



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 17, 2021 – 07:06 PM JST

PDB ID : 6M0P  
Title : Hydroxylamine oxidoreductase in complex with juglone  
Authors : Fujiwara, T.; Fujimoto, Z.; Nishigaya, Y.; Yamazaki, T.  
Deposited on : 2020-02-22  
Resolution : 2.78 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

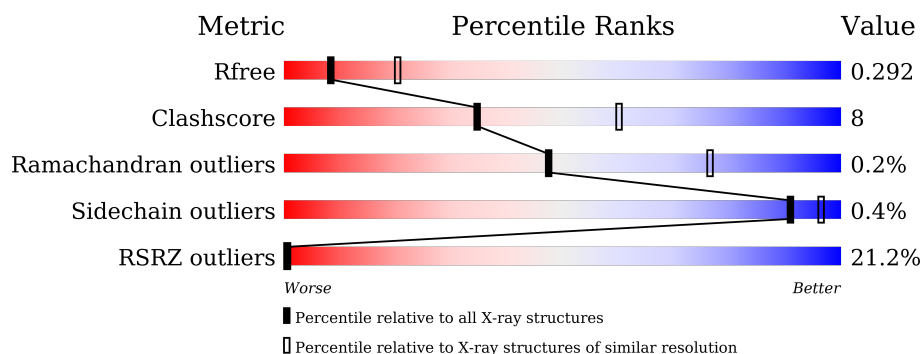
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.78 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	570	<div> <div>16%</div> <div> <div></div> <div>71%</div> <div>18%</div> <div>12%</div> </div> </div>
1	C	570	<div> <div>19%</div> <div> <div></div> <div>71%</div> <div>17%</div> <div>12%</div> </div> </div>
1	E	570	<div> <div>16%</div> <div> <div></div> <div>71%</div> <div>16%</div> <div>12%</div> </div> </div>
2	B	91	<div> <div>27%</div> <div> <div></div> <div>58%</div> <div>•</div> <div>38%</div> </div> </div>
2	D	91	<div> <div>15%</div> <div> <div></div> <div>56%</div> <div>5%</div> <div>38%</div> </div> </div>
2	F	91	<div> <div>34%</div> <div> <div></div> <div>56%</div> <div>5%</div> <div>38%</div> </div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14521 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.

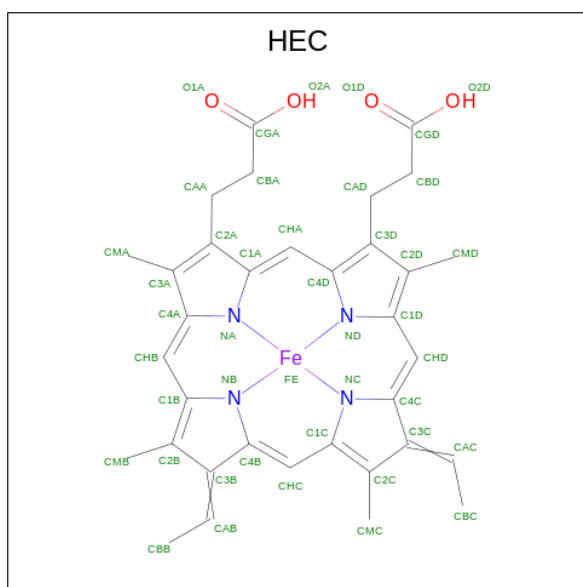
- Molecule 1 is a protein called Aerobic hydroxylamine oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	503	Total	C	N	O	S	0	0	0
			4009	2493	711	773	32			
1	C	503	Total	C	N	O	S	0	0	0
			4009	2493	711	773	32			
1	E	503	Total	C	N	O	S	0	0	0
			4009	2493	711	773	32			

- Molecule 2 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	56	Total	C	N	O	S	0	0	0
			423	263	75	82	3			
2	D	56	Total	C	N	O	S	0	0	0
			425	264	75	83	3			
2	F	56	Total	C	N	O	S	0	0	0
			425	264	75	83	3			

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

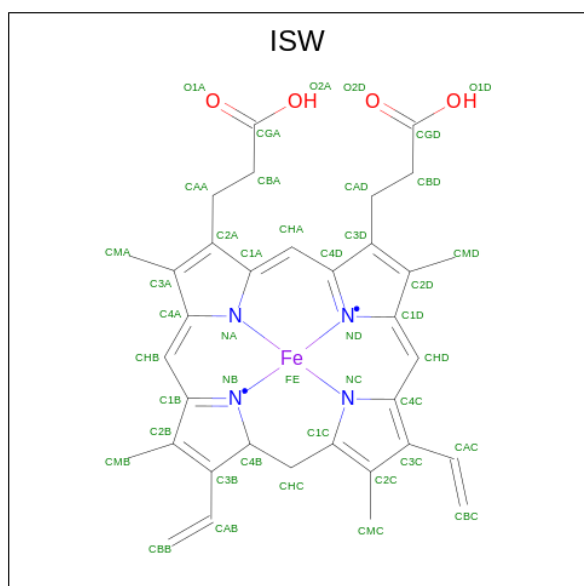
[illegible]

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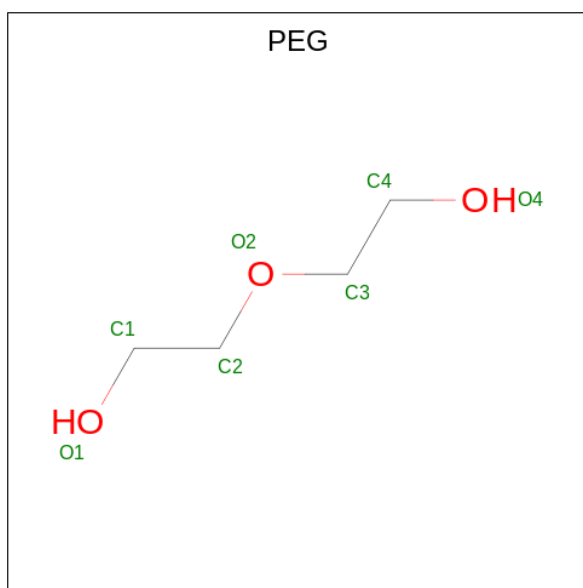
[illegible]

- 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 ]dipropanoato(2-)}iron (three-letter code: ISW) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).



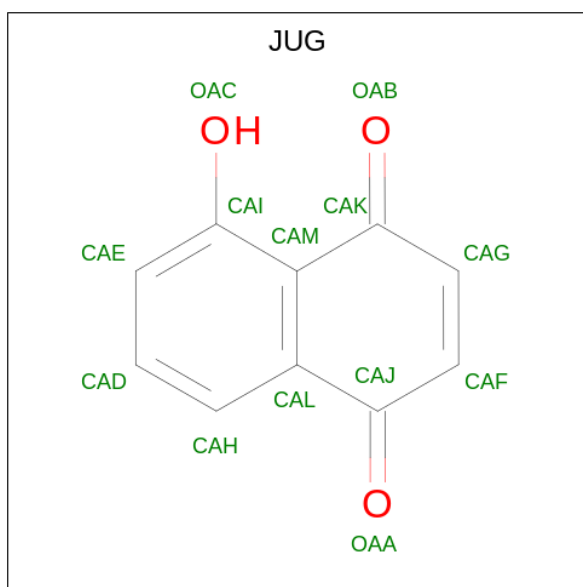
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



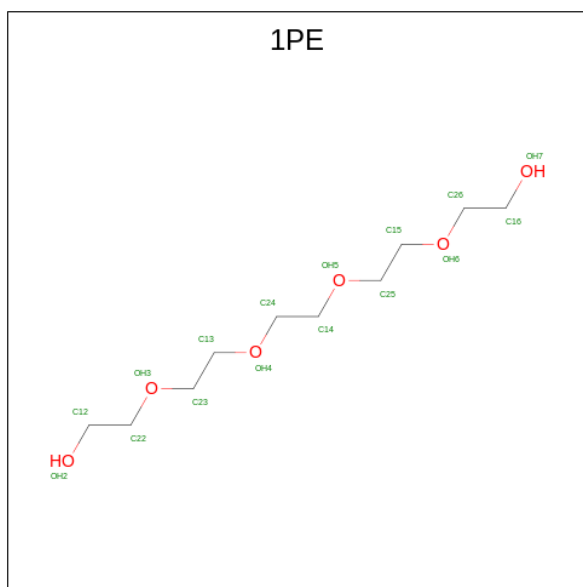
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	E	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is 5-hydroxynaphthalene-1,4-dione (three-letter code: JUG) (formula:  $C_{10}H_6O_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			13	10	3		
6	E	1	Total	C	O	0	0
			13	10	3		

- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			12	8	4		
7	C	1	Total	C	O	0	0
			16	10	6		

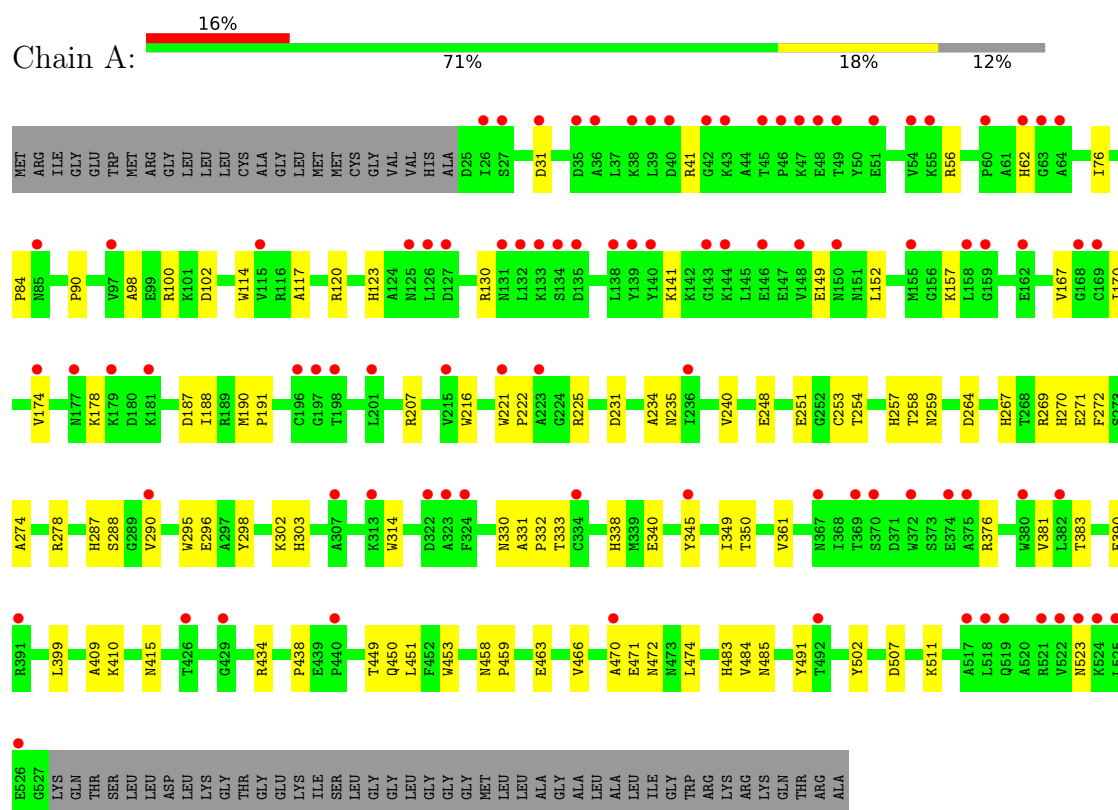
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	44	Total	O	0	0
			44	44		
8	B	5	Total	O	0	0
			5	5		
8	C	31	Total	O	0	0
			31	31		
8	D	7	Total	O	0	0
			7	7		
8	E	26	Total	O	0	0
			26	26		
8	F	1	Total	O	0	0
			1	1		

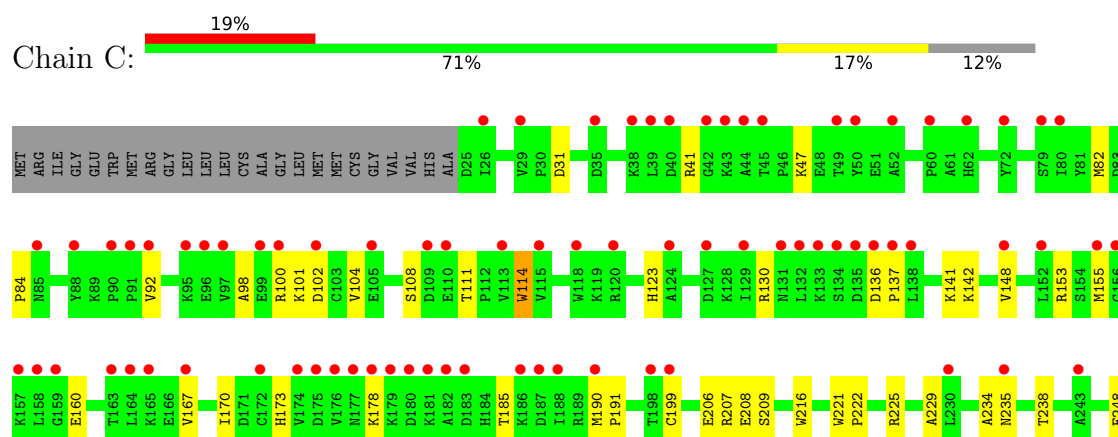
### 3 Residue-property plots [i](#)

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

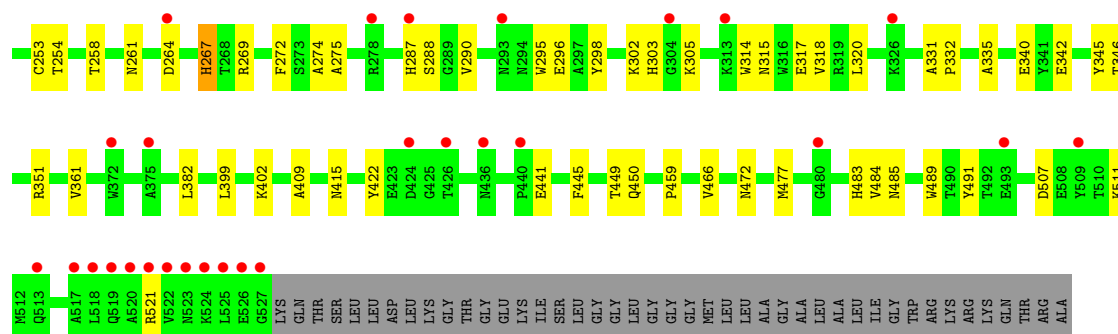
- Molecule 1: Aerobic hydroxylamine oxidoreductase



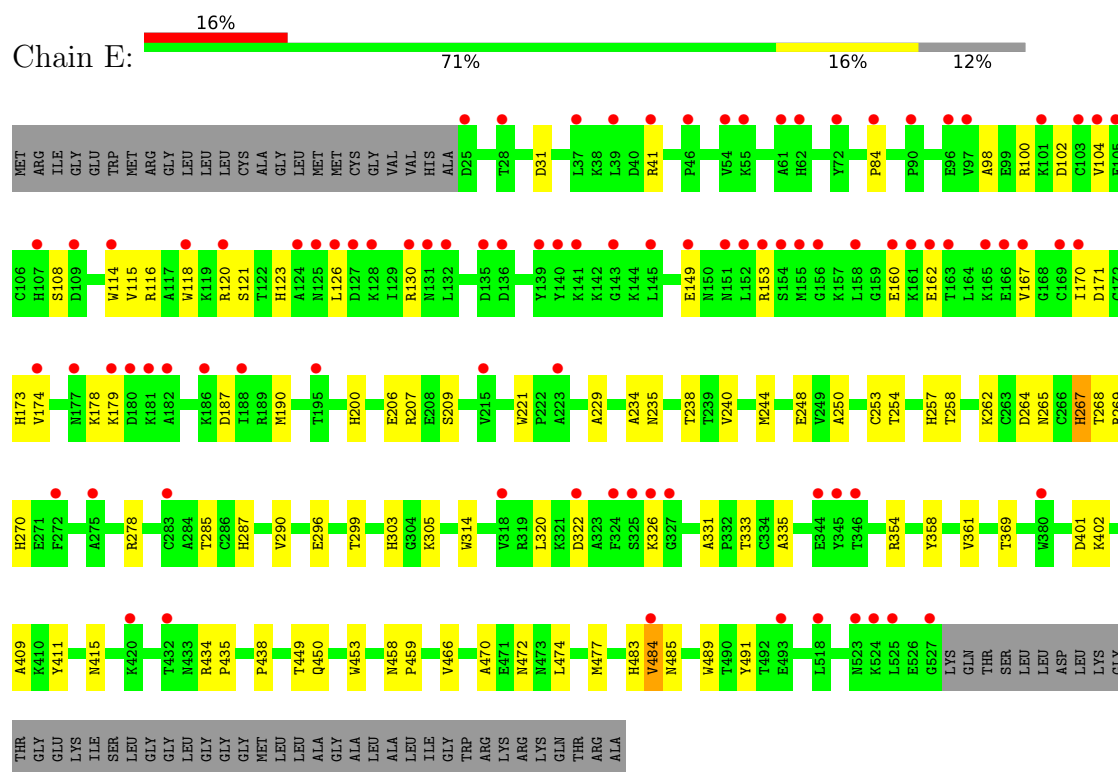
- Molecule 1: Aerobic hydroxylamine oxidoreductase



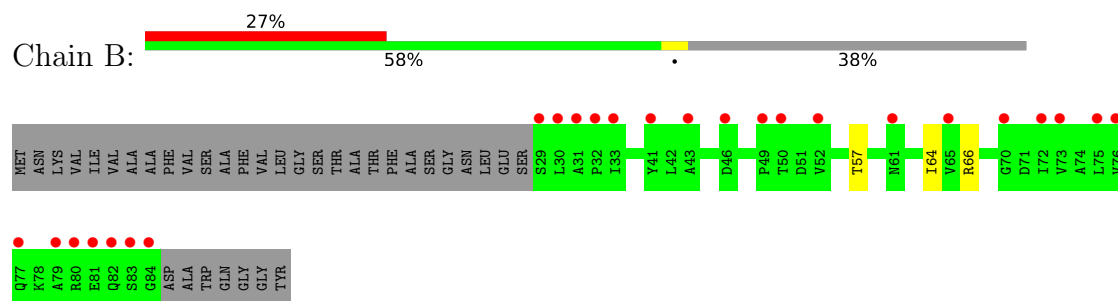




• Molecule 1: Aerobic hydroxylamine oxidoreductase

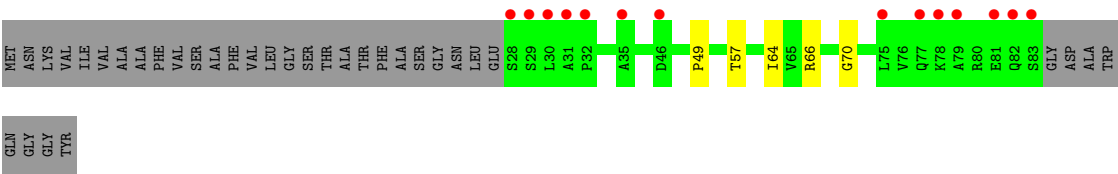


• Molecule 2: Uncharacterized protein

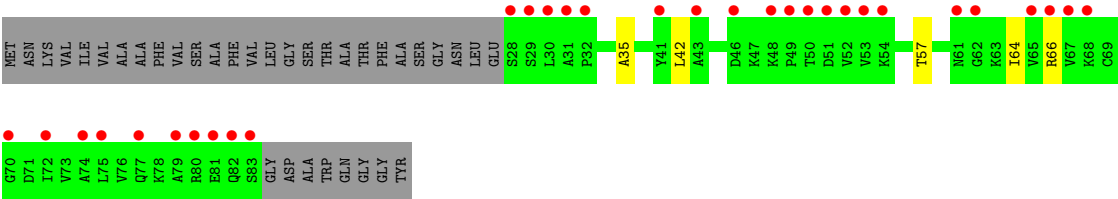


• Molecule 2: Uncharacterized protein





● Molecule 2: Uncharacterized protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.34Å 141.07Å 106.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.77 – 2.78 46.77 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.77-2.78) 100.0 (46.77-2.78)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.256 , 0.292 0.256 , 0.292	Depositor DCC
$R_{free}$ test set	2661 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.3	Xtriage
Anisotropy	0.729	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 58.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.010 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	14521	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: JUG, HEC, PEG, 1PE, 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	0.24	0/4112	0.39	0/5572
1	C	0.24	0/4112	0.39	0/5572
1	E	0.24	0/4112	0.39	0/5572
2	B	0.23	0/426	0.39	0/571
2	D	0.23	0/428	0.39	0/574
2	F	0.22	0/428	0.39	0/574
All	All	0.24	0/13618	0.39	0/18435

