



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 10:23 AM EDT

PDB ID : 2RF7  
Title : Crystal structure of the escherichia coli nrfa mutant Q263E  
Authors : Clarke, T.A.; Richardson, D.J.; Hemmings, A.M.  
Deposited on : 2007-09-28  
Resolution : 2.04 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.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

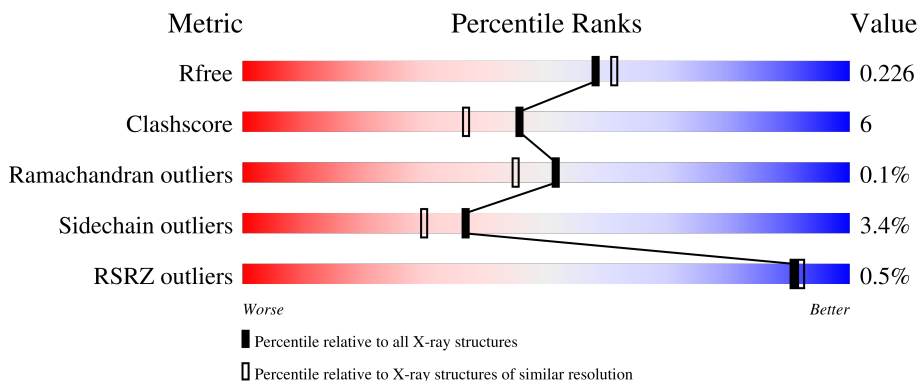
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


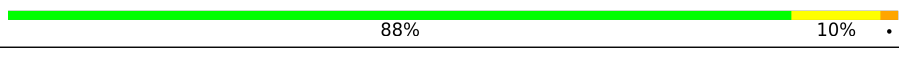
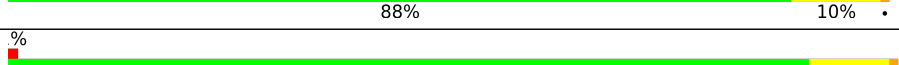

The reported resolution of this entry is 2.04 Å.

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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	441	 88% 10% .
1	B	441	 88% 10% .
1	C	441	 88% 10% .
1	D	441	 % 90% 9% .

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16697 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 Cytochrome c-552.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	441	3500	2193	620	665	22	0	4	0
1	B	441	3500	2196	621	660	23	0	4	0
1	C	441	3482	2181	619	660	22	3	1	0
1	D	441	3505	2198	622	663	22	0	5	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	263	GLU	GLN	engineered mutation	UNP P0ABK9
B	263	GLU	GLN	engineered mutation	UNP P0ABK9
C	263	GLU	GLN	engineered mutation	UNP P0ABK9
D	263	GLU	GLN	engineered mutation	UNP P0ABK9

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Ca 2	0	0
2	B	2	Total 2	Ca 2	0	0
2	C	2	Total 2	Ca 2	0	0
2	D	2	Total 2	Ca 2	0	0

- Molecule 3 is HEME C (three-letter code: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).



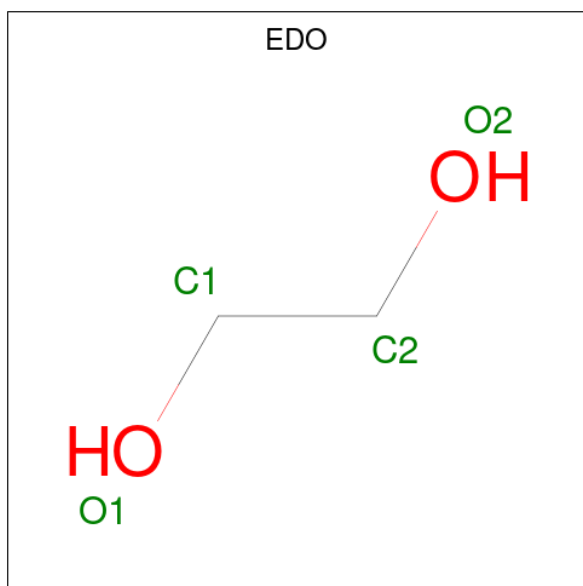
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B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

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

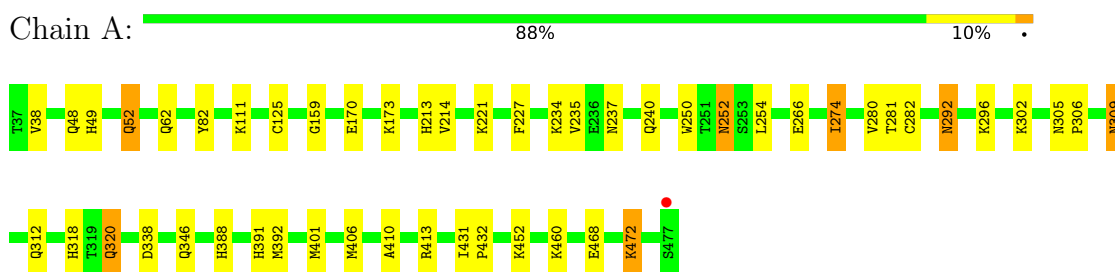
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	447	Total O 447 447	0	0
5	B	494	Total O 494 494	0	0
5	C	516	Total O 516 516	0	0
5	D	325	Total O 325 325	0	0

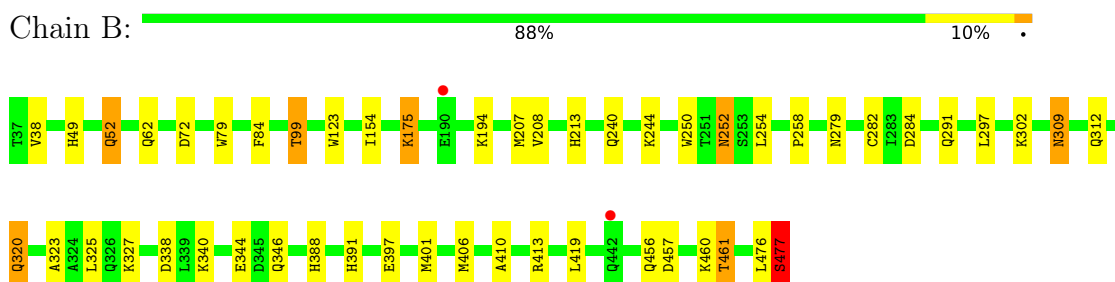
### 3 Residue-property plots

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.

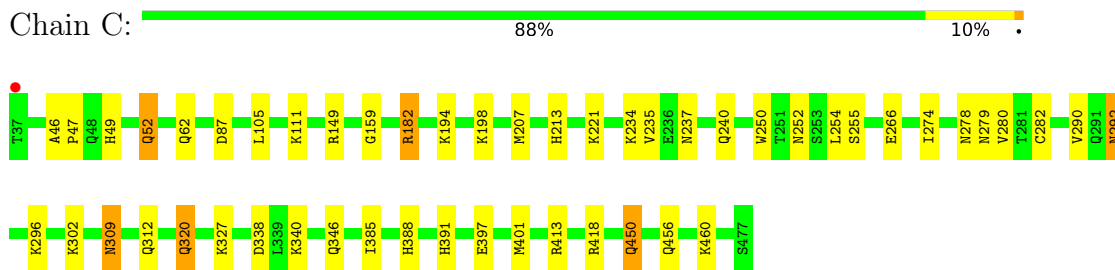
- Molecule 1: Cytochrome c-552



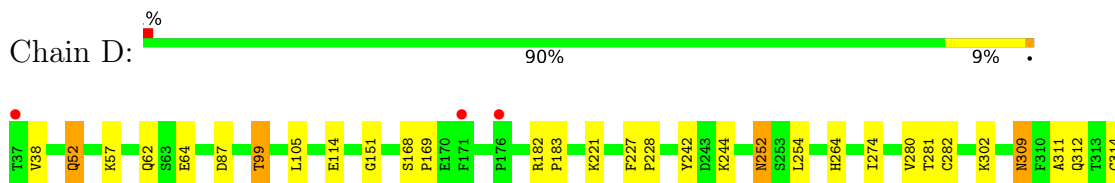
- Molecule 1: Cytochrome c-552



- Molecule 1: Cytochrome c-552



- Molecule 1: Cytochrome c-552







## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.29Å 91.20Å 295.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.31 – 2.04 79.28 – 2.04	Depositor EDS
% Data completeness (in resolution range)	96.8 (79.31-2.04) 96.8 (79.28-2.04)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.95 (at 2.03Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.171 , 0.226 0.172 , 0.226	Depositor DCC
$R_{free}$ test set	6940 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.5	Xtrriage
Anisotropy	0.053	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 59.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16697	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5392e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: EDO, HEC, CA

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	0.76	0/3596	0.69	0/4862
1	B	0.80	0/3596	0.70	1/4859 (0.0%)
1	C	0.82	0/3569	0.71	1/4826 (0.0%)
1	D	0.67	0/3604	0.65	0/4871
All	All	0.77	0/14365	0.69	2/19418 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	182	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	B	477	SER	N-CA-CB	5.55	118.82	110.50

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	3500	0	3389	49	0
1	B	3500	0	3405	44	0
1	C	3482	0	3368	37	0
1	D	3505	0	3406	28	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	215	0	151	18	0
3	B	215	0	150	12	0
3	C	215	0	150	10	0
3	D	215	0	150	13	0
4	A	12	0	18	1	0
4	B	28	0	42	5	0
4	C	12	0	18	2	0
4	D	8	0	12	2	0
5	A	447	0	0	9	0
5	B	494	0	0	11	0
5	C	516	0	0	5	0
5	D	325	0	0	6	0
All	All	16697	0	14259	186	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 6.

All (186) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ASN:OD1	1:A:312:GLN:HG3	1.42	1.19
1:A:125:CYS:SG	3:A:1:HEC:CAC	2.31	1.19
1:A:111:LYS:HG3	5:A:798:HOH:O	1.43	1.16
1:B:338:ASP:HB2	5:B:758:HOH:O	1.63	0.97
1:A:338:ASP:HB2	5:A:851:HOH:O	1.67	0.91
1:A:320:GLN:HE21	1:A:320:GLN:H	1.29	0.81
1:C:338:ASP:HB2	5:C:1095:HOH:O	1.83	0.79
1:B:309:ASN:ND2	1:B:312[B]:GLN:HG3	1.99	0.78
1:B:279:ASN:HB2	5:B:811:HOH:O	1.86	0.76
4:D:480:EDO:H12	5:D:786:HOH:O	1.88	0.72
1:B:240:GLN:O	1:B:244:LYS:HG2	1.90	0.71
1:B:456:GLN:O	1:B:460:LYS:HG2	1.92	0.70
1:D:320:GLN:HE21	1:D:320:GLN:H	1.39	0.69
1:A:62:GLN:HE21	1:A:302:LYS:HZ3	1.38	0.68
3:C:4:HEC:HMC1	3:C:4:HEC:HBC3	1.75	0.68
1:A:49:HIS:HD2	5:A:557:HOH:O	1.77	0.68
1:A:62:GLN:HE21	1:A:302:LYS:NZ	1.92	0.68
1:A:125:CYS:SG	3:A:1:HEC:C3C	2.82	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ASN:CG	1:A:312:GLN:HG3	2.14	0.68
3:B:4:HEC:HMC1	3:B:4:HEC:HBC3	1.73	0.67
1:B:99:THR:HG22	4:B:8:EDO:H22	1.77	0.67
1:D:52:GLN:H	1:D:52:GLN:NE2	1.92	0.67
1:C:290:VAL:HG12	1:C:312:GLN:HG2	1.77	0.67
1:B:99:THR:HG23	5:B:521:HOH:O	1.94	0.66
4:B:8:EDO:H21	5:B:853:HOH:O	1.95	0.66
1:B:320:GLN:HE21	1:B:320:GLN:H	1.43	0.66
3:B:1:HEC:HMC1	3:B:1:HEC:HBC3	1.79	0.65
1:D:320:GLN:H	1:D:320:GLN:NE2	1.94	0.65
1:D:311:ALA:H	4:D:480:EDO:H11	1.61	0.65
3:C:5:HEC:HMB1	3:C:5:HEC:HBB3	1.79	0.64
1:D:52:GLN:H	1:D:52:GLN:HE21	1.44	0.64
1:B:309:ASN:HD21	1:B:312[B]:GLN:HG3	1.61	0.63
1:B:320:GLN:H	1:B:320:GLN:NE2	1.96	0.63
1:B:391:HIS:HE1	3:B:4:HEC:O2D	1.81	0.62
1:C:346:GLN:NE2	1:C:413:ARG:HH11	1.96	0.62
1:C:62:GLN:HE21	1:C:302:LYS:NZ	1.98	0.61
1:A:320:GLN:H	1:A:320:GLN:NE2	1.96	0.61
1:D:252:ASN:ND2	1:D:254:LEU:H	1.98	0.61
1:B:323:ALA:O	1:B:327[A]:LYS:HG3	2.00	0.61
1:B:62:GLN:HE21	1:B:302:LYS:NZ	1.99	0.61
1:D:57:LYS:HE3	5:D:623:HOH:O	2.00	0.61
1:A:388:HIS:HD2	5:A:796:HOH:O	1.85	0.60
1:C:62:GLN:HE21	1:C:302:LYS:HZ3	1.49	0.60
1:A:391:HIS:HE1	3:A:4:HEC:O2D	1.84	0.60
3:C:1:HEC:HMC1	3:C:1:HEC:HBC3	1.83	0.60
1:A:292:ASN:C	1:A:292:ASN:HD22	2.05	0.59
1:A:460:LYS:HG2	5:A:676:HOH:O	2.01	0.59
3:D:3:HEC:HBC3	3:D:3:HEC:HMC1	1.83	0.59
1:B:309:ASN:CG	1:B:312[B]:GLN:HG3	2.23	0.59
1:D:309:ASN:ND2	1:D:312:GLN:HG2	2.18	0.59
1:B:327[A]:LYS:HE3	5:B:771:HOH:O	2.01	0.59
1:C:320:GLN:NE2	1:C:320:GLN:H	2.01	0.58
1:D:391:HIS:HE1	3:D:4:HEC:O2D	1.87	0.58
1:A:125:CYS:SG	3:A:1:HEC:CBC	2.92	0.58
1:A:280:VAL:HG13	3:A:5:HEC:HBC2	1.86	0.58
1:C:320:GLN:H	1:C:320:GLN:HE21	1.50	0.58
1:A:52:GLN:NE2	1:A:52:GLN:H	2.01	0.57
3:A:2:HEC:HMC1	3:A:2:HEC:HBC3	1.85	0.57
1:B:388:HIS:HE1	5:B:482:HOH:O	1.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ASN:ND2	1:A:254:LEU:H	2.02	0.57
3:D:2:HEC:HMC1	3:D:2:HEC:HBC3	1.87	0.57
1:C:340:LYS:HD2	1:C:385:ILE:HG21	1.88	0.56
1:B:52:GLN:NE2	1:B:52:GLN:H	2.04	0.55
1:A:292:ASN:ND2	1:A:296:LYS:H	2.05	0.55
1:A:125:CYS:SG	3:A:1:HEC:HAC	2.39	0.55
1:D:476:LEU:HG	1:D:477:SER:N	2.22	0.55
3:B:5:HEC:HMB1	3:B:5:HEC:HBB3	1.89	0.54
1:B:346:GLN:NE2	1:B:413:ARG:HH11	2.05	0.54
1:B:397:GLU:O	1:B:401[A]:MET:HG3	2.07	0.54
1:B:291:GLN:HG3	1:B:297:LEU:HD12	1.90	0.53
3:C:4:HEC:HMB1	3:C:4:HEC:HBB3	1.91	0.53
1:C:49:HIS:HD2	5:C:969:HOH:O	1.92	0.53
1:D:87:ASP:HB2	1:D:105:LEU:HB2	1.90	0.52
3:A:4:HEC:HMC1	3:A:4:HEC:HBC3	1.90	0.52
3:D:1:HEC:HBC3	3:D:1:HEC:HMC1	1.91	0.52
1:A:388:HIS:HE1	5:A:490:HOH:O	1.92	0.51
1:A:292:ASN:HD21	1:A:296:LYS:H	1.58	0.51
3:B:3:HEC:HMC1	3:B:3:HEC:HBC3	1.93	0.51
1:B:476:LEU:O	1:B:477:SER:HB2	2.10	0.51
1:A:346:GLN:NE2	1:A:413:ARG:HH11	2.09	0.51
1:C:52:GLN:NE2	1:C:52:GLN:H	2.08	0.51
1:C:391:HIS:HE1	3:C:4:HEC:O2D	1.93	0.51
3:B:5:HEC:HBC3	4:B:15:EDO:H11	1.92	0.50
1:B:49:HIS:HE1	5:B:594:HOH:O	1.95	0.50
1:C:456:GLN:HE21	1:C:460:LYS:HG3	1.75	0.50
1:B:340:LYS:CE	5:B:606:HOH:O	2.60	0.50
1:A:170:GLU:HA	1:A:173:LYS:HD2	1.94	0.50
1:C:418:ARG:HH22	4:C:11:EDO:C1	2.25	0.50
1:C:397:GLU:O	1:C:401:MET:HG3	2.12	0.49
1:A:52:GLN:H	1:A:52:GLN:HE21	1.60	0.49
3:A:3:HEC:HMC1	3:A:3:HEC:HBC3	1.93	0.49
1:B:62:GLN:HE21	1:B:302:LYS:HZ3	1.59	0.49
1:C:418:ARG:HH22	4:C:11:EDO:H11	1.77	0.48
3:B:4:HEC:HMB1	3:B:4:HEC:HBB3	1.95	0.48
1:C:388:HIS:HE1	5:C:1330:HOH:O	1.97	0.48
1:A:392:MET:HG2	3:A:4:HEC:C2D	2.45	0.47
1:C:252:ASN:ND2	1:C:254:LEU:H	2.12	0.47
1:B:457:ASP:O	1:B:461:THR:HG23	2.15	0.47
1:C:235:VAL:HB	1:C:401:MET:HE3	1.97	0.47
1:D:99:THR:HG23	5:D:535:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4:HEC:HMC1	3:D:4:HEC:HBC3	1.95	0.47
1:B:258:PRO:HG2	4:B:12:EDO:H21	1.97	0.47
1:B:284:ASP:OD1	4:B:15:EDO:H12	2.14	0.47
1:C:46:ALA:HB3	1:C:47:PRO:HD3	1.97	0.47
1:D:281:THR:HG22	5:D:565:HOH:O	2.14	0.47
1:D:282:CYS:HA	3:D:4:HEC:CHC	2.45	0.46
1:B:194:LYS:HB3	1:B:207:MET:CE	2.45	0.46
3:A:1:HEC:HMC1	3:A:1:HEC:HBC3	1.97	0.46
1:B:309:ASN:OD1	1:B:312[B]:GLN:HG3	2.15	0.46
1:A:227:PHE:CD2	1:A:227:PHE:N	2.84	0.46
1:B:244:LYS:HG3	5:B:762:HOH:O	2.15	0.46
1:A:406:MET:HB3	1:B:406:MET:HG2	1.97	0.46
1:A:213:HIS:HB3	1:A:266:GLU:HB2	1.97	0.45
1:A:214:VAL:HG21	1:A:227:PHE:CZ	2.51	0.45
1:C:213:HIS:HB3	1:C:266:GLU:HB2	1.99	0.45
1:C:292:ASN:HD21	1:C:296:LYS:H	1.64	0.45
1:C:159:GLY:O	3:C:2:HEC:HMC3	2.17	0.45
3:B:2:HEC:HMC1	3:B:2:HEC:HBC3	1.99	0.45
1:D:62:GLN:HE21	1:D:302:LYS:NZ	2.15	0.45
1:D:391:HIS:H	1:D:391:HIS:CD2	2.35	0.45
1:B:194:LYS:HB3	1:B:207:MET:HE1	1.99	0.45
1:C:234:LYS:H	1:C:237:ASN:HD22	1.64	0.45
1:C:280:VAL:HG13	3:C:5:HEC:HBC2	1.98	0.45
3:D:5:HEC:HMC1	3:D:5:HEC:HBC3	1.98	0.45
1:C:87:ASP:HB2	1:C:105:LEU:HB2	1.99	0.44
3:D:4:HEC:HMB1	3:D:4:HEC:HBB3	1.99	0.44
1:A:48:GLN:HB2	5:A:539:HOH:O	2.17	0.44
3:A:5:HEC:HBC3	3:A:5:HEC:HMC1	1.99	0.44
3:C:5:HEC:HBA2	3:D:5:HEC:HBA2	2.00	0.44
1:D:346:GLN:NE2	1:D:413:ARG:HH11	2.16	0.43
1:A:431:ILE:HG22	1:A:432:PRO:O	2.17	0.43
3:A:5:HEC:HMB1	3:A:5:HEC:HBB3	1.98	0.43
1:D:227:PHE:CD2	1:D:227:PHE:N	2.87	0.43
1:A:282:CYS:HA	3:A:4:HEC:CHC	2.48	0.43
1:D:228:PRO:HG3	1:D:242:TYR:OH	2.19	0.43
1:A:391:HIS:H	1:A:391:HIS:CD2	2.37	0.43
1:A:452:LYS:NZ	5:A:919:HOH:O	2.52	0.43
1:B:309:ASN:HD21	1:B:312[A]:GLN:HG2	1.82	0.43
1:D:182:ARG:HA	1:D:183:PRO:HD3	1.89	0.43
1:B:240:GLN:NE2	5:B:762:HOH:O	2.51	0.43
1:B:52:GLN:H	1:B:52:GLN:HE21	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:ALA:HB2	1:B:410:ALA:HB2	2.01	0.42
1:A:235:VAL:HB	1:A:401:MET:HE3	2.00	0.42
1:A:159:GLY:O	3:A:2:HEC:HMC3	2.20	0.42
1:B:49:HIS:HD2	5:B:654:HOH:O	2.01	0.42
1:D:168:SER:HA	1:D:169:PRO:HD3	1.91	0.42
1:D:327[A]:LYS:HG3	5:D:560:HOH:O	2.20	0.42
1:C:49:HIS:HE1	5:C:991:HOH:O	2.03	0.42
1:D:151:GLY:HA3	1:D:466:TRP:CE2	2.55	0.42
1:B:123:TRP:CG	1:B:154:ILE:HD13	2.55	0.42
1:C:194:LYS:HB3	1:C:207:MET:HE3	2.02	0.42
1:D:281:THR:O	3:D:4:HEC:HMC3	2.19	0.42
3:A:5:HEC:HBA2	3:B:5:HEC:HBA2	2.01	0.42
1:C:182:ARG:HG3	5:C:908:HOH:O	2.19	0.42
1:A:281:THR:HG22	5:A:580:HOH:O	2.20	0.41
1:A:309:ASN:CG	1:A:312:GLN:CG	2.86	0.41
1:D:280:VAL:HG13	3:D:5:HEC:HBC2	2.02	0.41
1:B:72:ASP:OD2	1:B:344:GLU:OE1	2.38	0.41
1:B:213:HIS:CE1	3:B:1:HEC:HMD1	2.54	0.41
3:B:2:HEC:HBC1	3:B:3:HEC:HHC	2.01	0.41
1:A:234:LYS:H	1:A:237:ASN:HD22	1.67	0.41
1:C:282:CYS:HA	3:C:4:HEC:CHC	2.49	0.41
1:A:305:ASN:HA	1:A:306:PRO:HD3	1.95	0.41
1:B:79:TRP:CE3	1:B:84:PHE:HB3	2.55	0.41
1:B:252:ASN:ND2	1:B:254:LEU:H	2.17	0.41
1:A:82:TYR:CD1	1:A:250:TRP:HB3	2.55	0.41
1:C:252:ASN:HD22	1:C:255:SER:H	1.68	0.41
1:C:292:ASN:ND2	1:C:296:LYS:H	2.19	0.41
3:D:5:HEC:HMB1	3:D:5:HEC:HBB3	2.03	0.41
1:A:472:LYS:N	1:A:472:LYS:HE3	2.35	0.41
1:B:175:LYS:HA	1:B:175:LYS:HD2	1.86	0.41
1:C:278:ASN:O	1:C:279[B]:ASN:CG	2.59	0.41
1:C:309:ASN:ND2	1:C:312:GLN:HE21	2.19	0.41
1:C:391:HIS:CD2	1:C:391:HIS:H	2.38	0.41
1:C:450:GLN:HE21	1:C:450:GLN:HB3	1.72	0.41
1:D:314:CYS:HA	3:D:5:HEC:CHC	2.51	0.41
1:D:388:HIS:HE1	5:D:485:HOH:O	2.04	0.41
1:A:392:MET:HG2	3:A:4:HEC:C1D	2.51	0.40
1:C:309:ASN:HD21	1:C:312:GLN:HE21	1.67	0.40
1:A:318:HIS:HB3	1:A:320:GLN:NE2	2.36	0.40
1:D:381:TRP:O	1:D:385:ILE:HG13	2.21	0.40
1:B:282:CYS:HA	3:B:4:HEC:CHC	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:5:HEC:HMC1	3:C:5:HEC:HBC3	2.03	0.40
1:A:274:ILE:HG21	3:A:5:HEC:HBA1	2.03	0.40
1:A:309:ASN:HA	4:A:480:EDO:H22	2.02	0.40
1:C:198:LYS:HE3	1:C:198:LYS:HB3	1.78	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	443/441 (100%)	433 (98%)	10 (2%)	0	100	100
1	B	443/441 (100%)	433 (98%)	10 (2%)	0	100	100
1	C	440/441 (100%)	431 (98%)	9 (2%)	0	100	100
1	D	444/441 (101%)	427 (96%)	16 (4%)	1 (0%)	47	39
All	All	1770/1764 (100%)	1724 (97%)	45 (2%)	1 (0%)	51	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	264	HIS

