



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 17, 2021 – 07:27 PM JST

PDB ID : 6M0Q
Title : Hydroxylamine oxidoreductase from Nitrosomonas europaea
Authors : Fujiwara, T.; Fujimoto, Z.; Nishigaya, Y.; Yamazaki, T.
Deposited on : 2020-02-22
Resolution : 1.99 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.18
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)	:	2.18

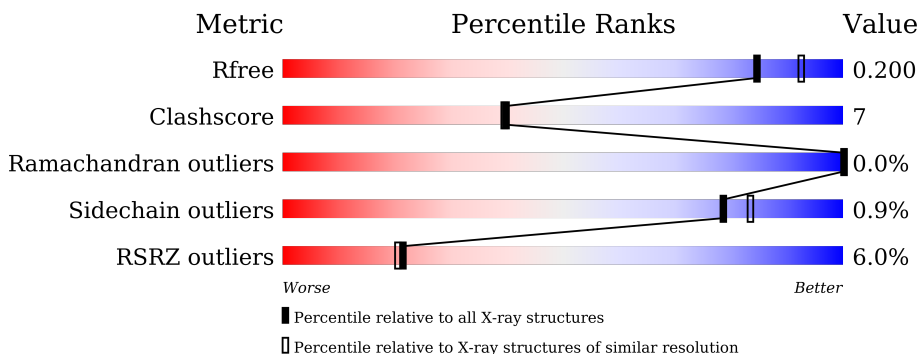
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 ≥ 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	570	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>9%</div> <div>12%</div> </div> </div>
1	C	570	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>9%</div> <div>12%</div> </div> </div>
1	E	570	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>9%</div> <div>12%</div> </div> </div>
1	G	570	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>7%</div> <div>12%</div> </div> </div>
1	I	570	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>11%</div> <div>12%</div> </div> </div>
1	K	570	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>11%</div> <div>12%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	B	91	
2	D	91	
2	F	91	
2	H	91	
2	J	91	
2	L	91	

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
6	PGE	G	611	-	-	X	-
6	PGE	I	609	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 31763 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.

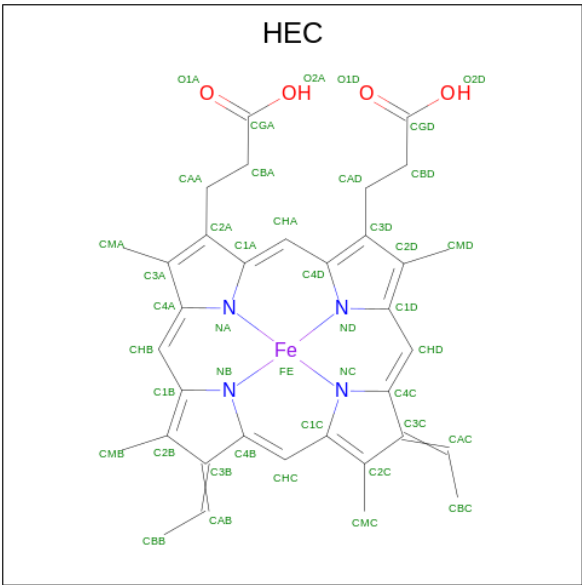
- Molecule 1 is a protein called Aerobic hydroxylamine oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	0	0
			4018	2499	713	774	32			
1	C	504	Total	C	N	O	S	0	0	0
			4018	2499	713	774	32			
1	E	504	Total	C	N	O	S	0	0	0
			4018	2499	713	774	32			
1	G	504	Total	C	N	O	S	0	0	0
			4018	2499	713	774	32			
1	I	504	Total	C	N	O	S	0	0	0
			4018	2499	713	774	32			
1	K	504	Total	C	N	O	S	0	0	0
			4018	2499	713	774	32			

- Molecule 2 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	64	Total	C	N	O	S	0	0	0
			486	302	85	96	3			
2	D	64	Total	C	N	O	S	0	0	0
			486	302	85	96	3			
2	F	64	Total	C	N	O	S	0	0	0
			486	302	85	96	3			
2	H	64	Total	C	N	O	S	0	0	0
			486	302	85	96	3			
2	J	64	Total	C	N	O	S	0	0	0
			486	302	85	96	3			
2	L	64	Total	C	N	O	S	0	0	0
			486	302	85	96	3			

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



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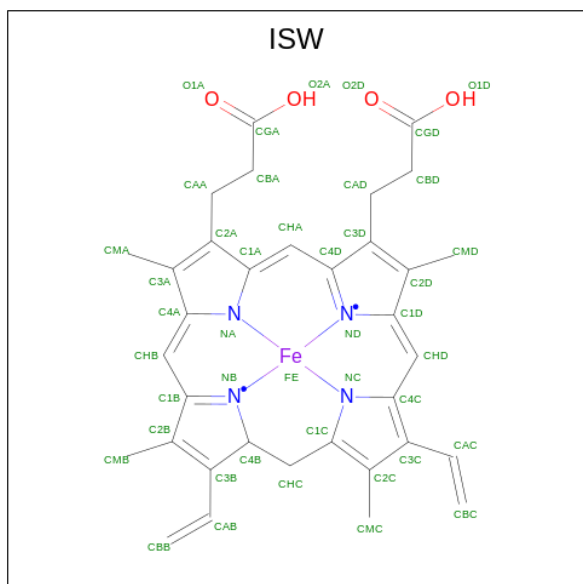
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0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

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

- Molecule 4 is {3,3'-[(9S)-8,13-diethenyl-3,7,12,17-tetramethyl-9,10-dihydroporphyrin-2,18-diyl-kappa 4 N 21 ,N 22 ,N 23 ,N 24]dipropionoato(2-)}iron (three-letter code: ISW) (formula: C₃₄H₃₄FeN₄O₄).



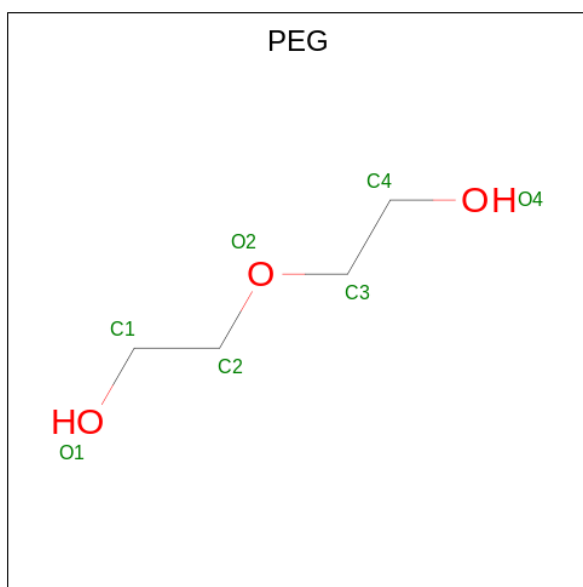
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
4	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
4	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	

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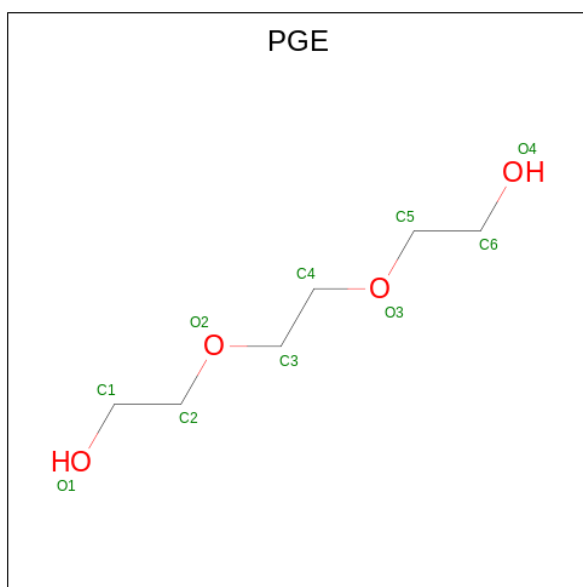
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	G	1	Total	C	Fe	N	O	
			43	34	1	4	4	
4	G	1	Total	C	Fe	N	O	
			43	34	1	4	4	
4	I	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



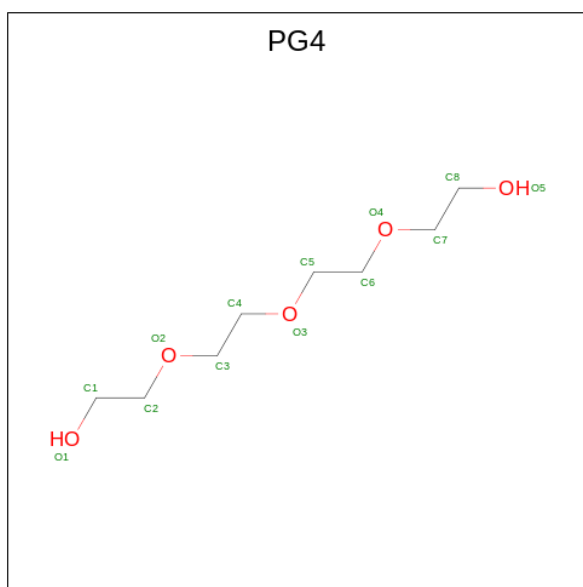
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O		
			7	4	3		
5	C	1	Total	C	O		
			7	4	3		
5	G	1	Total	C	O		
			7	4	3		
5	J	1	Total	C	O		
			7	4	3		
5	K	1	Total	C	O		
			7	4	3		
5	K	1	Total	C	O		
			7	4	3		

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		
6	C	1	Total	C	O	0	0
			10	6	4		
6	E	1	Total	C	O	0	0
			10	6	4		
6	E	1	Total	C	O	0	0
			10	6	4		
6	G	1	Total	C	O	0	0
			10	6	4		
6	G	1	Total	C	O	0	0
			10	6	4		
6	I	1	Total	C	O	0	0
			10	6	4		
6	I	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	8	5		
7	C	1	Total	C	O	0	0
			13	8	5		
7	E	1	Total	C	O	0	0
			13	8	5		
7	K	1	Total	C	O	0	0
			13	8	5		

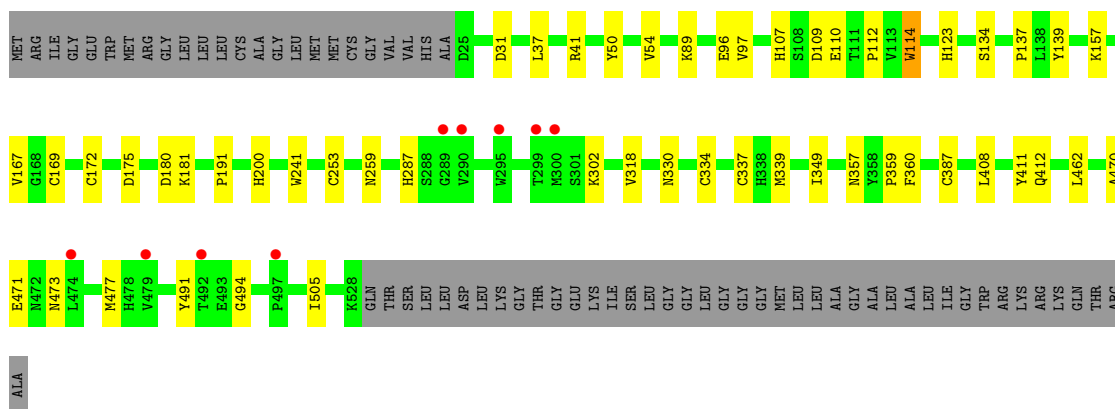
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	422	Total	O	0	0
			422	422		
8	B	49	Total	O	0	0
			49	49		
8	C	383	Total	O	0	0
			383	383		
8	D	66	Total	O	0	0
			66	66		
8	E	393	Total	O	0	0
			393	393		
8	F	42	Total	O	0	0
			42	42		
8	G	351	Total	O	0	0
			351	351		
8	H	40	Total	O	0	0
			40	40		

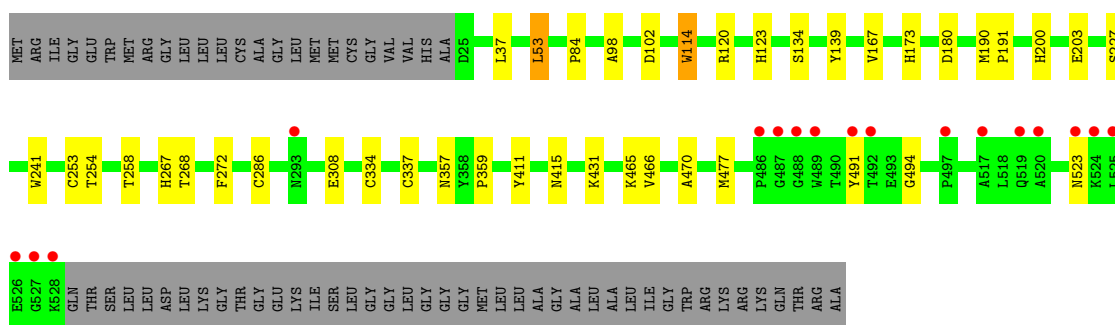
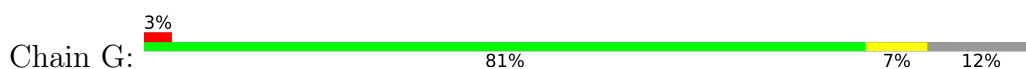
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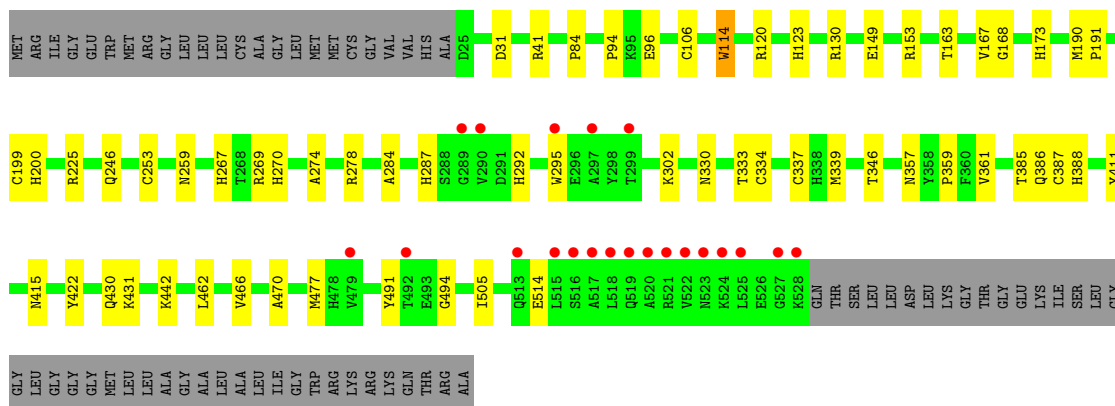
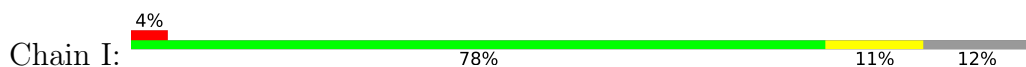
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	I	313	Total 313	O 313	0	0
8	J	58	Total 58	O 58	0	0
8	K	351	Total 351	O 351	0	0
8	L	33	Total 33	O 33	0	0



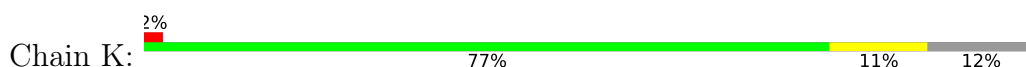
- Molecule 1: Aerobic hydroxylamine oxidoreductase

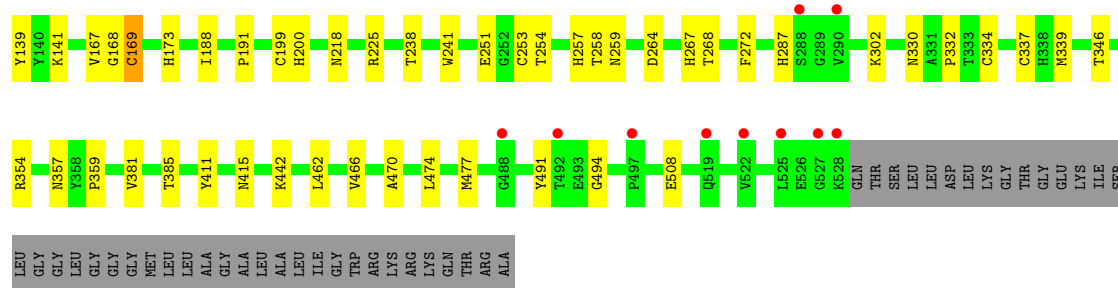


- Molecule 1: Aerobic hydroxylamine oxidoreductase

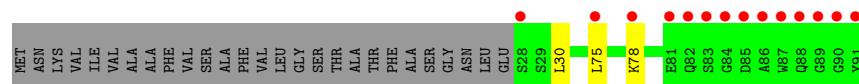


- Molecule 1: Aerobic hydroxylamine oxidoreductase

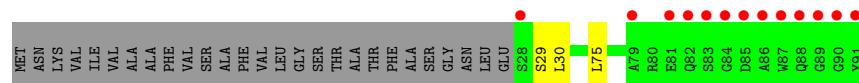




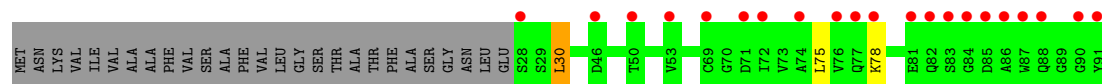
- Molecule 2: Uncharacterized protein



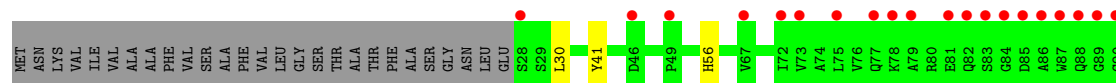
- Molecule 2: Uncharacterized protein



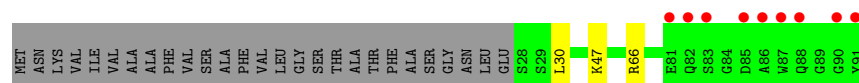
- Molecule 2: Uncharacterized protein



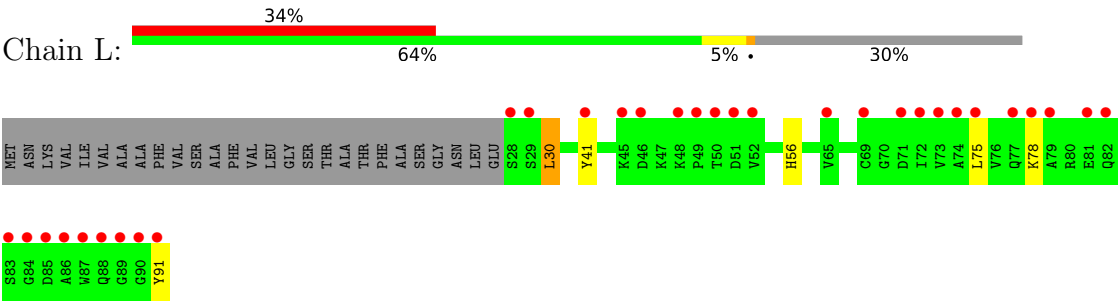
- Molecule 2: Uncharacterized protein



- Molecule 2: Uncharacterized protein



● Molecule 2: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	141.23Å 141.91Å 213.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.18 – 1.99 48.73 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.18-1.99) 99.9 (48.73-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.163 , 0.200 0.163 , 0.200	Depositor DCC
R_{free} test set	14603 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	31763	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, PGE, PG4, PEG, ISW

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	0.49	0/4121	0.62	0/5583
1	C	0.48	0/4121	0.62	0/5583
1	E	0.50	0/4121	0.62	0/5583
1	G	0.48	0/4121	0.59	0/5583
1	I	0.46	0/4121	0.59	0/5583
1	K	0.48	0/4121	0.61	1/5583 (0.0%)
2	B	0.45	0/492	0.62	0/660
2	D	0.42	0/492	0.64	1/660 (0.2%)
2	F	0.38	0/492	0.56	0/660
2	H	0.41	0/492	0.56	0/660
2	J	0.41	0/492	0.65	1/660 (0.2%)
2	L	0.34	0/492	0.55	0/660
All	All	0.47	0/27678	0.61	3/37458 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	354	ARG	NE-CZ-NH2	-7.36	116.62	120.30
2	J	66	ARG	NE-CZ-NH1	-5.12	117.74	120.30
2	D	75	LEU	CA-CB-CG	5.07	126.96	115.30

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	4018	0	3822	46	0
1	C	4018	0	3823	52	0
1	E	4018	0	3822	47	0
1	G	4018	0	3822	40	0
1	I	4018	0	3824	64	0
1	K	4018	0	3822	51	0
2	B	486	0	491	1	0
2	D	486	0	491	0	0
2	F	486	0	491	2	0
2	H	486	0	491	2	0
2	J	486	0	491	1	0
2	L	486	0	491	4	0
3	A	301	0	212	26	0
3	C	301	0	212	28	0
3	E	301	0	211	27	0
3	G	301	0	211	24	0
3	I	301	0	214	33	0
3	K	301	0	211	29	0
4	A	86	0	56	22	0
4	C	43	0	28	11	0
4	G	86	0	56	21	0
4	I	43	0	28	7	0
5	A	7	0	10	0	0
5	C	7	0	10	1	0
5	G	7	0	10	0	0
5	J	7	0	10	2	0
5	K	14	0	20	2	0
6	A	10	0	14	1	0
6	C	10	0	14	2	0
6	E	20	0	28	3	0
6	G	20	0	28	8	0
6	I	20	0	28	11	0
7	A	13	0	18	2	0
7	C	13	0	18	3	0
7	E	13	0	18	1	0
7	K	13	0	18	0	0
8	A	422	0	0	5	0
8	B	49	0	0	0	0
8	C	383	0	0	5	0
8	D	66	0	0	0	0
8	E	393	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	42	0	0	0	0
8	G	351	0	0	4	0
8	H	40	0	0	0	0
8	I	313	0	0	6	0
8	J	58	0	0	1	0
8	K	351	0	0	2	0
8	L	33	0	0	0	0
All	All	31763	0	27564	393	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 393 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)
4:G:608:ISW:C4B	1:I:491:TYR:OH	1.74	1.21
1:I:337:CYS:SG	3:I:605:HEC:HAC	1.81	1.18
4:A:608:ISW:C4B	1:C:491:TYR:OH	1.75	1.15
1:C:337:CYS:SG	3:C:605:HEC:HAC	1.87	1.09
1:G:337:CYS:SG	3:G:605:HEC:HAC	1.82	1.09

There are no symmetry-related clashes.

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	502/570 (88%)	487 (97%)	15 (3%)	0	100	100
1	C	502/570 (88%)	489 (97%)	13 (3%)	0	100	100
1	E	502/570 (88%)	488 (97%)	14 (3%)	0	100	100
1	G	502/570 (88%)	486 (97%)	16 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	502/570 (88%)	489 (97%)	12 (2%)	1 (0%)	47	44
1	K	502/570 (88%)	488 (97%)	14 (3%)	0	100	100
2	B	62/91 (68%)	61 (98%)	1 (2%)	0	100	100
2	D	62/91 (68%)	61 (98%)	1 (2%)	0	100	100
2	F	62/91 (68%)	61 (98%)	1 (2%)	0	100	100
2	H	62/91 (68%)	61 (98%)	1 (2%)	0	100	100
2	J	62/91 (68%)	61 (98%)	1 (2%)	0	100	100
2	L	62/91 (68%)	61 (98%)	1 (2%)	0	100	100
All	All	3384/3966 (85%)	3293 (97%)	90 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	292	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	430/477 (90%)	426 (99%)	4 (1%)	78	83
1	C	430/477 (90%)	428 (100%)	2 (0%)	88	92
1	E	430/477 (90%)	428 (100%)	2 (0%)	88	92
1	G	430/477 (90%)	426 (99%)	4 (1%)	78	83
1	I	430/477 (90%)	428 (100%)	2 (0%)	88	92
1	K	430/477 (90%)	426 (99%)	4 (1%)	78	83
2	B	53/73 (73%)	52 (98%)	1 (2%)	57	61
2	D	53/73 (73%)	51 (96%)	2 (4%)	33	31
2	F	53/73 (73%)	52 (98%)	1 (2%)	57	61
2	H	53/73 (73%)	52 (98%)	1 (2%)	57	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	53/73 (73%)	52 (98%)	1 (2%)	57	61
2	L	53/73 (73%)	52 (98%)	1 (2%)	57	61
All	All	2898/3300 (88%)	2873 (99%)	25 (1%)	78	83

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	267	HIS
1	I	114	TRP
2	L	30	LEU
2	H	30	LEU
1	I	267	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	56	HIS
2	L	61	ASN

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](#)

66 ligands are modelled in this entry.

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	K	601	1	26,50,50	2.04	3 (11%)	18,82,82	2.51	7 (38%)
3	HEC	E	601	1	26,50,50	2.22	4 (15%)	18,82,82	2.57	7 (38%)
3	HEC	C	601	1	26,50,50	2.28	3 (11%)	18,82,82	2.33	6 (33%)
3	HEC	A	604	1	26,50,50	2.17	3 (11%)	18,82,82	2.38	5 (27%)
3	HEC	C	605	1	26,50,50	2.45	4 (15%)	18,82,82	2.23	5 (27%)
6	PGE	E	608	-	9,9,9	0.36	0	8,8,8	0.31	0
3	HEC	G	603	1	26,50,50	2.01	3 (11%)	18,82,82	2.98	7 (38%)
4	ISW	A	609	8,1	30,50,50	4.40	12 (40%)	20,82,82	5.23	14 (70%)
3	HEC	G	605	1	26,50,50	2.29	3 (11%)	18,82,82	2.42	7 (38%)
3	HEC	E	602	1	26,50,50	2.32	4 (15%)	18,82,82	2.28	8 (44%)
3	HEC	G	604	1	26,50,50	2.42	4 (15%)	18,82,82	1.87	5 (27%)
4	ISW	G	608	1	30,50,50	4.45	12 (40%)	20,82,82	5.38	12 (60%)
3	HEC	E	605	1	26,50,50	2.25	3 (11%)	18,82,82	2.27	7 (38%)
5	PEG	J	101	-	6,6,6	0.48	0	5,5,5	0.52	0
6	PGE	I	610	-	9,9,9	0.29	0	8,8,8	0.24	0
3	HEC	E	604	1	26,50,50	2.25	5 (19%)	18,82,82	2.00	6 (33%)
5	PEG	K	608	-	6,6,6	0.42	0	5,5,5	0.33	0
3	HEC	G	606	1	26,50,50	2.28	3 (11%)	18,82,82	2.86	8 (44%)
4	ISW	G	609	8,1	30,50,50	4.43	14 (46%)	20,82,82	4.75	12 (60%)
6	PGE	G	612	-	9,9,9	0.39	0	8,8,8	0.41	0
3	HEC	I	607	1	26,50,50	2.39	3 (11%)	18,82,82	2.53	7 (38%)
3	HEC	A	607	1	26,50,50	2.41	3 (11%)	18,82,82	2.26	7 (38%)
7	PG4	E	610	-	12,12,12	0.52	0	11,11,11	0.32	0
3	HEC	K	607	1	26,50,50	2.28	3 (11%)	18,82,82	2.52	7 (38%)
6	PGE	C	610	-	9,9,9	0.36	0	8,8,8	0.31	0
6	PGE	E	609	-	9,9,9	0.31	0	8,8,8	0.50	0
3	HEC	I	605	1	26,50,50	2.36	3 (11%)	18,82,82	2.48	7 (38%)
3	HEC	A	606	1	26,50,50	2.32	5 (19%)	18,82,82	2.48	8 (44%)
6	PGE	I	609	-	9,9,9	0.32	0	8,8,8	0.25	0
3	HEC	A	603	1	26,50,50	2.25	5 (19%)	18,82,82	2.61	8 (44%)
3	HEC	I	601	1	26,50,50	2.30	3 (11%)	18,82,82	1.88	5 (27%)
3	HEC	A	605	1	26,50,50	2.25	3 (11%)	18,82,82	2.33	7 (38%)
3	HEC	I	603	1	26,50,50	2.36	5 (19%)	18,82,82	2.27	8 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEC	I	604	1	26,50,50	2.40	4 (15%)	18,82,82	1.82	4 (22%)
4	ISW	A	608	8,1	30,50,50	4.51	11 (36%)	20,82,82	4.89	12 (60%)
3	HEC	E	607	1	26,50,50	2.24	4 (15%)	18,82,82	2.57	7 (38%)
3	HEC	E	603	1	26,50,50	2.28	5 (19%)	18,82,82	2.57	6 (33%)
3	HEC	K	603	1	26,50,50	2.17	4 (15%)	18,82,82	2.34	6 (33%)
3	HEC	K	604	1	26,50,50	2.37	3 (11%)	18,82,82	1.95	7 (38%)
3	HEC	C	603	1	26,50,50	2.07	3 (11%)	18,82,82	2.37	6 (33%)
7	PG4	K	610	-	12,12,12	0.56	0	11,11,11	0.34	0
3	HEC	G	601	1	26,50,50	2.16	4 (15%)	18,82,82	2.26	6 (33%)
3	HEC	K	605	1	26,50,50	2.27	4 (15%)	18,82,82	2.33	7 (38%)
4	ISW	C	608	8,1	30,50,50	4.58	11 (36%)	20,82,82	4.91	14 (70%)
7	PG4	A	612	-	12,12,12	0.53	0	11,11,11	0.31	0
3	HEC	C	606	1	26,50,50	2.31	4 (15%)	18,82,82	2.45	6 (33%)
3	HEC	E	606	1	26,50,50	2.30	3 (11%)	18,82,82	2.21	8 (44%)
3	HEC	C	604	1	26,50,50	2.50	5 (19%)	18,82,82	2.18	8 (44%)
4	ISW	I	608	8,1	30,50,50	4.59	11 (36%)	20,82,82	4.66	11 (55%)
3	HEC	K	606	1	26,50,50	2.39	4 (15%)	18,82,82	2.40	9 (50%)
7	PG4	C	611	-	12,12,12	0.52	0	11,11,11	0.29	0
6	PGE	G	611	-	9,9,9	0.34	0	8,8,8	0.40	0
5	PEG	C	609	-	6,6,6	0.48	0	5,5,5	0.38	0
5	PEG	K	609	-	6,6,6	0.47	0	5,5,5	0.41	0
3	HEC	I	602	1	26,50,50	2.33	3 (11%)	18,82,82	2.39	8 (44%)
3	HEC	A	602	1	26,50,50	2.27	5 (19%)	18,82,82	2.31	5 (27%)
3	HEC	C	607	1	26,50,50	2.45	7 (26%)	18,82,82	2.51	9 (50%)
3	HEC	G	602	1	26,50,50	2.28	4 (15%)	18,82,82	2.20	5 (27%)
5	PEG	G	610	-	6,6,6	0.50	0	5,5,5	0.25	0
3	HEC	G	607	1	26,50,50	2.33	5 (19%)	18,82,82	2.23	5 (27%)
6	PGE	A	611	-	9,9,9	0.35	0	8,8,8	0.35	0
5	PEG	A	610	-	6,6,6	0.50	0	5,5,5	0.41	0
3	HEC	K	602	1	26,50,50	2.23	4 (15%)	18,82,82	2.15	5 (27%)
3	HEC	I	606	1	26,50,50	2.26	3 (11%)	18,82,82	2.39	5 (27%)
3	HEC	A	601	1	26,50,50	1.94	3 (11%)	18,82,82	2.67	6 (33%)
3	HEC	C	602	1	26,50,50	2.28	3 (11%)	18,82,82	2.50	7 (38%)

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	K	601	1	-	0/6/54/54	-
3	HEC	E	601	1	-	1/6/54/54	-
3	HEC	C	601	1	-	0/6/54/54	-
3	HEC	A	604	1	-	2/6/54/54	-
3	HEC	C	605	1	-	1/6/54/54	-
6	PGE	E	608	-	-	4/7/7/7	-
3	HEC	G	603	1	-	0/6/54/54	-
4	ISW	A	609	8,1	-	1/8/74/74	-
3	HEC	G	605	1	-	1/6/54/54	-
3	HEC	E	602	1	-	0/6/54/54	-
3	HEC	G	604	1	-	2/6/54/54	-
4	ISW	G	608	1	-	0/8/74/74	-
3	HEC	E	605	1	-	1/6/54/54	-
5	PEG	J	101	-	-	2/4/4/4	-
6	PGE	I	610	-	-	6/7/7/7	-
3	HEC	E	604	1	-	2/6/54/54	-
5	PEG	K	608	-	-	2/4/4/4	-
3	HEC	G	606	1	-	0/6/54/54	-
4	ISW	G	609	8,1	-	1/8/74/74	-
6	PGE	G	612	-	-	5/7/7/7	-
3	HEC	I	607	1	-	0/6/54/54	-
3	HEC	A	607	1	-	0/6/54/54	-
7	PG4	E	610	-	-	3/10/10/10	-
3	HEC	K	607	1	-	0/6/54/54	-
6	PGE	C	610	-	-	4/7/7/7	-
6	PGE	E	609	-	-	2/7/7/7	-
3	HEC	I	605	1	-	1/6/54/54	-
3	HEC	A	606	1	-	0/6/54/54	-
6	PGE	I	609	-	-	5/7/7/7	-
3	HEC	A	603	1	-	0/6/54/54	-
3	HEC	I	601	1	-	0/6/54/54	-
3	HEC	A	605	1	-	1/6/54/54	-
3	HEC	I	603	1	-	0/6/54/54	-
3	HEC	I	604	1	-	2/6/54/54	-
4	ISW	A	608	8,1	-	1/8/74/74	-
3	HEC	E	607	1	-	0/6/54/54	-
3	HEC	E	603	1	-	0/6/54/54	-
3	HEC	K	603	1	-	0/6/54/54	-
3	HEC	K	604	1	-	2/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	C	603	1	-	0/6/54/54	-
7	PG4	K	610	-	-	5/10/10/10	-
3	HEC	G	601	1	-	0/6/54/54	-
3	HEC	K	605	1	-	1/6/54/54	-
4	ISW	C	608	8,1	-	1/8/74/74	-
7	PG4	A	612	-	-	7/10/10/10	-
3	HEC	C	606	1	-	0/6/54/54	-
3	HEC	E	606	1	-	0/6/54/54	-
3	HEC	C	604	1	-	2/6/54/54	-
4	ISW	I	608	8,1	-	1/8/74/74	-
3	HEC	K	606	1	-	0/6/54/54	-
7	PG4	C	611	-	-	6/10/10/10	-
6	PGE	G	611	-	-	6/7/7/7	-
5	PEG	C	609	-	-	2/4/4/4	-
5	PEG	K	609	-	-	2/4/4/4	-
3	HEC	I	602	1	-	0/6/54/54	-
3	HEC	A	602	1	-	0/6/54/54	-
3	HEC	C	607	1	-	0/6/54/54	-
3	HEC	G	602	1	-	0/6/54/54	-
5	PEG	G	610	-	-	3/4/4/4	-
3	HEC	G	607	1	-	0/6/54/54	-
6	PGE	A	611	-	-	3/7/7/7	-
5	PEG	A	610	-	-	3/4/4/4	-
3	HEC	K	602	1	-	0/6/54/54	-
3	HEC	I	606	1	-	0/6/54/54	-
3	HEC	A	601	1	-	0/6/54/54	-
3	HEC	C	602	1	-	0/6/54/54	-

The worst 5 of 230 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	608	ISW	CHC-C4B	-14.98	1.30	1.53
4	I	608	ISW	CHC-C4B	-14.90	1.30	1.53
4	A	608	ISW	CHC-C4B	-14.51	1.30	1.53
4	G	608	ISW	CHC-C4B	-14.50	1.31	1.53
4	A	609	ISW	CHC-C4B	-13.77	1.32	1.53

The worst 5 of 352 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	608	ISW	CHB-C1B-C2B	-14.57	102.22	124.98
4	A	609	ISW	CHB-C1B-C2B	-9.89	109.53	124.98
4	C	608	ISW	CAD-CBD-CGD	-9.87	96.12	112.67
4	G	609	ISW	CHB-C1B-C2B	-9.59	110.00	124.98
4	A	609	ISW	CAD-CBD-CGD	-9.57	96.62	112.67

There are no chirality outliers.

5 of 94 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	605	HEC	C2A-CAA-CBA-CGA
3	I	604	HEC	C1A-C2A-CAA-CBA
3	I	604	HEC	C3A-C2A-CAA-CBA
3	K	604	HEC	C1A-C2A-CAA-CBA
3	K	604	HEC	C3A-C2A-CAA-CBA

There are no ring outliers.