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4009	0	3808	77	0
1	C	4009	0	3808	70	0
1	E	4009	0	3808	76	0
2	B	423	0	444	2	0
2	D	425	0	446	3	0
2	F	425	0	446	4	0
3	A	301	0	210	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	301	0	209	17	0
3	E	301	0	210	16	0
4	A	86	0	56	14	0
4	C	43	0	28	9	0
5	A	14	0	20	1	0
5	E	7	0	10	0	0
6	C	13	0	6	1	0
6	E	13	0	6	2	0
7	C	28	0	37	1	0
8	A	44	0	0	2	0
8	B	5	0	0	0	0
8	C	31	0	0	1	0
8	D	7	0	0	0	0
8	E	26	0	0	1	0
8	F	1	0	0	0	0
All	All	14521	0	13552	232	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (232) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:HIS:HB3	1:C:167:VAL:HB	1.69	0.75
1:A:100:ARG:HG2	1:A:170:ILE:HG21	1.70	0.72
1:C:264:ASP:OD2	1:C:269:ARG:NH1	2.23	0.71
1:A:123:HIS:CD2	3:A:602:HEC:ND	2.60	0.69
1:A:123:HIS:HB3	1:A:167:VAL:HB	1.75	0.68
1:E:238:THR:HG23	6:E:608:JUG:HAD	1.75	0.66
1:A:120:ARG:NH2	8:A:701:HOH:O	2.28	0.66
4:A:608:ISW:HHB	1:E:235:ASN:HA	1.78	0.65
1:C:100:ARG:HG2	1:C:170:ILE:HG21	1.77	0.65
1:A:130:ARG:NH2	8:A:702:HOH:O	2.28	0.65
1:A:130:ARG:NH1	1:A:149:GLU:OE2	2.30	0.65
1:C:235:ASN:HA	4:C:611:ISW:HHB	1.79	0.63
1:A:330:ASN:HB3	1:E:120:ARG:HH12	1.64	0.62
1:C:153:ARG:HD3	1:C:160:GLU:HA	1.81	0.61
1:A:303:HIS:CD2	3:A:607:HEC:ND	2.68	0.61
1:A:235:ASN:HA	4:A:611:ISW:HHB	1.83	0.61
1:C:82:MET:O	1:C:261:ASN:ND2	2.30	0.60
1:E:130:ARG:NH2	1:E:149:GLU:OE2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:VAL:HG13	1:E:187:ASP:HB3	1.84	0.60
1:E:173:HIS:HE1	3:E:604:HEC:ND	1.99	0.60
1:E:126:LEU:HD11	1:E:167:VAL:HG23	1.82	0.60
1:E:167:VAL:HG13	3:E:602:HEC:HBC2	1.85	0.59
1:C:207:ARG:HH21	1:C:229:ALA:HA	1.68	0.58
1:C:483:HIS:O	1:C:485:ASN:N	2.37	0.58
1:A:120:ARG:NH1	1:A:271:GLU:OE1	2.36	0.58
1:E:287:HIS:HE1	3:E:606:HEC:NA	2.02	0.58
2:F:64:ILE:HB	2:F:66:ARG:HH12	1.67	0.58
1:E:483:HIS:O	1:E:485:ASN:N	2.37	0.58
4:A:608:ISW:HMAB	1:E:234:ALA:HB1	1.85	0.58
1:C:114:TRP:NE1	3:C:604:HEC:O1A	2.36	0.57
2:D:64:ILE:O	2:D:66:ARG:NH1	2.37	0.57
1:A:221:TRP:CZ3	4:A:611:ISW:HBA	2.39	0.56
1:A:483:HIS:O	1:A:485:ASN:N	2.37	0.56
1:A:152:LEU:HB3	1:A:157:LYS:HB2	1.88	0.56
1:A:31:ASP:OD1	1:A:41:ARG:NH1	2.39	0.56
1:A:207:ARG:NH1	1:A:259:ASN:O	2.29	0.56
1:C:253:CYS:SG	4:C:611:ISW:HHC	2.44	0.56
5:A:610:PEG:H32	4:A:611:ISW:HAA	1.88	0.55
1:C:238:THR:HG23	6:C:608:JUG:HAD	1.88	0.55
1:C:346:THR:OG1	1:C:351:ARG:NH2	2.40	0.55
1:C:234:ALA:HB1	4:C:611:ISW:HMAB	1.88	0.55
1:C:302:LYS:NZ	8:C:703:HOH:O	2.38	0.55
2:B:64:ILE:O	2:B:66:ARG:NH2	2.40	0.55
1:A:84:PRO:HB3	1:A:190:MET:HB2	1.89	0.55
4:C:611:ISW:HMCA	1:E:491:TYR:HD2	1.72	0.54
1:A:338:HIS:HE1	3:A:605:HEC:ND	2.05	0.54
4:A:608:ISW:HHC	1:E:253:CYS:SG	2.47	0.54
1:E:123:HIS:HD2	1:E:167:VAL:HG11	1.73	0.54
1:C:141:LYS:NZ	3:C:601:HEC:O2A	2.38	0.54
1:E:264:ASP:OD2	1:E:269:ARG:NH1	2.39	0.54
1:C:191:PRO:HB2	3:C:604:HEC:HMD3	1.88	0.54
1:A:234:ALA:HB1	4:A:611:ISW:HMAB	1.90	0.53
1:C:221:TRP:CZ2	1:C:361:VAL:HG21	2.43	0.53
1:A:450:GLN:HB3	1:A:459:PRO:HG3	1.90	0.53
1:C:207:ARG:NH2	1:C:208:GLU:OE2	2.42	0.53
1:C:98:ALA:HB2	3:C:603:HEC:HMC2	1.89	0.53
1:E:450:GLN:HB3	1:E:459:PRO:HG3	1.90	0.53
1:C:148:VAL:HG13	1:C:199:CYS:HB3	1.91	0.53
3:E:605:HEC:HBA1	3:E:606:HEC:HMA3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:611:ISW:HMCA	1:C:491:TYR:HD2	1.74	0.52
1:C:415:ASN:HA	1:C:466:VAL:HG21	1.91	0.52
1:C:287:HIS:CD2	3:C:606:HEC:NC	2.74	0.51
1:C:167:VAL:HG22	3:C:602:HEC:HBC2	1.92	0.51
1:A:253:CYS:SG	4:A:611:ISW:HHC	2.50	0.51
1:E:170:ILE:HD11	1:E:178:LYS:HD3	1.93	0.51
1:E:262:LYS:NZ	1:E:265:ASN:OD1	2.43	0.51
1:A:287:HIS:HE1	3:A:606:HEC:NA	2.05	0.51
1:A:330:ASN:HB3	1:E:120:ARG:NH1	2.25	0.50
1:E:162:GLU:OE2	1:E:179:LYS:NZ	2.31	0.50
1:C:31:ASP:HA	1:C:41:ARG:HH12	1.76	0.49
1:E:290:VAL:HG22	1:E:472:ASN:HB3	1.94	0.49
1:E:415:ASN:HA	1:E:466:VAL:HG21	1.94	0.49
1:C:221:TRP:CZ3	4:C:611:ISW:HBA	2.47	0.49
1:C:84:PRO:HB3	1:C:190:MET:HB2	1.93	0.49
1:C:47:LYS:HD2	1:C:155:MET:HA	1.95	0.49
1:C:441:GLU:OE2	1:C:449:THR:OG1	2.25	0.49
1:A:507:ASP:OD1	1:A:511:LYS:NZ	2.33	0.49
1:C:290:VAL:HG22	1:C:472:ASN:HB3	1.94	0.49
1:A:491:TYR:HD2	4:A:608:ISW:HMCA	1.78	0.49
1:C:173:HIS:HE1	3:C:604:HEC:ND	2.07	0.48
1:A:287:HIS:CD2	3:A:606:HEC:NC	2.78	0.48
1:A:170:ILE:HD11	1:A:178:LYS:HD3	1.94	0.48
1:A:314:TRP:HH2	1:A:331:ALA:HB3	1.79	0.48
1:A:98:ALA:HB1	1:A:102:ASP:HB2	1.94	0.48
1:C:173:HIS:HE1	3:C:604:HEC:C4D	2.27	0.48
1:C:450:GLN:HB3	1:C:459:PRO:HG3	1.94	0.48
1:E:84:PRO:HB3	1:E:190:MET:HB2	1.96	0.48
1:E:221:TRP:CZ2	1:E:361:VAL:HG21	2.49	0.48
1:A:167:VAL:HG22	3:A:602:HEC:HBC2	1.96	0.48
1:C:206:GLU:O	1:C:209:SER:OG	2.24	0.48
1:E:477:MET:HG3	1:E:489:TRP:HB2	1.96	0.48
1:A:231:ASP:HB3	3:A:606:HEC:HBD2	1.95	0.47
1:A:381:VAL:HG11	1:A:390:GLU:HG3	1.96	0.47
1:A:415:ASN:HA	1:A:466:VAL:HG21	1.95	0.47
1:E:314:TRP:HH2	1:E:331:ALA:HB3	1.79	0.47
1:E:470:ALA:HA	1:E:474:LEU:HB3	1.96	0.47
1:C:248:GLU:HG2	1:E:402:LYS:HB2	1.96	0.47
1:A:221:TRP:CZ2	1:A:361:VAL:HG21	2.49	0.47
1:E:153:ARG:HD3	1:E:160:GLU:HA	1.96	0.47
1:E:287:HIS:CD2	3:E:606:HEC:NC	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:PRO:N	3:A:607:HEC:HBC2	2.30	0.47
1:A:269:ARG:HA	1:A:270:HIS:HA	1.67	0.46
1:E:358:TYR:CZ	6:E:608:JUG:HAF	2.50	0.46
1:C:477:MET:HG3	1:C:489:TRP:HB2	1.96	0.46
1:C:298:TYR:CE1	3:C:605:HEC:HMC2	2.51	0.46
1:E:100:ARG:NH2	1:E:171:ASP:OD1	2.45	0.46
1:A:191:PRO:HG2	3:A:604:HEC:CHD	2.46	0.46
1:E:153:ARG:HB3	1:E:160:GLU:OE2	2.16	0.46
1:C:303:HIS:CD2	3:C:607:HEC:ND	2.84	0.46
7:C:609:1PE:H252	7:C:609:1PE:H242	1.76	0.46
1:E:435:PRO:O	1:E:458:ASN:ND2	2.44	0.46
1:A:409:ALA:HB3	2:B:57:THR:HG21	1.98	0.45
1:A:222:PRO:HB2	1:A:225:ARG:HD3	1.98	0.45
1:E:98:ALA:HB2	3:E:603:HEC:HMC2	1.98	0.45
1:C:254:THR:O	1:C:258:THR:HG23	2.17	0.45
1:C:315:ASN:O	1:C:318:VAL:HG22	2.16	0.45
1:E:303:HIS:CD2	3:E:607:HEC:ND	2.81	0.45
1:E:320:LEU:HD11	1:E:335:ALA:HB1	1.99	0.45
1:C:287:HIS:HE1	3:C:606:HEC:NA	2.11	0.45
1:E:322:ASP:HB3	1:E:326:LYS:HB2	1.99	0.45
1:A:90:PRO:HG3	1:A:188:ILE:O	2.17	0.45
1:C:272:PHE:CE2	3:C:604:HEC:HBC2	2.51	0.45
1:E:369:THR:HG21	2:F:42:LEU:HD11	1.99	0.45
1:E:409:ALA:HB3	2:F:57:THR:HG21	1.99	0.45
1:E:267:HIS:HE1	3:E:601:HEC:NB	2.07	0.44
1:C:320:LEU:HD11	1:C:335:ALA:HB1	1.98	0.44
1:A:272:PHE:CE2	3:A:604:HEC:HBC2	2.52	0.44
4:A:608:ISW:HBA	1:E:221:TRP:CZ3	2.52	0.44
1:C:288:SER:HB3	1:C:295:TRP:HB3	1.99	0.44
1:E:207:ARG:HH11	1:E:229:ALA:HA	1.81	0.44
1:A:270:HIS:HD2	3:A:604:HEC:NC	2.15	0.44
1:C:98:ALA:HB1	1:C:102:ASP:HB2	2.00	0.44
1:E:98:ALA:HB1	1:E:102:ASP:HB2	1.99	0.44
1:A:76:ILE:HD11	1:A:251:GLU:HG2	1.99	0.44
1:A:340:GLU:OE1	1:A:383:THR:OG1	2.29	0.44
3:A:606:HEC:HMD3	4:A:611:ISW:CHD	2.48	0.44
1:C:111:THR:HB	1:C:114:TRP:HB2	2.00	0.44
1:A:56:ARG:HG3	1:A:62:HIS:CG	2.53	0.44
1:C:104:VAL:O	1:C:108:SER:OG	2.22	0.44
1:C:136:ASP:OD1	1:C:137:PRO:HD2	2.18	0.44
1:C:314:TRP:HH2	1:C:331:ALA:HB3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:507:ASP:OD1	1:C:511:LYS:NZ	2.33	0.44
1:E:200:HIS:CE1	3:E:602:HEC:ND	2.86	0.44
1:E:269:ARG:HA	1:E:270:HIS:HA	1.67	0.44
2:D:49:PRO:O	2:D:70:GLY:N	2.51	0.43
1:A:350:THR:O	1:A:376:ARG:NH1	2.40	0.43
1:A:399:LEU:HG	1:E:248:GLU:HG3	1.99	0.43
1:A:470:ALA:HA	1:A:474:LEU:HB3	2.00	0.43
3:A:605:HEC:HMA3	3:A:606:HEC:C3A	2.48	0.43
1:E:244:MET:SD	1:E:250:ALA:HB2	2.58	0.43
1:A:240:VAL:HB	1:A:449:THR:HA	2.01	0.43
1:A:298:TYR:CE1	3:A:605:HEC:HMC2	2.53	0.43
1:C:409:ALA:HB3	2:D:57:THR:HG21	2.01	0.43
1:A:257:HIS:CE1	3:A:606:HEC:HMD1	2.53	0.43
1:A:451:LEU:HD11	1:A:471:GLU:HG2	2.01	0.43
1:E:434:ARG:HG3	1:E:458:ASN:HB2	2.00	0.43
1:A:141:LYS:NZ	3:A:601:HEC:O2A	2.50	0.43
1:A:167:VAL:HG13	3:A:602:HEC:HBC2	2.01	0.43
1:A:248:GLU:HG3	1:C:399:LEU:HG	2.01	0.43
3:C:605:HEC:HMA2	4:C:611:ISW:O1D	2.19	0.43
1:E:206:GLU:O	1:E:209:SER:OG	2.24	0.43
1:E:296:GLU:OE1	1:E:296:GLU:N	2.44	0.43
1:C:275:ALA:HB2	1:C:317:GLU:HA	2.01	0.43
1:E:240:VAL:HB	1:E:449:THR:HA	2.00	0.43
3:A:605:HEC:HBA1	3:A:606:HEC:HMA3	2.01	0.43
1:A:349:ILE:HD13	3:A:606:HEC:C3A	2.49	0.42
1:C:101:LYS:HD3	1:C:101:LYS:HA	1.86	0.42
1:C:267:HIS:HE1	3:C:601:HEC:NB	2.15	0.42
1:A:174:VAL:HG13	1:A:187:ASP:HB3	2.00	0.42
1:A:248:GLU:HG2	1:C:402:LYS:HB2	2.00	0.42
1:A:296:GLU:OE1	1:A:296:GLU:N	2.43	0.42
1:E:173:HIS:HE1	3:E:604:HEC:C4D	2.32	0.42
4:A:608:ISW:HHA	4:A:608:ISW:HAAA	2.00	0.42
1:E:118:TRP:O	1:E:121:SER:OG	2.22	0.42
1:A:274:ALA:O	1:A:278:ARG:HG3	2.20	0.42
3:C:606:HEC:HMD3	4:C:611:ISW:CHD	2.49	0.42
1:A:290:VAL:HG22	1:A:472:ASN:HB3	2.00	0.42
1:C:340:GLU:HB2	1:C:345:TYR:CE2	2.54	0.42
4:C:611:ISW:HHA	4:C:611:ISW:HAAA	1.99	0.42
1:E:104:VAL:HG13	1:E:115:VAL:HG13	2.01	0.42
1:A:98:ALA:HB2	3:A:603:HEC:HMC2	2.02	0.42
1:A:434:ARG:HH22	1:A:463:GLU:CD	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:PRO:HB2	1:C:225:ARG:HD3	2.02	0.42
1:C:296:GLU:OE1	1:C:296:GLU:N	2.43	0.42
1:E:116:ARG:O	1:E:120:ARG:HG3	2.19	0.42
3:E:603:HEC:HMD1	3:E:603:HEC:HBD2	2.02	0.42
1:E:305:LYS:HD3	1:E:305:LYS:HA	1.89	0.42
1:A:333:THR:O	3:A:605:HEC:HMC3	2.20	0.42
1:C:216:TRP:NE1	1:C:221:TRP:HB2	2.35	0.41
1:C:92:VAL:HA	1:C:185:THR:HG23	2.03	0.41
4:C:611:ISW:HMCA	1:E:491:TYR:CD2	2.54	0.41
1:A:450:GLN:NE2	1:A:463:GLU:OE2	2.46	0.41
3:A:607:HEC:HBA2	1:E:269:ARG:HH22	1.85	0.41
1:C:207:ARG:NH2	1:C:229:ALA:HA	2.33	0.41
1:C:274:ALA:H	3:C:602:HEC:HBA1	1.86	0.41
1:E:254:THR:O	1:E:258:THR:HG23	2.20	0.41
1:A:117:ALA:HB1	1:A:271:GLU:HG3	2.02	0.41
1:A:302:LYS:HD3	1:A:302:LYS:HA	1.94	0.41
1:A:434:ARG:HG3	1:A:458:ASN:HB2	2.01	0.41
1:A:523:ASN:OD1	1:C:521:ARG:NH1	2.51	0.41
1:E:354:ARG:NH2	1:E:401:ASP:OD1	2.53	0.41
1:E:31:ASP:OD1	1:E:41:ARG:NH2	2.54	0.41
1:E:278:ARG:NE	3:E:601:HEC:O2D	2.34	0.41
1:A:216:TRP:CD1	1:A:221:TRP:HB2	2.55	0.41
3:A:605:HEC:HMA2	4:A:611:ISW:O1D	2.21	0.41
1:C:130:ARG:HA	1:C:142:LYS:HE2	2.02	0.41
1:C:332:PRO:N	3:C:607:HEC:HBC2	2.36	0.41
1:E:104:VAL:O	1:E:108:SER:OG	2.28	0.41
1:E:257:HIS:CE1	3:E:606:HEC:HMD1	2.56	0.41
1:E:411:TYR:CE1	1:E:470:ALA:HB2	2.56	0.41
1:E:438:PRO:HD3	1:E:453:TRP:CE2	2.56	0.41
1:A:254:THR:O	1:A:258:THR:HG23	2.21	0.41
1:E:333:THR:O	3:E:605:HEC:HMC3	2.21	0.41
1:A:288:SER:HB3	1:A:295:TRP:HB3	2.03	0.41
1:A:410:LYS:HE3	1:A:502:TYR:CG	2.55	0.41
1:E:31:ASP:HA	1:E:41:ARG:HH22	1.86	0.41
1:E:409:ALA:HB2	2:F:35:ALA:HB3	2.02	0.41
1:E:411:TYR:CE1	1:E:415:ASN:HB2	2.56	0.41
1:C:170:ILE:HD11	1:C:178:LYS:HD3	2.03	0.41
1:E:299:THR:O	1:E:305:LYS:HG2	2.20	0.41
1:E:484:VAL:HG11	3:E:607:HEC:HMA2	2.02	0.41
1:A:31:ASP:HA	1:A:41:ARG:HH22	1.87	0.40
3:A:607:HEC:HBD1	1:E:268:THR:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:LYS:HA	1:C:305:LYS:HD3	1.90	0.40
1:E:265:ASN:HB3	3:E:606:HEC:HBC3	2.03	0.40
1:A:191:PRO:HB2	3:A:604:HEC:HMD3	2.03	0.40
1:A:264:ASP:OD2	1:A:269:ARG:NH1	2.49	0.40
1:C:422:TYR:CE1	1:C:445:PHE:HB2	2.56	0.40
1:A:340:GLU:HB2	1:A:345:TYR:CE2	2.56	0.40
1:E:285:THR:HB	8:E:720:HOH:O	2.21	0.40
1:A:438:PRO:HD3	1:A:453:TRP:CE2	2.56	0.40
1:C:342:GLU:HA	1:C:382:LEU:HD23	2.04	0.40

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	501/570 (88%)	479 (96%)	21 (4%)	1 (0%)	47	76
1	C	501/570 (88%)	479 (96%)	21 (4%)	1 (0%)	47	76
1	E	501/570 (88%)	479 (96%)	21 (4%)	1 (0%)	47	76
2	B	54/91 (59%)	53 (98%)	1 (2%)	0	100	100
2	D	54/91 (59%)	53 (98%)	1 (2%)	0	100	100
2	F	54/91 (59%)	53 (98%)	1 (2%)	0	100	100
All	All	1665/1983 (84%)	1596 (96%)	66 (4%)	3 (0%)	47	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	484	VAL
1	C	484	VAL
1	E	484	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	429/477 (90%)	427 (100%)	2 (0%)	88	95
1	C	429/477 (90%)	427 (100%)	2 (0%)	88	95
1	E	429/477 (90%)	427 (100%)	2 (0%)	88	95
2	B	48/73 (66%)	48 (100%)	0	100	100
2	D	49/73 (67%)	49 (100%)	0	100	100
2	F	49/73 (67%)	49 (100%)	0	100	100
All	All	1433/1650 (87%)	1427 (100%)	6 (0%)	91	96

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	TRP
1	A	267	HIS
1	C	114	TRP
1	C	267	HIS
1	E	114	TRP
1	E	267	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

31 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	A	605	1	26,50,50	2.41	3 (11%)	18,82,82	1.67	4 (22%)
3	HEC	E	605	1	26,50,50	2.42	4 (15%)	18,82,82	1.63	3 (16%)
4	ISW	A	611	8,1	30,50,50	4.89	14 (46%)	20,82,82	4.67	10 (50%)
3	HEC	C	605	1	26,50,50	2.41	4 (15%)	18,82,82	1.64	3 (16%)
3	HEC	E	604	1	26,50,50	2.35	3 (11%)	18,82,82	1.59	3 (16%)
3	HEC	C	604	1	26,50,50	2.36	3 (11%)	18,82,82	1.58	4 (22%)
7	1PE	C	609	-	11,11,15	0.55	0	10,10,14	0.25	0
3	HEC	A	607	1	26,50,50	2.30	3 (11%)	18,82,82	1.68	5 (27%)
3	HEC	E	607	1	26,50,50	2.33	3 (11%)	18,82,82	1.62	4 (22%)
3	HEC	A	604	1	26,50,50	2.38	3 (11%)	18,82,82	1.57	4 (22%)
3	HEC	E	602	1	26,50,50	2.33	3 (11%)	18,82,82	1.42	1 (5%)
6	JUG	C	608	-	14,14,14	2.79	7 (50%)	20,20,20	1.02	1 (5%)
7	1PE	C	610	-	15,15,15	0.53	0	14,14,14	0.23	0
3	HEC	C	602	1	26,50,50	2.33	3 (11%)	18,82,82	1.47	2 (11%)
5	PEG	A	610	-	6,6,6	0.49	0	5,5,5	0.24	0
3	HEC	A	603	1	26,50,50	2.32	4 (15%)	18,82,82	1.62	4 (22%)
3	HEC	E	606	1	26,50,50	2.35	3 (11%)	18,82,82	1.57	2 (11%)
5	PEG	E	609	-	6,6,6	0.49	0	5,5,5	0.28	0
3	HEC	C	606	1	26,50,50	2.33	3 (11%)	18,82,82	1.53	2 (11%)
3	HEC	A	601	1	26,50,50	2.34	3 (11%)	18,82,82	1.50	3 (16%)
4	ISW	C	611	8,1	30,50,50	4.90	14 (46%)	20,82,82	4.55	10 (50%)
3	HEC	A	606	1	26,50,50	2.35	3 (11%)	18,82,82	1.50	2 (11%)
3	HEC	A	602	1	26,50,50	2.37	4 (15%)	18,82,82	1.44	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PEG	A	609	-	6,6,6	0.49	0	5,5,5	0.28	0
3	HEC	C	607	1	26,50,50	2.37	3 (11%)	18,82,82	1.50	3 (16%)
3	HEC	E	603	1	26,50,50	2.36	4 (15%)	18,82,82	1.67	4 (22%)
3	HEC	C	603	1	26,50,50	2.33	3 (11%)	18,82,82	1.64	5 (27%)
3	HEC	C	601	1	26,50,50	2.34	3 (11%)	18,82,82	1.59	5 (27%)
3	HEC	E	601	1	26,50,50	2.35	3 (11%)	18,82,82	1.48	3 (16%)
4	ISW	A	608	8,1	30,50,50	4.90	14 (46%)	20,82,82	4.47	10 (50%)
6	JUG	E	608	-	14,14,14	2.78	8 (57%)	20,20,20	1.05	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	A	605	1	-	3/6/54/54	-
3	HEC	E	605	1	-	3/6/54/54	-
4	ISW	A	611	8,1	-	4/8/74/74	-
3	HEC	C	605	1	-	3/6/54/54	-
3	HEC	E	604	1	-	2/6/54/54	-
3	HEC	C	604	1	-	3/6/54/54	-
7	1PE	C	609	-	-	4/9/9/13	-
3	HEC	A	607	1	-	2/6/54/54	-
3	HEC	E	607	1	-	0/6/54/54	-
3	HEC	A	604	1	-	2/6/54/54	-
3	HEC	E	602	1	-	0/6/54/54	-
6	JUG	C	608	-	-	-	0/2/2/2
7	1PE	C	610	-	-	4/13/13/13	-
3	HEC	C	602	1	-	0/6/54/54	-
5	PEG	A	610	-	-	2/4/4/4	-
3	HEC	A	603	1	-	0/6/54/54	-
3	HEC	E	606	1	-	0/6/54/54	-
5	PEG	E	609	-	-	2/4/4/4	-
3	HEC	C	606	1	-	0/6/54/54	-
3	HEC	A	601	1	-	0/6/54/54	-
4	ISW	C	611	8,1	-	2/8/74/74	-
3	HEC	A	606	1	-	0/6/54/54	-
3	HEC	A	602	1	-	2/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	A	609	-	-	0/4/4/4	-
3	HEC	C	607	1	-	0/6/54/54	-
3	HEC	E	603	1	-	2/6/54/54	-
3	HEC	C	603	1	-	0/6/54/54	-
3	HEC	C	601	1	-	0/6/54/54	-
3	HEC	E	601	1	-	0/6/54/54	-
4	ISW	A	608	8,1	-	2/8/74/74	-
6	JUG	E	608	-	-	-	0/2/2/2

All (125) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	611	ISW	CHC-C4B	-15.01	1.30	1.53
4	A	608	ISW	CHC-C4B	-14.87	1.30	1.53
4	A	611	ISW	CHC-C4B	-14.75	1.30	1.53
4	A	608	ISW	C4C-CHD	11.50	1.73	1.41
4	A	611	ISW	C4C-CHD	11.42	1.72	1.41
4	C	611	ISW	C4C-CHD	11.41	1.72	1.41
4	A	611	ISW	C4D-CHA	10.14	1.69	1.41
4	C	611	ISW	C4D-CHA	10.07	1.69	1.41
4	A	608	ISW	C4D-CHA	10.06	1.69	1.41
4	A	611	ISW	CHB-C1B	9.26	1.67	1.41
4	C	611	ISW	CHB-C1B	9.23	1.67	1.41
4	A	608	ISW	CHB-C1B	9.22	1.67	1.41
3	E	605	HEC	C3B-C2B	-6.51	1.34	1.40
3	C	607	HEC	C3B-C2B	-6.49	1.34	1.40
3	A	605	HEC	C3C-C2C	-6.45	1.34	1.40
3	C	605	HEC	C3B-C2B	-6.43	1.34	1.40
3	A	605	HEC	C3B-C2B	-6.34	1.34	1.40
3	E	606	HEC	C3C-C2C	-6.32	1.34	1.40
3	A	606	HEC	C3B-C2B	-6.27	1.34	1.40
3	A	604	HEC	C3C-C2C	-6.26	1.34	1.40
3	C	601	HEC	C3C-C2C	-6.24	1.34	1.40
3	A	604	HEC	C3B-C2B	-6.23	1.34	1.40
3	E	605	HEC	C3C-C2C	-6.21	1.34	1.40
3	E	601	HEC	C3C-C2C	-6.19	1.34	1.40
3	A	601	HEC	C3C-C2C	-6.19	1.34	1.40
3	A	602	HEC	C3B-C2B	-6.19	1.34	1.40
3	E	602	HEC	C3B-C2B	-6.18	1.34	1.40
3	E	603	HEC	C3B-C2B	-6.17	1.34	1.40
3	C	602	HEC	C3B-C2B	-6.16	1.34	1.40
3	A	606	HEC	C3C-C2C	-6.15	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	606	HEC	C3C-C2C	-6.15	1.34	1.40
3	C	605	HEC	C3C-C2C	-6.14	1.34	1.40
3	E	606	HEC	C3B-C2B	-6.14	1.34	1.40
3	E	604	HEC	C3C-C2C	-6.13	1.34	1.40
3	E	607	HEC	C3B-C2B	-6.10	1.34	1.40
3	C	601	HEC	C3B-C2B	-6.08	1.34	1.40
3	C	606	HEC	C3B-C2B	-6.07	1.34	1.40
3	E	601	HEC	C3B-C2B	-6.06	1.34	1.40
3	C	604	HEC	C3C-C2C	-6.05	1.34	1.40
3	E	604	HEC	C3B-C2B	-6.03	1.34	1.40
3	A	601	HEC	C3B-C2B	-6.02	1.34	1.40
3	C	604	HEC	C3B-C2B	-6.01	1.34	1.40
3	C	603	HEC	C3C-C2C	-6.00	1.34	1.40
3	A	607	HEC	C3B-C2B	-5.98	1.34	1.40
3	A	603	HEC	C3C-C2C	-5.97	1.34	1.40
3	C	603	HEC	C3B-C2B	-5.96	1.34	1.40
6	C	608	JUG	CAG-CAF	5.96	1.48	1.35
6	E	608	JUG	CAG-CAF	5.95	1.48	1.35
3	A	602	HEC	C3C-C2C	-5.93	1.34	1.40
3	A	603	HEC	C3B-C2B	-5.90	1.34	1.40
3	E	603	HEC	C3C-C2C	-5.87	1.34	1.40
3	C	607	HEC	C3C-C2C	-5.87	1.34	1.40
3	C	602	HEC	C3C-C2C	-5.81	1.34	1.40
3	E	602	HEC	C3C-C2C	-5.80	1.34	1.40
3	E	607	HEC	C3C-C2C	-5.79	1.34	1.40
3	E	603	HEC	C3D-C2D	5.75	1.54	1.37
4	A	608	ISW	C1D-C2D	5.69	1.55	1.42
3	E	605	HEC	C3D-C2D	5.66	1.54	1.37
4	A	611	ISW	CHC-C1C	5.65	1.65	1.51
4	A	611	ISW	C1D-C2D	5.63	1.55	1.42
4	C	611	ISW	C1D-C2D	5.63	1.55	1.42
3	C	605	HEC	C3D-C2D	5.63	1.54	1.37
3	C	604	HEC	C3D-C2D	5.61	1.54	1.37
3	A	607	HEC	C3C-C2C	-5.59	1.34	1.40
3	A	605	HEC	C3D-C2D	5.59	1.54	1.37
4	A	608	ISW	CHC-C1C	5.57	1.65	1.51
3	A	602	HEC	C3D-C2D	5.56	1.54	1.37
3	A	607	HEC	C3D-C2D	5.55	1.54	1.37
3	A	603	HEC	C3D-C2D	5.54	1.54	1.37
3	C	603	HEC	C3D-C2D	5.52	1.54	1.37
3	E	607	HEC	C3D-C2D	5.51	1.54	1.37
3	C	602	HEC	C3D-C2D	5.50	1.54	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	608	ISW	C4D-ND	5.50	1.47	1.36
4	C	611	ISW	CHC-C1C	5.49	1.64	1.51
3	C	607	HEC	C3D-C2D	5.48	1.53	1.37
3	E	602	HEC	C3D-C2D	5.47	1.53	1.37
3	A	601	HEC	C3D-C2D	5.45	1.53	1.37
3	E	601	HEC	C3D-C2D	5.43	1.53	1.37
3	A	604	HEC	C3D-C2D	5.42	1.53	1.37
3	E	604	HEC	C3D-C2D	5.42	1.53	1.37
3	C	601	HEC	C3D-C2D	5.42	1.53	1.37
6	C	608	JUG	CAL-CAJ	5.40	1.57	1.48
4	C	611	ISW	C4D-ND	5.40	1.47	1.36
6	E	608	JUG	CAL-CAJ	5.38	1.57	1.48
3	E	606	HEC	C3D-C2D	5.37	1.53	1.37
3	C	606	HEC	C3D-C2D	5.34	1.53	1.37
4	A	611	ISW	C4D-ND	5.33	1.47	1.36
3	A	606	HEC	C3D-C2D	5.32	1.53	1.37
4	A	608	ISW	C1B-C2B	4.26	1.52	1.44
4	C	611	ISW	C1B-C2B	4.25	1.52	1.44
4	A	611	ISW	C1B-C2B	4.20	1.52	1.44
6	C	608	JUG	CAM-CAK	4.18	1.57	1.46
6	E	608	JUG	CAM-CAK	4.06	1.57	1.46
4	C	611	ISW	C3C-CAC	3.24	1.54	1.47
4	A	611	ISW	C3C-C2C	3.23	1.44	1.40
4	A	611	ISW	C3C-CAC	3.17	1.54	1.47
4	A	608	ISW	C4B-NB	3.15	1.53	1.48
4	A	611	ISW	C4B-NB	3.13	1.53	1.48
4	A	608	ISW	C3C-C2C	3.12	1.44	1.40
4	A	608	ISW	C3C-CAC	3.12	1.54	1.47
4	C	611	ISW	C4B-NB	3.08	1.53	1.48
4	C	611	ISW	C3C-C2C	3.07	1.44	1.40
4	A	611	ISW	C3D-C2D	2.82	1.46	1.37
4	C	611	ISW	C3D-C2D	2.68	1.45	1.37
4	A	608	ISW	C3D-C2D	2.64	1.45	1.37
4	A	611	ISW	C4C-NC	-2.60	1.30	1.36
4	A	611	ISW	CAD-C3D	2.58	1.55	1.52
4	C	611	ISW	CAD-C3D	2.57	1.55	1.52
4	A	608	ISW	CAD-C3D	2.51	1.55	1.52
4	A	608	ISW	C4C-NC	-2.48	1.31	1.36
6	E	608	JUG	OAB-CAK	-2.48	1.18	1.24
4	C	611	ISW	C4C-NC	-2.47	1.31	1.36
3	A	602	HEC	CAD-C3D	2.45	1.55	1.52
6	C	608	JUG	OAA-CAJ	-2.45	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	608	JUG	OAA-CAJ	-2.44	1.19	1.24
6	C	608	JUG	OAB-CAK	-2.44	1.19	1.24
3	E	603	HEC	CAD-C3D	2.32	1.55	1.52
6	C	608	JUG	CAF-CAJ	2.15	1.51	1.46
3	C	605	HEC	CAD-C3D	2.12	1.55	1.52
6	E	608	JUG	CAF-CAJ	2.12	1.50	1.46
6	C	608	JUG	CAG-CAK	2.11	1.50	1.46
6	E	608	JUG	CAG-CAK	2.10	1.50	1.46
3	A	603	HEC	CAD-C3D	2.10	1.55	1.52
3	E	605	HEC	CAD-C3D	2.07	1.55	1.52
6	E	608	JUG	OAC-CAI	2.00	1.40	1.36

