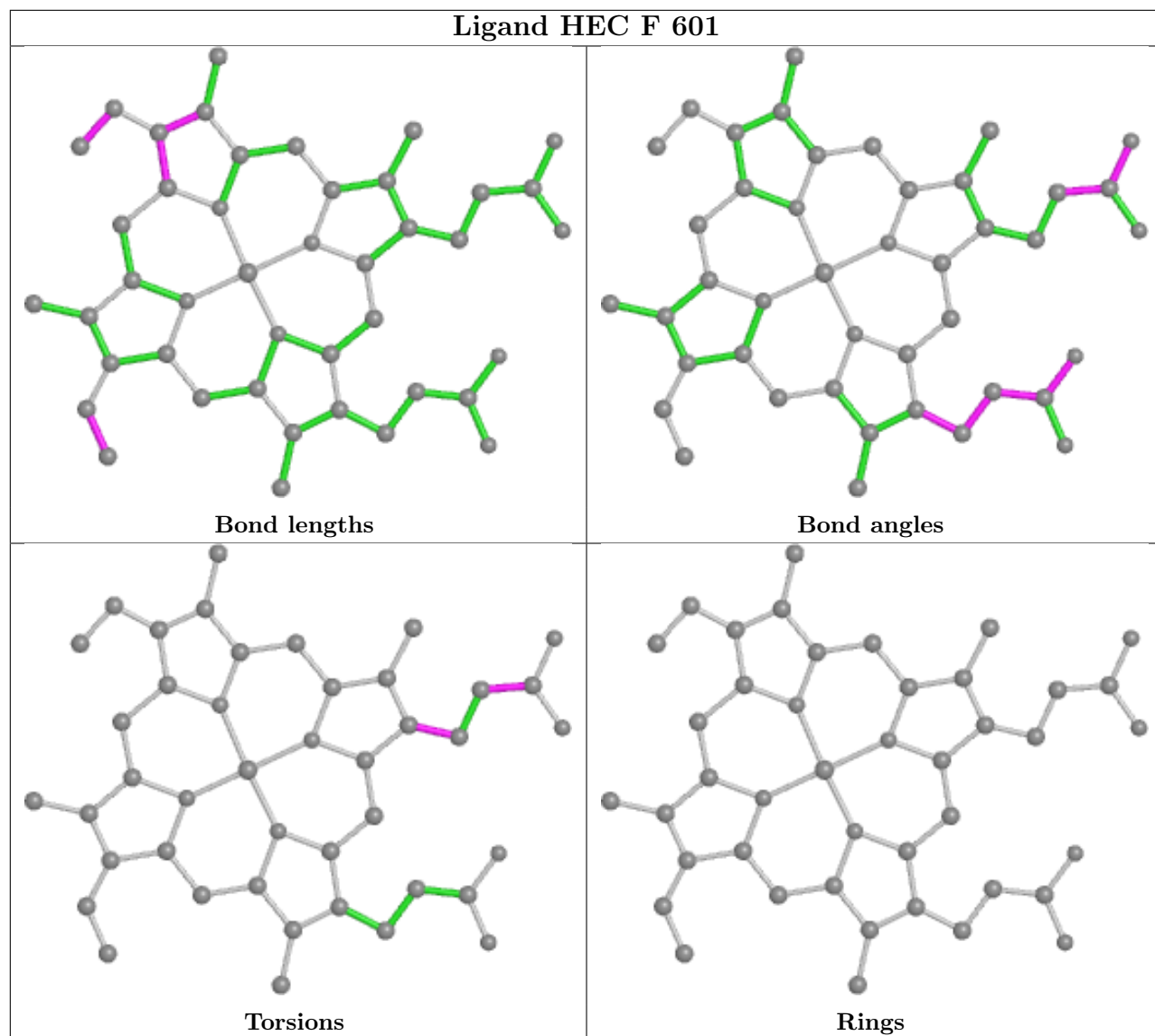


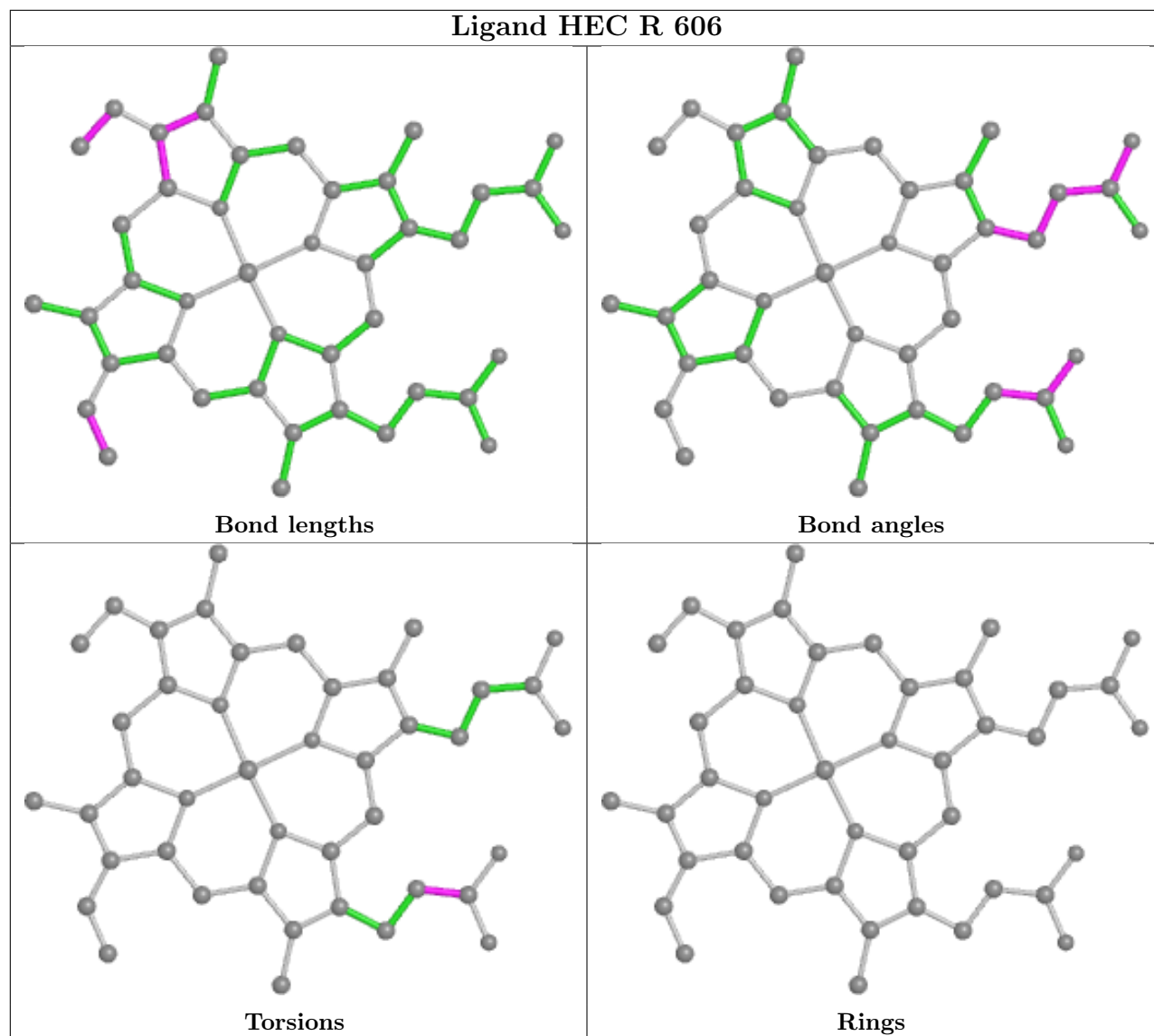


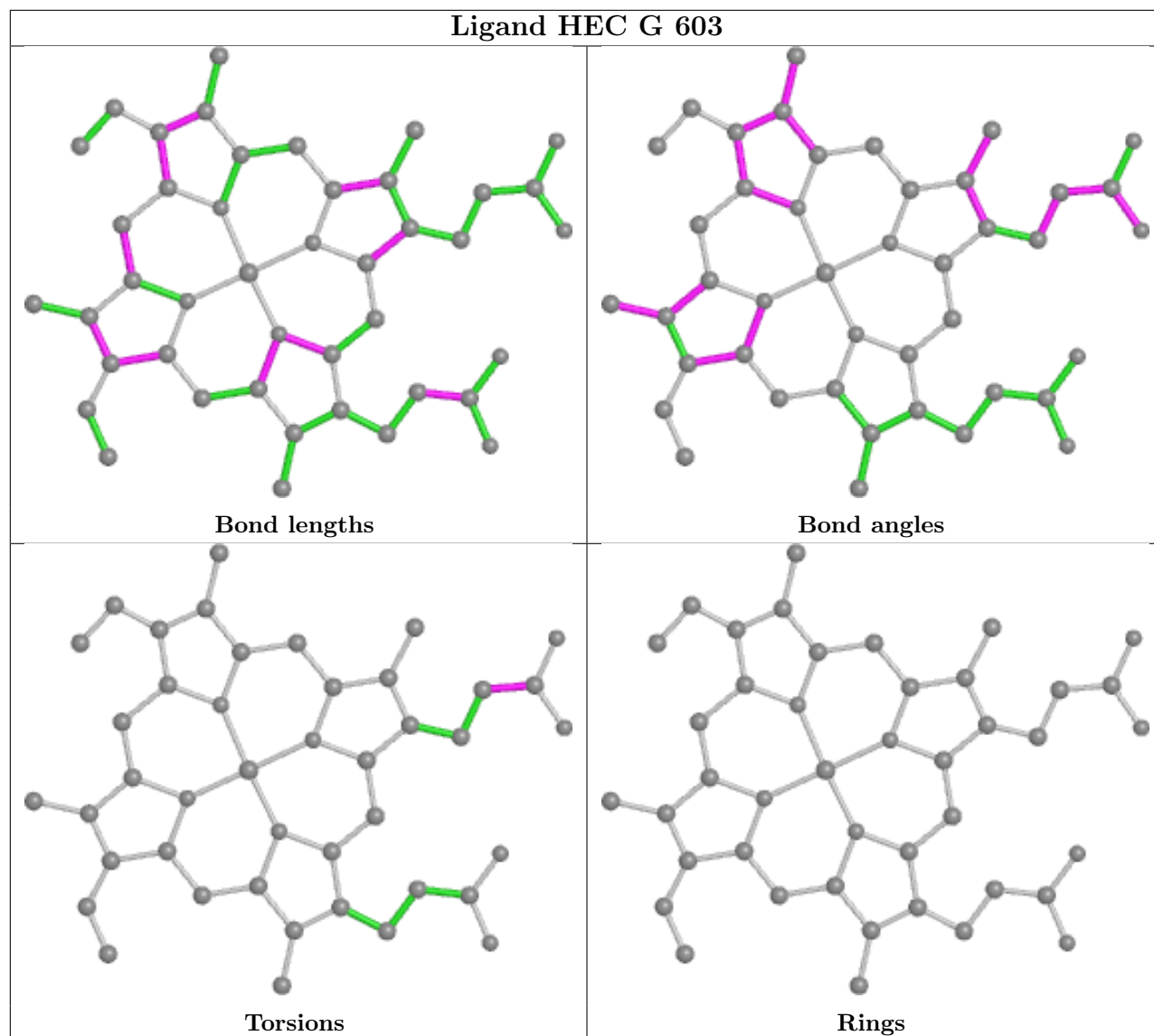


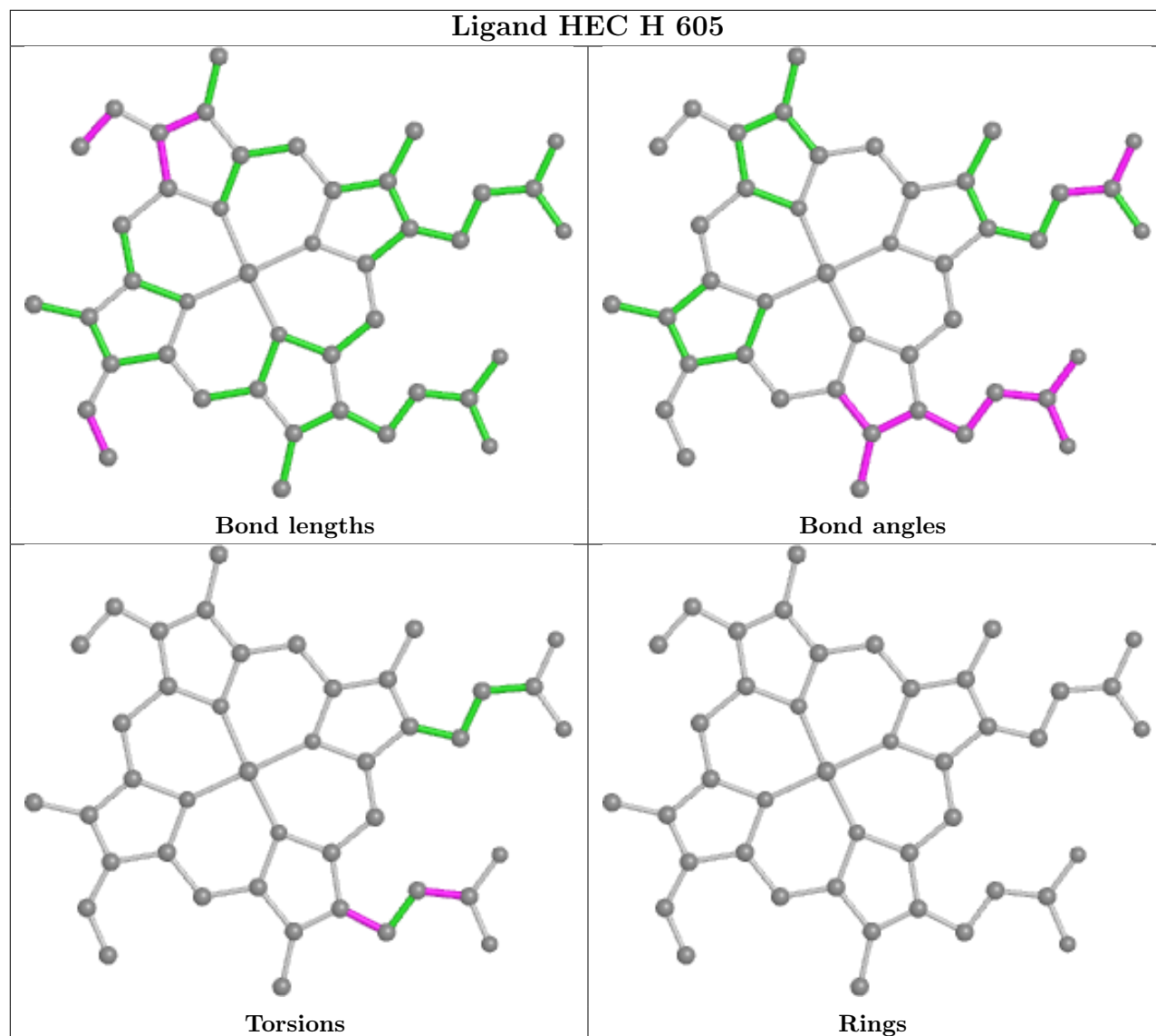


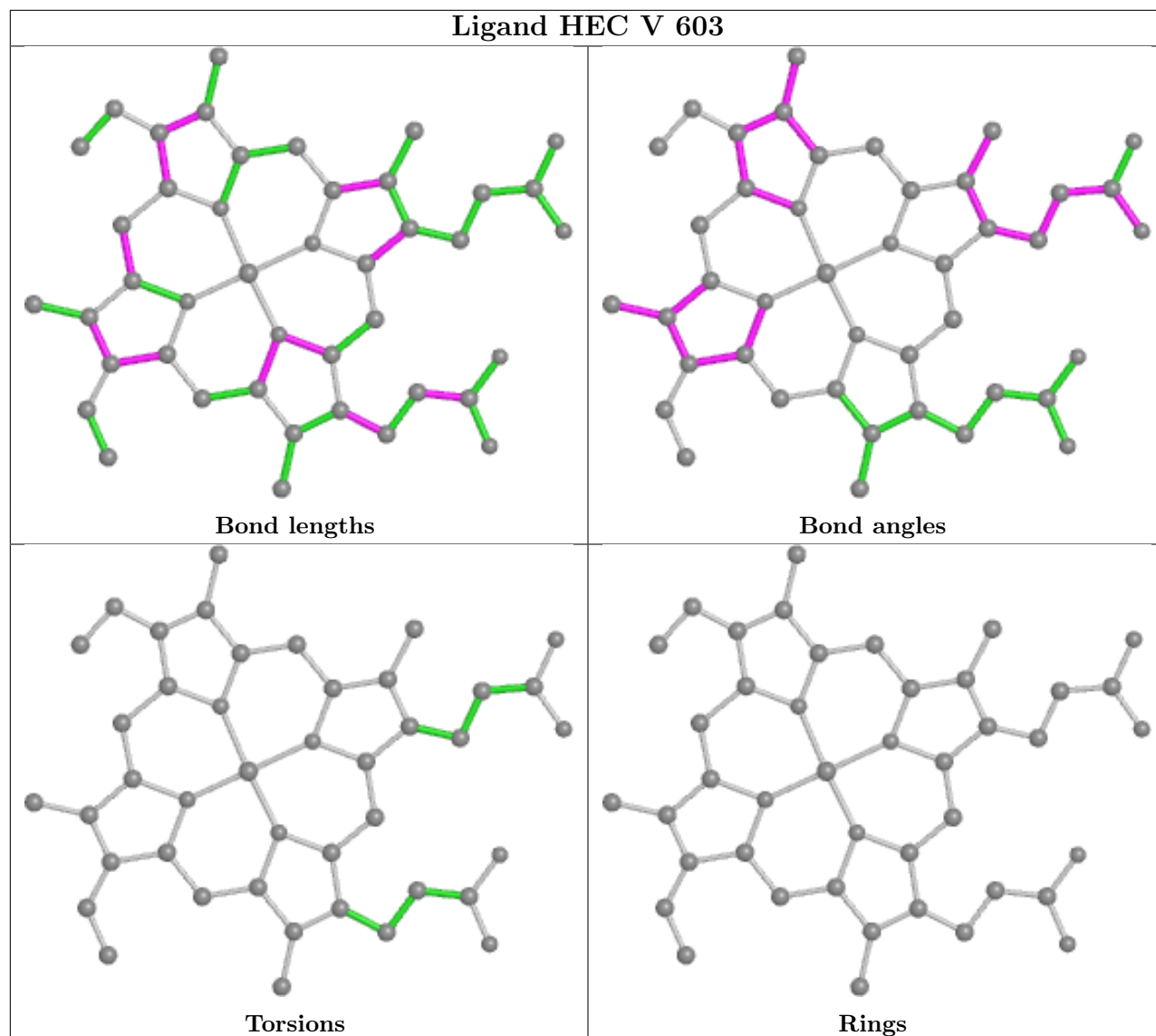




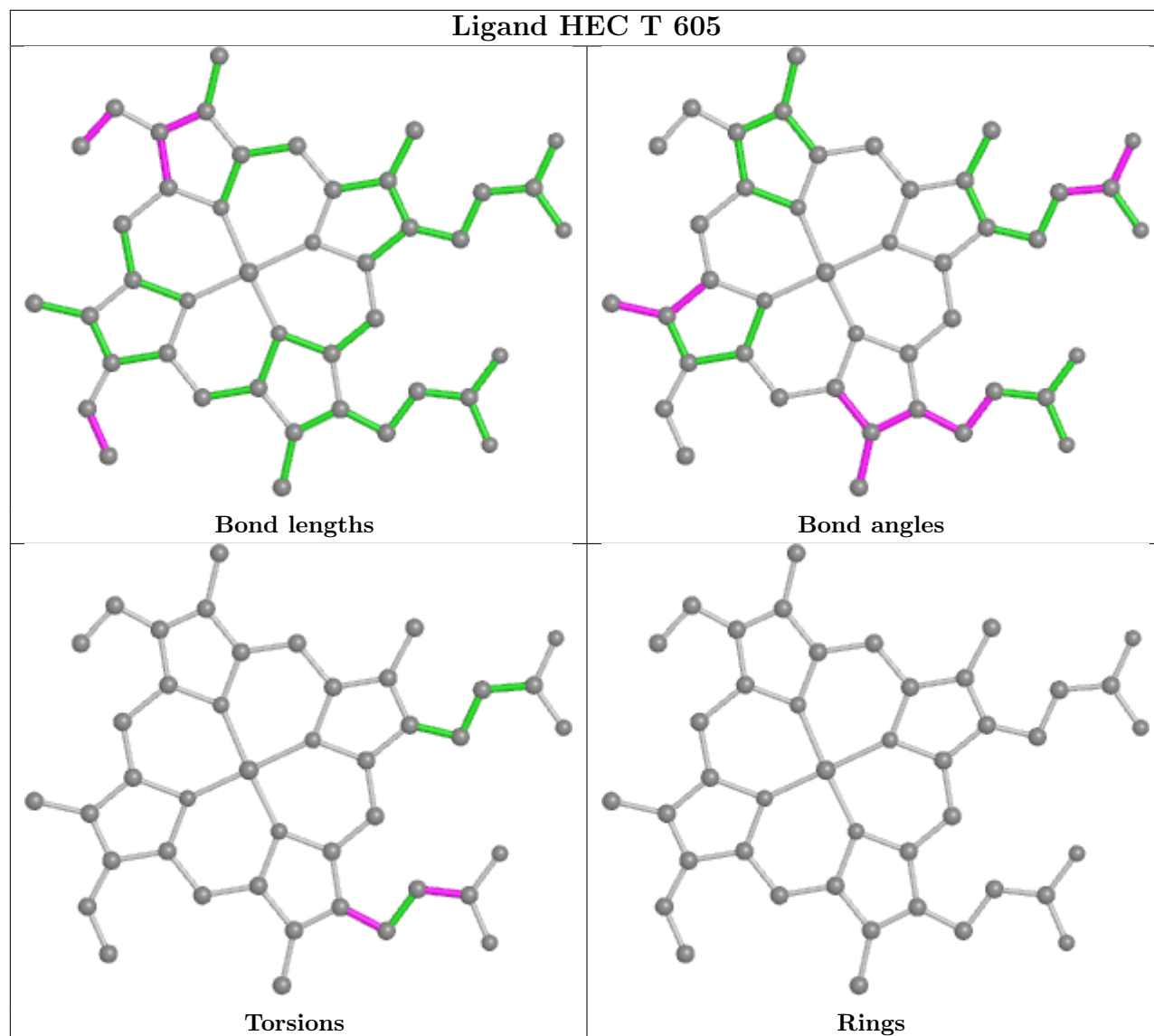


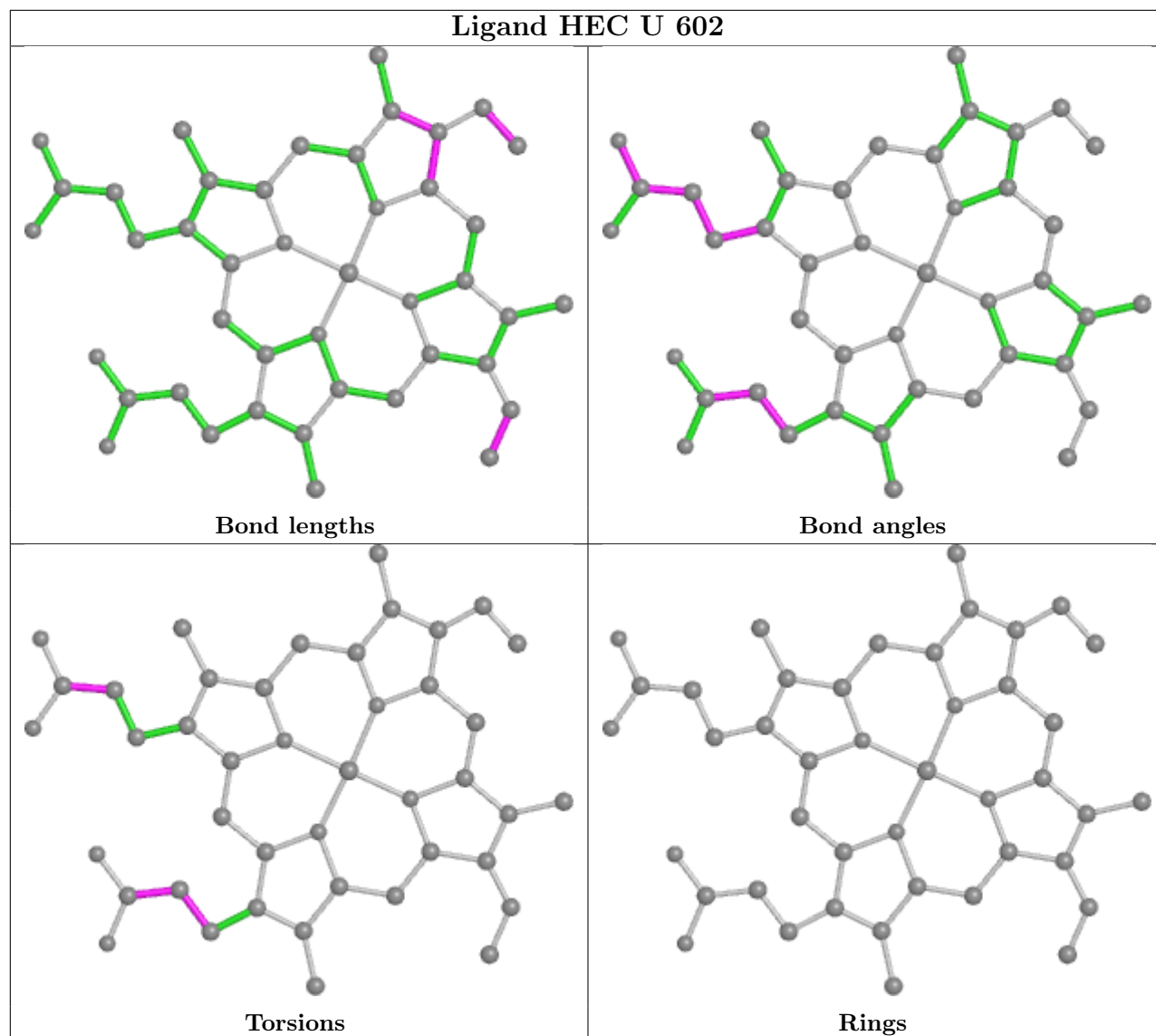


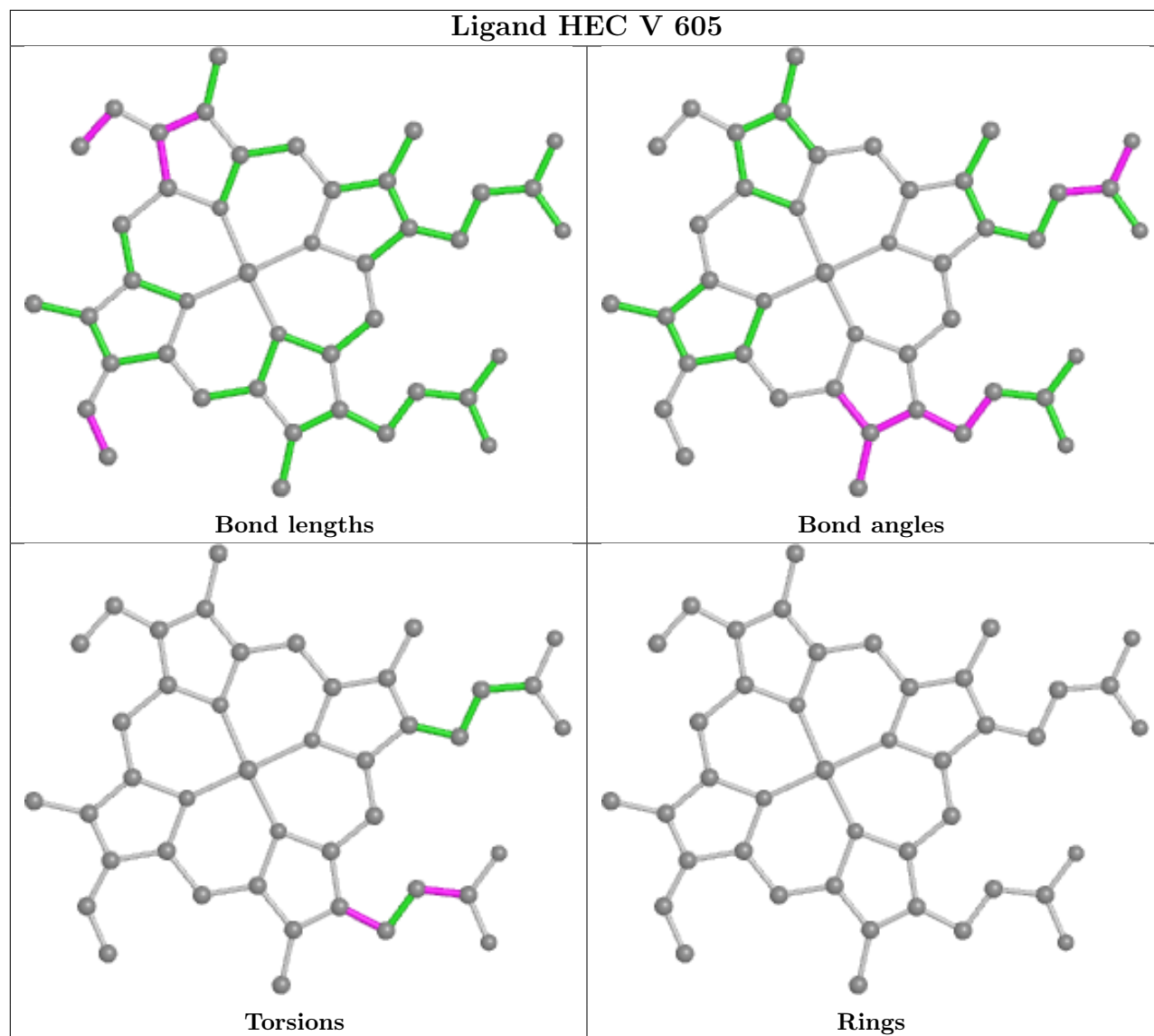


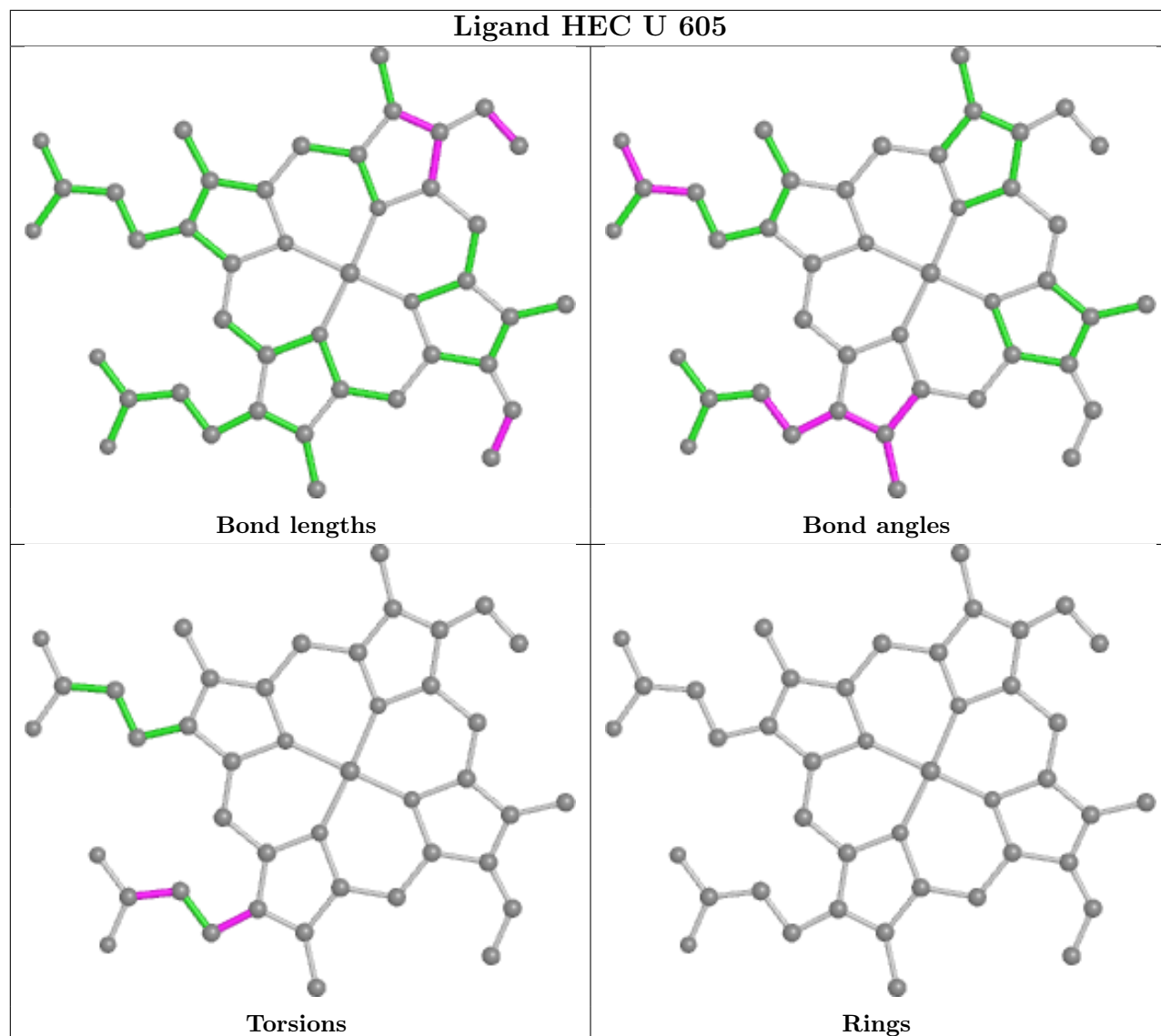


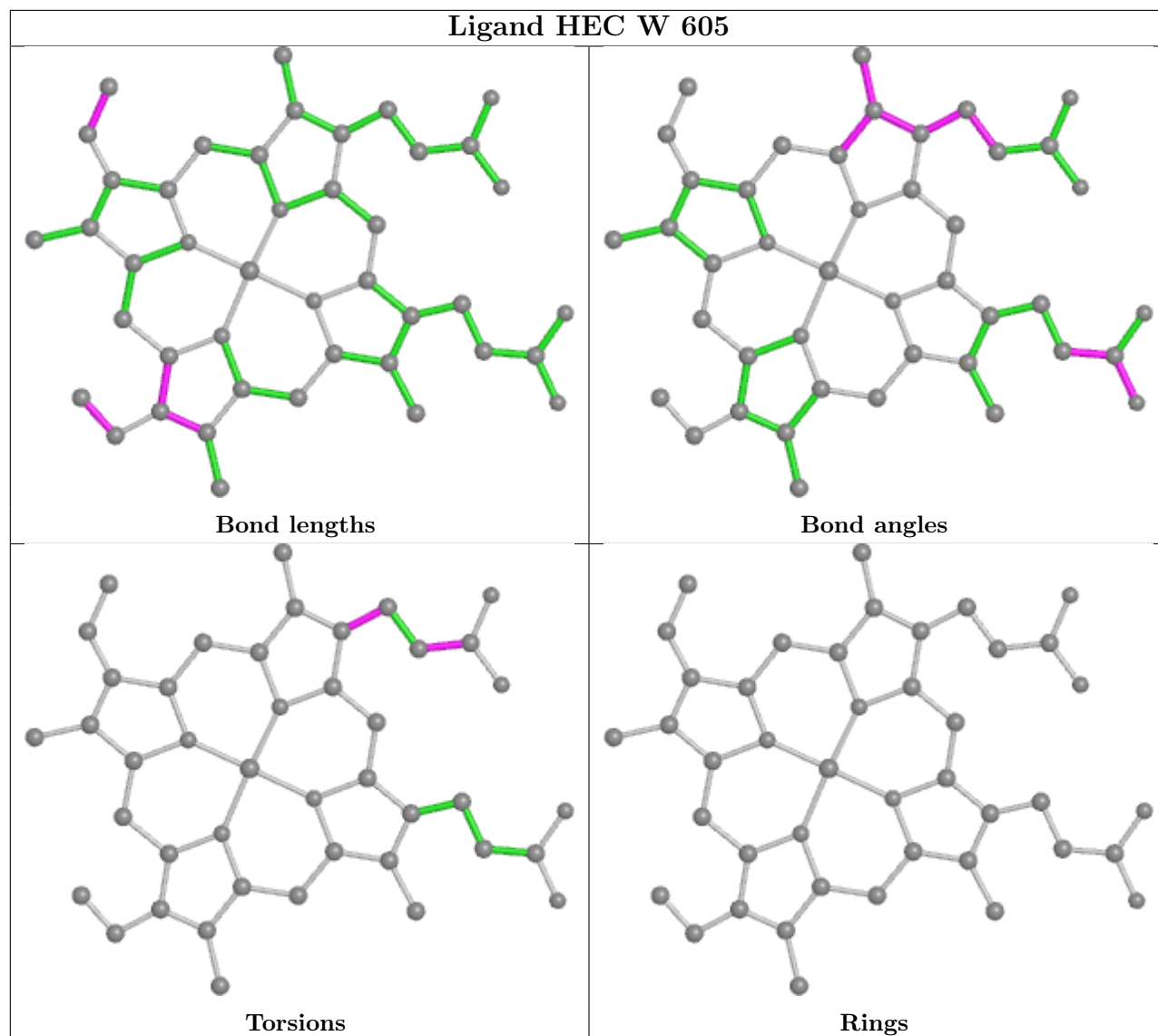


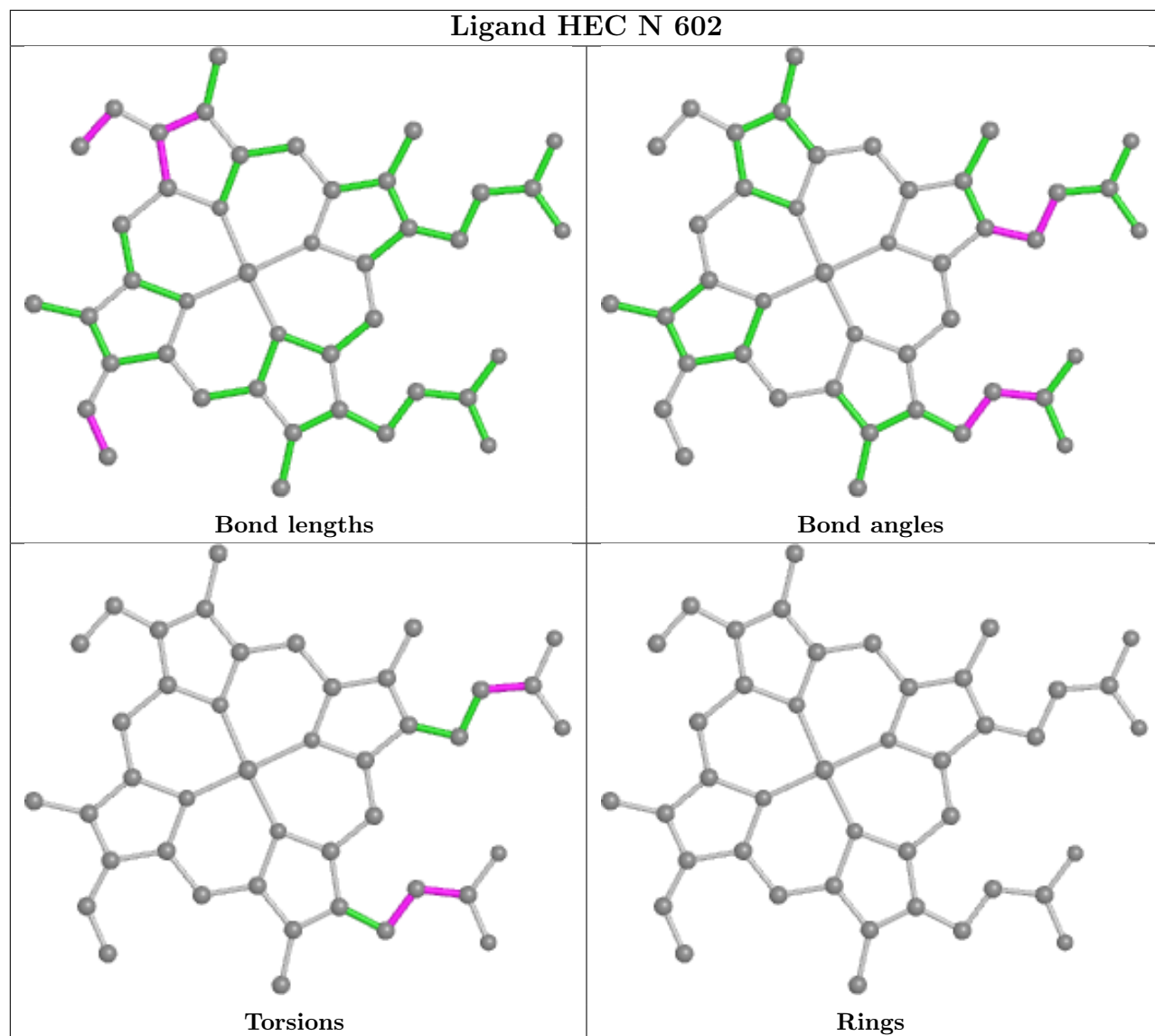


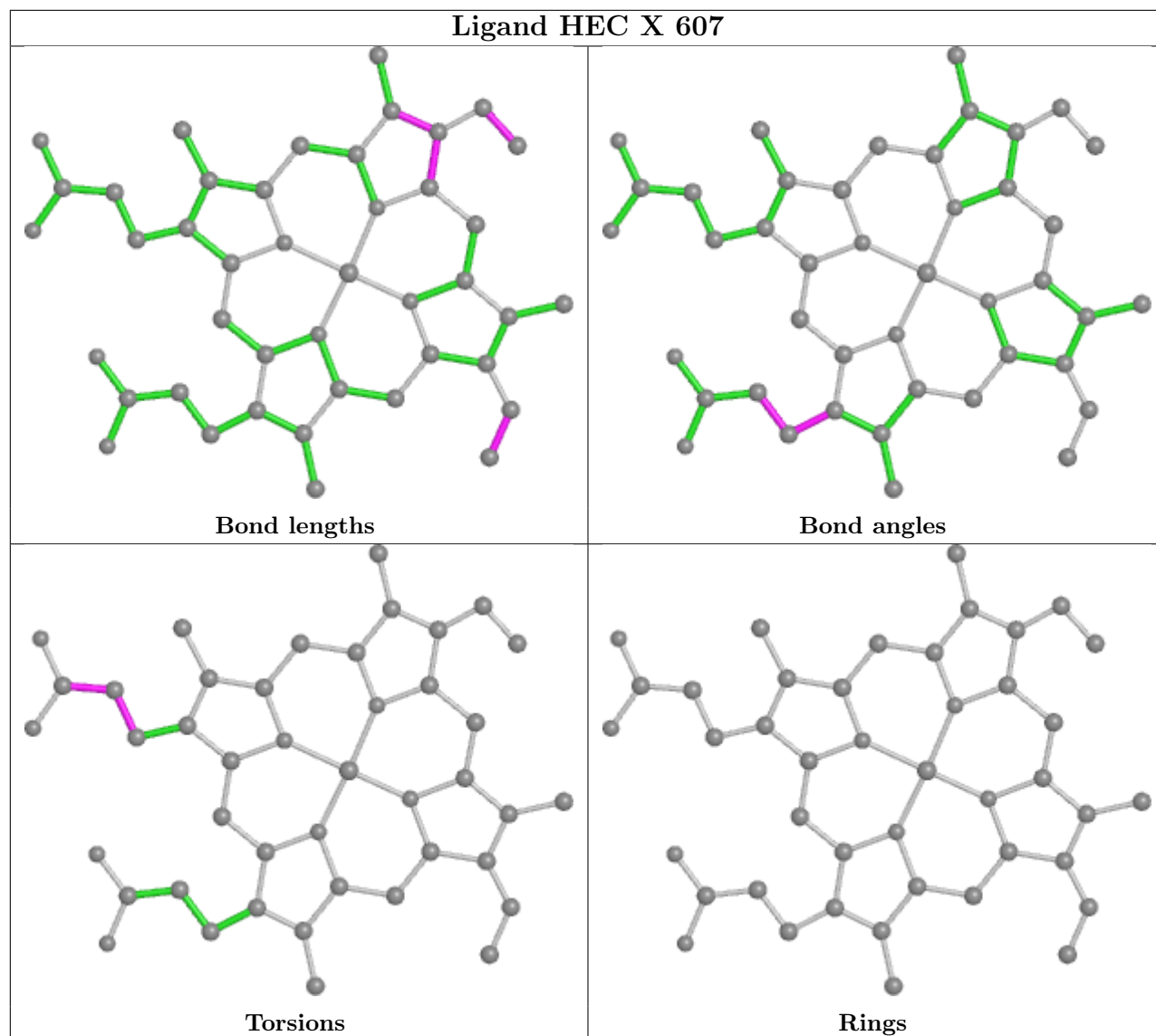


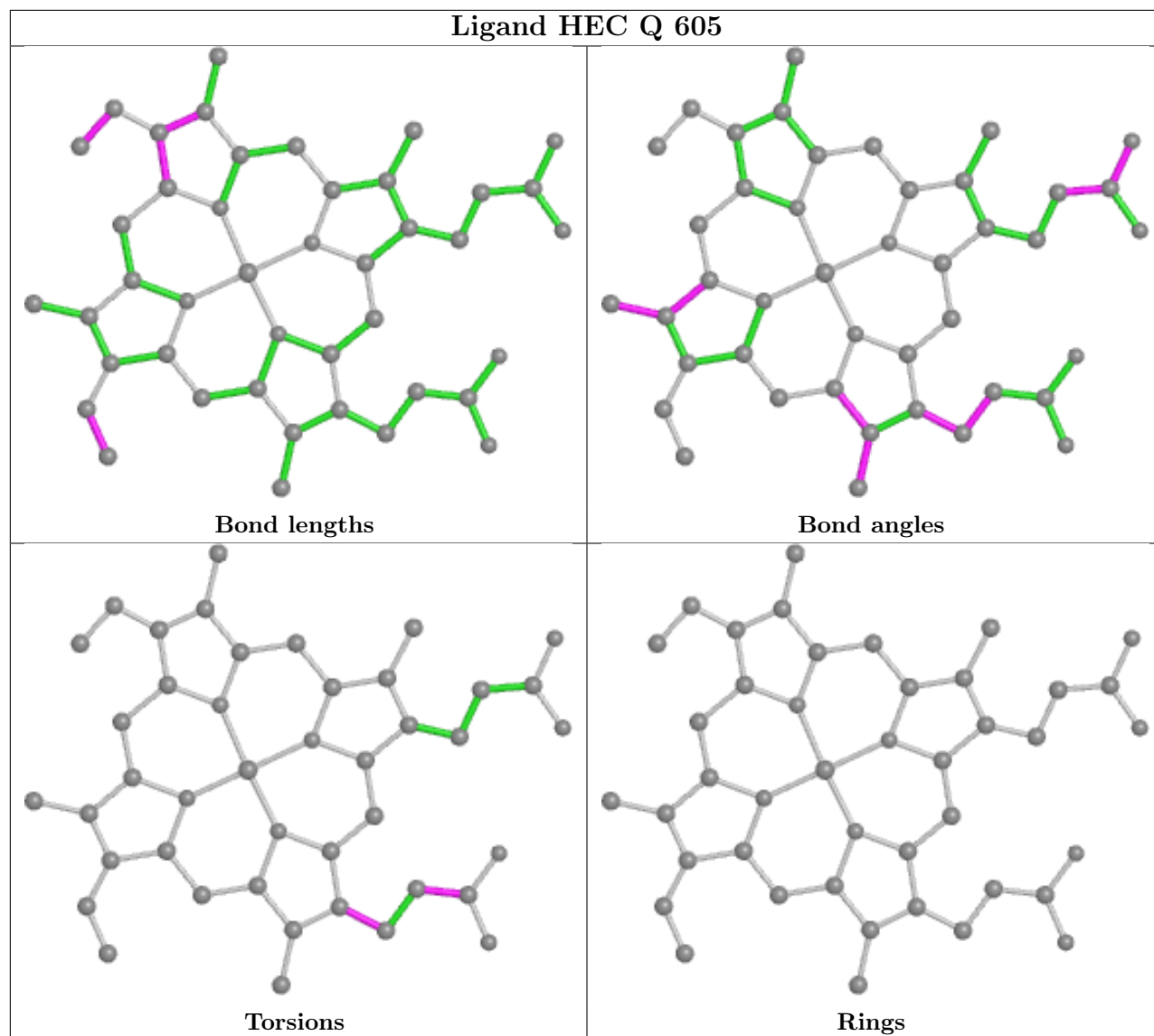




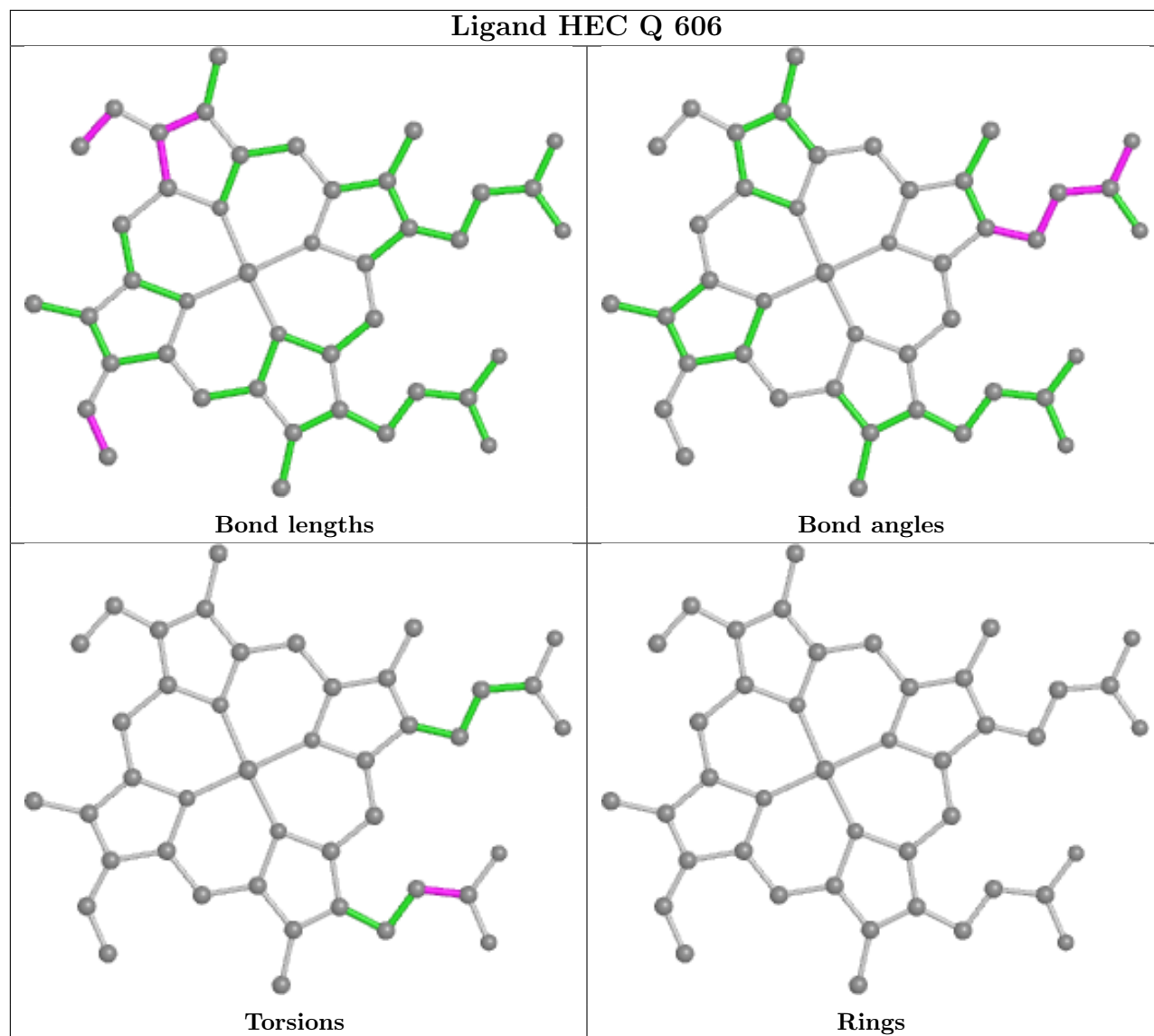


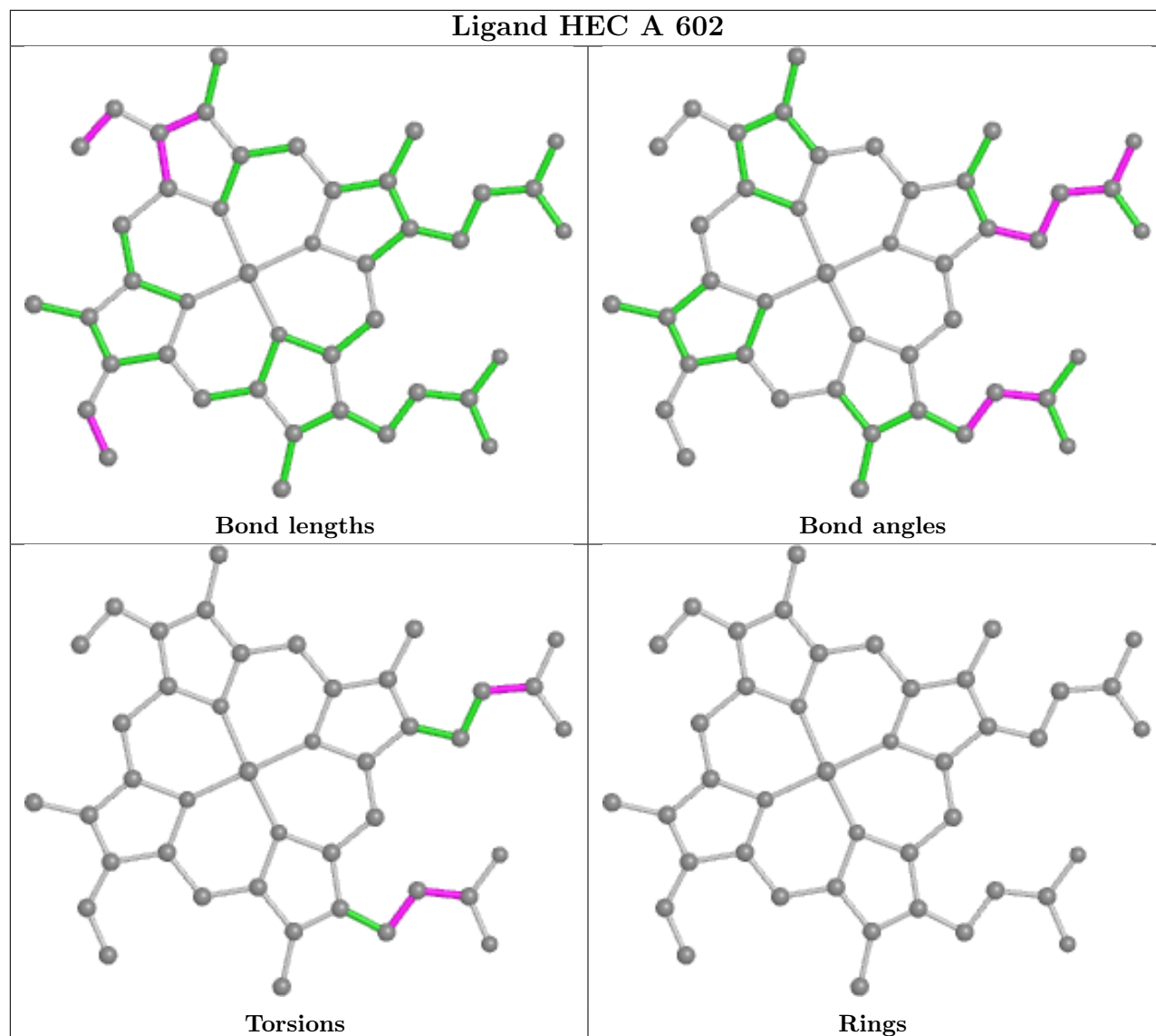


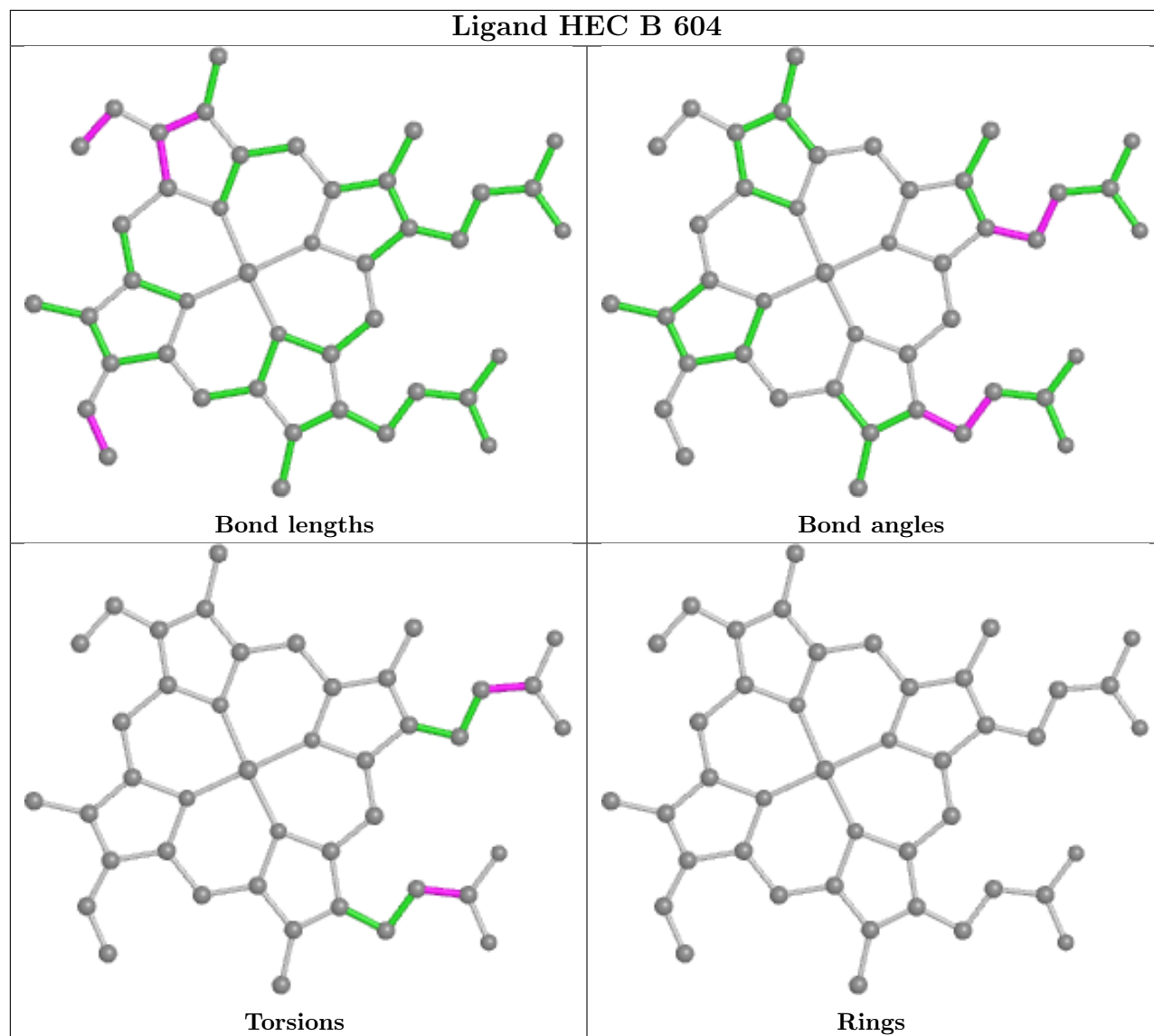


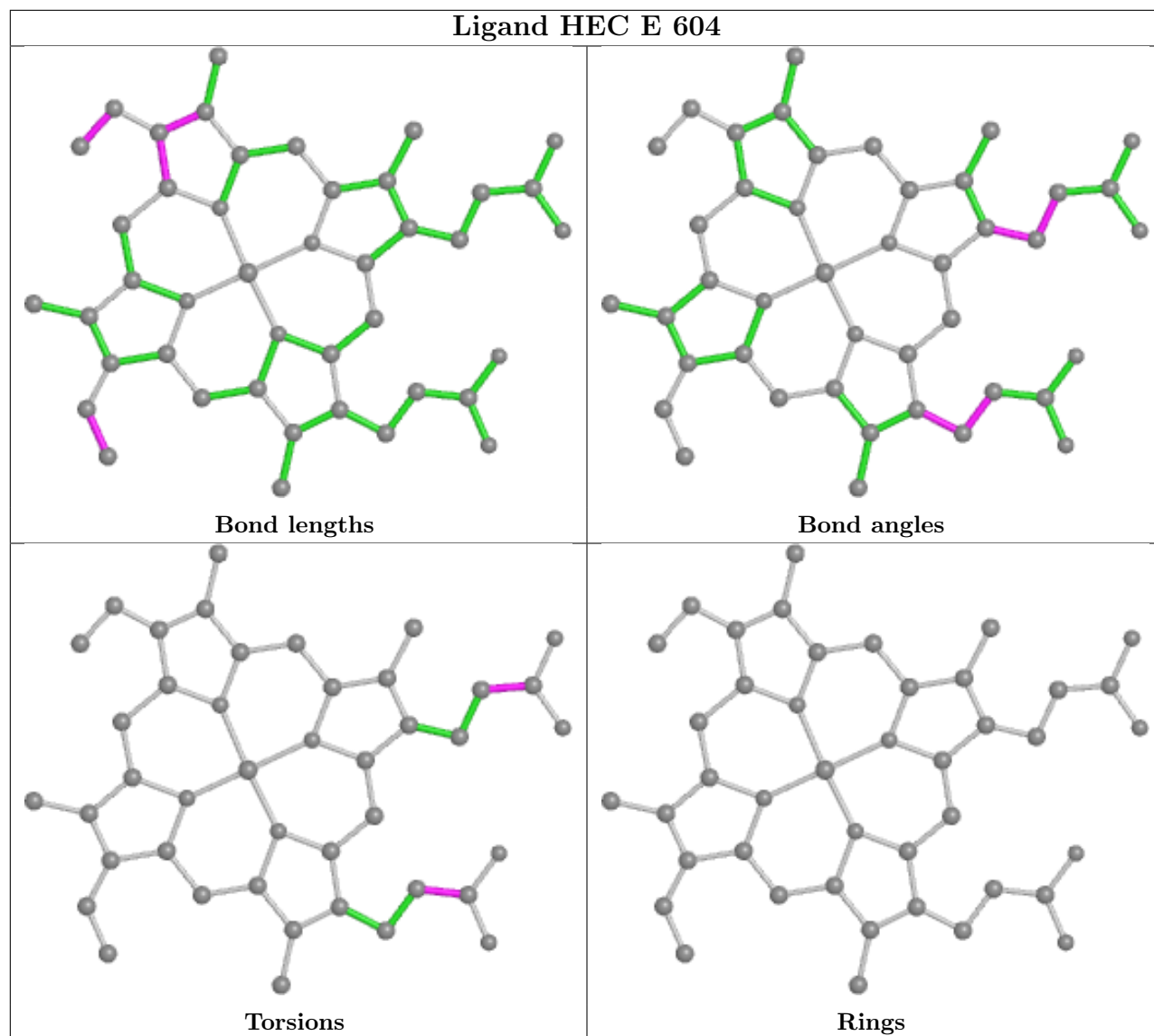


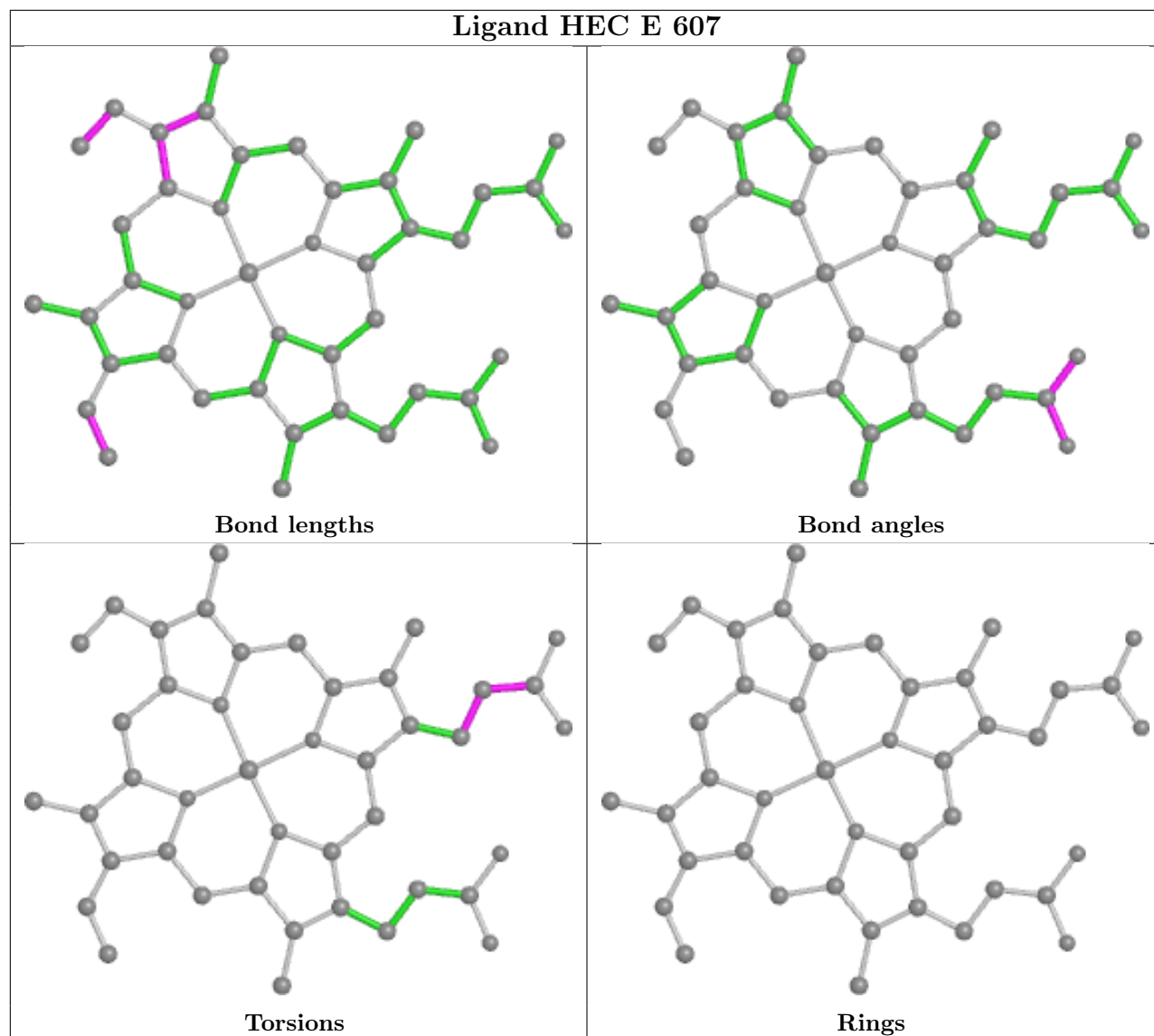


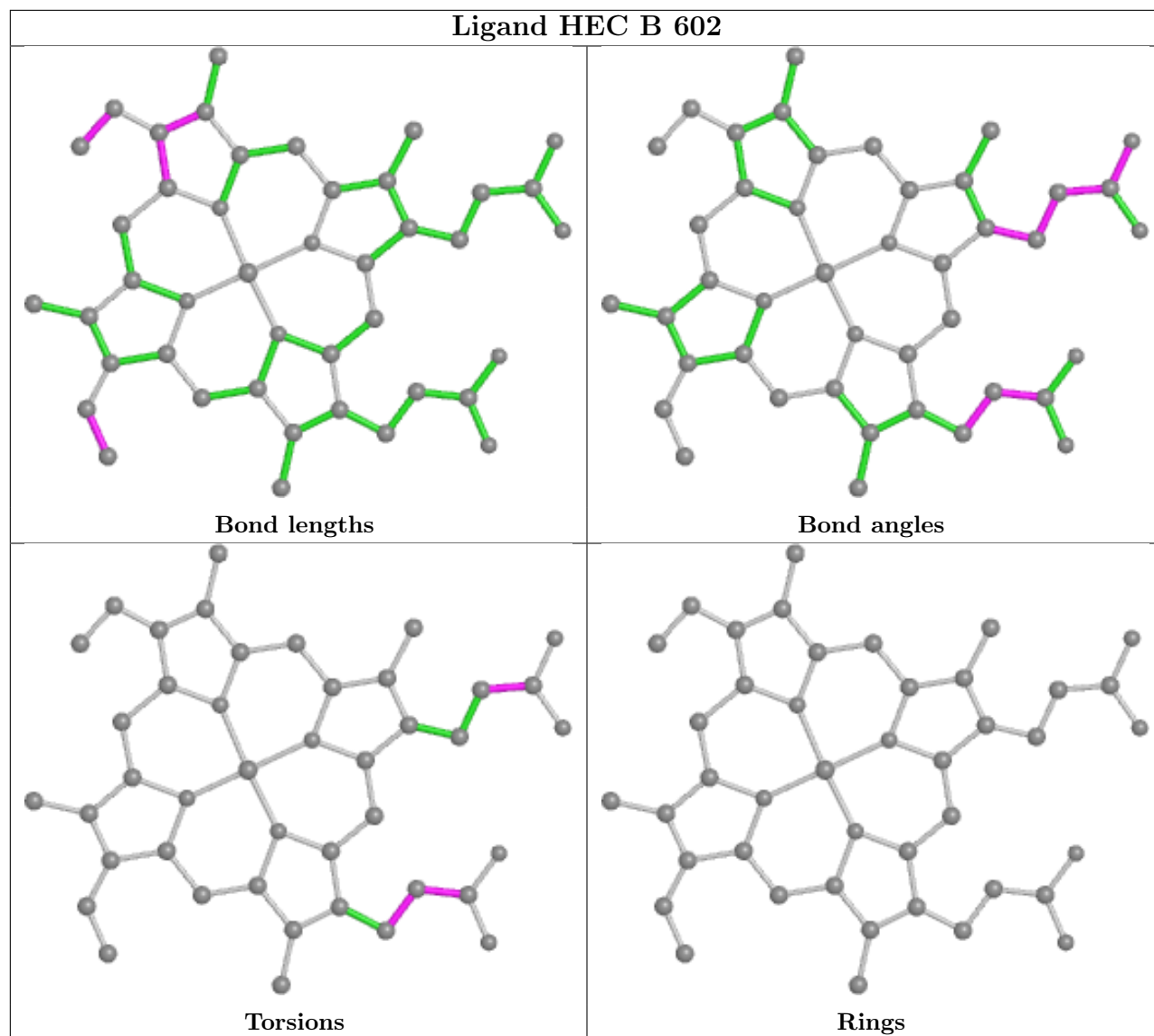


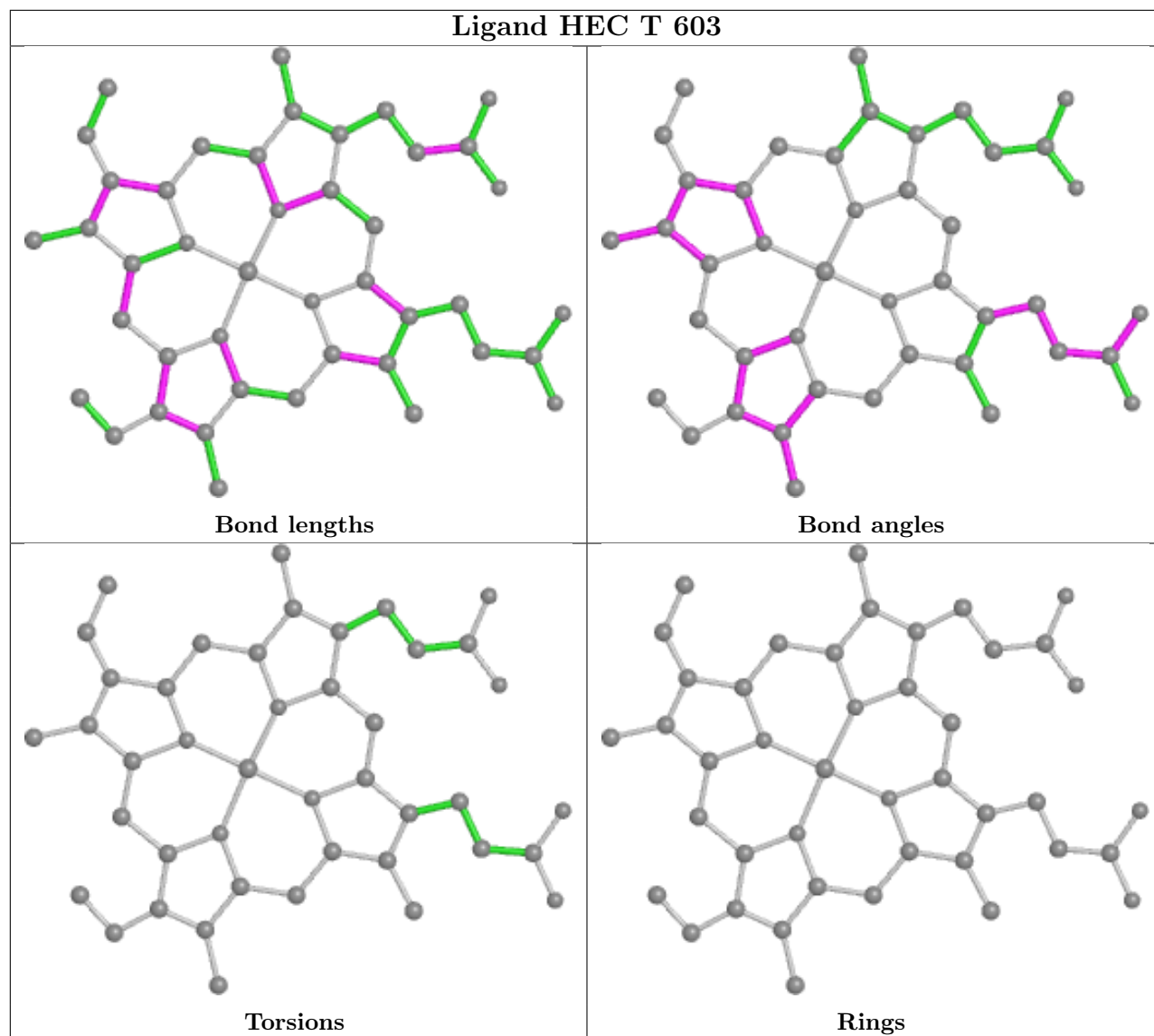


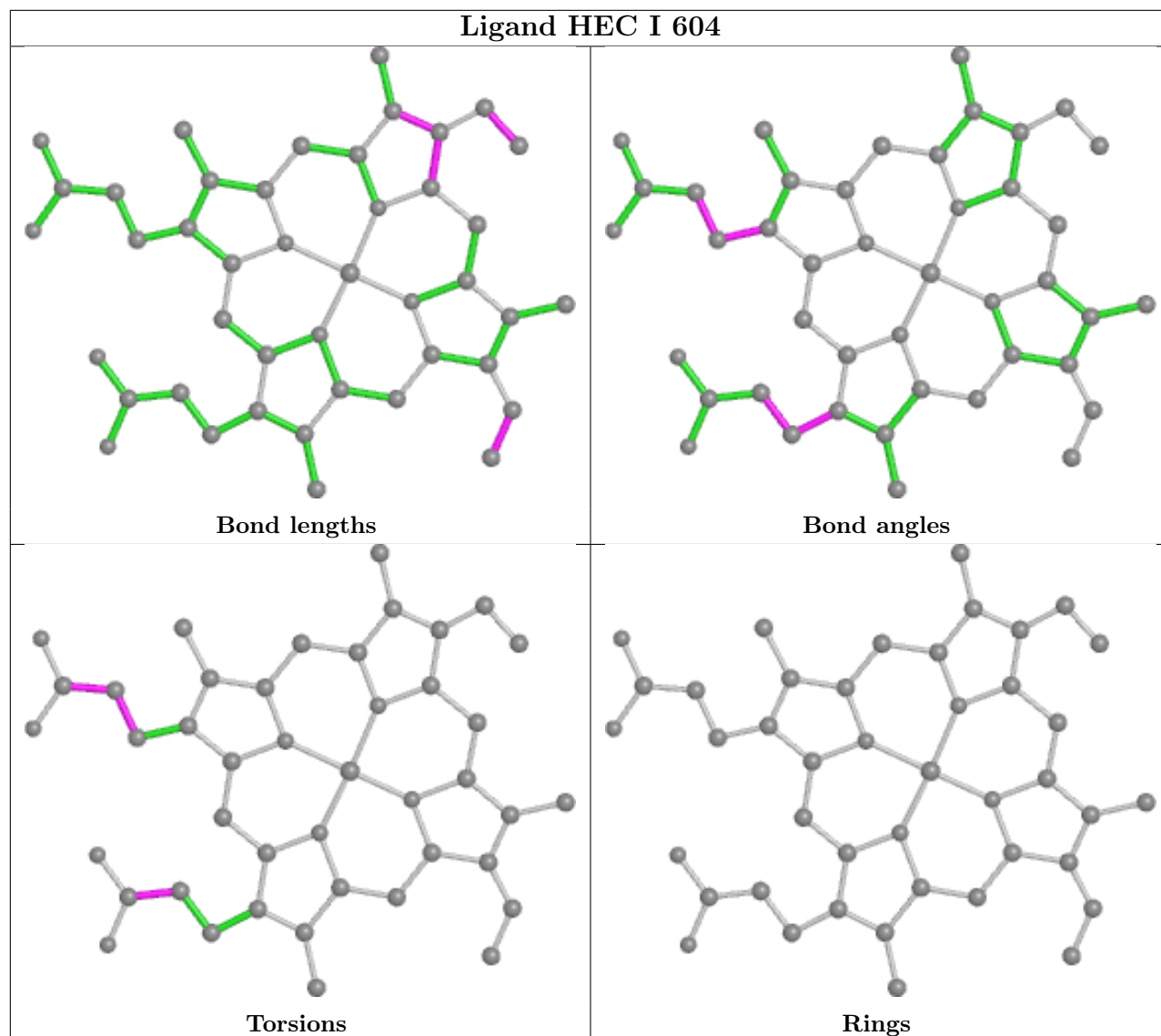




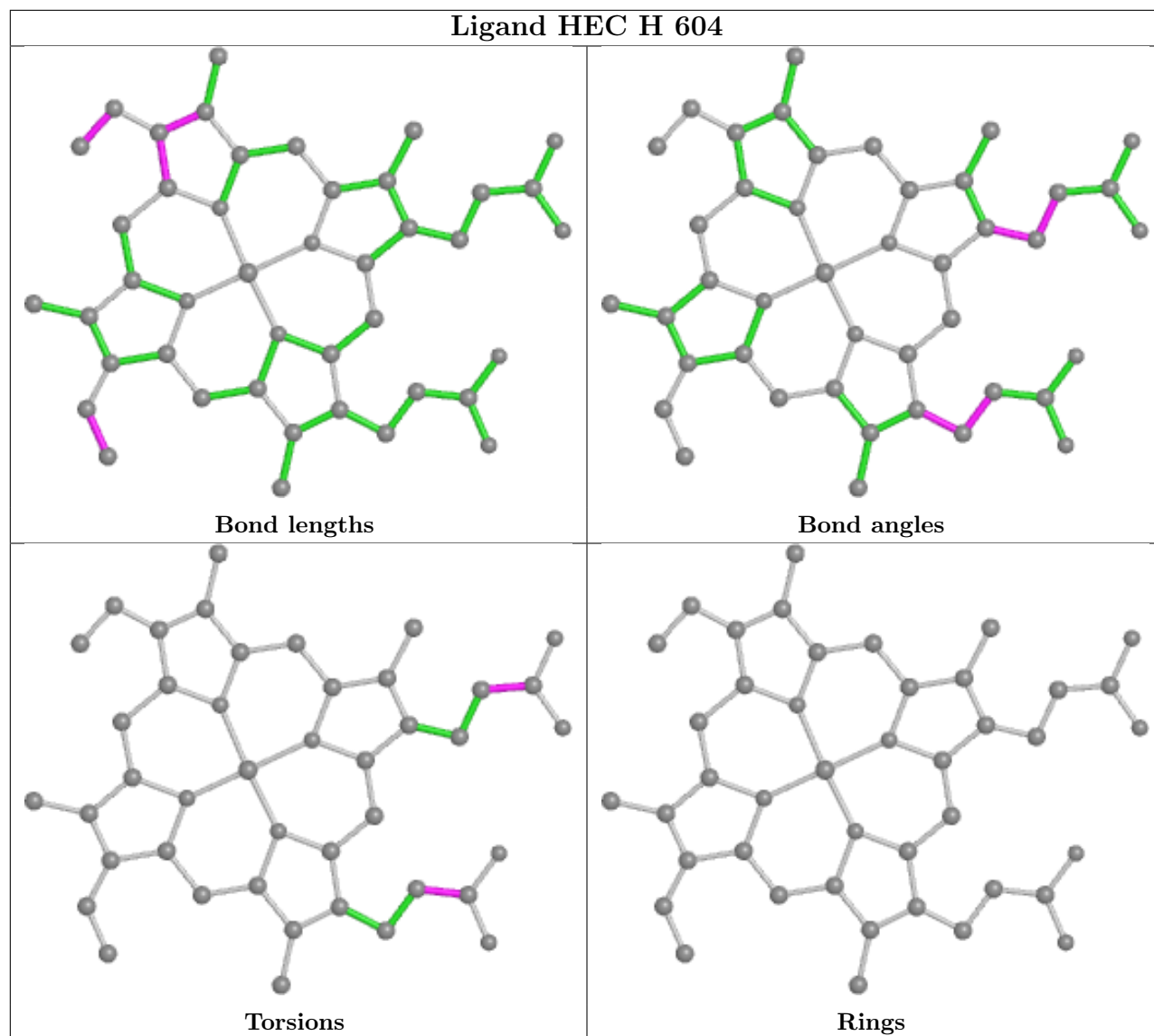


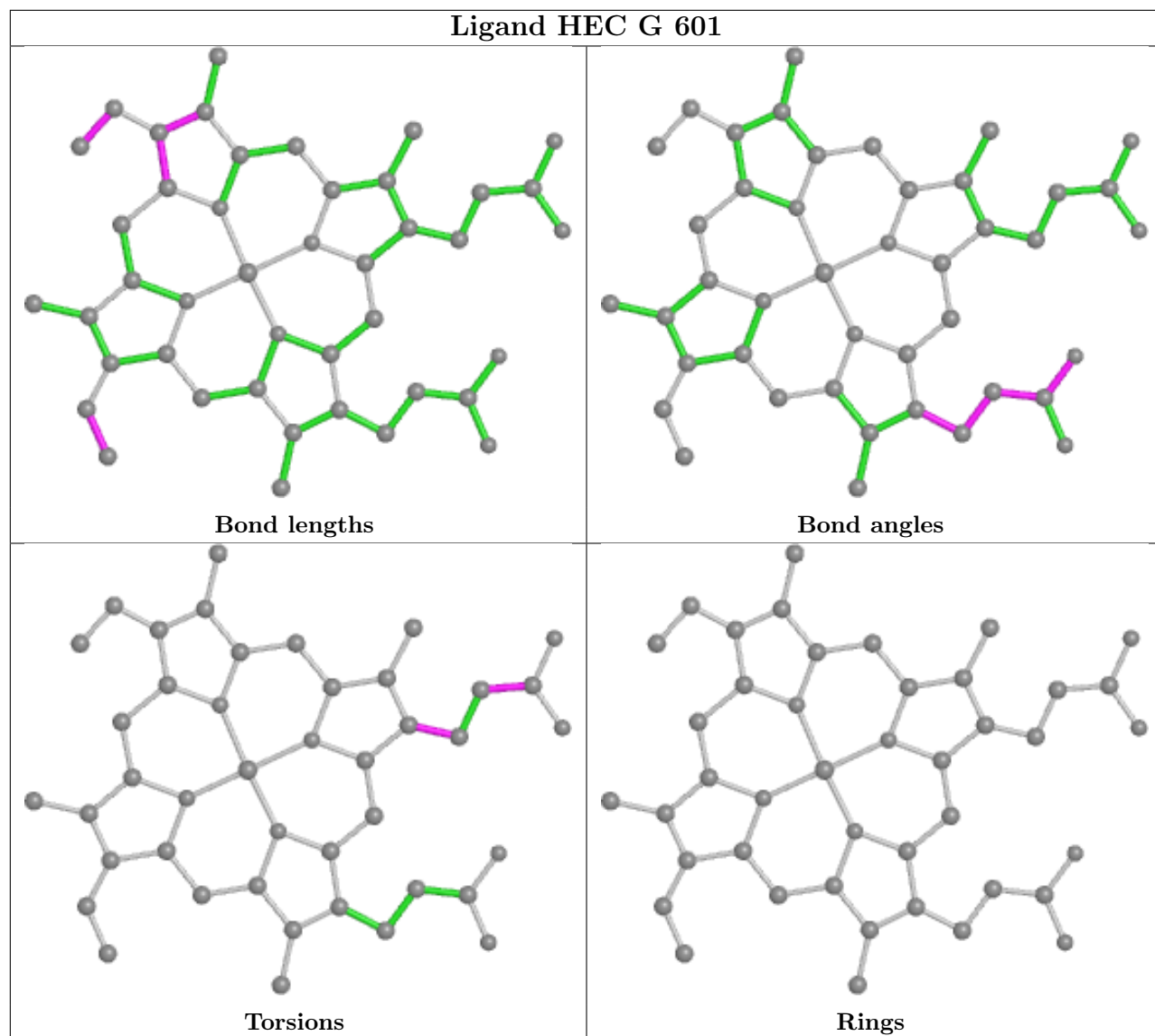


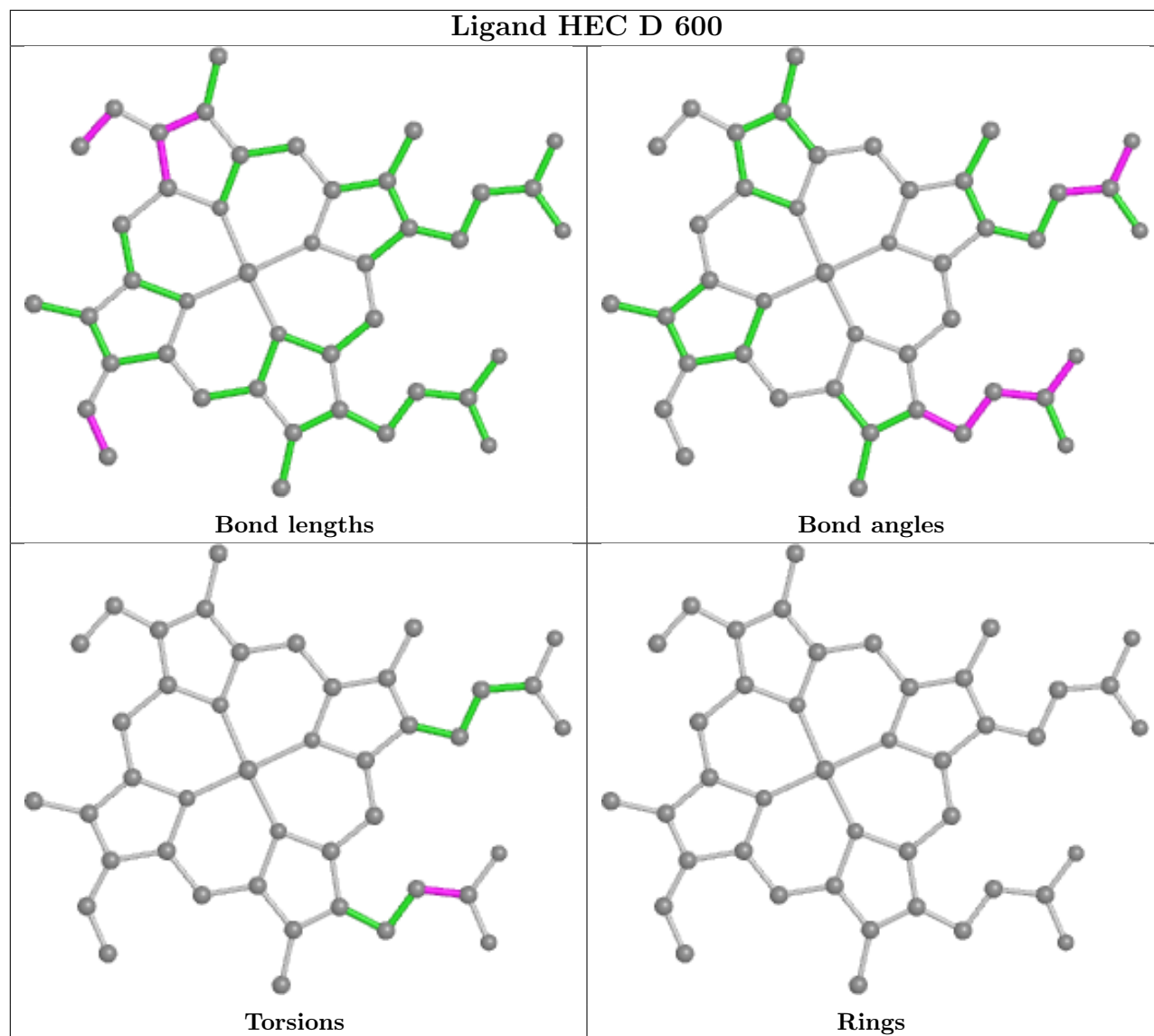


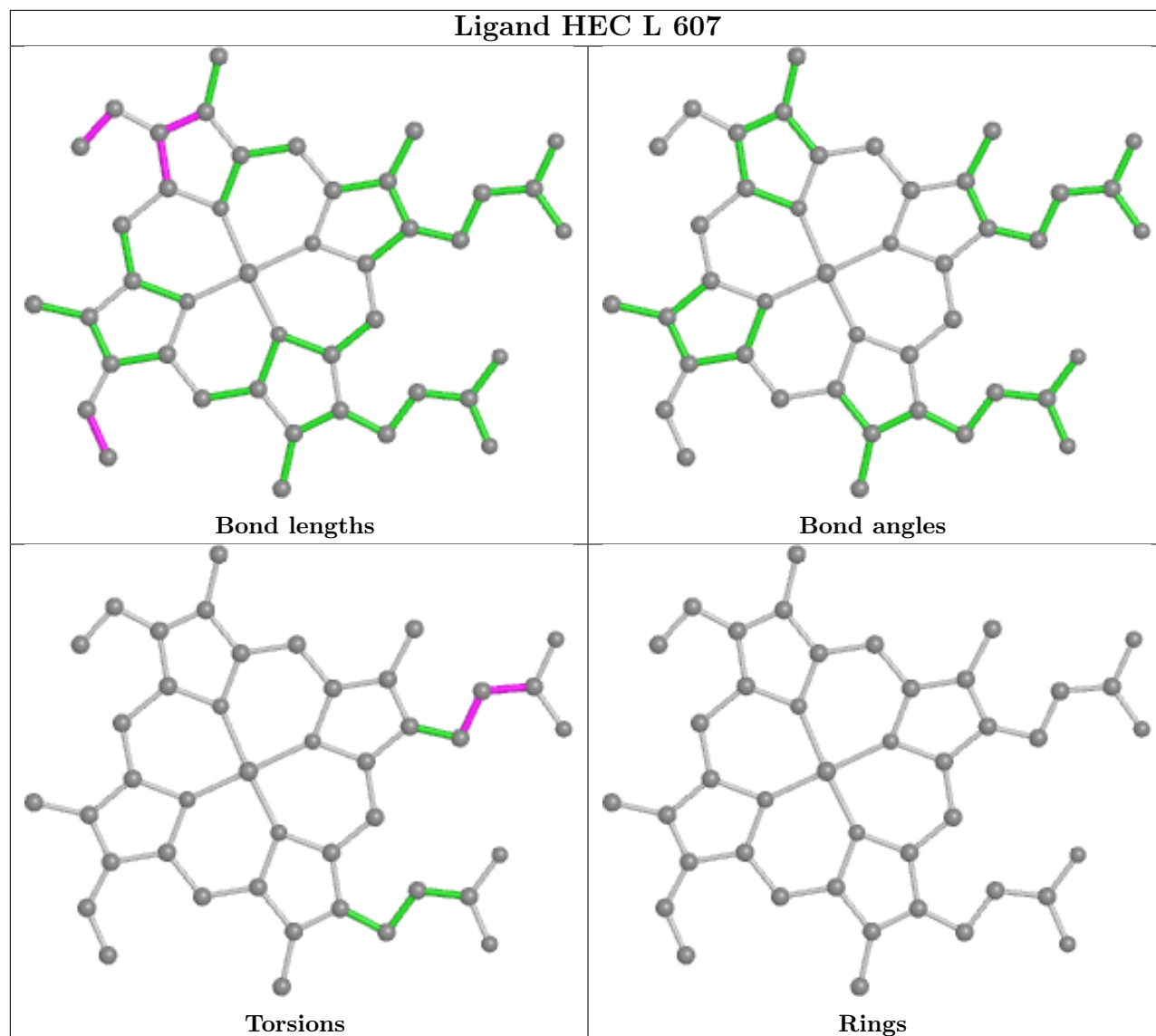


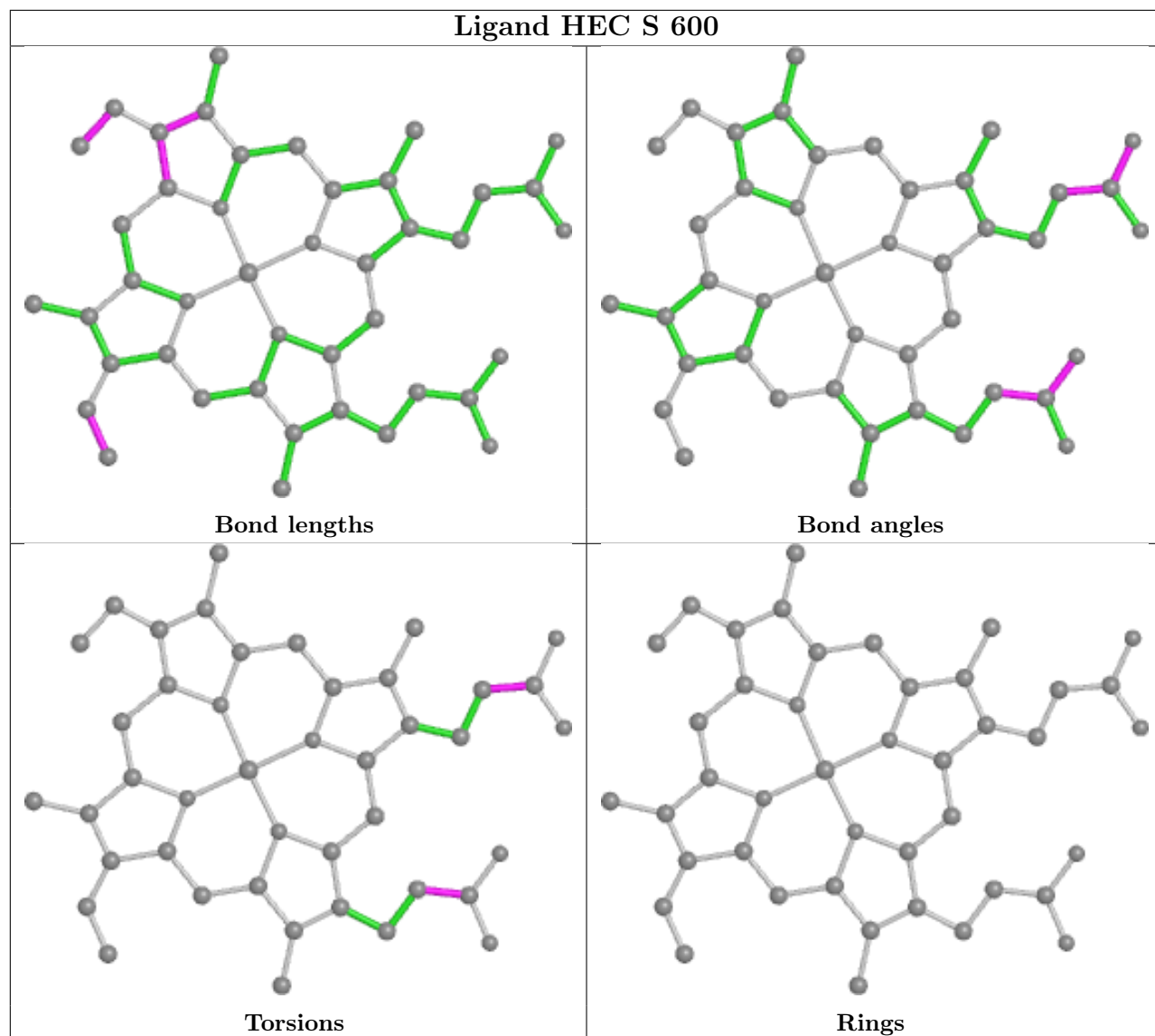


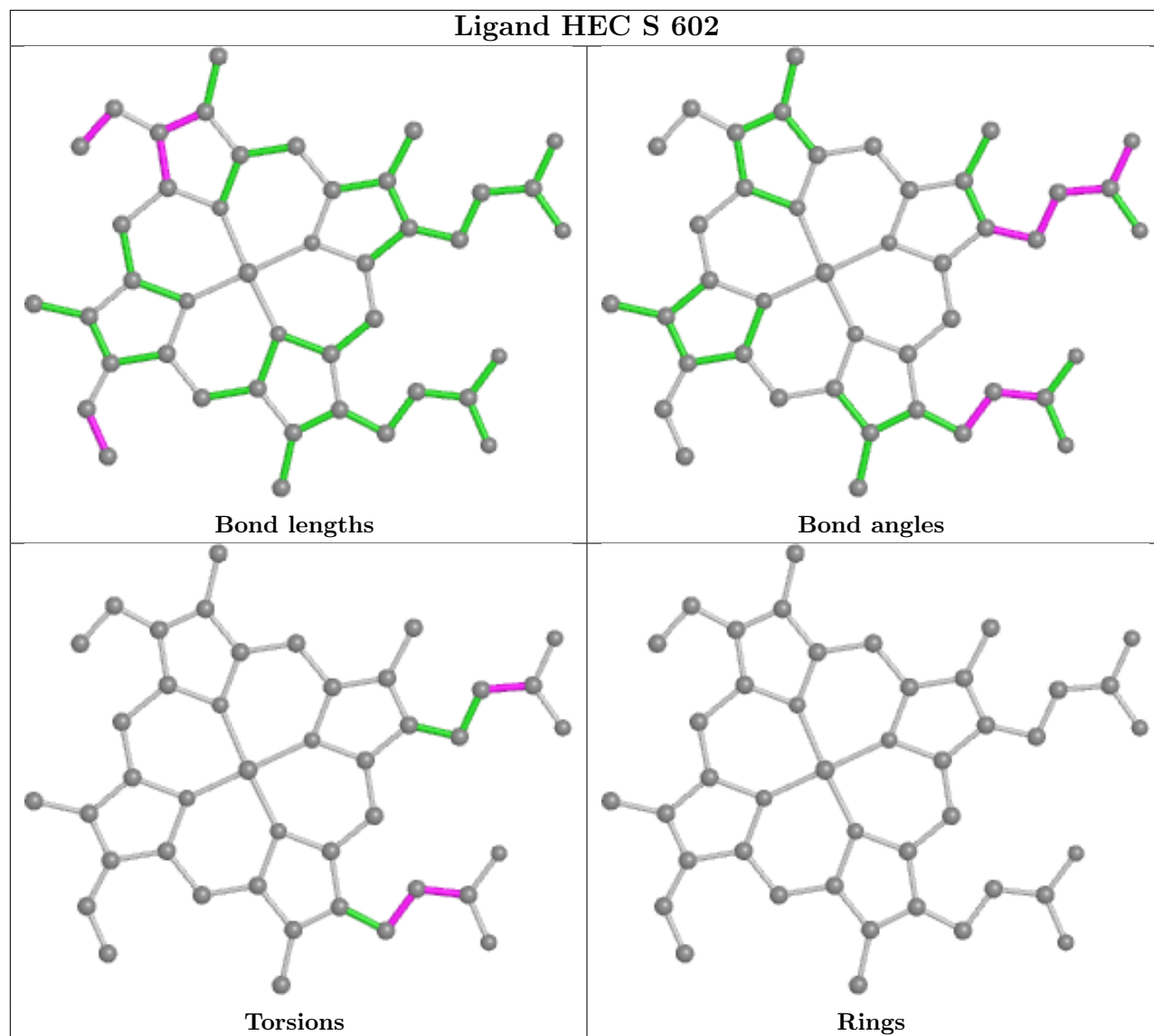


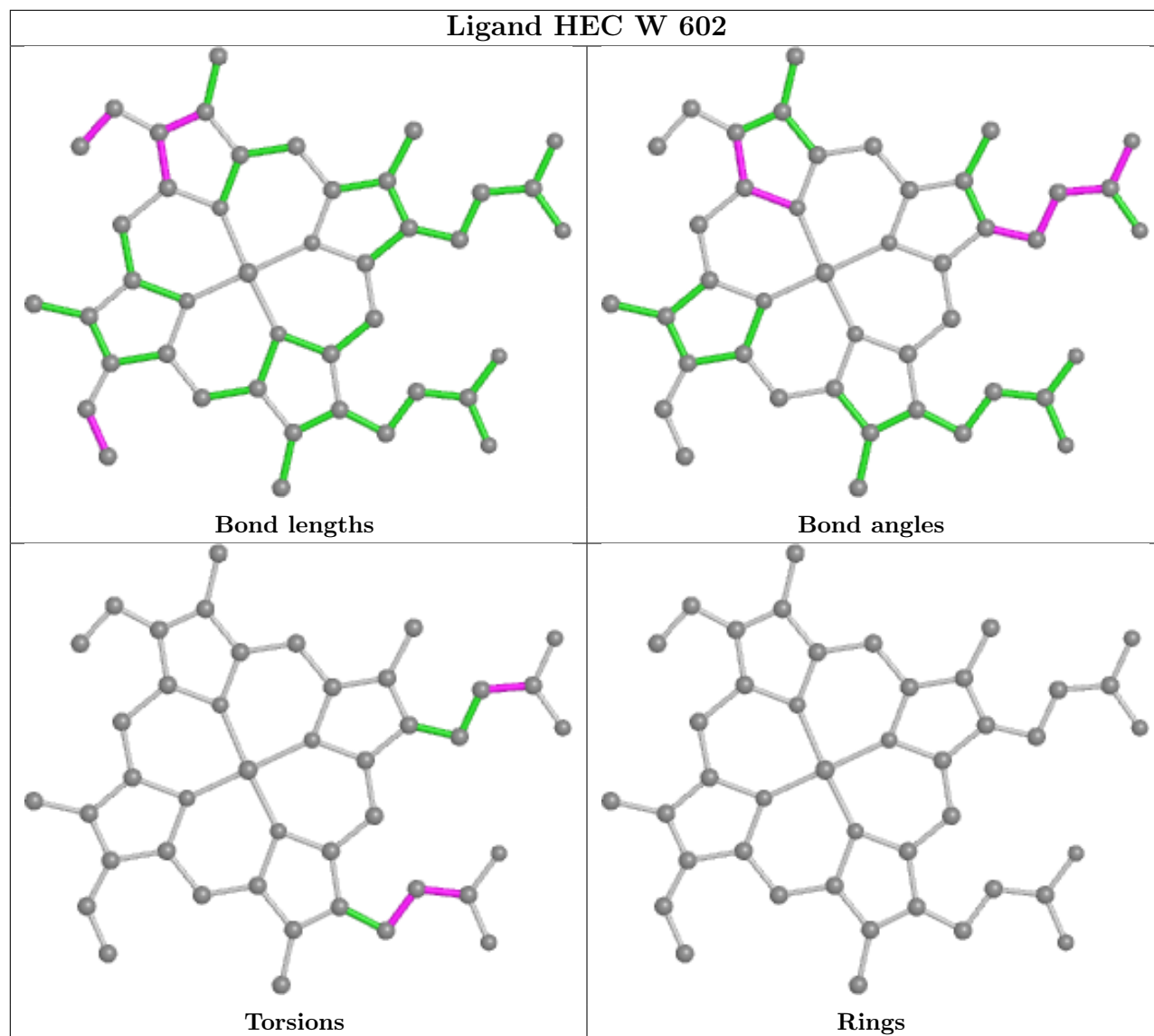


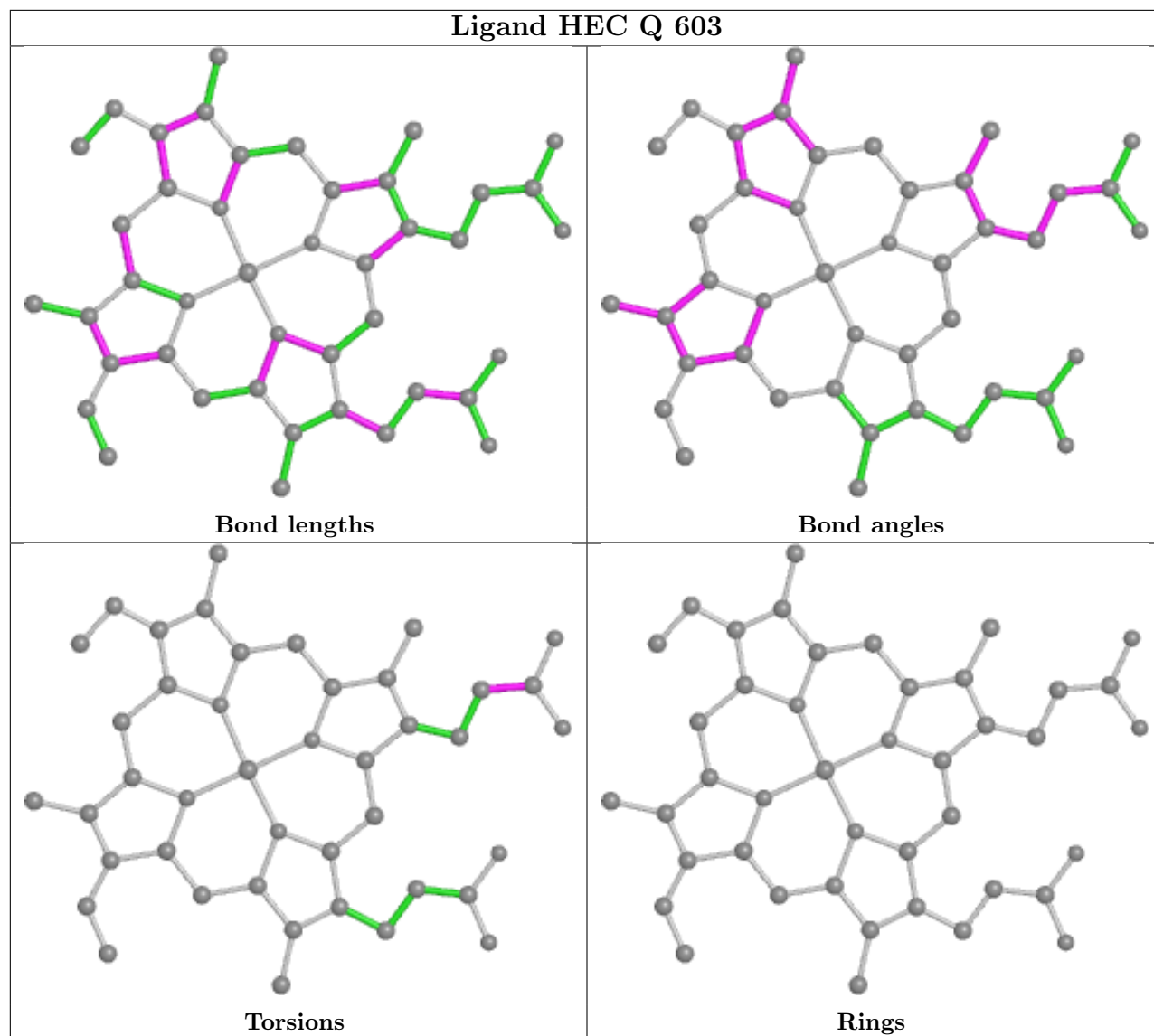




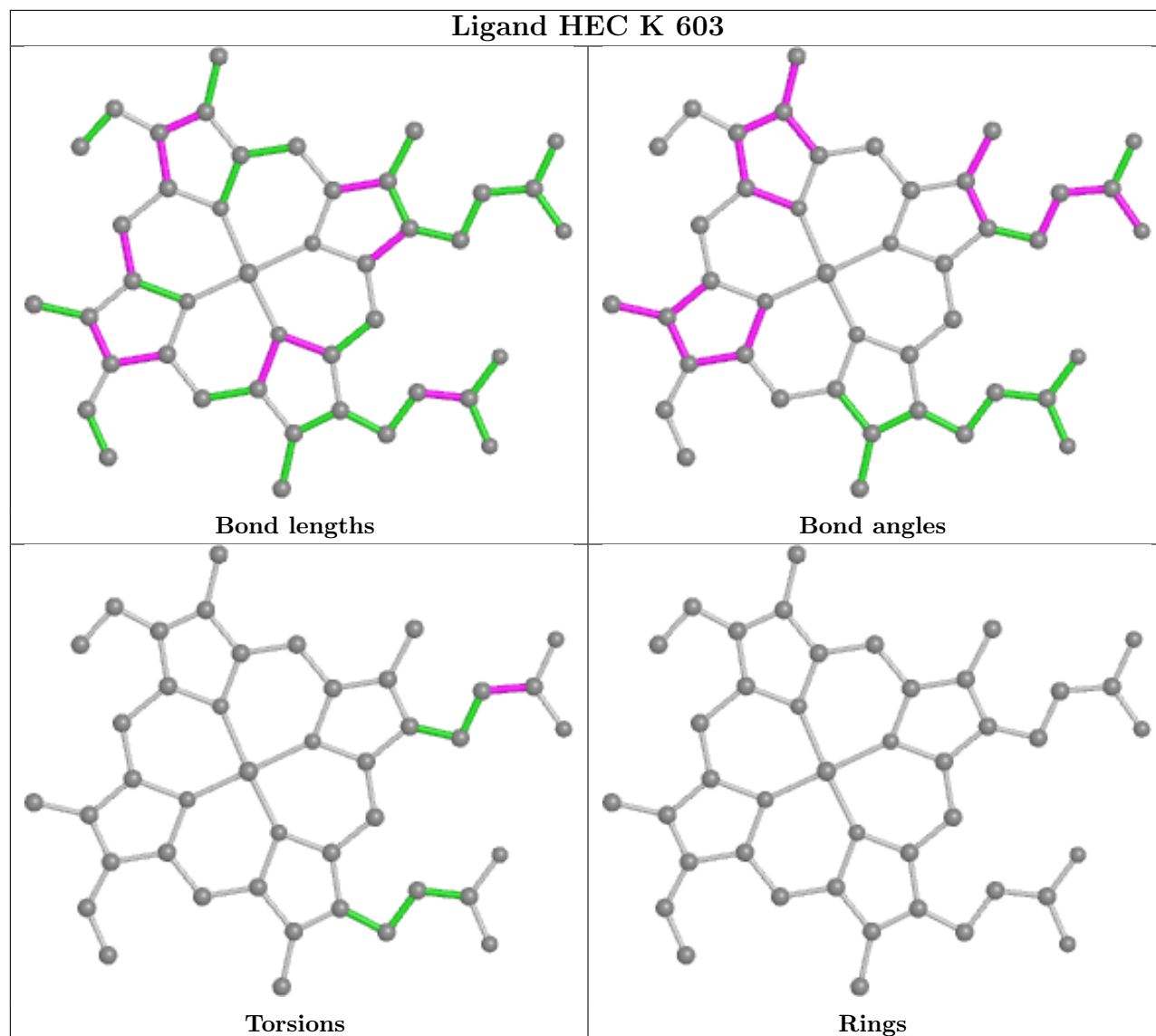


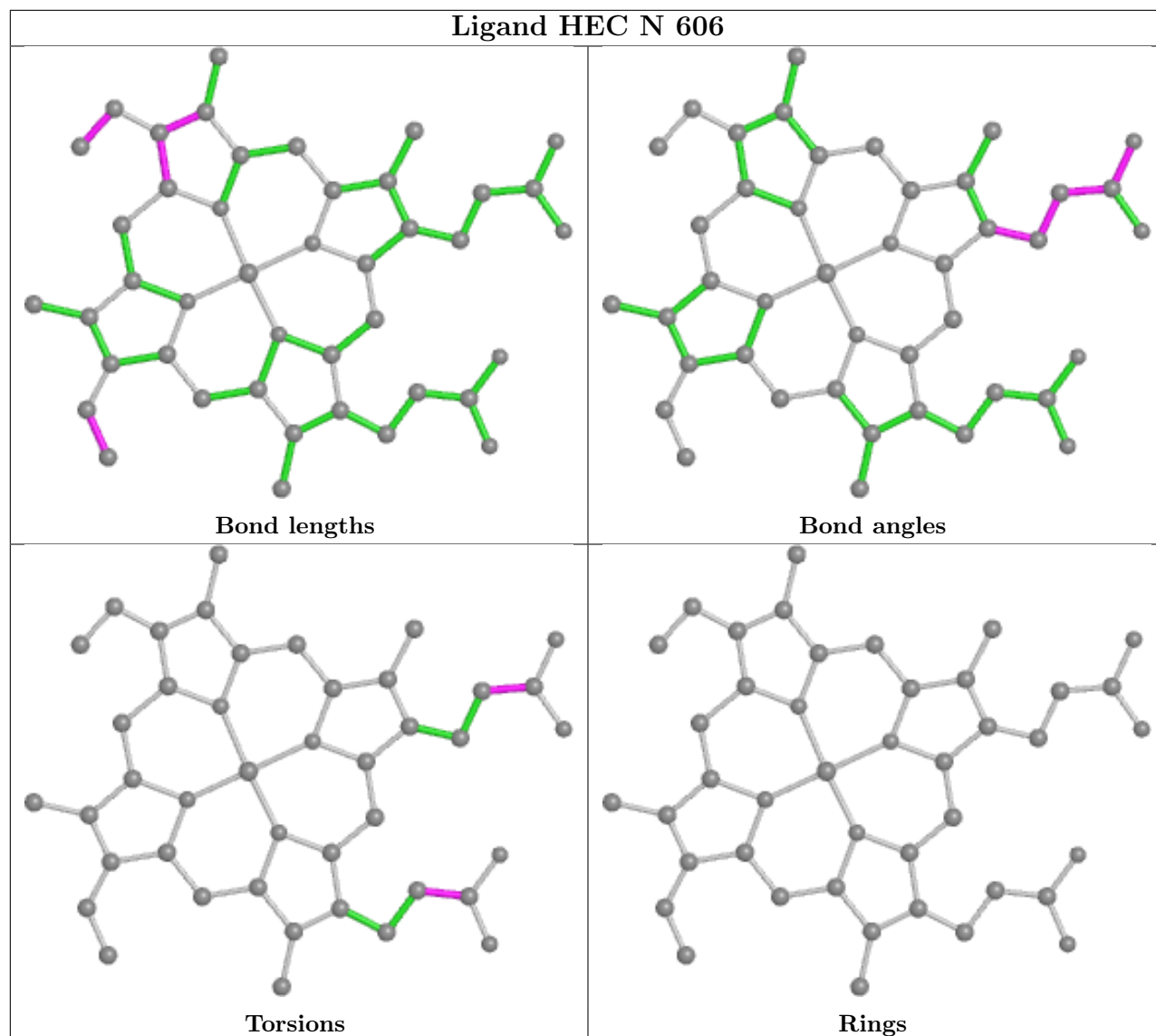


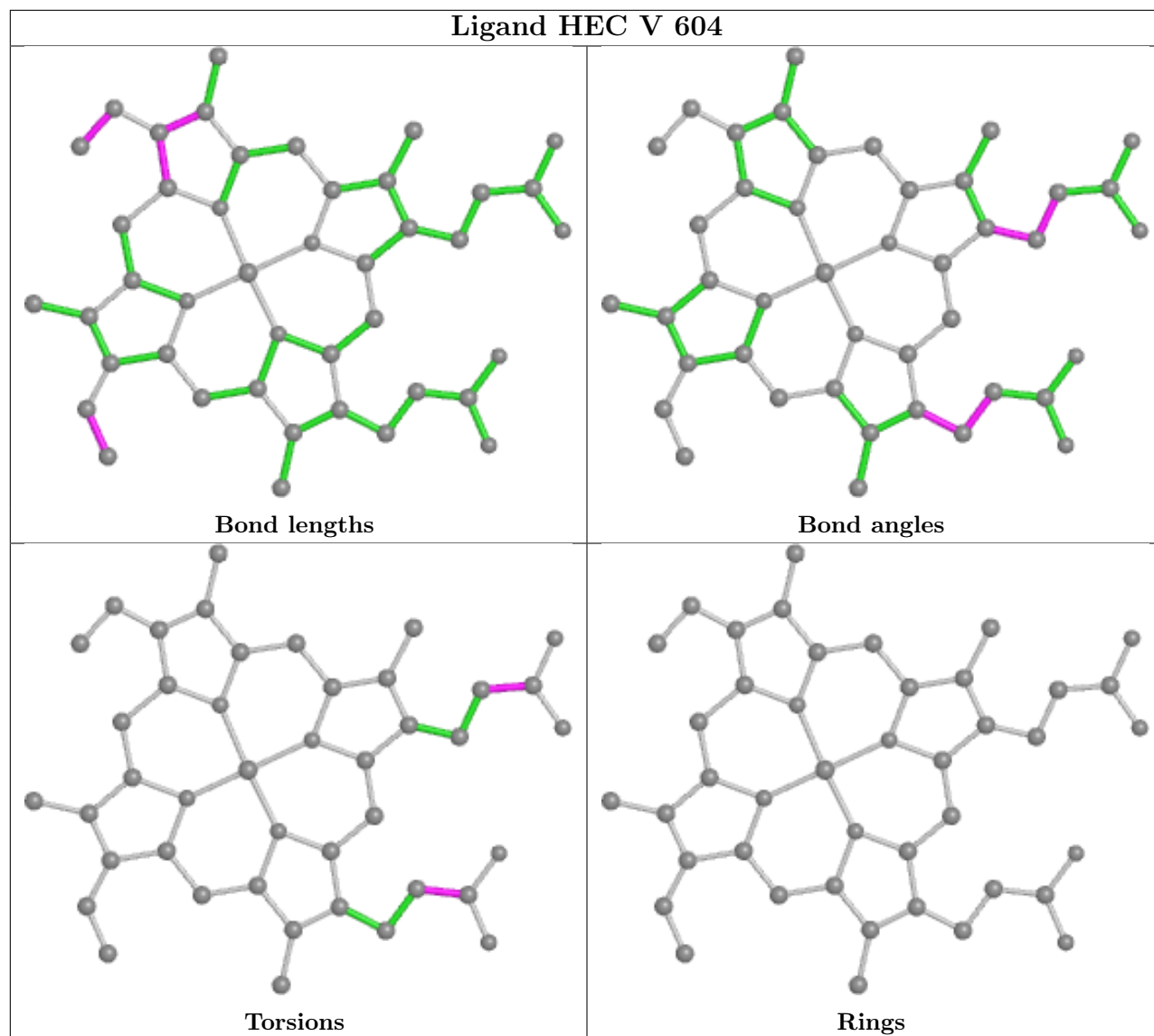


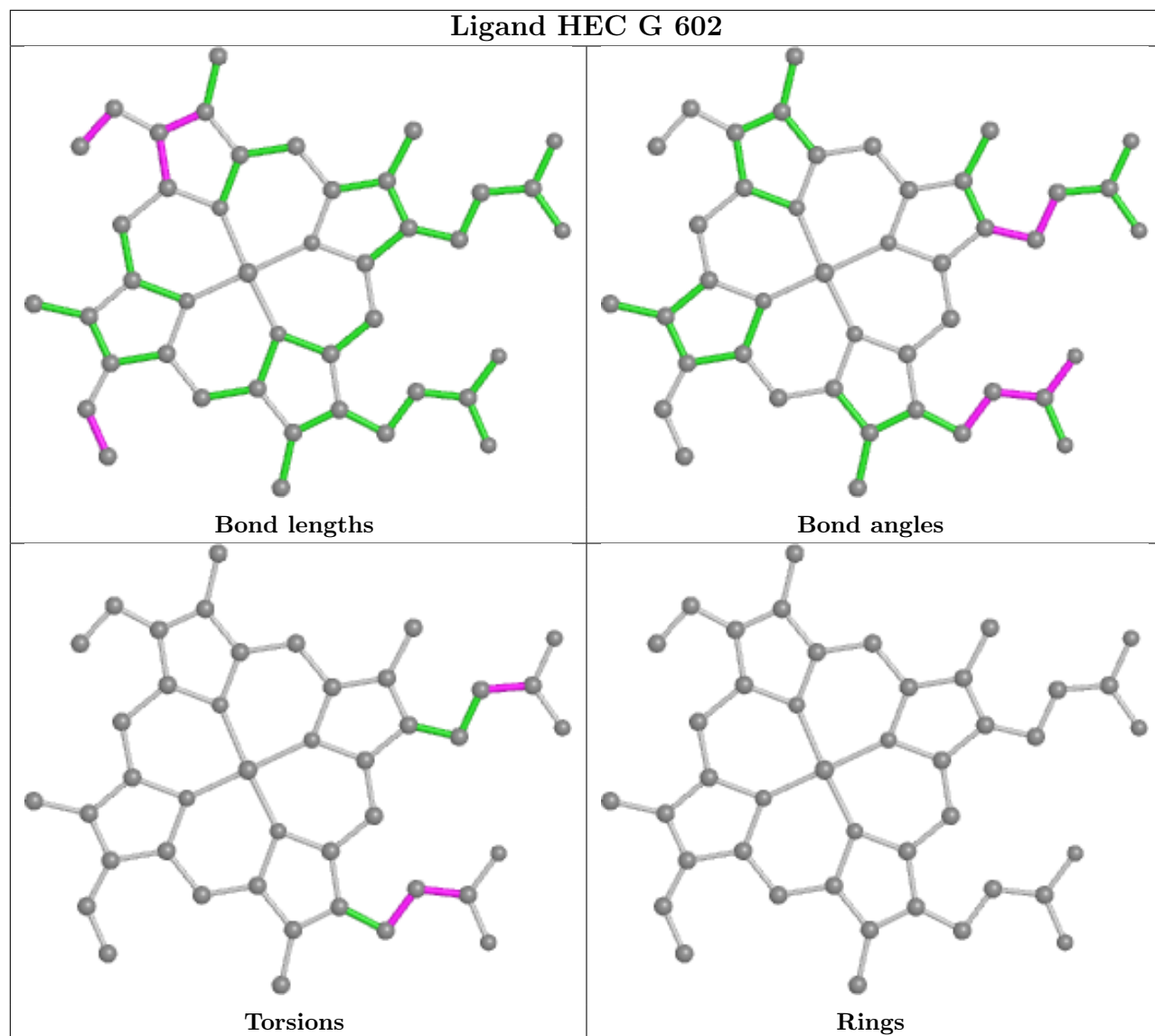


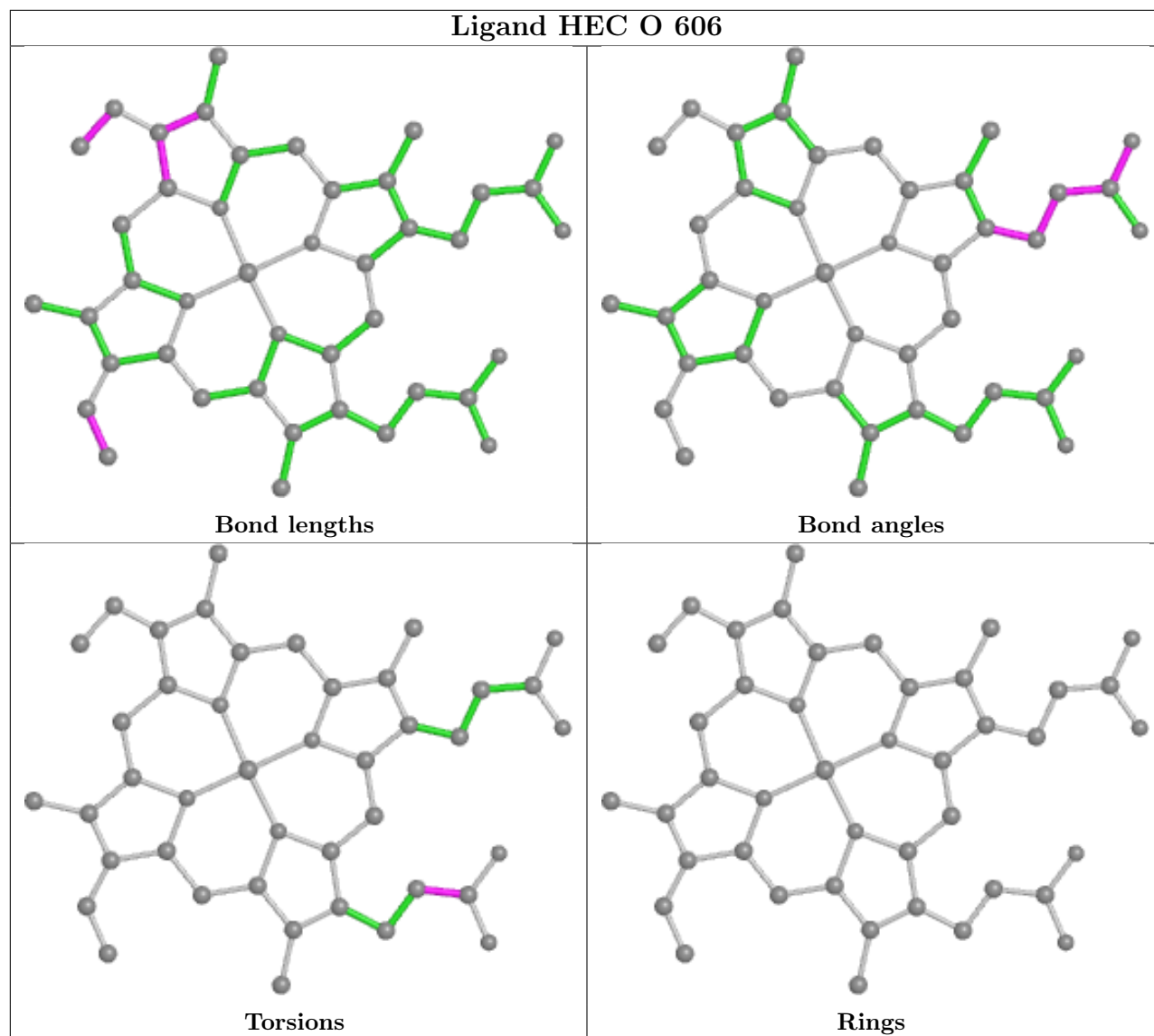


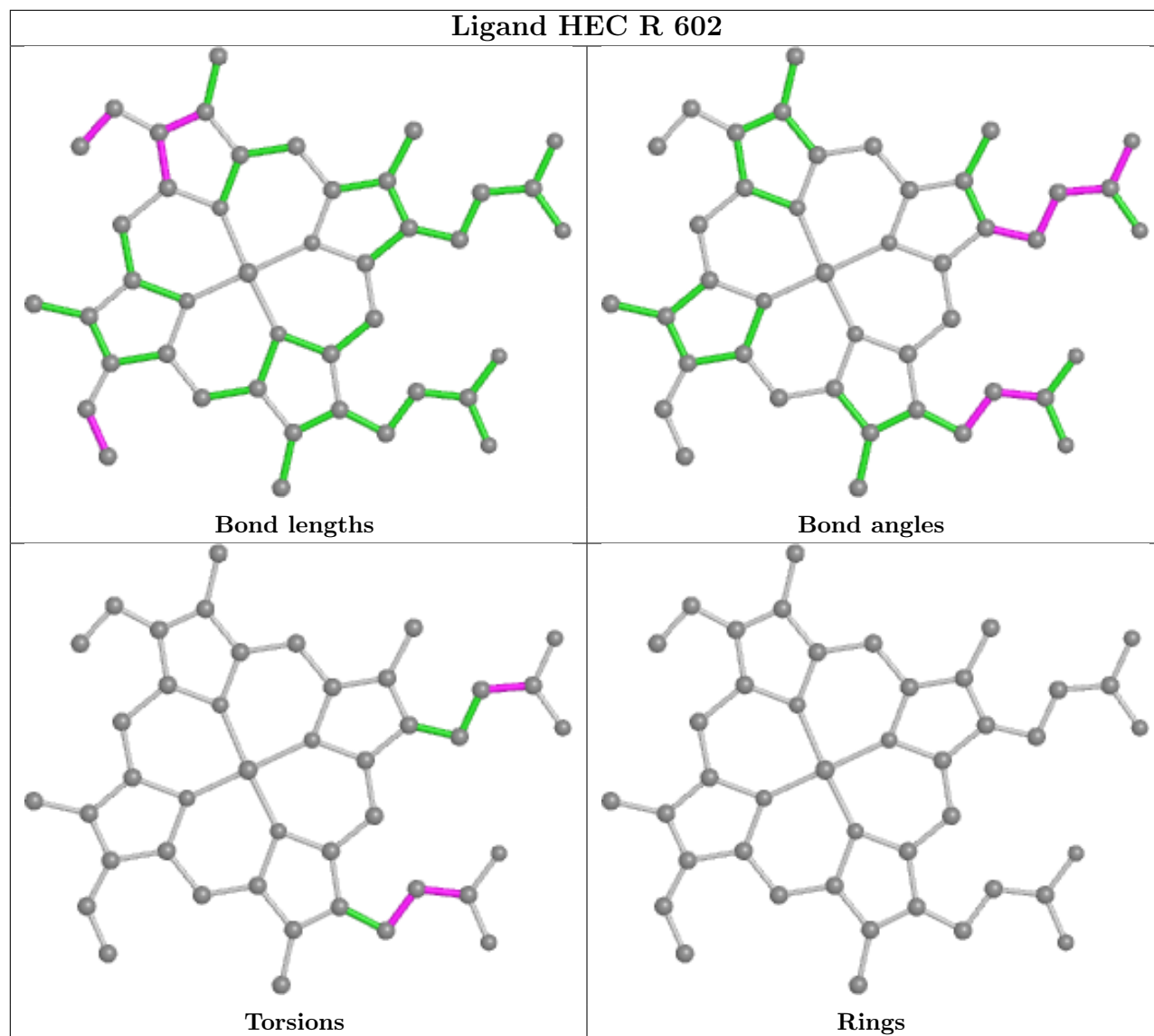


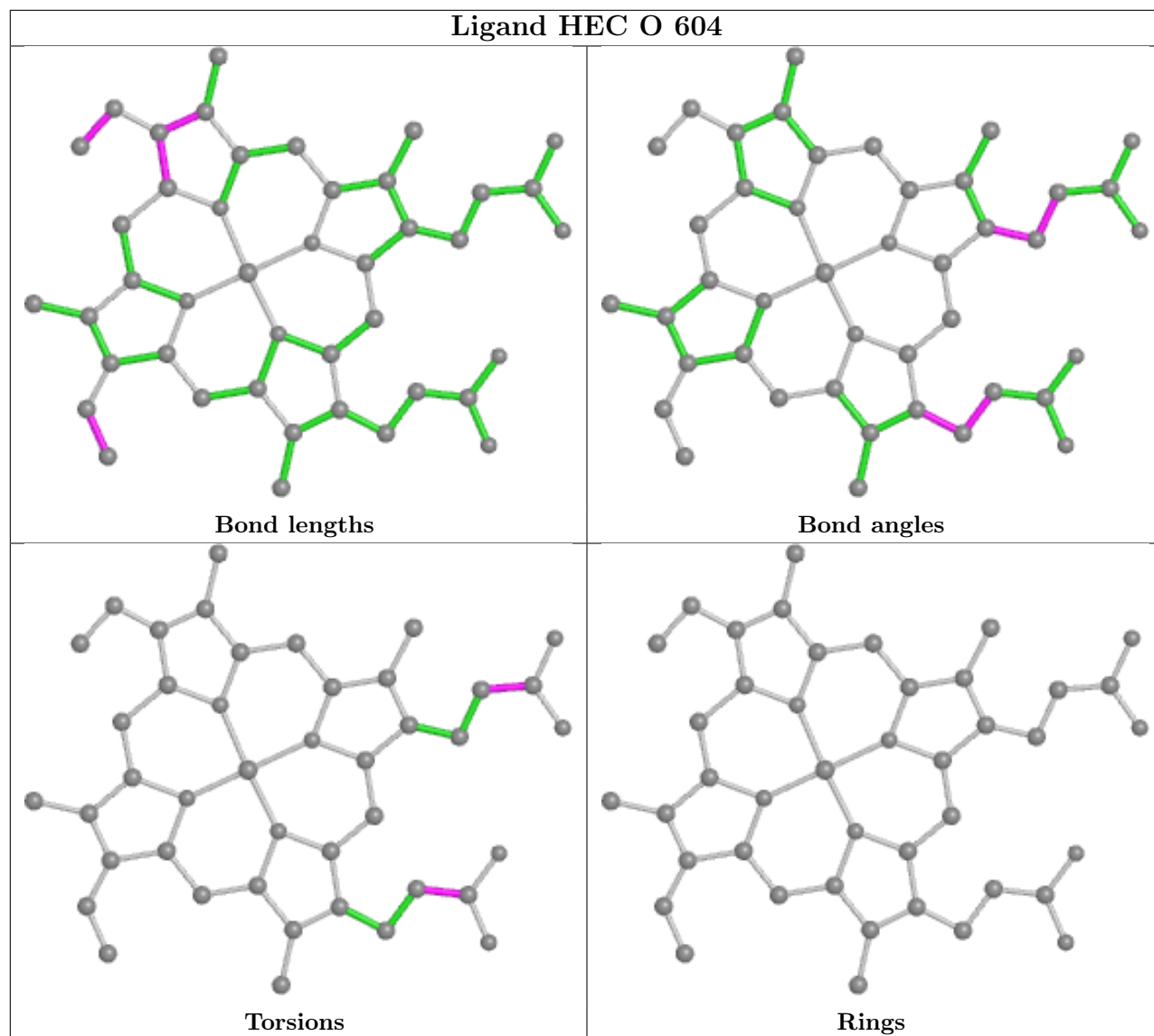


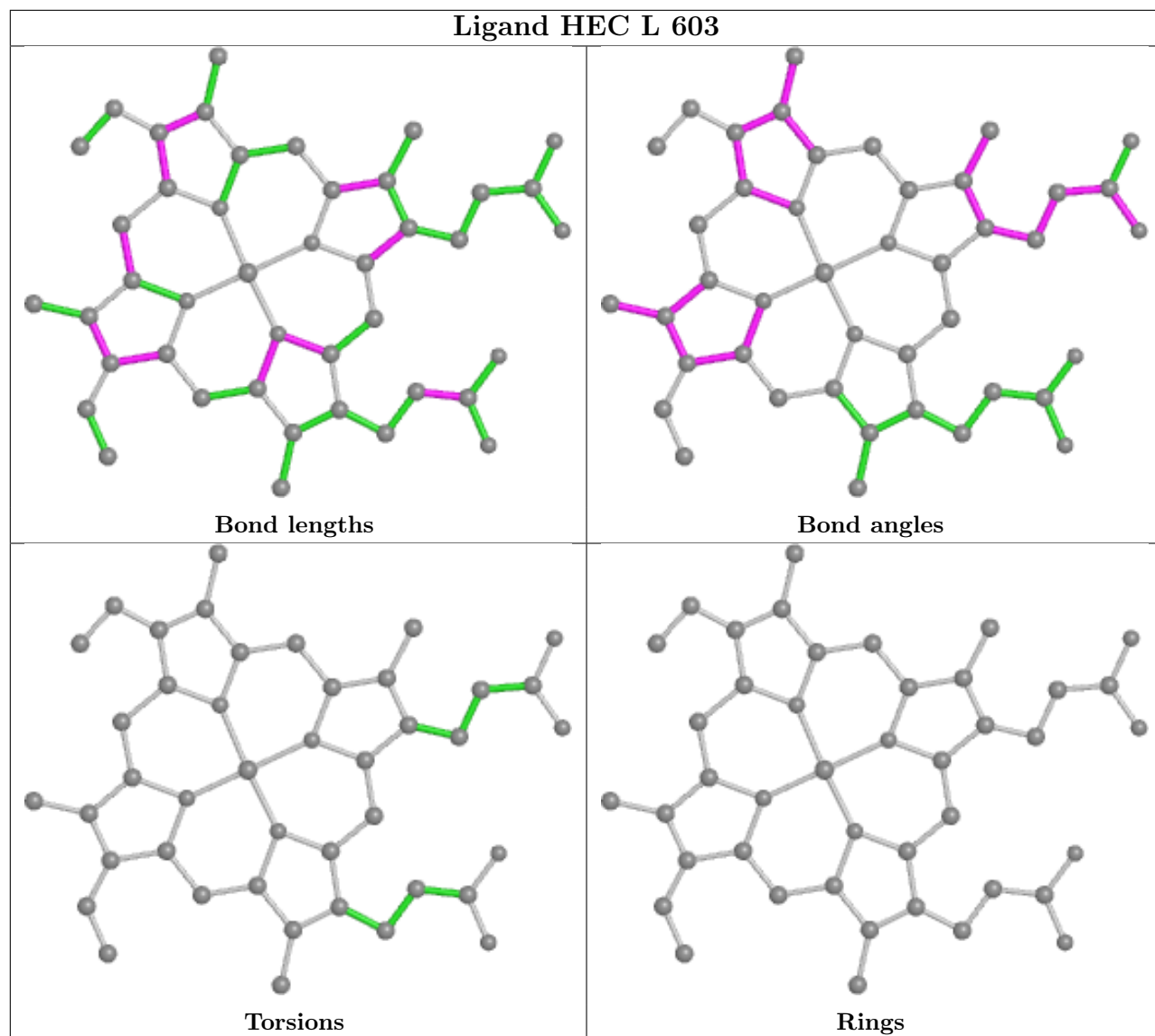




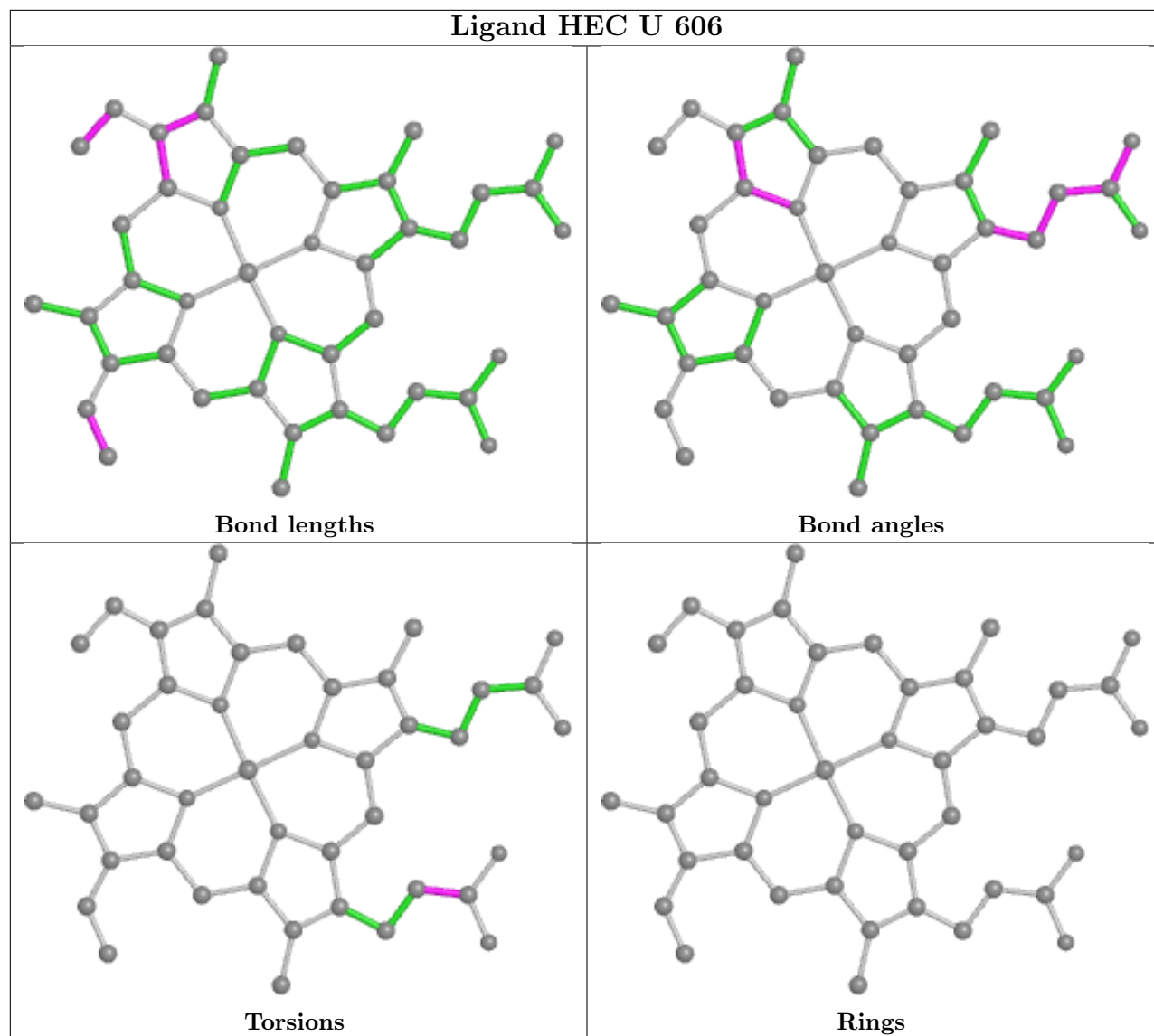


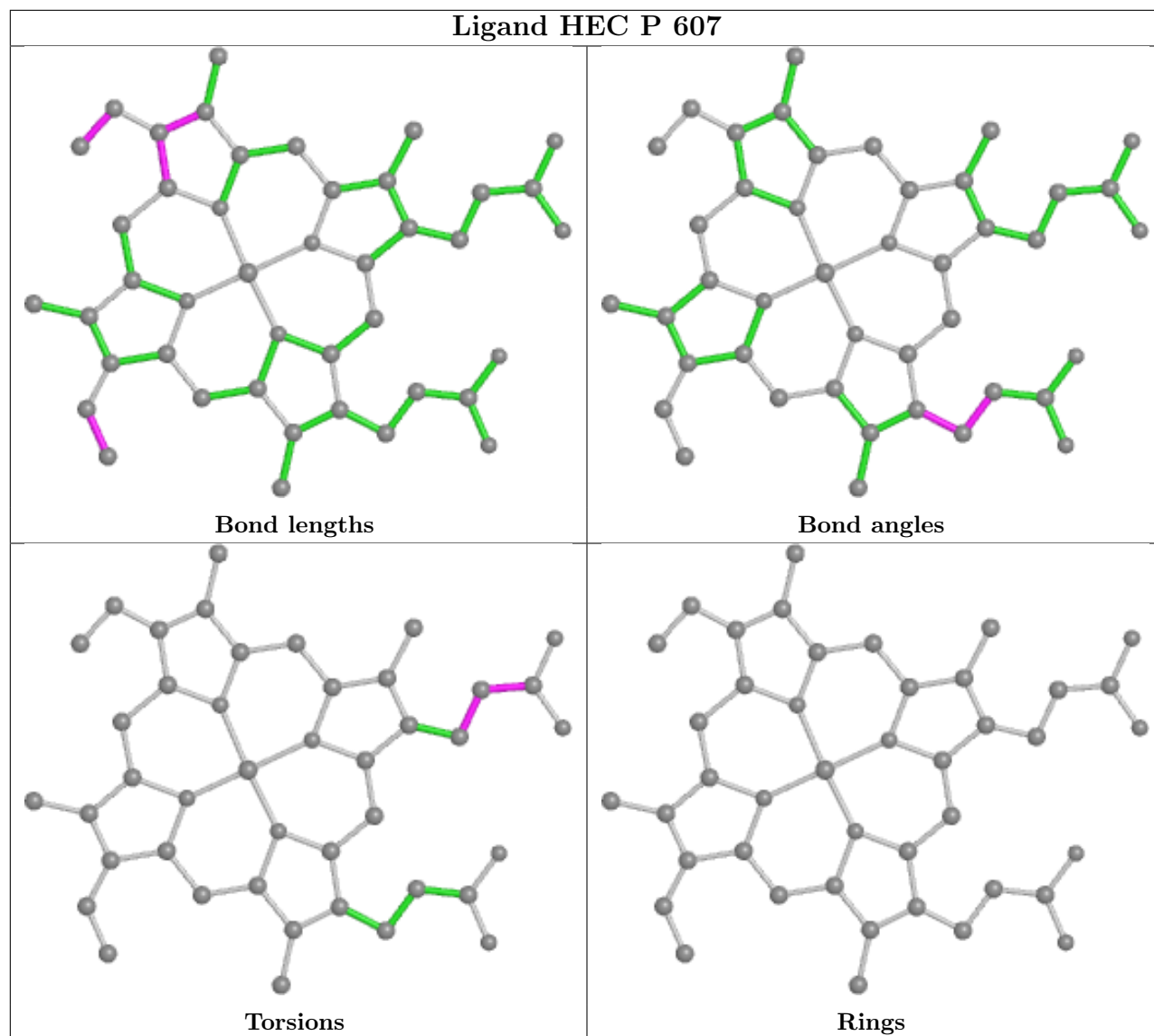


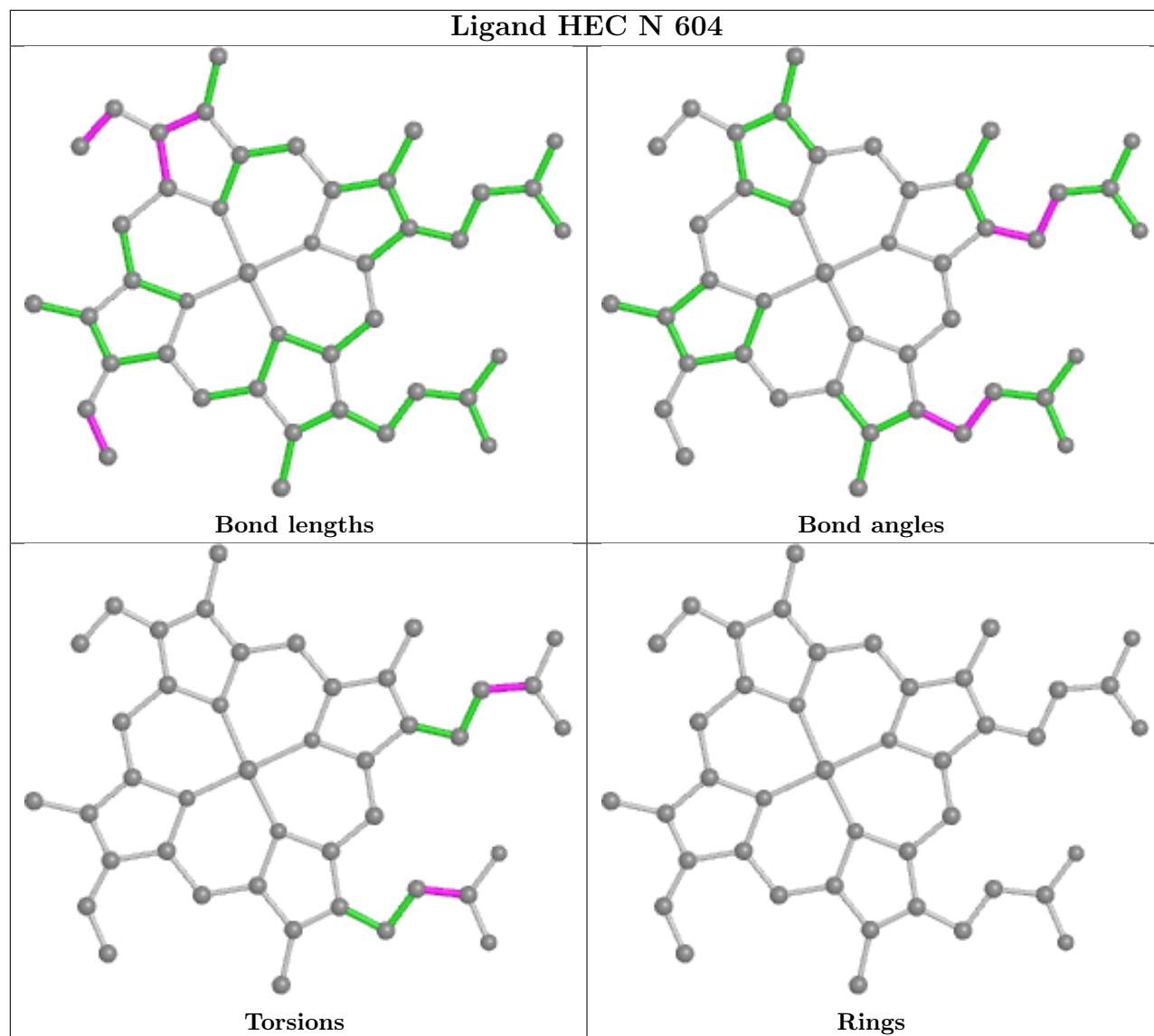


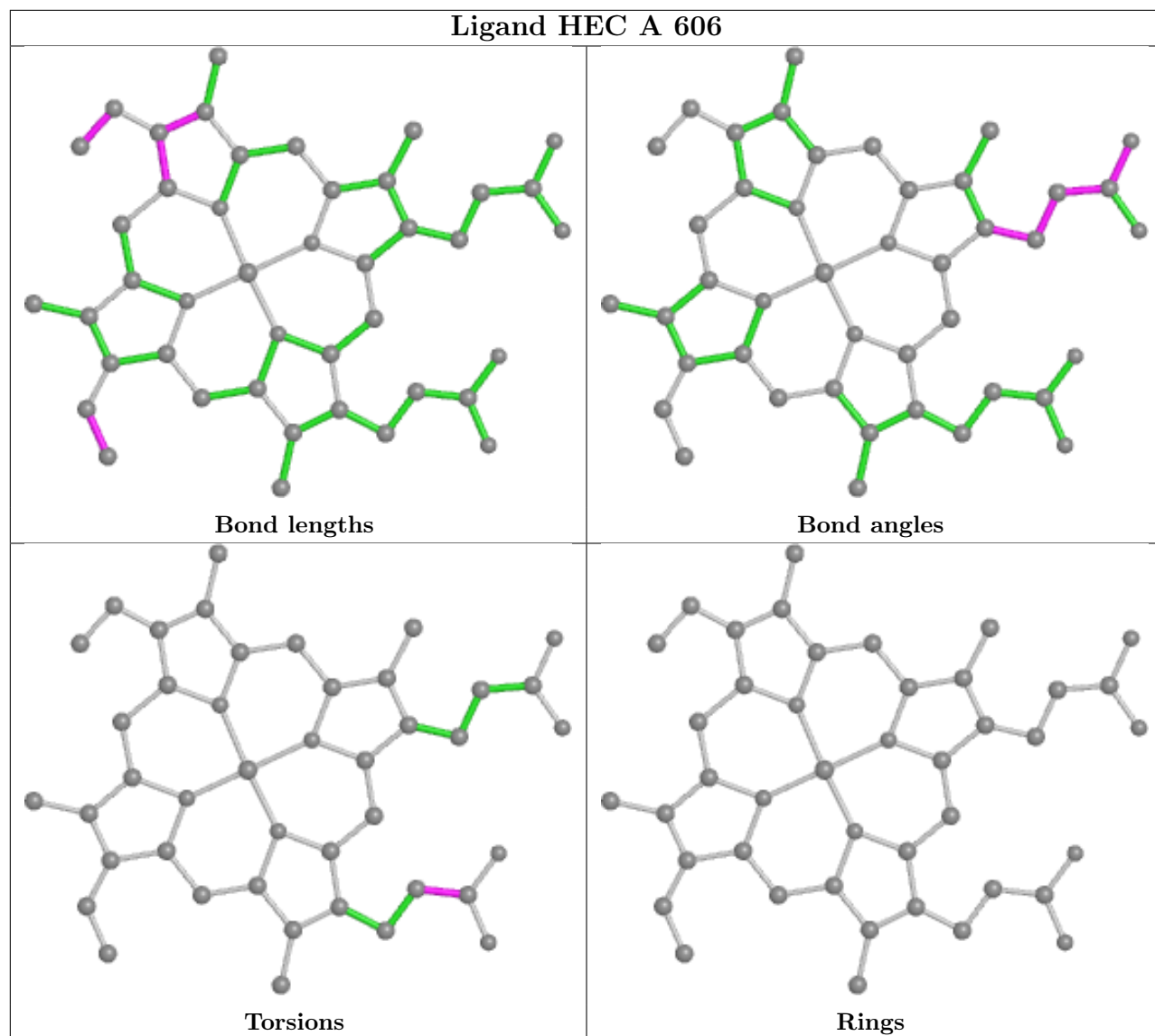


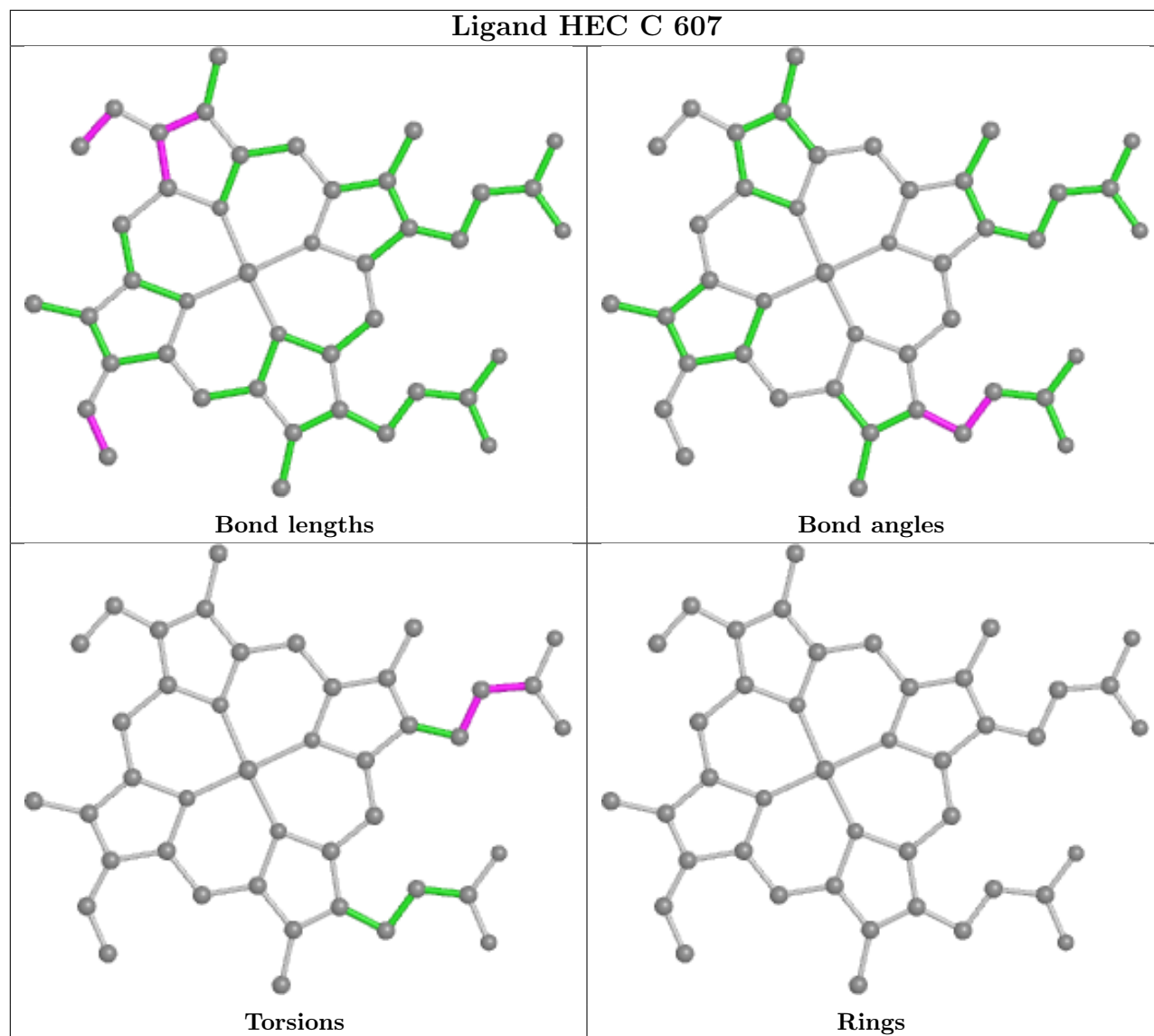


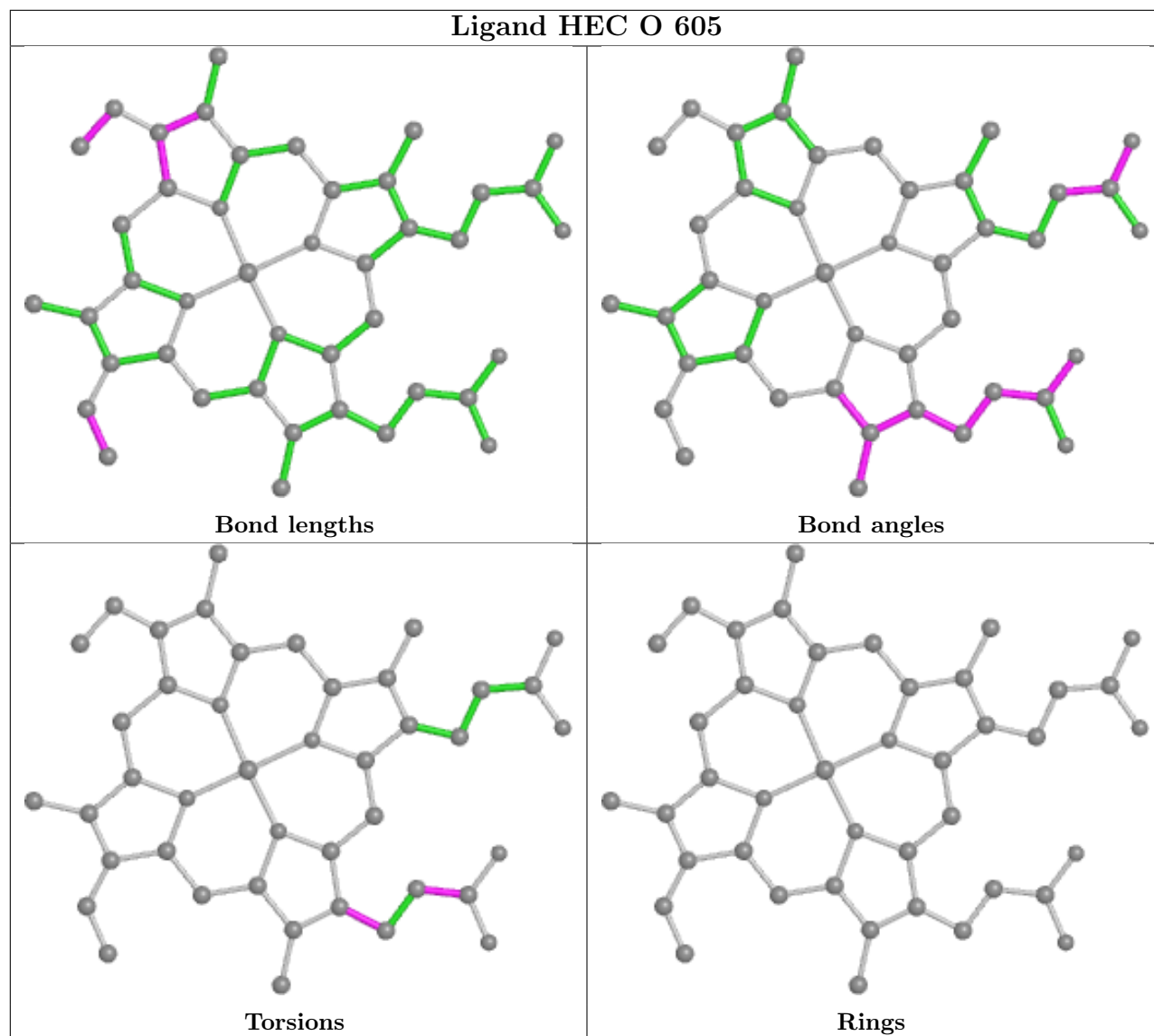


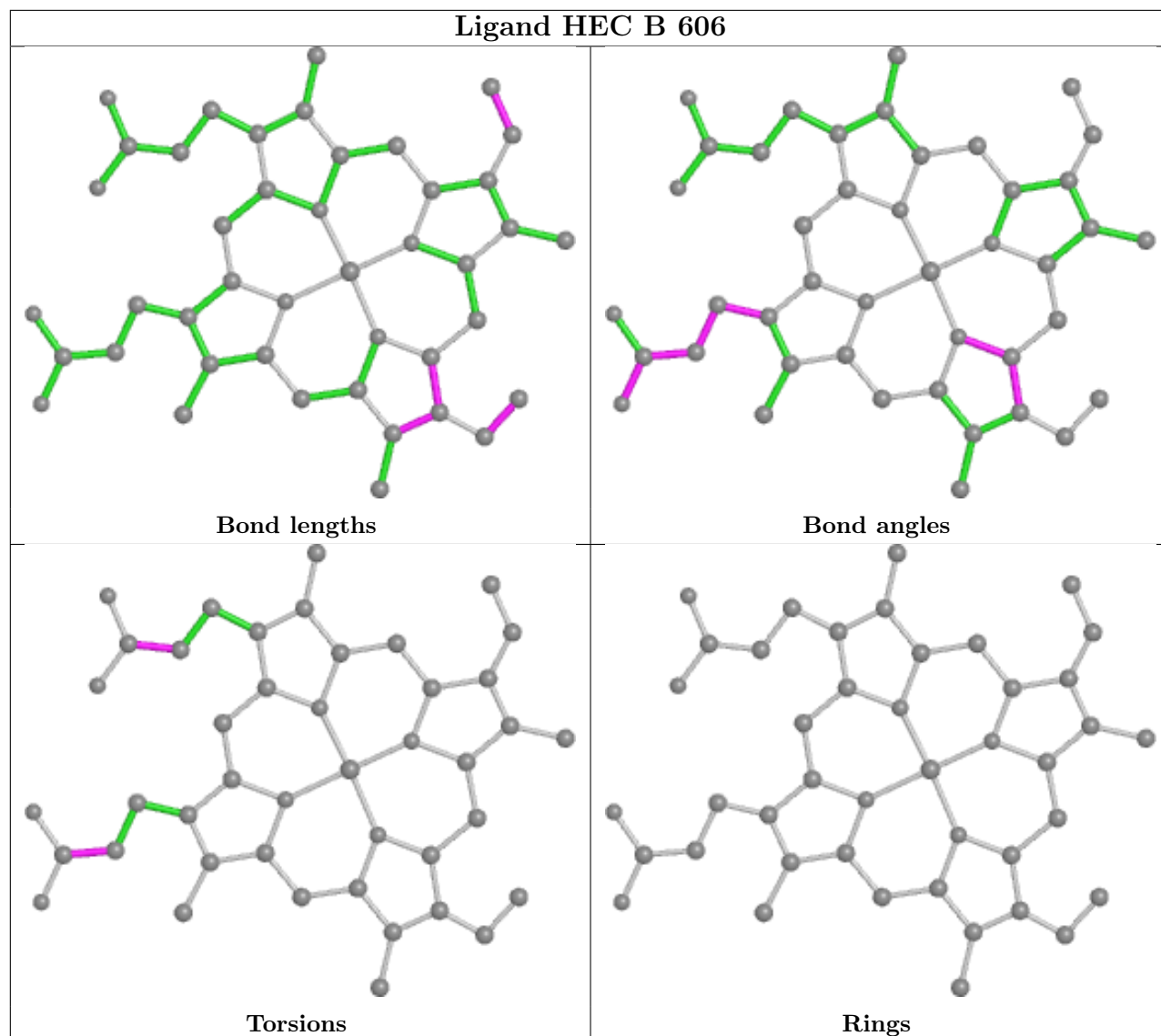


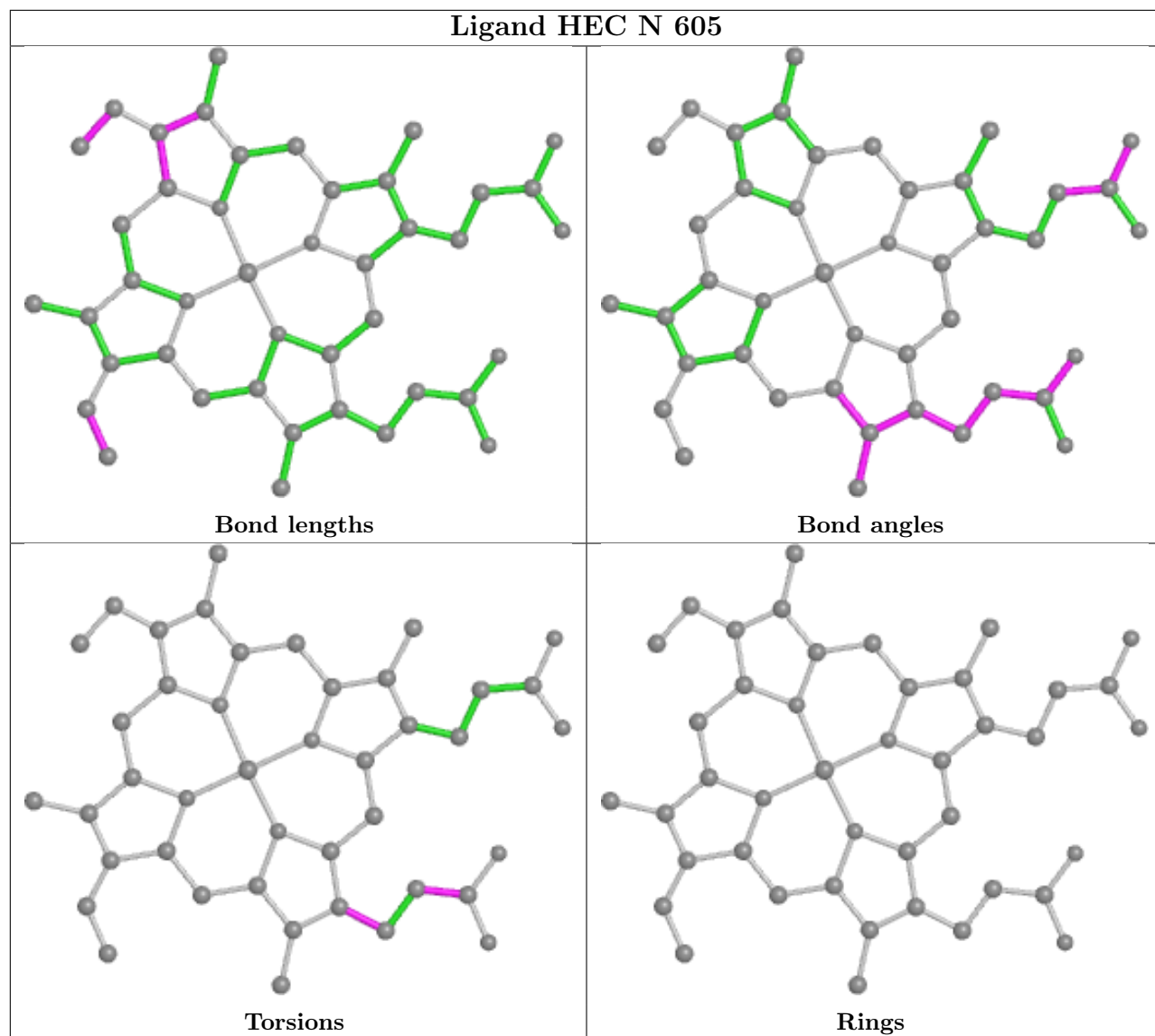




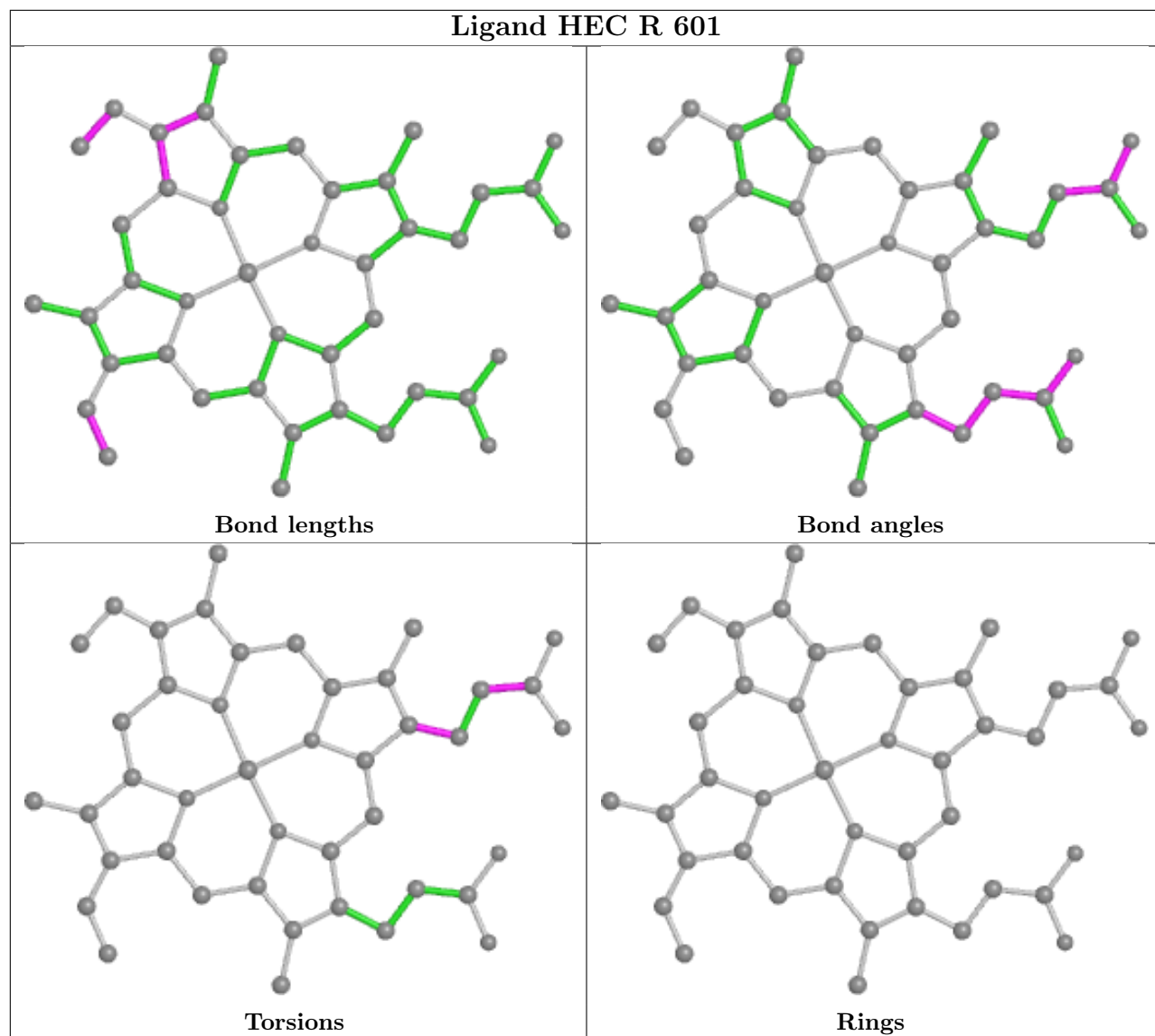


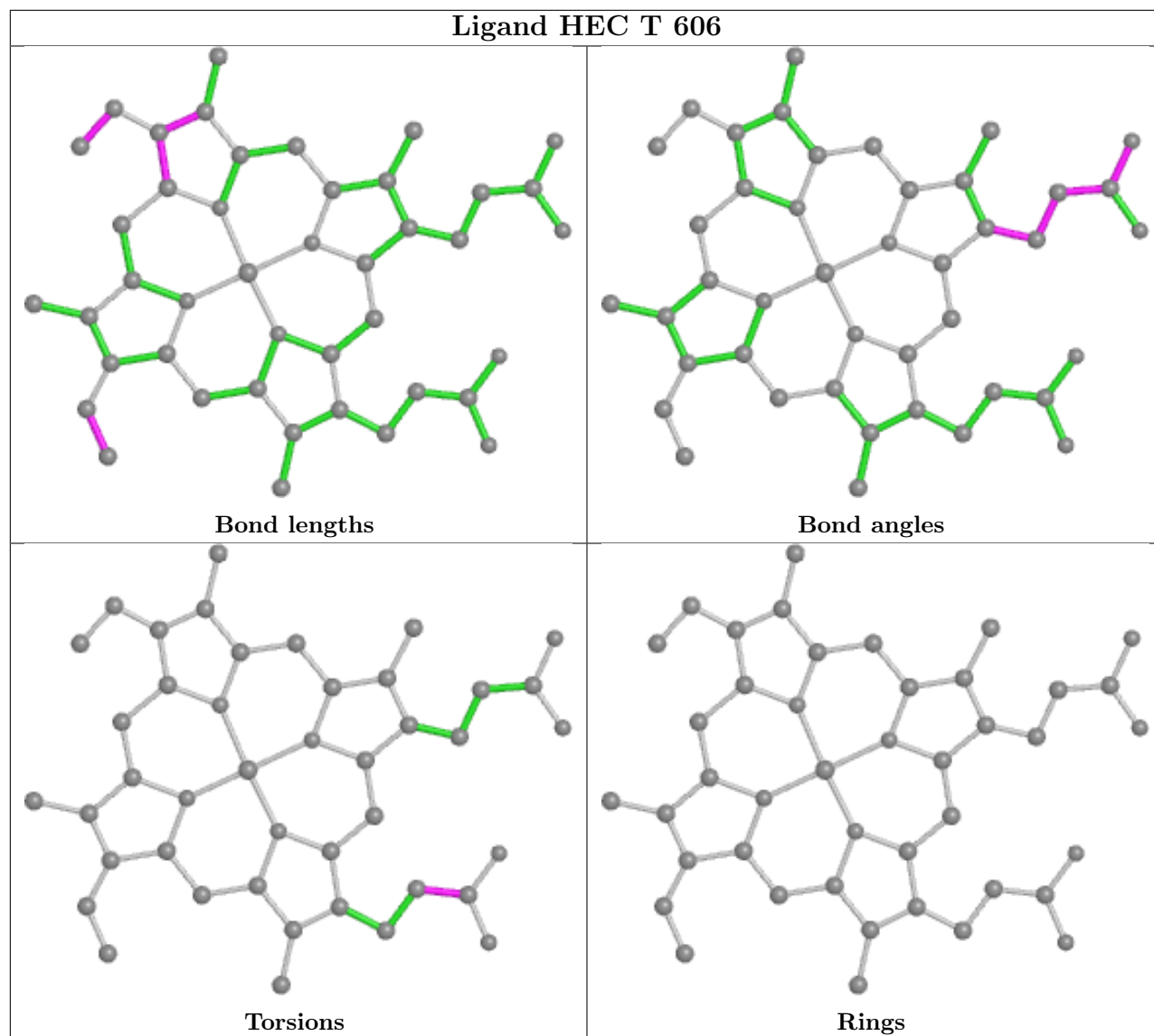


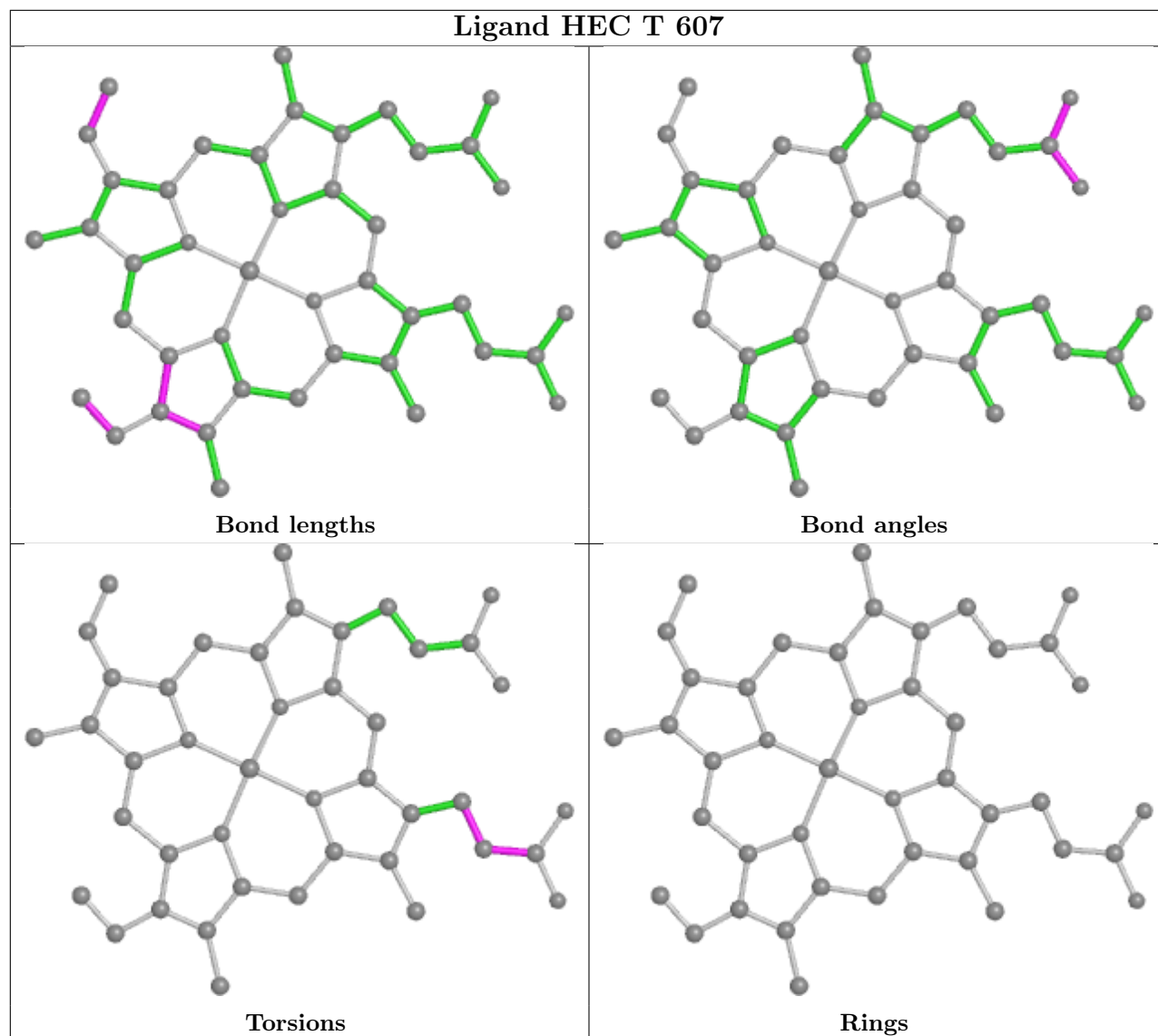


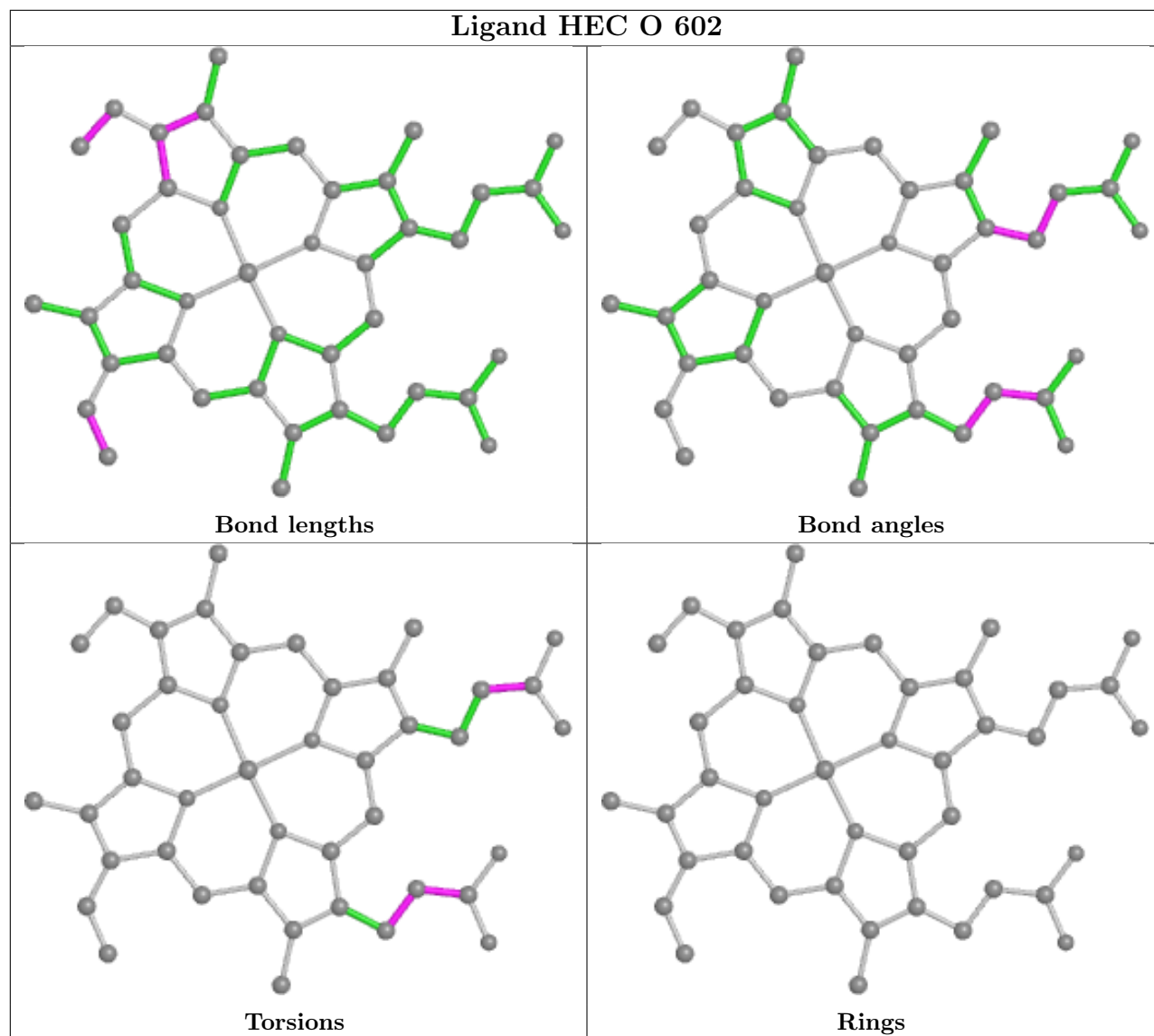


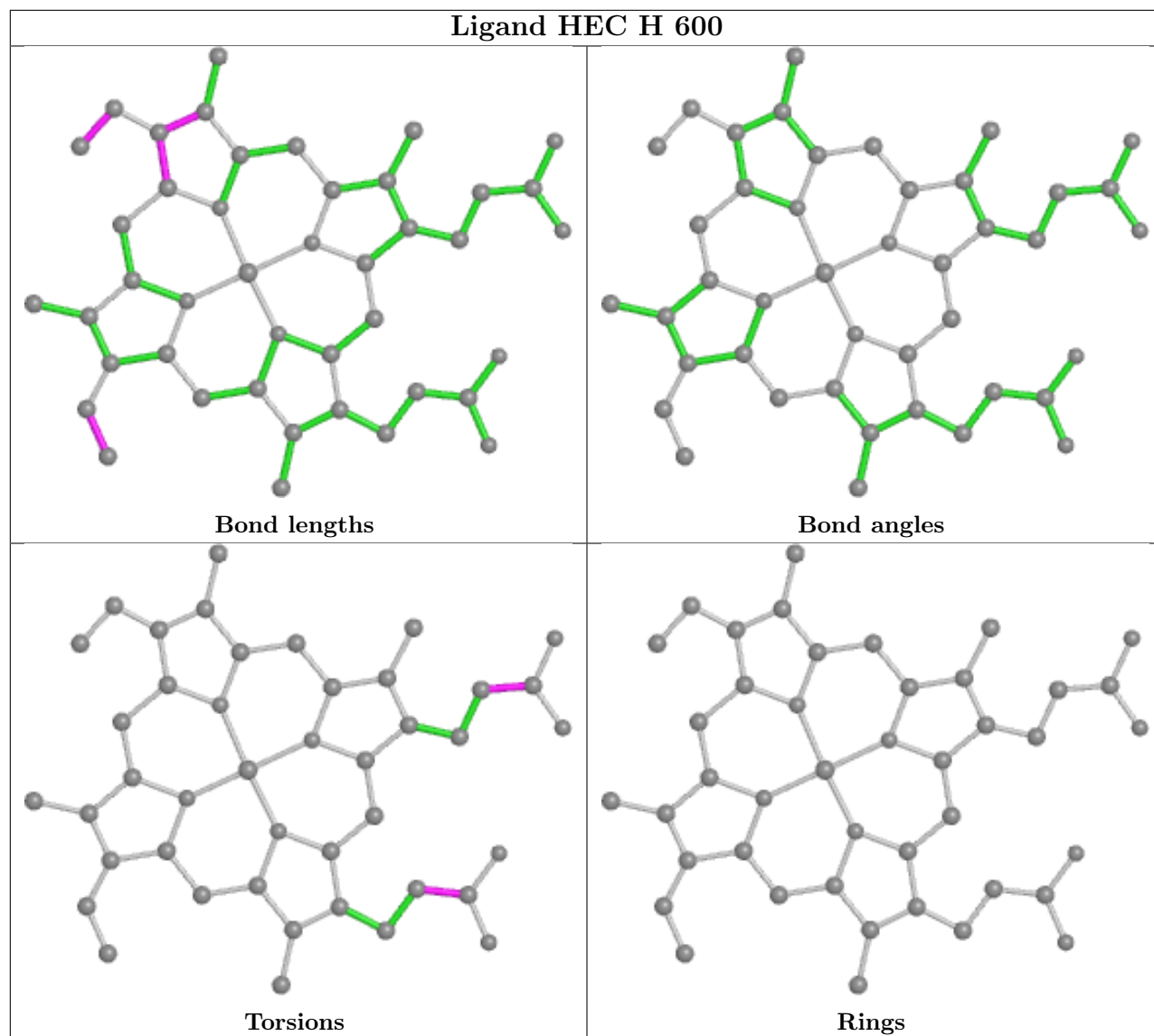


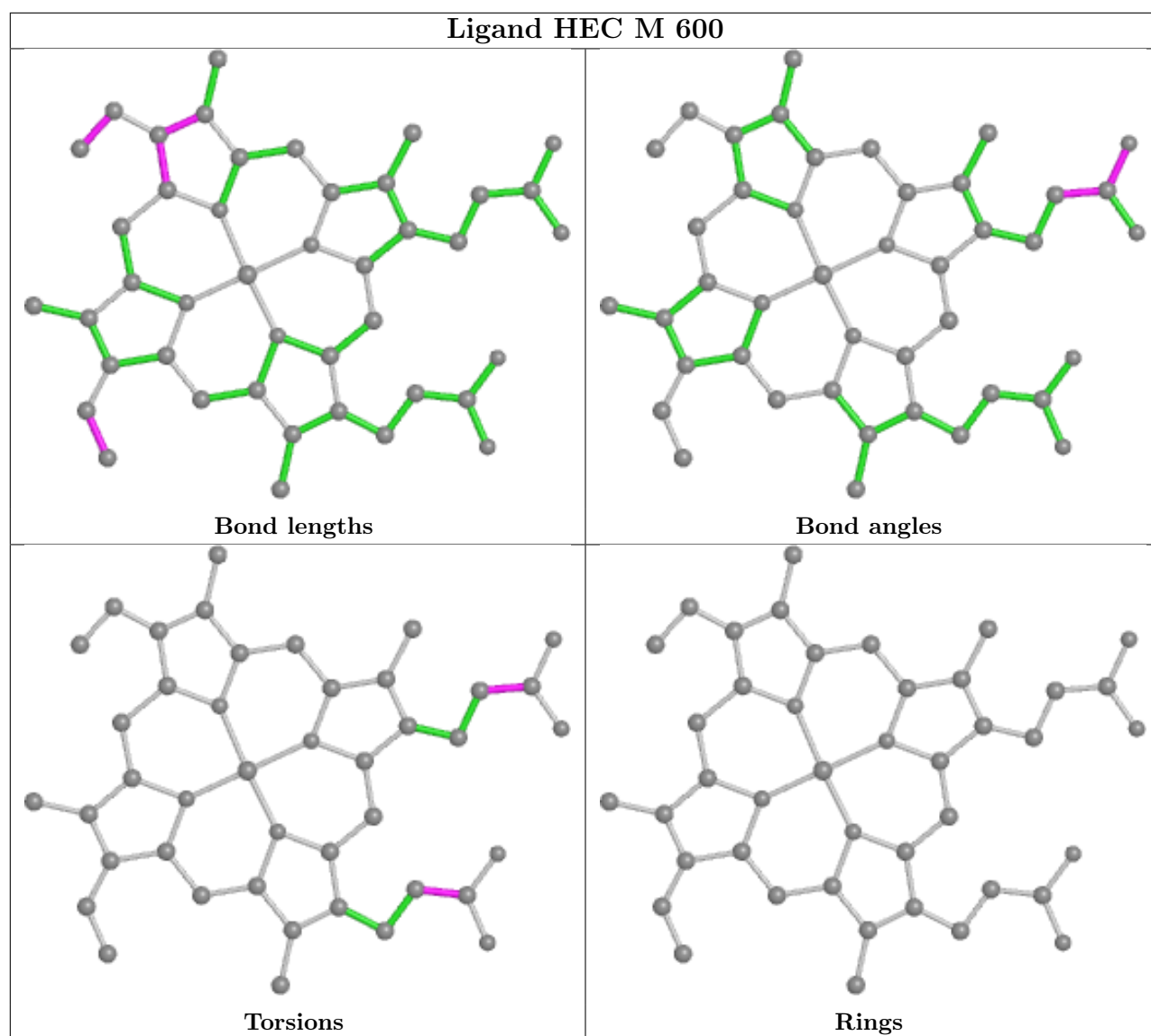


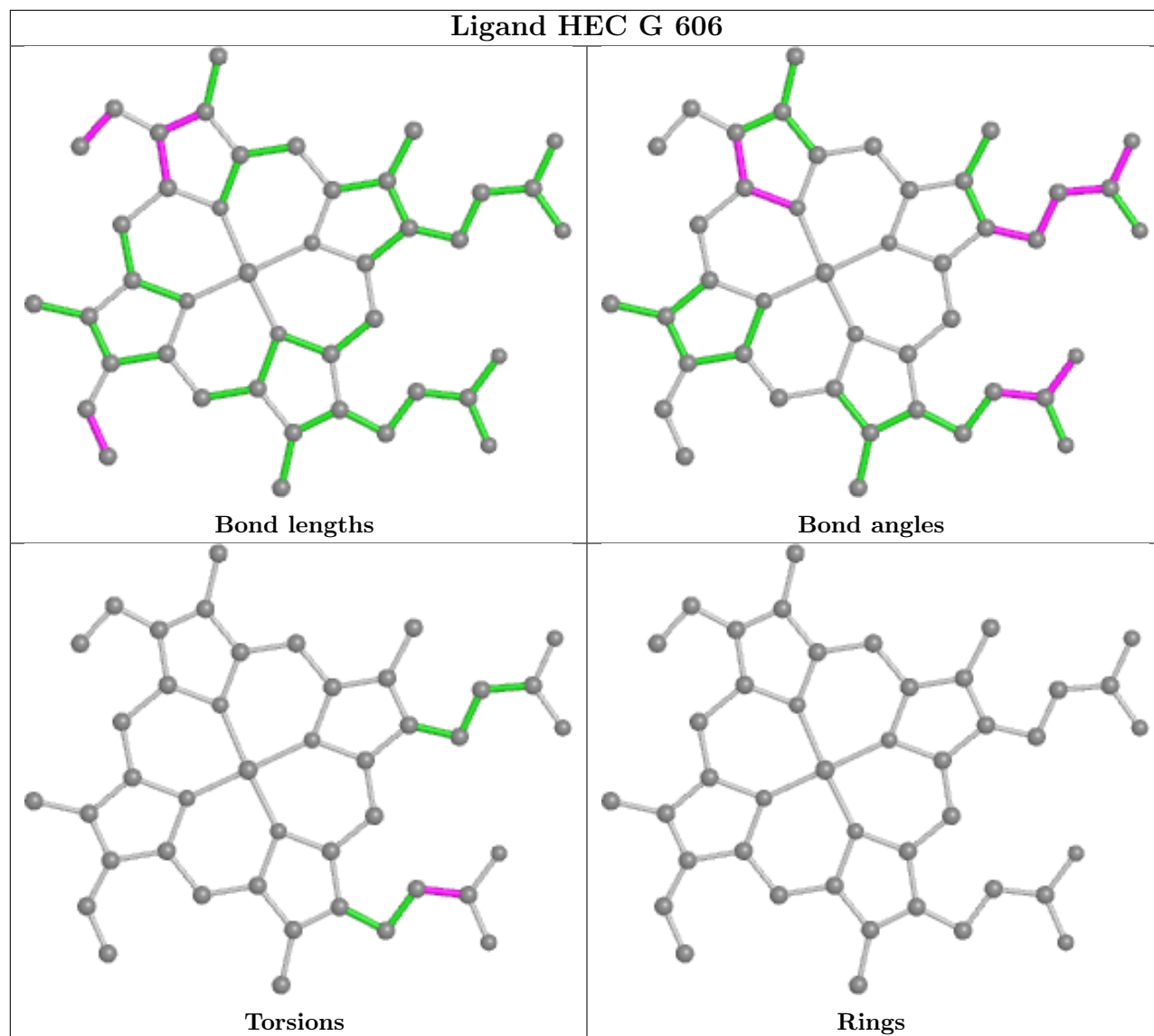


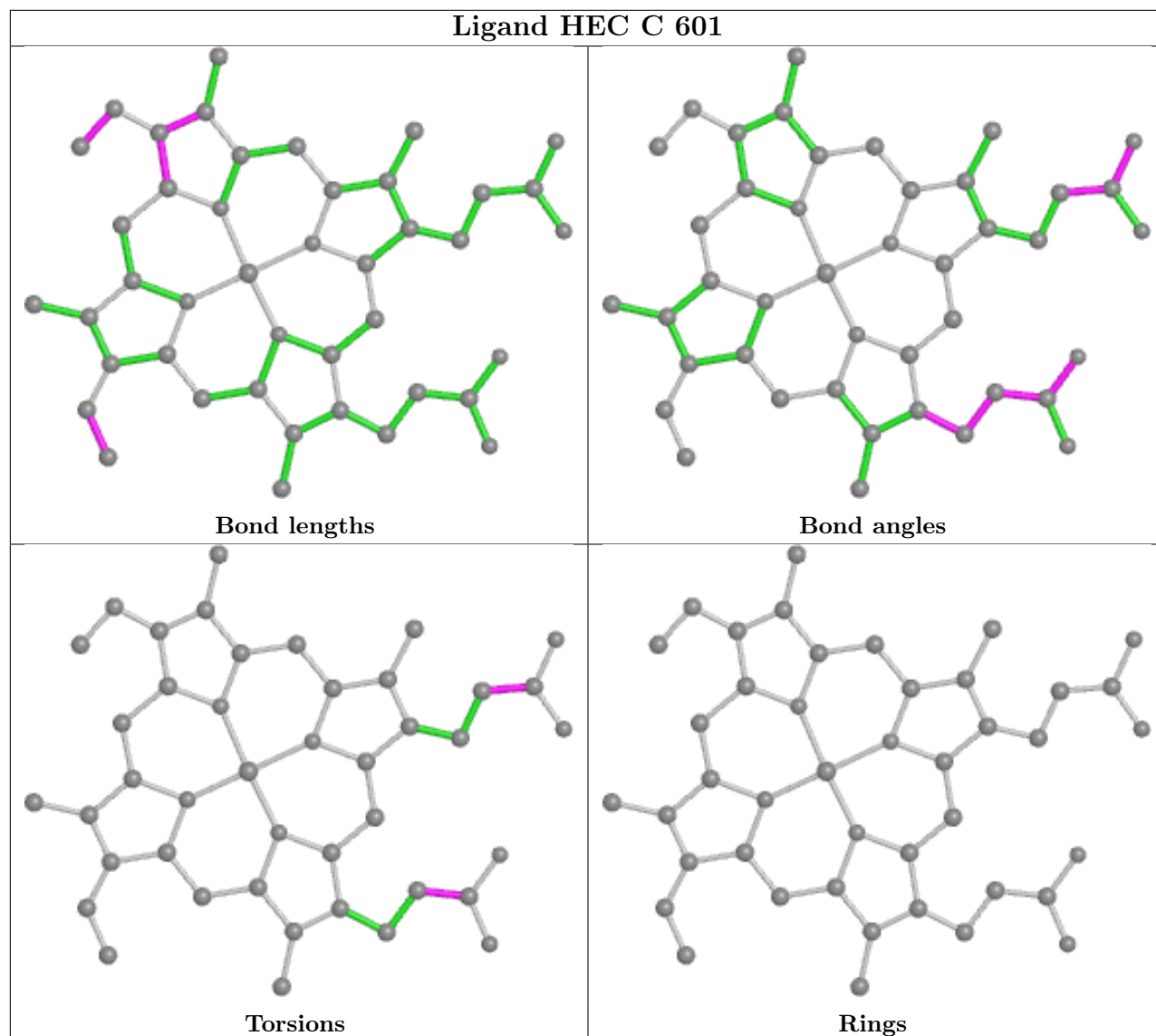




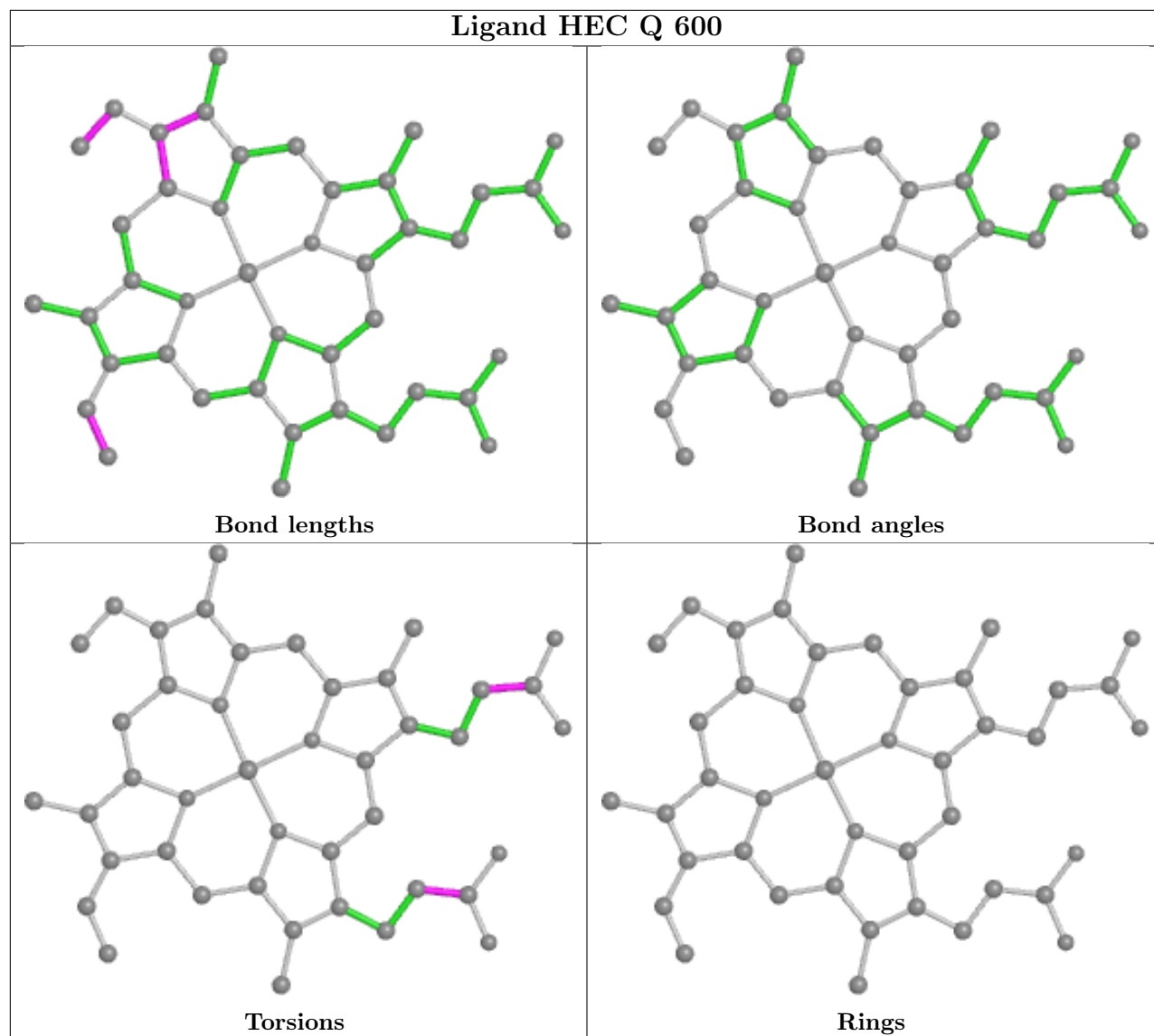


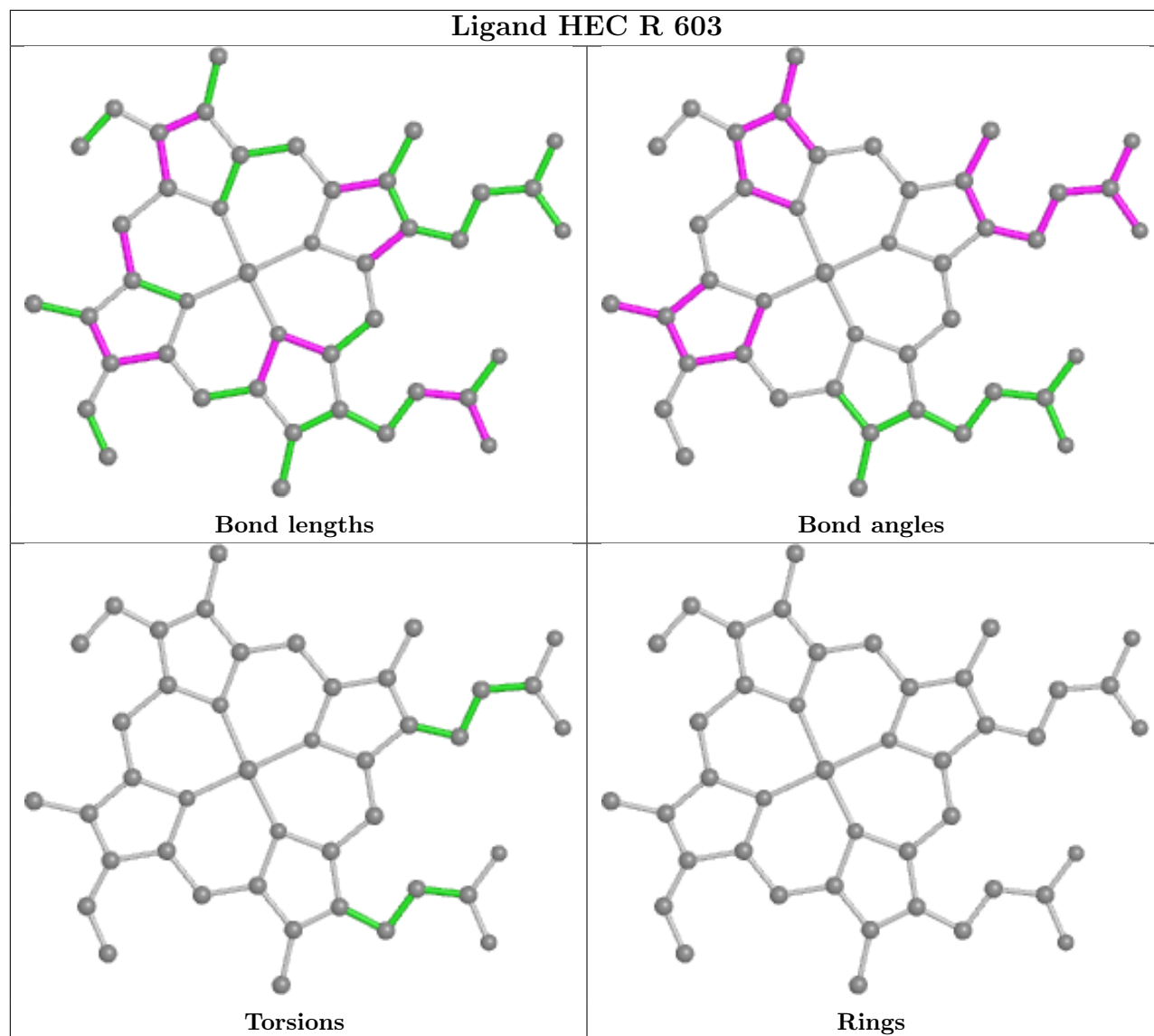


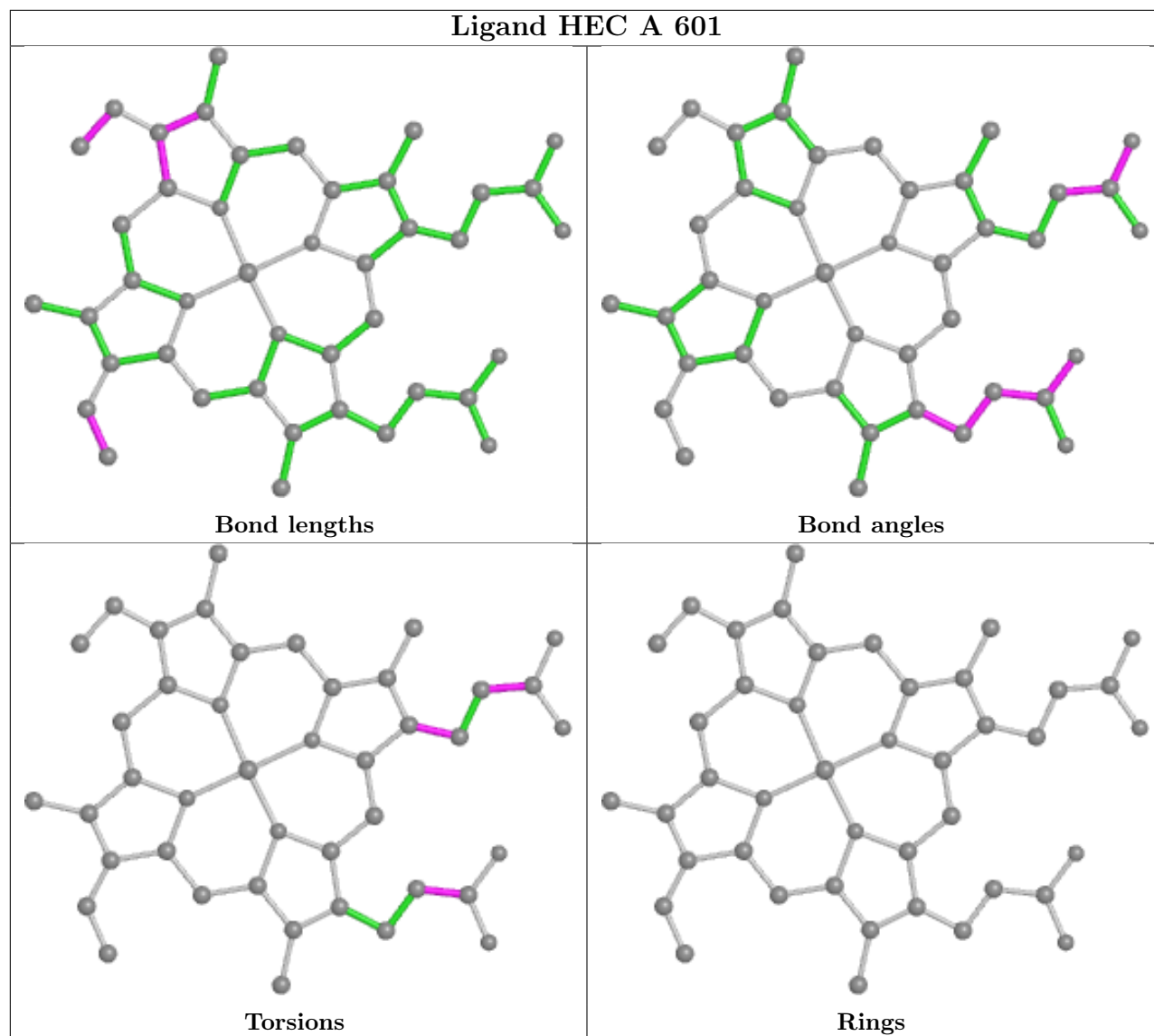


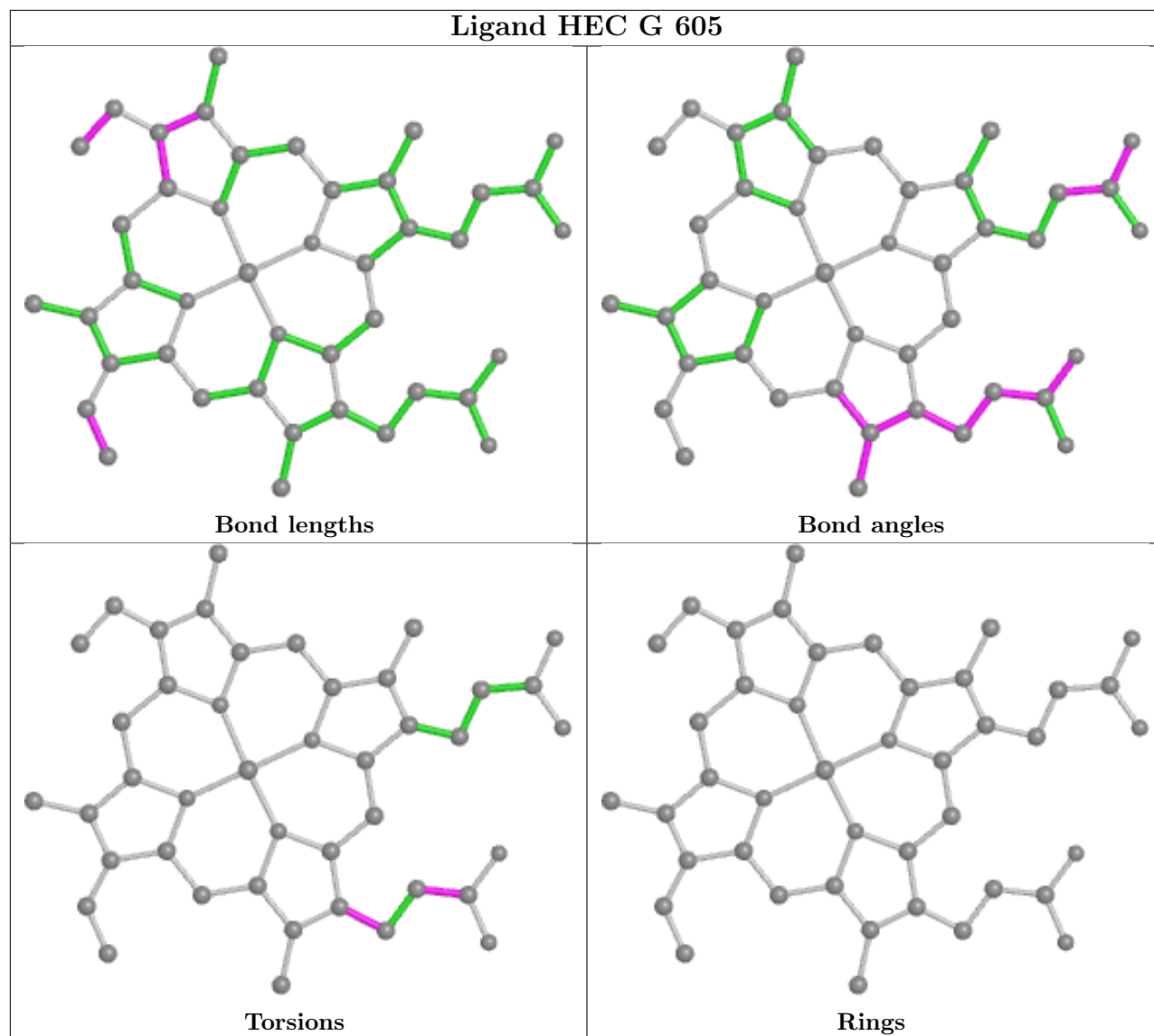


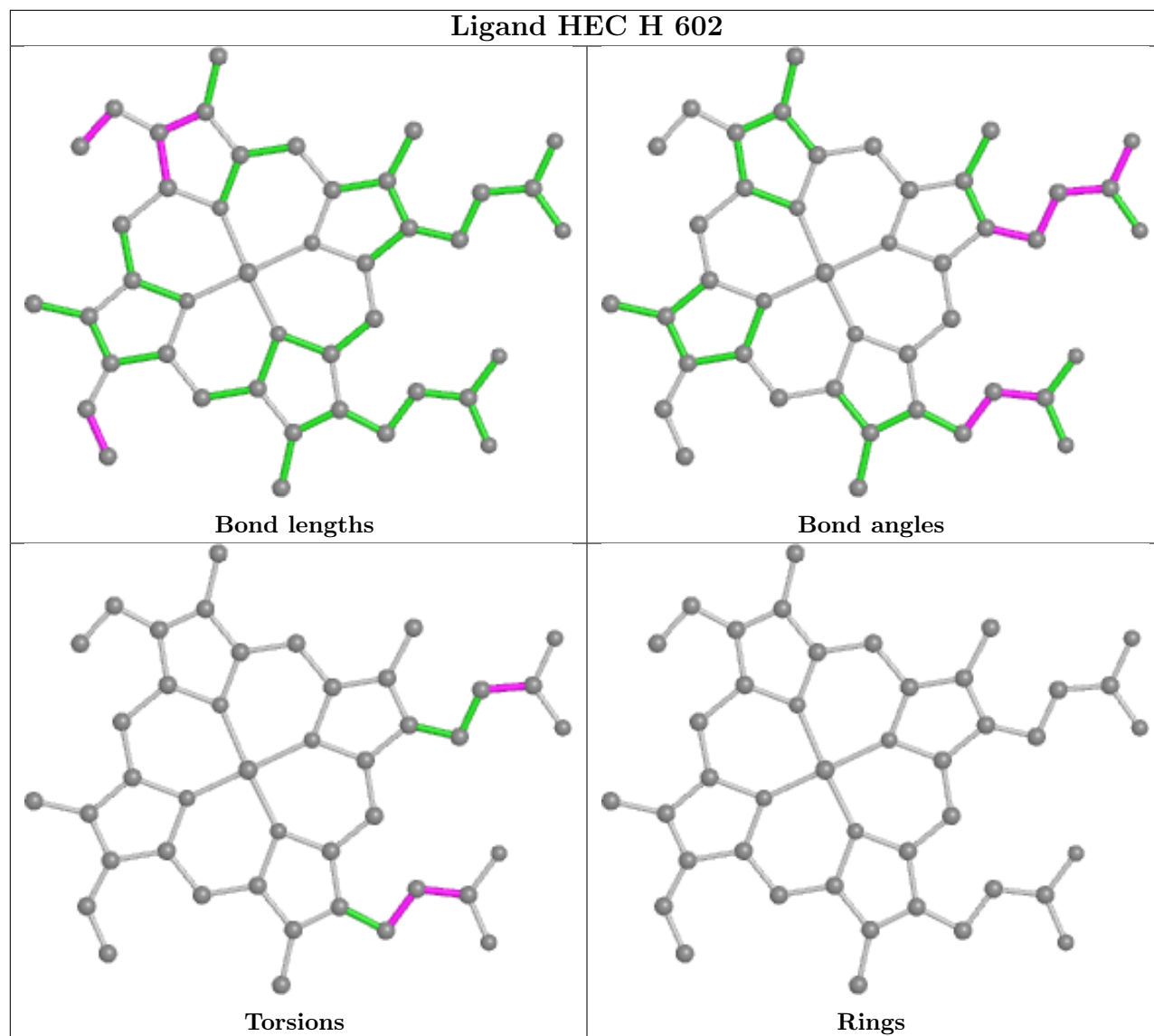


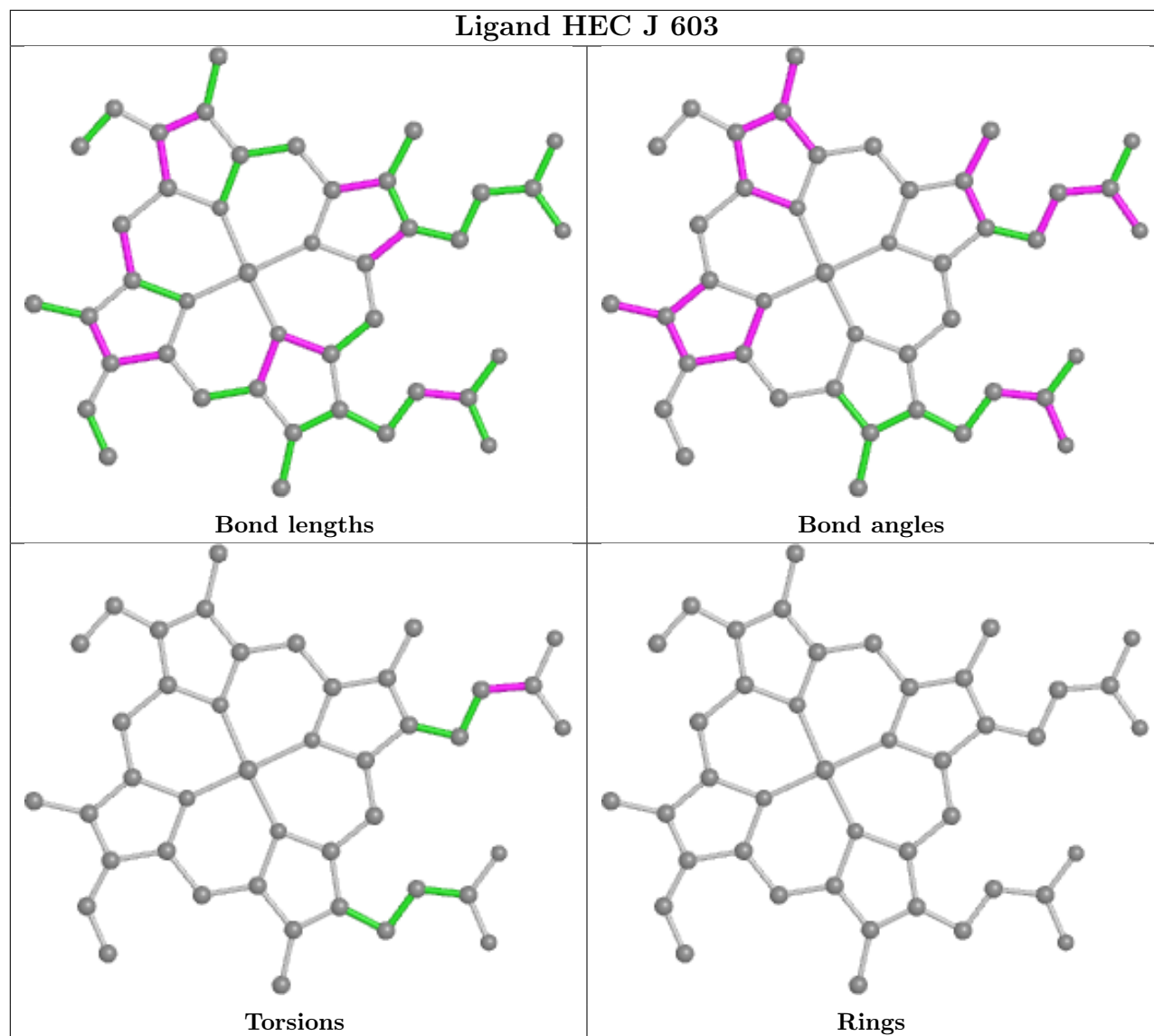


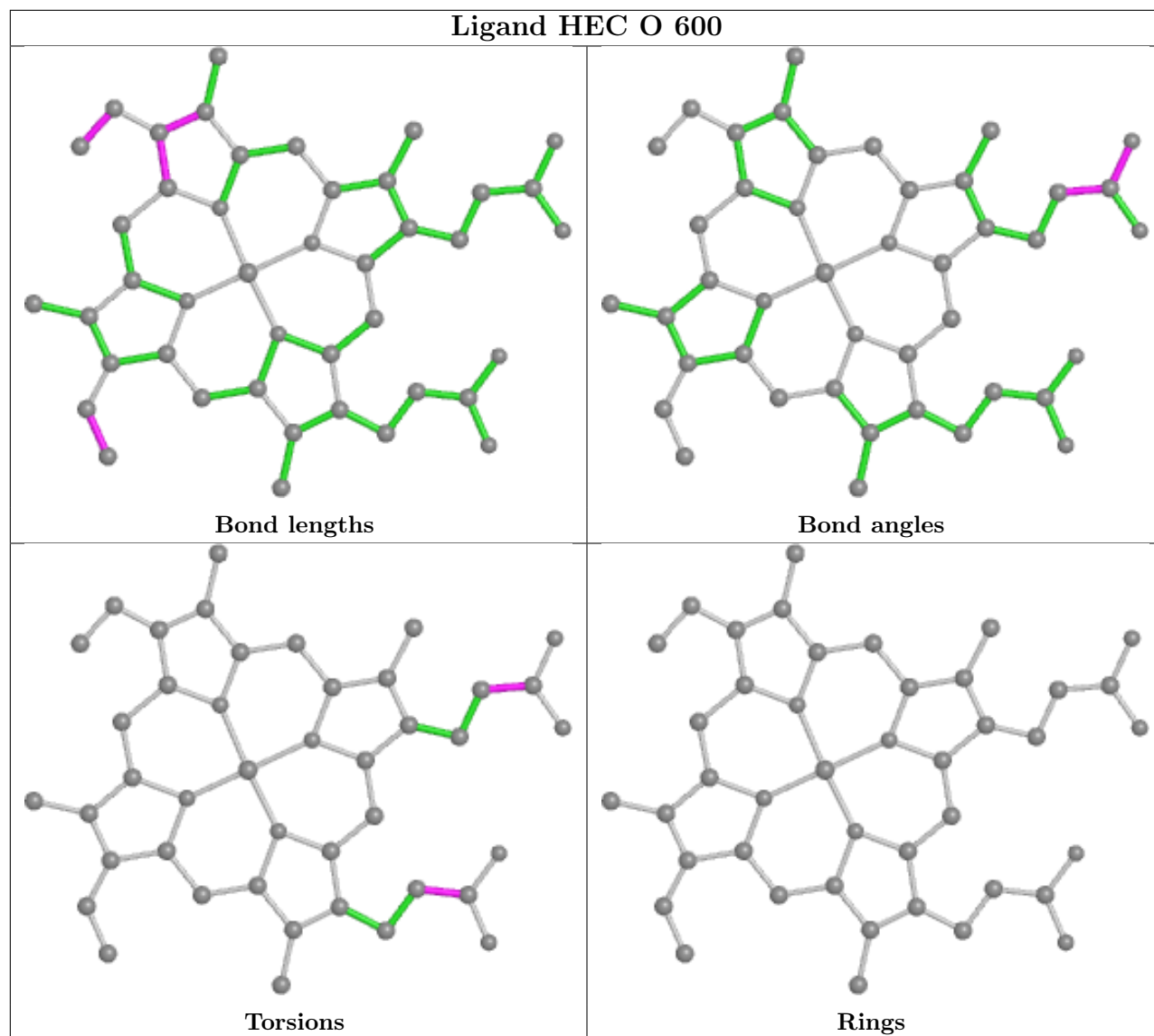


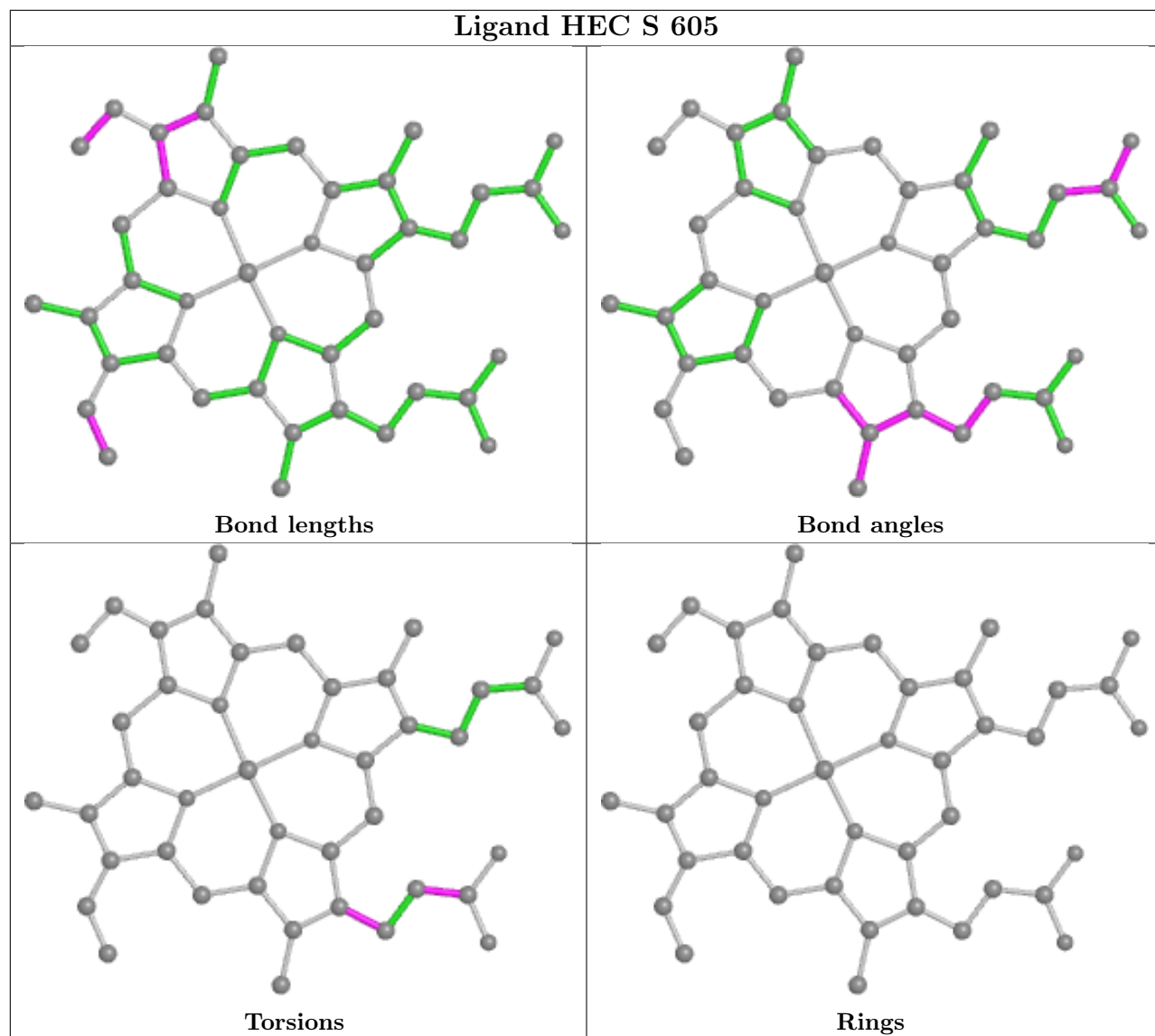




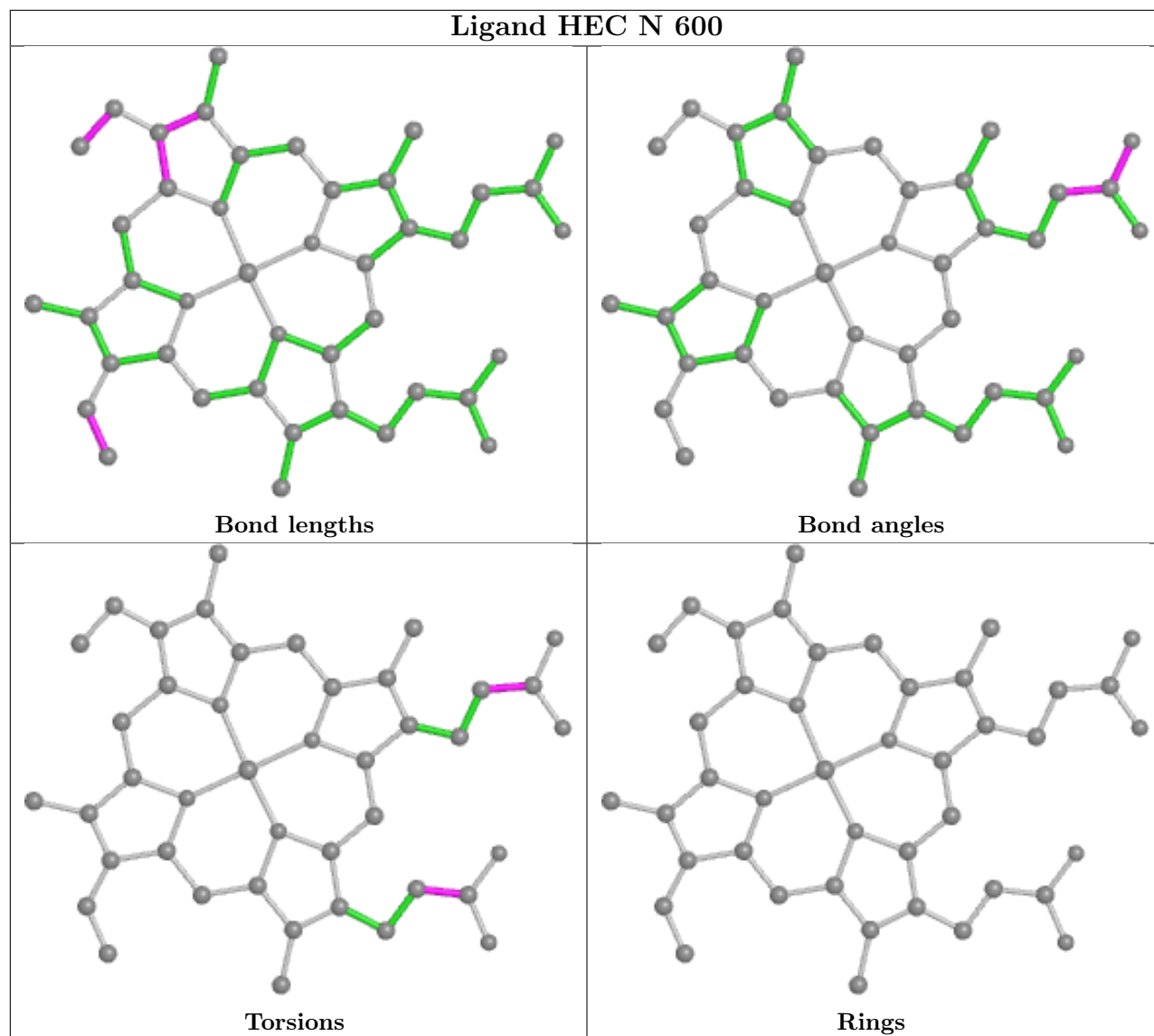


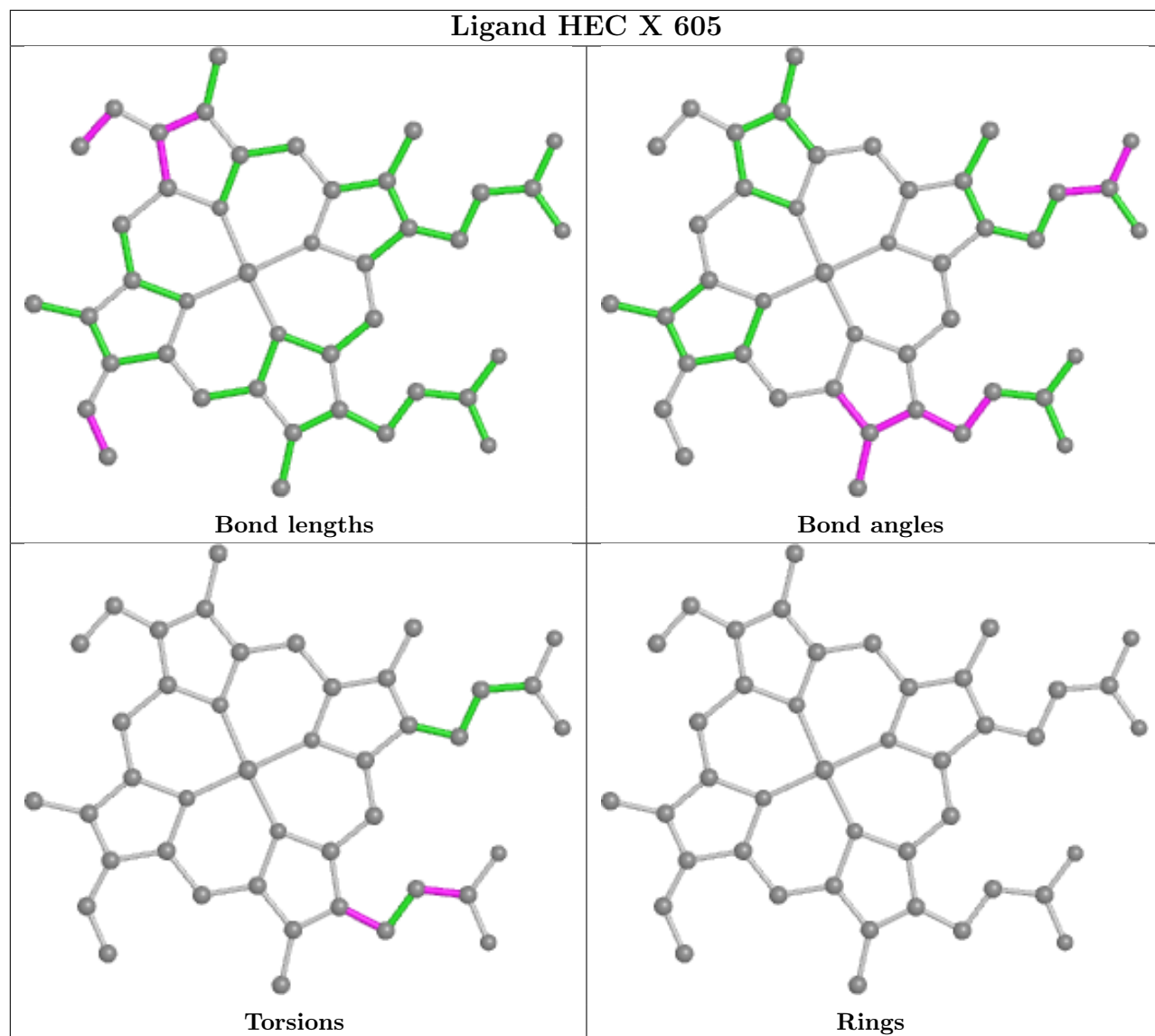


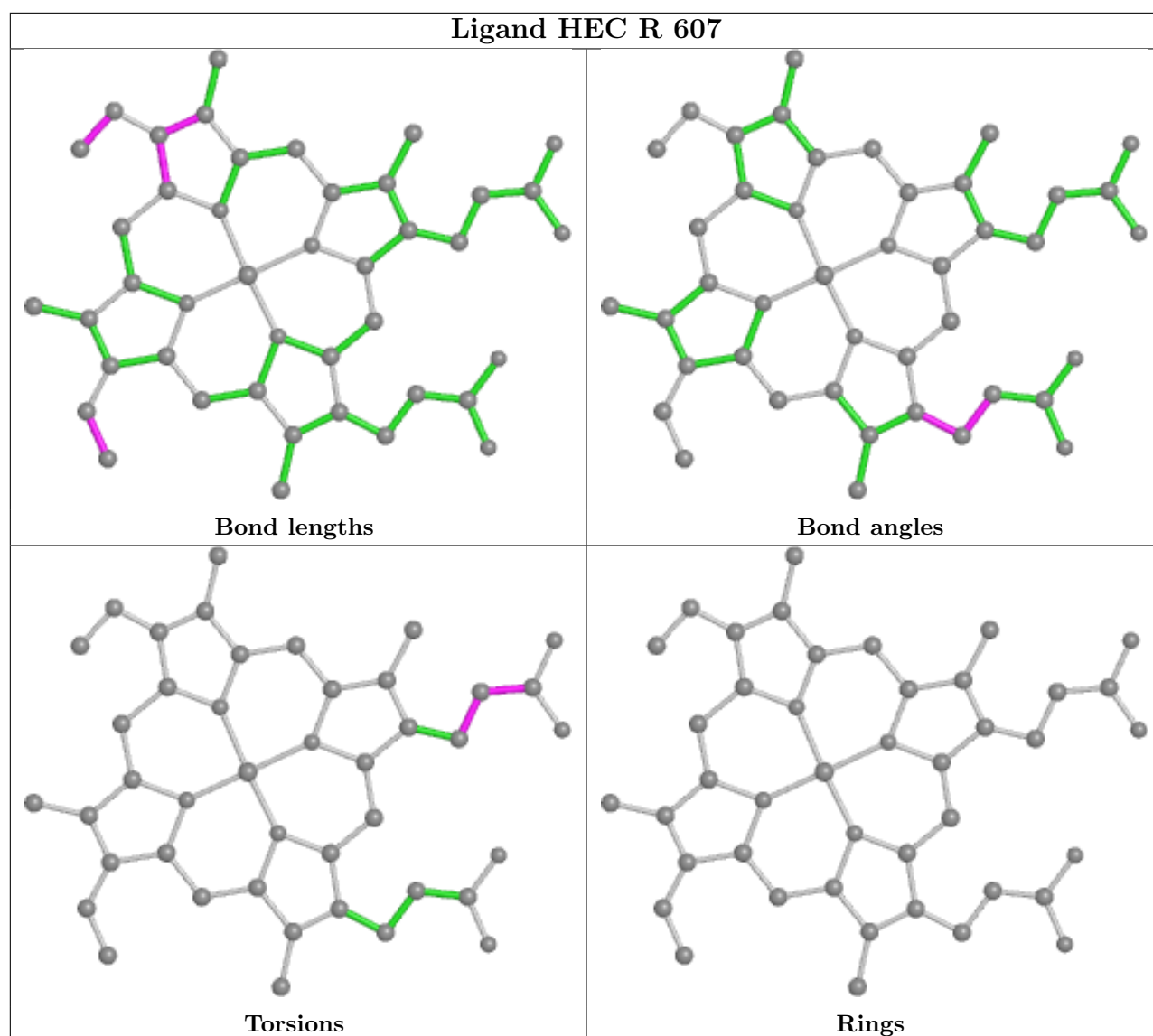


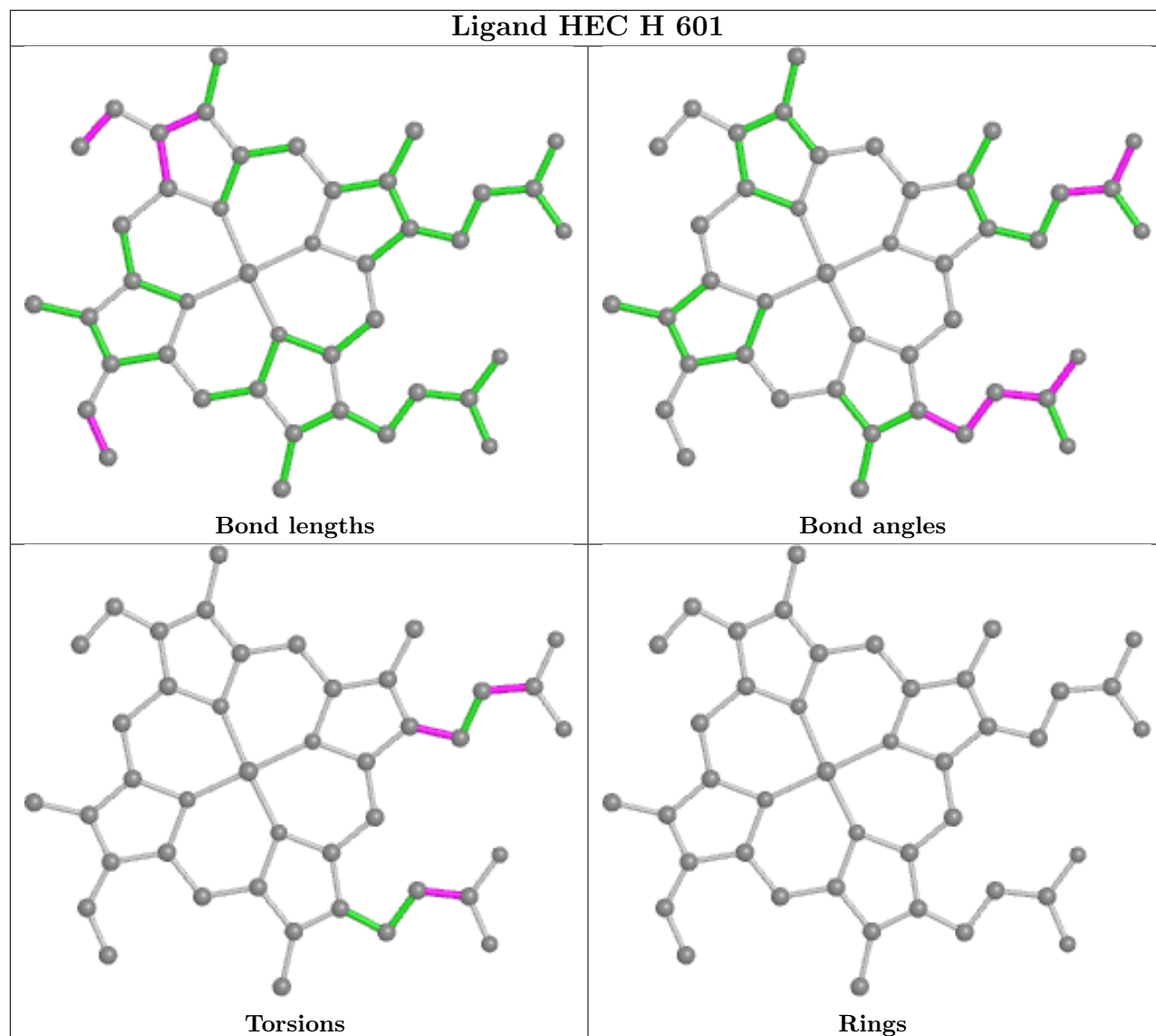


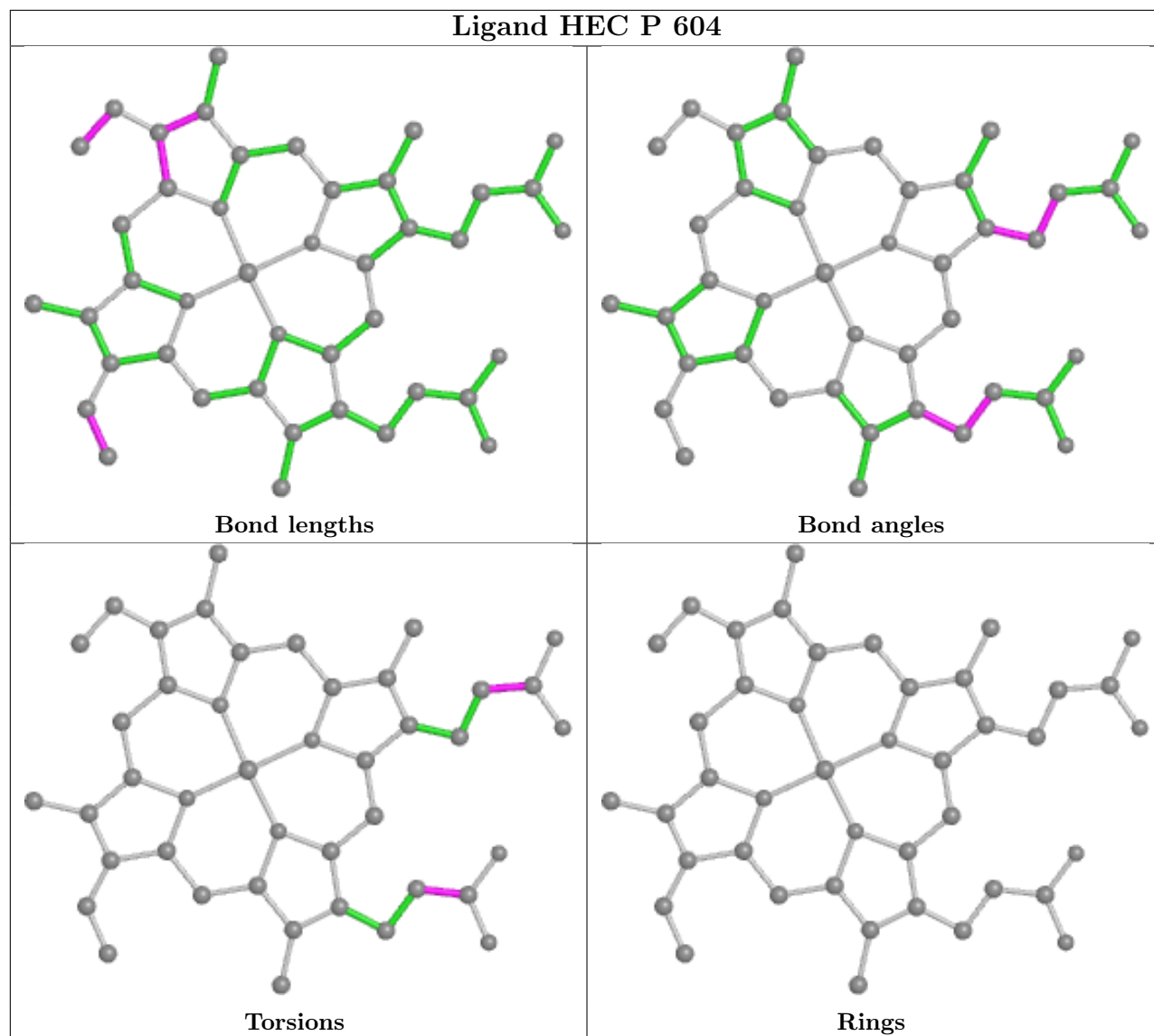


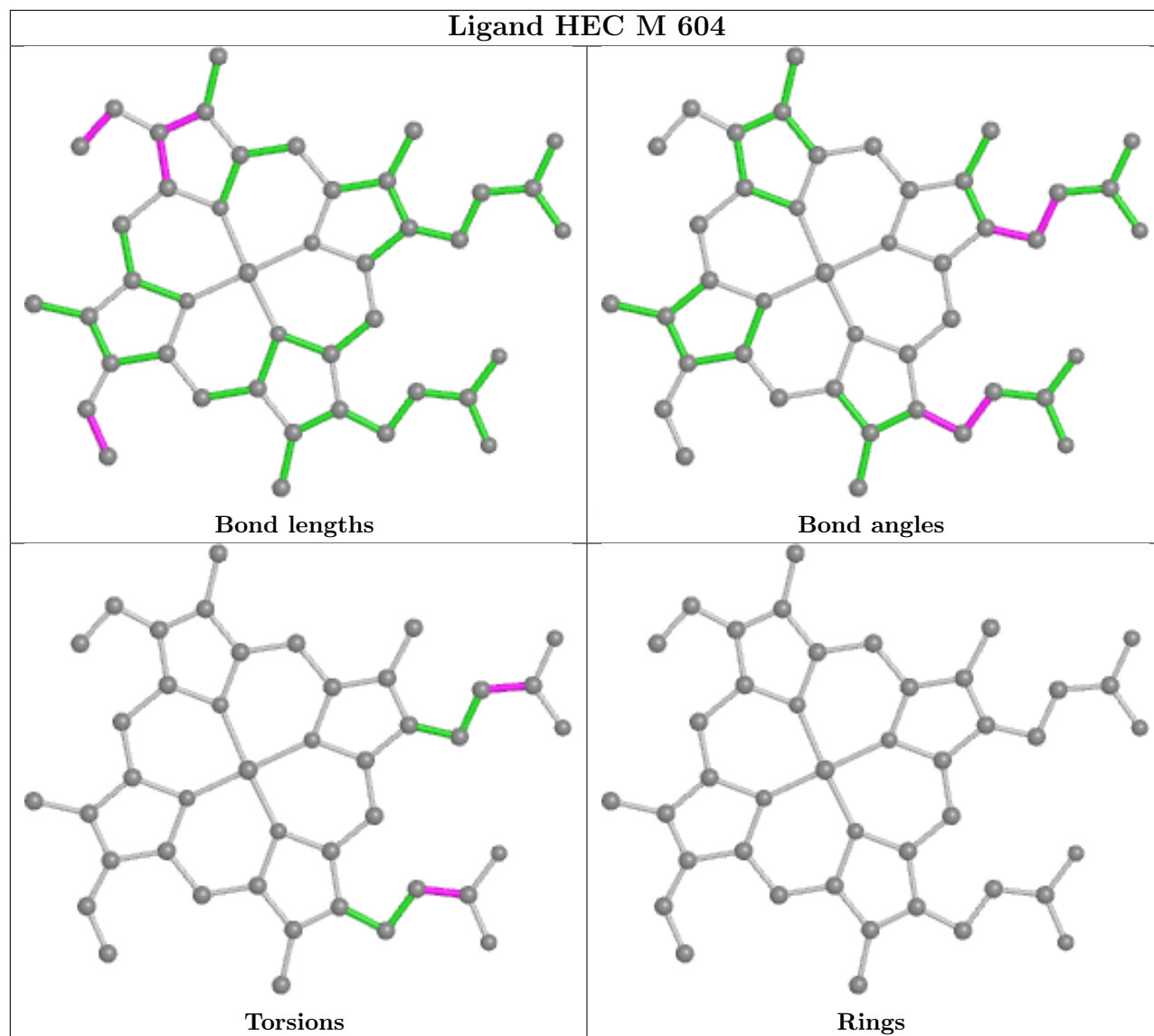


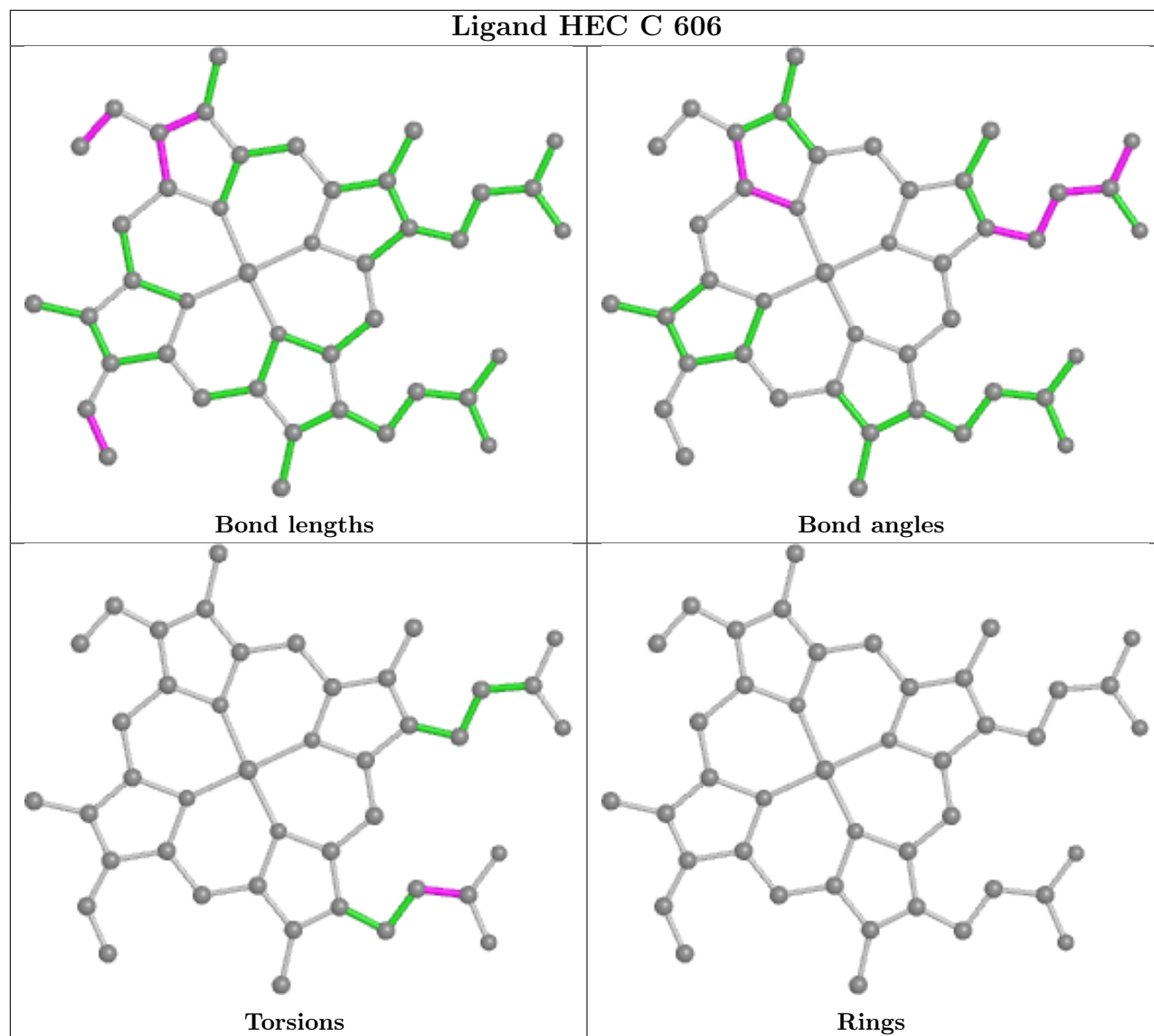


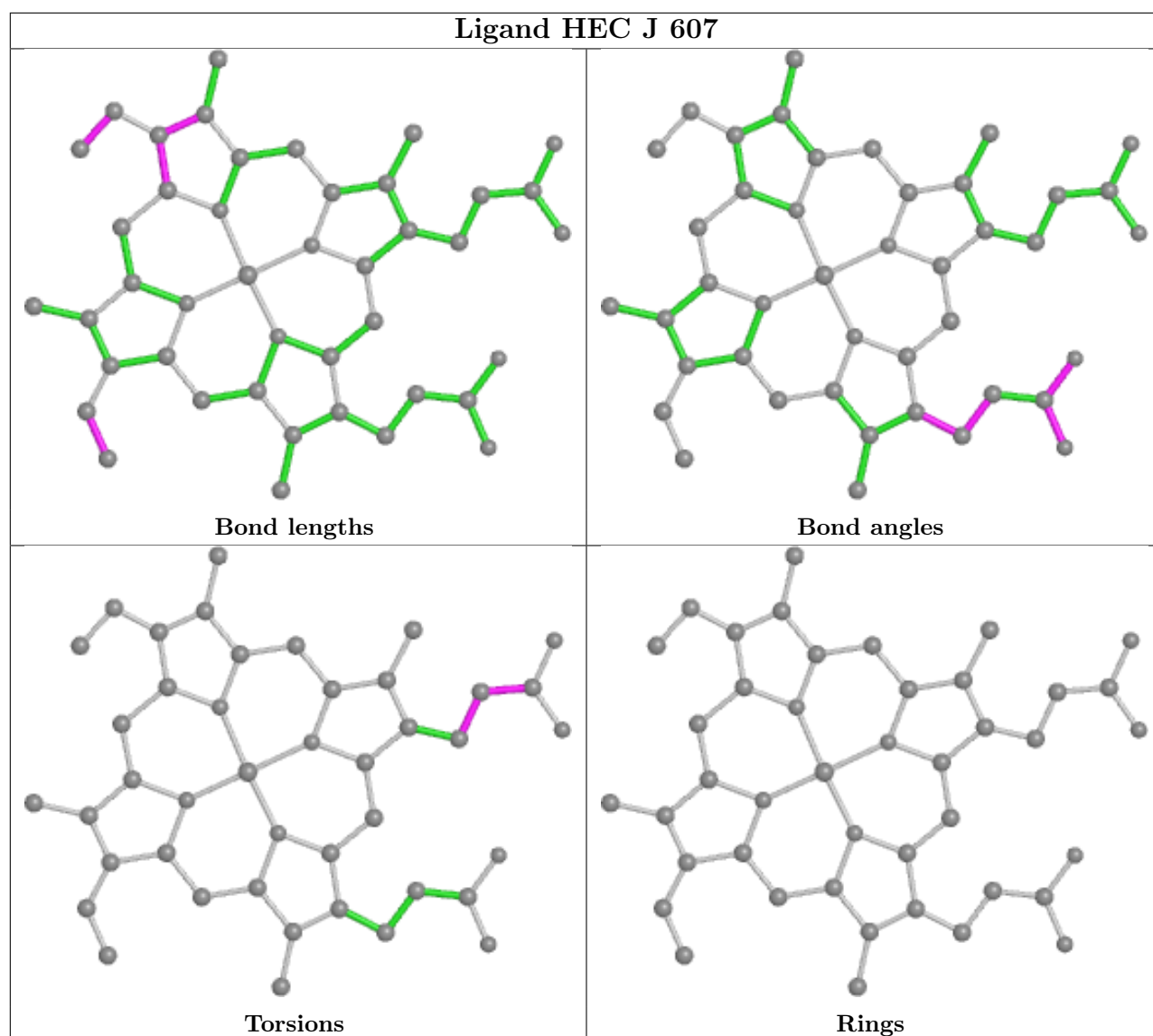




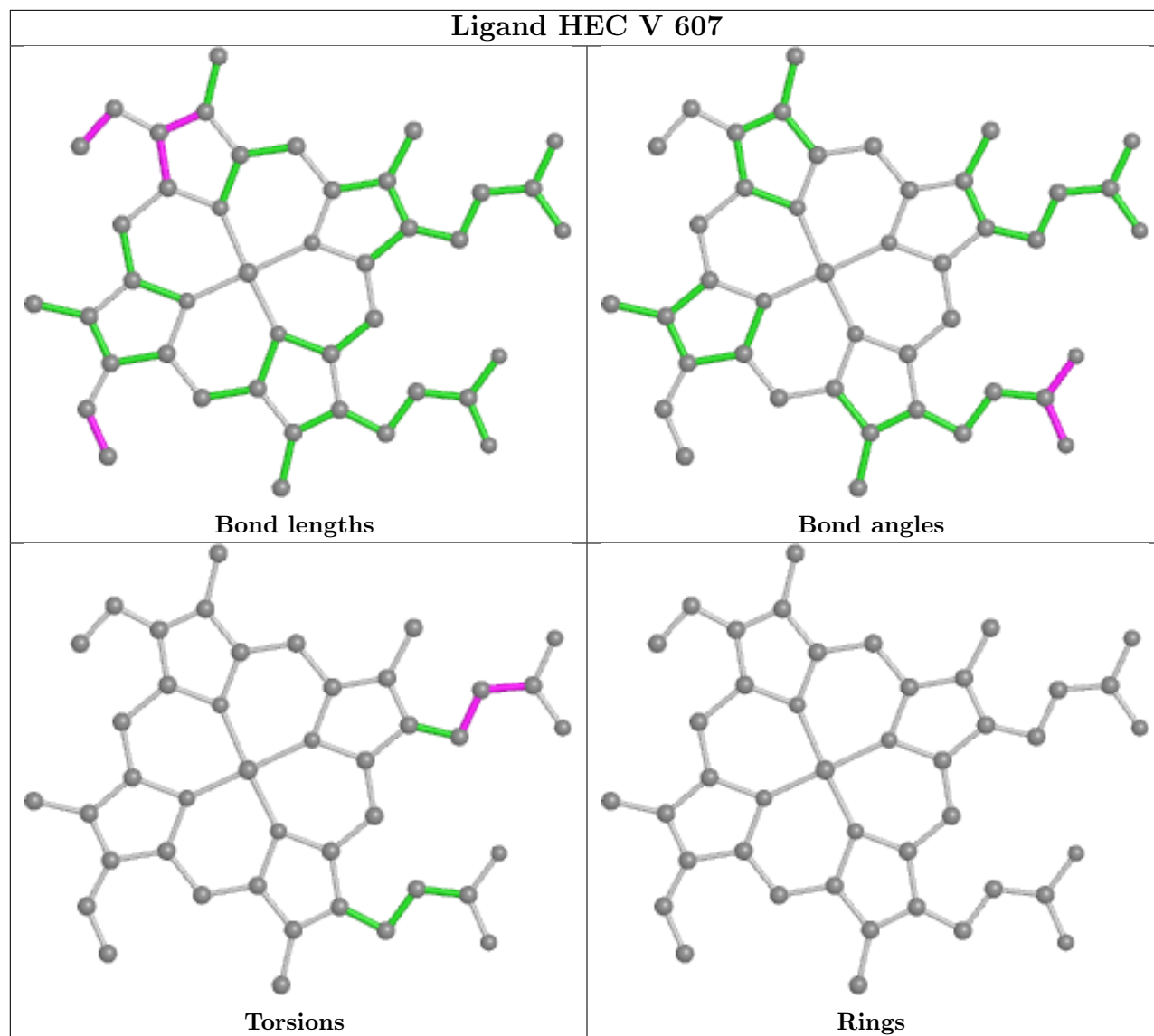


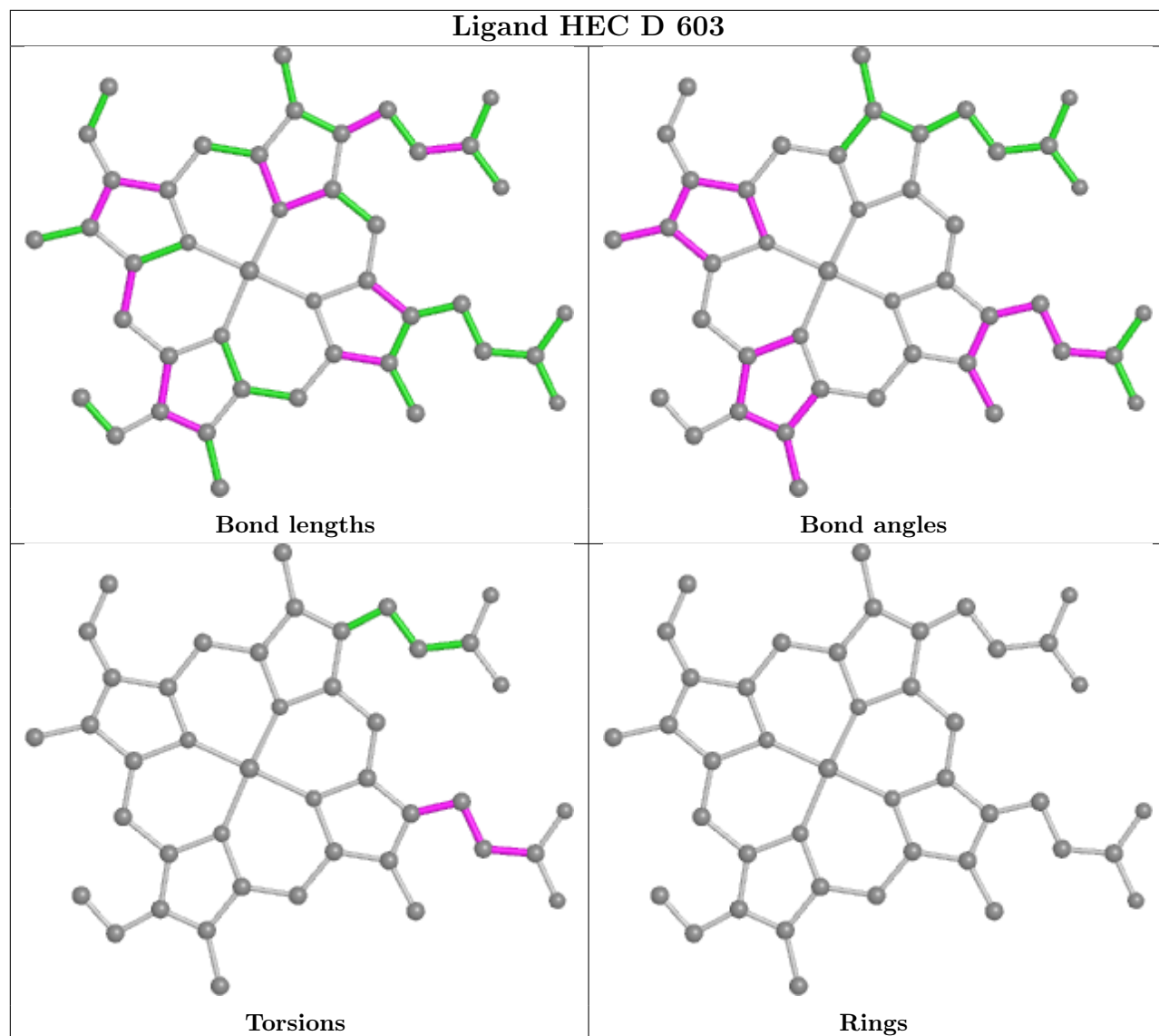


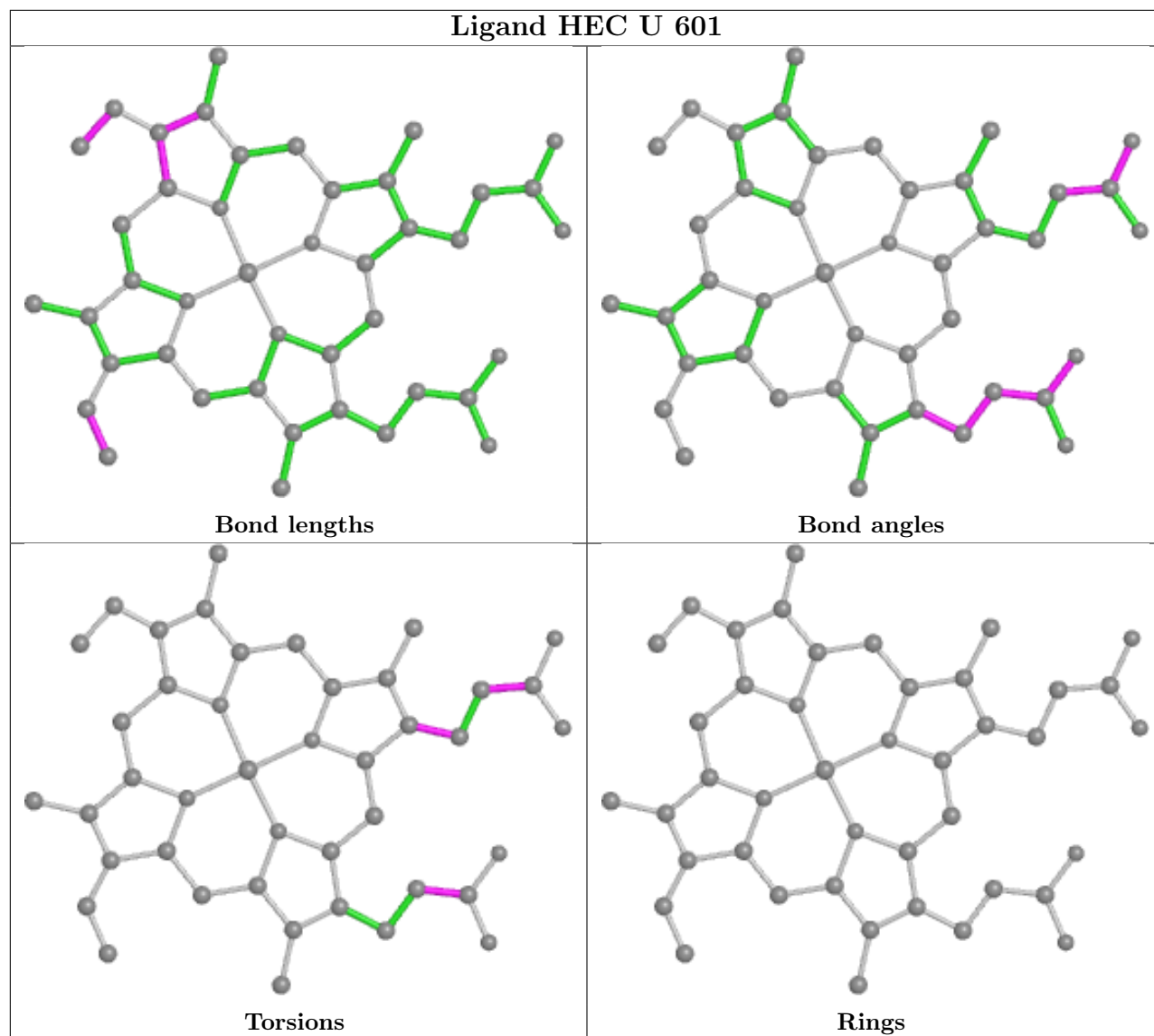


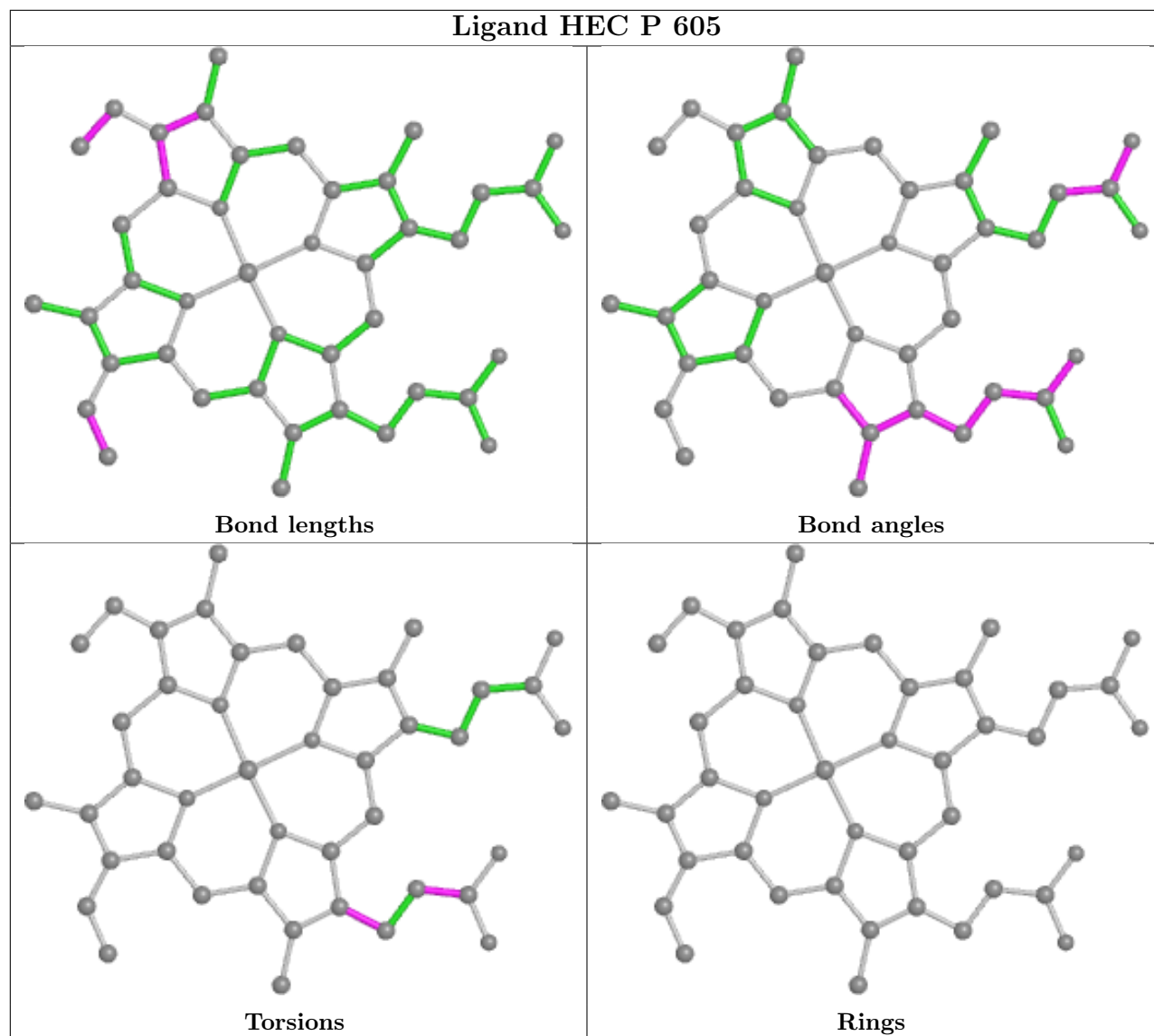


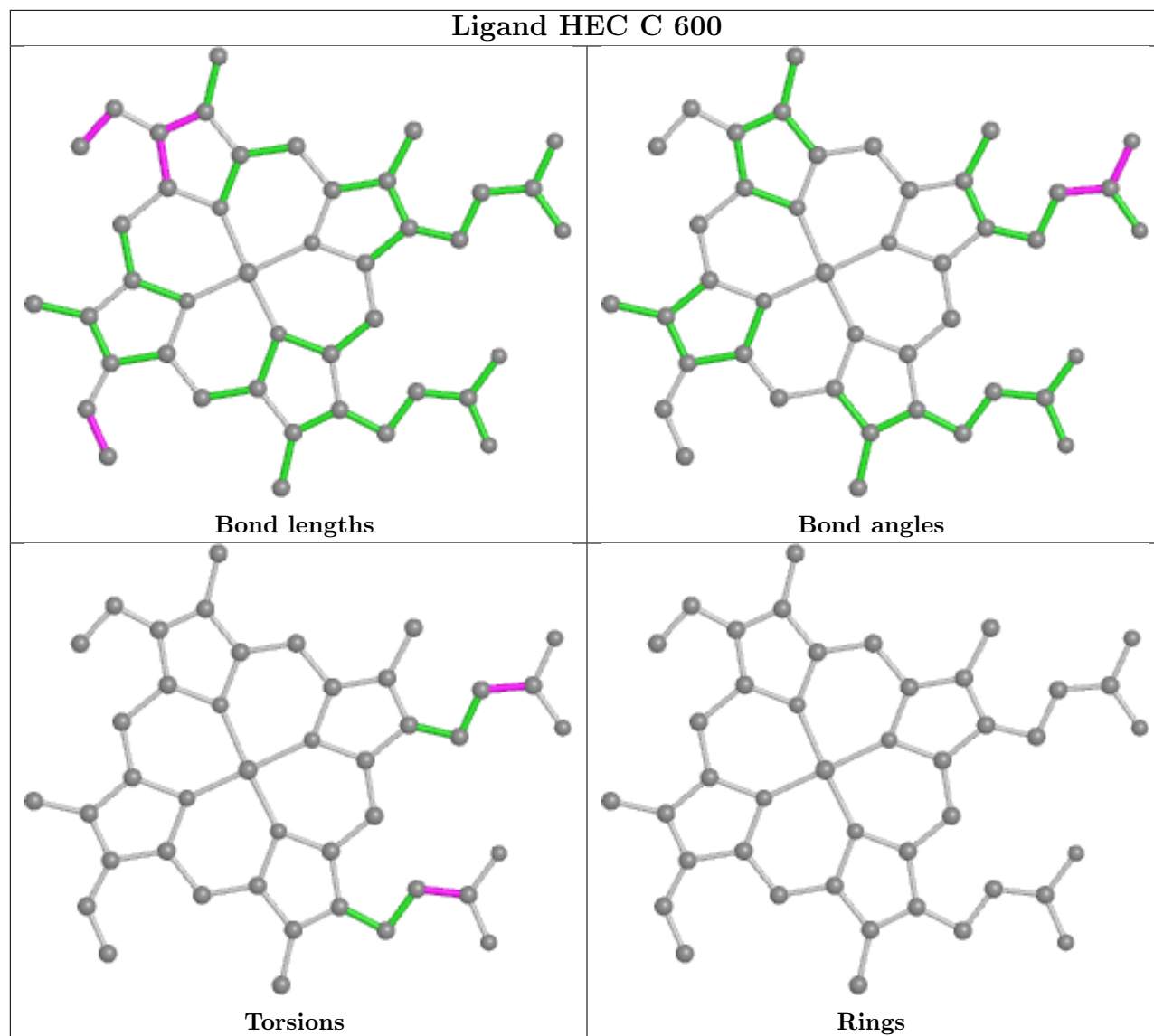


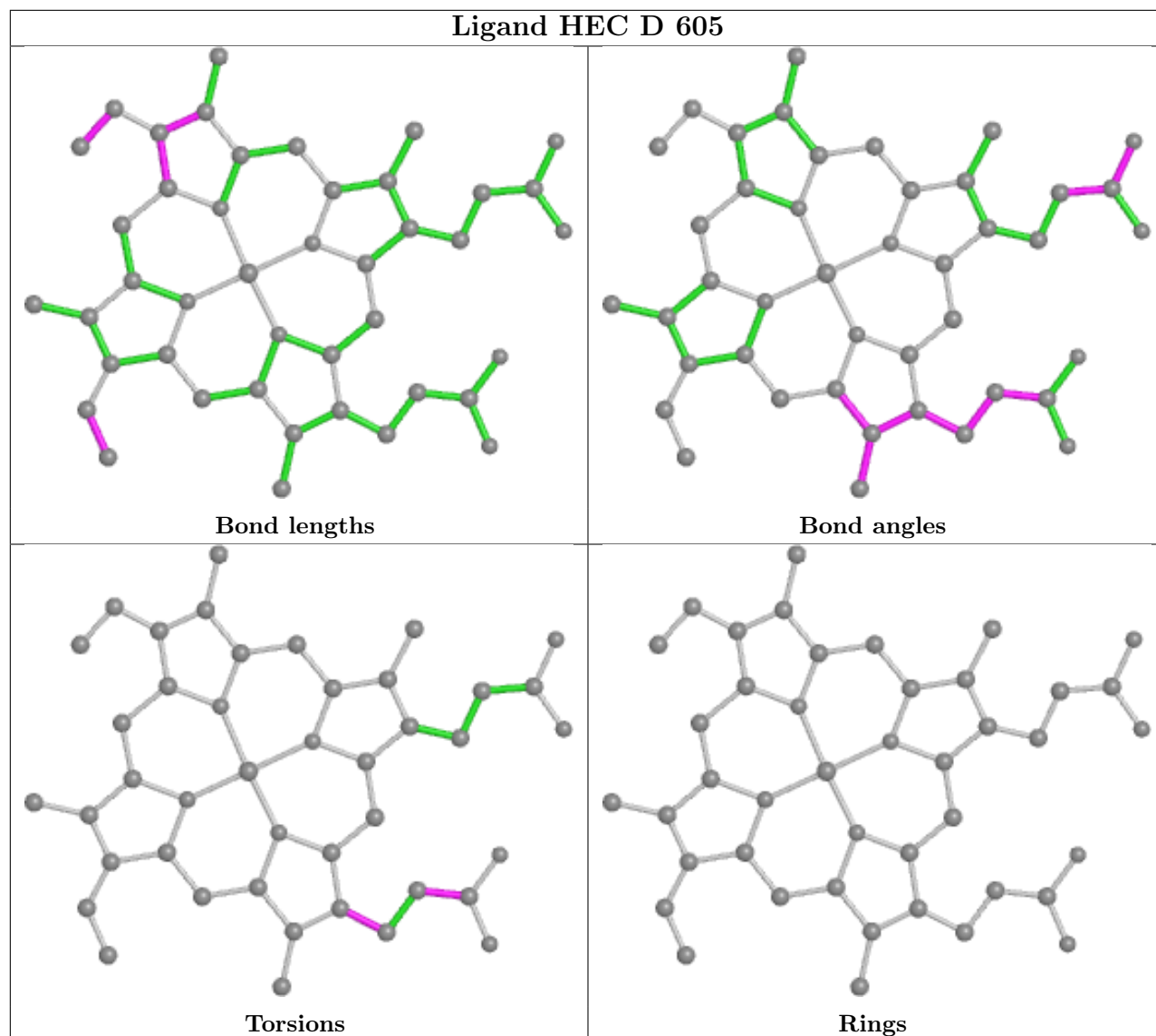


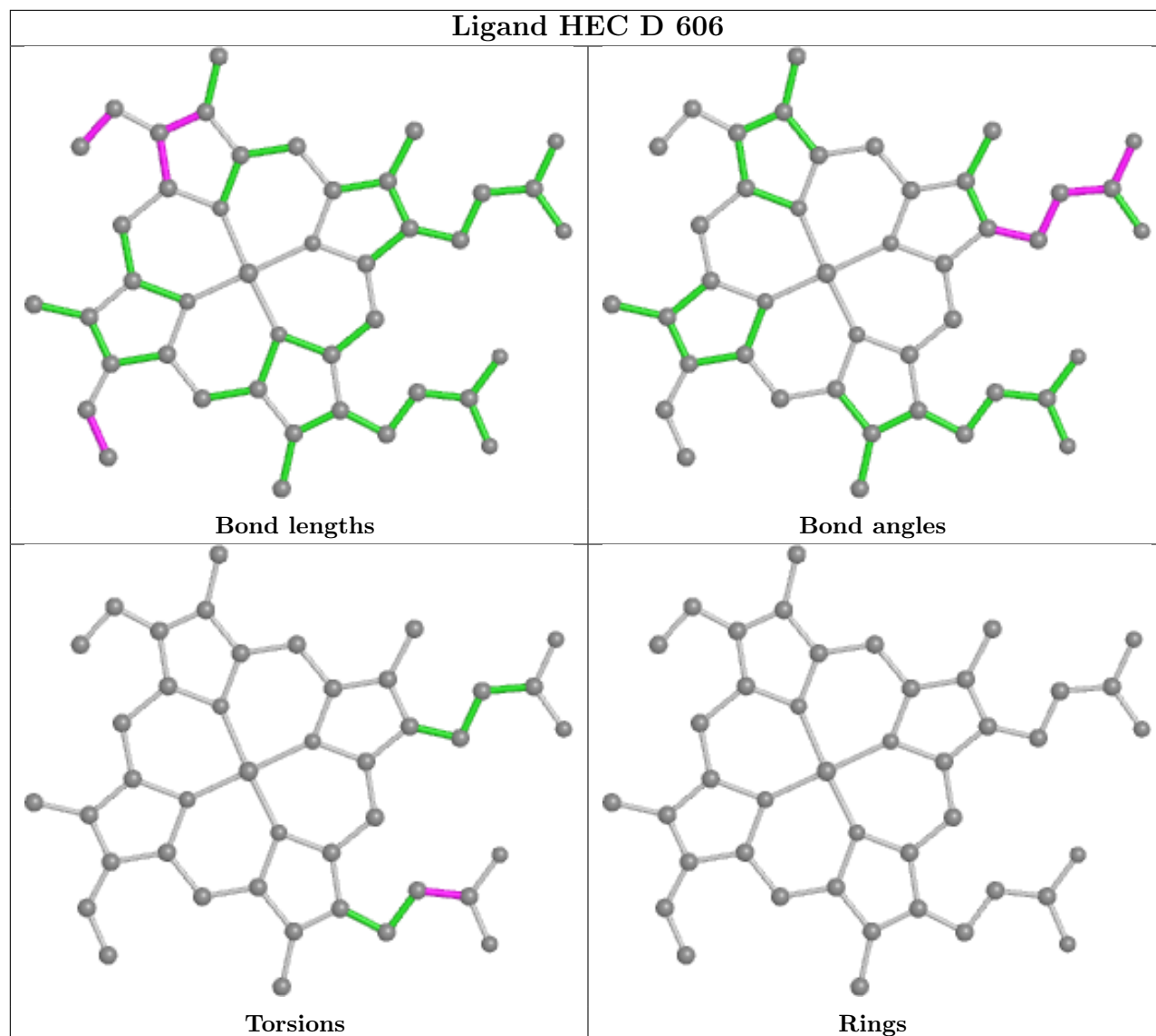


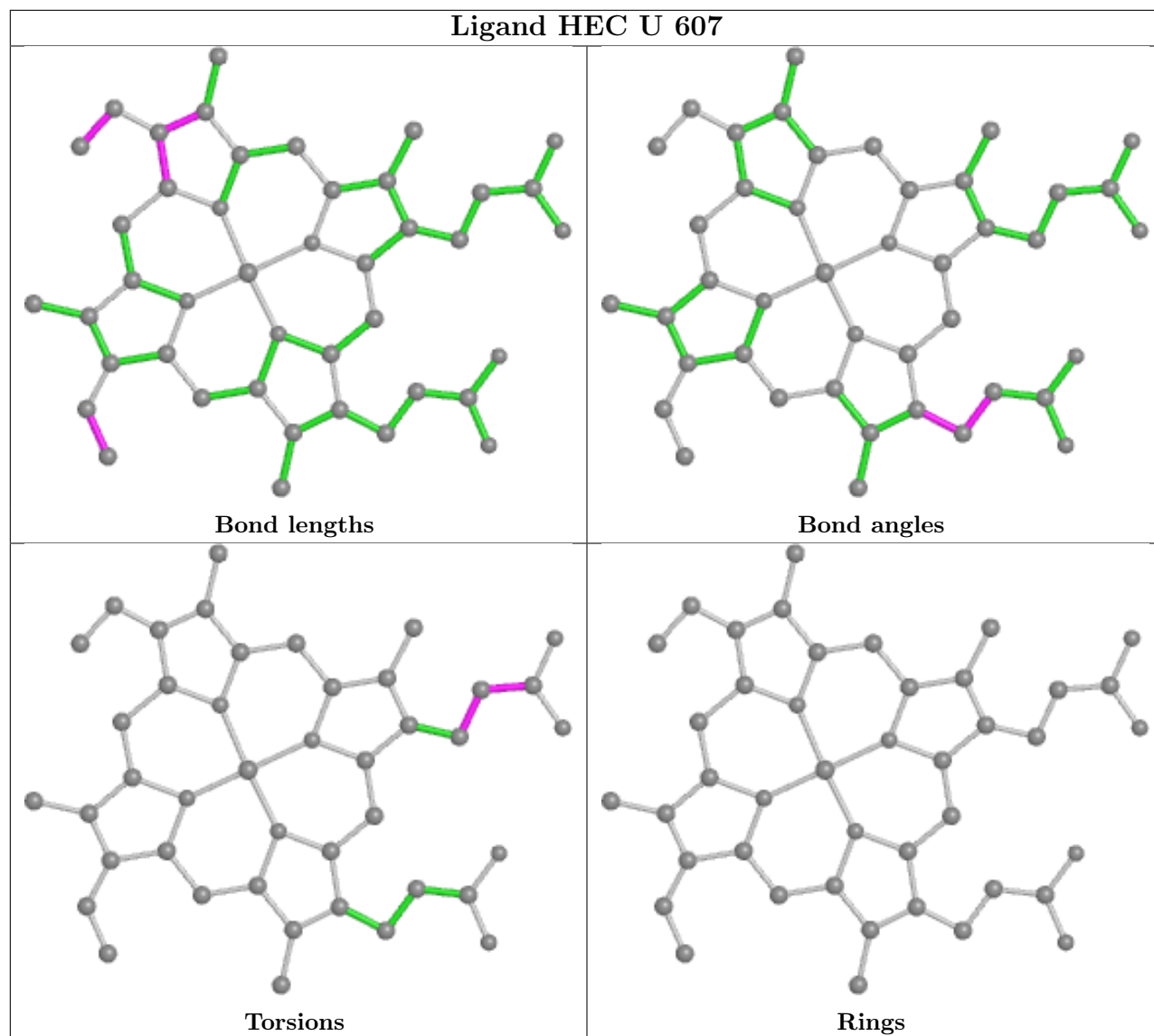




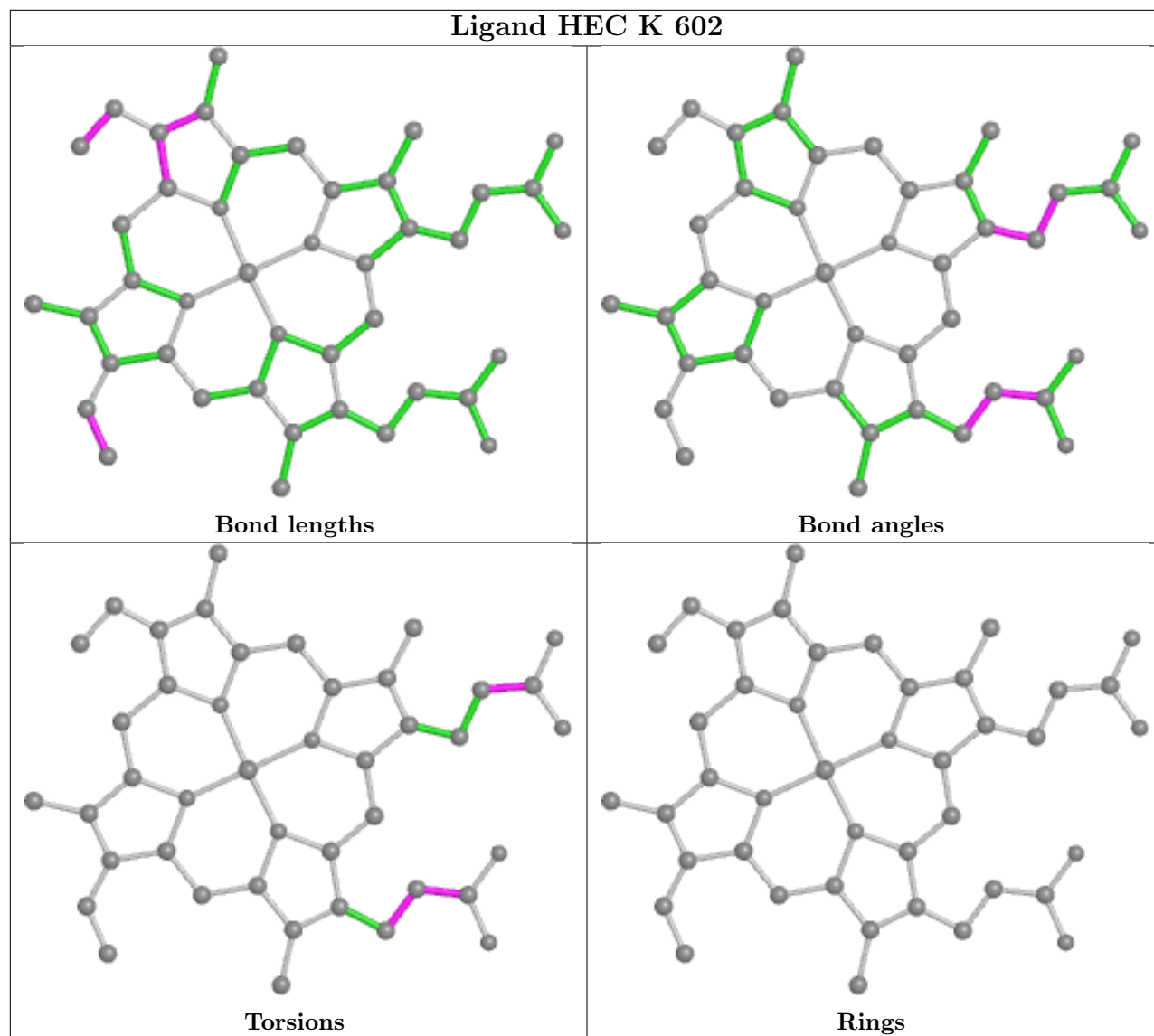


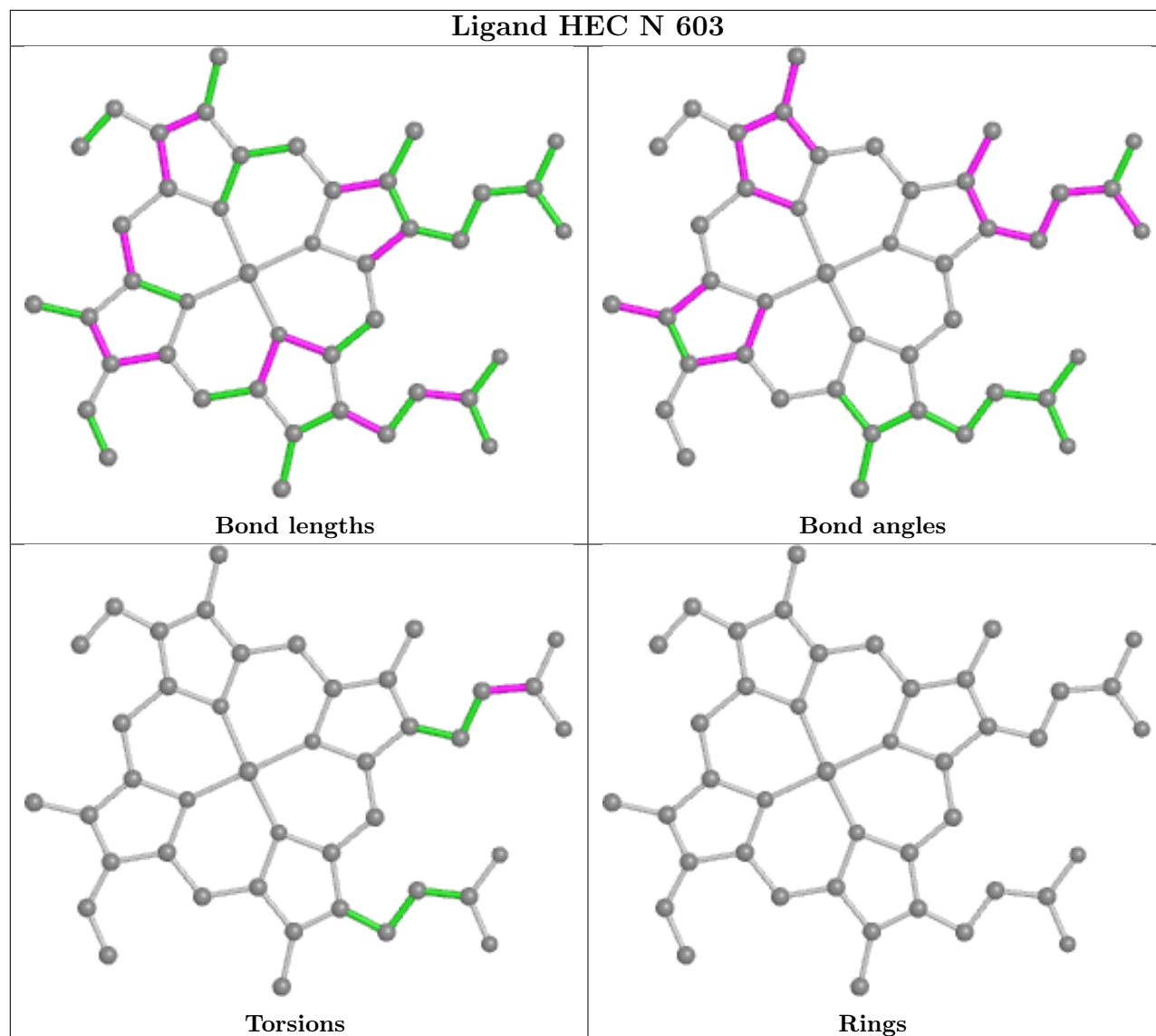


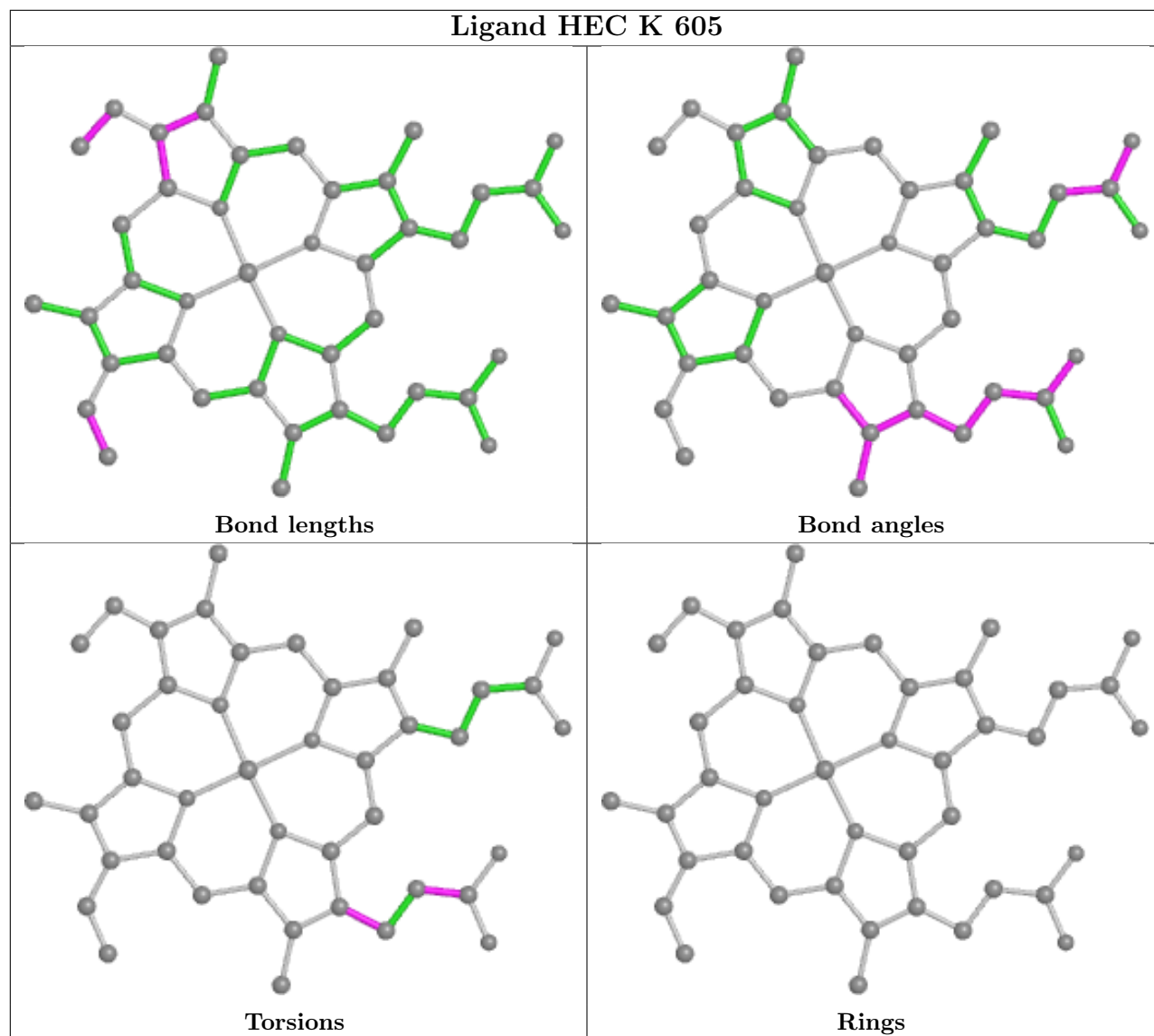


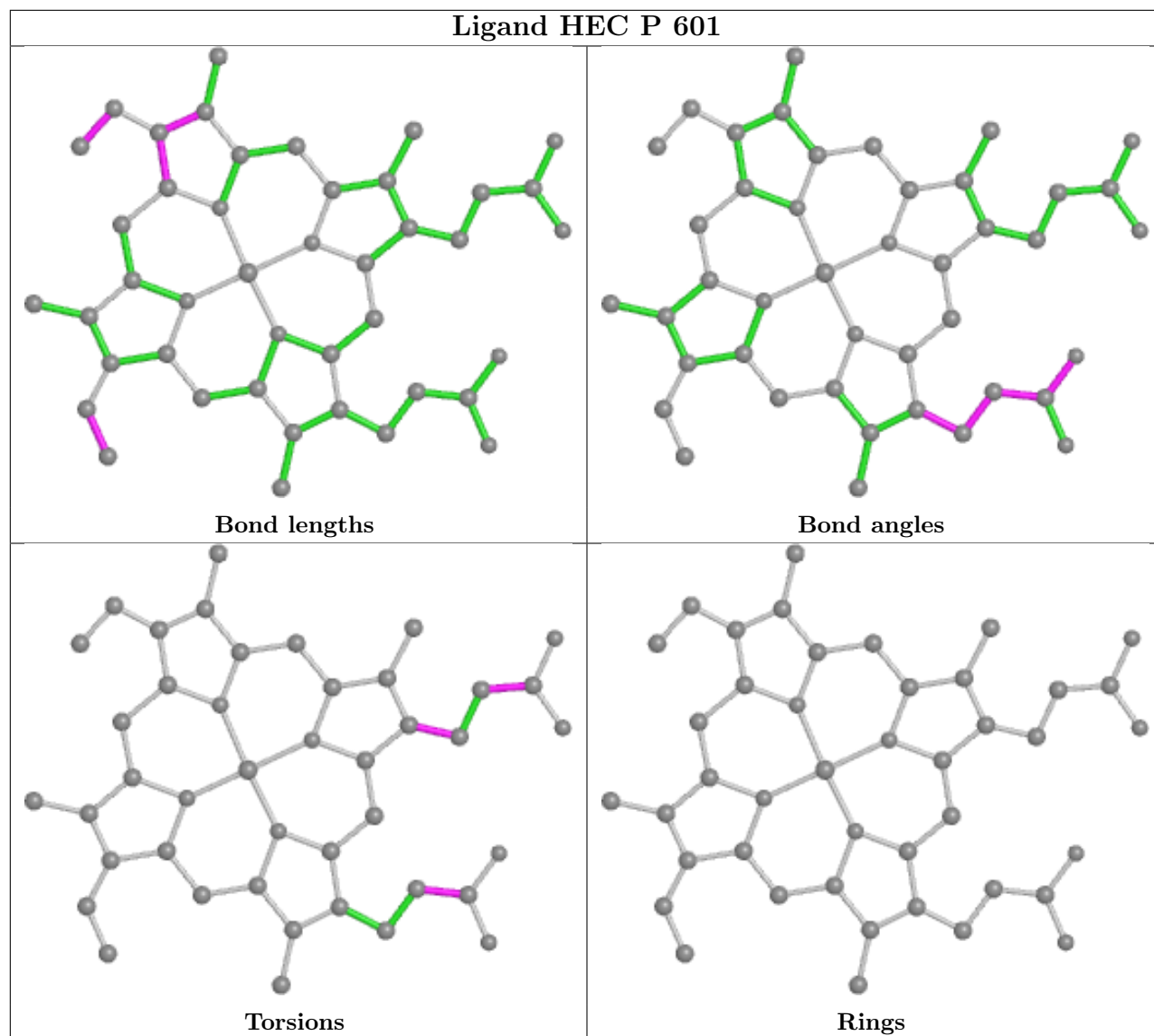


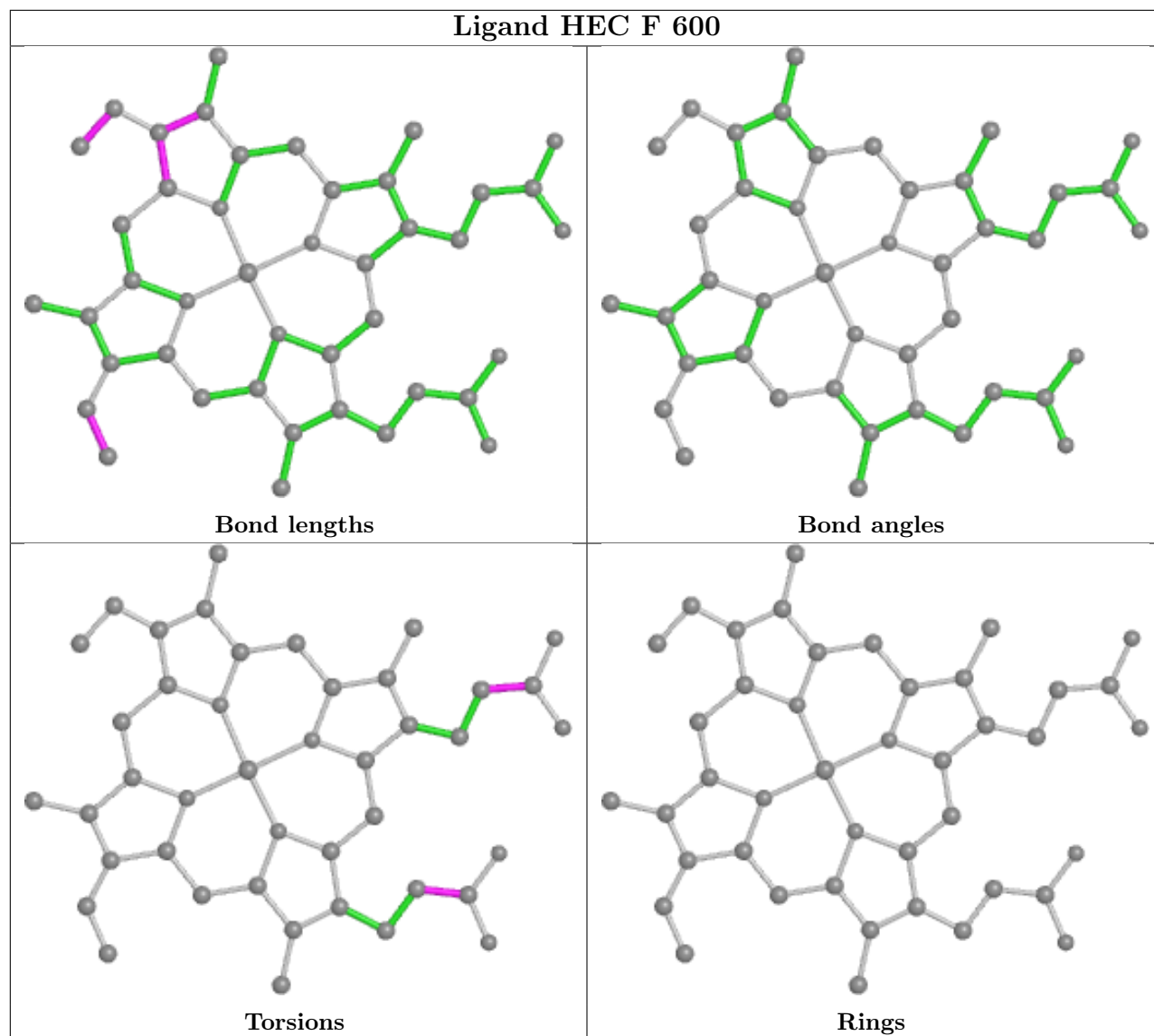


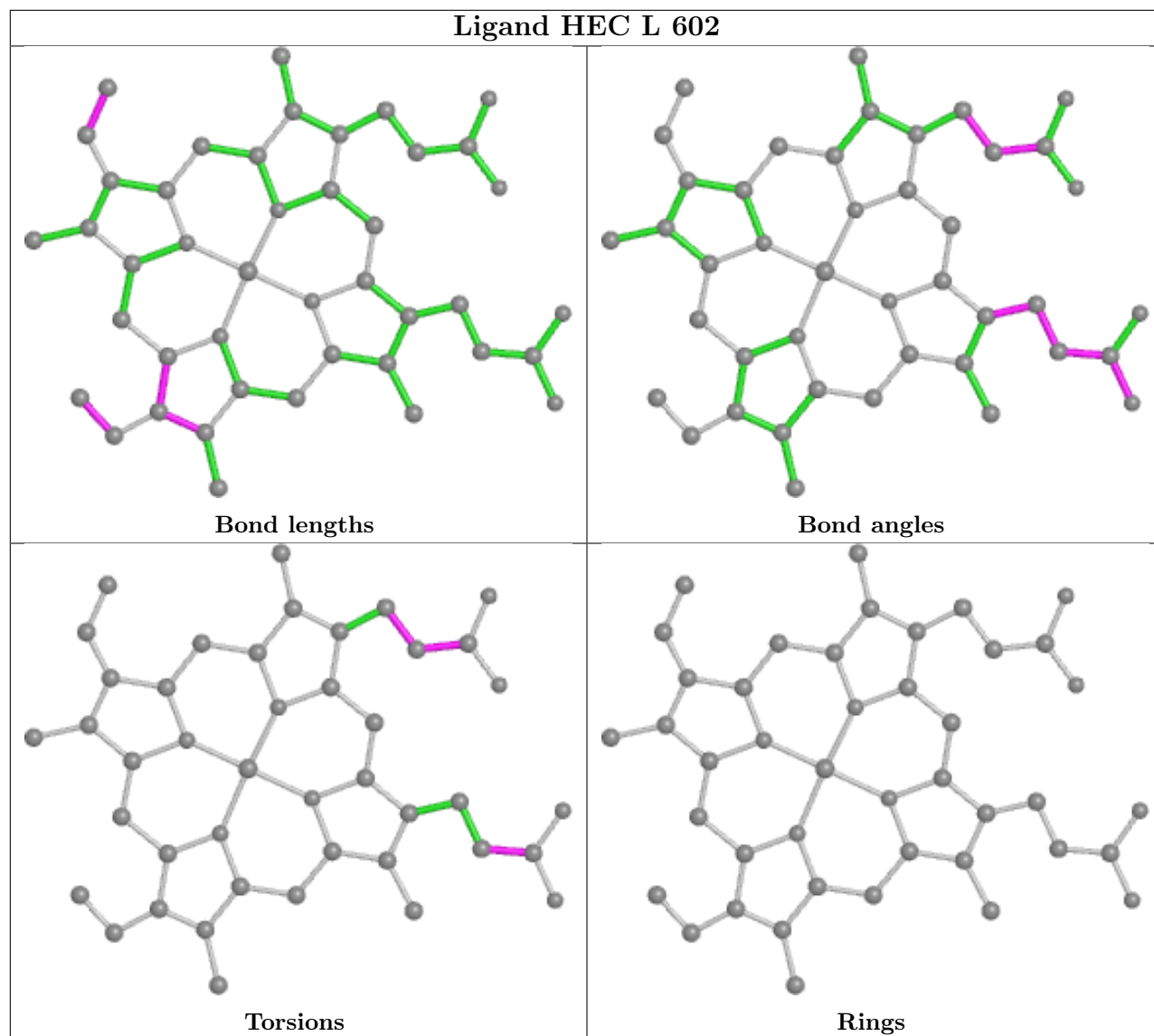


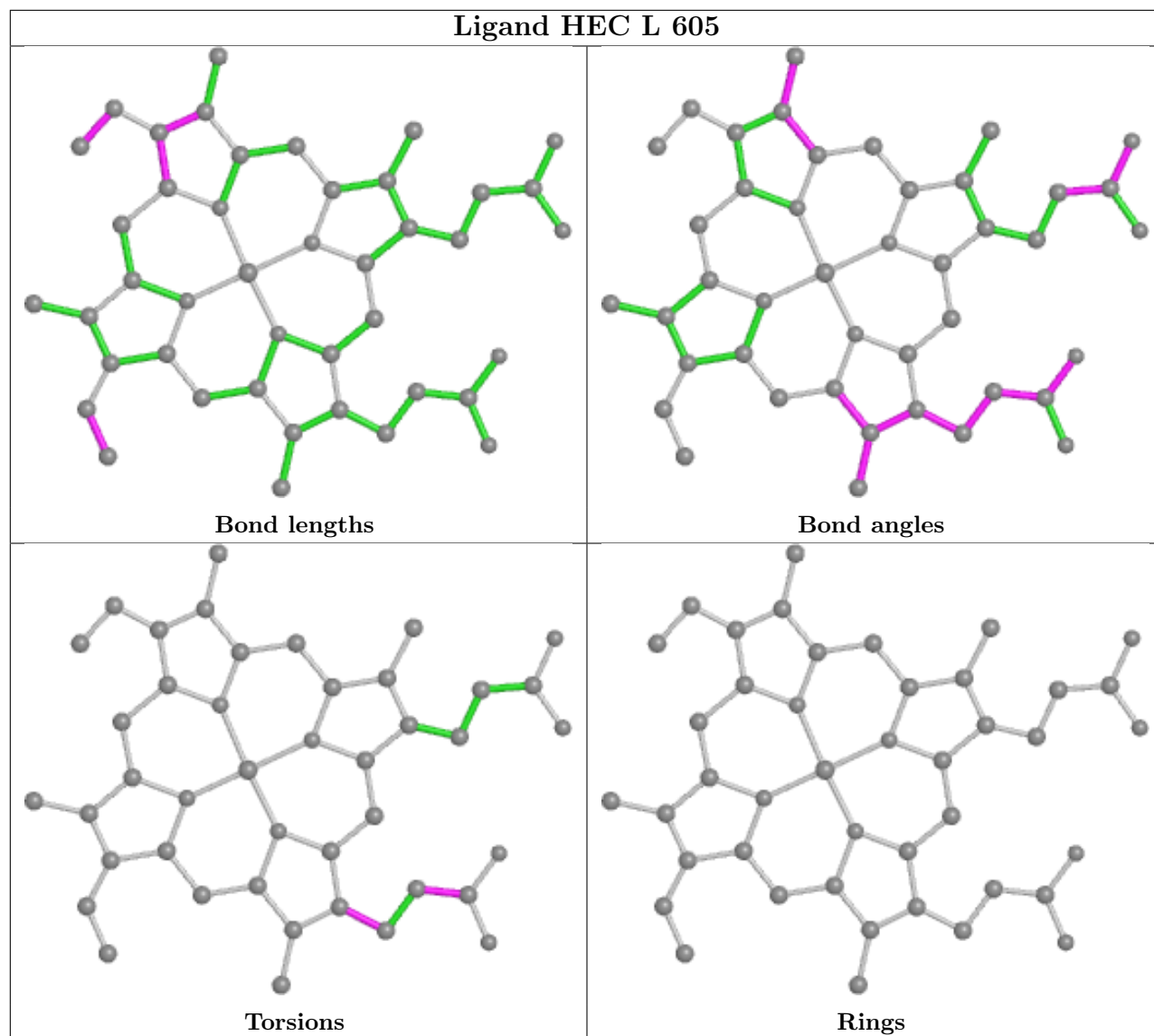


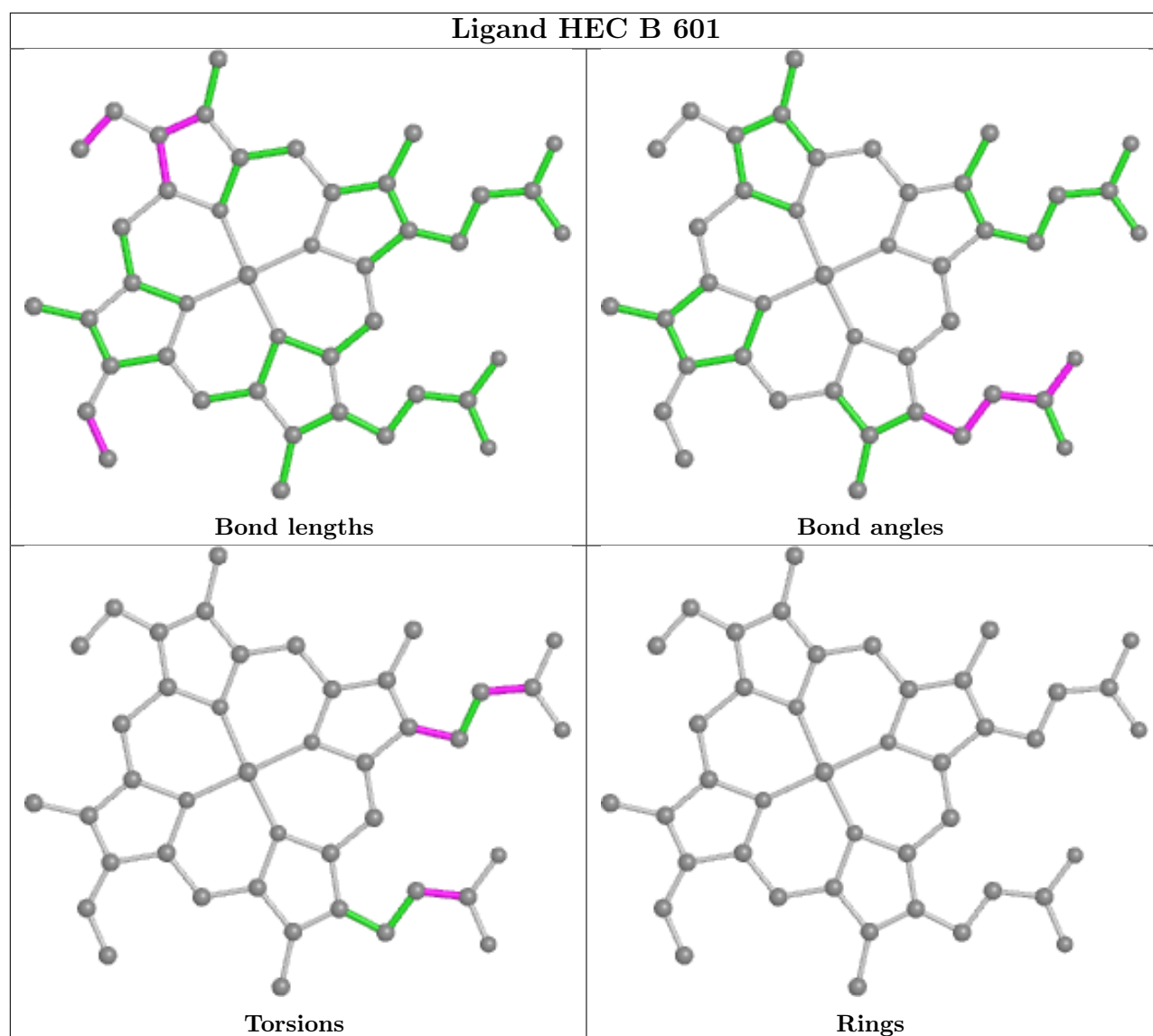












## 5.7 Other polymers [\(i\)](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

*Continued on next page...*

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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

The worst 5 of 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

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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
6	K	K	616	1/1	0.69	0.11	85,85,85,85	0
5	GOL	J	612	6/6	0.69	0.28	58,64,67,67	0
4	SO4	S	609	5/5	0.69	0.18	129,133,135,135	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
4	SO4	L	610	5/5	0.71	0.24	142,143,145,150	0
5	GOL	A	612	6/6	0.71	0.25	76,78,79,81	0
5	GOL	H	615	6/6	0.76	0.68	78,86,90,100	0
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	Q	611	5/5	0.80	0.16	112,118,119,119	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	F	610	5/5	0.81	0.21	135,136,139,139	0
4	SO4	c	201	5/5	0.81	0.15	132,133,135,135	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
5	GOL	K	612	6/6	0.83	0.36	76,80,86,90	0