62 monomers are involved in 253 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	601	HEC	5	0
3	E	601	HEC	4	0
3	C	601	HEC	4	0
3	A	604	HEC	4	0
3	C	605	HEC	8	0
6	E	608	PGE	1	0
3	G	603	HEC	1	0
4	A	609	ISW	10	0
3	G	605	HEC	8	0
3	E	602	HEC	2	0
3	G	604	HEC	3	0
4	G	608	ISW	9	0
3	E	605	HEC	7	0
5	J	101	PEG	2	0
6	I	610	PGE	4	0
3	E	604	HEC	7	0
3	G	606	HEC	5	0
4	G	609	ISW	12	0
6	G	612	PGE	2	0
3	I	607	HEC	5	0
3	A	607	HEC	1	0
7	E	610	PG4	1	0

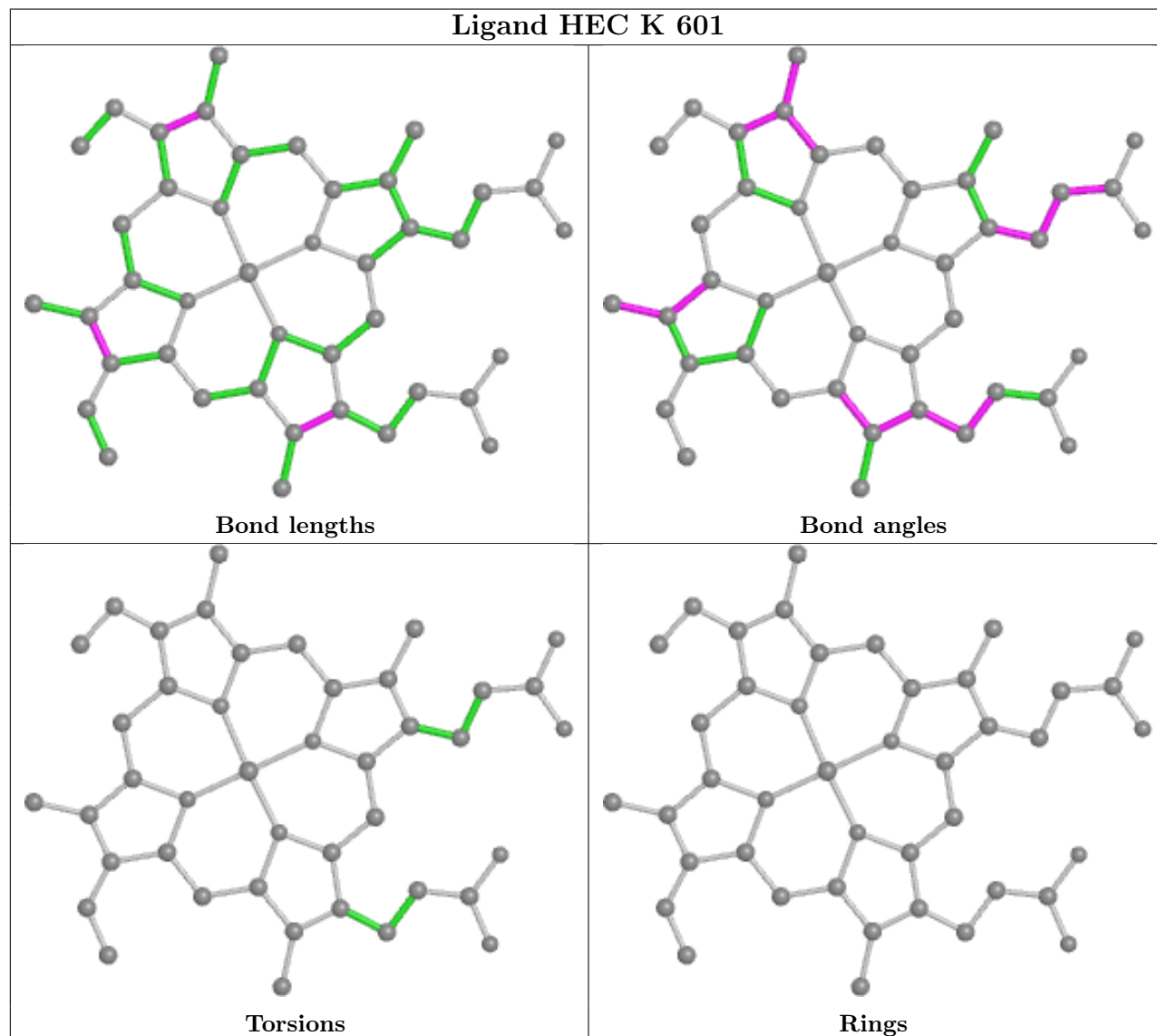
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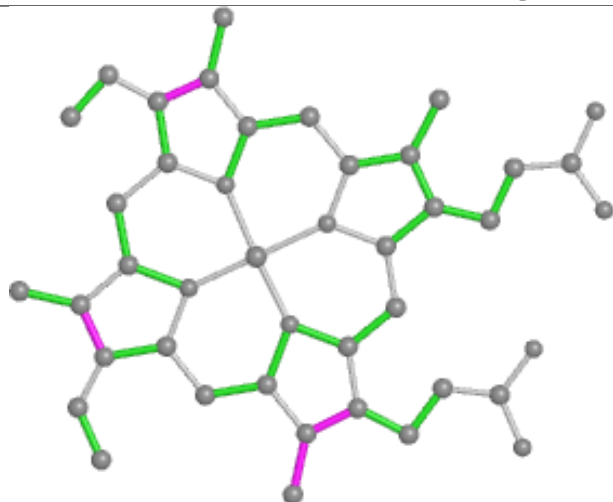
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	607	HEC	2	0
6	C	610	PGE	2	0
6	E	609	PGE	2	0
3	I	605	HEC	9	0
3	A	606	HEC	4	0
6	I	609	PGE	7	0
3	A	603	HEC	2	0
3	I	601	HEC	2	0
3	A	605	HEC	8	0
3	I	603	HEC	5	0
3	I	604	HEC	6	0
4	A	608	ISW	12	0
3	E	607	HEC	3	0
3	E	603	HEC	2	0
3	K	603	HEC	2	0
3	K	604	HEC	6	0
3	C	603	HEC	5	0
3	G	601	HEC	4	0
3	K	605	HEC	8	0
4	C	608	ISW	11	0
7	A	612	PG4	2	0
3	C	606	HEC	4	0
3	E	606	HEC	4	0
3	C	604	HEC	1	0
4	I	608	ISW	7	0
3	K	606	HEC	5	0
7	C	611	PG4	3	0
6	G	611	PGE	6	0
5	C	609	PEG	1	0
5	K	609	PEG	2	0
3	I	602	HEC	5	0
3	A	602	HEC	7	0
3	C	607	HEC	3	0
3	G	602	HEC	4	0
3	G	607	HEC	1	0
6	A	611	PGE	1	0
3	K	602	HEC	4	0
3	I	606	HEC	3	0
3	A	601	HEC	1	0
3	C	602	HEC	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

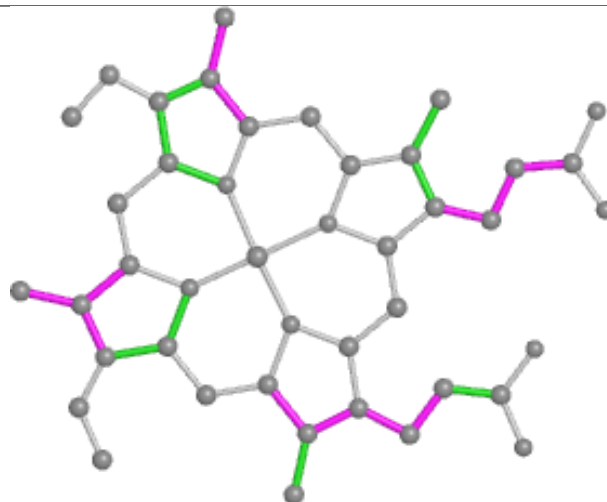
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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