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	611	ISW	C4A-CHB-C1B	-13.07	105.31	122.56
4	C	611	ISW	C4A-CHB-C1B	-12.59	105.94	122.56
4	A	608	ISW	C4A-CHB-C1B	-12.48	106.09	122.56
4	A	611	ISW	CMA-C3A-C2A	9.33	142.53	124.94
4	C	611	ISW	CMA-C3A-C2A	9.22	142.33	124.94
4	A	611	ISW	CBA-CAA-C2A	9.10	129.24	112.48
4	A	608	ISW	CMA-C3A-C2A	9.06	142.03	124.94
4	C	611	ISW	CBA-CAA-C2A	8.50	128.14	112.48
4	A	608	ISW	CBA-CAA-C2A	8.48	128.10	112.48
4	C	611	ISW	C3C-C4C-NC	5.03	115.72	109.21
4	A	611	ISW	C3C-C4C-NC	4.85	115.48	109.21
4	A	608	ISW	C3C-C4C-NC	4.72	115.32	109.21
4	A	608	ISW	CHB-C1B-C2B	-4.06	118.64	124.98
4	C	611	ISW	CHB-C1B-C2B	-4.02	118.70	124.98
4	A	611	ISW	CAD-CBD-CGD	-3.72	106.43	112.67
4	A	611	ISW	CHB-C1B-C2B	-3.67	119.25	124.98
3	E	605	HEC	CMC-C2C-C1C	-3.38	123.26	128.46
3	C	605	HEC	CMC-C2C-C1C	-3.33	123.34	128.46
3	C	602	HEC	CMC-C2C-C1C	-3.33	123.34	128.46
3	E	603	HEC	CMC-C2C-C1C	-3.33	123.35	128.46
4	C	611	ISW	CAD-CBD-CGD	-3.30	107.13	112.67
4	A	608	ISW	C2B-C1B-NB	3.20	113.72	109.88
3	C	606	HEC	CMC-C2C-C1C	-3.19	123.56	128.46
3	E	606	HEC	CMC-C2C-C1C	-3.16	123.61	128.46
3	E	607	HEC	CMC-C2C-C1C	-3.15	123.62	128.46
4	C	611	ISW	C2B-C1B-NB	3.14	113.64	109.88
3	A	602	HEC	CMC-C2C-C1C	-3.13	123.65	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	607	HEC	CMC-C2C-C1C	-3.11	123.69	128.46
3	E	604	HEC	CMC-C2C-C1C	-3.09	123.71	128.46
3	C	603	HEC	CMC-C2C-C1C	-3.03	123.81	128.46
4	A	611	ISW	C2B-C1B-NB	3.00	113.48	109.88
3	E	602	HEC	CMC-C2C-C1C	-2.98	123.89	128.46
3	A	605	HEC	CMC-C2C-C1C	-2.96	123.91	128.46
3	C	604	HEC	CMC-C2C-C1C	-2.93	123.97	128.46
3	A	603	HEC	CMC-C2C-C1C	-2.91	123.99	128.46
3	A	606	HEC	CMC-C2C-C1C	-2.91	123.99	128.46
3	C	607	HEC	CMC-C2C-C1C	-2.91	124.00	128.46
4	C	611	ISW	CHB-C1B-NB	2.90	127.58	124.43
3	A	604	HEC	CMC-C2C-C1C	-2.90	124.01	128.46
4	A	608	ISW	CHB-C1B-NB	2.87	127.55	124.43
4	A	608	ISW	CAD-CBD-CGD	-2.87	107.85	112.67
3	C	601	HEC	CMC-C2C-C1C	-2.76	124.23	128.46
3	A	601	HEC	CMC-C2C-C1C	-2.72	124.29	128.46
3	C	601	HEC	CBD-CAD-C3D	-2.71	107.48	112.49
3	E	604	HEC	CMB-C2B-C1B	-2.71	124.30	128.46
3	C	604	HEC	CAD-CBD-CGD	-2.65	108.22	112.67
3	C	604	HEC	CMB-C2B-C1B	-2.64	124.40	128.46
3	E	601	HEC	CMC-C2C-C1C	-2.64	124.41	128.46
3	A	605	HEC	CMB-C2B-C1B	-2.59	124.48	128.46
3	A	604	HEC	CMB-C2B-C1B	-2.57	124.52	128.46
3	C	605	HEC	CMB-C2B-C1B	-2.55	124.54	128.46
3	A	603	HEC	CBA-CAA-C2A	-2.55	107.78	112.48
4	A	611	ISW	CHB-C1B-NB	2.54	127.19	124.43
3	A	605	HEC	CBA-CAA-C2A	-2.50	107.86	112.48
3	A	607	HEC	C1D-C2D-C3D	-2.50	105.26	107.00
3	C	606	HEC	CMB-C2B-C1B	-2.49	124.64	128.46
3	E	606	HEC	CMB-C2B-C1B	-2.49	124.64	128.46
4	A	608	ISW	C1B-C2B-C3B	-2.47	103.84	106.80
4	C	611	ISW	C1B-C2B-C3B	-2.47	103.85	106.80
3	E	607	HEC	CMB-C2B-C1B	-2.45	124.69	128.46
3	A	607	HEC	CMB-C2B-C1B	-2.45	124.71	128.46
3	C	603	HEC	CAD-CBD-CGD	-2.42	108.60	112.67
3	A	603	HEC	CMB-C2B-C1B	-2.39	124.80	128.46
3	A	606	HEC	CMB-C2B-C1B	-2.31	124.91	128.46
3	C	603	HEC	CMB-C2B-C1B	-2.31	124.92	128.46
3	A	603	HEC	C1D-C2D-C3D	-2.31	105.39	107.00
4	A	611	ISW	C1B-C2B-C3B	-2.30	104.05	106.80
3	C	604	HEC	C1D-C2D-C3D	-2.30	105.40	107.00
3	E	607	HEC	CAA-CBA-CGA	-2.28	108.85	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	611	ISW	CAA-C2A-C3A	2.25	133.70	127.25
4	A	611	ISW	CAA-C2A-C3A	2.24	133.69	127.25
3	E	601	HEC	CMB-C2B-C1B	-2.24	125.02	128.46
3	A	601	HEC	CAA-CBA-CGA	-2.23	108.93	112.67
3	A	605	HEC	C1D-C2D-C3D	-2.22	105.45	107.00
3	E	605	HEC	CMB-C2B-C1B	-2.22	125.05	128.46
3	A	604	HEC	C1D-C2D-C3D	-2.21	105.46	107.00
3	A	601	HEC	CMB-C2B-C1B	-2.18	125.12	128.46
3	C	601	HEC	C1D-C2D-C3D	-2.17	105.49	107.00
4	A	608	ISW	CAA-C2A-C3A	2.15	133.42	127.25
3	E	603	HEC	CAD-CBD-CGD	-2.15	109.07	112.67
3	C	601	HEC	CMB-C2B-C1B	-2.14	125.17	128.46
3	C	607	HEC	C1D-C2D-C3D	-2.13	105.52	107.00
3	E	605	HEC	CBA-CAA-C2A	-2.13	108.56	112.48
3	E	603	HEC	C1D-C2D-C3D	-2.12	105.52	107.00
3	E	607	HEC	C1D-C2D-C3D	-2.12	105.52	107.00
3	A	607	HEC	CAD-CBD-CGD	-2.11	109.13	112.67
3	C	607	HEC	CAA-CBA-CGA	-2.10	109.16	112.67
3	E	603	HEC	CMB-C2B-C1B	-2.09	125.26	128.46
3	C	605	HEC	C1D-C2D-C3D	-2.08	105.55	107.00
3	E	601	HEC	C1D-C2D-C3D	-2.04	105.57	107.00
3	C	601	HEC	CAA-CBA-CGA	-2.04	109.25	112.67
3	C	603	HEC	CAA-CBA-CGA	-2.04	109.26	112.67
3	A	602	HEC	CMB-C2B-C1B	-2.03	125.35	128.46
3	C	603	HEC	C1D-C2D-C3D	-2.02	105.59	107.00
3	E	604	HEC	C1D-C2D-C3D	-2.02	105.59	107.00
3	A	607	HEC	CMC-C2C-C3C	2.02	128.19	125.82
3	C	602	HEC	CMB-C2B-C1B	-2.00	125.38	128.46
3	A	604	HEC	CMA-C3A-C2A	2.00	128.72	124.94
6	C	608	JUG	CAL-CAJ-CAF	2.00	120.04	116.99

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	HEC	C2D-C3D-CAD-CBD
3	A	602	HEC	C4D-C3D-CAD-CBD
3	A	605	HEC	C2A-CAA-CBA-CGA
3	A	607	HEC	C1A-C2A-CAA-CBA
3	C	605	HEC	C2A-CAA-CBA-CGA
3	E	603	HEC	C2D-C3D-CAD-CBD
3	E	603	HEC	C4D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
7	C	609	1PE	OH5-C14-C24-OH4
7	C	609	1PE	OH6-C15-C25-OH5
7	C	610	1PE	OH5-C14-C24-OH4
4	A	608	ISW	C4B-C3B-CAB-CBB
4	A	611	ISW	C4B-C3B-CAB-CBB
4	C	611	ISW	C4B-C3B-CAB-CBB
7	C	609	1PE	C24-C14-OH5-C25
7	C	610	1PE	OH6-C15-C25-OH5
4	A	611	ISW	C2B-C3B-CAB-CBB
3	A	604	HEC	C1A-C2A-CAA-CBA
3	A	604	HEC	C3A-C2A-CAA-CBA
3	A	605	HEC	C2D-C3D-CAD-CBD
3	A	605	HEC	C4D-C3D-CAD-CBD
3	A	607	HEC	C3A-C2A-CAA-CBA
3	C	604	HEC	C2D-C3D-CAD-CBD
3	C	604	HEC	C4D-C3D-CAD-CBD
3	C	605	HEC	C2D-C3D-CAD-CBD
3	C	605	HEC	C4D-C3D-CAD-CBD
3	E	604	HEC	C1A-C2A-CAA-CBA
3	E	604	HEC	C3A-C2A-CAA-CBA
3	E	605	HEC	C2D-C3D-CAD-CBD
3	E	605	HEC	C4D-C3D-CAD-CBD
4	A	611	ISW	C2D-C3D-CAD-CBD
4	A	611	ISW	C4D-C3D-CAD-CBD
5	E	609	PEG	C1-C2-O2-C3
7	C	610	1PE	C25-C15-OH6-C26
3	E	605	HEC	C2A-CAA-CBA-CGA
7	C	609	1PE	C15-C25-OH5-C14
4	C	611	ISW	C2B-C3B-CAB-CBB
5	A	610	PEG	O2-C3-C4-O4
5	E	609	PEG	C4-C3-O2-C2
5	A	610	PEG	C1-C2-O2-C3
4	A	608	ISW	C2B-C3B-CAB-CBB
3	C	604	HEC	C2A-CAA-CBA-CGA
7	C	610	1PE	OH4-C13-C23-OH3

There are no ring outliers.

28 monomers are involved in 81 short contacts:

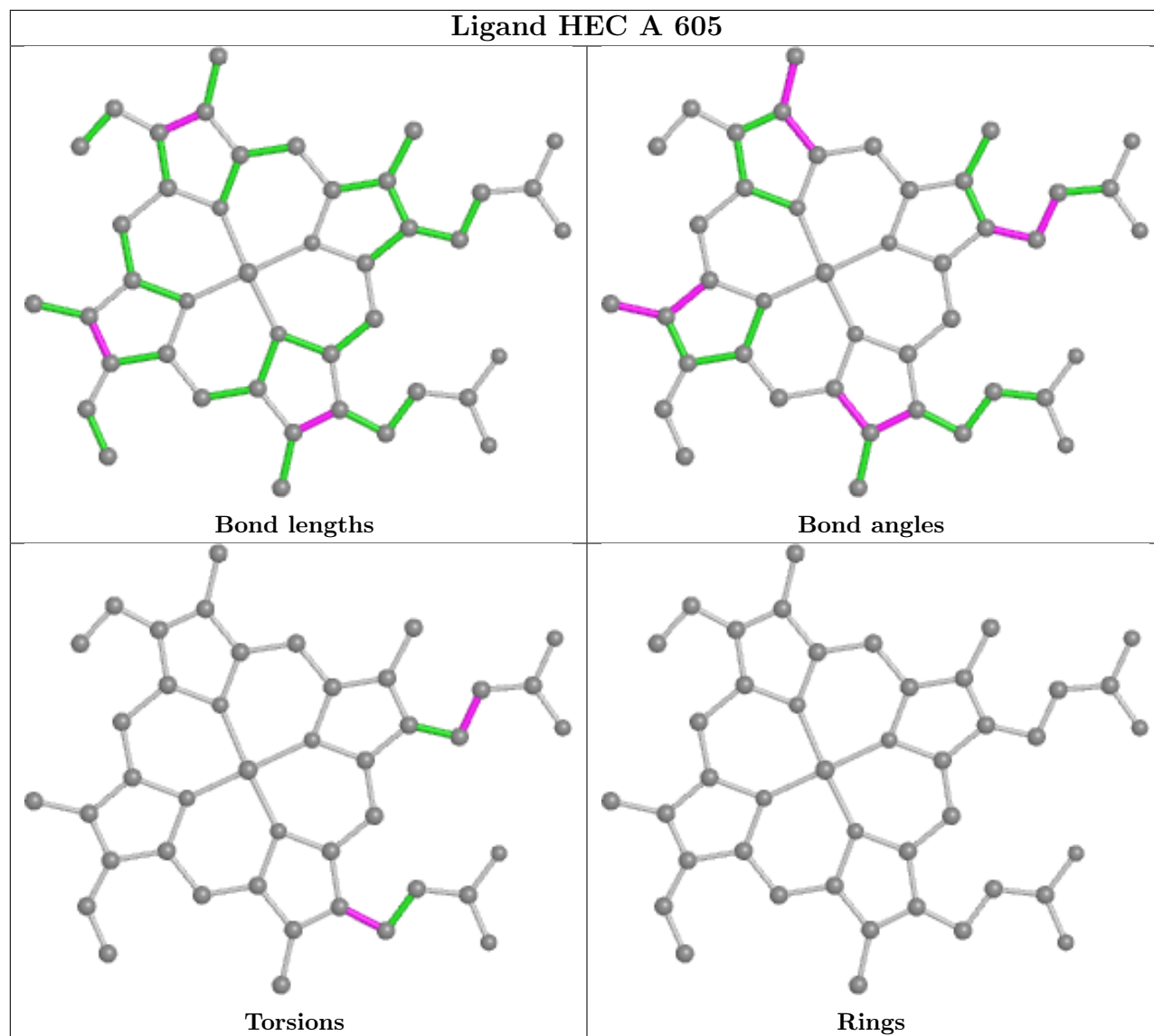
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	605	HEC	6	0
3	E	605	HEC	2	0

*Continued on next page...*

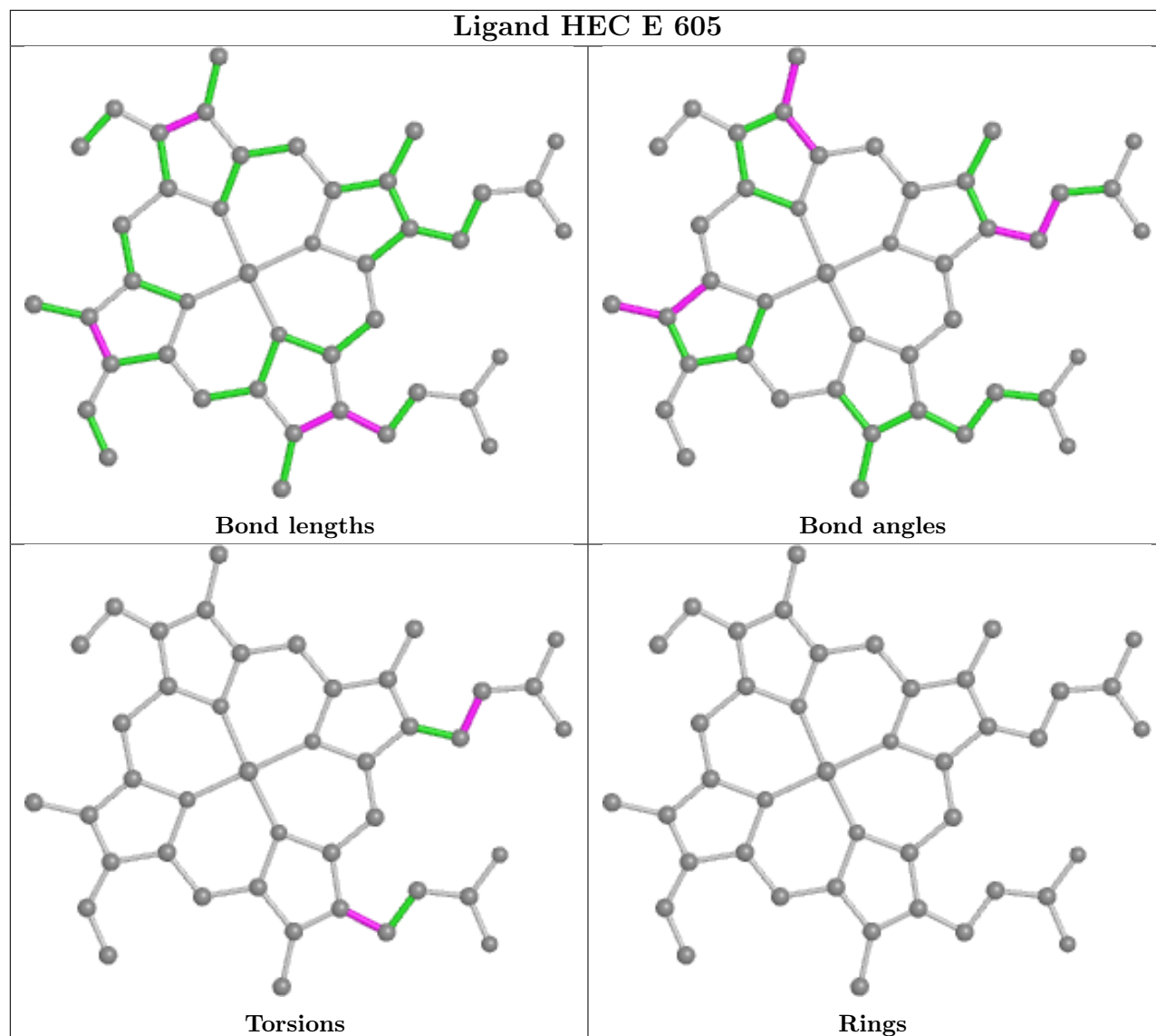
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	611	ISW	8	0
3	C	605	HEC	2	0
3	E	604	HEC	2	0
3	C	604	HEC	5	0
7	C	609	1PE	1	0
3	A	607	HEC	4	0
3	E	607	HEC	2	0
3	A	604	HEC	4	0
3	E	602	HEC	2	0
6	C	608	JUG	1	0
3	C	602	HEC	2	0
5	A	610	PEG	1	0
3	A	603	HEC	1	0
3	E	606	HEC	5	0
3	C	606	HEC	3	0
3	A	601	HEC	1	0
4	C	611	ISW	9	0
3	A	606	HEC	8	0
3	A	602	HEC	3	0
3	C	607	HEC	2	0
3	E	603	HEC	2	0
3	C	603	HEC	1	0
3	C	601	HEC	2	0
3	E	601	HEC	2	0
4	A	608	ISW	6	0
6	E	608	JUG	2	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.