### 5.3.2 Protein sidechains [i](#)

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

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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	366/362 (101%)	354 (97%)	12 (3%)	38	31
1	B	366/362 (101%)	353 (96%)	13 (4%)	35	28
1	C	363/362 (100%)	351 (97%)	12 (3%)	38	31
1	D	367/362 (101%)	354 (96%)	13 (4%)	36	29
All	All	1462/1448 (101%)	1412 (97%)	50 (3%)	37	30

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	VAL
1	A	52	GLN
1	A	221	LYS
1	A	240[A]	GLN
1	A	240[B]	GLN
1	A	252	ASN
1	A	274	ILE
1	A	292	ASN
1	A	309	ASN
1	A	320	GLN
1	A	468	GLU
1	A	472	LYS
1	B	38	VAL
1	B	52	GLN
1	B	99	THR
1	B	175	LYS
1	B	208	VAL
1	B	250	TRP
1	B	252	ASN
1	B	309	ASN
1	B	320	GLN
1	B	325	LEU
1	B	419	LEU
1	B	461	THR
1	B	477	SER
1	C	52	GLN
1	C	111	LYS
1	C	149	ARG
1	C	221	LYS
1	C	240	GLN
1	C	250	TRP
1	C	274	ILE
1	C	292	ASN

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Mol	Chain	Res	Type
1	C	309	ASN
1	C	320	GLN
1	C	327	LYS
1	C	450	GLN
1	D	38	VAL
1	D	52	GLN
1	D	64	GLU
1	D	99	THR
1	D	114	GLU
1	D	221	LYS
1	D	244	LYS
1	D	252	ASN
1	D	274	ILE
1	D	309	ASN
1	D	320	GLN
1	D	325	LEU
1	D	419	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	52	GLN
1	A	62	GLN
1	A	237	ASN
1	A	252	ASN
1	A	291	GLN
1	A	292	ASN
1	A	309	ASN
1	A	320	GLN
1	A	346	GLN
1	A	371	GLN
1	A	388	HIS
1	A	391	HIS
1	A	430	GLN
1	A	469	GLN
1	B	49	HIS
1	B	52	GLN
1	B	62	GLN
1	B	240	GLN
1	B	252	ASN
1	B	309	ASN

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Mol	Chain	Res	Type
1	B	320	GLN
1	B	346	GLN
1	B	371	GLN
1	B	388	HIS
1	B	391	HIS
1	B	469	GLN
1	C	49	HIS
1	C	52	GLN
1	C	62	GLN
1	C	237	ASN
1	C	240	GLN
1	C	252	ASN
1	C	292	ASN
1	C	309	ASN
1	C	320	GLN
1	C	326	GLN
1	C	337	ASN
1	C	346	GLN
1	C	371	GLN
1	C	388	HIS
1	C	391	HIS
1	C	450	GLN
1	C	456	GLN
1	C	469	GLN
1	D	52	GLN
1	D	62	GLN
1	D	237	ASN
1	D	252	ASN
1	D	291	GLN
1	D	309	ASN
1	D	320	GLN
1	D	346	GLN
1	D	371	GLN
1	D	388	HIS
1	D	391	HIS
1	D	450	GLN

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 43 ligands modelled in this entry, 8 are monoatomic - leaving 35 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HEC	D	4	2,1	32,50,50	2.09	8 (25%)	24,82,82	1.98	4 (16%)
3	HEC	B	1	5,1	32,50,50	1.84	6 (18%)	24,82,82	1.71	5 (20%)
3	HEC	B	4	1	32,50,50	2.23	8 (25%)	24,82,82	2.10	4 (16%)
4	EDO	C	9	-	3,3,3	0.44	0	2,2,2	0.55	0
3	HEC	A	1	5,1	32,50,50	2.08	6 (18%)	24,82,82	1.87	7 (29%)
3	HEC	A	2	1	32,50,50	1.98	8 (25%)	24,82,82	1.70	3 (12%)
3	HEC	C	3	2,1	32,50,50	2.28	10 (31%)	24,82,82	1.88	6 (25%)
4	EDO	A	480	-	3,3,3	0.27	0	2,2,2	1.47	0
4	EDO	B	6	-	3,3,3	0.52	0	2,2,2	0.26	0
3	HEC	C	5	1	32,50,50	2.19	8 (25%)	24,82,82	1.70	7 (29%)
4	EDO	B	14	-	3,3,3	0.47	0	2,2,2	0.36	0
3	HEC	C	4	2,1	32,50,50	2.33	10 (31%)	24,82,82	1.90	7 (29%)
4	EDO	B	8	-	3,3,3	0.35	0	2,2,2	0.74	0
4	EDO	A	10	-	3,3,3	0.41	0	2,2,2	0.67	0
4	EDO	D	481	-	3,3,3	0.31	0	2,2,2	0.71	0
4	EDO	D	480	-	3,3,3	0.37	0	2,2,2	0.85	0
4	EDO	A	7	-	3,3,3	0.70	0	2,2,2	0.27	0
3	HEC	A	4	2,1	32,50,50	2.12	6 (18%)	24,82,82	2.11	4 (16%)
3	HEC	D	3	2,1	32,50,50	1.93	6 (18%)	24,82,82	2.15	7 (29%)
3	HEC	B	2	1	32,50,50	1.96	4 (12%)	24,82,82	2.21	8 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	B	12	-	3,3,3	0.48	0	2,2,2	0.37	0
3	HEC	D	5	1	32,50,50	2.24	6 (18%)	24,82,82	1.83	5 (20%)
4	EDO	B	15	-	3,3,3	0.37	0	2,2,2	0.45	0
3	HEC	C	2	1	32,50,50	2.03	10 (31%)	24,82,82	1.82	5 (20%)
3	HEC	C	1	5,1	32,50,50	2.06	8 (25%)	24,82,82	1.66	3 (12%)
4	EDO	B	481	-	3,3,3	0.44	0	2,2,2	0.40	0
3	HEC	D	2	1	32,50,50	2.05	7 (21%)	24,82,82	1.68	4 (16%)
3	HEC	D	1	1	32,50,50	2.00	6 (18%)	24,82,82	1.65	4 (16%)
4	EDO	C	13	-	3,3,3	0.47	0	2,2,2	0.44	0
4	EDO	C	11	-	3,3,3	0.38	0	2,2,2	0.96	0
3	HEC	A	5	1	32,50,50	2.03	7 (21%)	24,82,82	1.53	3 (12%)
3	HEC	B	5	1	32,50,50	3.31	8 (25%)	24,82,82	2.07	8 (33%)
4	EDO	B	480	-	3,3,3	0.18	0	2,2,2	1.08	0
3	HEC	A	3	2,1	32,50,50	2.13	8 (25%)	24,82,82	2.04	6 (25%)
3	HEC	B	3	2,1	32,50,50	2.05	7 (21%)	24,82,82	2.40	6 (25%)

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	D	4	2,1	-	0/10/54/54	-
3	HEC	B	1	5,1	-	2/10/54/54	-
3	HEC	B	4	1	-	1/10/54/54	-
4	EDO	C	9	-	-	1/1/1/1	-
3	HEC	A	1	5,1	-	2/10/54/54	-
3	HEC	A	2	1	-	2/10/54/54	-
3	HEC	C	3	2,1	-	0/10/54/54	-
4	EDO	A	480	-	-	0/1/1/1	-
4	EDO	B	6	-	-	0/1/1/1	-
3	HEC	C	5	1	-	5/10/54/54	-
4	EDO	B	14	-	-	0/1/1/1	-
3	HEC	C	4	2,1	-	3/10/54/54	-
4	EDO	B	8	-	-	0/1/1/1	-
4	EDO	A	10	-	-	0/1/1/1	-
4	EDO	D	481	-	-	0/1/1/1	-
4	EDO	D	480	-	-	1/1/1/1	-
4	EDO	A	7	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	A	4	2,1	-	3/10/54/54	-
3	HEC	D	3	2,1	-	0/10/54/54	-
3	HEC	B	2	1	-	2/10/54/54	-
4	EDO	B	12	-	-	0/1/1/1	-
3	HEC	D	5	1	-	5/10/54/54	-
4	EDO	B	15	-	-	1/1/1/1	-
3	HEC	C	2	1	-	2/10/54/54	-
3	HEC	C	1	5,1	-	2/10/54/54	-
4	EDO	B	481	-	-	1/1/1/1	-
3	HEC	D	2	1	-	4/10/54/54	-
3	HEC	D	1	1	-	3/10/54/54	-
4	EDO	C	13	-	-	1/1/1/1	-
4	EDO	C	11	-	-	0/1/1/1	-
3	HEC	A	5	1	-	4/10/54/54	-
3	HEC	B	5	1	-	5/10/54/54	-
4	EDO	B	480	-	-	1/1/1/1	-
3	HEC	A	3	2,1	-	0/10/54/54	-
3	HEC	B	3	2,1	-	0/10/54/54	-

All (147) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5	HEC	C1B-NB	13.99	1.65	1.36
3	C	4	HEC	C2B-C3B	-7.23	1.33	1.40
3	B	5	HEC	C2B-C3B	-6.99	1.33	1.40
3	A	4	HEC	C2B-C3B	-6.94	1.33	1.40
3	D	5	HEC	C2B-C3B	-6.92	1.33	1.40
3	B	4	HEC	C2B-C3B	-6.91	1.33	1.40
3	C	5	HEC	C3C-C2C	-6.18	1.34	1.40
3	D	2	HEC	C3D-C2D	5.88	1.55	1.37
3	C	3	HEC	C2B-C3B	-5.86	1.34	1.40
3	C	4	HEC	C3C-C2C	-5.83	1.34	1.40
3	A	3	HEC	C2B-C3B	-5.81	1.34	1.40
3	D	1	HEC	C3D-C2D	5.69	1.54	1.37
3	C	5	HEC	C2B-C3B	-5.66	1.34	1.40
3	A	5	HEC	C2B-C3B	-5.60	1.34	1.40
3	A	1	HEC	C3D-C2D	5.55	1.54	1.37
3	D	4	HEC	C3D-C2D	5.54	1.54	1.37
3	A	2	HEC	C3D-C2D	5.49	1.53	1.37
3	D	3	HEC	C3D-C2D	5.44	1.53	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	HEC	C3D-C2D	5.41	1.53	1.37
3	C	3	HEC	C3C-C2C	-5.37	1.35	1.40
3	C	2	HEC	C3C-C2C	-5.36	1.35	1.40
3	A	3	HEC	C3C-C2C	-5.27	1.35	1.40
3	C	1	HEC	C3D-C2D	5.27	1.53	1.37
3	B	5	HEC	C3D-C2D	5.27	1.53	1.37
3	D	5	HEC	C3D-C2D	5.21	1.53	1.37
3	B	4	HEC	C3C-C2C	-5.18	1.35	1.40
3	A	3	HEC	C3D-C2D	5.15	1.52	1.37
3	C	5	HEC	C3D-C2D	5.11	1.52	1.37
3	D	5	HEC	C3C-C2C	-5.10	1.35	1.40
3	B	2	HEC	C3D-C2D	5.08	1.52	1.37
3	A	4	HEC	C3D-C2D	5.05	1.52	1.37
3	A	1	HEC	C3C-C2C	-5.04	1.35	1.40
3	B	3	HEC	C2B-C3B	-5.03	1.35	1.40
3	D	4	HEC	C3C-C2C	-5.03	1.35	1.40
3	C	1	HEC	C2B-C3B	-5.02	1.35	1.40
3	C	4	HEC	C3D-C2D	5.01	1.52	1.37
3	A	5	HEC	C3D-C2D	4.94	1.52	1.37
3	B	2	HEC	C3C-C2C	-4.90	1.35	1.40
3	B	3	HEC	C3D-C2D	4.90	1.52	1.37
3	C	3	HEC	C3D-C2D	4.86	1.52	1.37
3	B	1	HEC	C3D-C2D	4.84	1.52	1.37
3	D	1	HEC	C3C-C2C	-4.80	1.35	1.40
3	B	5	HEC	C3C-C2C	-4.75	1.35	1.40
3	D	3	HEC	C3C-C2C	-4.73	1.35	1.40
3	D	2	HEC	C2B-C3B	-4.72	1.35	1.40
3	C	1	HEC	C3C-C2C	-4.54	1.36	1.40
3	D	4	HEC	C2B-C3B	-4.51	1.36	1.40
3	A	2	HEC	C2B-C3B	-4.48	1.36	1.40
3	B	4	HEC	C3D-C2D	4.43	1.50	1.37
3	D	3	HEC	C2B-C3B	-4.35	1.36	1.40
3	D	2	HEC	C3C-C2C	-4.31	1.36	1.40
3	B	3	HEC	C4B-C3B	4.30	1.50	1.43
3	B	2	HEC	C2B-C3B	-4.19	1.36	1.40
3	D	1	HEC	C2B-C3B	-4.15	1.36	1.40
3	B	1	HEC	C2B-C3B	-4.04	1.36	1.40
3	A	4	HEC	C3C-C2C	-3.96	1.36	1.40
3	A	2	HEC	C3C-C2C	-3.91	1.36	1.40
3	B	3	HEC	C3C-C2C	-3.84	1.36	1.40
3	A	1	HEC	CAD-C3D	3.80	1.57	1.52
3	A	5	HEC	C3C-C2C	-3.58	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	HEC	C2B-C3B	-3.55	1.37	1.40
3	B	1	HEC	C3C-C2C	-3.55	1.37	1.40
3	C	3	HEC	C4D-ND	3.27	1.42	1.36
3	D	5	HEC	CAD-C3D	3.14	1.56	1.52
3	C	3	HEC	CAD-C3D	3.03	1.56	1.52
3	C	2	HEC	C2B-C3B	-2.99	1.37	1.40
3	C	5	HEC	CAD-C3D	2.95	1.56	1.52
3	C	4	HEC	CMD-C2D	2.92	1.57	1.51
3	D	4	HEC	C3C-C4C	2.91	1.48	1.43
3	C	3	HEC	C1D-ND	2.89	1.42	1.36
3	C	4	HEC	CAD-C3D	2.88	1.56	1.52
3	C	3	HEC	CMA-C3A	2.87	1.58	1.51
3	B	5	HEC	CAD-C3D	2.84	1.56	1.52
3	B	4	HEC	CMB-C2B	2.84	1.58	1.51
3	C	2	HEC	C4B-C3B	2.83	1.48	1.43
3	C	1	HEC	C3C-C4C	2.80	1.48	1.43
3	A	5	HEC	CAD-C3D	2.79	1.56	1.52
3	C	1	HEC	CAD-C3D	2.77	1.56	1.52
3	C	2	HEC	C3C-C4C	2.76	1.48	1.43
3	C	5	HEC	C1D-ND	2.72	1.41	1.36
3	B	5	HEC	C1D-ND	2.68	1.41	1.36
3	B	5	HEC	C4D-ND	2.64	1.41	1.36
3	A	3	HEC	CMA-C3A	2.63	1.57	1.51
3	A	5	HEC	C3C-C4C	2.59	1.47	1.43
3	D	4	HEC	C1D-ND	2.57	1.41	1.36
3	A	4	HEC	C3C-C4C	2.55	1.47	1.43
3	C	1	HEC	CAA-C2A	2.53	1.56	1.52
3	B	2	HEC	CAD-C3D	2.50	1.55	1.52
3	A	2	HEC	C1D-ND	2.46	1.41	1.36
3	A	1	HEC	C3C-C4C	2.46	1.47	1.43
3	D	5	HEC	C3C-C4C	2.43	1.47	1.43
3	A	4	HEC	CMA-C3A	2.42	1.57	1.51
3	C	4	HEC	CMB-C2B	2.41	1.57	1.51
3	D	2	HEC	C3C-C4C	2.40	1.47	1.43
3	A	3	HEC	C3C-C4C	2.37	1.47	1.43
3	A	2	HEC	C4B-C3B	2.37	1.47	1.43
3	D	5	HEC	C4D-ND	2.36	1.41	1.36
3	B	4	HEC	CAD-C3D	2.36	1.55	1.52
3	D	1	HEC	CAD-C3D	2.35	1.55	1.52
3	A	3	HEC	CAD-C3D	2.34	1.55	1.52
3	A	3	HEC	CMD-C2D	2.32	1.56	1.51
3	A	5	HEC	C4D-ND	2.31	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4	HEC	CAD-C3D	2.30	1.55	1.52
3	D	4	HEC	C4D-ND	2.30	1.40	1.36
3	C	5	HEC	CMD-C2D	2.29	1.56	1.51
3	D	2	HEC	CAD-C3D	2.29	1.55	1.52
3	C	1	HEC	C4B-C3B	2.27	1.47	1.43
3	C	4	HEC	CAA-C2A	2.26	1.56	1.52
3	A	2	HEC	C4D-ND	2.23	1.40	1.36
3	B	4	HEC	CAA-C2A	2.22	1.56	1.52
3	A	2	HEC	C3C-C4C	2.22	1.47	1.43
3	C	5	HEC	CMC-C2C	2.19	1.56	1.51
3	D	1	HEC	CAA-C2A	2.18	1.56	1.52
3	B	1	HEC	CMC-C2C	2.17	1.56	1.51
3	B	3	HEC	C1C-NC	2.17	1.40	1.36
3	C	2	HEC	CAD-C3D	2.17	1.55	1.52
3	D	3	HEC	C1C-NC	2.15	1.40	1.36
3	D	3	HEC	CMA-C3A	2.15	1.56	1.51
3	D	4	HEC	CMB-C2B	2.14	1.56	1.51
3	C	5	HEC	C3C-C4C	2.14	1.46	1.43
3	D	2	HEC	C4B-C3B	2.12	1.46	1.43
3	C	2	HEC	CMA-C3A	2.12	1.56	1.51
3	C	3	HEC	CMD-C2D	2.12	1.56	1.51
3	C	3	HEC	CMC-C2C	2.11	1.56	1.51
3	B	1	HEC	C4B-C3B	2.11	1.46	1.43
3	C	4	HEC	CBB-CAB	2.10	1.57	1.49
3	C	2	HEC	CAA-C2A	2.09	1.55	1.52
3	B	5	HEC	O2D-CGD	-2.09	1.23	1.30
3	C	1	HEC	C4D-ND	2.07	1.40	1.36
3	C	2	HEC	C4D-ND	2.07	1.40	1.36
3	A	2	HEC	CAA-C2A	2.06	1.55	1.52
3	D	3	HEC	C1D-ND	2.05	1.40	1.36
3	A	1	HEC	CAA-C2A	2.05	1.55	1.52
3	C	4	HEC	CMA-C3A	2.04	1.56	1.51
3	D	1	HEC	C4B-C3B	2.04	1.46	1.43
3	A	3	HEC	CMC-C2C	2.04	1.56	1.51
3	A	4	HEC	C1D-ND	2.04	1.40	1.36
3	B	4	HEC	C1D-ND	2.04	1.40	1.36
3	A	5	HEC	CMC-C2C	2.03	1.56	1.51
3	C	2	HEC	C1D-ND	2.03	1.40	1.36
3	C	4	HEC	CMC-C2C	2.03	1.56	1.51
3	D	2	HEC	C2A-C1A	2.03	1.47	1.42
3	B	3	HEC	CBB-CAB	2.03	1.57	1.49
3	B	4	HEC	CBB-CAB	2.01	1.57	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	HEC	CBB-CAB	2.01	1.57	1.49
3	B	3	HEC	CMD-C2D	2.00	1.55	1.51
3	B	1	HEC	C3C-C4C	2.00	1.46	1.43

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3	HEC	C2B-C3B-C4B	-7.62	98.12	106.35
3	B	4	HEC	CBA-CAA-C2A	-6.83	101.09	112.60
3	A	4	HEC	CBA-CAA-C2A	-5.90	102.66	112.60
3	B	2	HEC	CMB-C2B-C1B	-5.80	119.55	128.46
3	C	3	HEC	CMC-C2C-C1C	-5.62	119.83	128.46
3	B	2	HEC	CMC-C2C-C1C	-5.39	120.18	128.46
3	D	4	HEC	CBA-CAA-C2A	-5.24	103.77	112.60
3	D	4	HEC	CMC-C2C-C1C	-5.16	120.54	128.46
3	D	3	HEC	CBA-CAA-C2A	-5.12	103.97	112.60
3	A	3	HEC	CBA-CAA-C2A	-5.11	103.98	112.60
3	A	2	HEC	CMC-C2C-C1C	-5.00	120.78	128.46
3	B	4	HEC	CMC-C2C-C1C	-4.72	121.21	128.46
3	C	2	HEC	CMC-C2C-C1C	-4.67	121.29	128.46
3	D	5	HEC	CMC-C2C-C1C	-4.66	121.30	128.46
3	B	5	HEC	C3B-C4B-NB	4.61	119.64	110.94
3	C	4	HEC	CMC-C2C-C1C	-4.55	121.47	128.46
3	C	2	HEC	CMB-C2B-C1B	-4.55	121.47	128.46
3	A	1	HEC	CMC-C2C-C1C	-4.54	121.49	128.46
3	A	4	HEC	CMB-C2B-C1B	-4.50	121.54	128.46
3	A	3	HEC	CMC-C2C-C1C	-4.43	121.66	128.46
3	A	5	HEC	CMC-C2C-C1C	-4.43	121.66	128.46
3	A	4	HEC	CMC-C2C-C1C	-4.41	121.68	128.46
3	C	1	HEC	CMB-C2B-C1B	-4.33	121.80	128.46
3	D	3	HEC	CMB-C2B-C1B	-4.30	121.85	128.46
3	D	5	HEC	CBA-CAA-C2A	-4.18	105.57	112.60
3	B	1	HEC	CMB-C2B-C1B	-3.94	122.41	128.46
3	B	5	HEC	CMB-C2B-C1B	-3.90	122.47	128.46
3	D	1	HEC	CMC-C2C-C1C	-3.83	122.58	128.46
3	D	2	HEC	CMC-C2C-C1C	-3.80	122.63	128.46
3	C	4	HEC	CBA-CAA-C2A	-3.75	106.29	112.60
3	D	1	HEC	CMB-C2B-C1B	-3.74	122.71	128.46
3	D	4	HEC	CMC-C2C-C3C	3.73	130.21	125.82
3	C	1	HEC	CMC-C2C-C1C	-3.68	122.81	128.46
3	D	2	HEC	CBA-CAA-C2A	-3.64	106.47	112.60
3	B	3	HEC	CMC-C2C-C1C	-3.63	122.88	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3	HEC	CBD-CAD-C3D	-3.59	106.49	112.62
3	B	5	HEC	CMC-C2C-C1C	-3.57	122.98	128.46
3	B	1	HEC	CBA-CAA-C2A	-3.55	106.62	112.60
3	C	5	HEC	CMB-C2B-C1B	-3.55	123.01	128.46
3	B	3	HEC	CMB-C2B-C1B	-3.52	123.05	128.46
3	B	5	HEC	CBA-CAA-C2A	-3.43	106.83	112.60
3	A	3	HEC	CMB-C2B-C1B	-3.40	123.24	128.46
3	B	3	HEC	CBA-CAA-C2A	-3.34	106.97	112.60
3	D	3	HEC	CMC-C2C-C1C	-3.32	123.36	128.46
3	C	4	HEC	C1D-C2D-C3D	-3.26	104.73	107.00
3	A	1	HEC	CMB-C2B-C3B	3.19	129.57	125.82
3	C	4	HEC	CMB-C2B-C1B	-3.16	123.61	128.46
3	A	1	HEC	CMB-C2B-C1B	-3.11	123.68	128.46
3	D	5	HEC	CMC-C2C-C3C	3.10	129.47	125.82
3	B	1	HEC	CMC-C2C-C1C	-3.09	123.71	128.46
3	A	1	HEC	CMC-C2C-C3C	3.05	129.41	125.82
3	B	5	HEC	CAA-CBA-CGA	-2.98	105.41	113.76
3	C	5	HEC	CBA-CAA-C2A	-2.93	107.66	112.60
3	C	5	HEC	CAA-CBA-CGA	-2.89	105.65	113.76
3	B	3	HEC	CBD-CAD-C3D	-2.88	107.71	112.62
3	D	3	HEC	CMB-C2B-C3B	2.87	129.19	125.82
3	A	5	HEC	CMB-C2B-C1B	-2.85	124.08	128.46
3	C	5	HEC	CMC-C2C-C1C	-2.85	124.08	128.46
3	A	2	HEC	CMB-C2B-C1B	-2.83	124.12	128.46
3	C	3	HEC	CBA-CAA-C2A	-2.82	107.84	112.60
3	B	2	HEC	CMB-C2B-C3B	2.82	129.13	125.82
3	B	4	HEC	CMC-C2C-C3C	2.81	129.13	125.82
3	C	2	HEC	CMC-C2C-C3C	2.79	129.10	125.82
3	A	5	HEC	CBA-CAA-C2A	-2.78	107.92	112.60
3	A	3	HEC	CBD-CAD-C3D	-2.78	107.88	112.62
3	C	3	HEC	CMB-C2B-C1B	-2.74	124.25	128.46
3	C	5	HEC	CMA-C3A-C2A	2.72	130.07	124.94
3	B	5	HEC	CBD-CAD-C3D	-2.70	108.01	112.62
3	C	3	HEC	CMC-C2C-C3C	2.70	129.00	125.82
3	D	2	HEC	CMB-C2B-C1B	-2.70	124.32	128.46
3	A	1	HEC	C2B-C3B-C4B	2.69	109.25	106.35
3	C	4	HEC	CAD-CBD-CGD	-2.65	106.32	113.76
3	B	2	HEC	CBD-CAD-C3D	-2.63	108.13	112.62
3	C	1	HEC	CMA-C3A-C2A	2.62	129.89	124.94
3	D	3	HEC	C1D-C2D-C3D	-2.62	105.17	107.00
3	A	2	HEC	CBA-CAA-C2A	-2.60	108.22	112.60
3	B	5	HEC	C1D-C2D-C3D	-2.52	105.24	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	HEC	CMB-C2B-C3B	2.51	128.77	125.82
3	B	3	HEC	C1D-C2D-C3D	-2.44	105.30	107.00
3	C	2	HEC	CMA-C3A-C2A	2.42	129.51	124.94
3	D	1	HEC	C1D-C2D-C3D	-2.42	105.31	107.00
3	A	3	HEC	C1D-C2D-C3D	-2.42	105.31	107.00
3	D	4	HEC	CMB-C2B-C1B	-2.39	124.79	128.46
3	B	2	HEC	C1D-C2D-C3D	-2.38	105.34	107.00
3	A	3	HEC	O2A-CGA-CBA	2.36	121.63	114.03
3	C	5	HEC	C1D-C2D-C3D	-2.36	105.35	107.00
3	B	2	HEC	O2A-CGA-CBA	2.34	121.56	114.03
3	D	2	HEC	C3C-C4C-NC	-2.33	106.55	110.94
3	D	5	HEC	CAD-CBD-CGD	-2.32	107.25	113.76
3	B	1	HEC	C1D-C2D-C3D	-2.31	105.39	107.00
3	D	3	HEC	C3B-C4B-NB	-2.26	106.68	110.94
3	B	2	HEC	CMA-C3A-C2A	2.26	129.19	124.94
3	C	5	HEC	CMC-C2C-C3C	2.22	128.43	125.82
3	A	1	HEC	CBA-CAA-C2A	-2.20	108.90	112.60
3	C	4	HEC	CMC-C2C-C3C	2.17	128.38	125.82
3	B	5	HEC	CMA-C3A-C2A	2.17	129.04	124.94
3	C	3	HEC	C3C-C4C-NC	-2.09	106.99	110.94
3	B	4	HEC	O1A-CGA-CBA	-2.09	116.36	123.08
3	D	5	HEC	CMA-C3A-C2A	2.08	128.87	124.94
3	A	1	HEC	C3B-C4B-NB	-2.07	107.03	110.94
3	C	2	HEC	O2A-CGA-CBA	2.06	120.65	114.03
3	B	2	HEC	O2A-CGA-O1A	-2.06	118.17	123.30
3	A	4	HEC	CBD-CAD-C3D	-2.05	109.12	112.62
3	B	1	HEC	CMA-C3A-C2A	2.03	128.77	124.94
3	C	3	HEC	CBD-CAD-C3D	-2.03	109.16	112.62
3	C	4	HEC	CBD-CAD-C3D	-2.01	109.20	112.62

