



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2023 – 08:20 PM EDT

PDB ID : 4FAS
Title : Complex crystal structure of hydroxylamine oxidoreductase and NE1300 from *Nitrosomonas europaea*
Authors : Cedervall, P.E.; Wilmot, C.M.
Deposited on : 2012-05-22
Resolution : 2.10 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

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>.

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)
Xtrriage (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

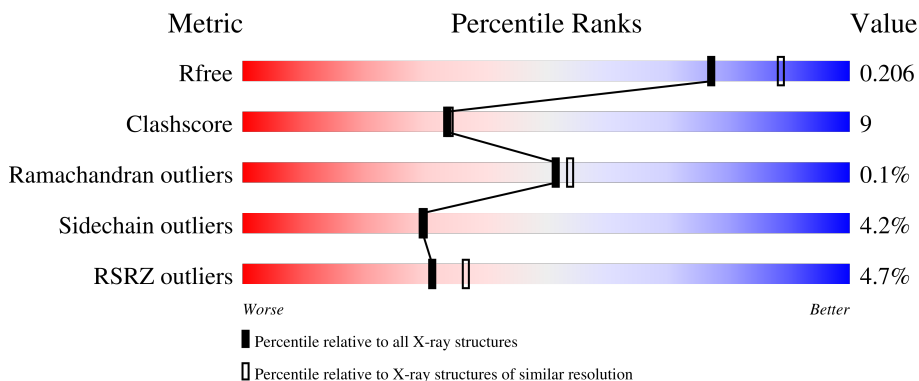
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	546	
1	B	546	
1	C	546	
2	D	69	
2	E	69	

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Mol	Chain	Length	Quality of chain
2	F	69	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment (16%), a green segment (54%), a yellow segment (14%), and a grey segment (29%). A small black dot is located on the yellow segment.</p>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 15197 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.

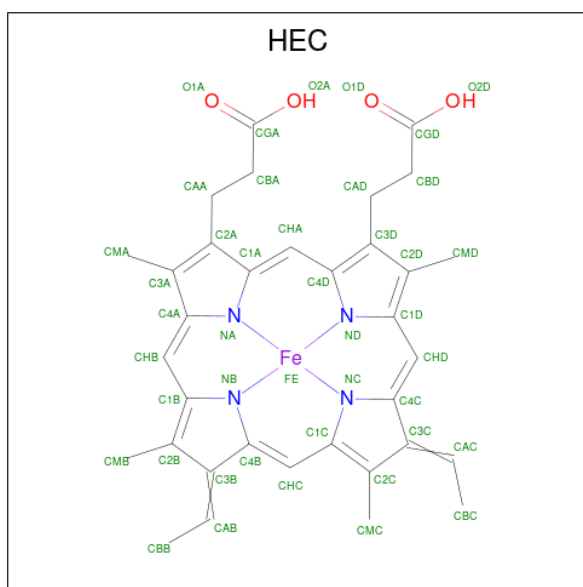
- Molecule 1 is a protein called Hydroxylamine oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	502	Total 4013	C 2495	N 711	O 775	S 32	0	1	0
1	B	502	Total 4005	C 2491	N 710	O 772	S 32	0	1	0
1	C	502	Total 4005	C 2491	N 710	O 772	S 32	0	0	0

- Molecule 2 is a protein called NE1300.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	49	Total 370	C 233	N 63	O 71	S 3	0	0	0
2	E	49	Total 370	C 233	N 63	O 71	S 3	0	0	0
2	F	49	Total 370	C 233	N 63	O 71	S 3	0	0	0

- Molecule 3 is HEME C (three-letter code: HEC) (formula: C₃₄H₃₄FeN₄O₄).



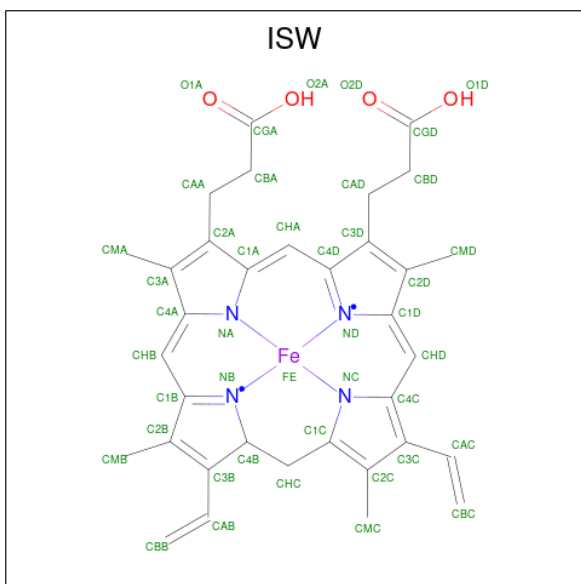
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A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

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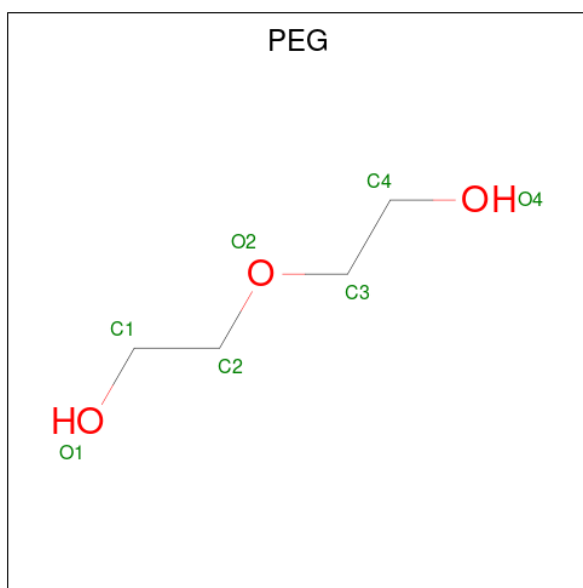
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



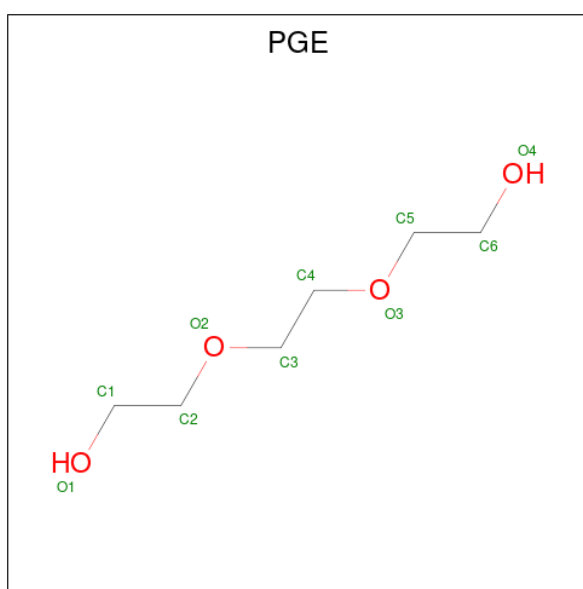
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0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

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

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



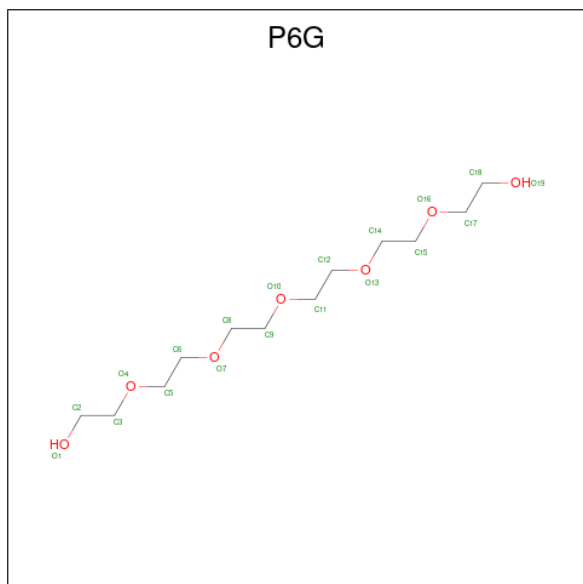
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0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

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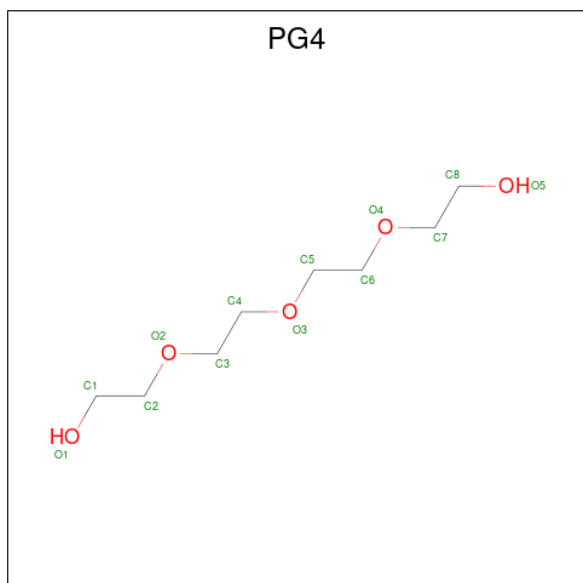
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).



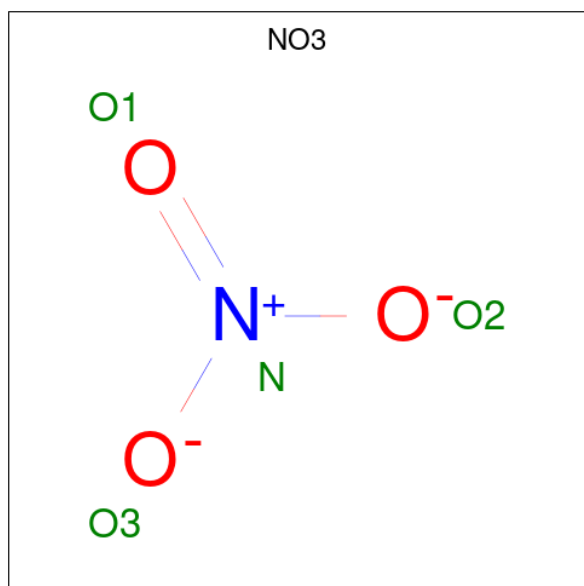
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			19	12	7		

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 10 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	N	O	0	0
			4	1	3		
10	B	1	Total	N	O	0	0
			4	1	3		
10	C	1	Total	N	O	0	0
			4	1	3		
10	F	1	Total	N	O	0	0
			4	1	3		

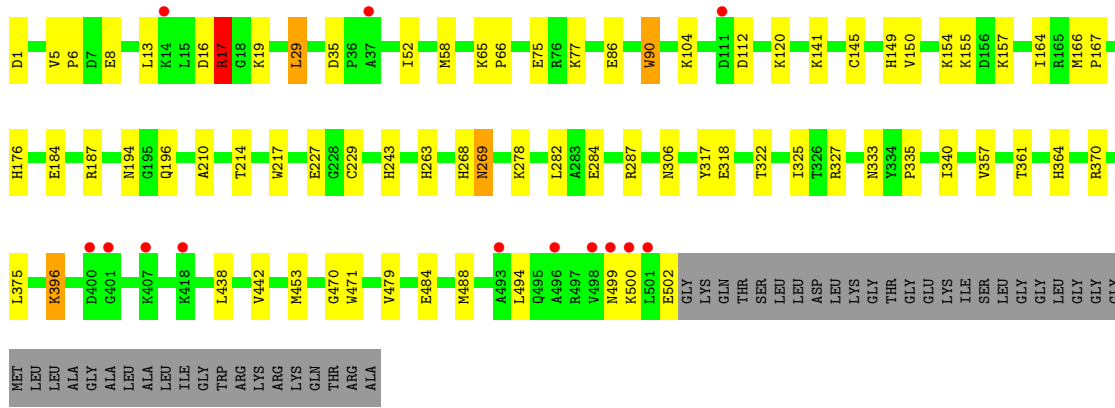
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	237	Total	O	0	0
			237	237		
11	B	258	Total	O	0	0
			258	258		
11	C	244	Total	O	0	0
			244	244		
11	D	14	Total	O	0	0
			14	14		
11	E	10	Total	O	0	0
			10	10		

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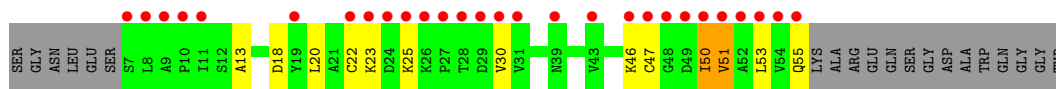
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	F	22	Total	O	0	0
			22	22		



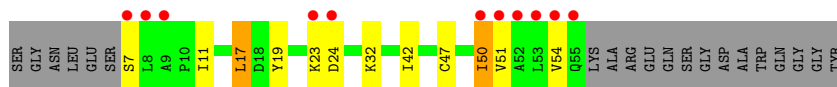
• Molecule 2: NE1300



• Molecule 2: NE1300



• Molecule 2: NE1300



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	140.73Å 142.62Å 107.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.89 – 2.10 42.89 – 2.10	Depositor EDS
% Data completeness (in resolution range)	79.9 (42.89-2.10) 79.9 (42.89-2.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.165 , 0.206 0.166 , 0.206	Depositor DCC
R_{free} test set	5071 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtrriage
Anisotropy	0.603	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.015 for k,h,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15197	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ISW, PG4, PEG, EDO, PGE, HEC, P6G, NO3

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	1.07	5/4116 (0.1%)	0.92	8/5578 (0.1%)
1	B	1.10	8/4108 (0.2%)	0.96	11/5567 (0.2%)
1	C	1.07	1/4108 (0.0%)	0.92	5/5567 (0.1%)
2	D	0.78	0/373	0.87	0/502
2	E	0.76	0/373	0.86	0/502
2	F	0.87	0/373	0.96	1/502 (0.2%)
All	All	1.06	14/13451 (0.1%)	0.93	25/18218 (0.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	272	GLU	CG-CD	5.90	1.60	1.51
1	B	266	VAL	CB-CG1	-5.85	1.40	1.52
1	B	272	GLU	CG-CD	5.78	1.60	1.51
1	B	242	CYS	CB-SG	-5.52	1.72	1.81
1	A	148	CYS	CB-SG	-5.45	1.73	1.81
1	B	320	GLU	CG-CD	5.42	1.60	1.51
1	B	208	TYR	CD1-CE1	5.28	1.47	1.39
1	C	471	TRP	CE3-CZ3	5.26	1.47	1.38
1	A	293	GLU	CG-CD	5.25	1.59	1.51
1	A	72	GLU	CG-CD	5.21	1.59	1.51
1	A	320	GLU	CG-CD	5.18	1.59	1.51
1	B	356	TRP	CE3-CZ3	5.15	1.47	1.38
1	B	272	GLU	CB-CG	5.14	1.61	1.52
1	B	278	LYS	CB-CG	-5.07	1.38	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	ARG	NE-CZ-NH1	6.10	123.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	295	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	C	58	MET	CG-SD-CE	5.93	109.69	100.20
1	A	254	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	B	17	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	B	315	MET	CG-SD-CE	5.90	109.63	100.20
1	B	266	VAL	CB-CA-C	-5.88	100.22	111.40
1	A	17	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	177	LEU	CB-CG-CD2	5.73	120.75	111.00
1	C	112	ASP	CB-CG-OD1	5.72	123.45	118.30
1	B	111	ASP	CB-CG-OD2	5.65	123.38	118.30
1	A	476	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	B	352	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	B	438	LEU	CA-CB-CG	5.44	127.82	115.30
1	C	438	LEU	CB-CG-CD1	-5.44	101.75	111.00
2	F	17	LEU	CB-CG-CD1	5.44	120.25	111.00
1	A	29	LEU	CA-CB-CG	5.41	127.73	115.30
1	B	240	ASP	CB-CG-OD1	5.41	123.17	118.30
1	B	58	MET	CG-SD-CE	5.39	108.83	100.20
1	A	240	ASP	CB-CG-OD1	5.37	123.13	118.30
1	B	327	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	106	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	B	254	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	C	35	ASP	CB-CG-OD1	5.11	122.90	118.30
1	C	17	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4013	0	3811	59	0
1	B	4005	0	3807	66	0
1	C	4005	0	3808	64	0
2	D	370	0	391	1	0
2	E	370	0	391	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	370	0	391	8	0
3	A	301	0	210	15	0
3	B	301	0	210	17	0
3	C	301	0	210	20	0
4	A	43	0	28	11	0
4	B	43	0	28	14	0
4	C	43	0	28	11	0
5	A	42	0	60	5	0
5	B	28	0	40	4	0
5	C	42	0	60	4	0
5	F	7	0	10	1	0
6	A	10	0	14	2	0
6	C	10	0	14	4	0
7	A	16	0	24	2	0
7	B	20	0	30	0	0
7	C	24	0	36	3	0
8	B	19	0	26	1	0
9	B	13	0	18	1	0
10	B	8	0	0	0	0
10	C	4	0	0	0	0
10	F	4	0	0	0	0
11	A	237	0	0	4	0
11	B	258	0	0	1	0
11	C	244	0	0	3	0
11	D	14	0	0	0	0
11	E	10	0	0	0	0
11	F	22	0	0	1	0
All	All	15197	0	13645	239	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 9.