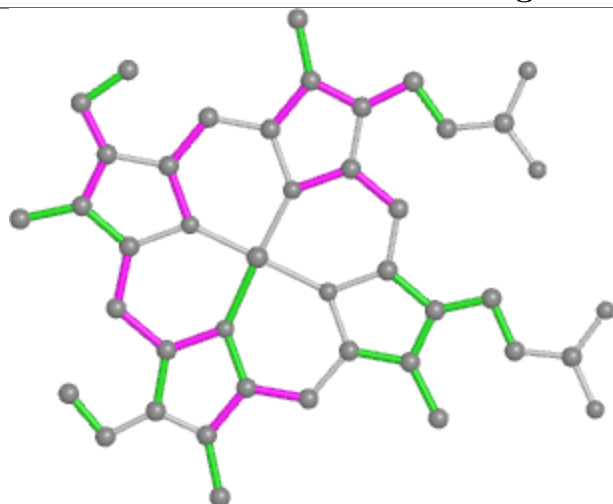


## Ligand HEC E 605

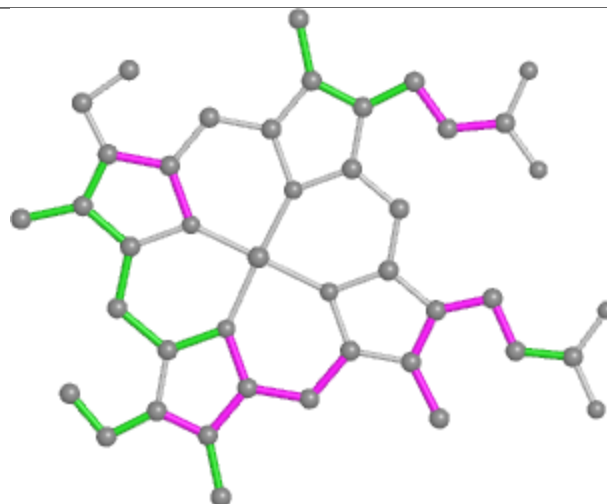




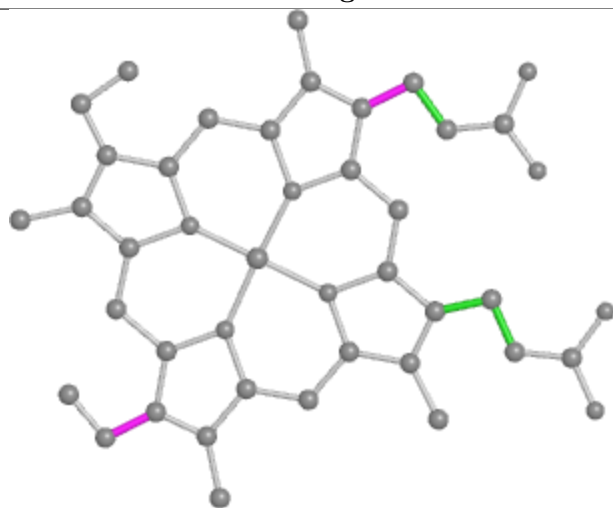
## Ligand ISW A 611



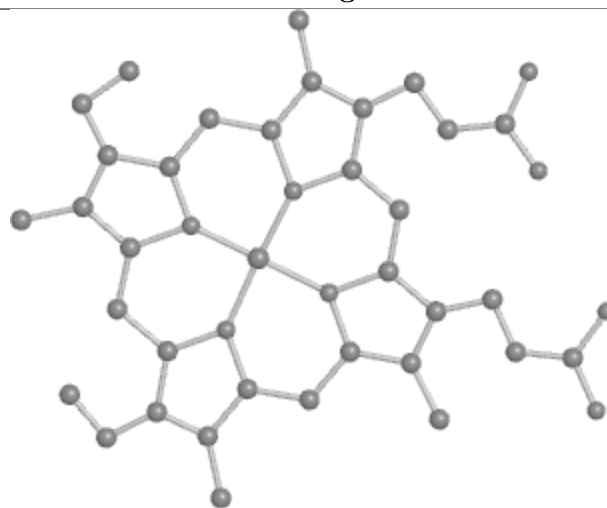
Bond lengths



Bond angles

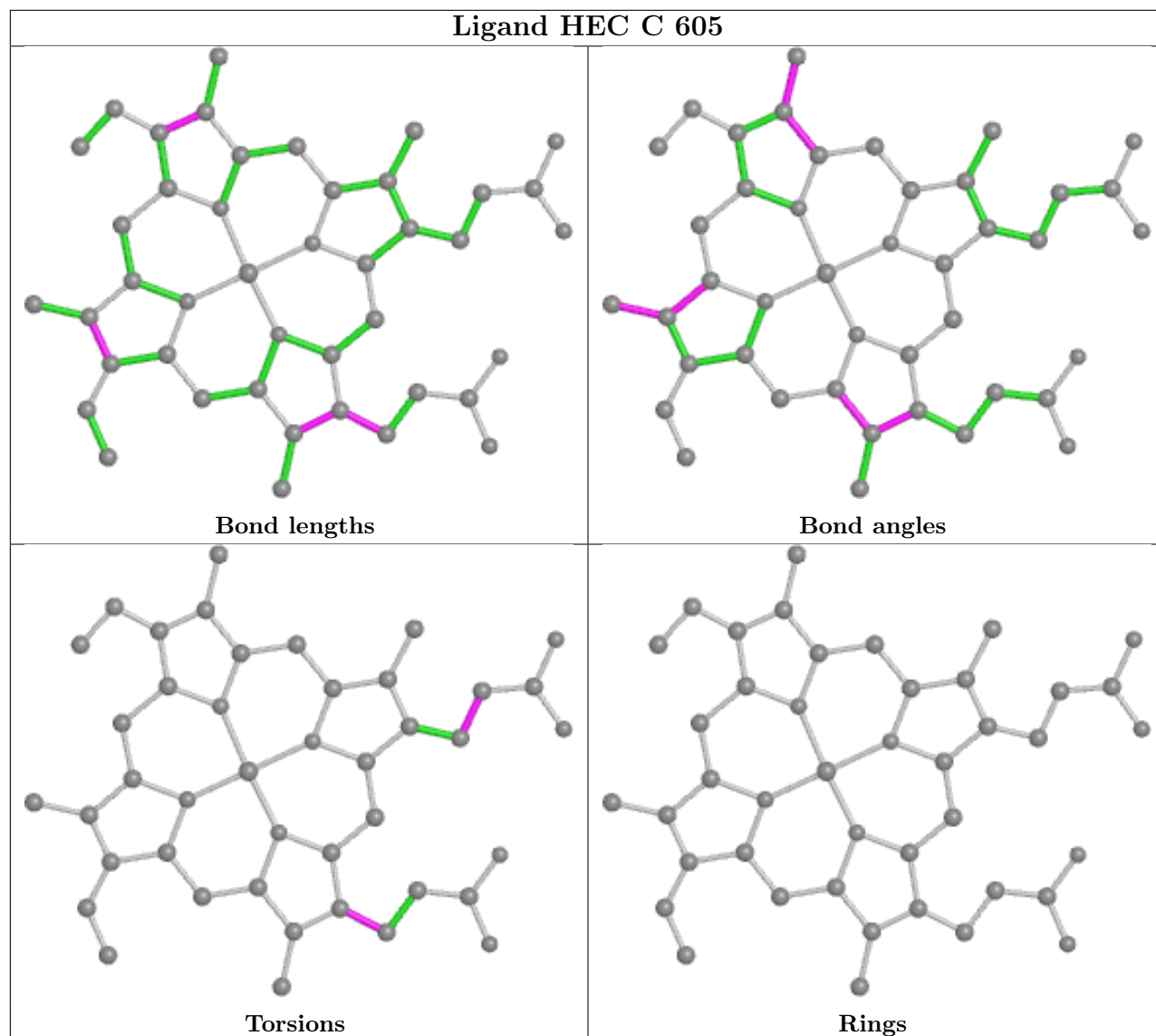


Torsions

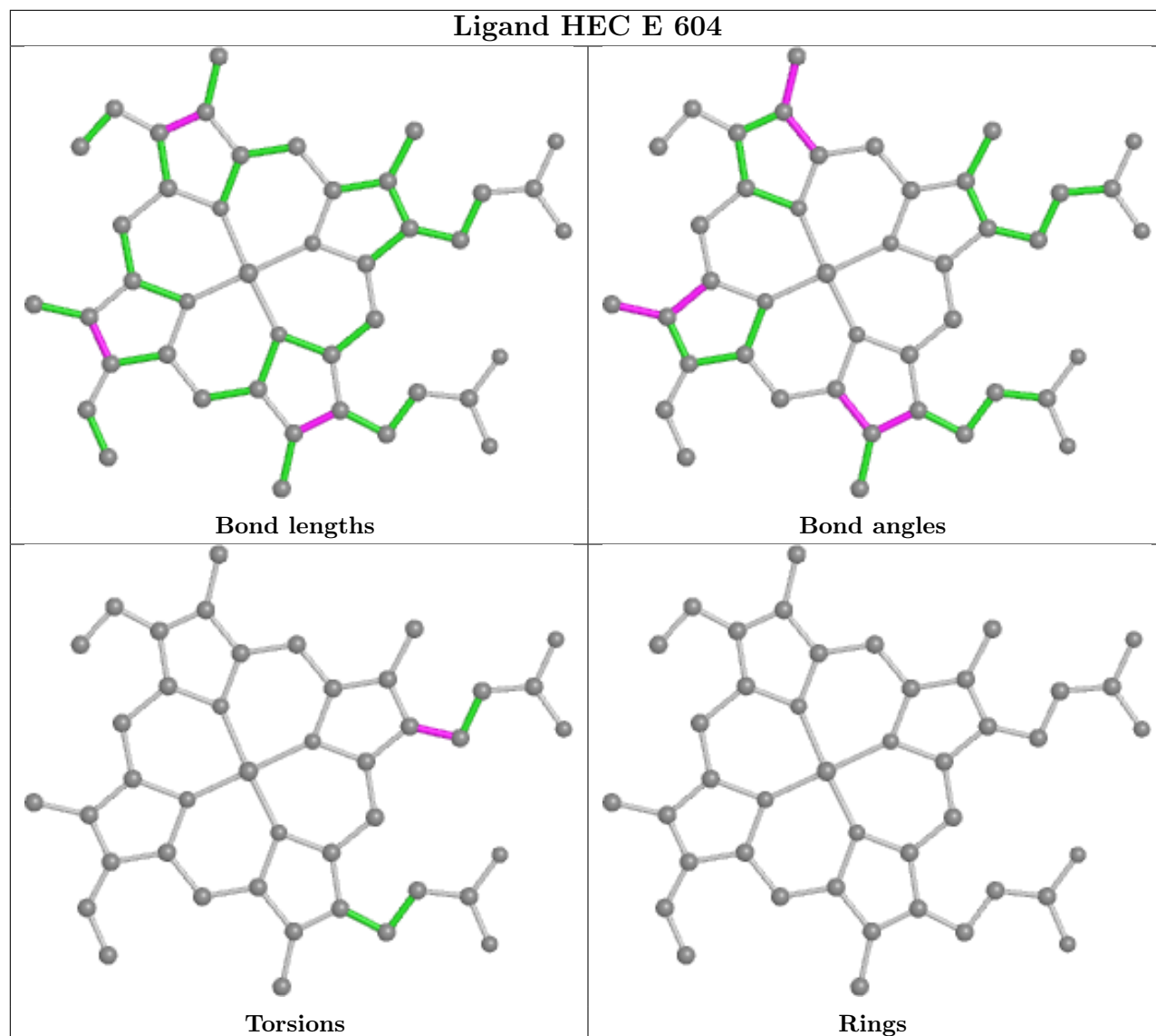


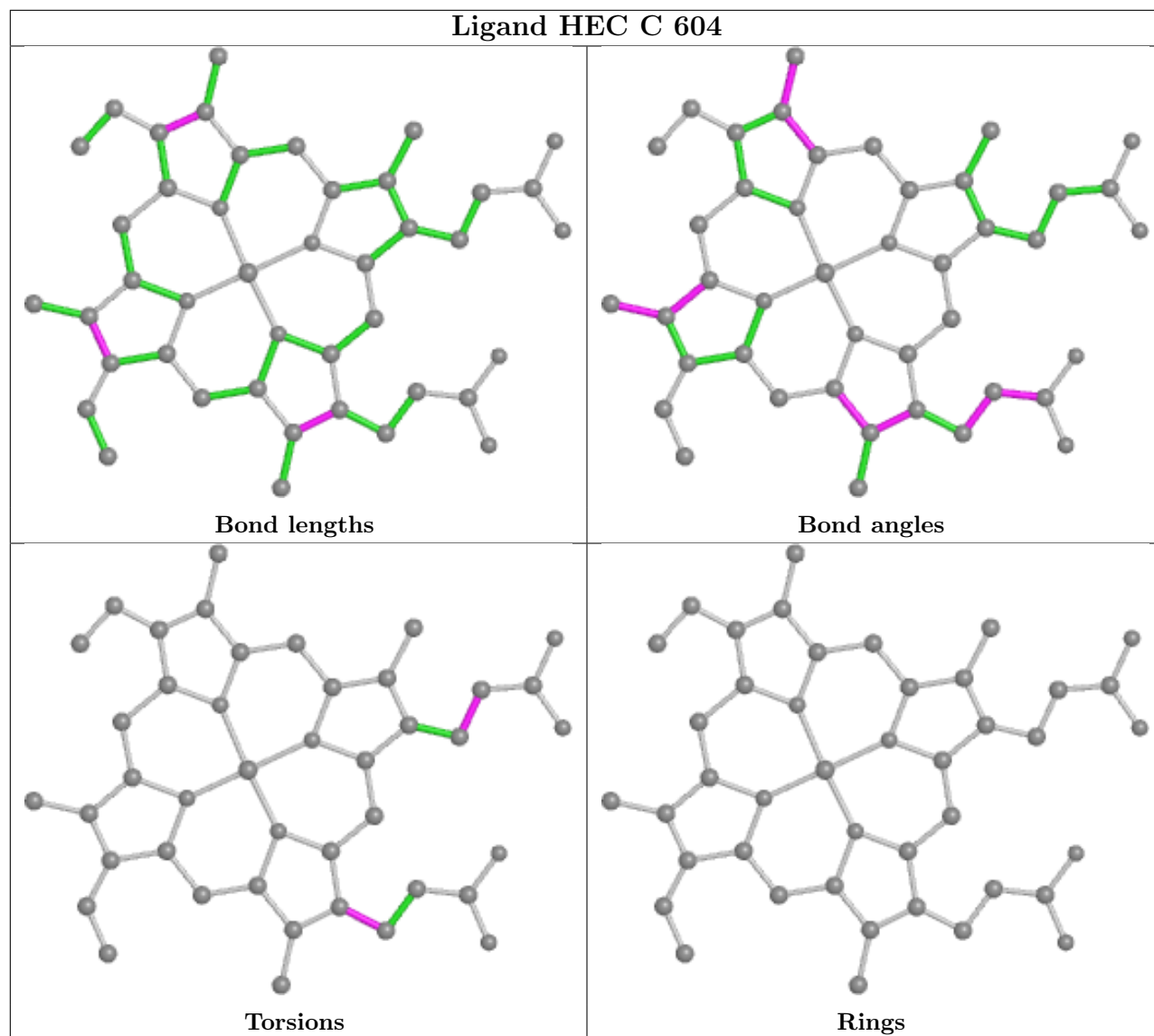
Rings

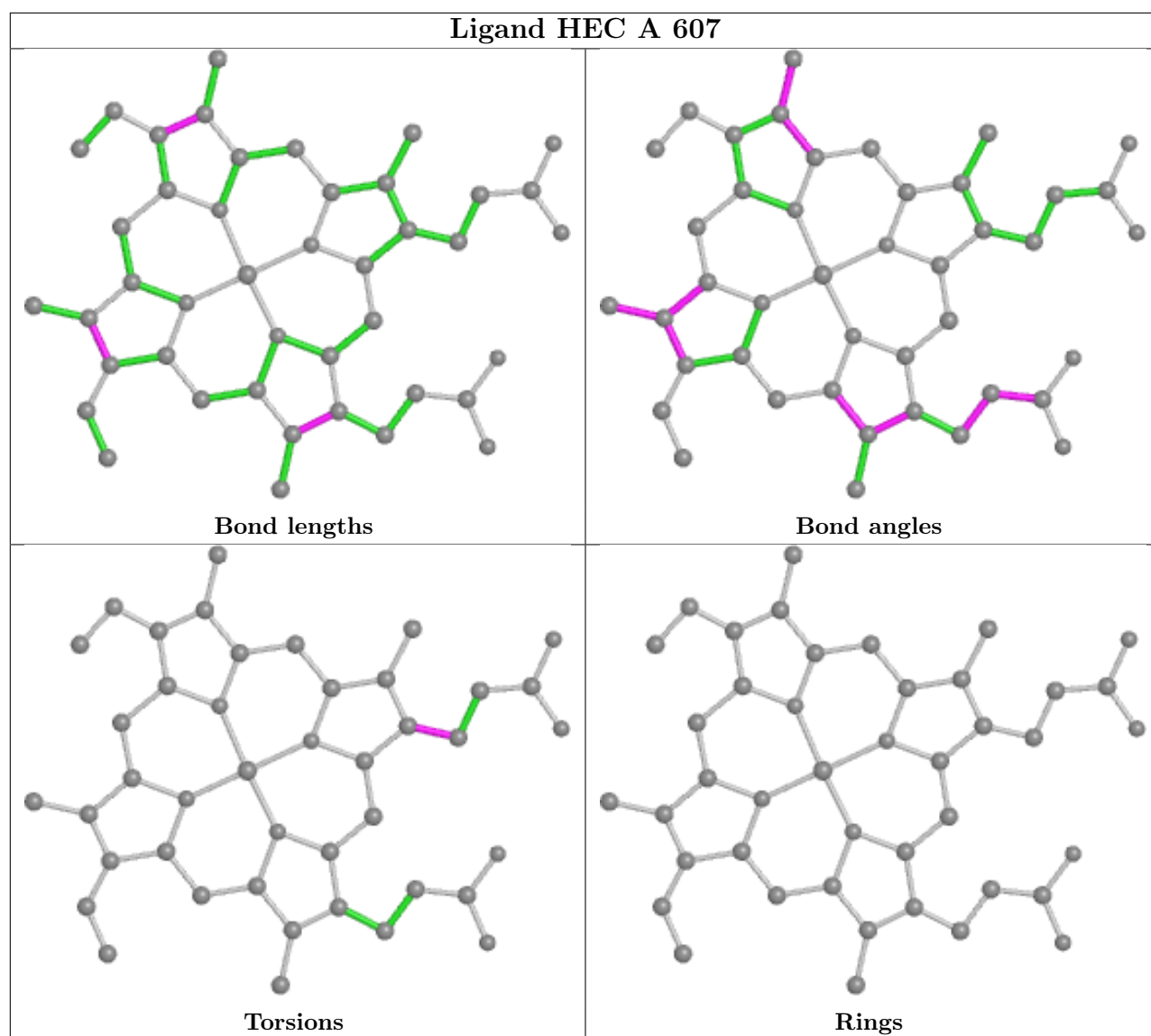
## Ligand HEC C 605



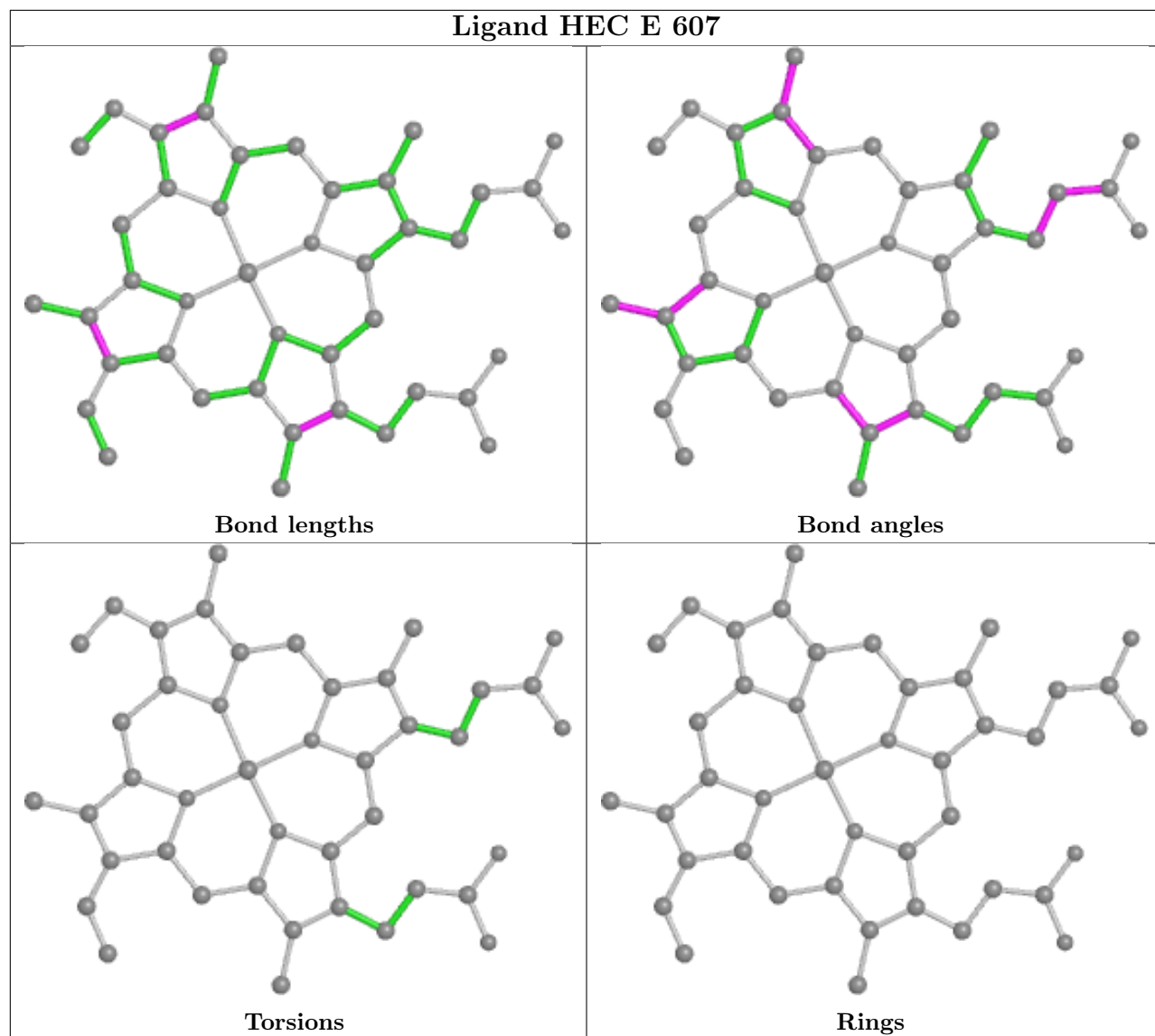
## Ligand HEC E 604

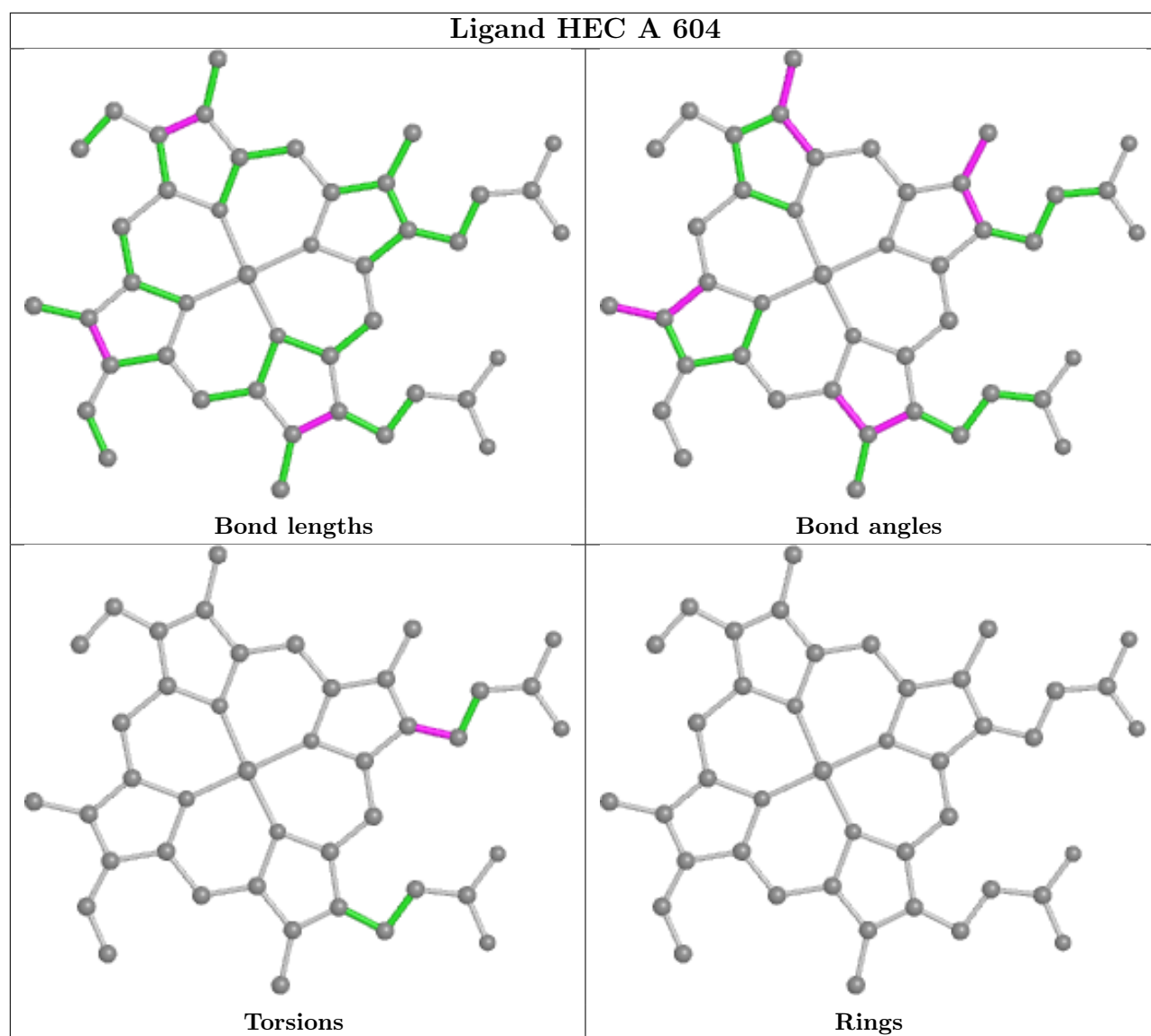




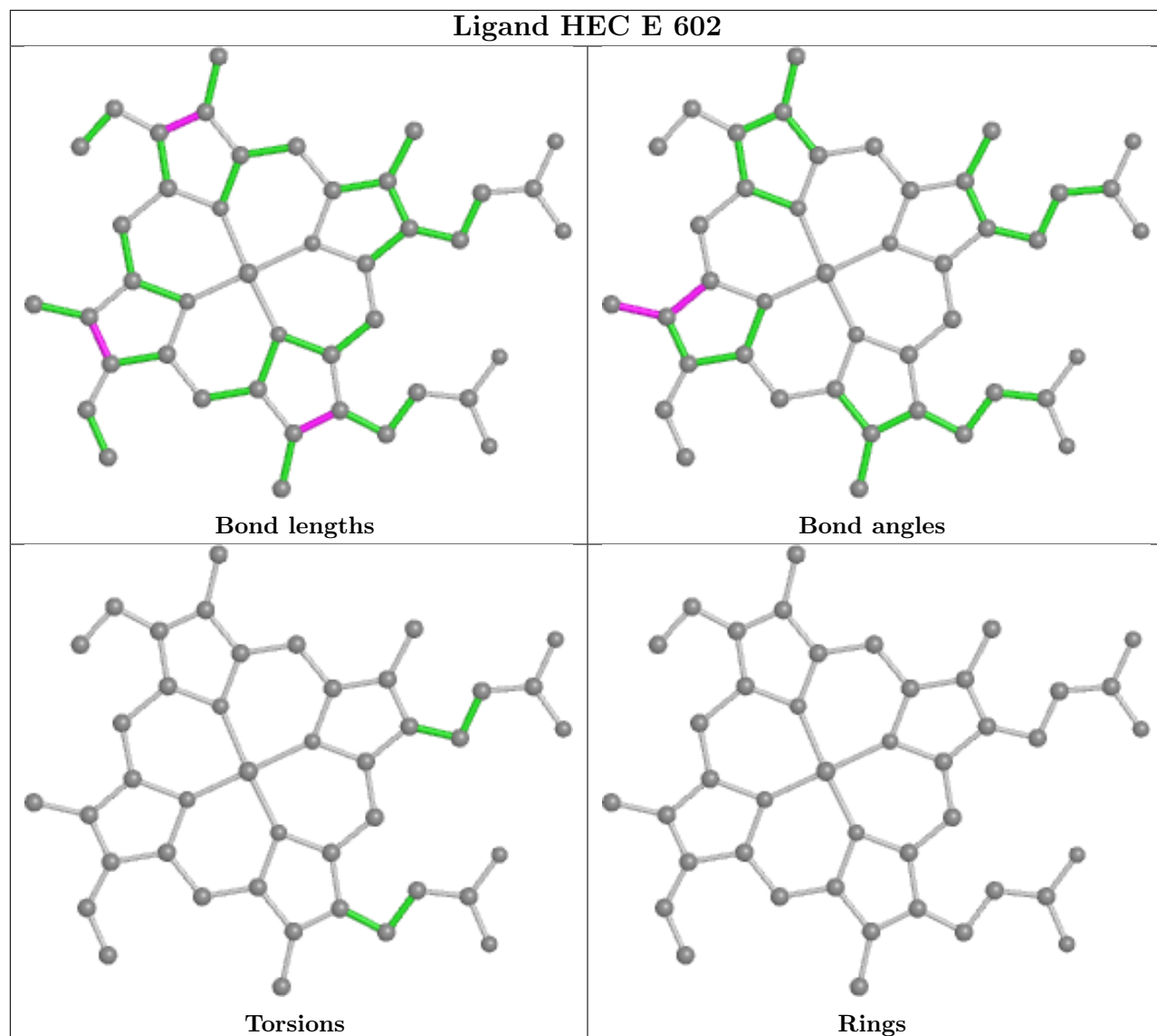


## Ligand HEC E 607



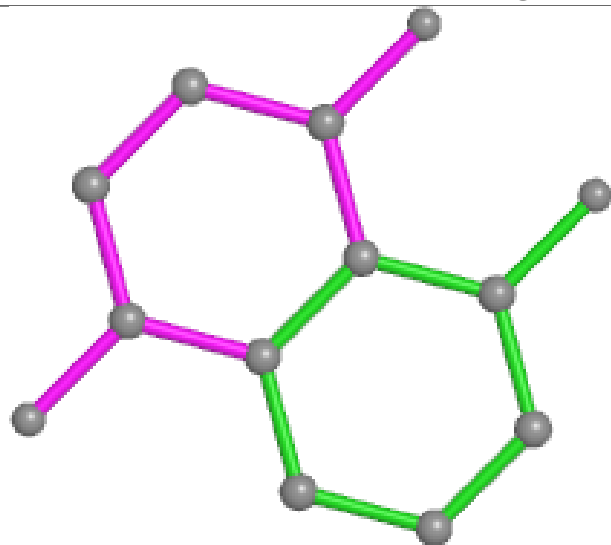


## Ligand HEC E 602

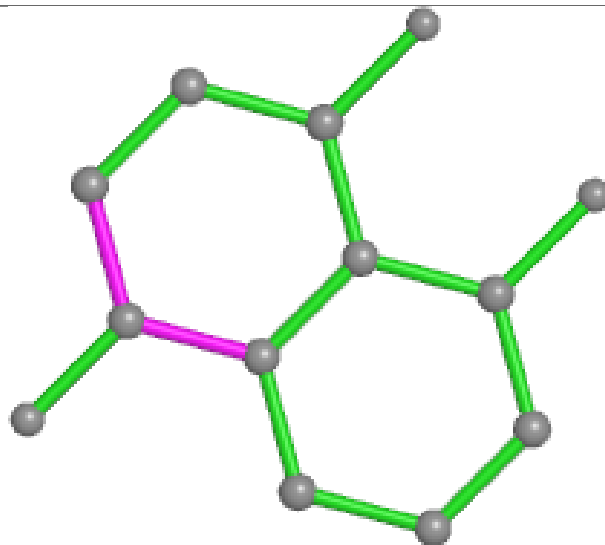




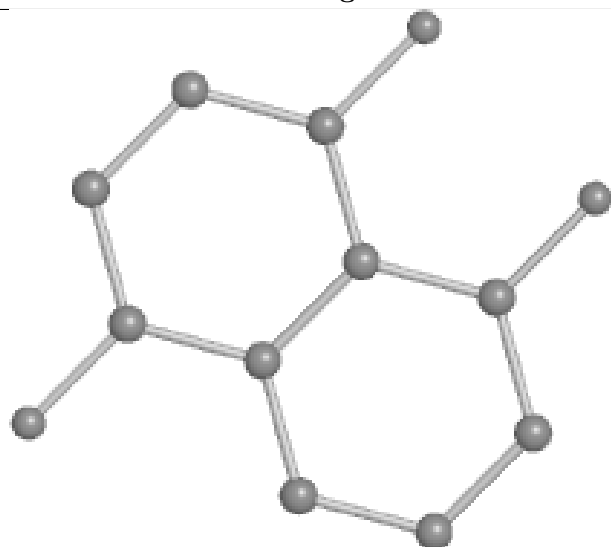
## Ligand JUG C 608



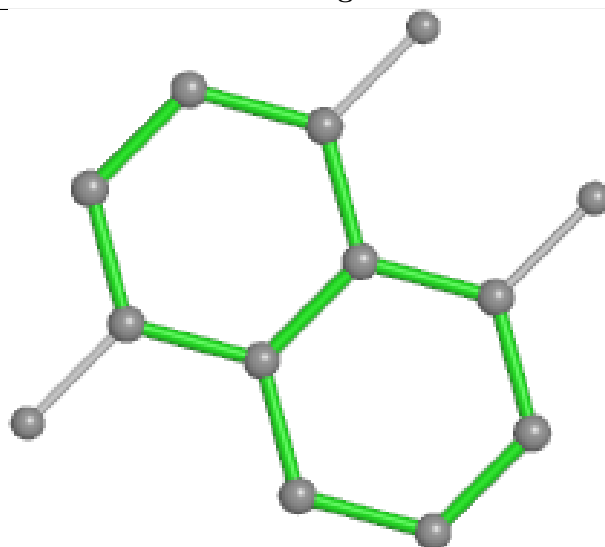
Bond lengths



Bond angles

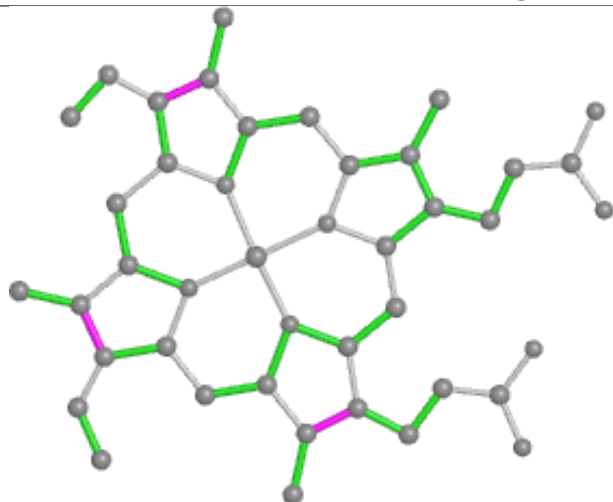


Torsions