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4	HEC	C2A-CAA-CBA-CGA
3	B	5	HEC	C2A-CAA-CBA-CGA
3	D	5	HEC	C2A-CAA-CBA-CGA
4	C	13	EDO	O1-C1-C2-O2
3	C	5	HEC	C2A-CAA-CBA-CGA
4	B	481	EDO	O1-C1-C2-O2
4	C	9	EDO	O1-C1-C2-O2
4	B	480	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	D	5	HEC	CAA-CBA-CGA-O1A
3	B	2	HEC	CAA-CBA-CGA-O1A
3	A	5	HEC	CAA-CBA-CGA-O1A
3	B	5	HEC	CAD-CBD-CGD-O2D
3	A	2	HEC	CAA-CBA-CGA-O2A
3	C	2	HEC	CAA-CBA-CGA-O2A
3	C	5	HEC	CAA-CBA-CGA-O1A
3	A	2	HEC	CAA-CBA-CGA-O1A
3	A	4	HEC	CAA-CBA-CGA-O1A
3	D	2	HEC	CAA-CBA-CGA-O1A
3	A	5	HEC	CAD-CBD-CGD-O2D
3	B	1	HEC	CAA-CBA-CGA-O1A
3	C	5	HEC	CAD-CBD-CGD-O1D
3	A	5	HEC	CAD-CBD-CGD-O1D
3	B	5	HEC	CAA-CBA-CGA-O1A
3	C	1	HEC	CAA-CBA-CGA-O2A
3	D	5	HEC	CAA-CBA-CGA-O2A
3	B	1	HEC	CAA-CBA-CGA-O2A
3	D	5	HEC	CAD-CBD-CGD-O1D
3	A	5	HEC	CAA-CBA-CGA-O2A
3	C	2	HEC	CAA-CBA-CGA-O1A
3	C	5	HEC	CAA-CBA-CGA-O2A
3	B	5	HEC	CAD-CBD-CGD-O1D
3	C	1	HEC	CAA-CBA-CGA-O1A
3	D	1	HEC	CAA-CBA-CGA-O1A
3	D	1	HEC	CAA-CBA-CGA-O2A
3	B	5	HEC	CAA-CBA-CGA-O2A
3	C	5	HEC	CAD-CBD-CGD-O2D
3	D	2	HEC	CAA-CBA-CGA-O2A
3	A	4	HEC	CAA-CBA-CGA-O2A
3	D	5	HEC	CAD-CBD-CGD-O2D
3	B	2	HEC	CAA-CBA-CGA-O2A
3	A	1	HEC	CAA-CBA-CGA-O2A
3	D	1	HEC	C3D-CAD-CBD-CGD
3	A	1	HEC	CAA-CBA-CGA-O1A
4	B	15	EDO	O1-C1-C2-O2
3	B	4	HEC	CAA-CBA-CGA-O2A
4	D	480	EDO	O1-C1-C2-O2
3	C	4	HEC	CAD-CBD-CGD-O2D
3	D	2	HEC	CAD-CBD-CGD-O2D
3	D	2	HEC	CAD-CBD-CGD-O1D
3	C	4	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
3	C	4	HEC	CAA-CBA-CGA-O2A

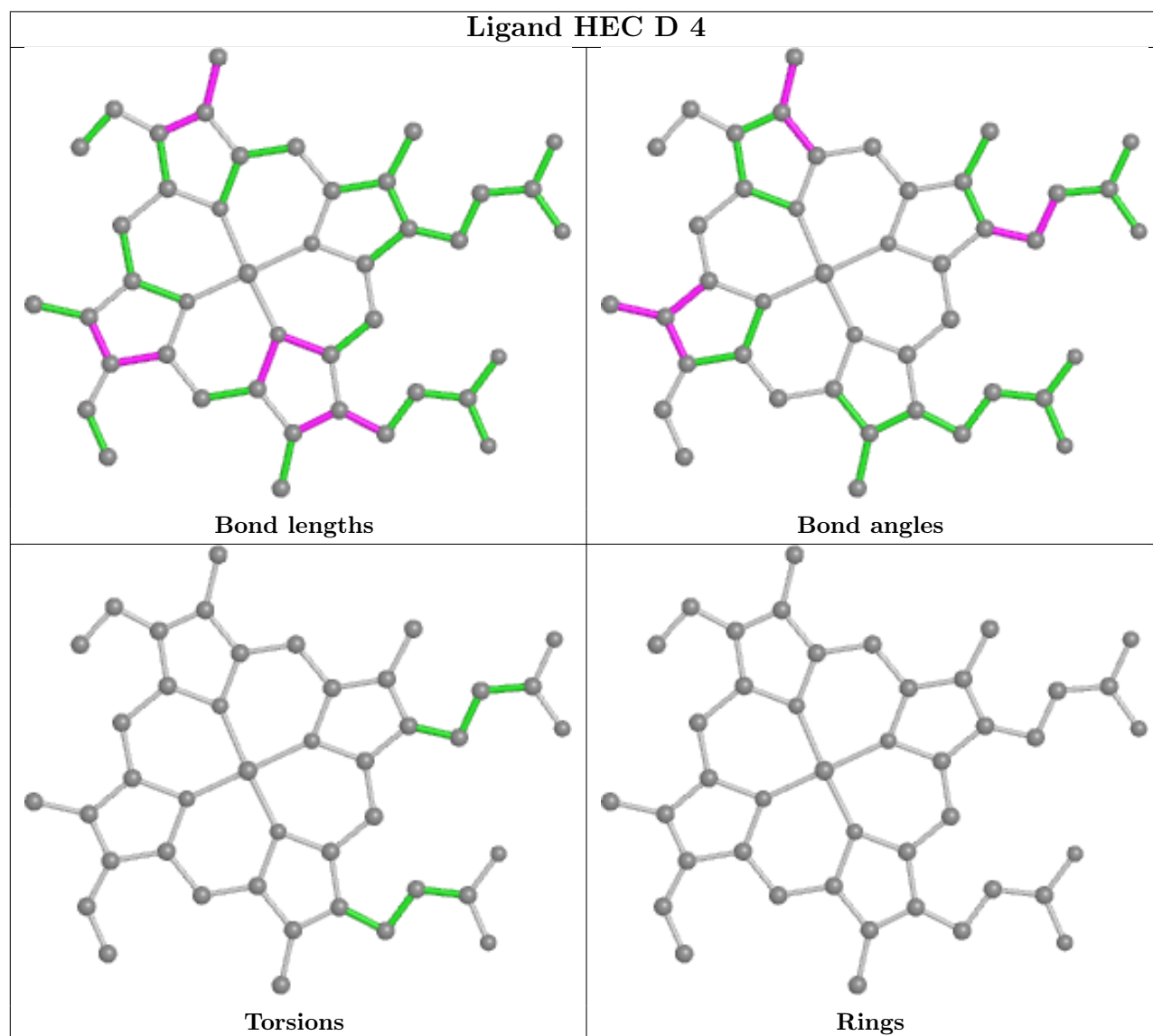
There are no ring outliers.

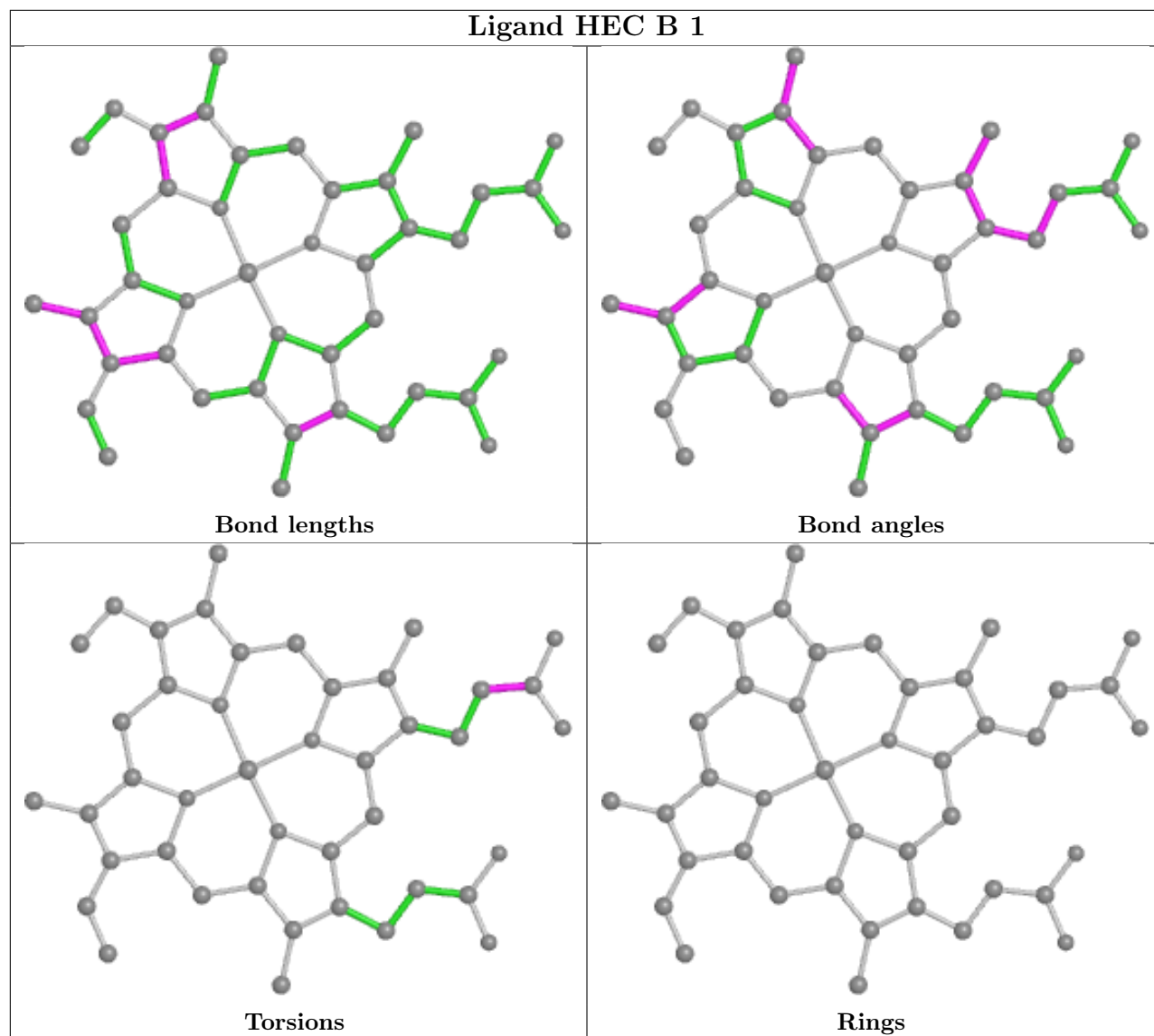
25 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	4	HEC	5	0
3	B	1	HEC	2	0
3	B	4	HEC	4	0
3	A	1	HEC	5	0
3	A	2	HEC	2	0
4	A	480	EDO	1	0
3	C	5	HEC	4	0
3	C	4	HEC	4	0
4	B	8	EDO	2	0
4	D	480	EDO	2	0
3	A	4	HEC	5	0
3	D	3	HEC	1	0
3	B	2	HEC	2	0
4	B	12	EDO	1	0
3	D	5	HEC	5	0
4	B	15	EDO	2	0
3	C	2	HEC	1	0
3	C	1	HEC	1	0
3	D	2	HEC	1	0
3	D	1	HEC	1	0
4	C	11	EDO	2	0
3	A	5	HEC	5	0
3	B	5	HEC	3	0
3	A	3	HEC	1	0
3	B	3	HEC	2	0

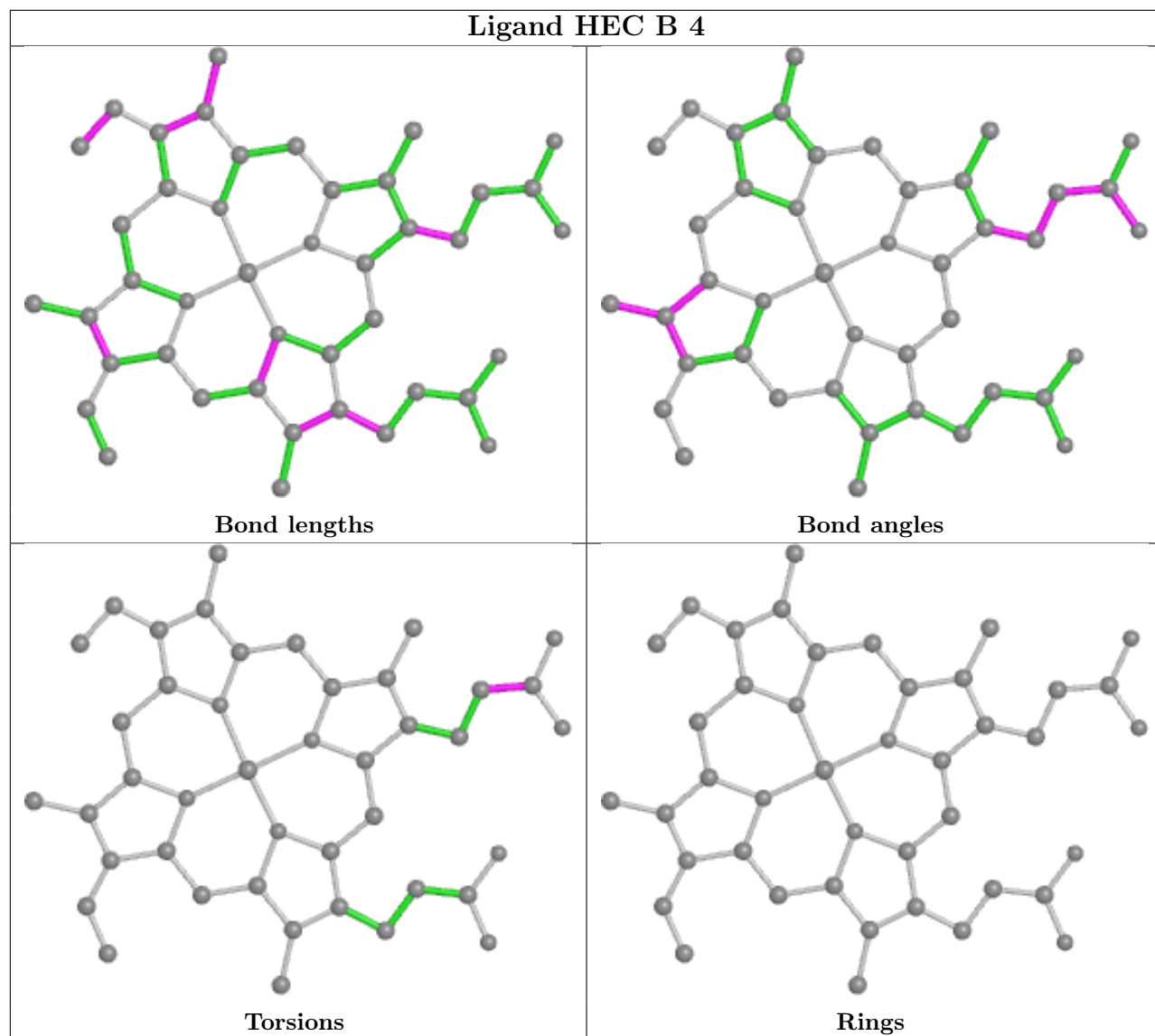
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

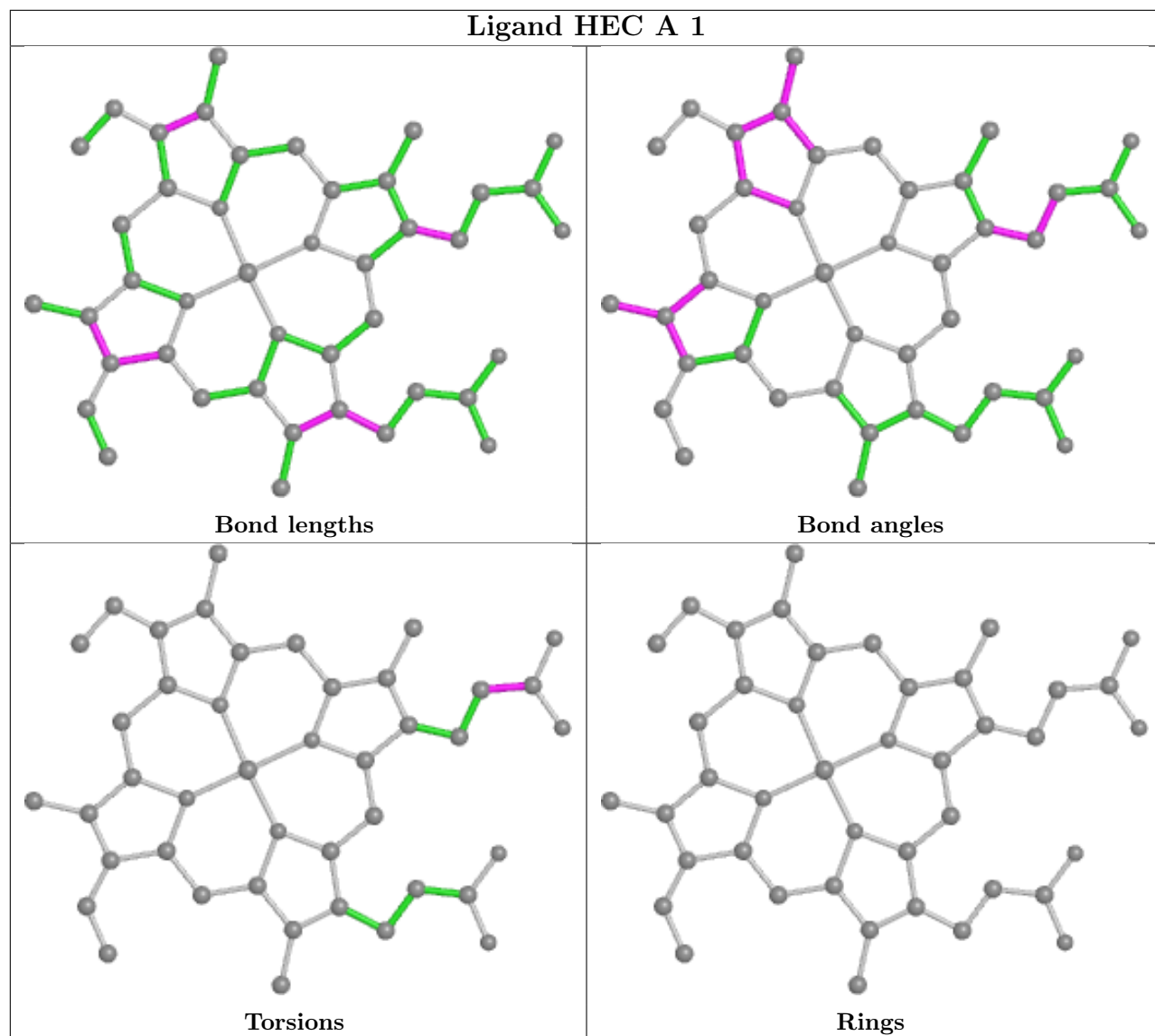
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