All (239) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:608:ISW:HBAA	3:B:605:HEC:O1D	1.65	0.96
4:B:608:ISW:HBAA	3:C:606:HEC:O1D	1.66	0.95
1:B:497:ARG:HB2	1:B:497:ARG:HH11	1.31	0.95
1:B:497:ARG:HH11	1:B:497:ARG:CB	1.80	0.94
5:A:614:PEG:H42	4:C:601:ISW:HMAA	1.49	0.93
1:B:13:LEU:HD21	1:B:29:LEU:HD13	1.49	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LEU:HD11	1:A:29:LEU:HD13	1.55	0.89
1:B:104:LYS:HE3	5:B:609:PEG:H22	1.54	0.87
1:A:495:GLN:HG2	1:C:494:LEU:HD13	1.61	0.81
1:C:13:LEU:HD11	1:C:29:LEU:HD13	1.64	0.80
1:B:104:LYS:CE	5:B:609:PEG:H22	2.12	0.79
2:E:30:VAL:HG22	2:E:46:LYS:HA	1.64	0.79
3:C:608:HEC:HMB1	3:C:608:HEC:HBB3	1.65	0.78
3:A:605:HEC:O1D	4:C:601:ISW:HBAA	1.83	0.77
1:B:497:ARG:HH11	1:B:497:ARG:CG	1.96	0.77
1:B:119:GLY:HA3	8:B:613:P6G:H61	1.68	0.75
1:A:407:LYS:HE3	5:A:613:PEG:H11	1.69	0.74
4:A:608:ISW:HBB	4:A:608:ISW:HMB	1.70	0.74
1:B:497:ARG:HB2	1:B:497:ARG:NH1	2.03	0.73
1:C:269:ASN:HD22	1:C:269:ASN:H	1.36	0.71
1:A:405:GLY:HA2	1:A:408:THR:CG2	2.21	0.70
1:A:407:LYS:CE	5:A:613:PEG:H11	2.21	0.70
2:D:46:LYS:HB3	2:D:49:ASP:OD2	1.90	0.70
1:A:405:GLY:HA2	1:A:408:THR:HG22	1.73	0.69
3:B:601:HEC:CAA	3:B:602:HEC:HMA3	2.22	0.69
1:B:497:ARG:CB	1:B:497:ARG:NH1	2.56	0.69
1:C:396:LYS:HE2	1:C:396:LYS:HA	1.74	0.69
1:A:8:GLU:N	1:A:8:GLU:OE1	2.28	0.67
3:C:602:HEC:HMC1	3:C:602:HEC:HBC3	1.78	0.66
1:A:431:LYS:HE3	11:F:212:HOH:O	1.95	0.66
1:B:8:GLU:OE1	1:B:8:GLU:N	2.20	0.66
1:C:104:LYS:NZ	6:C:614:PGE:H42	2.11	0.65
3:C:602:HEC:CAA	3:C:603:HEC:HMA3	2.26	0.65
1:A:498:VAL:O	1:A:502:GLU:HG3	1.96	0.64
3:B:606:HEC:HMC1	3:B:606:HEC:HBC3	1.80	0.64
1:B:248:PHE:O	3:B:603:HEC:HBA1	1.98	0.64
1:A:214:THR:HG21	4:C:601:ISW:HMBA	1.81	0.63
1:C:13:LEU:CD1	1:C:29:LEU:HD13	2.28	0.62
1:B:13:LEU:CD2	1:B:29:LEU:HD13	2.27	0.62
1:C:90:TRP:HA	1:C:90:TRP:CE3	2.33	0.62
1:A:34:LYS:NZ	11:A:832:HOH:O	2.32	0.62
3:A:605:HEC:O2A	4:C:601:ISW:O2D	2.18	0.62
3:B:601:HEC:HMB1	3:B:601:HEC:HBB3	1.82	0.62
4:B:608:ISW:HBB	4:B:608:ISW:HMB	1.81	0.62
3:B:607:HEC:HMB1	3:B:607:HEC:HBB3	1.82	0.61
1:B:374:ASP:OD1	1:B:378:LYS:HE2	2.01	0.61
1:A:316:GLU:HB2	1:A:321:TYR:CE2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ASN:HD22	1:A:269:ASN:H	1.48	0.60
1:C:333:ASN:O	1:C:335:PRO:HD3	2.01	0.60
1:C:19:LYS:NZ	7:C:617:EDO:H21	2.17	0.59
1:C:86:GLU:HG3	3:C:602:HEC:HMD3	1.84	0.59
3:B:601:HEC:HAA2	3:B:602:HEC:HMA3	1.84	0.59
4:A:608:ISW:HHC	1:B:229:CYS:SG	2.42	0.59
4:B:608:ISW:HMBA	1:C:214:THR:HG21	1.84	0.59
1:C:13:LEU:HD11	1:C:29:LEU:CD1	2.31	0.59
1:B:387:TYR:CE1	1:B:446:ALA:HB2	2.38	0.58
1:B:269:ASN:H	1:B:269:ASN:HD22	1.50	0.58
1:C:194:ASN:HB3	2:F:7:SER:HB3	1.86	0.57
1:A:201:ARG:NE	4:C:601:ISW:O1A	2.29	0.57
1:A:229:CYS:SG	4:C:601:ISW:HHC	2.45	0.57
3:C:606:HEC:HMB1	3:C:606:HEC:HBB3	1.87	0.56
1:C:90:TRP:HA	1:C:90:TRP:HE3	1.71	0.56
2:F:11:ILE:HD13	2:F:54:VAL:HG22	1.87	0.56
1:B:23:LYS:HG3	1:B:131:MET:HA	1.88	0.55
4:C:601:ISW:HMB	4:C:601:ISW:HBB	1.87	0.55
1:A:495:GLN:HG2	1:C:494:LEU:CD1	2.32	0.55
3:C:608:HEC:HBB3	3:C:608:HEC:CMB	2.37	0.55
3:A:601:HEC:CAA	3:A:602:HEC:HMA3	2.37	0.55
1:B:501:LEU:HD11	1:C:502:GLU:HG2	1.88	0.54
4:B:608:ISW:HHC	1:C:229:CYS:SG	2.46	0.54
1:A:407:LYS:NZ	5:A:613:PEG:H11	2.21	0.54
1:A:501:LEU:HD11	1:B:502:GLU:HG3	1.88	0.54
1:C:104:LYS:HZ2	6:C:614:PGE:H42	1.72	0.54
1:B:90:TRP:HA	1:B:90:TRP:CE3	2.43	0.54
4:A:608:ISW:O2A	1:B:201:ARG:NE	2.35	0.53
1:B:497:ARG:HH11	1:B:497:ARG:HG3	1.71	0.53
1:A:75:GLU:OE2	1:A:157:LYS:HE2	2.09	0.53
4:B:608:ISW:C3A	5:C:610:PEG:H32	2.39	0.53
1:B:316:GLU:HB2	1:B:321:TYR:CE2	2.43	0.52
4:A:608:ISW:HMBA	1:B:214:THR:HG21	1.92	0.52
1:B:357:VAL:O	1:B:361:THR:HG23	2.10	0.52
1:C:1:ASP:HB3	1:C:17:ARG:O	2.10	0.52
3:A:602:HEC:HMC1	3:A:602:HEC:HBC3	1.92	0.52
4:A:608:ISW:HBB	4:A:608:ISW:CMB	2.38	0.51
1:C:19:LYS:HZ1	7:C:617:EDO:H21	1.74	0.51
1:C:484:GLU:HG2	1:C:488:MET:HE2	1.92	0.51
1:B:1:ASP:OD2	9:B:614:PG4:O1	2.27	0.51
3:C:603:HEC:HMC1	3:C:603:HEC:HBC3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:608:ISW:HMD	1:C:263:HIS:CE1	2.45	0.51
1:C:75:GLU:HG3	1:C:157:LYS:HG2	1.93	0.51
1:B:453:MET:SD	1:B:474:MET:CE	2.99	0.51
4:A:608:ISW:HMB	4:A:608:ISW:CBB	2.40	0.50
1:B:453:MET:HB2	1:B:470:GLY:HA2	1.93	0.50
1:C:488:MET:HE1	11:C:877:HOH:O	2.11	0.50
1:A:104:LYS:NZ	6:A:615:PGE:H1	2.26	0.50
2:F:32:LYS:HD2	5:F:102:PEG:H22	1.94	0.50
1:B:90:TRP:HA	1:B:90:TRP:HE3	1.77	0.50
1:A:427:LEU:HD11	1:A:447:GLU:HG3	1.92	0.49
1:B:479:VAL:HG22	11:C:726:HOH:O	2.11	0.49
2:E:50:ILE:HD13	2:E:50:ILE:O	2.12	0.49
3:C:603:HEC:HBB3	3:C:603:HEC:HMB1	1.95	0.49
1:B:203:SER:O	3:B:605:HEC:HBD1	2.13	0.49
3:B:604:HEC:HBC3	3:B:604:HEC:HMC1	1.95	0.49
1:A:217:TRP:HB2	4:C:601:ISW:HMB	1.94	0.49
3:A:602:HEC:HMB1	3:A:602:HEC:HBB3	1.94	0.49
3:C:605:HEC:HMC1	3:C:605:HEC:HBC3	1.93	0.49
1:A:309:THR:C	3:A:606:HEC:HMC3	2.33	0.49
3:A:601:HEC:HMC1	3:A:601:HEC:CBC	2.42	0.49
1:B:496:ALA:O	1:B:500:LYS:HE2	2.13	0.48
1:C:184:GLU:OE1	1:C:187:ARG:NE	2.43	0.48
4:A:608:ISW:O1A	1:B:201:ARG:NH1	2.35	0.48
1:C:453:MET:HB2	1:C:470:GLY:HA2	1.95	0.48
4:A:608:ISW:HMB	1:B:217:TRP:HB2	1.95	0.48
1:B:176:HIS:CG	3:B:604:HEC:HMA1	2.49	0.48
1:A:387:TYR:CE1	1:A:446:ALA:HB2	2.49	0.48
1:B:60:PRO:HB3	1:B:166:MET:HB2	1.95	0.48
1:C:484:GLU:HG2	1:C:488:MET:CE	2.44	0.48
1:C:8:GLU:OE1	1:C:8:GLU:N	2.46	0.47
1:C:66:PRO:HB3	1:C:164:ILE:HB	1.96	0.47
1:B:431:LYS:NZ	11:B:914:HOH:O	2.44	0.47
1:A:453:MET:SD	1:A:474:MET:CE	3.03	0.47
1:B:271:TRP:O	1:B:275:THR:HG23	2.14	0.47
1:C:484:GLU:CG	1:C:488:MET:HE2	2.44	0.47
3:C:602:HEC:HMC1	3:C:602:HEC:CBC	2.44	0.47
1:A:453:MET:HB2	1:A:470:GLY:HA2	1.96	0.47
1:A:104:LYS:HZ3	6:A:615:PGE:H1	1.80	0.47
1:C:141:LYS:HB3	5:C:612:PEG:H22	1.97	0.47
1:A:495:GLN:CG	1:C:494:LEU:HD13	2.39	0.47
3:A:604:HEC:HHA	3:A:604:HEC:HAA2	1.69	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:608:ISW:HMD	1:B:263:HIS:CE1	2.49	0.47
1:C:269:ASN:HD22	1:C:269:ASN:N	2.05	0.47
2:F:50:ILE:O	2:F:50:ILE:HD13	2.14	0.47
1:C:120:LYS:HE2	3:C:605:HEC:HAA1	1.97	0.46
1:B:233:HIS:CE1	3:B:605:HEC:HMD1	2.50	0.46
1:C:284:GLU:O	1:C:287:ARG:HG2	2.15	0.46
1:A:150:VAL:HG11	1:A:154:LYS:HD3	1.97	0.46
2:F:19:TYR:CE2	2:F:23:LYS:HE2	2.50	0.46
3:A:603:HEC:CAA	3:A:604:HEC:HBA1	2.46	0.46
1:B:110:SER:HA	1:B:115:TYR:CG	2.51	0.46
1:A:13:LEU:CD1	1:A:29:LEU:HD13	2.38	0.46
1:C:375:LEU:HD23	1:C:375:LEU:C	2.36	0.46
1:A:106:ARG:NH2	1:A:139:THR:HB	2.31	0.45
1:A:106:ARG:HG3	1:A:121:LEU:HD21	1.97	0.45
1:A:411:PRO:HG3	1:A:431:LYS:HG3	1.98	0.45
1:B:74:ALA:HB1	1:B:78:ASP:HB2	1.99	0.45
1:A:50:GLU:OE1	2:F:32:LYS:NZ	2.48	0.45
1:C:196:GLN:HG2	1:C:340:ILE:HD13	1.98	0.45
1:A:21:THR:OG1	1:A:24:GLU:HG3	2.17	0.45
1:A:302:LYS:NZ	7:A:617:EDO:H12	2.32	0.45
1:B:13:LEU:HG	1:B:28:ALA:HB1	1.98	0.45
1:A:467:TYR:HD2	4:A:608:ISW:HMCA	1.81	0.45
1:B:407:LYS:HD3	1:B:407:LYS:HA	1.71	0.45
1:C:1:ASP:OD1	1:C:17:ARG:NE	2.40	0.45
3:C:607:HEC:HMB1	3:C:607:HEC:HBB3	1.99	0.44
2:F:47:CYS:O	2:F:51:VAL:HG23	2.17	0.44
3:B:605:HEC:HMC1	3:B:605:HEC:HBC3	1.99	0.44
1:C:176:HIS:CG	3:C:605:HEC:HMA1	2.52	0.44
4:B:608:ISW:O2D	3:C:606:HEC:O2A	2.35	0.44
2:E:30:VAL:HG22	2:E:46:LYS:CA	2.42	0.44
1:A:146:ILE:O	1:A:150:VAL:HB	2.18	0.44
1:A:263:HIS:CE1	4:C:601:ISW:HMD	2.52	0.44
1:B:269:ASN:HD22	1:B:269:ASN:N	2.12	0.44
1:B:162:LYS:HB2	1:B:162:LYS:HE3	1.77	0.44
4:B:608:ISW:C3A	5:C:610:PEG:C3	2.96	0.44
1:C:52:ILE:HD11	1:C:227:GLU:HG2	2.00	0.44
1:A:156:ASP:OD1	1:A:156:ASP:N	2.49	0.44
1:B:167:PRO:HG2	3:B:602:HEC:CHD	2.48	0.44
3:A:601:HEC:HMC1	3:A:601:HEC:HBC3	2.00	0.43
1:B:384:LEU:HD23	2:E:13:ALA:HB2	2.00	0.43
1:C:243:HIS:CE1	3:C:605:HEC:NB	2.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:608:ISW:HMB	1:C:217:TRP:HB2	2.00	0.43
1:C:361:THR:HA	1:C:364:HIS:O	2.18	0.43
1:C:484:GLU:OE2	1:C:488:MET:HE2	2.17	0.43
3:A:601:HEC:HMB1	3:A:601:HEC:HBB3	2.01	0.43
3:A:605:HEC:HBB3	3:A:605:HEC:HMB1	2.00	0.43
1:A:176:HIS:HA	11:A:804:HOH:O	2.18	0.43
1:A:221:PRO:HB3	2:F:42:ILE:HG12	2.00	0.43
11:A:775:HOH:O	1:C:479:VAL:HG22	2.17	0.43
1:B:491:LEU:O	1:B:491:LEU:HD13	2.18	0.43
1:C:396:LYS:HE2	1:C:396:LYS:CA	2.34	0.43
1:C:453:MET:HB2	1:C:470:GLY:CA	2.48	0.43
1:A:96:ARG:HH22	1:C:306:ASN:HB3	1.83	0.43
1:B:104:LYS:NZ	5:B:609:PEG:H22	2.34	0.43
1:A:157:LYS:CD	1:A:157:LYS:H	2.31	0.43
1:B:23:LYS:O	1:B:27:GLU:HG3	2.19	0.43
1:B:42:LYS:HD2	1:B:63:PHE:CZ	2.53	0.43
1:A:110:SER:HA	1:A:115:TYR:CG	2.54	0.43
1:A:203:SER:O	3:A:605:HEC:HBD1	2.18	0.43
1:B:275:THR:O	1:B:281:LYS:HG2	2.18	0.43
1:C:104:LYS:HZ3	6:C:614:PGE:H42	1.83	0.43
4:B:608:ISW:HMAB	1:C:210:ALA:HB1	2.01	0.42
2:E:22:CYS:O	2:E:23:LYS:C	2.57	0.42
1:C:166:MET:HA	1:C:167:PRO:HD3	1.93	0.42
1:C:278:LYS:HA	1:C:278:LYS:HD3	1.80	0.42
1:A:113:PRO:HA	5:A:612:PEG:H21	2.00	0.42
1:A:167:PRO:HG2	3:A:602:HEC:CHD	2.49	0.42
2:E:47:CYS:O	2:E:51:VAL:HB	2.19	0.42
1:C:145:CYS:O	1:C:149:HIS:HB2	2.20	0.42
2:E:20:LEU:HD23	2:E:20:LEU:HA	1.68	0.42
1:C:150:VAL:HG11	1:C:154:LYS:HE2	2.01	0.42
1:A:96:ARG:NH2	1:C:306:ASN:HB3	2.34	0.42
1:B:176:HIS:CD2	3:B:603:HEC:NB	2.86	0.42
1:B:453:MET:SD	1:B:474:MET:HE1	2.60	0.42
3:B:606:HEC:HBB3	3:B:606:HEC:HMB1	2.02	0.42
1:C:327:ARG:HB2	11:C:727:HOH:O	2.19	0.42
1:C:370:ARG:HB3	7:C:616:EDO:H21	2.02	0.42
1:C:104:LYS:HD2	6:C:614:PGE:H2	2.00	0.41
1:A:214:THR:CG2	4:C:601:ISW:HMBA	2.50	0.41
1:B:278:LYS:HA	1:B:278:LYS:HD3	1.60	0.41
1:B:245:ARG:HA	1:B:246:HIS:HA	1.87	0.41
4:B:608:ISW:HMBA	1:C:214:THR:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:VAL:O	1:C:361:THR:HG23	2.20	0.41
3:C:604:HEC:HMC1	3:C:604:HEC:HBC3	2.02	0.41
2:E:18:ASP:HB2	2:E:50:ILE:HG13	2.02	0.41
1:B:143:VAL:HG22	3:B:603:HEC:HBC2	2.02	0.41
1:B:467:TYR:HD2	4:B:608:ISW:HMCA	1.86	0.41
1:C:317:TYR:O	1:C:318:GLU:C	2.57	0.41
1:A:252:GLU:OE2	1:C:282:LEU:HD21	2.20	0.41
4:B:608:ISW:HBAA	3:C:606:HEC:CGD	2.44	0.41
5:B:612:PEG:H41	5:B:612:PEG:H21	1.59	0.41
1:A:429:TRP:CZ2	1:A:431:LYS:HB3	2.56	0.41
1:A:416:PRO:O	7:A:619:EDO:H11	2.21	0.41
3:A:604:HEC:HMC1	3:A:604:HEC:HBC3	2.02	0.41
1:B:143:VAL:HG21	3:B:603:HEC:CHD	2.51	0.41
1:A:152:VAL:HG23	11:A:720:HOH:O	2.21	0.41
1:A:491:LEU:CD2	1:B:491:LEU:HD21	2.51	0.41
1:B:42:LYS:HD2	1:B:63:PHE:HZ	1.85	0.40
1:B:240:ASP:O	1:B:244:THR:HA	2.21	0.40
1:C:325:ILE:HD13	3:C:606:HEC:C3A	2.51	0.40
2:E:55:GLN:N	2:E:55:GLN:CD	2.74	0.40
1:A:441:LYS:HE3	1:A:441:LYS:HB2	1.90	0.40
1:C:5:VAL:HA	1:C:6:PRO:HD3	1.83	0.40
3:C:602:HEC:HHB	3:C:602:HEC:HMA1	1.92	0.40
1:A:491:LEU:HD21	1:B:491:LEU:HD21	2.03	0.40
1:A:201:ARG:HH21	4:C:601:ISW:CGA	2.33	0.40
1:B:271:TRP:CZ2	1:B:275:THR:HG21	2.57	0.40
4:B:608:ISW:HMAA	5:C:610:PEG:H31	2.04	0.40
1:A:282:LEU:HD23	1:A:282:LEU:HA	1.87	0.40
1:B:13:LEU:HD21	1:B:29:LEU:CD1	2.34	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	501/546 (92%)	482 (96%)	19 (4%)	0	100	100
1	B	500/546 (92%)	483 (97%)	16 (3%)	1 (0%)	47	49
1	C	500/546 (92%)	478 (96%)	21 (4%)	1 (0%)	47	49
2	D	47/69 (68%)	45 (96%)	2 (4%)	0	100	100
2	E	47/69 (68%)	44 (94%)	3 (6%)	0	100	100
2	F	47/69 (68%)	45 (96%)	2 (4%)	0	100	100
All	All	1642/1845 (89%)	1577 (96%)	63 (4%)	2 (0%)	51	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	268	HIS
1	C	268	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	430/459 (94%)	414 (96%)	16 (4%)	34	35
1	B	429/459 (94%)	410 (96%)	19 (4%)	28	28
1	C	429/459 (94%)	416 (97%)	13 (3%)	41	44
2	D	43/57 (75%)	39 (91%)	4 (9%)	9	6
2	E	43/57 (75%)	39 (91%)	4 (9%)	9	6
2	F	43/57 (75%)	40 (93%)	3 (7%)	15	12
All	All	1417/1548 (92%)	1358 (96%)	59 (4%)	30	30

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	65	LYS
1	A	67	PRO

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Mol	Chain	Res	Type
1	A	90	TRP
1	A	137	LYS
1	A	145	CYS
1	A	157	LYS
1	A	177	LEU
1	A	247	GLU
1	A	269	ASN
1	A	301	SER
1	A	418	LYS
1	A	442	VAL
1	A	443	LEU
1	A	491	LEU
1	A	497	ARG
1	B	13	LEU
1	B	14	LYS
1	B	23	LYS
1	B	29	LEU
1	B	42	LYS
1	B	88	PRO
1	B	90	TRP
1	B	177	LEU
1	B	266	VAL
1	B	269	ASN
1	B	278	LYS
1	B	287	ARG
1	B	342	GLU
1	B	358	LEU
1	B	396	LYS
1	B	443	LEU
1	B	497	ARG
1	B	499	ASN
1	B	500	LYS
1	C	16	ASP
1	C	17	ARG
1	C	29	LEU
1	C	65	LYS
1	C	77	LYS
1	C	90	TRP
1	C	155	LYS
1	C	269	ASN
1	C	322	THR
1	C	396	LYS

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Mol	Chain	Res	Type
1	C	442	VAL
1	C	499	ASN
1	C	500	LYS
2	D	17	LEU
2	D	23	LYS
2	D	44	ARG
2	D	50	ILE
2	E	25	LYS
2	E	50	ILE
2	E	51	VAL
2	E	53	LEU
2	F	17	LEU
2	F	24	ASP
2	F	50	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	269	ASN
1	A	343	ASN
1	A	448	ASN
1	A	461	ASN
1	A	489	GLN
1	B	269	ASN
1	B	448	ASN
1	B	461	ASN
1	C	269	ASN
1	C	448	ASN
1	C	461	ASN
1	C	495	GLN
1	C	499	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

64 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
5	PEG	A	609	-	6,6,6	0.22	0	5,5,5	1.01	0
7	EDO	C	620	-	3,3,3	0.83	0	2,2,2	0.43	0
3	HEC	C	607	1	32,50,50	1.33	3 (9%)	24,82,82	1.94	7 (29%)
3	HEC	B	603	1	32,50,50	1.17	2 (6%)	24,82,82	2.12	10 (41%)
10	NO3	B	618	-	1,3,3	4.10	1 (100%)	0,3,3	-	-
7	EDO	C	615	-	3,3,3	0.45	0	2,2,2	0.25	0
3	HEC	B	607	1	32,50,50	1.32	4 (12%)	24,82,82	2.20	7 (29%)
7	EDO	A	619	-	3,3,3	0.56	0	2,2,2	0.32	0
5	PEG	C	609	-	6,6,6	0.48	0	5,5,5	0.40	0
5	PEG	A	611	-	6,6,6	0.64	0	5,5,5	0.48	0
5	PEG	C	610	-	6,6,6	0.75	0	5,5,5	0.69	0
7	EDO	A	618	-	3,3,3	0.46	0	2,2,2	0.22	0
3	HEC	A	601	1	32,50,50	1.21	2 (6%)	24,82,82	2.12	7 (29%)
5	PEG	C	612	-	6,6,6	0.46	0	5,5,5	0.84	0
6	PGE	C	614	-	9,9,9	0.36	0	8,8,8	1.02	0
3	HEC	A	604	1	32,50,50	1.16	3 (9%)	24,82,82	2.60	7 (29%)
4	ISW	A	608	1	40,50,50	2.97	18 (45%)	38,82,82	2.91	18 (47%)
5	PEG	A	610	-	6,6,6	0.27	0	5,5,5	1.05	0
5	PEG	B	610	-	6,6,6	0.50	0	5,5,5	0.48	0
5	PEG	C	613	-	6,6,6	0.65	0	5,5,5	0.91	0
7	EDO	B	615	-	3,3,3	0.63	0	2,2,2	0.07	0
7	EDO	C	618	-	3,3,3	0.74	0	2,2,2	0.22	0
3	HEC	C	606	1	32,50,50	1.22	2 (6%)	24,82,82	1.66	7 (29%)
3	HEC	B	601	1	32,50,50	1.31	3 (9%)	24,82,82	2.20	9 (37%)
7	EDO	A	617	-	3,3,3	0.68	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEC	A	602	1	32,50,50	1.67	7 (21%)	24,82,82	1.62	3 (12%)
7	EDO	C	617	-	3,3,3	0.52	0	2,2,2	0.34	0
9	PG4	B	614	-	12,12,12	0.61	0	11,11,11	0.91	0
3	HEC	C	603	1	32,50,50	1.40	4 (12%)	24,82,82	1.93	7 (29%)
7	EDO	C	621	-	3,3,3	0.56	0	2,2,2	0.43	0
3	HEC	B	606	1	32,50,50	1.47	6 (18%)	24,82,82	1.80	4 (16%)
10	NO3	F	101	-	1,3,3	3.83	1 (100%)	0,3,3	-	-
7	EDO	B	620	-	3,3,3	0.74	0	2,2,2	0.44	0
7	EDO	B	621	-	3,3,3	0.49	0	2,2,2	0.17	0
3	HEC	C	602	1	32,50,50	1.18	2 (6%)	24,82,82	2.30	10 (41%)
5	PEG	F	102	-	6,6,6	0.59	0	5,5,5	0.68	0
6	PGE	A	615	-	9,9,9	0.67	0	8,8,8	0.80	0
3	HEC	B	602	1	32,50,50	1.33	3 (9%)	24,82,82	1.48	4 (16%)
5	PEG	A	612	-	6,6,6	0.53	0	5,5,5	0.35	0
10	NO3	B	617	-	1,3,3	3.00	1 (100%)	0,3,3	-	-
5	PEG	C	622	-	6,6,6	0.96	0	5,5,5	1.21	0
7	EDO	C	616	-	3,3,3	0.19	0	2,2,2	0.74	0
5	PEG	A	614	-	6,6,6	0.76	0	5,5,5	0.85	0
7	EDO	B	616	-	3,3,3	0.49	0	2,2,2	0.41	0
3	HEC	A	606	1	32,50,50	1.51	7 (21%)	24,82,82	2.18	6 (25%)
5	PEG	B	609	-	6,6,6	0.46	0	5,5,5	0.94	0
5	PEG	B	612	-	6,6,6	0.69	0	5,5,5	0.71	0
4	ISW	C	601	1	40,50,50	3.07	17 (42%)	38,82,82	2.46	16 (42%)
5	PEG	A	613	-	6,6,6	0.55	0	5,5,5	0.53	0
5	PEG	C	611	-	6,6,6	0.55	0	5,5,5	0.62	0
7	EDO	B	619	-	3,3,3	0.25	0	2,2,2	0.71	0
4	ISW	B	608	1	40,50,50	3.28	19 (47%)	38,82,82	2.68	15 (39%)
10	NO3	C	619	-	1,3,3	3.66	1 (100%)	0,3,3	-	-
3	HEC	C	604	1	32,50,50	1.29	4 (12%)	24,82,82	1.78	3 (12%)
3	HEC	A	605	1	32,50,50	1.16	2 (6%)	24,82,82	2.24	9 (37%)
3	HEC	B	605	1	32,50,50	1.29	2 (6%)	24,82,82	1.89	9 (37%)
5	PEG	B	611	-	6,6,6	0.34	0	5,5,5	0.96	0
8	P6G	B	613	-	18,18,18	0.48	0	17,17,17	0.75	0
3	HEC	B	604	1	32,50,50	1.12	3 (9%)	24,82,82	2.04	6 (25%)
3	HEC	C	608	1	32,50,50	1.27	2 (6%)	24,82,82	2.31	8 (33%)
3	HEC	A	603	1	32,50,50	1.09	0	24,82,82	1.58	5 (20%)
3	HEC	C	605	1	32,50,50	1.42	3 (9%)	24,82,82	2.02	8 (33%)
7	EDO	A	616	-	3,3,3	0.63	0	2,2,2	1.03	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEC	A	607	1	32,50,50	1.49	5 (15%)	24,82,82	2.82	10 (41%)