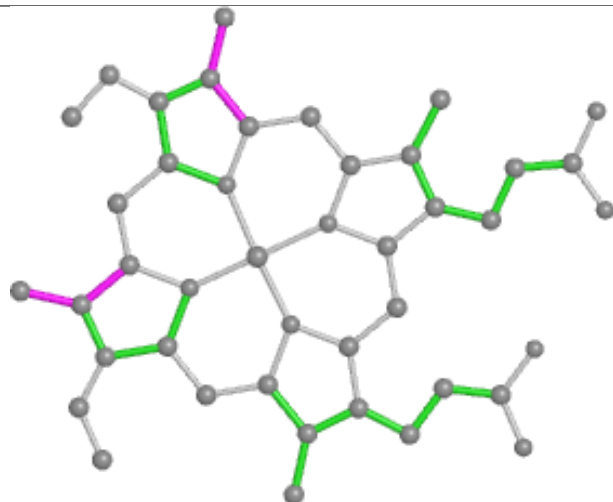


Rings

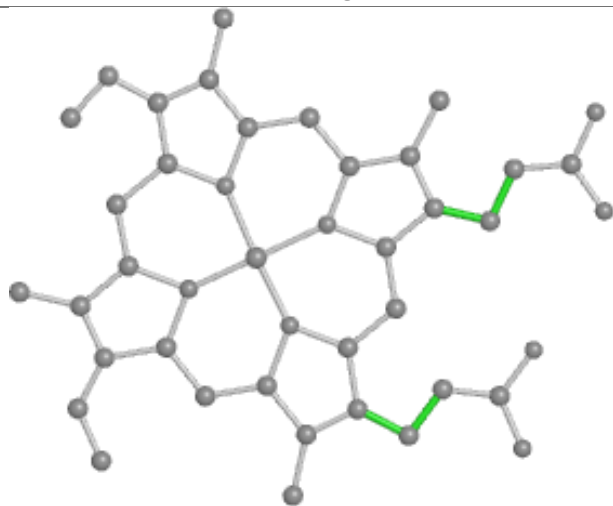
## Ligand HEC C 602



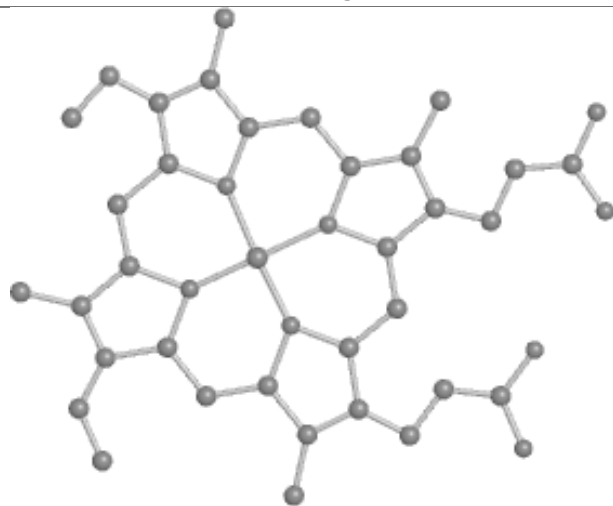
Bond lengths



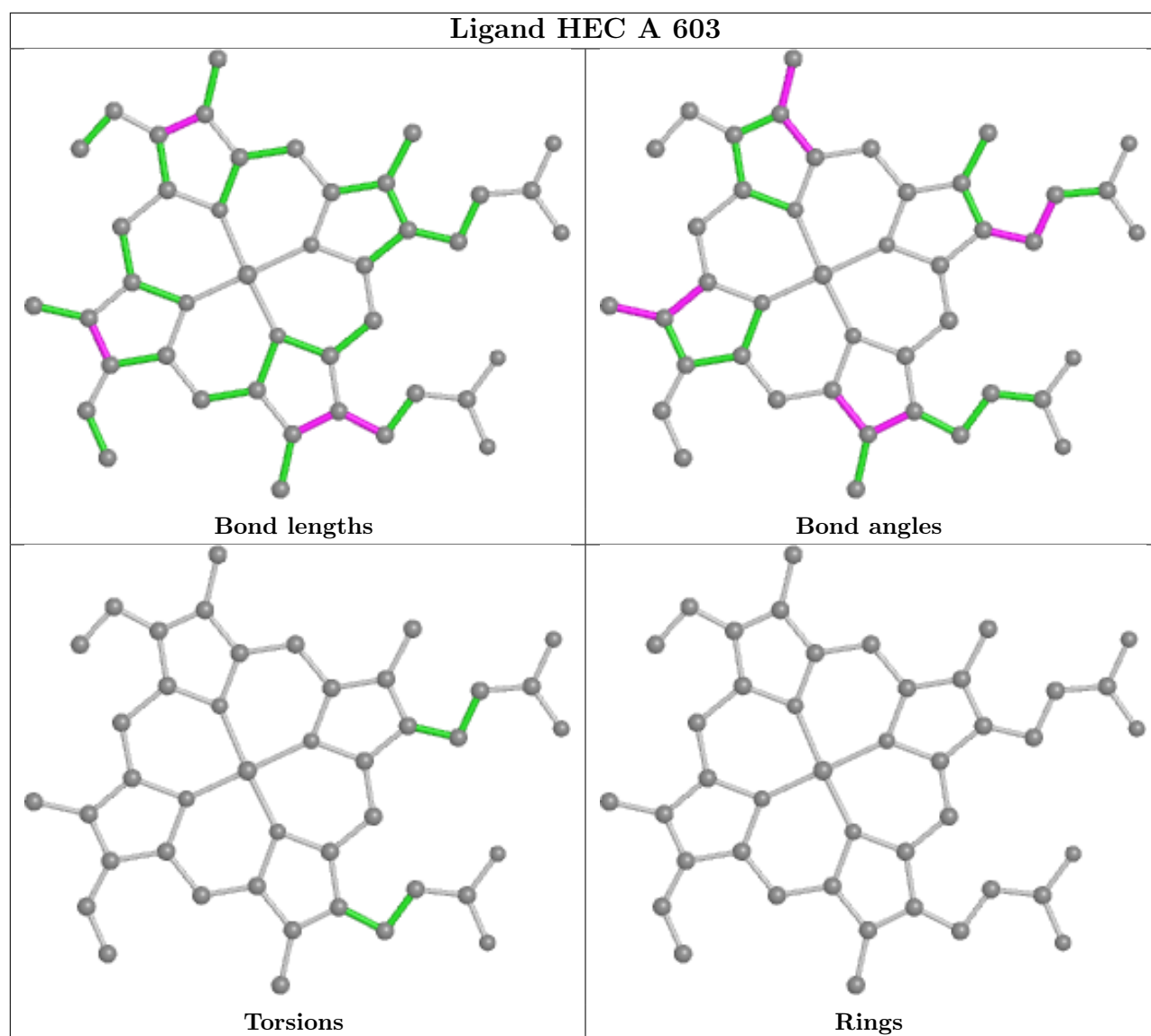
Bond angles



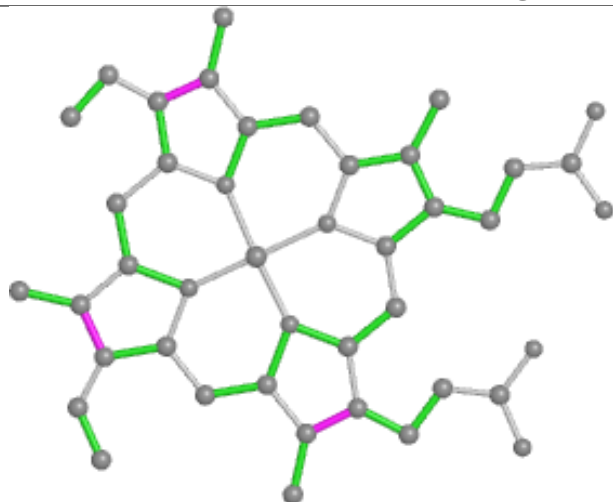
Torsions



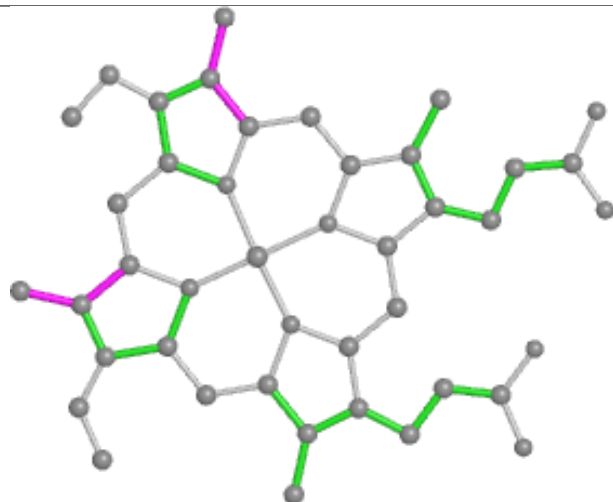
Rings



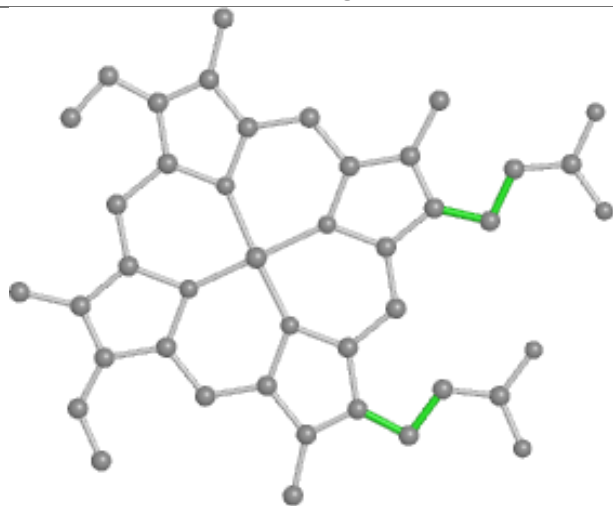
## Ligand HEC E 606



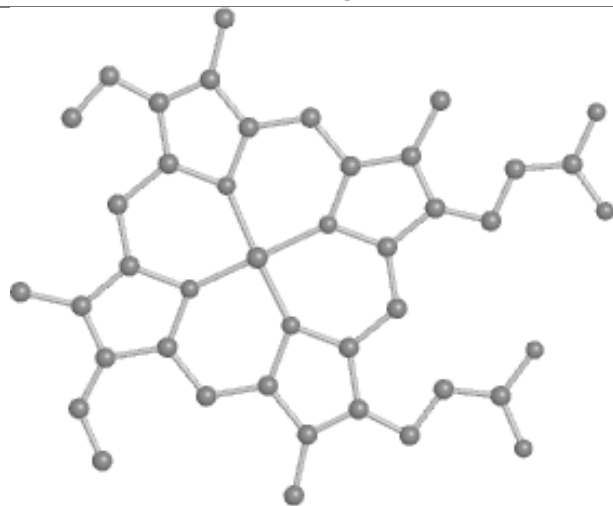
Bond lengths



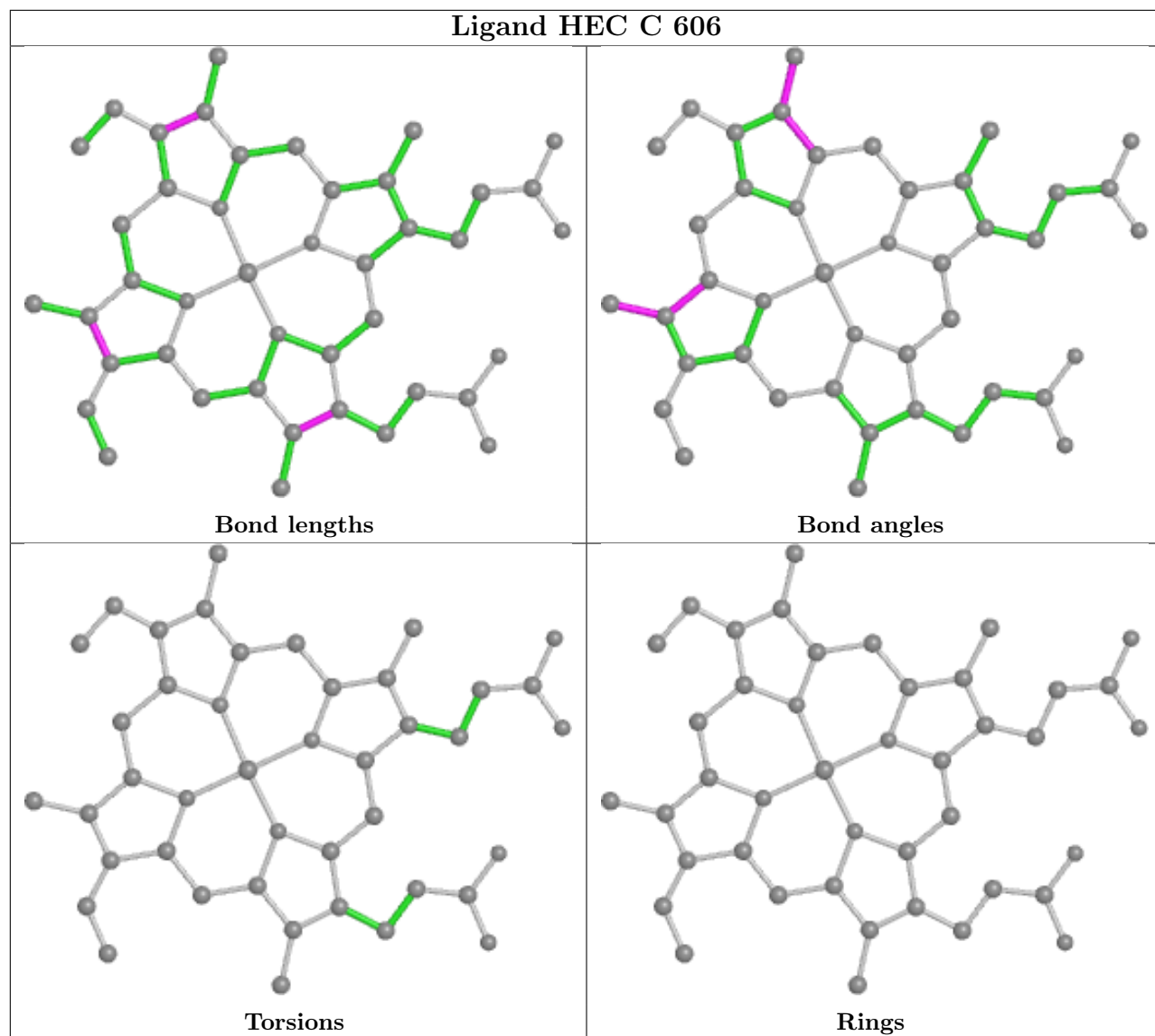
Bond angles

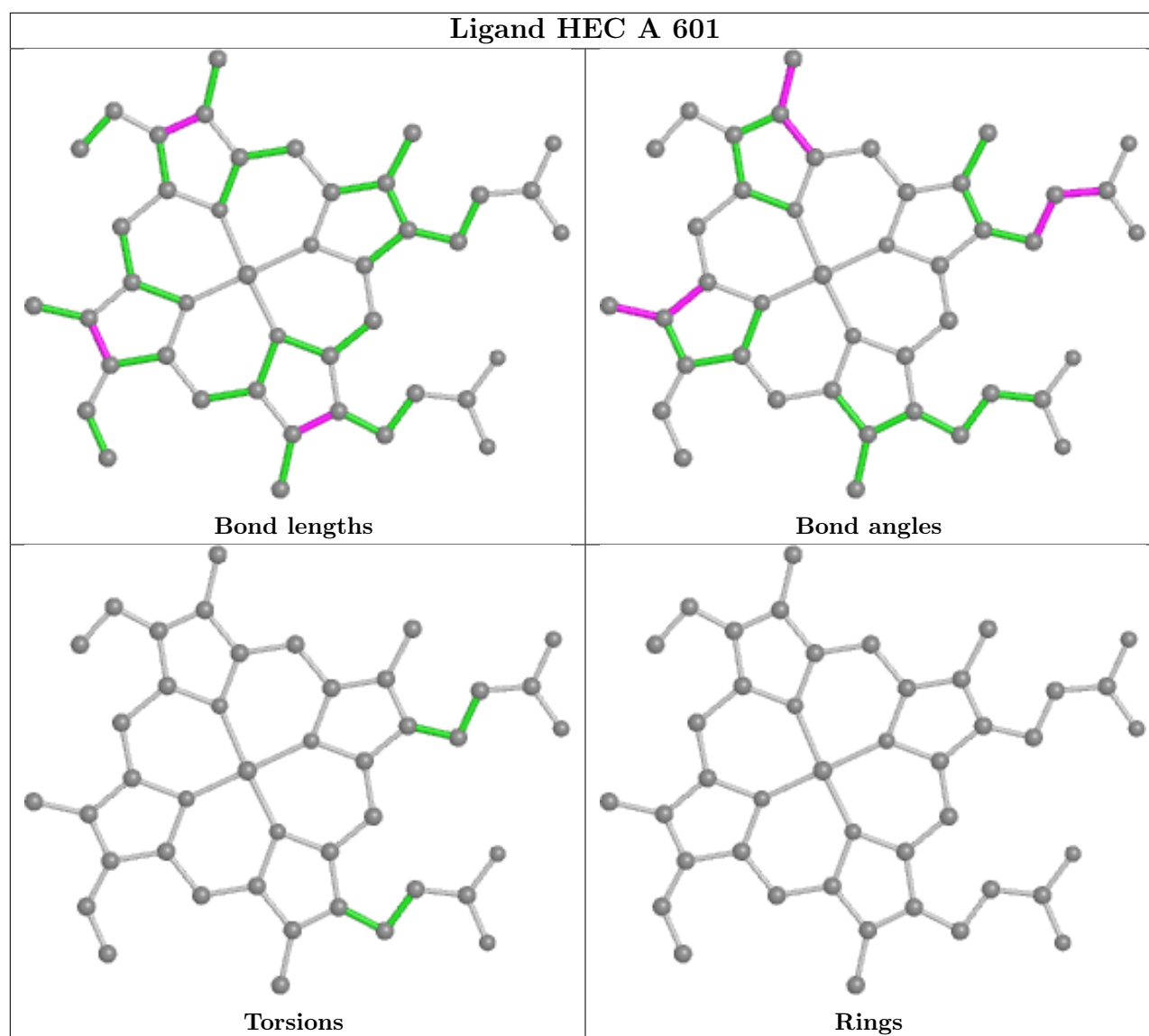


Torsions

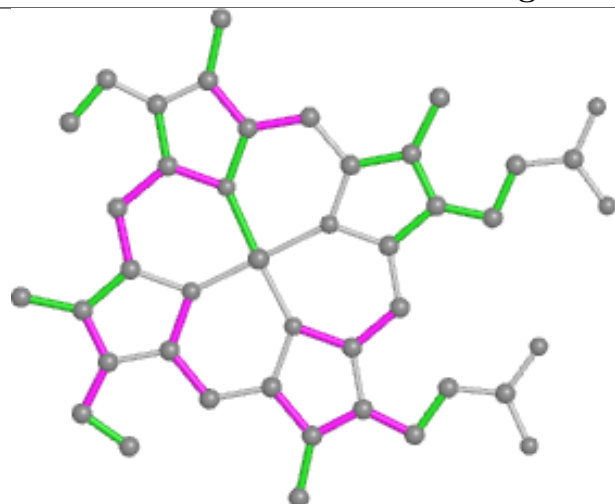


Rings

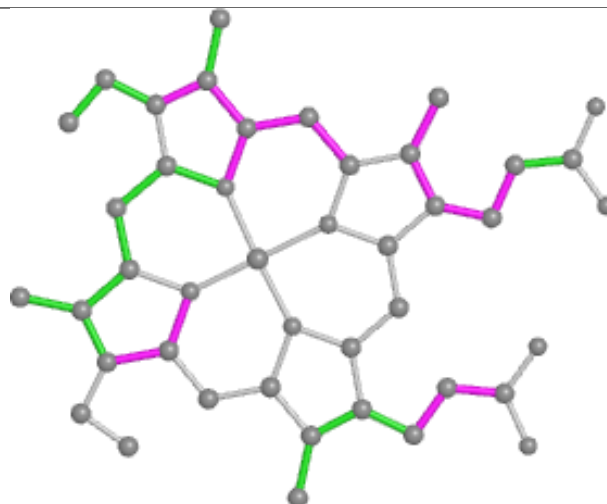




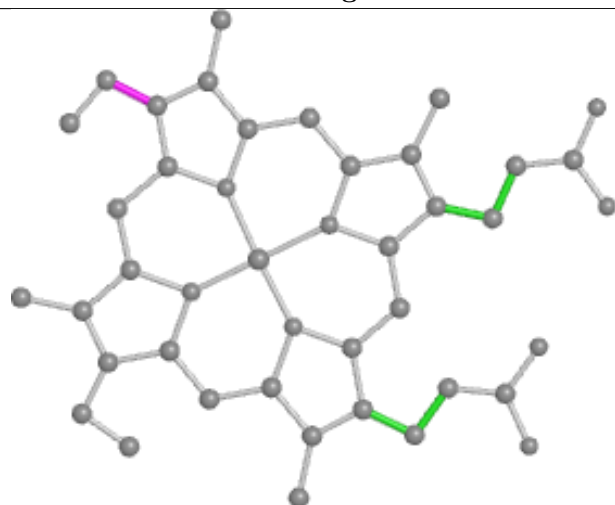
## Ligand ISW C 611



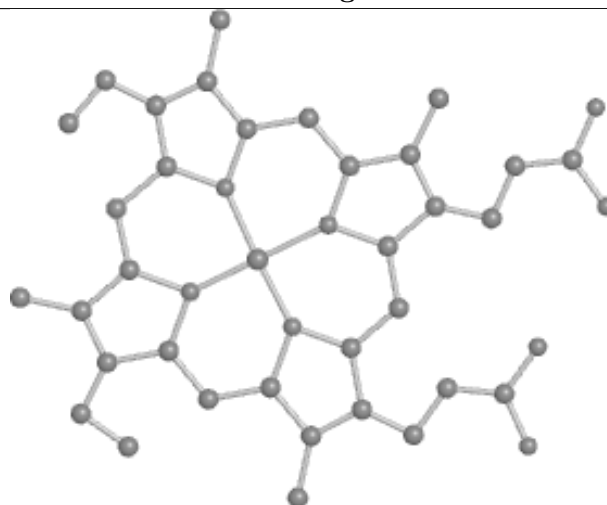
Bond lengths



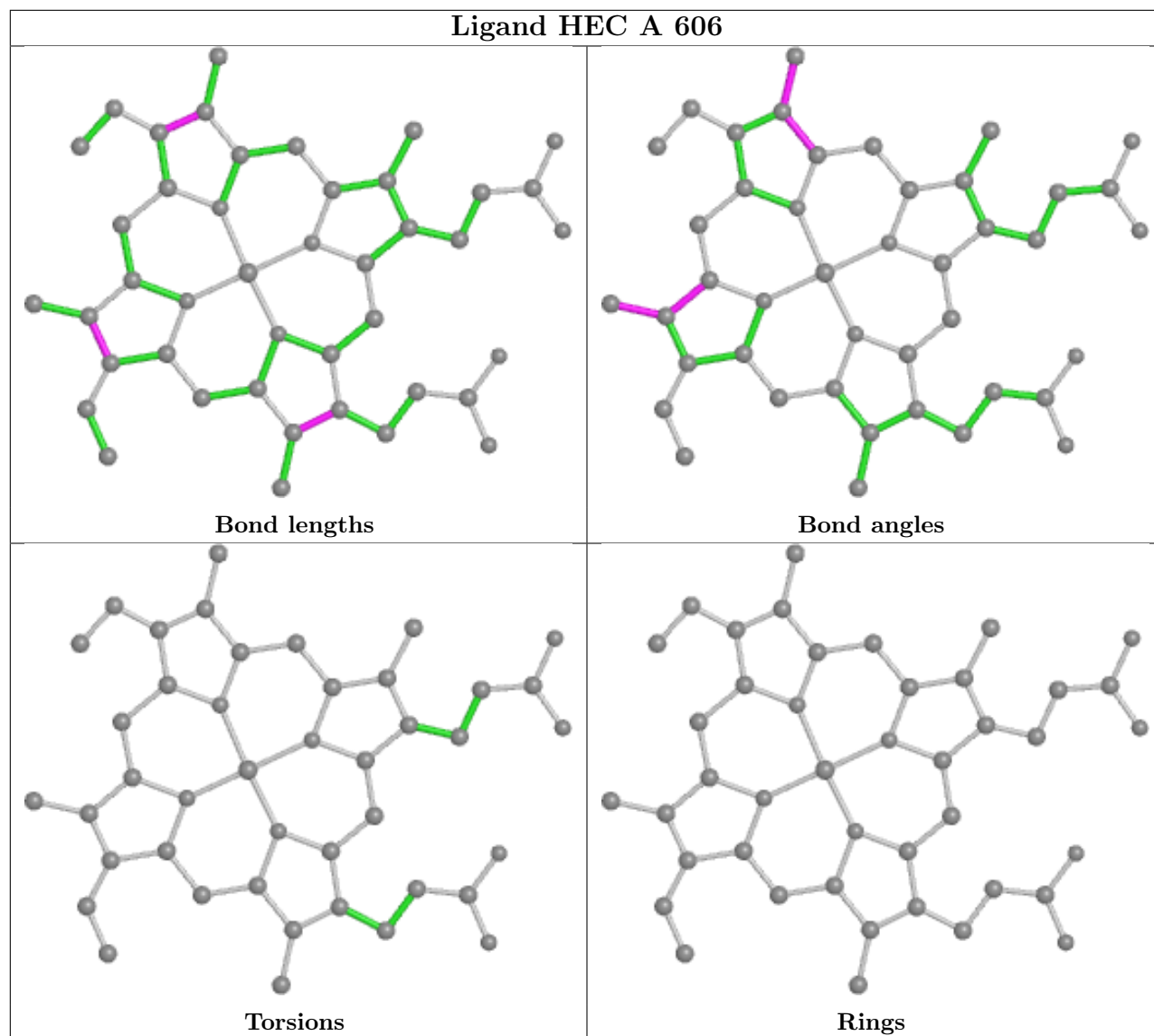
Bond angles



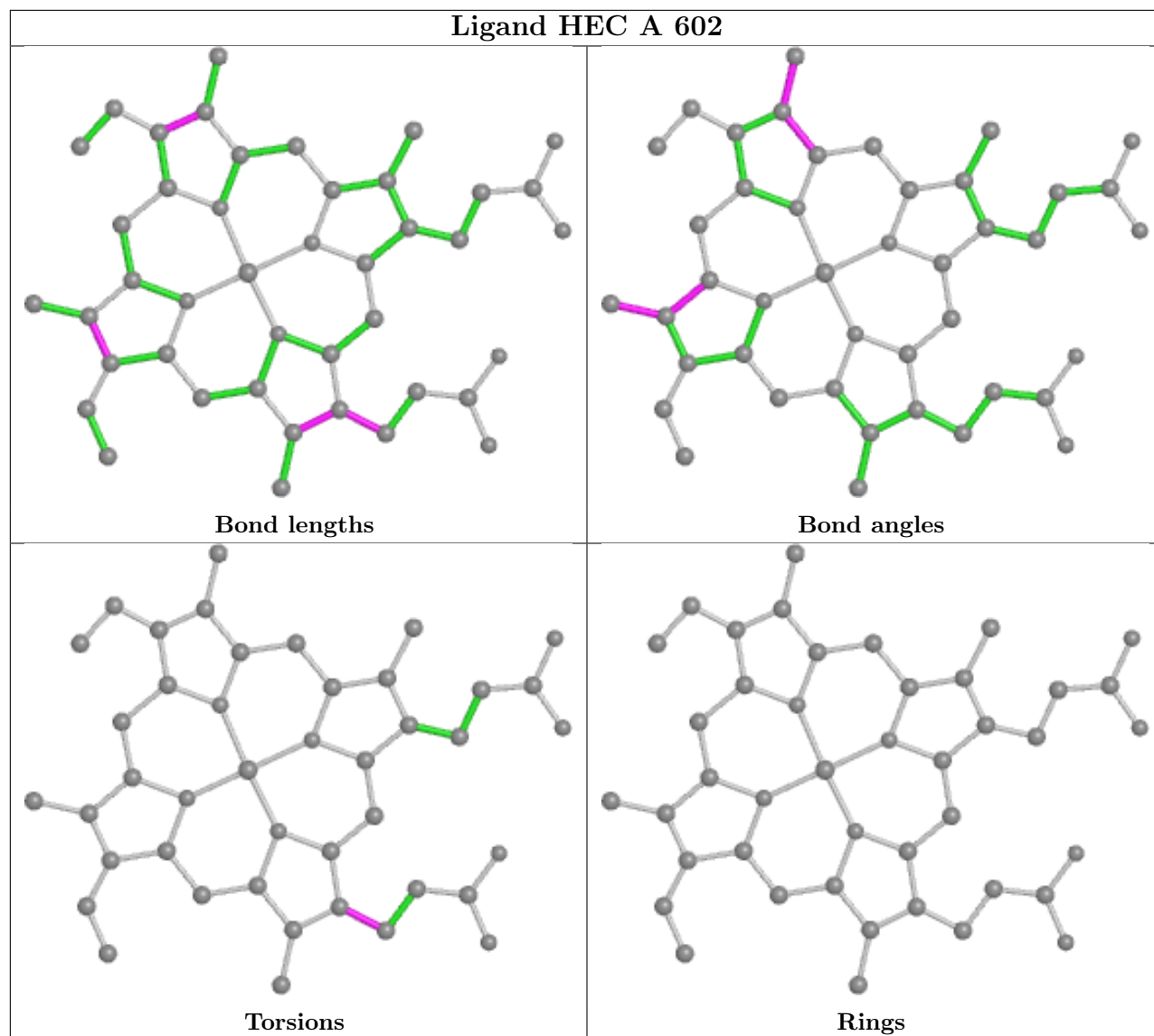
Torsions



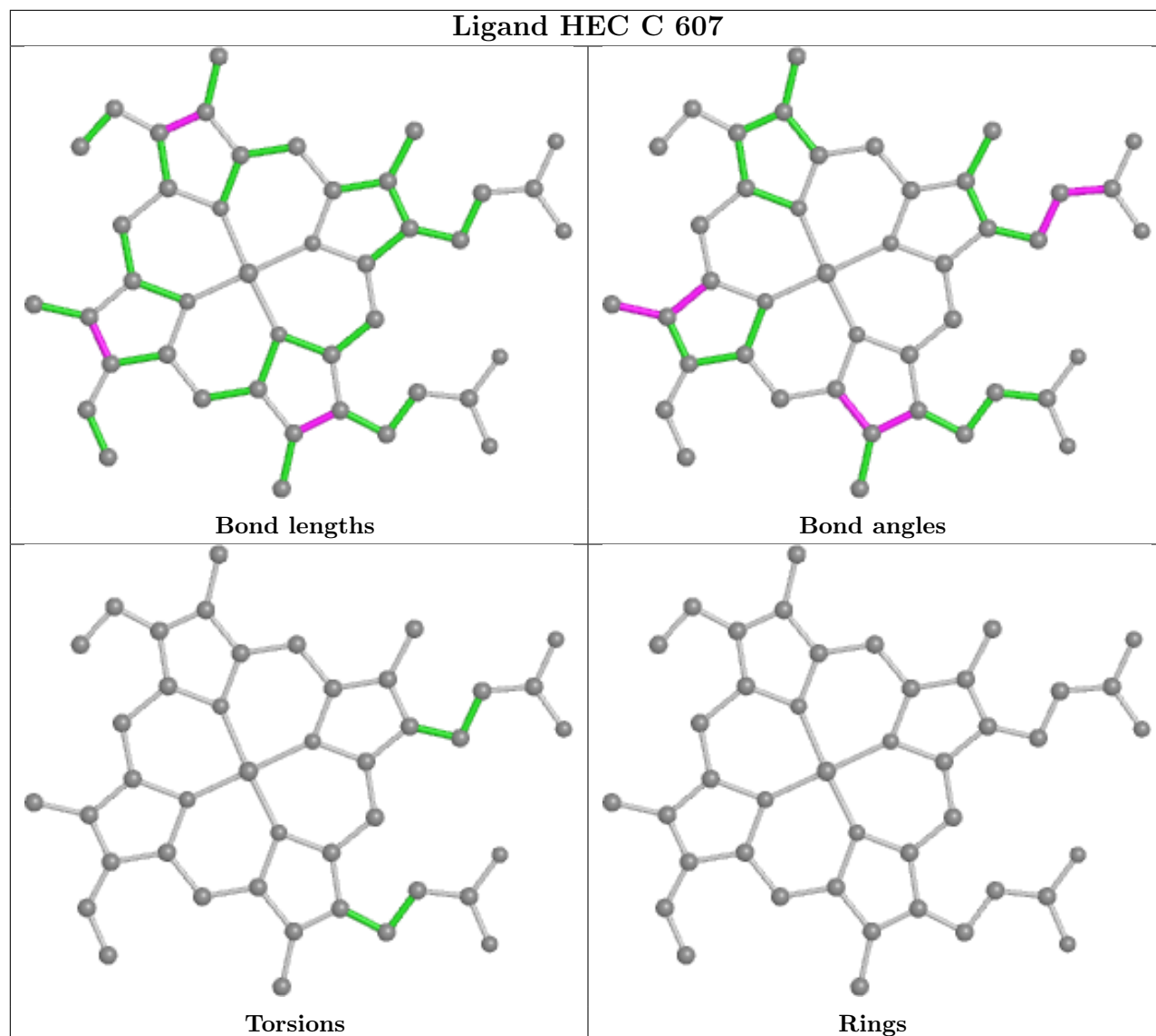
Rings