4	SO4	M	612	5/5	0.83	0.18	121,122,123,125	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	N	611	5/5	0.83	0.18	123,126,127,129	0
4	SO4	M	610	5/5	0.84	0.49	134,135,138,139	0
4	SO4	Y	202	5/5	0.84	0.17	130,130,132,136	0
4	SO4	L	611	5/5	0.84	0.14	116,119,121,122	0
4	SO4	O	610	5/5	0.84	0.21	109,111,112,112	0
4	SO4	C	611	5/5	0.85	0.31	111,111,114,116	0
4	SO4	I	612	5/5	0.85	0.20	120,121,124,125	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
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	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	O	611	5/5	0.87	0.13	114,114,119,120	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	J	613	6/6	0.91	0.27	58,61,62,63	0
4	SO4	K	611	5/5	0.91	0.22	102,104,105,105	0
5	GOL	I	613	6/6	0.91	0.23	59,64,66,73	0
4	SO4	F	609	5/5	0.91	0.12	95,99,102,104	0
4	SO4	U	610	5/5	0.91	0.19	99,101,103,104	0
5	GOL	H	614	6/6	0.91	0.74	56,63,64,68	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	P	609	5/5	0.93	0.17	95,95,96,98	0
5	GOL	K	613	6/6	0.93	0.23	45,51,52,53	0
4	SO4	N	610	5/5	0.93	0.16	101,105,107,109	0
4	SO4	V	610	5/5	0.93	0.16	94,97,98,99	0
4	SO4	H	609	5/5	0.93	0.15	78,81,82,83	0
4	SO4	C	609	5/5	0.93	0.16	96,102,106,108	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	G	610	5/5	0.94	0.42	104,106,107,108	0
5	GOL	K	615	6/6	0.94	0.65	53,55,58,59	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
4	SO4	A	610	5/5	0.94	0.14	73,77,79,80	0
4	SO4	Q	609	5/5	0.94	0.09	84,87,88,89	0
3	HEC	X	606	43/43	0.95	0.25	69,83,87,90	0
5	GOL	K	614	6/6	0.95	0.65	49,56,57,59	0
5	GOL	G	616	6/6	0.95	0.19	37,40,41,41	0
3	HEC	V	602	43/43	0.95	0.24	68,73,87,100	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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	HEC	T	607	43/43	0.96	0.26	49,57,60,62	0
3	HEC	U	600	43/43	0.96	0.18	58,64,71,72	0
3	HEC	U	602	43/43	0.96	0.27	60,69,94,116	0
3	HEC	U	604	43/43	0.96	0.23	52,60,72,81	0
3	HEC	U	606	43/43	0.96	0.29	65,72,88,96	0
3	HEC	A	604	43/43	0.96	0.22	47,50,61,73	0
3	HEC	V	604	43/43	0.96	0.28	59,71,81,85	0
4	SO4	J	609	5/5	0.96	0.19	77,79,80,80	0
3	HEC	V	603	43/43	0.96	0.25	51,65,82,86	0
3	HEC	W	603	43/43	0.96	0.27	67,77,85,89	0
3	HEC	W	602	43/43	0.96	0.23	54,58,83,99	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	X	604	43/43	0.96	0.21	63,73,78,80	0
3	HEC	A	606	43/43	0.96	0.26	45,60,73,78	0
3	HEC	B	602	43/43	0.96	0.22	49,56,80,99	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	E	602	43/43	0.96	0.24	48,53,73,94	0
3	HEC	E	605	43/43	0.96	0.23	53,63,75,82	0
3	HEC	E	606	43/43	0.96	0.26	55,60,68,75	0
3	HEC	F	603	43/43	0.96	0.22	62,70,74,79	0
3	HEC	F	602	43/43	0.96	0.23	64,75,85,96	0
3	HEC	H	602	43/43	0.96	0.23	35,44,64,77	0
3	HEC	N	606	43/43	0.96	0.22	47,51,60,64	0
3	HEC	P	602	43/43	0.96	0.20	41,45,63,76	0
3	HEC	Q	602	43/43	0.96	0.23	64,68,88,97	0
3	HEC	Q	604	43/43	0.96	0.25	54,60,68,76	0
3	HEC	S	602	43/43	0.96	0.23	63,71,86,104	0
3	HEC	S	604	43/43	0.96	0.23	59,66,75,86	0
3	HEC	S	605	43/43	0.96	0.30	63,72,82,83	0
3	HEC	S	603	43/43	0.96	0.25	72,77,88,94	0
4	SO4	S	610	5/5	0.96	0.09	92,93,94,95	0
3	HEC	T	602	43/43	0.96	0.23	59,68,83,97	0
3	HEC	W	606	43/43	0.97	0.31	64,76,88,96	0
3	HEC	W	607	43/43	0.97	0.25	63,68,71,71	0
3	HEC	X	603	43/43	0.97	0.24	70,80,103,109	0
3	HEC	X	600	43/43	0.97	0.19	57,63,75,81	0
3	HEC	X	601	43/43	0.97	0.23	62,69,78,82	0
3	HEC	A	602	43/43	0.97	0.23	51,56,79,99	0
3	HEC	E	607	43/43	0.97	0.27	47,54,60,62	0
3	HEC	G	600	43/43	0.97	0.21	40,42,45,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	HEC	F	600	43/43	0.97	0.21	46,52,62,68	0
3	HEC	X	607	43/43	0.97	0.23	57,61,65,67	0
3	HEC	F	601	43/43	0.97	0.25	51,55,68,70	0
3	HEC	A	605	43/43	0.97	0.26	50,59,63,64	0
3	HEC	F	604	43/43	0.97	0.23	58,65,74,84	0
3	HEC	F	605	43/43	0.97	0.25	54,60,69,78	0
4	SO4	G	613	5/5	0.97	0.18	63,63,64,66	0
3	HEC	F	606	43/43	0.97	0.24	50,56,67,76	0
3	HEC	F	607	43/43	0.97	0.27	49,56,57,60	0
3	HEC	G	601	43/43	0.97	0.21	37,41,43,48	0
3	HEC	I	602	43/43	0.97	0.21	37,42,59,70	0
3	HEC	J	600	43/43	0.97	0.22	37,41,52,60	0
3	HEC	J	602	43/43	0.97	0.22	38,41,67,86	0
3	HEC	K	600	43/43	0.97	0.22	38,40,46,55	0
3	HEC	K	602	43/43	0.97	0.22	44,47,65,81	0
3	HEC	K	604	43/43	0.97	0.20	36,41,49,57	0
4	SO4	E	609	5/5	0.97	0.15	50,51,53,53	0
3	HEC	L	600	43/43	0.97	0.22	41,44,50,51	0
3	HEC	L	601	43/43	0.97	0.22	36,40,45,46	0
3	HEC	L	602	43/43	0.97	0.22	42,45,57,72	0
3	HEC	L	604	43/43	0.97	0.22	35,41,48,58	0
3	HEC	M	600	43/43	0.97	0.21	44,48,56,62	0
3	HEC	M	602	43/43	0.97	0.23	44,48,72,89	0
3	HEC	M	604	43/43	0.97	0.24	40,43,51,62	0
3	HEC	M	605	43/43	0.97	0.27	36,38,46,51	0
4	SO4	I	610	5/5	0.97	0.11	67,67,69,69	0
3	HEC	M	607	43/43	0.97	0.23	36,39,52,62	0
3	HEC	M	603	43/43	0.97	0.24	42,46,49,50	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	N	602	43/43	0.97	0.23	48,52,75,92	0
3	HEC	A	607	43/43	0.97	0.21	41,45,50,53	0
3	HEC	O	603	43/43	0.97	0.20	40,44,49,51	0