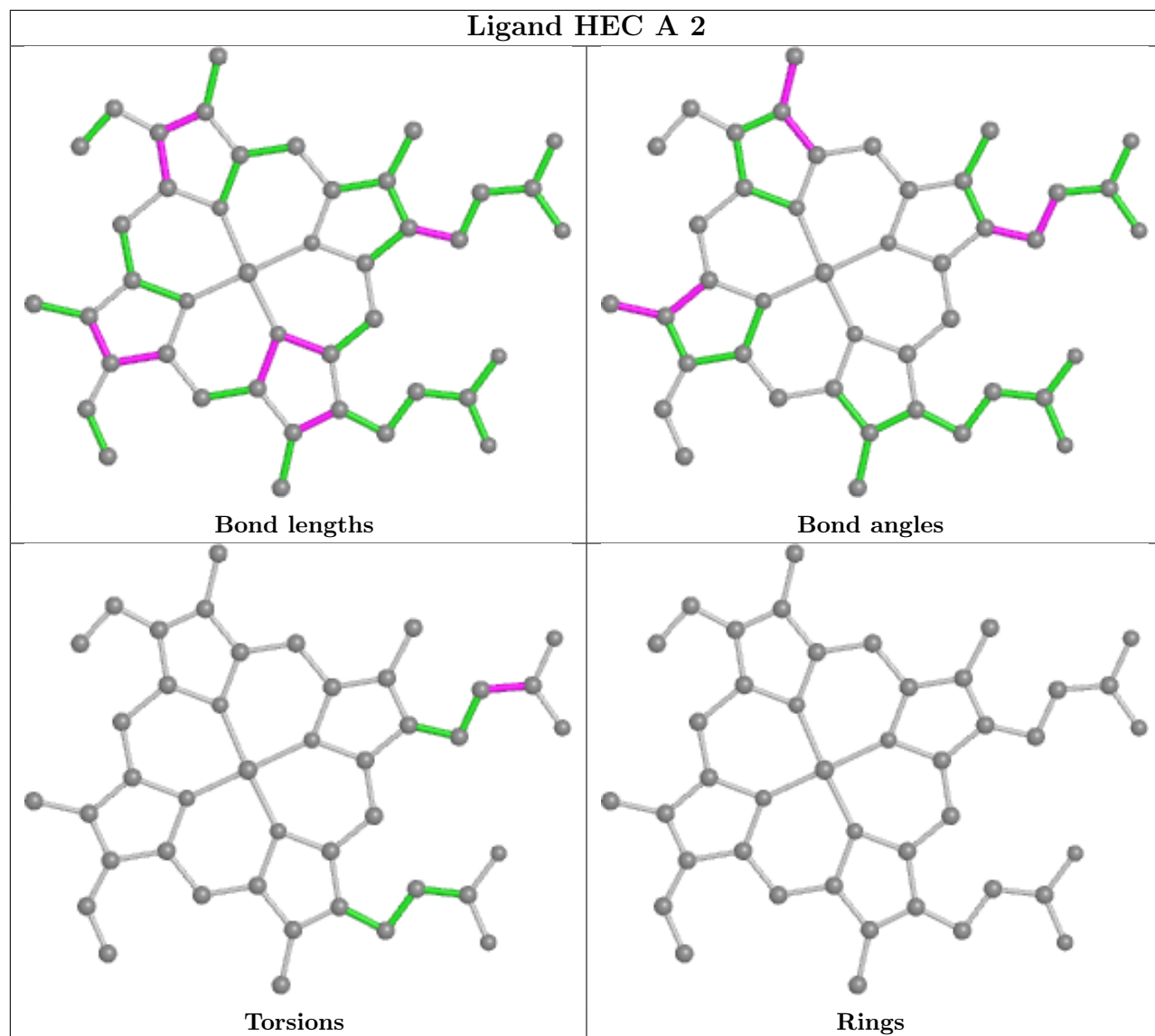


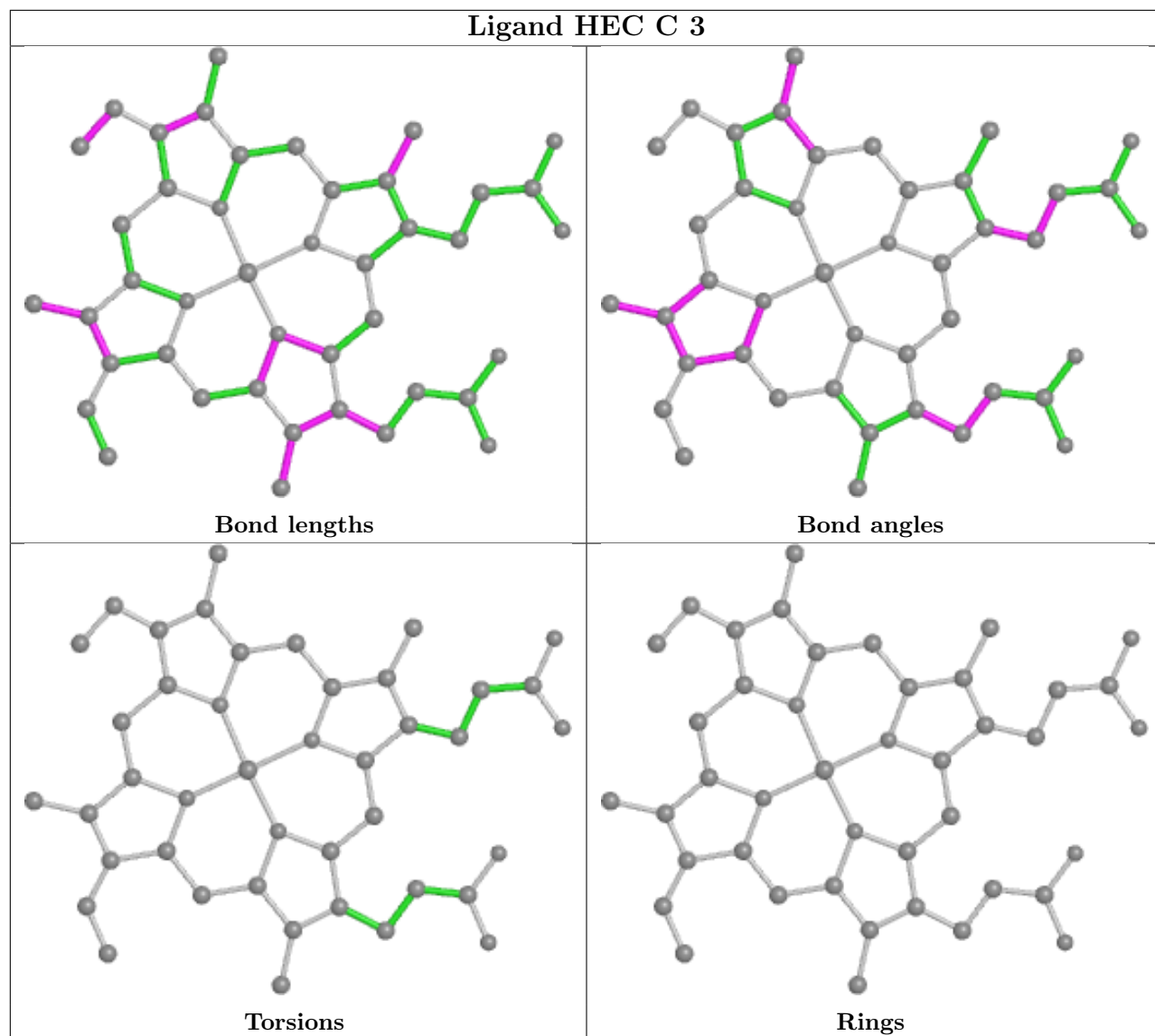


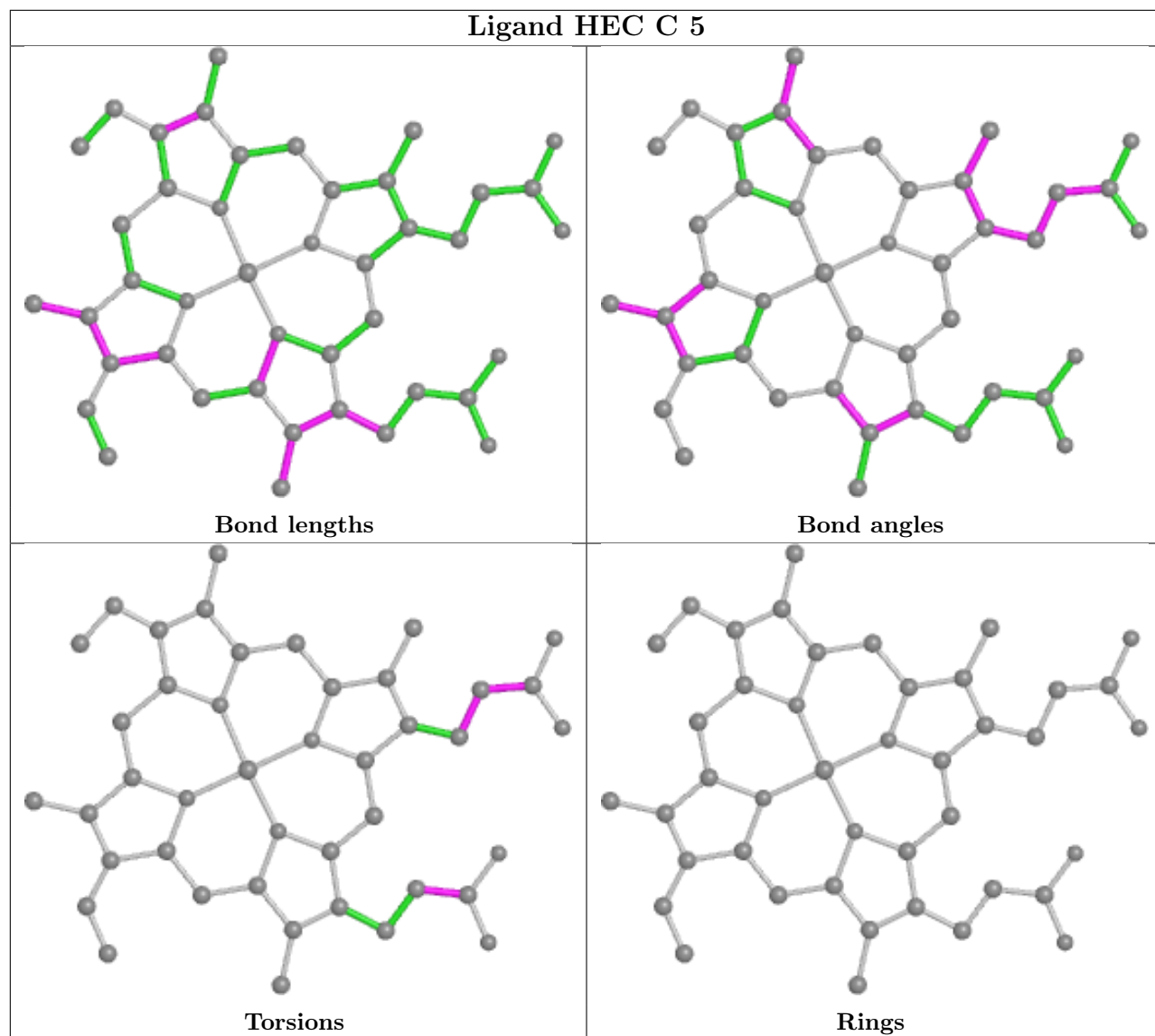


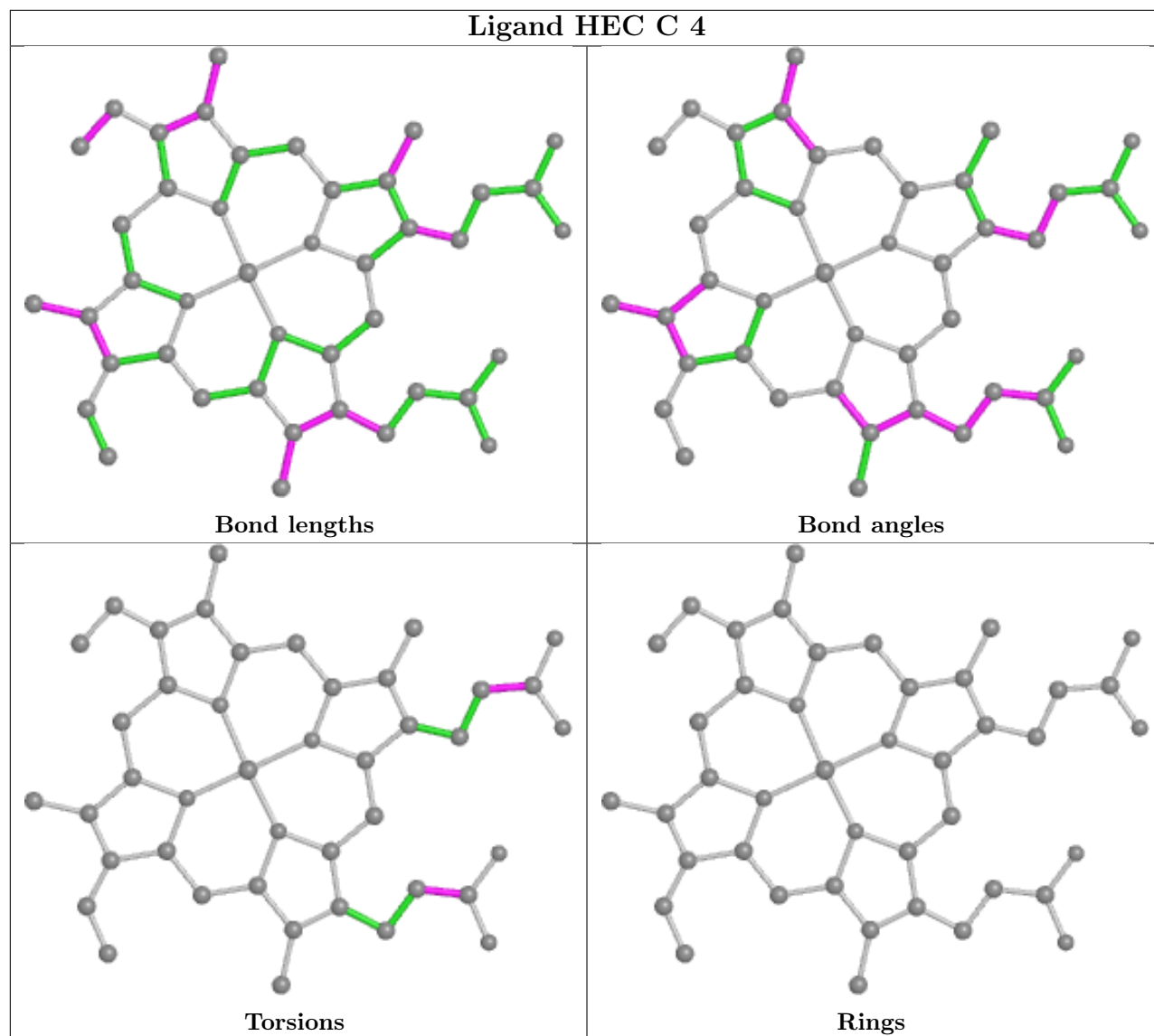


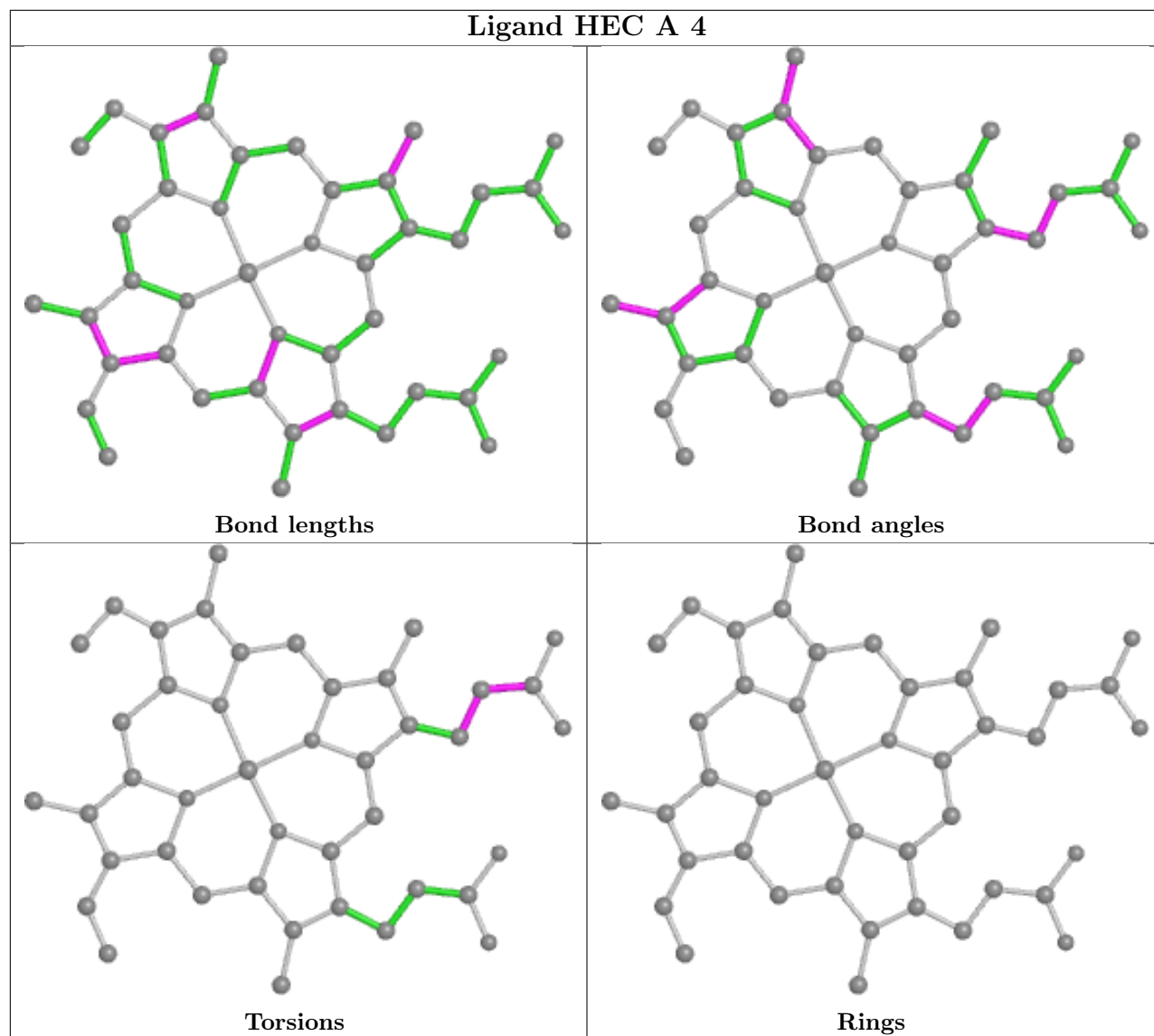


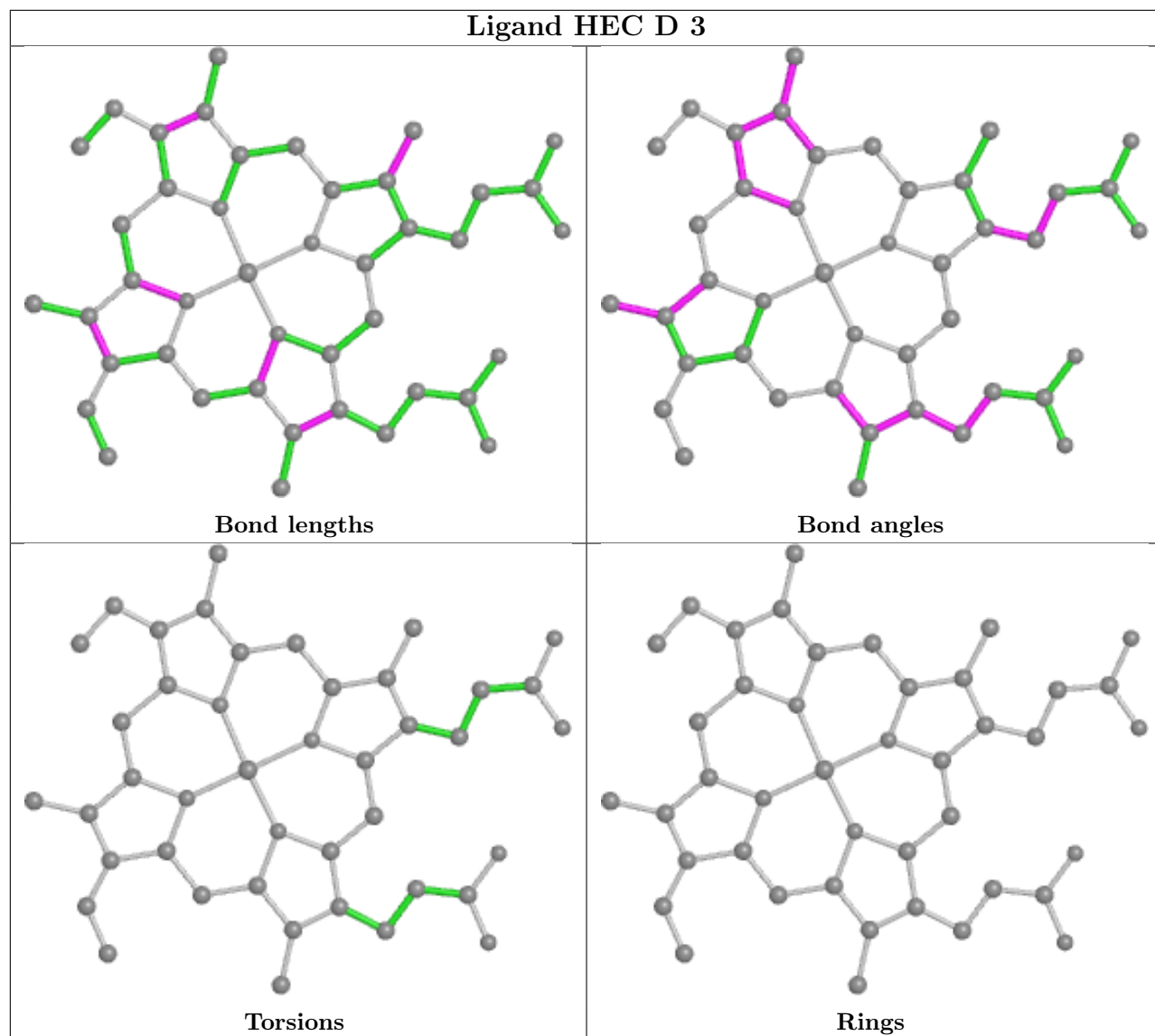




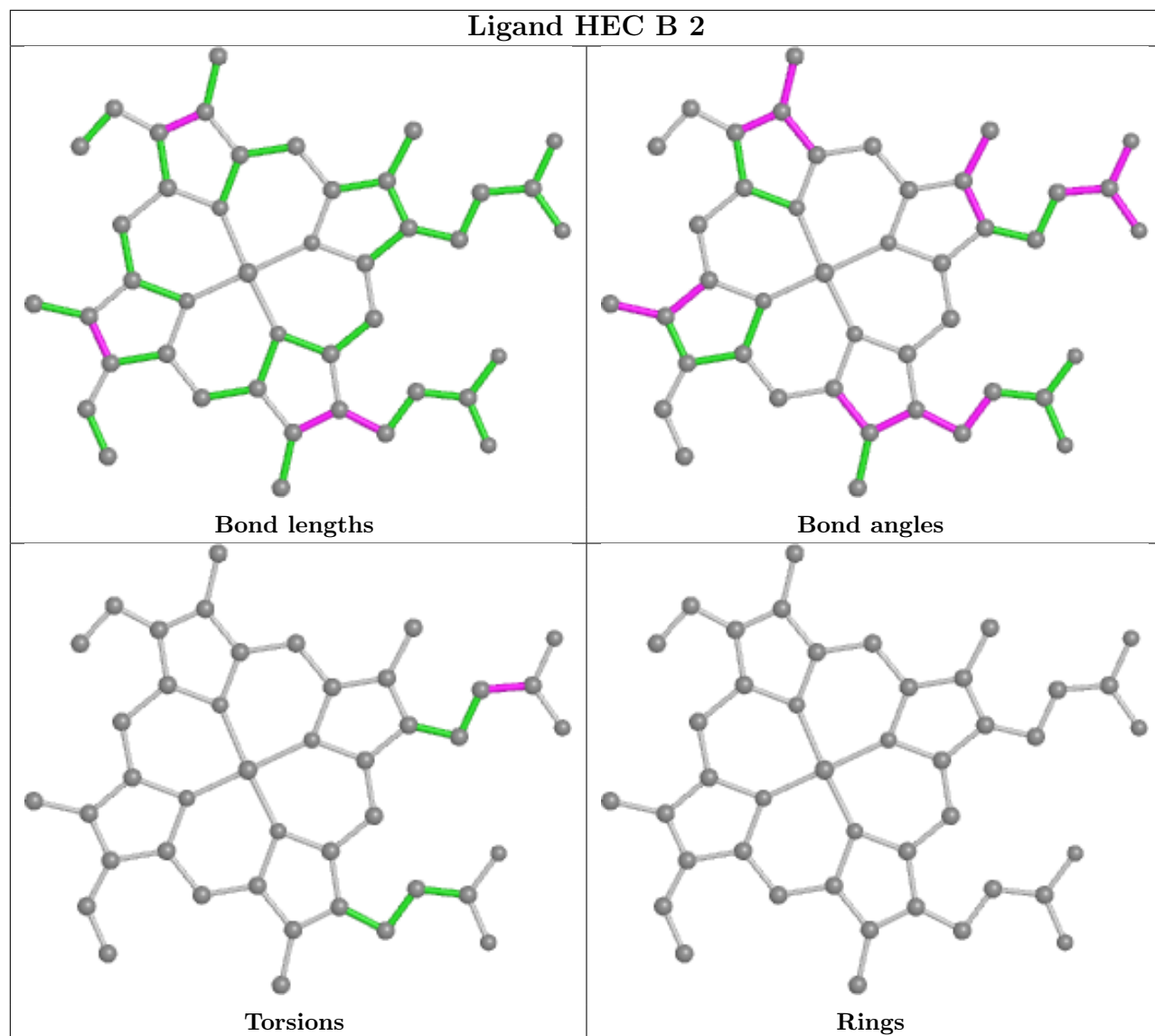


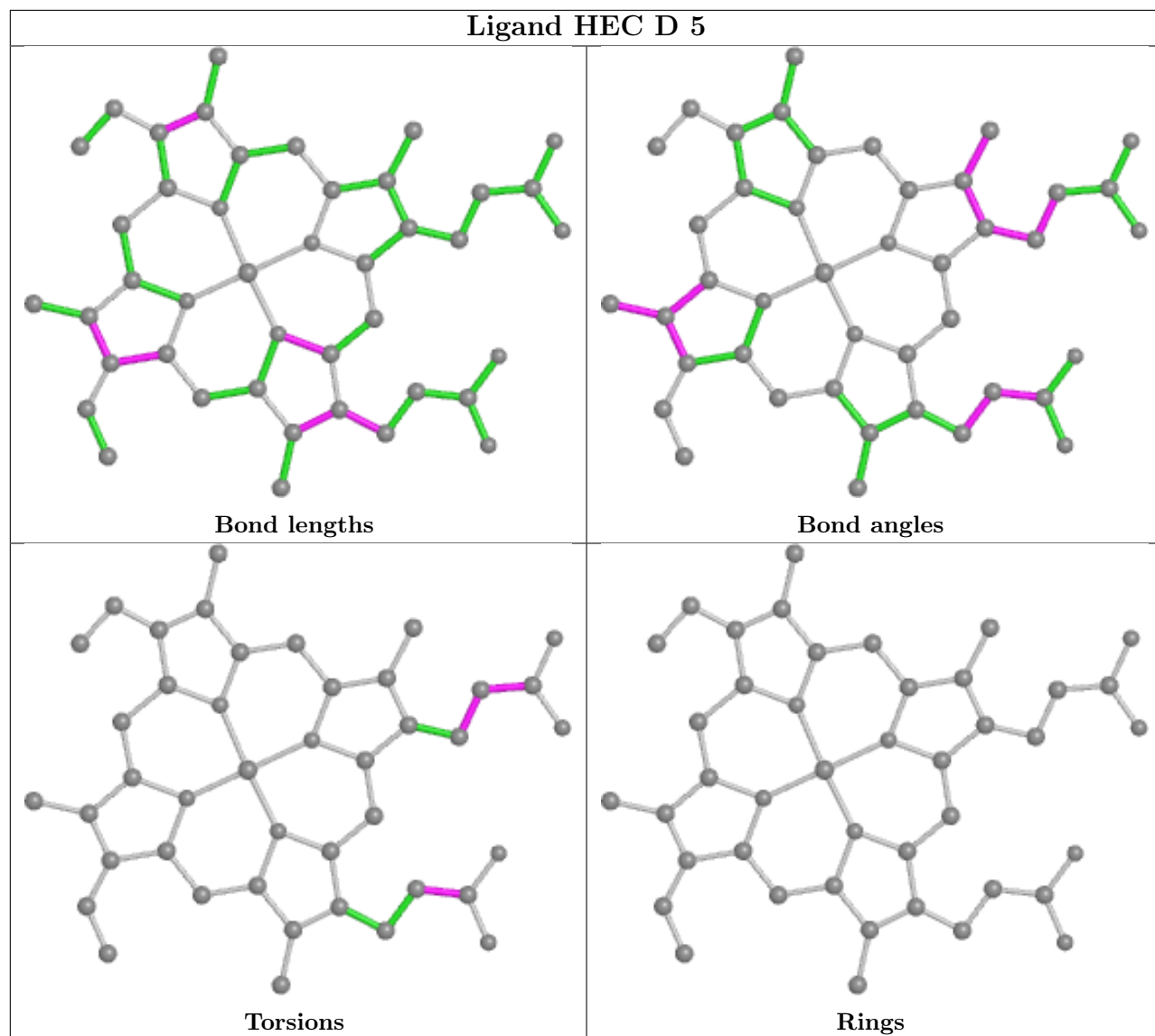


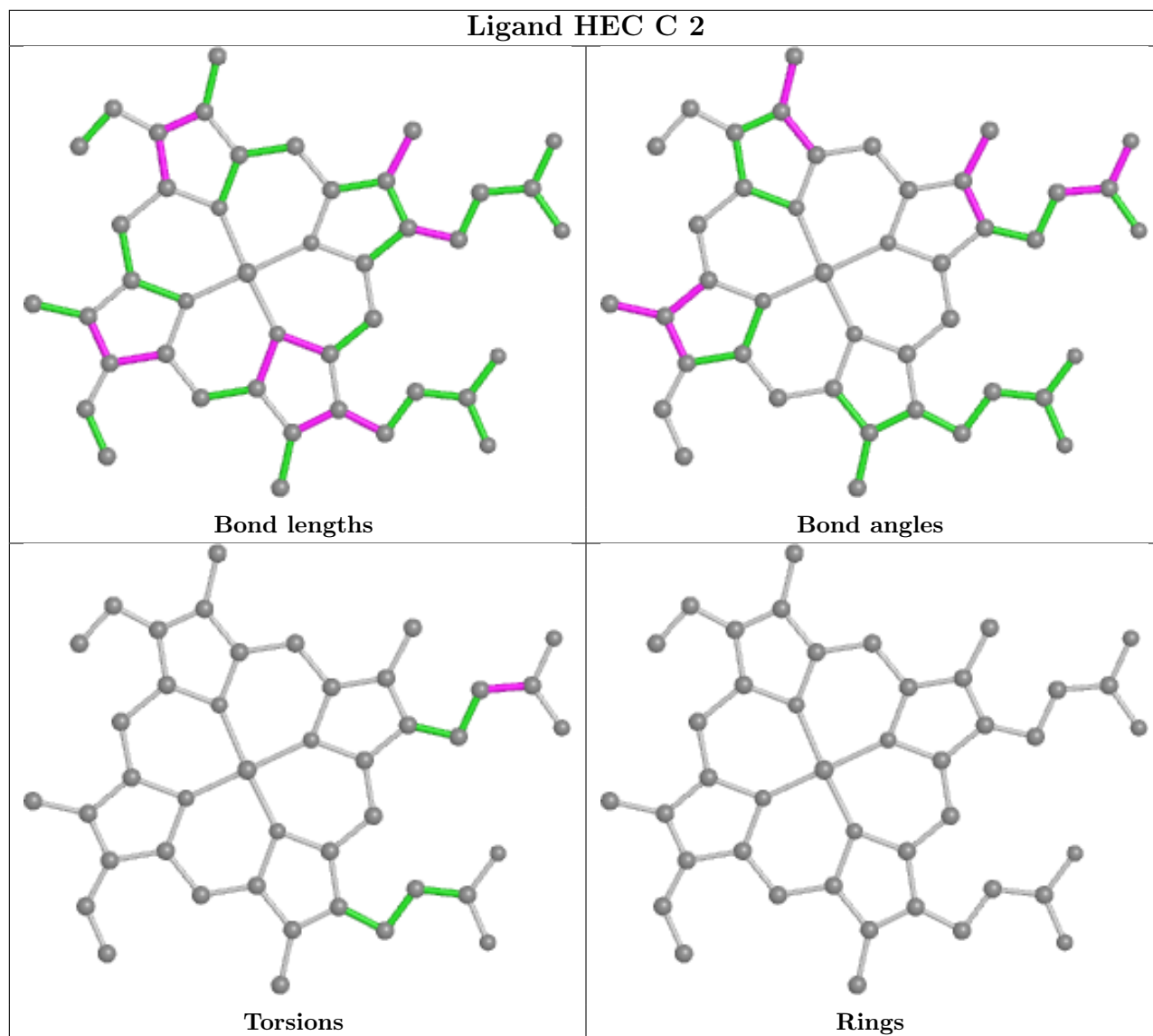


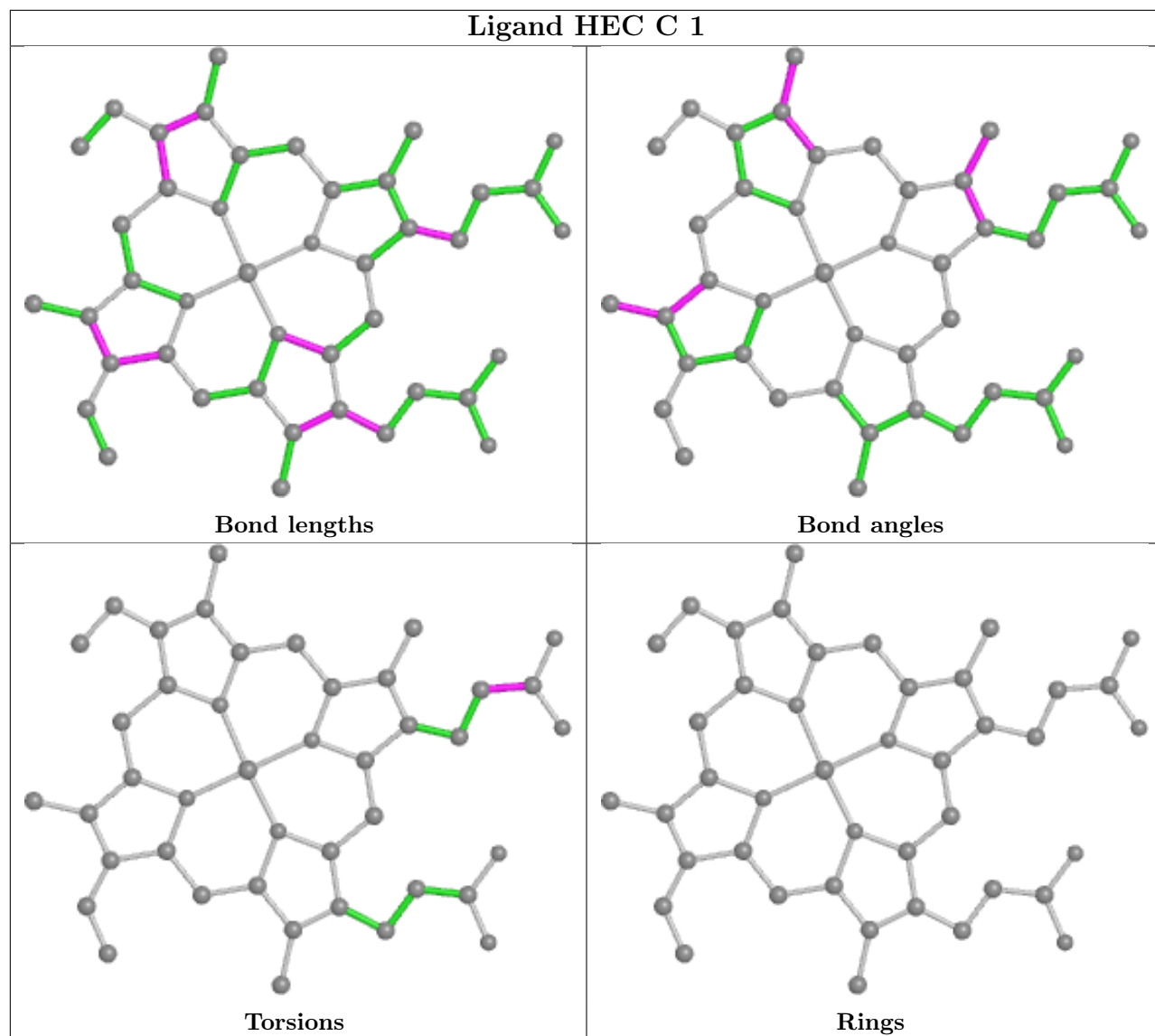


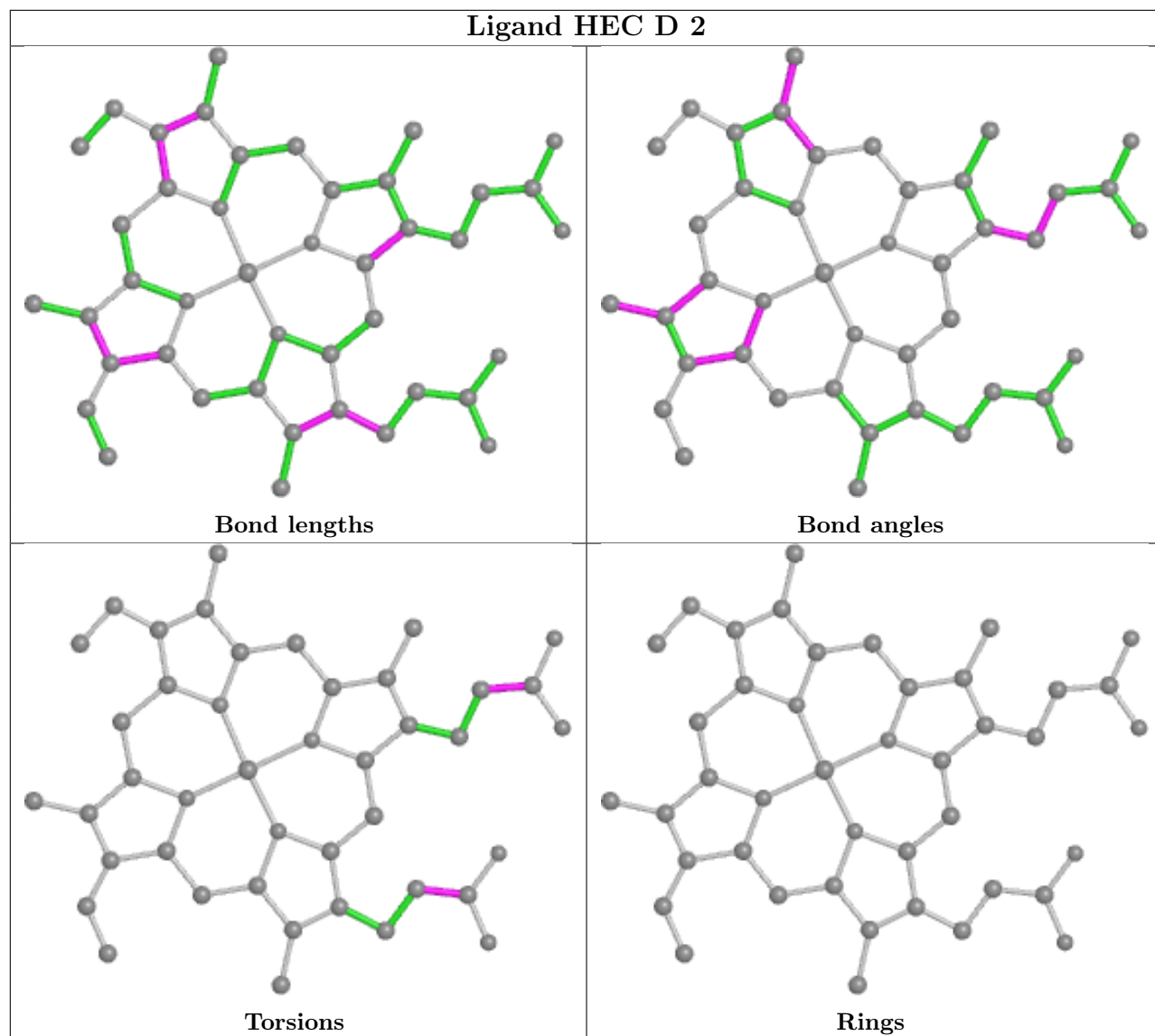


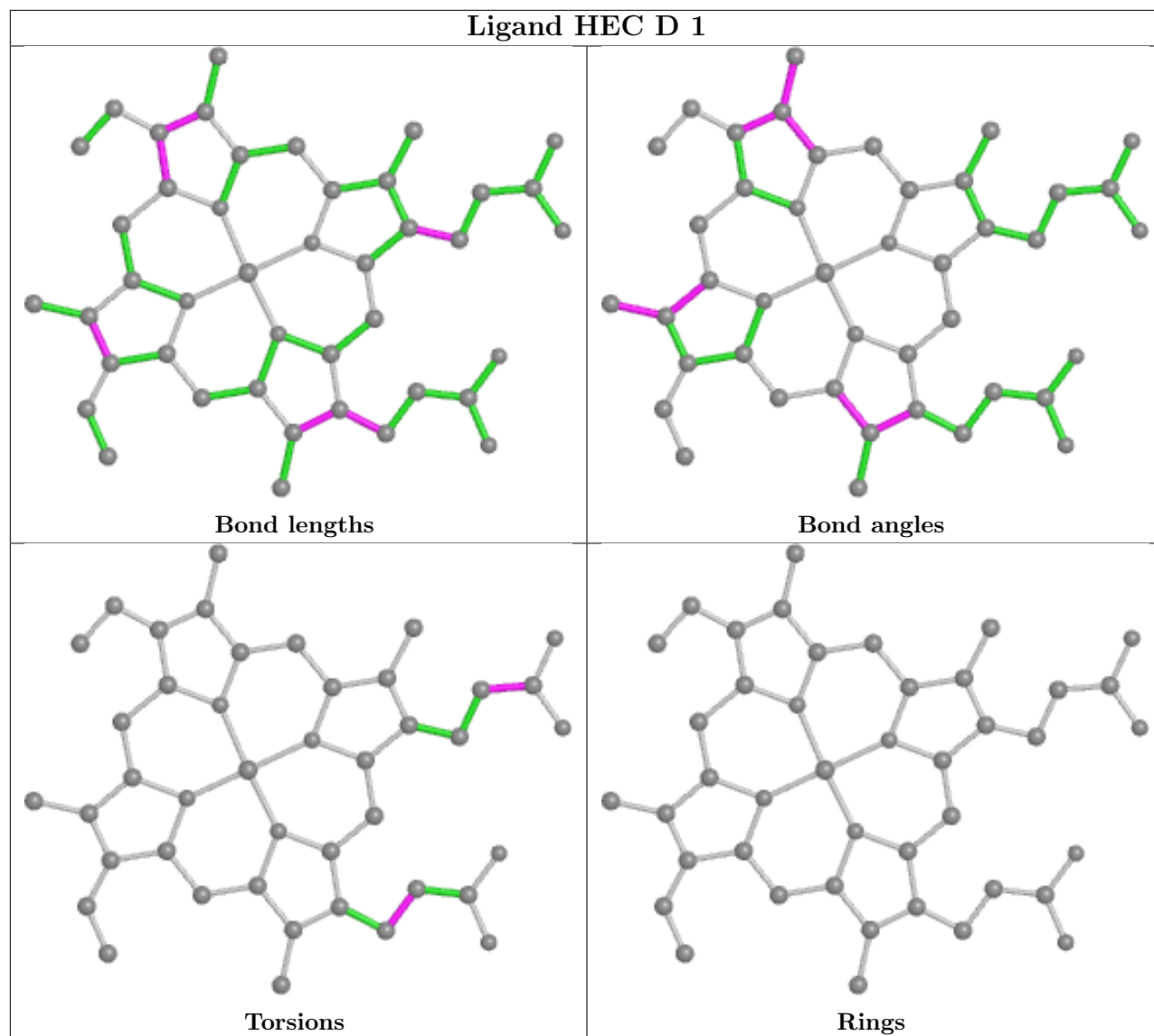


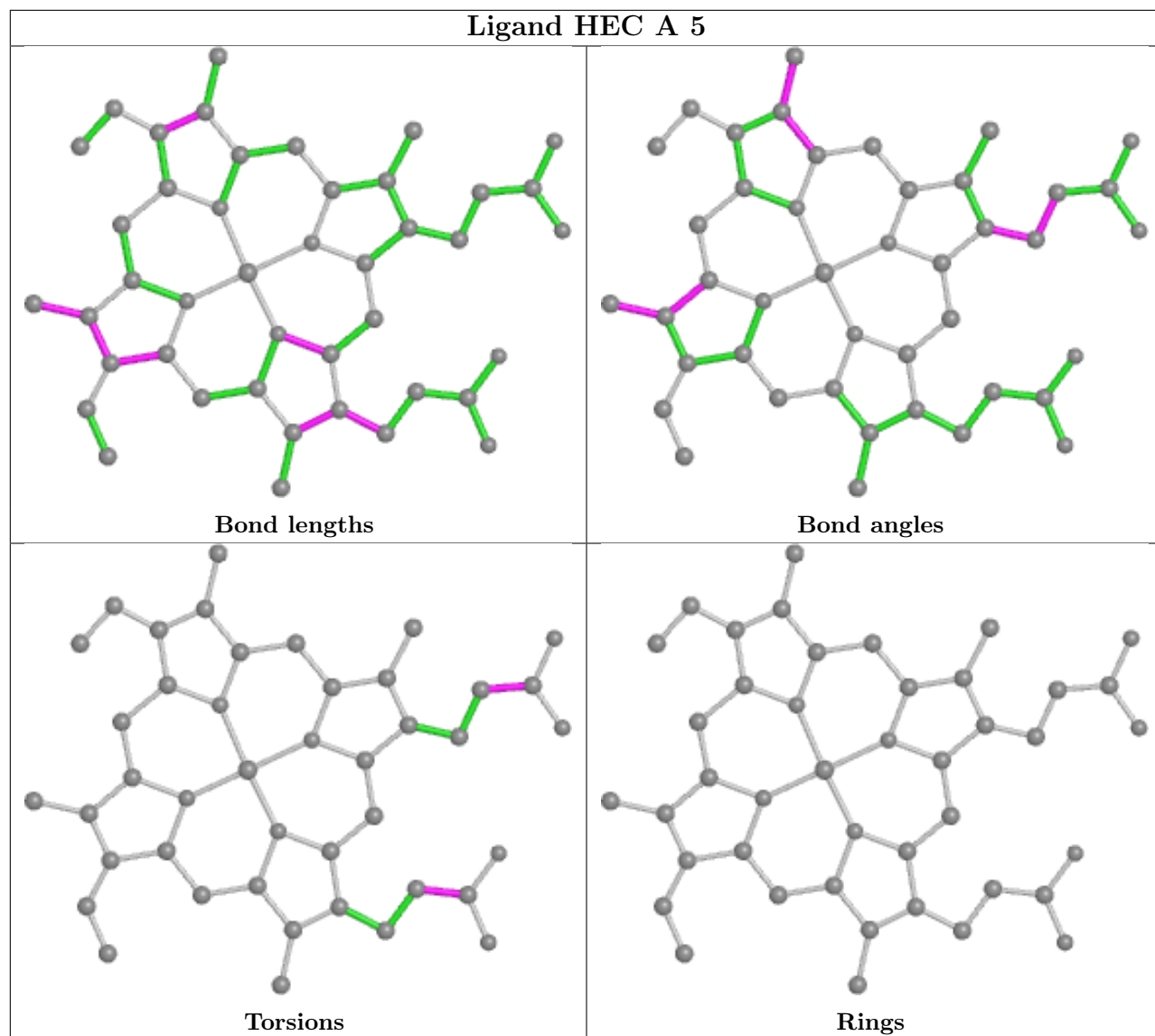


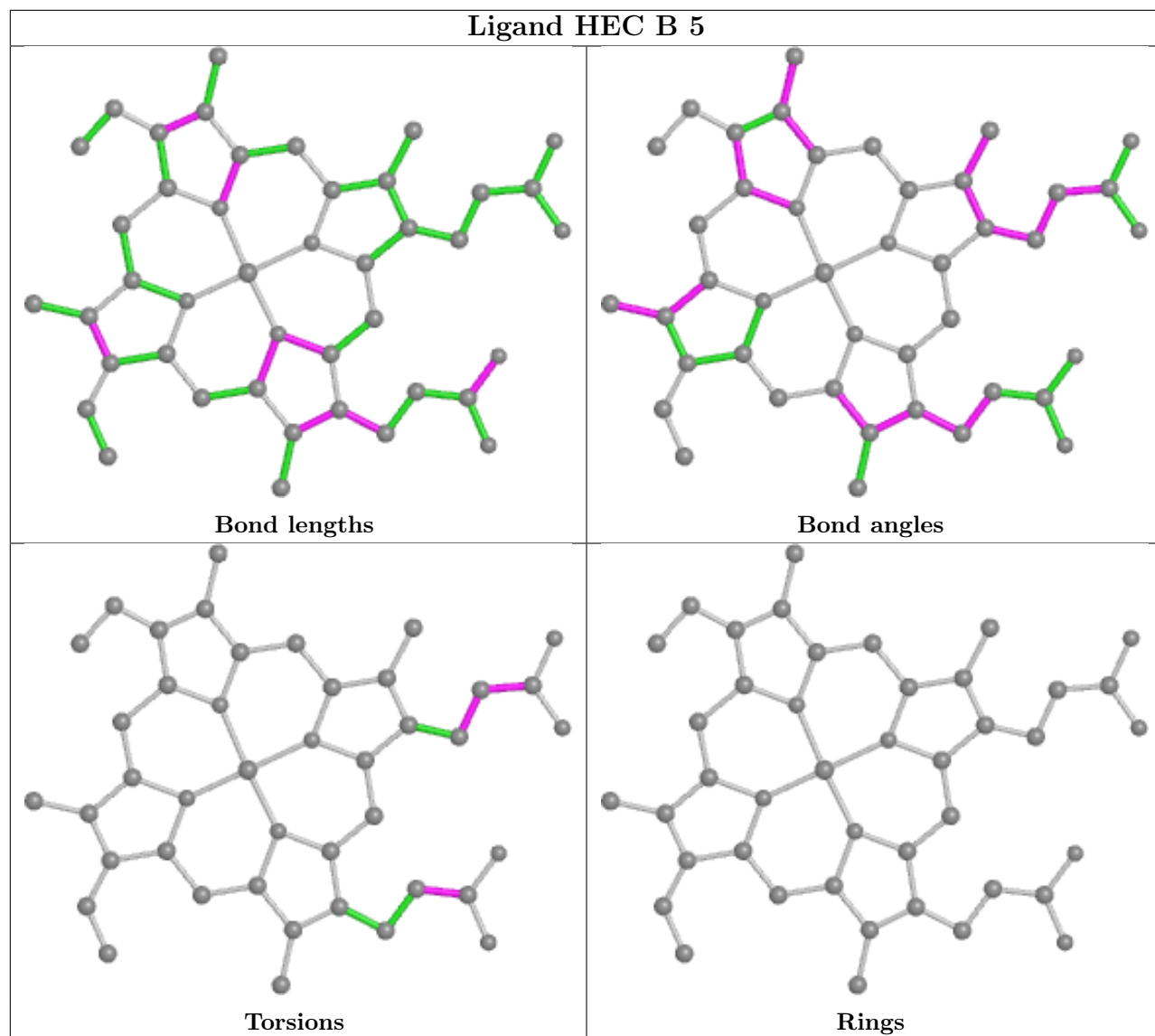




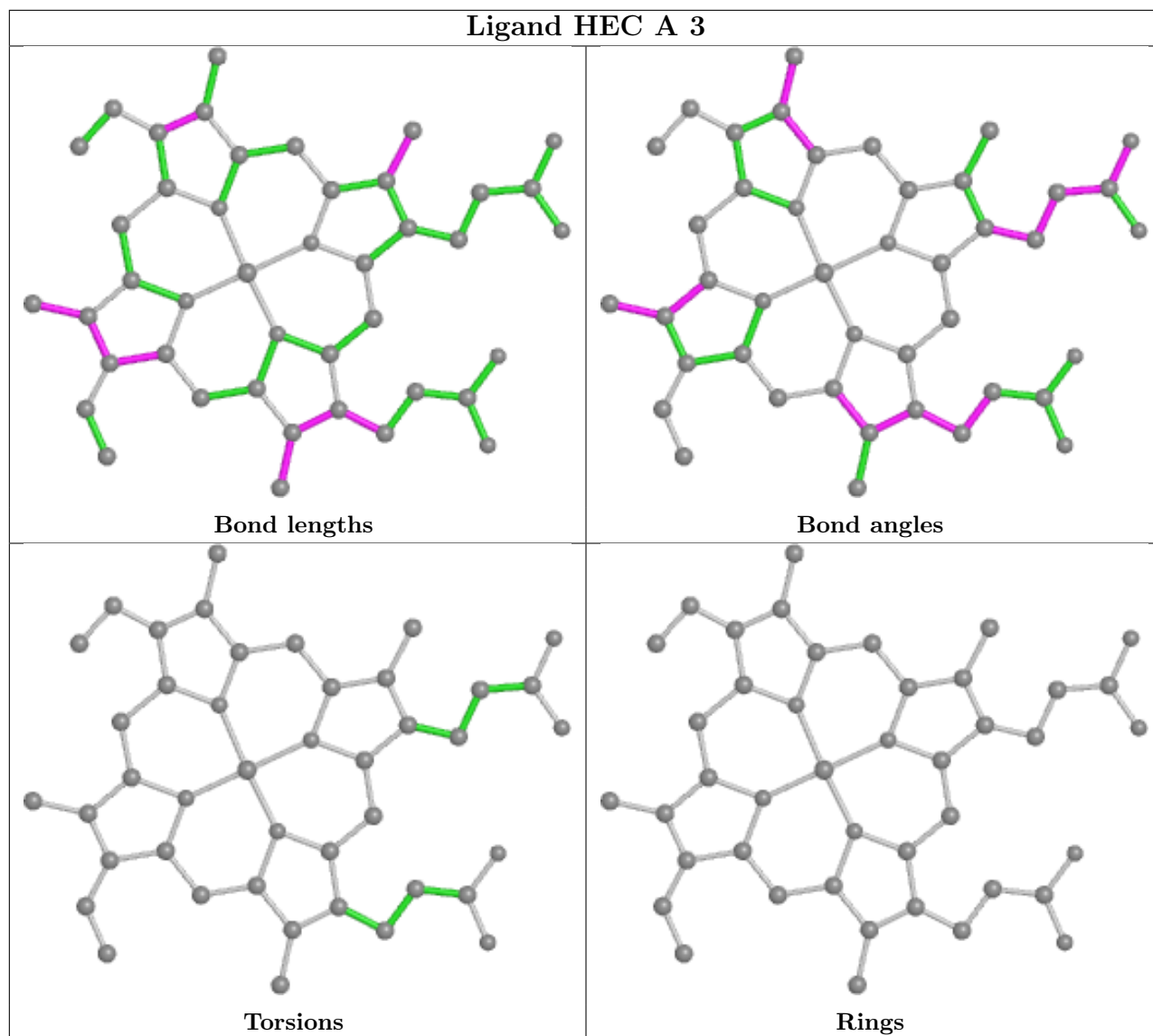


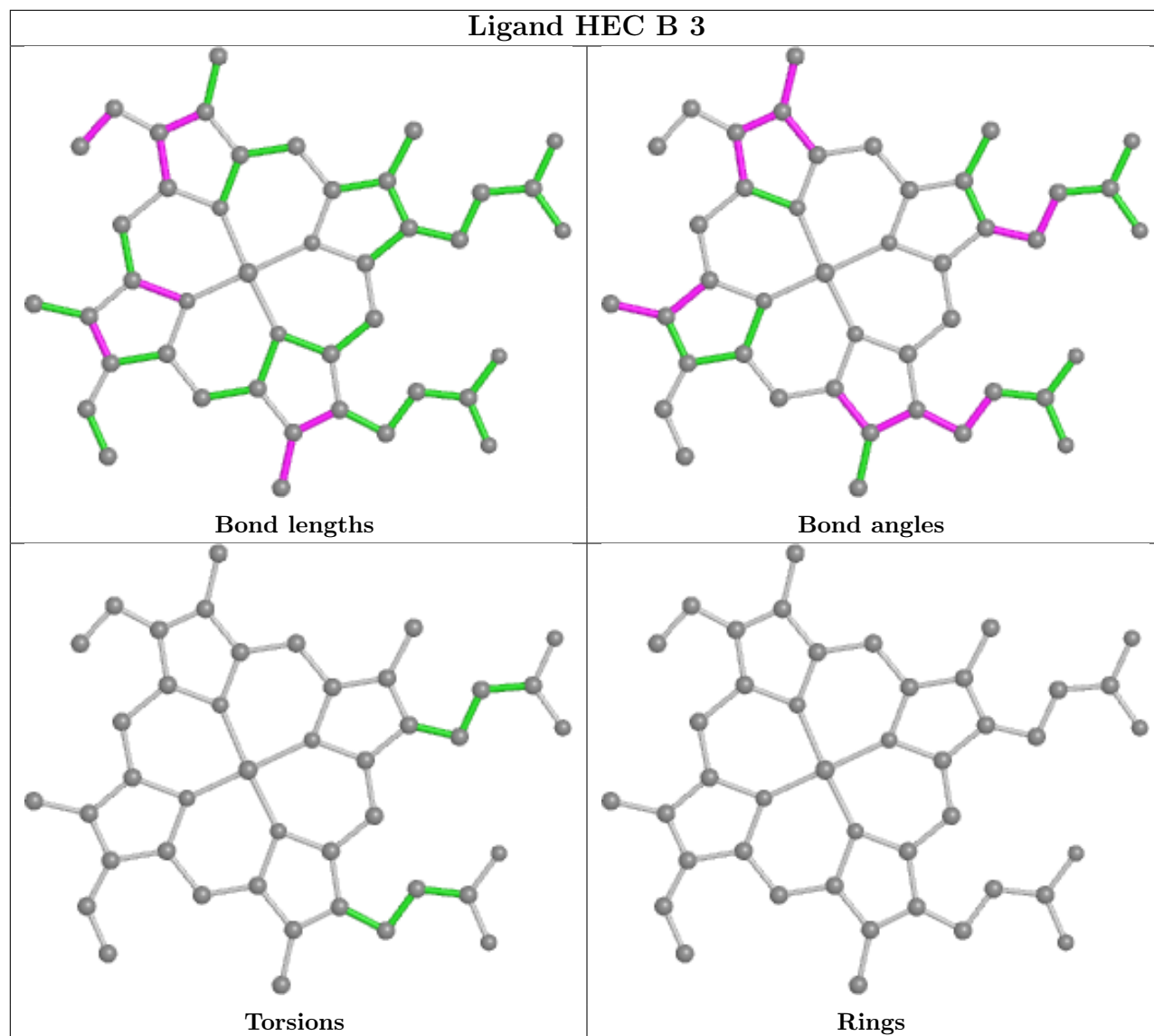












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	441/441 (100%)	-0.25	1 (0%) 95   95	10, 20, 35, 45	10 (2%)
1	B	441/441 (100%)	-0.35	2 (0%) 91   92	9, 17, 29, 40	11 (2%)
1	C	441/441 (100%)	-0.39	1 (0%) 95   95	9, 16, 28, 43	6 (1%)
1	D	441/441 (100%)	0.08	4 (0%) 84   86	13, 26, 47, 54	12 (2%)
All	All	1764/1764 (100%)	-0.23	8 (0%) 91   92	9, 19, 37, 54	39 (2%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	37	THR	4.1
1	B	442	GLN	2.5
1	D	37	THR	2.5
1	A	477	SER	2.4
1	B	190	GLU	2.2
1	D	171	PHE	2.1
1	D	476	LEU	2.1
1	D	176	PRO	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.

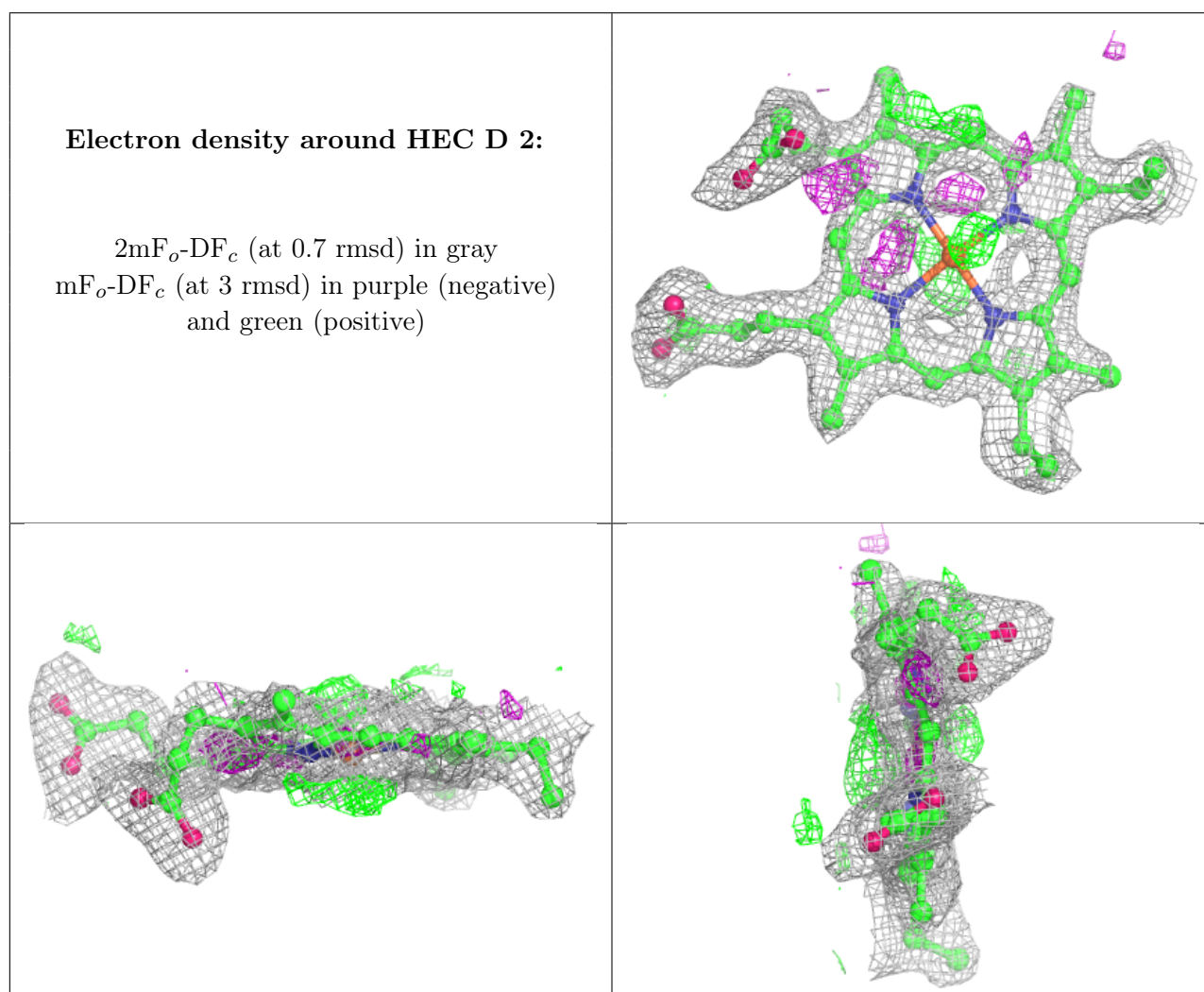