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
5	PEG	A	609	-	-	2/4/4/4	-
7	EDO	C	620	-	-	1/1/1/1	-
3	HEC	C	607	1	-	5/10/54/54	-
3	HEC	B	603	1	-	4/10/54/54	-
7	EDO	C	615	-	-	0/1/1/1	-
3	HEC	B	607	1	-	2/10/54/54	-
7	EDO	A	619	-	-	1/1/1/1	-
5	PEG	C	609	-	-	1/4/4/4	-
5	PEG	A	611	-	-	2/4/4/4	-
5	PEG	C	610	-	-	4/4/4/4	-
7	EDO	A	618	-	-	1/1/1/1	-
3	HEC	A	601	1	-	2/10/54/54	-
5	PEG	C	612	-	-	2/4/4/4	-
6	PGE	C	614	-	-	6/7/7/7	-
3	HEC	A	604	1	-	4/10/54/54	-
4	ISW	A	608	1	-	3/12/74/74	-
5	PEG	A	610	-	-	1/4/4/4	-
5	PEG	B	610	-	-	1/4/4/4	-
5	PEG	C	613	-	-	3/4/4/4	-
7	EDO	B	615	-	-	1/1/1/1	-
7	EDO	C	618	-	-	0/1/1/1	-
3	HEC	C	606	1	-	2/10/54/54	-
3	HEC	B	601	1	-	2/10/54/54	-
7	EDO	A	617	-	-	1/1/1/1	-
3	HEC	A	602	1	-	2/10/54/54	-
7	EDO	C	617	-	-	1/1/1/1	-
9	PG4	B	614	-	-	4/10/10/10	-
3	HEC	C	603	1	-	4/10/54/54	-
7	EDO	C	621	-	-	1/1/1/1	-
3	HEC	B	606	1	-	4/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	B	620	-	-	0/1/1/1	-
7	EDO	B	621	-	-	1/1/1/1	-
3	HEC	C	602	1	-	0/10/54/54	-
5	PEG	F	102	-	-	3/4/4/4	-
6	PGE	A	615	-	-	5/7/7/7	-
3	HEC	B	602	1	-	2/10/54/54	-
5	PEG	A	612	-	-	1/4/4/4	-
5	PEG	C	622	-	-	3/4/4/4	-
7	EDO	C	616	-	-	1/1/1/1	-
5	PEG	A	614	-	-	3/4/4/4	-
7	EDO	B	616	-	-	0/1/1/1	-
3	HEC	A	606	1	-	4/10/54/54	-
5	PEG	B	609	-	-	2/4/4/4	-
5	PEG	B	612	-	-	4/4/4/4	-
4	ISW	C	601	1	-	2/12/74/74	-
5	PEG	A	613	-	-	4/4/4/4	-
5	PEG	C	611	-	-	4/4/4/4	-
7	EDO	B	619	-	-	1/1/1/1	-
4	ISW	B	608	1	-	2/12/74/74	-
3	HEC	C	604	1	-	4/10/54/54	-
3	HEC	A	605	1	-	2/10/54/54	-
3	HEC	B	605	1	-	2/10/54/54	-
5	PEG	B	611	-	-	2/4/4/4	-
8	P6G	B	613	-	-	10/16/16/16	-
3	HEC	B	604	1	-	2/10/54/54	-
3	HEC	C	608	1	-	2/10/54/54	-
3	HEC	A	603	1	-	4/10/54/54	-
3	HEC	C	605	1	-	0/10/54/54	-
7	EDO	A	616	-	-	0/1/1/1	-
3	HEC	A	607	1	-	2/10/54/54	-

All (127) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	608	ISW	C1C-C2C	10.60	1.52	1.38
4	C	601	ISW	C1C-C2C	9.19	1.50	1.38
4	A	608	ISW	C1C-C2C	7.82	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	608	ISW	C3D-C2D	6.77	1.51	1.36
4	B	608	ISW	C3C-C2C	6.57	1.49	1.40
4	C	601	ISW	C3C-C2C	5.64	1.48	1.40
4	B	608	ISW	C1B-NB	5.63	1.33	1.28
4	A	608	ISW	CHD-C1D	5.54	1.49	1.35
4	C	601	ISW	C3D-C2D	5.47	1.48	1.36
4	B	608	ISW	C3D-C2D	5.43	1.48	1.36
4	C	601	ISW	CHD-C1D	5.41	1.48	1.35
4	C	601	ISW	C1B-NB	5.40	1.32	1.28
4	B	608	ISW	C2A-C3A	5.14	1.52	1.37
4	B	608	ISW	CHD-C1D	4.93	1.47	1.35
4	A	608	ISW	CBB-CAB	4.83	1.54	1.30
4	C	601	ISW	CBB-CAB	4.57	1.53	1.30
4	A	608	ISW	C2A-C3A	4.53	1.51	1.37
4	A	608	ISW	C2A-C1A	4.49	1.52	1.42
4	A	608	ISW	C3A-C4A	4.44	1.52	1.42
4	A	608	ISW	C3C-C2C	4.33	1.46	1.40
4	B	608	ISW	CHA-C4D	4.19	1.53	1.41
4	C	601	ISW	C2A-C3A	4.17	1.50	1.37
10	B	618	NO3	O1-N	4.10	1.43	1.24
3	C	605	HEC	C3C-C2C	-4.09	1.36	1.40
3	A	602	HEC	C4B-C3B	-4.07	1.35	1.43
4	C	601	ISW	C1D-ND	-4.04	1.33	1.40
3	B	602	HEC	C2B-C3B	-4.02	1.36	1.40
3	A	607	HEC	C2B-C3B	-3.98	1.36	1.40
4	B	608	ISW	C4D-C3D	3.94	1.51	1.45
3	C	607	HEC	C2B-C3B	-3.93	1.36	1.40
4	A	608	ISW	C1B-NB	3.91	1.31	1.28
4	C	601	ISW	CBC-CAC	3.90	1.55	1.29
4	B	608	ISW	C2A-C1A	3.88	1.51	1.42
4	B	608	ISW	CBB-CAB	3.87	1.49	1.30
3	A	605	HEC	C2B-C3B	-3.84	1.36	1.40
3	B	605	HEC	C3C-C2C	-3.83	1.36	1.40
10	F	101	NO3	O1-N	3.83	1.41	1.24
4	B	608	ISW	C1D-ND	-3.81	1.33	1.40
4	A	608	ISW	CHA-C4D	3.78	1.52	1.41
4	B	608	ISW	CBC-CAC	3.77	1.54	1.29
10	C	619	NO3	O1-N	3.66	1.40	1.24
4	C	601	ISW	C3A-C4A	3.64	1.50	1.42
3	A	602	HEC	C2B-C3B	-3.56	1.37	1.40
4	A	608	ISW	C4C-CHD	3.43	1.50	1.41
4	C	601	ISW	CHA-C4D	3.40	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	606	HEC	C2B-C3B	-3.25	1.37	1.40
3	C	604	HEC	C2B-C3B	-3.24	1.37	1.40
4	C	601	ISW	C2A-C1A	3.22	1.49	1.42
4	B	608	ISW	FE-NB	3.22	2.12	1.96
3	C	603	HEC	C4B-C3B	-3.19	1.37	1.43
4	C	601	ISW	FE-NB	3.15	2.12	1.96
3	A	602	HEC	C3C-C2C	-3.10	1.37	1.40
4	B	608	ISW	C4C-CHD	3.08	1.49	1.41
4	A	608	ISW	C4D-C3D	3.08	1.50	1.45
3	B	606	HEC	O1A-CGA	3.06	1.32	1.22
4	B	608	ISW	C3A-C4A	3.02	1.49	1.42
10	B	617	NO3	O1-N	3.00	1.37	1.24
3	B	601	HEC	C1D-CHD	2.97	1.49	1.41
4	A	608	ISW	CBC-CAC	2.96	1.48	1.29
3	B	606	HEC	C3C-C4C	-2.86	1.37	1.43
3	B	607	HEC	C3C-C2C	-2.81	1.37	1.40
4	A	608	ISW	C1B-C2B	2.77	1.49	1.44
3	A	604	HEC	C3C-C2C	-2.75	1.37	1.40
3	B	601	HEC	C3C-C2C	-2.75	1.37	1.40
3	C	603	HEC	C3C-C2C	-2.75	1.37	1.40
3	A	601	HEC	C3C-C4C	-2.74	1.38	1.43
3	C	608	HEC	C1B-NB	-2.73	1.30	1.36
3	A	602	HEC	C3D-C2D	2.73	1.45	1.37
4	A	608	ISW	FE-NB	2.67	2.10	1.96
4	C	601	ISW	C1B-C2B	2.66	1.49	1.44
3	A	604	HEC	CAD-C3D	2.63	1.55	1.52
3	C	606	HEC	O1A-CGA	2.63	1.30	1.22
4	B	608	ISW	C4B-C3B	-2.62	1.48	1.52
4	B	608	ISW	FE-ND	2.62	2.09	1.96
3	A	606	HEC	CAA-C2A	2.59	1.56	1.52
3	B	606	HEC	C3D-C2D	2.58	1.45	1.37
3	A	606	HEC	CMD-C2D	2.58	1.57	1.51
3	A	607	HEC	C1C-CHC	2.57	1.48	1.41
3	A	607	HEC	CMD-C2D	2.54	1.56	1.51
3	A	606	HEC	C1B-NB	-2.53	1.31	1.36
3	B	606	HEC	C1C-CHC	2.52	1.48	1.41
3	B	602	HEC	C1C-NC	-2.48	1.31	1.36
3	A	607	HEC	C4D-ND	-2.45	1.31	1.36
3	B	604	HEC	O2A-CGA	-2.44	1.22	1.30
4	C	601	ISW	C3C-CAC	2.42	1.52	1.47
3	B	605	HEC	C2B-C3B	-2.41	1.38	1.40
3	C	607	HEC	C1D-CHD	2.41	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	606	HEC	C2B-C3B	-2.37	1.38	1.40
3	C	605	HEC	C4D-CHA	2.37	1.47	1.41
3	B	607	HEC	C3D-C2D	2.35	1.44	1.37
4	C	601	ISW	FE-ND	2.34	2.08	1.96
4	A	608	ISW	FE-ND	2.34	2.08	1.96
4	B	608	ISW	CHB-C1B	2.30	1.47	1.41
4	A	608	ISW	CBA-CGA	2.30	1.55	1.50
3	B	603	HEC	C1D-CHD	2.30	1.47	1.41
3	C	604	HEC	C3C-C2C	2.29	1.43	1.40
3	B	604	HEC	C3D-C2D	2.29	1.44	1.37
3	A	602	HEC	C1B-NB	-2.29	1.31	1.36
3	B	607	HEC	C4B-C3B	-2.28	1.38	1.43
3	A	602	HEC	O1D-CGD	2.28	1.29	1.22
3	B	604	HEC	C3C-C2C	-2.28	1.38	1.40
3	C	603	HEC	C4D-CHA	2.28	1.47	1.41
3	A	601	HEC	C4B-C3B	-2.27	1.38	1.43
3	C	605	HEC	C4B-C3B	-2.27	1.38	1.43
4	A	608	ISW	C1D-ND	-2.24	1.36	1.40
3	C	607	HEC	O1A-CGA	2.24	1.29	1.22
3	B	602	HEC	C3C-C2C	-2.24	1.38	1.40
3	C	602	HEC	C1C-CHC	2.22	1.47	1.41
3	C	604	HEC	C1B-CHB	2.21	1.47	1.41
3	A	606	HEC	C3C-C2C	-2.21	1.38	1.40
3	B	601	HEC	C1C-CHC	2.21	1.47	1.41
3	A	606	HEC	C4D-ND	-2.19	1.31	1.36
3	A	607	HEC	O2A-CGA	-2.18	1.23	1.30
4	B	608	ISW	O1D-CGD	-2.18	1.23	1.30
3	B	606	HEC	CBA-CGA	2.16	1.55	1.50
3	C	608	HEC	C2B-C3B	-2.16	1.38	1.40
3	A	602	HEC	CAA-C2A	2.14	1.56	1.52
3	B	607	HEC	O1D-CGD	2.11	1.29	1.22
3	A	604	HEC	C4B-C3B	-2.11	1.39	1.43
4	C	601	ISW	C4D-C3D	2.10	1.48	1.45
3	B	603	HEC	C1B-CHB	2.10	1.46	1.41
3	B	606	HEC	CAA-C2A	2.07	1.55	1.52
3	A	605	HEC	C4D-CHA	2.07	1.46	1.41
3	A	606	HEC	CMA-C3A	2.05	1.56	1.51
3	C	602	HEC	C3C-C4C	-2.02	1.39	1.43
3	C	604	HEC	C4B-C3B	-2.02	1.39	1.43
3	C	603	HEC	C1B-CHB	2.01	1.46	1.41