3	HEC	O	601	43/43	0.97	0.23	40,44,49,56	0
3	HEC	O	602	43/43	0.97	0.22	47,51,72,91	0
3	HEC	O	604	43/43	0.97	0.21	34,41,50,60	0
3	HEC	P	601	43/43	0.97	0.22	39,44,46,47	0
3	HEC	A	603	43/43	0.97	0.22	54,66,71,73	0
3	HEC	P	604	43/43	0.97	0.22	36,40,52,63	0
3	HEC	P	606	43/43	0.97	0.23	43,47,48,49	0
3	HEC	P	607	43/43	0.97	0.22	38,48,52,54	0
3	HEC	P	603	43/43	0.97	0.23	40,49,56,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	HEC	Q	600	43/43	0.97	0.23	47,52,59,65	0
3	HEC	Q	601	43/43	0.97	0.22	46,50,54,56	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	Q	606	43/43	0.97	0.23	44,55,65,69	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	R	600	43/43	0.97	0.21	49,54,62,64	0
3	HEC	R	602	43/43	0.97	0.24	45,48,74,89	0
3	HEC	R	604	43/43	0.97	0.21	38,43,53,61	0
3	HEC	S	600	43/43	0.97	0.22	60,65,73,75	0
3	HEC	S	601	43/43	0.97	0.25	67,70,81,85	0
3	HEC	B	604	43/43	0.97	0.21	44,51,62,67	0
3	HEC	C	603	43/43	0.97	0.22	44,48,58,63	0
3	HEC	C	600	43/43	0.97	0.22	49,52,56,58	0
3	HEC	S	606	43/43	0.97	0.26	61,69,74,79	0
3	HEC	S	607	43/43	0.97	0.24	51,57,59,60	0
3	HEC	C	602	43/43	0.97	0.21	45,48,66,80	0
3	HEC	T	603	43/43	0.97	0.23	60,66,71,73	0
3	HEC	T	600	43/43	0.97	0.20	53,60,68,69	0
3	HEC	C	604	43/43	0.97	0.22	42,47,53,60	0
3	HEC	T	604	43/43	0.97	0.23	59,65,70,80	0
3	HEC	T	605	43/43	0.97	0.24	54,60,74,76	0
3	HEC	T	606	43/43	0.97	0.27	52,56,65,74	0
3	HEC	C	605	43/43	0.97	0.22	38,43,53,57	0
3	HEC	U	603	43/43	0.97	0.24	61,72,83,85	0
3	HEC	C	607	43/43	0.97	0.22	44,48,49,52	0
3	HEC	U	601	43/43	0.97	0.23	54,57,67,73	0
3	HEC	D	600	43/43	0.97	0.22	54,60,68,74	0
3	HEC	D	602	43/43	0.97	0.19	45,48,65,79	0
3	HEC	U	605	43/43	0.97	0.27	62,68,80,87	0
3	HEC	D	605	43/43	0.97	0.26	48,53,61,66	0
3	HEC	U	607	43/43	0.97	0.29	53,70,73,74	0
3	HEC	V	600	43/43	0.97	0.23	67,70,84,91	0
3	HEC	V	601	43/43	0.97	0.20	52,63,65,67	0
3	HEC	E	603	43/43	0.97	0.23	56,66,92,96	0
3	HEC	E	600	43/43	0.97	0.21	39,41,53,55	0
3	HEC	V	605	43/43	0.97	0.26	56,65,73,76	0
3	HEC	V	606	43/43	0.97	0.26	57,60,76,81	0
3	HEC	V	607	43/43	0.97	0.29	54,66,69,70	0
3	HEC	E	601	43/43	0.97	0.22	39,43,47,55	0
3	HEC	G	604	43/43	0.97	0.23	31,34,49,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	HEC	W	600	43/43	0.97	0.23	61,68,74,77	0
3	HEC	W	601	43/43	0.97	0.27	61,70,77,80	0
3	HEC	E	604	43/43	0.97	0.21	40,45,53,63	0
3	HEC	W	604	43/43	0.97	0.21	50,57,67,74	0
3	HEC	A	600	43/43	0.97	0.22	47,49,56,59	0
3	HEC	K	605	43/43	0.98	0.23	35,38,43,48	0
3	HEC	K	606	43/43	0.98	0.23	33,39,42,46	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
3	HEC	B	601	43/43	0.98	0.21	43,47,56,68	0
3	HEC	T	601	43/43	0.98	0.22	55,58,61,63	0
3	HEC	C	606	43/43	0.98	0.22	41,43,59,65	0
3	HEC	G	603	43/43	0.98	0.20	34,36,39,42	0
3	HEC	G	605	43/43	0.98	0.22	33,36,41,43	0
3	HEC	L	605	43/43	0.98	0.23	35,37,41,45	0
3	HEC	L	606	43/43	0.98	0.21	35,37,43,47	0
3	HEC	L	607	43/43	0.98	0.23	32,34,35,36	0
3	HEC	D	601	43/43	0.98	0.23	51,59,61,62	0
3	HEC	M	601	43/43	0.98	0.23	41,44,47,51	0
3	HEC	B	605	43/43	0.98	0.22	42,45,53,59	0
3	HEC	D	604	43/43	0.98	0.21	44,47,54,60	0
3	HEC	B	606	43/43	0.98	0.23	39,42,50,57	0
3	HEC	M	606	43/43	0.98	0.25	37,40,50,55	0
3	HEC	D	606	43/43	0.98	0.27	46,51,62,66	0
3	HEC	D	607	43/43	0.98	0.23	40,45,55,61	0
3	HEC	N	603	43/43	0.98	0.20	47,56,60,62	0
3	HEC	H	603	43/43	0.98	0.22	31,34,42,48	0
3	HEC	H	600	43/43	0.98	0.20	32,37,42,44	0
3	HEC	H	601	43/43	0.98	0.21	34,36,41,47	0
3	HEC	N	604	43/43	0.98	0.23	42,47,56,59	0
3	HEC	N	605	43/43	0.98	0.24	48,52,66,73	0
3	HEC	D	603	43/43	0.98	0.22	54,66,69,72	0
3	HEC	N	607	43/43	0.98	0.20	37,41,44,46	0
3	HEC	H	604	43/43	0.98	0.21	38,43,53,64	0
3	HEC	O	600	43/43	0.98	0.21	44,48,58,60	0
3	HEC	H	605	43/43	0.98	0.23	28,32,34,35	0
4	SO4	U	609	5/5	0.98	0.18	57,58,60,64	0
3	HEC	H	606	43/43	0.98	0.22	32,34,39,44	0
3	HEC	H	607	43/43	0.98	0.21	28,30,32,35	0
4	SO4	V	609	5/5	0.98	0.20	56,59,60,62	0
3	HEC	O	605	43/43	0.98	0.21	36,41,49,52	0
3	HEC	O	606	43/43	0.98	0.21	37,41,49,52	0

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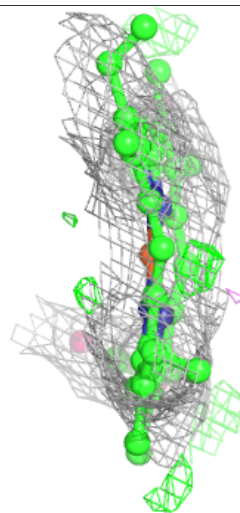
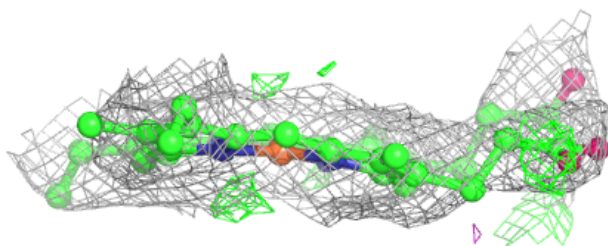
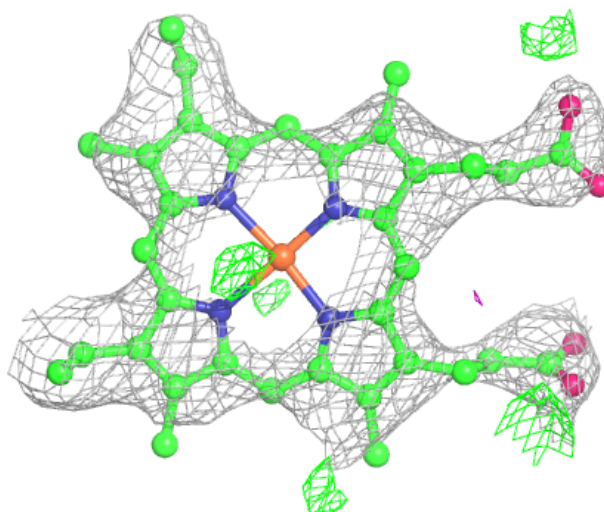
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	HEC	O	607	43/43	0.98	0.23	34,37,38,39	0
3	HEC	P	600	43/43	0.98	0.20	44,46,51,53	0
3	HEC	I	603	43/43	0.98	0.21	30,33,37,39	0
3	HEC	I	600	43/43	0.98	0.21	39,43,50,52	0
3	HEC	I	601	43/43	0.98	0.21	35,37,41,44	0
3	HEC	P	605	43/43	0.98	0.23	43,46,49,50	0
3	HEC	B	607	43/43	0.98	0.23	37,40,45,47	0
3	HEC	I	604	43/43	0.98	0.22	36,38,51,58	0
3	HEC	I	605	43/43	0.98	0.23	29,33,38,40	0
3	HEC	Q	603	43/43	0.98	0.23	52,55,58,59	0
3	HEC	I	606	43/43	0.98	0.22	34,35,44,47	0
3	HEC	I	607	43/43	0.98	0.21	32,34,36,38	0
3	HEC	A	601	43/43	0.98	0.23	44,47,53,54	0
3	HEC	J	601	43/43	0.98	0.21	34,37,41,47	0
3	HEC	Q	605	43/43	0.98	0.24	45,51,57,60	0
3	HEC	G	606	43/43	0.98	0.21	35,37,42,46	0