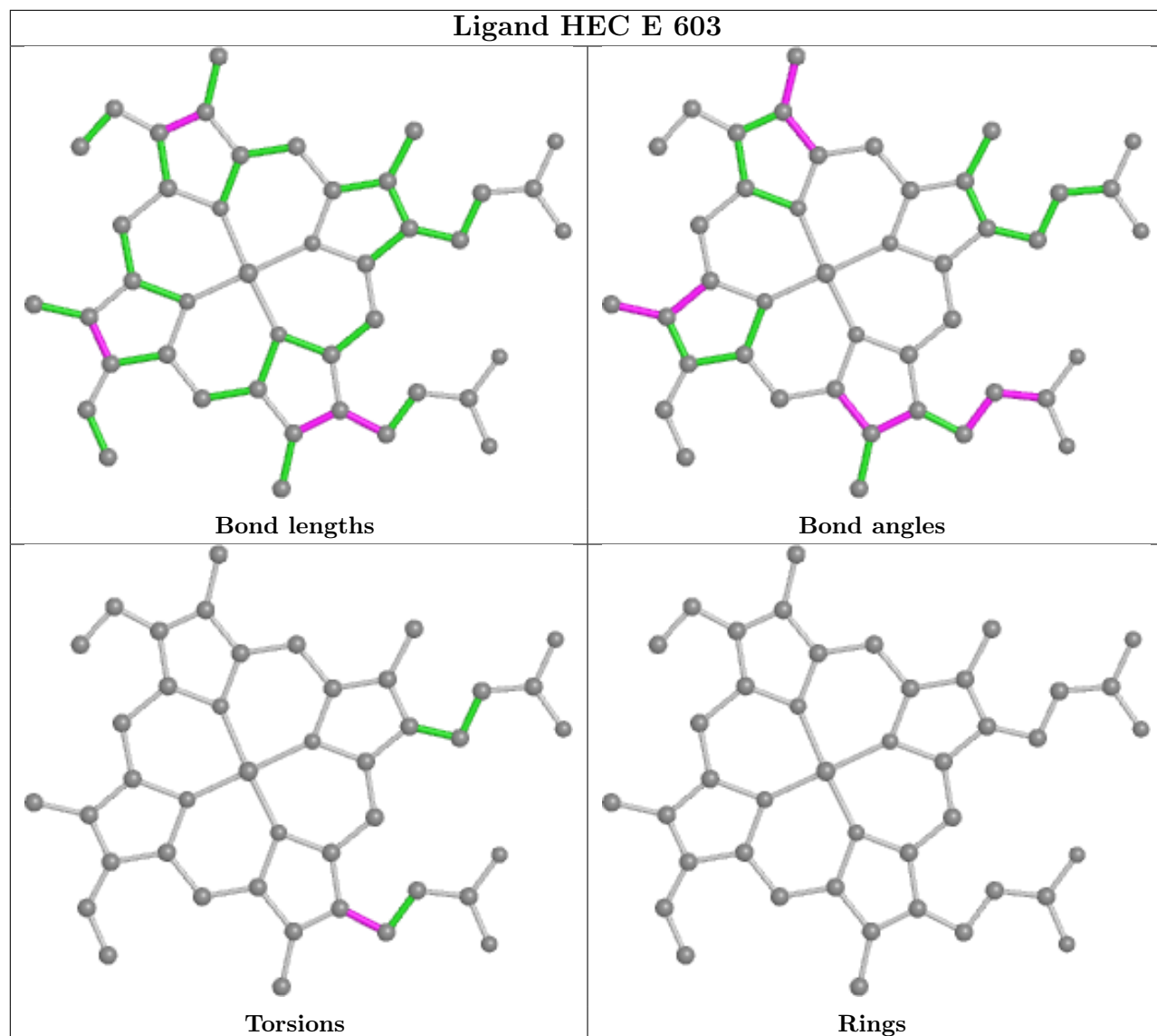




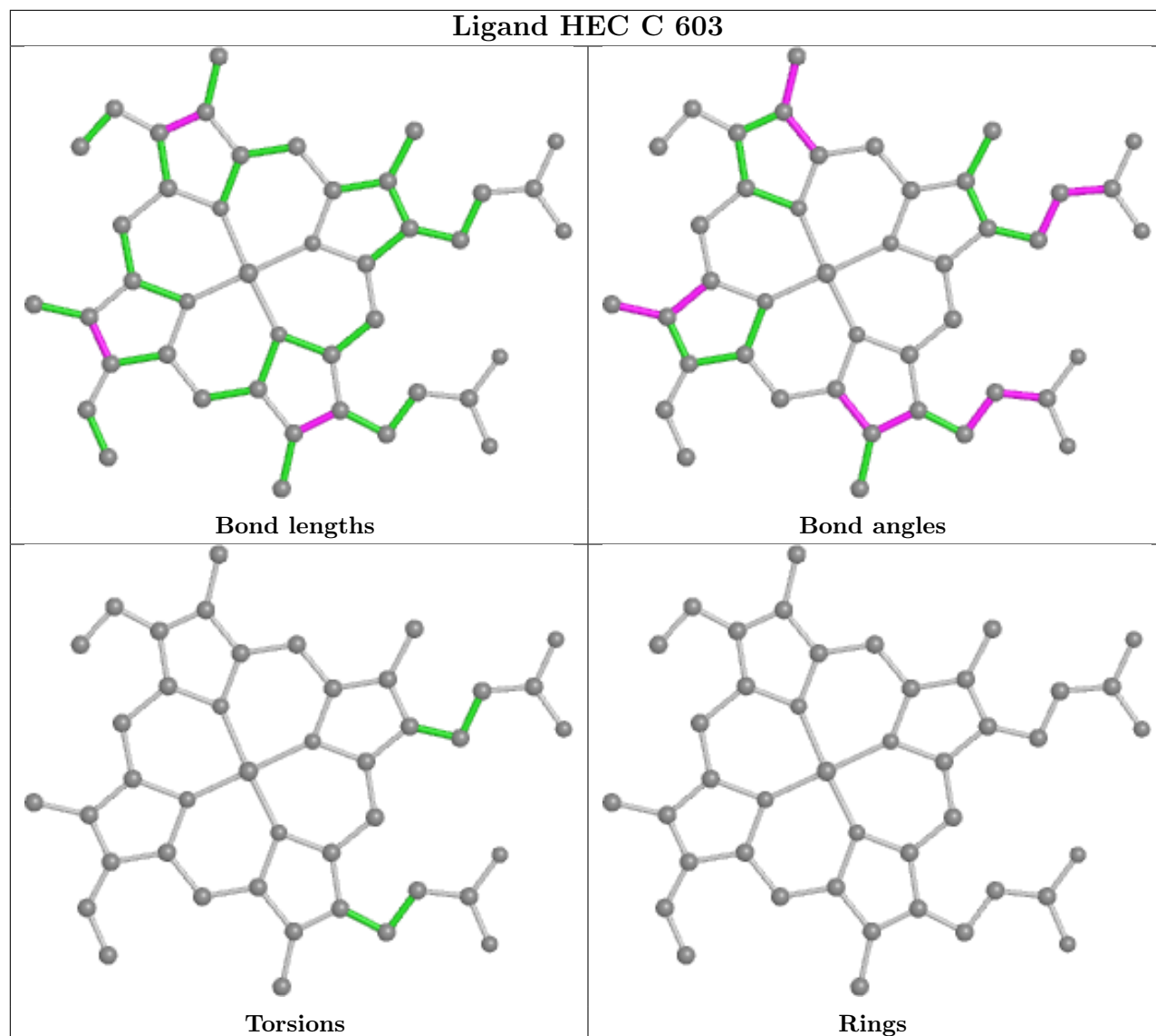
## Ligand HEC C 607



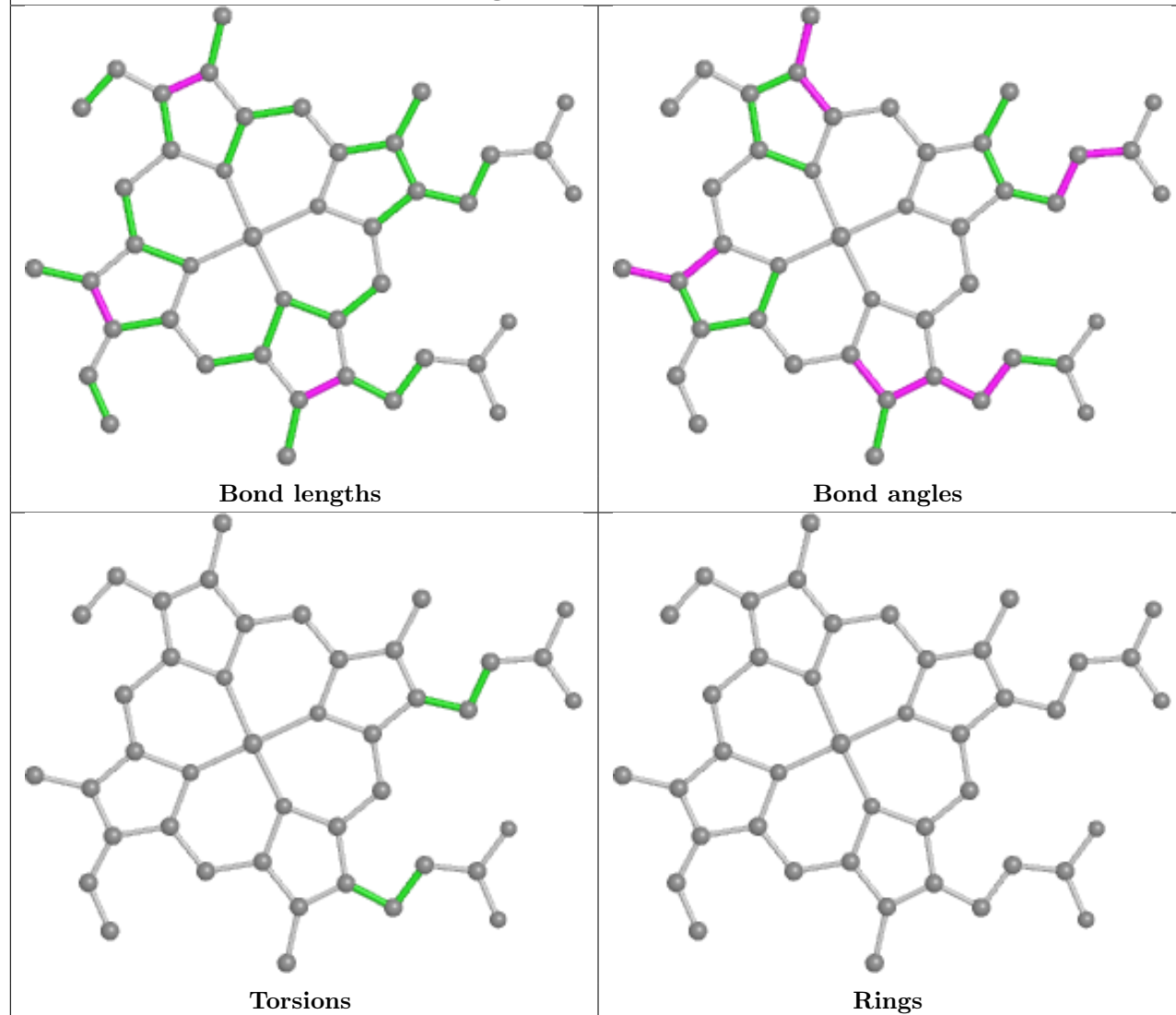
## Ligand HEC E 603



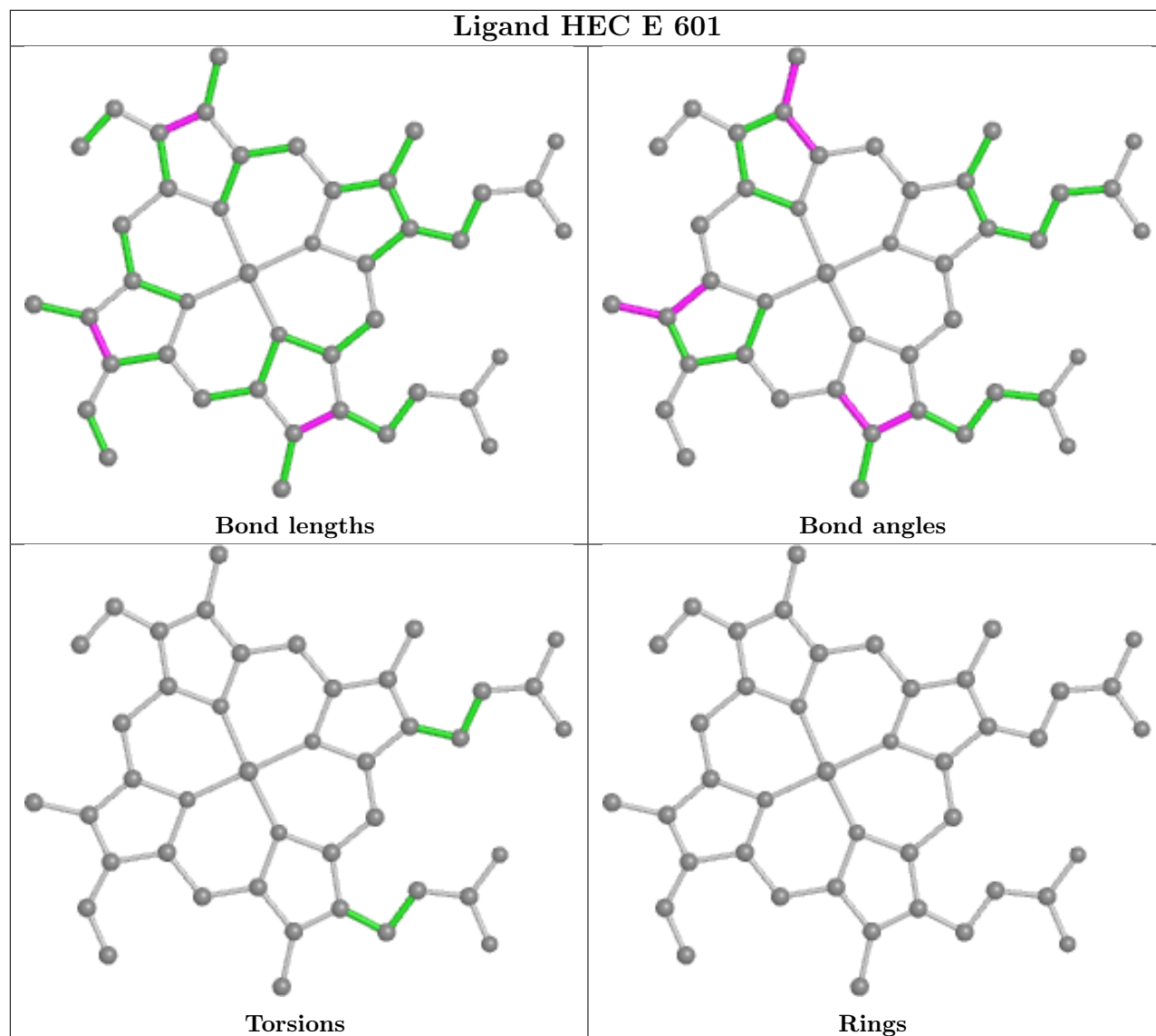
## Ligand HEC C 603



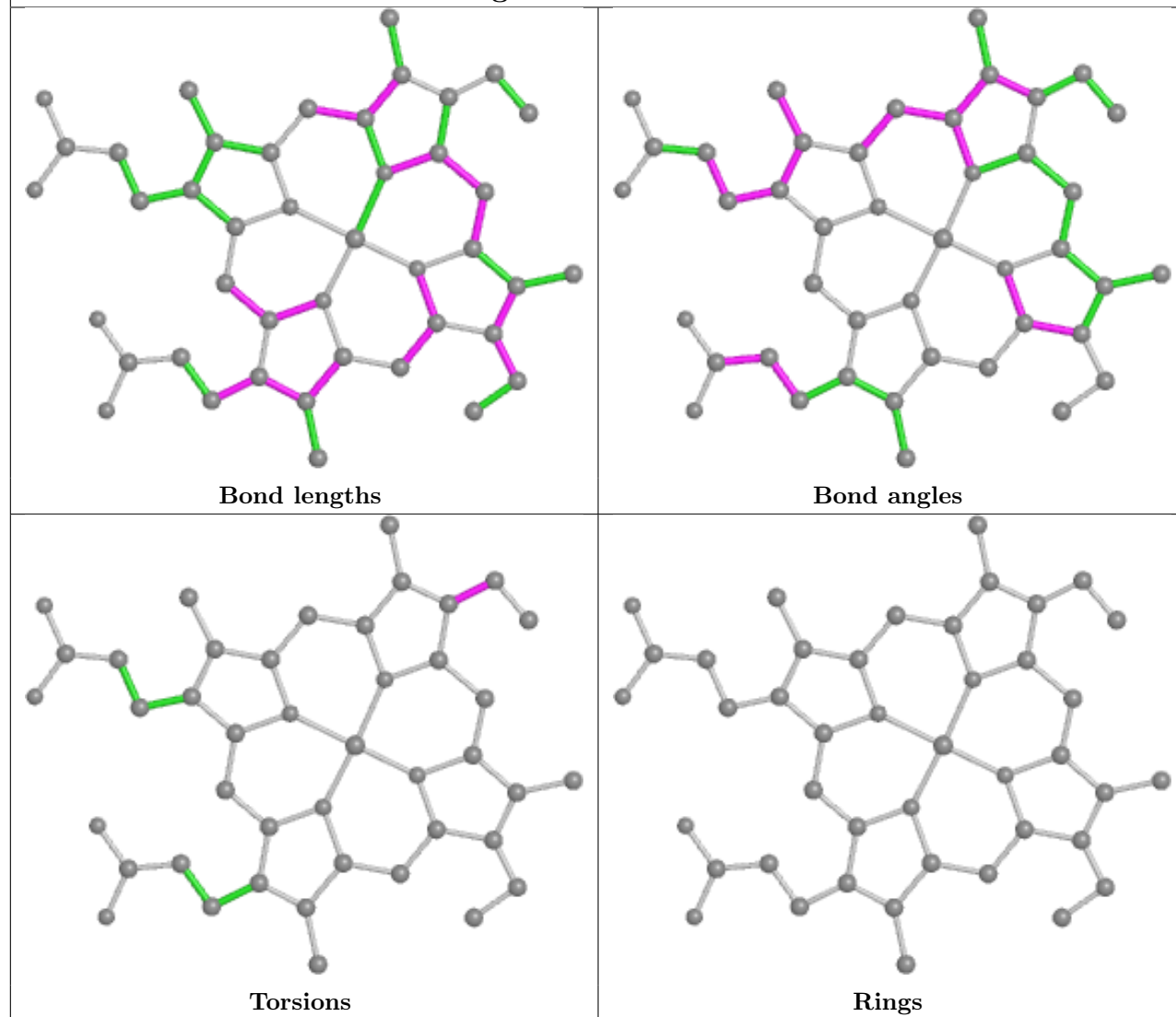
## Ligand HEC C 601

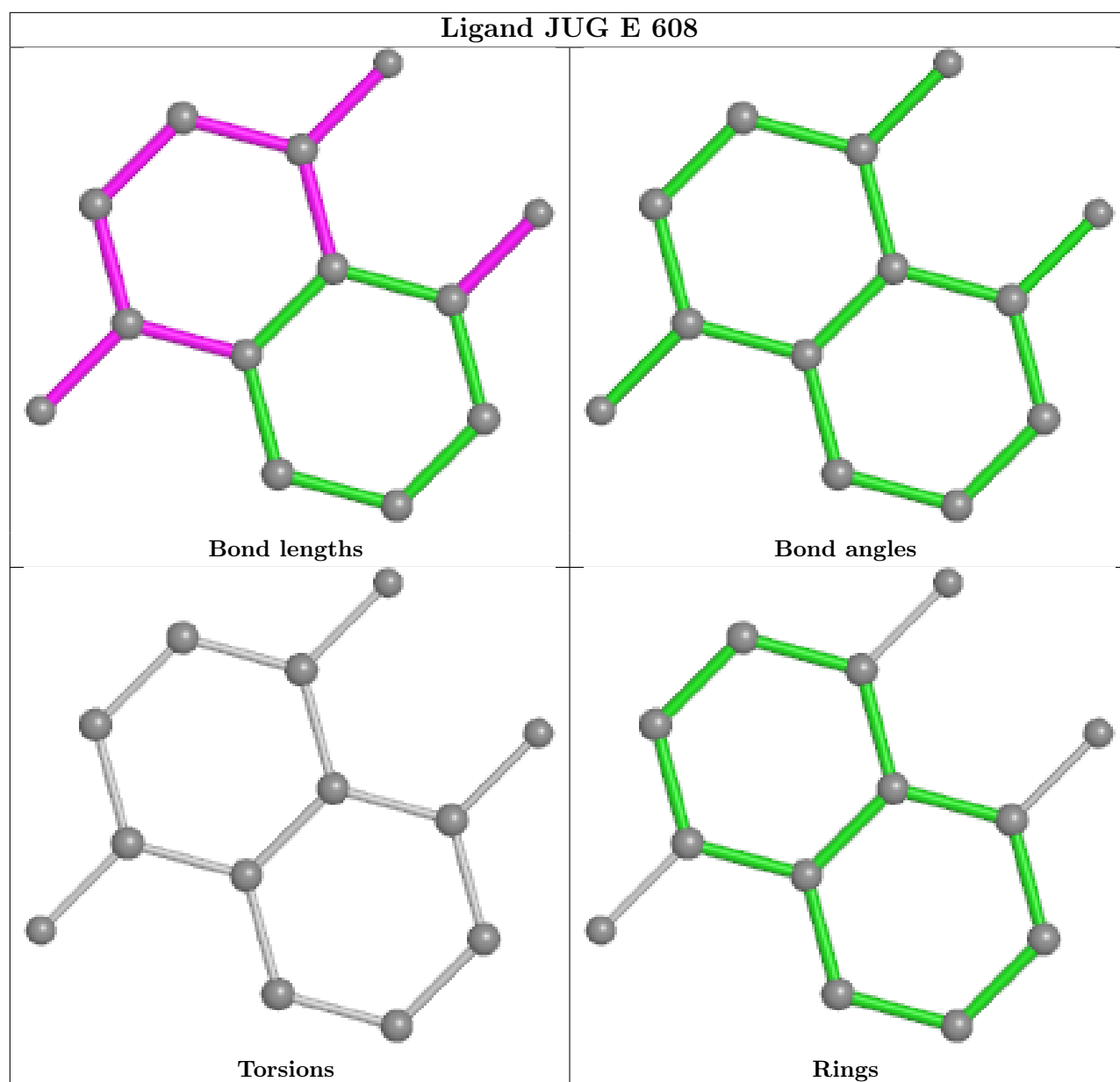


## Ligand HEC E 601



## Ligand ISW A 608





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	503/570 (88%)	1.22	90 (17%) <b>1</b> <b>1</b>	31, 60, 103, 142	0
1	C	503/570 (88%)	1.30	106 (21%) <b>1</b> <b>0</b>	22, 59, 103, 145	0
1	E	503/570 (88%)	1.18	89 (17%) <b>1</b> <b>1</b>	32, 61, 114, 171	0
2	B	56/91 (61%)	1.97	25 (44%) <b>0</b> <b>0</b>	48, 71, 121, 145	0
2	D	56/91 (61%)	1.32	14 (25%) <b>0</b> <b>0</b>	33, 48, 123, 156	0
2	F	56/91 (61%)	2.27	31 (55%) <b>0</b> <b>0</b>	53, 74, 133, 165	0
All	All	1677/1983 (84%)	1.30	355 (21%) <b>0</b> <b>0</b>	22, 61, 110, 171	0