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	D	1502	1/1	0.74	0.26	87,87,87,87	0
2	CA	A	1502	1/1	0.79	0.11	64,64,64,64	0
4	EDO	C	13	4/4	0.80	0.23	40,40,40,43	0
2	CA	B	1502	1/1	0.81	0.10	64,64,64,64	0
2	CA	C	1502	1/1	0.81	0.20	61,61,61,61	0
4	EDO	B	14	4/4	0.86	0.35	35,38,40,44	0
4	EDO	A	480	4/4	0.87	0.24	33,34,34,36	0
4	EDO	C	11	4/4	0.88	0.21	29,32,33,38	0
4	EDO	D	480	4/4	0.90	0.15	35,35,39,40	0
4	EDO	B	15	4/4	0.91	0.39	42,43,44,46	0
4	EDO	B	481	4/4	0.91	0.24	36,36,37,37	0
4	EDO	B	8	4/4	0.93	0.14	36,37,39,40	0
3	HEC	D	2	43/43	0.93	0.19	25,34,37,38	0
4	EDO	B	12	4/4	0.94	0.19	46,46,47,47	0
4	EDO	D	481	4/4	0.94	0.19	28,29,30,33	0
4	EDO	C	9	4/4	0.95	0.14	17,19,21,26	0
4	EDO	A	7	4/4	0.96	0.13	17,19,20,23	0
4	EDO	B	480	4/4	0.96	0.21	26,26,29,32	0
3	HEC	D	4	43/43	0.96	0.14	15,21,31,38	0
3	HEC	D	1	43/43	0.97	0.12	17,20,23,24	0
3	HEC	D	5	43/43	0.97	0.13	19,23,31,34	0
4	EDO	B	6	4/4	0.97	0.10	17,21,23,29	0
3	HEC	A	2	43/43	0.97	0.13	12,21,23,23	0
3	HEC	D	3	43/43	0.97	0.14	18,23,26,27	0
4	EDO	A	10	4/4	0.97	0.14	27,29,29,31	0
3	HEC	C	4	43/43	0.98	0.13	6,11,23,33	0
3	HEC	C	5	43/43	0.98	0.12	12,15,29,34	0
3	HEC	A	1	43/43	0.98	0.10	8,13,15,16	0
2	CA	D	1501	1/1	0.98	0.06	22,22,22,22	0
3	HEC	A	3	43/43	0.98	0.11	10,15,18,24	0
3	HEC	A	4	43/43	0.98	0.12	10,14,27,35	0
3	HEC	A	5	43/43	0.98	0.13	14,17,26,35	0
3	HEC	B	1	43/43	0.98	0.11	4,10,14,17	0