3	HEC	J	604	43/43	0.98	0.20	32,35,44,55	0
3	HEC	J	605	43/43	0.98	0.23	32,38,43,47	0
3	HEC	J	606	43/43	0.98	0.23	33,39,41,46	0
3	HEC	R	601	43/43	0.98	0.23	43,48,50,50	0
3	HEC	J	607	43/43	0.98	0.22	28,30,33,37	0
3	HEC	J	603	43/43	0.98	0.20	37,39,44,46	0
3	HEC	R	605	43/43	0.98	0.19	35,40,45,46	0
3	HEC	R	606	43/43	0.98	0.22	37,43,59,63	0
3	HEC	R	607	43/43	0.98	0.22	37,38,43,48	0
3	HEC	K	603	43/43	0.98	0.20	37,39,42,44	0
3	HEC	C	601	43/43	0.98	0.23	41,45,50,51	0
3	HEC	K	601	43/43	0.98	0.20	33,34,38,43	0
3	HEC	B	603	43/43	0.98	0.20	45,49,53,54	0
3	HEC	G	607	43/43	0.98	0.21	30,31,34,34	0
4	SO4	A	609	5/5	0.99	0.21	47,49,49,52	0
4	SO4	N	609	5/5	0.99	0.20	40,40,41,42	0
4	SO4	I	609	5/5	0.99	0.22	28,28,29,30	0
4	SO4	R	609	5/5	0.99	0.20	36,39,40,40	0
4	SO4	K	609	5/5	0.99	0.23	28,28,29,30	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.

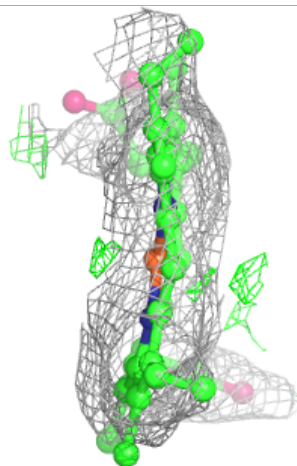
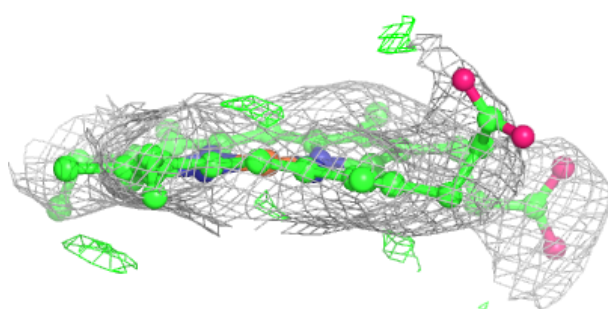
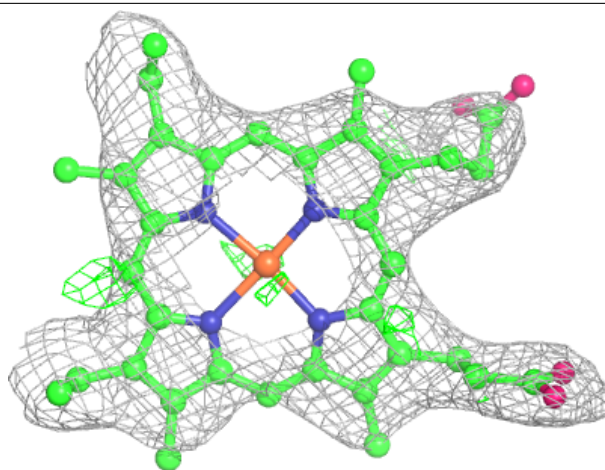
**Electron density around HEC X 606:**

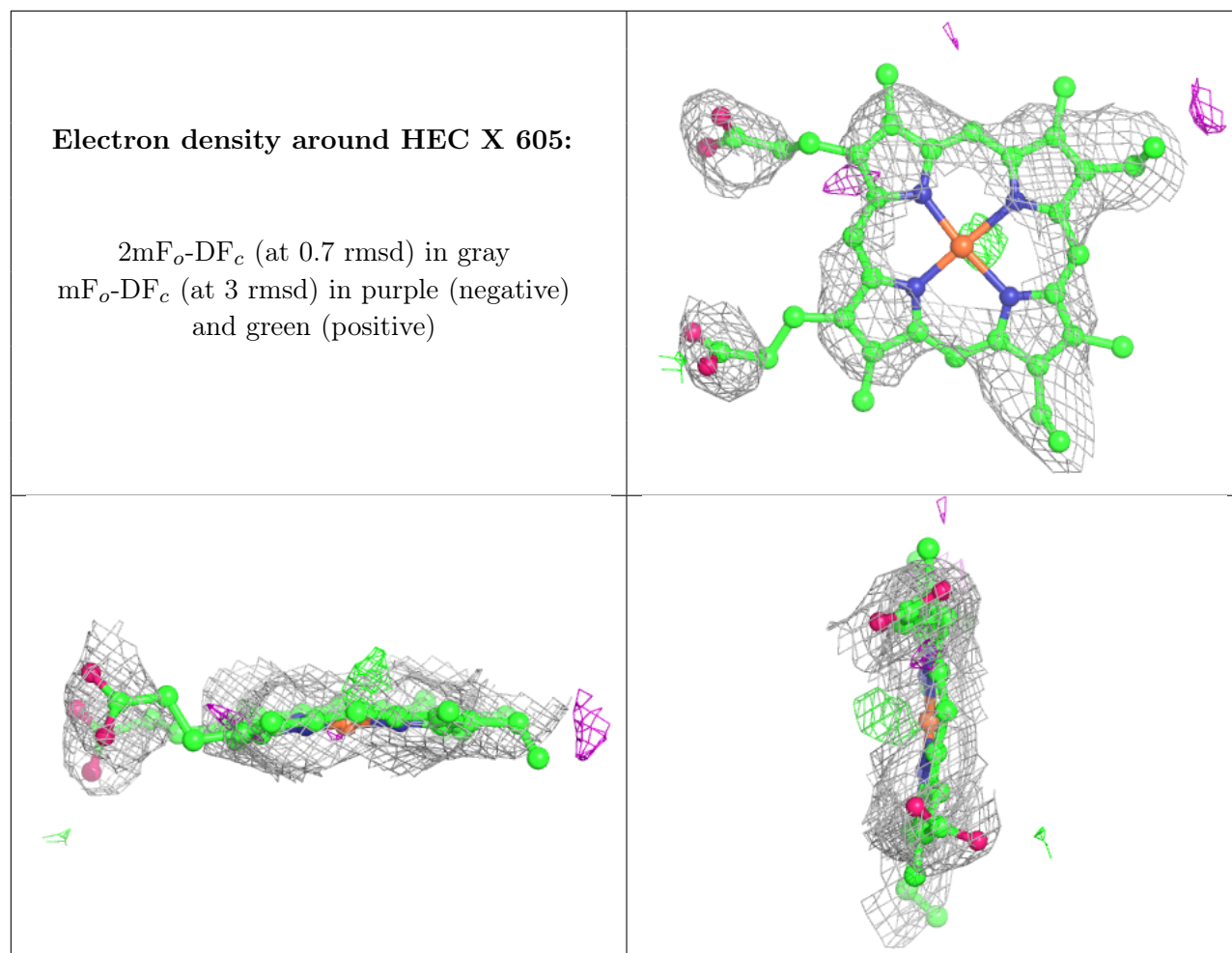
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC V 602:**

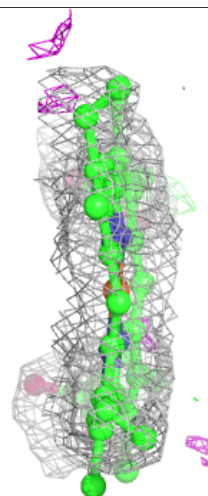
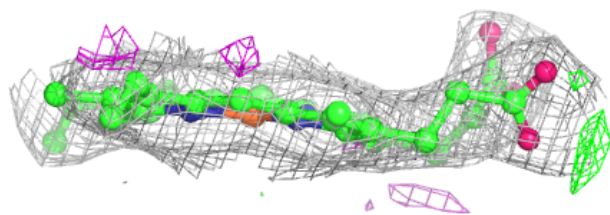
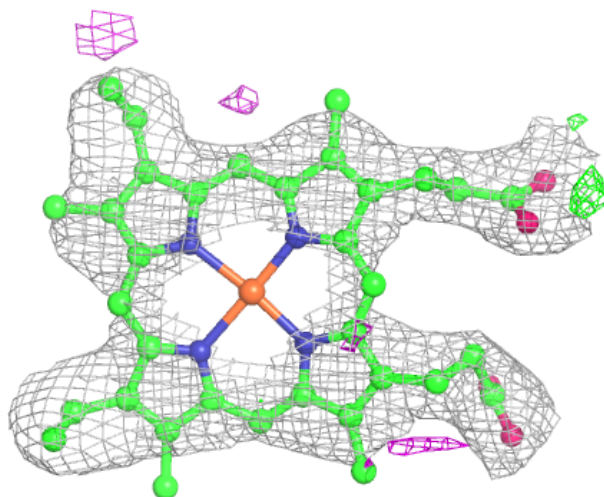
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





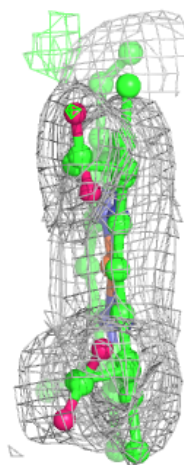
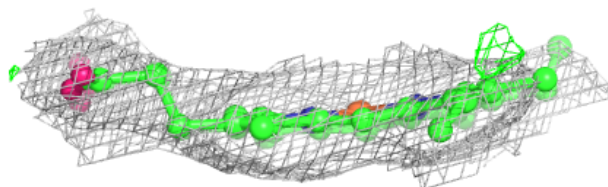
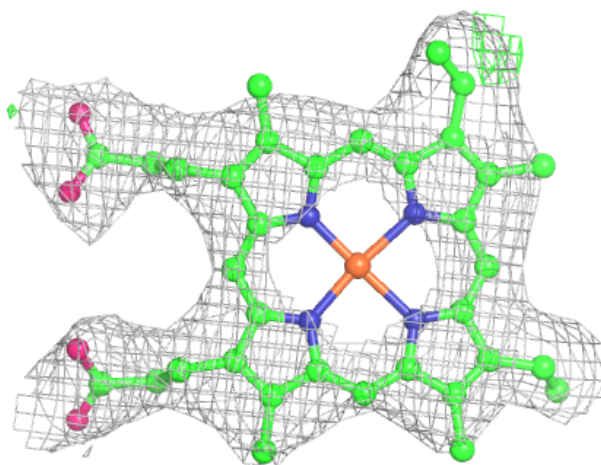
**Electron density around HEC T 607:**

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



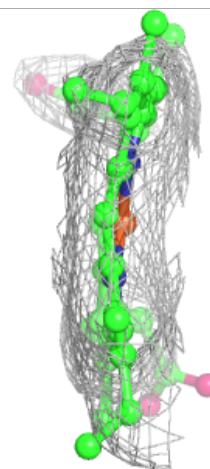
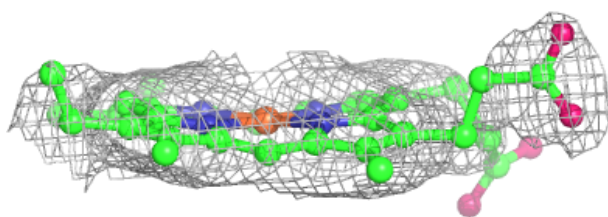
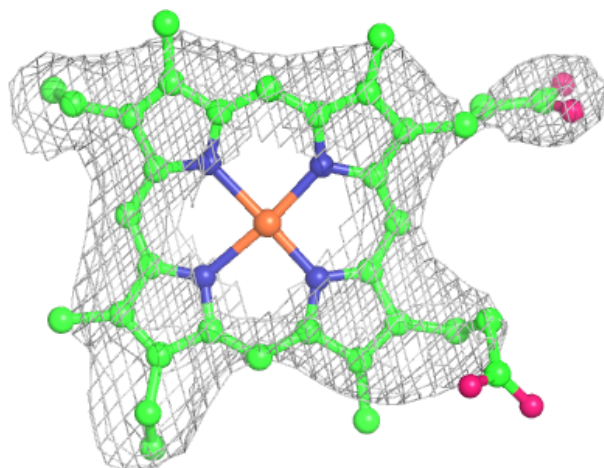
**Electron density around HEC U 600:**

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



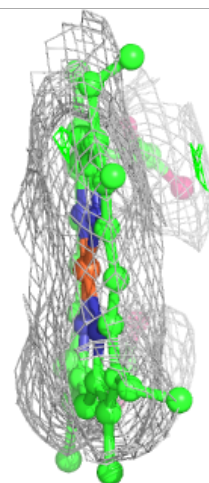
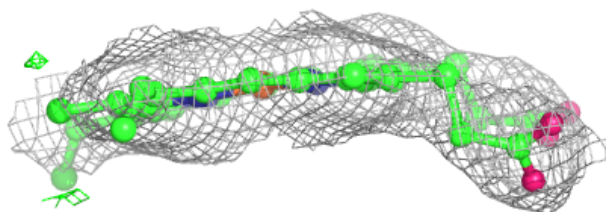
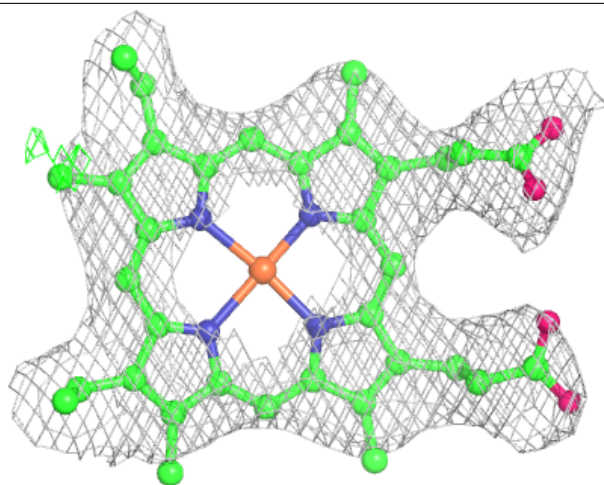
**Electron density around HEC U 602:**

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

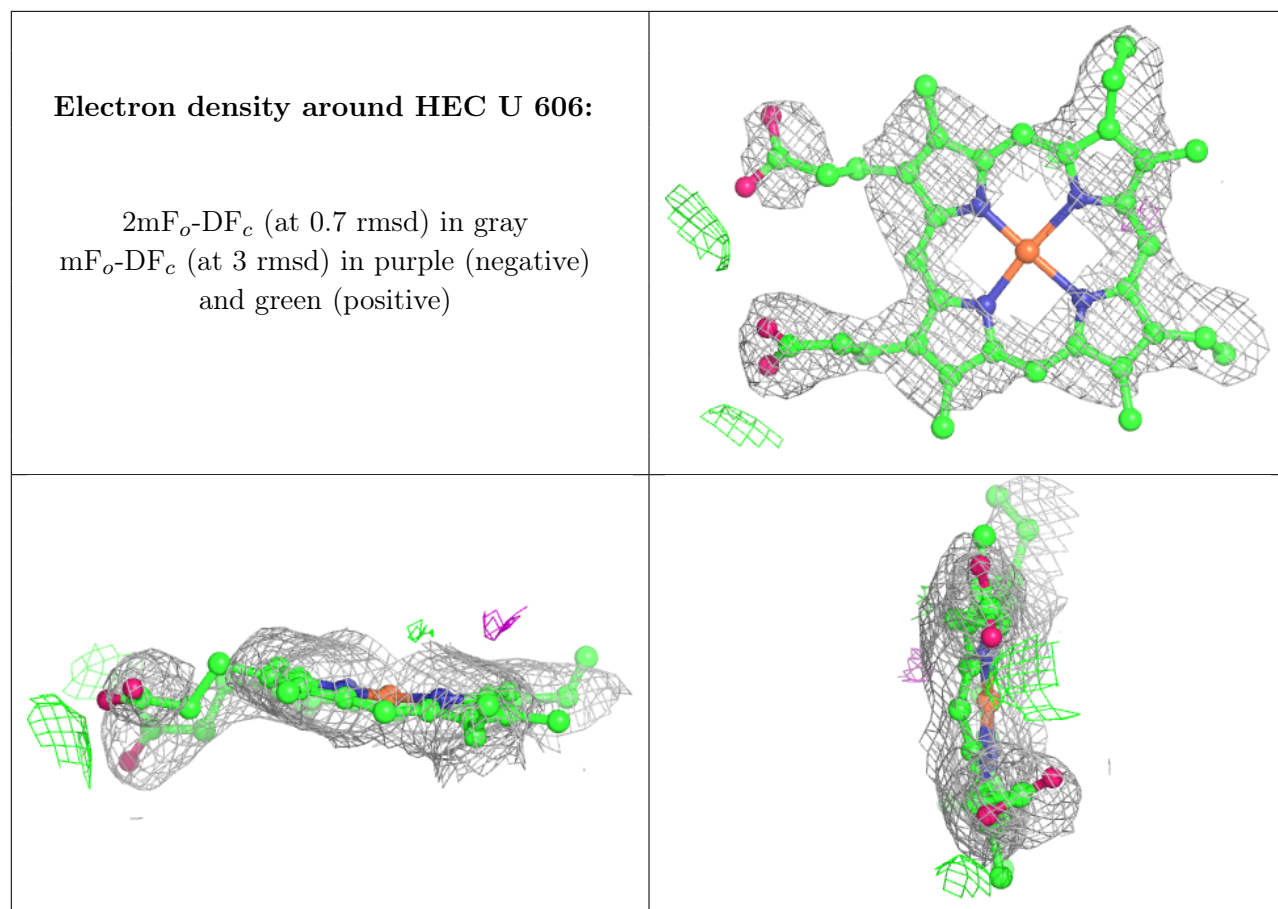


**Electron density around HEC U 604:**

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

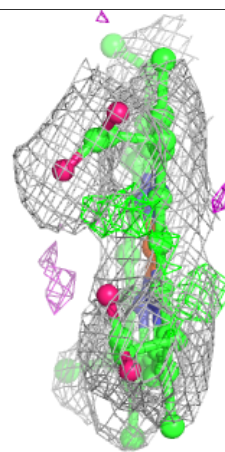
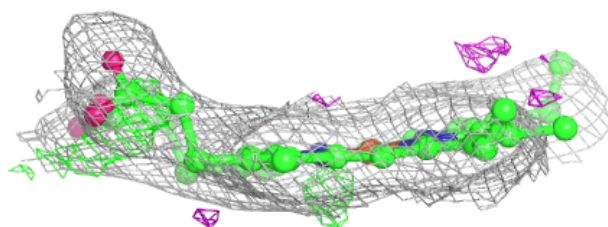
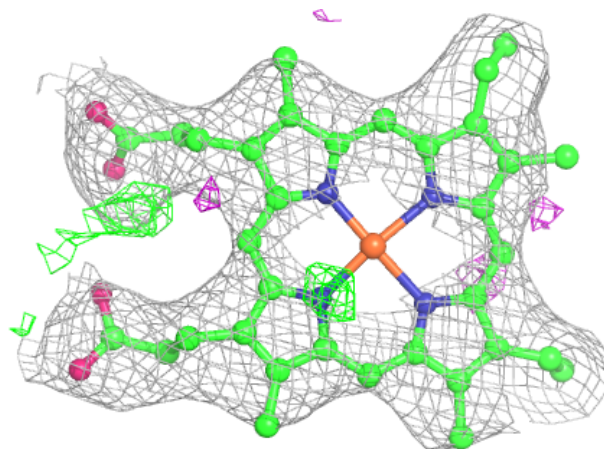






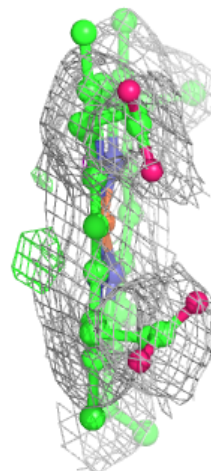
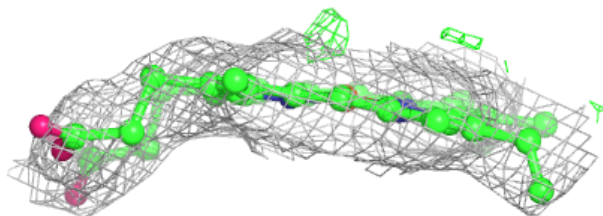
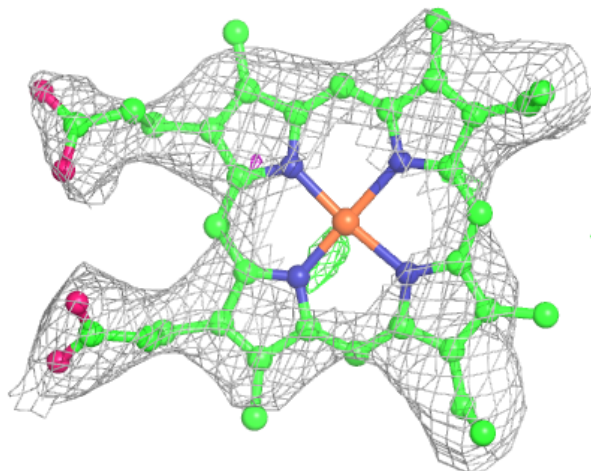
**Electron density around HEC A 604:**

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



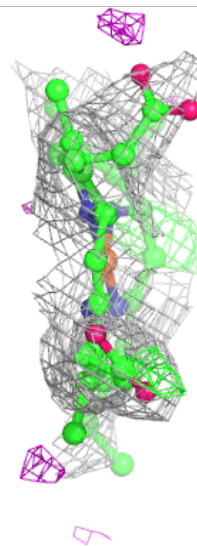
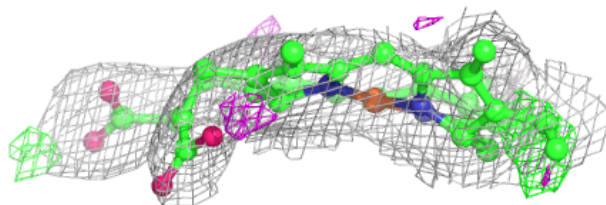
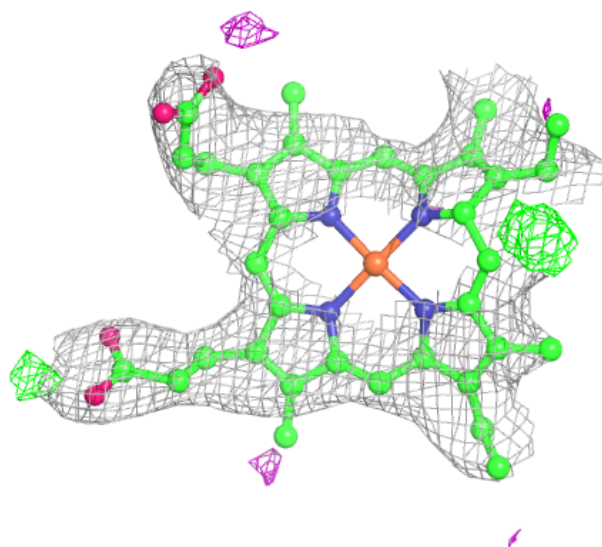
**Electron density around HEC V 604:**

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



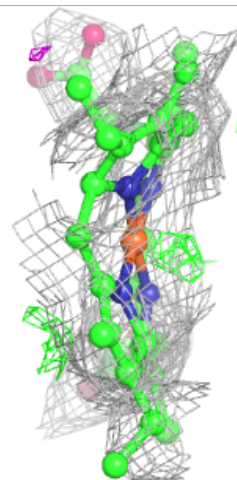
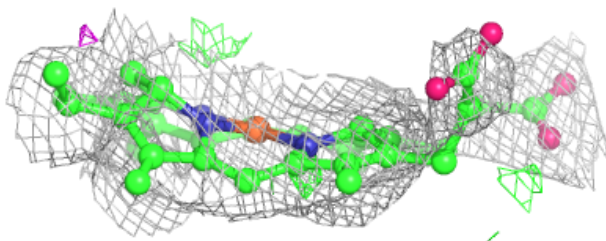
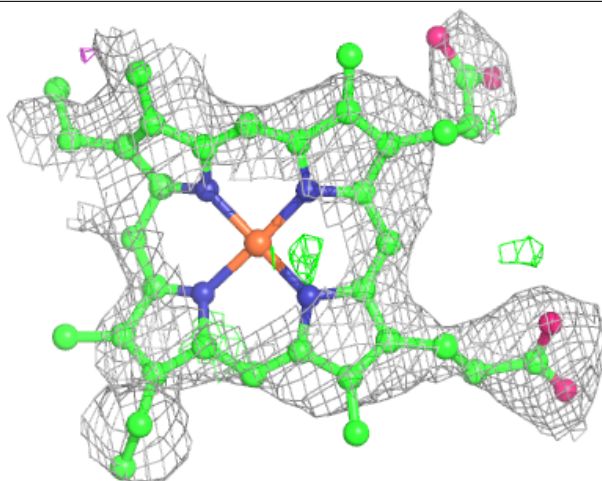
**Electron density around HEC V 603:**

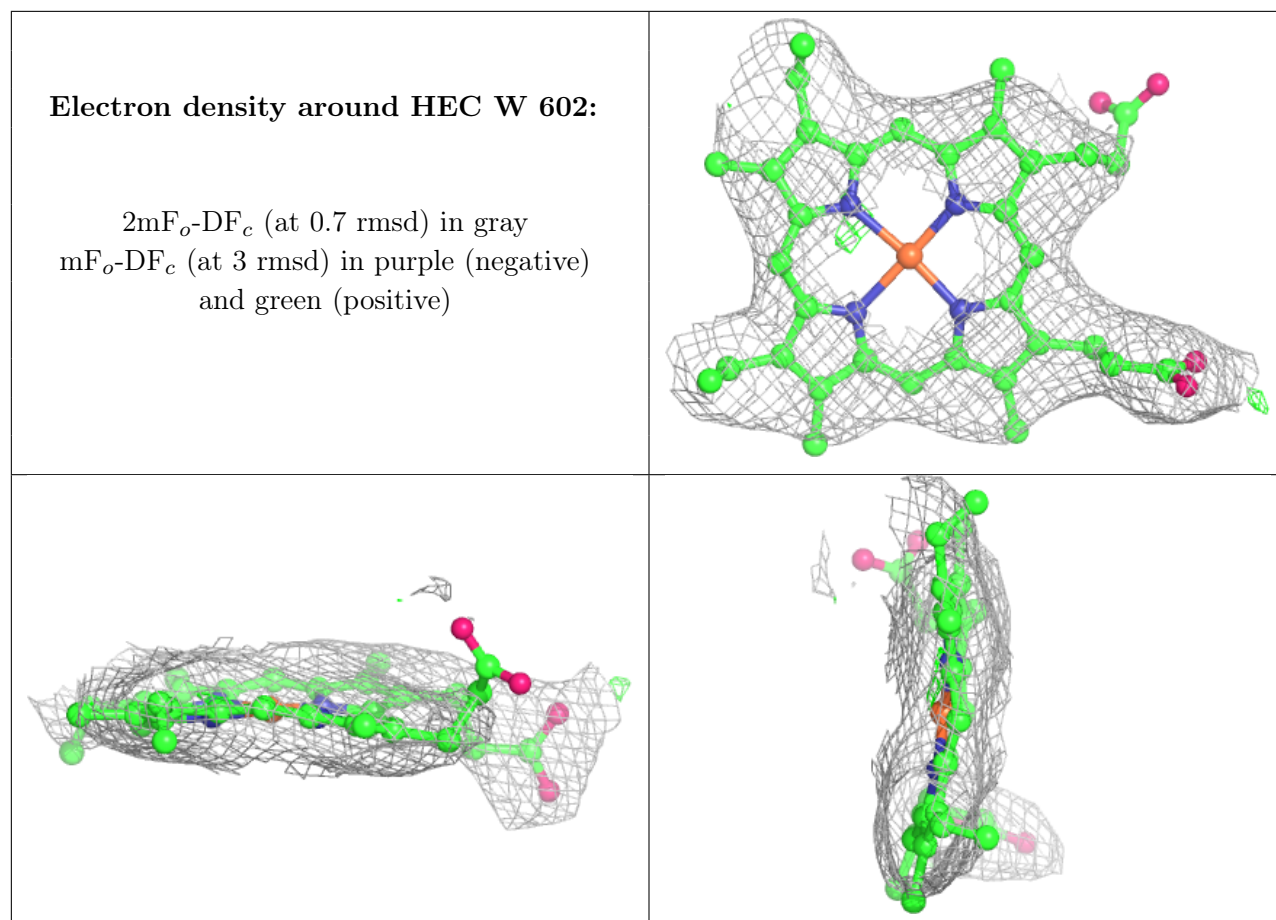
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC W 603:**

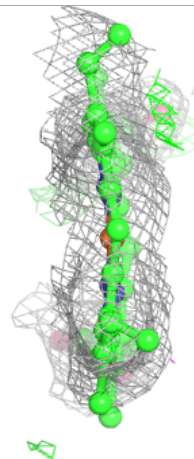
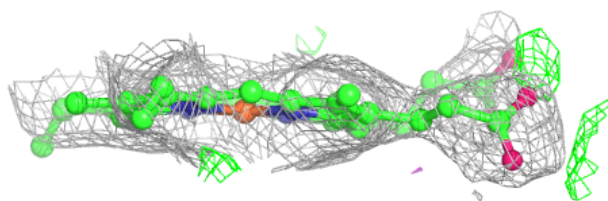
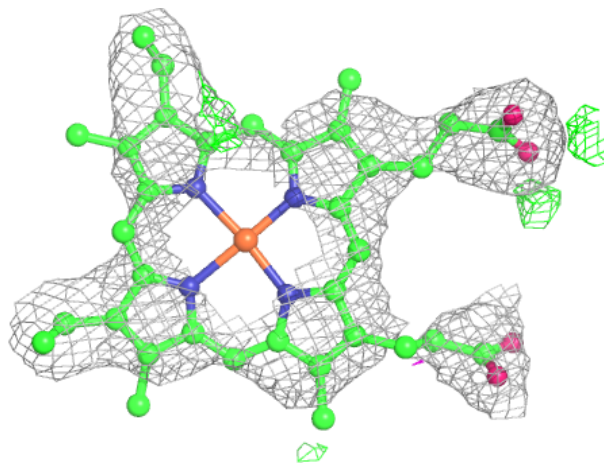
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





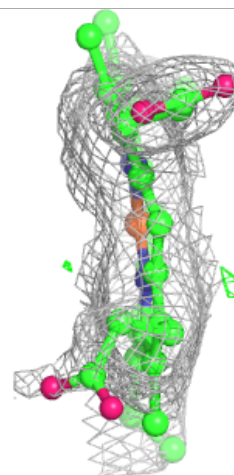
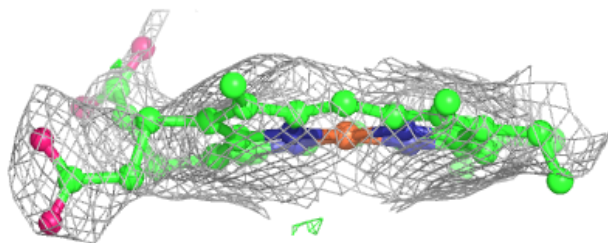
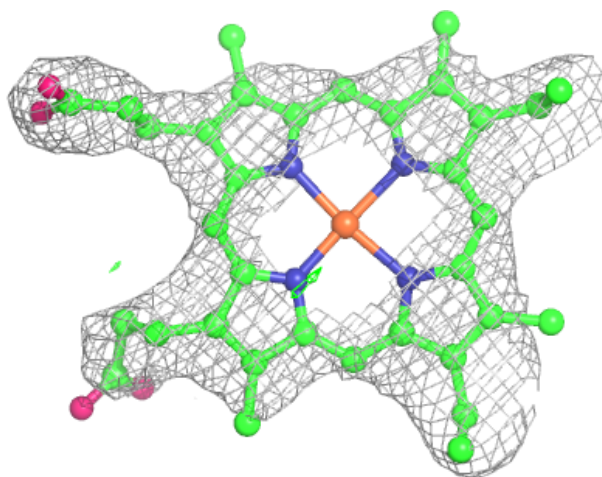
**Electron density around HEC W 605:**

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



**Electron density around HEC X 602:**

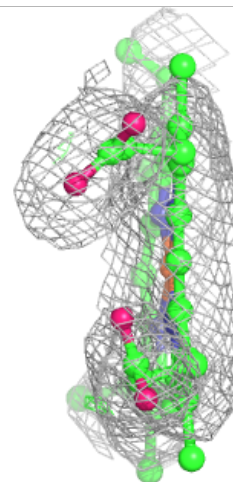
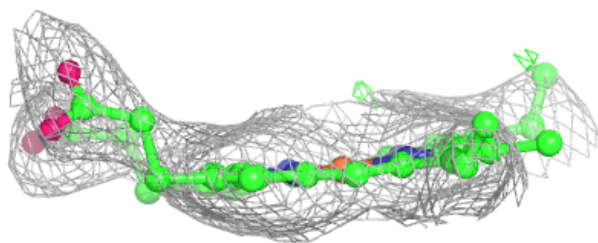
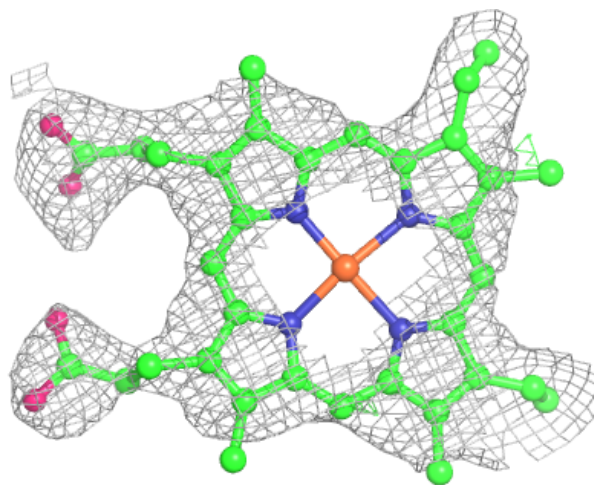
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





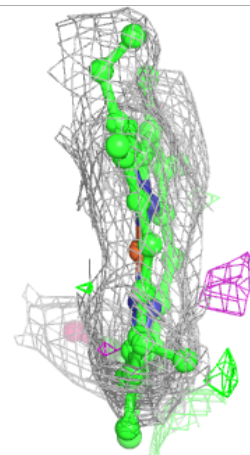
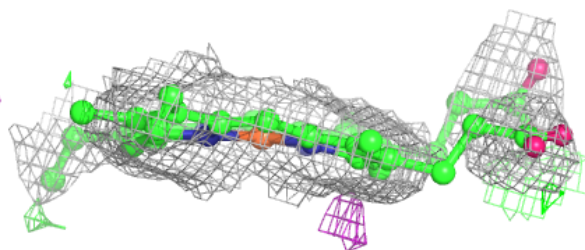
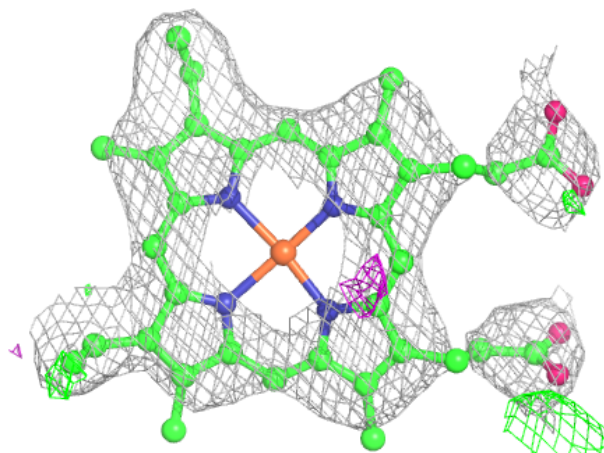
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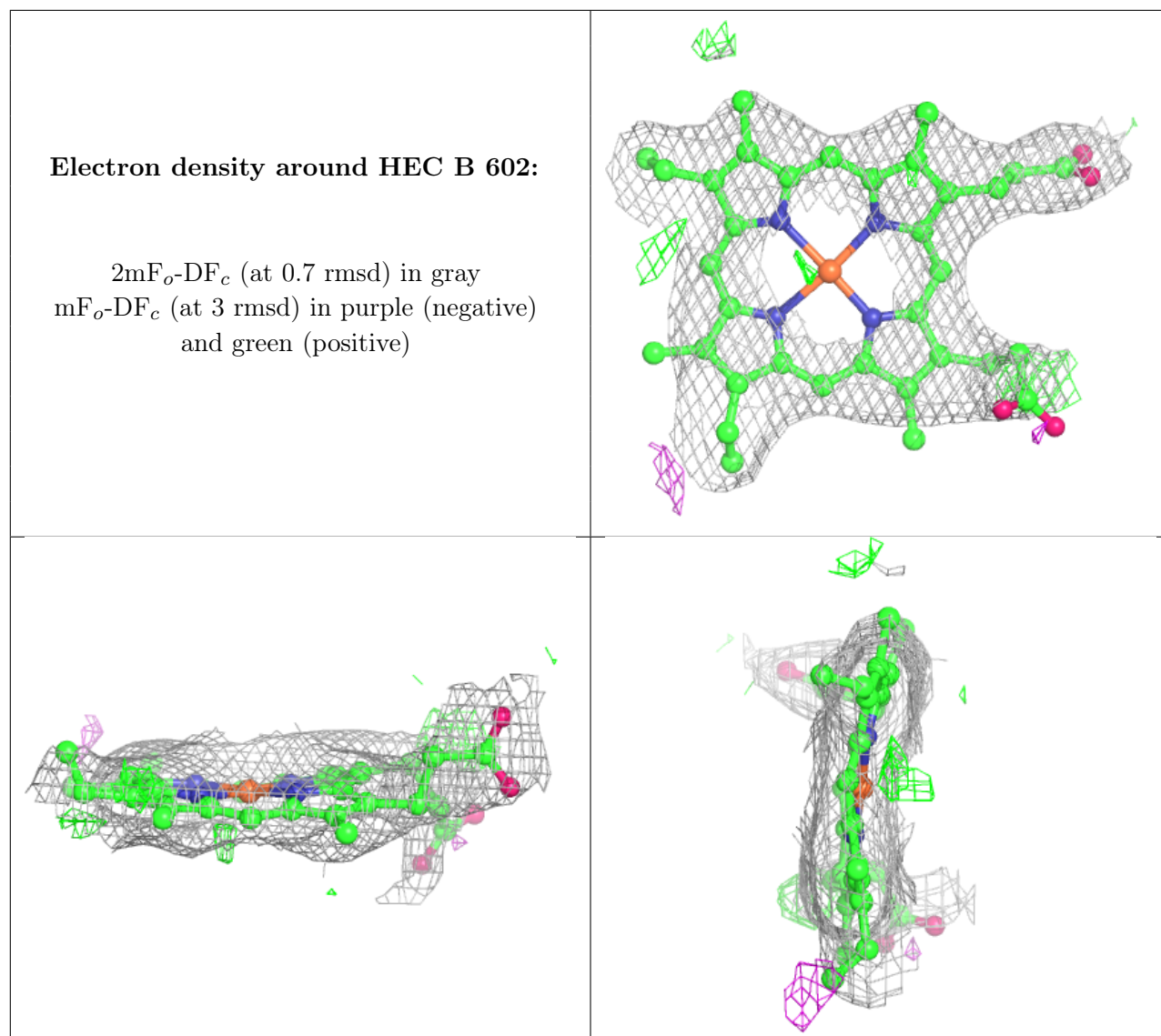
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC A 606:**

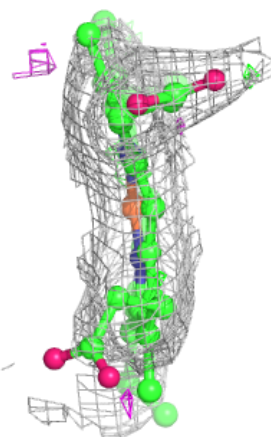
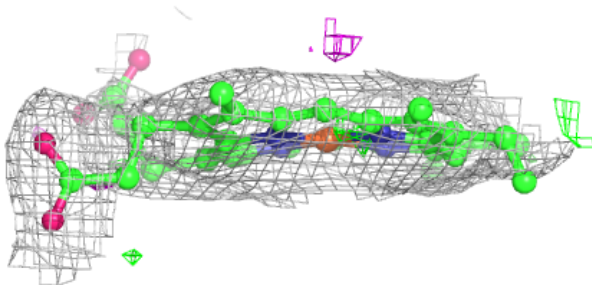
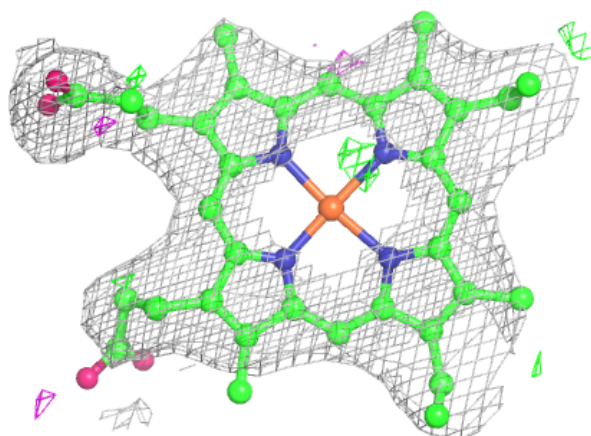
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
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and green (positive)

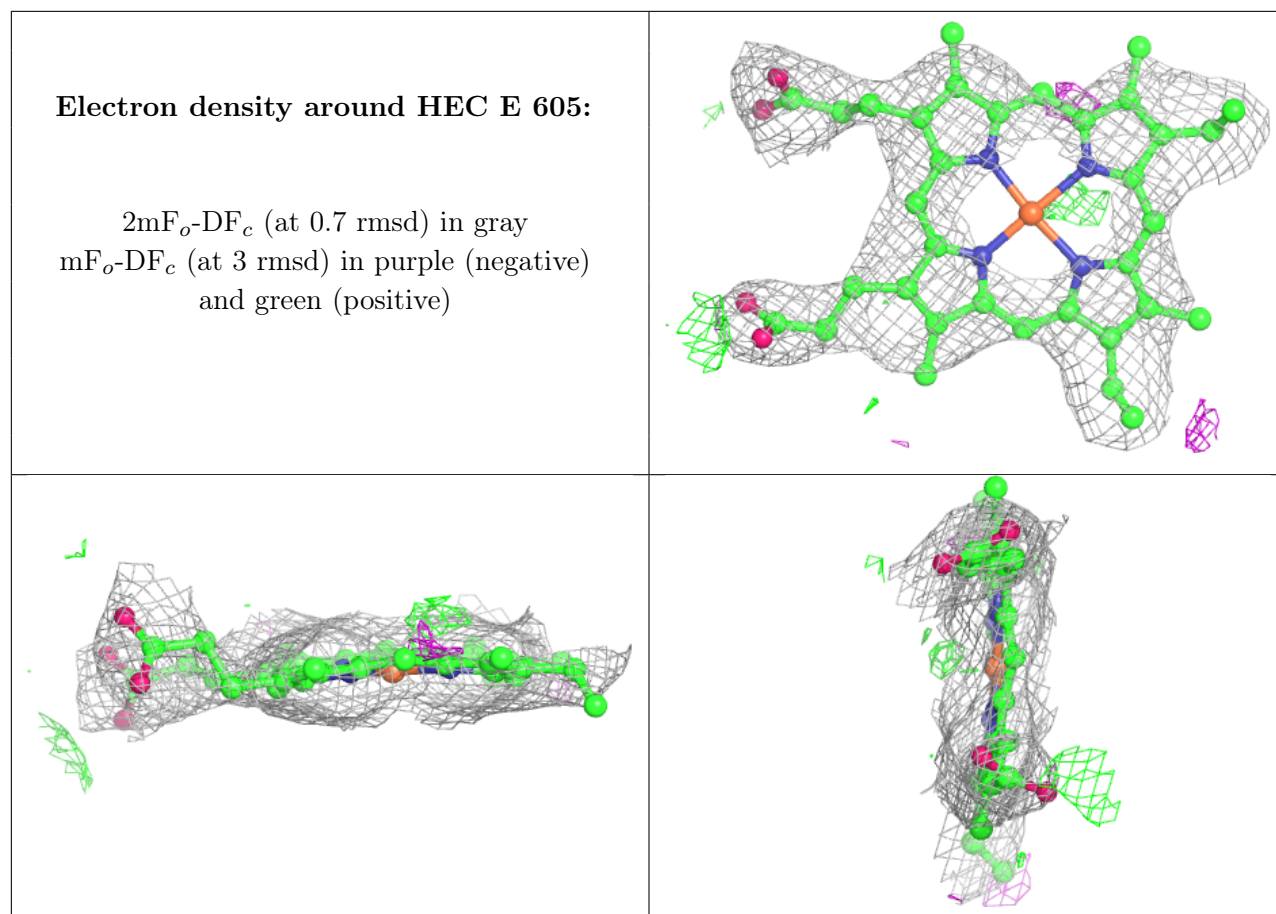




**Electron density around HEC E 602:**

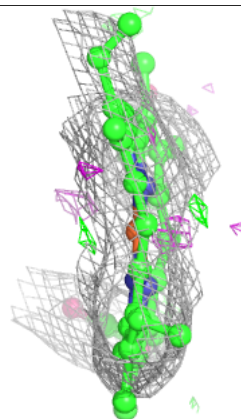
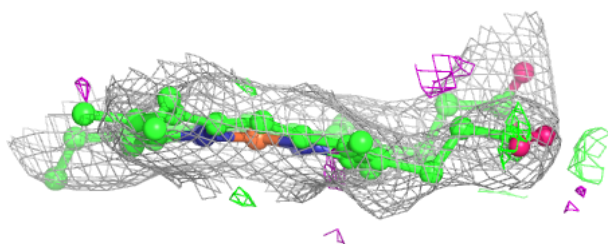
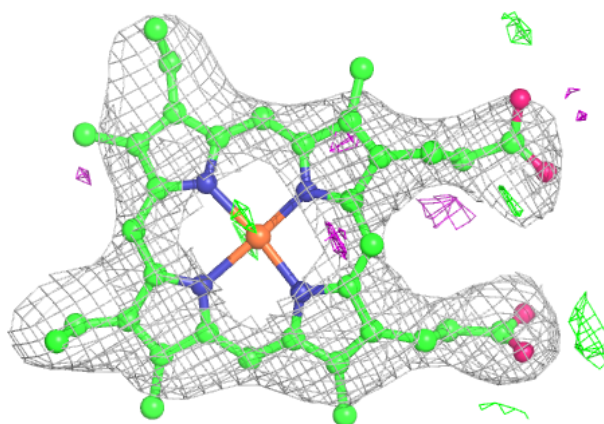
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





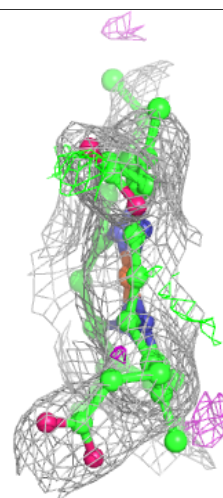
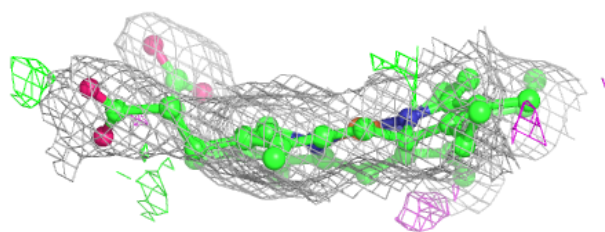
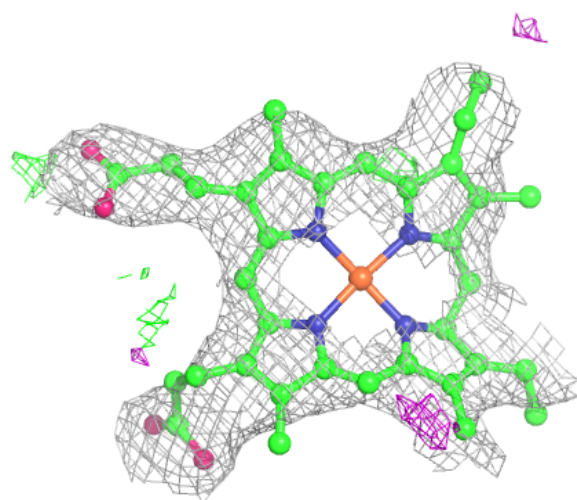
**Electron density around HEC E 606:**

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



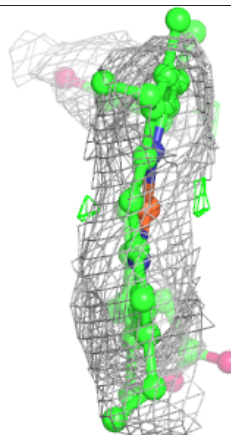
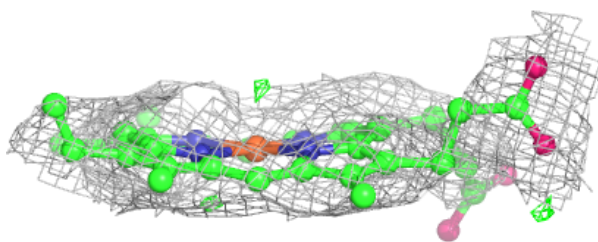
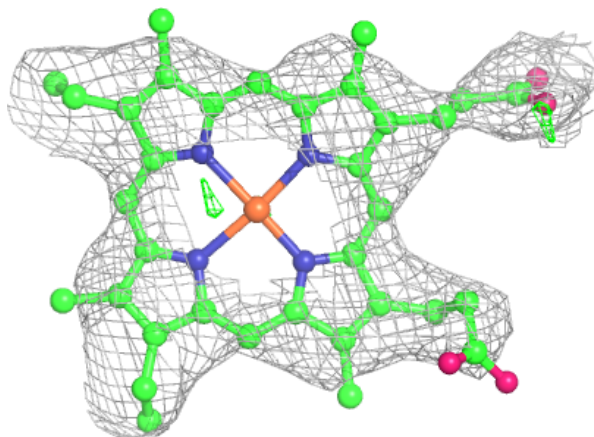
**Electron density around HEC F 603:**