All (195) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	607	HEC	C1D-C2D-C3D	-8.81	100.87	107.00
4	B	608	ISW	C4B-NB-C1B	7.41	115.13	107.63
4	A	608	ISW	C4B-NB-C1B	7.22	114.94	107.63
3	A	604	HEC	CBD-CAD-C3D	-7.02	100.64	112.62
3	B	604	HEC	CBD-CAD-C3D	-6.85	100.92	112.62
3	C	608	HEC	CMC-C2C-C3C	6.72	133.72	125.82
3	C	605	HEC	CBD-CAD-C3D	-6.21	102.02	112.62
4	A	608	ISW	C1B-C2B-C3B	-6.08	99.53	106.80
3	A	604	HEC	CMB-C2B-C3B	6.02	132.90	125.82
3	B	607	HEC	C1D-C2D-C3D	-5.97	102.84	107.00
3	A	601	HEC	CMC-C2C-C3C	5.86	132.71	125.82
4	C	601	ISW	C4B-NB-C1B	5.81	113.51	107.63
3	A	607	HEC	CMC-C2C-C3C	5.62	132.43	125.82
3	B	606	HEC	CMB-C2B-C3B	5.61	132.41	125.82
3	C	604	HEC	CMC-C2C-C3C	5.59	132.39	125.82
3	C	608	HEC	CMC-C2C-C1C	-5.52	119.98	128.46
4	C	601	ISW	C1B-C2B-C3B	-5.33	100.42	106.80
3	B	601	HEC	CBA-CAA-C2A	-5.30	103.67	112.60
3	A	606	HEC	C1D-C2D-C3D	-5.25	103.34	107.00
4	B	608	ISW	CAD-CBD-CGD	-5.22	102.37	113.60
4	A	608	ISW	CHC-C1C-C2C	-4.93	120.91	129.45
4	A	608	ISW	CAD-CBD-CGD	-4.92	103.01	113.60
3	A	605	HEC	CBA-CAA-C2A	-4.92	104.31	112.60
3	C	603	HEC	C1D-C2D-C3D	-4.83	103.64	107.00
4	C	601	ISW	CAD-CBD-CGD	-4.79	103.31	113.60
3	C	607	HEC	CBD-CAD-C3D	-4.75	104.52	112.62
3	B	607	HEC	CMB-C2B-C3B	4.71	131.36	125.82
3	A	601	HEC	CMC-C2C-C1C	-4.69	121.26	128.46
3	B	601	HEC	CMD-C2D-C1D	-4.66	121.31	128.46
3	A	606	HEC	CMB-C2B-C3B	4.62	131.26	125.82
3	A	604	HEC	CBA-CAA-C2A	4.52	120.22	112.60
4	A	608	ISW	CHA-C4D-ND	-4.49	119.56	124.43
3	A	606	HEC	CMB-C2B-C1B	-4.47	121.59	128.46
3	A	605	HEC	CMC-C2C-C1C	-4.44	121.64	128.46
4	B	608	ISW	C1B-C2B-C3B	-4.42	101.52	106.80
3	B	605	HEC	CBA-CAA-C2A	-4.32	105.32	112.60
4	B	608	ISW	CHC-C1C-C2C	-4.32	121.97	129.45
3	C	602	HEC	CMC-C2C-C3C	4.32	130.90	125.82
3	C	602	HEC	CBD-CAD-C3D	4.32	119.99	112.62
4	B	608	ISW	C1D-C2D-C3D	-4.31	102.42	106.96
3	B	603	HEC	CAA-CBA-CGA	-4.30	101.70	113.76
4	A	608	ISW	CBB-CAB-C3B	-4.29	112.28	127.20
3	B	606	HEC	CMB-C2B-C1B	-4.29	121.88	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	HEC	CBA-CAA-C2A	4.24	119.75	112.60
3	A	602	HEC	C1D-C2D-C3D	-4.21	104.07	107.00
4	A	608	ISW	CHB-C1B-NB	-4.19	119.88	124.43
4	A	608	ISW	C1D-C2D-C3D	-4.15	102.60	106.96
4	C	601	ISW	C3C-C4C-NC	4.11	114.52	109.21
4	B	608	ISW	C3C-C4C-NC	4.09	114.50	109.21
4	C	601	ISW	CHC-C1C-C2C	-4.06	122.42	129.45
3	C	602	HEC	O2A-CGA-CBA	4.03	126.99	114.03
3	A	607	HEC	CMC-C2C-C1C	-4.00	122.31	128.46
3	A	605	HEC	CMC-C2C-C3C	3.99	130.51	125.82
4	A	608	ISW	C1D-ND-C4D	3.99	109.19	105.07
4	C	601	ISW	C1D-ND-C4D	3.98	109.18	105.07
3	C	603	HEC	CMB-C2B-C1B	-3.97	122.36	128.46
4	B	608	ISW	CBB-CAB-C3B	-3.84	113.87	127.20
3	C	602	HEC	CMC-C2C-C1C	-3.82	122.59	128.46
3	A	604	HEC	CMB-C2B-C1B	-3.80	122.62	128.46
4	B	608	ISW	C1D-ND-C4D	3.78	108.98	105.07
4	B	608	ISW	C2D-C1D-ND	3.63	114.14	109.84
4	B	608	ISW	CMA-C3A-C2A	3.50	131.55	124.94
3	A	607	HEC	CMD-C2D-C3D	3.50	131.53	124.94
4	C	601	ISW	CBB-CAB-C3B	-3.46	115.16	127.20
4	A	608	ISW	CHA-C4D-C3D	3.45	129.91	124.84
3	C	602	HEC	CBA-CAA-C2A	-3.40	106.87	112.60
3	B	603	HEC	CBA-CAA-C2A	-3.37	106.93	112.60
3	A	606	HEC	CBD-CAD-C3D	-3.36	106.89	112.62
3	B	607	HEC	CMB-C2B-C1B	-3.35	123.31	128.46
3	B	601	HEC	CMD-C2D-C3D	3.31	131.18	124.94
3	A	605	HEC	C4C-C3C-C2C	-3.30	102.79	106.35
3	B	603	HEC	O2D-CGD-CBD	3.29	124.60	114.03
3	B	607	HEC	CBD-CAD-C3D	-3.28	107.03	112.62
3	A	601	HEC	CBA-CAA-C2A	-3.27	107.10	112.60
4	C	601	ISW	C1D-C2D-C3D	-3.25	103.54	106.96
3	C	604	HEC	CMC-C2C-C1C	-3.24	123.48	128.46
3	C	602	HEC	CMA-C3A-C2A	3.19	130.96	124.94
3	A	603	HEC	CMC-C2C-C3C	3.19	129.57	125.82
3	C	606	HEC	CBA-CAA-C2A	-3.19	107.23	112.60
3	A	605	HEC	CBD-CAD-C3D	-3.16	107.23	112.62
3	C	607	HEC	CMC-C2C-C3C	3.15	129.53	125.82
4	A	608	ISW	O2A-CGA-CBA	3.12	124.05	114.03
3	C	606	HEC	CBD-CAD-C3D	-3.08	107.37	112.62
3	A	607	HEC	CMB-C2B-C3B	3.06	129.42	125.82
3	A	607	HEC	CBA-CAA-C2A	-3.04	107.47	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	605	HEC	C1D-C2D-C3D	-3.04	104.88	107.00
3	B	602	HEC	CBD-CAD-C3D	-3.04	107.44	112.62
4	A	608	ISW	CMC-C2C-C3C	3.03	130.34	124.68
3	A	601	HEC	O2D-CGD-CBD	3.01	123.69	114.03
3	C	607	HEC	CBA-CAA-C2A	-3.00	107.55	112.60
3	A	606	HEC	CMD-C2D-C3D	3.00	130.59	124.94
3	B	603	HEC	CAD-CBD-CGD	-2.98	105.41	113.76
3	C	606	HEC	C1D-C2D-C3D	-2.97	104.93	107.00
3	B	604	HEC	CMB-C2B-C3B	2.95	129.29	125.82
3	C	607	HEC	CMB-C2B-C1B	-2.95	123.93	128.46
3	B	602	HEC	CBA-CAA-C2A	2.94	117.55	112.60
3	B	601	HEC	CAD-CBD-CGD	-2.93	105.54	113.76
3	B	607	HEC	CMD-C2D-C3D	2.90	130.42	124.94
3	C	603	HEC	O2A-CGA-CBA	2.89	123.32	114.03
3	B	603	HEC	CMB-C2B-C1B	-2.86	124.07	128.46
3	A	607	HEC	CMB-C2B-C1B	-2.84	124.11	128.46
3	C	602	HEC	CMB-C2B-C3B	2.83	129.15	125.82
3	B	604	HEC	CMB-C2B-C1B	-2.83	124.11	128.46
3	B	604	HEC	CBA-CAA-C2A	2.83	117.37	112.60
3	C	603	HEC	CMB-C2B-C3B	2.79	129.10	125.82
3	B	605	HEC	CMB-C2B-C3B	2.78	129.09	125.82
4	B	608	ISW	CHB-C1B-NB	-2.77	121.42	124.43
4	B	608	ISW	CHA-C4D-C3D	2.77	128.90	124.84
3	B	601	HEC	O1A-CGA-CBA	-2.76	114.21	123.08
3	B	606	HEC	C1D-C2D-C3D	-2.76	105.08	107.00
4	A	608	ISW	CMB-C2B-C1B	2.75	129.23	125.04
3	A	601	HEC	O2D-CGD-O1D	-2.74	116.46	123.30
3	B	601	HEC	CMB-C2B-C3B	2.74	129.04	125.82
3	C	605	HEC	CMA-C3A-C2A	2.73	130.09	124.94
3	C	605	HEC	O2D-CGD-CBD	2.73	122.79	114.03
3	C	606	HEC	CMC-C2C-C3C	2.70	128.99	125.82
3	B	605	HEC	O2D-CGD-CBD	2.70	122.69	114.03
3	C	608	HEC	CMB-C2B-C1B	-2.69	124.33	128.46
3	B	607	HEC	CMC-C2C-C1C	-2.69	124.33	128.46
3	B	603	HEC	CMC-C2C-C3C	2.68	128.97	125.82
3	C	604	HEC	CAA-CBA-CGA	-2.66	106.30	113.76
4	C	601	ISW	CAD-C3D-C4D	2.66	129.30	124.66
3	C	605	HEC	O1D-CGD-CBD	-2.65	114.57	123.08
3	B	605	HEC	C4C-C3C-C2C	-2.63	103.52	106.35
3	A	603	HEC	CMD-C2D-C1D	-2.62	124.44	128.46
4	A	608	ISW	C2D-C1D-ND	2.61	112.93	109.84
3	C	607	HEC	CMD-C2D-C1D	-2.61	124.46	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	603	HEC	CMD-C2D-C1D	-2.60	124.47	128.46
4	C	601	ISW	CMA-C3A-C2A	2.59	129.82	124.94
3	C	602	HEC	O1A-CGA-CBA	-2.58	114.81	123.08
4	B	608	ISW	CHA-C4D-ND	-2.55	121.66	124.43
3	C	605	HEC	CMB-C2B-C1B	-2.54	124.56	128.46
3	B	605	HEC	CMC-C2C-C1C	-2.53	124.58	128.46
3	C	606	HEC	CMA-C3A-C2A	2.52	129.69	124.94
3	C	608	HEC	C2B-C3B-C4B	-2.50	103.66	106.35
3	C	606	HEC	CMB-C2B-C3B	2.49	128.74	125.82
3	A	605	HEC	CMB-C2B-C1B	-2.47	124.67	128.46
3	A	603	HEC	CBD-CAD-C3D	-2.47	108.41	112.62
4	B	608	ISW	CMD-C2D-C3D	2.46	132.80	126.12
3	A	605	HEC	CMB-C2B-C3B	2.46	128.71	125.82
3	B	603	HEC	O1D-CGD-CBD	-2.44	115.24	123.08
4	A	608	ISW	CMD-C2D-C3D	2.41	132.65	126.12
3	A	601	HEC	CMA-C3A-C2A	2.40	129.47	124.94
3	A	604	HEC	C1D-C2D-C3D	-2.39	105.34	107.00
3	B	605	HEC	CAD-CBD-CGD	-2.38	107.08	113.76
3	B	605	HEC	CMC-C2C-C3C	2.38	128.62	125.82
3	B	603	HEC	CMA-C3A-C2A	2.38	129.43	124.94
4	C	601	ISW	O1D-CGD-CBD	2.37	121.66	114.03
3	A	607	HEC	O2D-CGD-CBD	2.36	121.62	114.03
3	B	602	HEC	C4C-C3C-C2C	-2.35	103.81	106.35
3	C	607	HEC	O2D-CGD-CBD	2.34	121.56	114.03
3	A	604	HEC	CAA-C2A-C3A	2.34	133.97	127.25
3	A	607	HEC	O1D-CGD-CBD	-2.34	115.58	123.08
3	C	608	HEC	CBA-CAA-C2A	-2.34	108.67	112.60
3	A	604	HEC	O2A-CGA-CBA	2.33	121.53	114.03
3	C	603	HEC	CMC-C2C-C3C	2.30	128.53	125.82
3	B	603	HEC	CMC-C2C-C1C	-2.30	124.93	128.46
3	A	603	HEC	O1A-CGA-CBA	-2.26	115.82	123.08
4	A	608	ISW	O2A-CGA-O1A	-2.26	117.67	123.30
3	A	607	HEC	CBD-CAD-C3D	-2.26	108.77	112.62
3	B	601	HEC	CBD-CAD-C3D	2.25	116.45	112.62
3	C	608	HEC	O1D-CGD-CBD	-2.24	115.87	123.08
3	B	606	HEC	CBD-CAD-C3D	-2.24	108.80	112.62
3	C	605	HEC	CMC-C2C-C1C	-2.23	125.03	128.46
3	B	605	HEC	O2D-CGD-O1D	-2.23	117.75	123.30
3	C	605	HEC	C1D-C2D-C3D	-2.22	105.45	107.00
4	C	601	ISW	C2D-C1D-ND	2.20	112.45	109.84
4	C	601	ISW	CMD-C2D-C1D	2.20	128.39	125.04
3	B	604	HEC	CMD-C2D-C1D	-2.17	125.12	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	HEC	CAA-CBA-CGA	-2.17	107.69	113.76
3	C	608	HEC	CBD-CAD-C3D	-2.16	108.94	112.62
3	A	603	HEC	CMC-C2C-C1C	-2.14	125.17	128.46
3	B	607	HEC	CMC-C2C-C3C	2.14	128.33	125.82
4	A	608	ISW	O2D-CGD-CBD	-2.13	116.23	123.08
3	C	607	HEC	CMA-C3A-C2A	2.12	128.94	124.94
3	B	601	HEC	O2A-CGA-CBA	2.11	120.81	114.03
3	C	603	HEC	CBD-CAD-C3D	-2.11	109.02	112.62
3	B	604	HEC	C2B-C3B-C4B	-2.11	104.08	106.35
4	C	601	ISW	CHB-C1B-NB	-2.10	122.15	124.43
3	C	602	HEC	CAD-CBD-CGD	-2.08	107.92	113.76
3	C	603	HEC	C2B-C3B-C4B	-2.08	104.11	106.35
3	C	605	HEC	CMC-C2C-C3C	2.08	128.26	125.82
4	C	601	ISW	CMC-C2C-C3C	2.07	128.55	124.68
4	B	608	ISW	CHB-C1B-C2B	2.06	128.20	124.98
3	C	606	HEC	O1D-CGD-CBD	-2.06	116.48	123.08
3	B	605	HEC	CMA-C3A-C2A	2.05	128.81	124.94
3	A	601	HEC	O2A-CGA-CBA	2.05	120.61	114.03
3	C	608	HEC	CMD-C2D-C1D	-2.05	125.32	128.46
4	C	601	ISW	C1C-CHC-C4B	2.05	121.22	114.75
3	A	606	HEC	CMA-C3A-C2A	2.05	128.80	124.94
3	C	602	HEC	O2A-CGA-O1A	-2.04	118.20	123.30
4	A	608	ISW	C2B-C1B-NB	2.04	112.32	109.88
3	A	605	HEC	O1D-CGD-CBD	-2.03	116.57	123.08
3	B	602	HEC	C2B-C3B-C4B	-2.03	104.17	106.35
3	B	601	HEC	O2D-CGD-CBD	2.01	120.48	114.03

There are no chirality outliers.

All (139) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	HEC	C1A-C2A-CAA-CBA
3	A	604	HEC	C1A-C2A-CAA-CBA
3	A	604	HEC	C3A-C2A-CAA-CBA
3	C	603	HEC	C1A-C2A-CAA-CBA
5	B	612	PEG	C4-C3-O2-C2
5	B	610	PEG	O1-C1-C2-O2
8	B	613	P6G	O16-C17-C18-O19
9	B	614	PG4	O1-C1-C2-O2
8	B	613	P6G	O4-C5-C6-O7
5	B	611	PEG	O1-C1-C2-O2
8	B	613	P6G	O7-C8-C9-O10

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Mol	Chain	Res	Type	Atoms
3	C	607	HEC	C2A-CAA-CBA-CGA
5	A	610	PEG	O2-C3-C4-O4
5	B	611	PEG	O2-C3-C4-O4
5	A	613	PEG	O2-C3-C4-O4
5	A	614	PEG	O1-C1-C2-O2
5	C	609	PEG	O1-C1-C2-O2
5	C	611	PEG	O1-C1-C2-O2
5	C	622	PEG	O1-C1-C2-O2
5	C	622	PEG	O2-C3-C4-O4
5	F	102	PEG	O2-C3-C4-O4
6	A	615	PGE	O1-C1-C2-O2
6	C	614	PGE	O1-C1-C2-O2
9	B	614	PG4	O3-C5-C6-O4
5	B	612	PEG	O1-C1-C2-O2
5	C	611	PEG	O2-C3-C4-O4
5	A	613	PEG	O1-C1-C2-O2
5	A	614	PEG	O2-C3-C4-O4
5	C	610	PEG	O1-C1-C2-O2
5	C	612	PEG	O1-C1-C2-O2
7	B	615	EDO	O1-C1-C2-O2
7	C	616	EDO	O1-C1-C2-O2
7	C	621	EDO	O1-C1-C2-O2
8	B	613	P6G	O13-C14-C15-O16
4	A	608	ISW	C2A-CAA-CBA-CGA
5	B	609	PEG	O2-C3-C4-O4
5	B	612	PEG	O2-C3-C4-O4
5	F	102	PEG	O1-C1-C2-O2
6	C	614	PGE	O3-C5-C6-O4
7	A	617	EDO	O1-C1-C2-O2
7	A	618	EDO	O1-C1-C2-O2
7	B	621	EDO	O1-C1-C2-O2
7	C	617	EDO	O1-C1-C2-O2
6	A	615	PGE	O2-C3-C4-O3
5	A	611	PEG	O1-C1-C2-O2
5	C	613	PEG	O2-C3-C4-O4
7	A	619	EDO	O1-C1-C2-O2
7	B	619	EDO	O1-C1-C2-O2
5	A	612	PEG	O1-C1-C2-O2
6	A	615	PGE	O3-C5-C6-O4
5	B	609	PEG	C1-C2-O2-C3
5	A	609	PEG	C4-C3-O2-C2
5	C	611	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
8	B	613	P6G	C6-C5-O4-C3
5	C	622	PEG	C1-C2-O2-C3
6	C	614	PGE	C4-C3-O2-C2
5	A	613	PEG	C1-C2-O2-C3
5	B	612	PEG	C1-C2-O2-C3
5	C	612	PEG	C1-C2-O2-C3
6	A	615	PGE	C1-C2-O2-C3
5	A	611	PEG	C4-C3-O2-C2
5	C	610	PEG	C1-C2-O2-C3
7	C	620	EDO	O1-C1-C2-O2
8	B	613	P6G	C9-C8-O7-C6
5	F	102	PEG	C4-C3-O2-C2
3	A	602	HEC	C3A-C2A-CAA-CBA
3	C	603	HEC	C3A-C2A-CAA-CBA
6	A	615	PGE	C6-C5-O3-C4
5	A	613	PEG	C4-C3-O2-C2
9	B	614	PG4	O4-C7-C8-O5
6	C	614	PGE	C3-C4-O3-C5
6	C	614	PGE	C6-C5-O3-C4
8	B	613	P6G	C8-C9-O10-C11
8	B	613	P6G	C12-C11-O10-C9
3	B	607	HEC	CAD-CBD-CGD-O1D
5	C	613	PEG	C4-C3-O2-C2
3	C	608	HEC	CAD-CBD-CGD-O1D
3	A	607	HEC	CAD-CBD-CGD-O1D
3	C	604	HEC	CAA-CBA-CGA-O1A
3	A	603	HEC	CAA-CBA-CGA-O1A
3	B	603	HEC	CAD-CBD-CGD-O1D
4	C	601	ISW	CAD-CBD-CGD-O1D
3	B	601	HEC	CAD-CBD-CGD-O1D
8	B	613	P6G	C14-C15-O16-C17
3	B	601	HEC	CAD-CBD-CGD-O2D
3	C	604	HEC	CAD-CBD-CGD-O1D
3	C	608	HEC	CAD-CBD-CGD-O2D
3	A	607	HEC	CAD-CBD-CGD-O2D
3	C	604	HEC	CAD-CBD-CGD-O2D
3	B	603	HEC	CAA-CBA-CGA-O2A
3	C	604	HEC	CAA-CBA-CGA-O2A
3	A	603	HEC	CAD-CBD-CGD-O2D
3	B	603	HEC	CAD-CBD-CGD-O2D
3	B	607	HEC	CAD-CBD-CGD-O2D
3	A	603	HEC	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
4	C	601	ISW	CAD-CBD-CGD-O2D
3	A	606	HEC	CAD-CBD-CGD-O2D
3	A	605	HEC	CAD-CBD-CGD-O2D
5	A	609	PEG	C1-C2-O2-C3
3	A	603	HEC	CAA-CBA-CGA-O2A
3	B	603	HEC	CAA-CBA-CGA-O1A
3	B	605	HEC	CAD-CBD-CGD-O2D
3	B	606	HEC	CAD-CBD-CGD-O2D
3	A	606	HEC	CAA-CBA-CGA-O2A
3	C	607	HEC	CAD-CBD-CGD-O1D
4	A	608	ISW	CAD-CBD-CGD-O1D
3	C	606	HEC	CAD-CBD-CGD-O2D
5	C	610	PEG	C4-C3-O2-C2
3	A	606	HEC	CAD-CBD-CGD-O1D
3	A	605	HEC	CAD-CBD-CGD-O1D
3	B	606	HEC	CAD-CBD-CGD-O1D
3	B	605	HEC	CAD-CBD-CGD-O1D
3	C	606	HEC	CAD-CBD-CGD-O1D
4	B	608	ISW	CAD-CBD-CGD-O1D
3	B	606	HEC	CAA-CBA-CGA-O2A
5	A	614	PEG	C4-C3-O2-C2
3	A	606	HEC	CAA-CBA-CGA-O1A
3	C	607	HEC	CAA-CBA-CGA-O2A
9	B	614	PG4	C8-C7-O4-C6
5	C	611	PEG	C1-C2-O2-C3
4	A	608	ISW	CAD-CBD-CGD-O2D
4	B	608	ISW	CAD-CBD-CGD-O2D
5	C	610	PEG	O2-C3-C4-O4
3	B	606	HEC	CAA-CBA-CGA-O1A
6	C	614	PGE	O2-C3-C4-O3
3	C	607	HEC	CAA-CBA-CGA-O1A
3	C	607	HEC	CAD-CBD-CGD-O2D
3	B	602	HEC	CAD-CBD-CGD-O2D
5	C	613	PEG	O1-C1-C2-O2
3	A	601	HEC	CAA-CBA-CGA-O2A
3	A	604	HEC	CAD-CBD-CGD-O1D
3	A	601	HEC	CAD-CBD-CGD-O2D
3	C	603	HEC	CAA-CBA-CGA-O2A
3	B	604	HEC	CAA-CBA-CGA-O2A
3	B	602	HEC	CAD-CBD-CGD-O1D
3	A	604	HEC	CAD-CBD-CGD-O2D
3	B	604	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
8	B	613	P6G	O10-C11-C12-O13
3	C	603	HEC	CAA-CBA-CGA-O1A

There are no ring outliers.

39 monomers are involved in 105 short contacts:

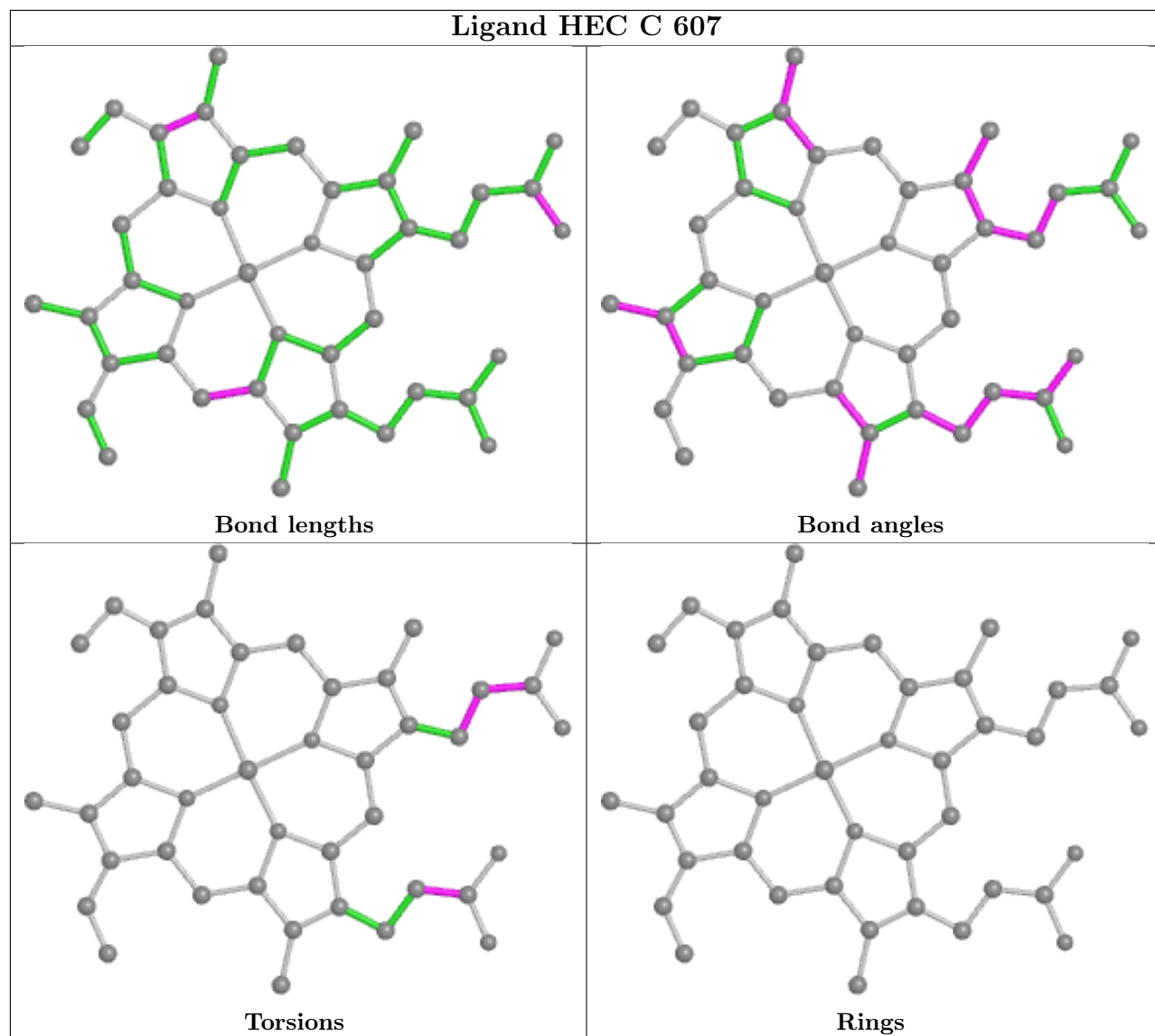
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	607	HEC	1	0
3	B	603	HEC	4	0
3	B	607	HEC	1	0
7	A	619	EDO	1	0
5	C	610	PEG	3	0
3	A	601	HEC	4	0
5	C	612	PEG	1	0
6	C	614	PGE	4	0
3	A	604	HEC	3	0
4	A	608	ISW	11	0
3	C	606	HEC	5	0
3	B	601	HEC	3	0
7	A	617	EDO	1	0
3	A	602	HEC	4	0
7	C	617	EDO	2	0
9	B	614	PG4	1	0
3	C	603	HEC	3	0
3	B	606	HEC	2	0
3	C	602	HEC	5	0
5	F	102	PEG	1	0
6	A	615	PGE	2	0
3	B	602	HEC	3	0
5	A	612	PEG	1	0
7	C	616	EDO	1	0
5	A	614	PEG	1	0
3	A	606	HEC	1	0
5	B	609	PEG	3	0
5	B	612	PEG	1	0
4	C	601	ISW	11	0
5	A	613	PEG	3	0
4	B	608	ISW	14	0
3	C	604	HEC	1	0
3	A	605	HEC	4	0
3	B	605	HEC	4	0
8	B	613	P6G	1	0