3	HEC	B	2	43/43	0.98	0.12	7,11,13,15	0
3	HEC	B	4	43/43	0.98	0.13	6,10,24,34	0
3	HEC	B	5	43/43	0.98	0.13	8,13,26,30	0
3	HEC	C	2	43/43	0.99	0.10	7,11,15,17	0

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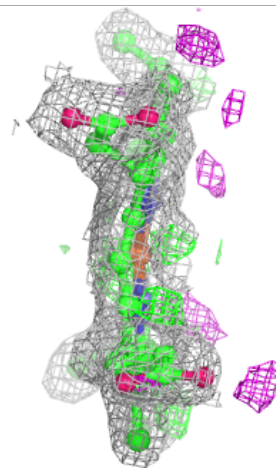
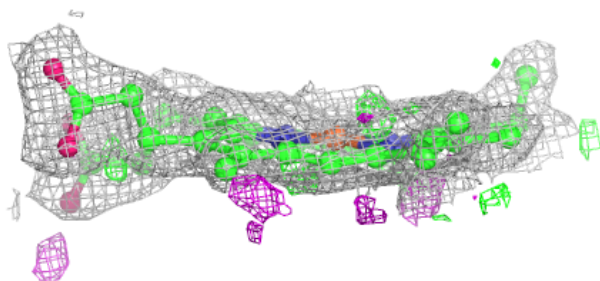
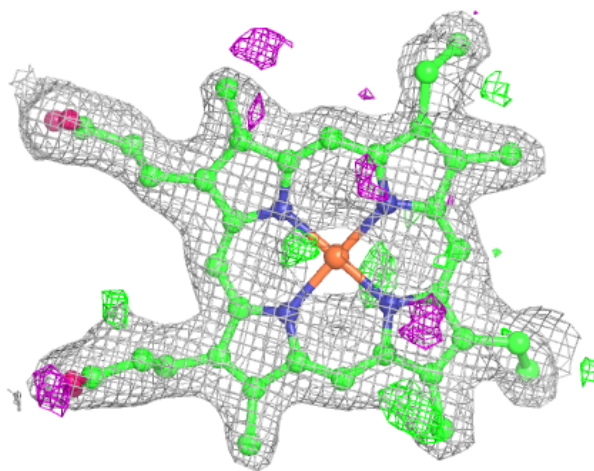
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	HEC	C	3	43/43	0.99	0.11	5,8,11,19	0
3	HEC	B	3	43/43	0.99	0.11	5,9,15,22	0
2	CA	B	1501	1/1	0.99	0.08	16,16,16,16	0
2	CA	A	1501	1/1	0.99	0.09	17,17,17,17	0
3	HEC	C	1	43/43	0.99	0.11	5,8,11,14	0
2	CA	C	1501	1/1	1.00	0.11	13,13,13,13	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



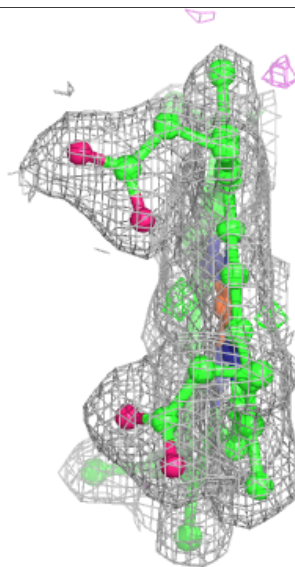
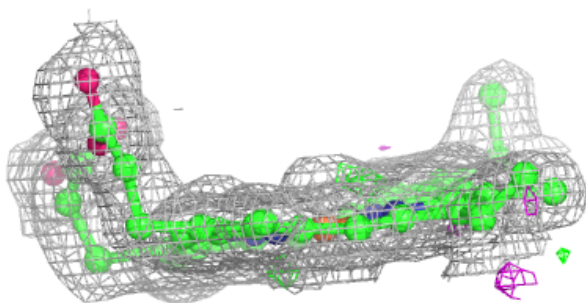
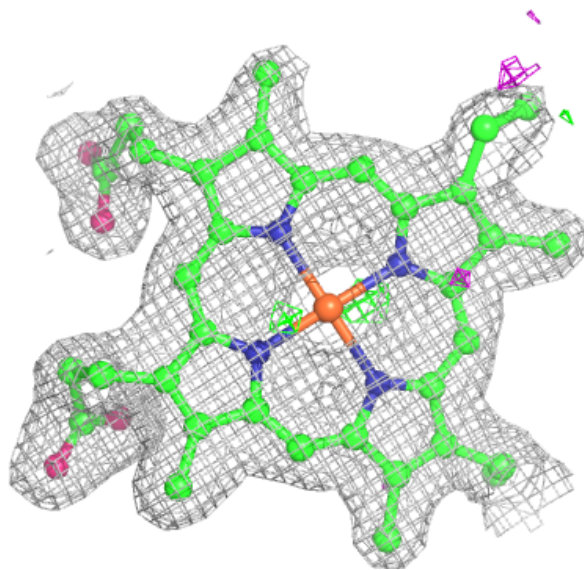
**Electron density around HEC D 4:**

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



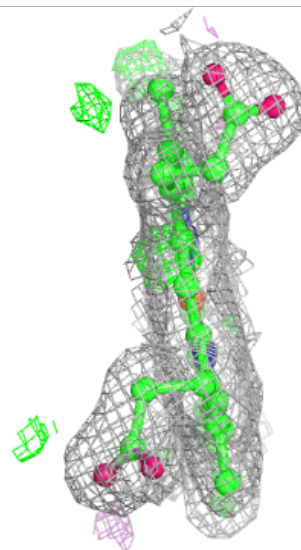
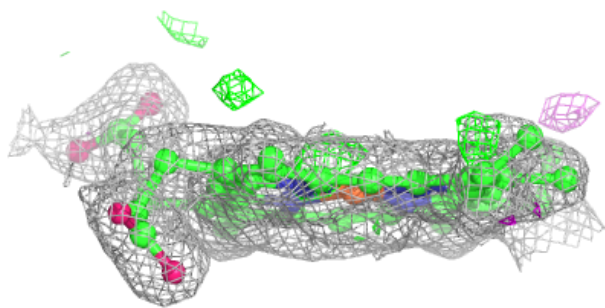
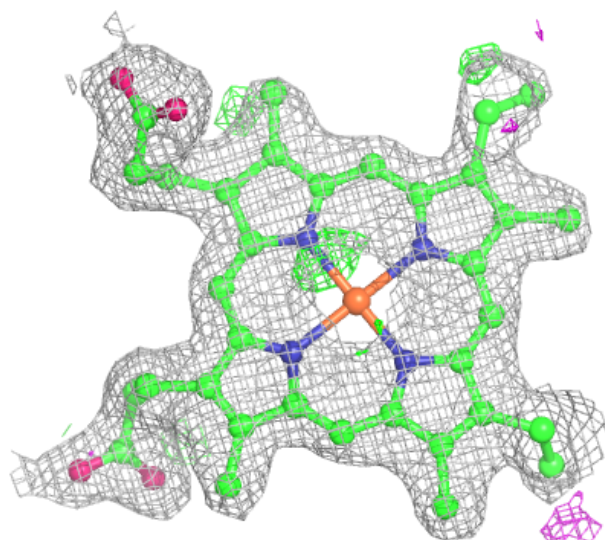
**Electron density around HEC D 1:**

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

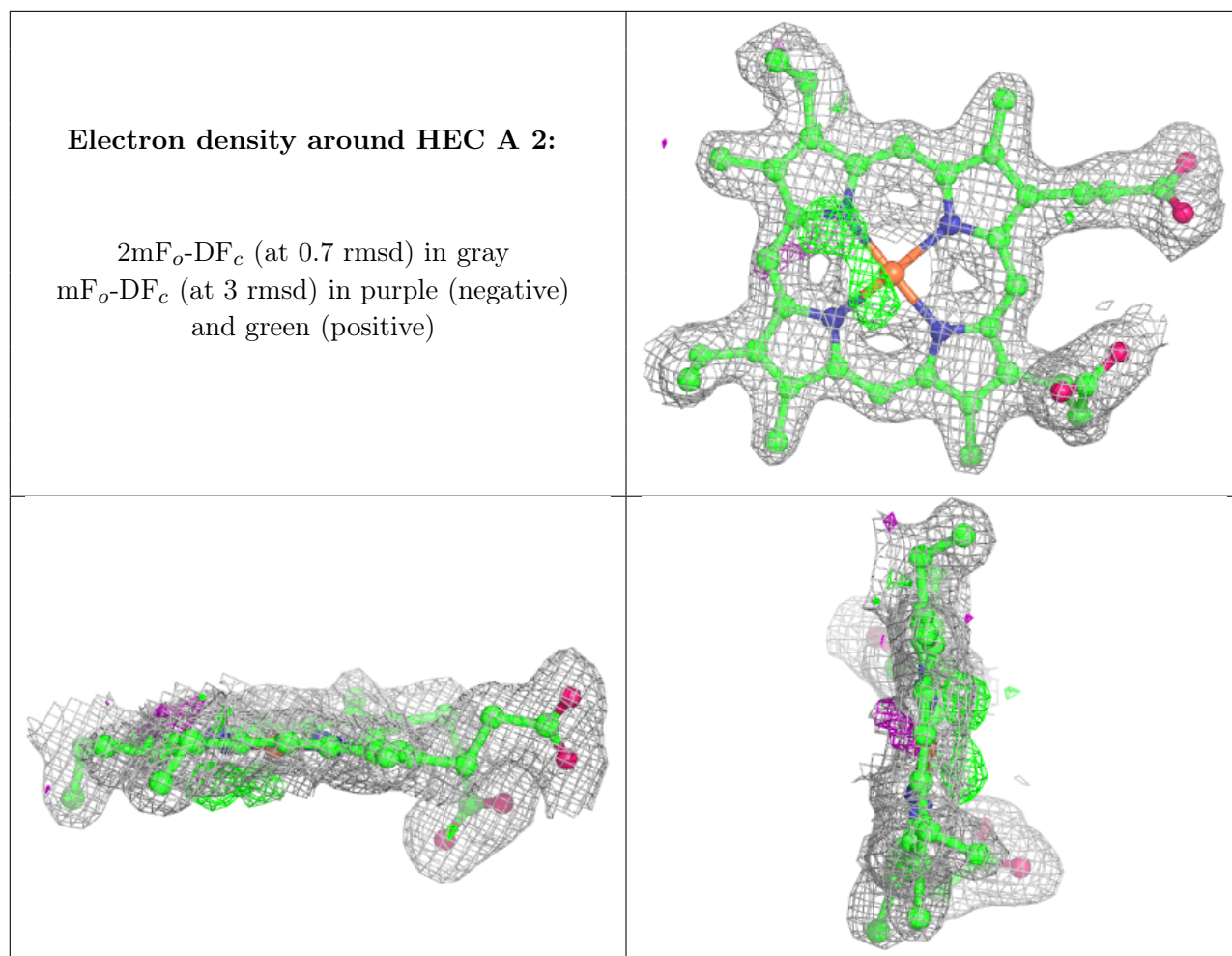


**Electron density around HEC D 5:**

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

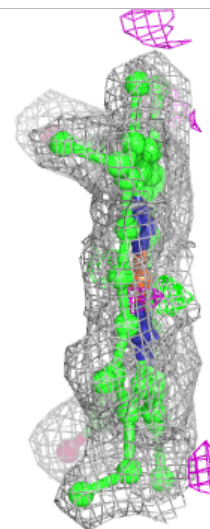
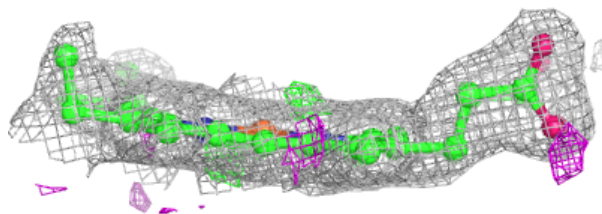
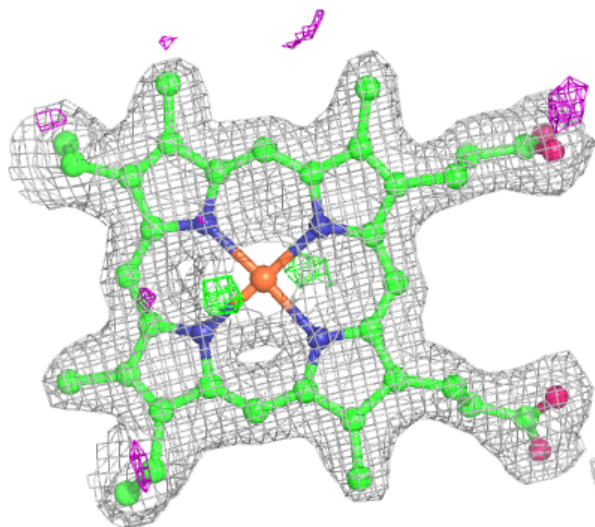