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



**Electron density around HEC F 602:**

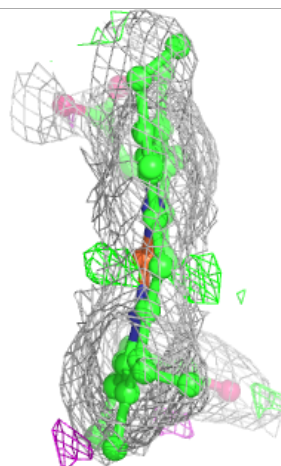
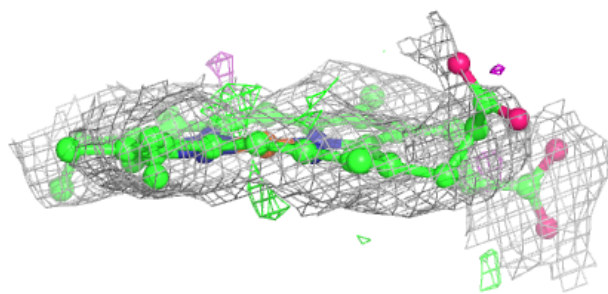
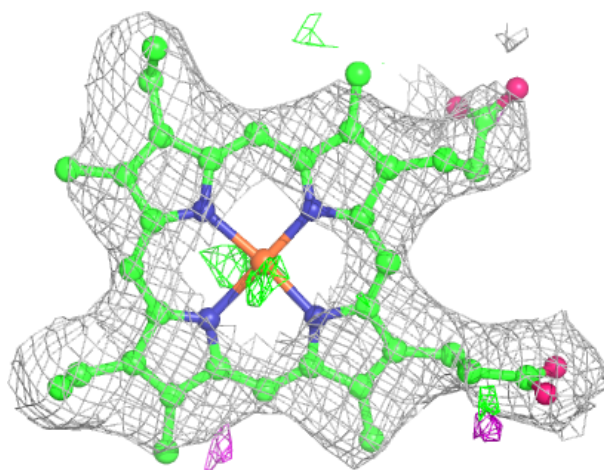
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

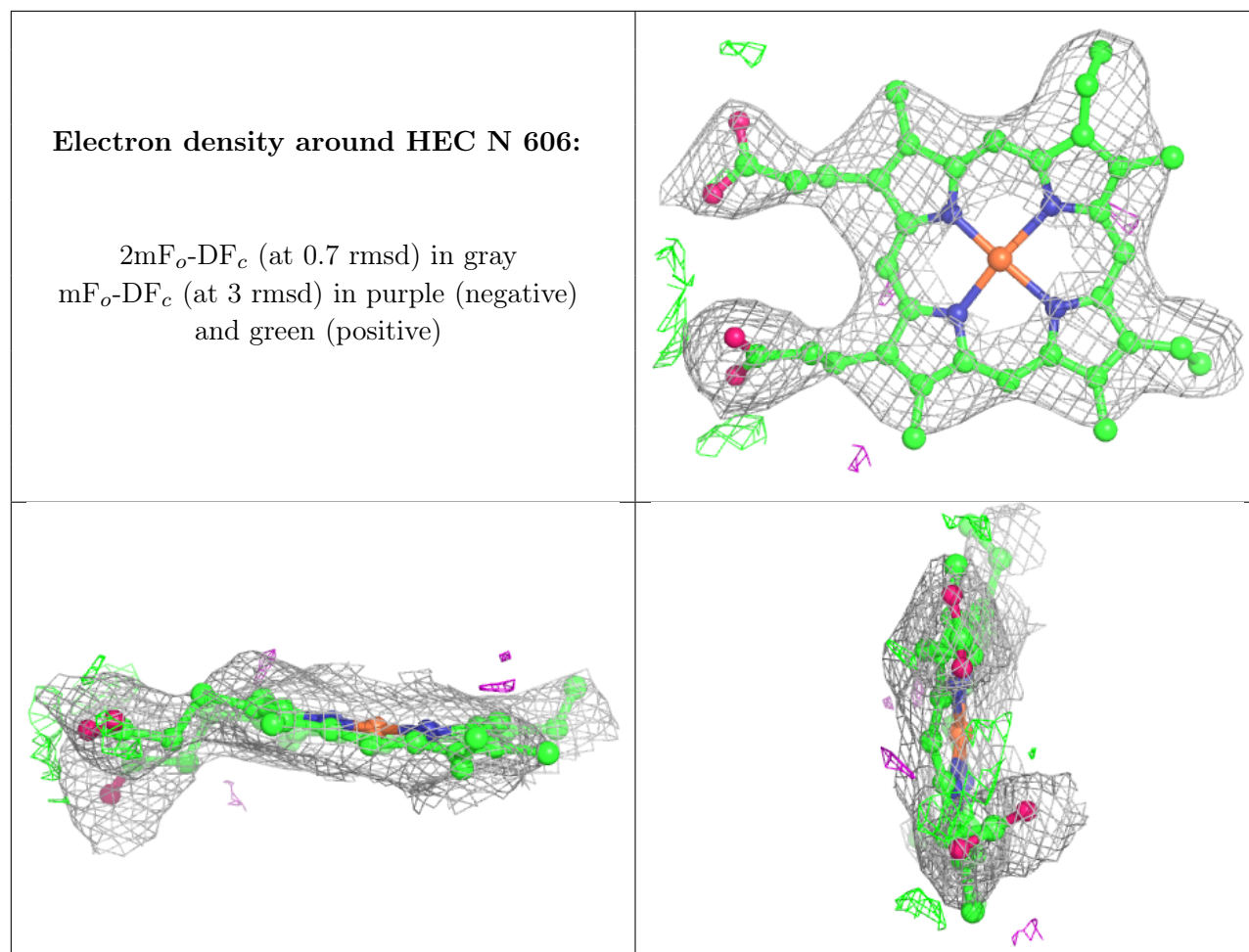




**Electron density around HEC H 602:**

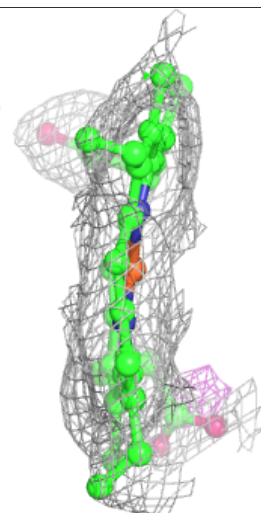
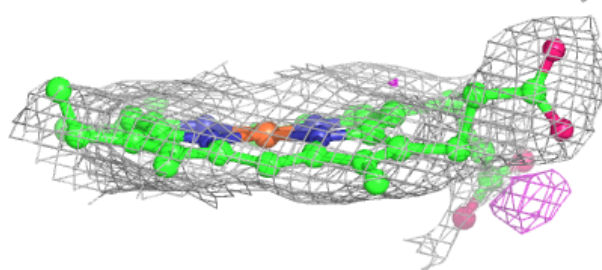
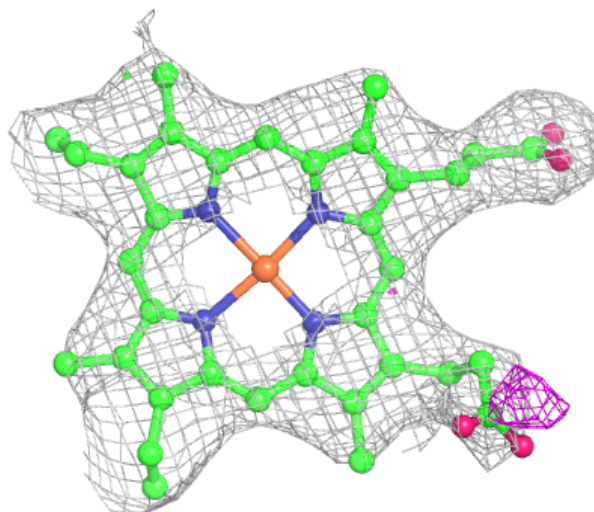
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

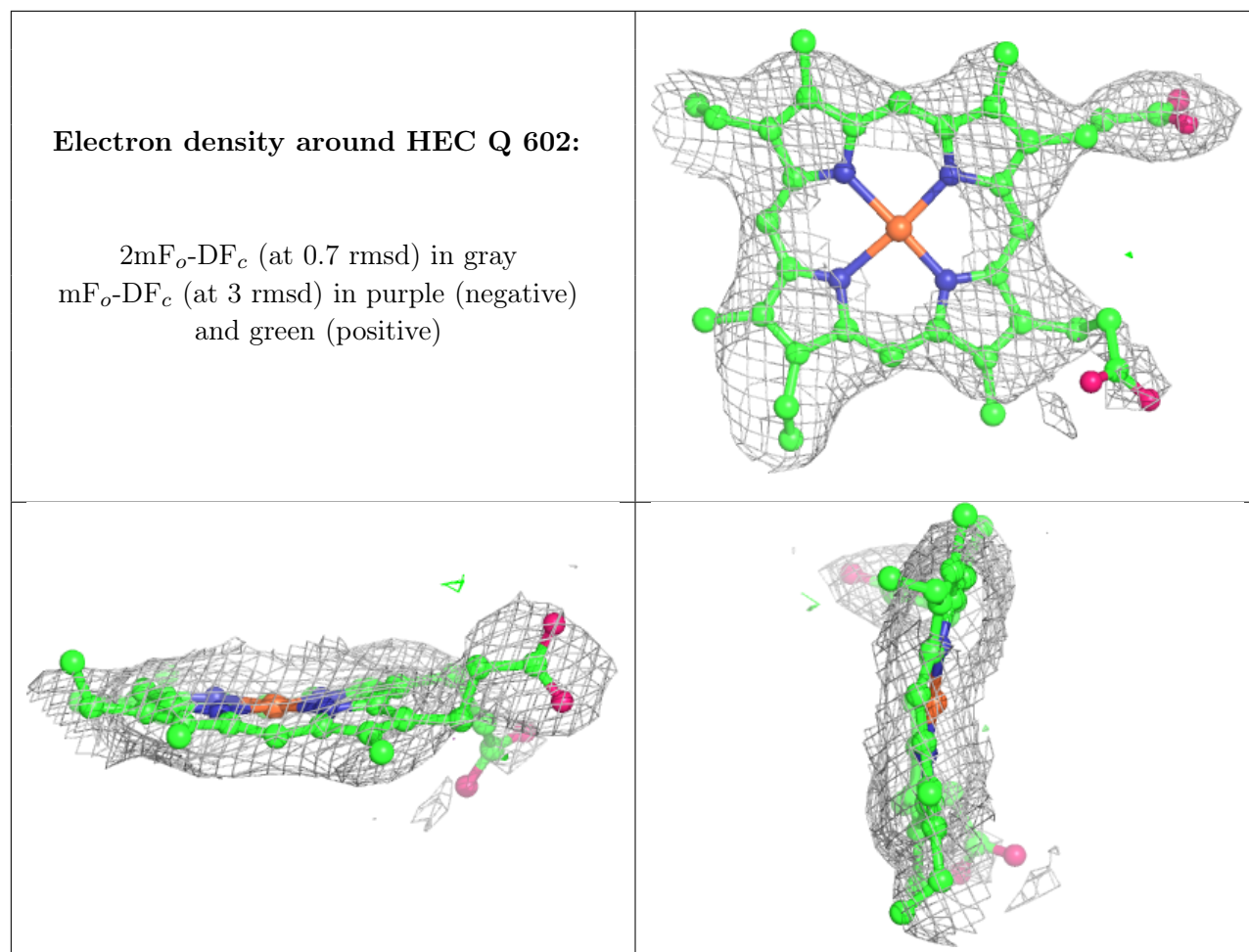




**Electron density around HEC P 602:**

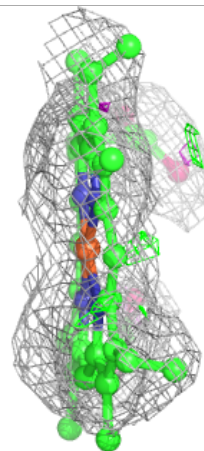
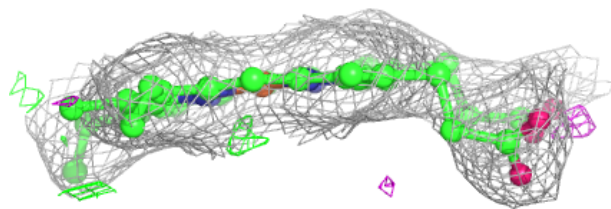
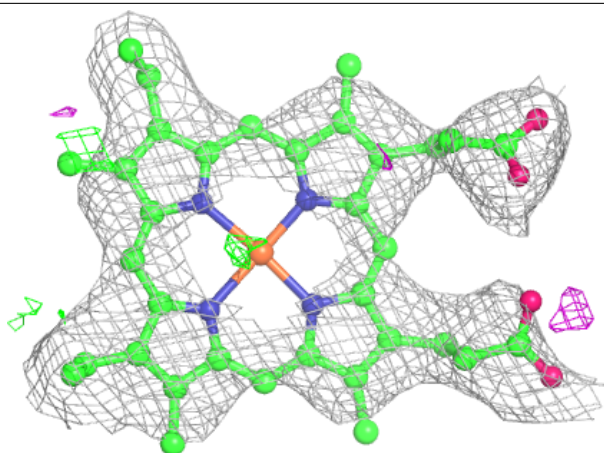
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





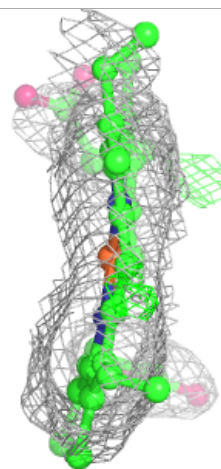
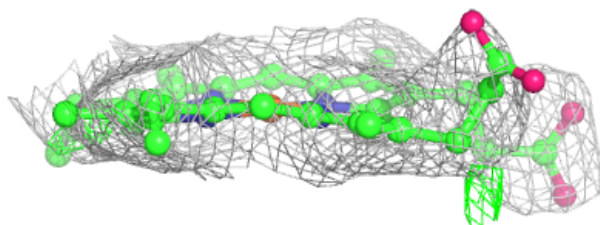
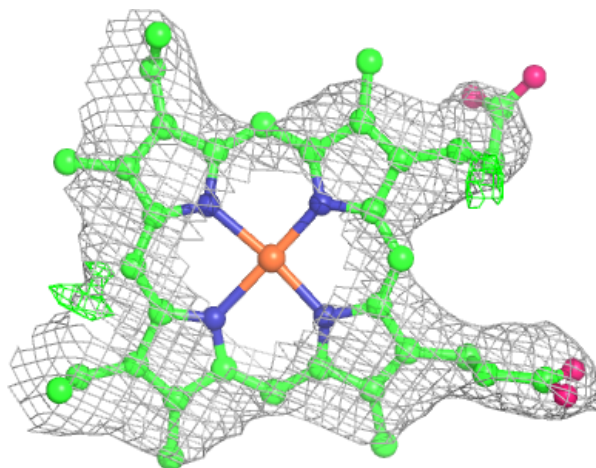
**Electron density around HEC Q 604:**

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



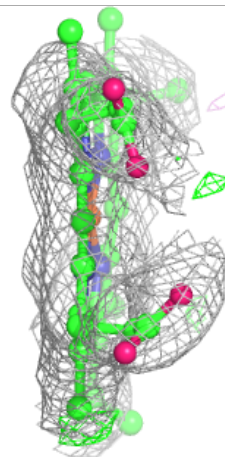
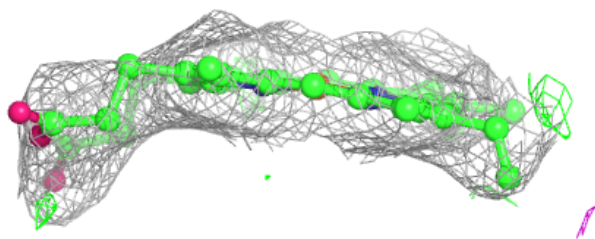
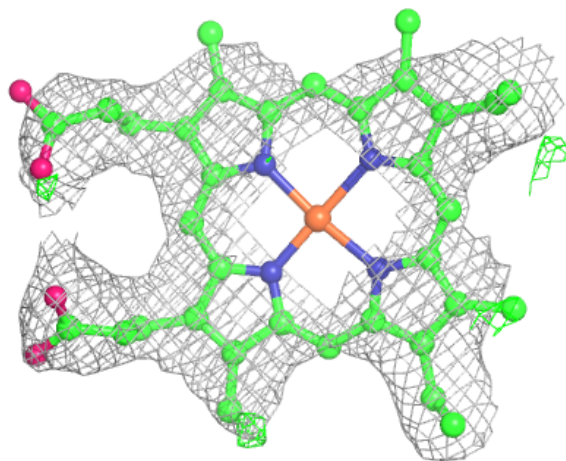
**Electron density around HEC S 602:**

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



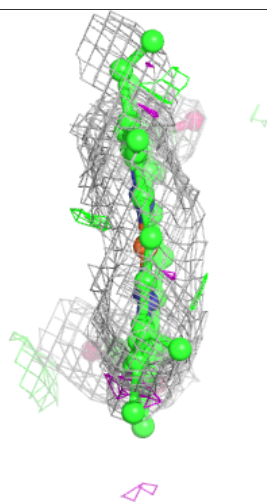
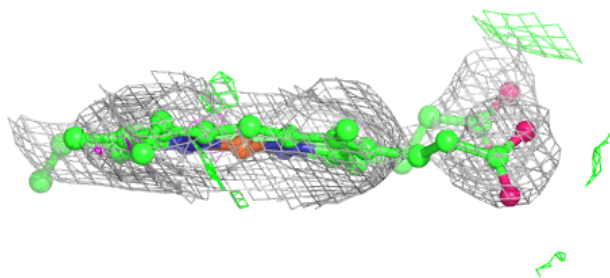
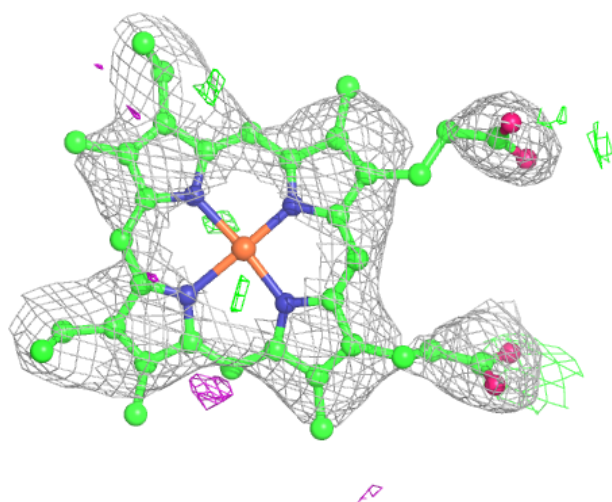
**Electron density around HEC S 604:**

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



**Electron density around HEC S 605:**

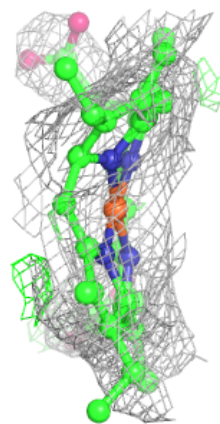
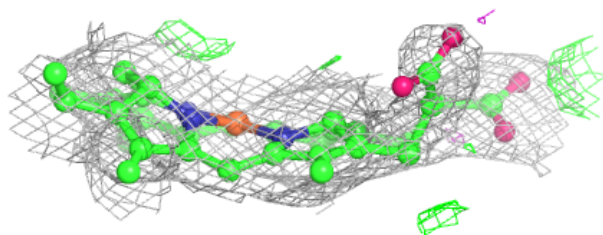
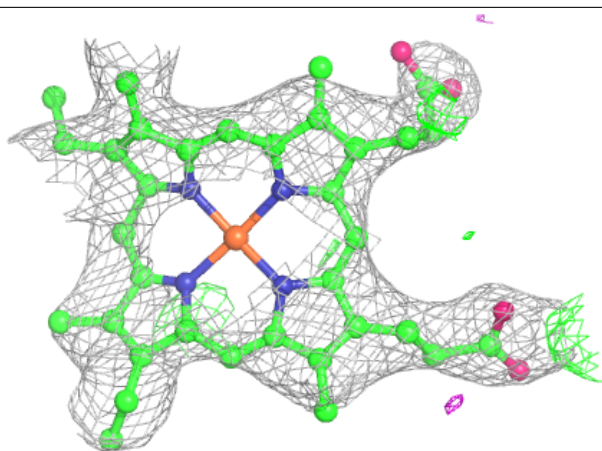
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

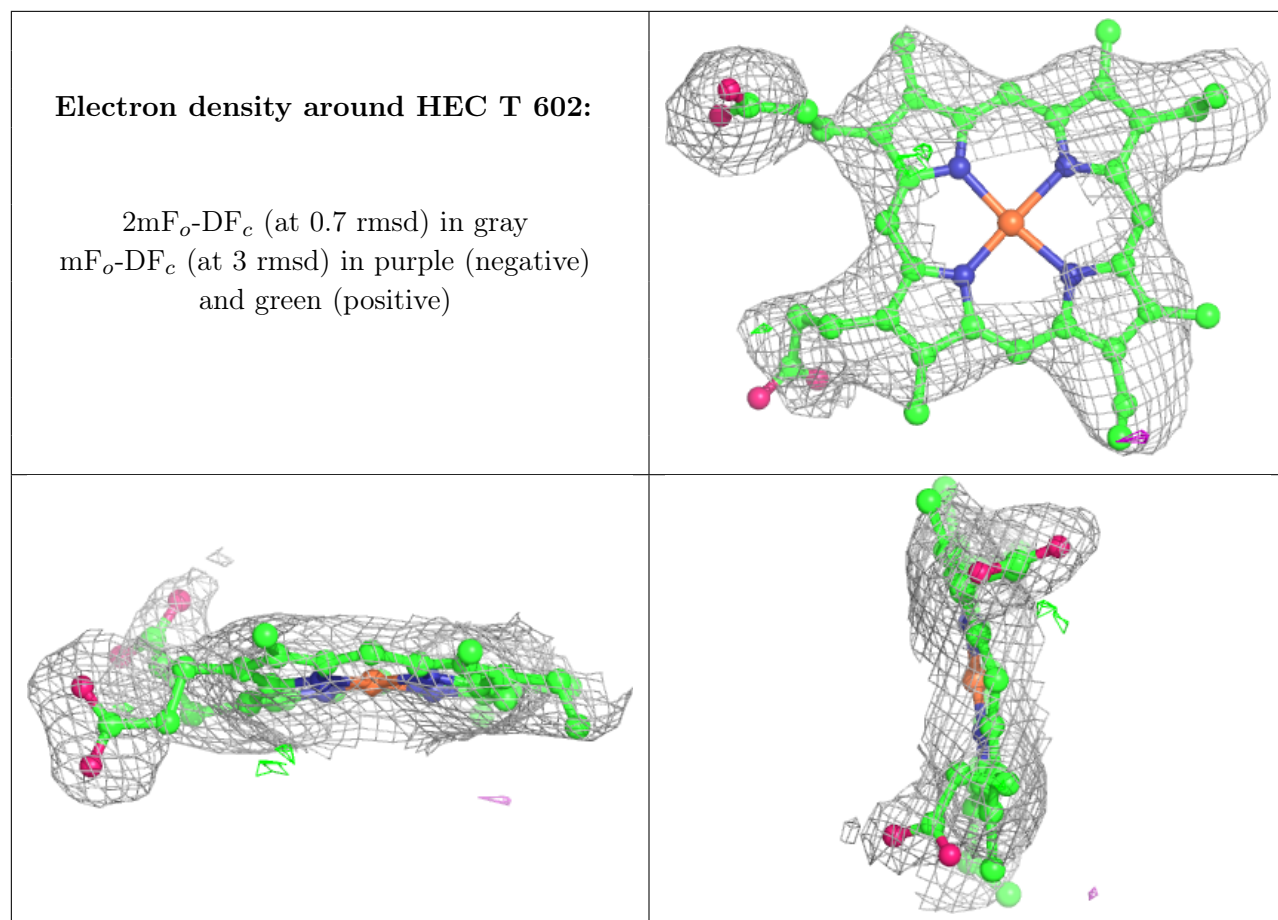


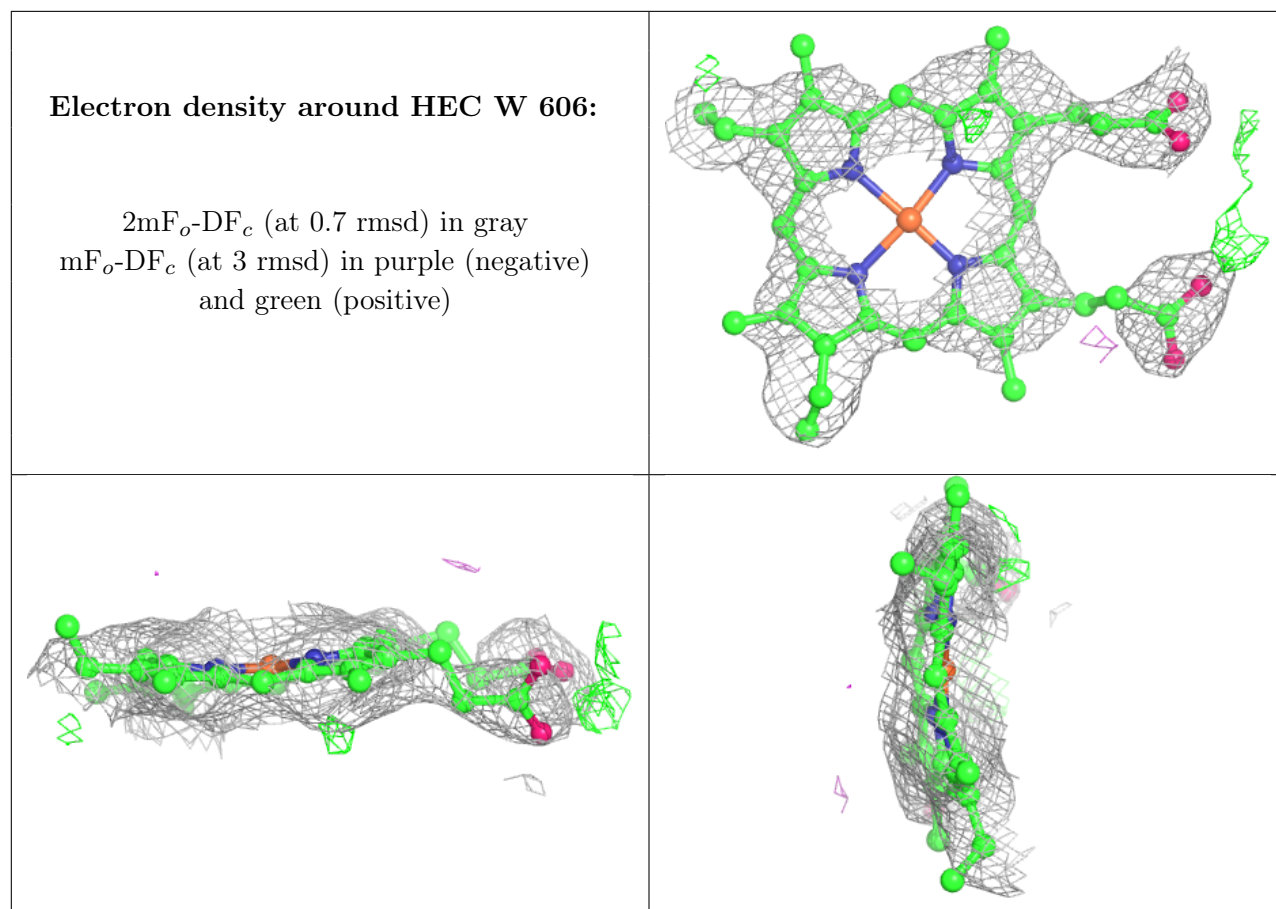


**Electron density around HEC S 603:**

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

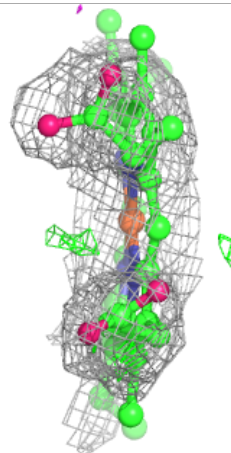
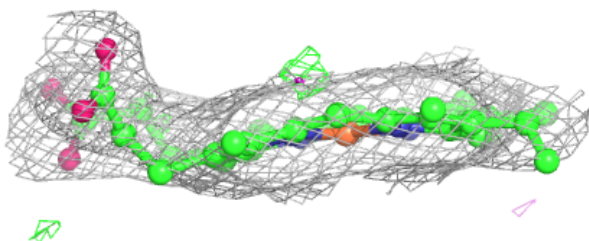
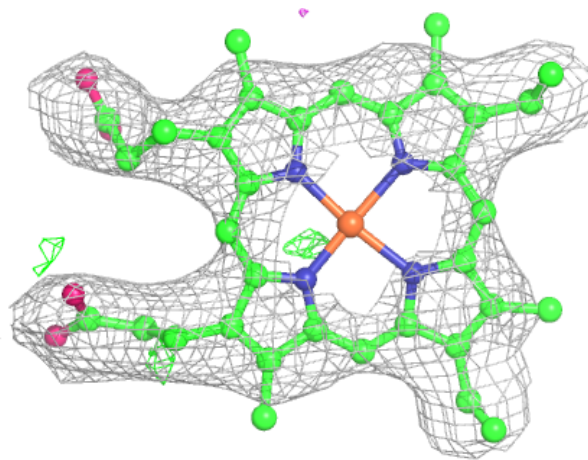


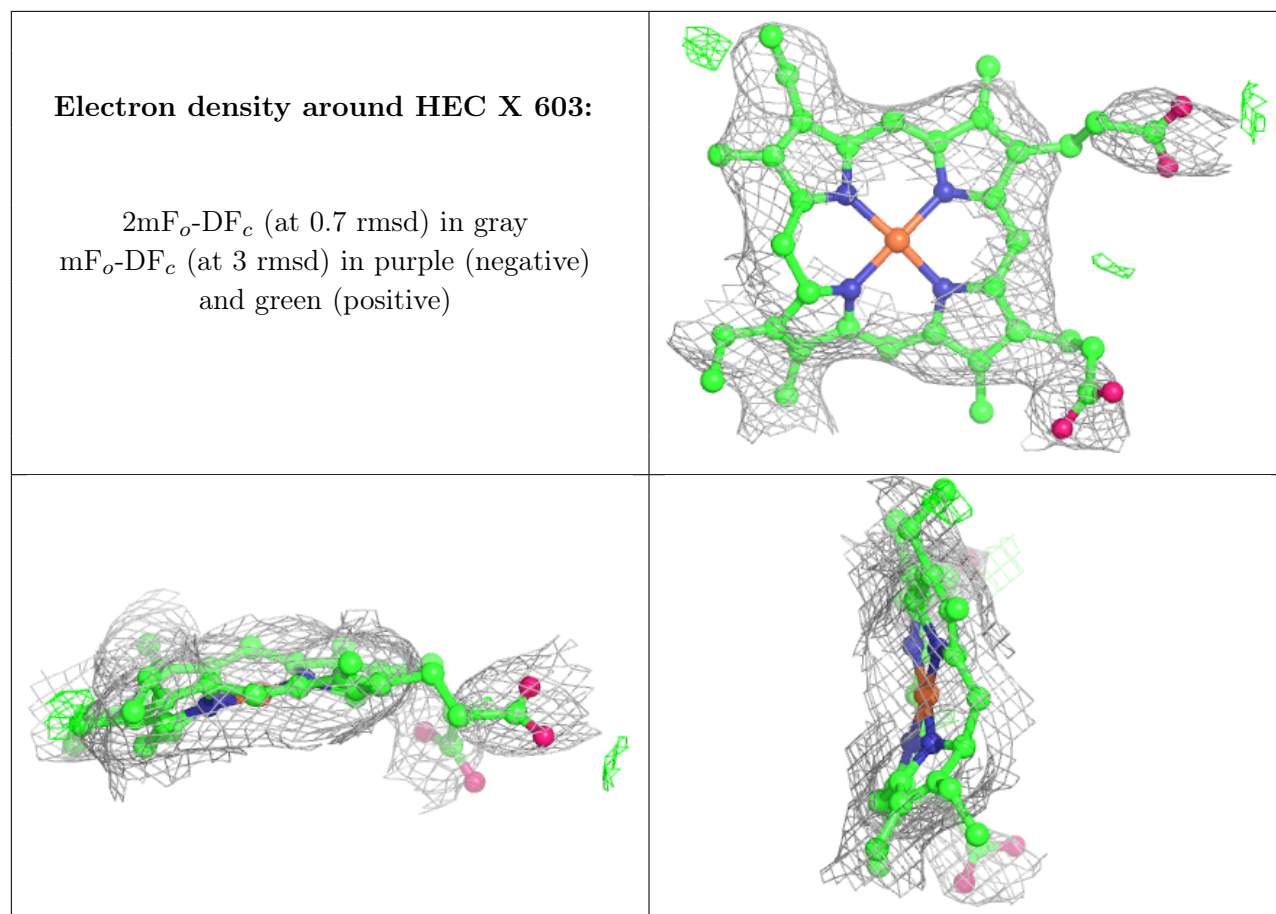




**Electron density around HEC W 607:**

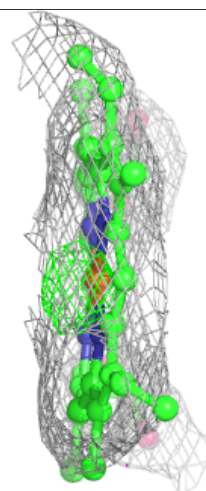
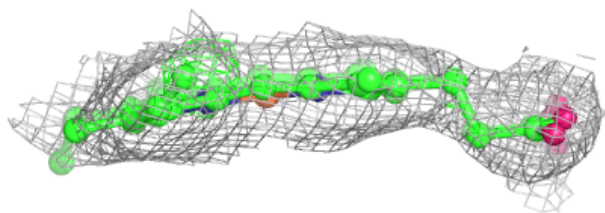
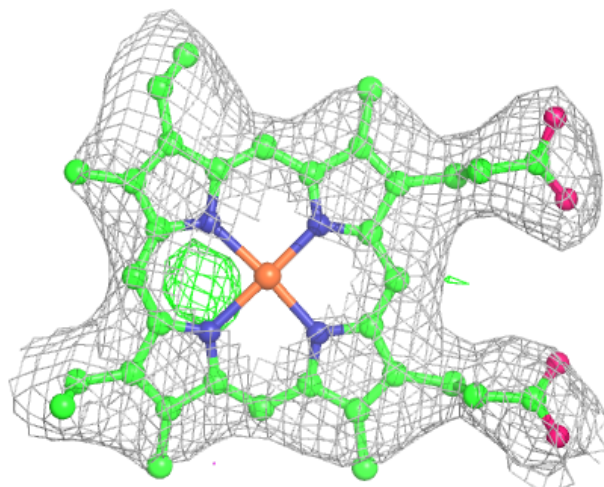
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





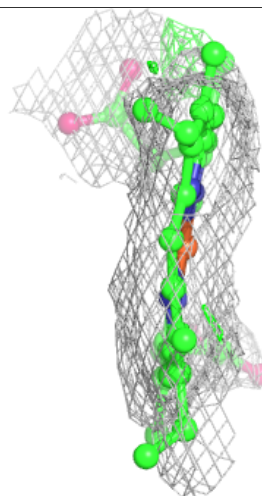
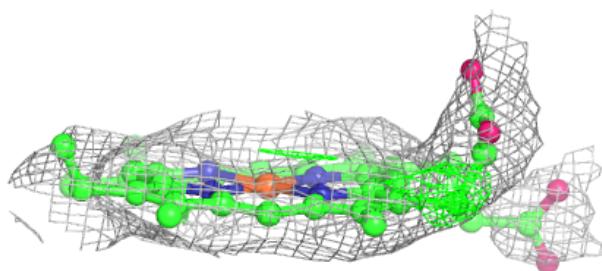
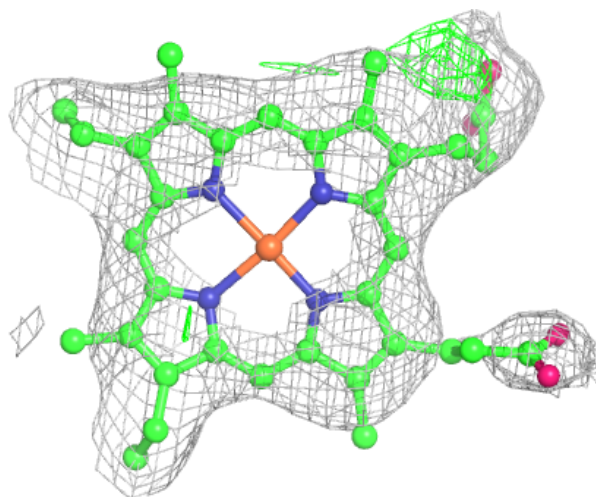
**Electron density around HEC X 600:**

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



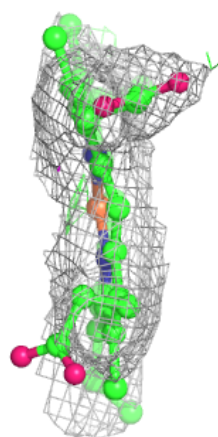
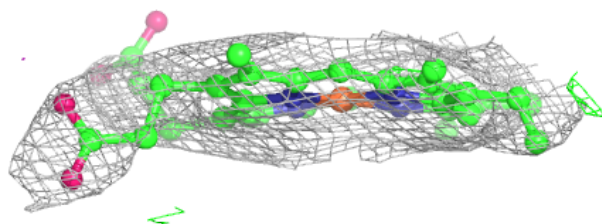
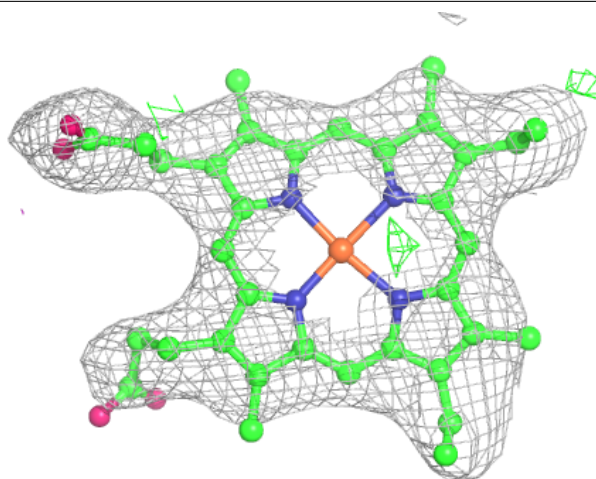
**Electron density around HEC X 601:**

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



**Electron density around HEC A 602:**

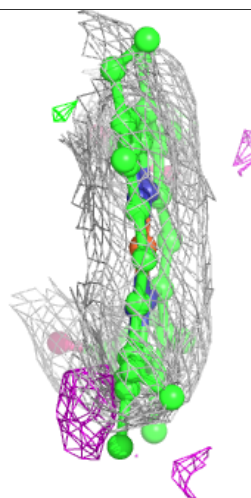
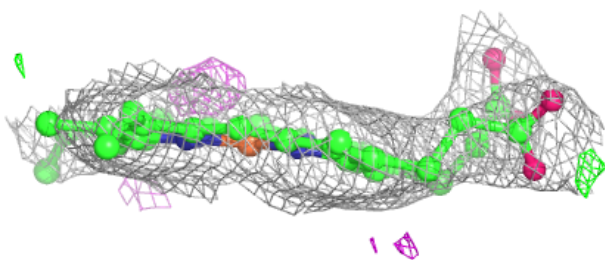
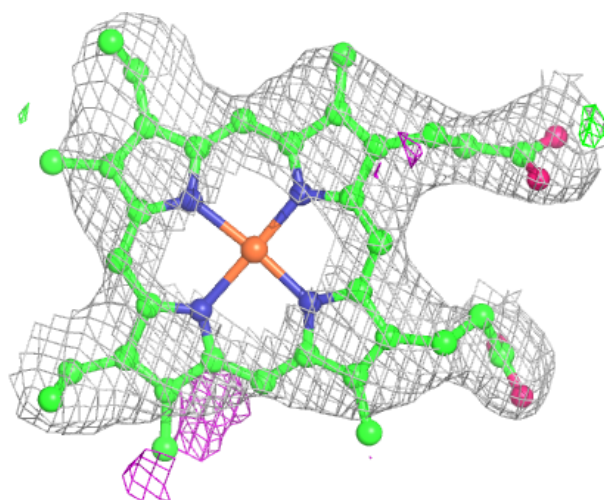
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





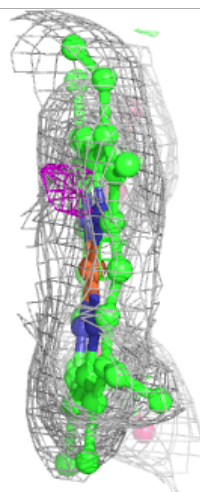
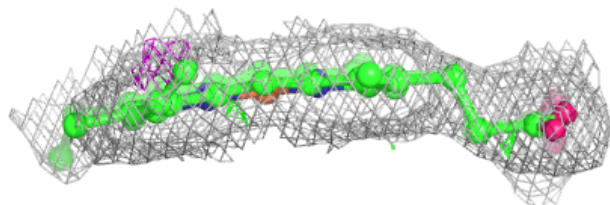
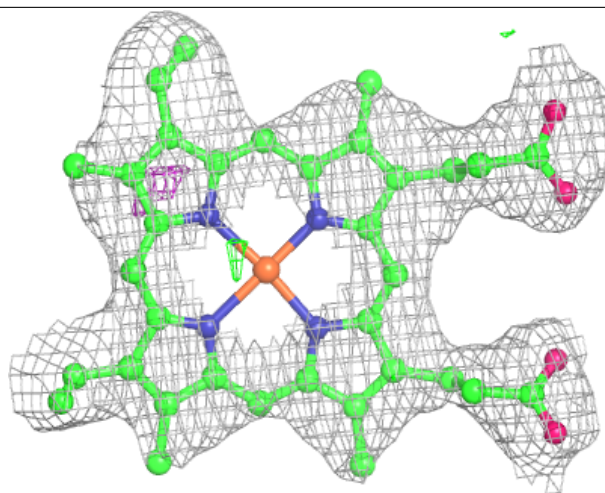
**Electron density around HEC E 607:**

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



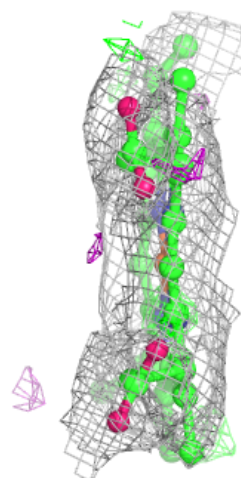
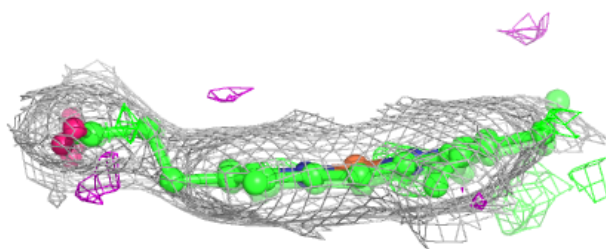
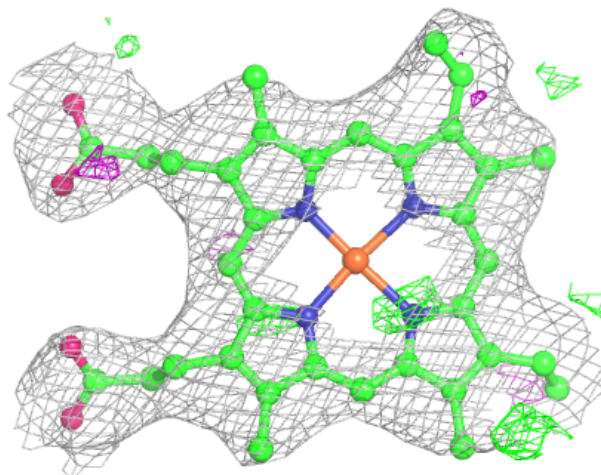
**Electron density around HEC G 600:**

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



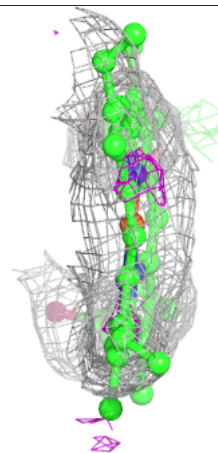
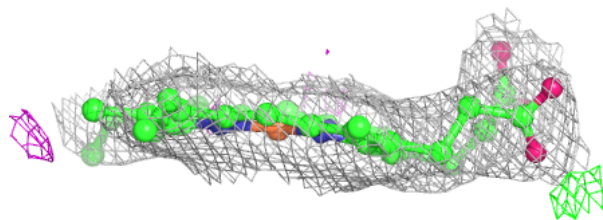
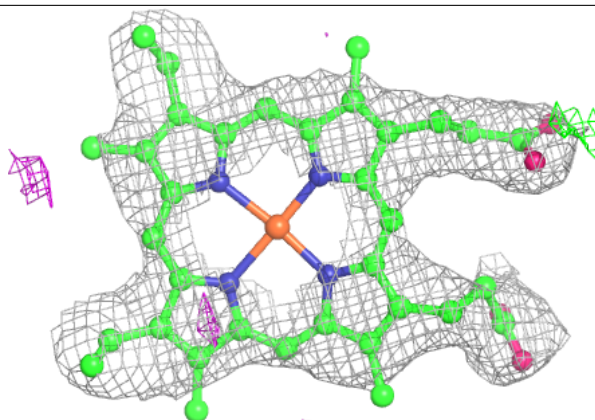
**Electron density around HEC F 600:**

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



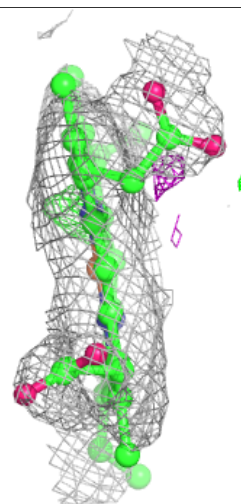
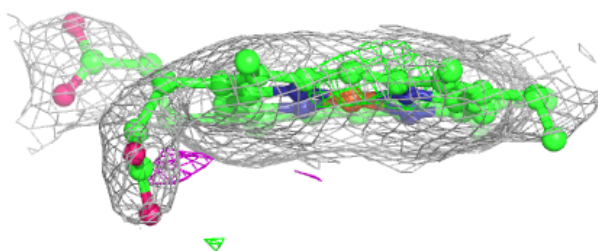
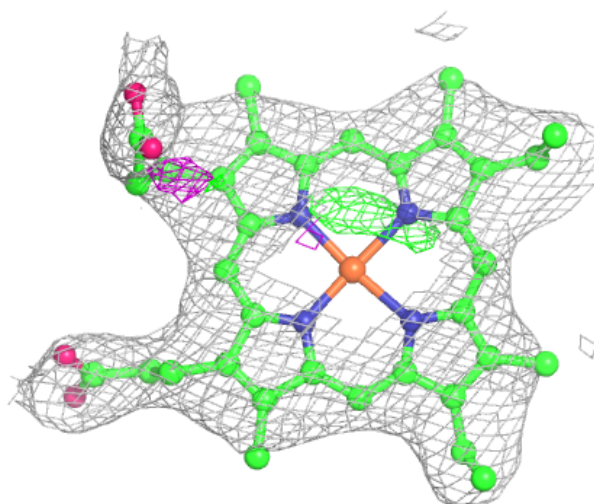
**Electron density around HEC X 607:**

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



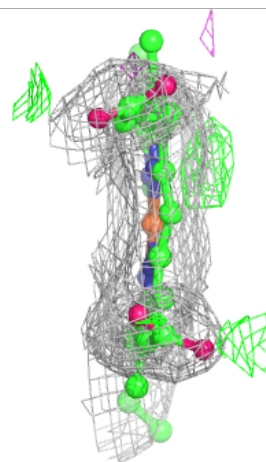
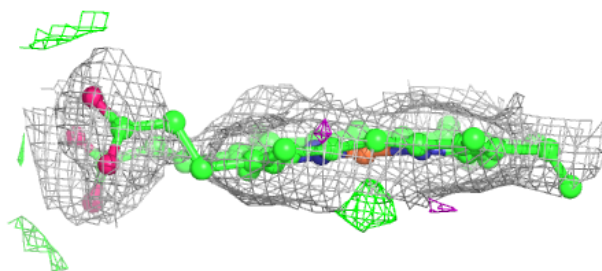
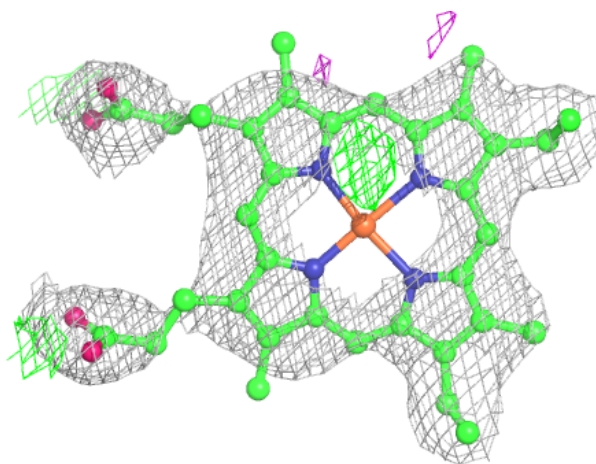
**Electron density around HEC F 601:**

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



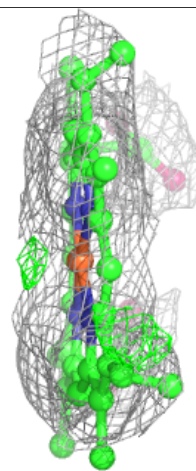
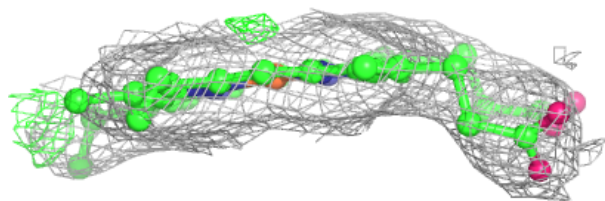
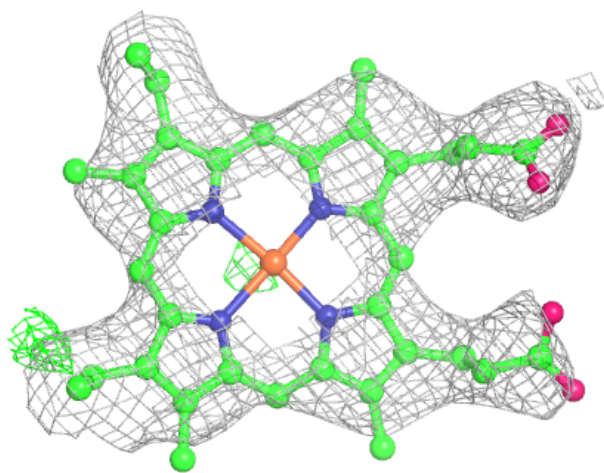
**Electron density around HEC A 605:**

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



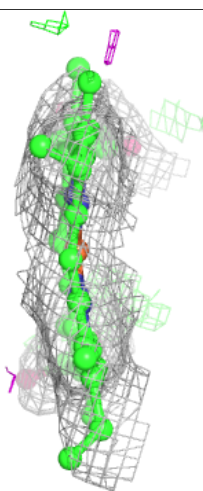
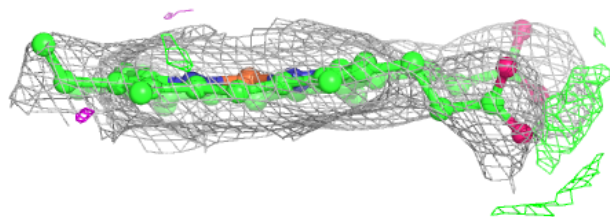
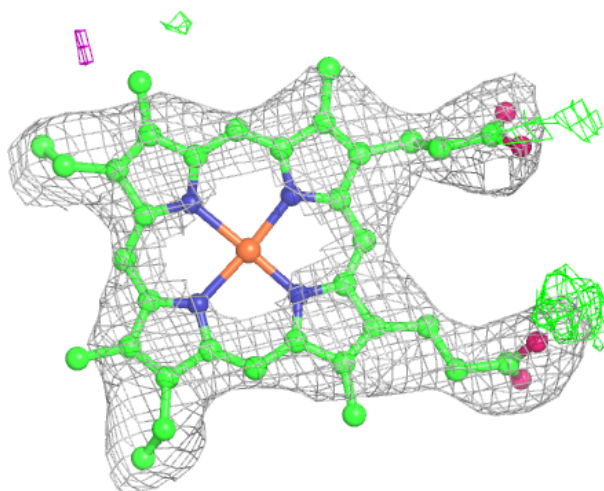
**Electron density around HEC F 604:**

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



**Electron density around HEC F 605:**

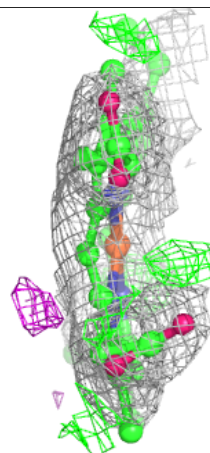
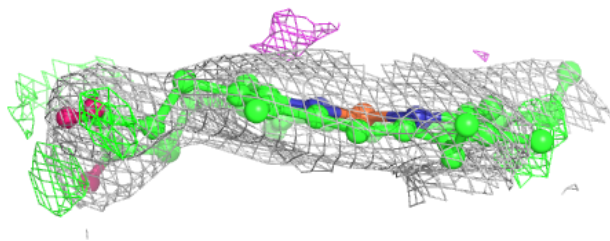
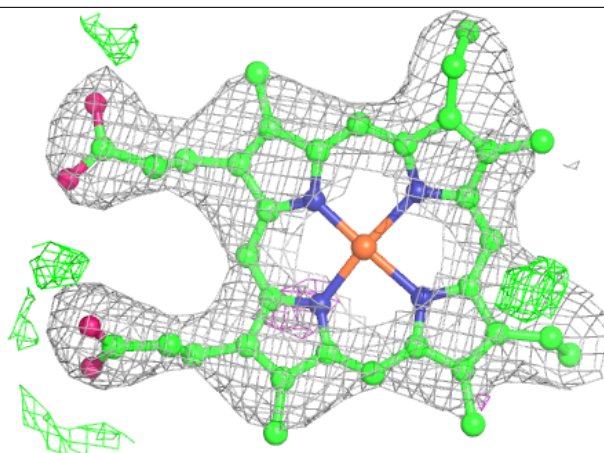
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





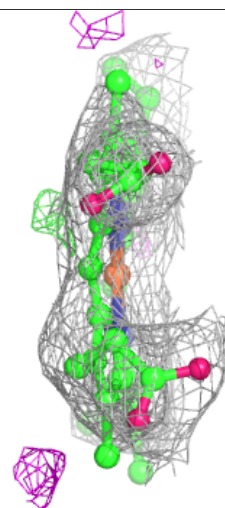
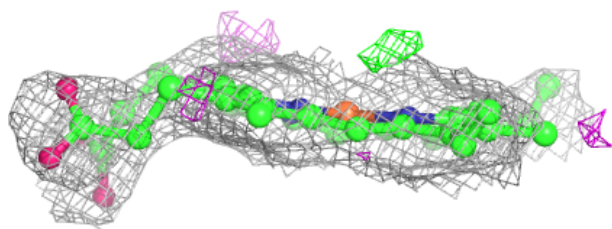
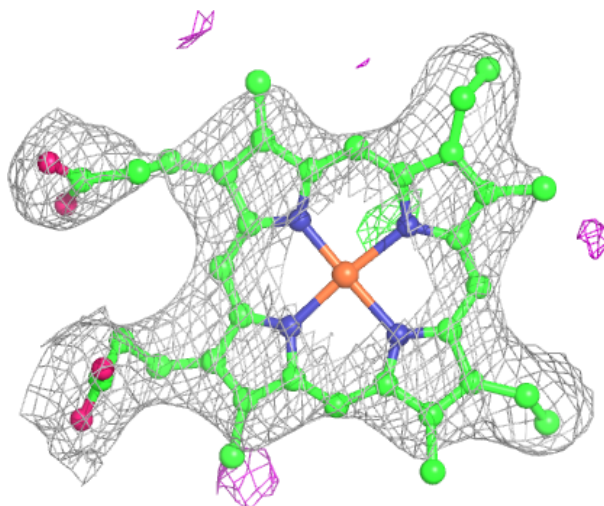
**Electron density around HEC F 606:**

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



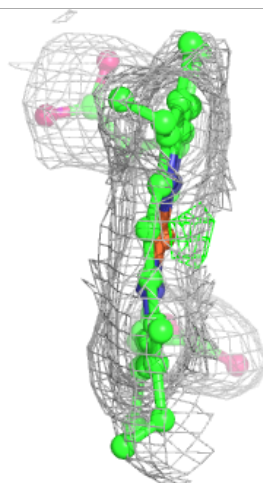
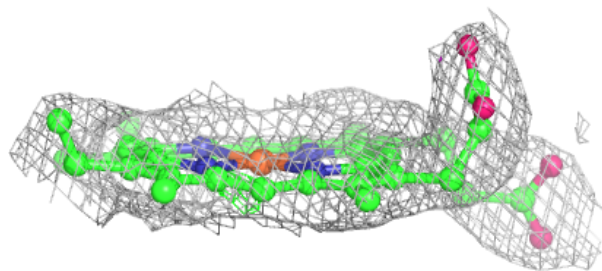
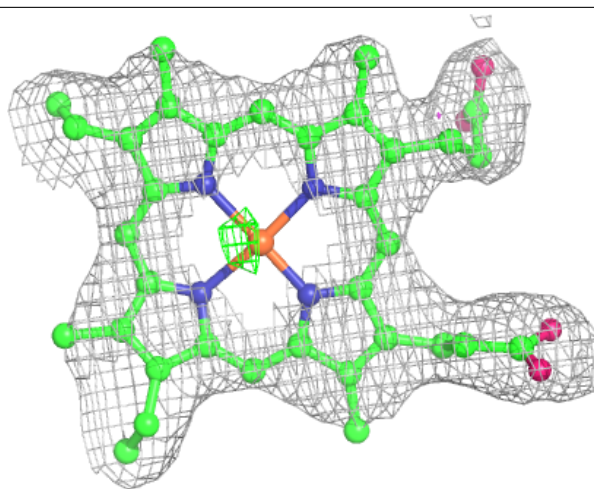
**Electron density around HEC F 607:**

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



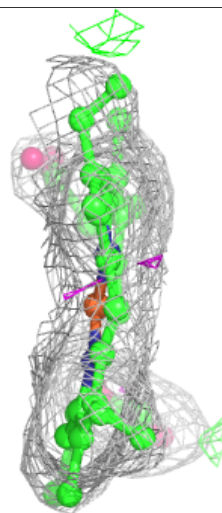
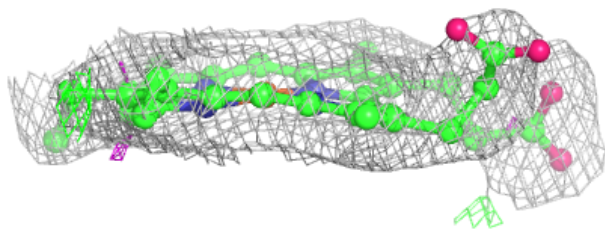
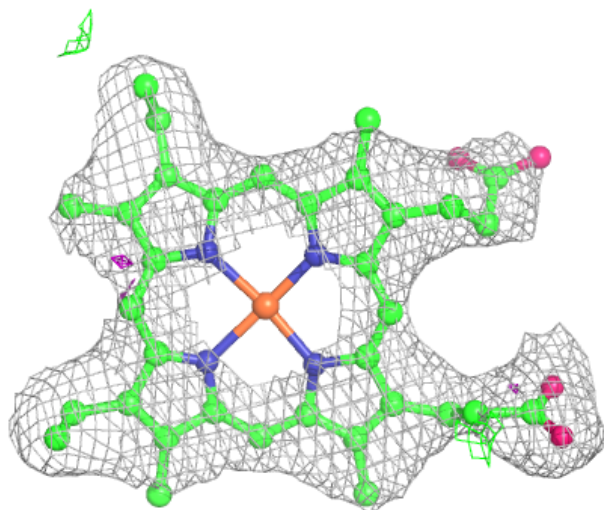
**Electron density around HEC G 601:**

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



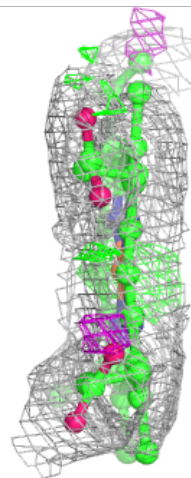
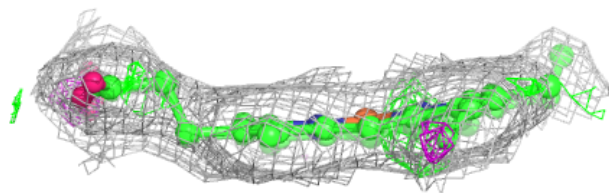
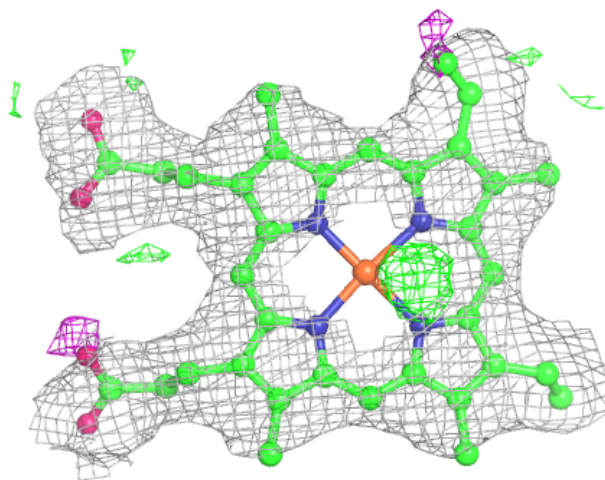
**Electron density around HEC I 602:**

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



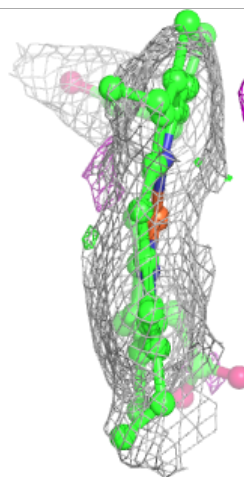
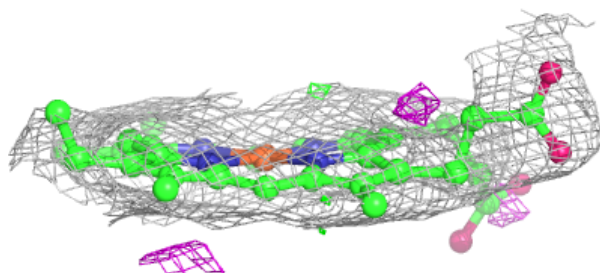
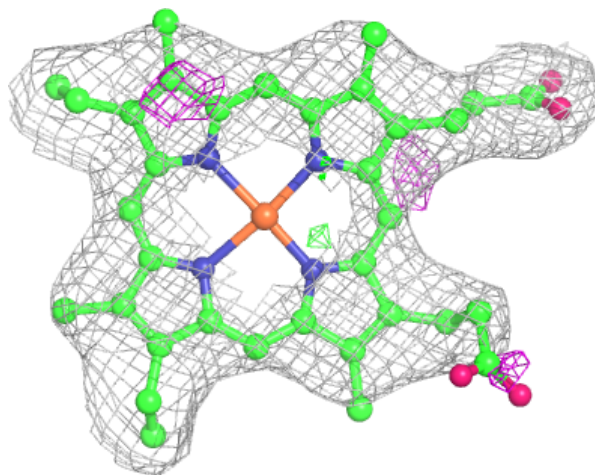
**Electron density around HEC J 600:**

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



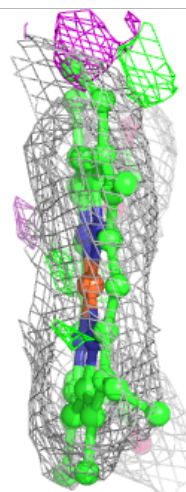
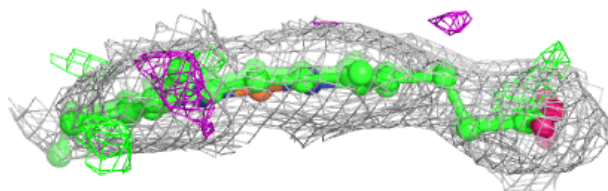
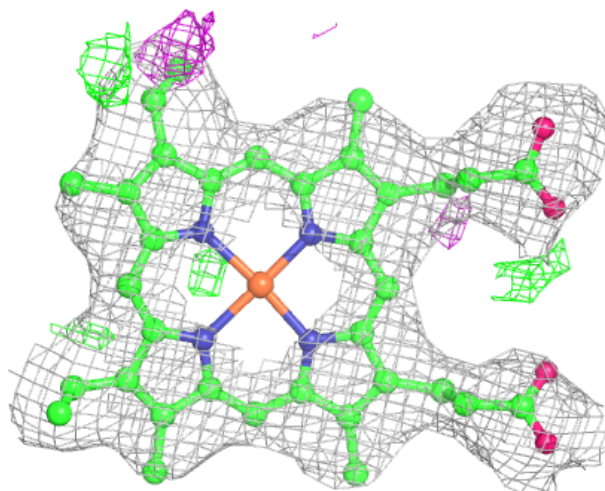
**Electron density around HEC J 602:**

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



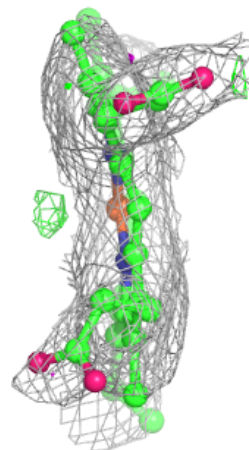
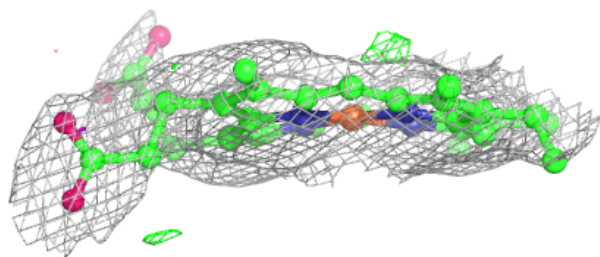
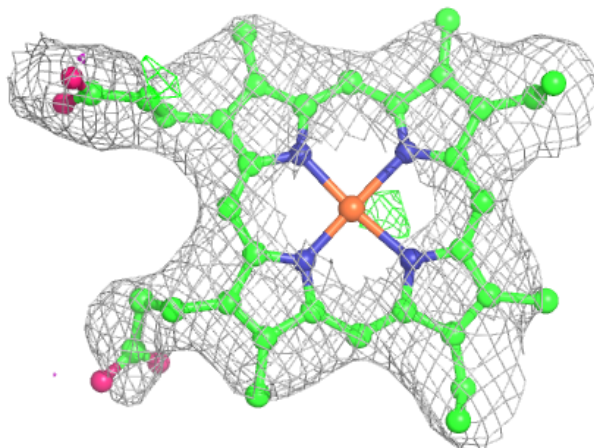
**Electron density around HEC K 600:**

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



**Electron density around HEC K 602:**

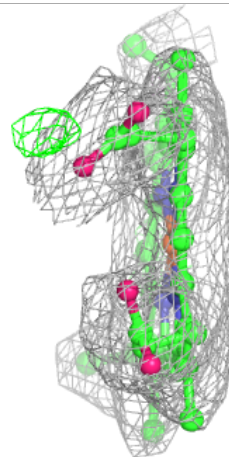
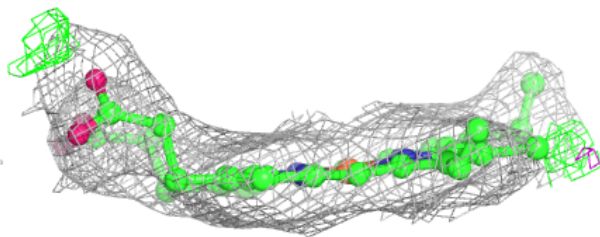
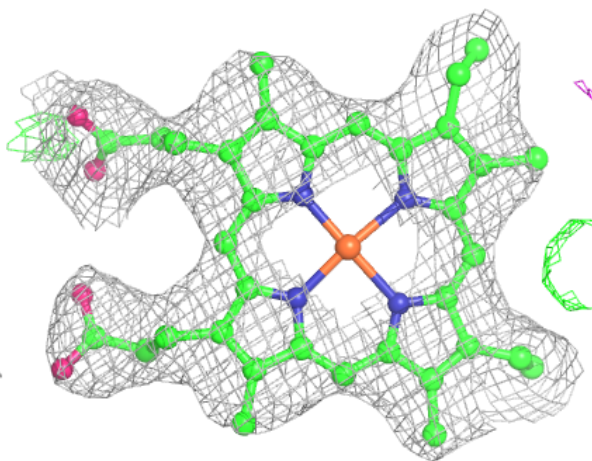
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





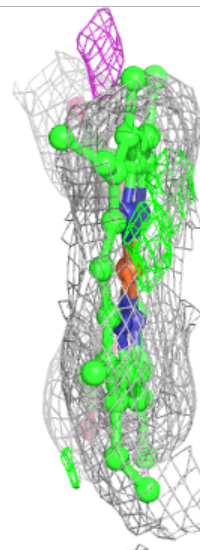
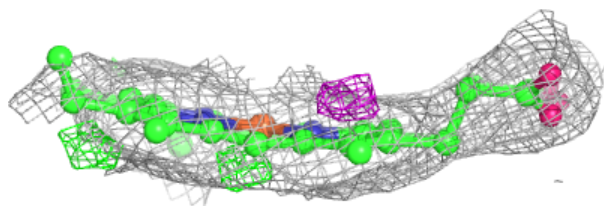
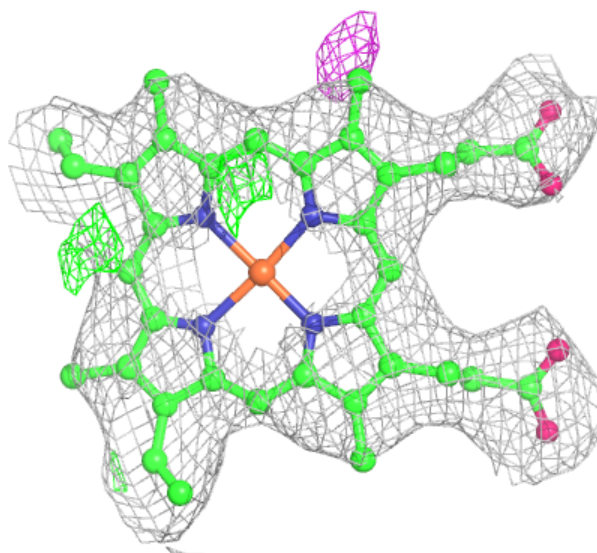
**Electron density around HEC K 604:**

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



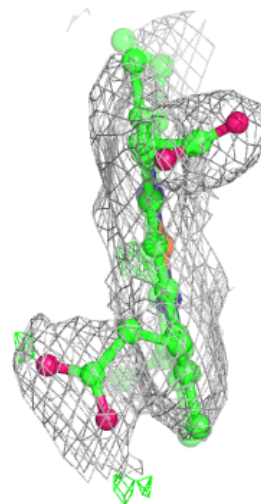
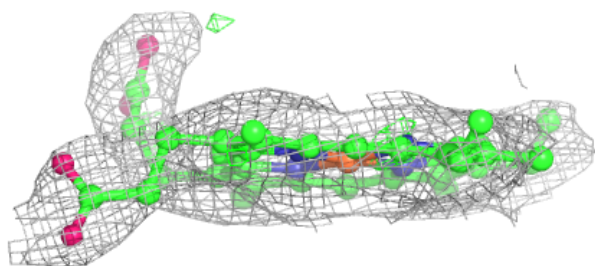
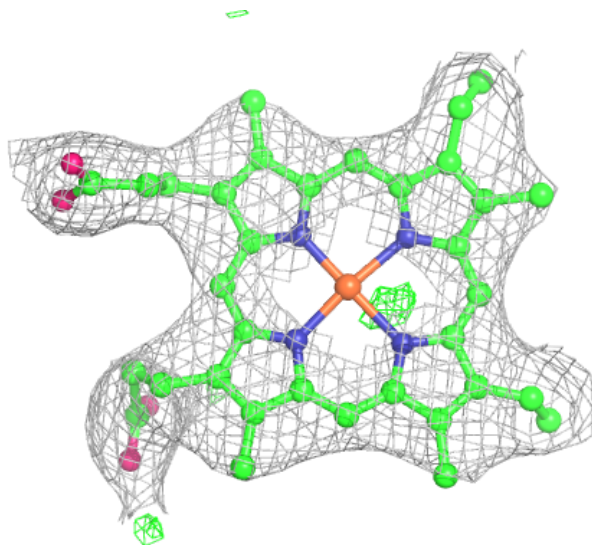
**Electron density around HEC L 600:**

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



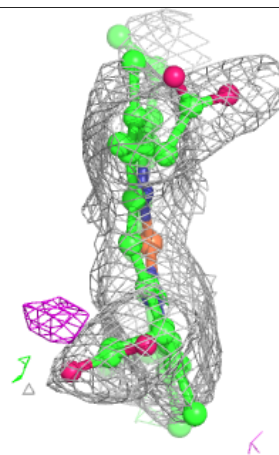
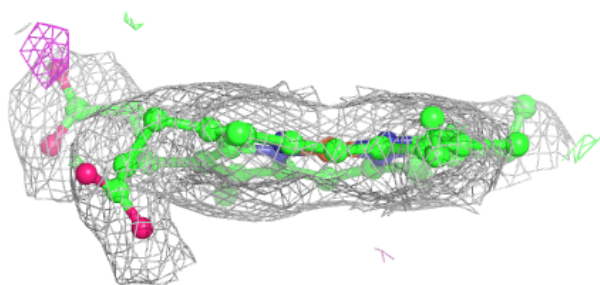
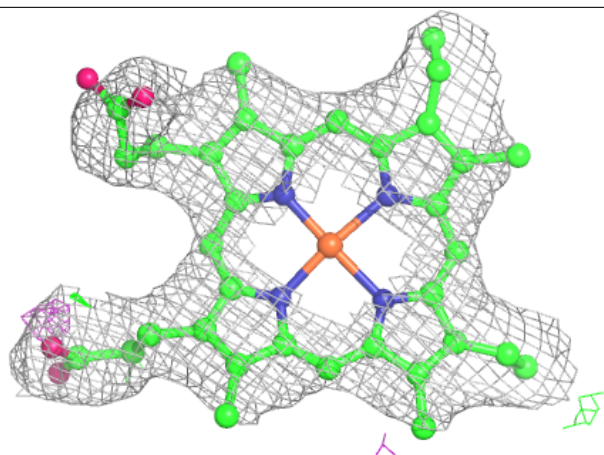
**Electron density around HEC L 601:**

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



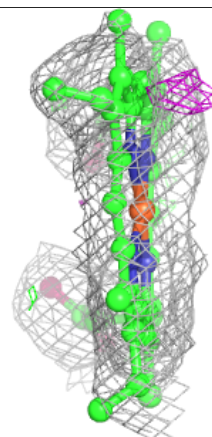
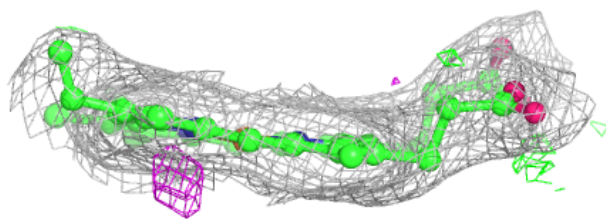
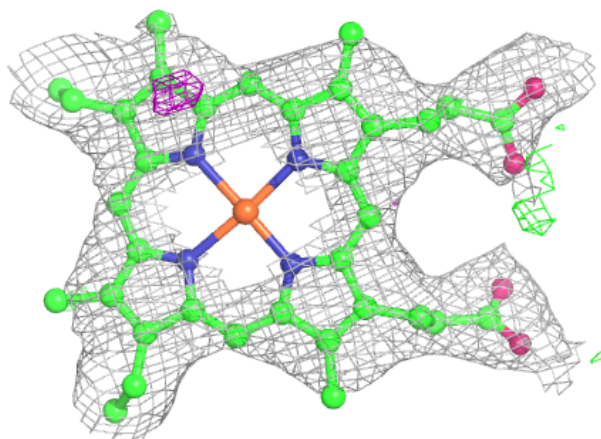
**Electron density around HEC L 602:**

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



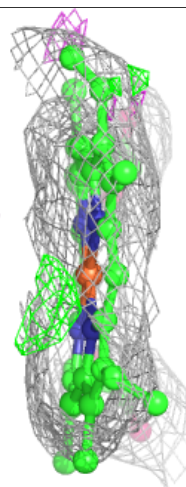
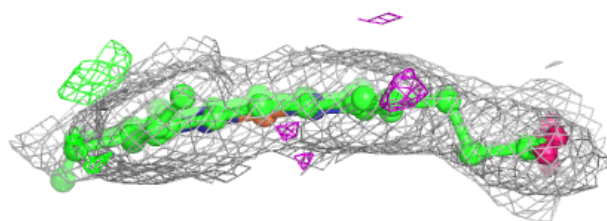
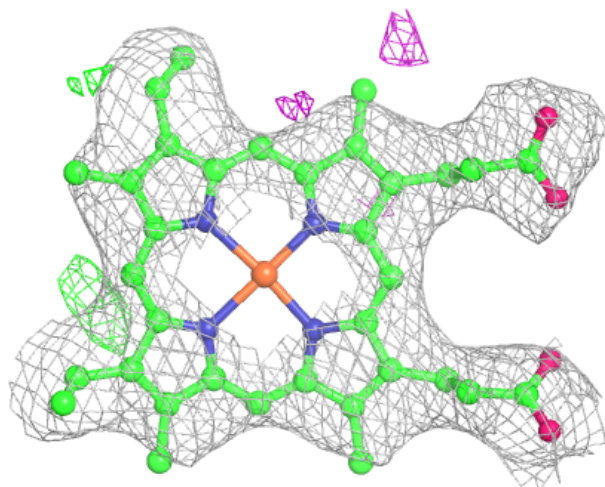
**Electron density around HEC L 604:**

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



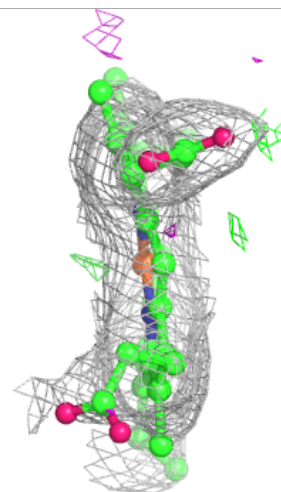
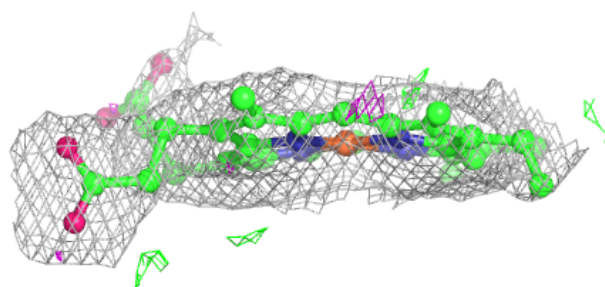
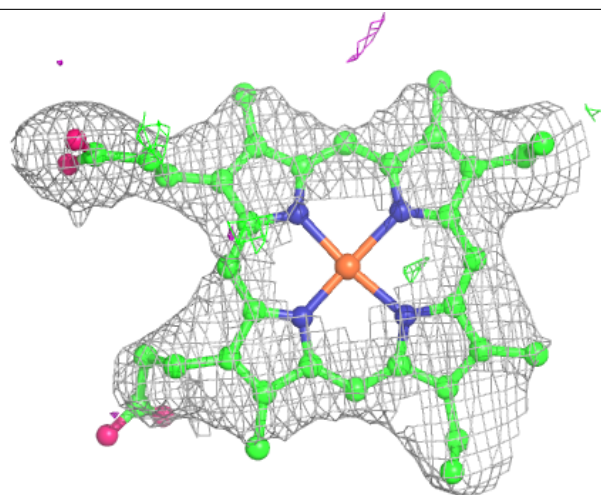
**Electron density around HEC M 600:**

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



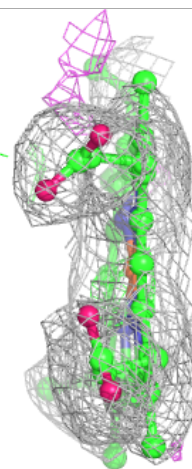
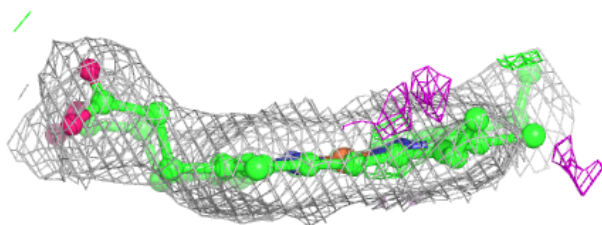
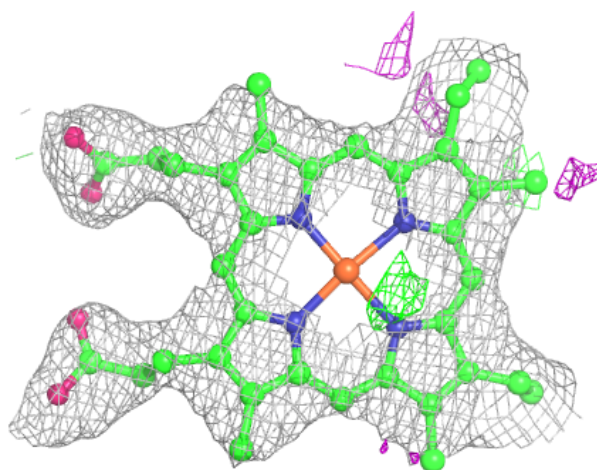
**Electron density around HEC M 602:**

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



**Electron density around HEC M 604:**

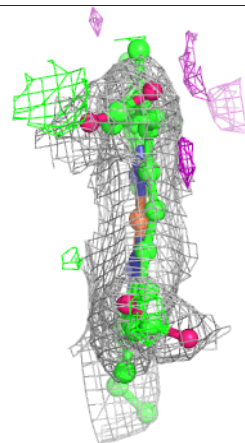
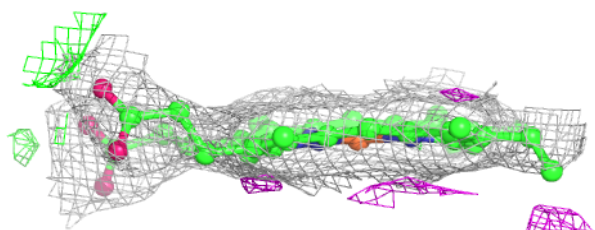
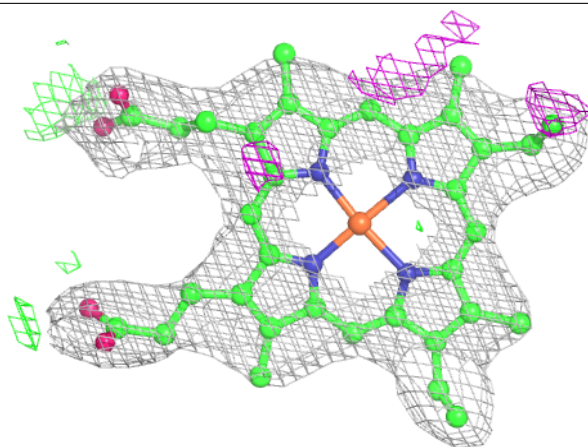
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





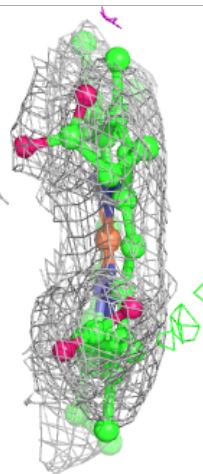
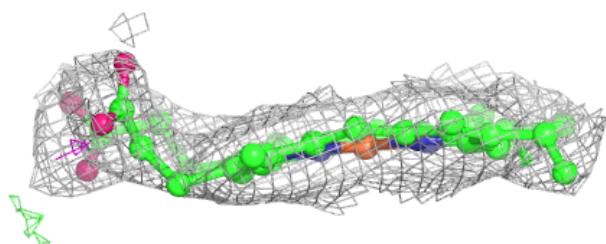
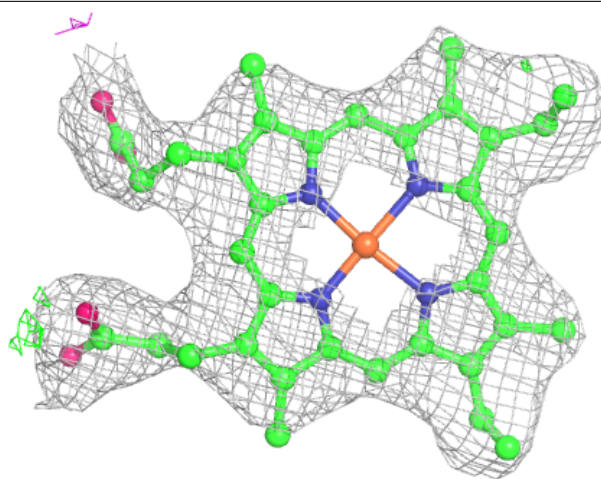
**Electron density around HEC M 605:**

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



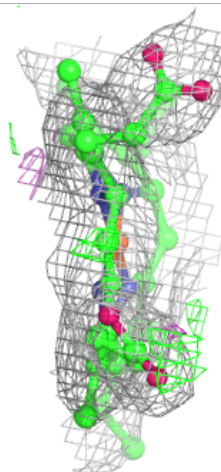
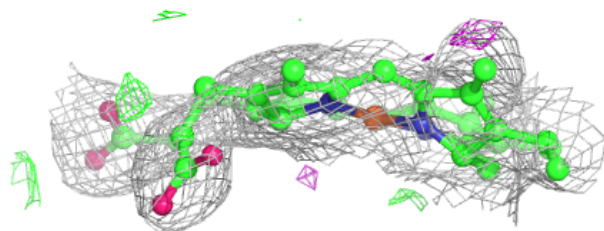
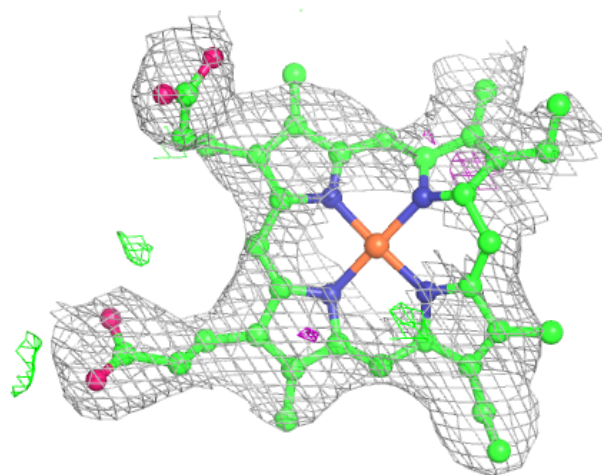
**Electron density around HEC M 607:**

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



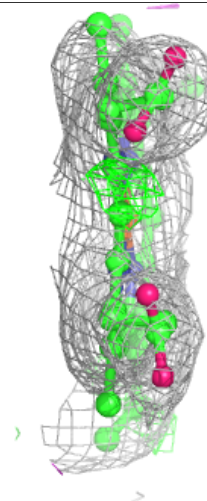
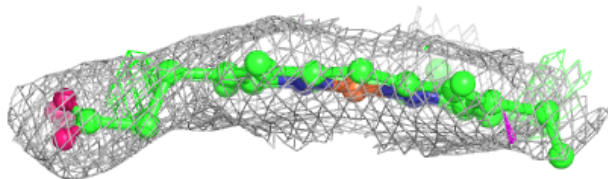
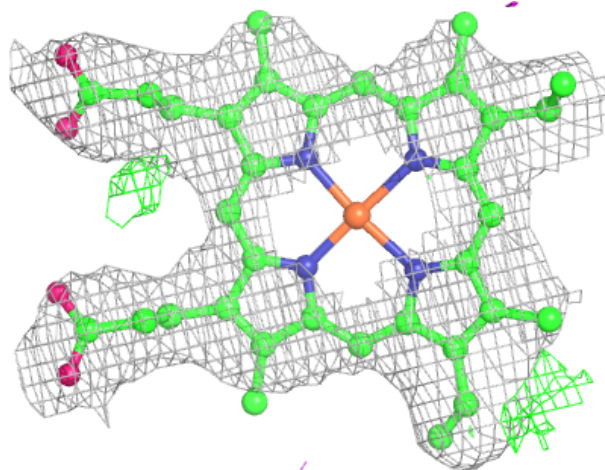
**Electron density around HEC M 603:**

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



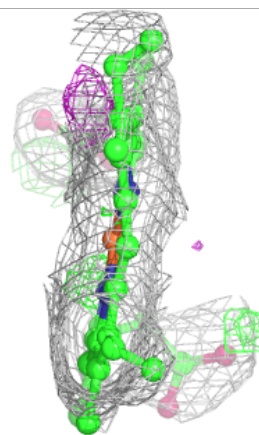
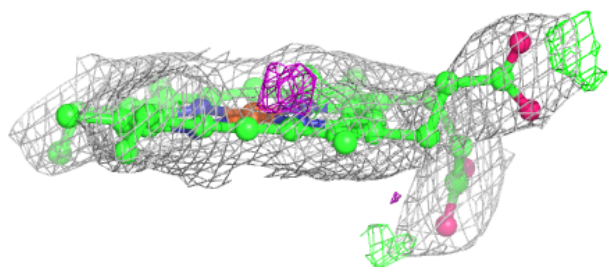
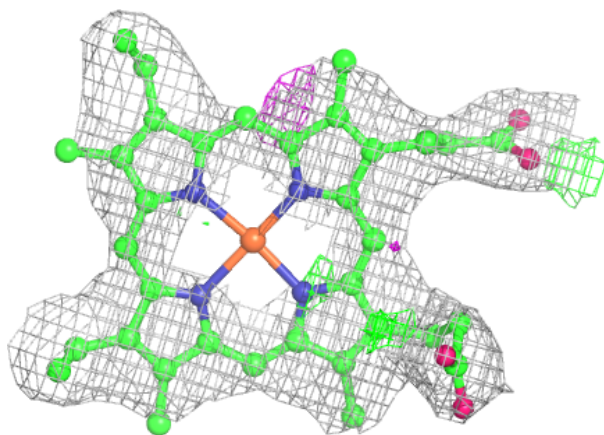
**Electron density around HEC N 600:**

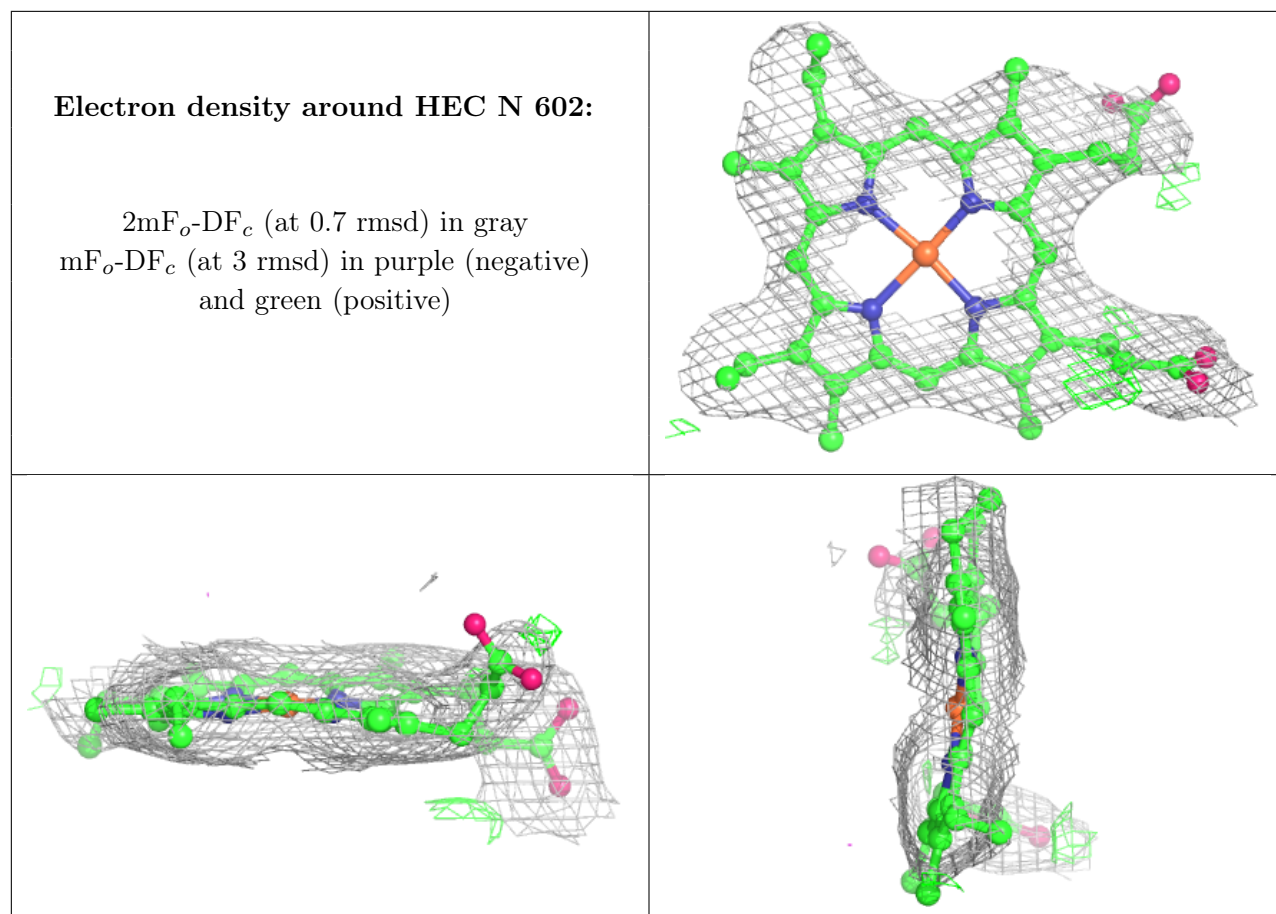
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