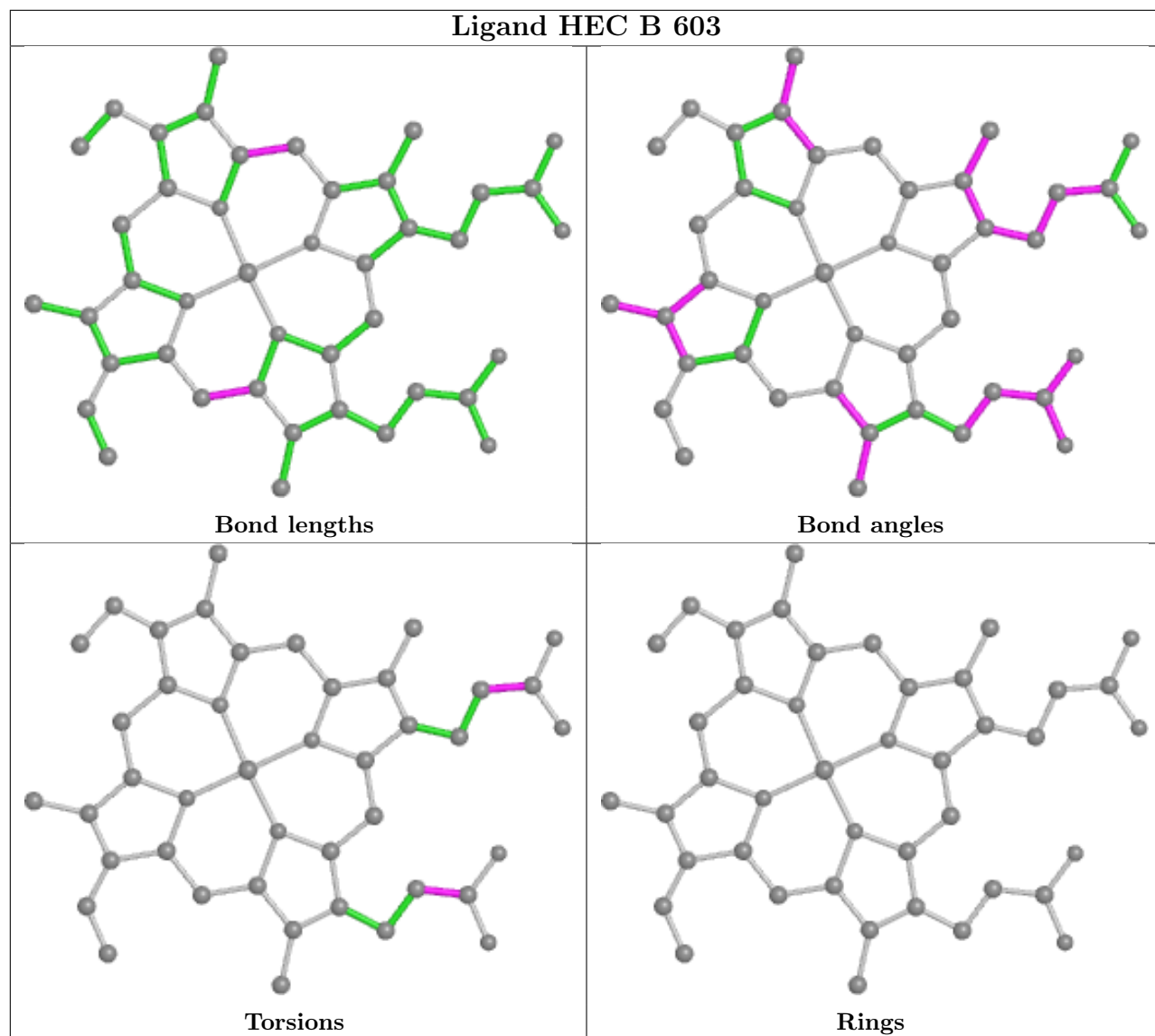
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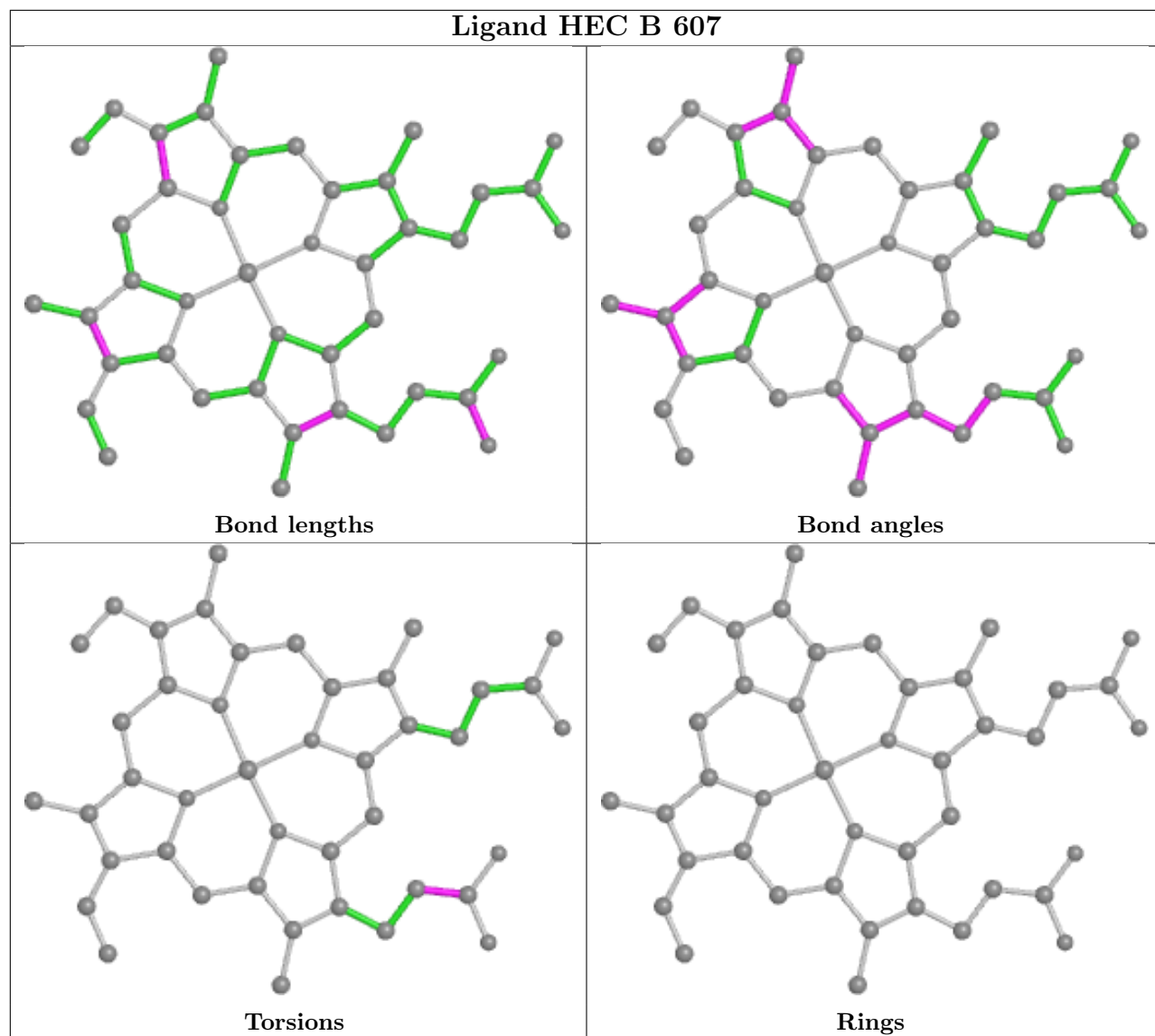
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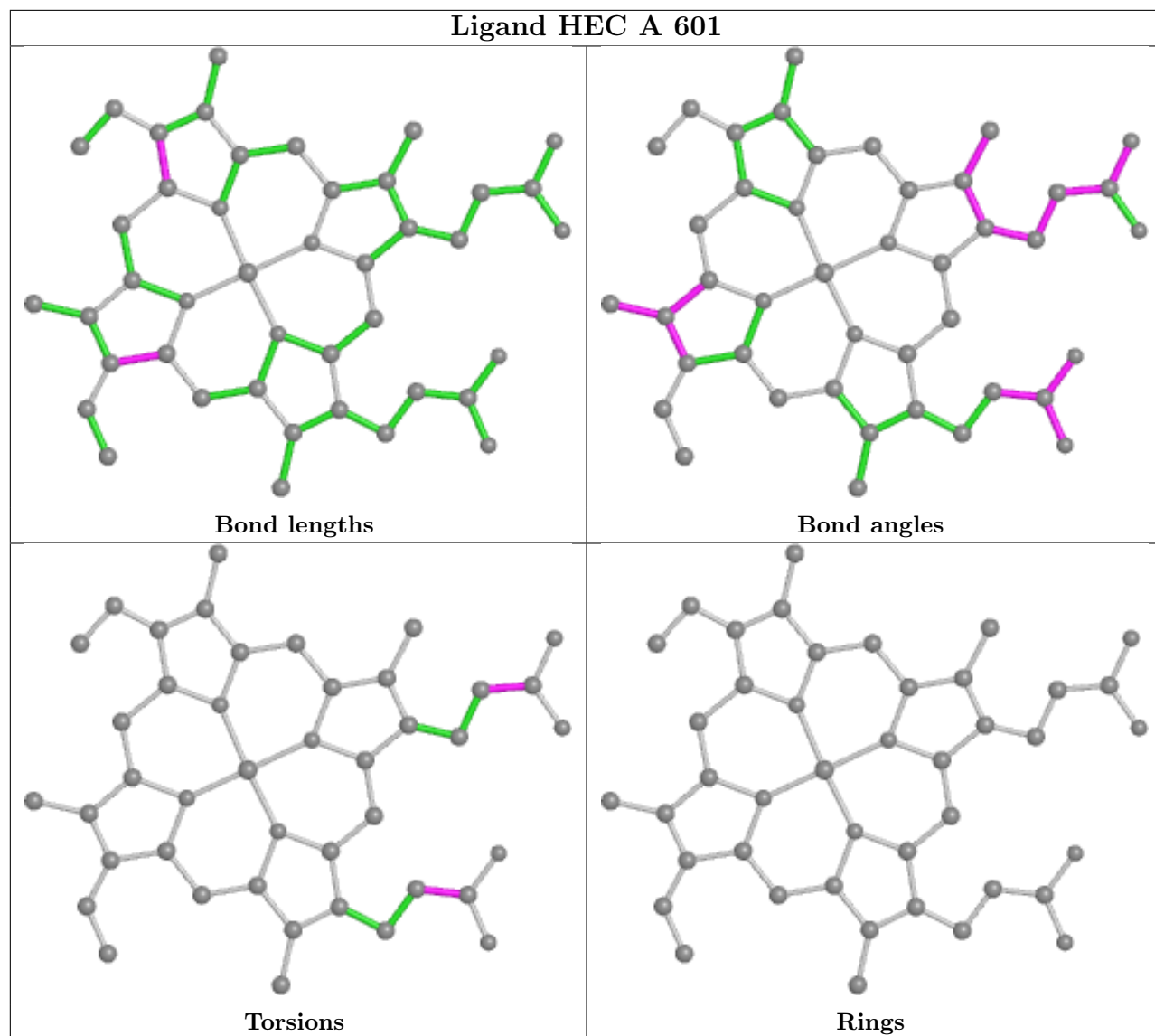
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	604	HEC	2	0
3	C	608	HEC	2	0
3	A	603	HEC	1	0
3	C	605	HEC	4	0

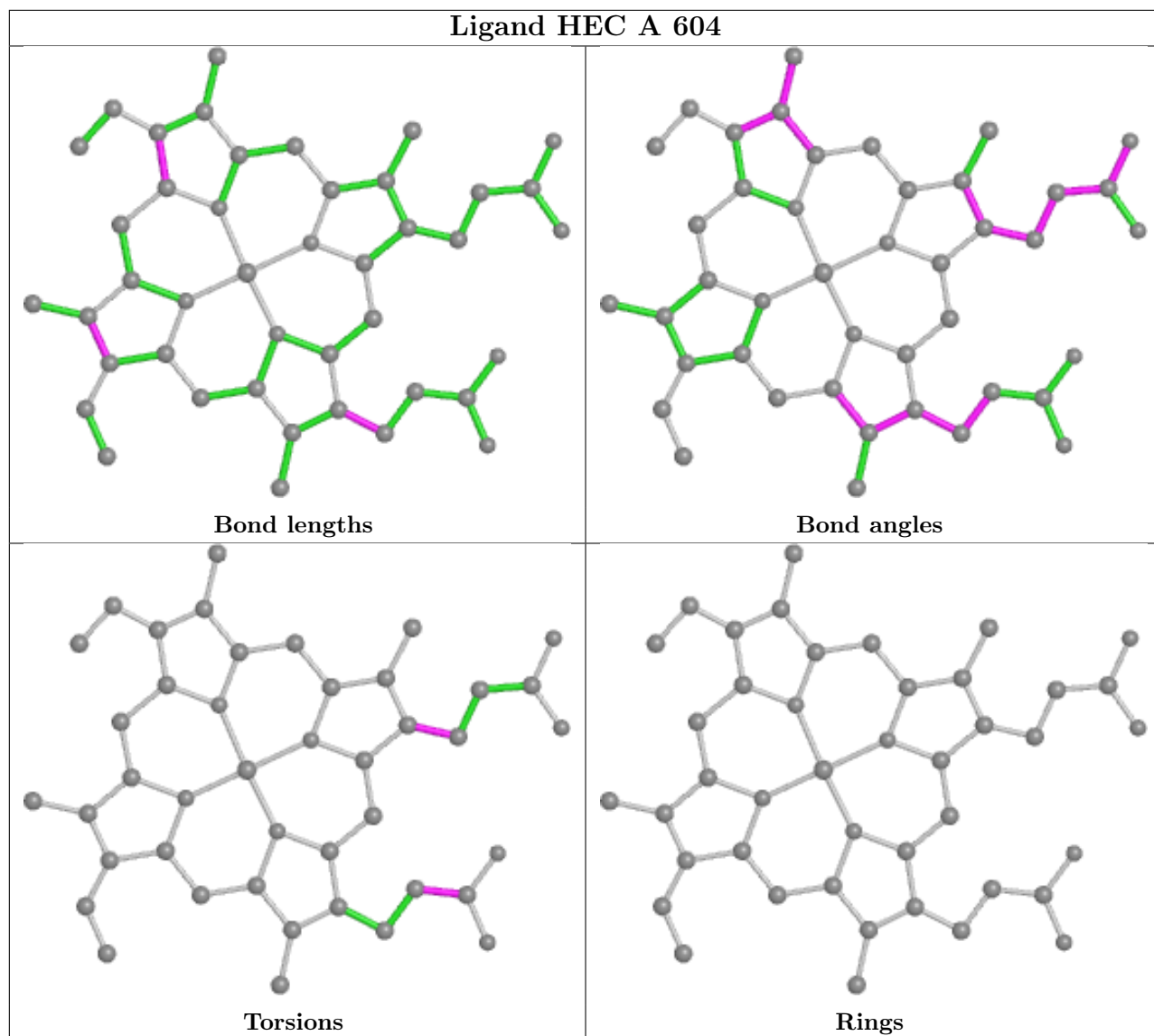
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