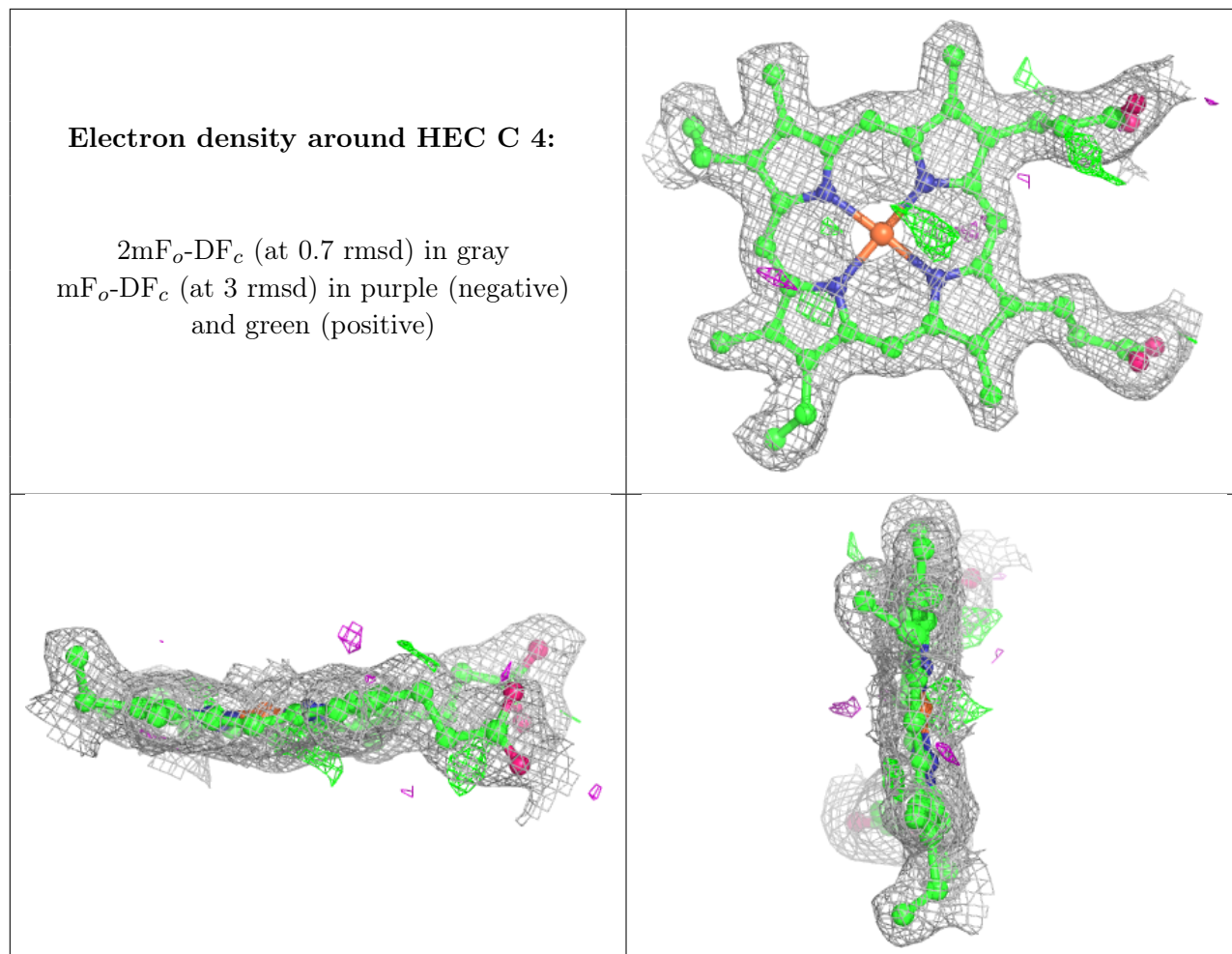


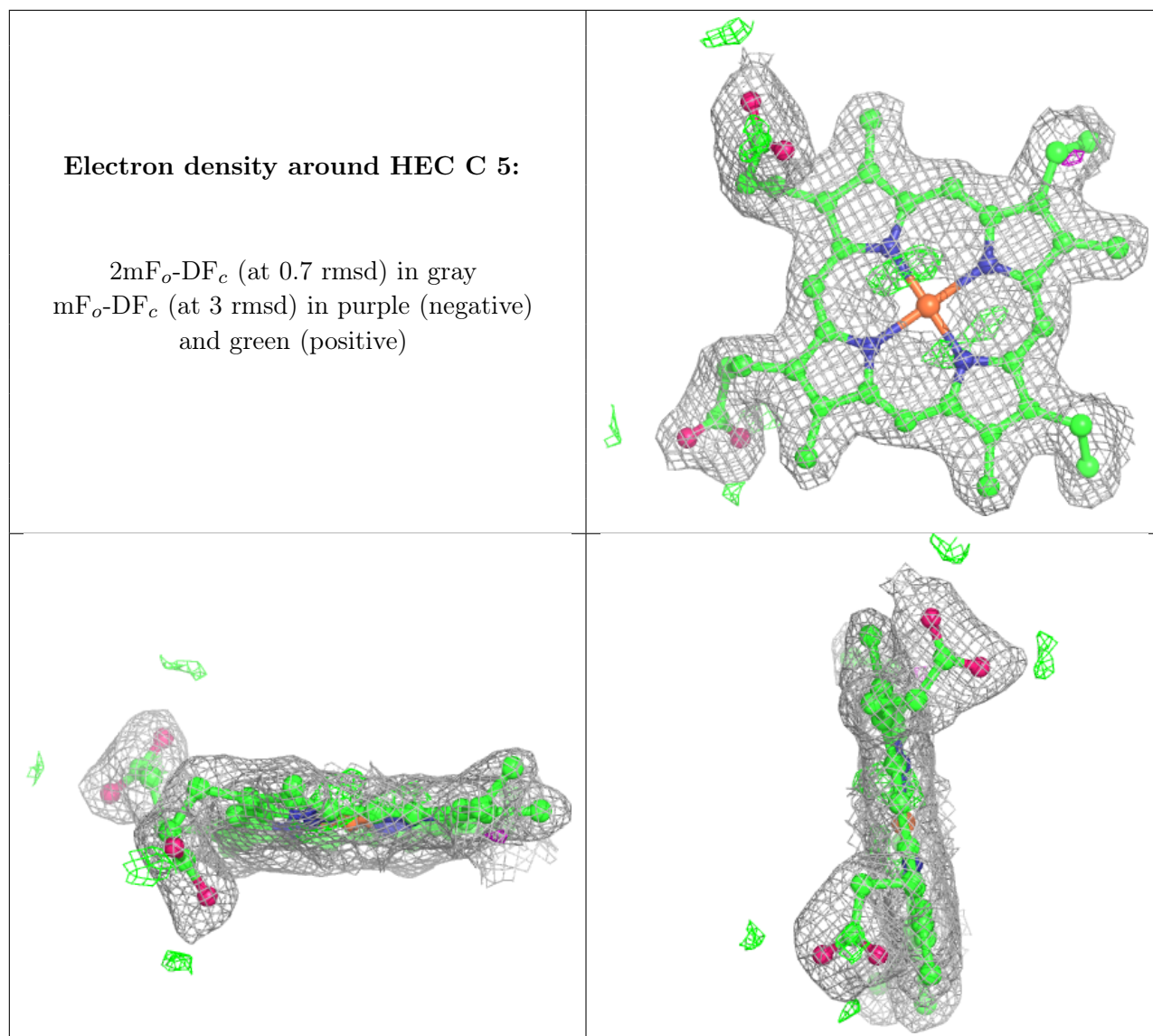


**Electron density around HEC D 3:**

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

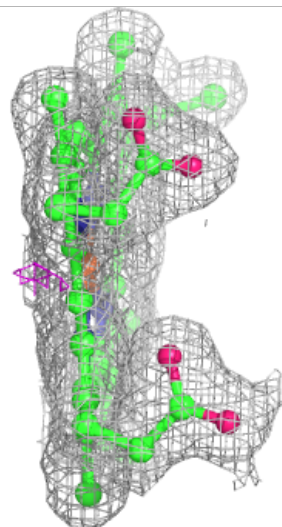
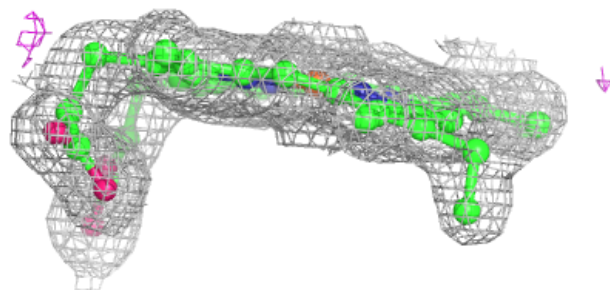
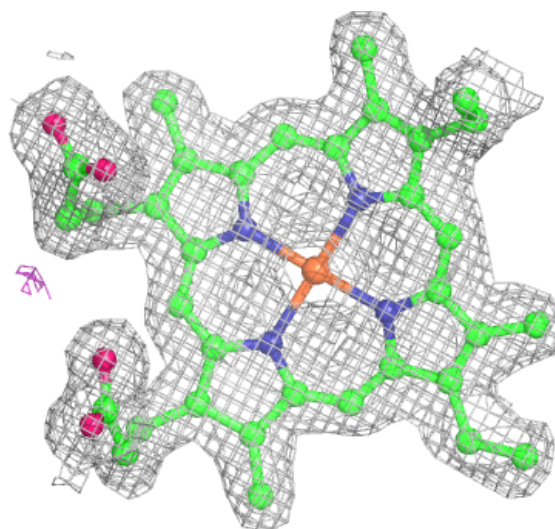


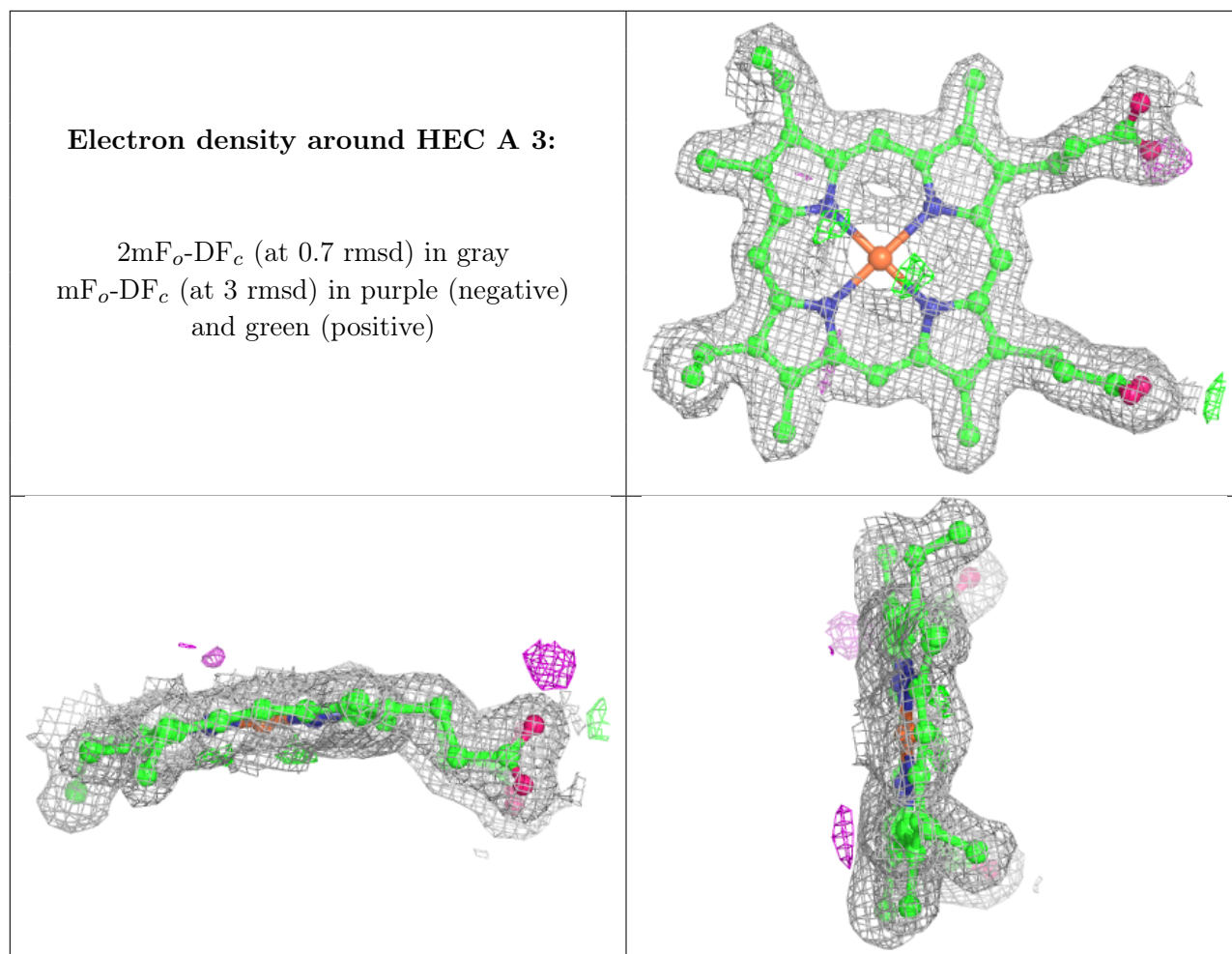




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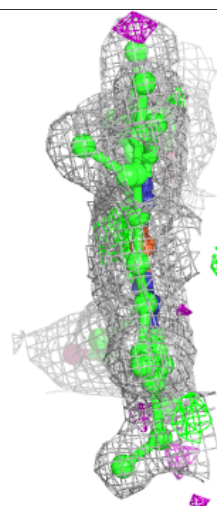
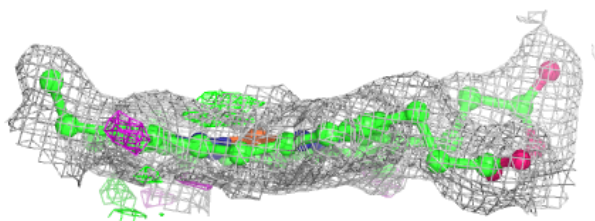
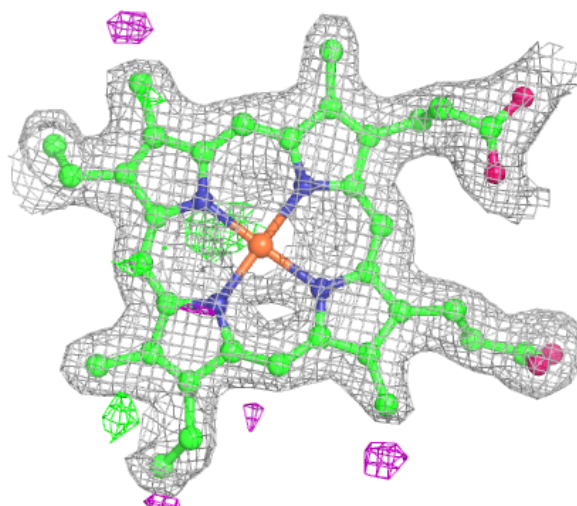
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





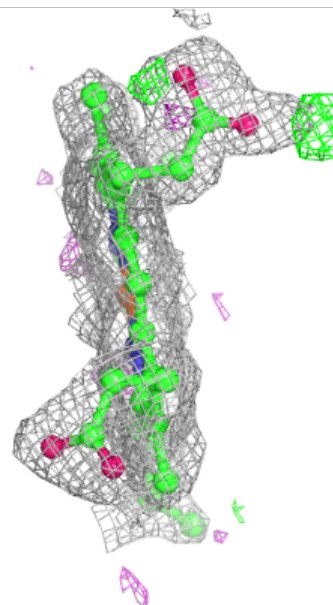
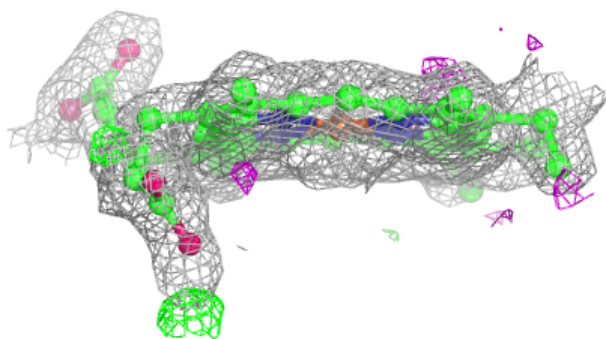
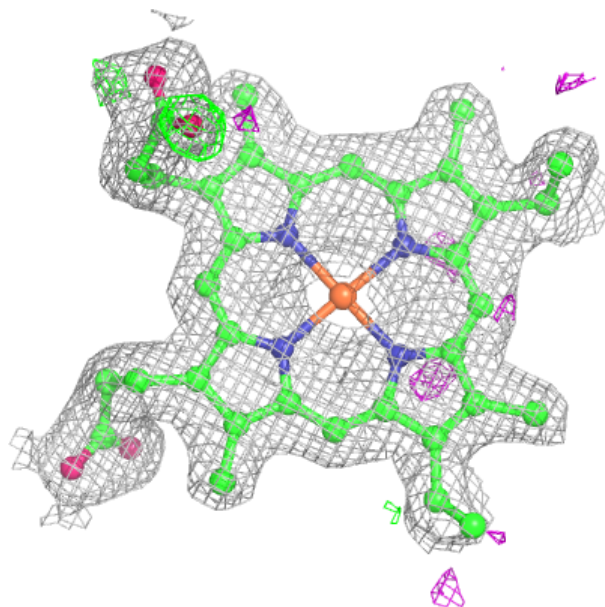
**Electron density around HEC A 4:**