All (355) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	187	ASP	7.7
1	C	155	MET	7.6
2	F	28	SER	7.5
2	D	83	SER	6.9
1	C	159	GLY	6.7
2	F	81	GLU	6.6
1	C	174	VAL	6.0
2	B	83	SER	6.0
1	E	139	TYR	5.9
1	C	131	ASN	5.7
1	E	165	LYS	5.6
1	C	179	LYS	5.5
2	D	28	SER	5.3
1	E	135	ASP	5.2
1	E	143	GLY	5.1
1	A	197	GLY	5.1
1	A	26	ILE	5.1
2	B	81	GLU	4.9
1	A	132	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	186	LYS	4.7
2	D	81	GLU	4.7
1	C	521	ARG	4.7
2	F	70	GLY	4.7
1	A	36	ALA	4.6
1	C	39	LEU	4.6
1	E	25	ASP	4.6
2	F	66	ARG	4.6
1	C	522	VAL	4.6
2	F	53	VAL	4.6
1	A	38	LYS	4.6
2	B	75	LEU	4.5
1	C	97	VAL	4.5
1	C	127	ASP	4.5
1	A	150	ASN	4.5
1	C	132	LEU	4.5
1	A	131	ASN	4.5
2	D	29	SER	4.5
1	E	109	ASP	4.4
1	C	181	LYS	4.4
2	B	29	SER	4.4
1	E	161	LYS	4.4
2	B	79	ALA	4.3
1	A	215	VAL	4.2
2	F	61	ASN	4.2
2	F	30	LEU	4.1
1	E	126	LEU	4.1
1	A	159	GLY	4.1
1	A	39	LEU	4.1
1	E	170	ILE	4.1
1	C	520	ALA	4.1
1	E	118	TRP	4.1
2	B	77	GLN	4.0
1	A	31	ASP	4.0
1	C	527	GLY	4.0
2	F	72	ILE	4.0
1	E	318	VAL	4.0
2	F	31	ALA	4.0
1	E	181	LYS	4.0
1	A	42	GLY	3.9
1	A	198	THR	3.9
1	E	39	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	30	LEU	3.9
2	D	75	LEU	3.8
1	C	517	ALA	3.8
1	C	49	THR	3.8
1	E	324	PHE	3.8
1	E	152	LEU	3.8
1	C	167	VAL	3.8
1	E	525	LEU	3.8
1	E	518	LEU	3.7
1	A	49	THR	3.7
1	C	99	GLU	3.7
1	E	163	THR	3.7
1	C	138	LEU	3.7
1	C	165	LYS	3.7
1	E	162	GLU	3.7
1	C	158	LEU	3.6
1	C	182	ALA	3.6
1	E	182	ALA	3.6
1	C	105	GLU	3.6
1	A	158	LEU	3.6
1	C	80	ILE	3.6
2	B	50	THR	3.6
1	C	518	LEU	3.6
2	B	33	ILE	3.6
1	C	157	LYS	3.6
1	C	44	ALA	3.5
1	C	52	ALA	3.5
1	A	134	SER	3.5
1	E	103	CYS	3.5
2	F	46	ASP	3.5
1	C	183	ASP	3.4
1	A	27	SER	3.4
2	F	75	LEU	3.4
1	C	172	CYS	3.4
1	E	188	ILE	3.4
1	C	177	ASN	3.4
1	E	275	ALA	3.4
2	D	79	ALA	3.4
1	E	145	LEU	3.4
1	C	525	LEU	3.3
2	F	77	GLN	3.3
1	E	223	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	133	LYS	3.3
1	C	91	PRO	3.3
2	F	54	LYS	3.3
1	E	160	GLU	3.3
1	A	127	ASP	3.3
1	E	136	ASP	3.3
1	C	92	VAL	3.3
2	F	29	SER	3.3
1	C	148	VAL	3.2
2	F	62	GLY	3.2
1	A	146	GLU	3.2
2	F	83	SER	3.2
1	C	90	PRO	3.2
1	E	432	THR	3.2
2	F	41	TYR	3.2
1	C	178	LYS	3.2
2	B	49	PRO	3.1
1	C	62	HIS	3.1
1	C	304	GLY	3.1
1	A	60	PRO	3.1
1	A	177	ASN	3.1
1	A	323	ALA	3.1
2	D	82	GLN	3.1
2	B	32	PRO	3.1
1	E	155	MET	3.1
2	F	32	PRO	3.1
1	A	521	ARG	3.0
1	C	45	THR	3.0
1	A	391	ARG	3.0
1	E	124	ALA	3.0
1	A	374	GLU	3.0
1	C	163	THR	3.0
2	B	61	ASN	3.0
1	A	524	LYS	3.0
1	C	43	LYS	3.0
1	C	60	PRO	3.0
1	A	43	LYS	3.0
2	B	70	GLY	3.0
1	A	162	GLU	3.0
2	F	80	ARG	3.0
2	F	82	GLN	3.0
1	E	153	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	523	ASN	3.0
1	C	102	ASP	3.0
1	C	180	ASP	3.0
1	C	152	LEU	3.0
1	E	215	VAL	3.0
2	B	31	ALA	3.0
2	F	49	PRO	3.0
1	E	179	LYS	3.0
1	A	518	LEU	2.9
1	A	139	TYR	2.9
1	C	164	LEU	2.9
1	C	176	VAL	2.9
2	F	65	VAL	2.9
2	B	72	ILE	2.9
1	E	167	VAL	2.9
2	B	76	VAL	2.9
1	A	35	ASP	2.9
1	A	143	GLY	2.9
1	E	61	ALA	2.9
1	E	90	PRO	2.9
2	F	67	VAL	2.8
1	A	223	ALA	2.8
2	B	80	ARG	2.8
1	E	141	LYS	2.8
1	C	175	ASP	2.8
1	A	63	GLY	2.8
1	C	50	TYR	2.8
1	C	513	GLN	2.8
1	A	382	LEU	2.8
1	C	293	ASN	2.8
1	E	166	GLU	2.8
1	E	105	GLU	2.7
2	D	35	ALA	2.7
1	E	107	HIS	2.7
1	C	26	ILE	2.7
1	E	131	ASN	2.7
1	C	526	GLU	2.7
1	E	101	LYS	2.7
1	A	221	TRP	2.7
1	C	113	VAL	2.7
1	A	48	GLU	2.7
1	A	324	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	84	GLY	2.7
1	A	46	PRO	2.7
2	D	30	LEU	2.7
1	A	135	ASP	2.7
1	C	135	ASP	2.7
1	E	127	ASP	2.7
1	E	41	ARG	2.7
1	E	97	VAL	2.7
2	B	65	VAL	2.7
1	A	525	LEU	2.7
1	E	158	LEU	2.7
1	E	493	GLU	2.7
1	A	426	THR	2.7
1	A	526	GLU	2.6
1	E	346	THR	2.6
1	E	174	VAL	2.6
2	B	52	VAL	2.6
1	E	151	ASN	2.6
2	F	74	ALA	2.6
1	A	97	VAL	2.6
1	C	38	LYS	2.6
1	E	54	VAL	2.6
1	C	156	GLY	2.6
1	E	527	GLY	2.6
1	E	104	VAL	2.6
1	A	155	MET	2.6
1	E	37	LEU	2.6
1	C	136	ASP	2.6
1	E	327	GLY	2.6
1	A	522	VAL	2.6
1	E	169	CYS	2.6
1	E	132	LEU	2.6
2	B	43	ALA	2.6
2	B	82	GLN	2.6
1	A	85	ASN	2.5
2	F	52	VAL	2.5
1	A	62	HIS	2.5
1	C	188	ILE	2.5
1	A	290	VAL	2.5
1	C	480	GLY	2.5
1	E	140	TYR	2.5
1	A	519	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	78	LYS	2.5
1	C	129	ILE	2.5
1	E	96	GLU	2.5
1	C	326	LYS	2.5
1	E	523	ASN	2.5
1	E	180	ASP	2.5
2	B	73	VAL	2.5
1	A	369	THR	2.5
2	D	77	GLN	2.5
1	A	174	VAL	2.5
1	C	40	ASP	2.5
1	C	519	GLN	2.4
1	A	492	THR	2.4
1	C	424	ASP	2.4
1	C	524	LYS	2.4
1	E	484	VAL	2.4
1	E	326	LYS	2.4
1	E	28	THR	2.4
2	F	43	ALA	2.4
1	C	109	ASP	2.4
1	E	114	TRP	2.4
2	B	46	ASP	2.4
2	F	51	ASP	2.4
1	A	440	PRO	2.4
1	C	124	ALA	2.4
1	A	370	SER	2.4
1	C	134	SER	2.4
1	C	436	ASN	2.4
2	F	68	LYS	2.4
1	C	230	LEU	2.4
1	A	372	TRP	2.4
1	C	372	TRP	2.4
1	C	96	GLU	2.4
2	B	41	TYR	2.4
1	C	243	ALA	2.4
1	A	236	ILE	2.4
1	E	524	LYS	2.4
1	C	278	ARG	2.4
1	A	345	TYR	2.3
1	C	88	TYR	2.3
1	A	138	LEU	2.3
2	F	79	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	380	TRP	2.3
1	A	140	TYR	2.3
1	E	195	THR	2.3
1	C	95	LYS	2.3
1	A	322	ASP	2.3
2	D	46	ASP	2.3
1	A	375	ALA	2.3
1	A	126	LEU	2.3
1	A	168	GLY	2.3
1	E	46	PRO	2.3
1	A	45	THR	2.3
1	C	29	VAL	2.3
1	C	287	HIS	2.3
1	A	201	LEU	2.3
1	C	313	LYS	2.3
1	C	426	THR	2.3
1	C	198	THR	2.3
1	A	54	VAL	2.3
1	A	144	LYS	2.3
1	C	137	PRO	2.2
1	E	62	HIS	2.2
1	E	120	ARG	2.2
1	A	470	ALA	2.2
1	C	375	ALA	2.2
1	C	72	TYR	2.2
1	C	509	TYR	2.2
1	E	344	GLU	2.2
1	E	128	LYS	2.2
2	F	48	LYS	2.2
1	C	79	SER	2.2
1	C	493	GLU	2.2
1	A	115	VAL	2.2
1	C	85	ASN	2.2
1	C	440	PRO	2.2
1	E	84	PRO	2.2
1	A	307	ALA	2.2
1	E	55	LYS	2.2
1	E	345	TYR	2.2
1	C	100	ARG	2.2
1	C	523	ASN	2.2
1	E	177	ASN	2.2
1	A	133	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	199	CYS	2.2
1	E	149	GLU	2.2
1	E	72	TYR	2.2
1	E	325	SER	2.2
1	E	420	LYS	2.2
1	A	380	TRP	2.2
1	A	47	LYS	2.1
2	D	31	ALA	2.1
1	C	190	MET	2.1
2	F	50	THR	2.1
1	C	118	TRP	2.1
1	C	110	GLU	2.1
1	A	196	CYS	2.1
1	A	367	ASN	2.1
1	E	154	SER	2.1
1	A	179	LYS	2.1
1	E	130	ARG	2.1
1	C	235	ASN	2.1
1	A	181	LYS	2.1
2	D	32	PRO	2.1
1	C	35	ASP	2.1
1	A	517	ALA	2.1
1	E	283	CYS	2.1
1	A	148	VAL	2.1
1	C	115	VAL	2.1
1	A	55	LYS	2.1
1	E	186	LYS	2.1
1	A	125	ASN	2.1
1	C	120	ARG	2.1
1	A	429	GLY	2.1
1	E	272	PHE	2.1
1	A	64	ALA	2.0
1	A	334	CYS	2.0
1	C	264	ASP	2.0
1	E	156	GLY	2.0
1	A	313	LYS	2.0
1	E	125	ASN	2.0
1	A	40	ASP	2.0
1	A	169	CYS	2.0
1	A	51	GLU	2.0
1	C	42	GLY	2.0
1	E	322	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

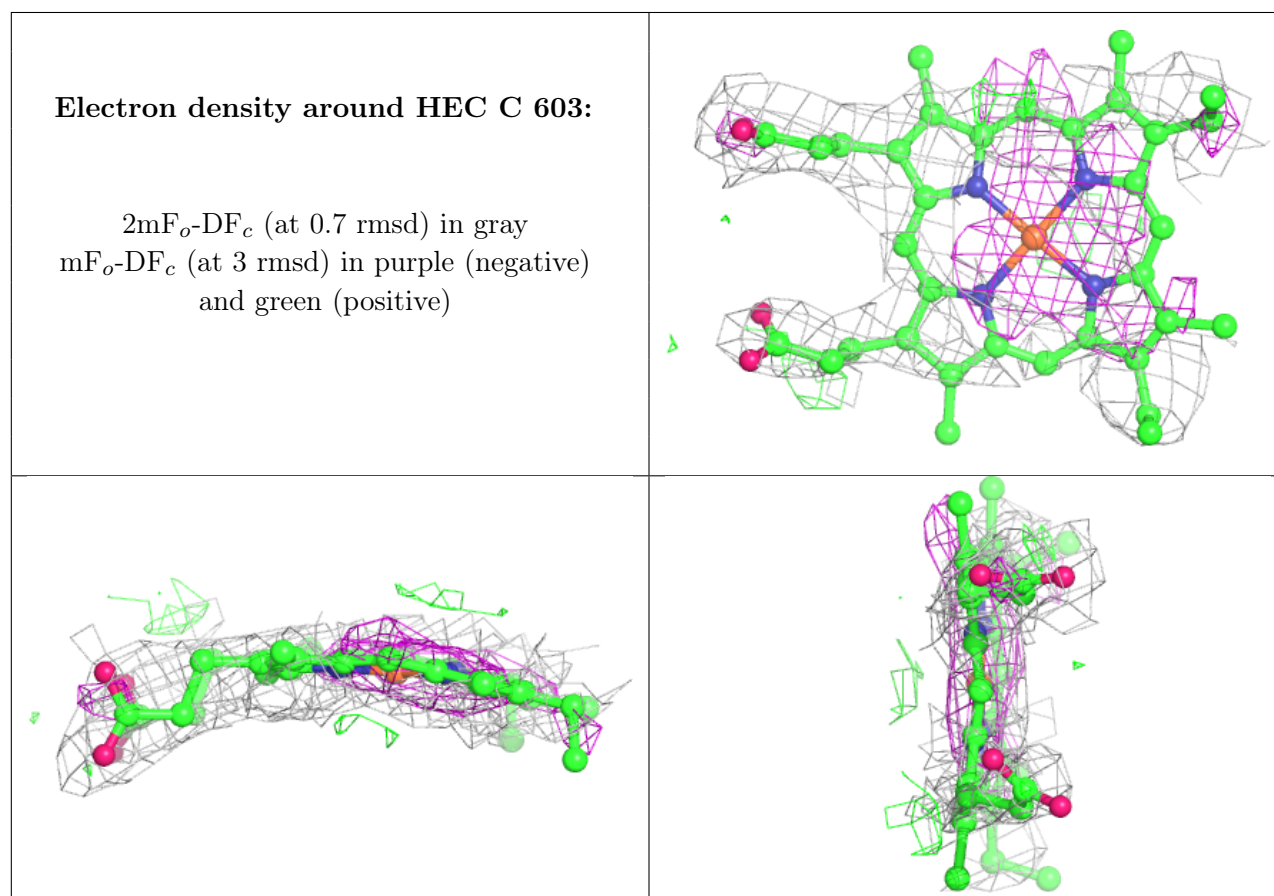
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	1PE	C	609	12/16	0.64	0.29	51,61,65,66	0
7	1PE	C	610	16/16	0.69	0.37	66,78,81,82	0
5	PEG	E	609	7/7	0.74	0.34	48,55,60,62	0
5	PEG	A	609	7/7	0.80	0.28	44,50,56,56	0
3	HEC	C	603	43/43	0.80	0.45	42,84,90,92	0
6	JUG	C	608	13/13	0.81	0.25	48,54,64,70	0
5	PEG	A	610	7/7	0.83	0.25	42,46,53,54	0
3	HEC	E	603	43/43	0.85	0.29	45,71,80,84	0
6	JUG	E	608	13/13	0.85	0.25	63,65,70,72	0
3	HEC	C	604	43/43	0.86	0.34	28,52,63,67	0
3	HEC	A	602	43/43	0.89	0.29	27,64,85,93	0
3	HEC	C	602	43/43	0.89	0.26	19,54,65,67	0
3	HEC	E	604	43/43	0.90	0.24	40,53,67,70	0
4	ISW	A	608	43/43	0.90	0.25	24,37,41,46	0
3	HEC	E	602	43/43	0.90	0.26	31,52,64,70	0
3	HEC	A	607	43/43	0.91	0.22	16,45,65,77	0
3	HEC	A	601	43/43	0.91	0.26	19,56,76,84	0
3	HEC	C	605	43/43	0.91	0.25	18,35,43,48	0
3	HEC	E	605	43/43	0.91	0.22	13,36,45,51	0
3	HEC	E	601	43/43	0.91	0.23	25,42,60,68	0
4	ISW	A	611	43/43	0.91	0.24	28,41,55,57	0
4	ISW	C	611	43/43	0.91	0.23	18,39,53,59	0
3	HEC	C	601	43/43	0.92	0.23	29,51,58,63	0
3	HEC	E	606	43/43	0.92	0.23	30,42,60,68	0
3	HEC	A	605	43/43	0.92	0.23	20,33,53,57	0
3	HEC	A	604	43/43	0.92	0.20	20,32,39,41	0
3	HEC	C	606	43/43	0.93	0.22	18,34,50,55	0

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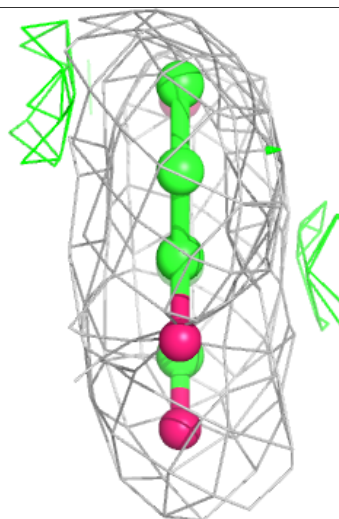
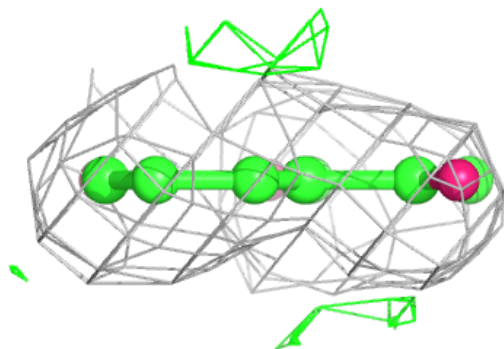
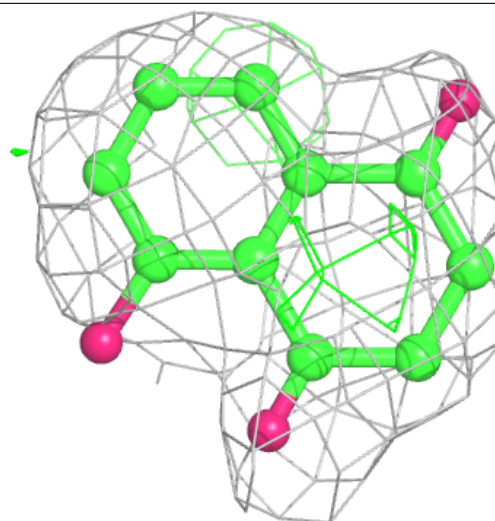
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	HEC	C	607	43/43	0.94	0.21	11,27,42,47	0
3	HEC	E	607	43/43	0.94	0.22	14,35,51,60	0
3	HEC	A	606	43/43	0.94	0.20	15,27,38,47	0
3	HEC	A	603	43/43	0.94	0.20	26,41,52,57	0

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.



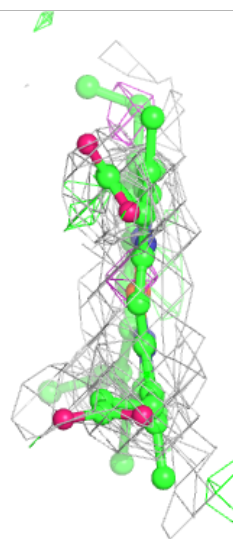
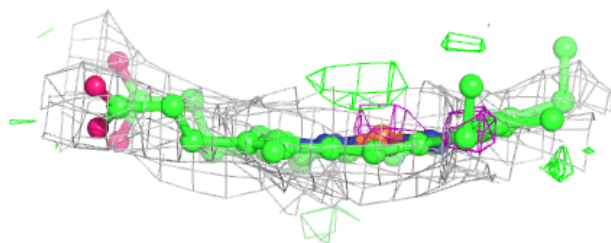
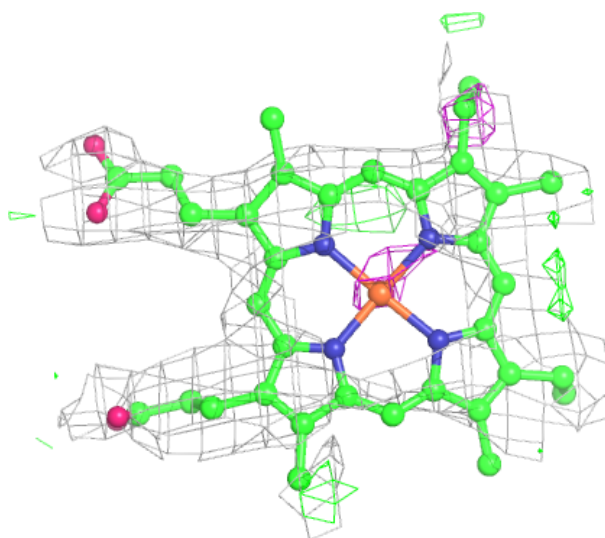
**Electron density around JUG C 608:**

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



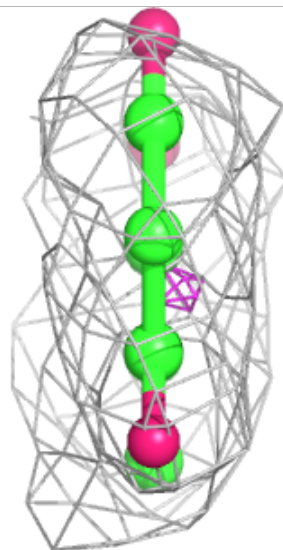
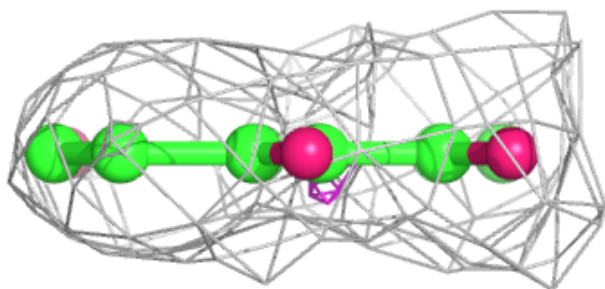
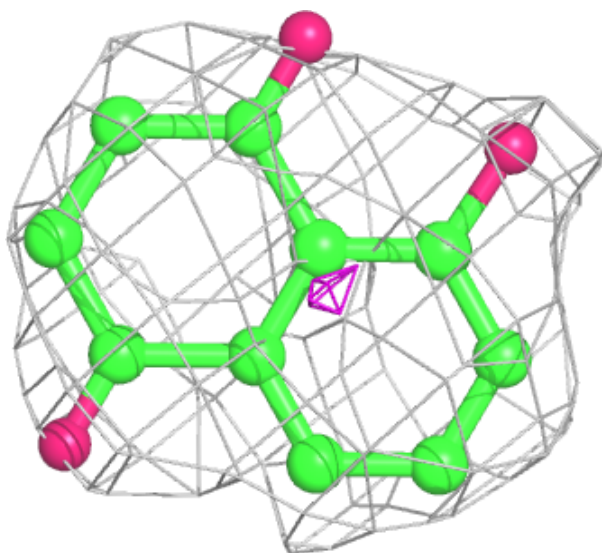
**Electron density around HEC E 603:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



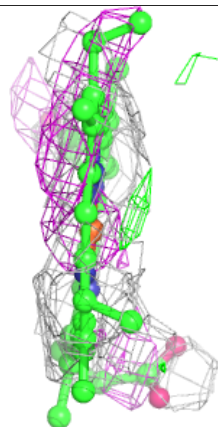
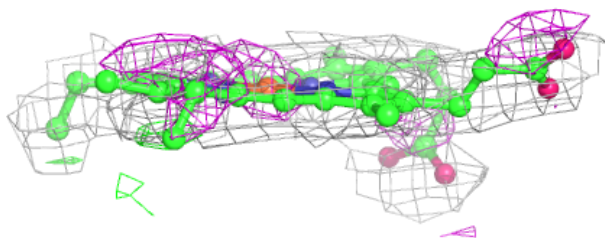
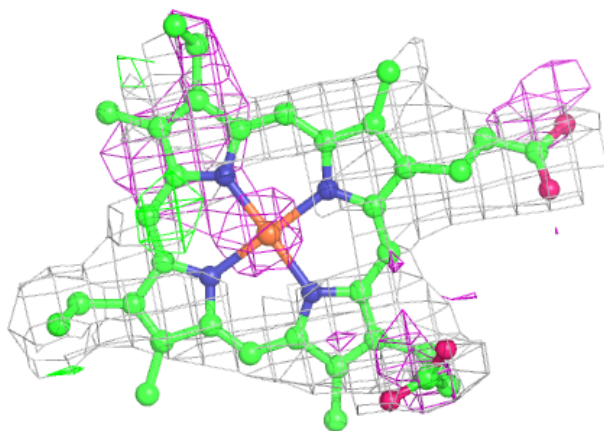
**Electron density around JUG E 608:**

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



**Electron density around HEC C 604:**

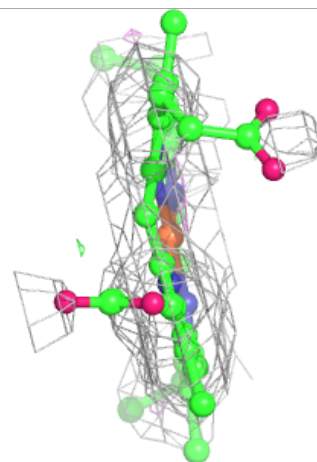
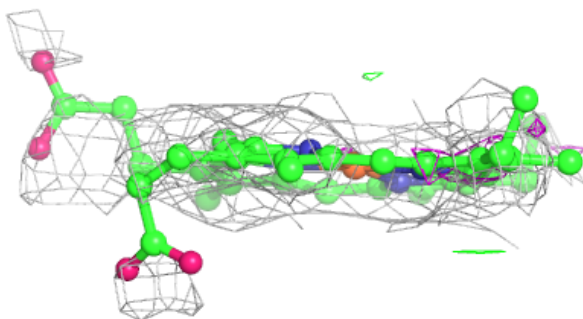
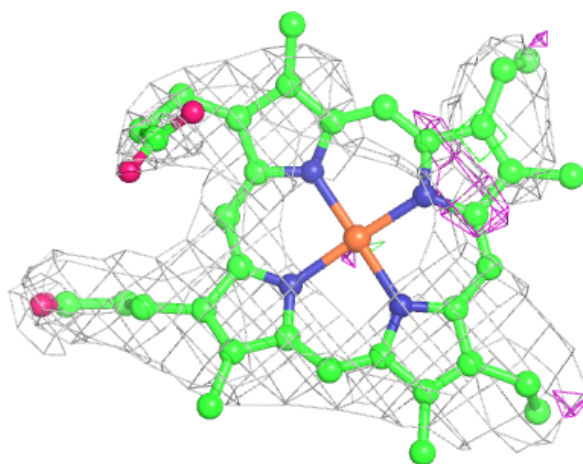
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC A 602:**

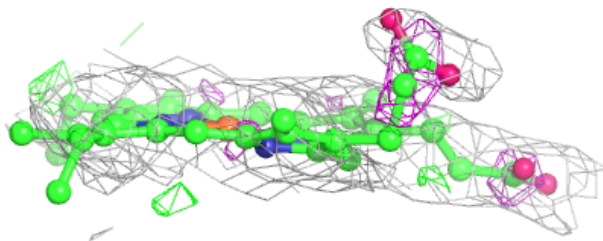
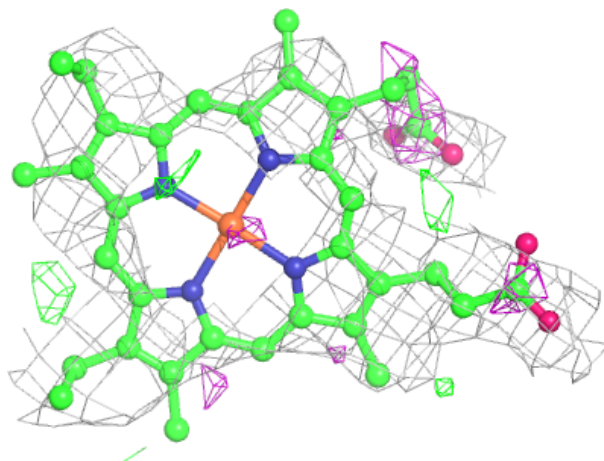
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





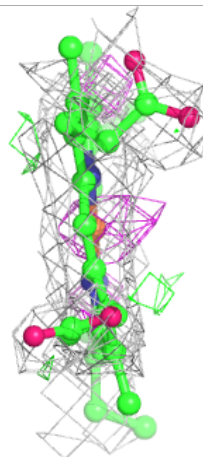
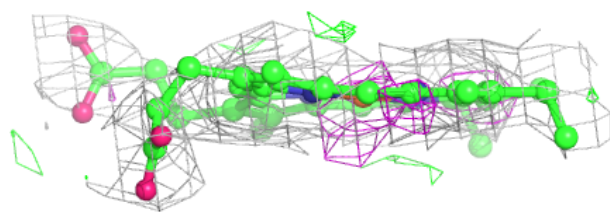
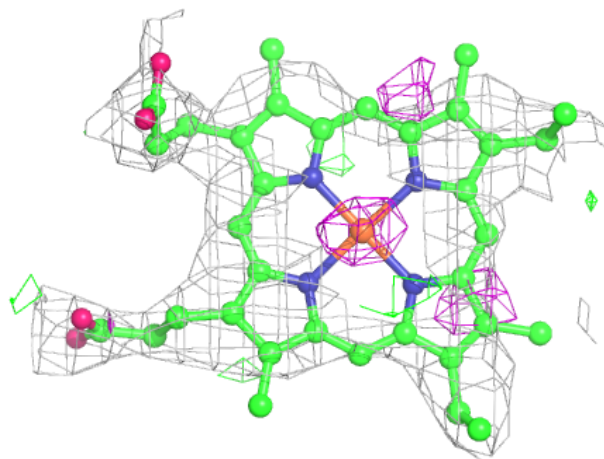
**Electron density around HEC C 602:**

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



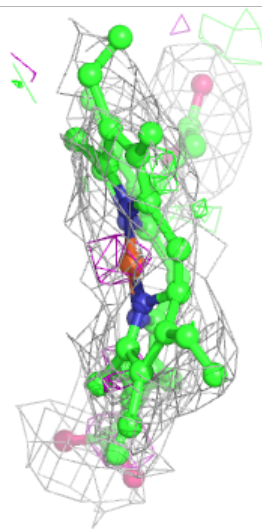
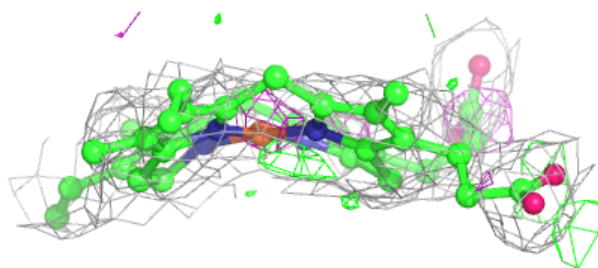
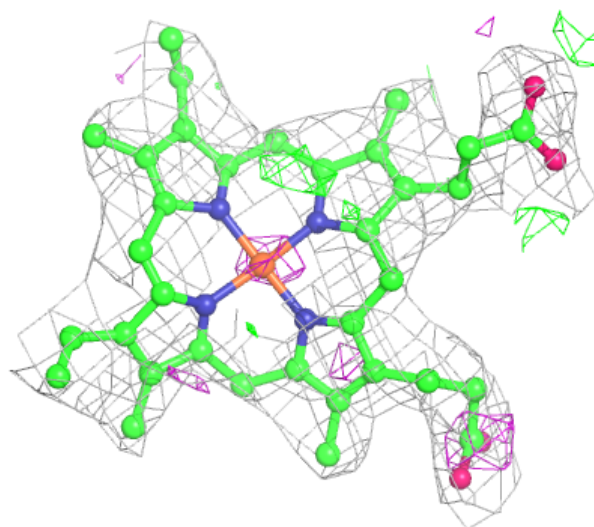
**Electron density around HEC E 604:**

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and green (positive)



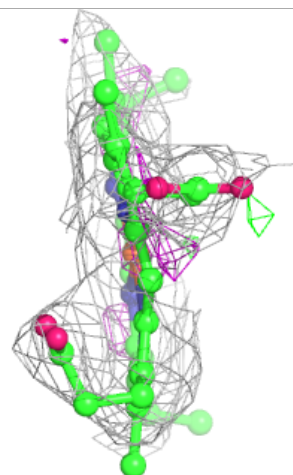
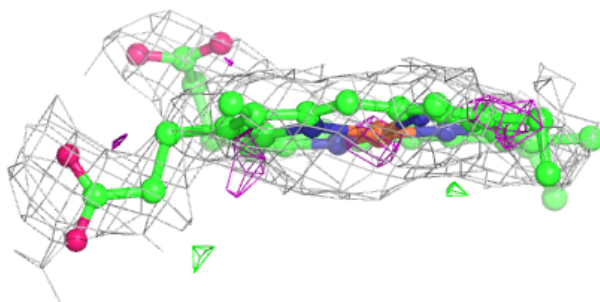
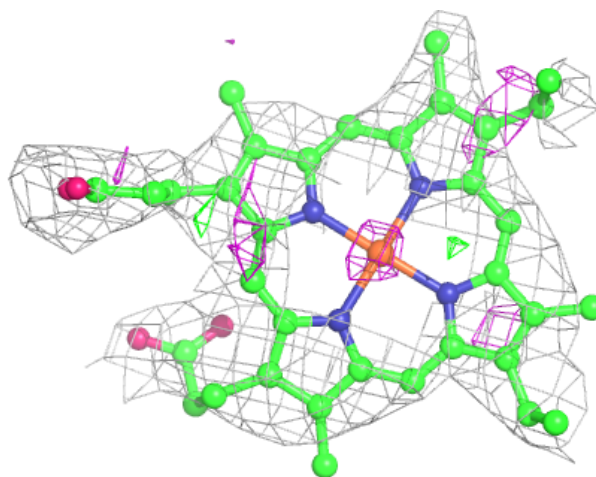
**Electron density around ISW A 608:**