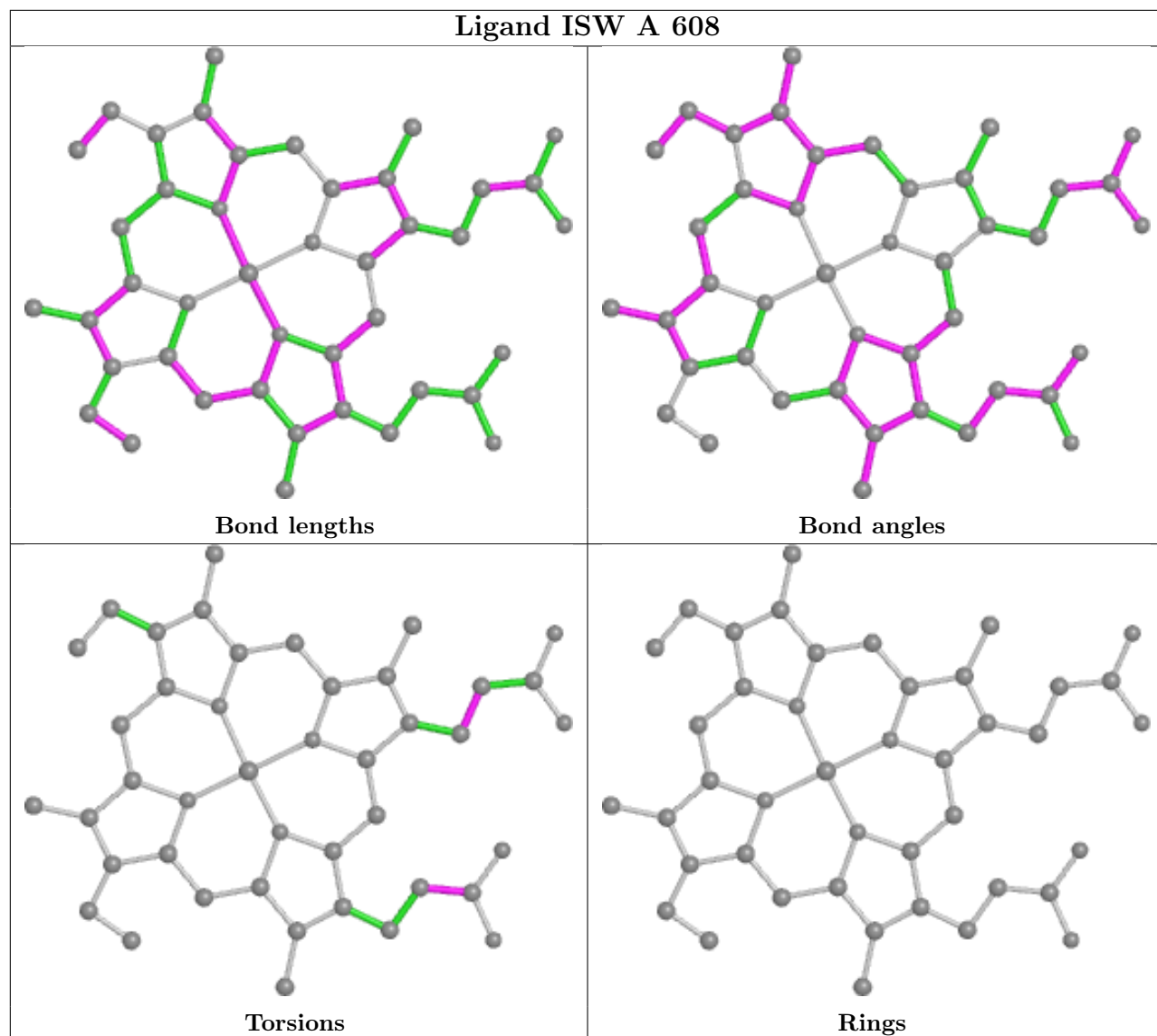


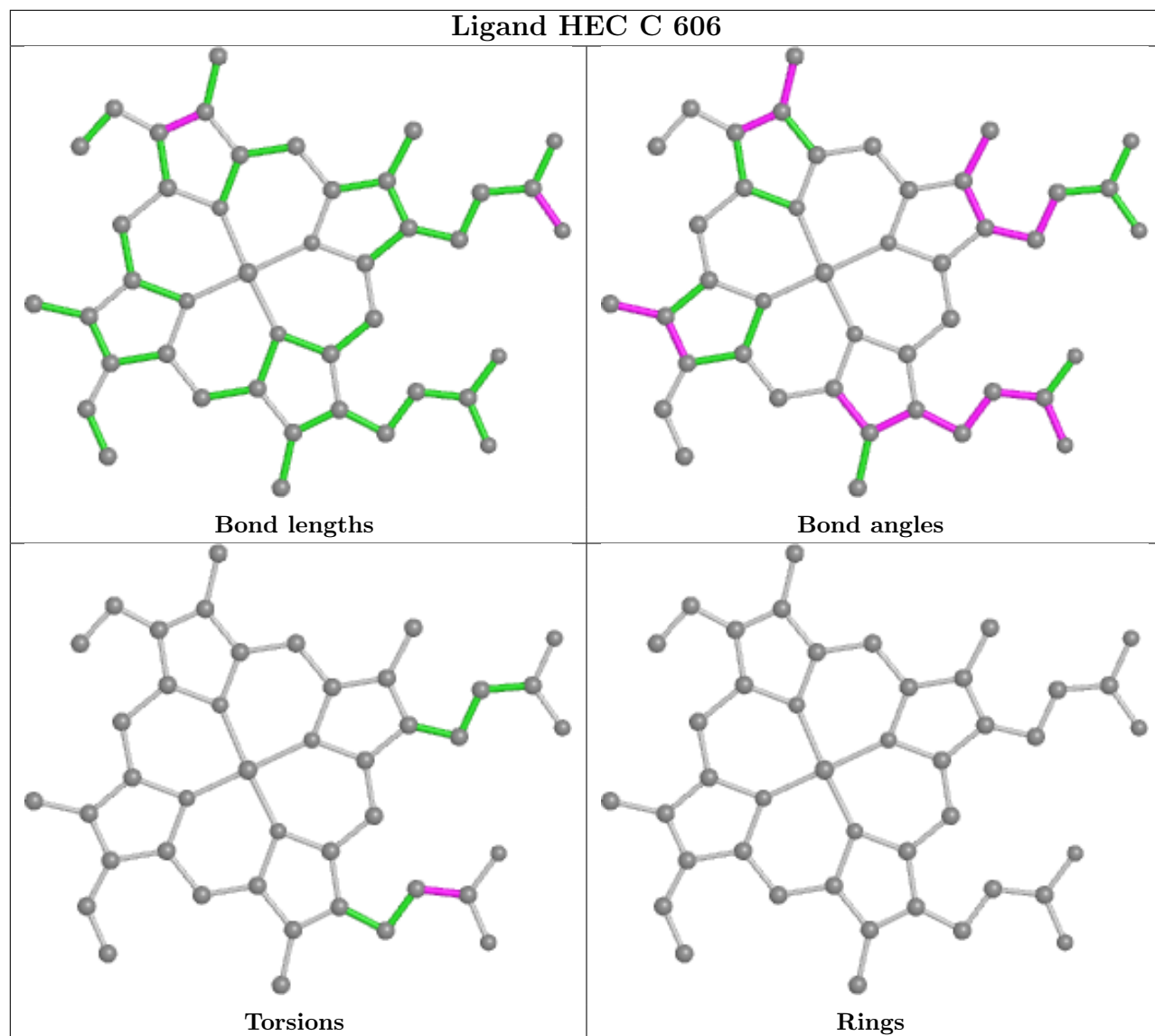


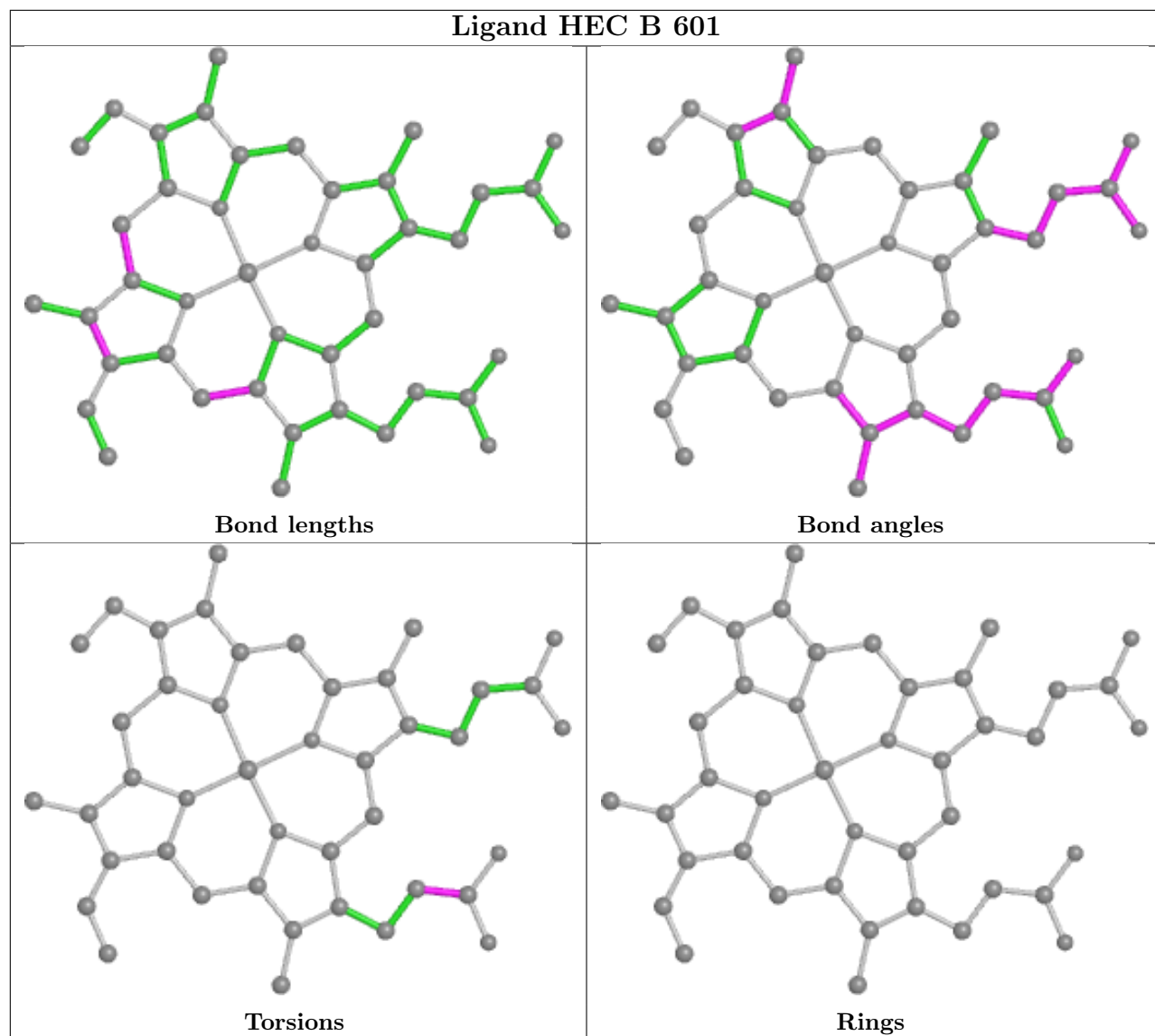


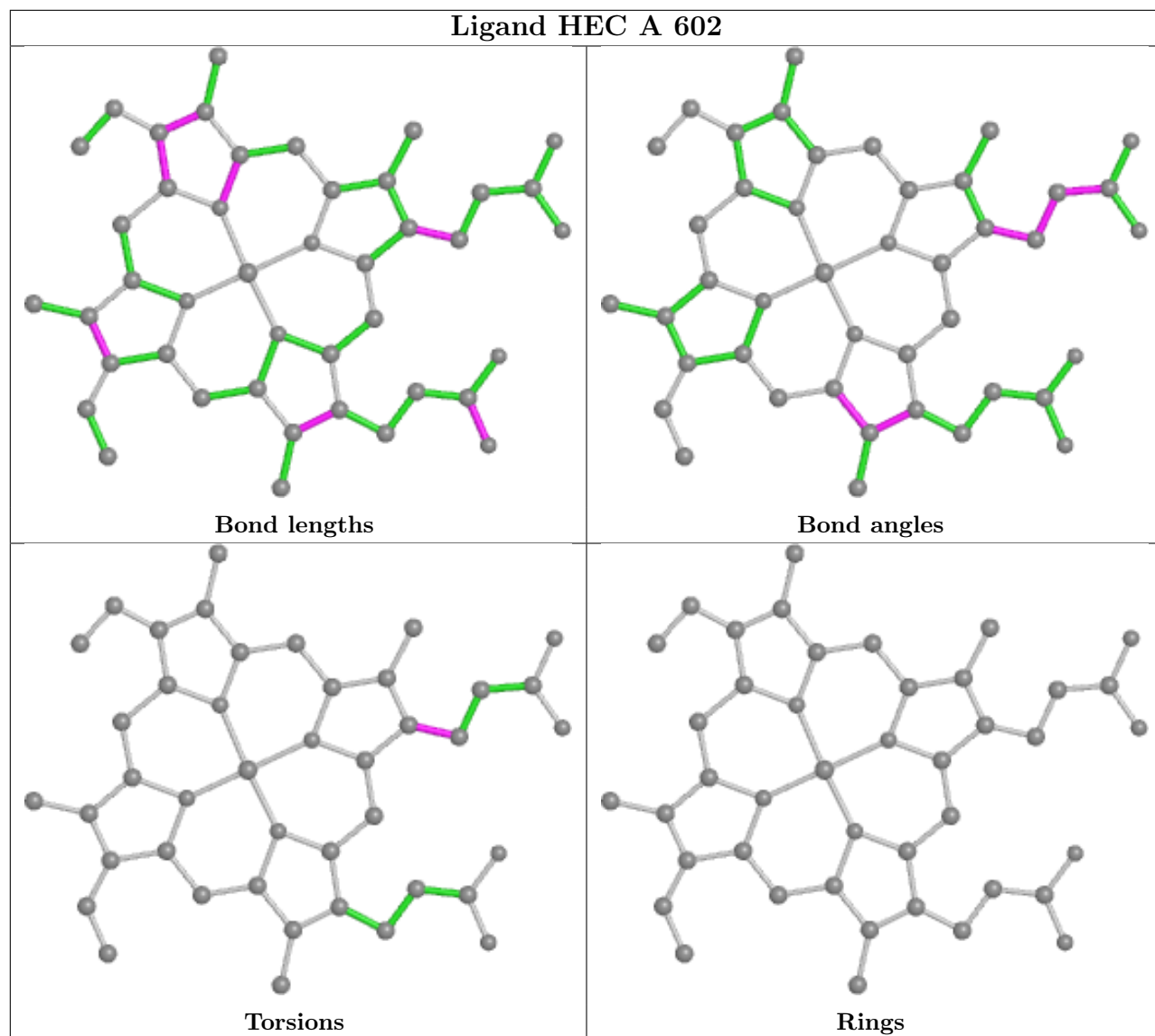


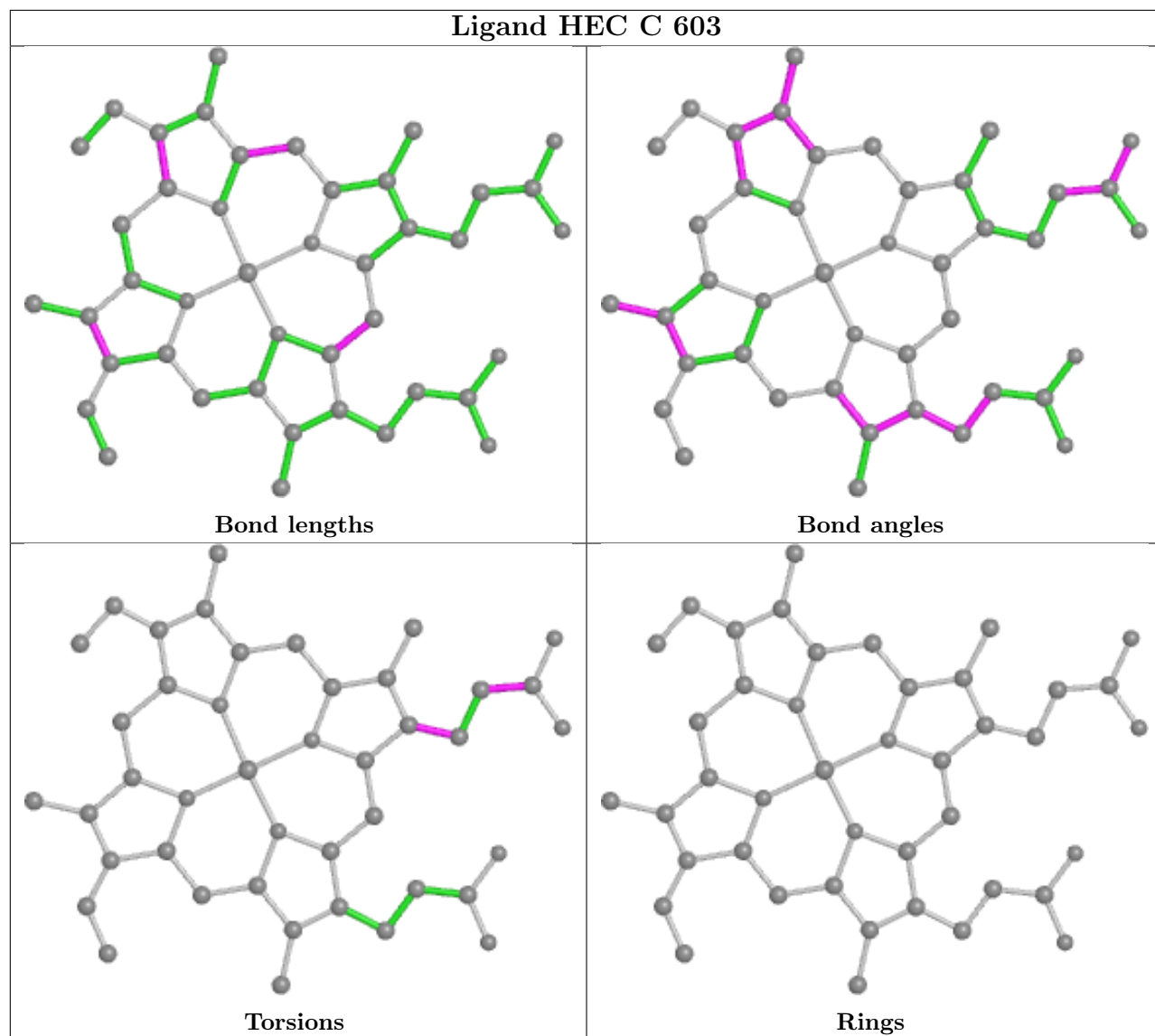


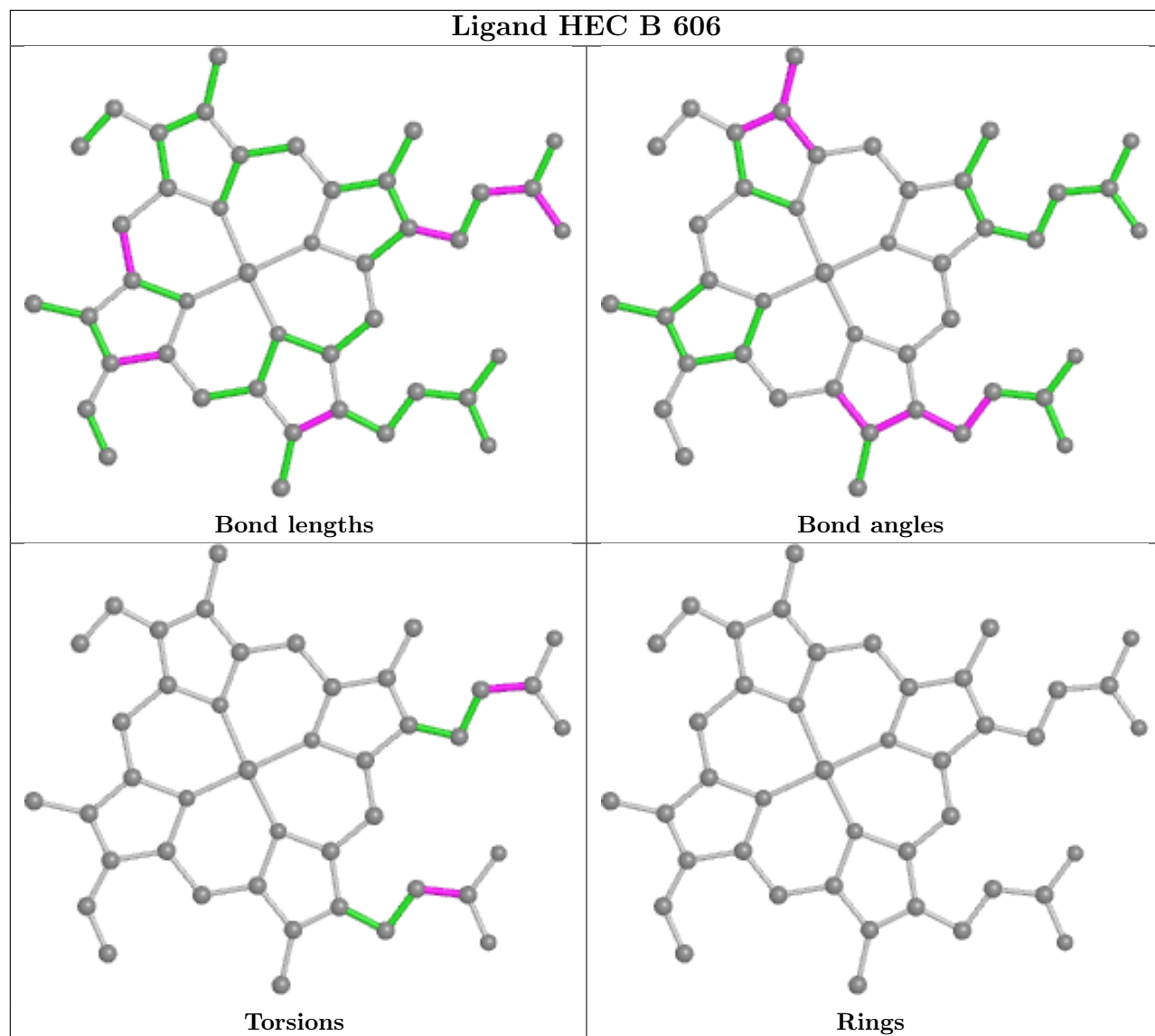


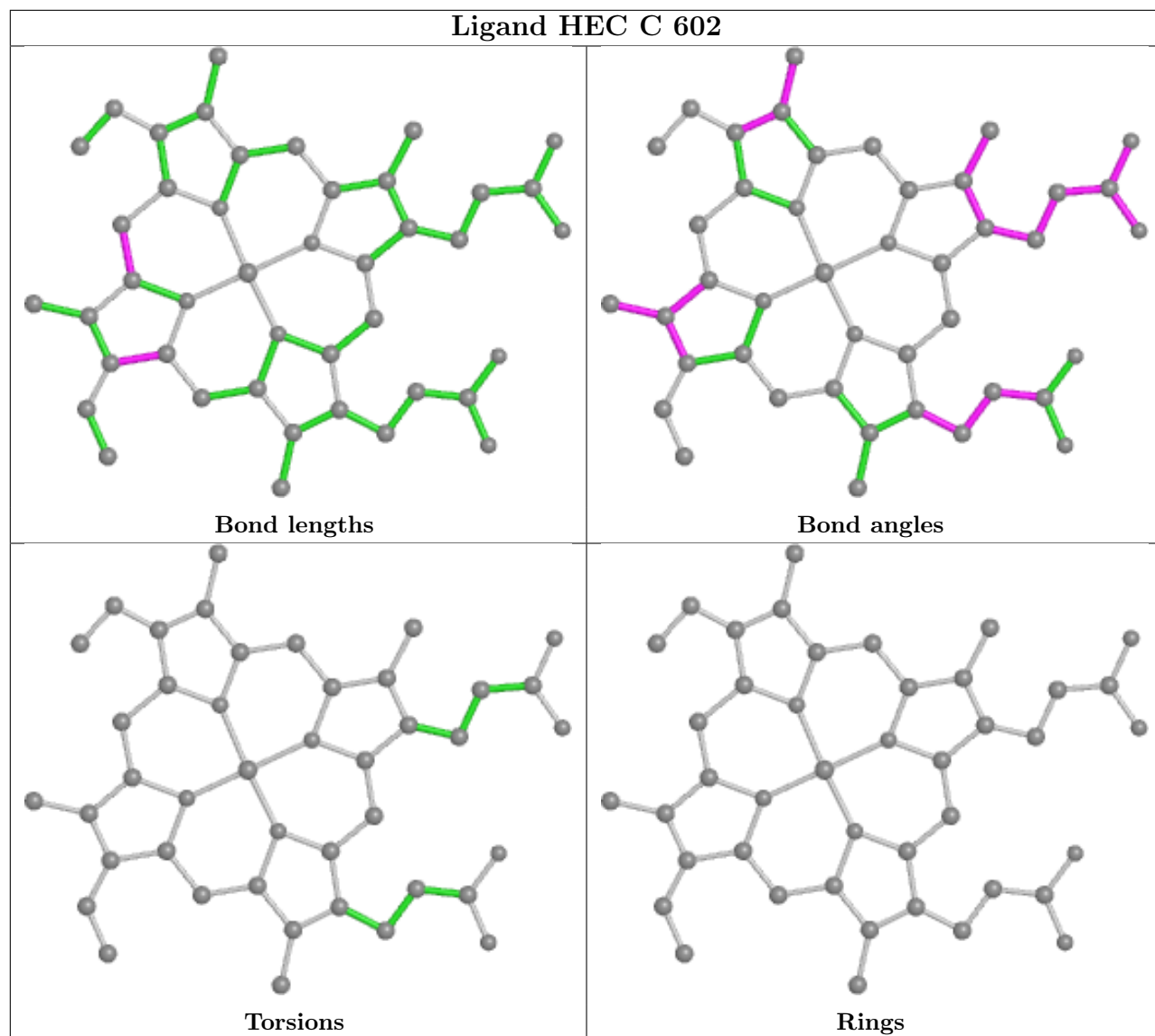


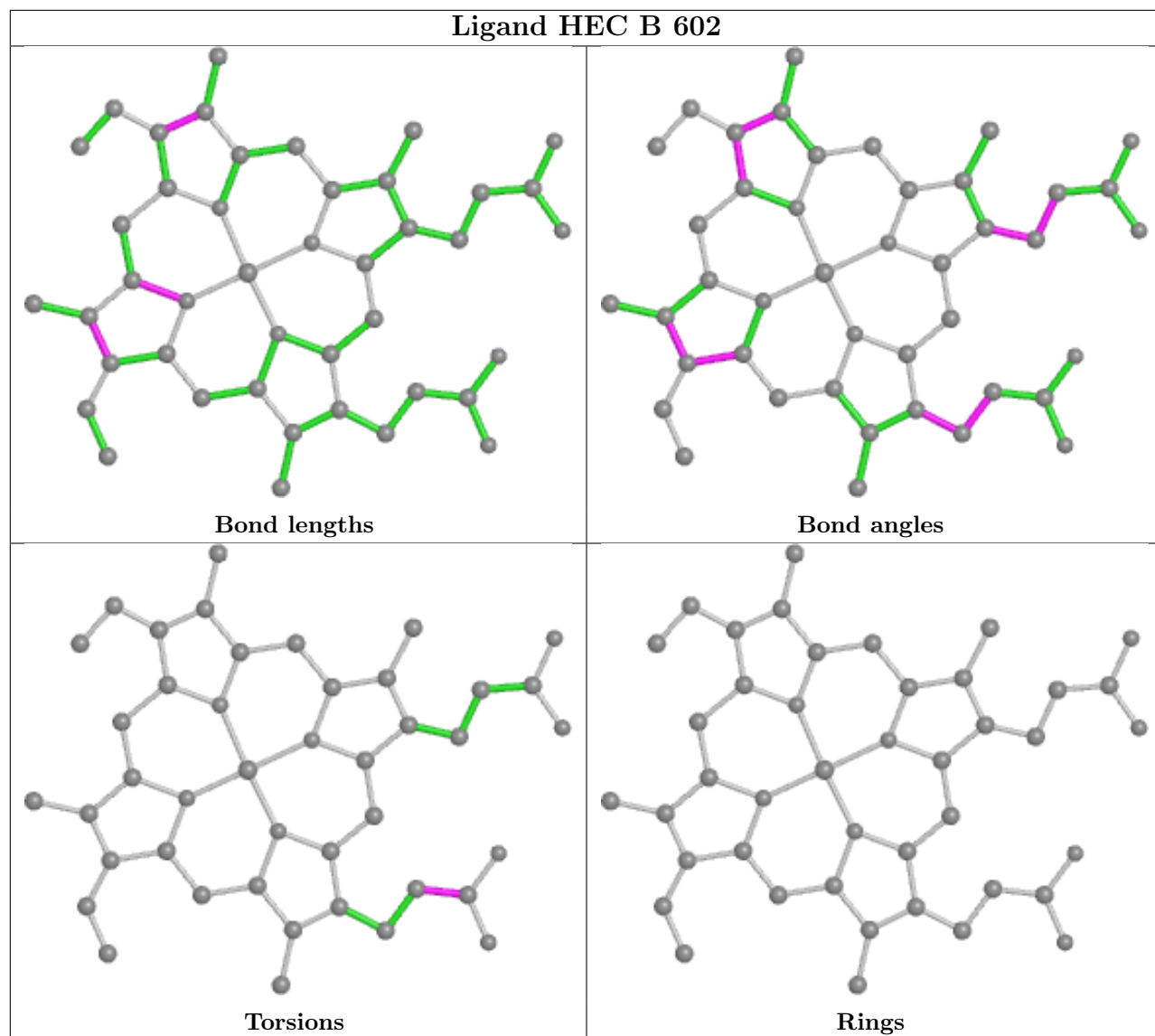


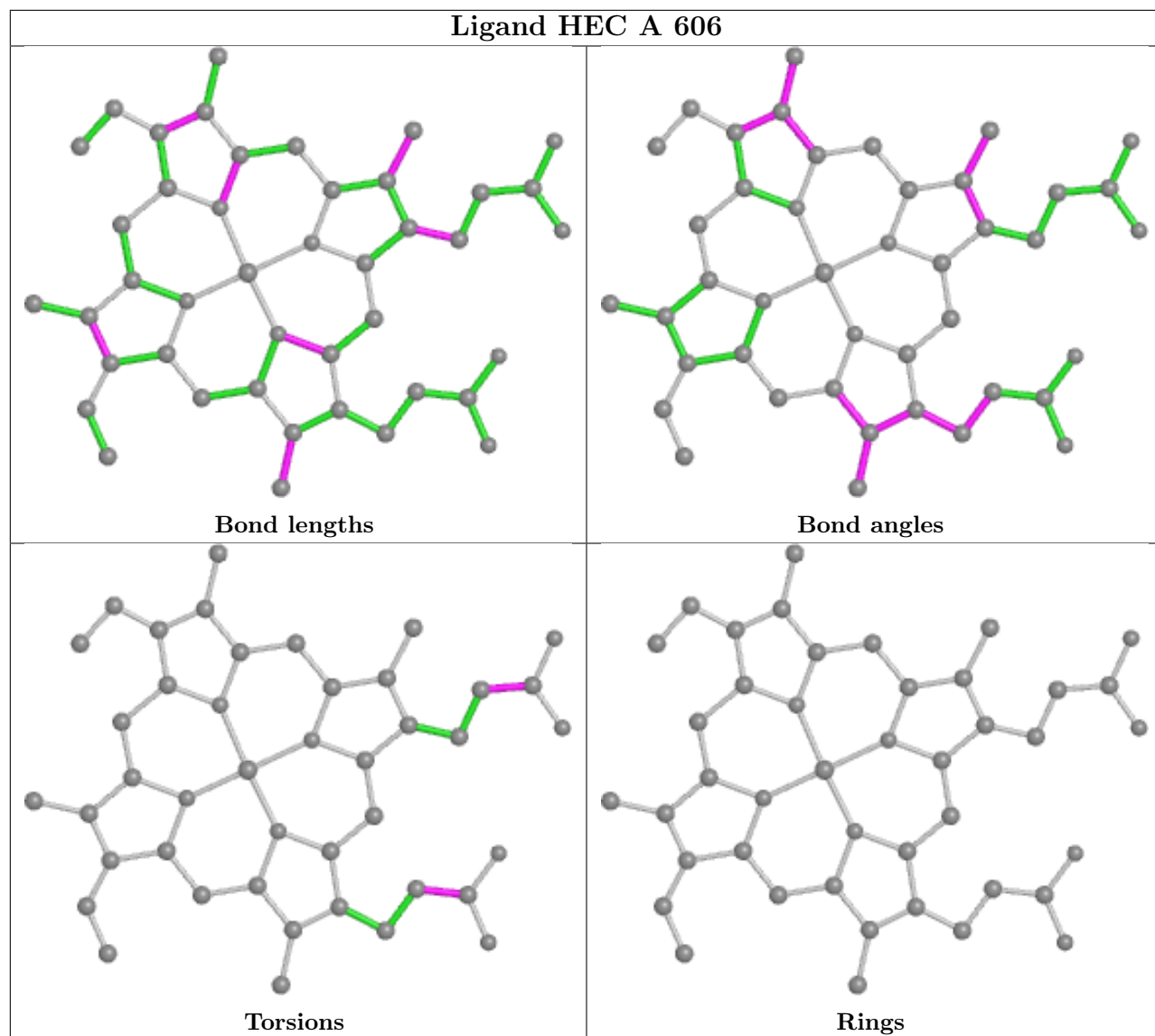


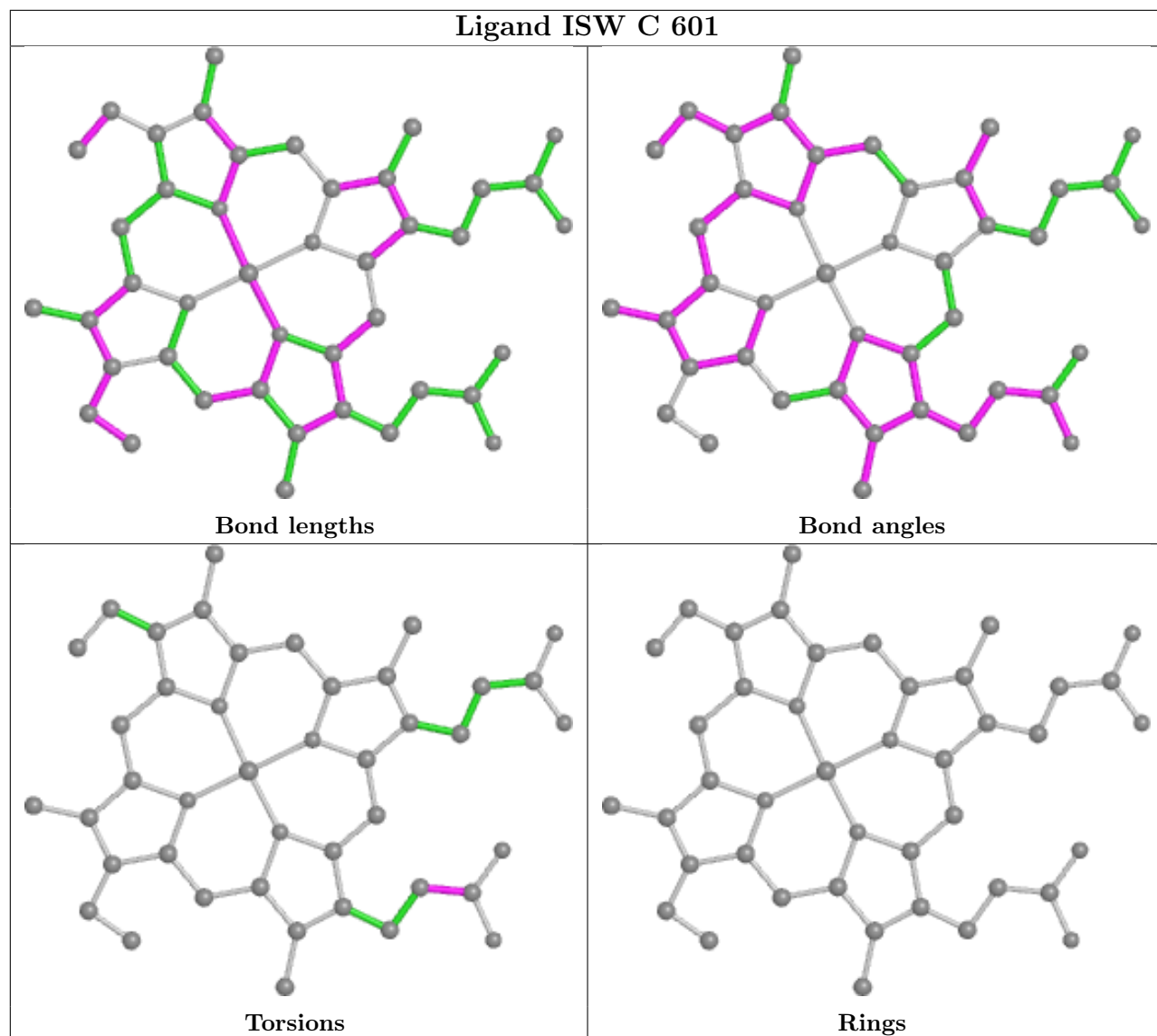


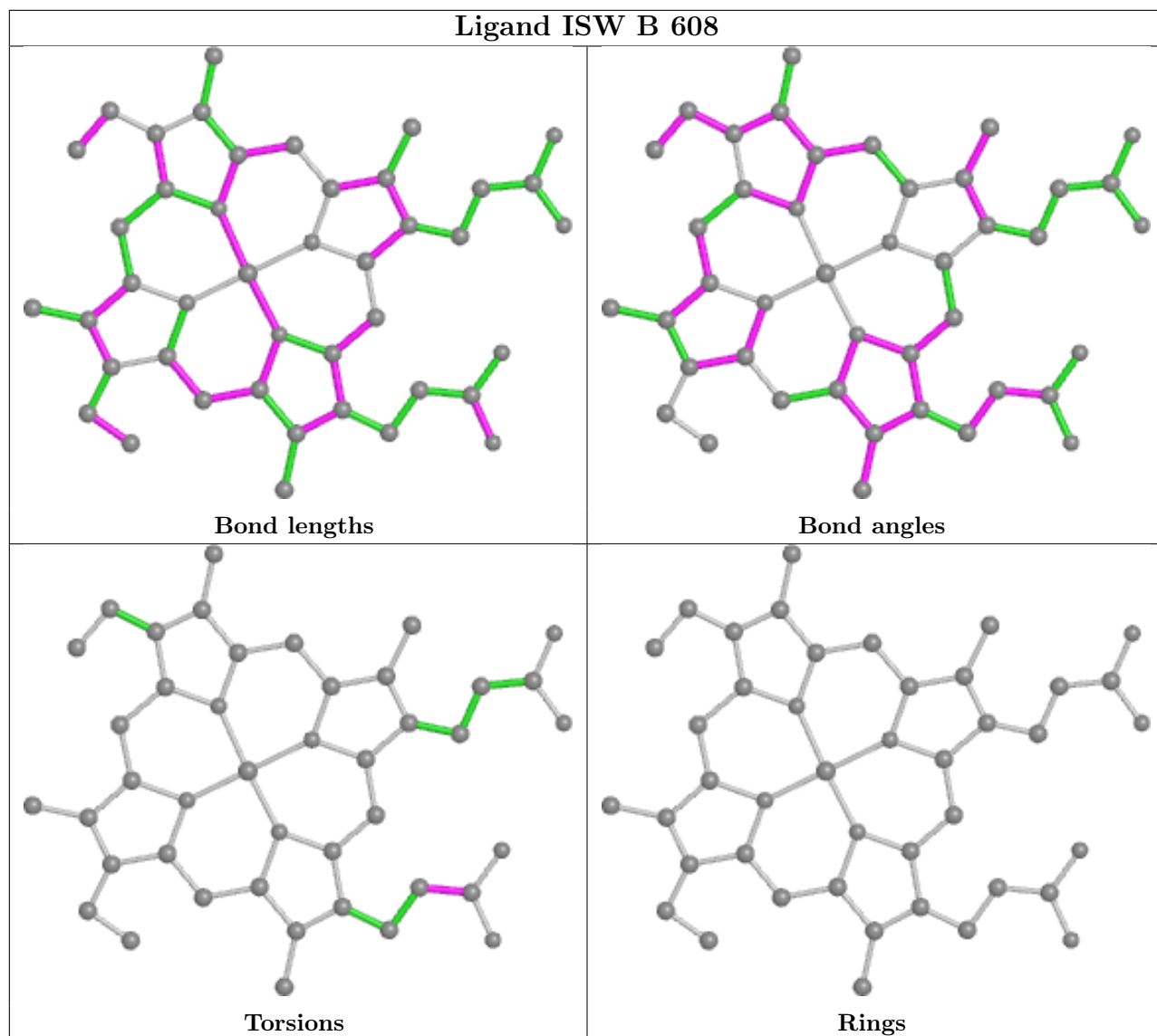


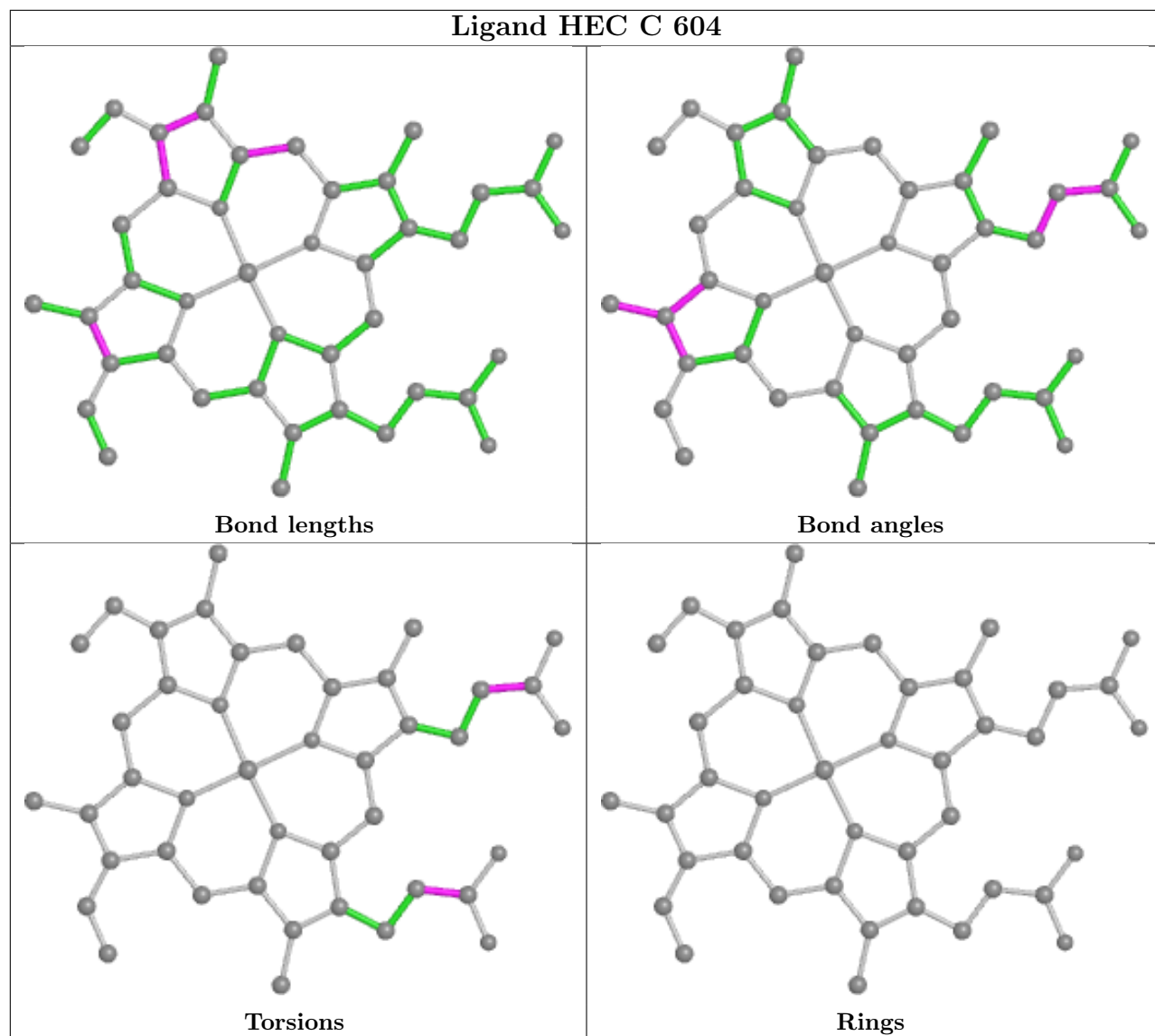


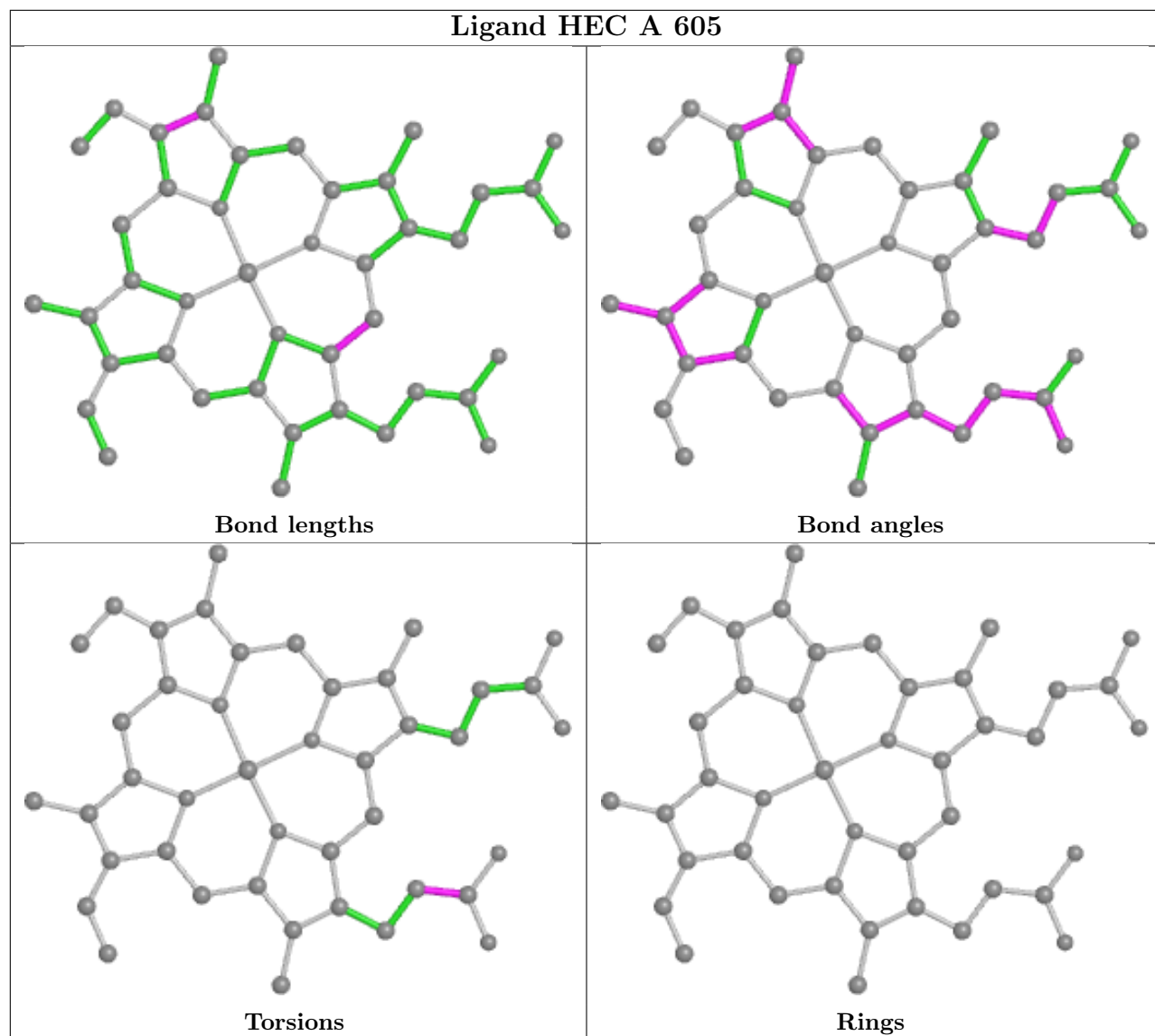


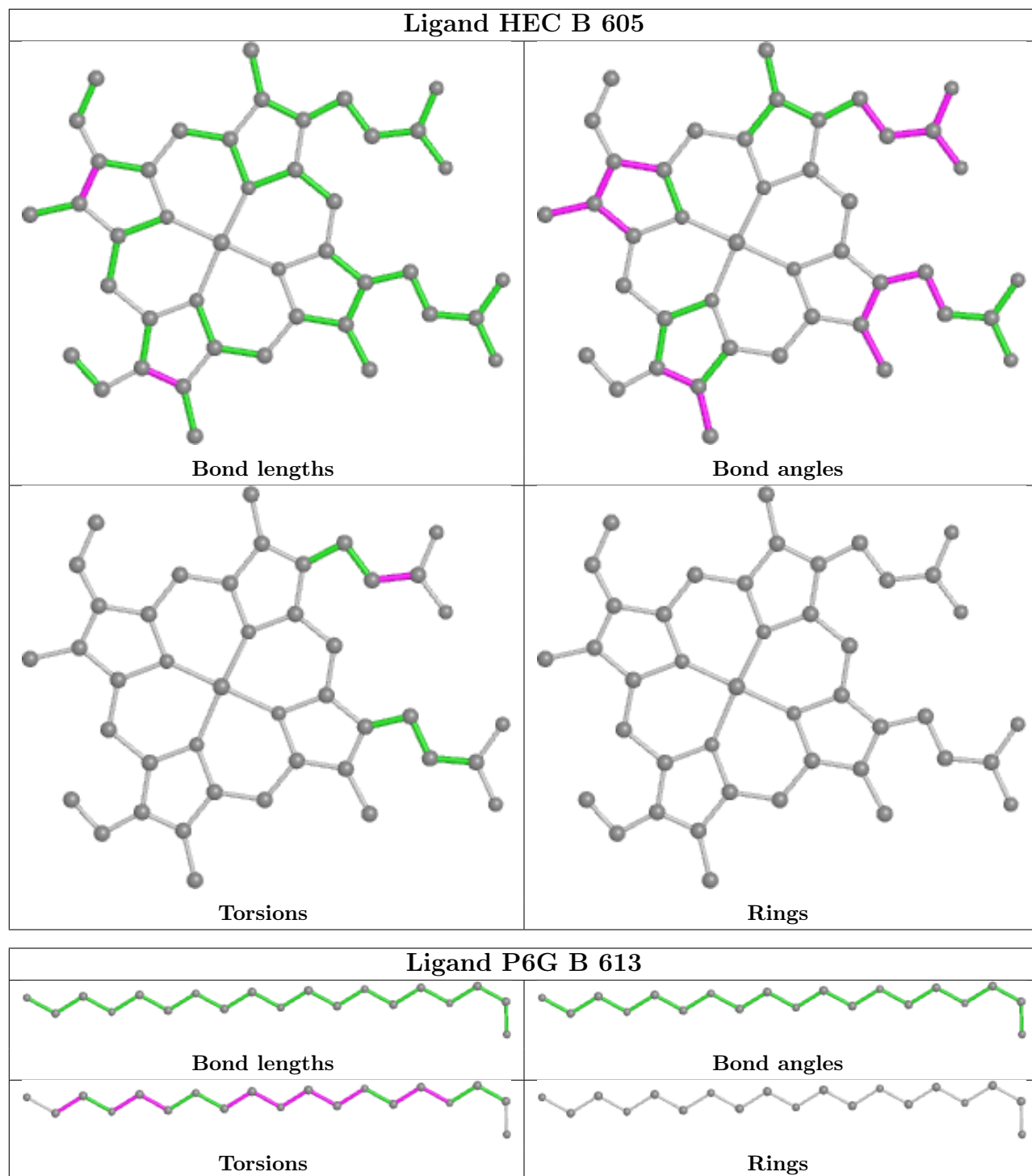


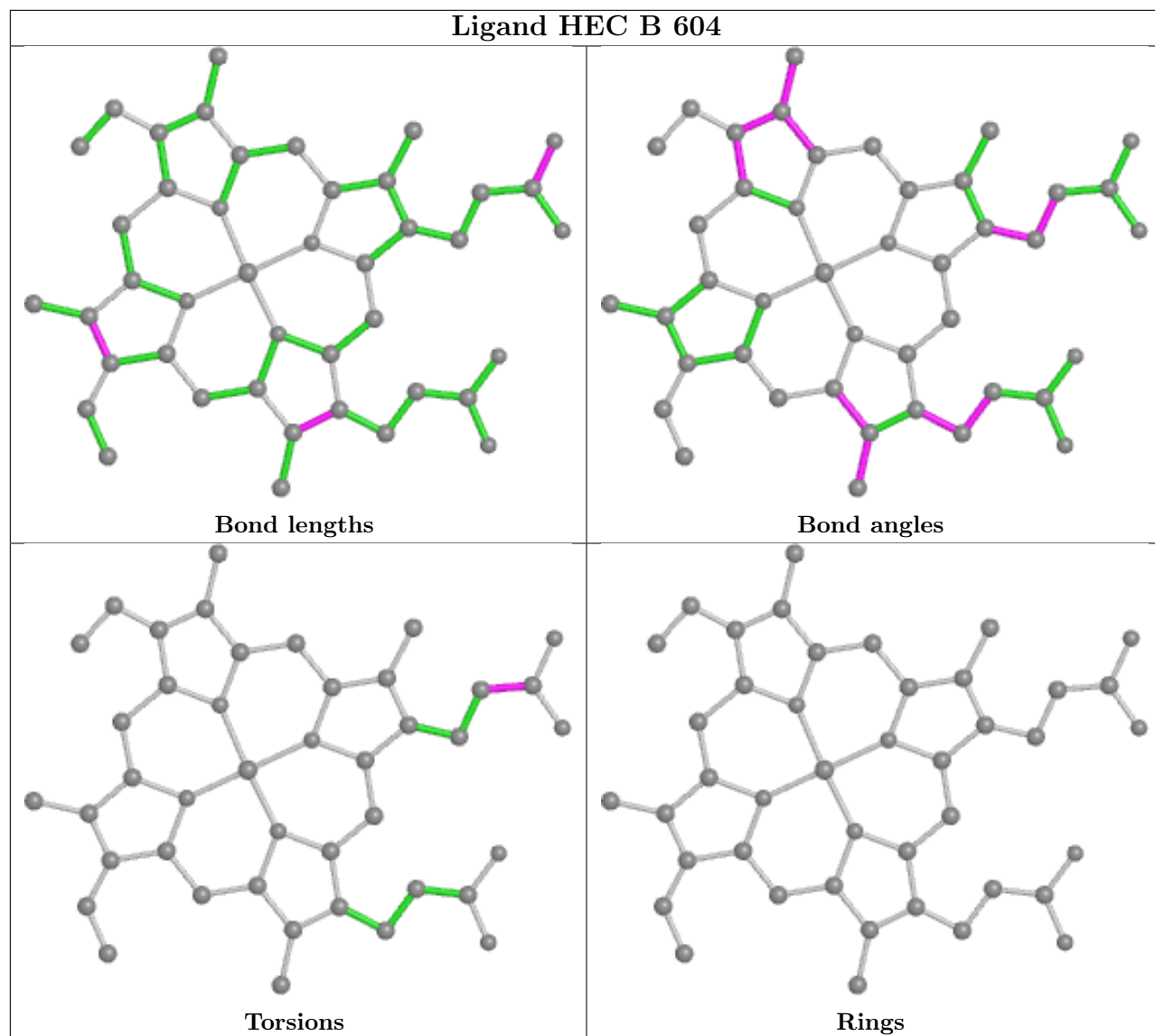


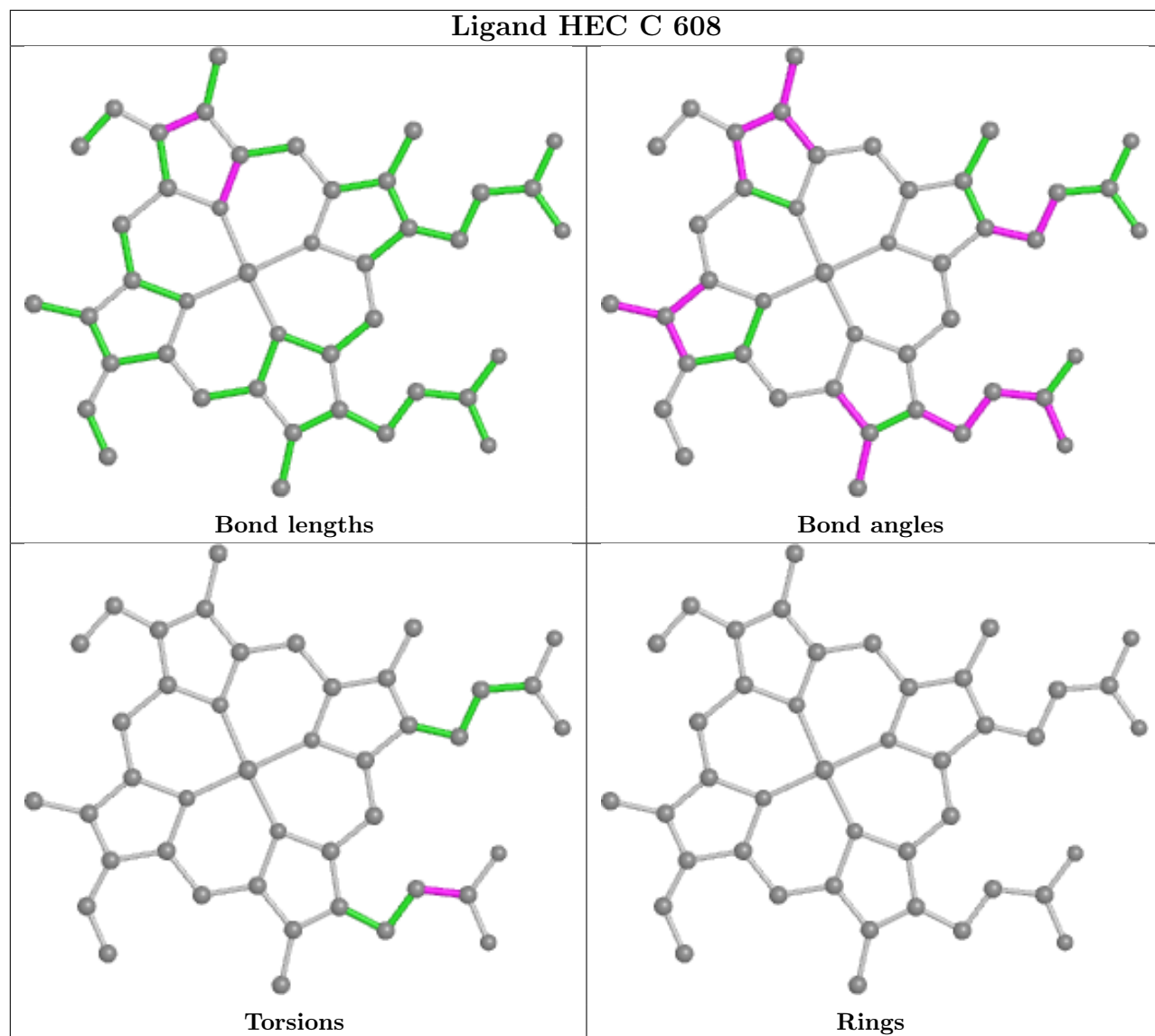


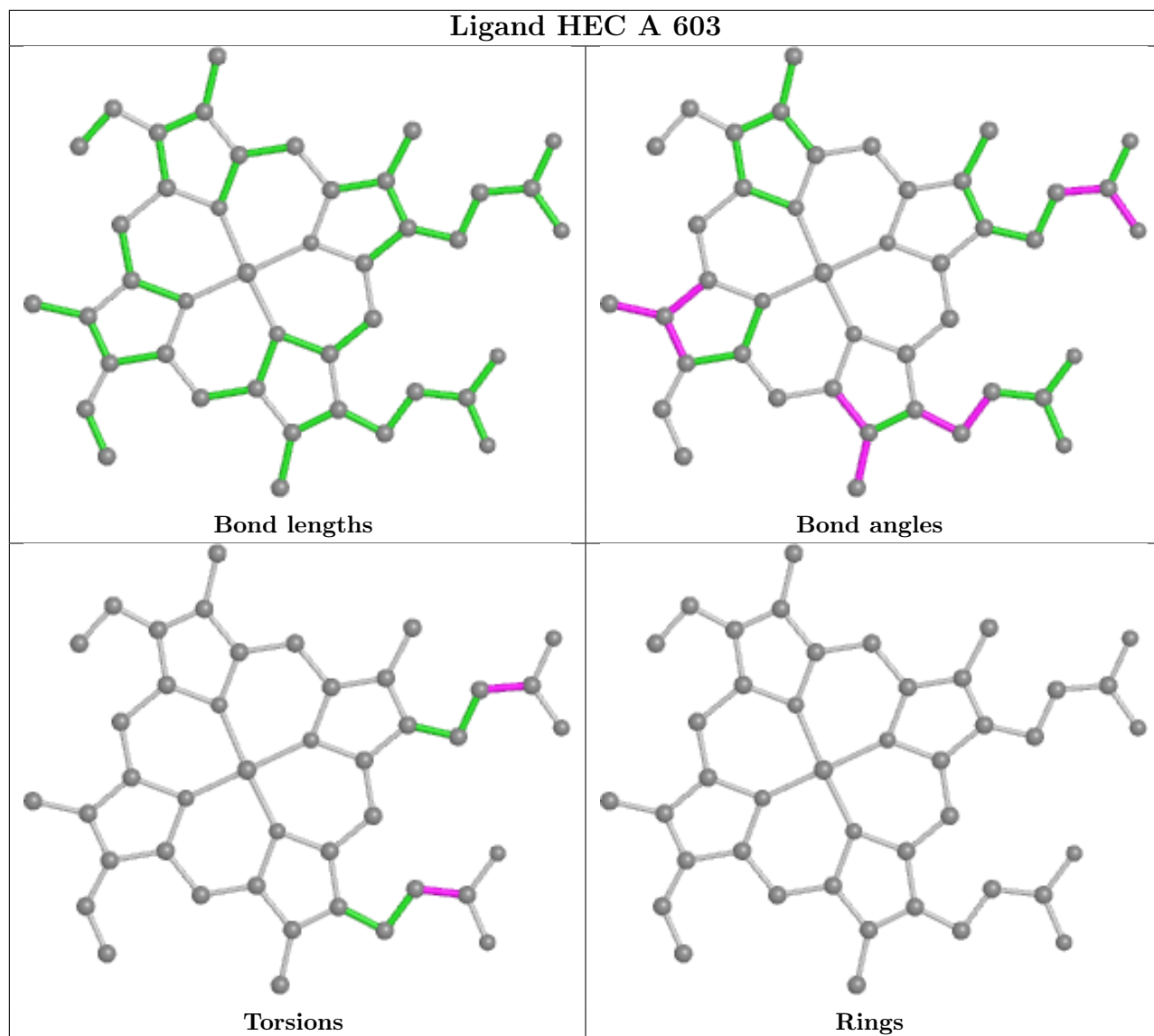


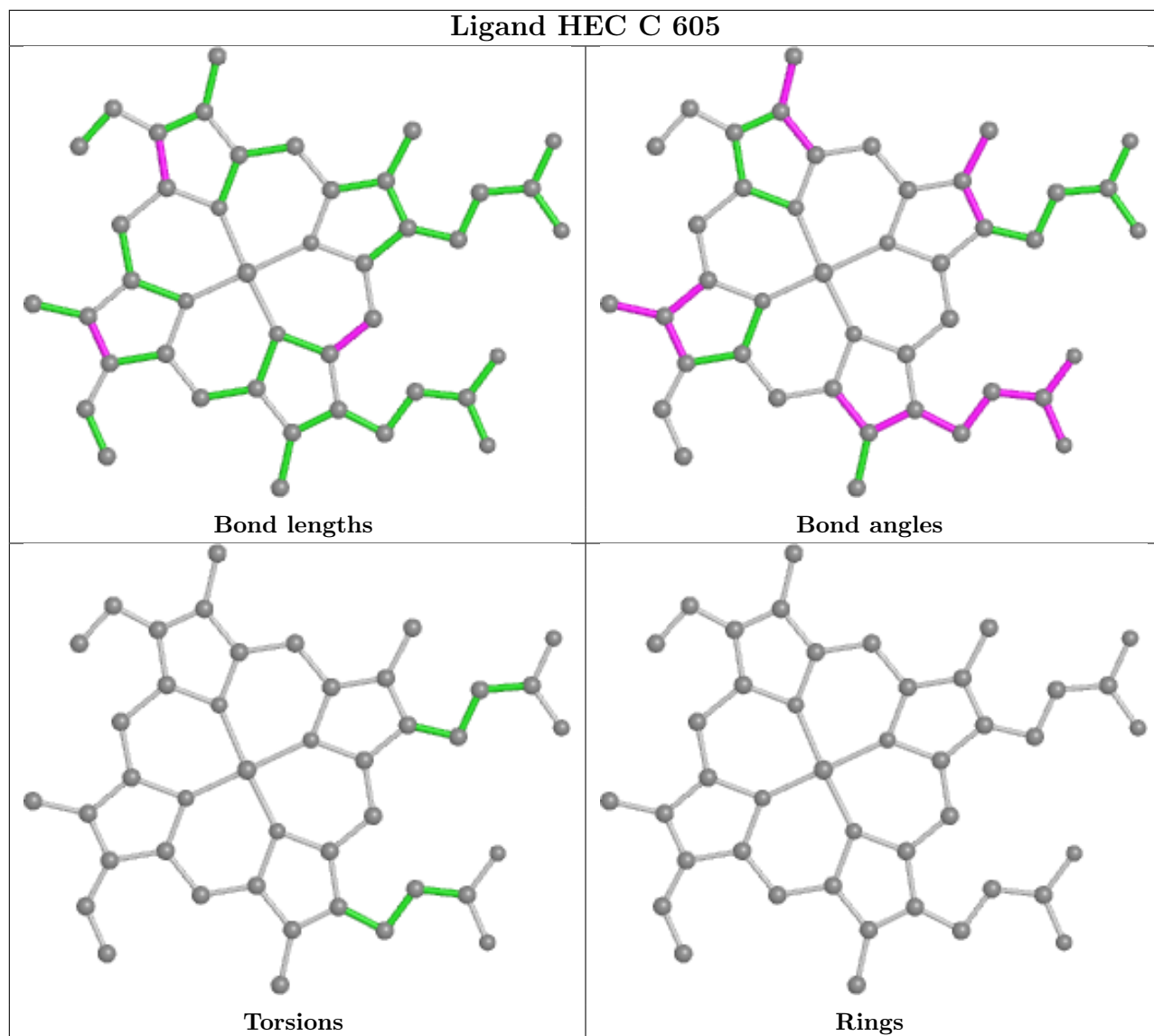


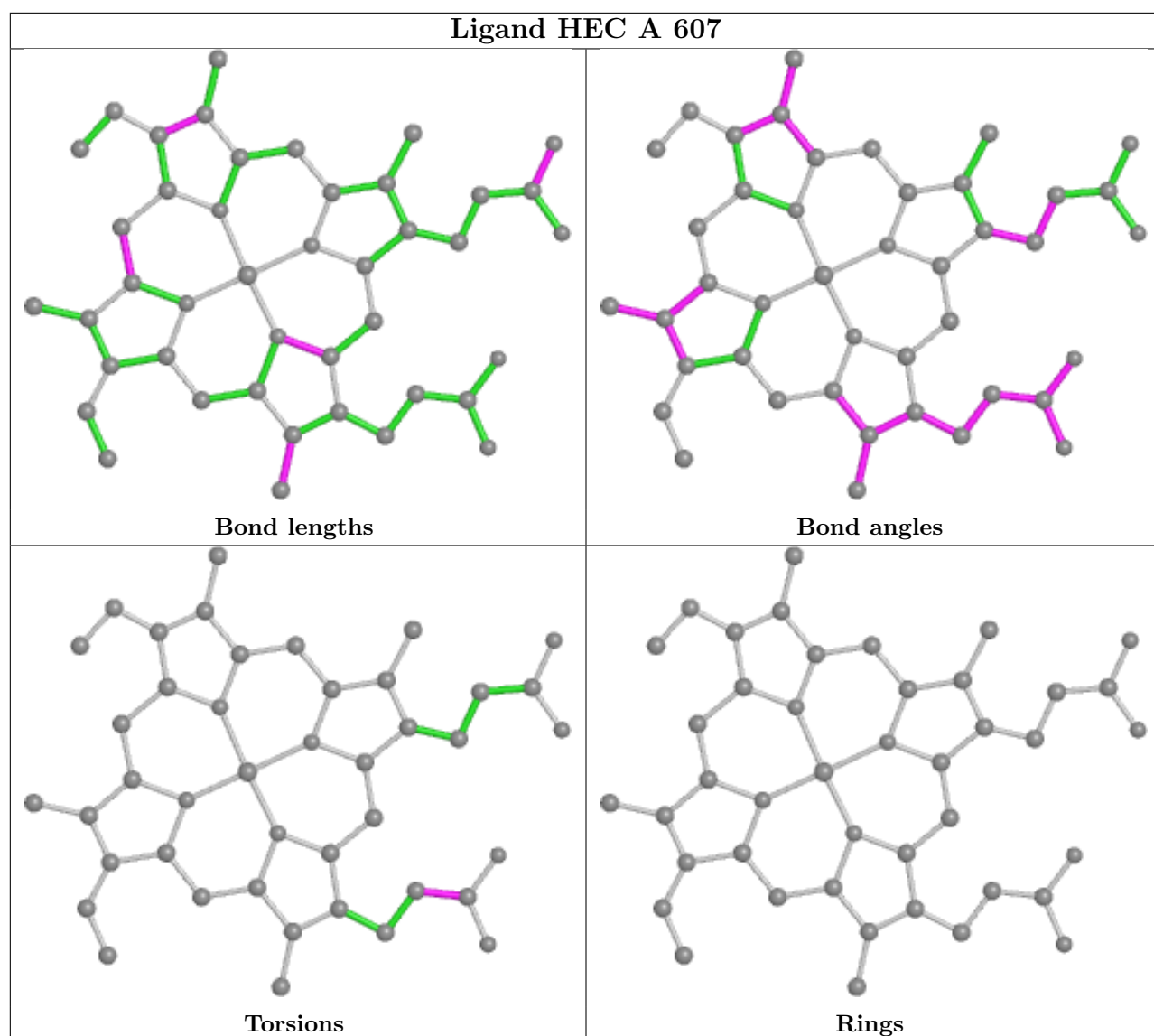












5.7 Other polymers [\(i\)](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	502/546 (91%)	-0.27	2 (0%) 92 93	17, 33, 52, 88	0