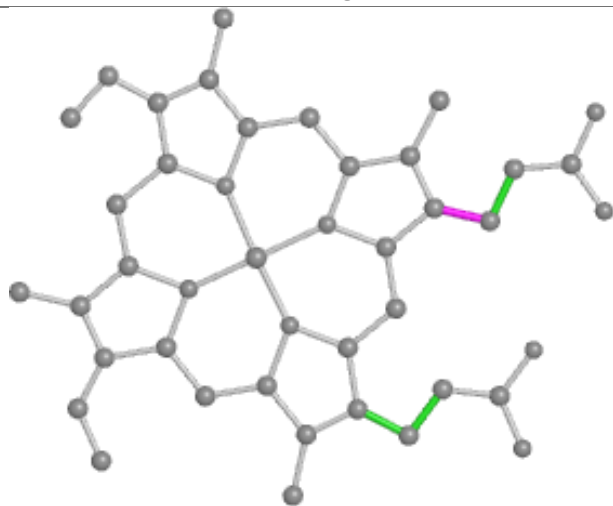
Ligand HEC E 601



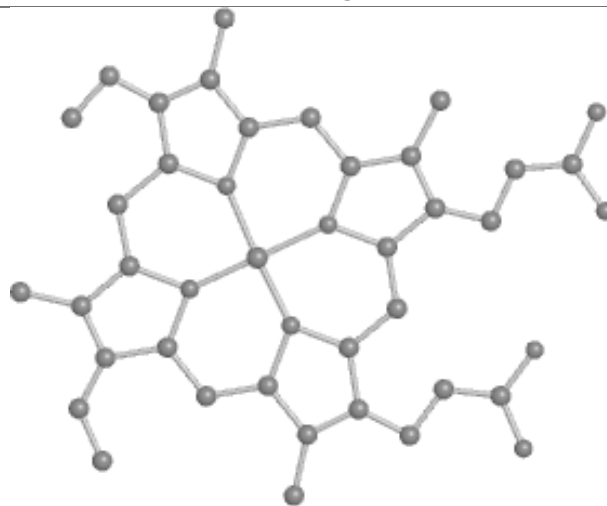
Bond lengths



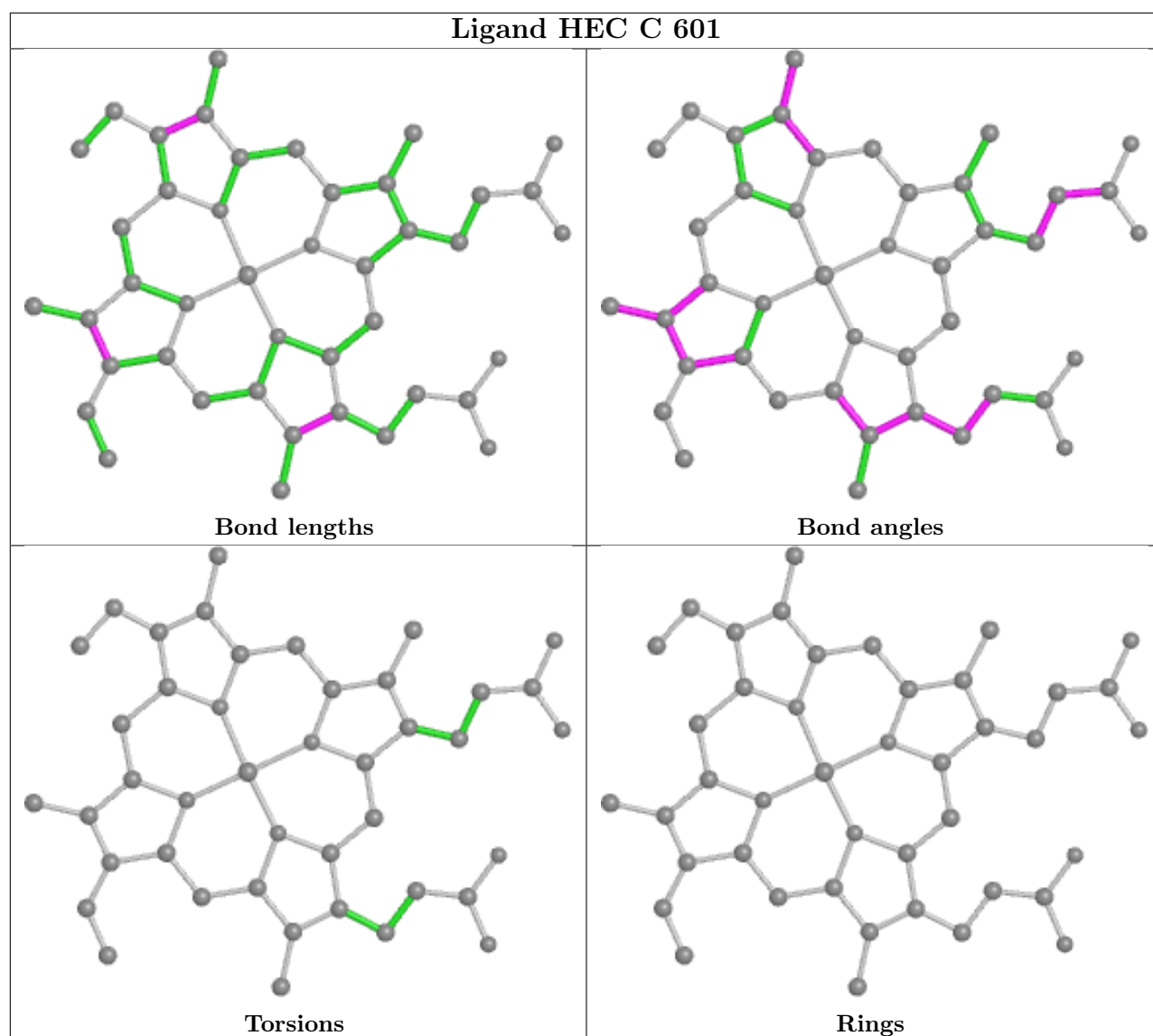
Bond angles

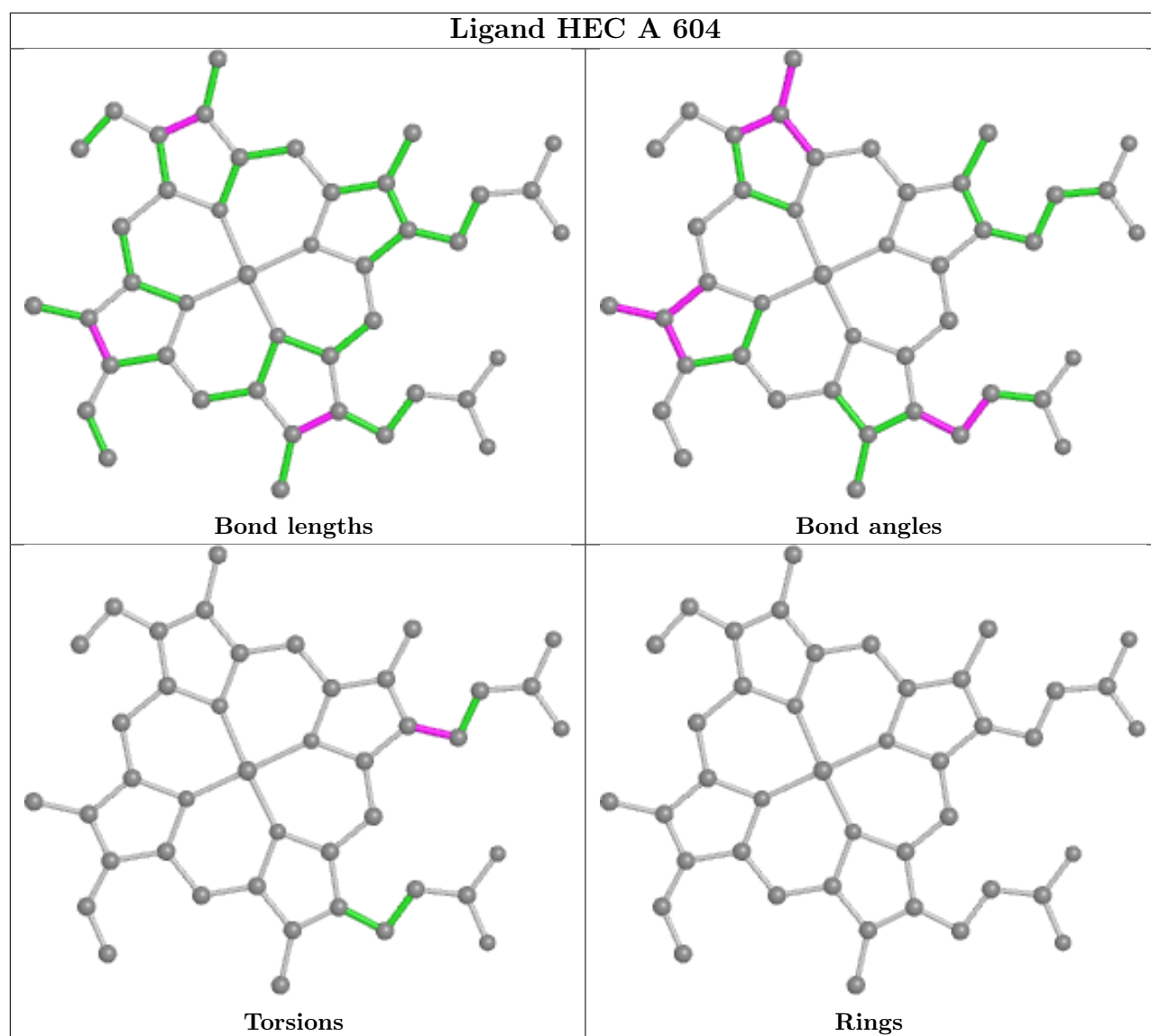


Torsions

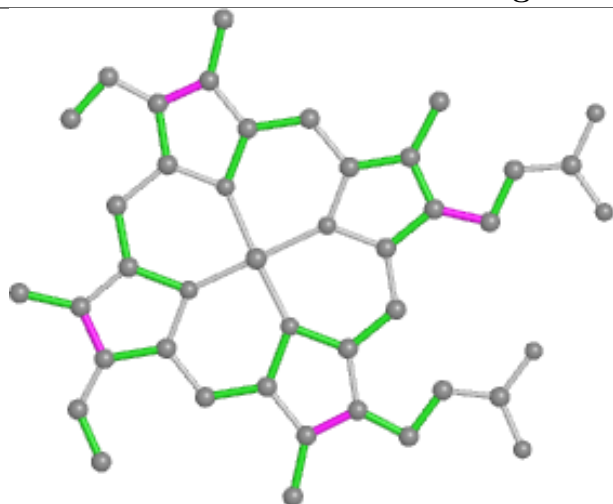


Rings

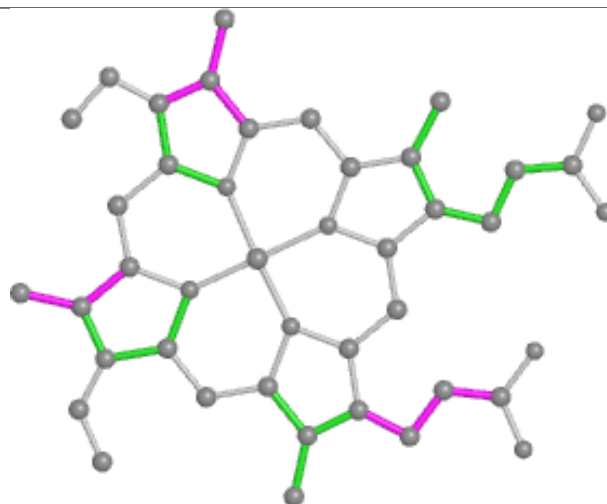




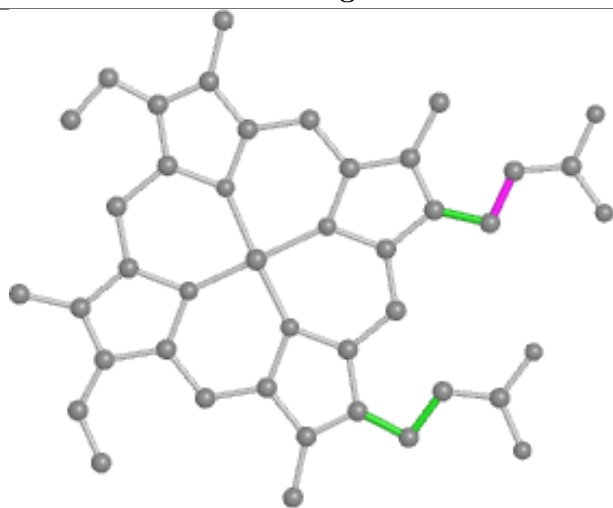
Ligand HEC C 605



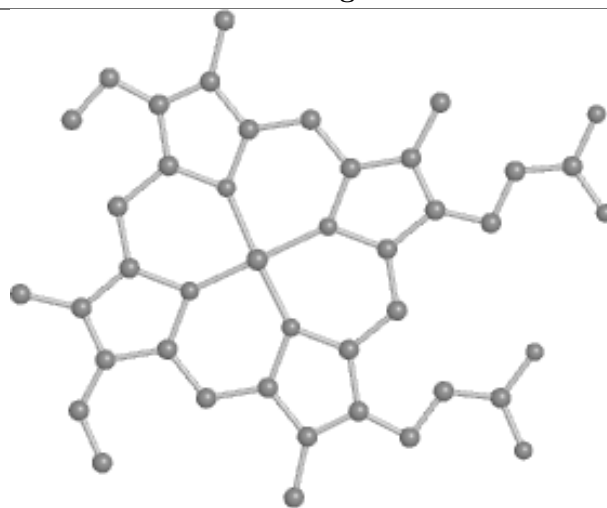
Bond lengths



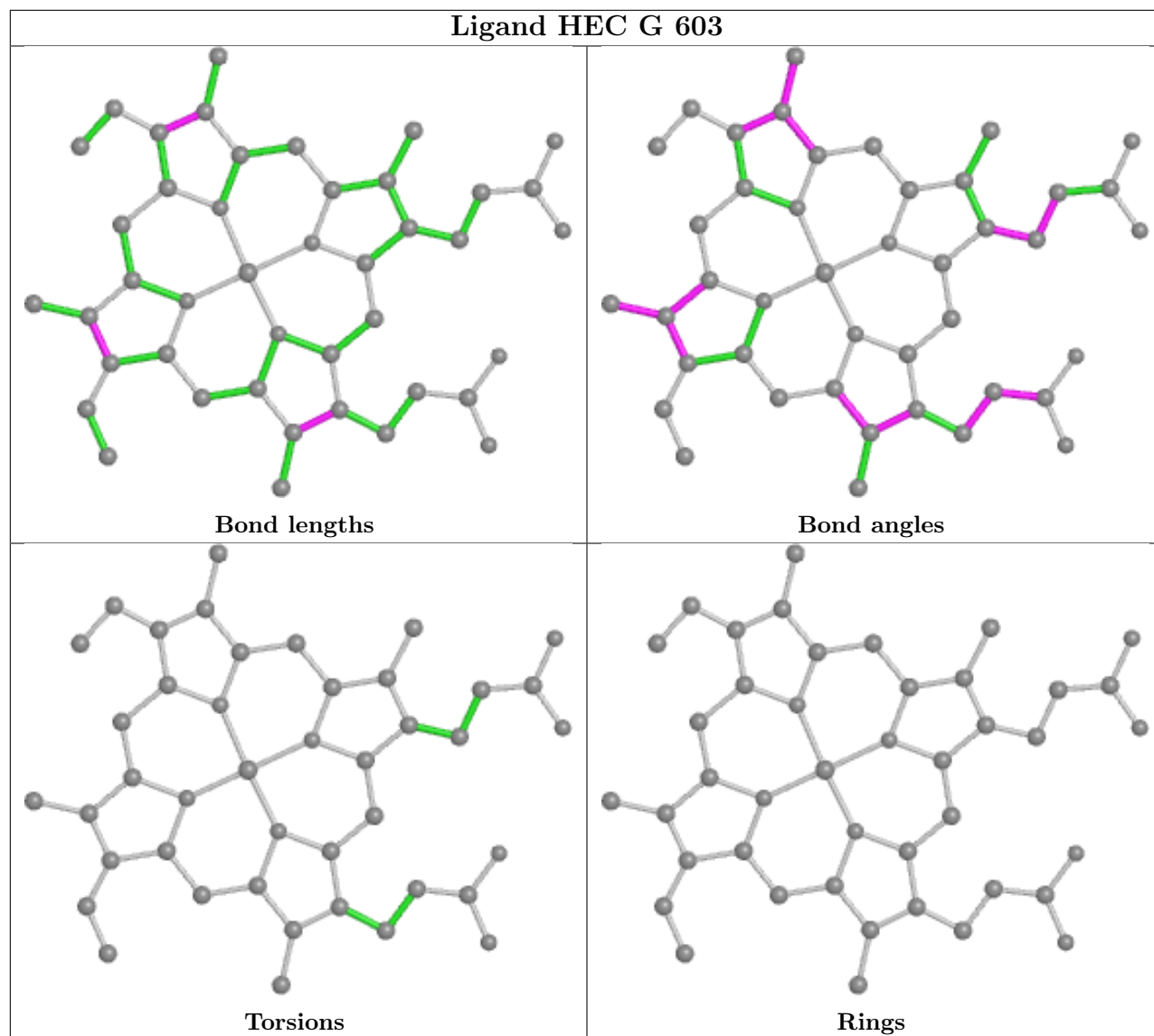
Bond angles



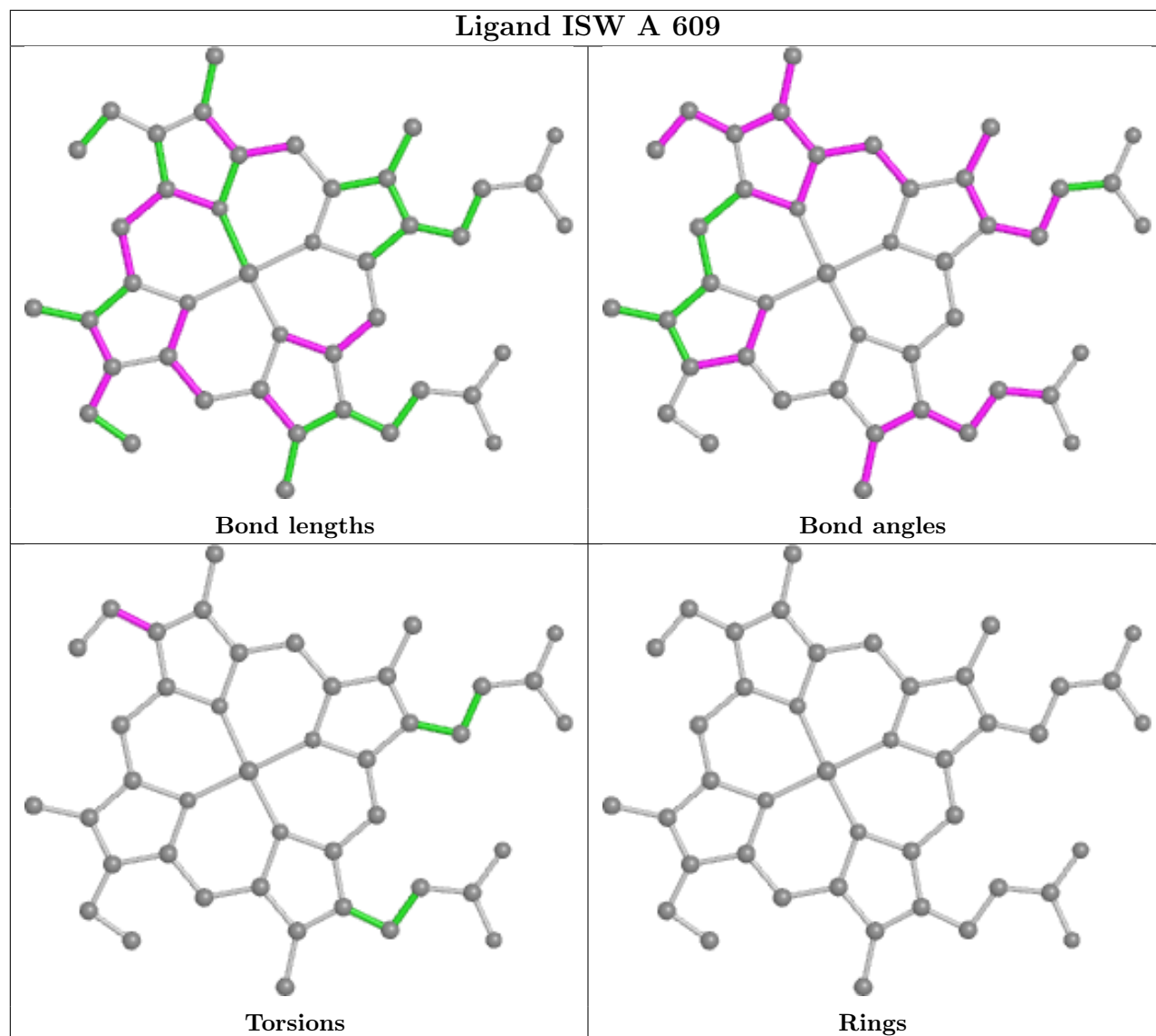
Torsions

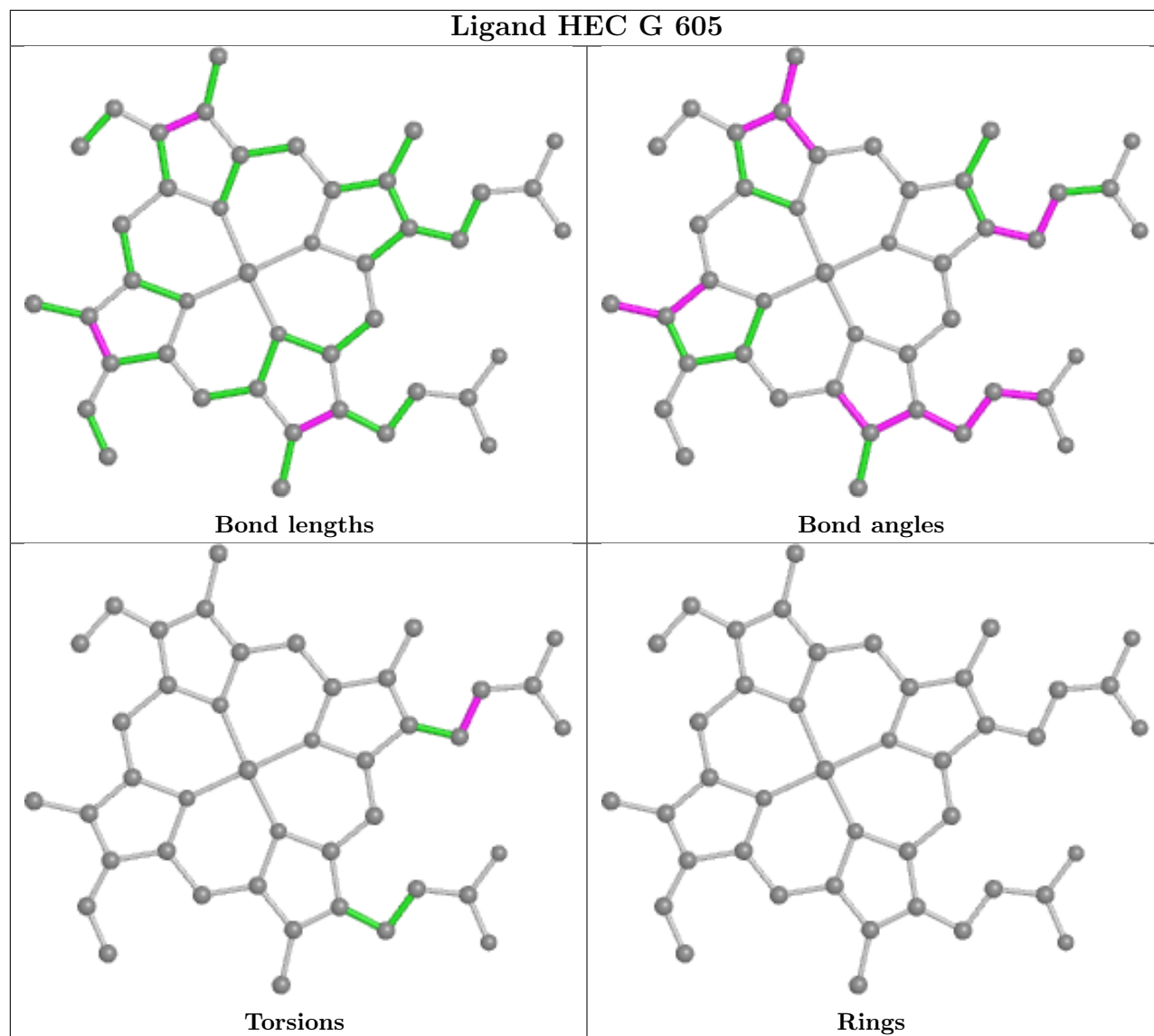


Rings

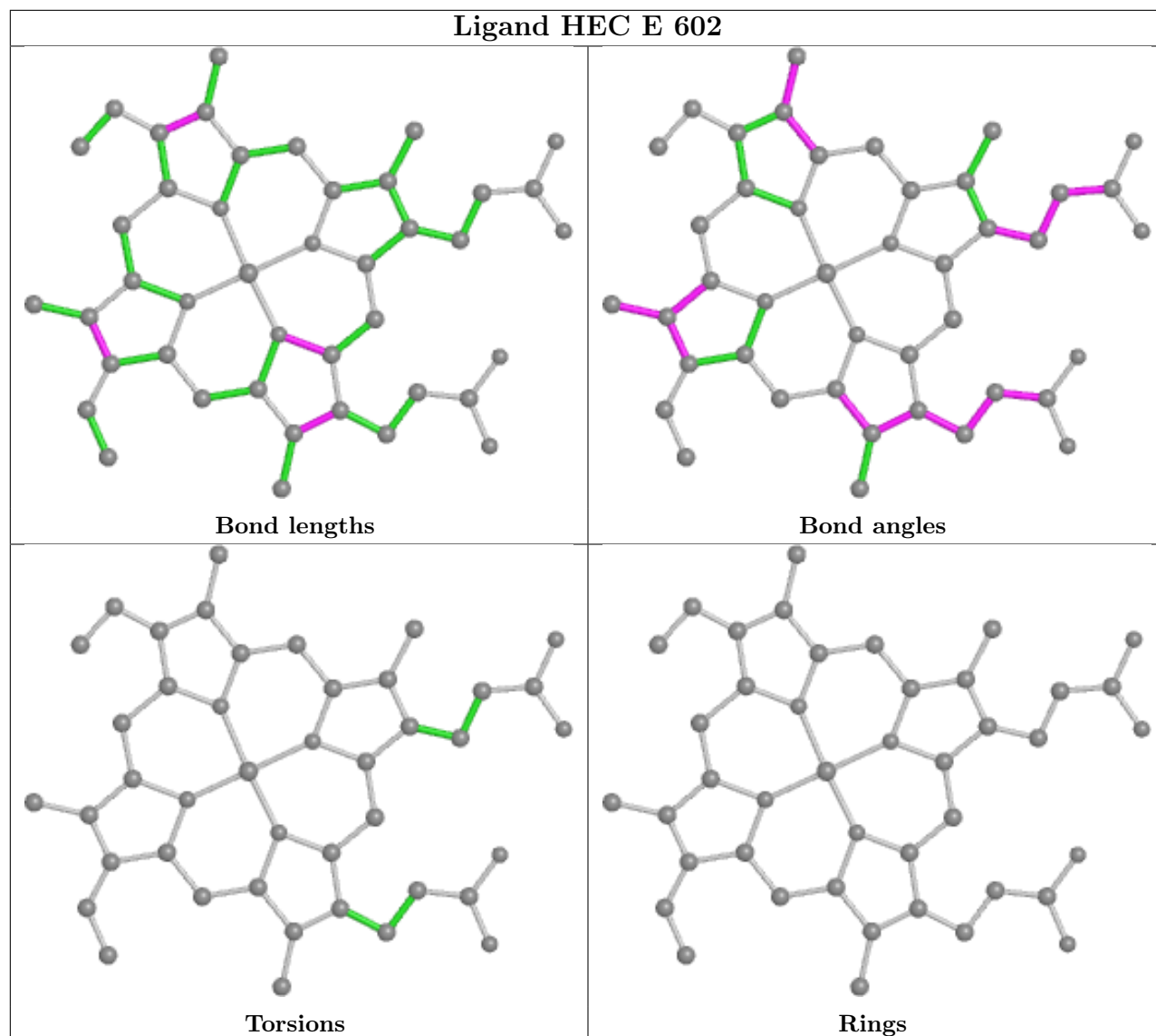


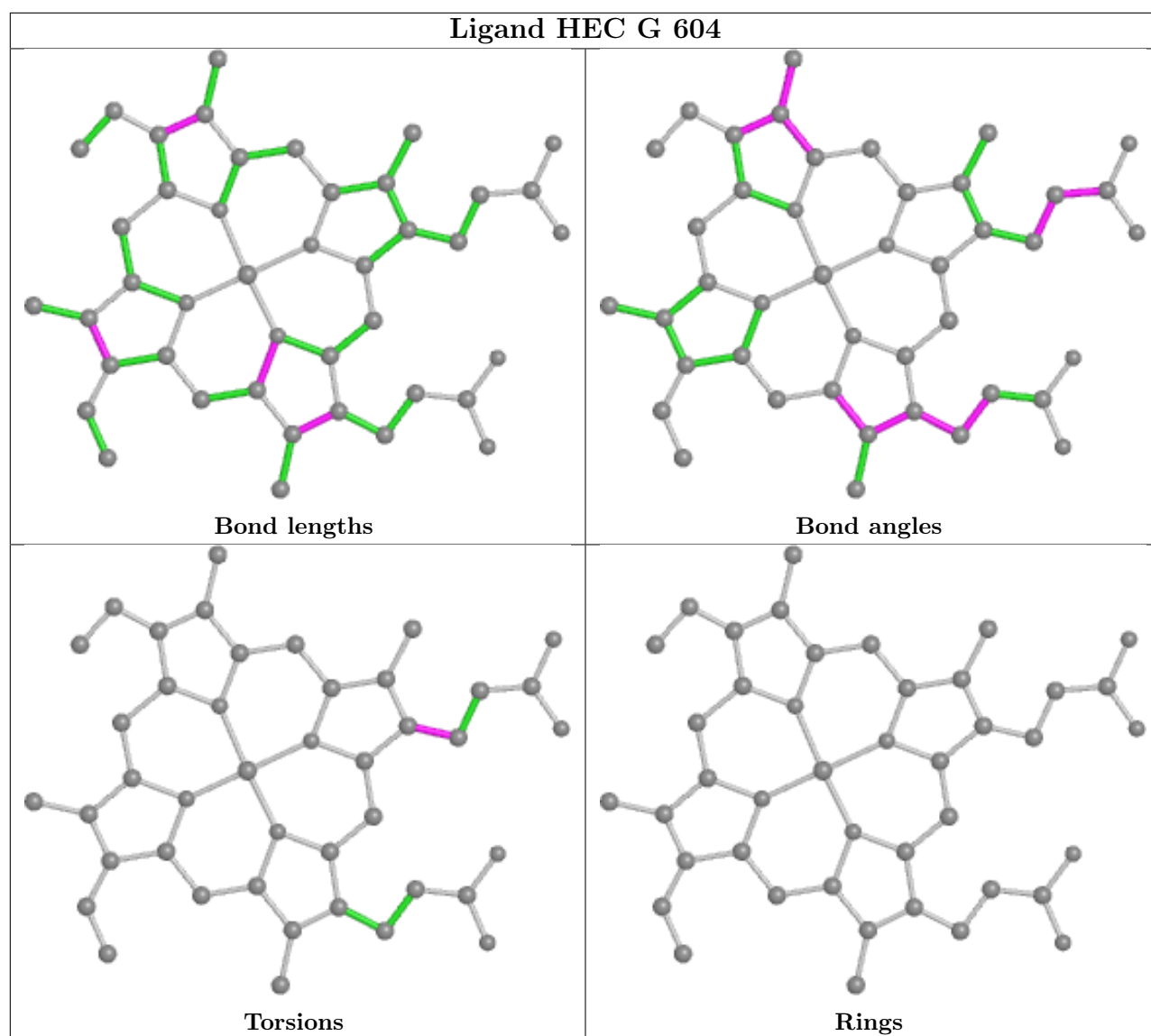
Ligand ISW A 609



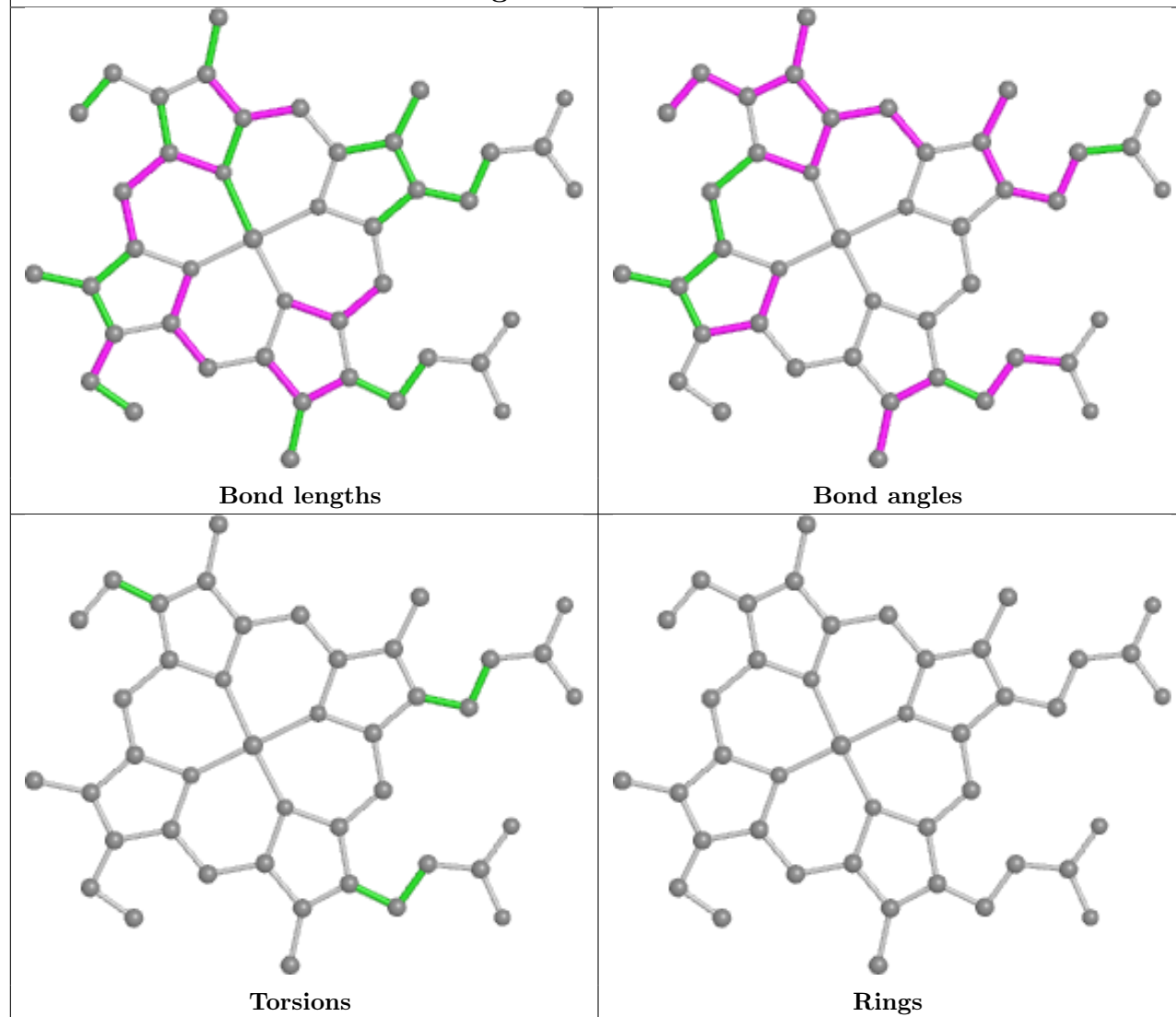


Ligand HEC E 602

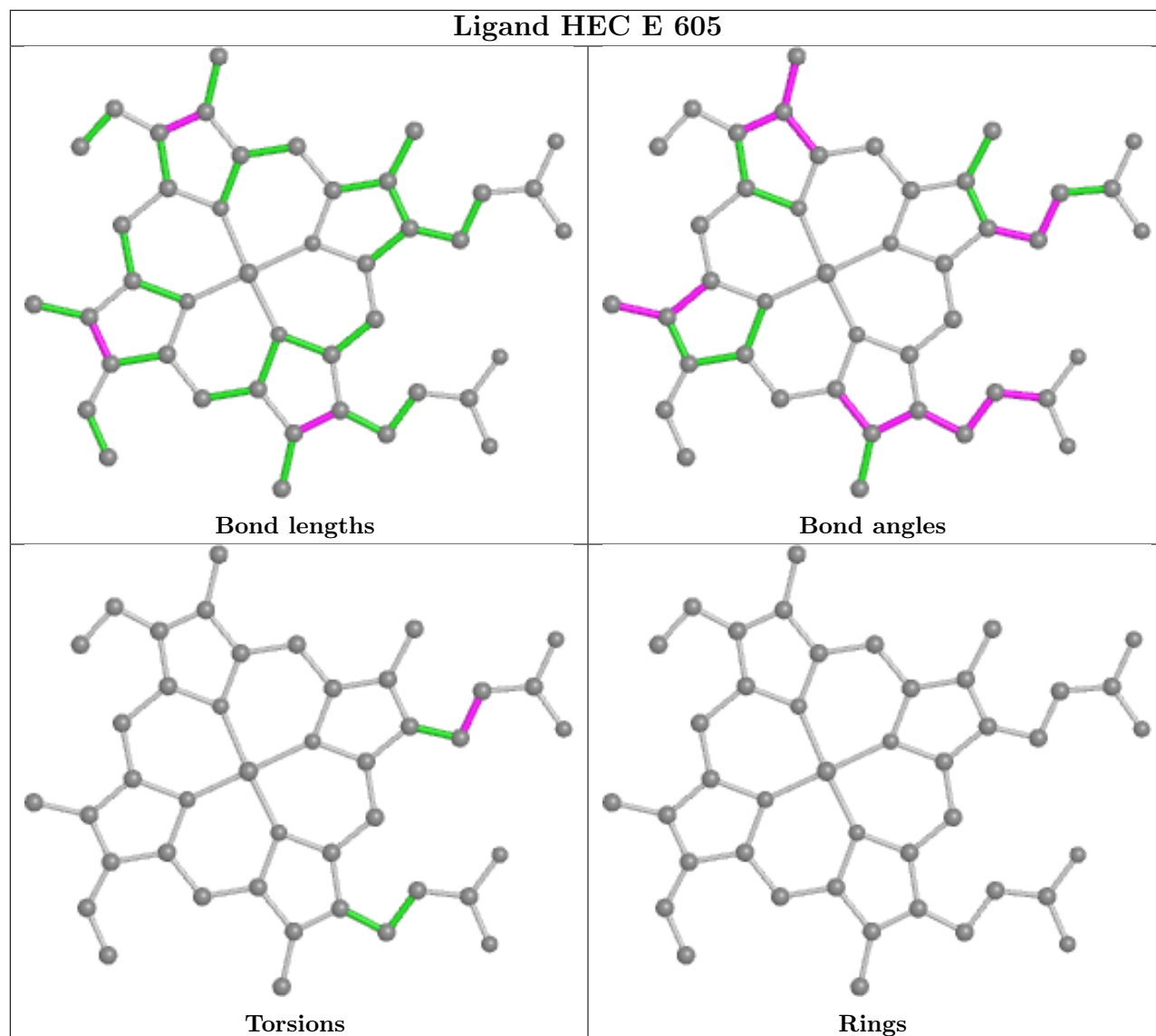




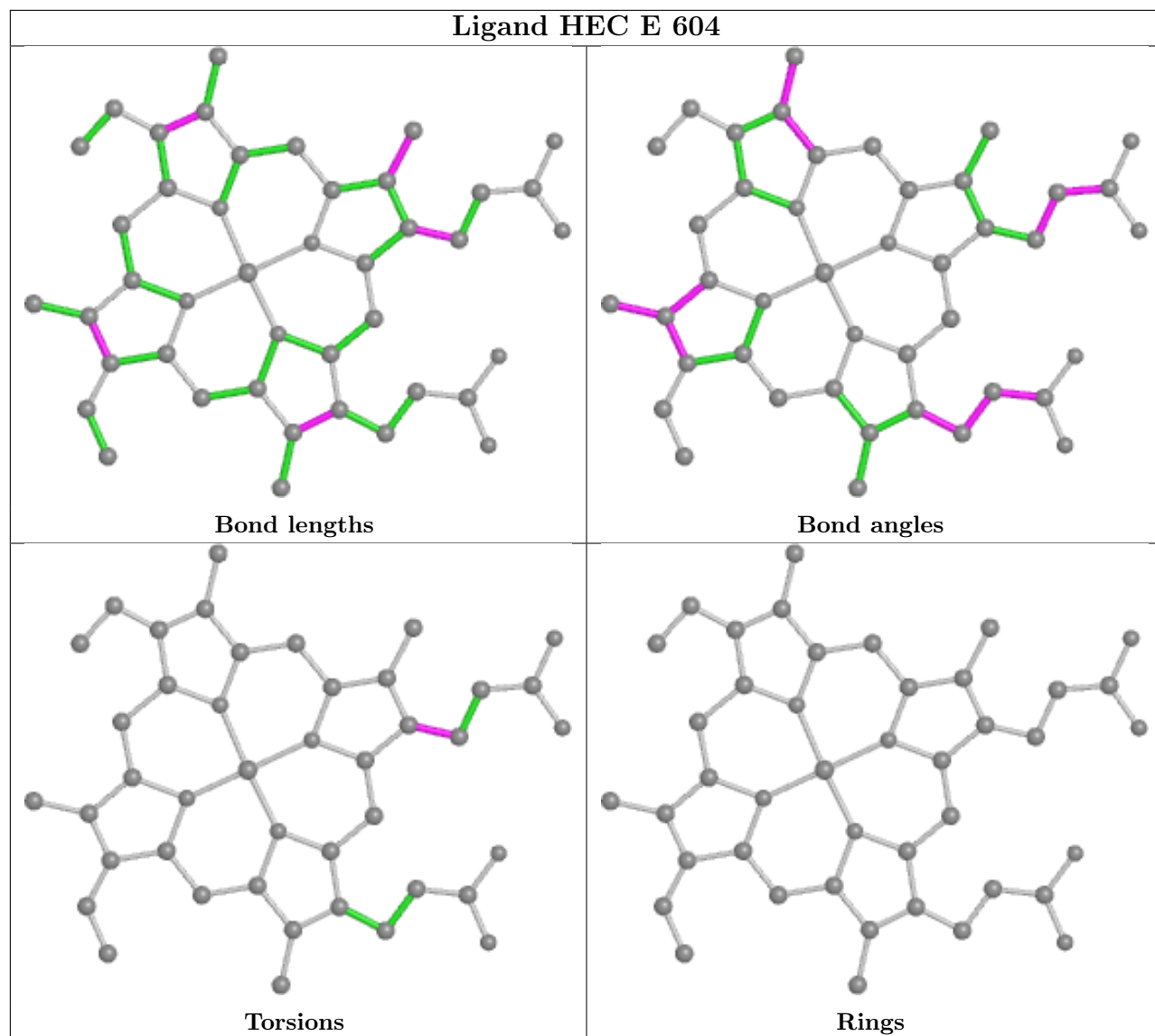
Ligand ISW G 608

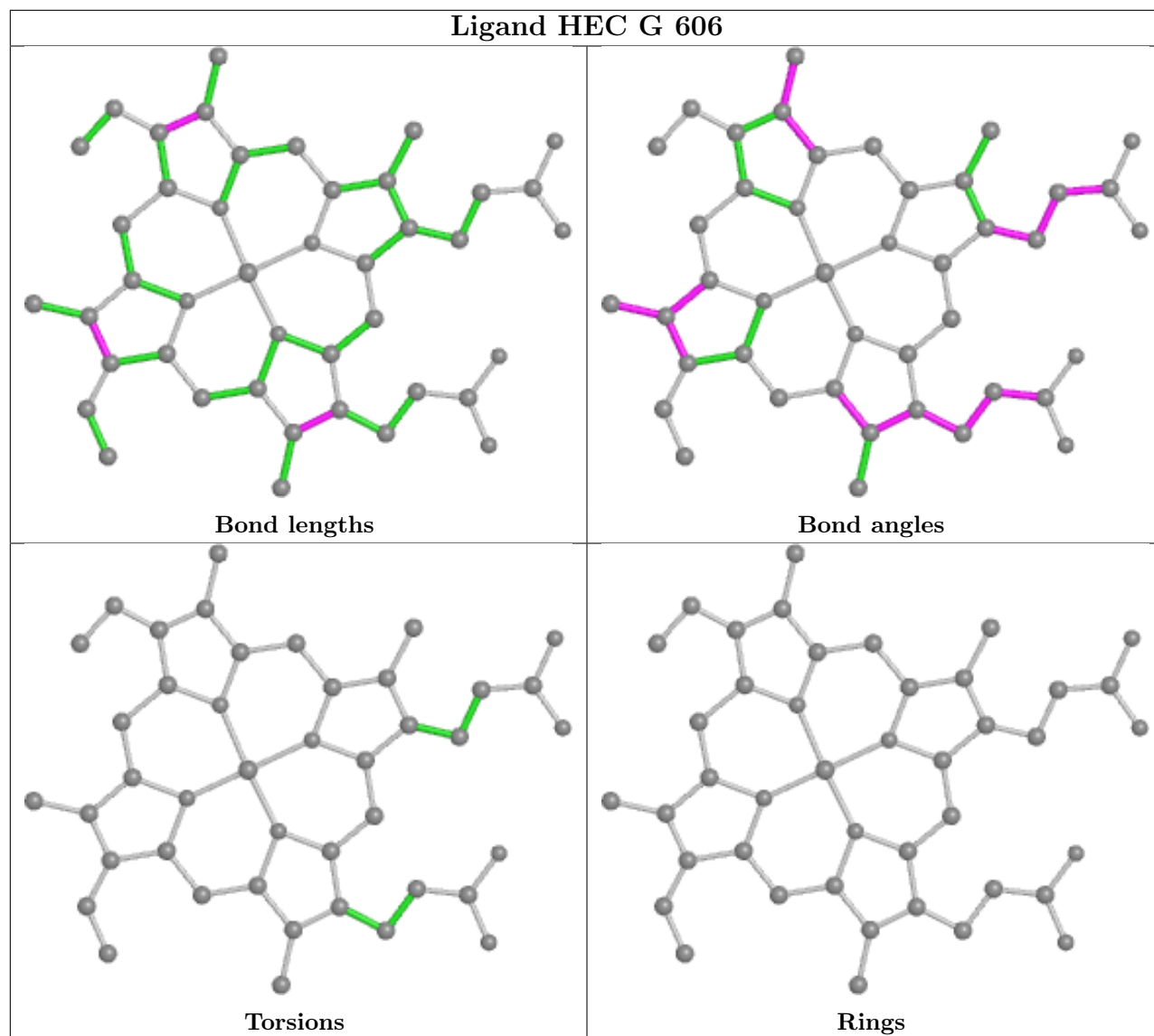


Ligand HEC E 605

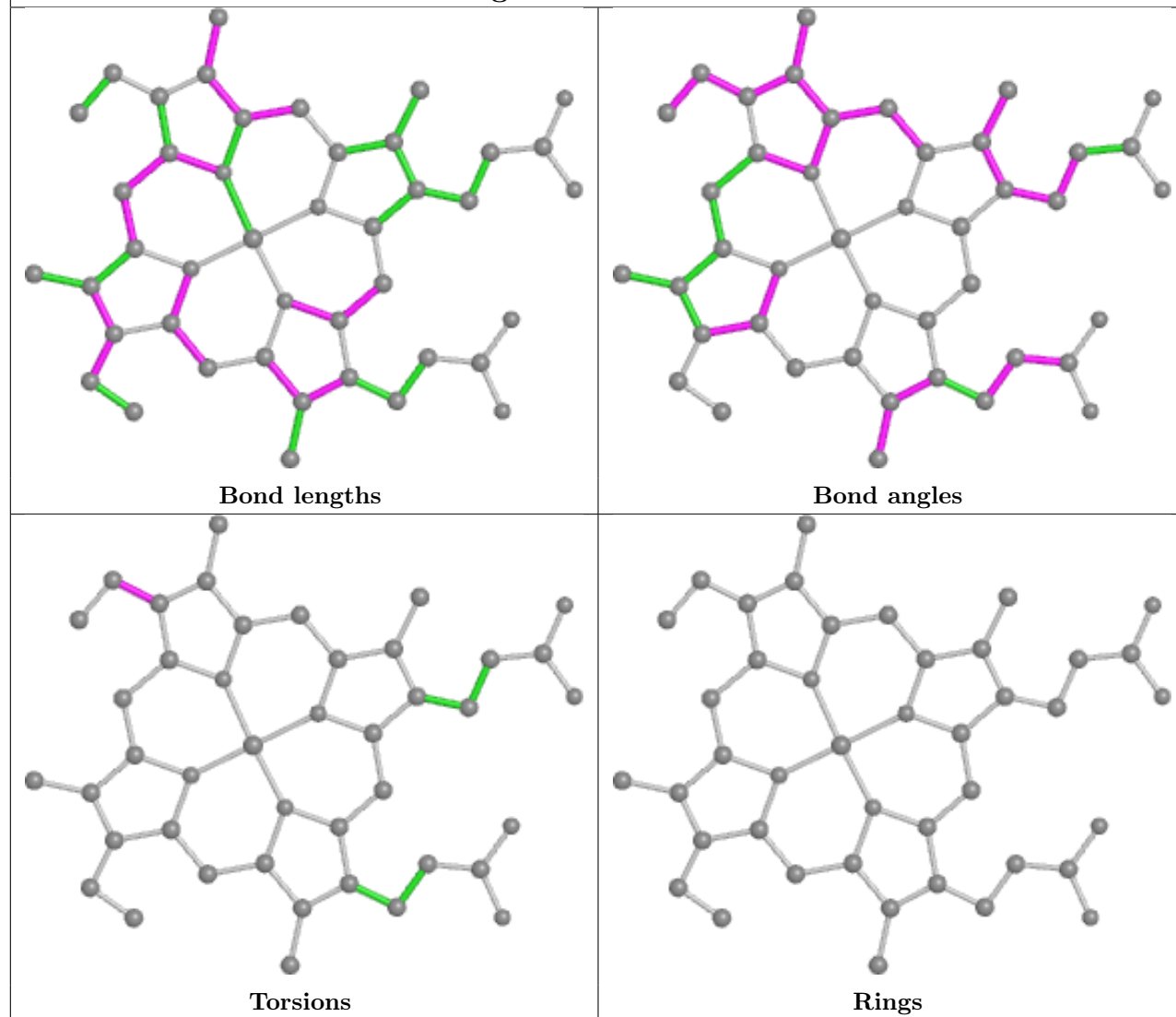


Ligand HEC E 604

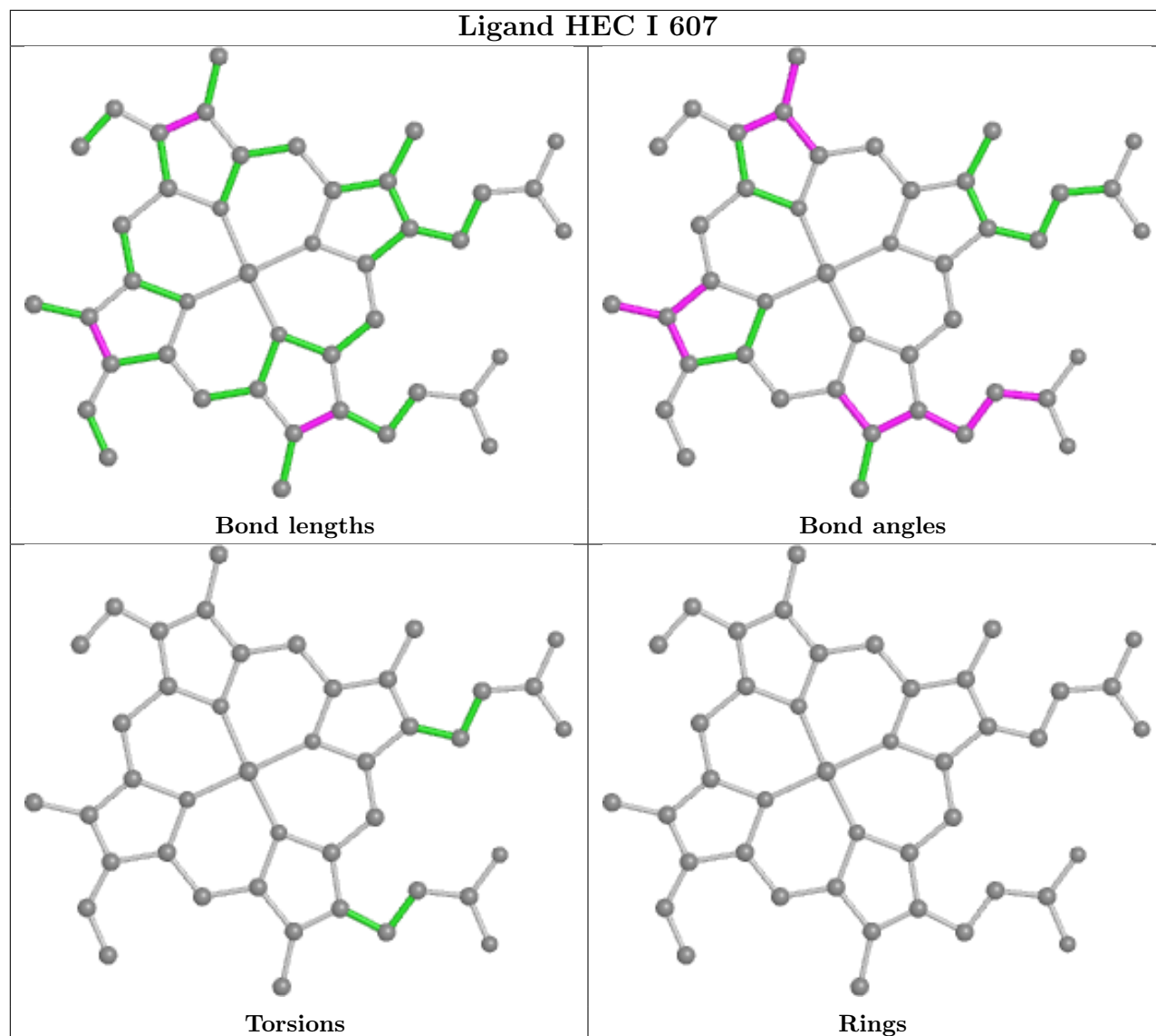


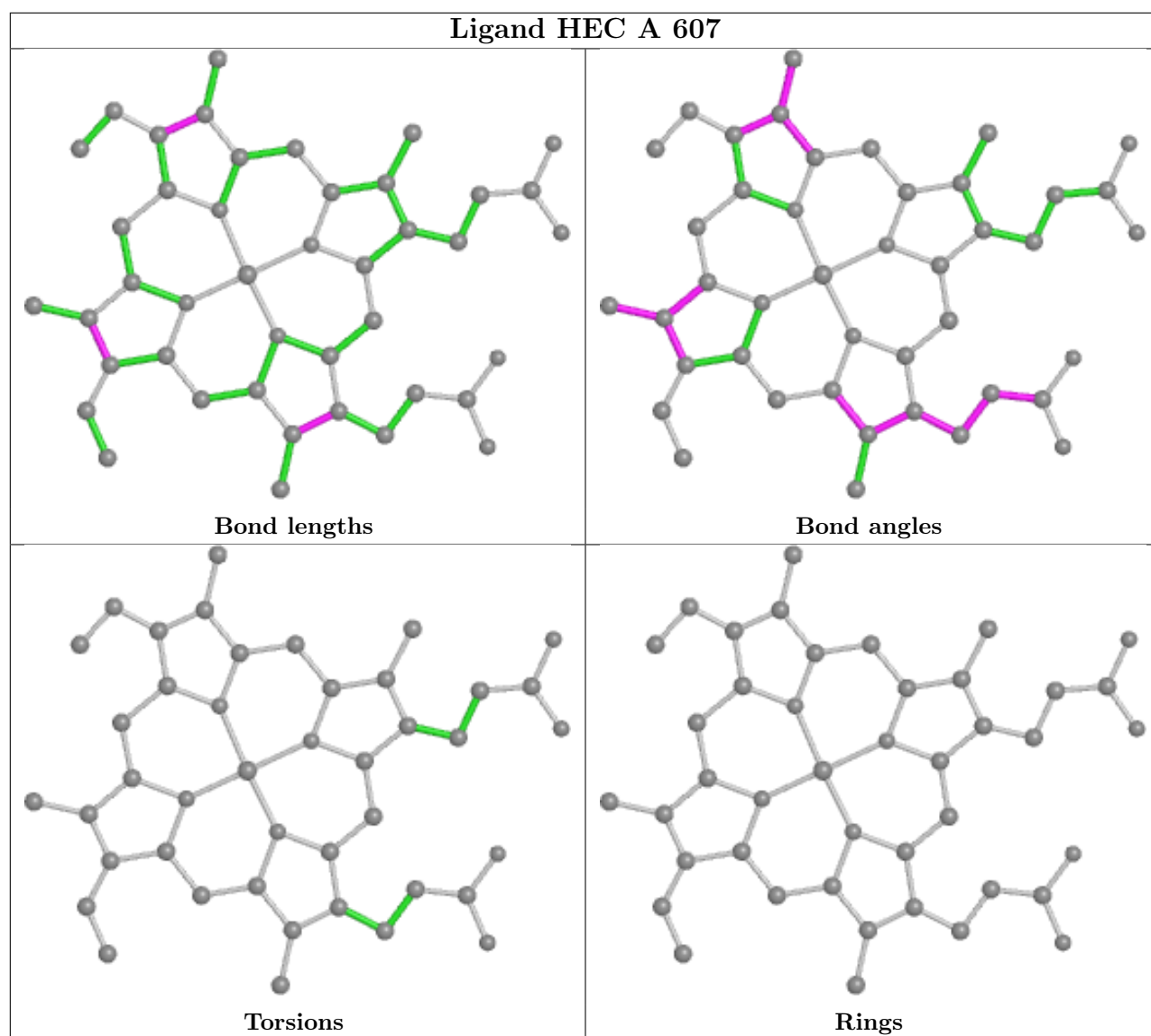


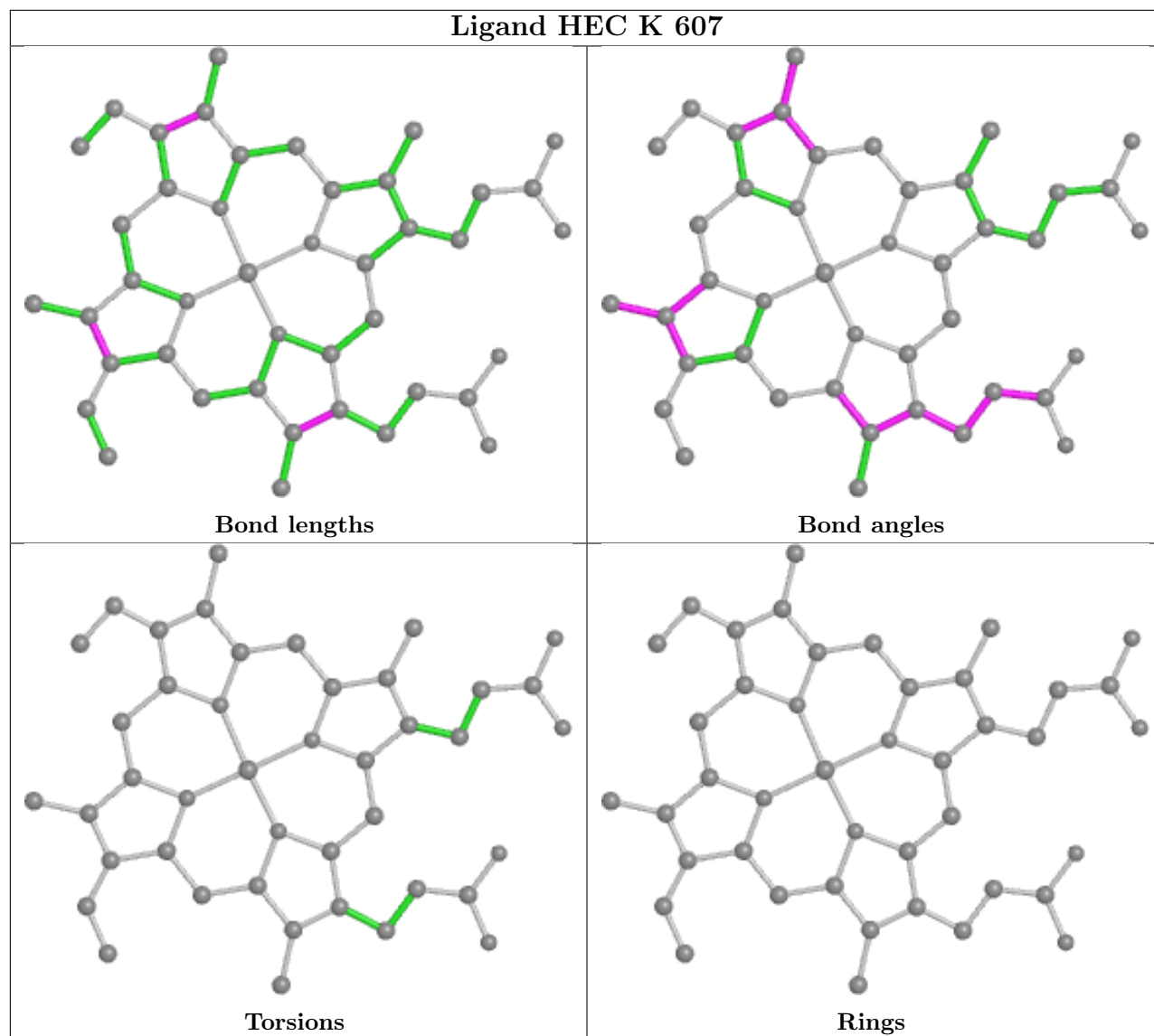
Ligand ISW G 609



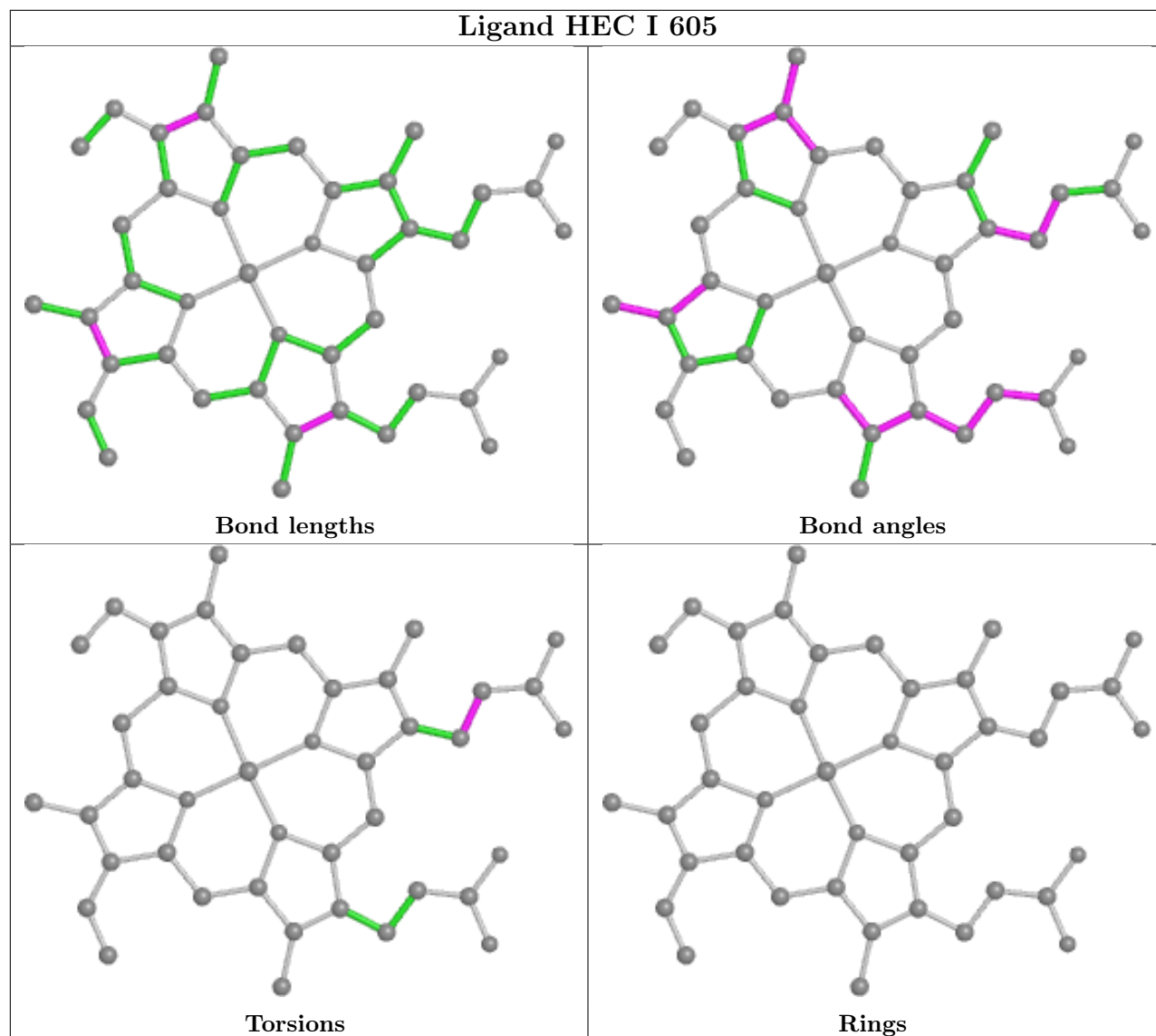