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



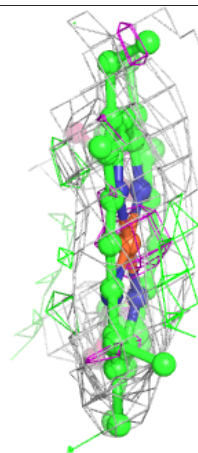
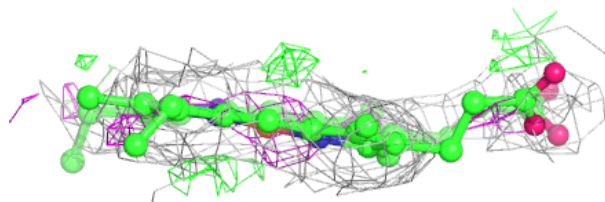
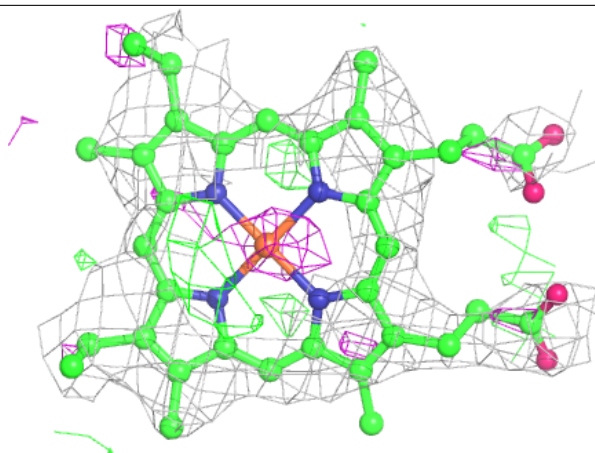
**Electron density around HEC E 602:**

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



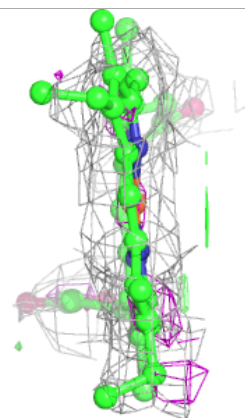
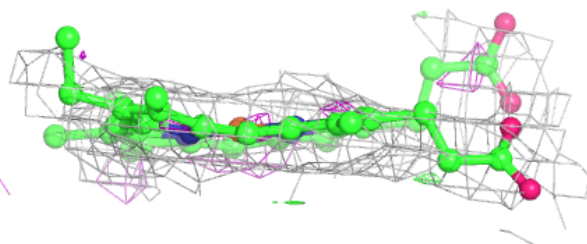
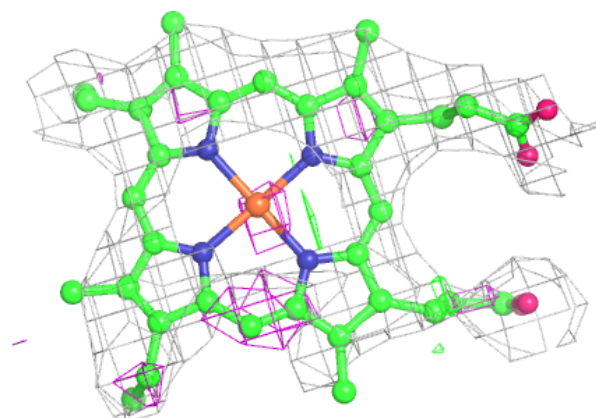
**Electron density around HEC A 607:**

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



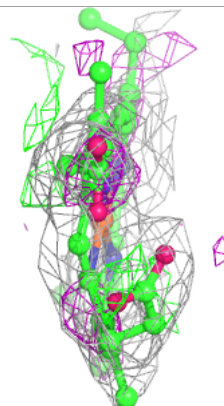
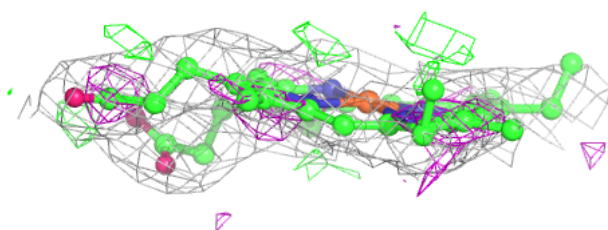
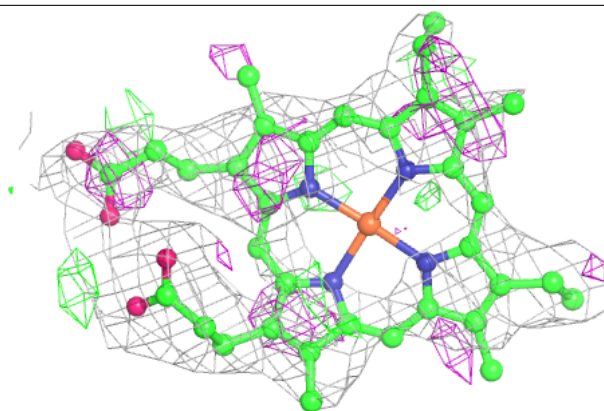
**Electron density around HEC A 601:**

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



**Electron density around HEC C 605:**

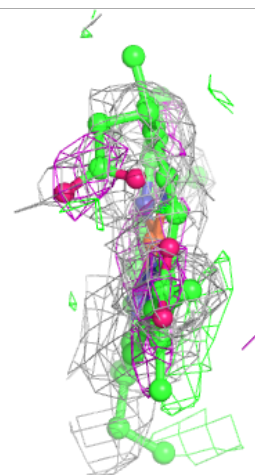
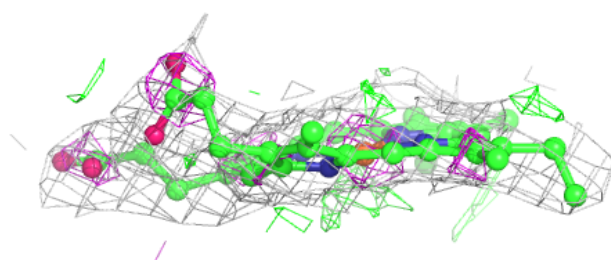
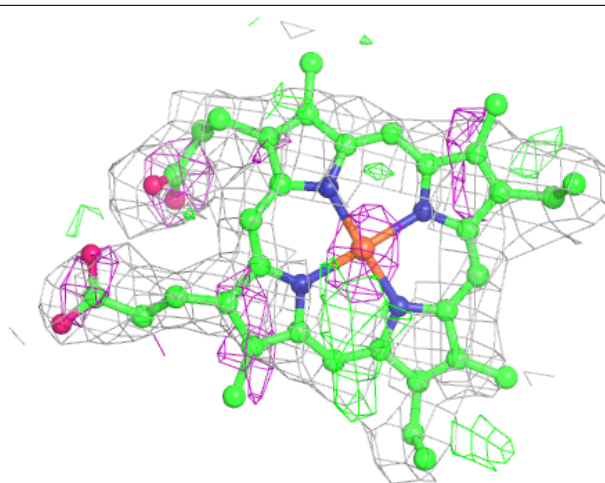
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and green (positive)





**Electron density around HEC E 605:**

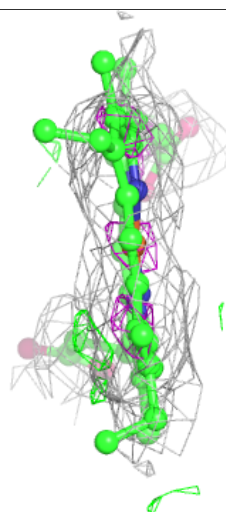
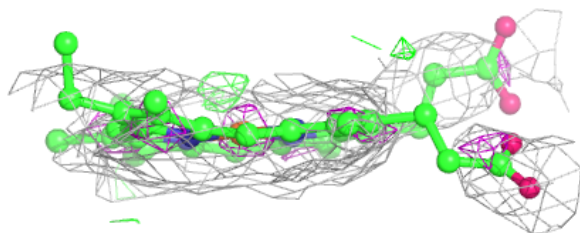
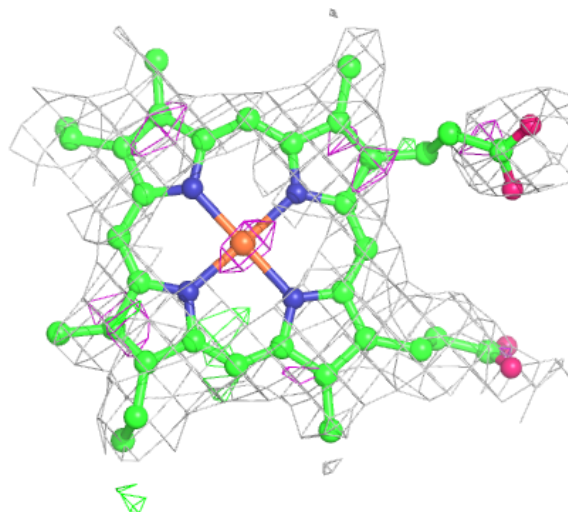
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and green (positive)





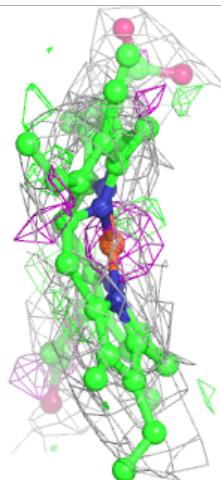
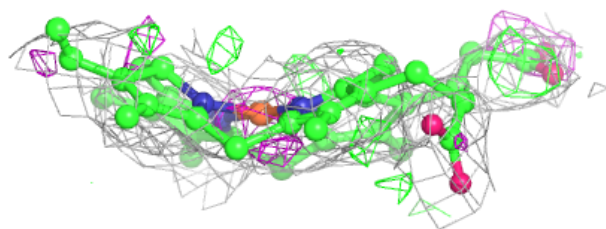
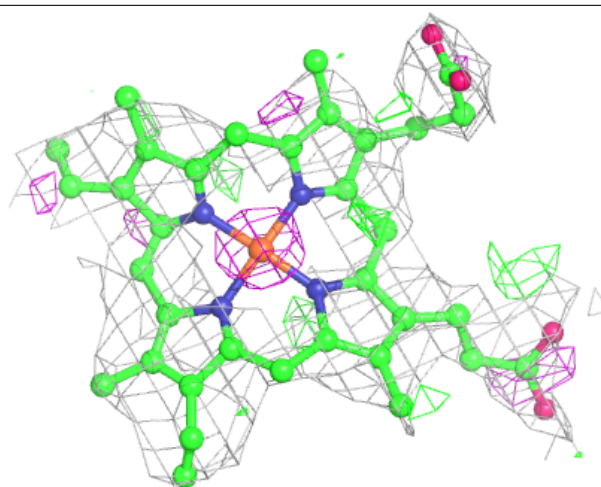
**Electron density around HEC E 601:**

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and green (positive)



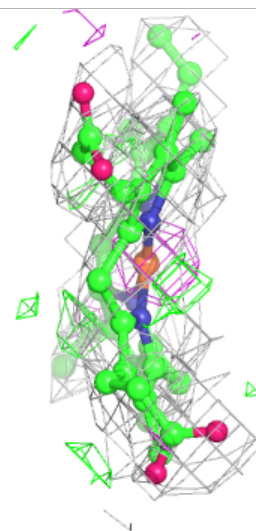
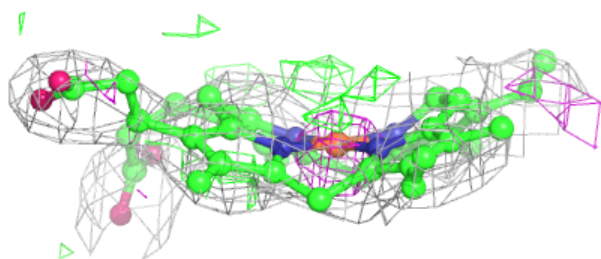
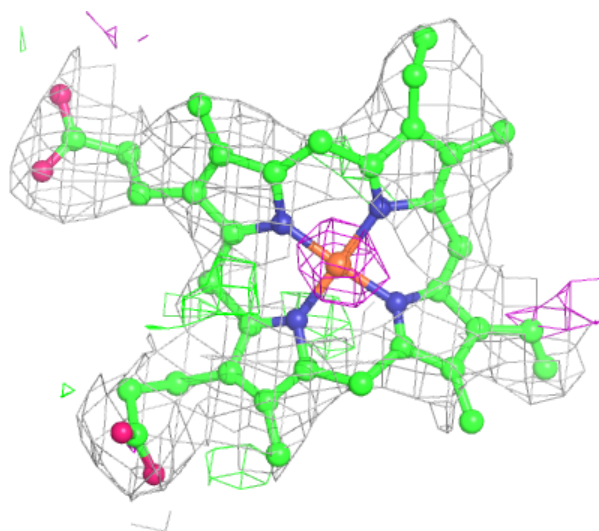
**Electron density around ISW A 611:**

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



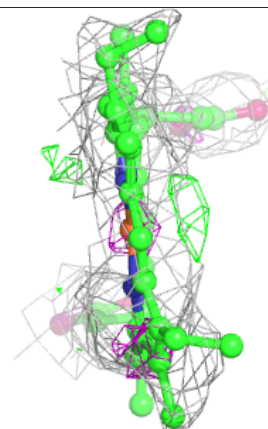
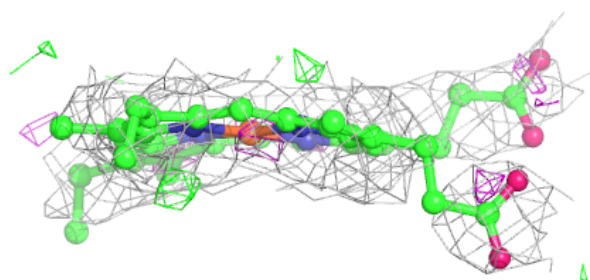
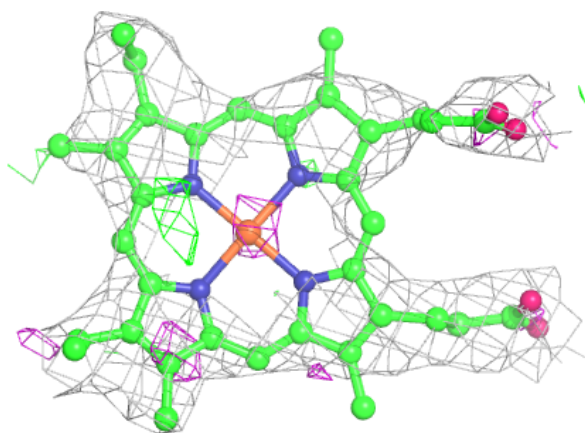
**Electron density around ISW C 611:**

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



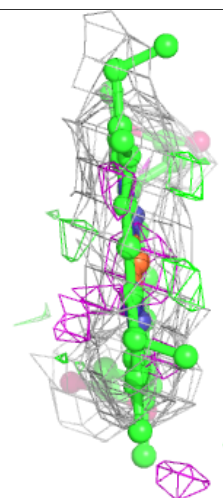
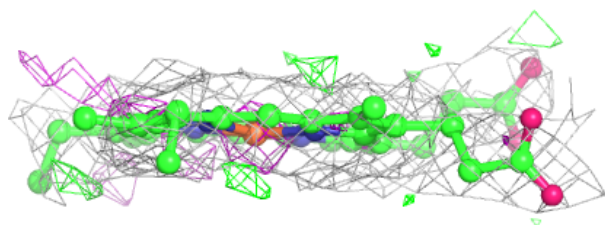
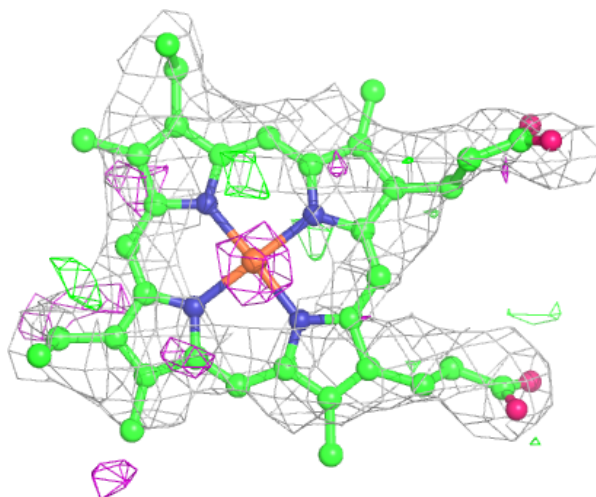
**Electron density around HEC C 601:**

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



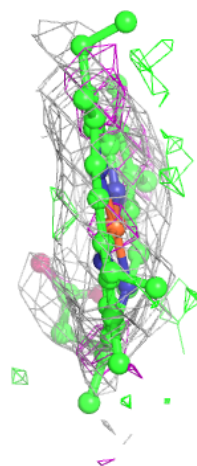
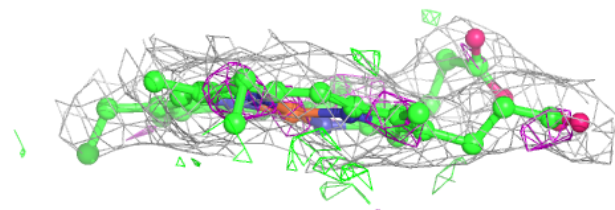
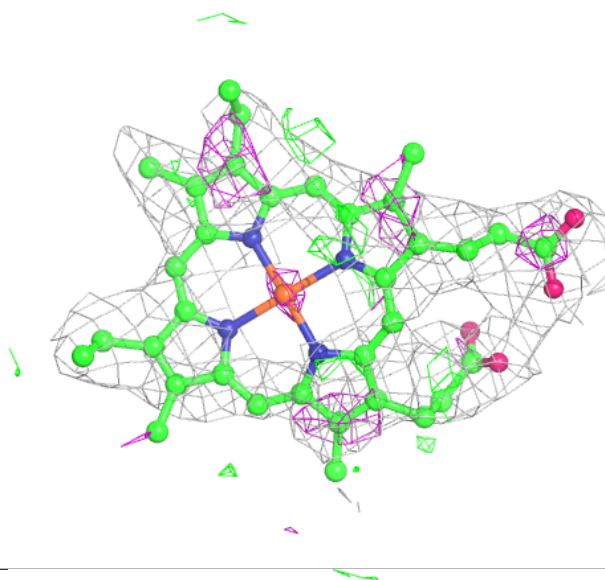
**Electron density around HEC E 606:**

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



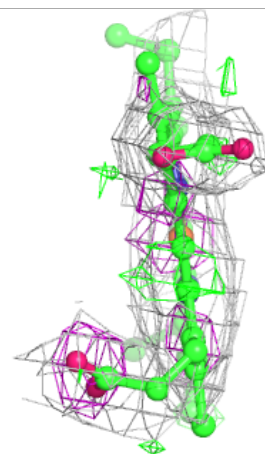
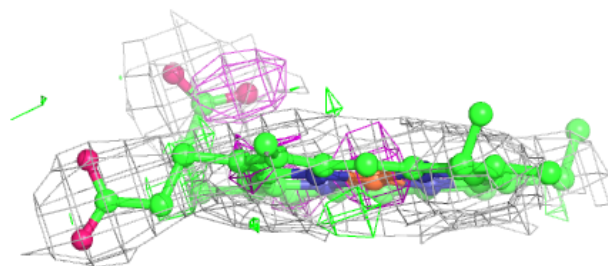
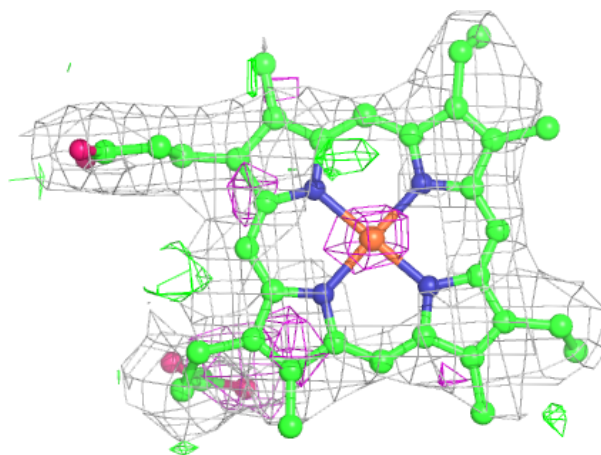
**Electron density around HEC A 605:**

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



**Electron density around HEC A 604:**

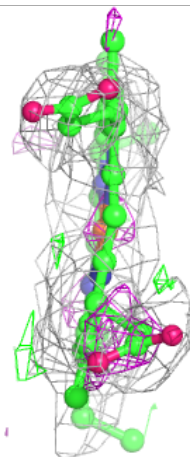
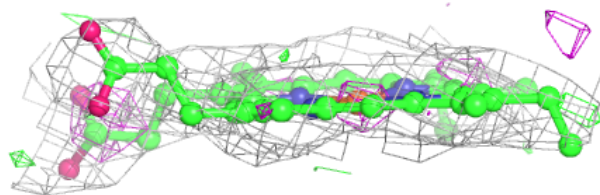
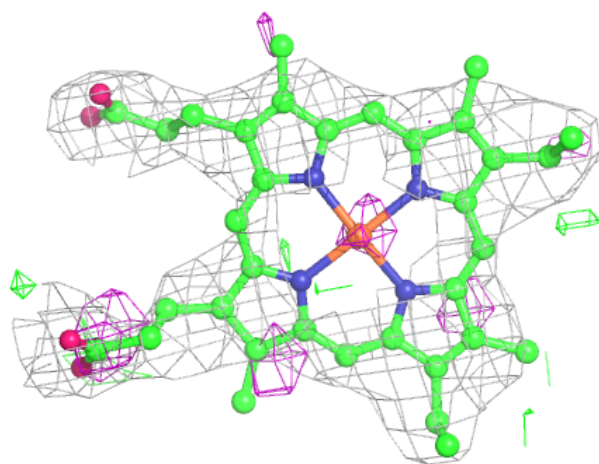
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC C 606:**

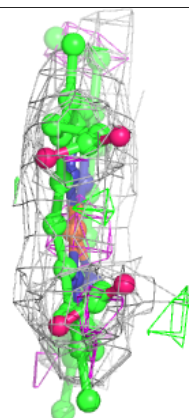
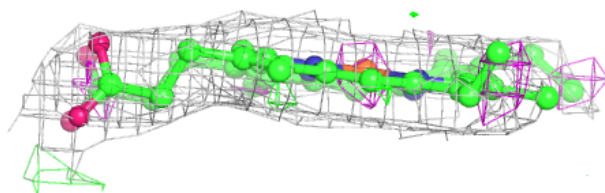
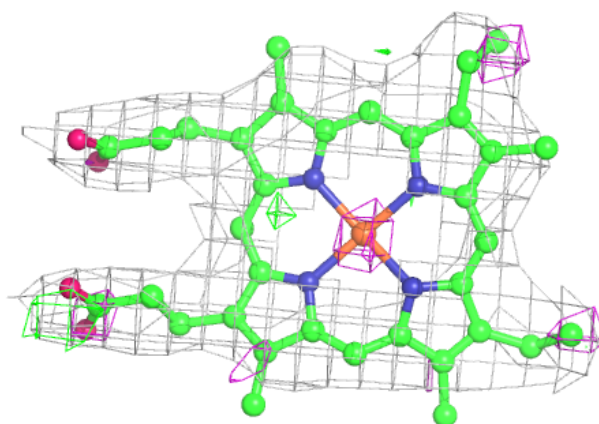
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





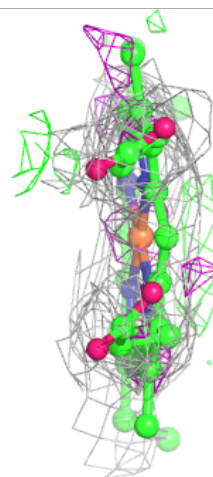
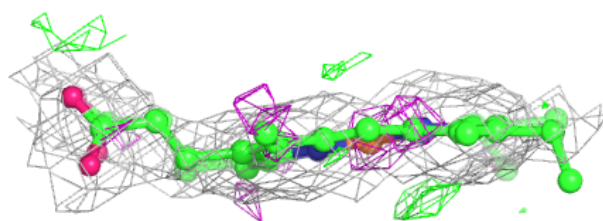
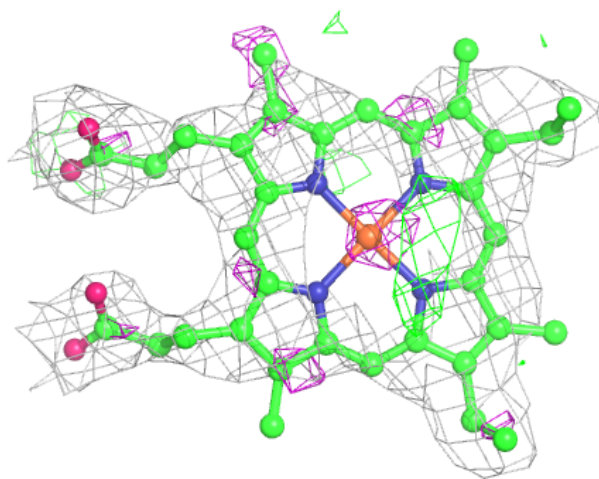
**Electron density around HEC C 607:**

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



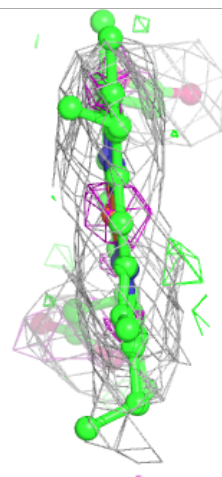
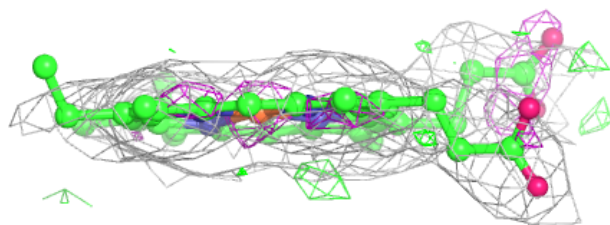
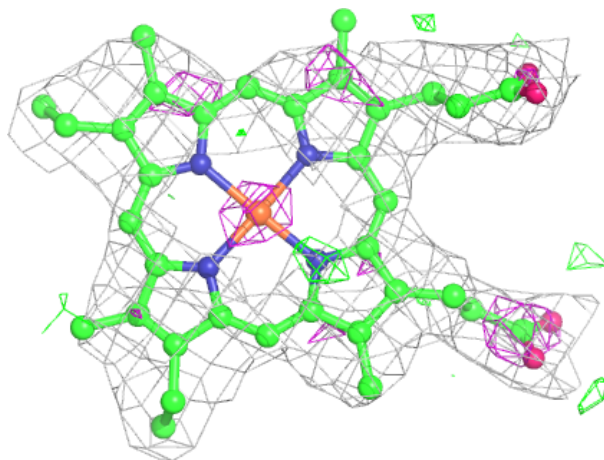
**Electron density around HEC E 607:**

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



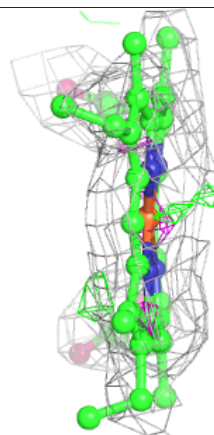
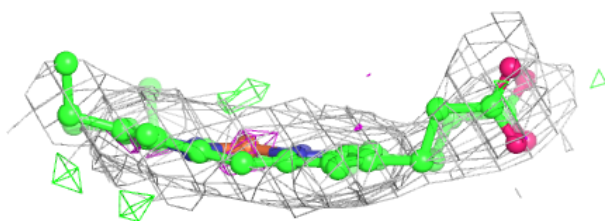
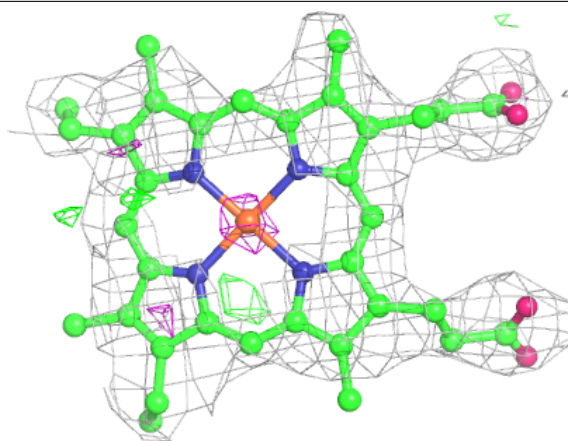
**Electron density around HEC A 606:**

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



**Electron density around HEC A 603:**

$2mF_o-DF_c$  (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.