1	B	502/546 (91%)	-0.32	5 (0%) 82 85	18, 34, 53, 80	0
1	C	502/546 (91%)	-0.09	13 (2%) 56 61	18, 35, 55, 82	0
2	D	49/69 (71%)	1.79	19 (38%) 0 0	39, 58, 89, 96	0
2	E	49/69 (71%)	2.38	28 (57%) 0 0	36, 64, 94, 101	0
2	F	49/69 (71%)	1.01	11 (22%) 0 0	35, 48, 72, 84	0
All	All	1653/1845 (89%)	-0.05	78 (4%) 31 37	17, 35, 63, 101	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	53	LEU	7.7
2	F	54	VAL	6.9
2	E	54	VAL	6.4
2	E	51	VAL	6.1
2	D	54	VAL	6.0
2	F	53	LEU	5.8
2	D	51	VAL	5.7
2	E	30	VAL	5.2
2	F	8	LEU	4.6
2	E	8	LEU	4.6
2	F	55	GLN	4.6
2	D	52	ALA	4.6
2	E	50	ILE	4.5
2	E	53	LEU	4.5
2	E	52	ALA	4.5
2	E	28	THR	4.4
1	C	496	ALA	4.3
2	E	55	GLN	4.3
2	D	55	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
2	E	11	ILE	4.0
2	E	9	ALA	3.9
2	D	27	PRO	3.9
2	E	19	TYR	3.9
2	E	24	ASP	3.8
2	D	8	LEU	3.8
1	C	500	LYS	3.7
2	D	7	SER	3.7
2	E	48	GLY	3.6
2	E	29	ASP	3.6
2	F	52	ALA	3.5
2	E	49	ASP	3.5
2	D	50	ILE	3.4
2	E	47	CYS	3.4
2	E	27	PRO	3.3
1	A	500	LYS	3.3
2	F	50	ILE	3.3
1	C	401	GLY	3.3
2	D	23	LYS	3.3
2	E	31	VAL	3.1