Ligand HEC I 607

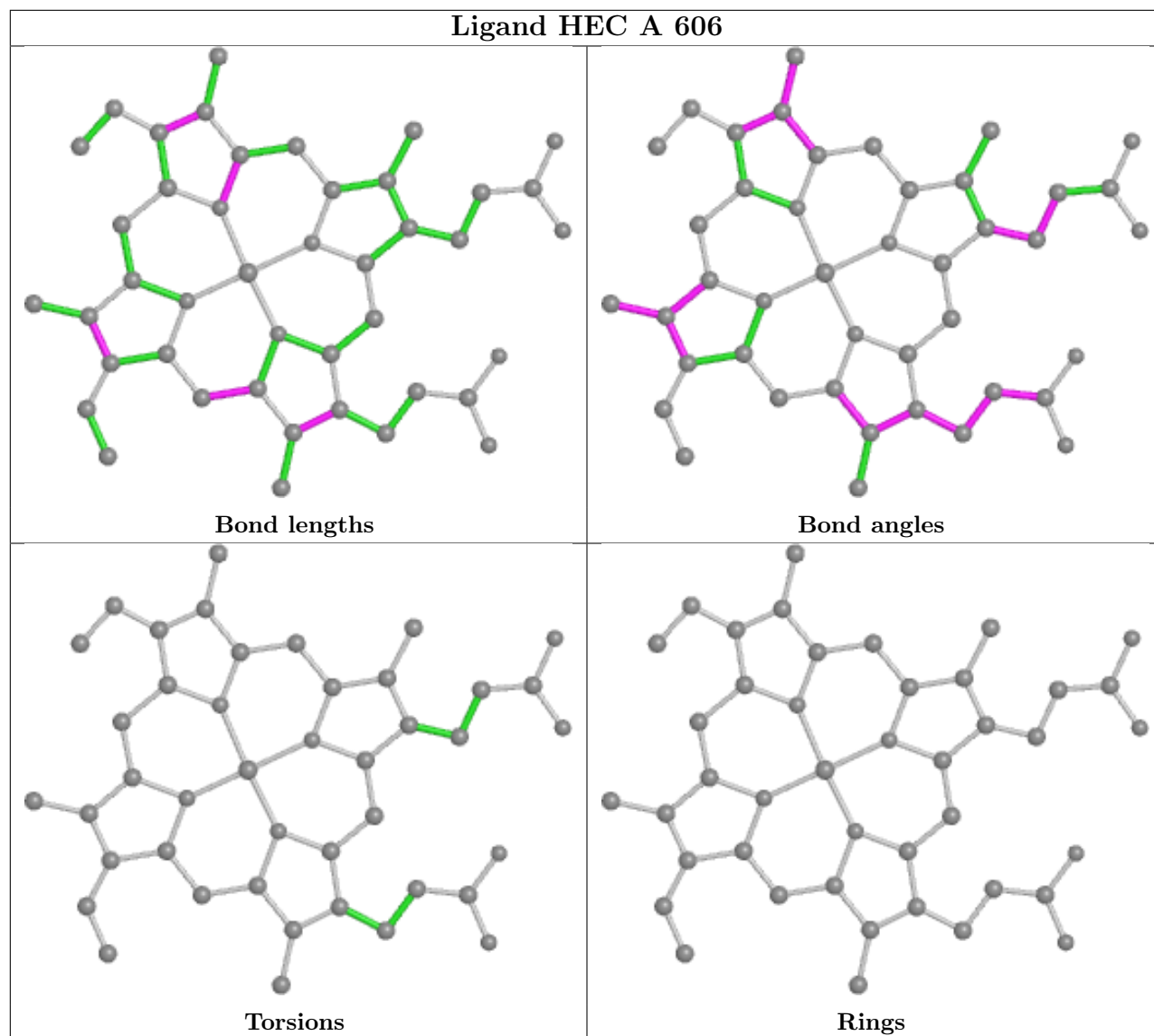


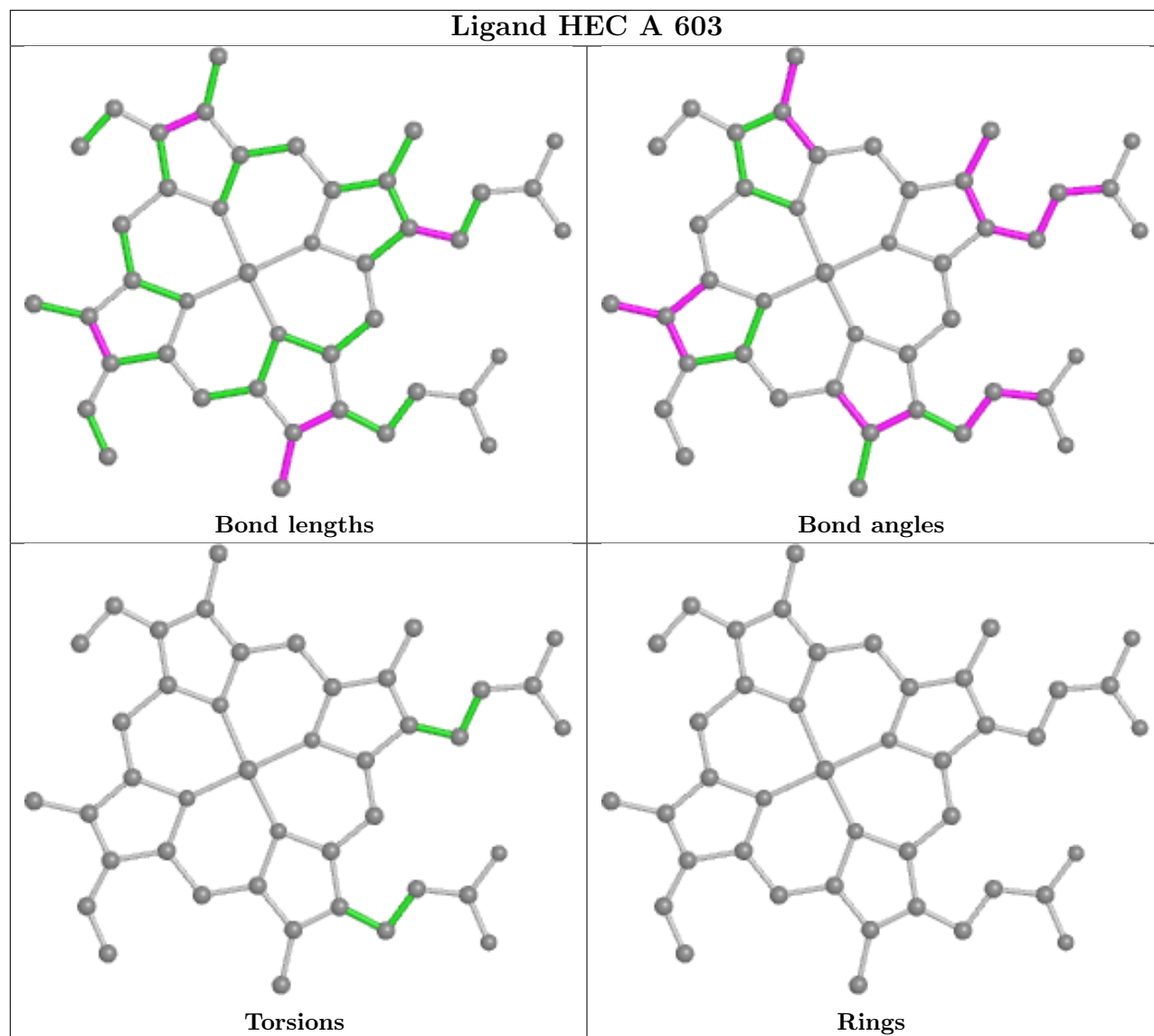




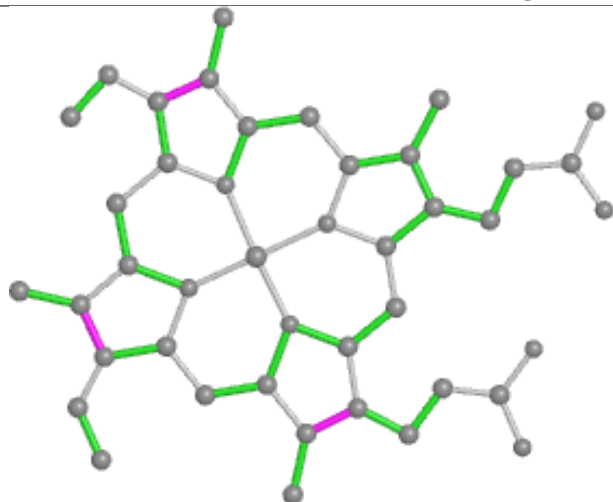
Ligand HEC I 605



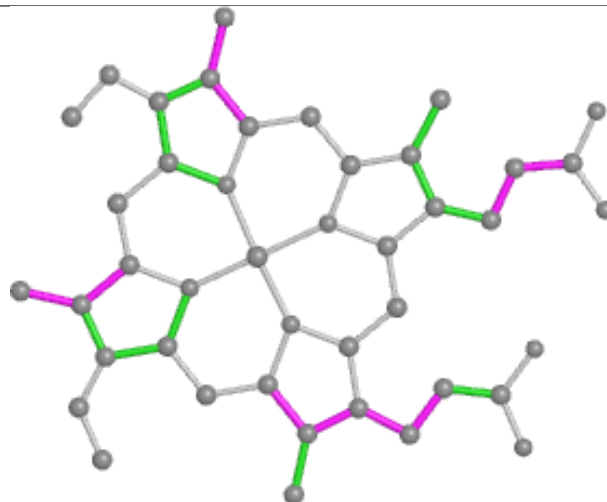




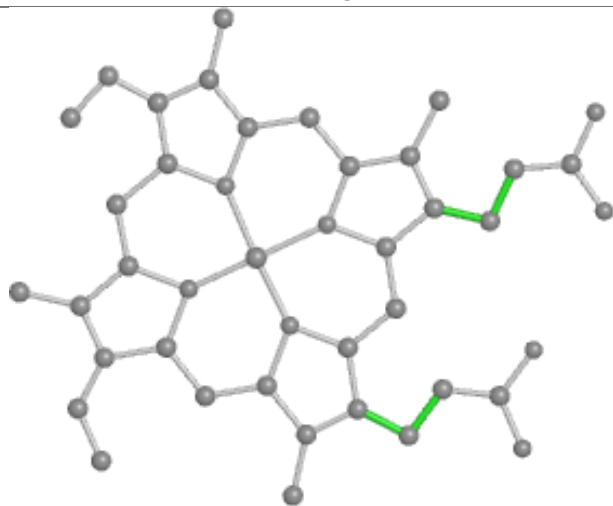
Ligand HEC I 601



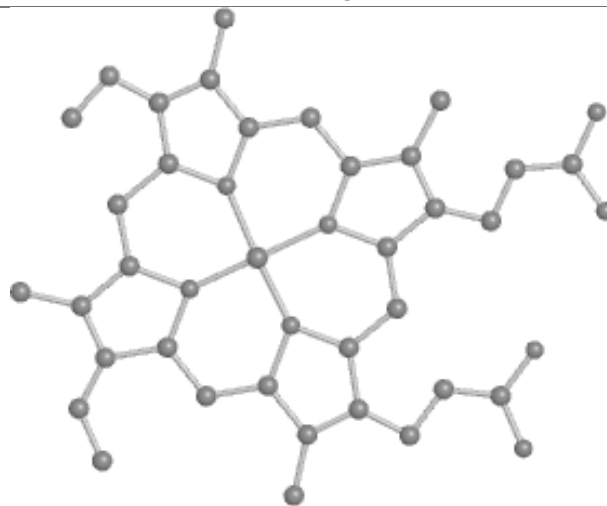
Bond lengths



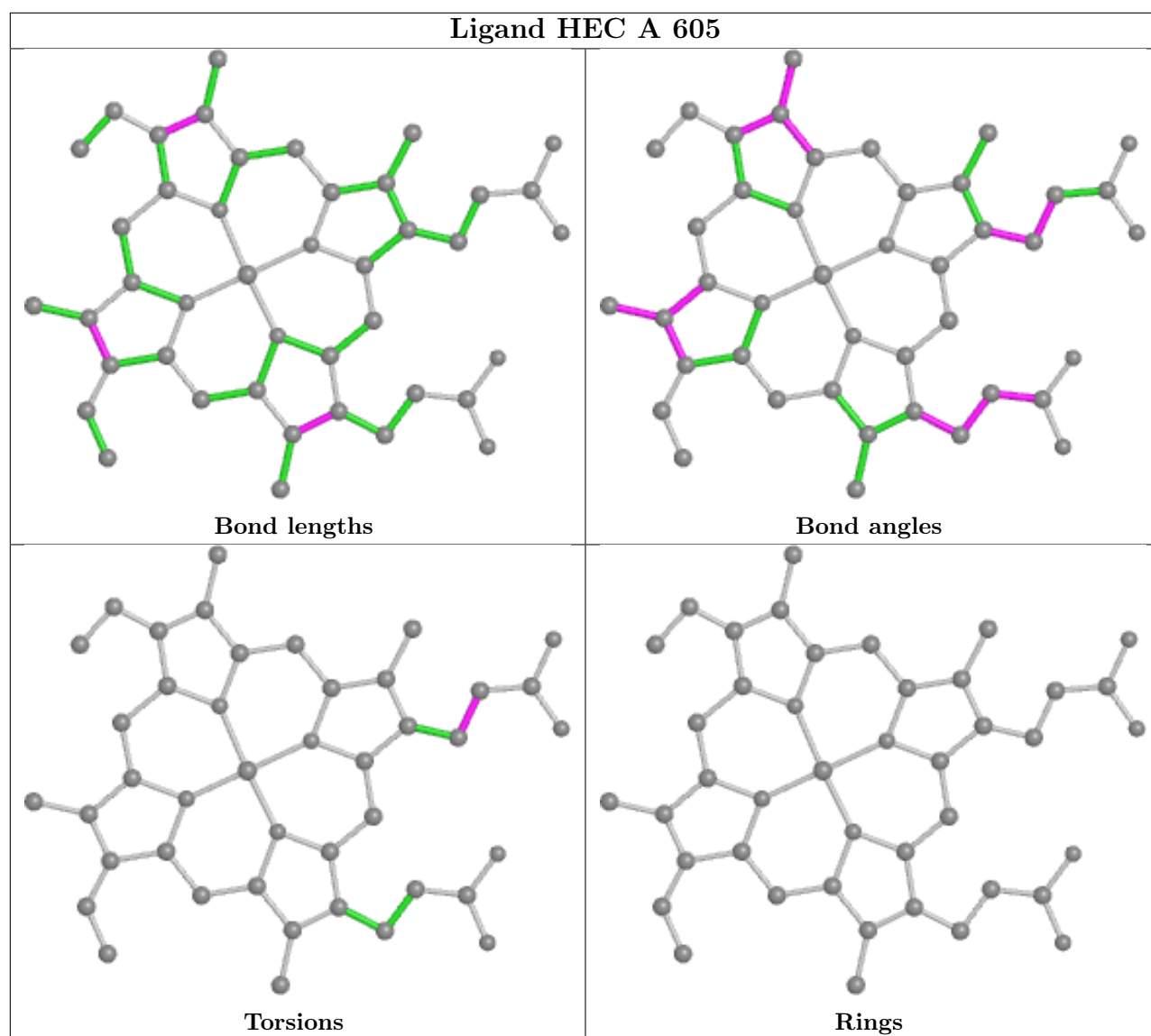
Bond angles



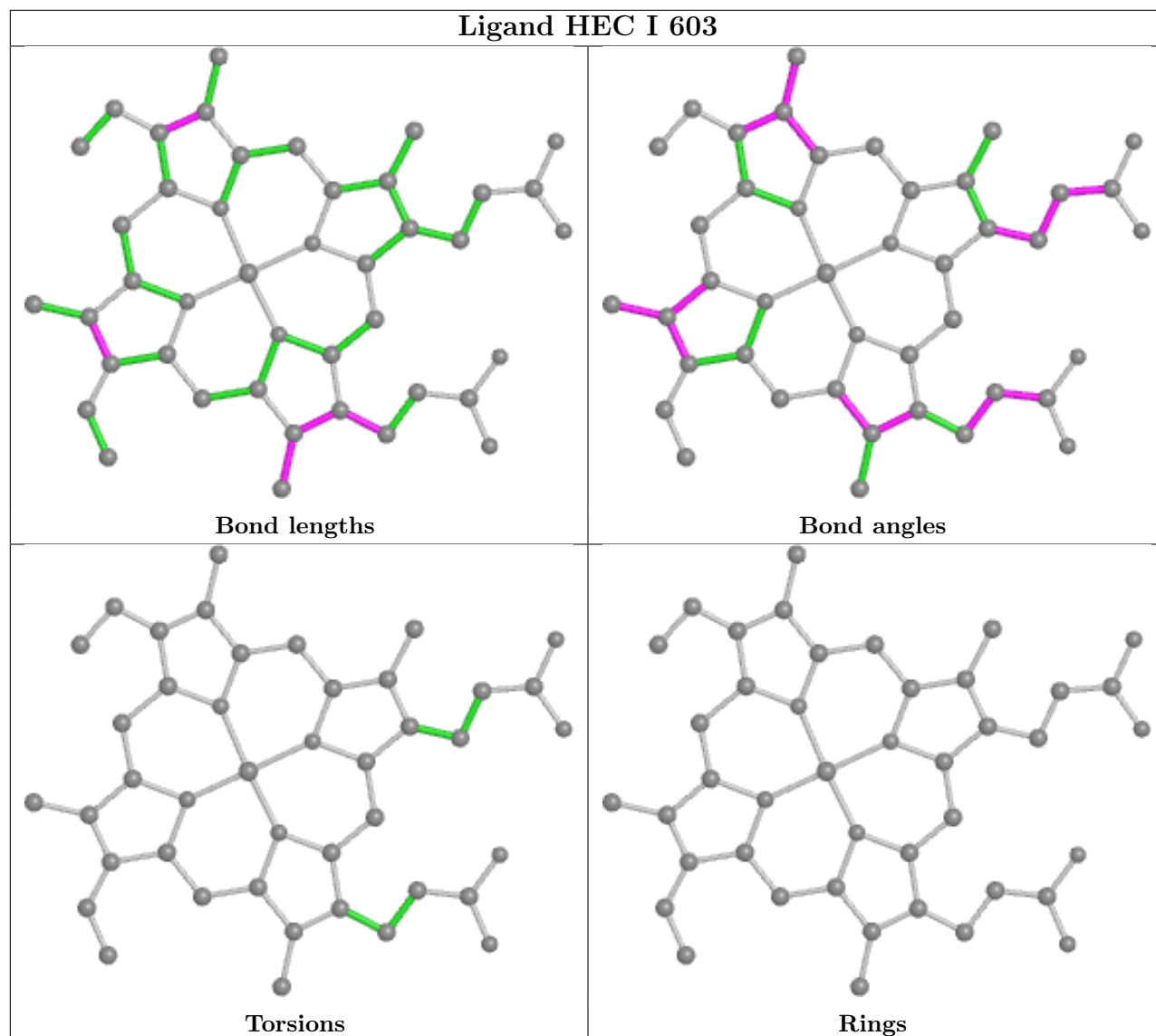
Torsions



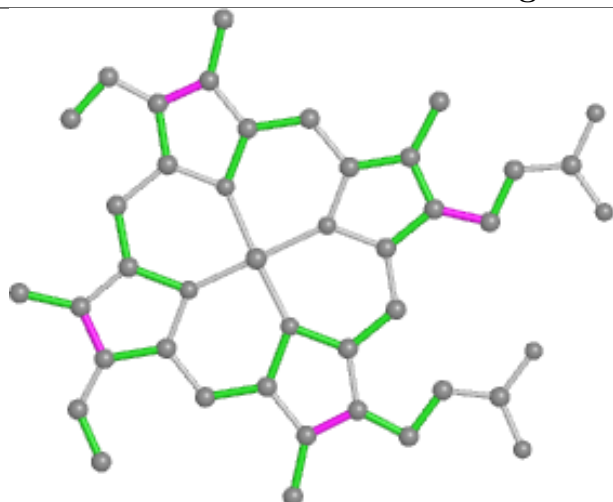
Rings



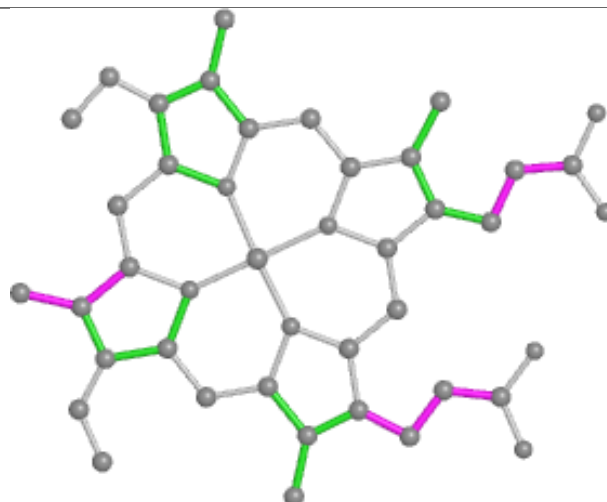
Ligand HEC I 603



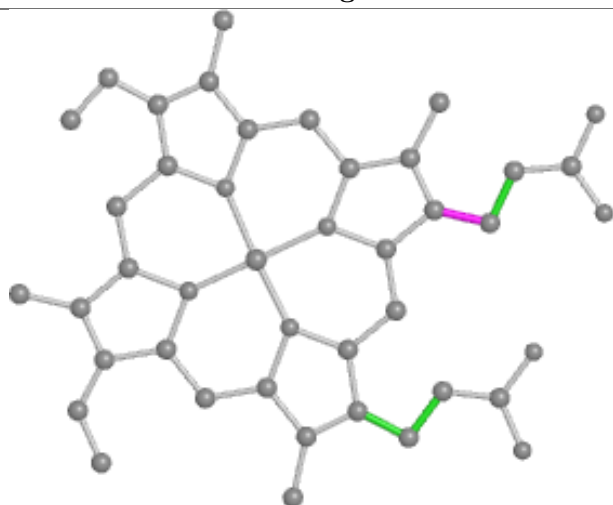
Ligand HEC I 604



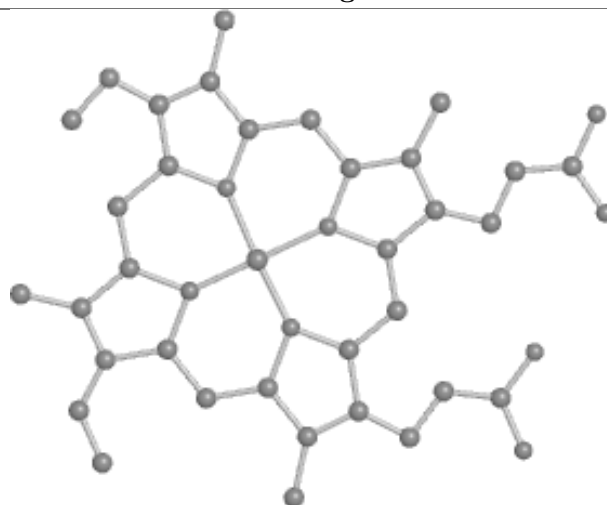
Bond lengths



Bond angles

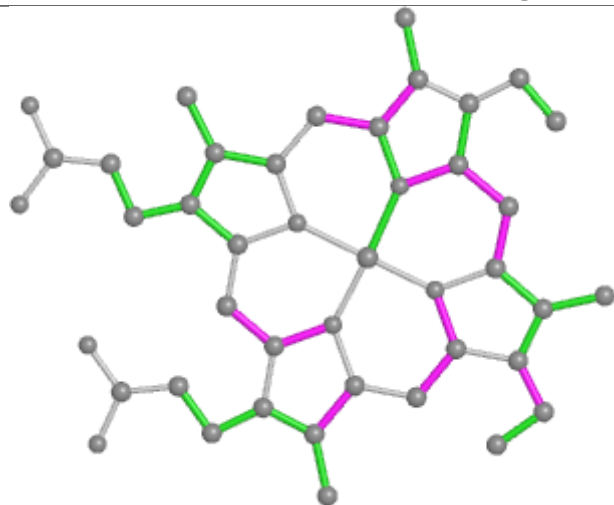


Torsions

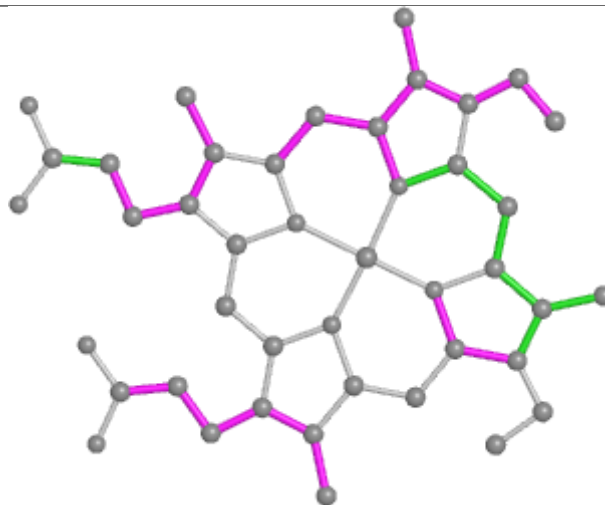


Rings

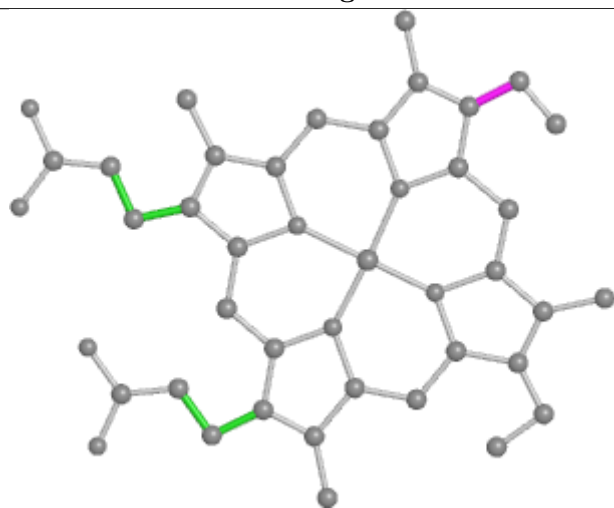
Ligand ISW A 608



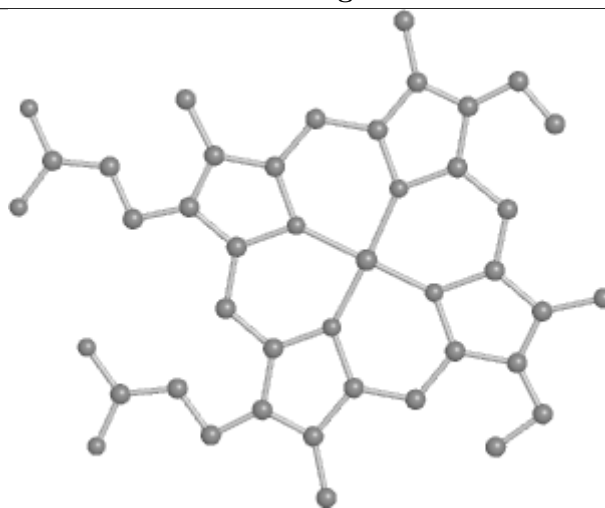
Bond lengths



Bond angles

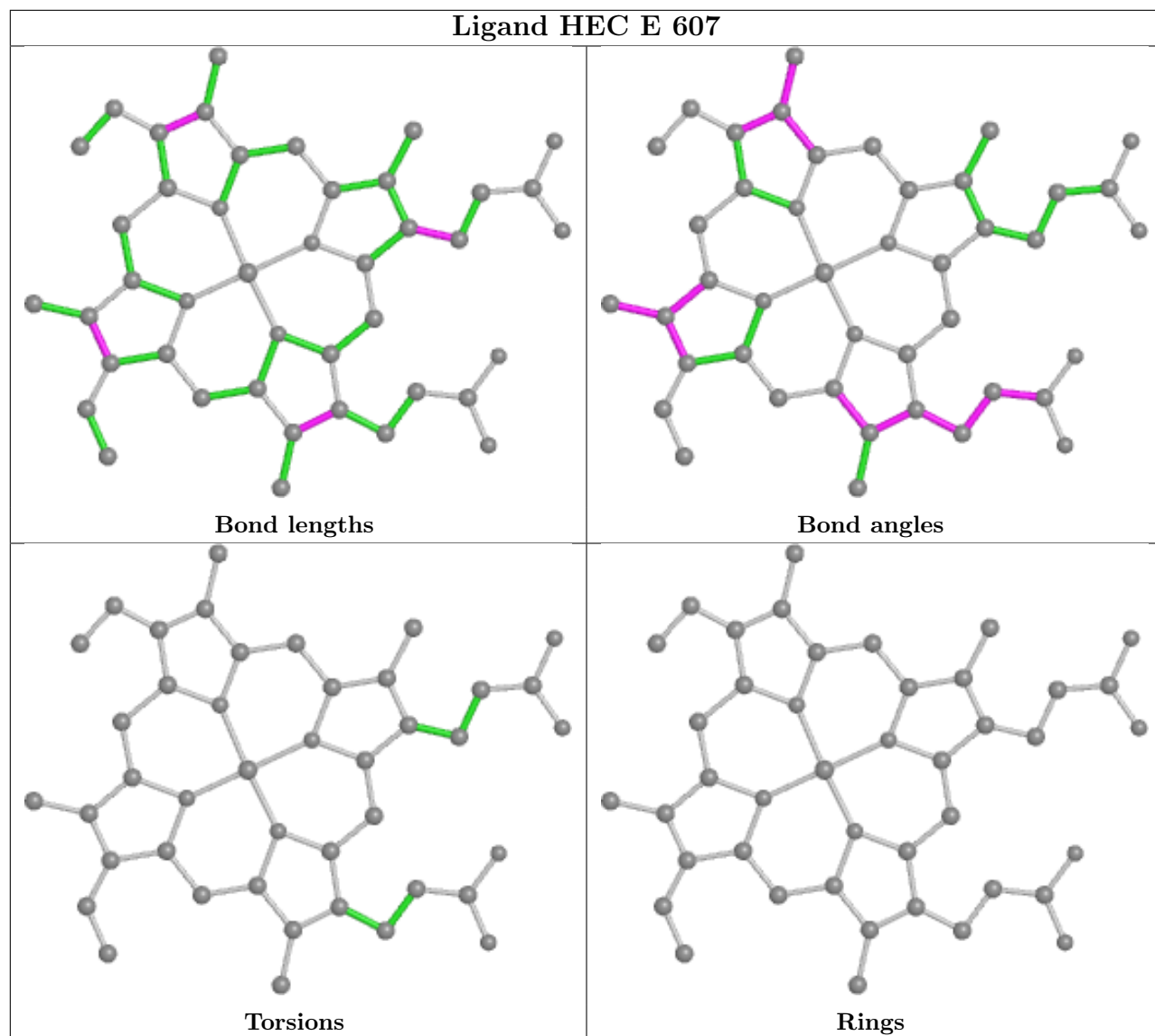


Torsions

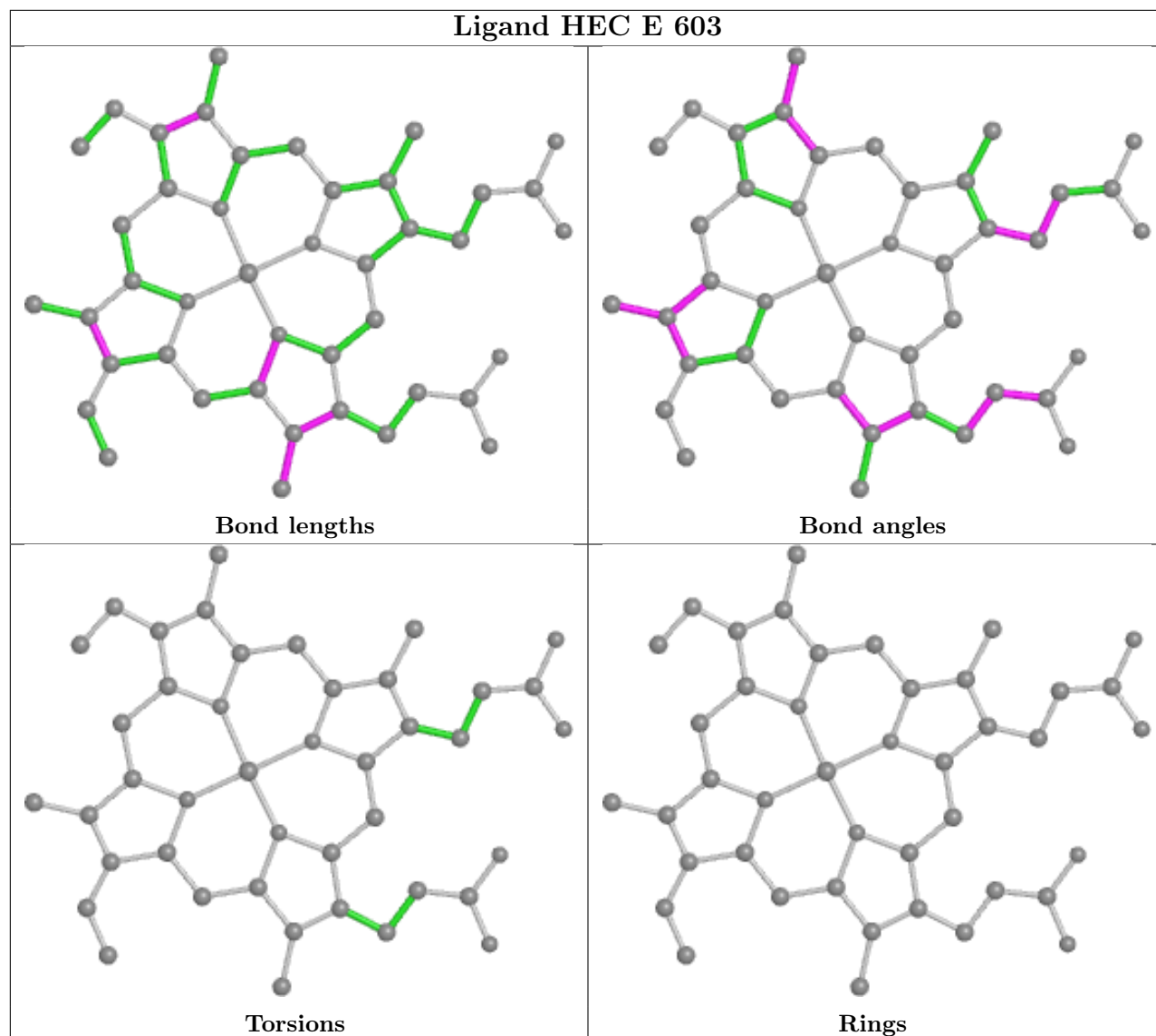


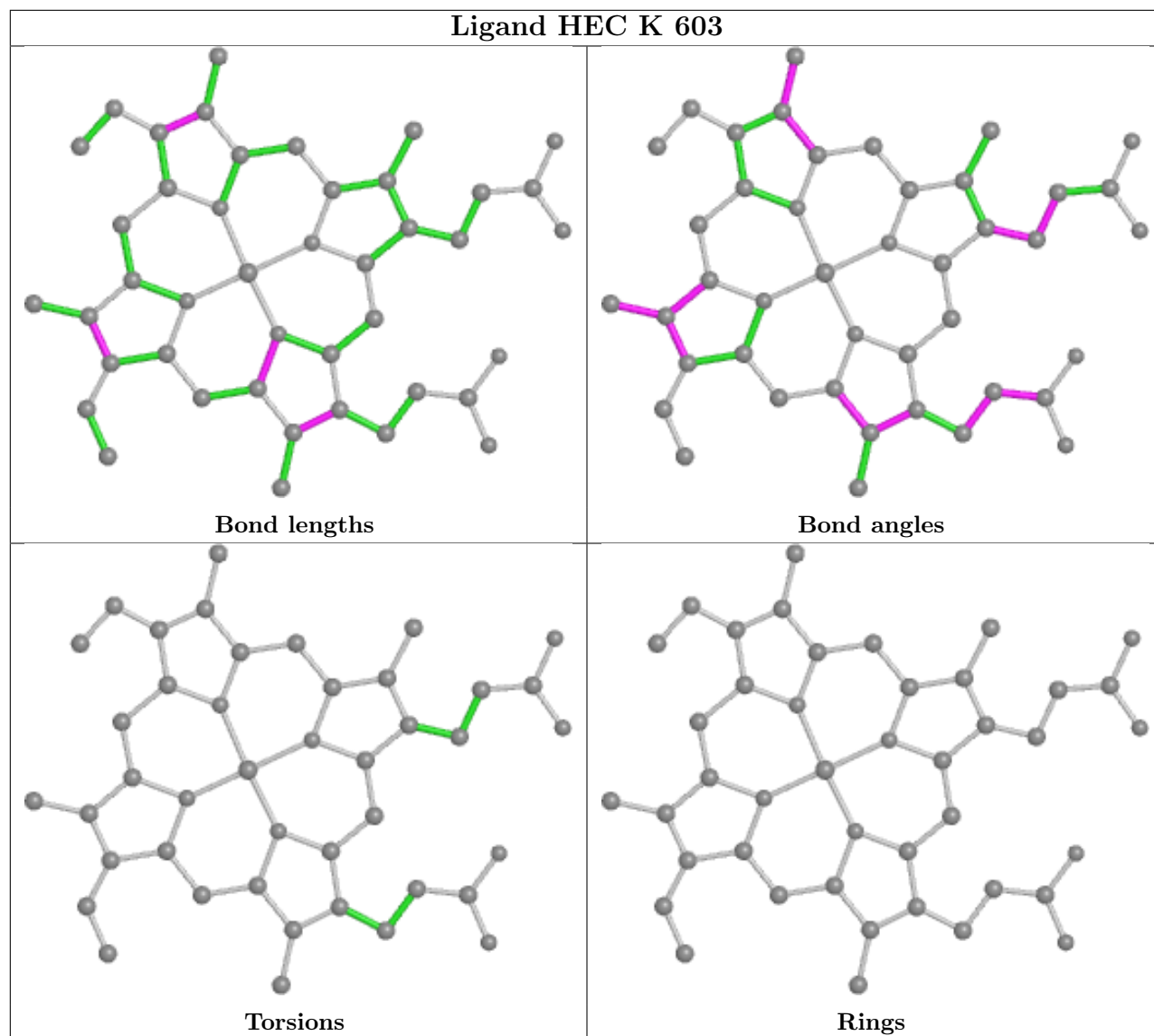
Rings

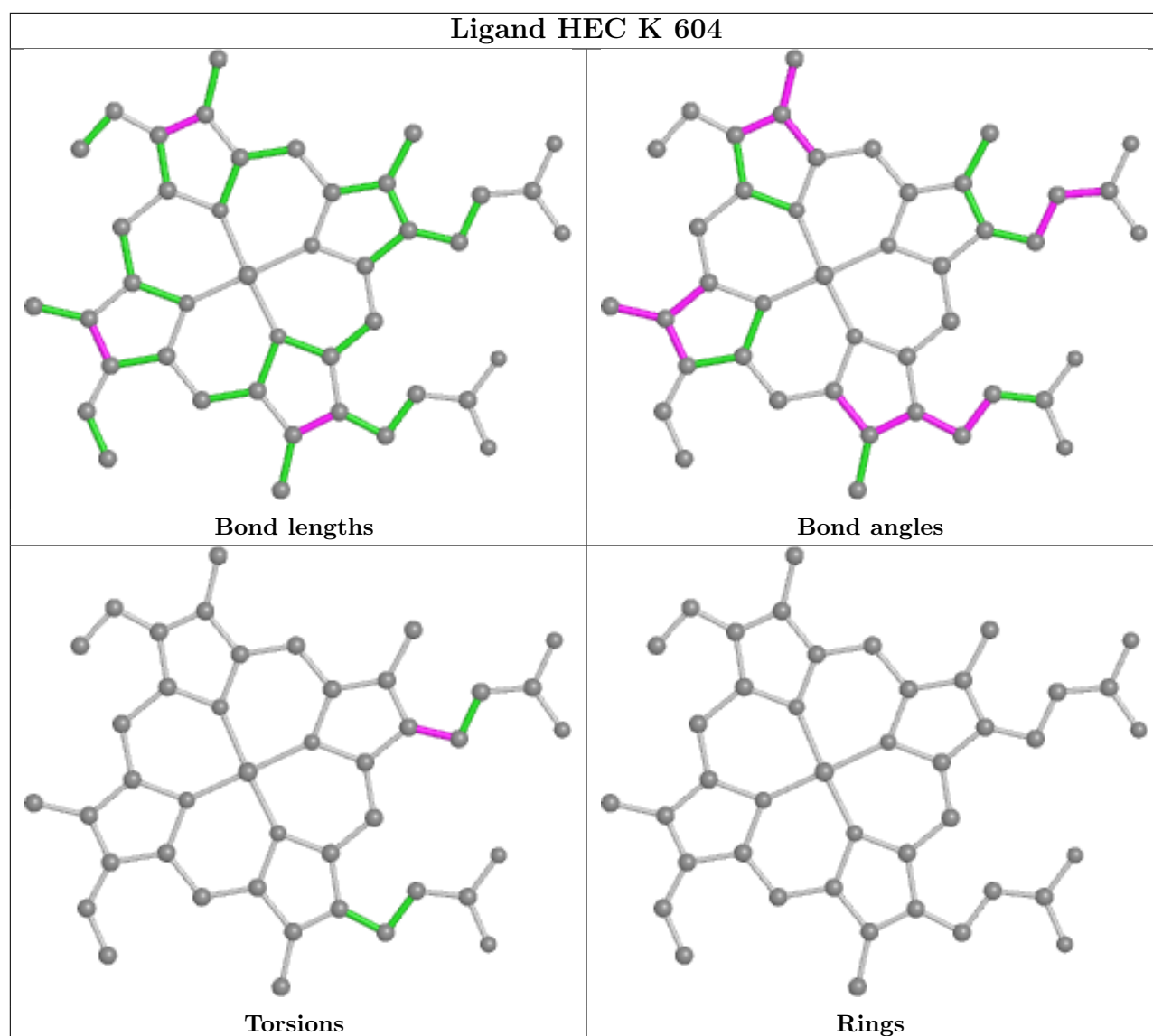
Ligand HEC E 607



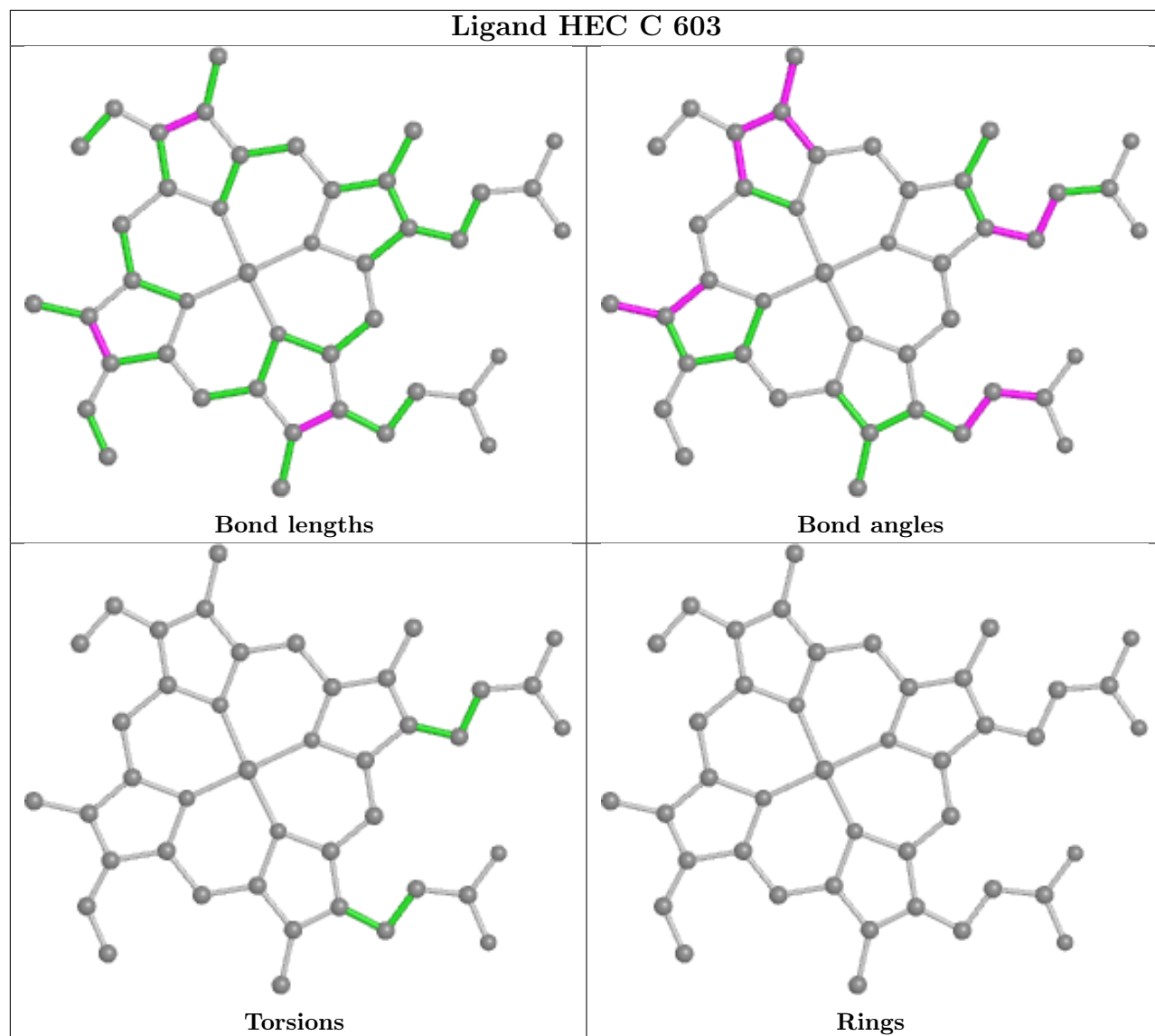
Ligand HEC E 603