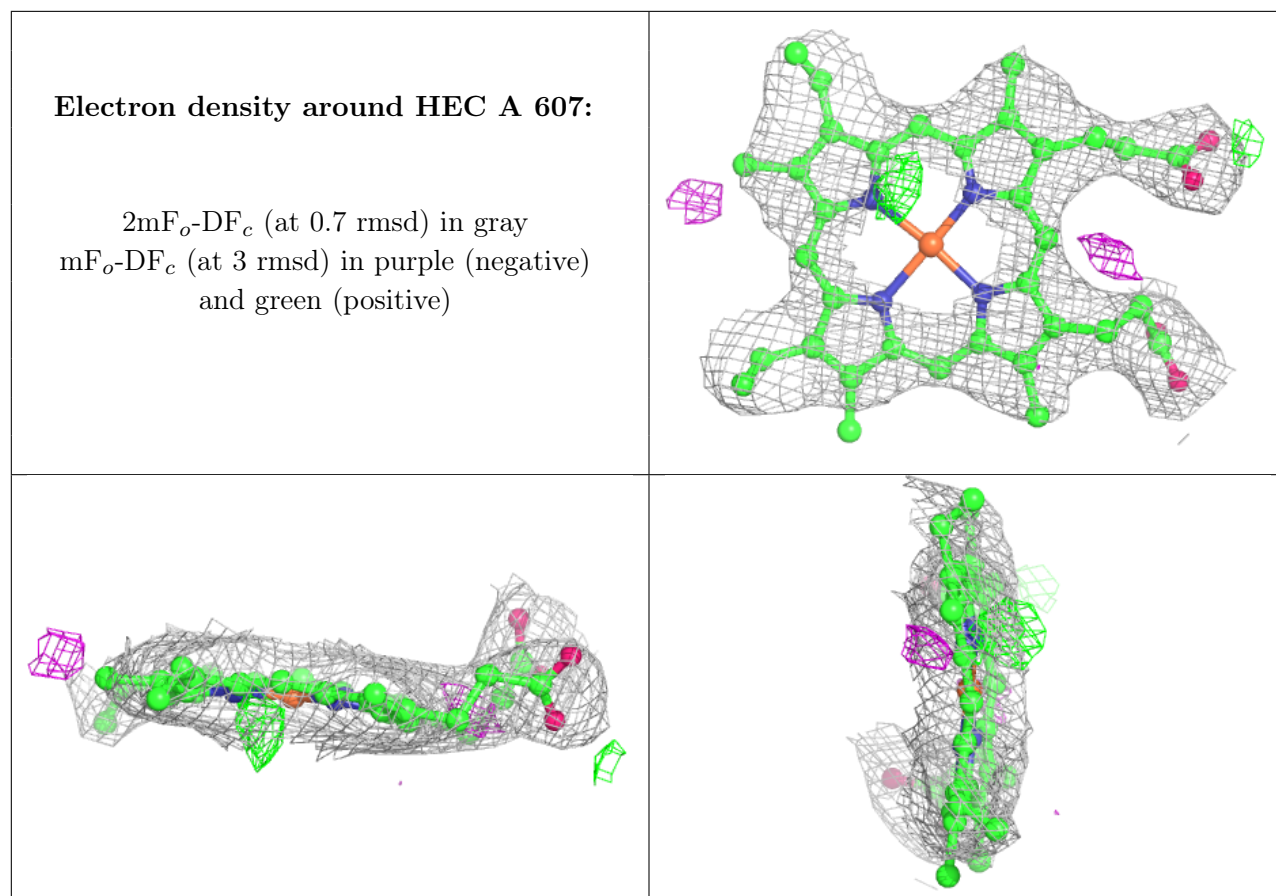


**Electron density around HEC N 601:**

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

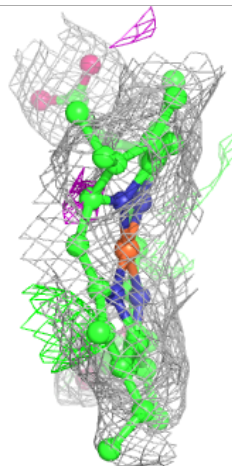
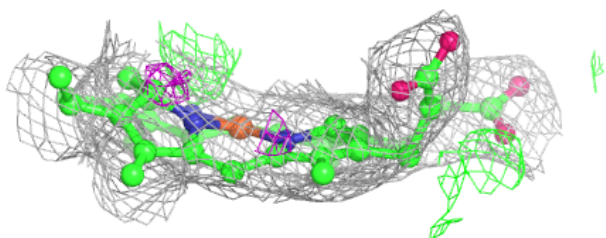
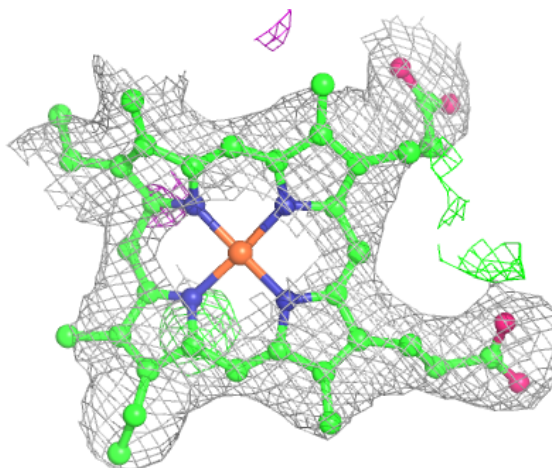






**Electron density around HEC O 603:**

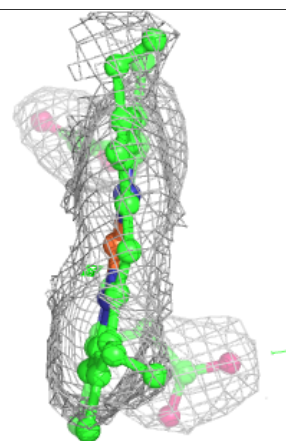
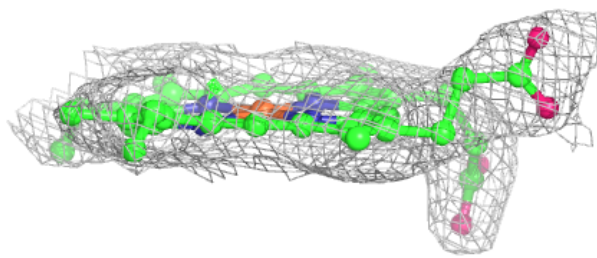
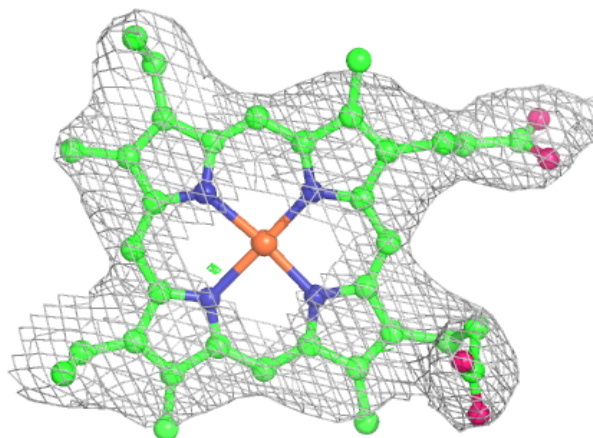
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

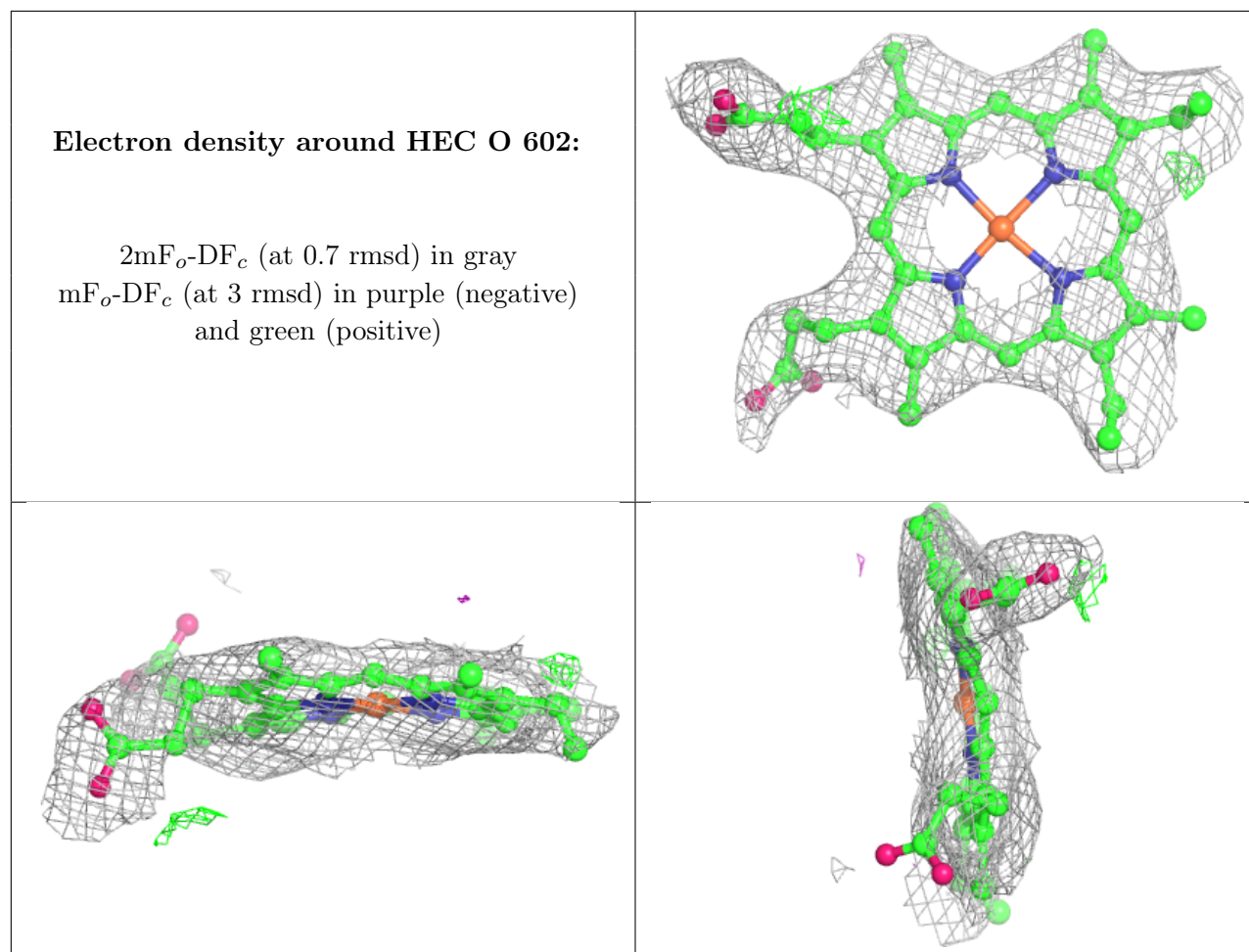




**Electron density around HEC O 601:**

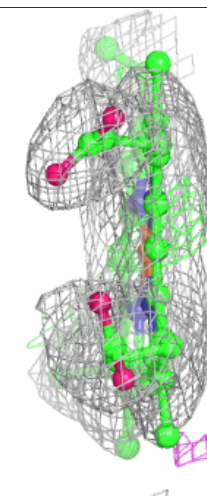
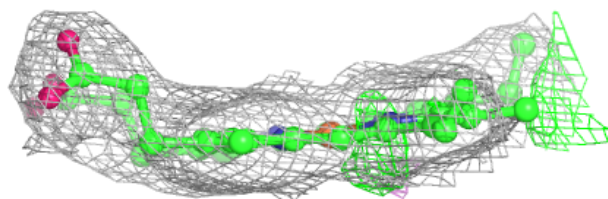
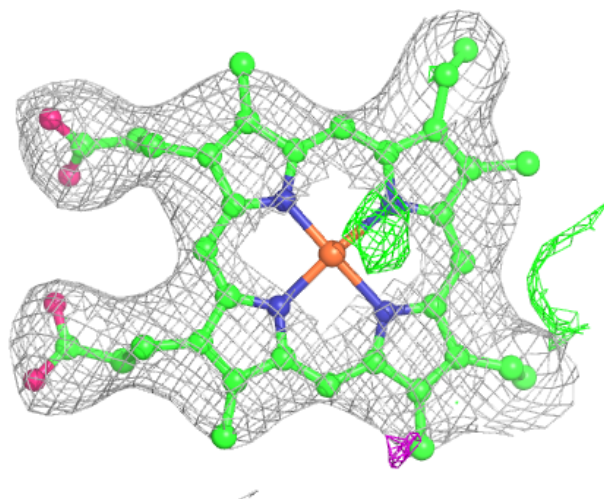
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





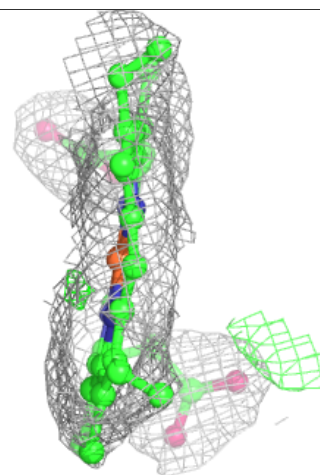
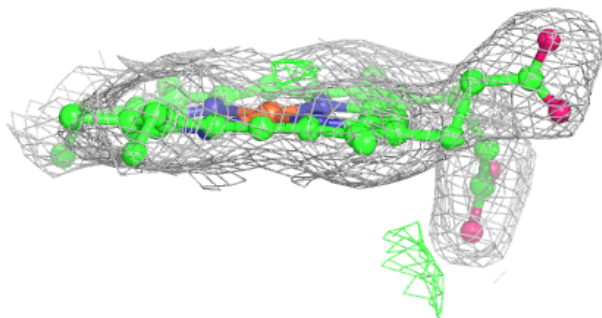
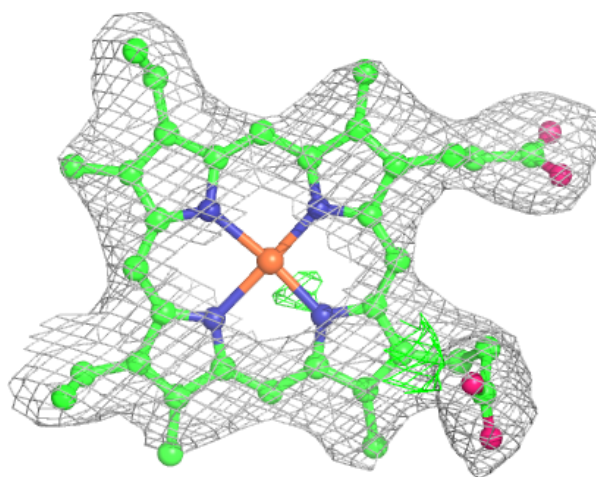
**Electron density around HEC O 604:**

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



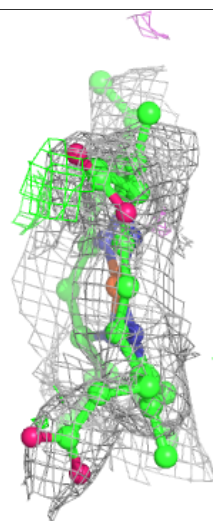
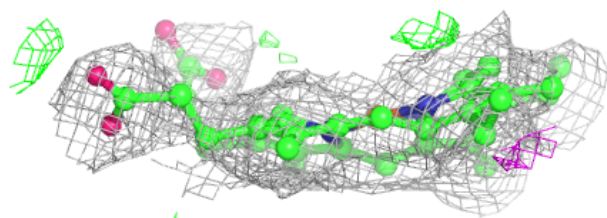
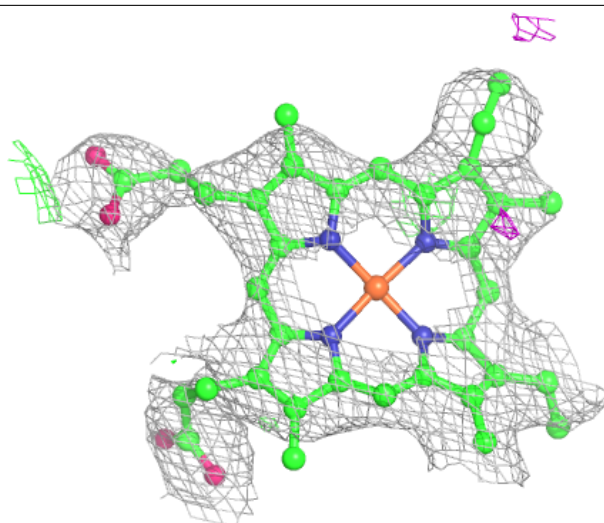
**Electron density around HEC P 601:**

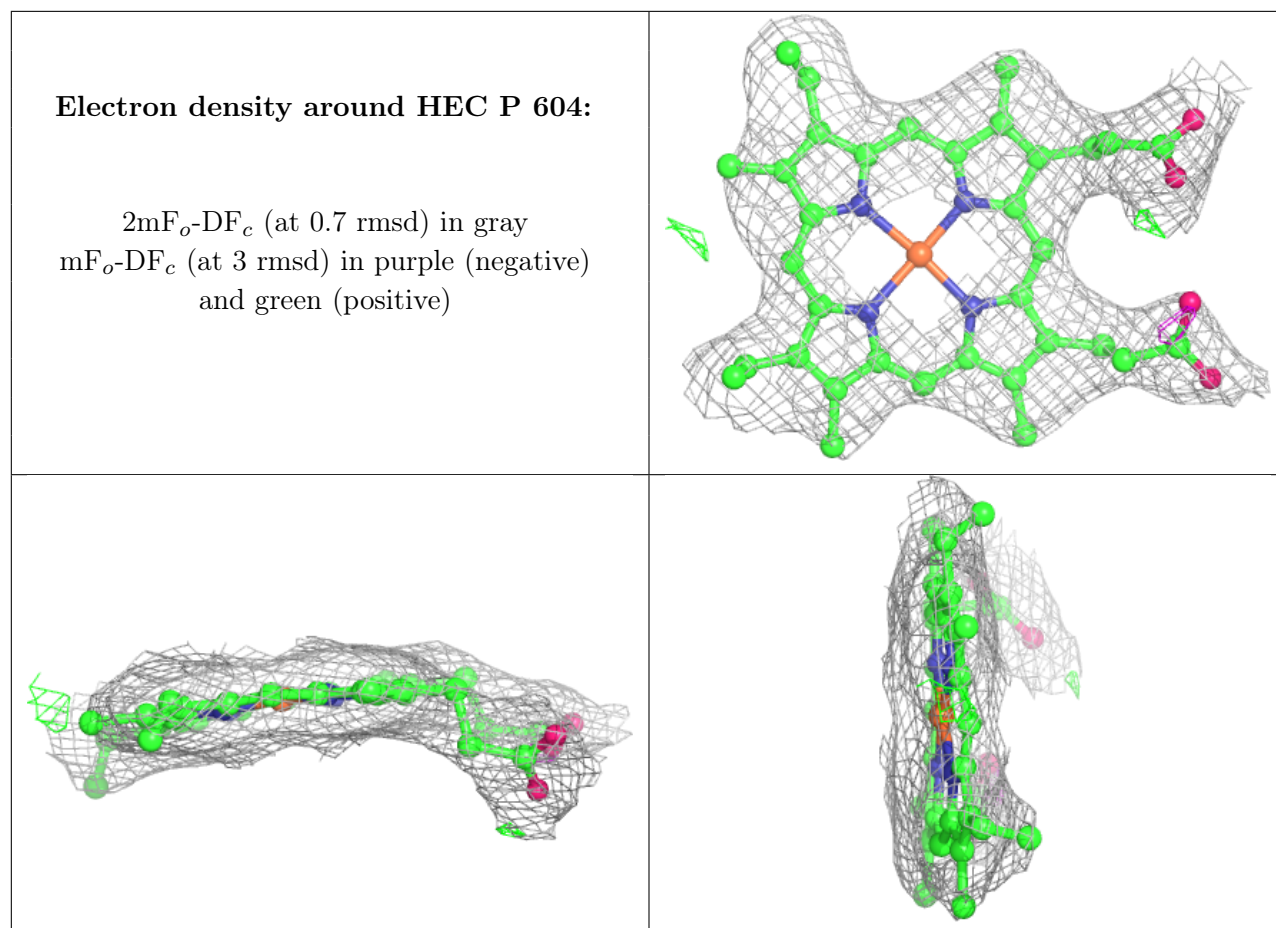
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

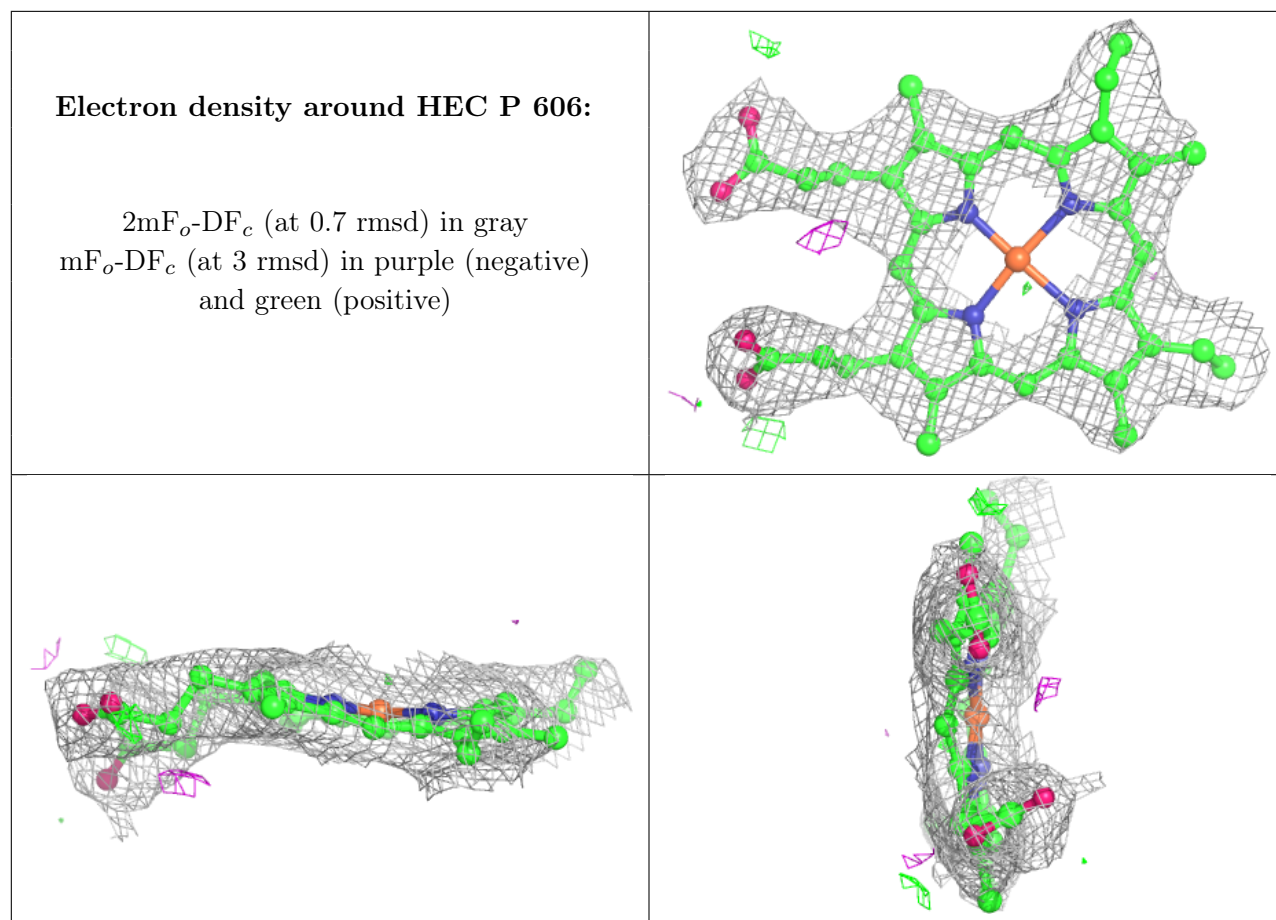


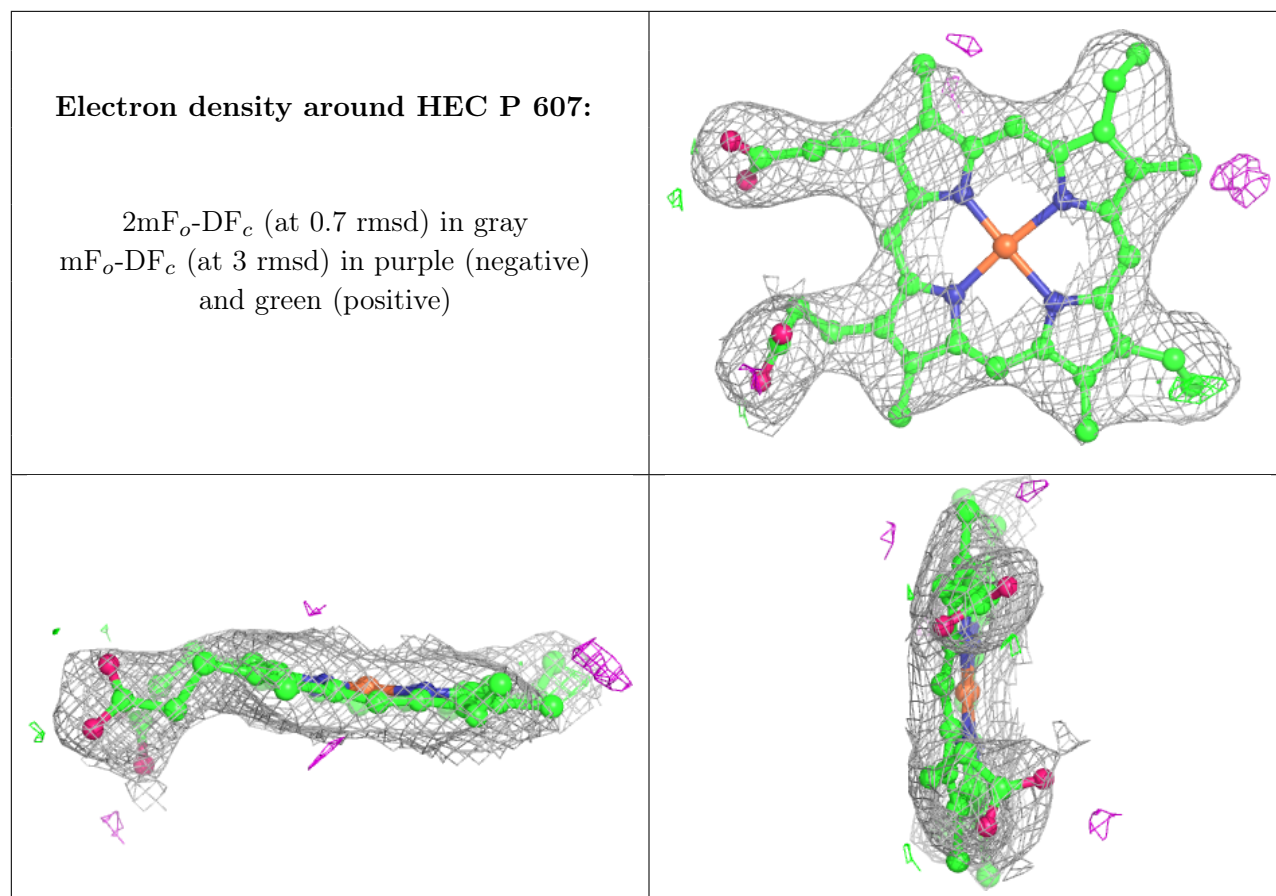
**Electron density around HEC A 603:**

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

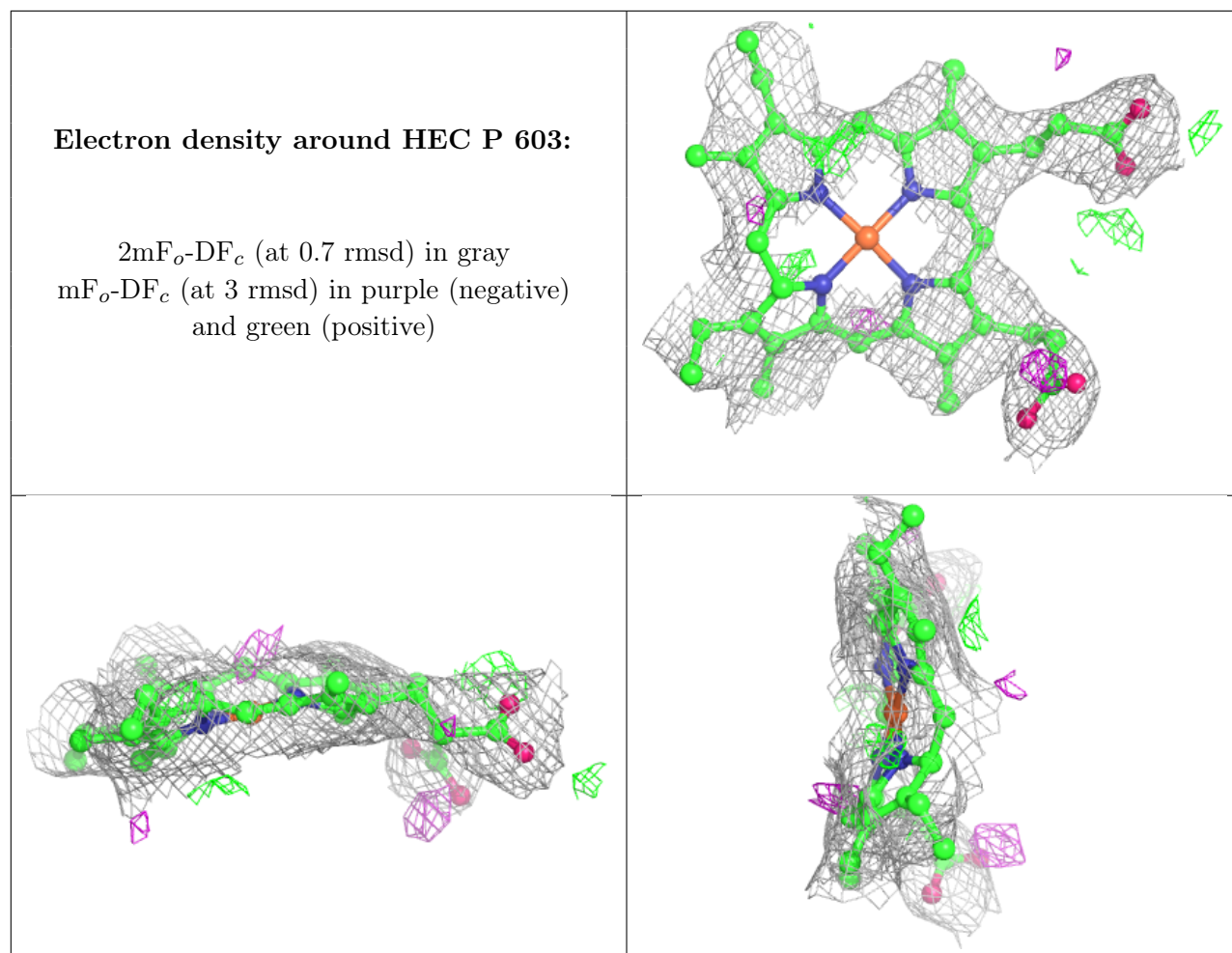


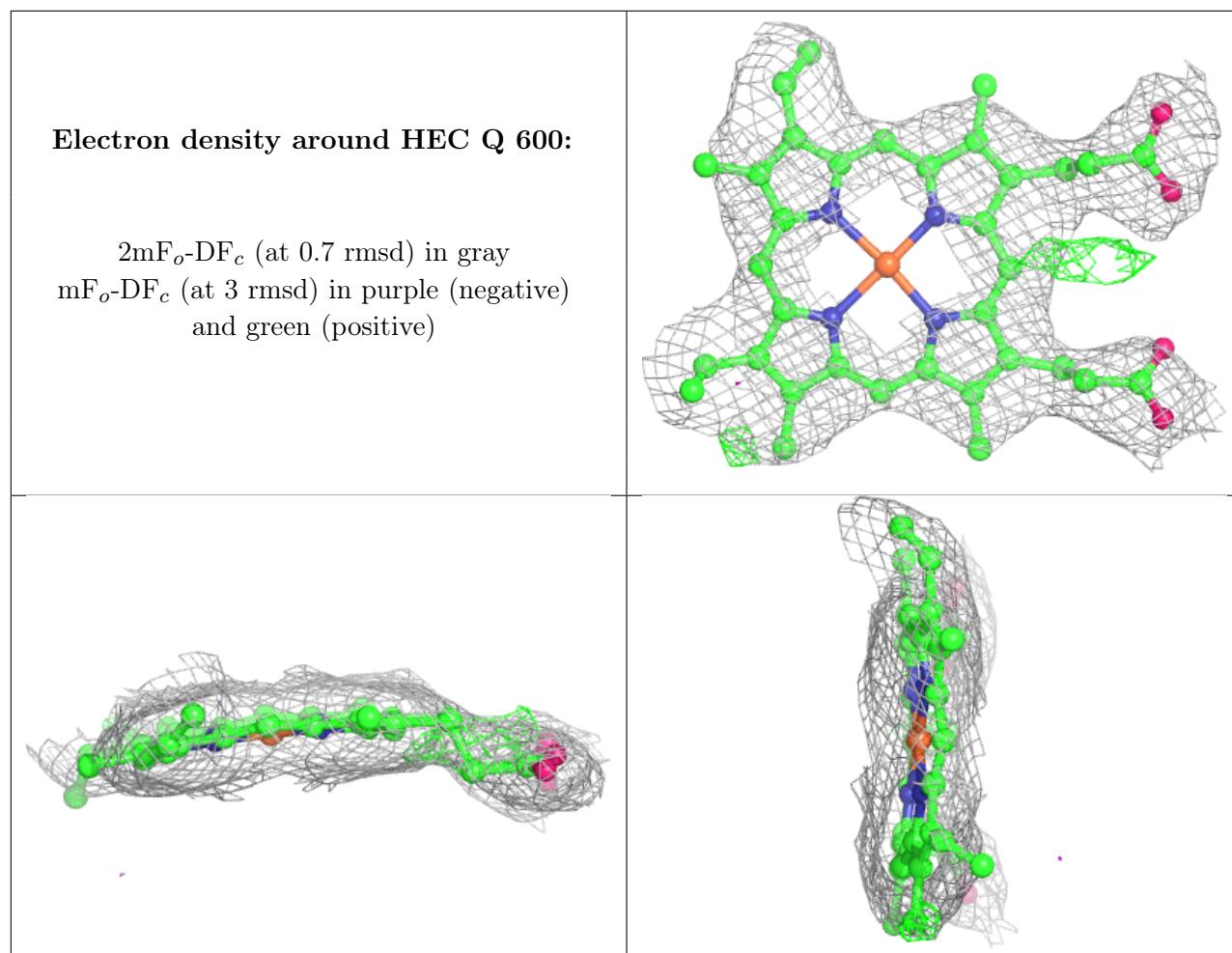






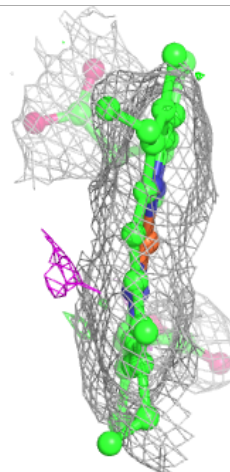
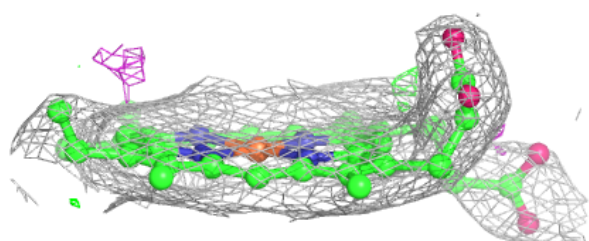
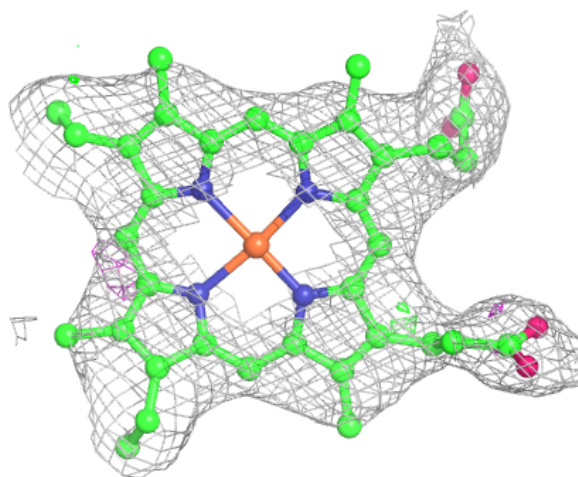






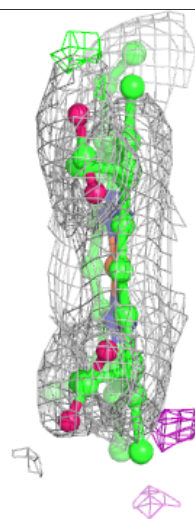
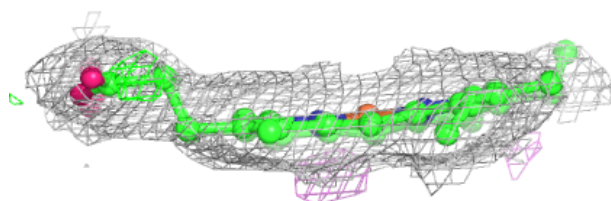
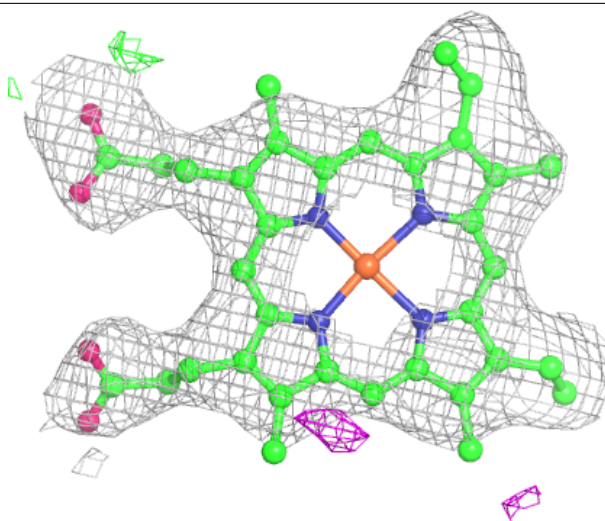
**Electron density around HEC Q 601:**

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



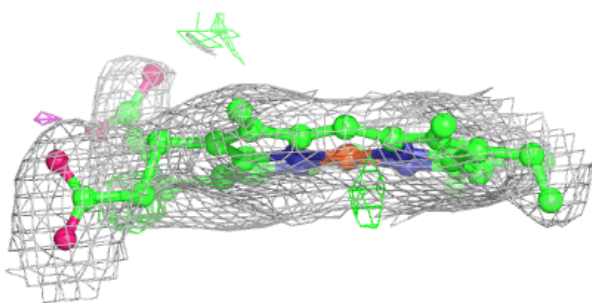
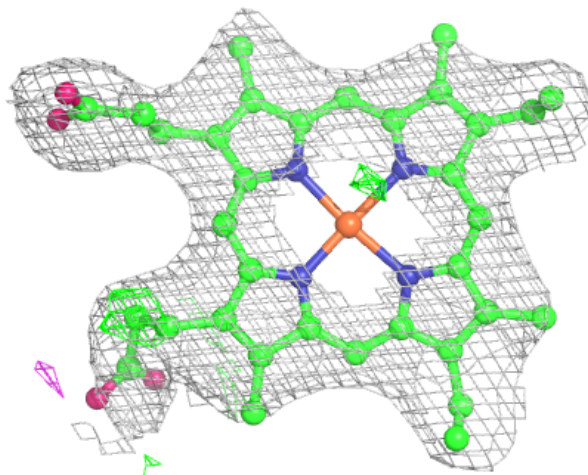
**Electron density around HEC B 600:**

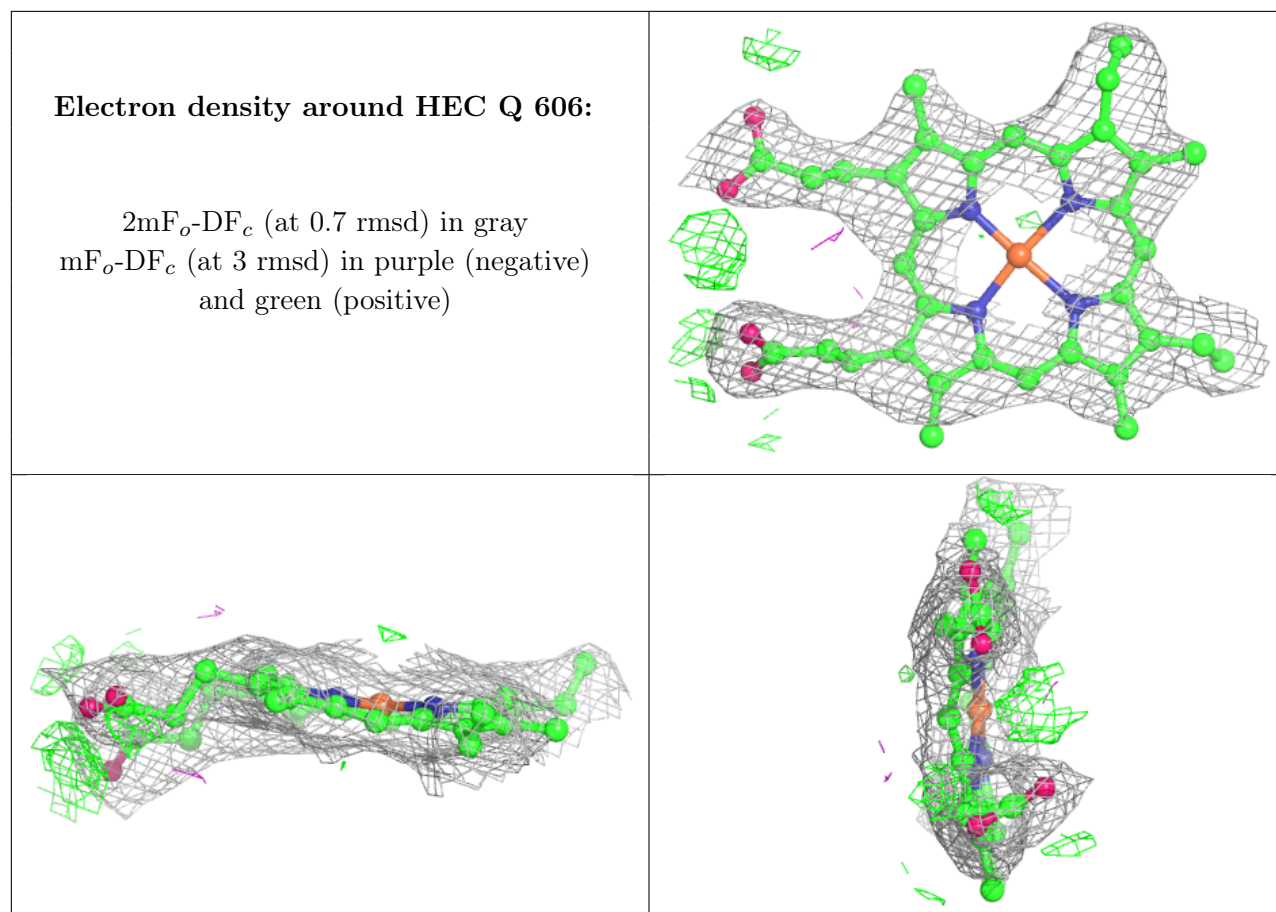
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC G 602:**

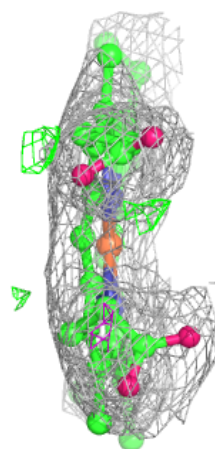
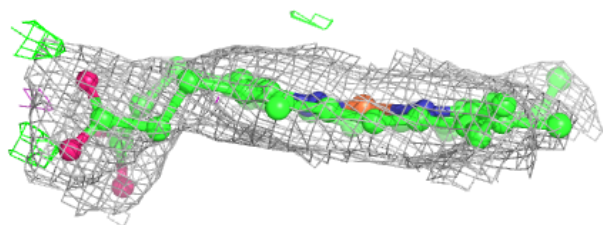
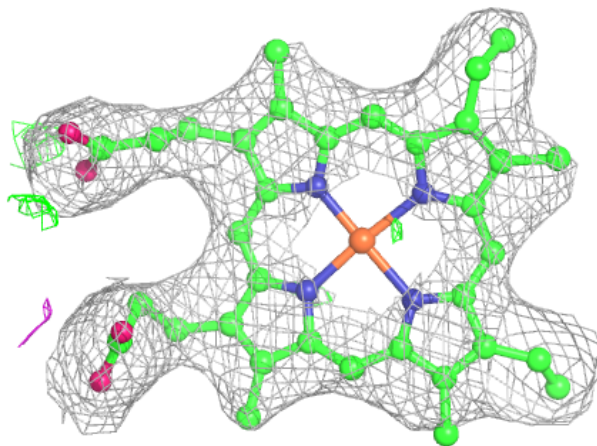
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





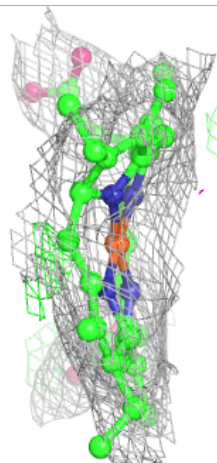
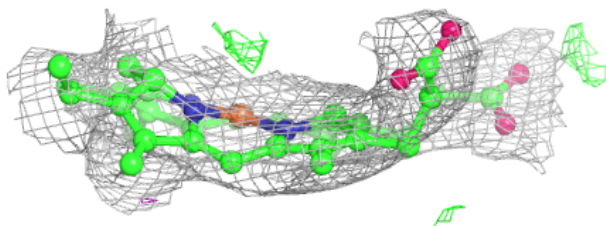
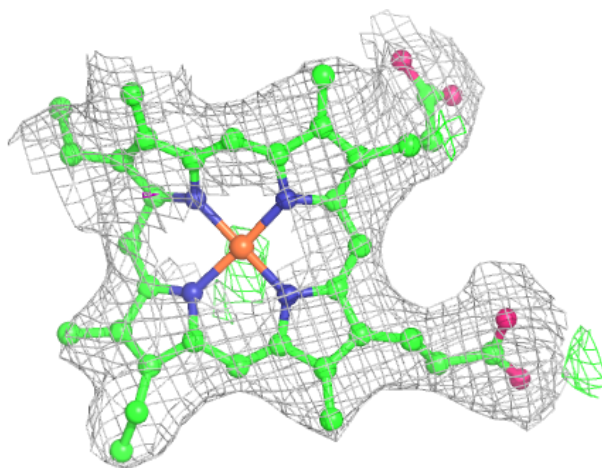
**Electron density around HEC Q 607:**

$2mF_o-DF_c$  (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:**

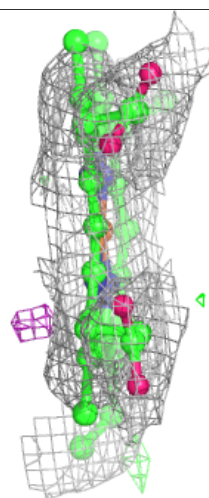
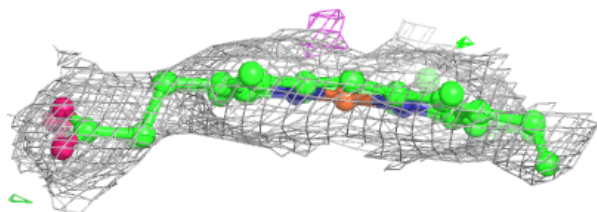
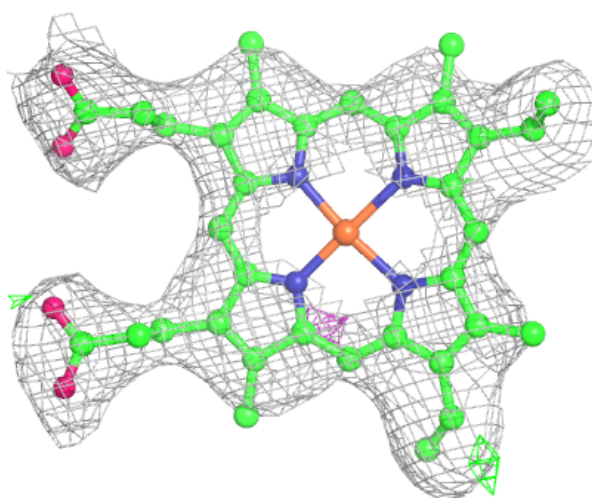
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





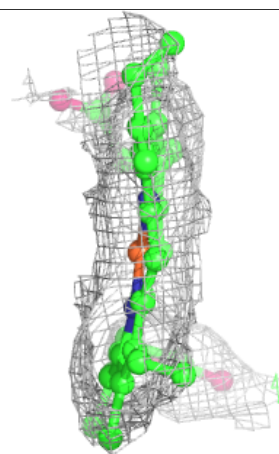
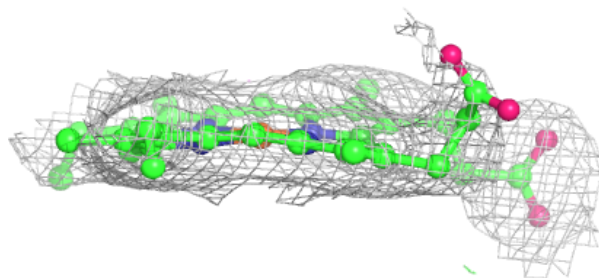
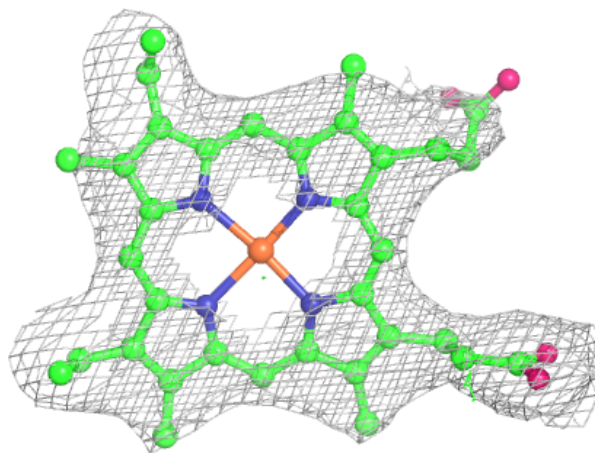
**Electron density around HEC R 600:**

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



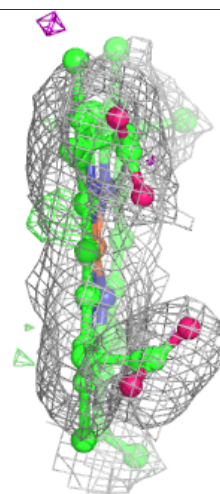
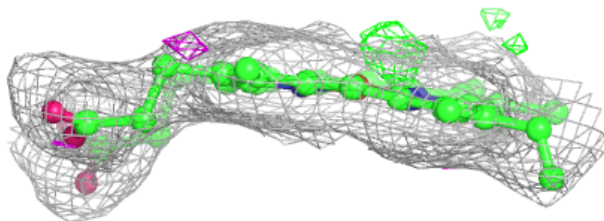
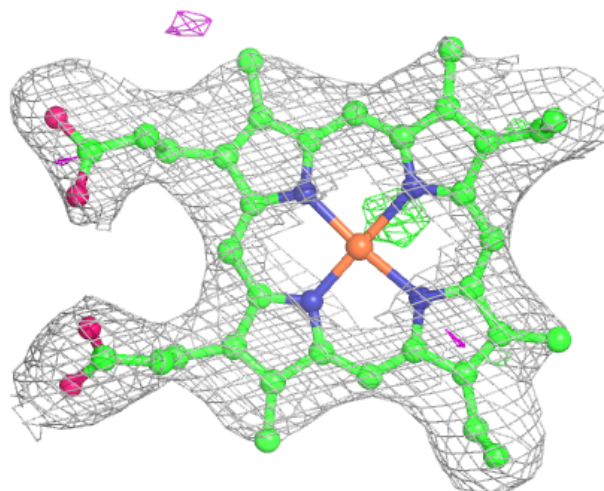
**Electron density around HEC R 602:**

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



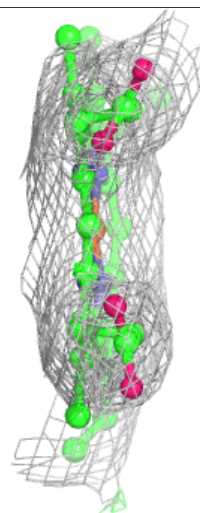
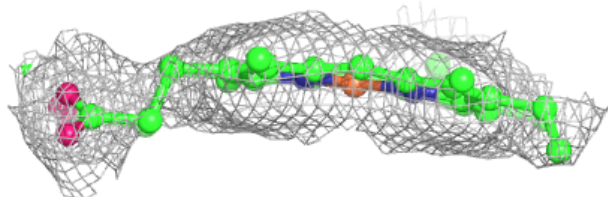
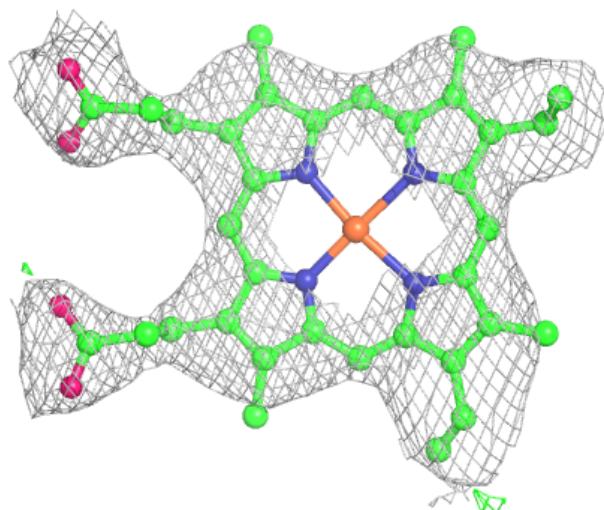
**Electron density around HEC R 604:**

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



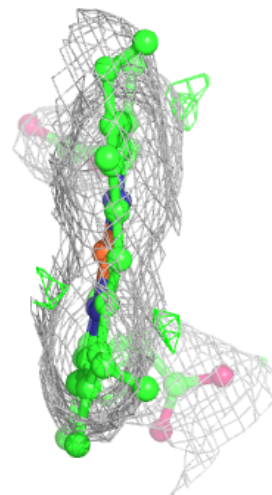
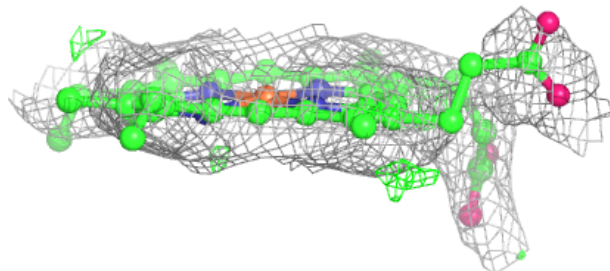
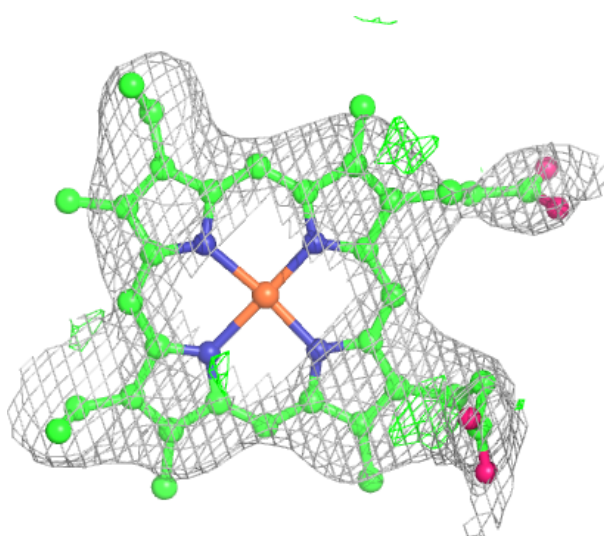
**Electron density around HEC S 600:**

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



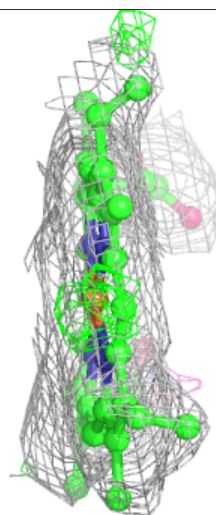
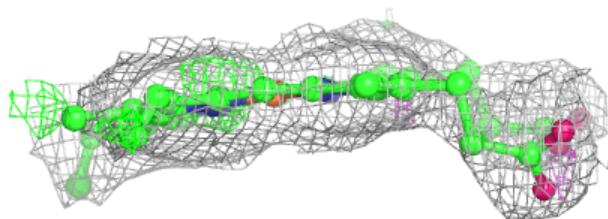
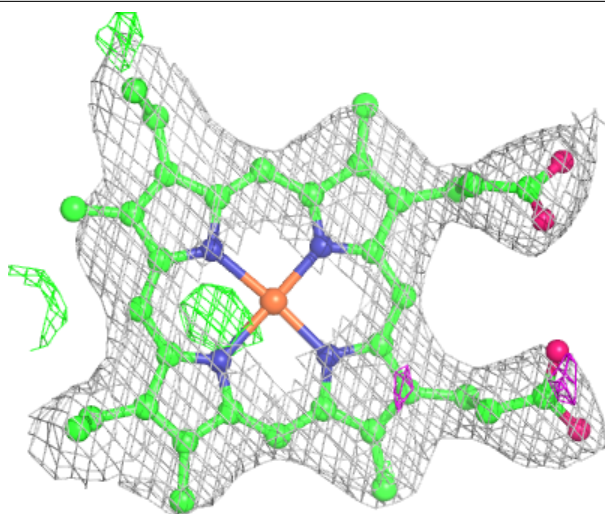
**Electron density around HEC S 601:**

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



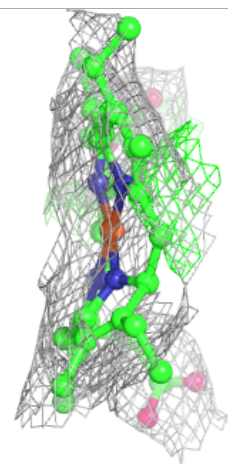
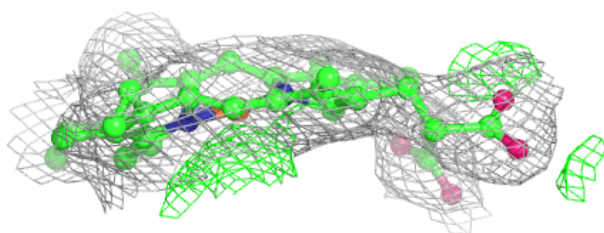
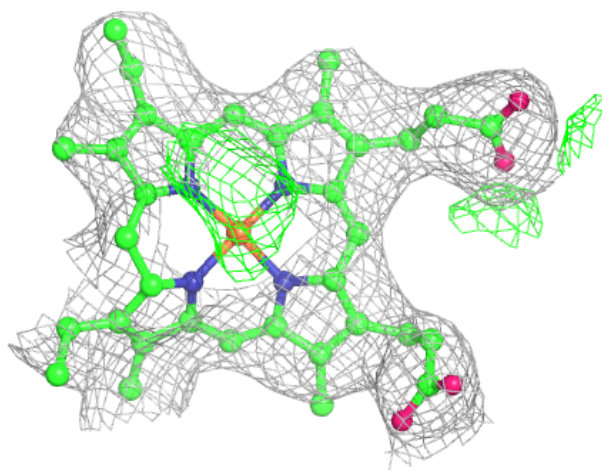
**Electron density around HEC B 604:**

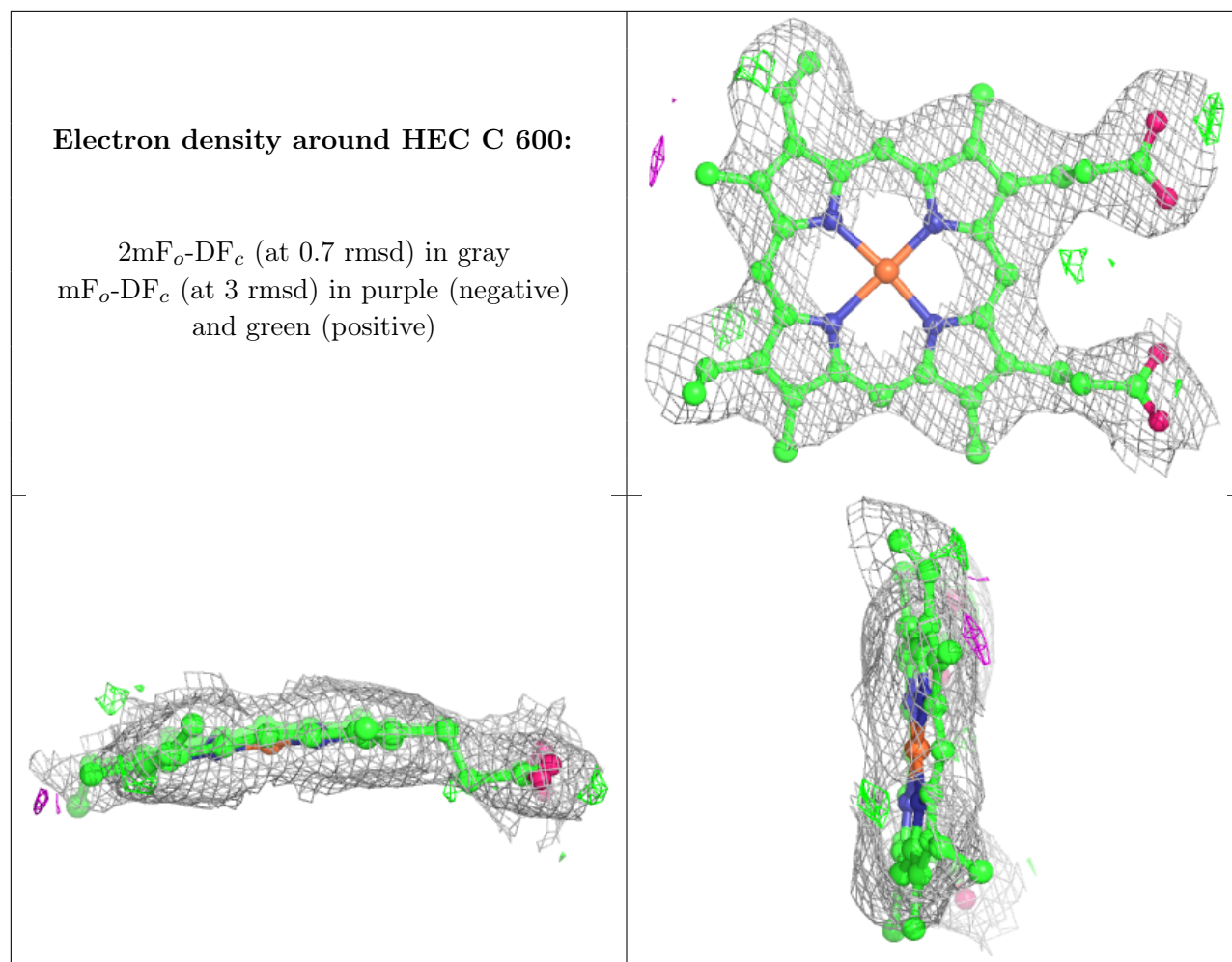
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC 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)

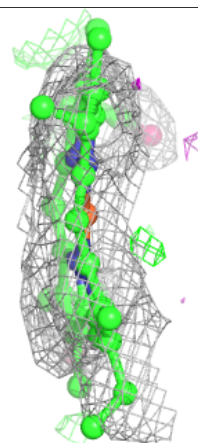
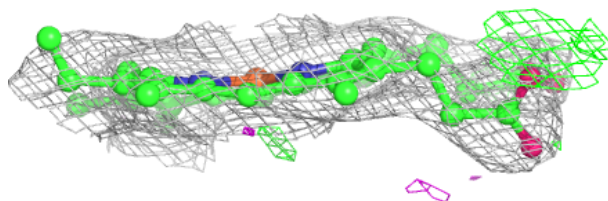
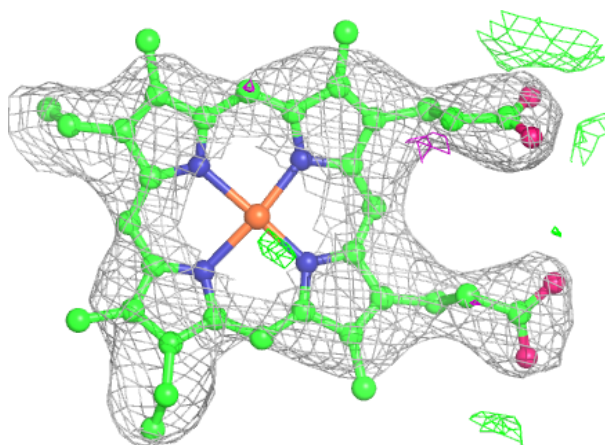






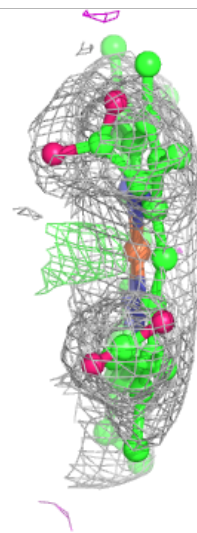
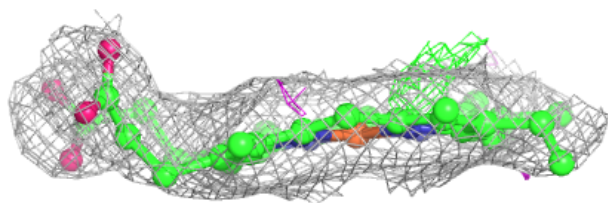
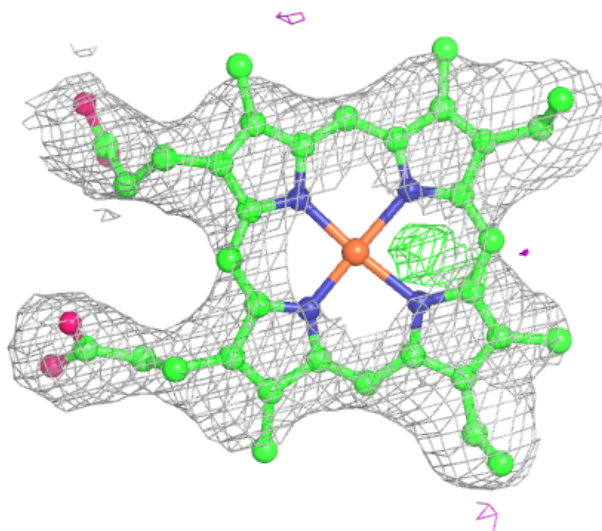
**Electron density around HEC S 606:**

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



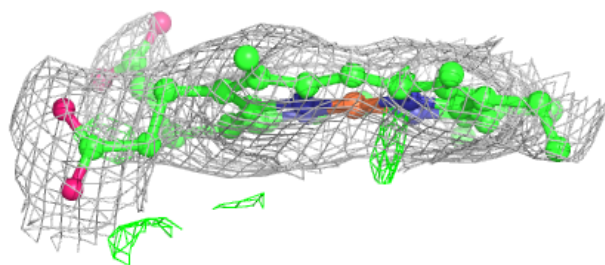
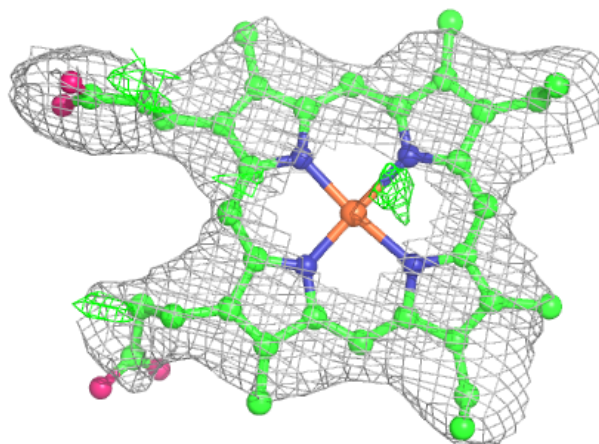
**Electron density around HEC S 607:**

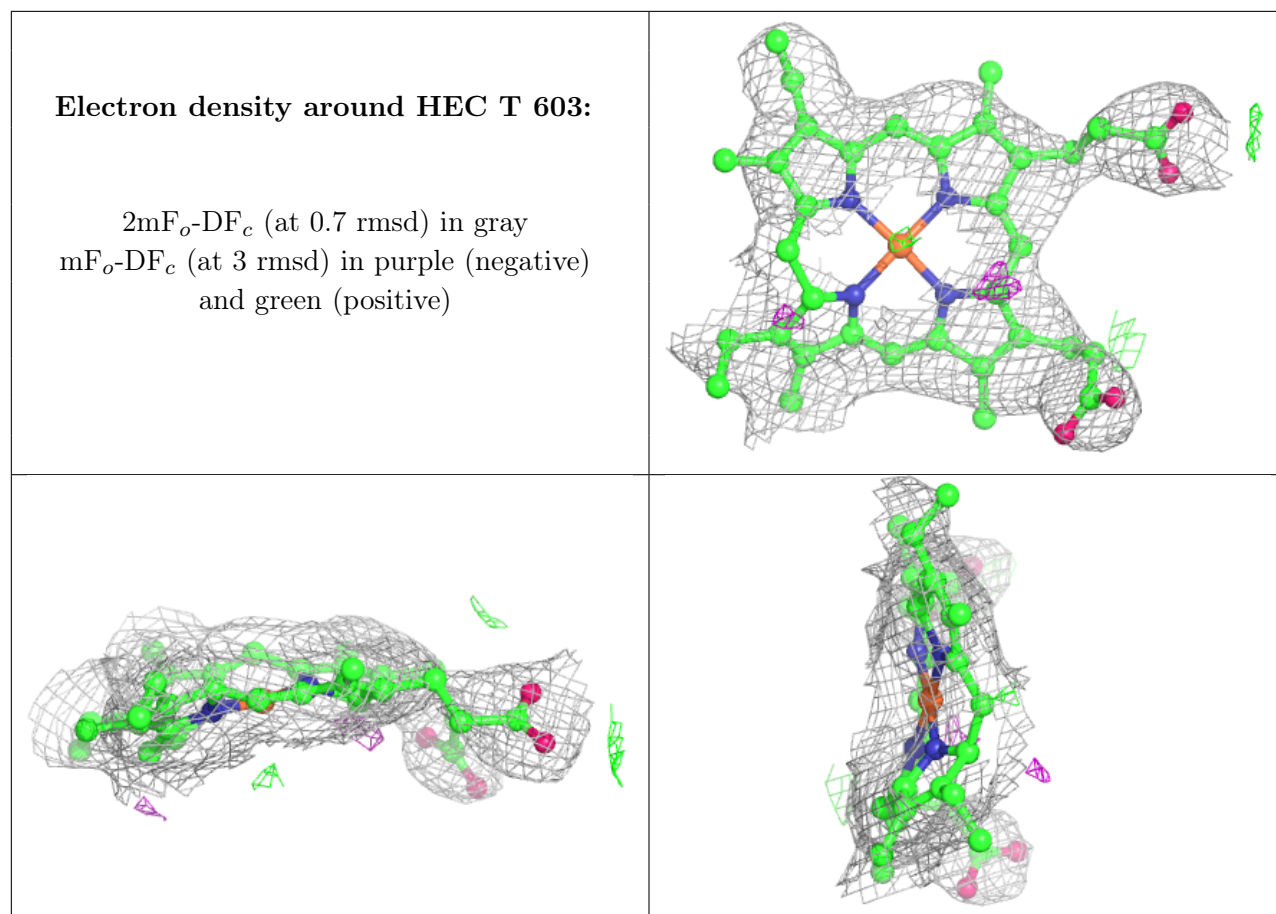
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

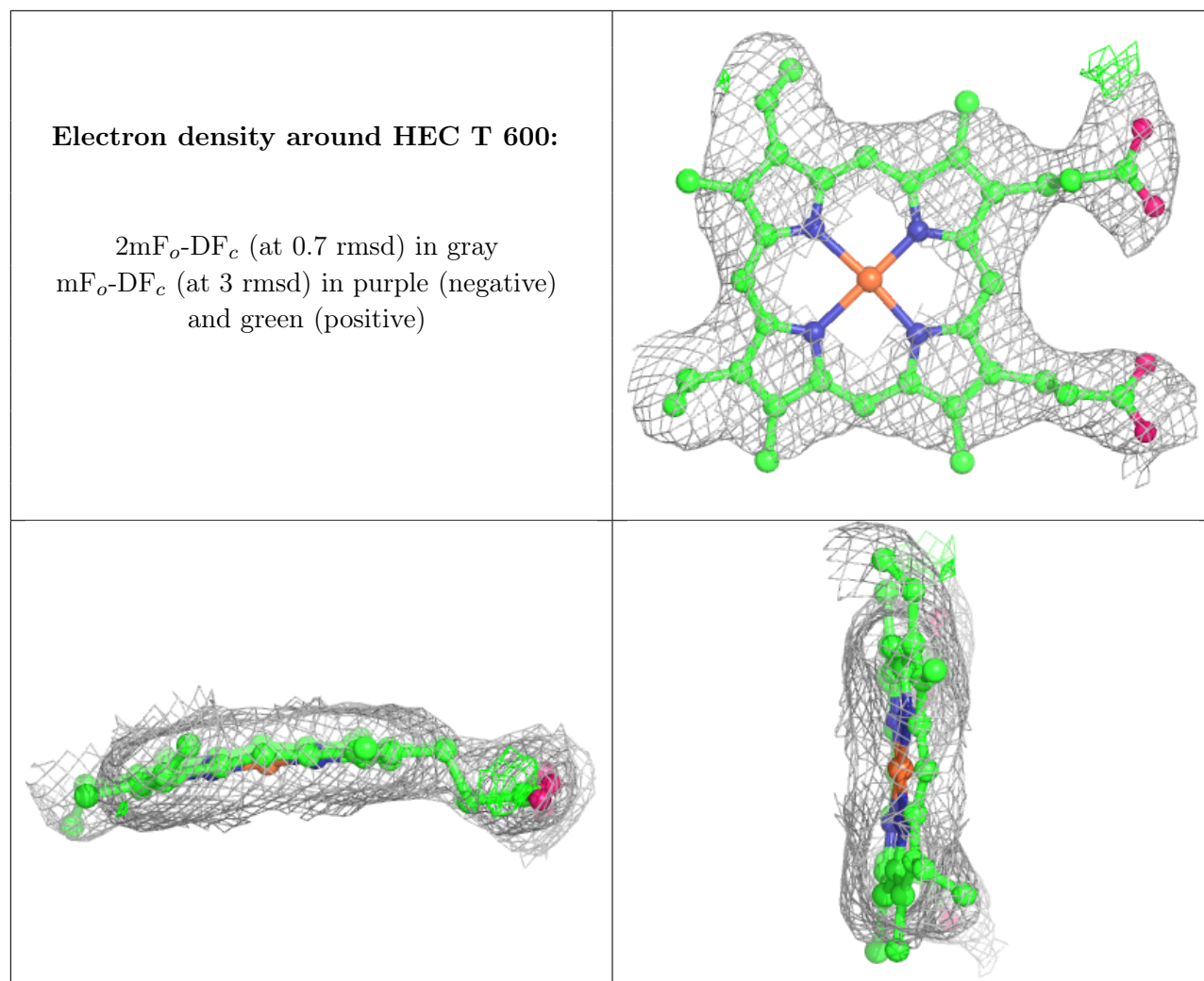


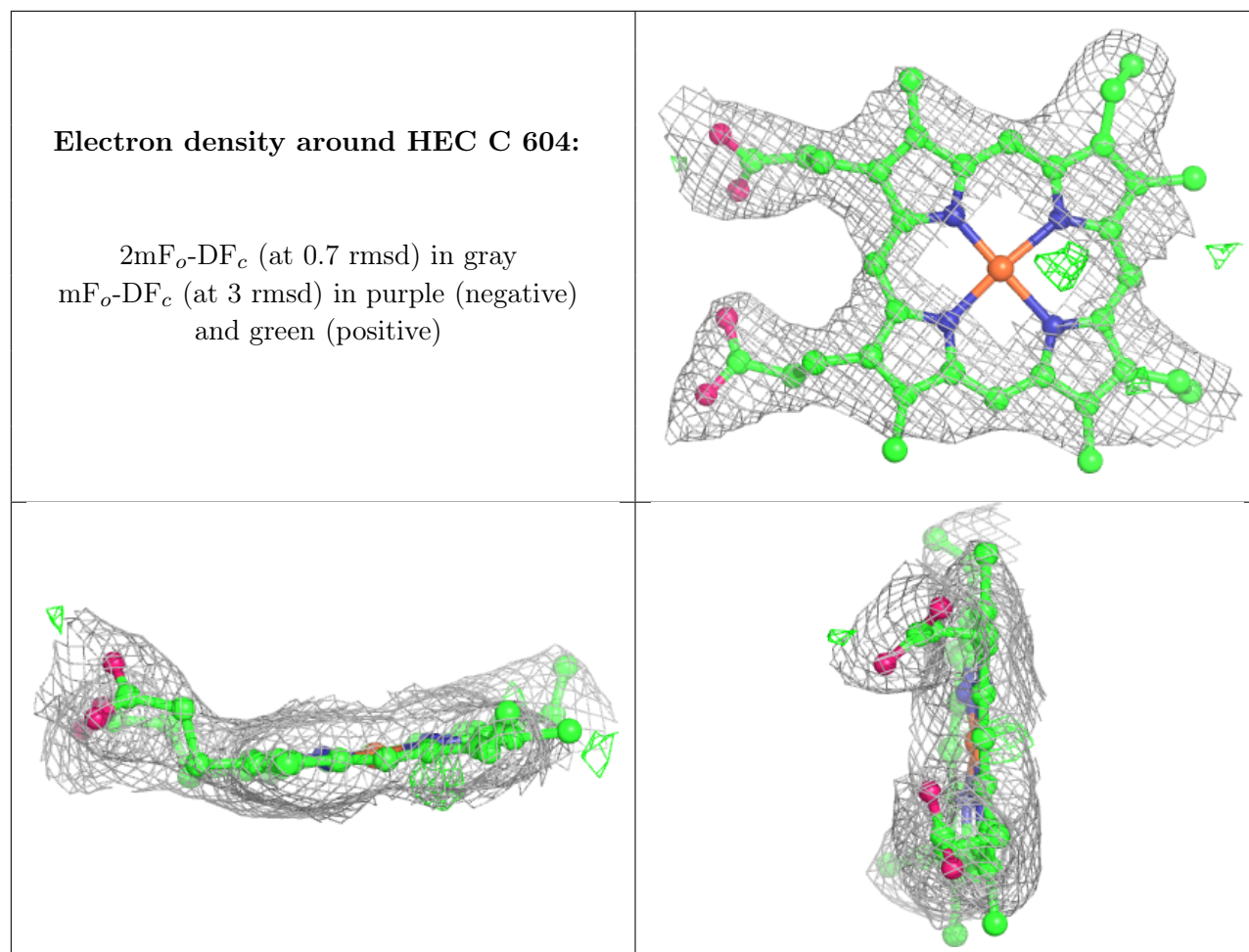
**Electron density around HEC C 602:**

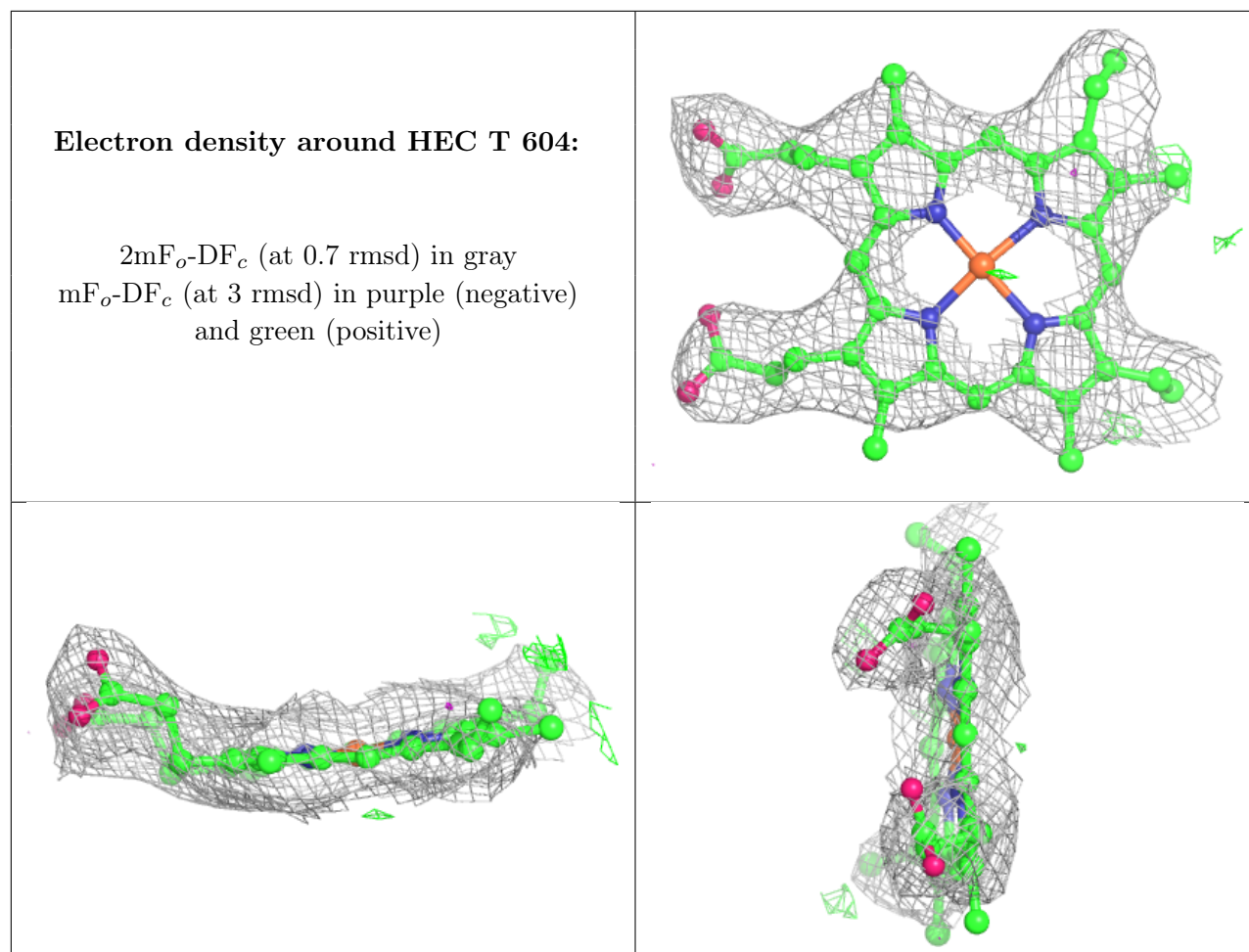
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

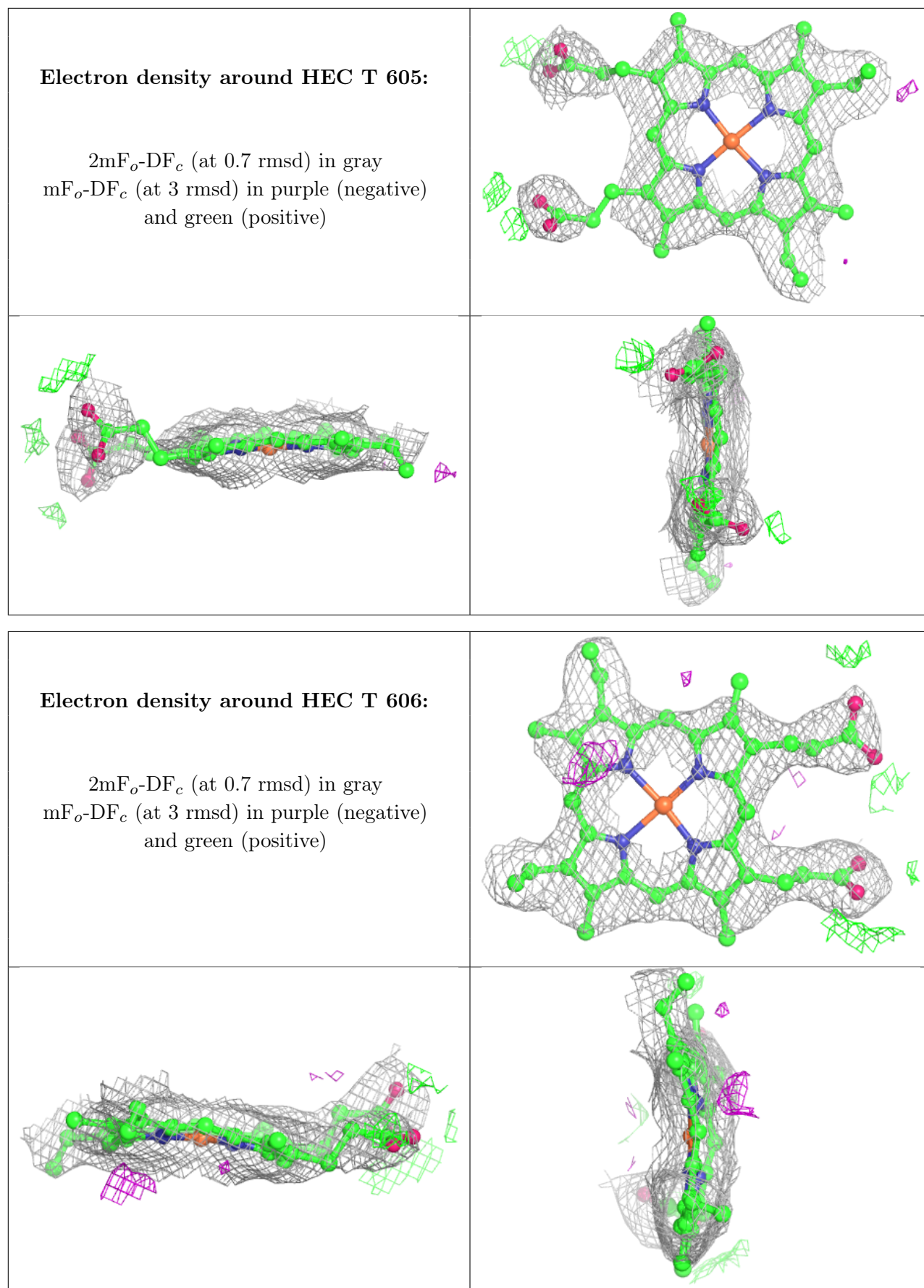




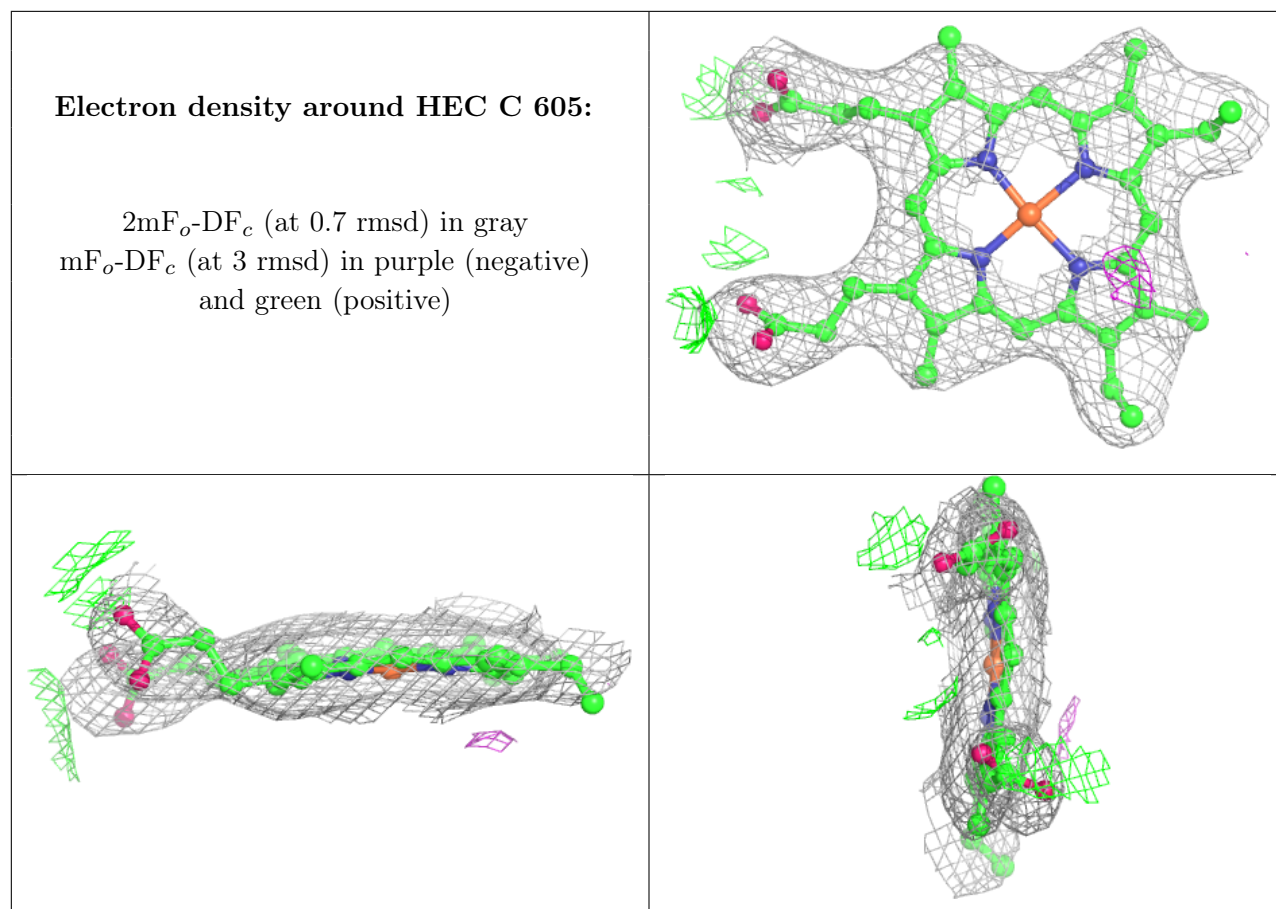






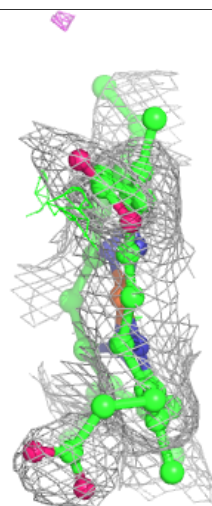
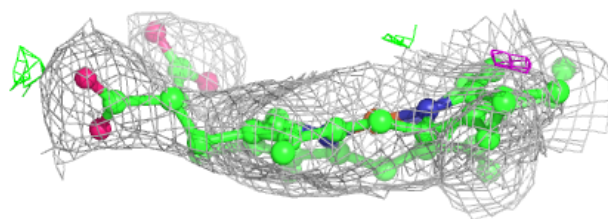
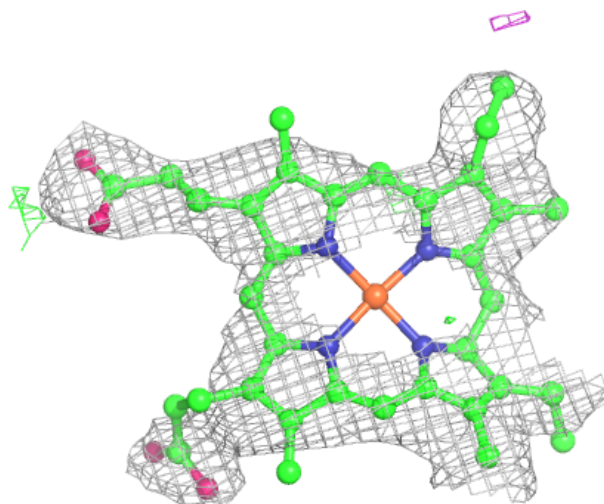


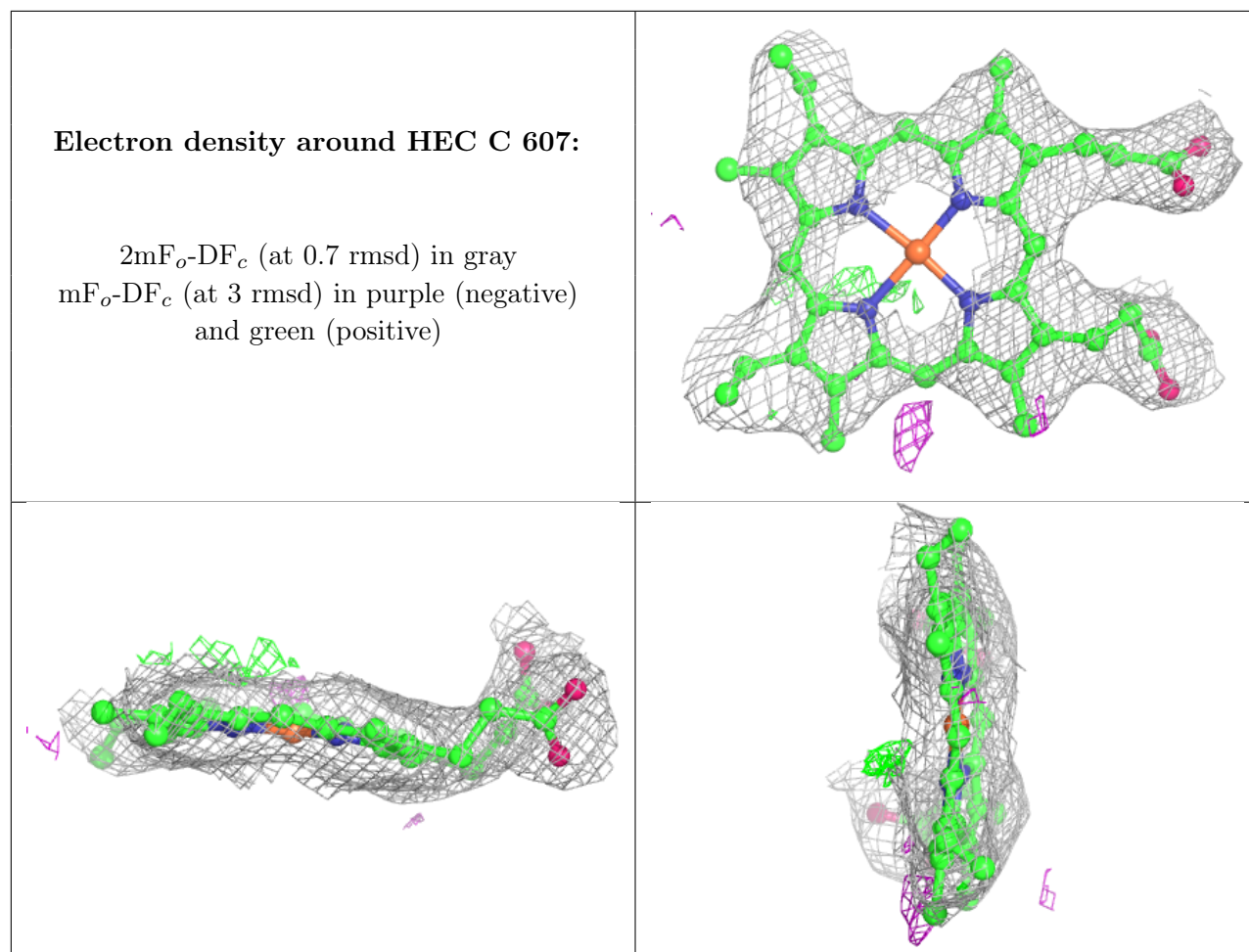




**Electron density around HEC U 603:**

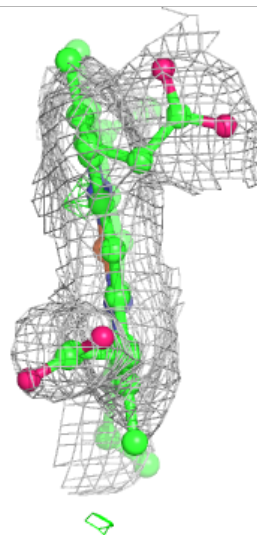
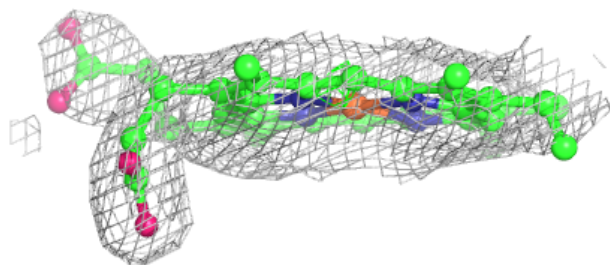
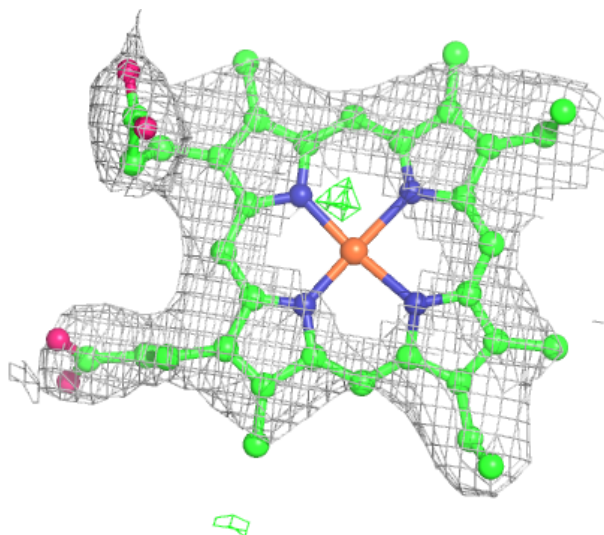
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