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

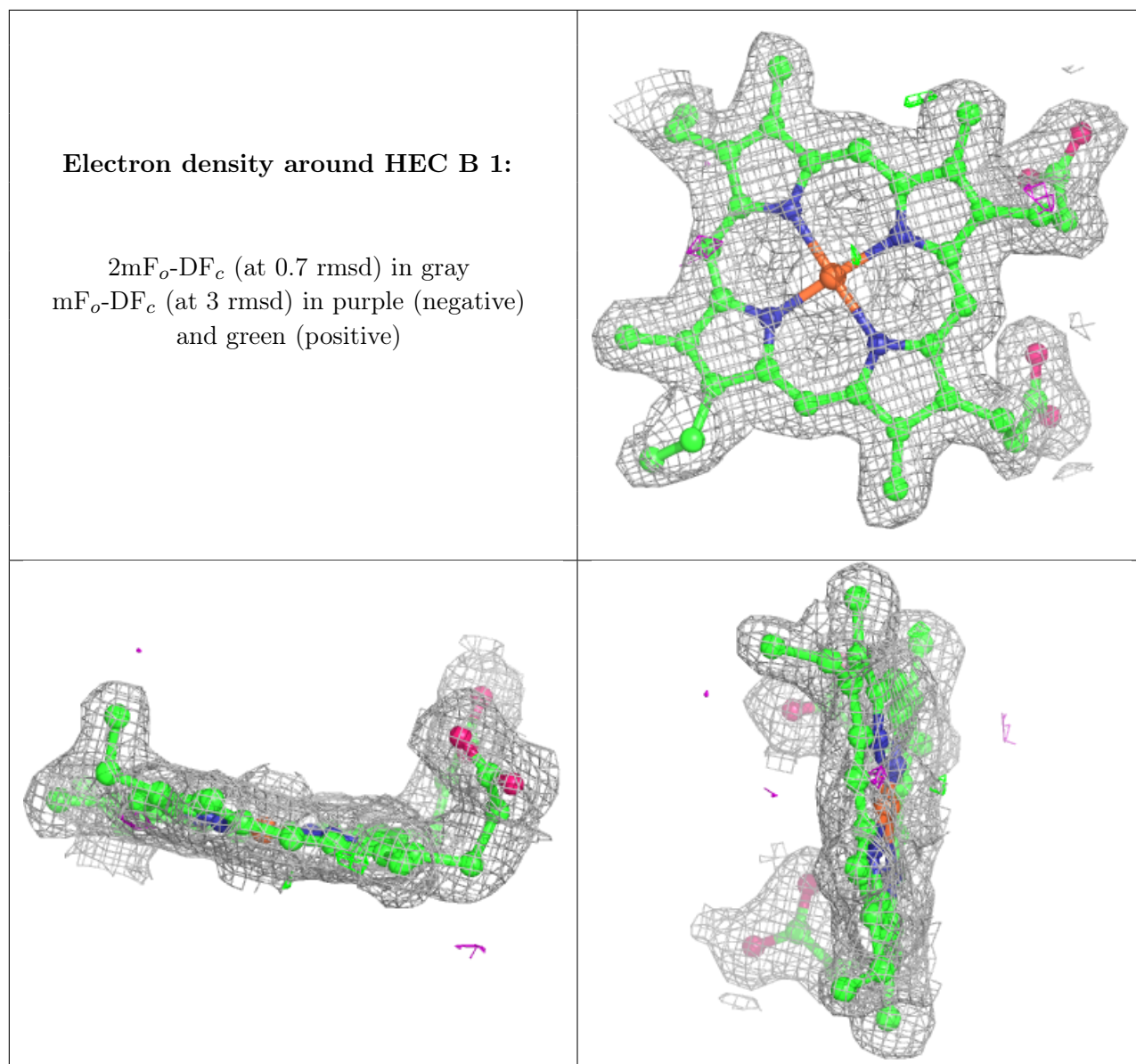


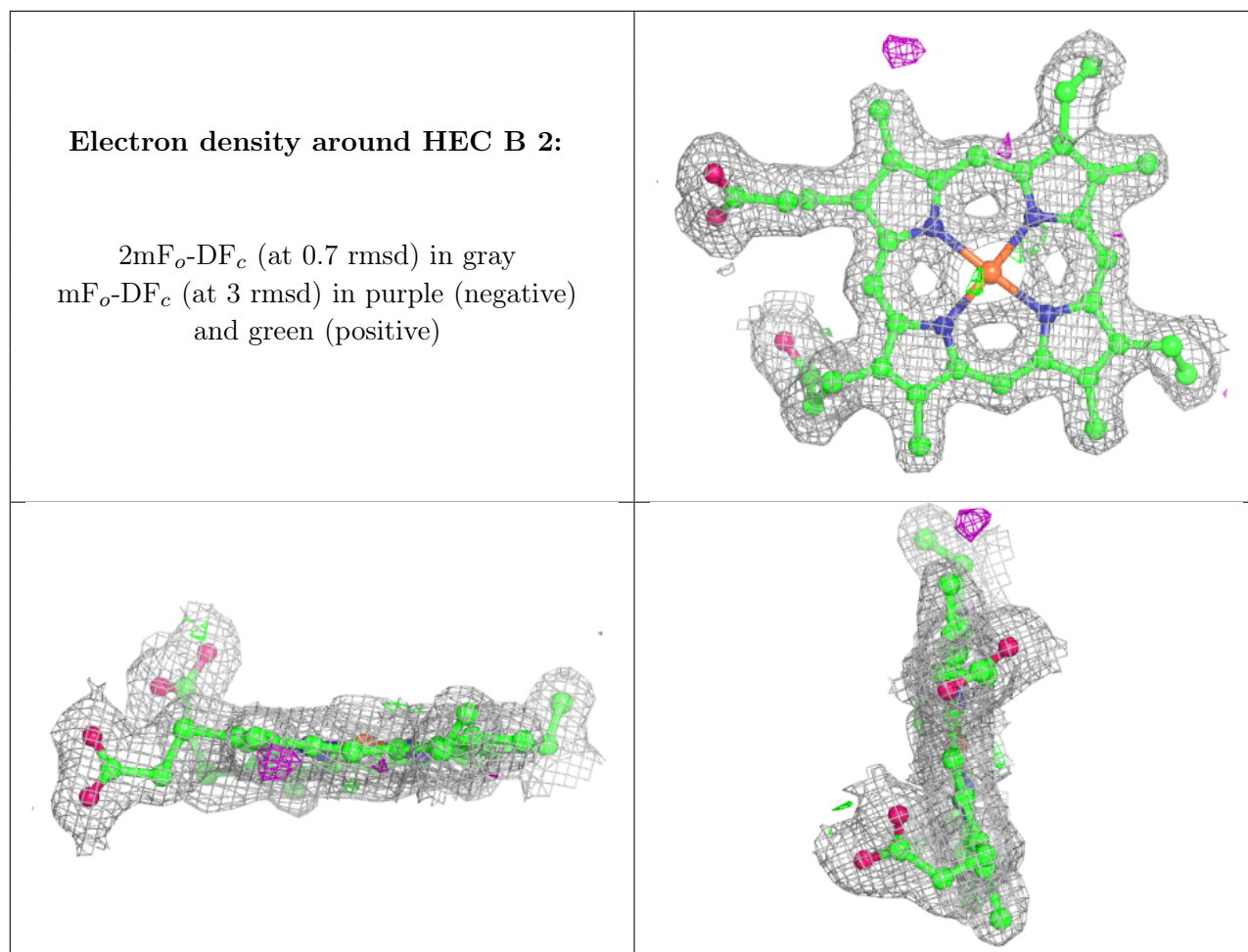
**Electron density around HEC A 5:**

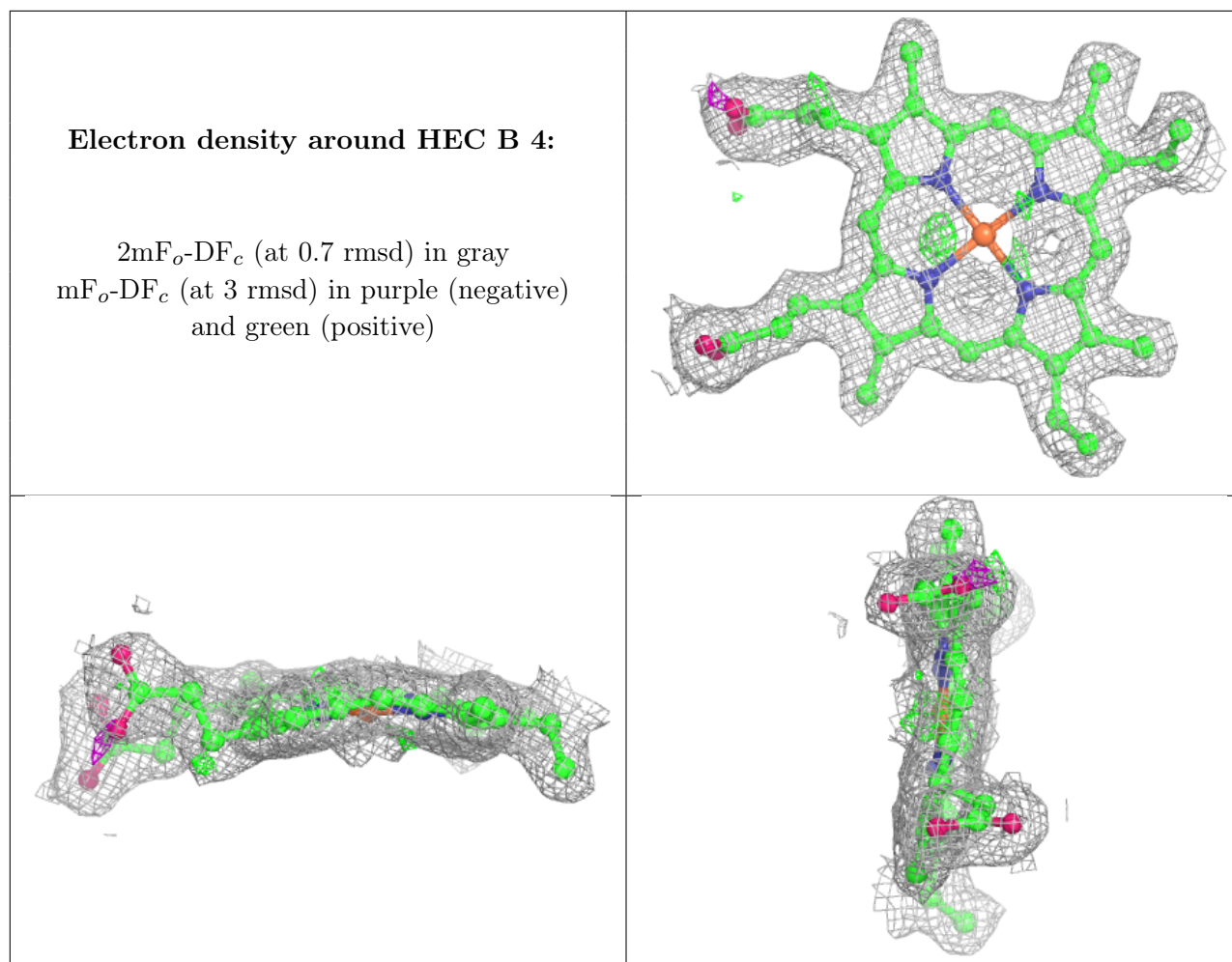
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

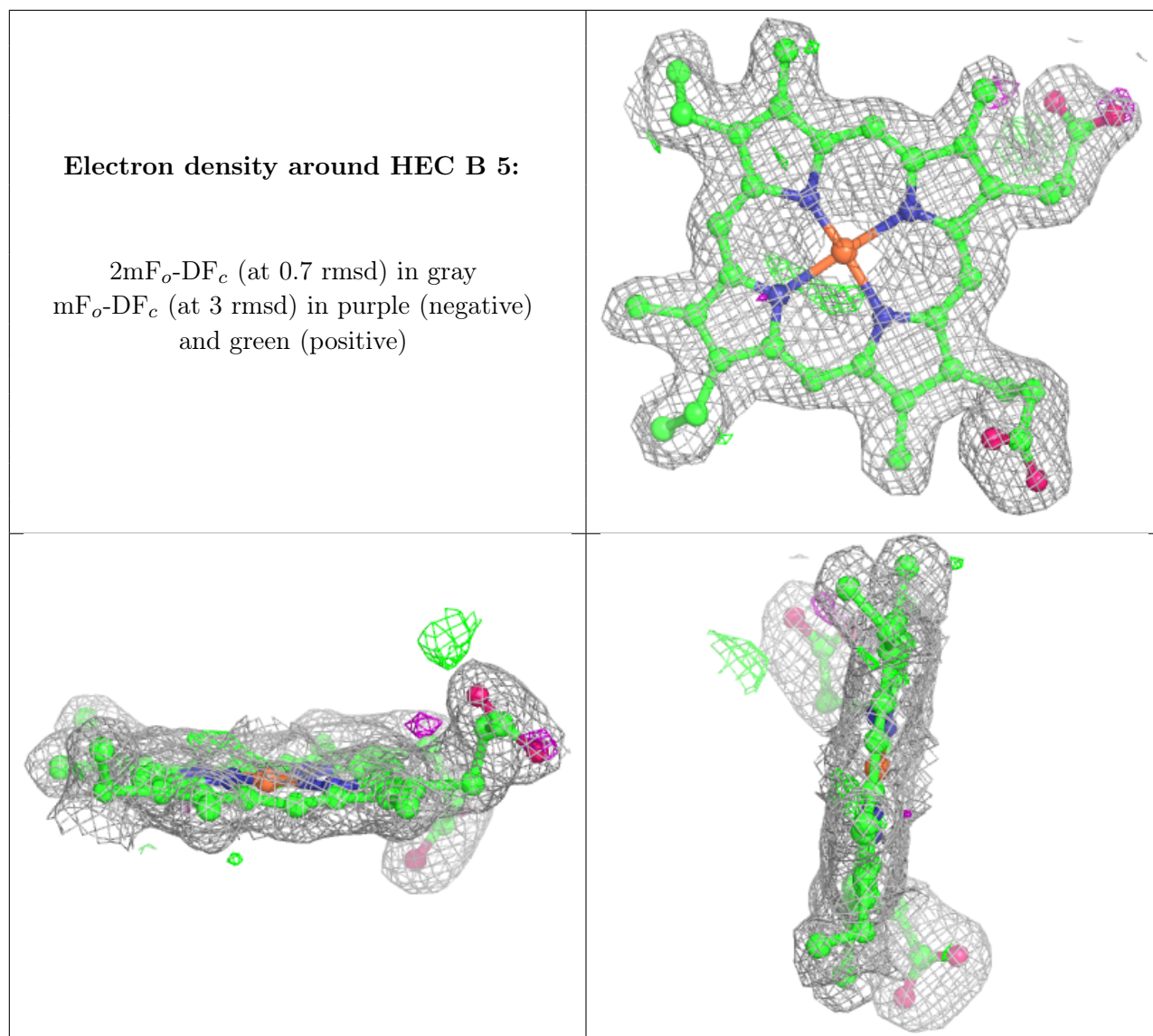


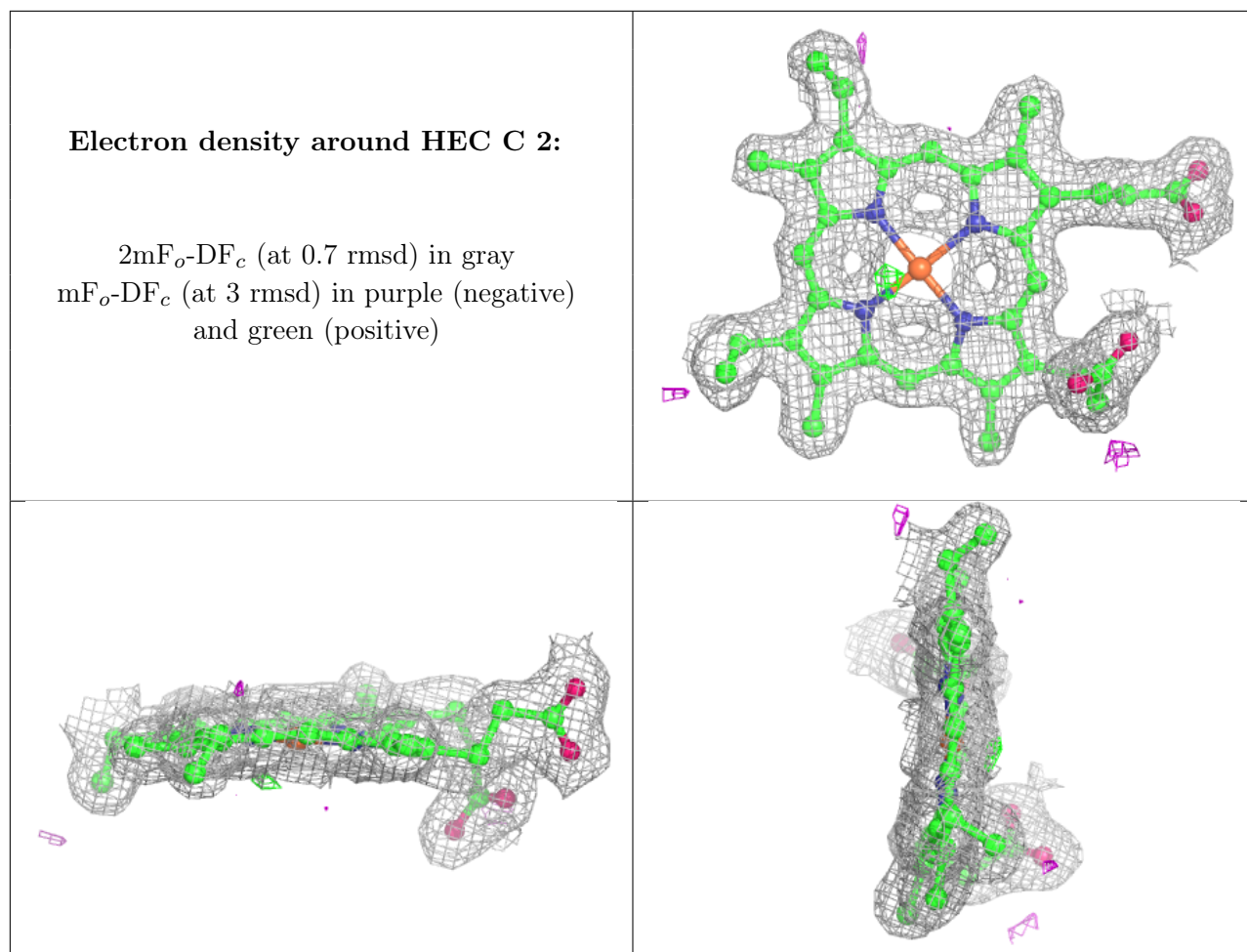


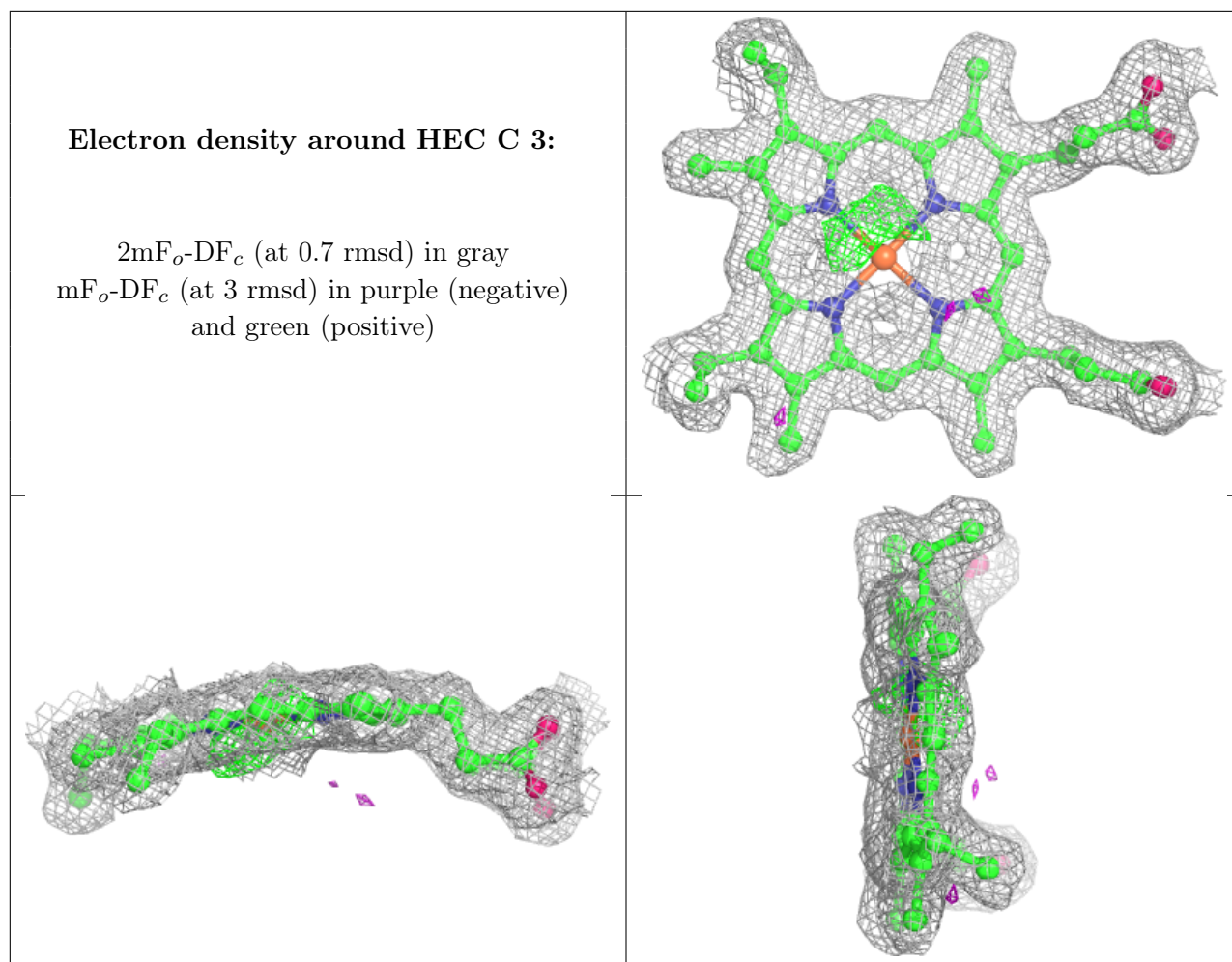


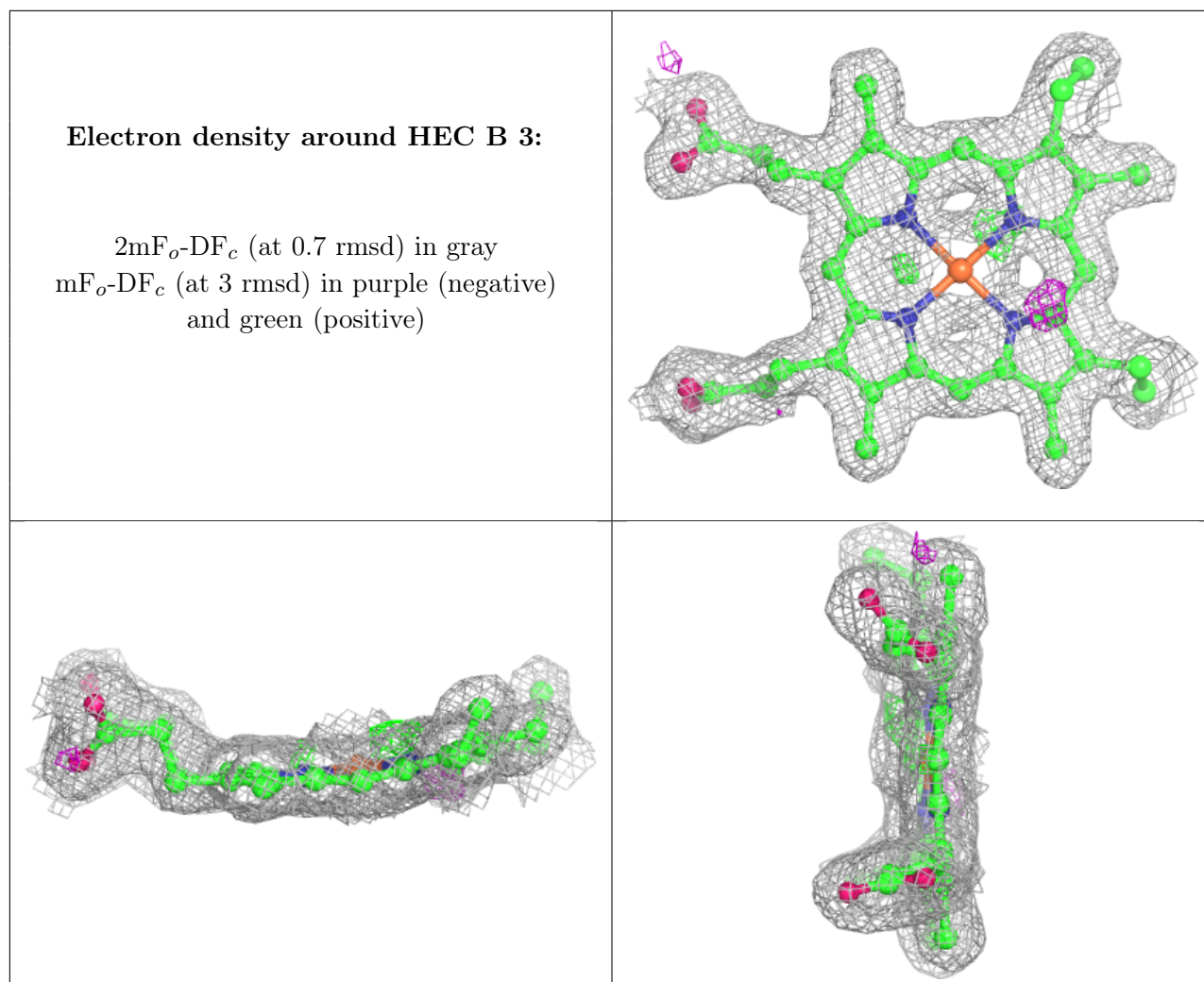


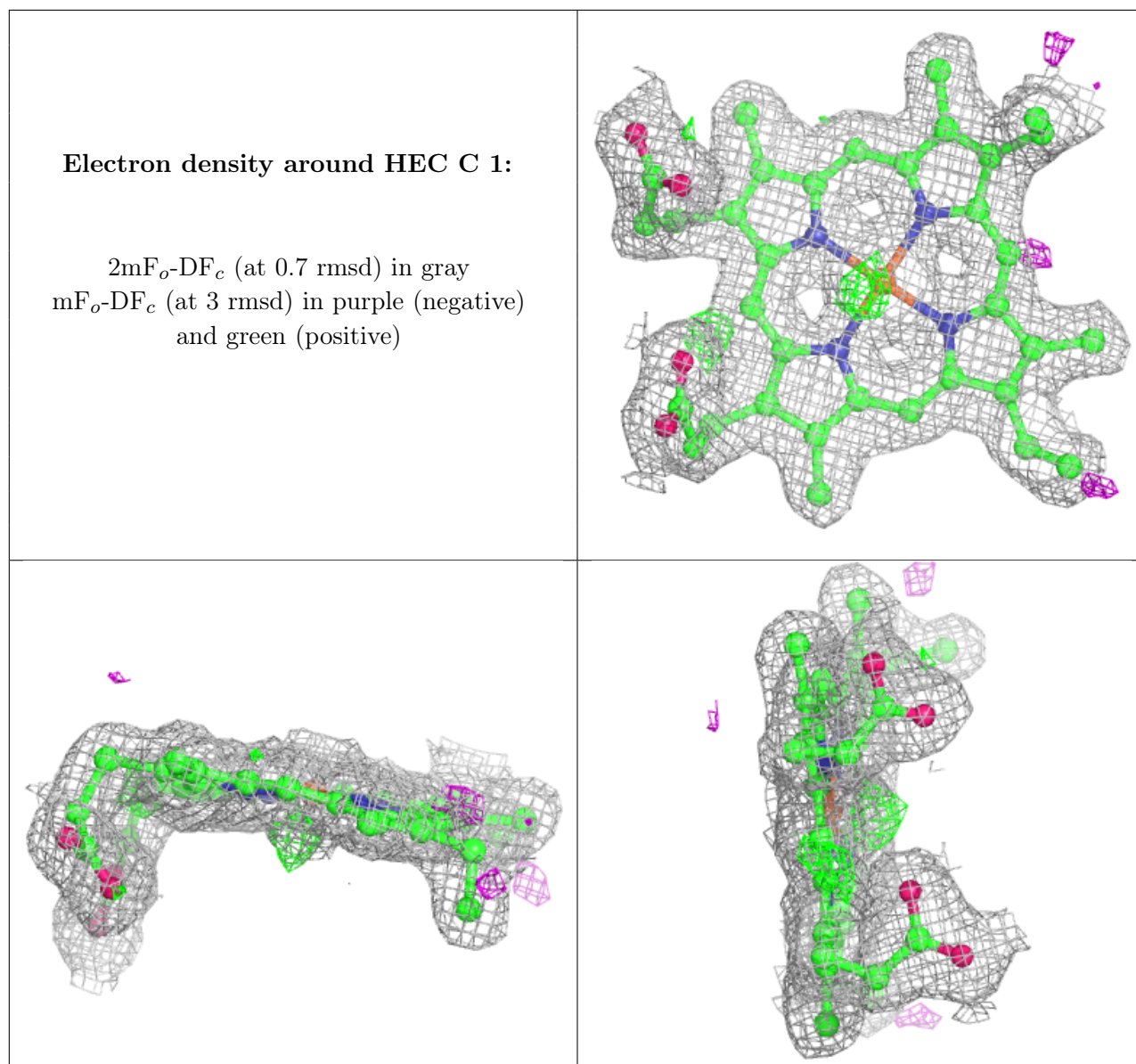












## 6.5 Other polymers [i](#)

There are no such residues in this entry.