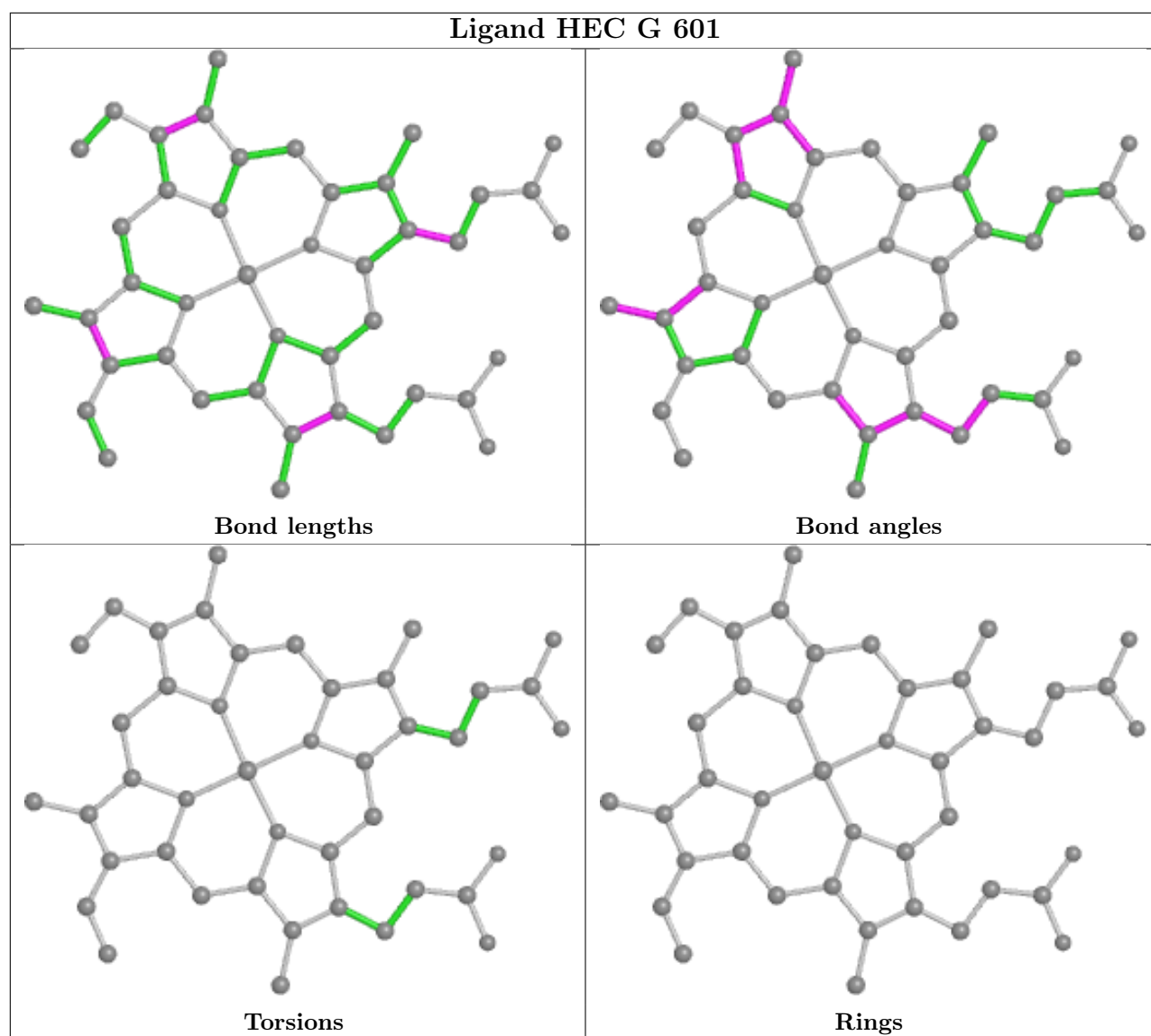


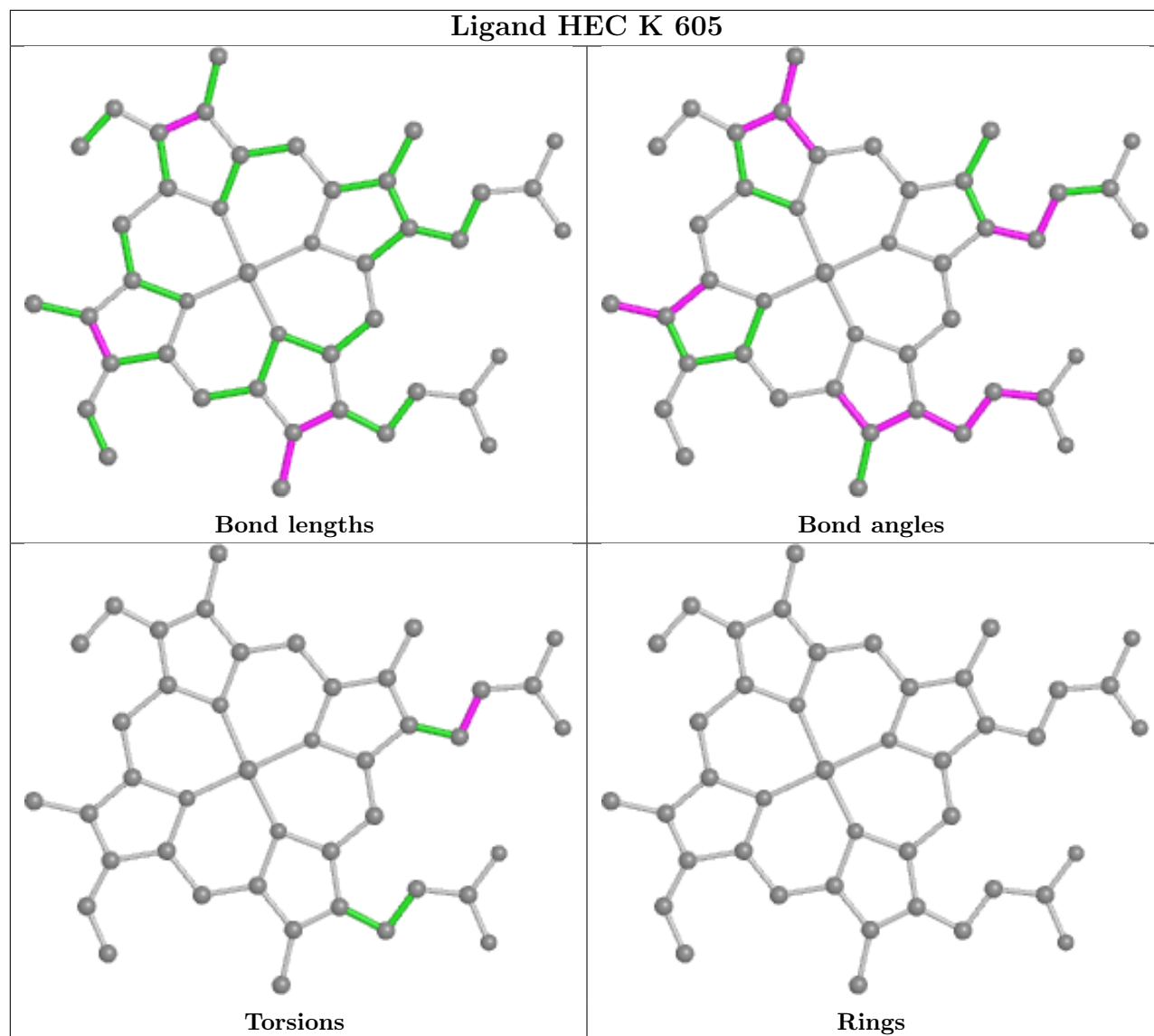




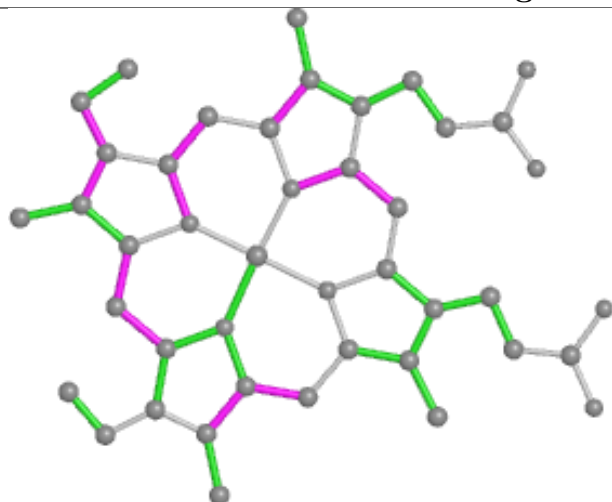
Ligand HEC C 603



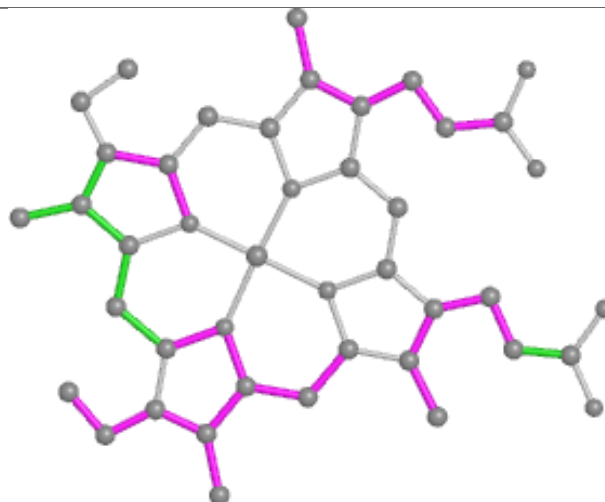




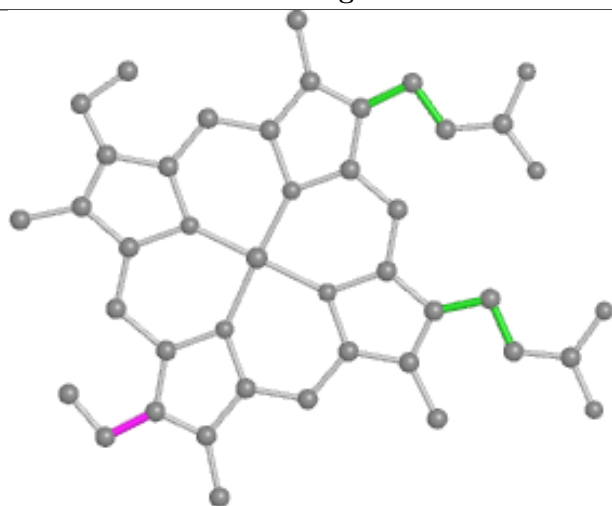
Ligand ISW C 608



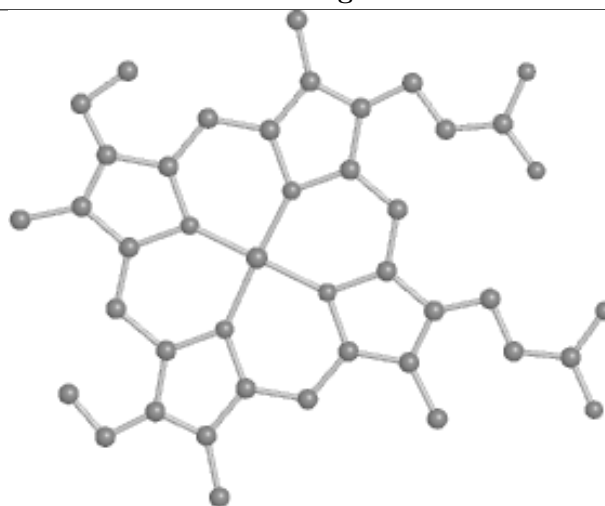
Bond lengths



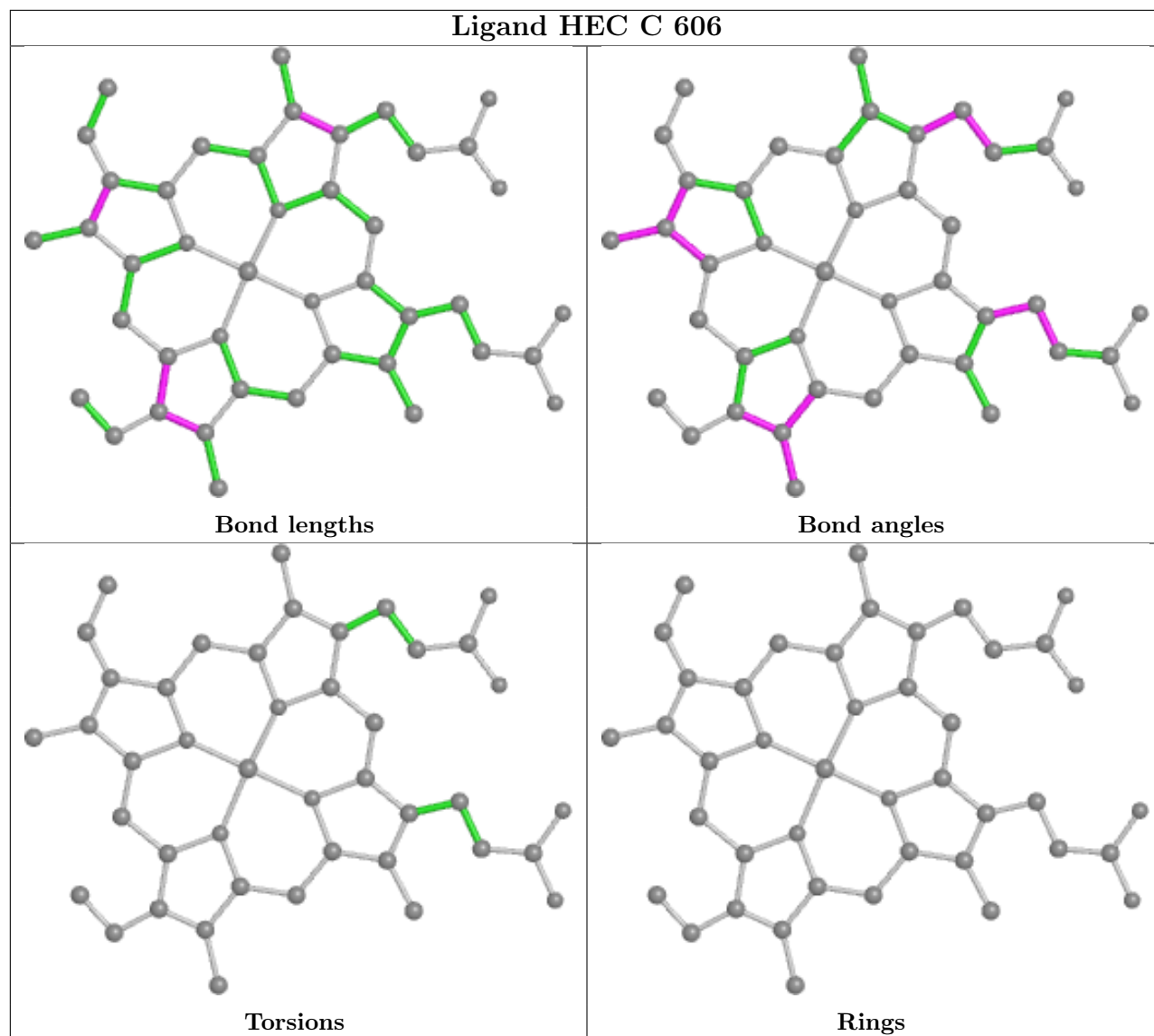
Bond angles



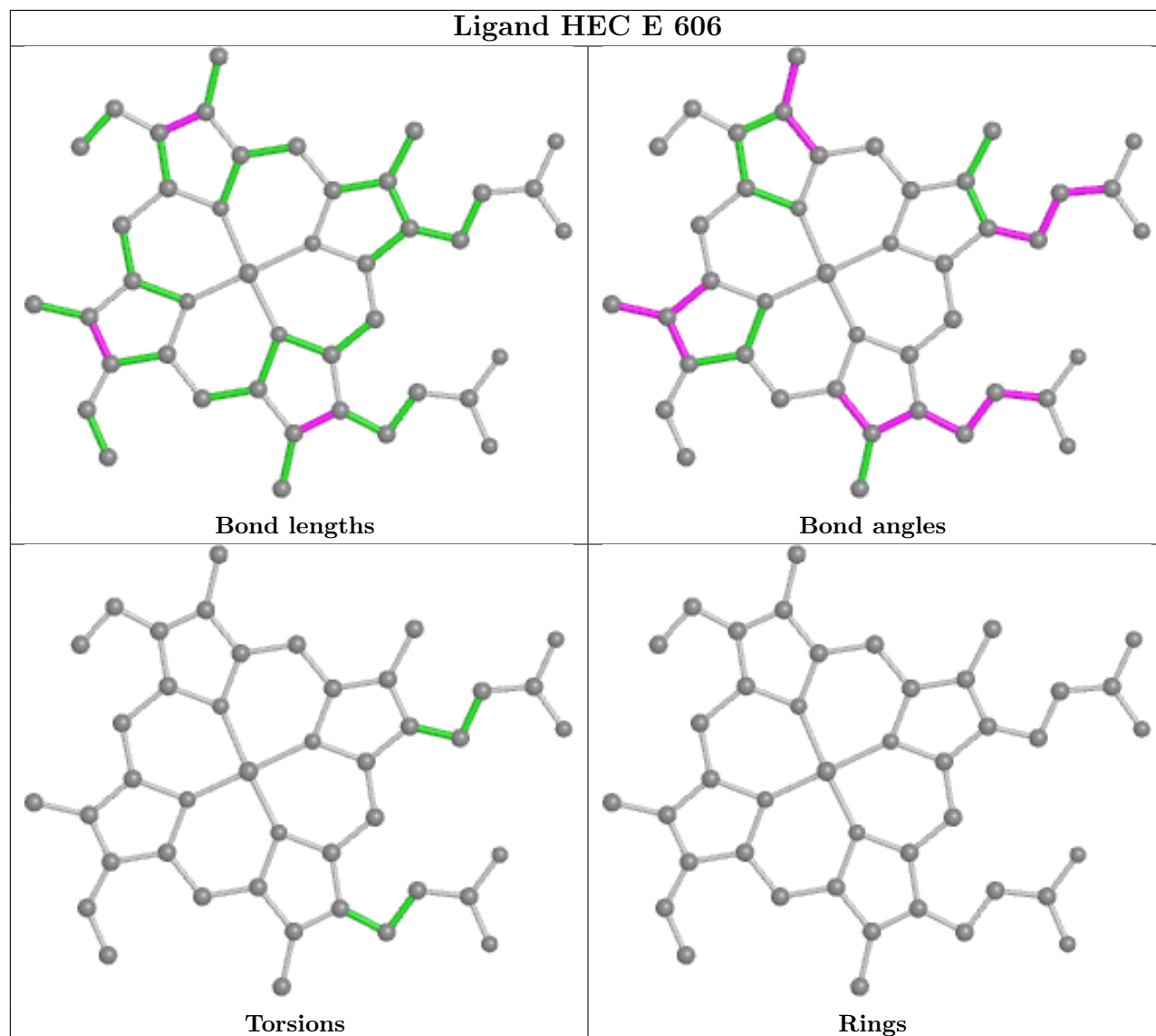
Torsions



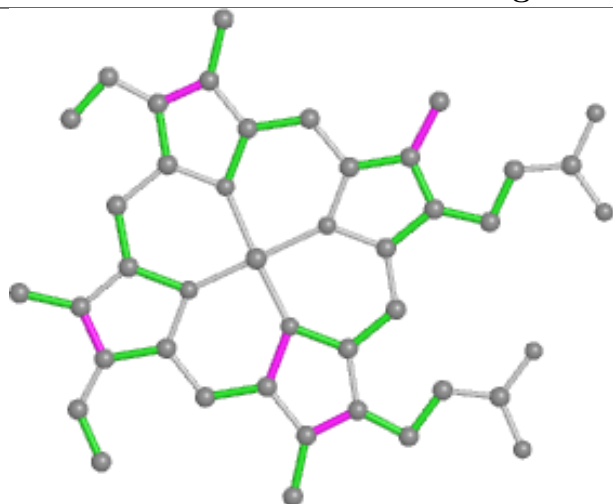
Rings



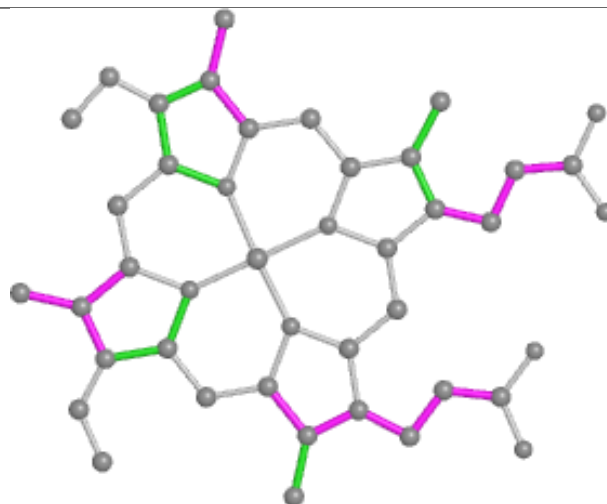
Ligand HEC E 606



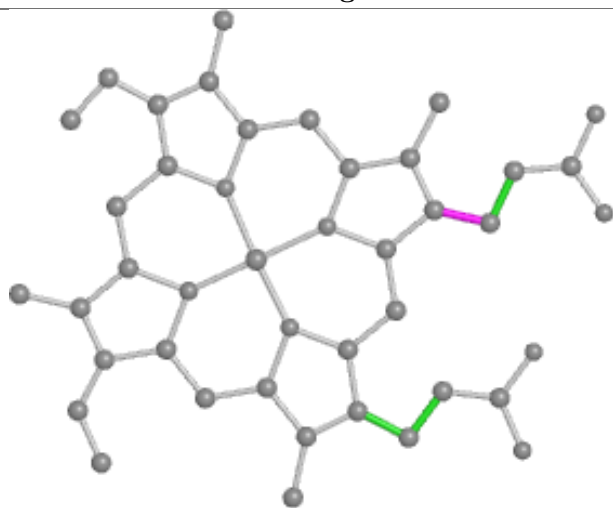
Ligand HEC C 604



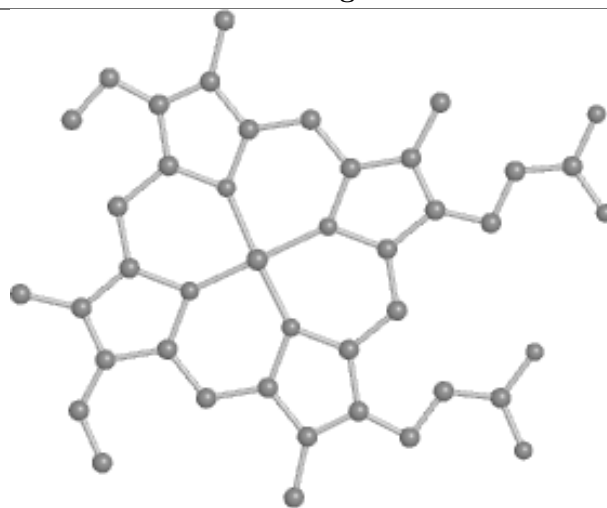
Bond lengths



Bond angles

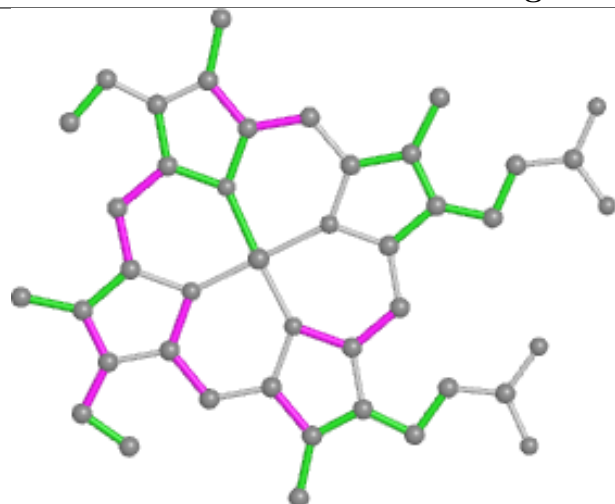


Torsions

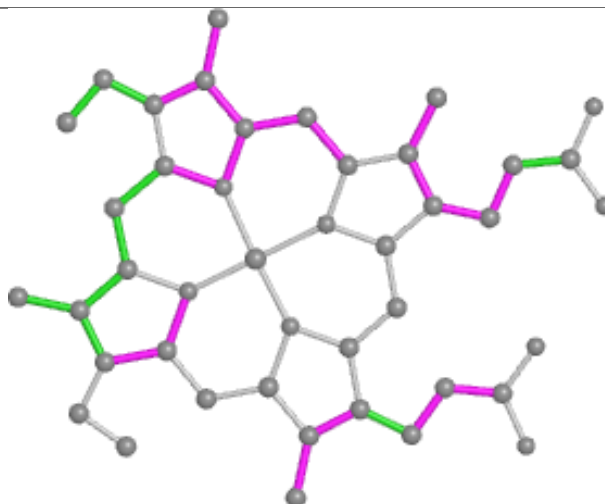


Rings

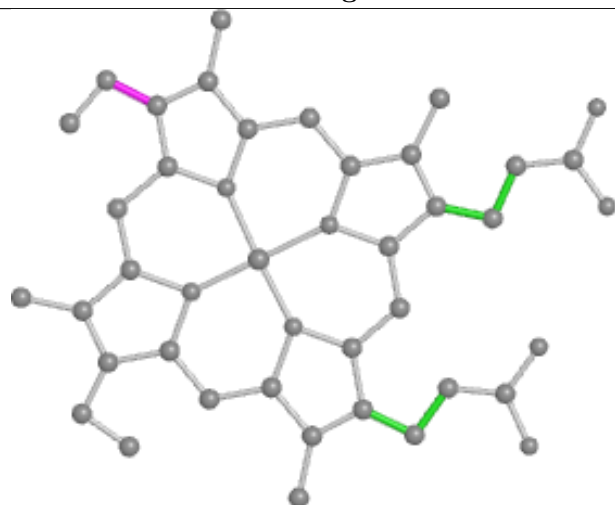
Ligand ISW I 608



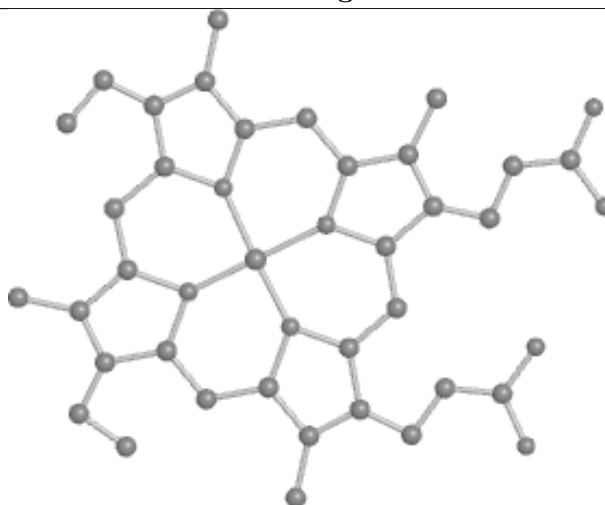
Bond lengths



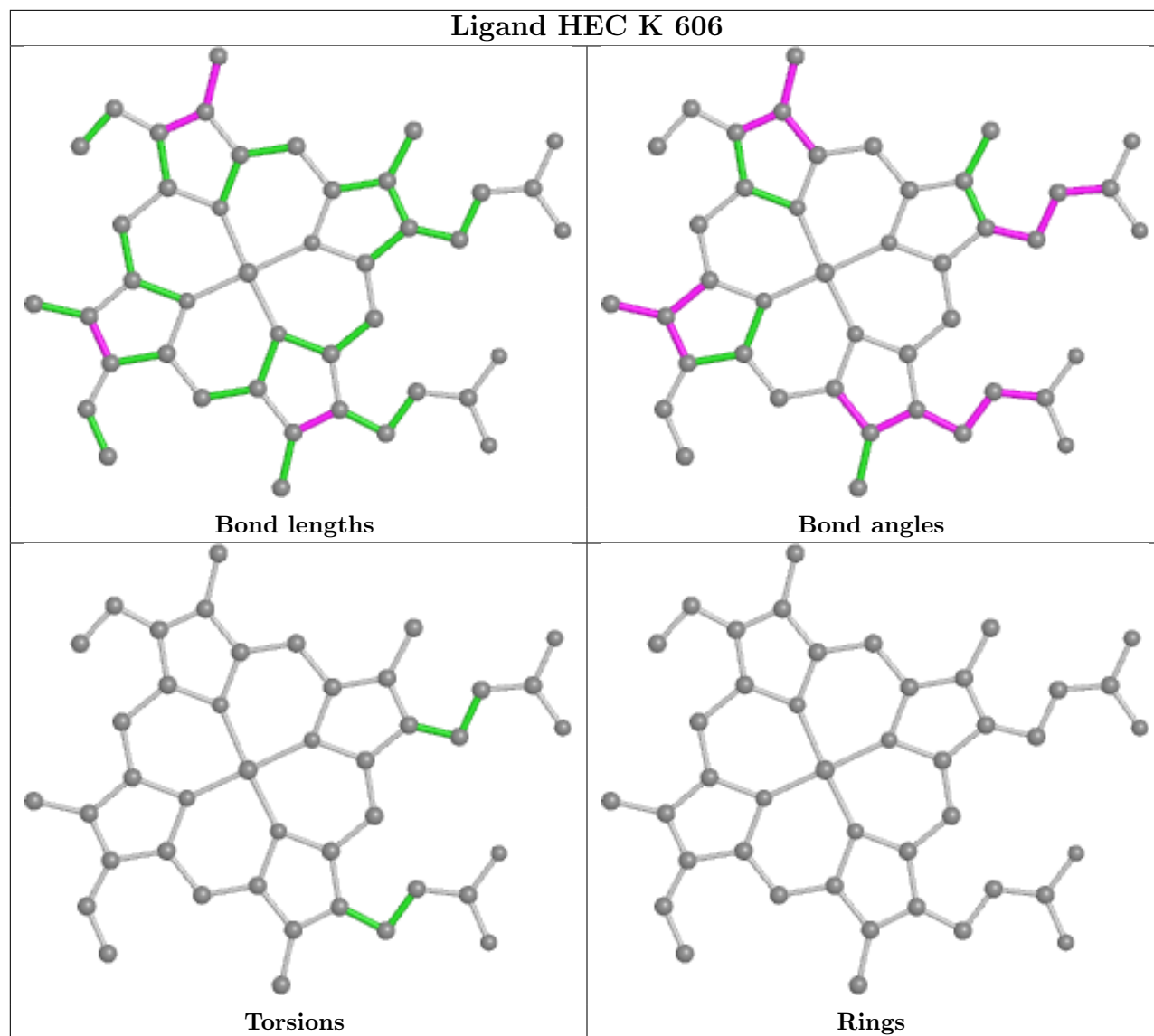
Bond angles



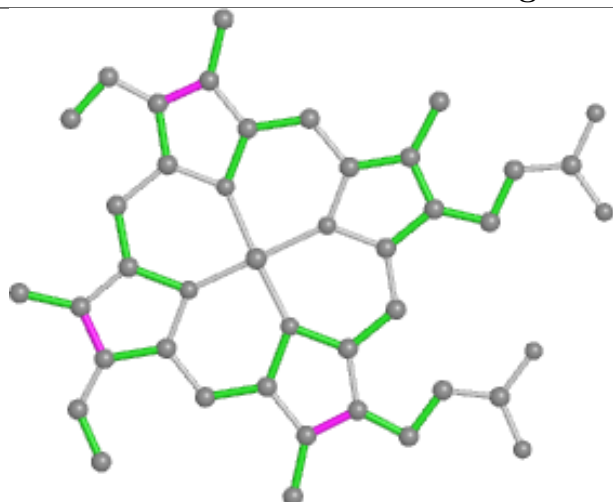
Torsions



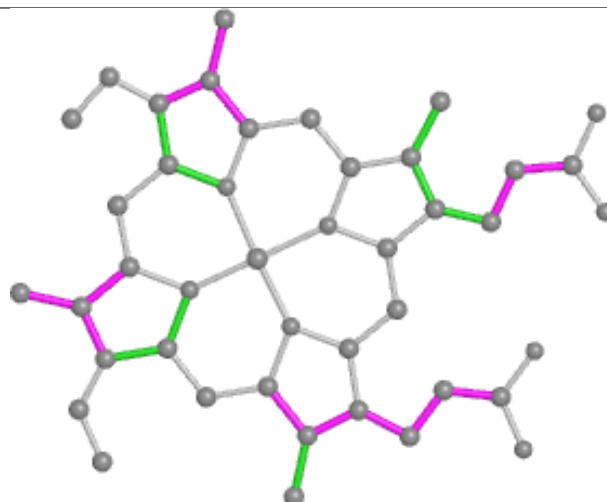
Rings



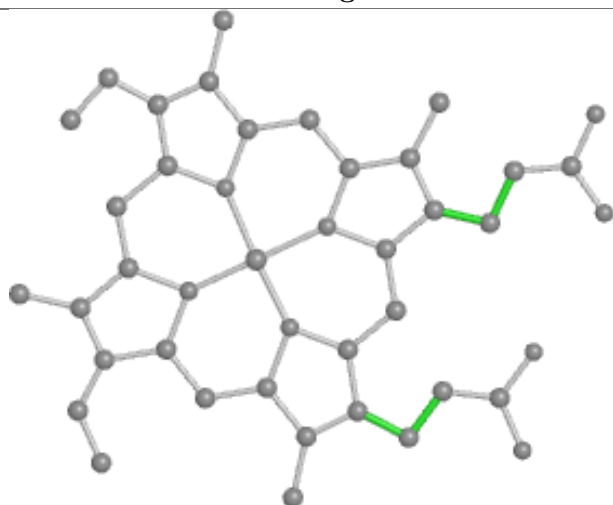
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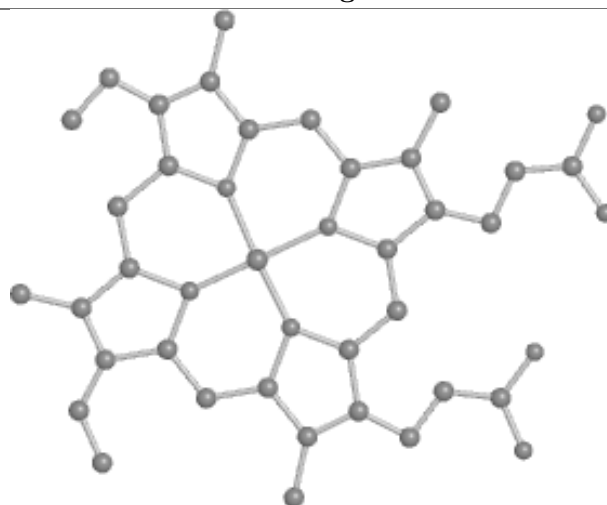
Bond lengths