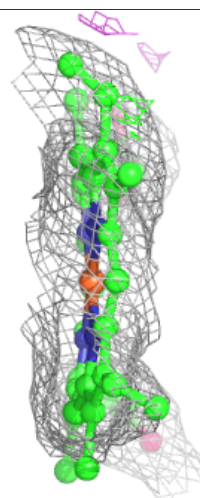
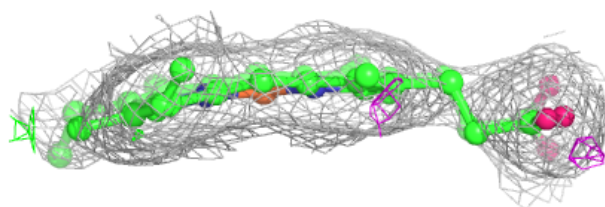
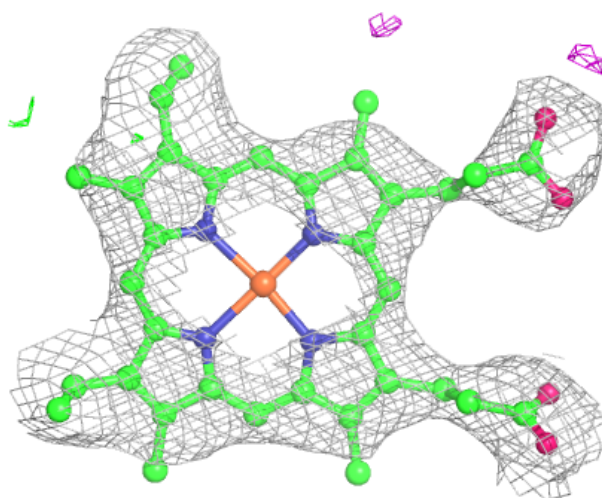
**Electron density around HEC U 601:**

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



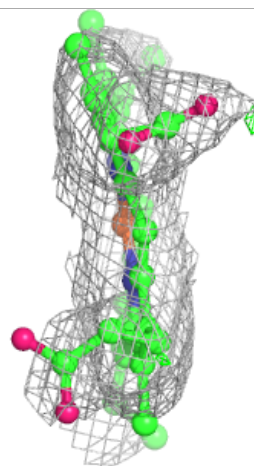
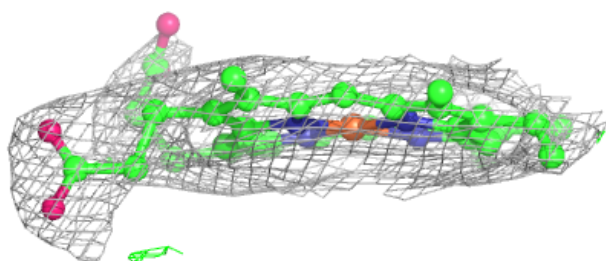
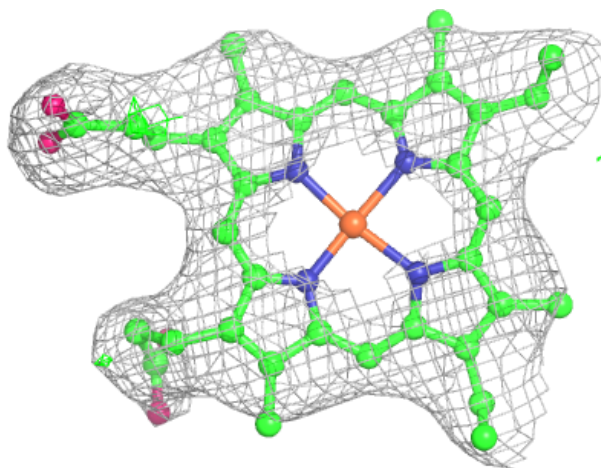
**Electron density around HEC D 600:**

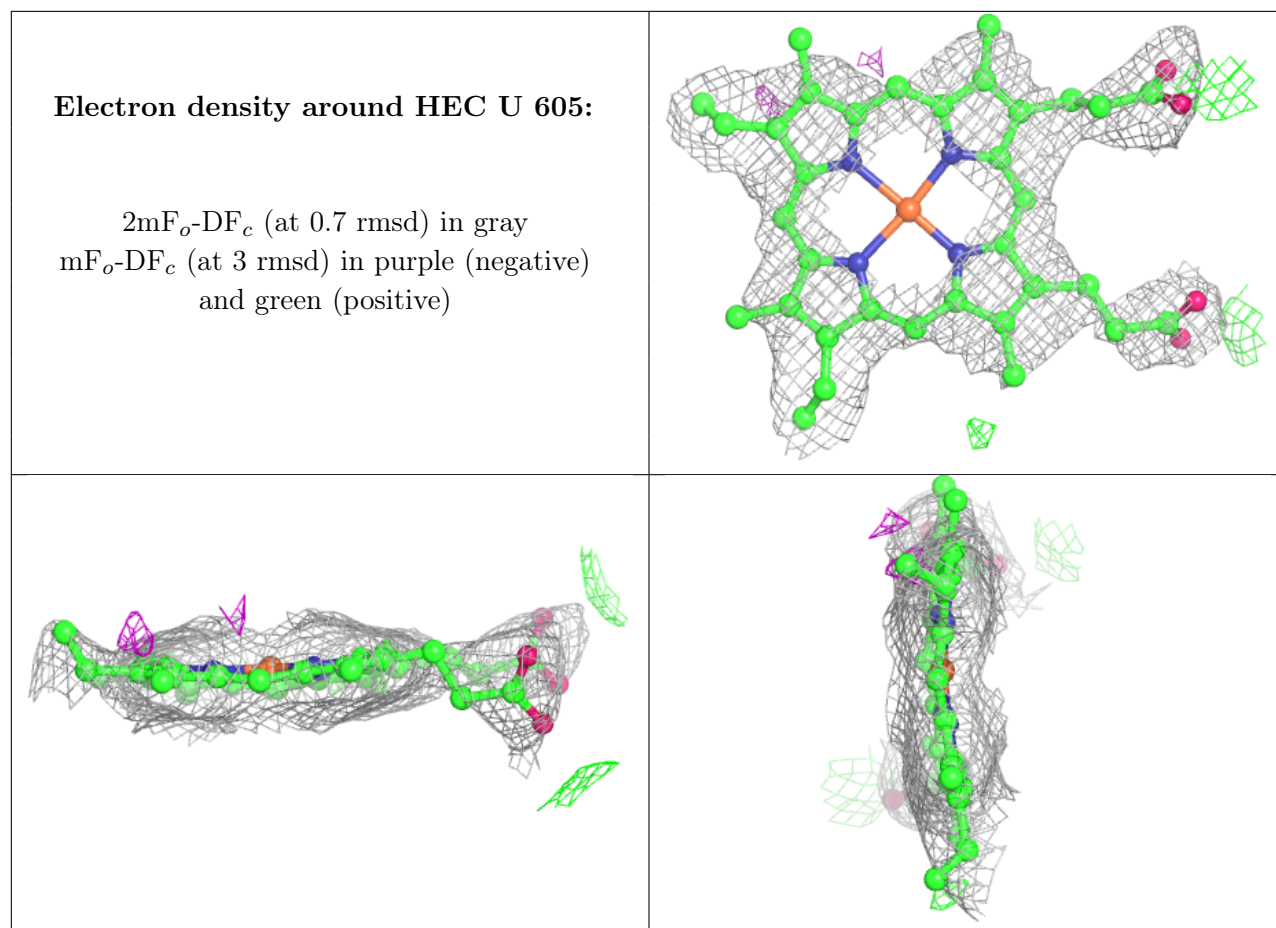
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC D 602:**

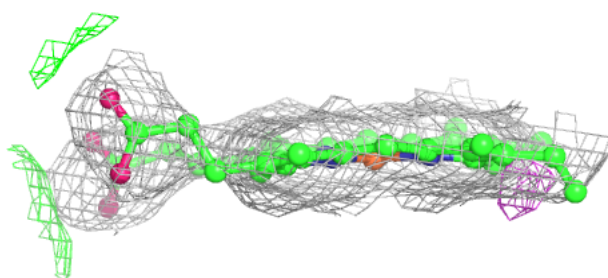
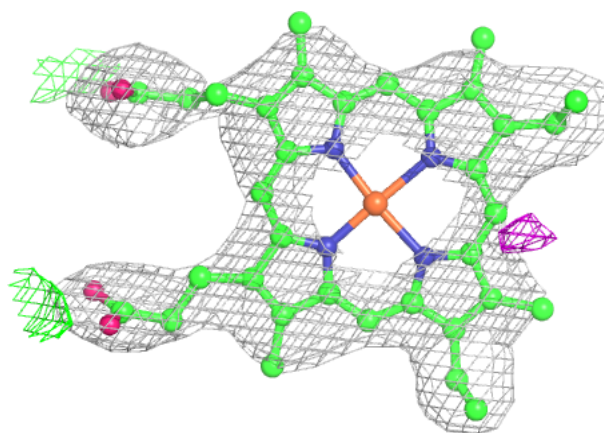
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC D 605:**

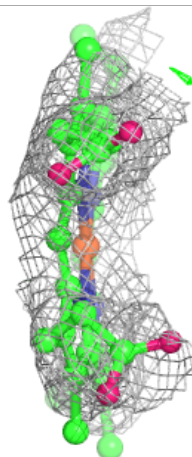
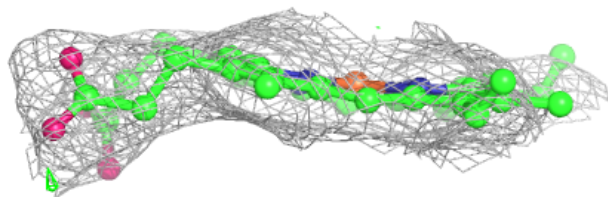
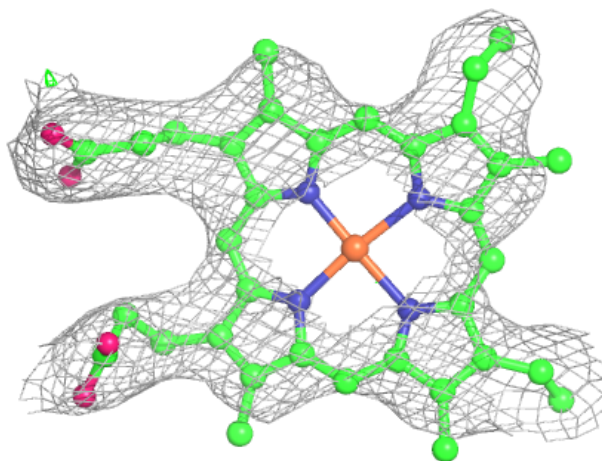
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





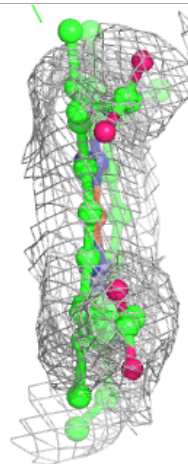
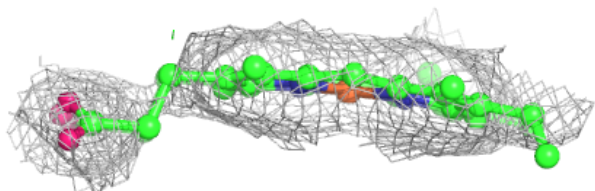
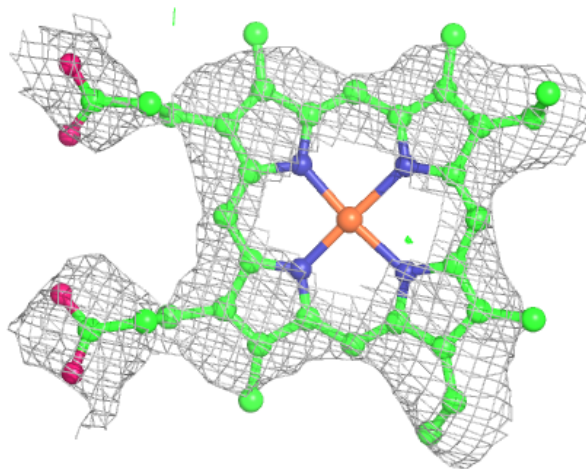
**Electron density around HEC U 607:**

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



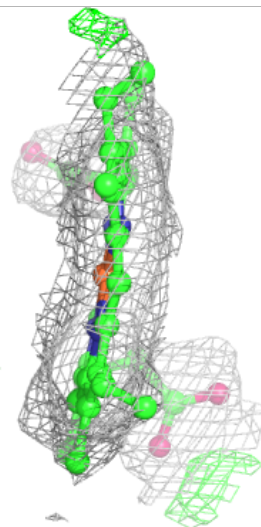
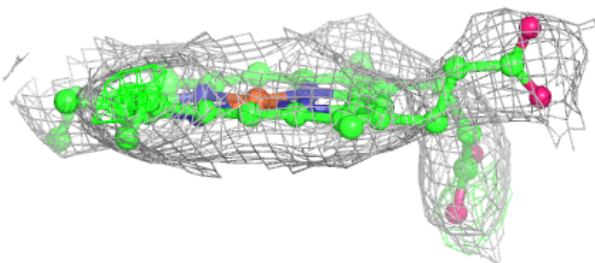
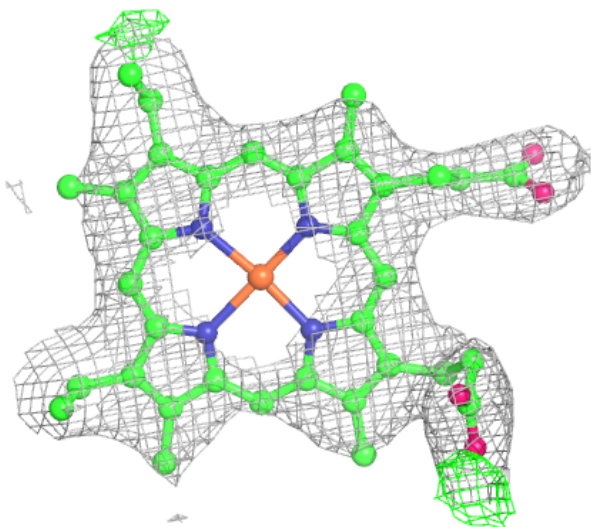
**Electron density around HEC V 600:**

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



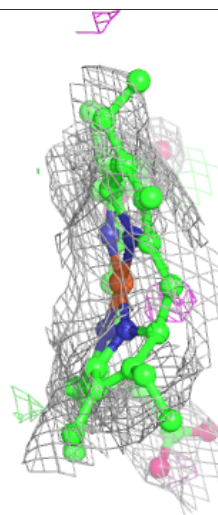
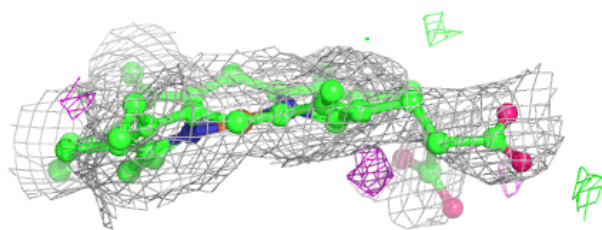
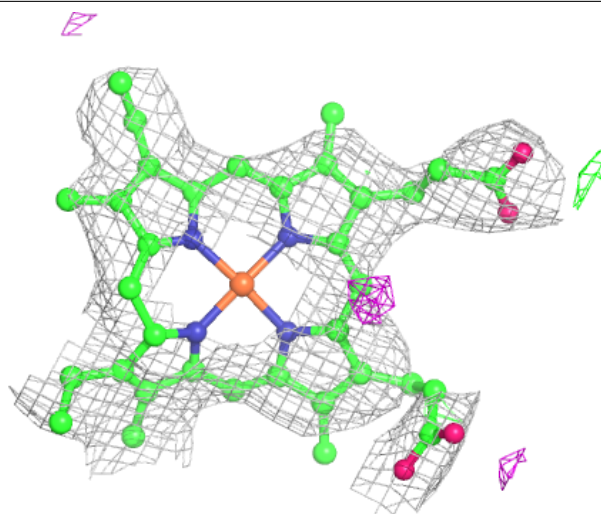
**Electron density around HEC V 601:**

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



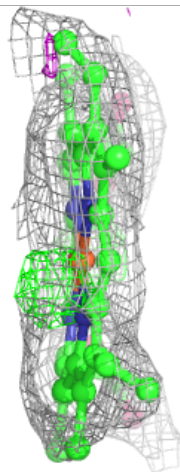
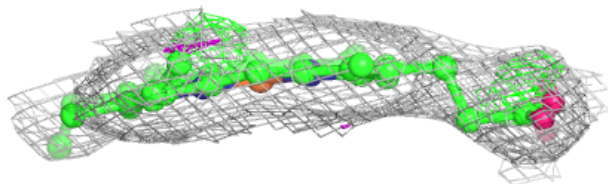
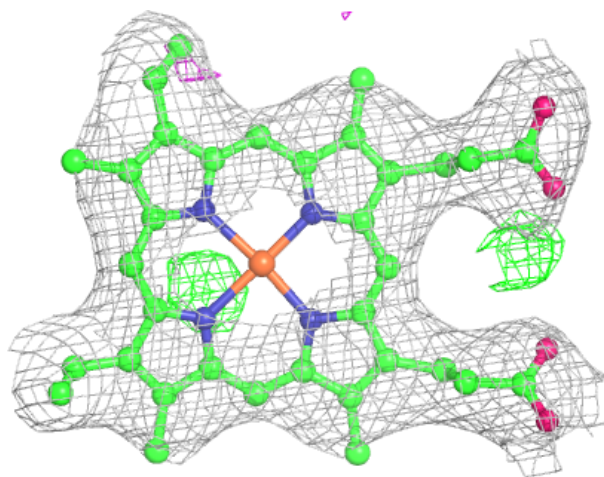
**Electron density around HEC E 603:**

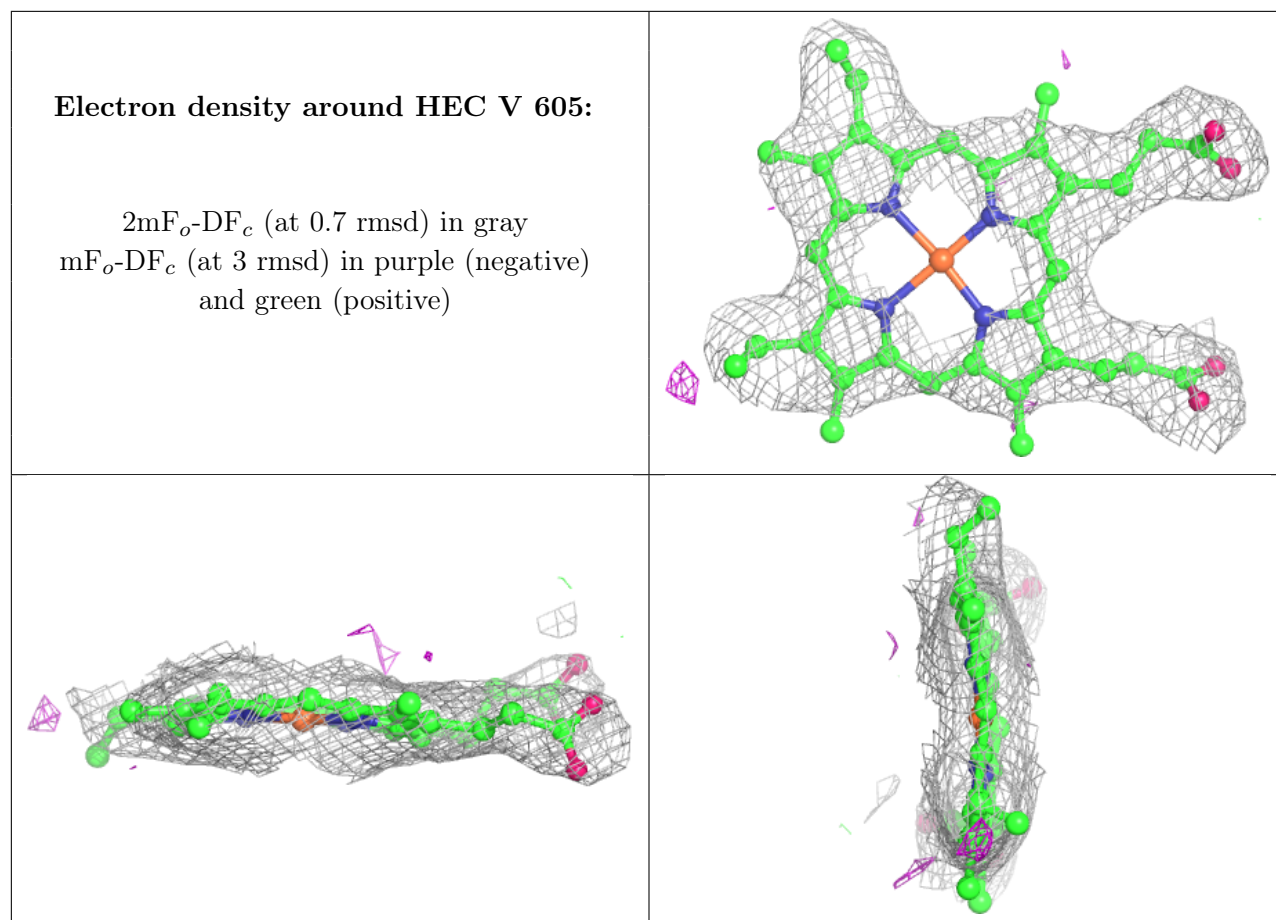
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

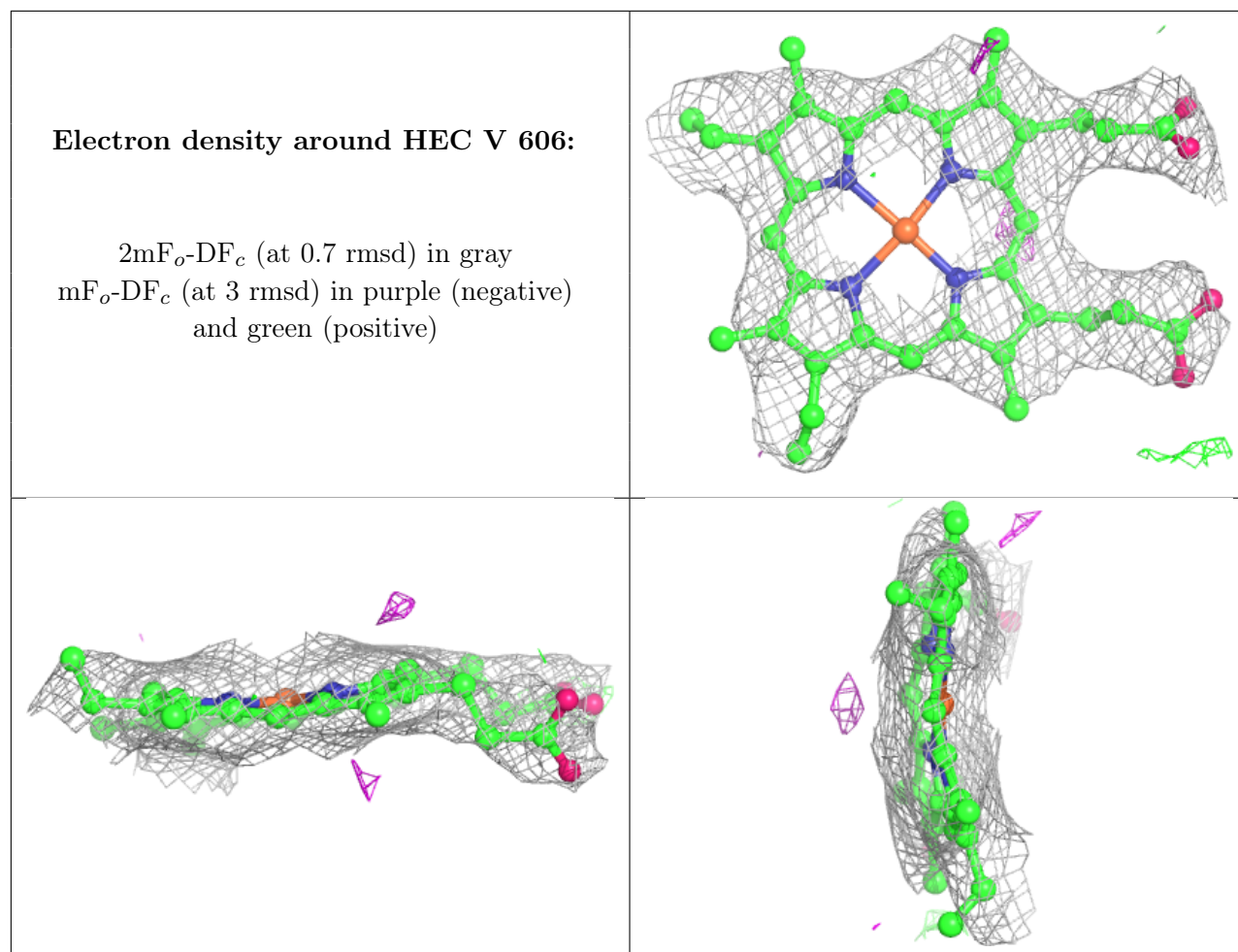


**Electron density around HEC E 600:**

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

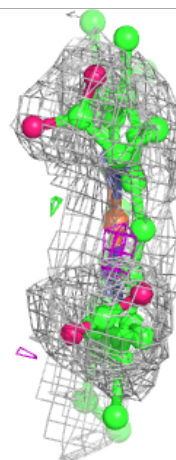
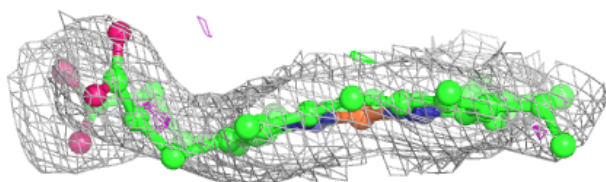
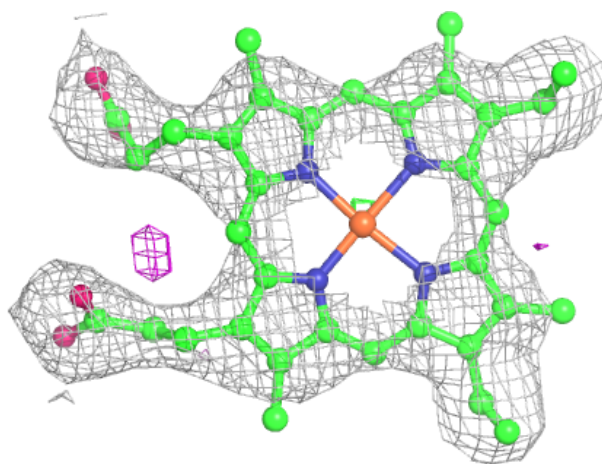






**Electron density around HEC V 607:**

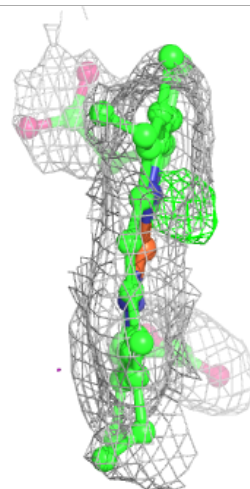
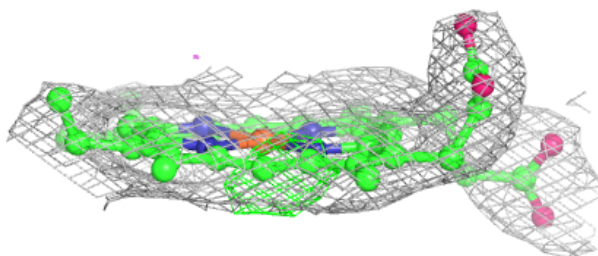
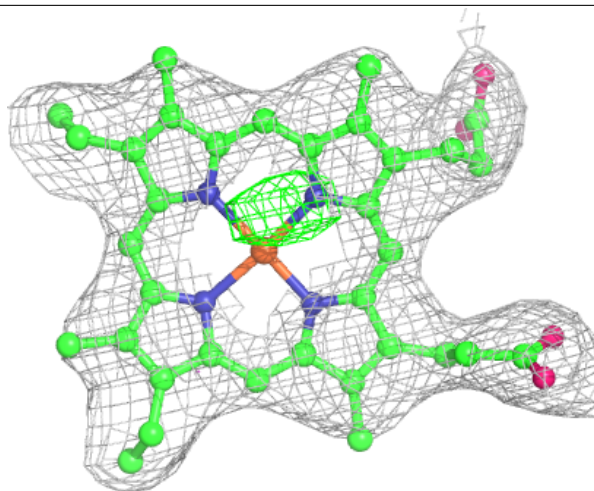
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





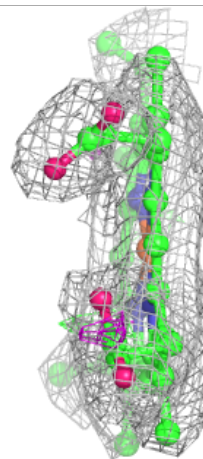
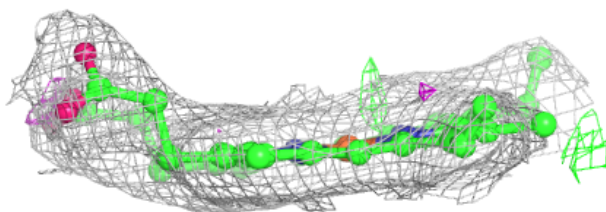
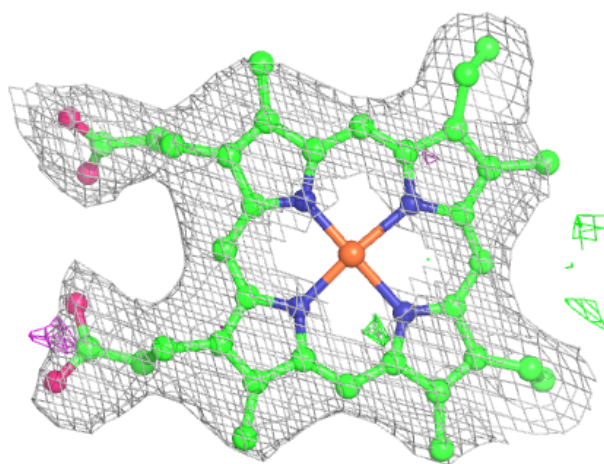
**Electron density around HEC E 601:**

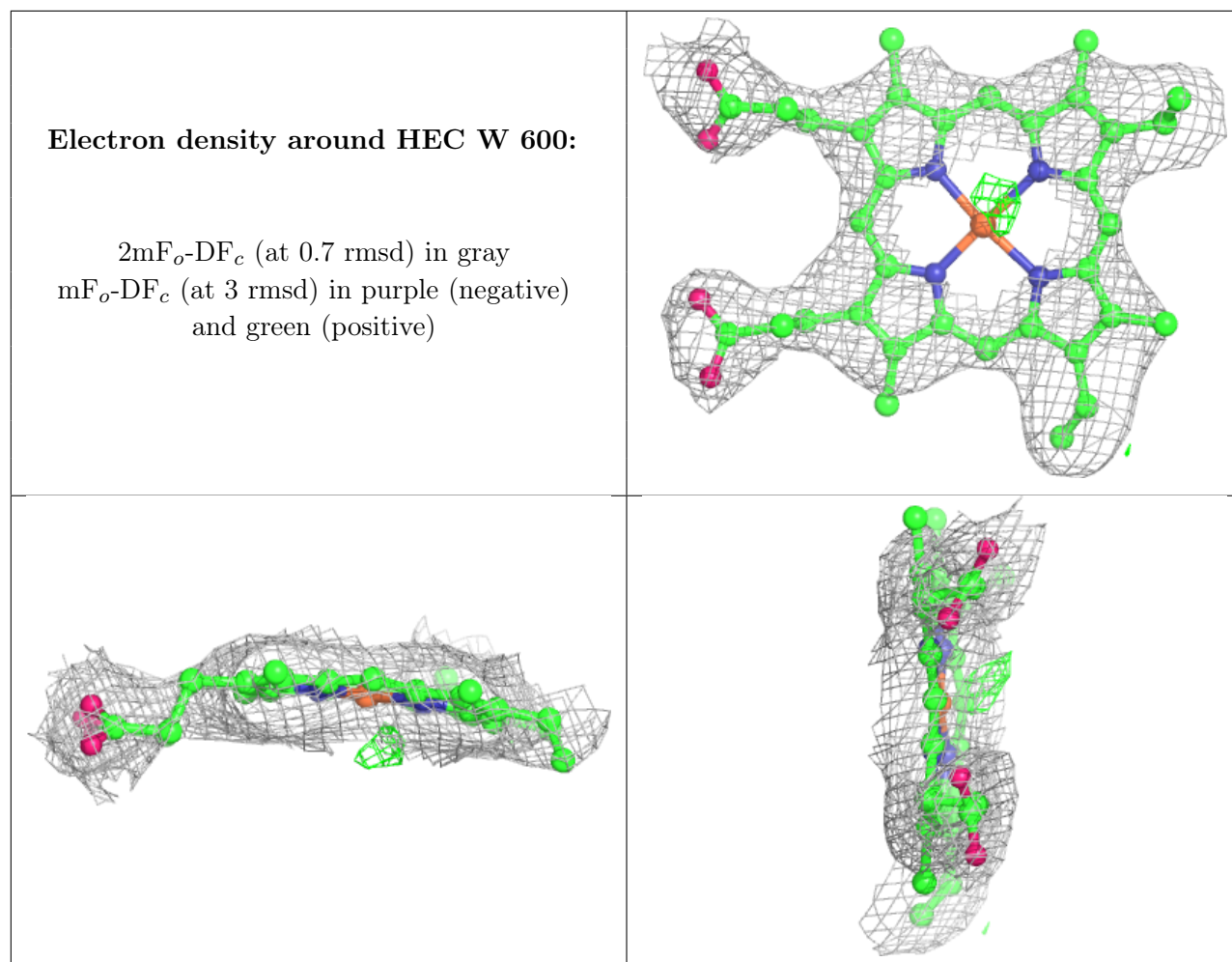
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC G 604:**

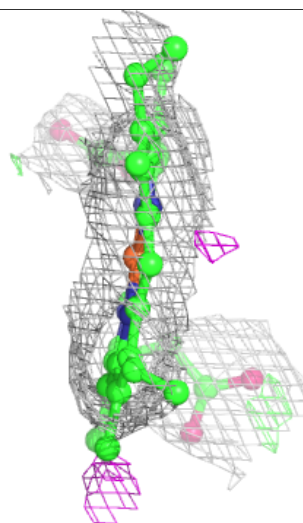
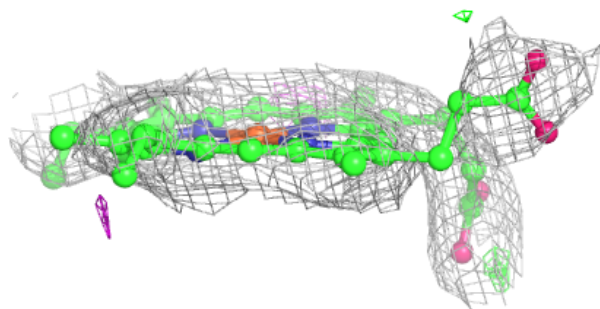
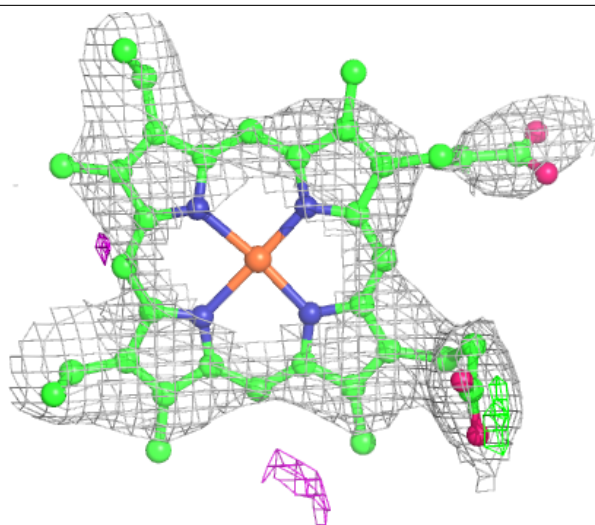
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





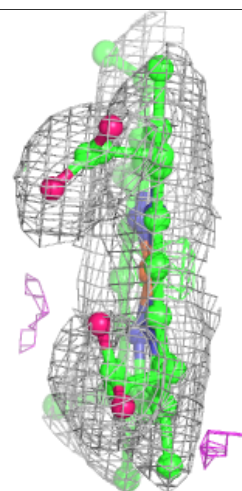
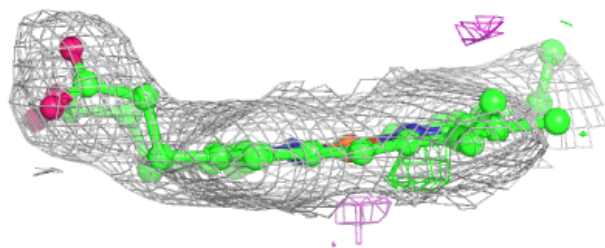
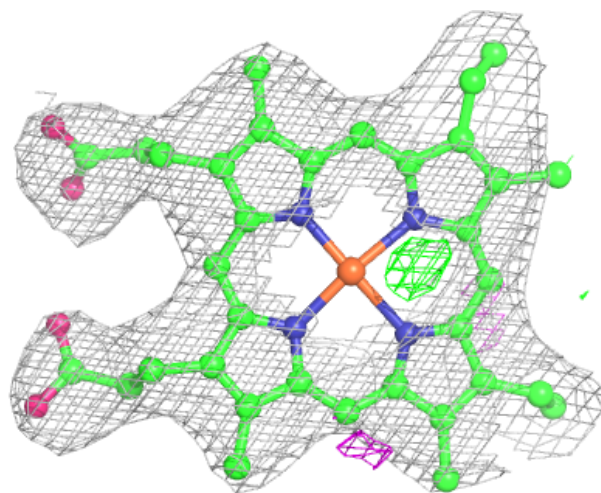
**Electron density around HEC W 601:**

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



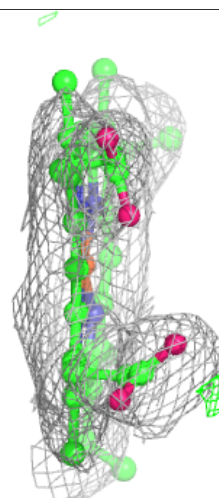
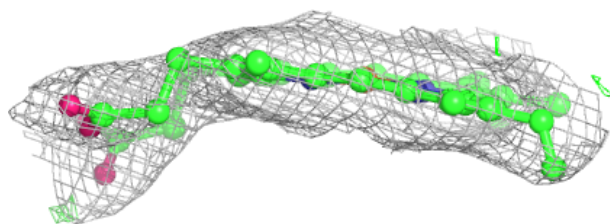
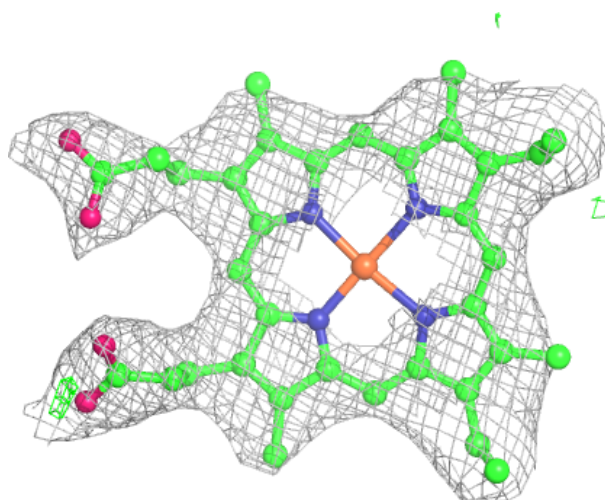
**Electron density around HEC E 604:**

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



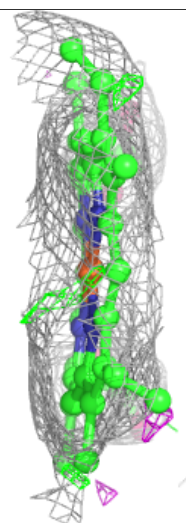
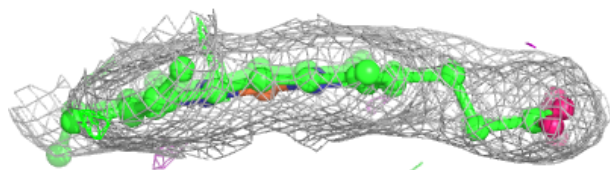
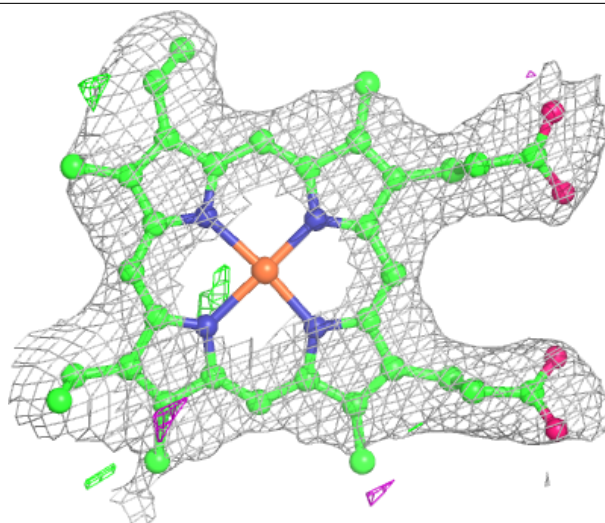
**Electron density around HEC W 604:**

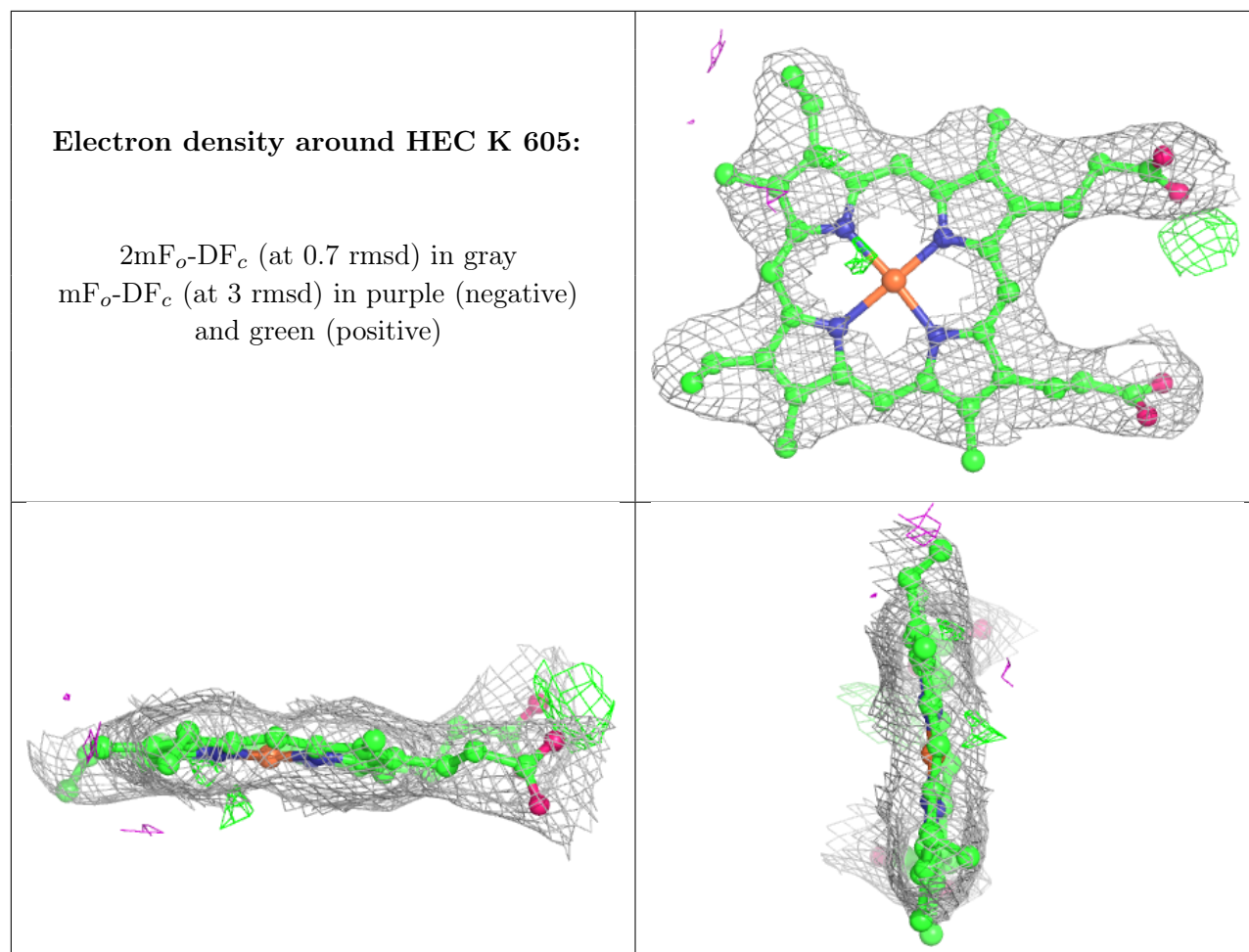
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC A 600:**

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

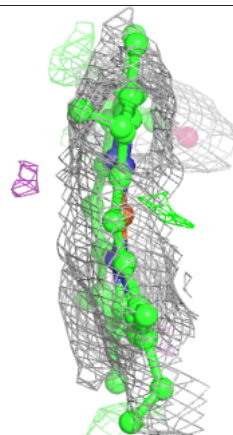
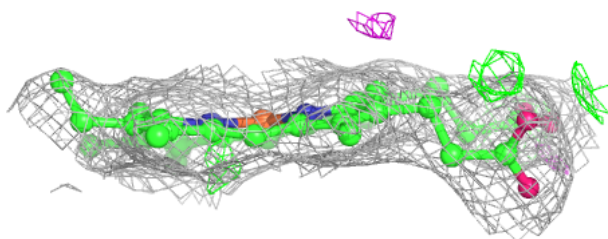
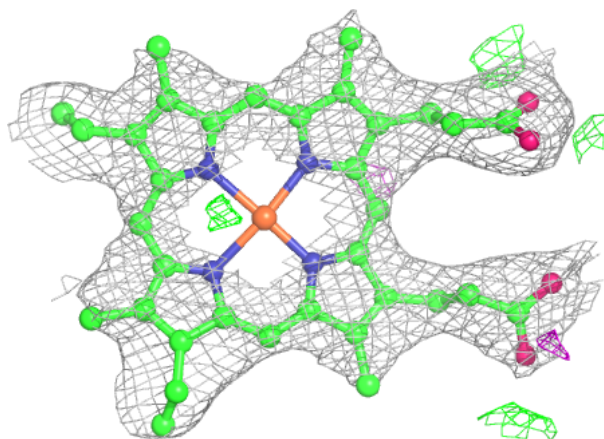






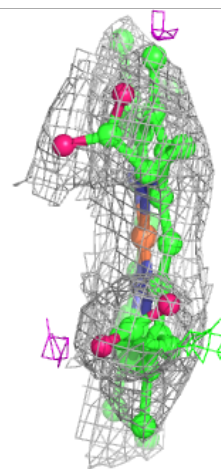
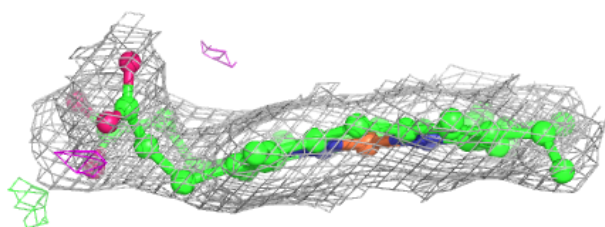
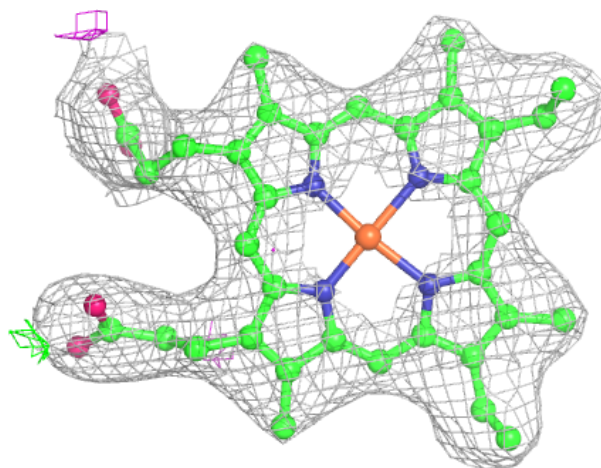
**Electron density around HEC K 606:**

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



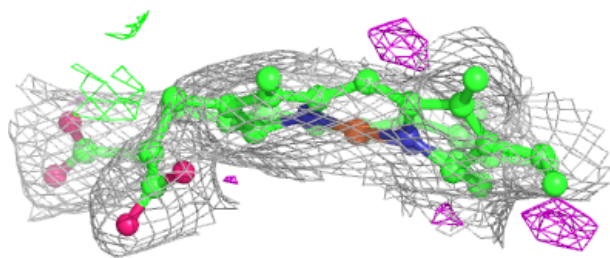
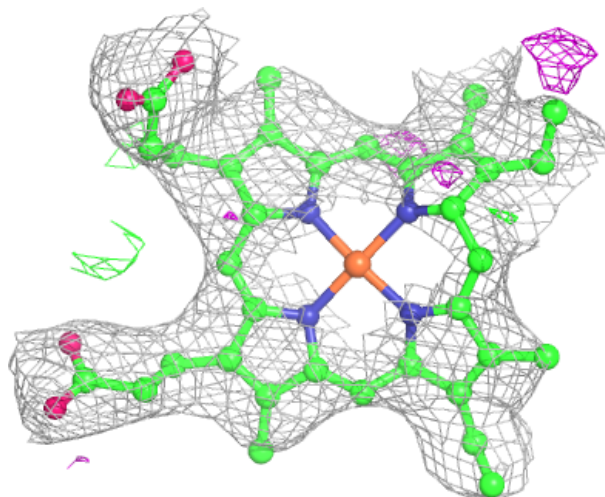
**Electron density around HEC K 607:**

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



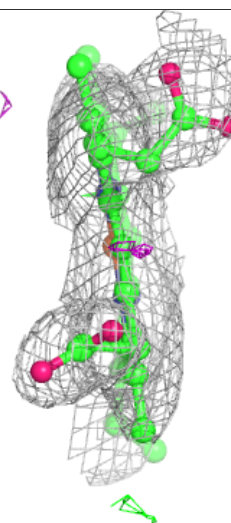
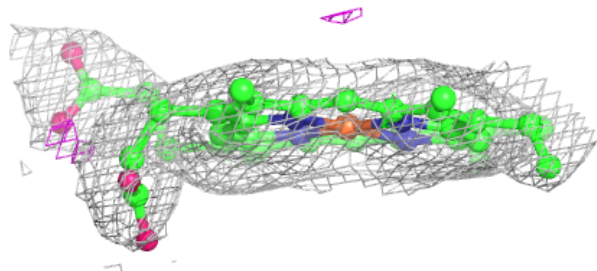
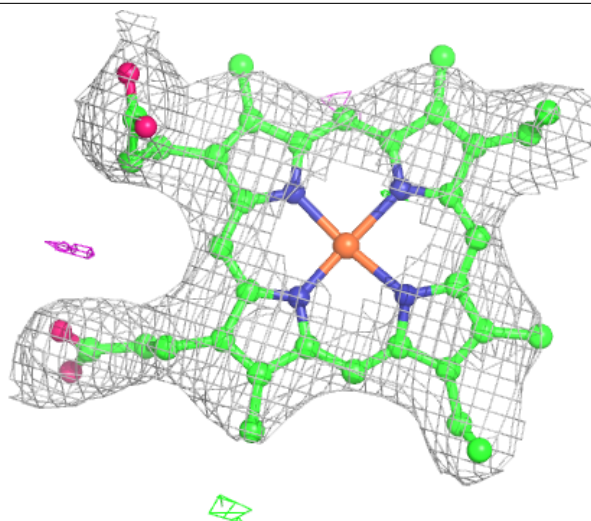
**Electron density around HEC L 603:**

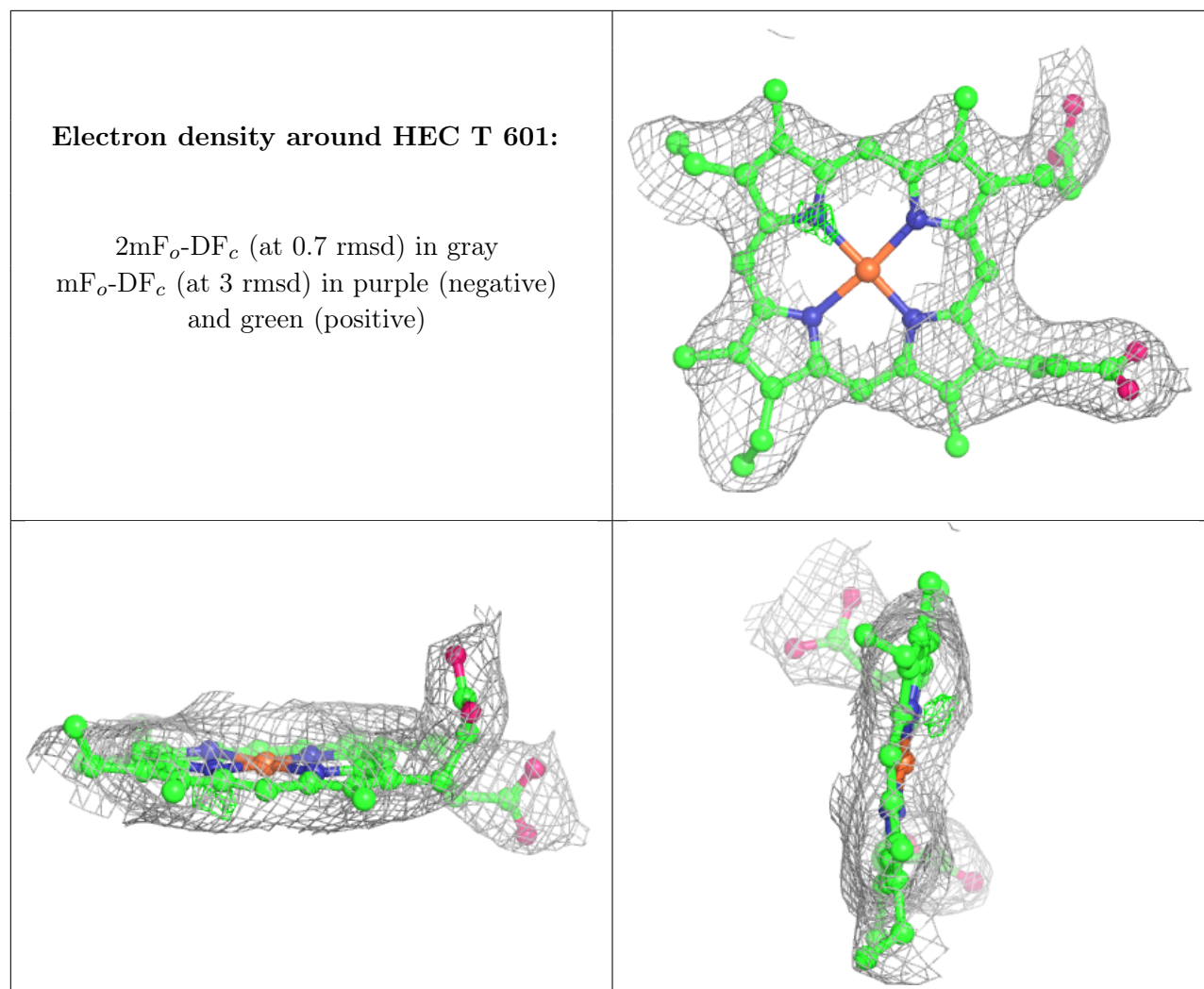
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

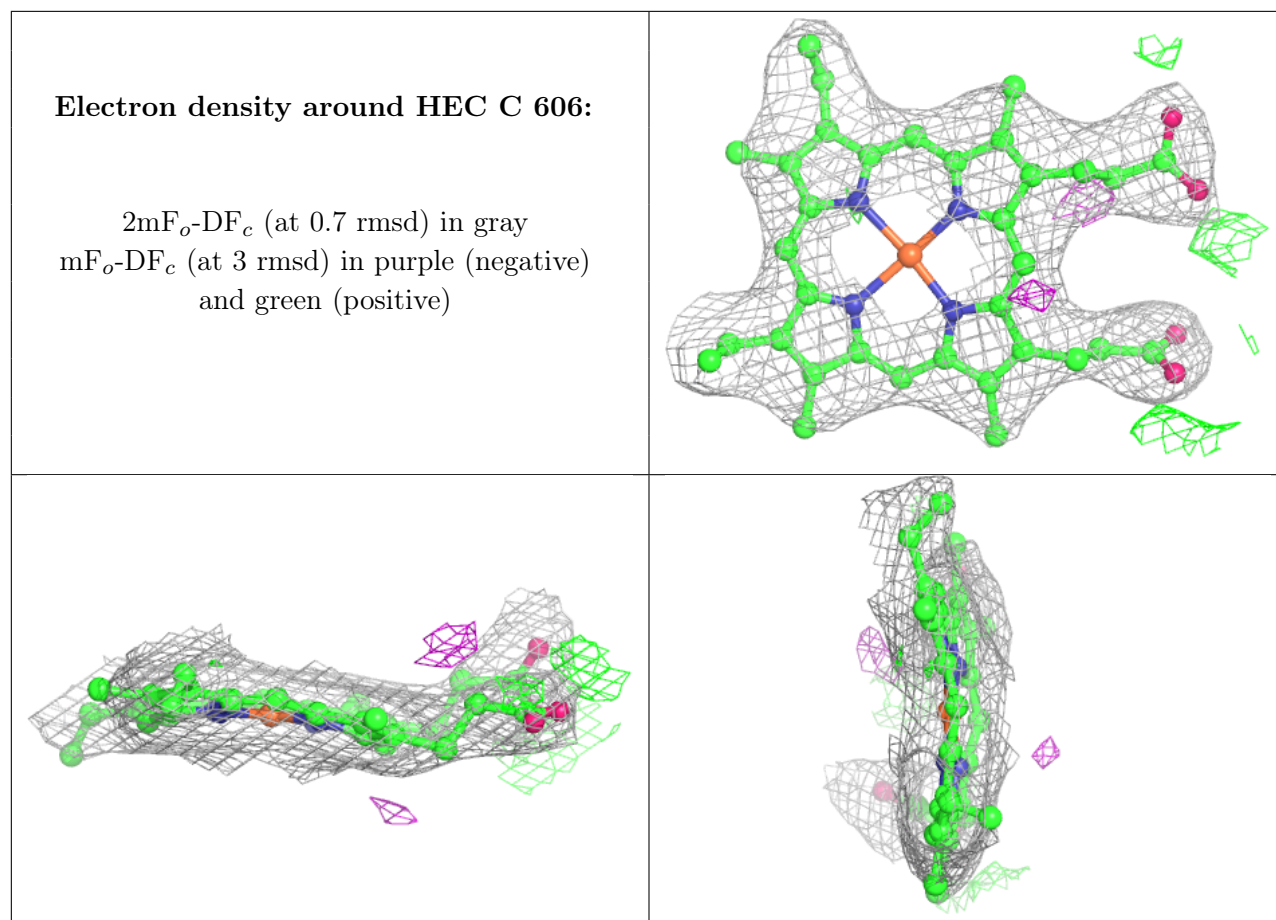


**Electron density around HEC B 601:**

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

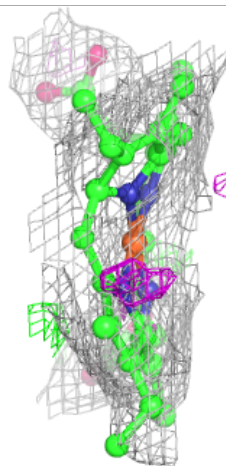
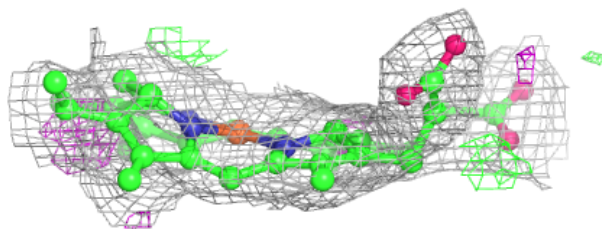
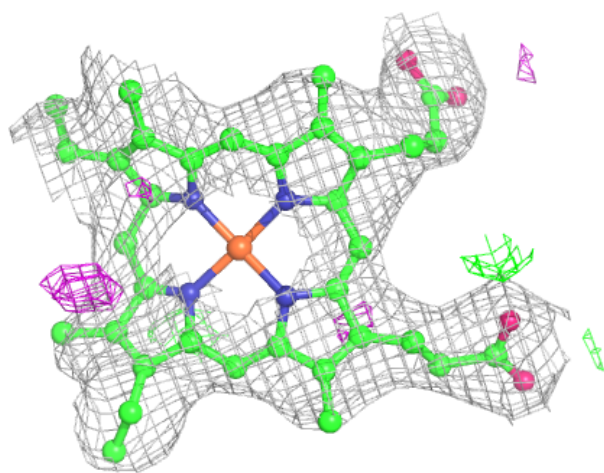






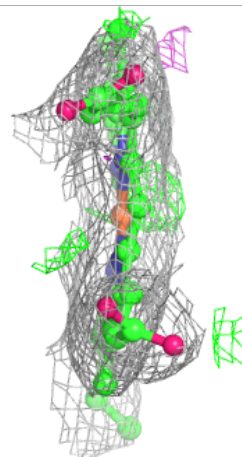
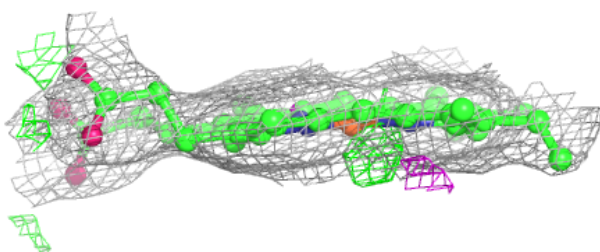
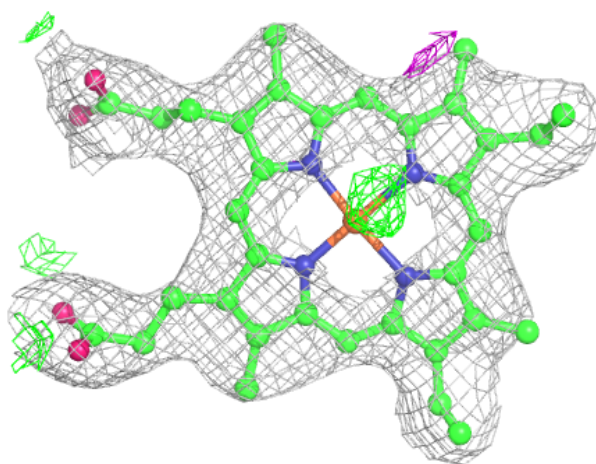
**Electron density around HEC G 603:**

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



**Electron density around HEC G 605:**

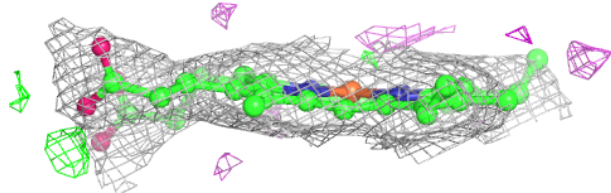
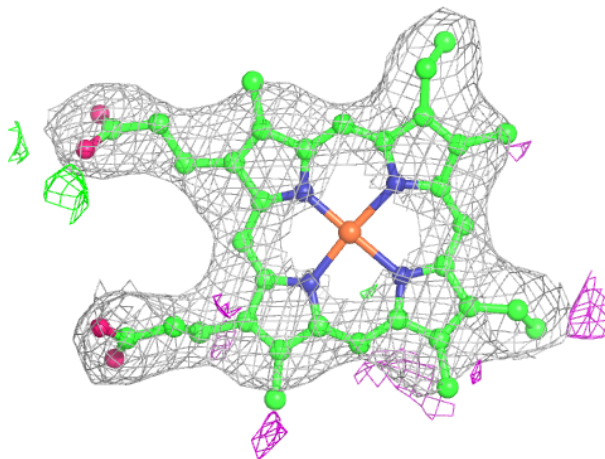
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





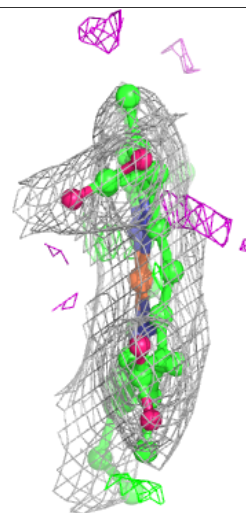
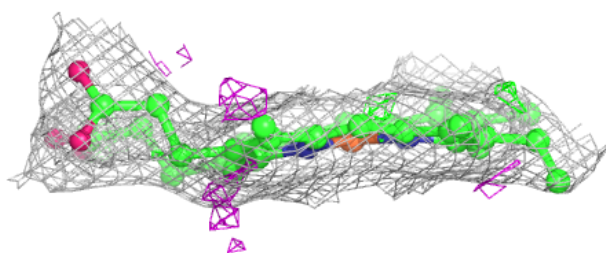
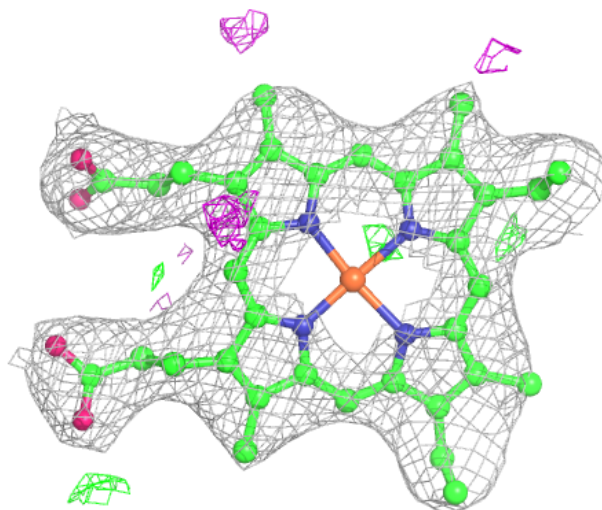
**Electron density around HEC L 605:**

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



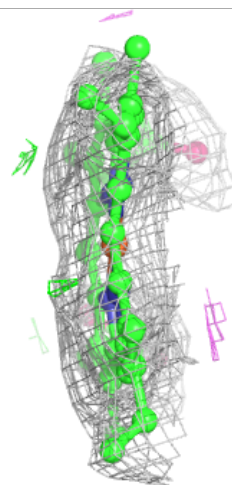
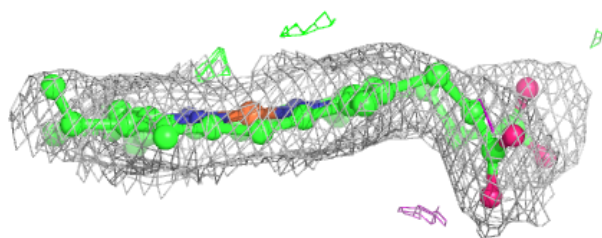
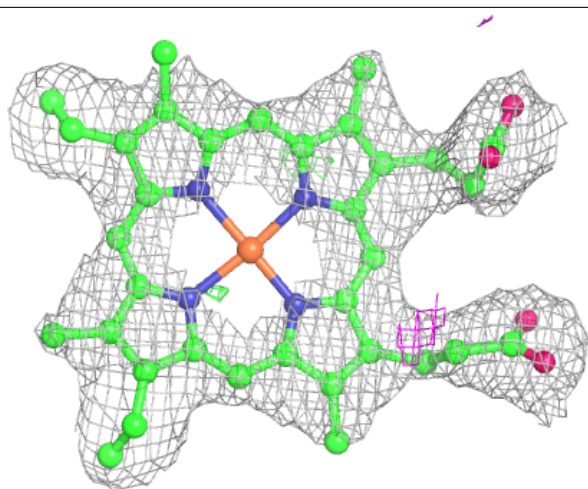
**Electron density around HEC L 606:**

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



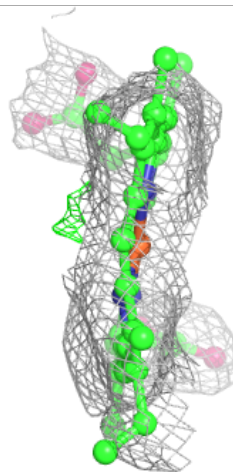
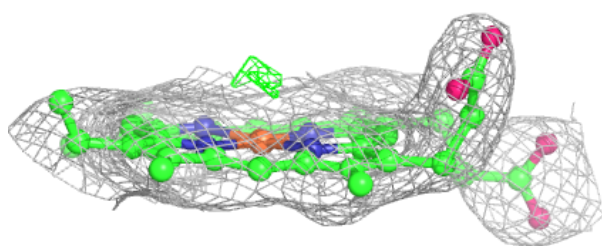
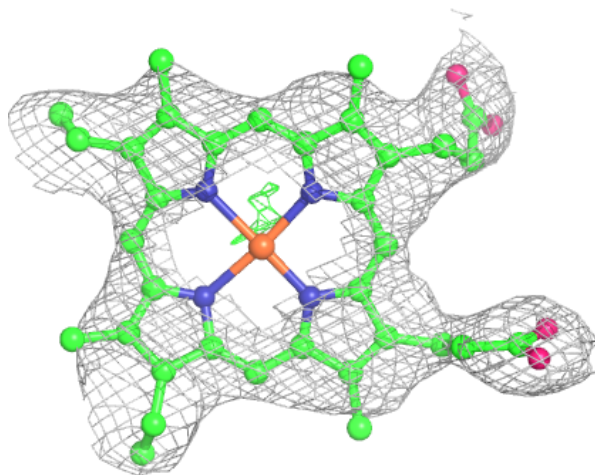
**Electron density around HEC L 607:**

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



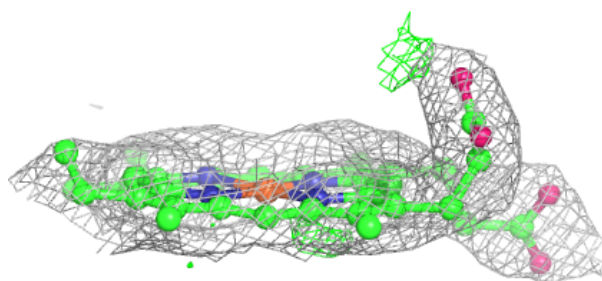
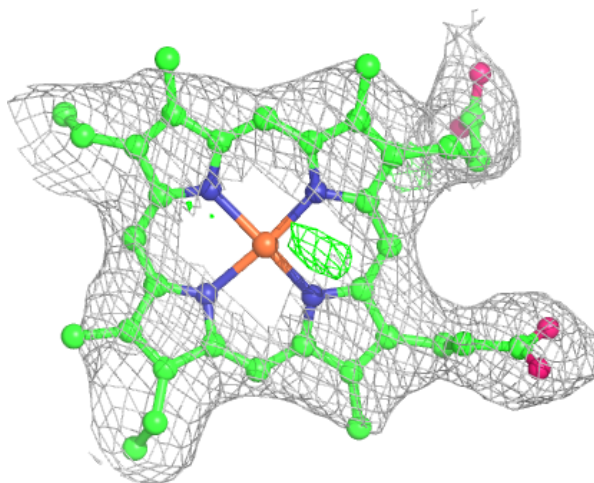
**Electron density around HEC D 601:**

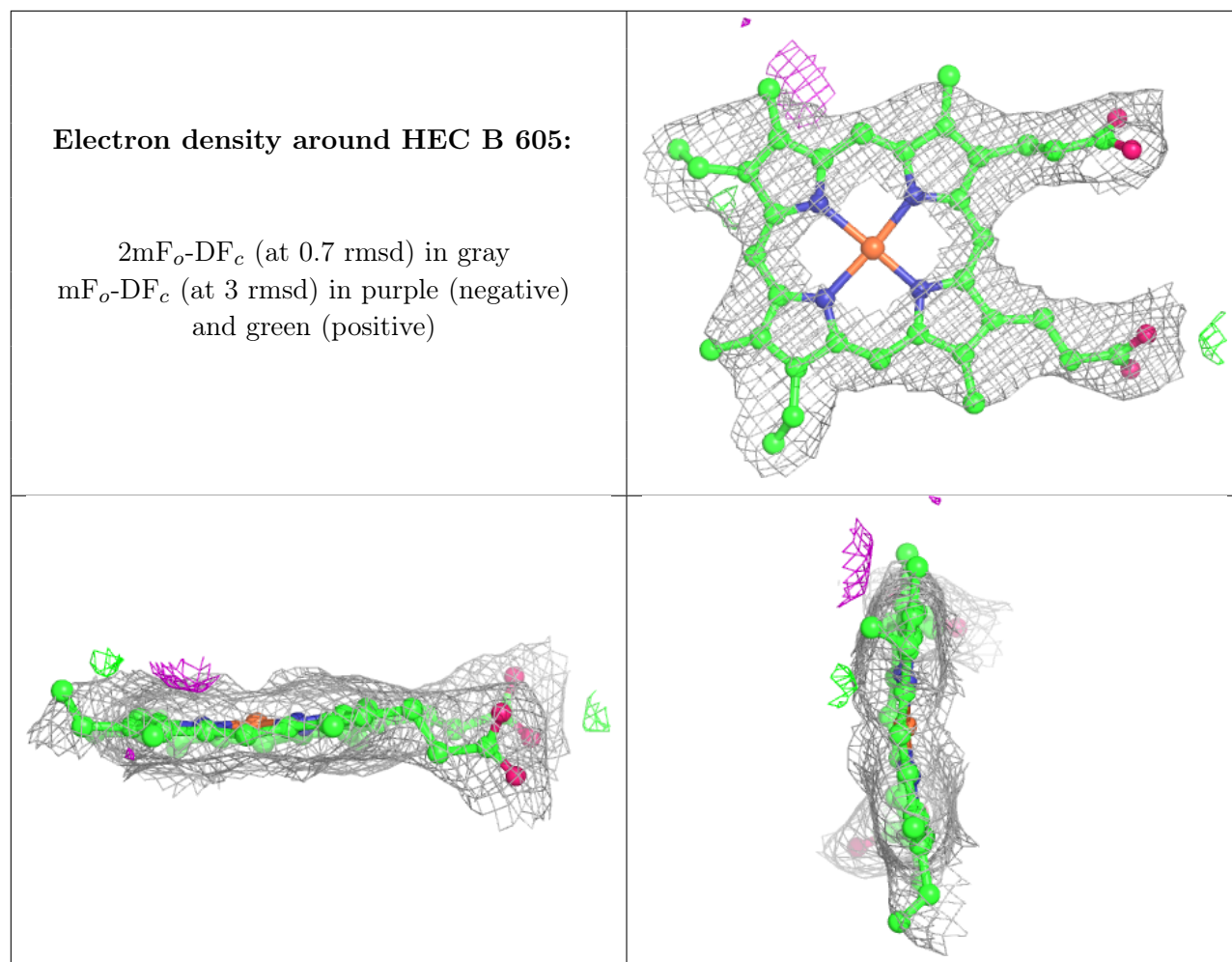
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC M 601:**

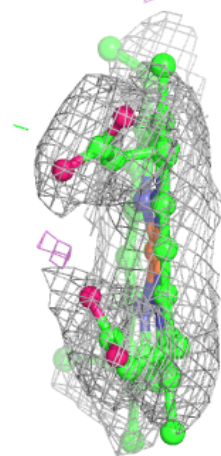
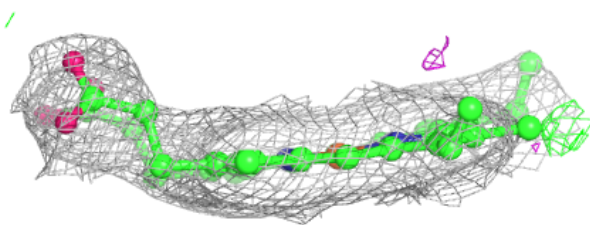
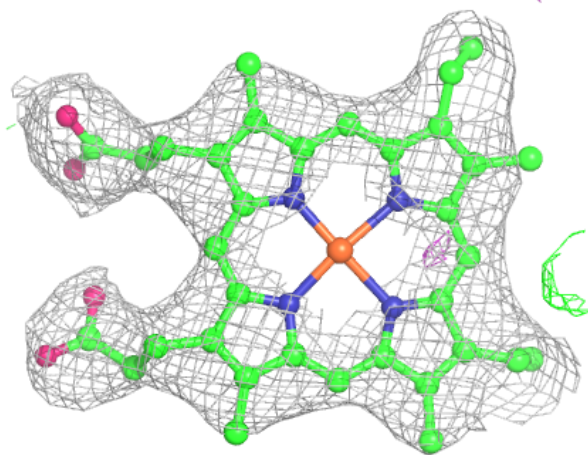
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

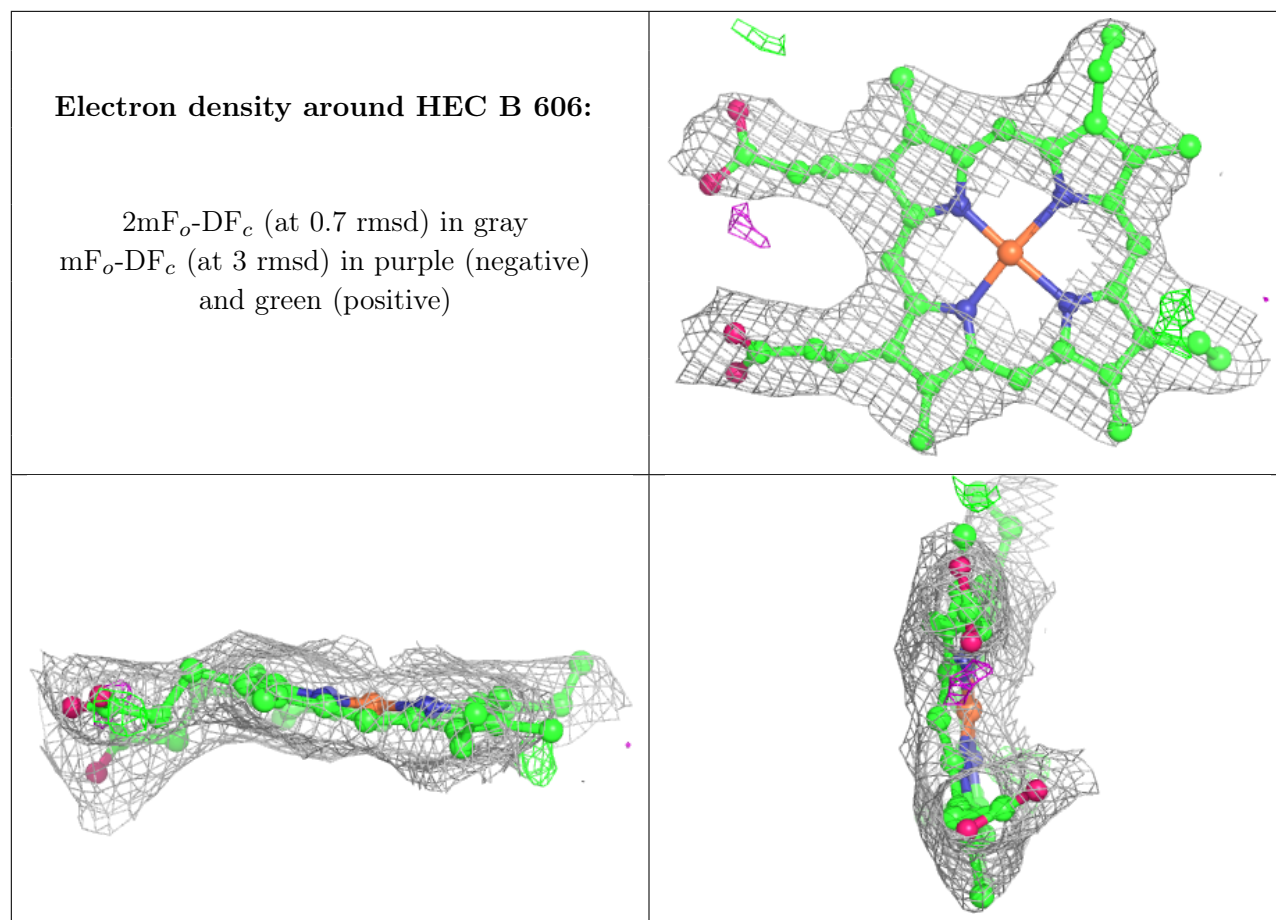




**Electron density around HEC D 604:**

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

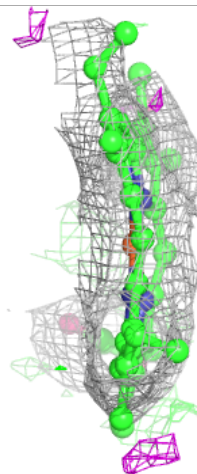
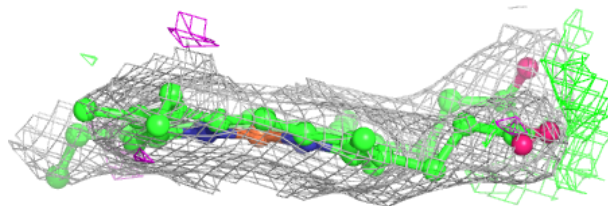
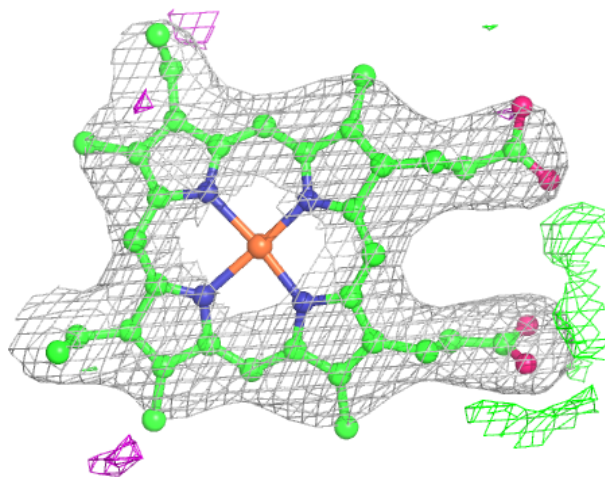


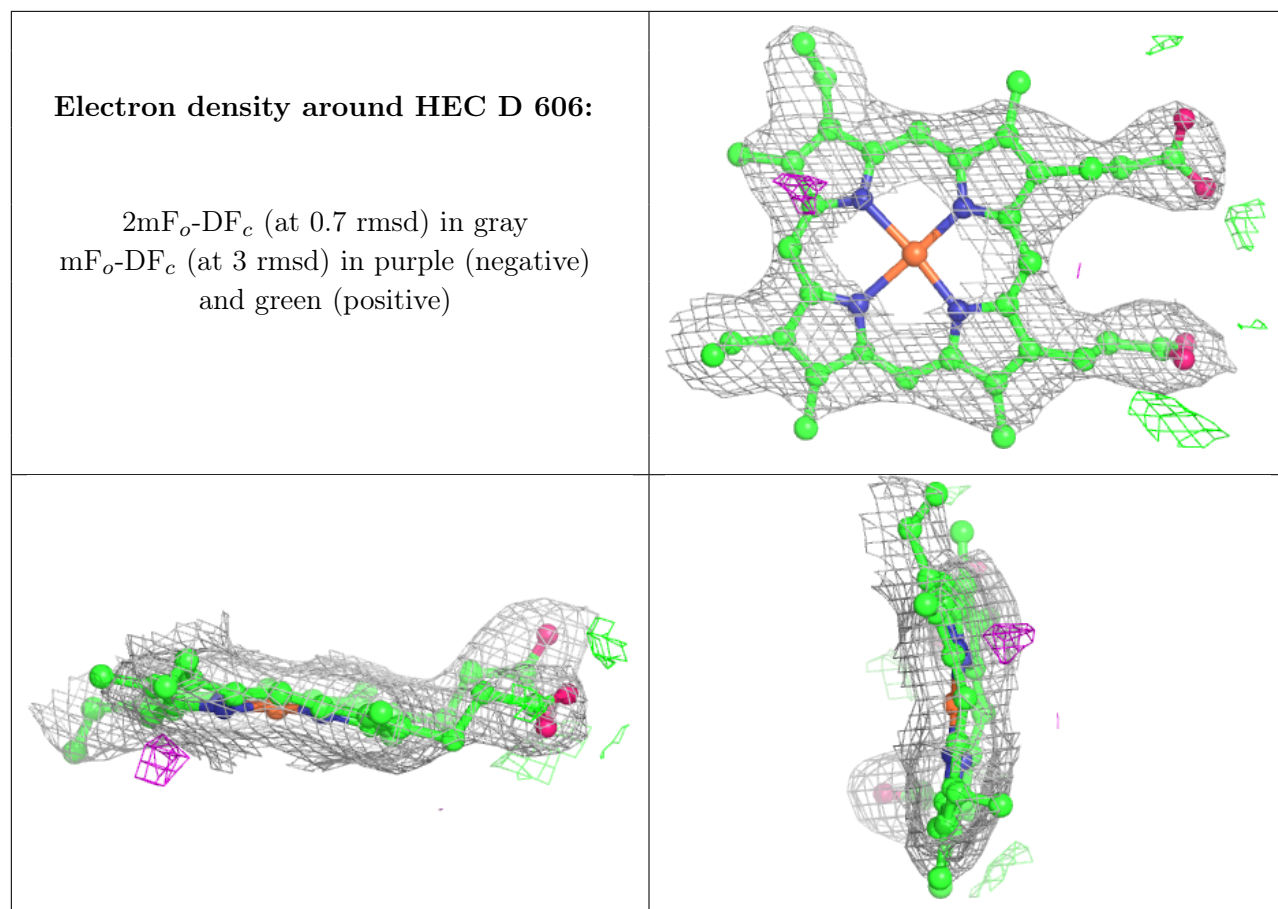


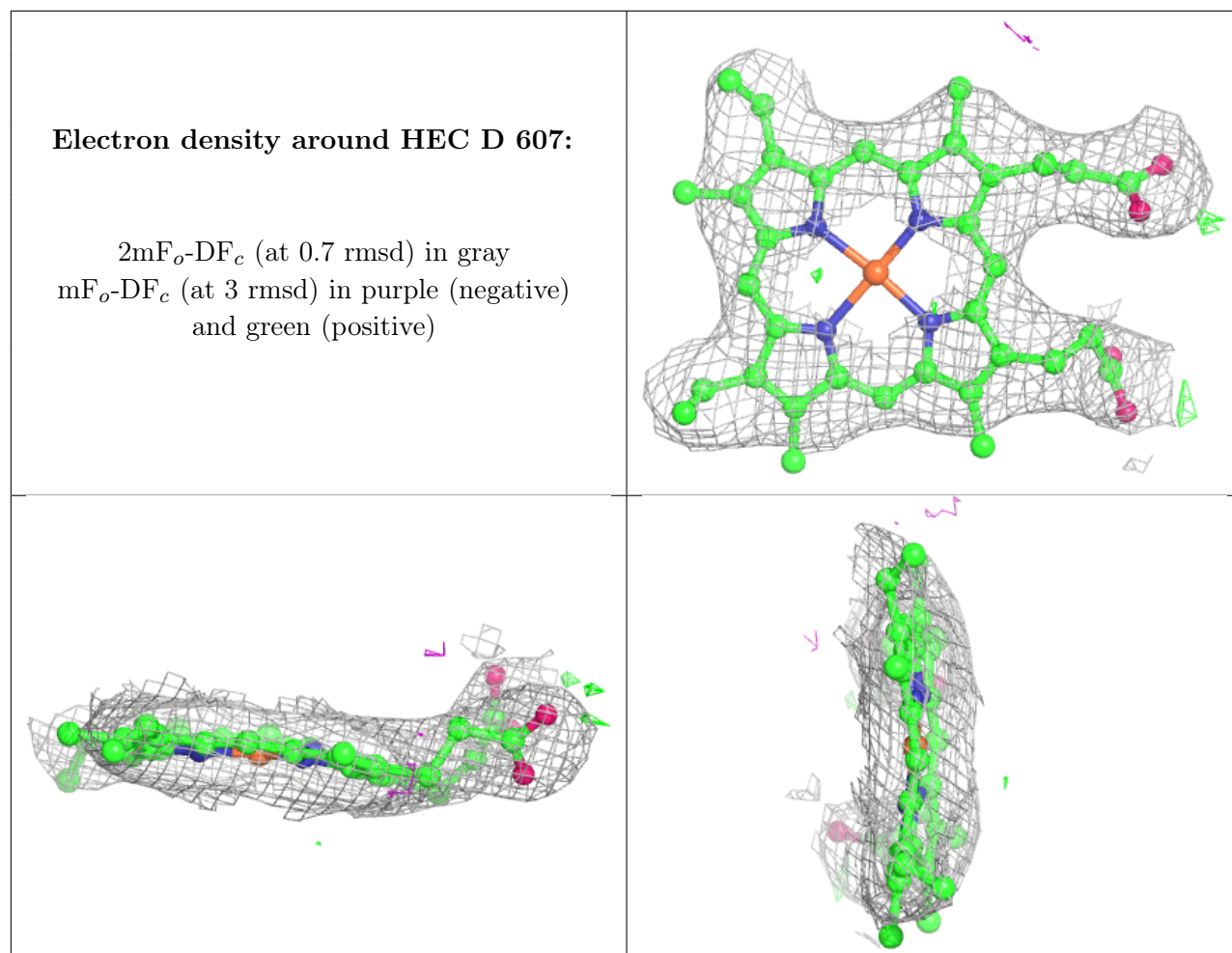


**Electron density around HEC M 606:**

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

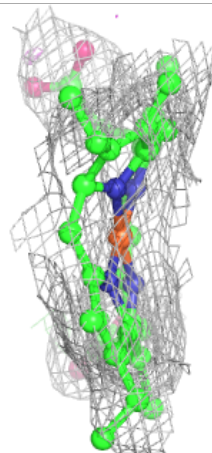
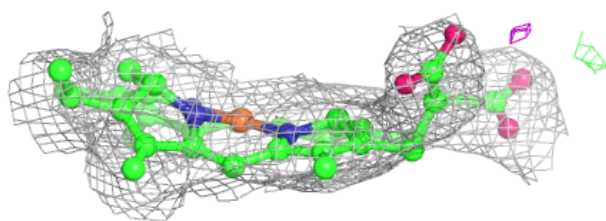
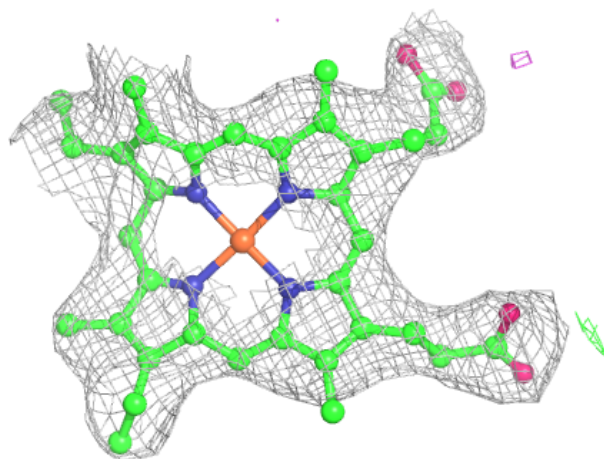






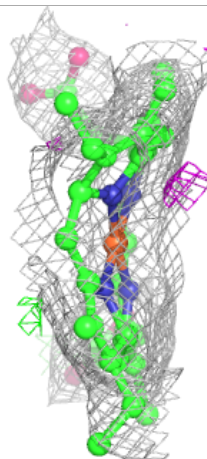
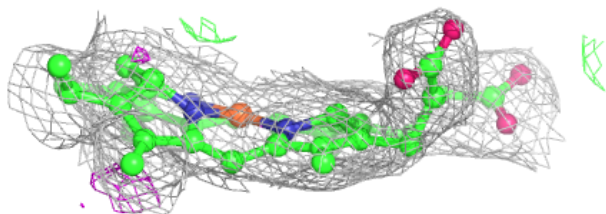
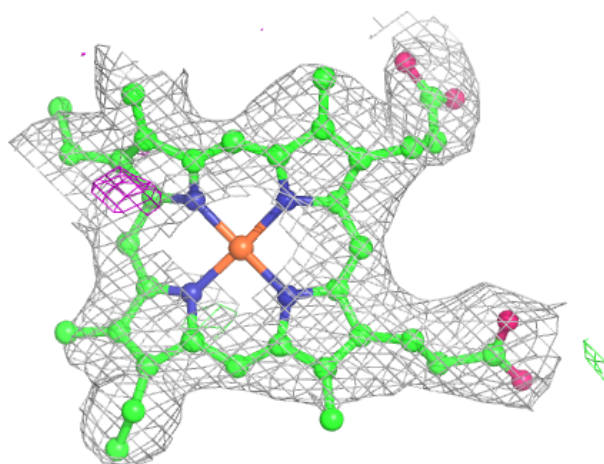
**Electron density around HEC N 603:**

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



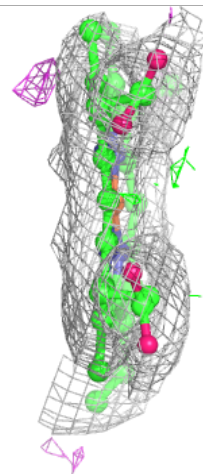
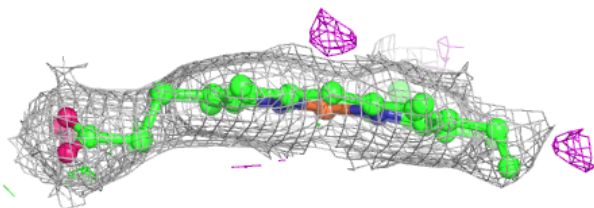
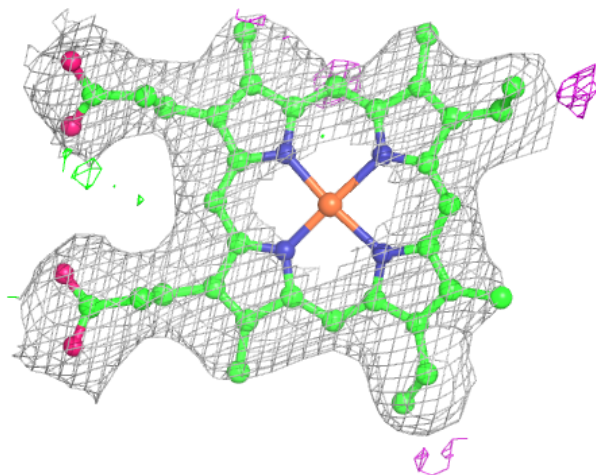
**Electron density around HEC H 603:**

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



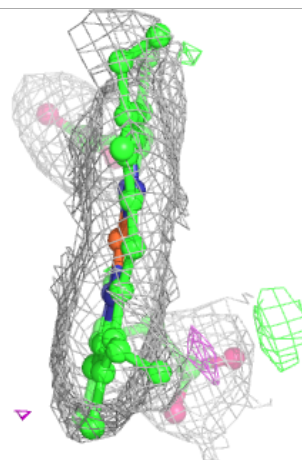
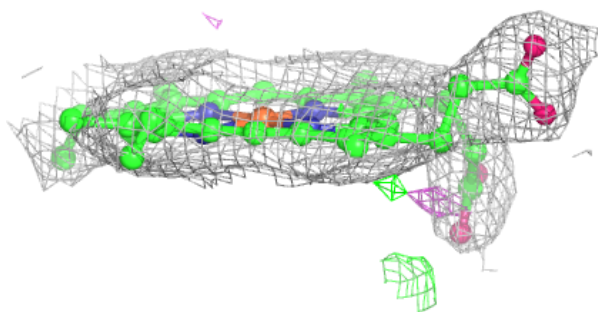
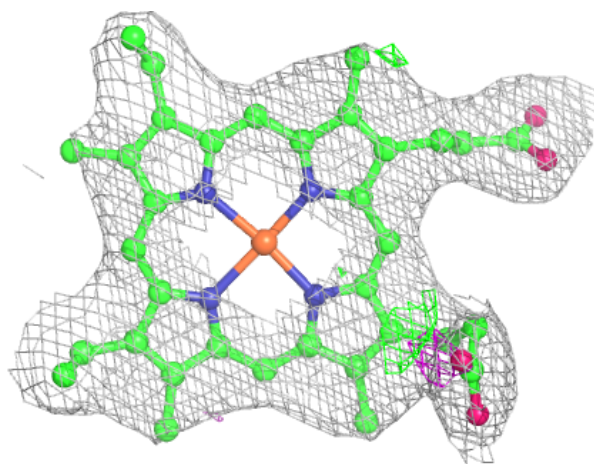
**Electron density around HEC H 600:**