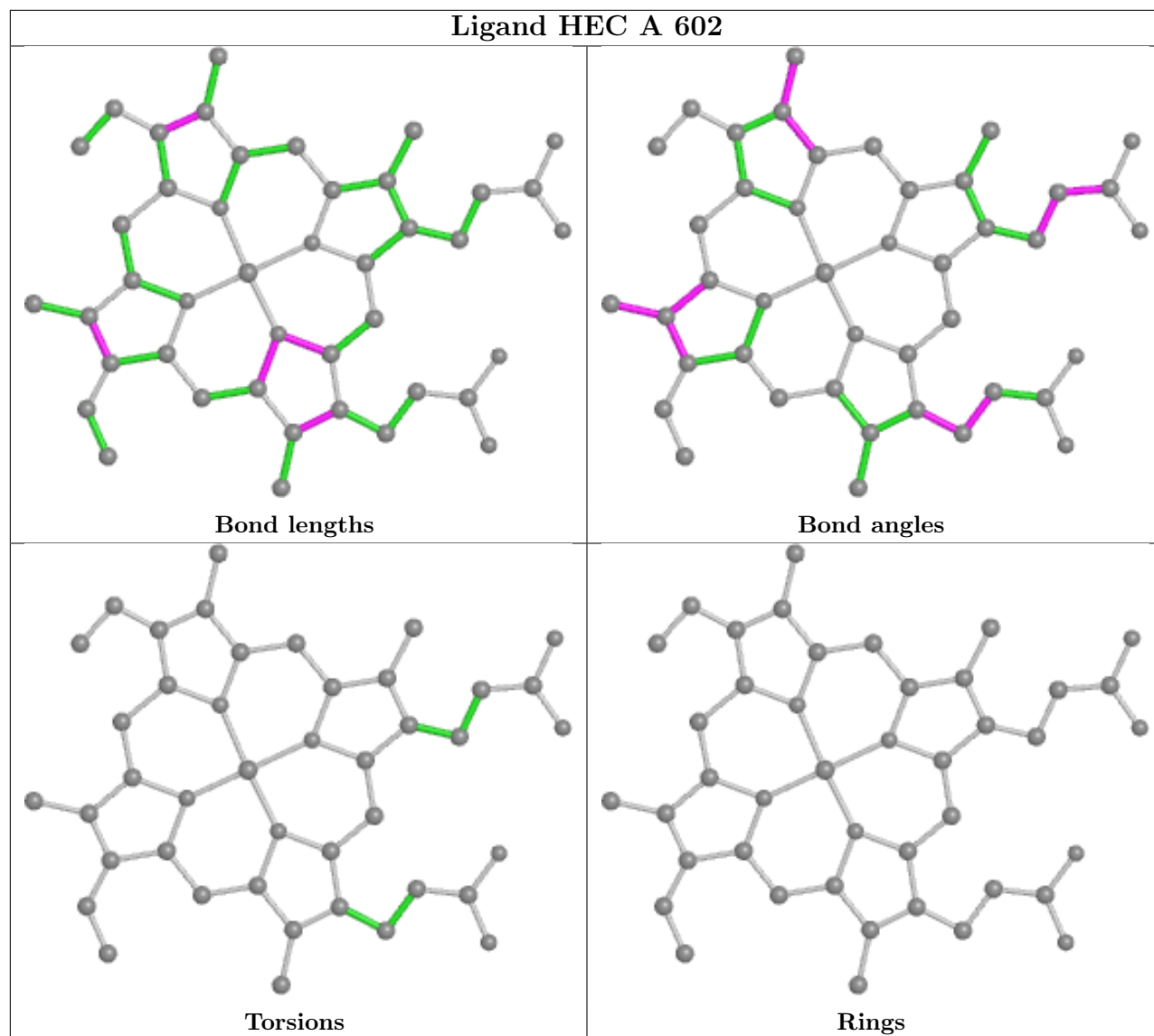
Bond angles



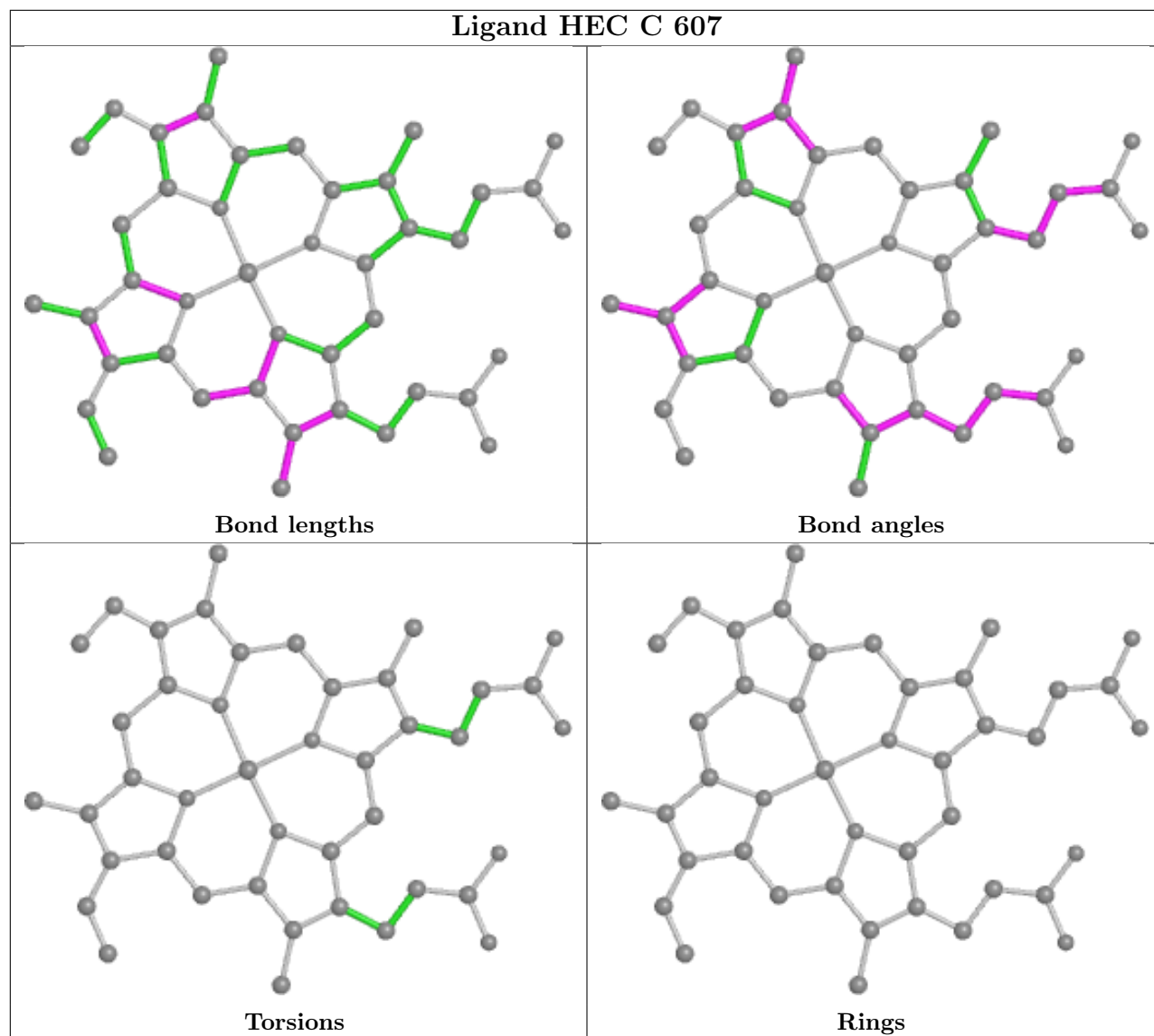
Torsions

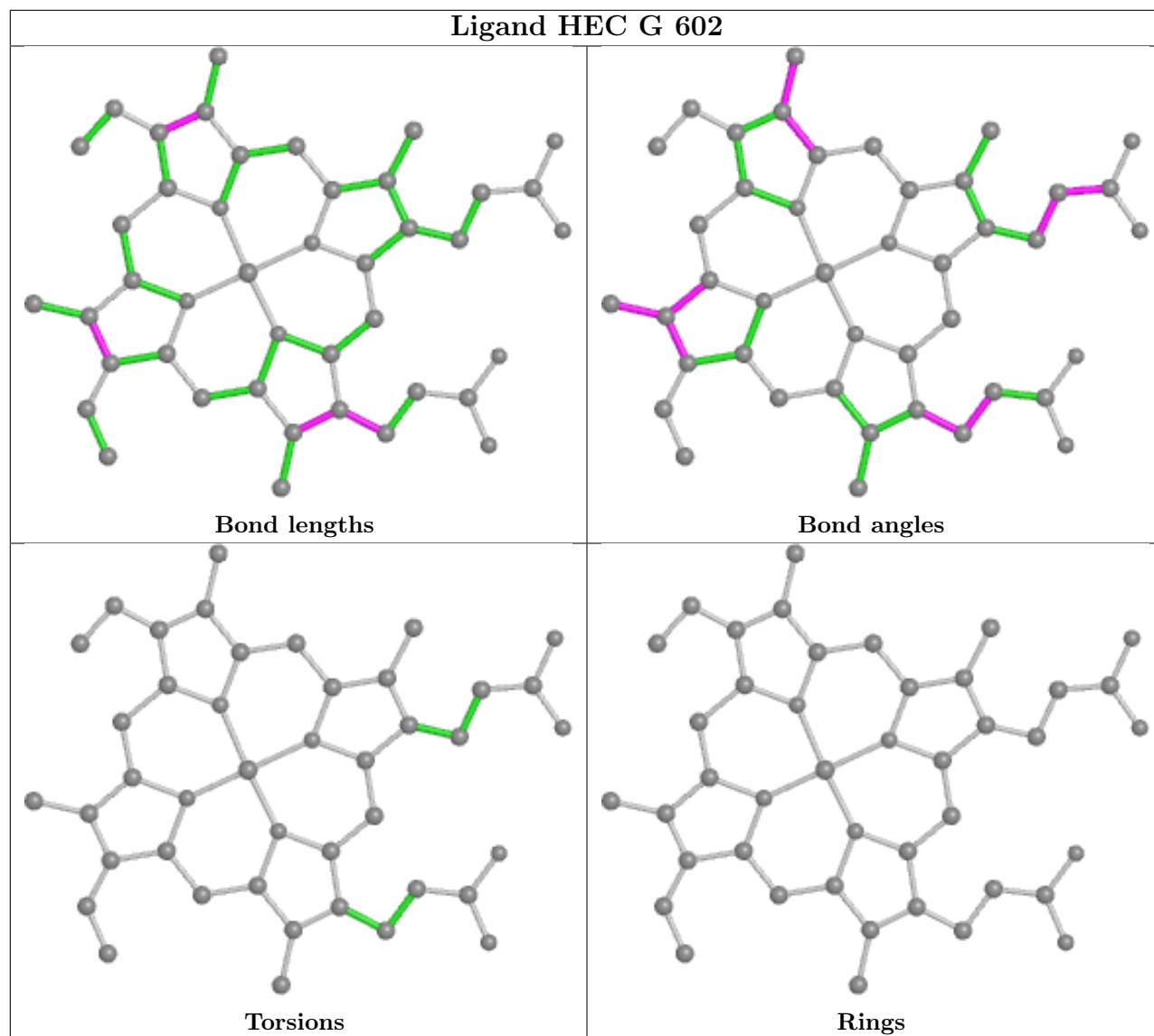


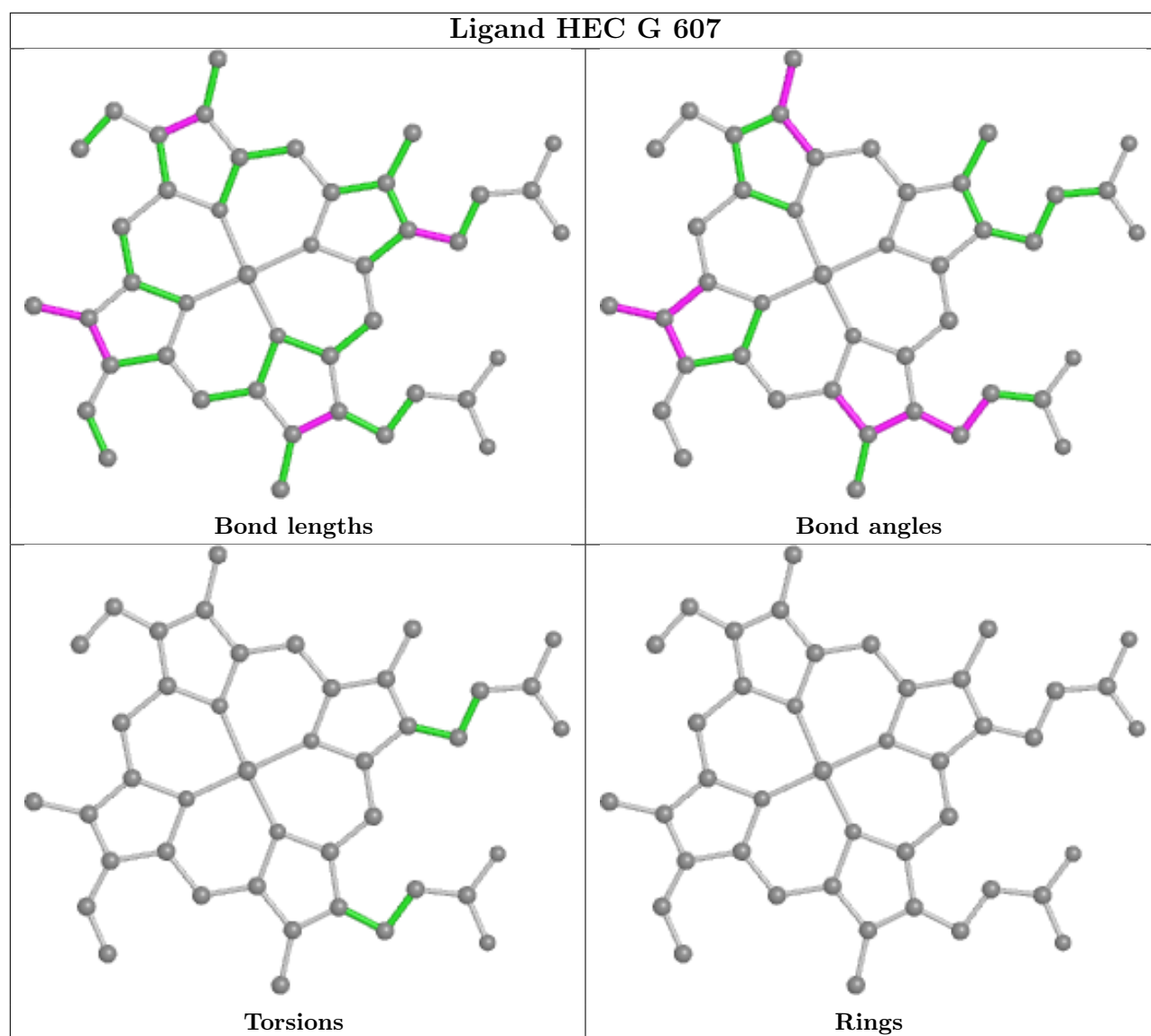
Rings

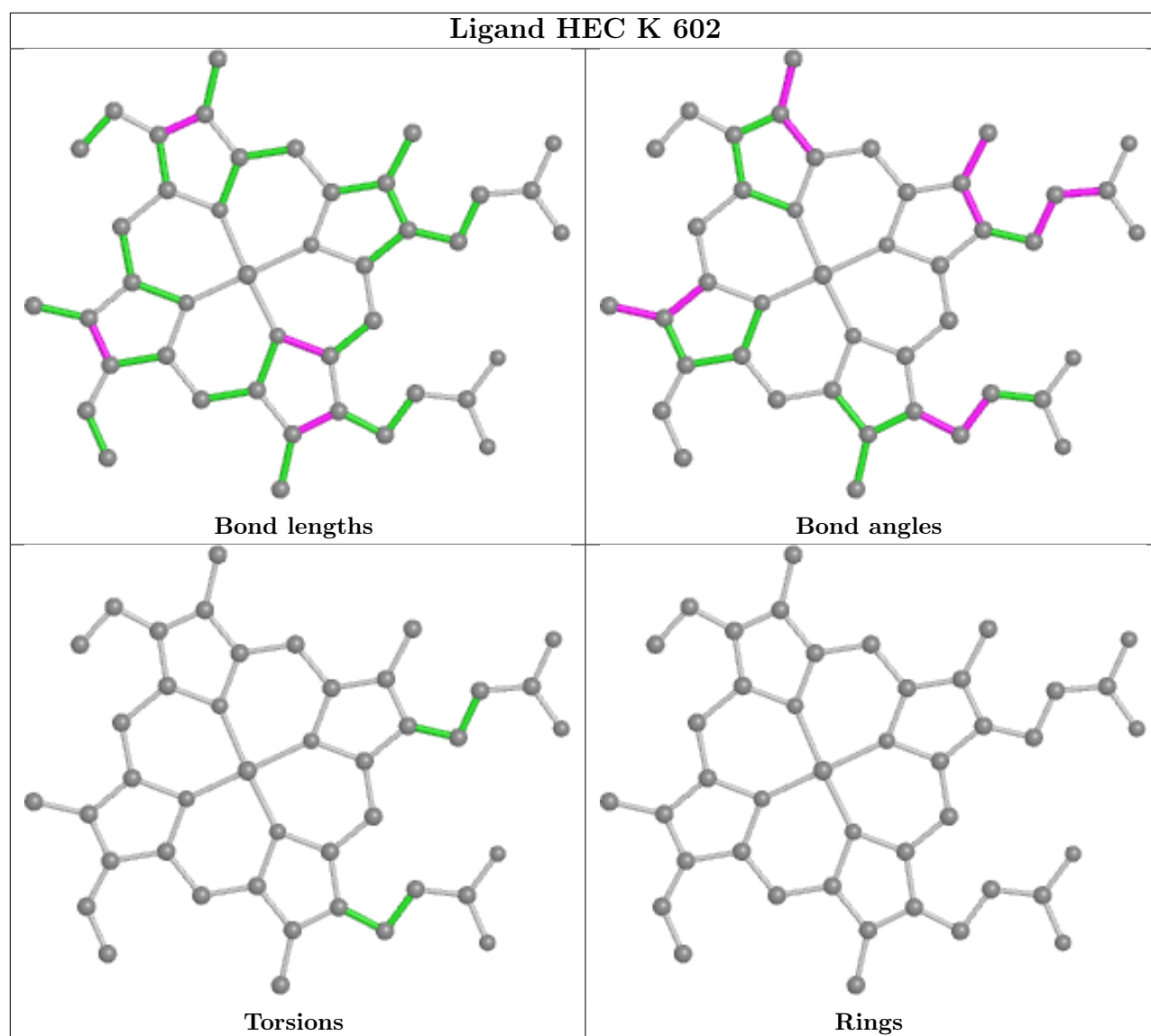


Ligand HEC C 607

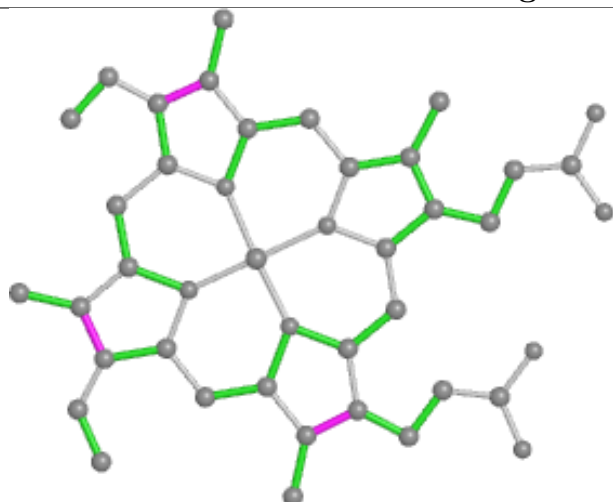




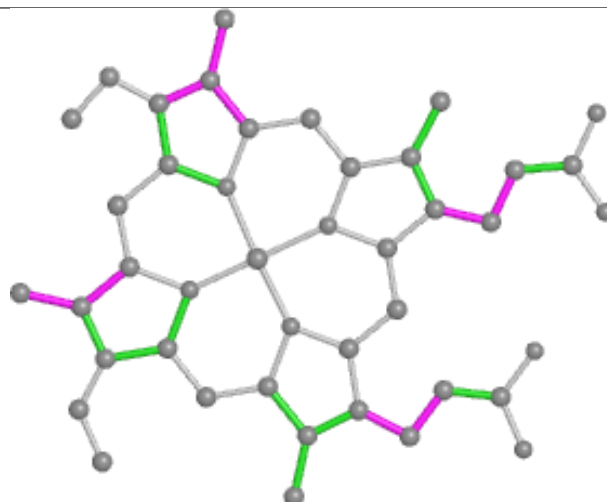




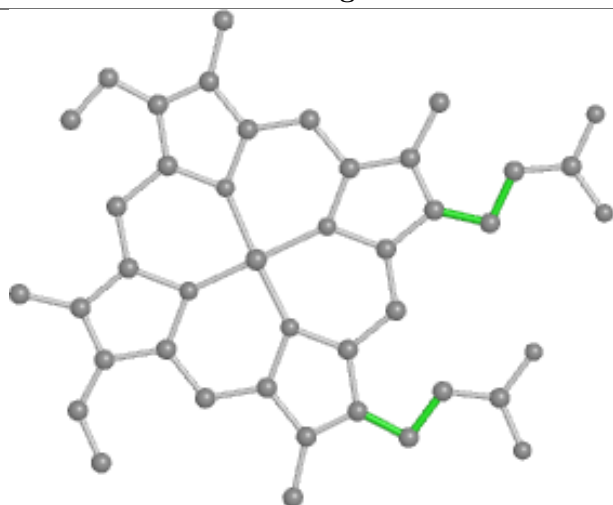
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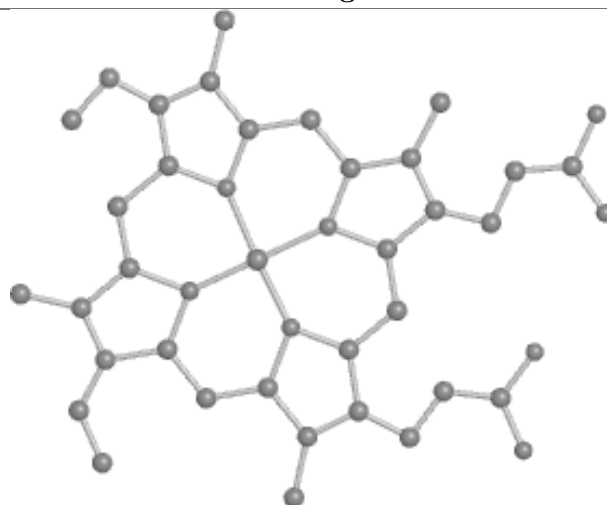
Bond lengths



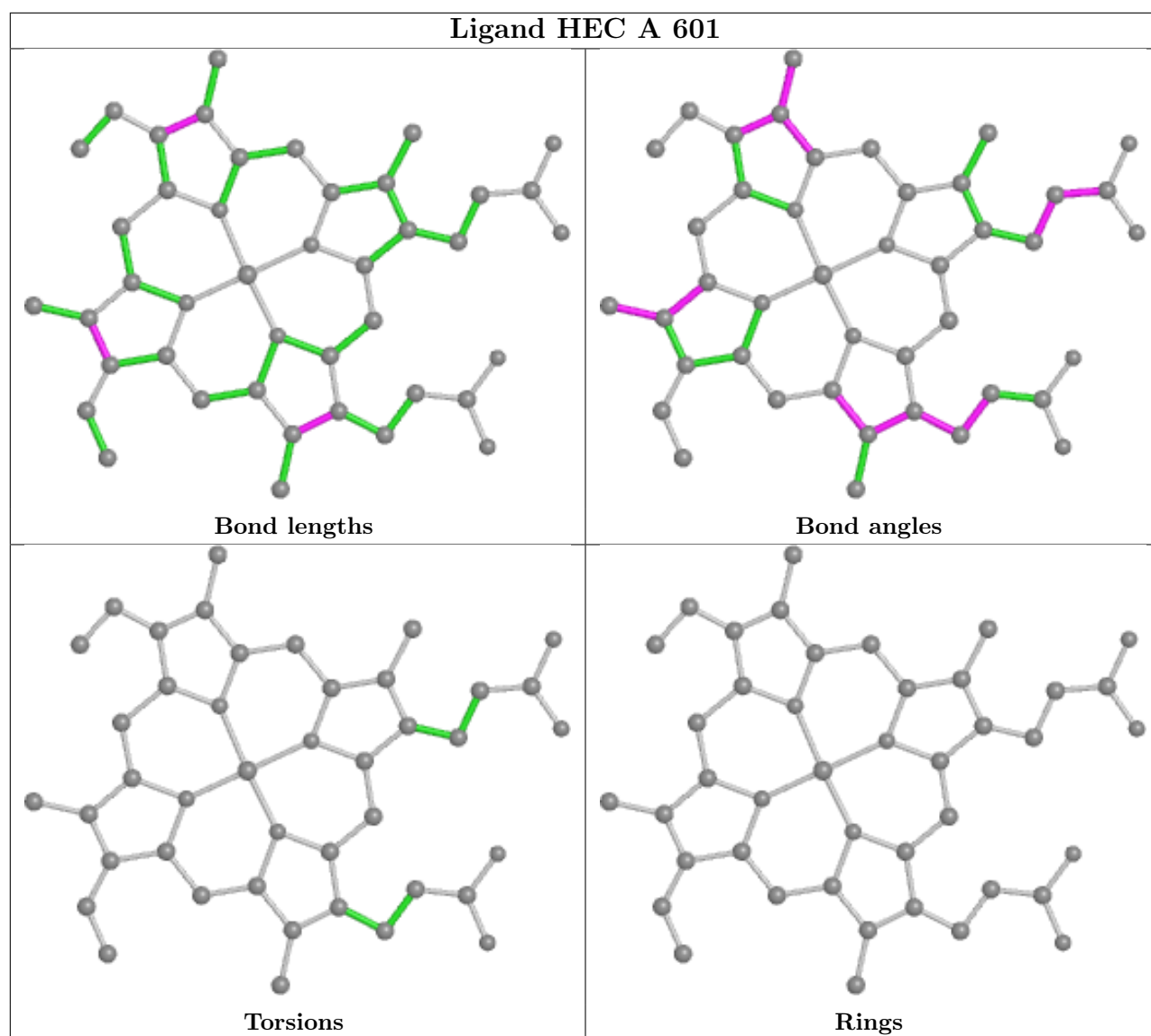
Bond angles

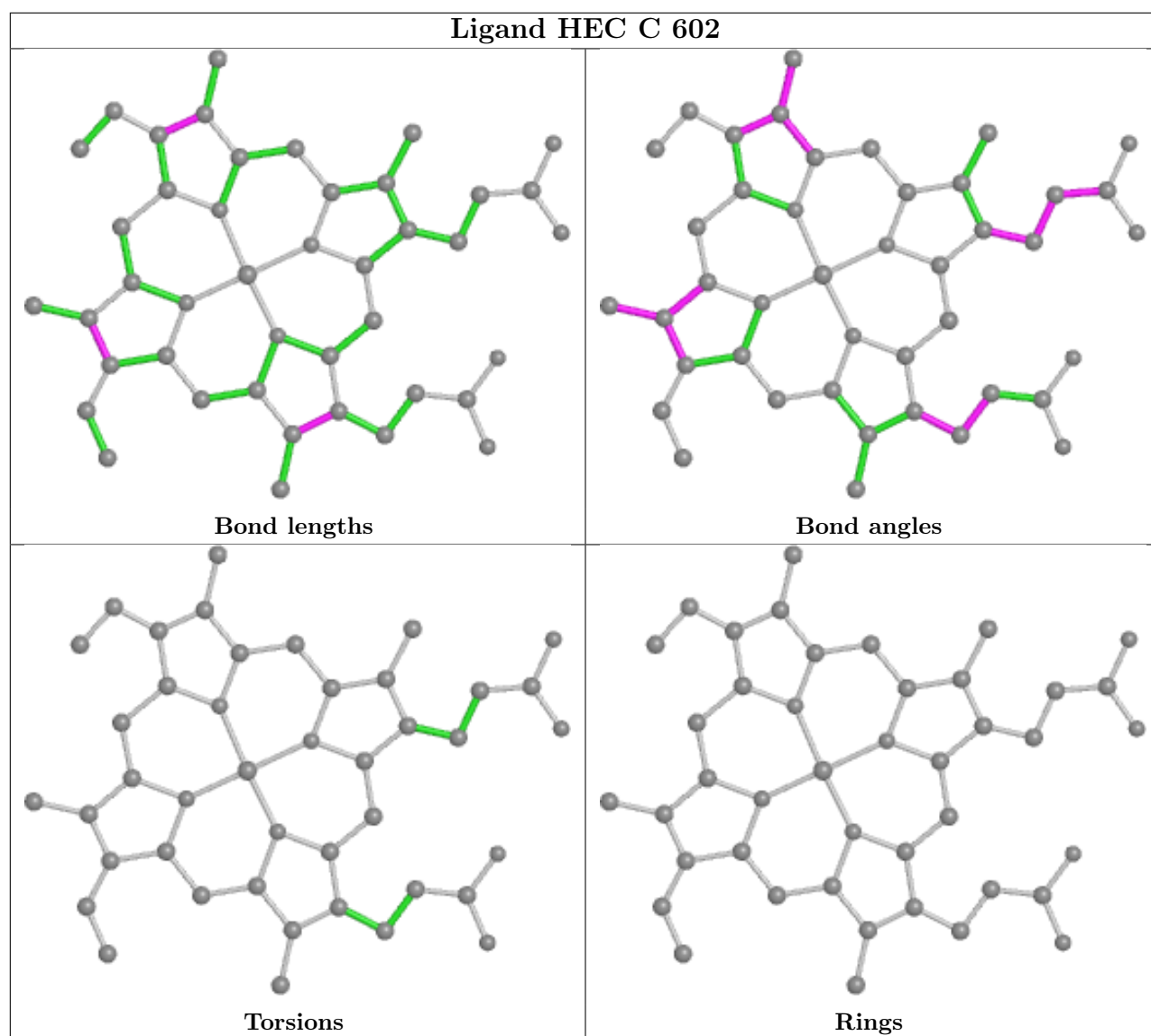


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	504/570 (88%)	0.02	19 (3%) 40 39	19, 27, 46, 69	0
1	C	504/570 (88%)	-0.02	16 (3%) 47 46	18, 29, 46, 82	0
1	E	504/570 (88%)	-0.02	9 (1%) 68 66	19, 27, 46, 76	0
1	G	504/570 (88%)	0.02	17 (3%) 45 44	20, 30, 52, 81	0
1	I	504/570 (88%)	0.09	21 (4%) 36 35	19, 32, 53, 90	0
1	K	504/570 (88%)	0.01	12 (2%) 59 57	21, 30, 50, 87	0
2	B	64/91 (70%)	1.05	14 (21%) 0 0	23, 43, 77, 85	0
2	D	64/91 (70%)	0.54	13 (20%) 1 0	25, 34, 69, 85	0
2	F	64/91 (70%)	1.54	21 (32%) 0 0	26, 45, 70, 87	0
2	H	64/91 (70%)	1.23	21 (32%) 0 0	25, 44, 73, 80	0
2	J	64/91 (70%)	0.40	9 (14%) 2 2	26, 37, 69, 90	0
2	L	64/91 (70%)	1.80	31 (48%) 0 0	30, 50, 81, 91	0
All	All	3408/3966 (85%)	0.14	203 (5%) 21 20	18, 30, 56, 91	0

The worst 5 of 203 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	87	TRP	6.1
2	J	85	ASP	5.9
2	L	85	ASP	5.5
2	B	91	TYR	5.5
2	L	91	TYR	5.4

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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PEG	J	101	7/7	0.80	0.19	58,59,61,61	0
6	PGE	E	608	10/10	0.80	0.16	60,62,65,66	0
7	PG4	C	611	13/13	0.80	0.21	60,64,67,67	0
6	PGE	G	612	10/10	0.81	0.21	49,52,56,58	0
5	PEG	K	608	7/7	0.82	0.29	49,51,54,55	0
7	PG4	A	612	13/13	0.84	0.21	50,56,60,60	0
7	PG4	K	610	13/13	0.85	0.18	48,55,61,63	0
6	PGE	A	611	10/10	0.86	0.17	46,50,61,63	0
5	PEG	K	609	7/7	0.86	0.14	49,51,55,56	0
7	PG4	E	610	13/13	0.87	0.16	61,63,64,65	0
6	PGE	I	610	10/10	0.87	0.20	49,53,55,55	0
6	PGE	E	609	10/10	0.90	0.22	52,52,55,56	0
5	PEG	G	610	7/7	0.90	0.12	50,51,52,53	0
6	PGE	I	609	10/10	0.90	0.21	56,58,60,60	0
5	PEG	C	609	7/7	0.90	0.14	42,44,52,54	0
6	PGE	C	610	10/10	0.93	0.19	53,55,57,57	0
5	PEG	A	610	7/7	0.93	0.10	43,46,50,51	0
6	PGE	G	611	10/10	0.94	0.17	52,53,55,55	0
4	ISW	A	608	43/43	0.95	0.14	16,25,36,39	0
4	ISW	A	609	43/43	0.95	0.15	16,25,34,37	0
4	ISW	G	608	43/43	0.95	0.12	21,27,36,38	0
4	ISW	C	608	43/43	0.96	0.12	14,27,37,38	0
4	ISW	G	609	43/43	0.96	0.14	19,28,35,37	0
4	ISW	I	608	43/43	0.96	0.13	20,28,40,41	0
3	HEC	K	605	43/43	0.98	0.12	14,21,25,27	0
3	HEC	K	606	43/43	0.98	0.10	17,22,34,37	0
3	HEC	K	607	43/43	0.98	0.10	16,21,35,36	0
3	HEC	A	602	43/43	0.98	0.09	18,22,28,35	0
3	HEC	A	603	43/43	0.98	0.09	19,27,31,33	0
3	HEC	A	605	43/43	0.98	0.15	15,19,22,24	0
3	HEC	A	606	43/43	0.98	0.12	14,20,28,32	0
3	HEC	C	603	43/43	0.98	0.09	22,26,29,36	0

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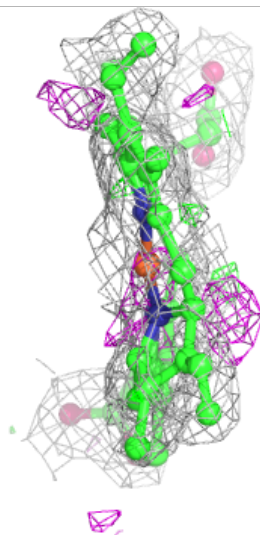
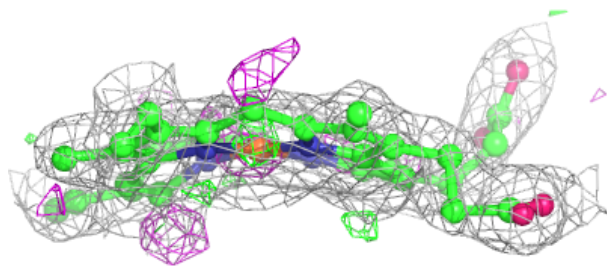
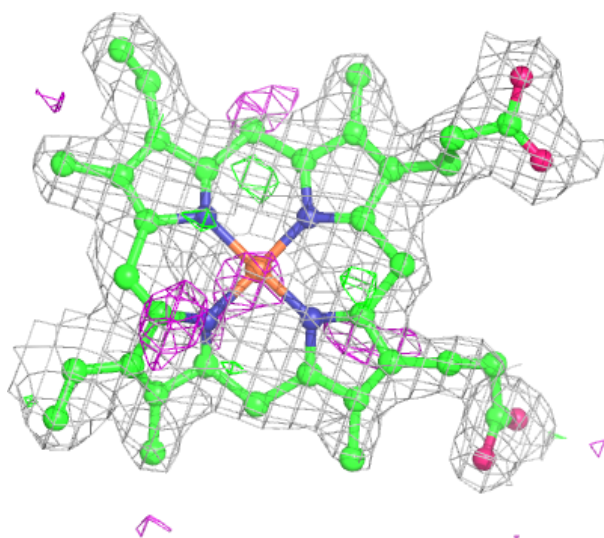
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	HEC	C	605	43/43	0.98	0.12	16,21,23,25	0
3	HEC	C	607	43/43	0.98	0.12	14,17,28,33	0
3	HEC	E	602	43/43	0.98	0.09	17,23,28,30	0
3	HEC	E	605	43/43	0.98	0.12	15,20,22,23	0
3	HEC	E	607	43/43	0.98	0.10	16,21,32,37	0
3	HEC	G	603	43/43	0.98	0.08	22,28,34,38	0
3	HEC	G	604	43/43	0.98	0.09	19,24,28,30	0
3	HEC	G	605	43/43	0.98	0.12	16,20,25,27	0
3	HEC	G	606	43/43	0.98	0.11	17,23,33,36	0
3	HEC	G	607	43/43	0.98	0.12	16,22,31,36	0
3	HEC	I	601	43/43	0.98	0.10	19,25,31,33	0
3	HEC	I	602	43/43	0.98	0.10	19,26,33,36	0
3	HEC	I	603	43/43	0.98	0.09	25,31,35,39	0
3	HEC	I	605	43/43	0.98	0.13	15,21,25,26	0
3	HEC	I	607	43/43	0.98	0.11	16,20,30,36	0
3	HEC	K	601	43/43	0.98	0.09	16,27,31,37	0
3	HEC	K	602	43/43	0.98	0.10	22,27,33,35	0
3	HEC	K	603	43/43	0.98	0.09	23,27,33,42	0
3	HEC	K	604	43/43	0.98	0.09	19,23,27,29	0
3	HEC	G	601	43/43	0.99	0.08	14,22,29,33	0
3	HEC	G	602	43/43	0.99	0.08	18,27,31,32	0
3	HEC	C	604	43/43	0.99	0.09	18,21,25,27	0
3	HEC	A	604	43/43	0.99	0.09	17,22,26,30	0
3	HEC	C	606	43/43	0.99	0.11	15,21,32,36	0
3	HEC	A	607	43/43	0.99	0.13	16,20,28,31	0
3	HEC	E	601	43/43	0.99	0.09	16,21,27,30	0
3	HEC	C	601	43/43	0.99	0.07	17,23,26,29	0
3	HEC	E	603	43/43	0.99	0.08	21,26,30,34	0
3	HEC	E	604	43/43	0.99	0.09	17,22,25,27	0
3	HEC	I	604	43/43	0.99	0.09	20,26,29,31	0
3	HEC	C	602	43/43	0.99	0.09	17,23,28,32	0
3	HEC	I	606	43/43	0.99	0.12	14,22,34,39	0
3	HEC	E	606	43/43	0.99	0.11	15,19,29,32	0
3	HEC	A	601	43/43	0.99	0.09	14,21,28,29	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.

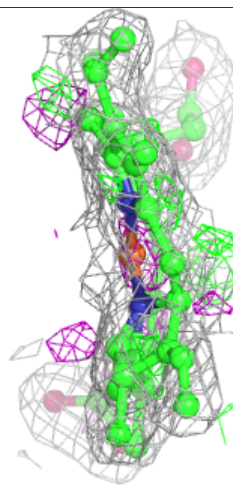
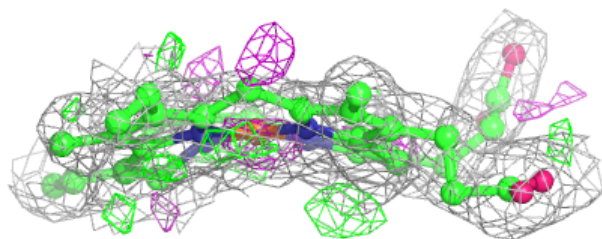
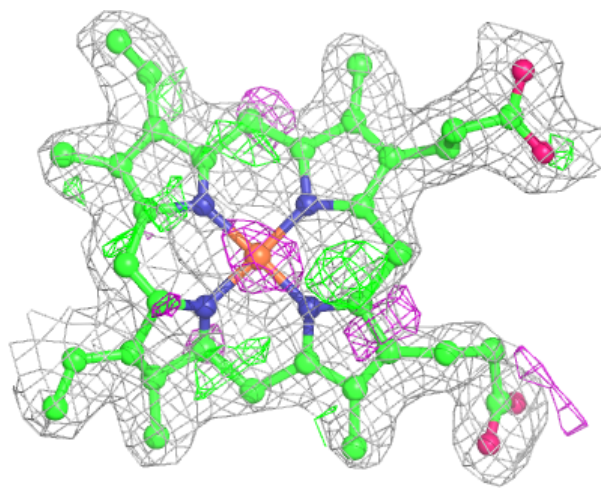
Electron density around ISW A 608:

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



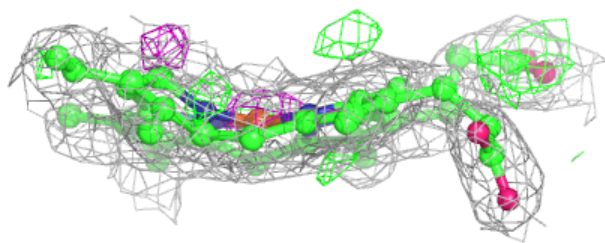
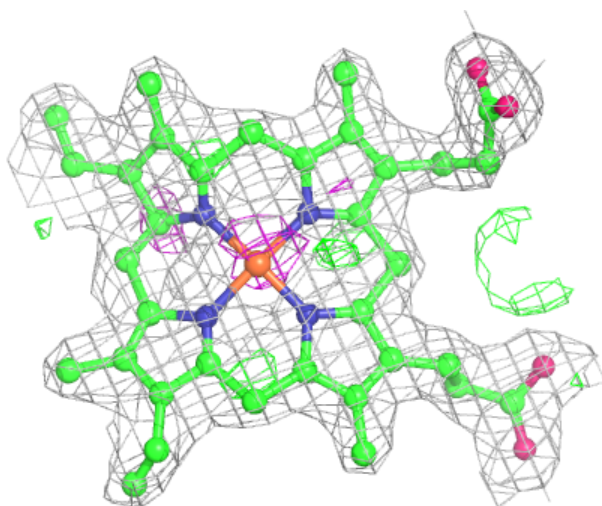
Electron density around ISW A 609:

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



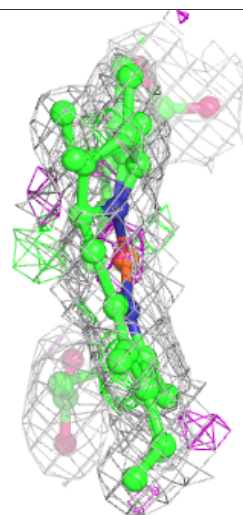
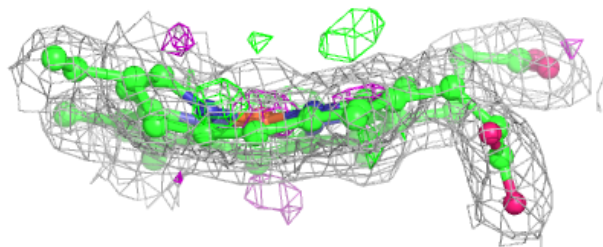
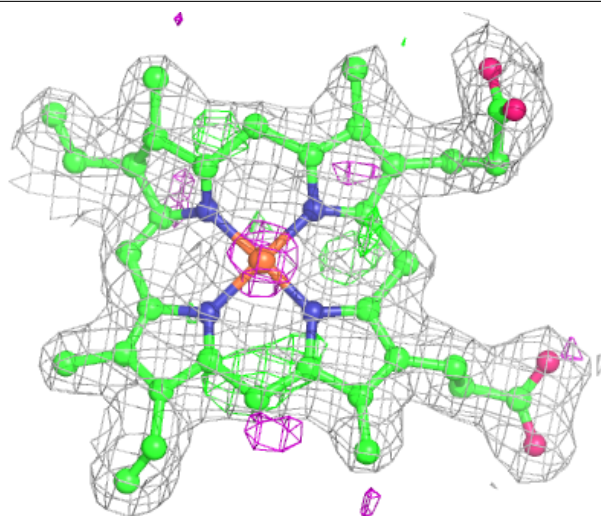
Electron density around ISW G 608:

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



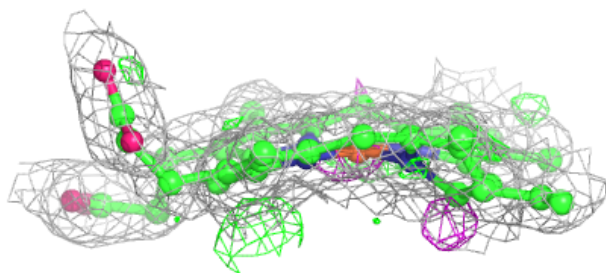
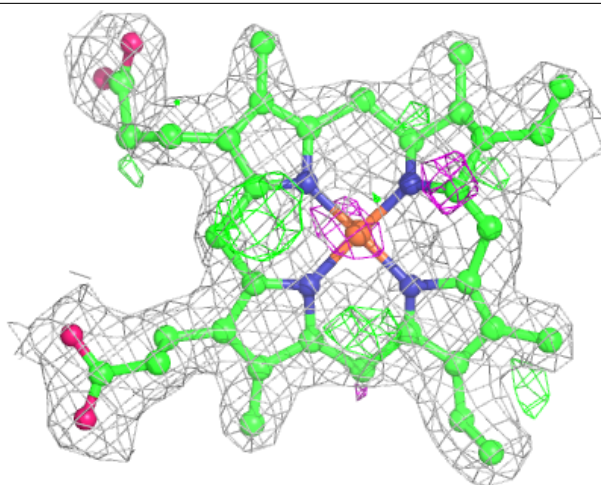
Electron density around ISW C 608:

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



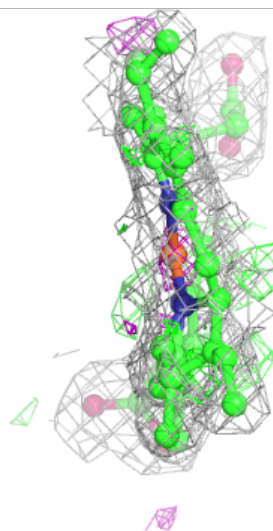
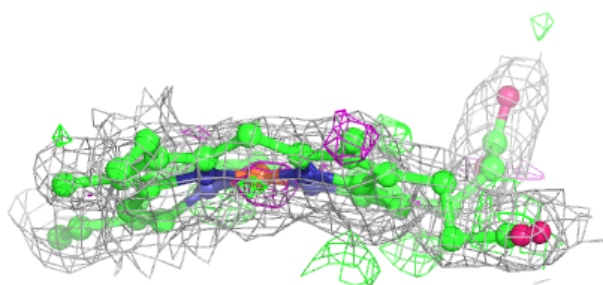
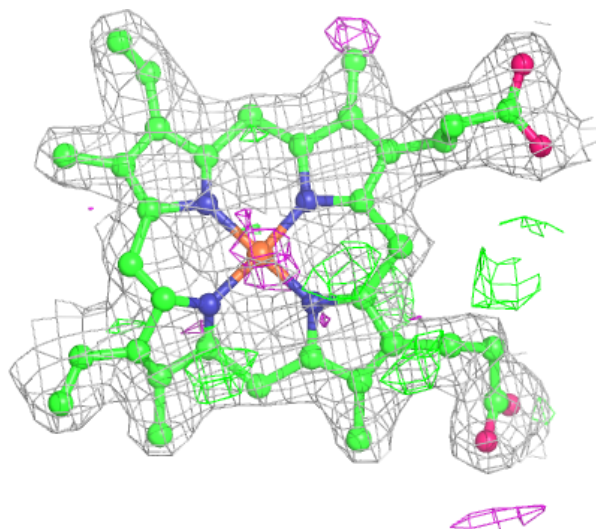
Electron density around ISW G 609:

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



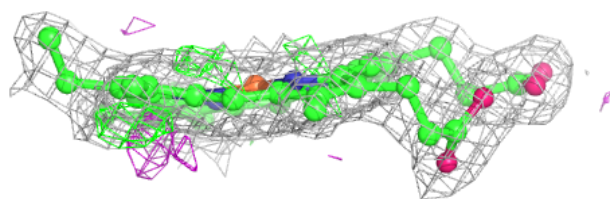
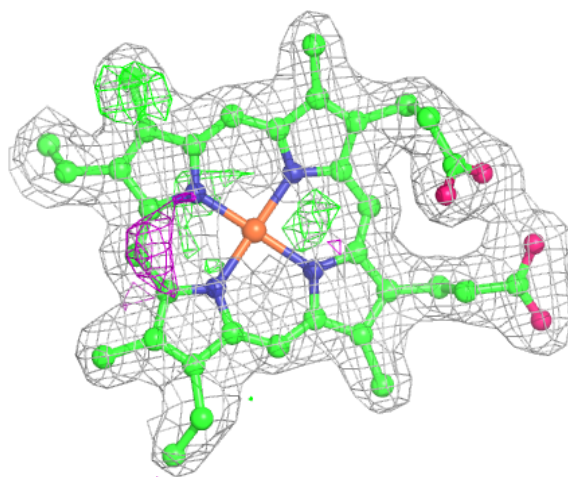
Electron density around ISW I 608:

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



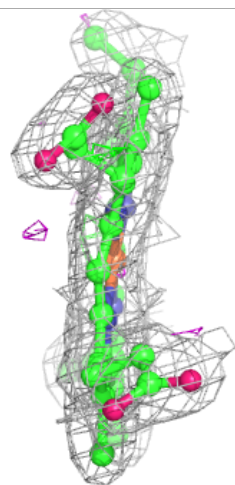
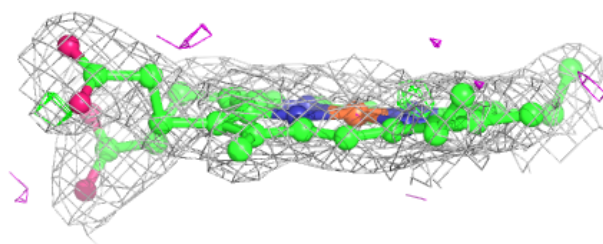
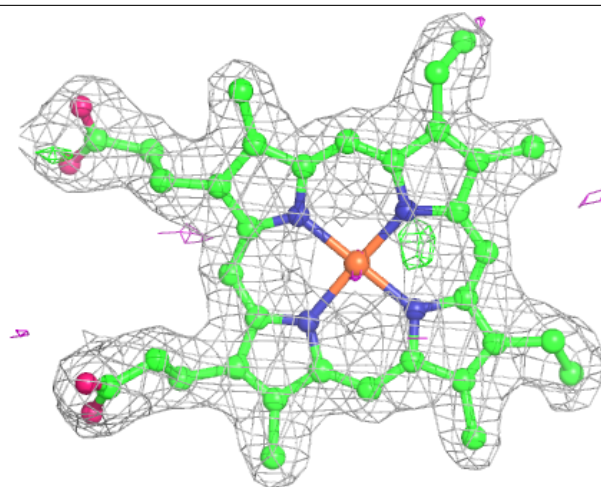
Electron density around HEC K 605:

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



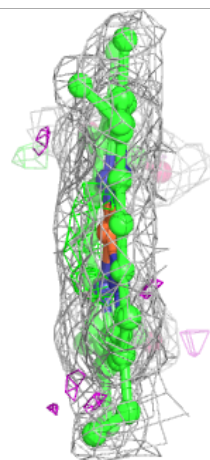
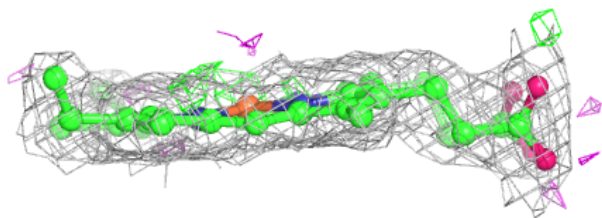
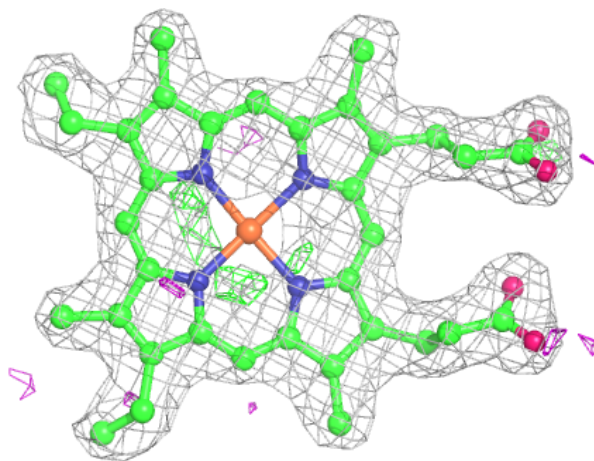
Electron density around HEC K 606:

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



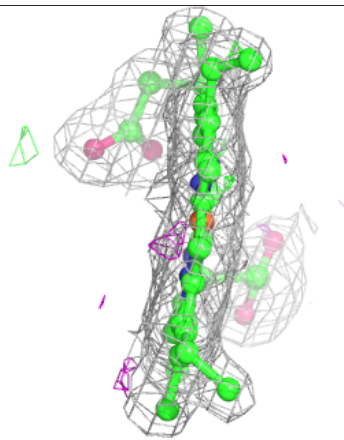
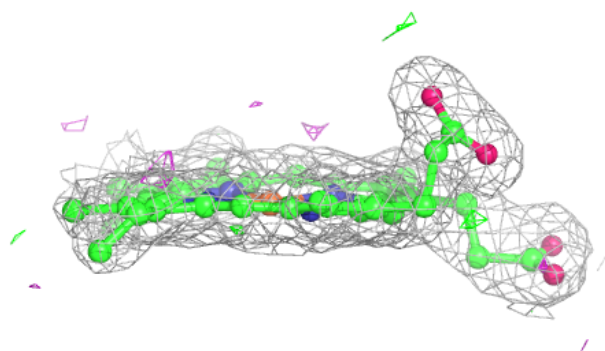
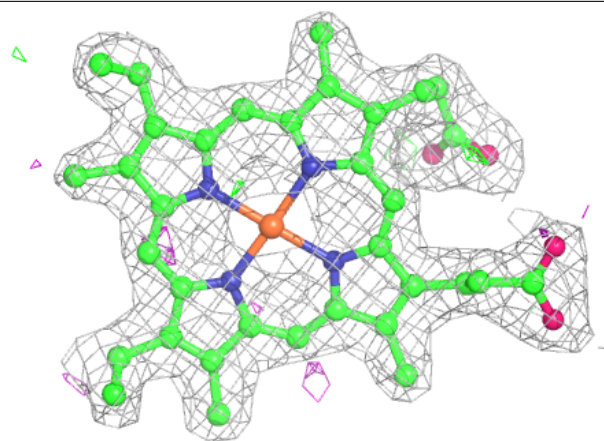
Electron density around HEC K 607:

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



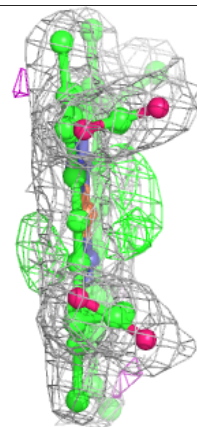
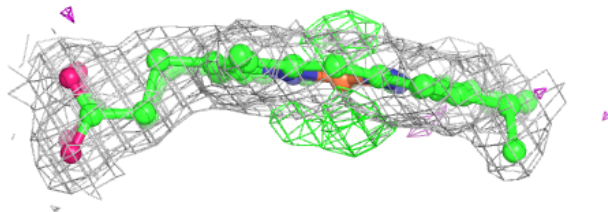
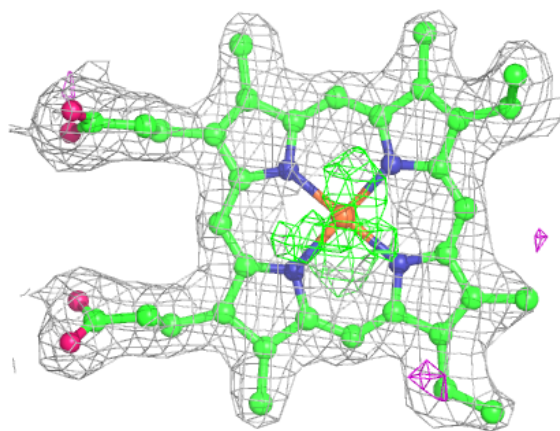
Electron density around HEC A 602:

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



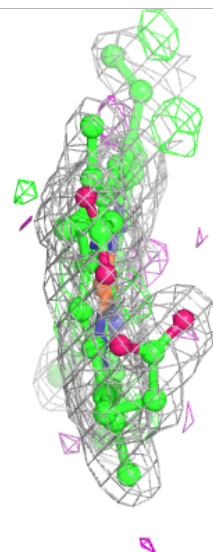
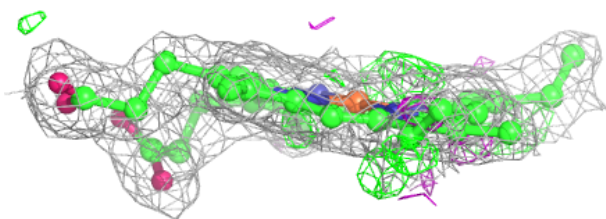
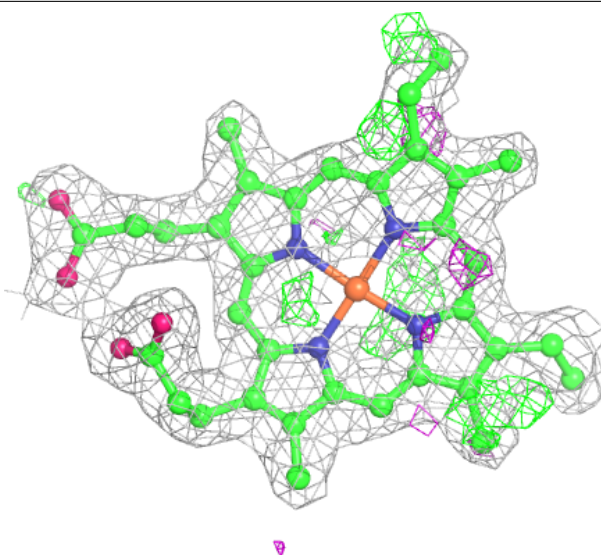
Electron density around HEC A 603:

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



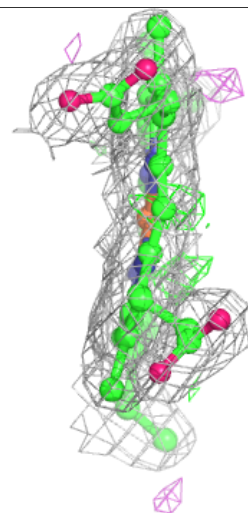
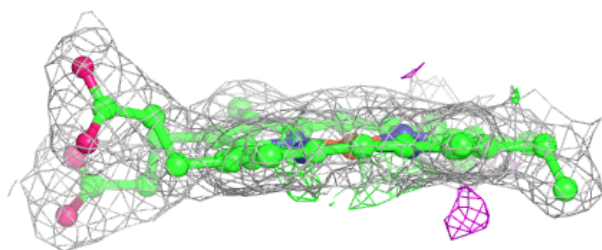
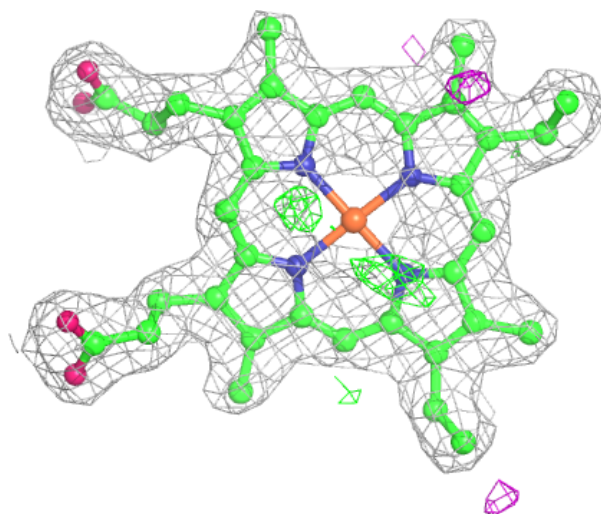
Electron density around HEC A 605:

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



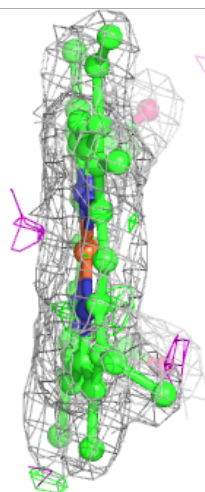
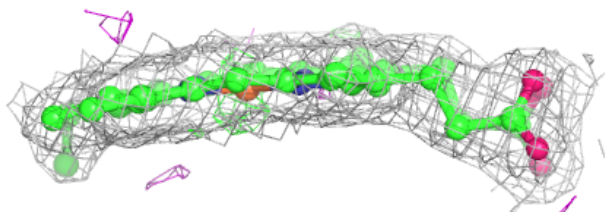
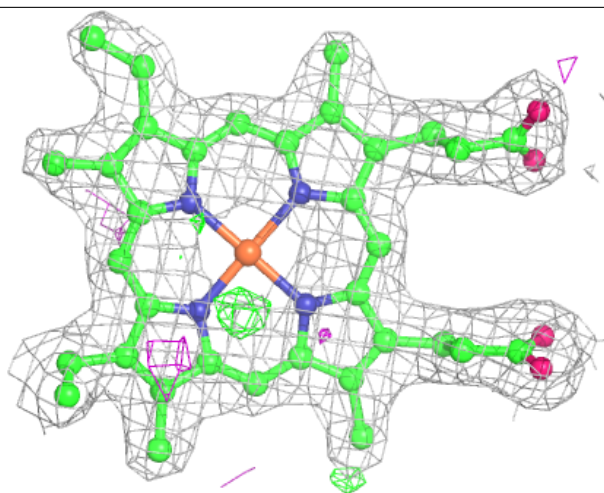
Electron density around HEC A 606:

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



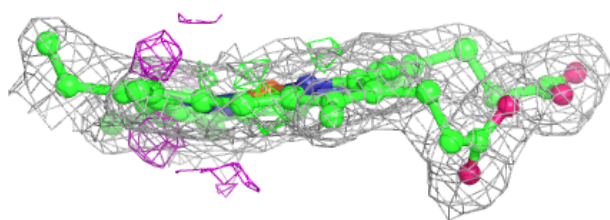
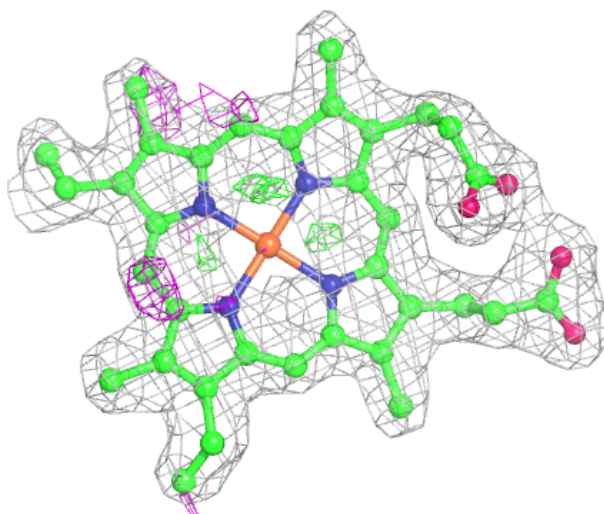
Electron density around HEC C 603:

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



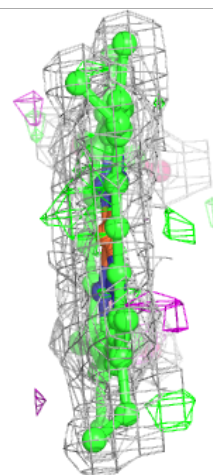
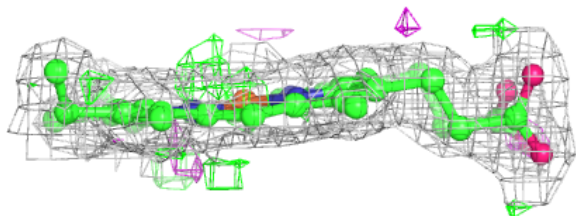
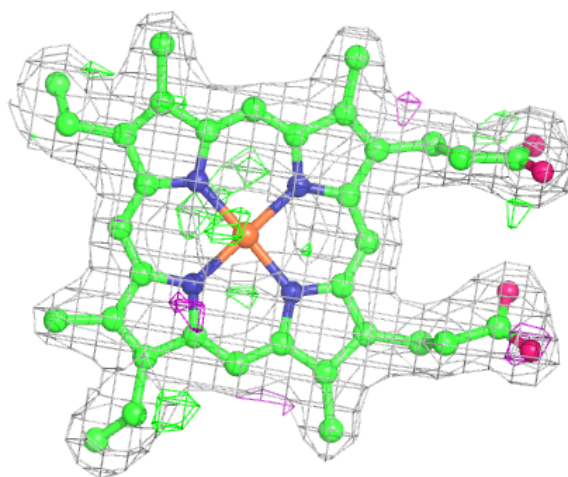
Electron density around HEC C 605:

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



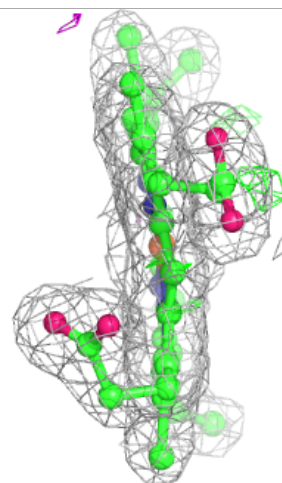
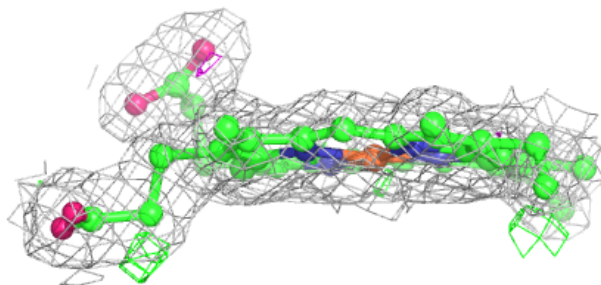
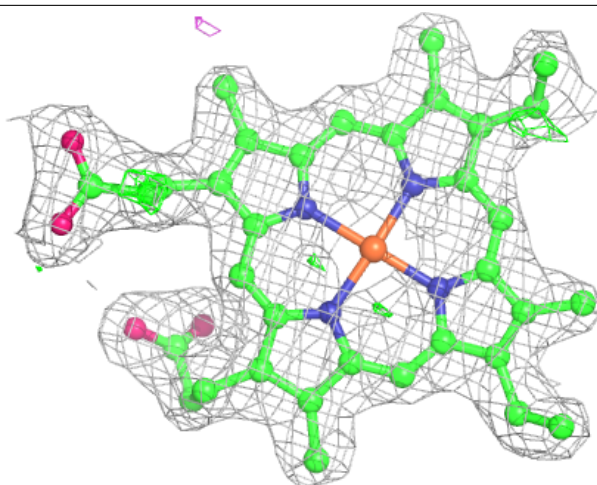
Electron density around HEC C 607:

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



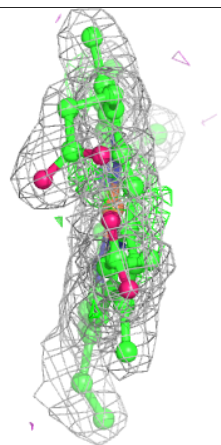
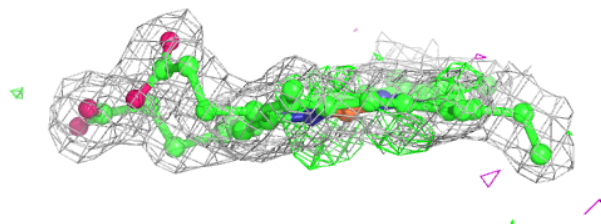
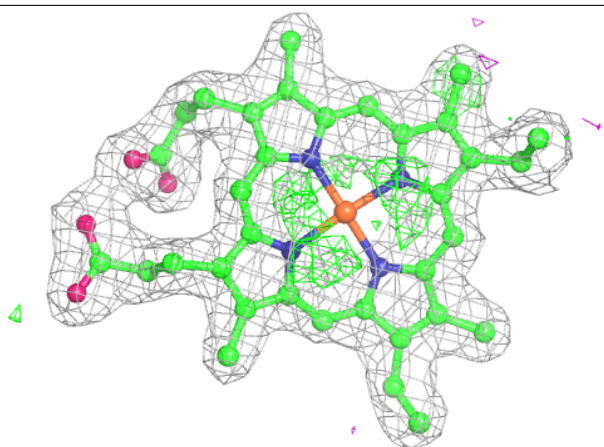
Electron density around HEC E 602:

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



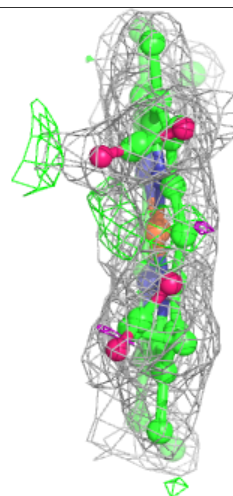
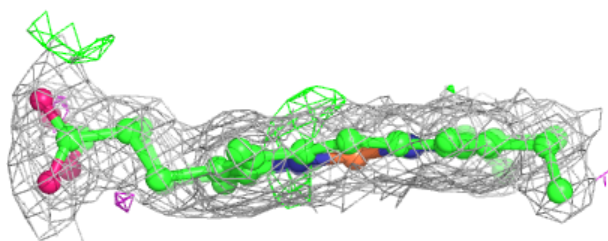
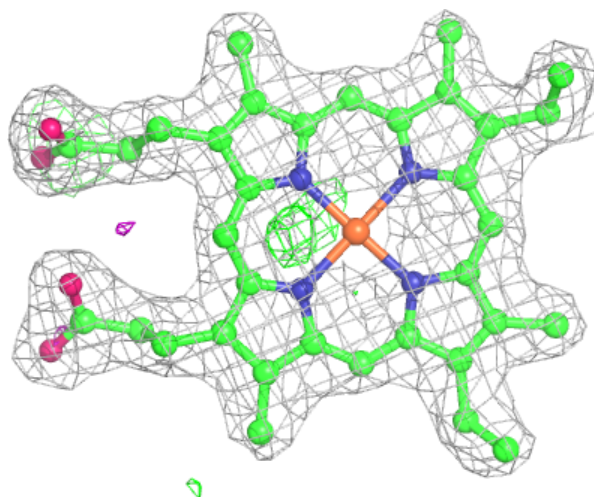
Electron density around HEC E 605:

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



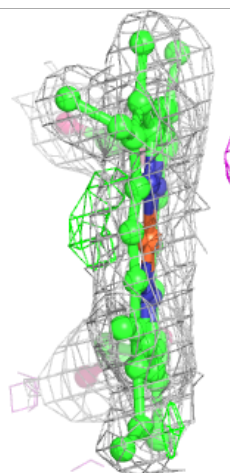
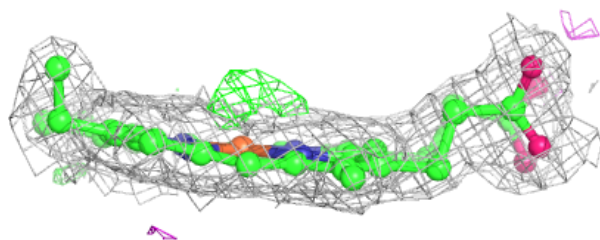
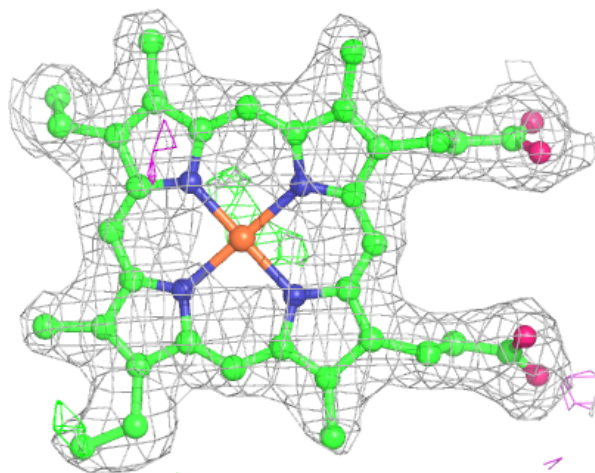
Electron density around HEC E 607:

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and green (positive)



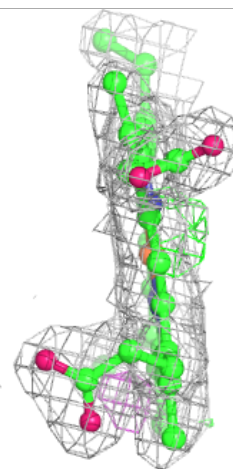
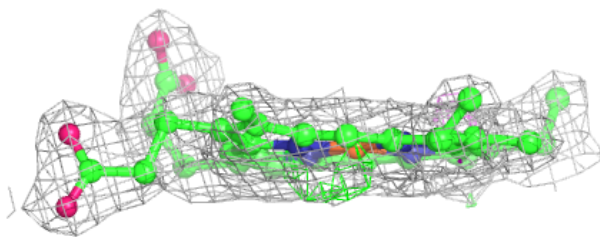
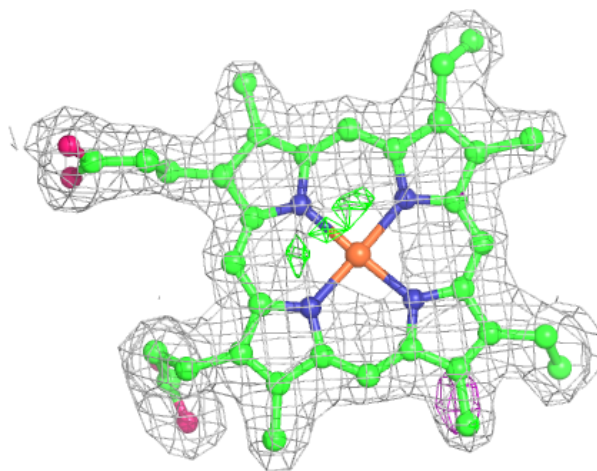
Electron density around HEC G 603:

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and green (positive)



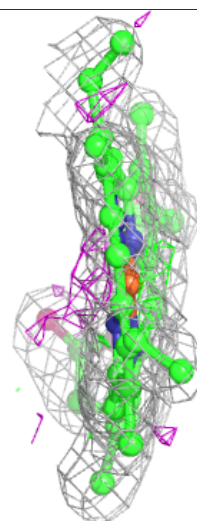
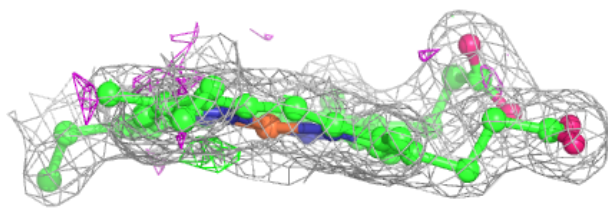
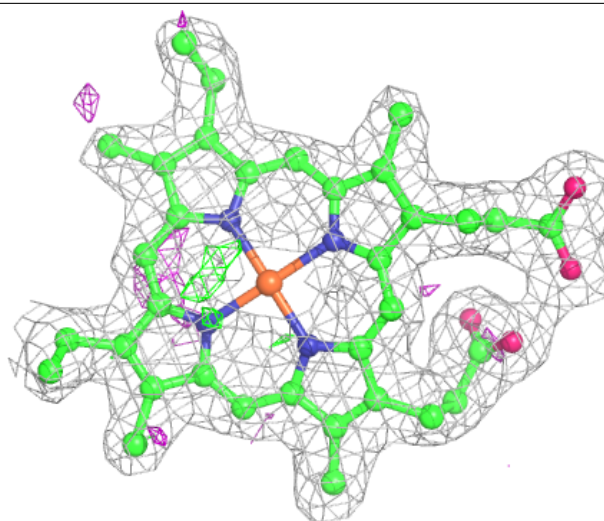
Electron density around HEC G 604:

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



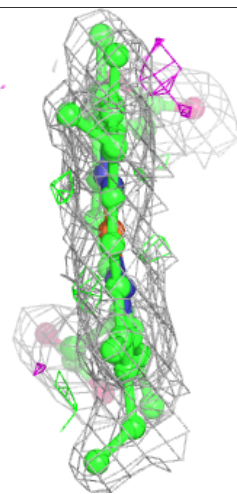
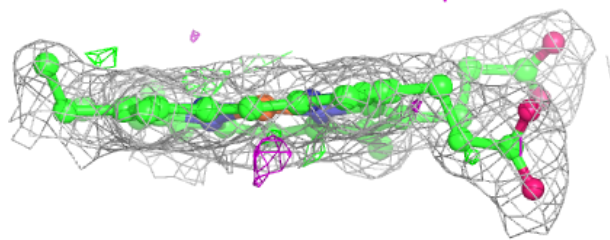
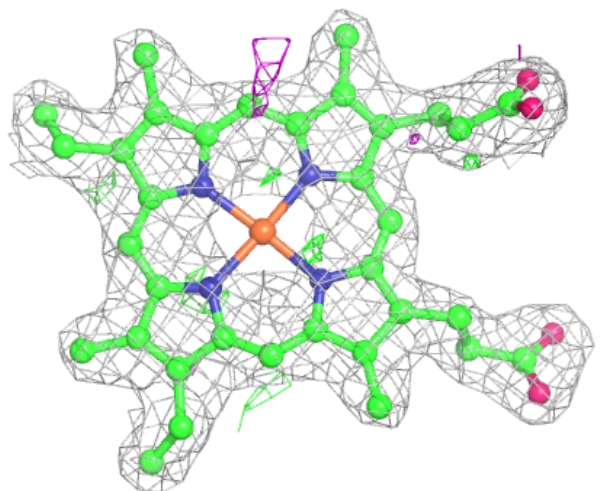
Electron density around HEC G 605:

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



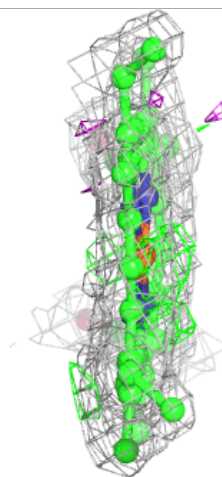
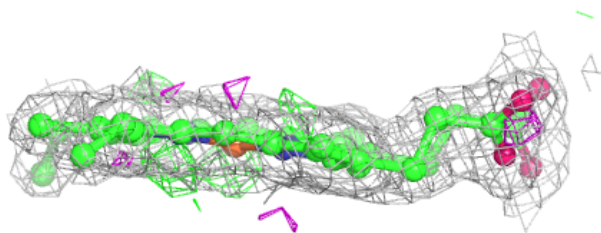
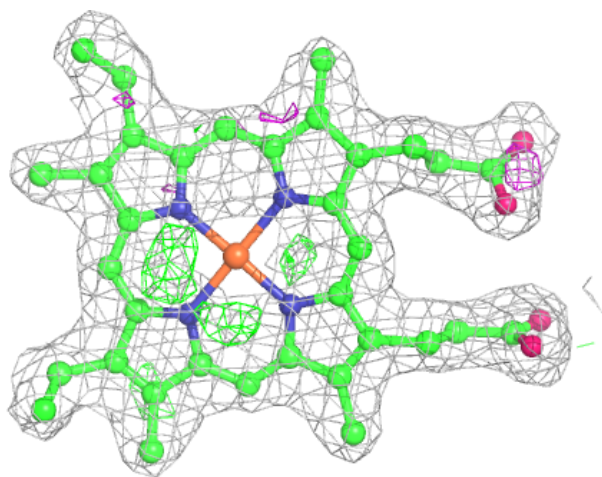
Electron density around HEC G 606:

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



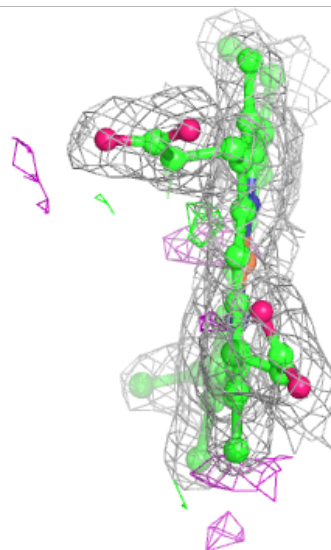
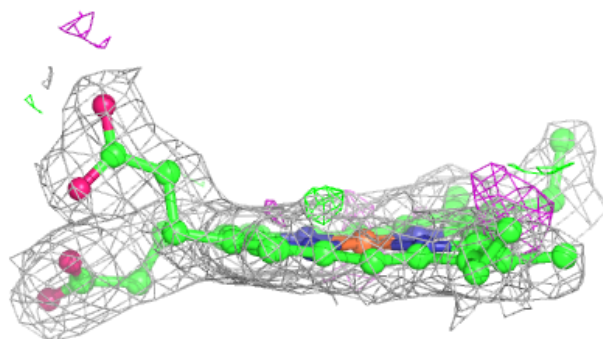
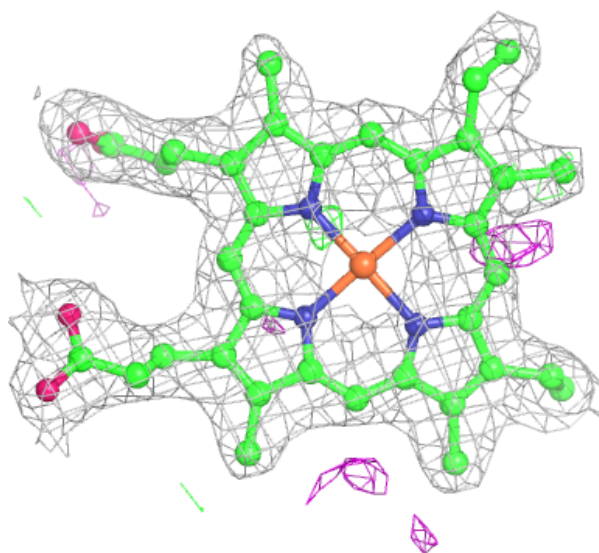
Electron density around HEC G 607:

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



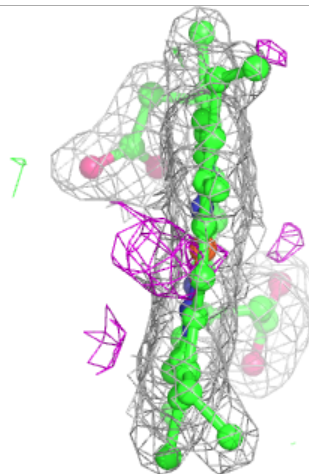
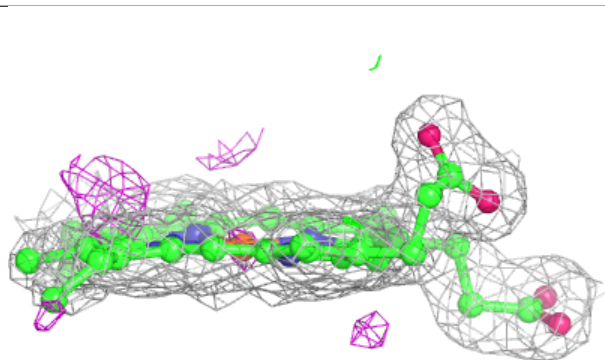
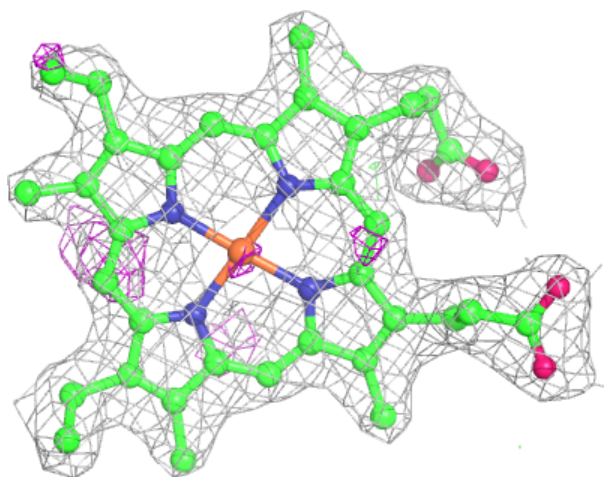
Electron density around HEC I 601:

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



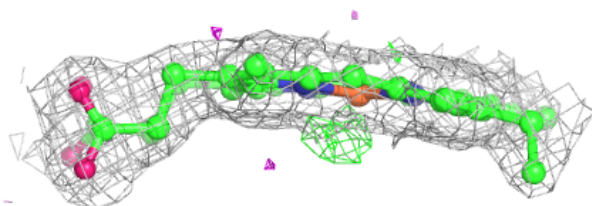
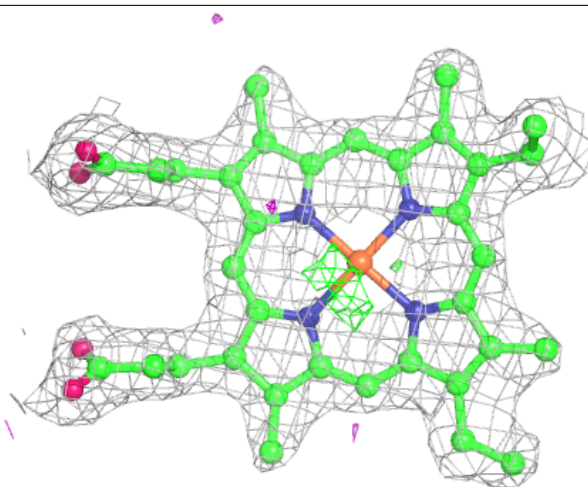
Electron density around HEC I 602:

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



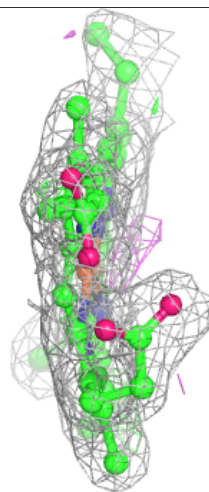
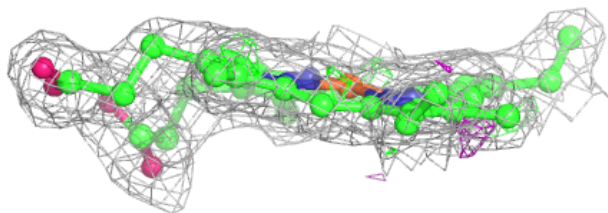
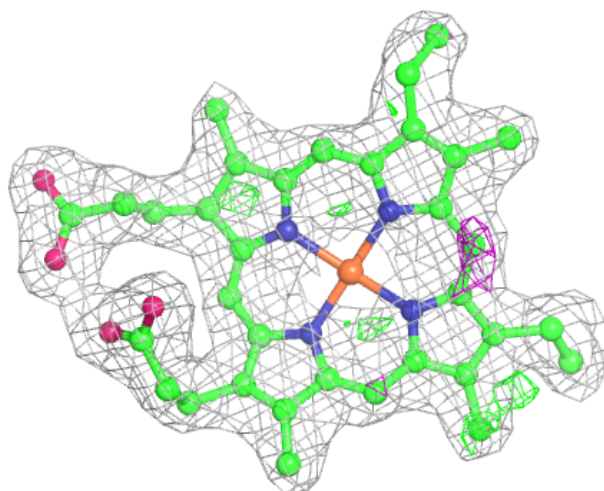
Electron density around HEC I 603:

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



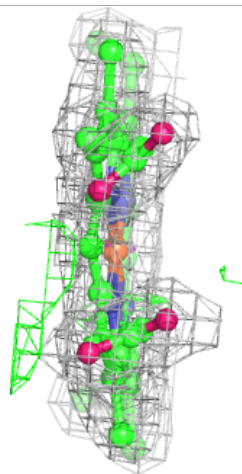
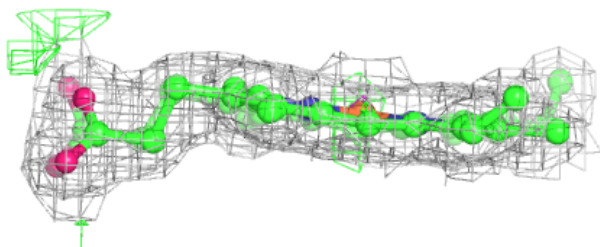
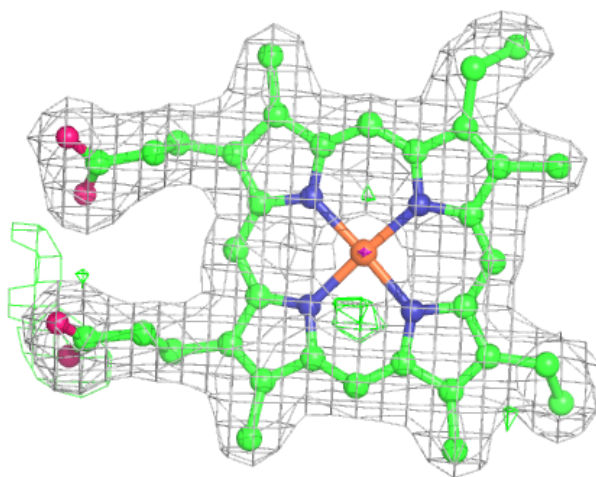
Electron density around HEC I 605:

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



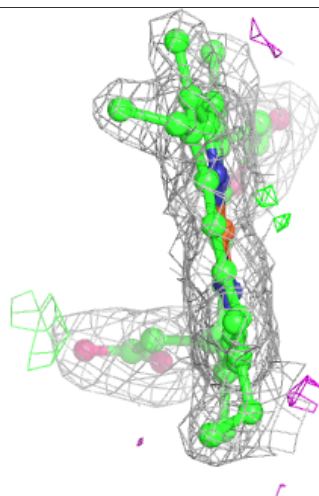
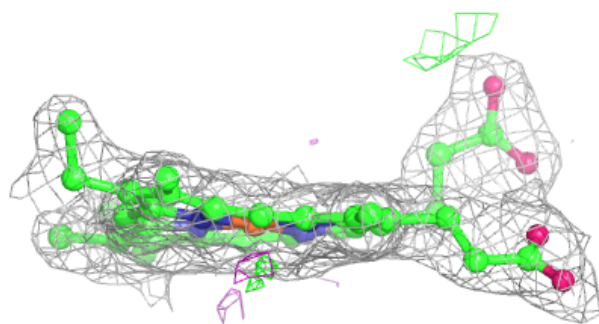
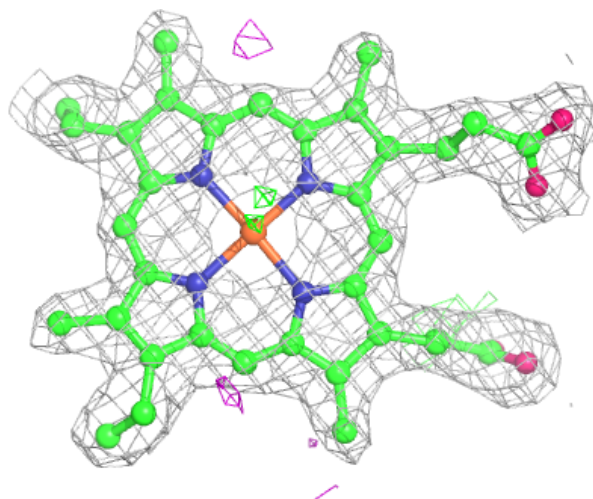
Electron density around HEC I 607:

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



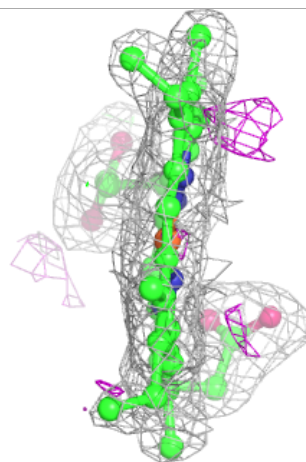
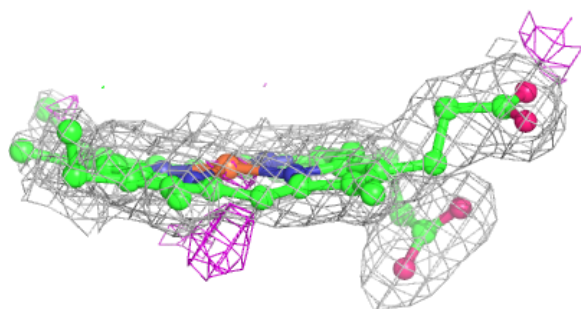
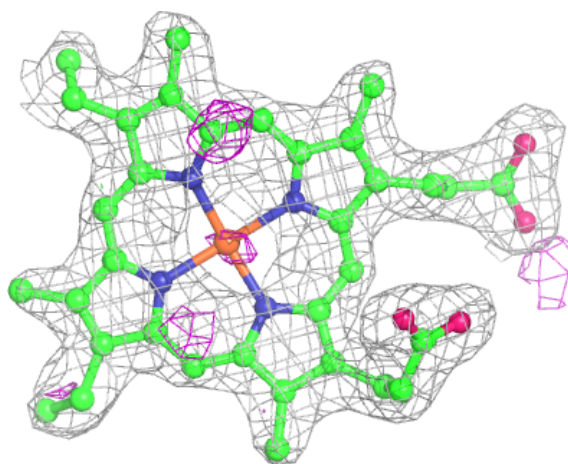
Electron density around HEC K 601:

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



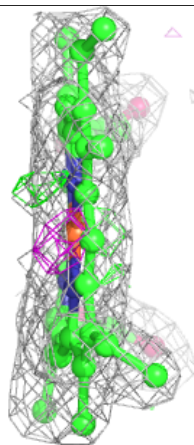
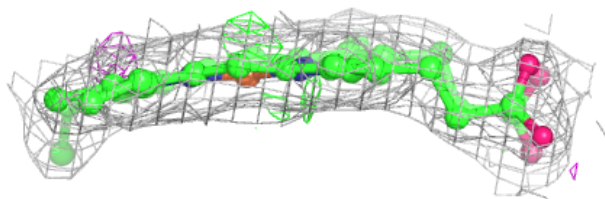
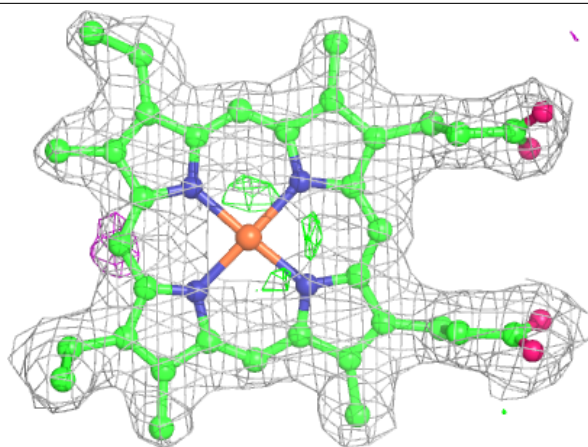
Electron density around HEC K 602:

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



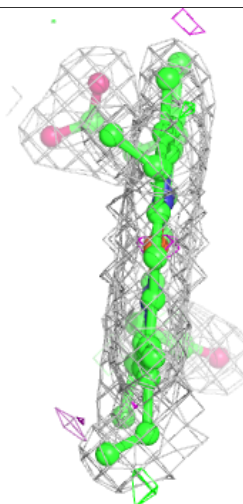
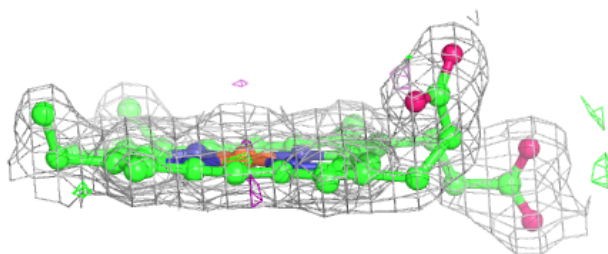
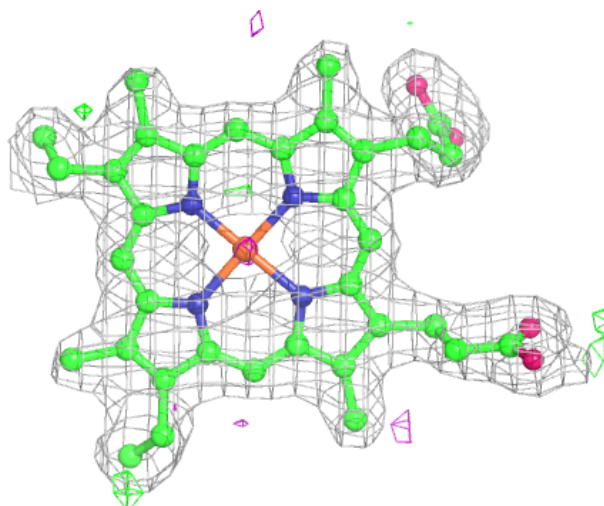
Electron density around HEC K 603:

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



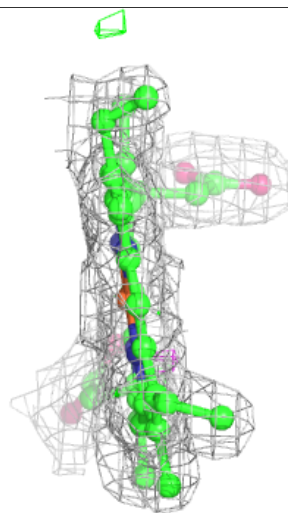
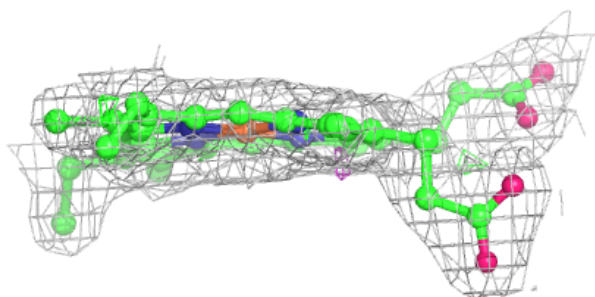
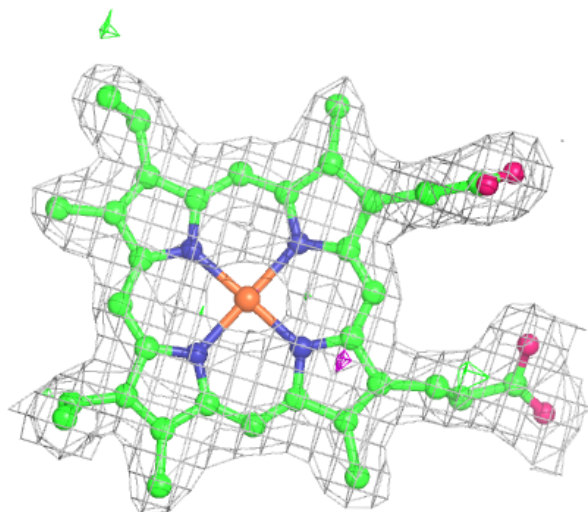
Electron density around HEC K 604:

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



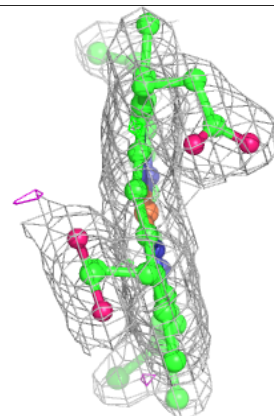
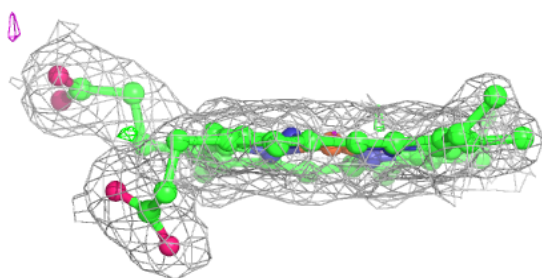
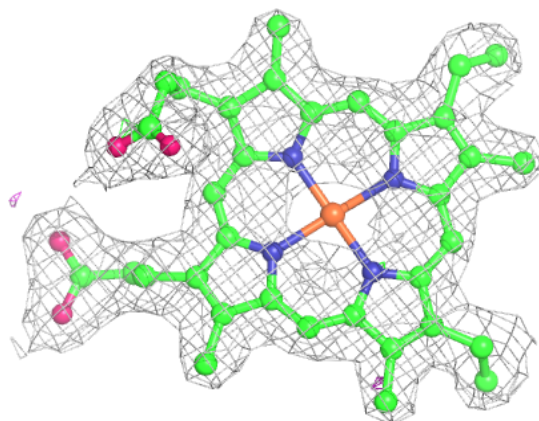
Electron density around HEC G 601:

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



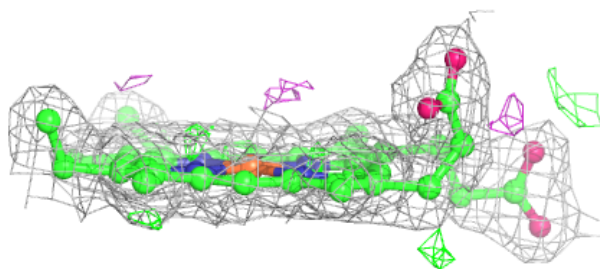
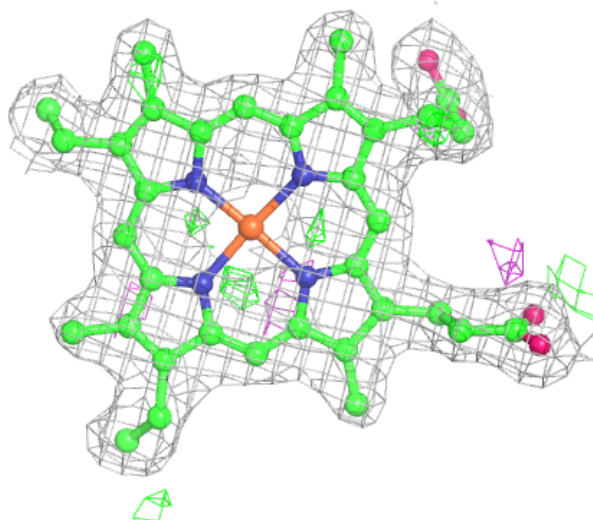
Electron density around HEC G 602:

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



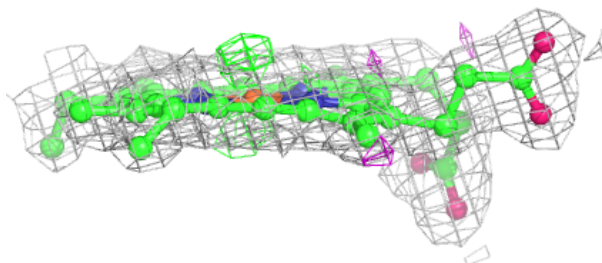
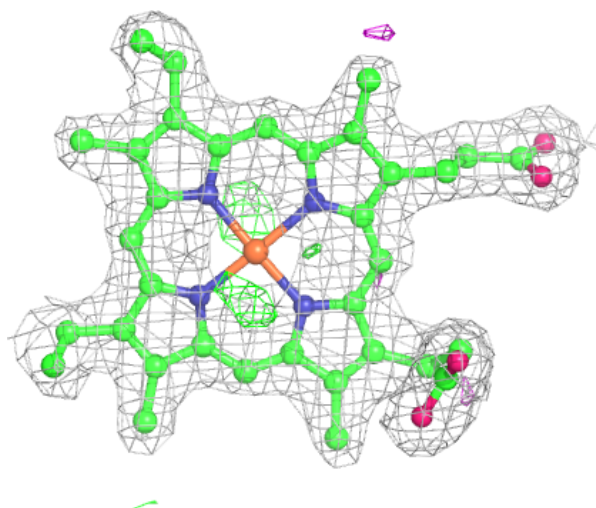
Electron density around HEC C 604:

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



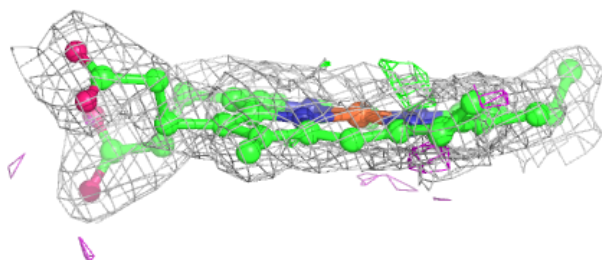
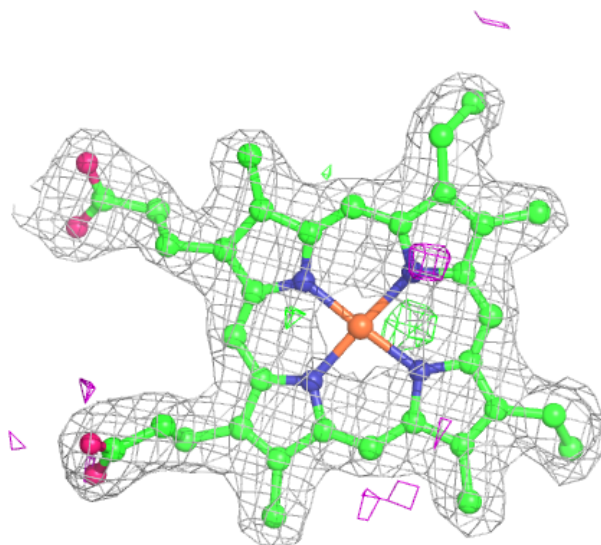
Electron density around HEC A 604:

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



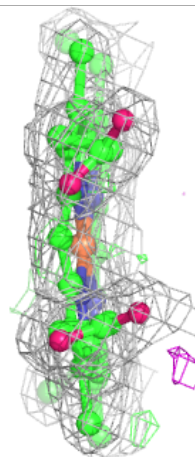
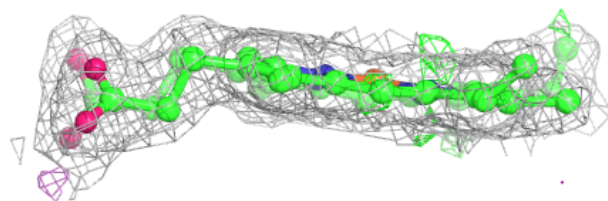
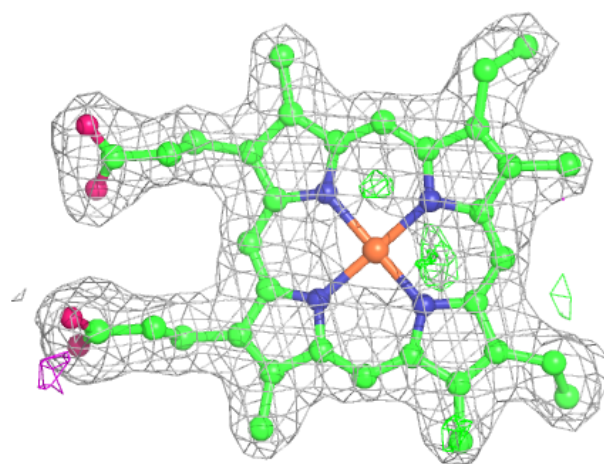
Electron density around HEC C 606:

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



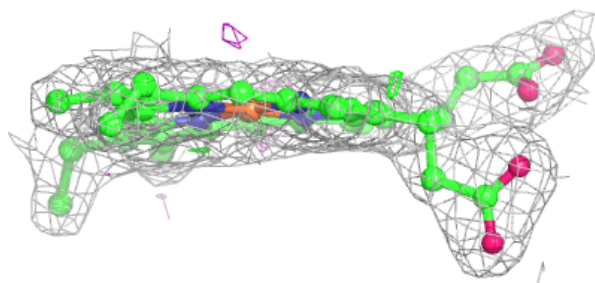
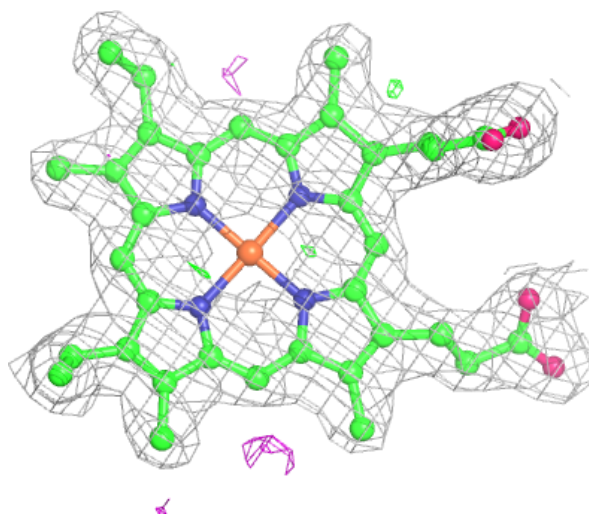
Electron density around HEC A 607:

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



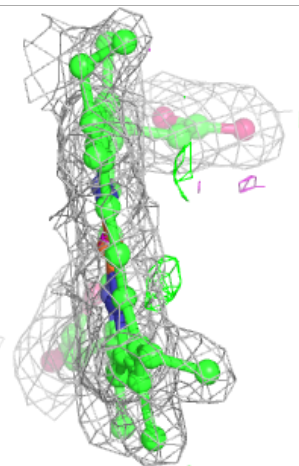
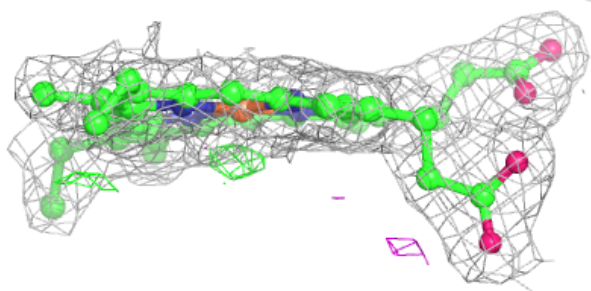
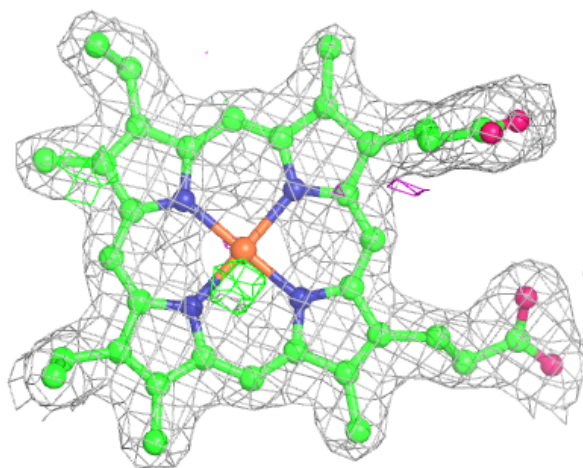
Electron density around HEC E 601:

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



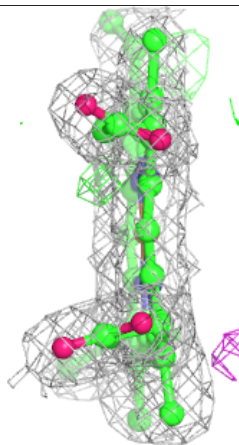
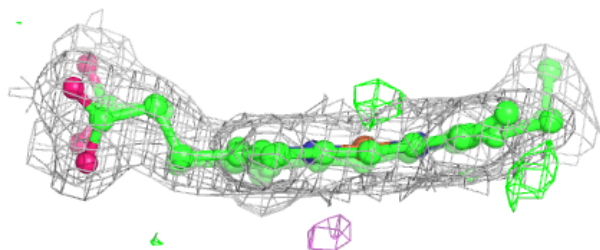
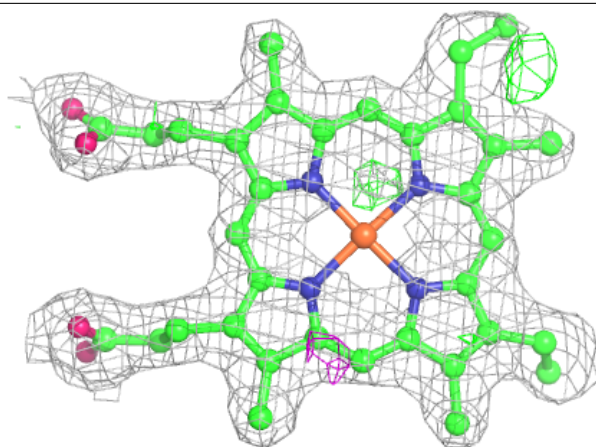
Electron density around HEC C 601:

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



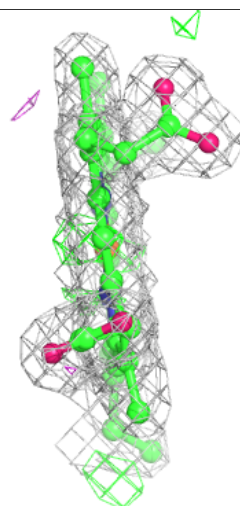
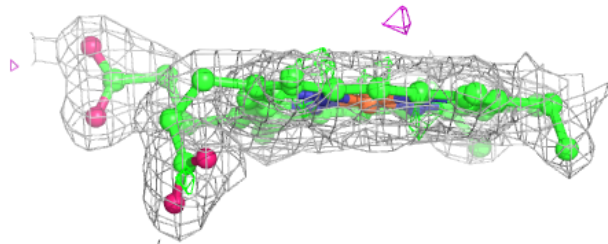
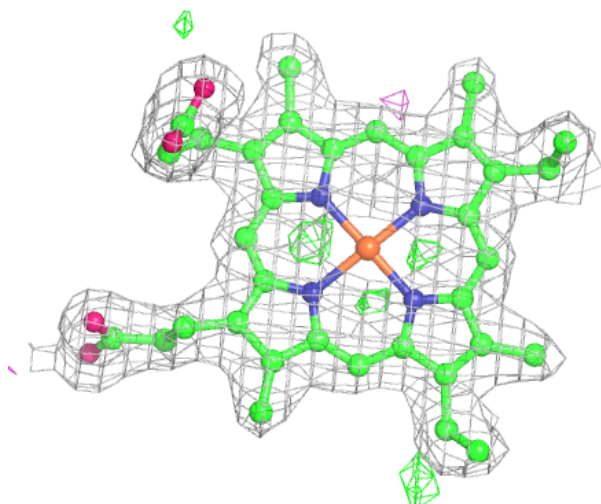
Electron density around HEC E 603:

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



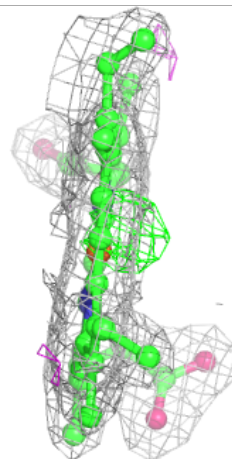
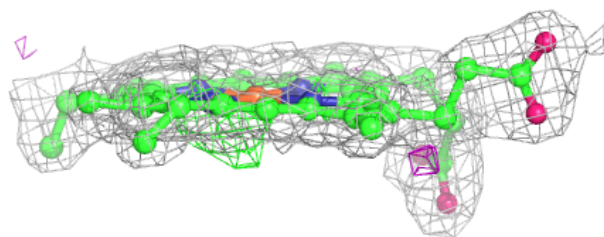
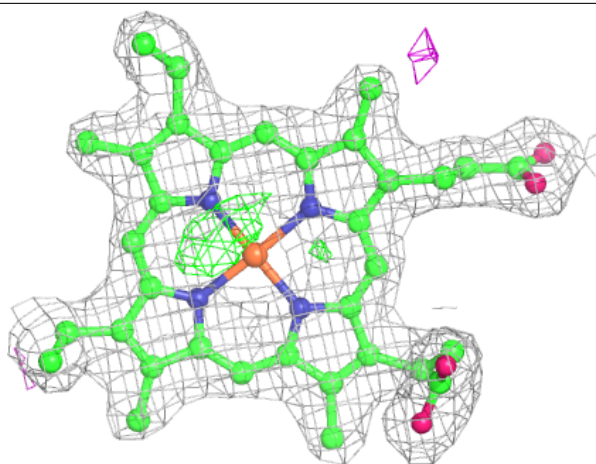
Electron density around HEC E 604:

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



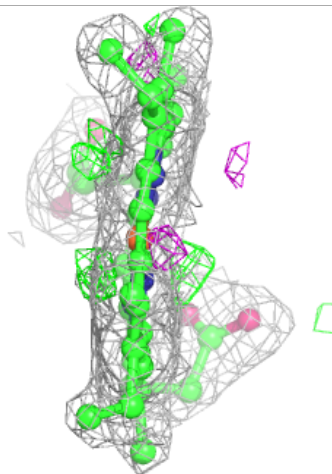
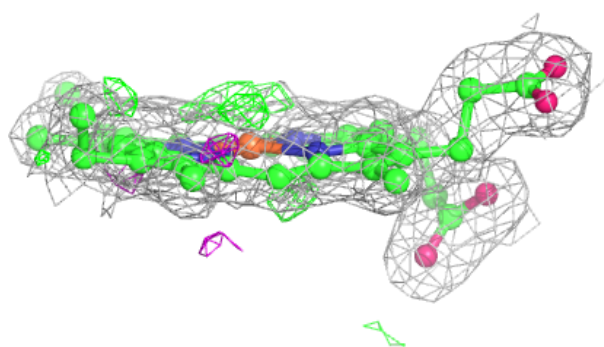
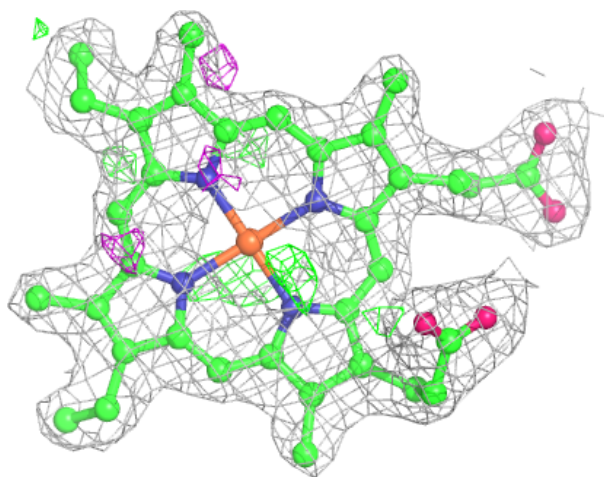
Electron density around HEC I 604:

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



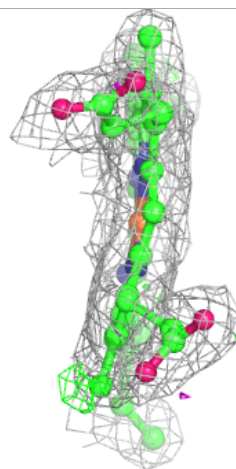
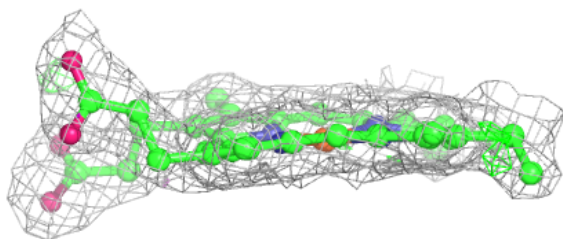
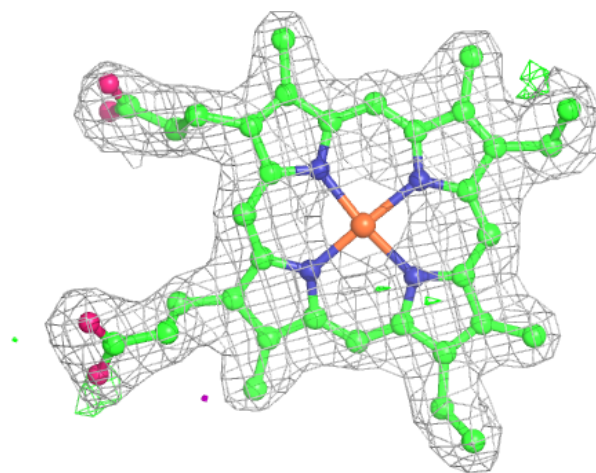
Electron density around HEC C 602:

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



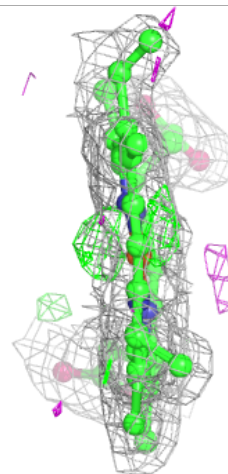
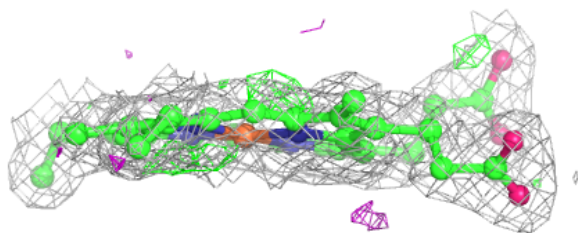
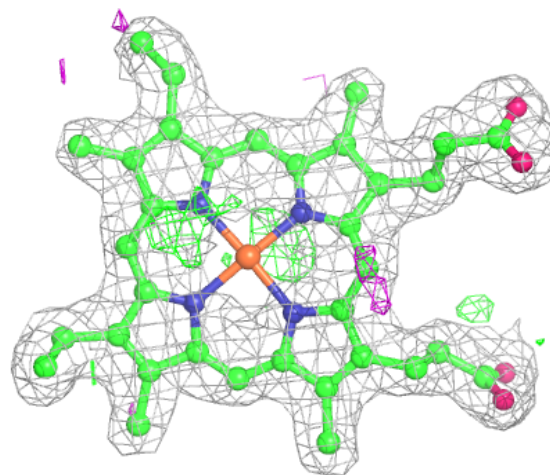
Electron density around HEC I 606:

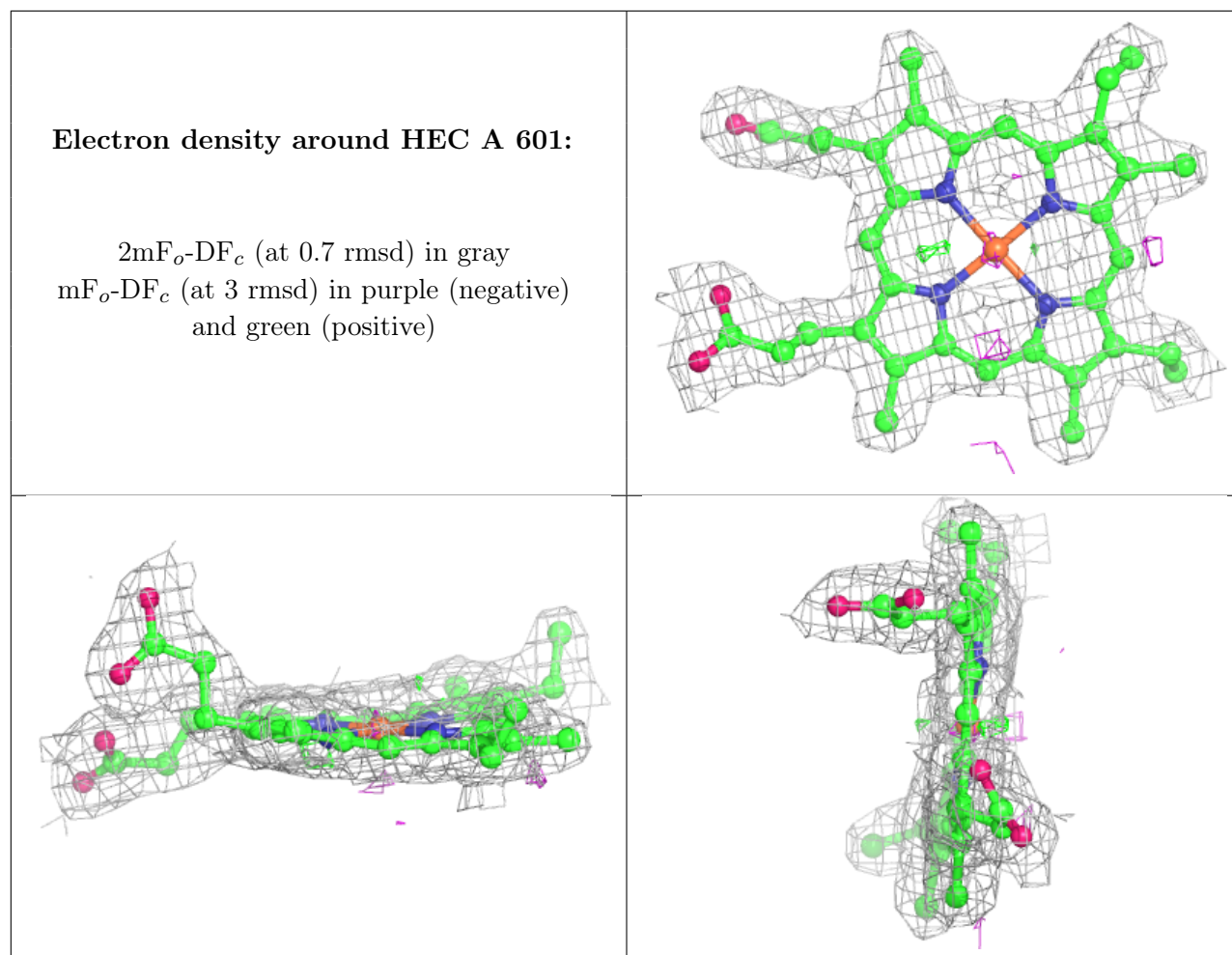
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC E 606:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.