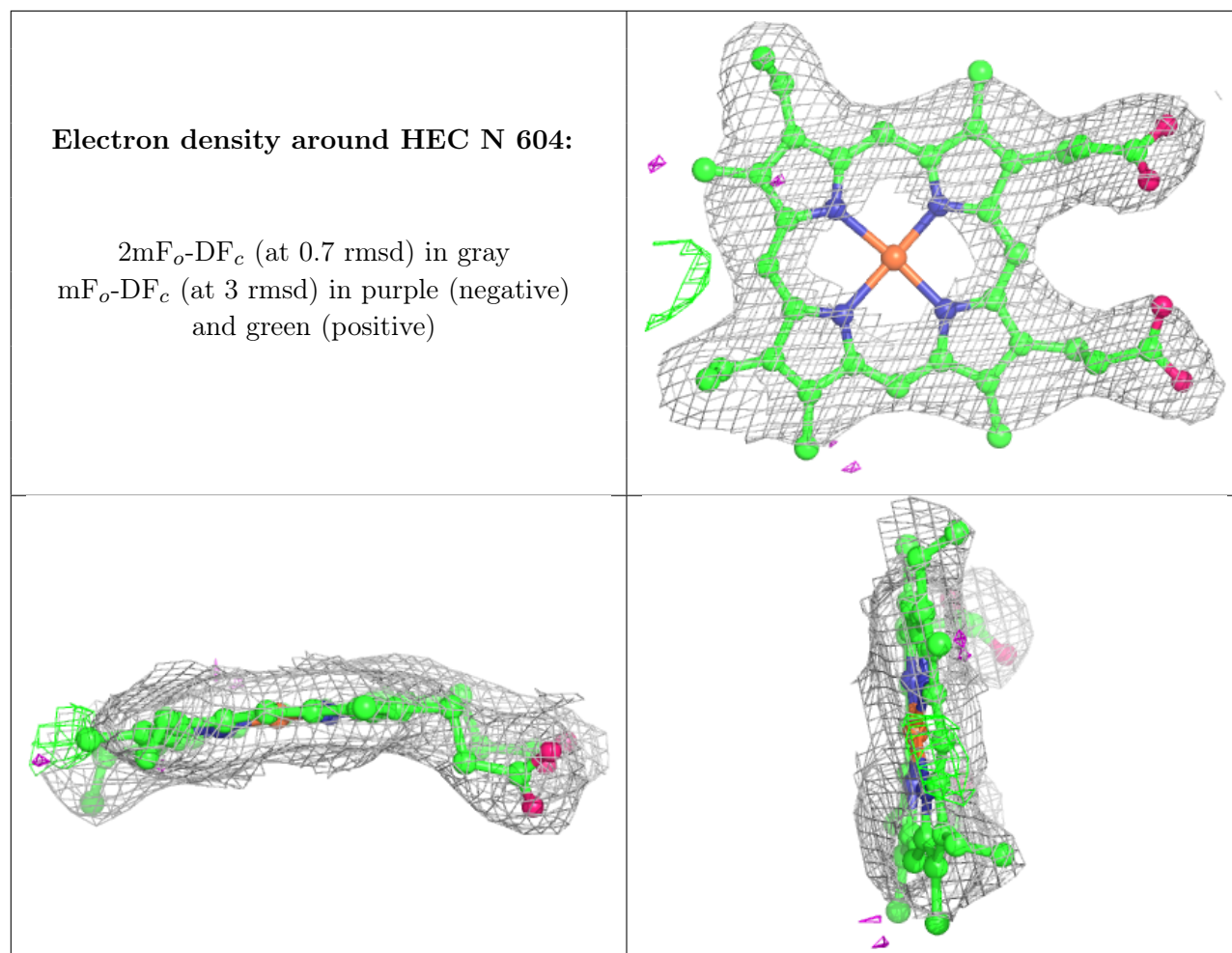
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



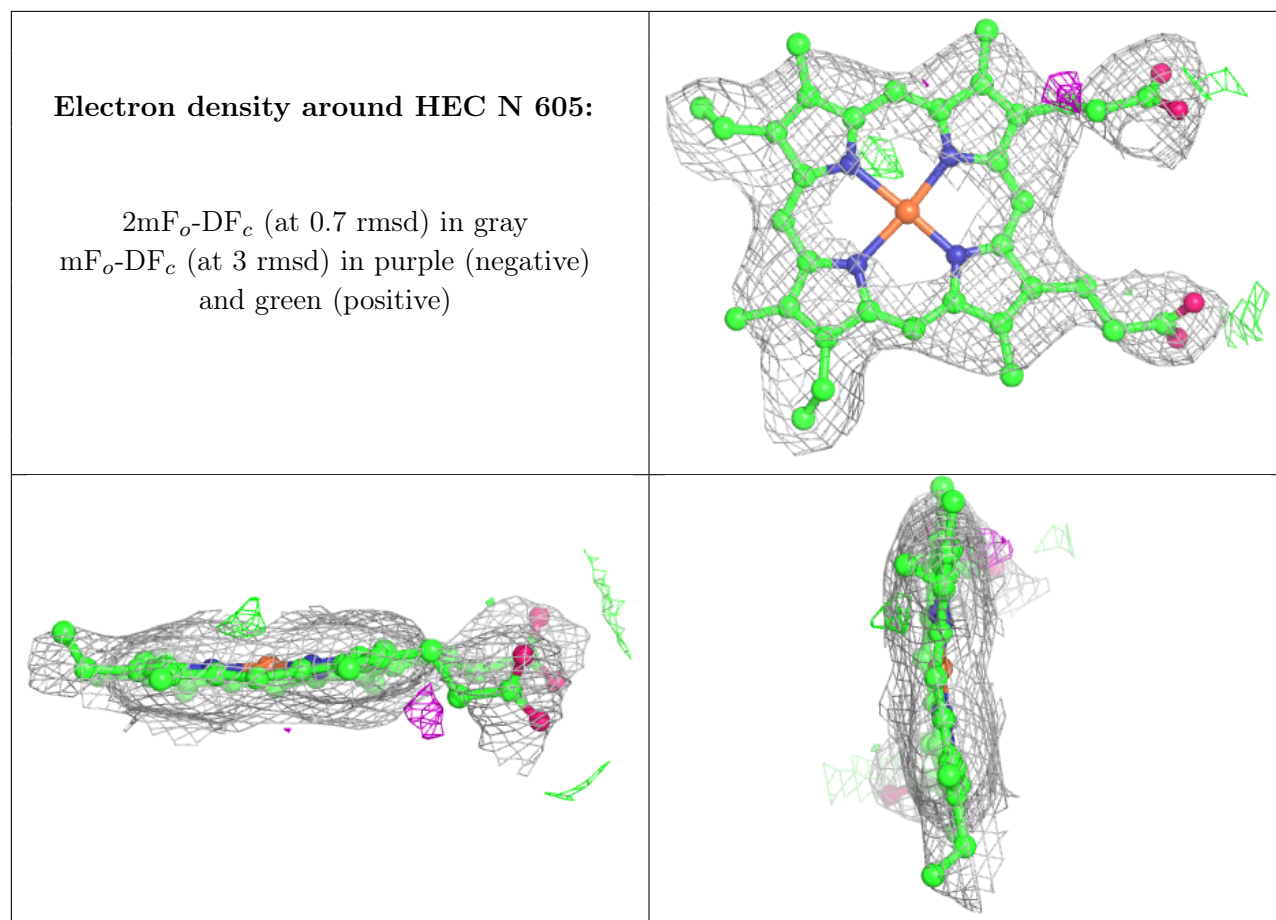
**Electron density around HEC H 601:**

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



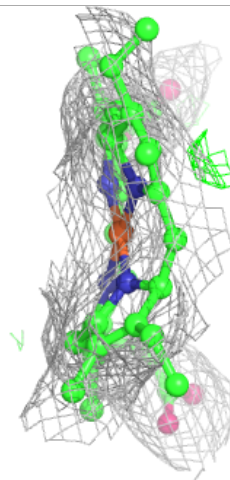
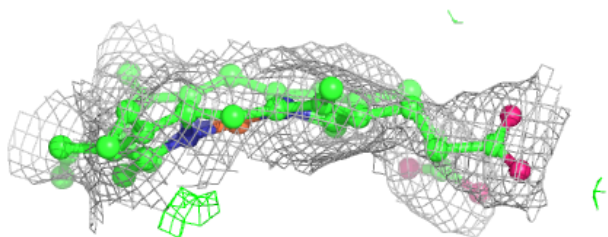
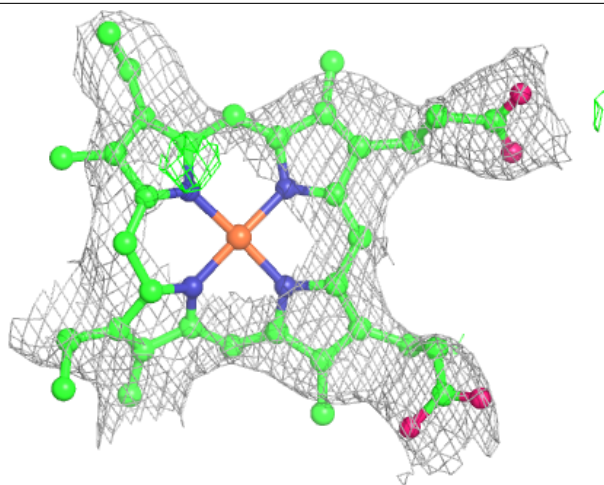






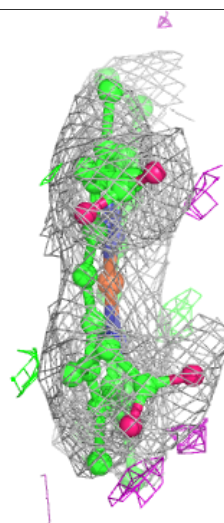
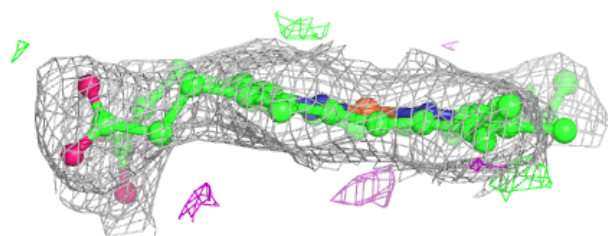
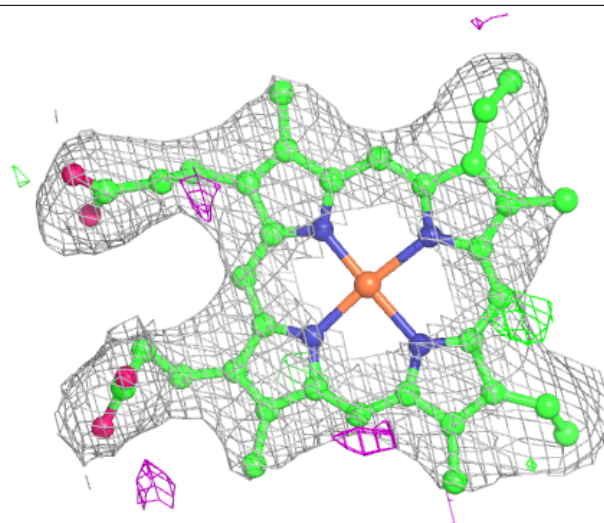
**Electron density around HEC D 603:**

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



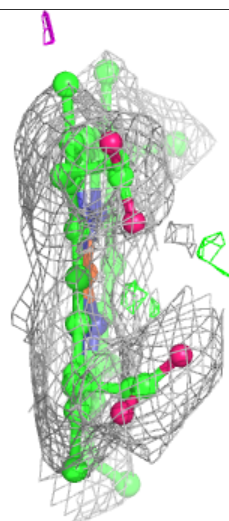
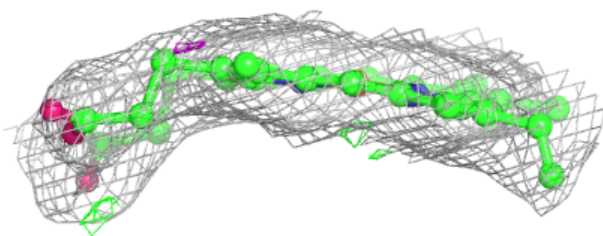
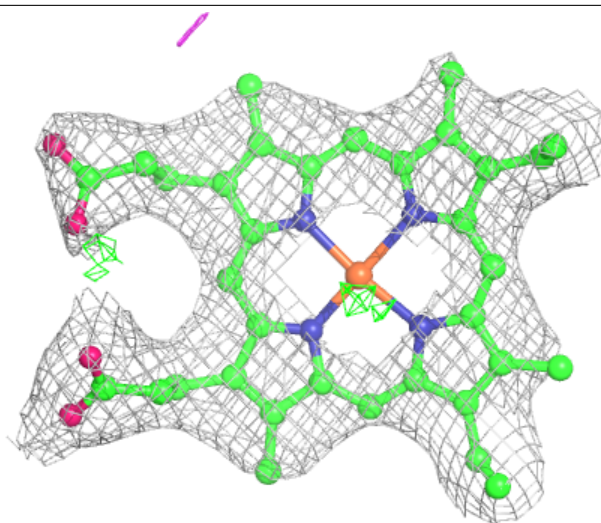
**Electron density around HEC N 607:**

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



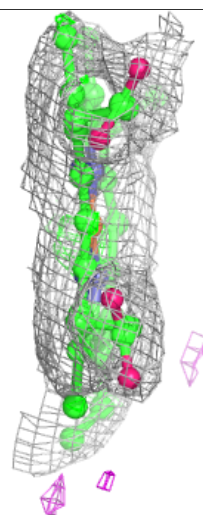
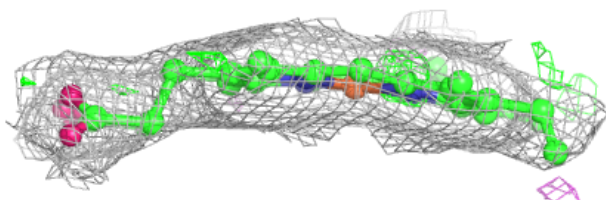
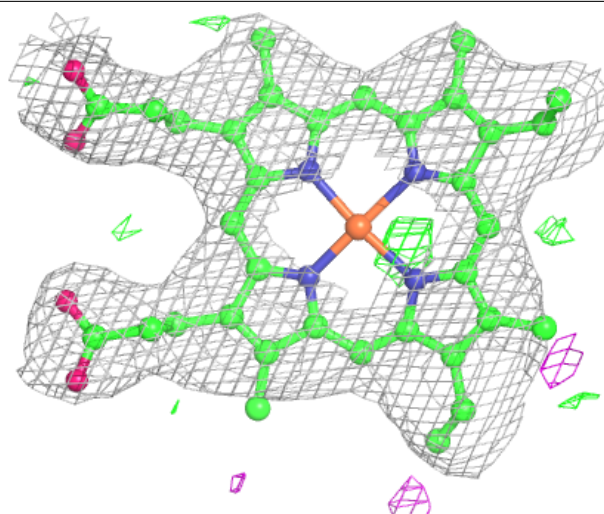
**Electron density around HEC H 604:**

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



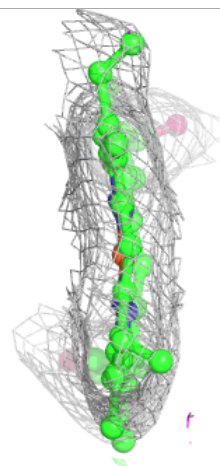
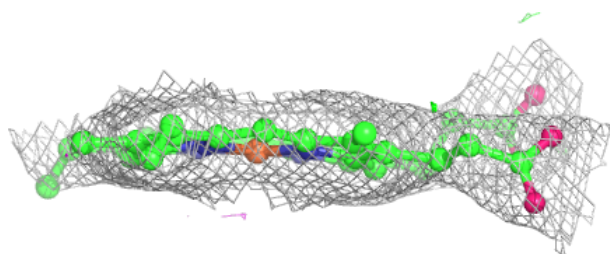
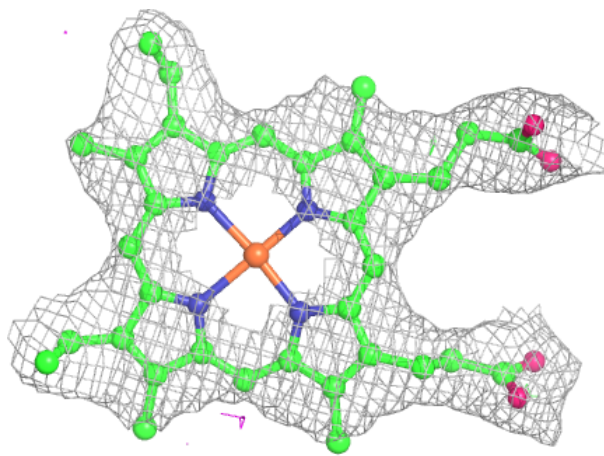
**Electron density around HEC O 600:**

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



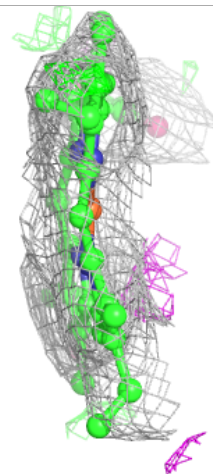
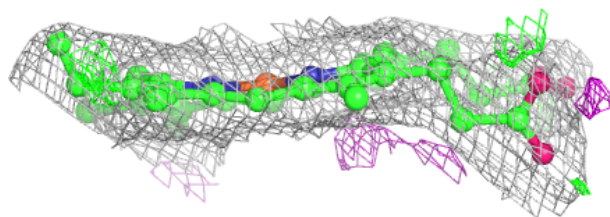
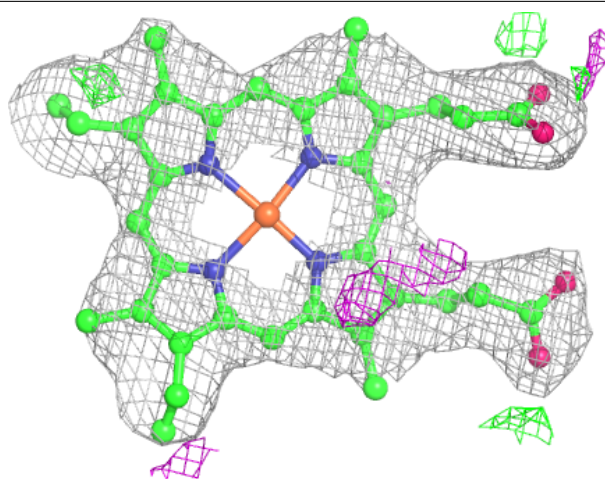
**Electron density around HEC H 605:**

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



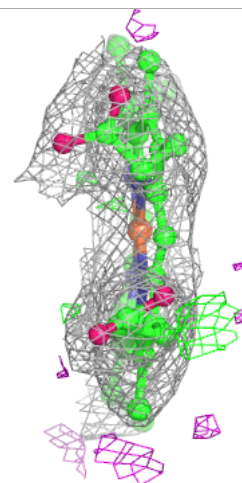
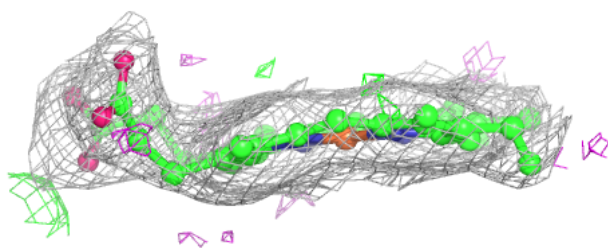
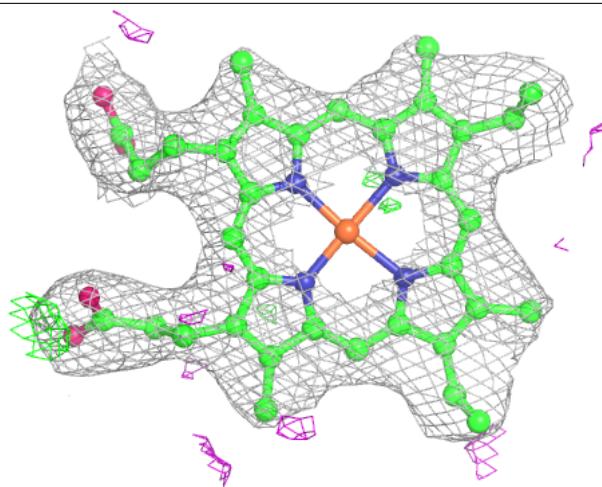
**Electron density around HEC H 606:**

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



**Electron density around HEC H 607:**

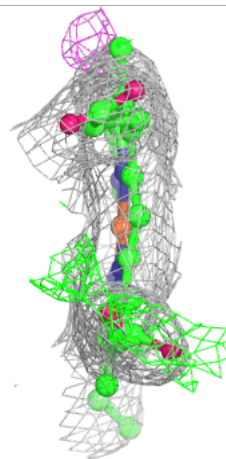
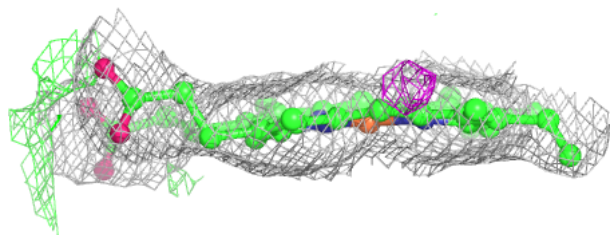
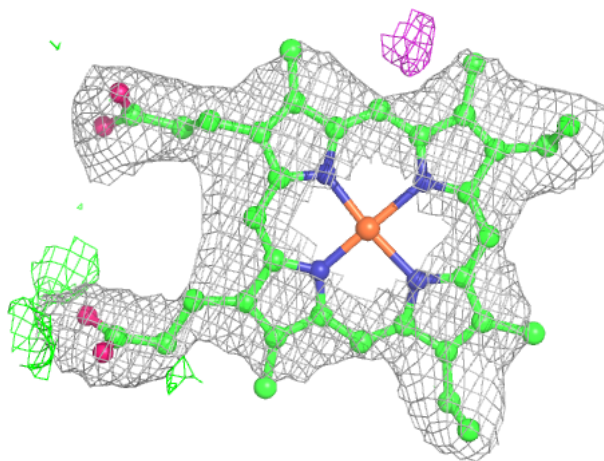
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





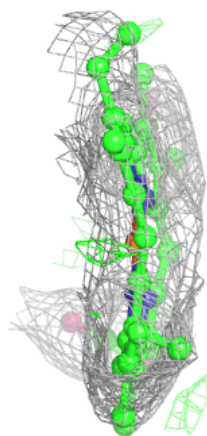
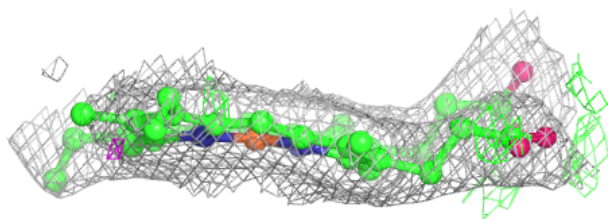
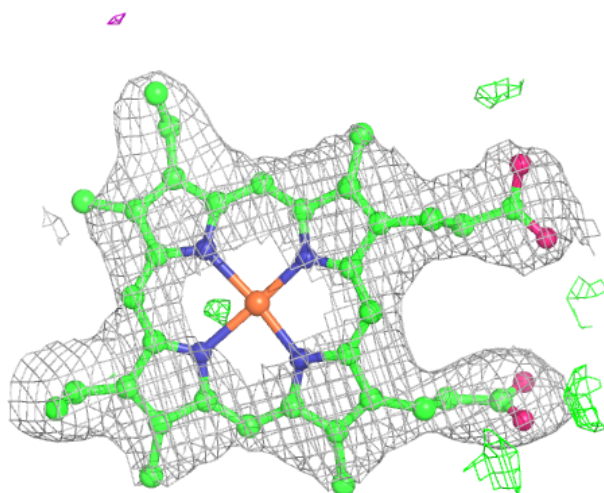
**Electron density around HEC O 605:**

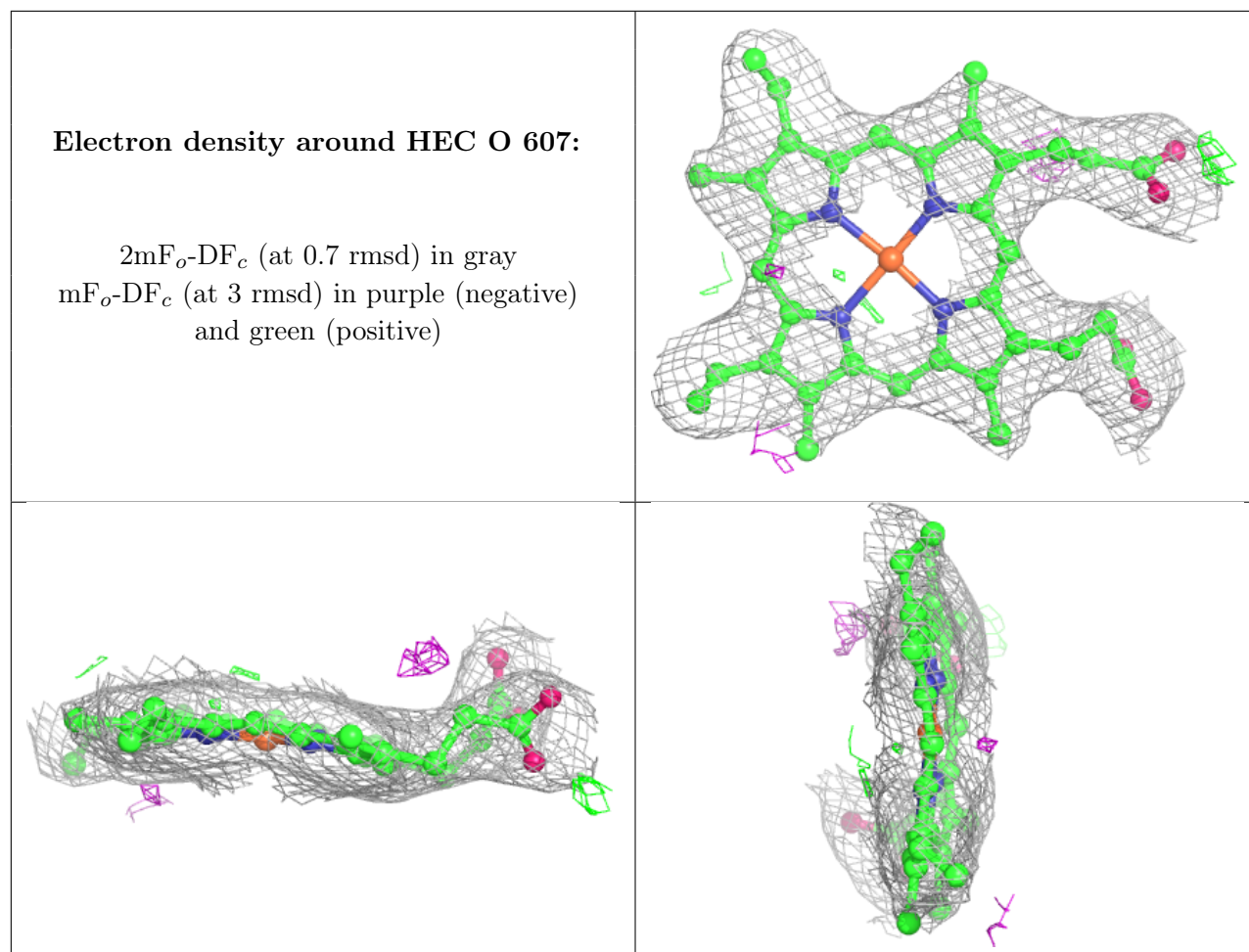
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

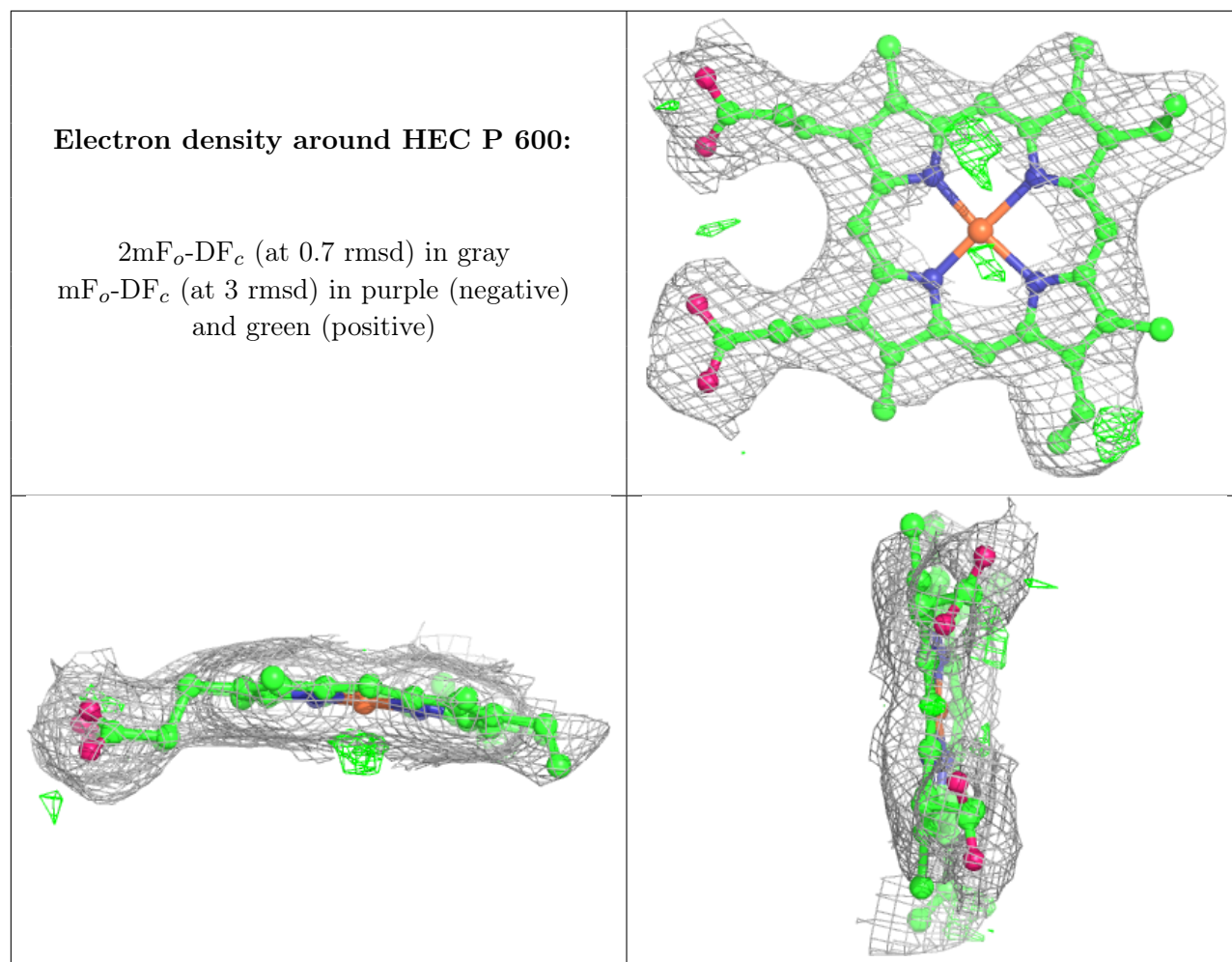


**Electron density around HEC O 606:**

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

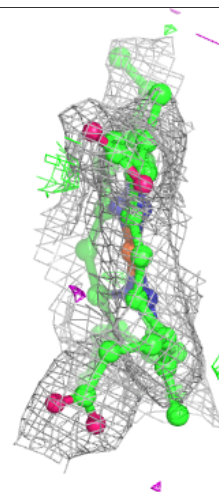
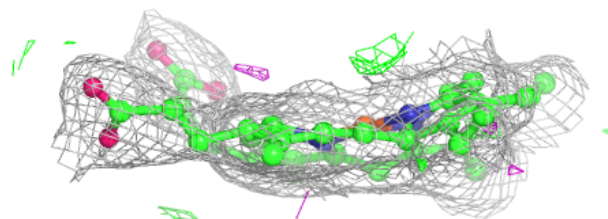
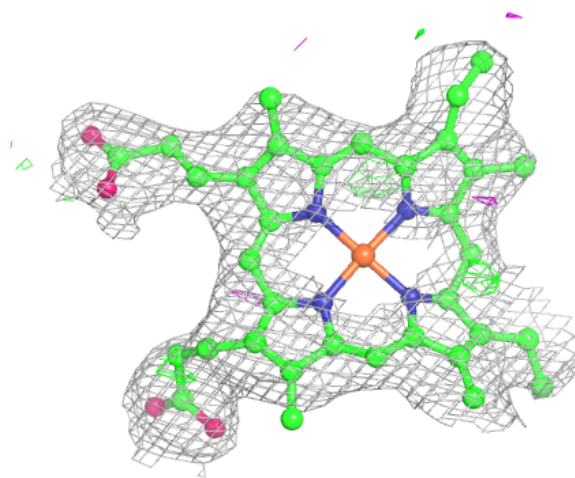






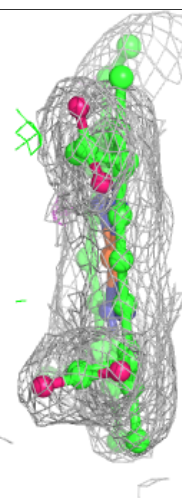
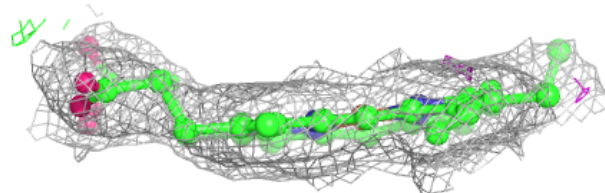
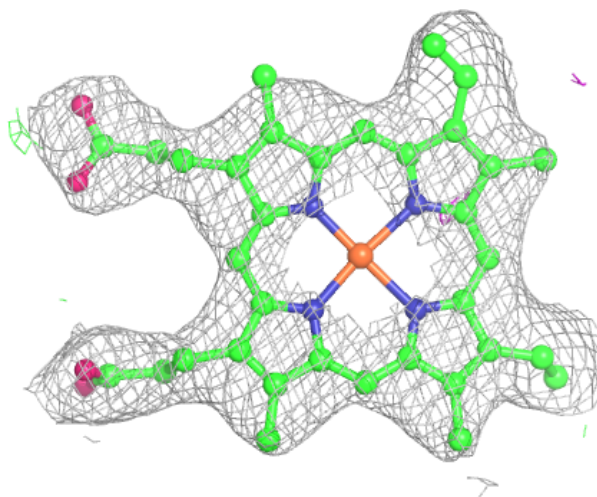
**Electron density around HEC I 603:**

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



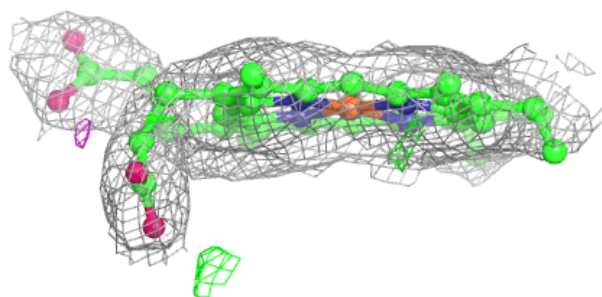
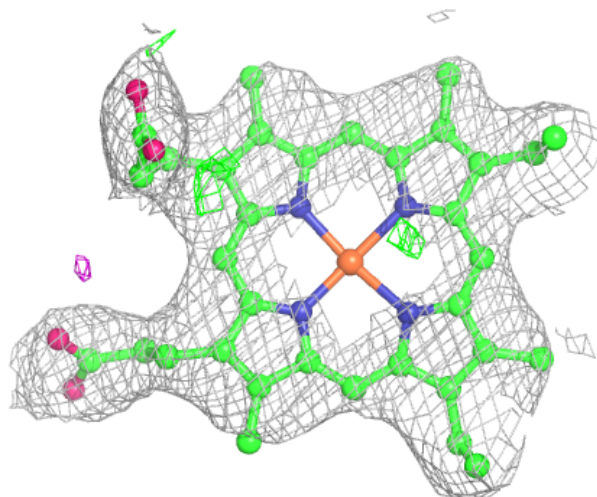
**Electron density around HEC I 600:**

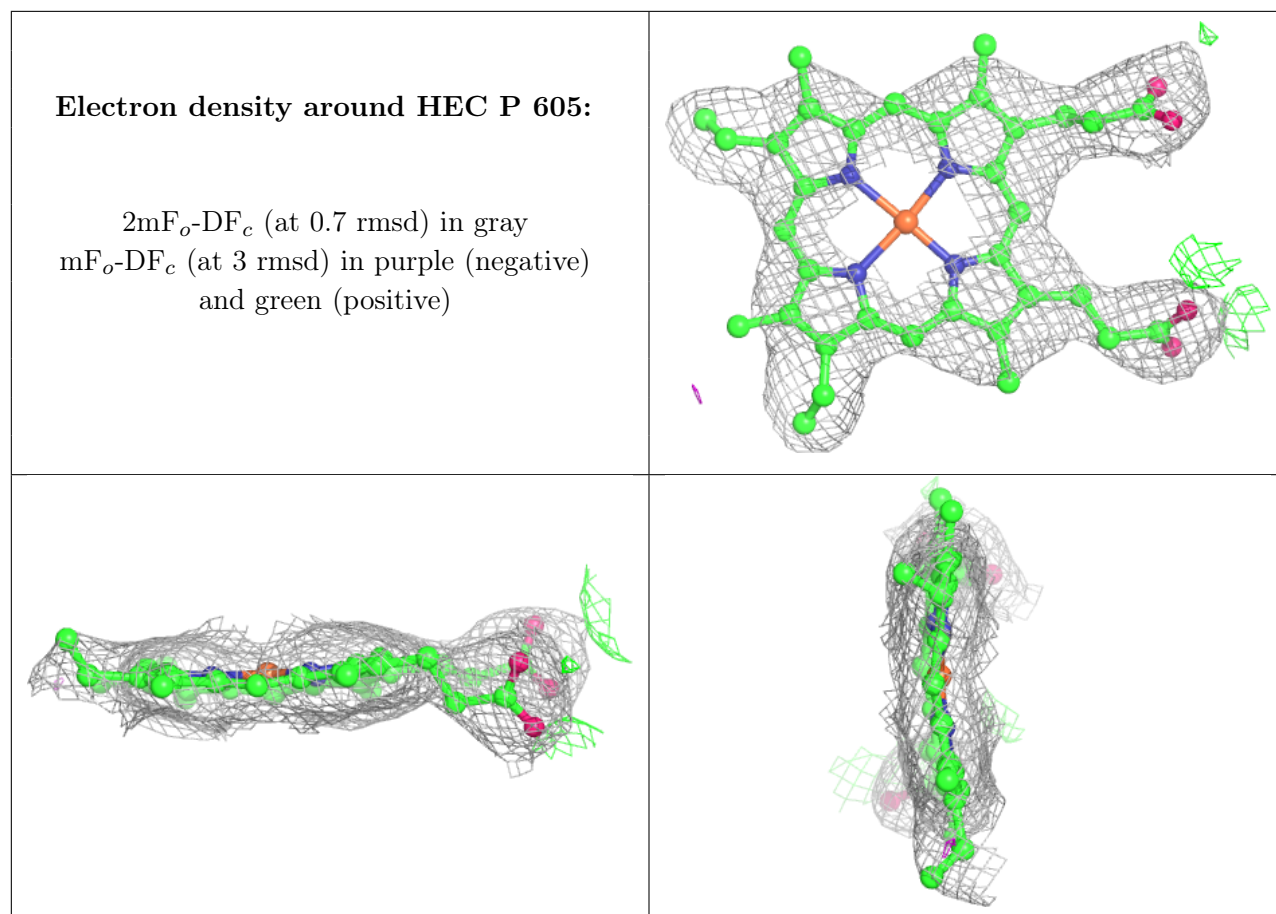
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



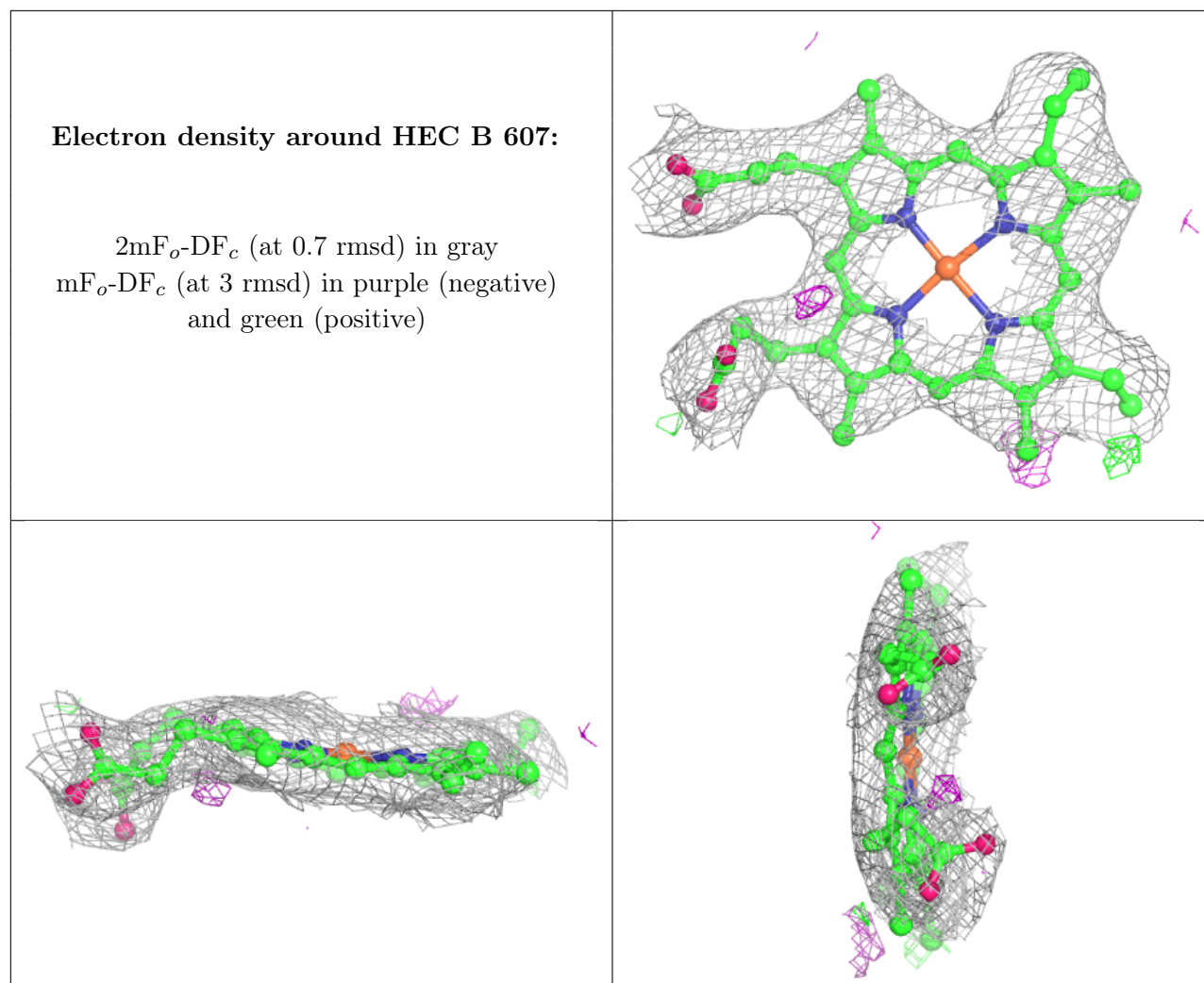
**Electron density around HEC I 601:**

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



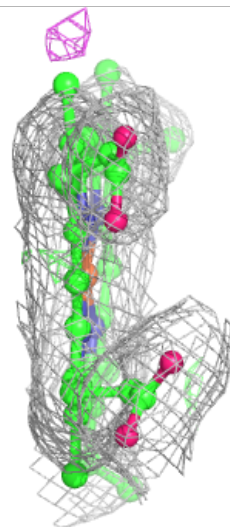
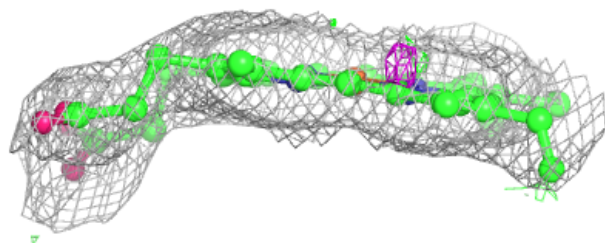
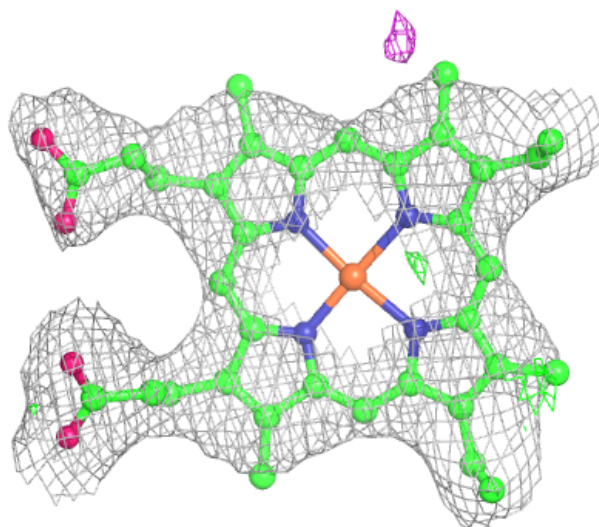






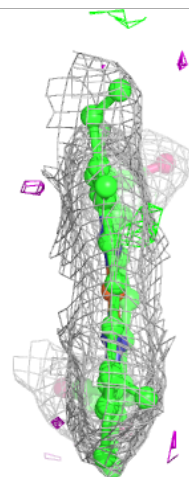
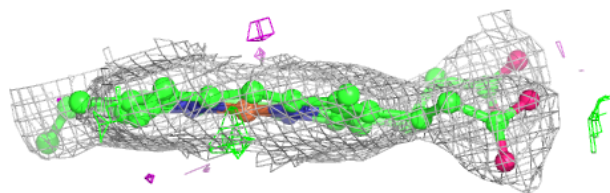
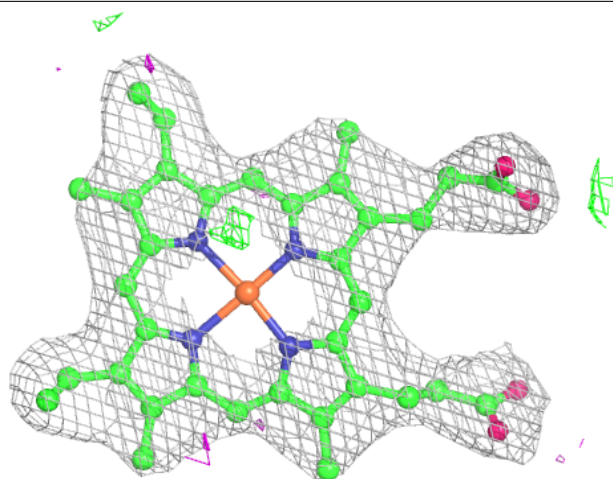
**Electron density around HEC I 604:**

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



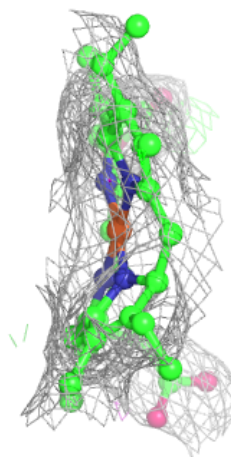
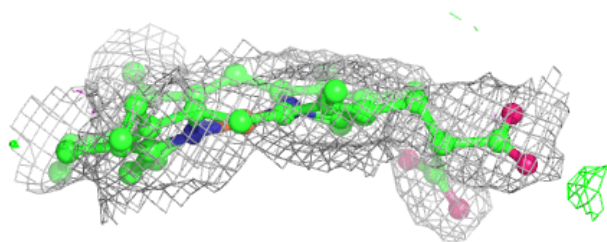
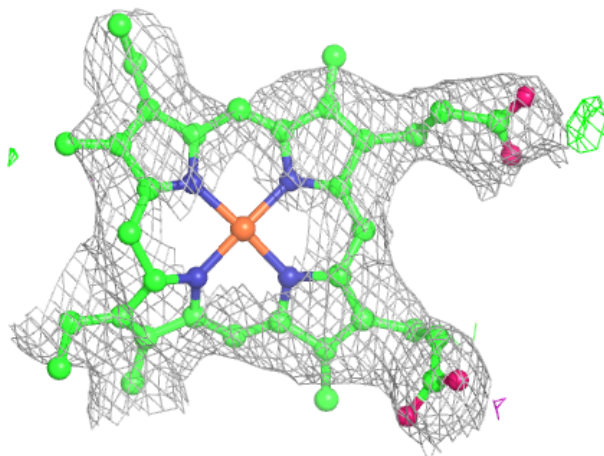
**Electron density around HEC I 605:**

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



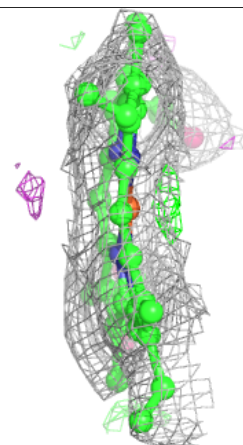
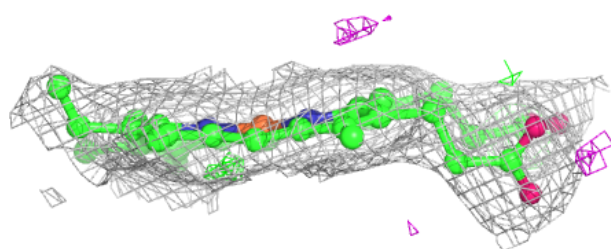
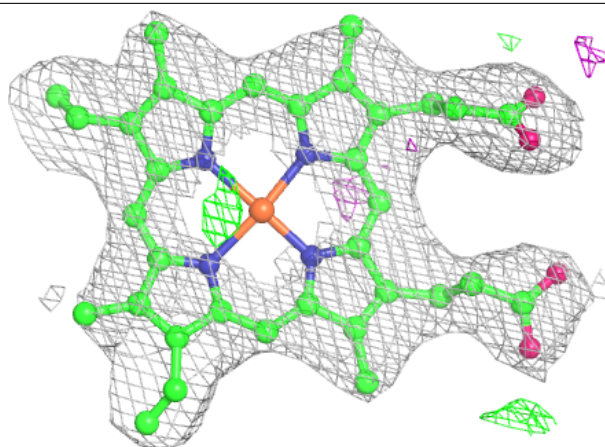
**Electron density around HEC Q 603:**

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



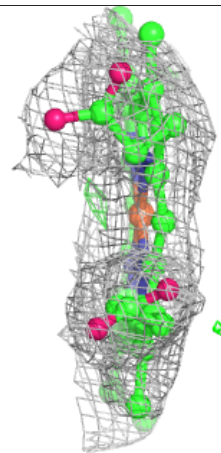
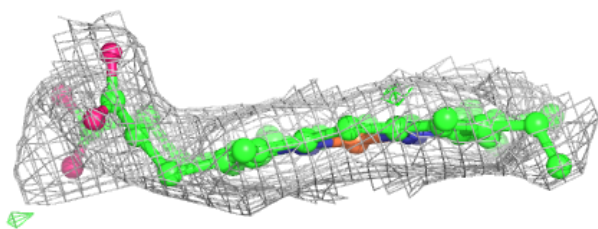
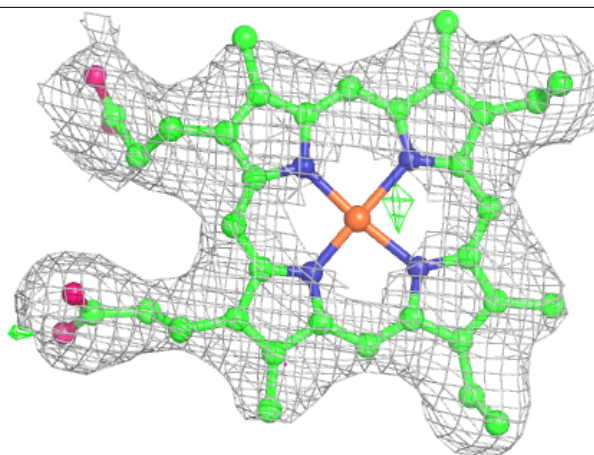
**Electron density around HEC I 606:**

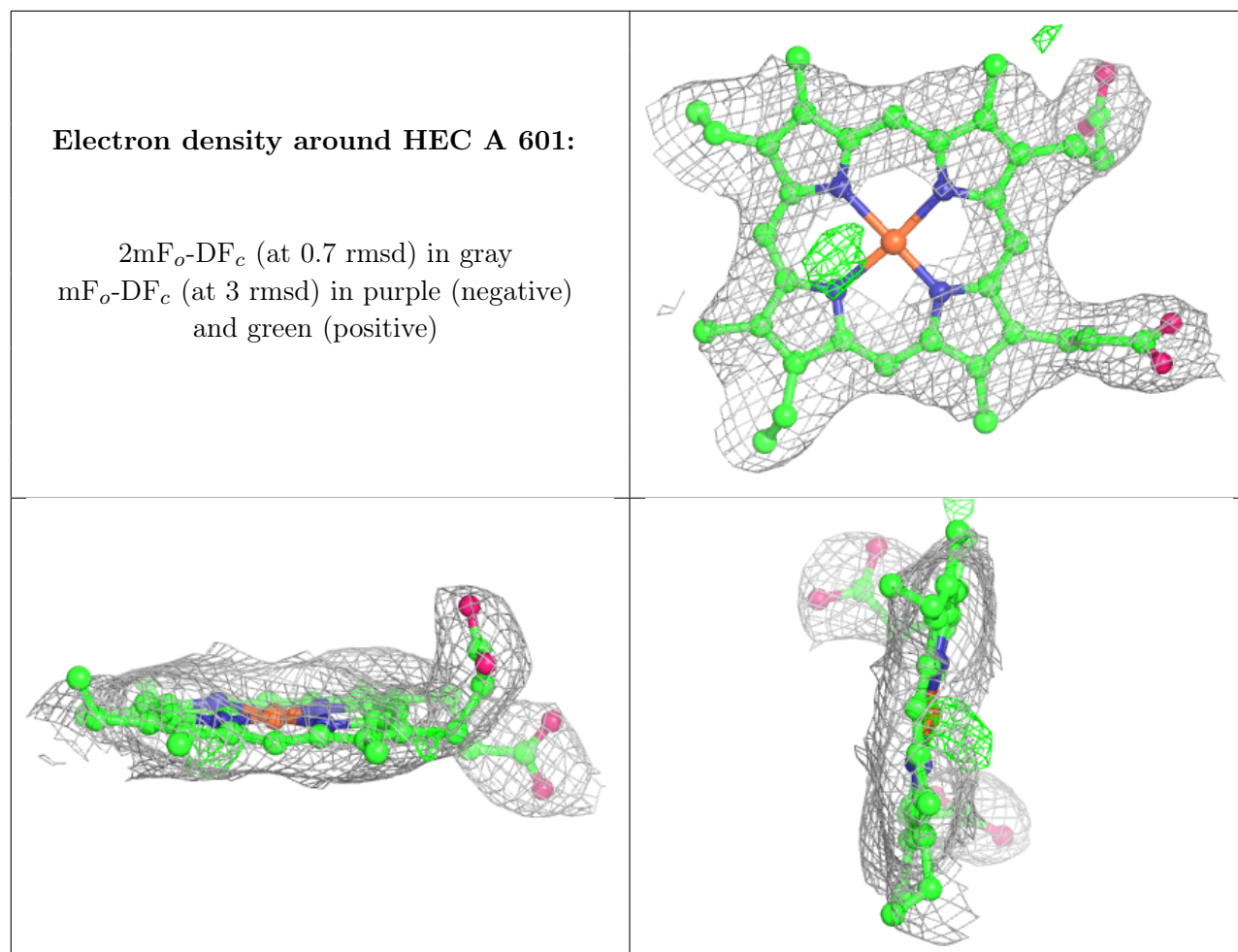
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC I 607:**

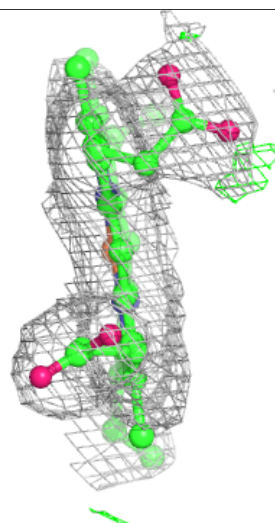
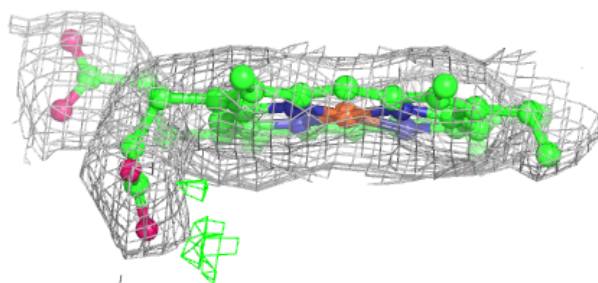
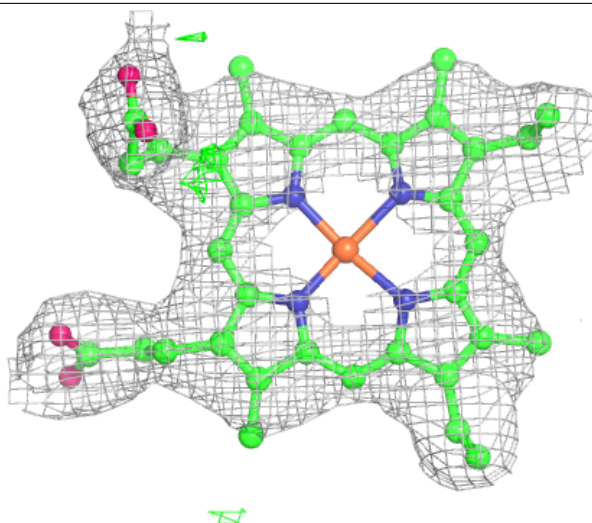
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC J 601:**

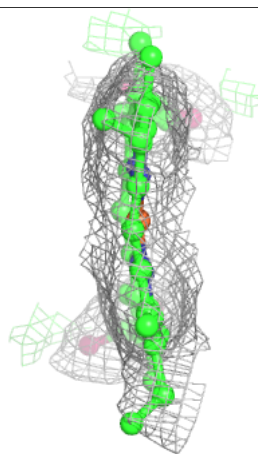
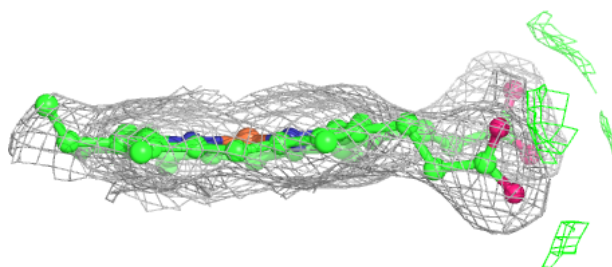
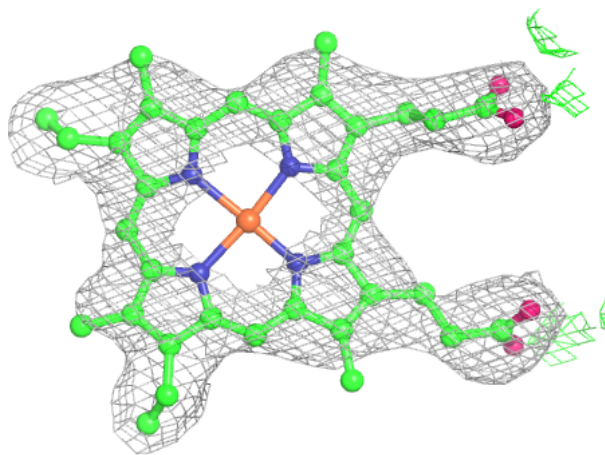
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

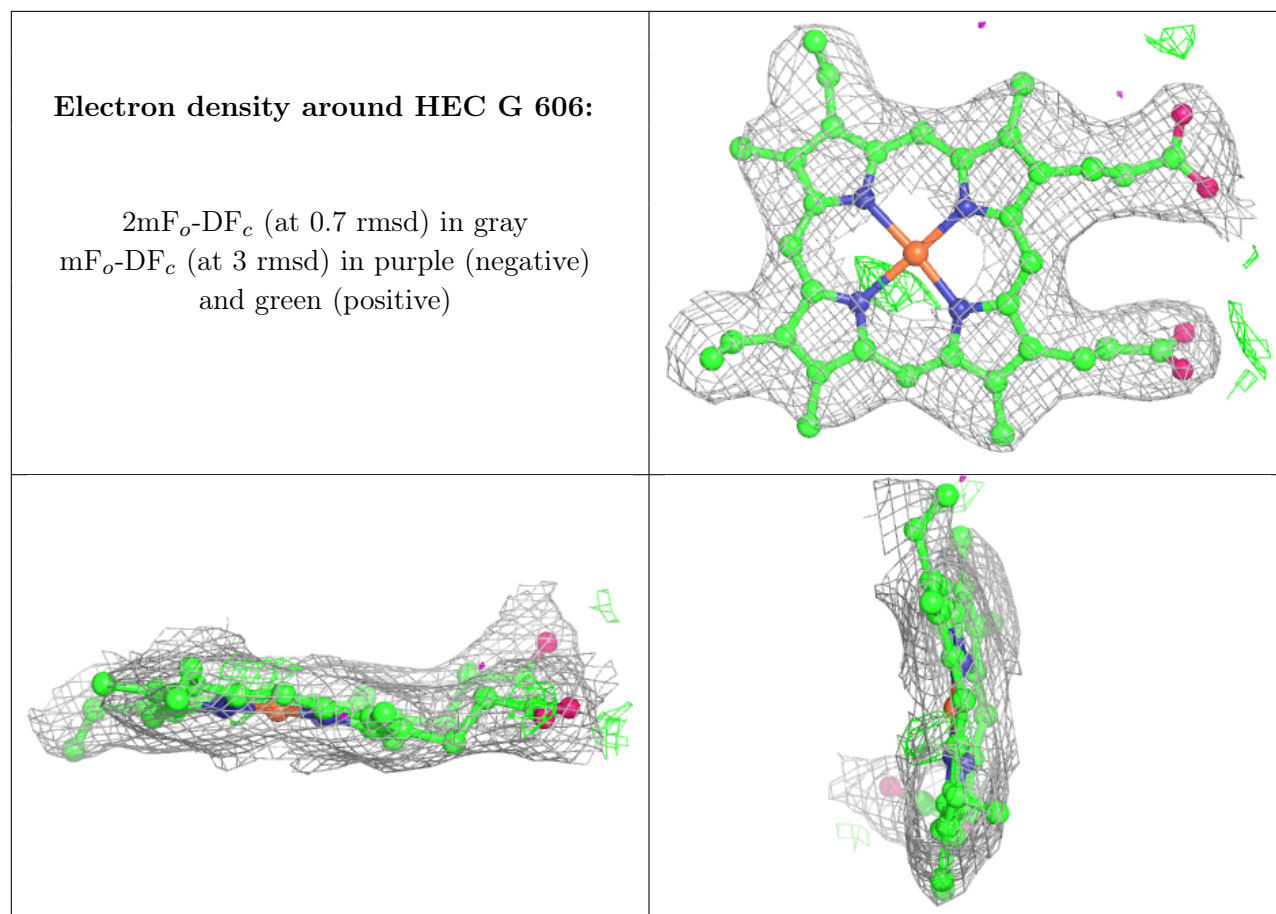




**Electron density around HEC Q 605:**

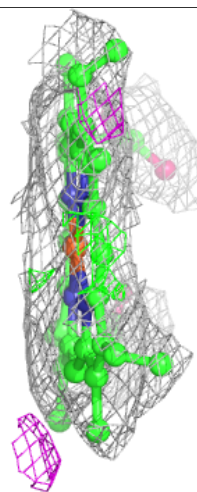
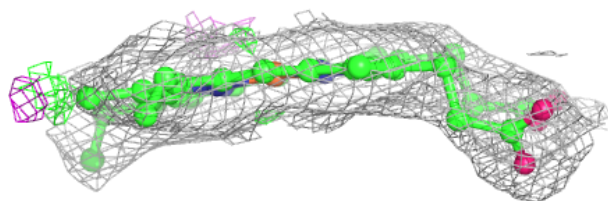
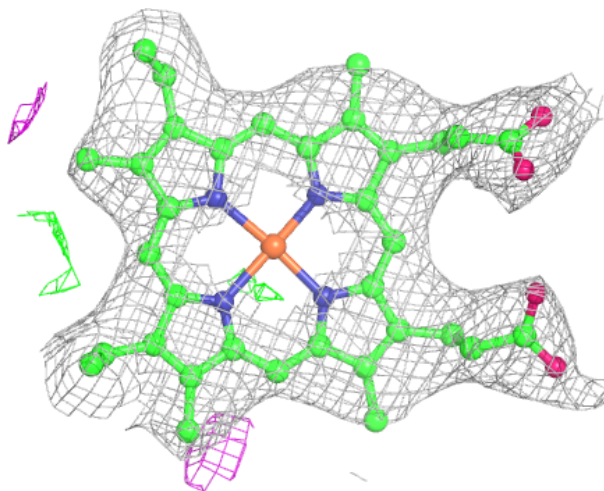
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





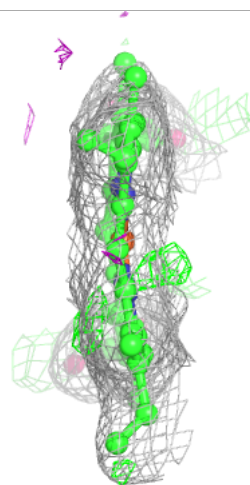
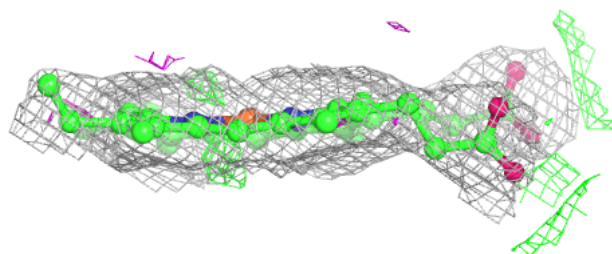
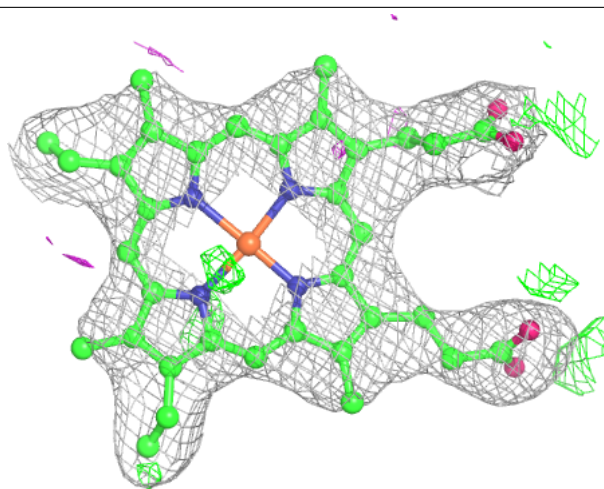
**Electron density around HEC J 604:**

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



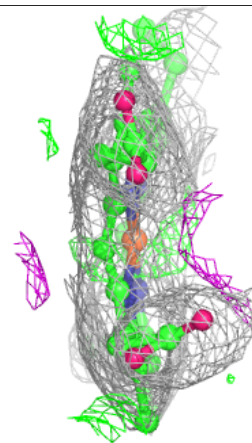
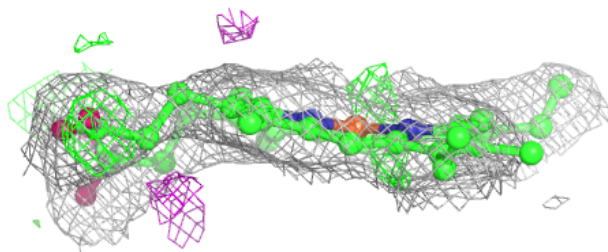
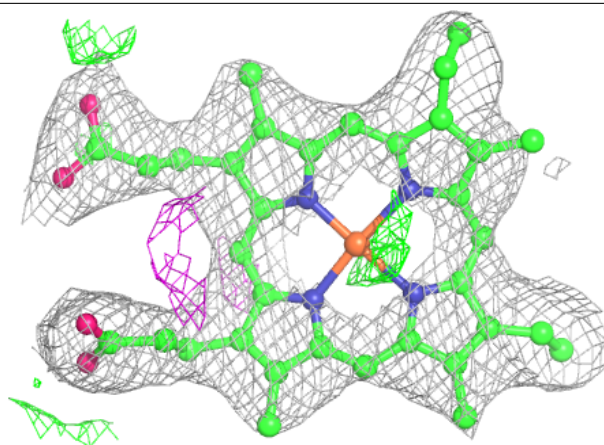
**Electron density around HEC J 605:**

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



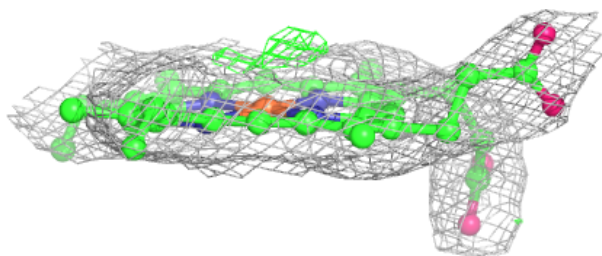
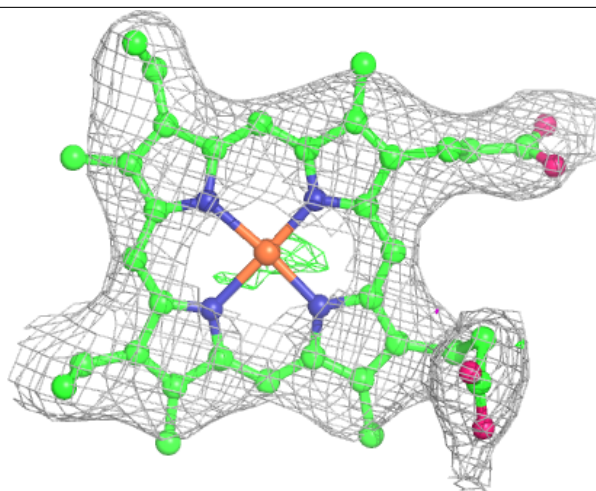
**Electron density around HEC J 606:**

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



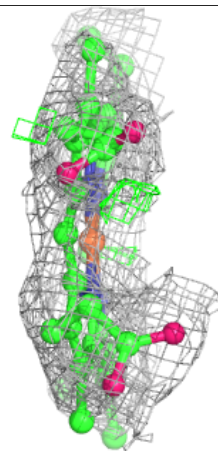
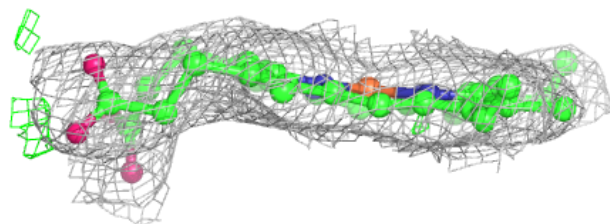
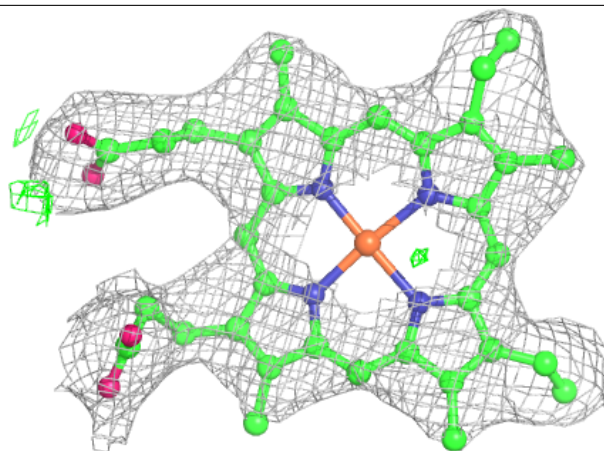
**Electron density around HEC R 601:**

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



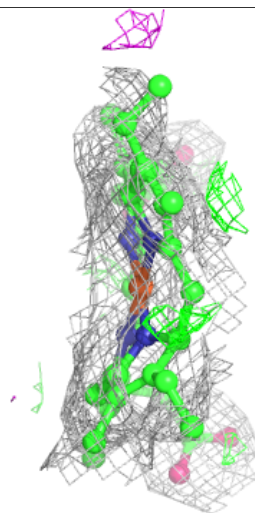
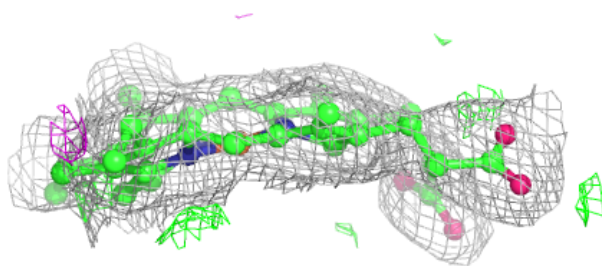
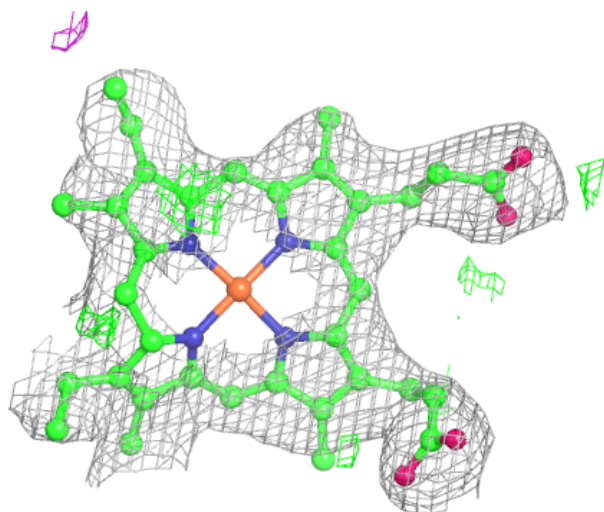
**Electron density around HEC J 607:**

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



**Electron density around HEC J 603:**

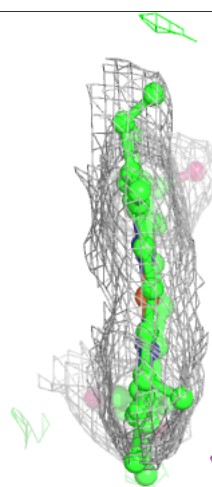
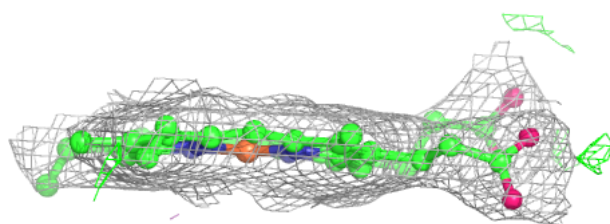
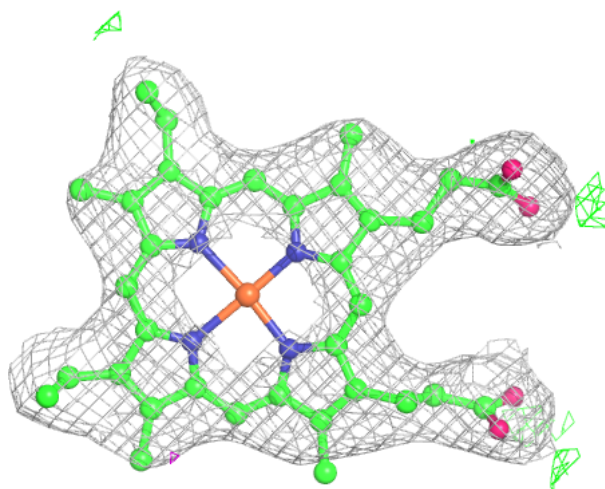
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

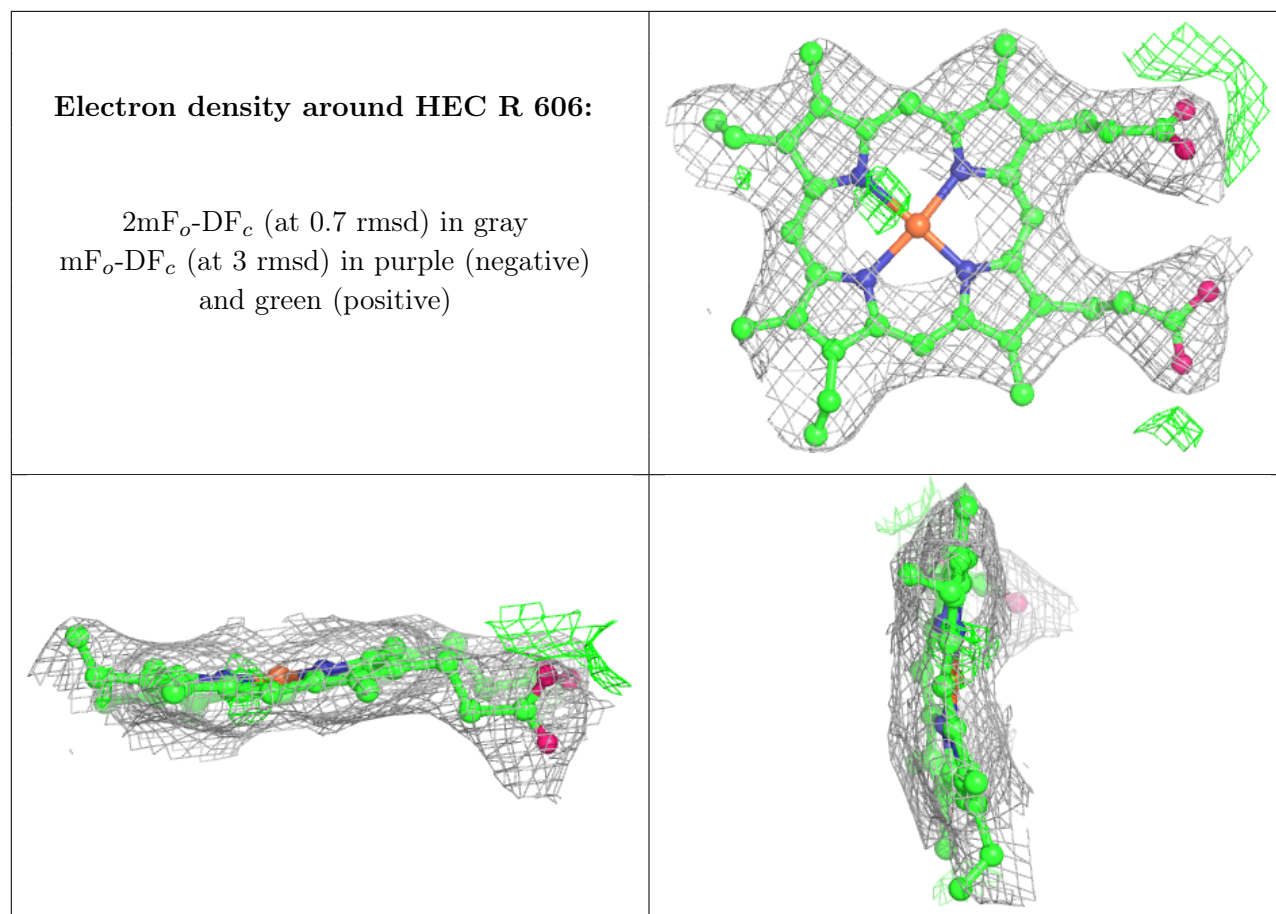


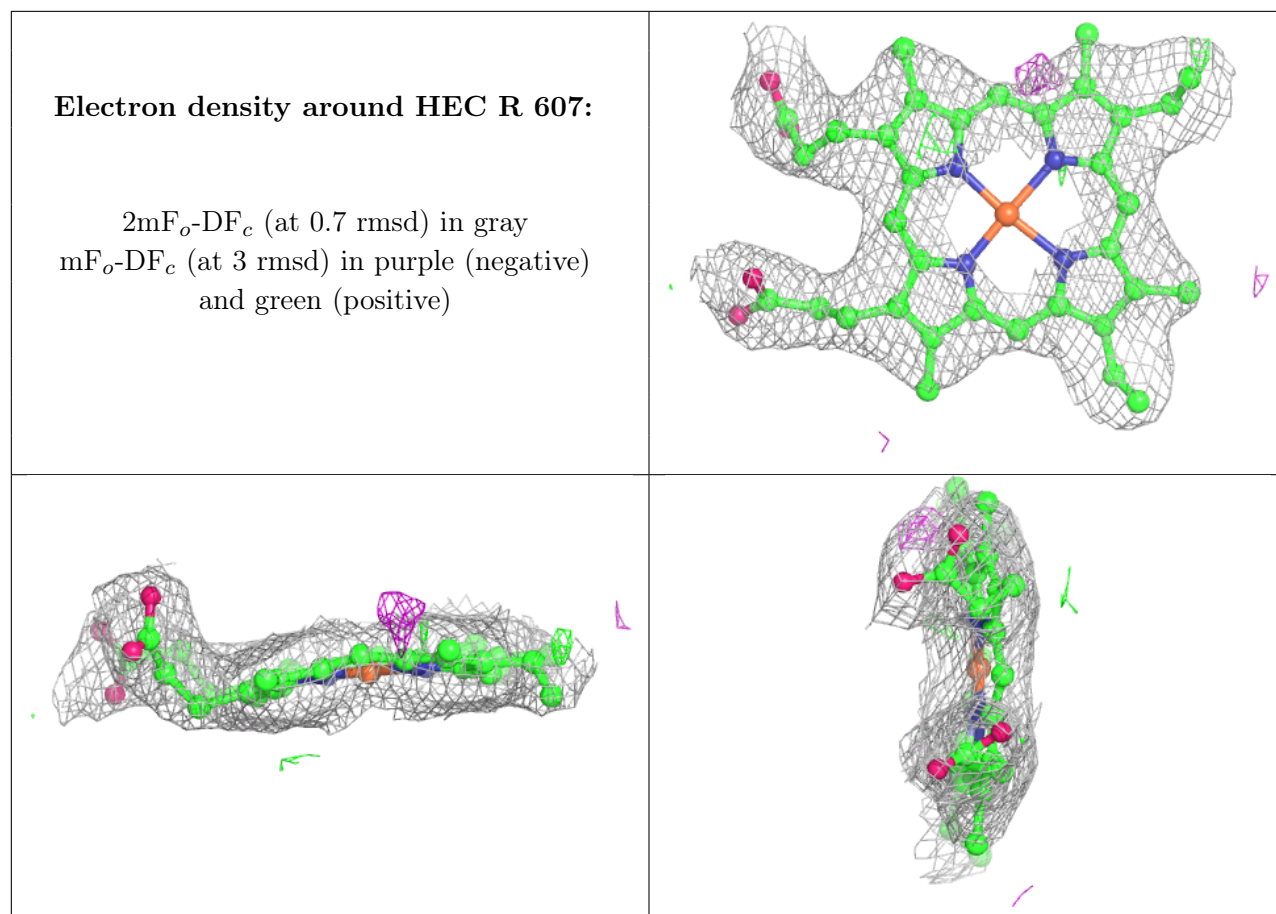


**Electron density around HEC R 605:**

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

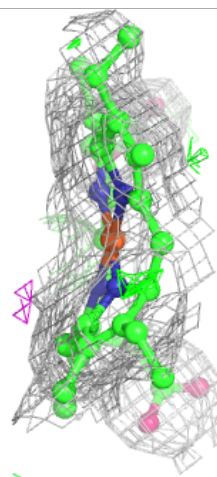
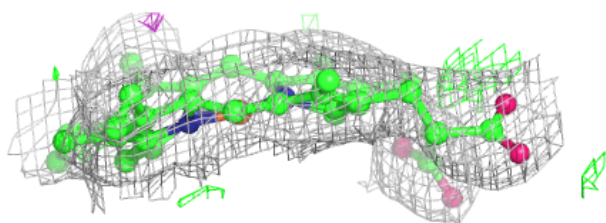
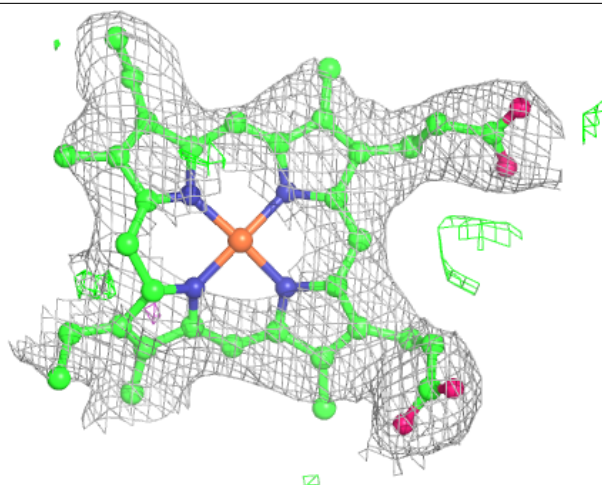






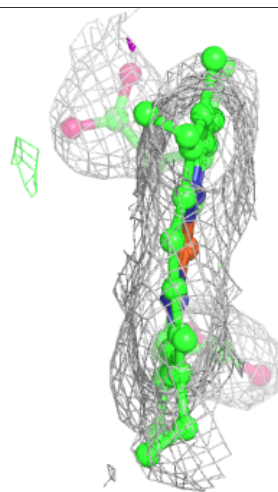
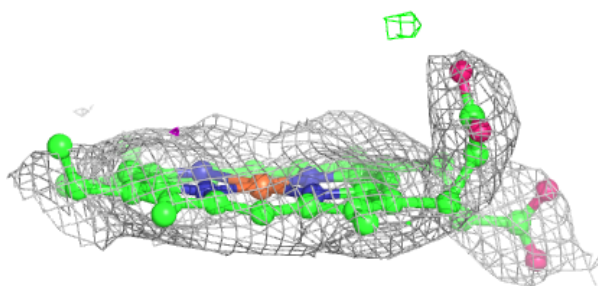
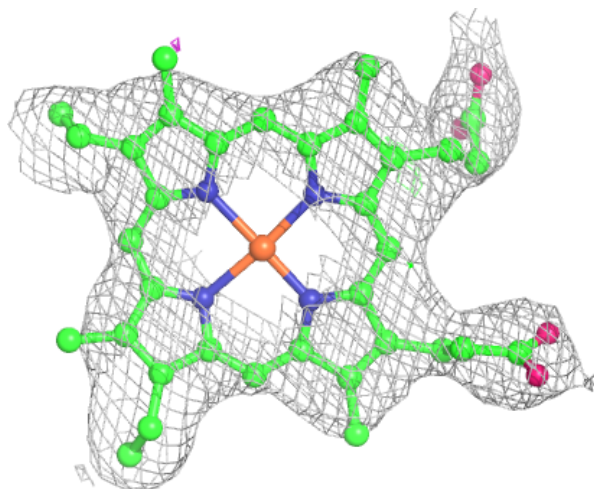
**Electron density around HEC K 603:**

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



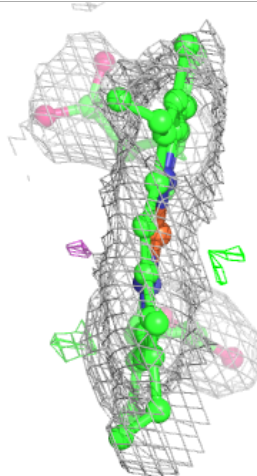
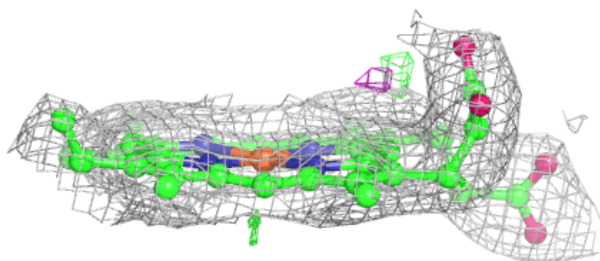
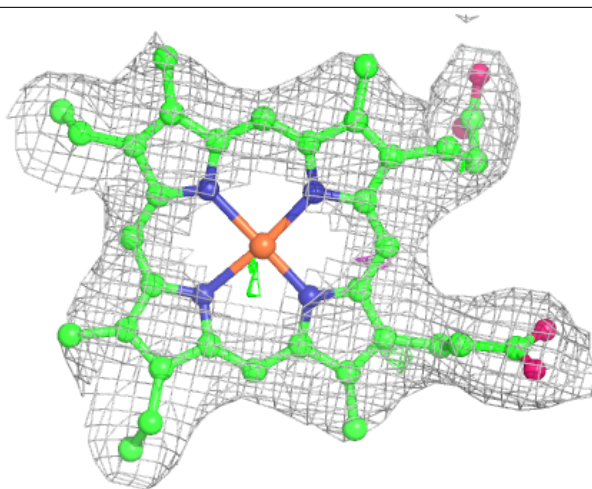
**Electron density around HEC C 601:**

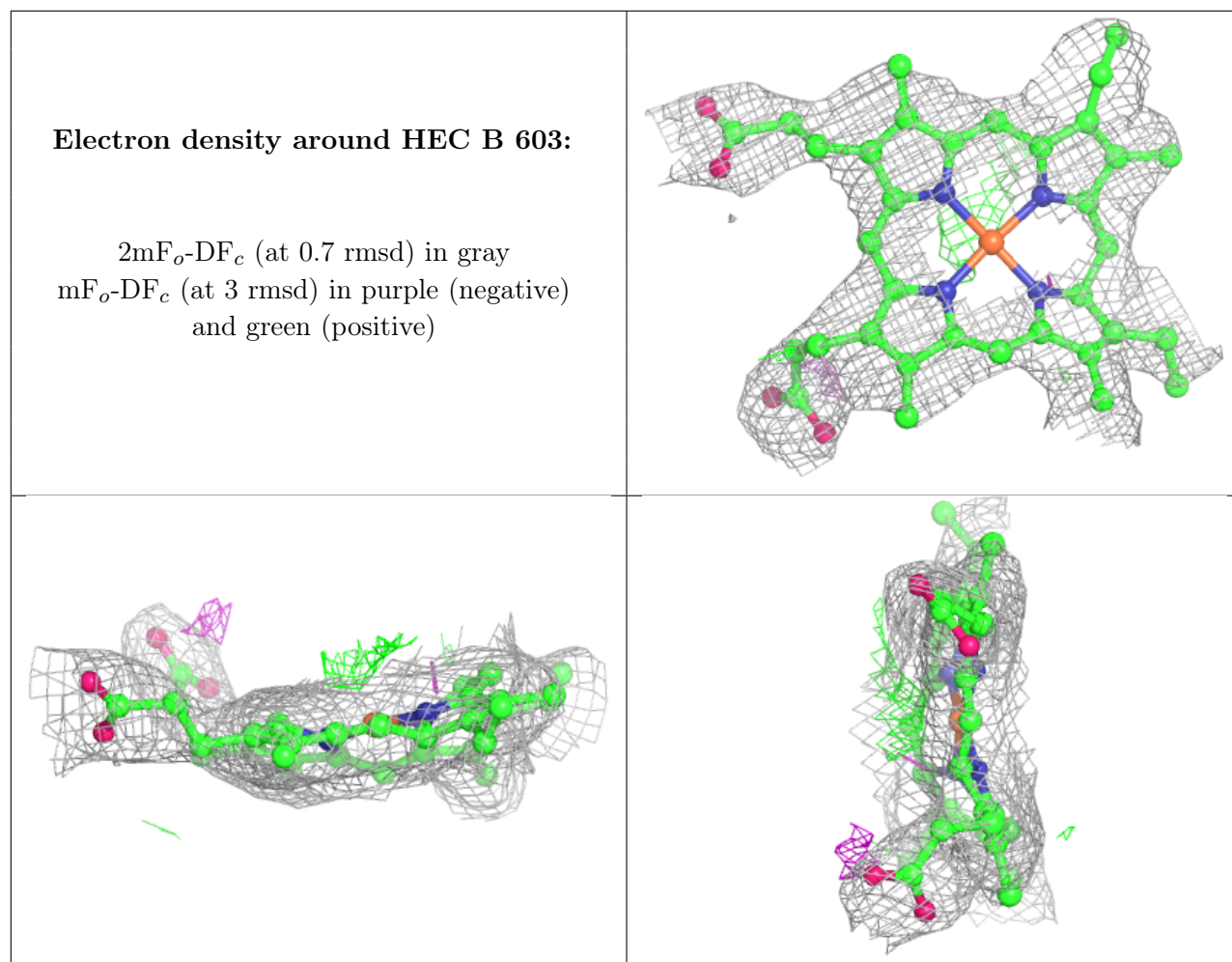
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

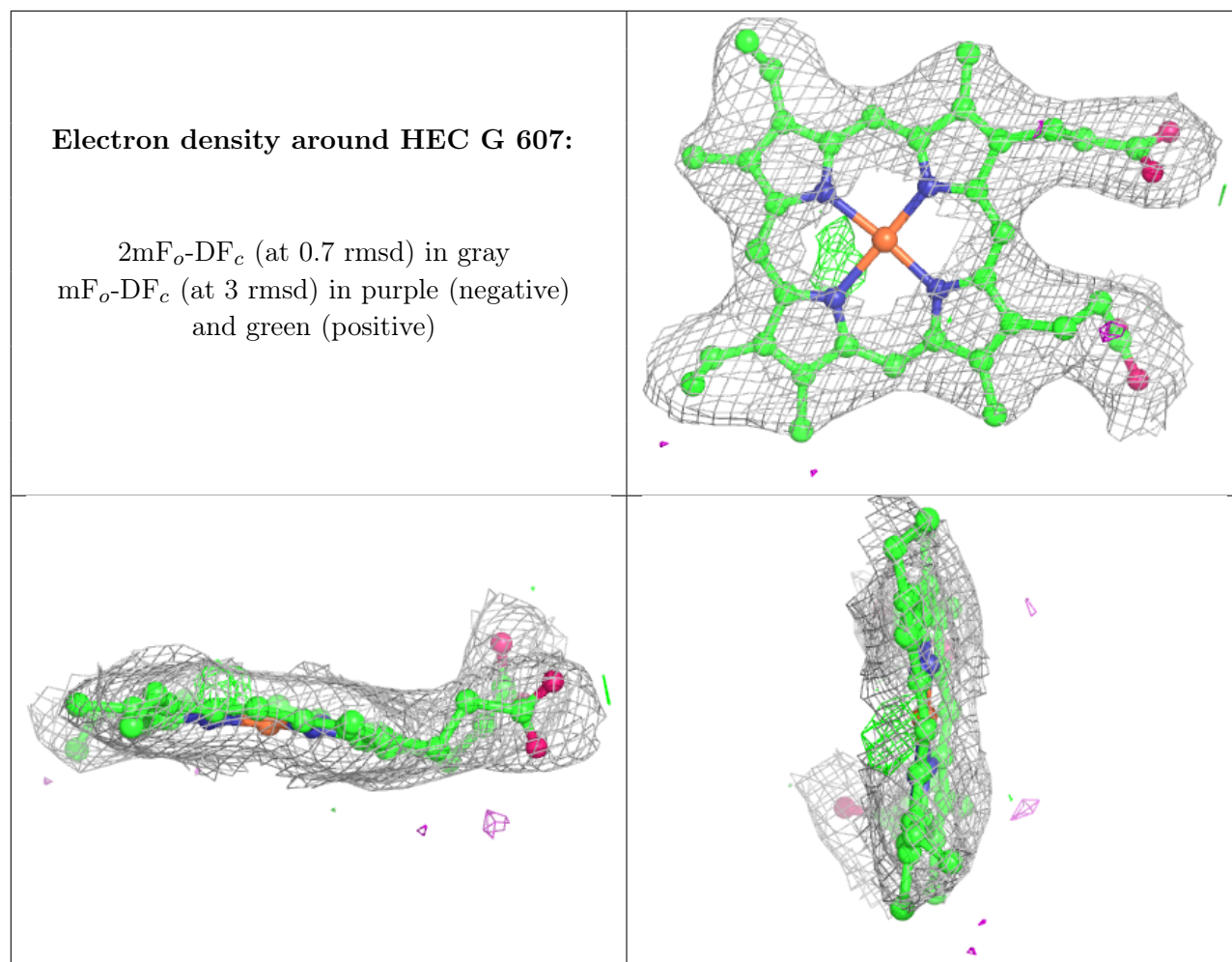


**Electron density around HEC K 601:**

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.