2	D	24	ASP	3.0
2	E	46	LYS	3.0
2	E	10	PRO	2.9
2	E	26	LYS	2.8
2	F	24	ASP	2.8
2	F	51	VAL	2.8
1	C	499	ASN	2.8
2	E	22	CYS	2.6
2	E	25	LYS	2.6
2	D	19	TYR	2.6
2	F	23	LYS	2.6
2	F	7	SER	2.6
1	B	499	ASN	2.6
1	A	501	LEU	2.6
2	E	43	VAL	2.6
2	D	28	THR	2.6
1	C	498	VAL	2.6
1	C	493	ALA	2.6
2	D	9	ALA	2.5
2	D	26	LYS	2.5
2	F	9	ALA	2.5
2	D	10	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	155	LYS	2.3
1	B	494	LEU	2.3
2	E	39	ASN	2.3
2	D	11	ILE	2.3
1	C	37	ALA	2.3
2	E	23	LYS	2.2
1	C	111	ASP	2.2
1	C	400	ASP	2.2
2	E	7	SER	2.2
1	B	137	LYS	2.2
1	C	418	LYS	2.1
1	C	407	LYS	2.1
2	D	31	VAL	2.1
1	B	500	LYS	2.1
2	D	48	GLY	2.1
1	C	501	LEU	2.1
1	C	14	LYS	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	EDO	A	617	4/4	0.74	0.25	63,63,63,65	0
5	PEG	B	612	7/7	0.78	0.24	63,68,69,71	0
10	NO3	B	618	4/4	0.78	0.25	67,68,68,69	0
7	EDO	B	620	4/4	0.79	0.14	46,51,52,55	0
5	PEG	A	614	7/7	0.80	0.26	54,61,63,64	0
7	EDO	B	616	4/4	0.80	0.20	60,61,62,63	0

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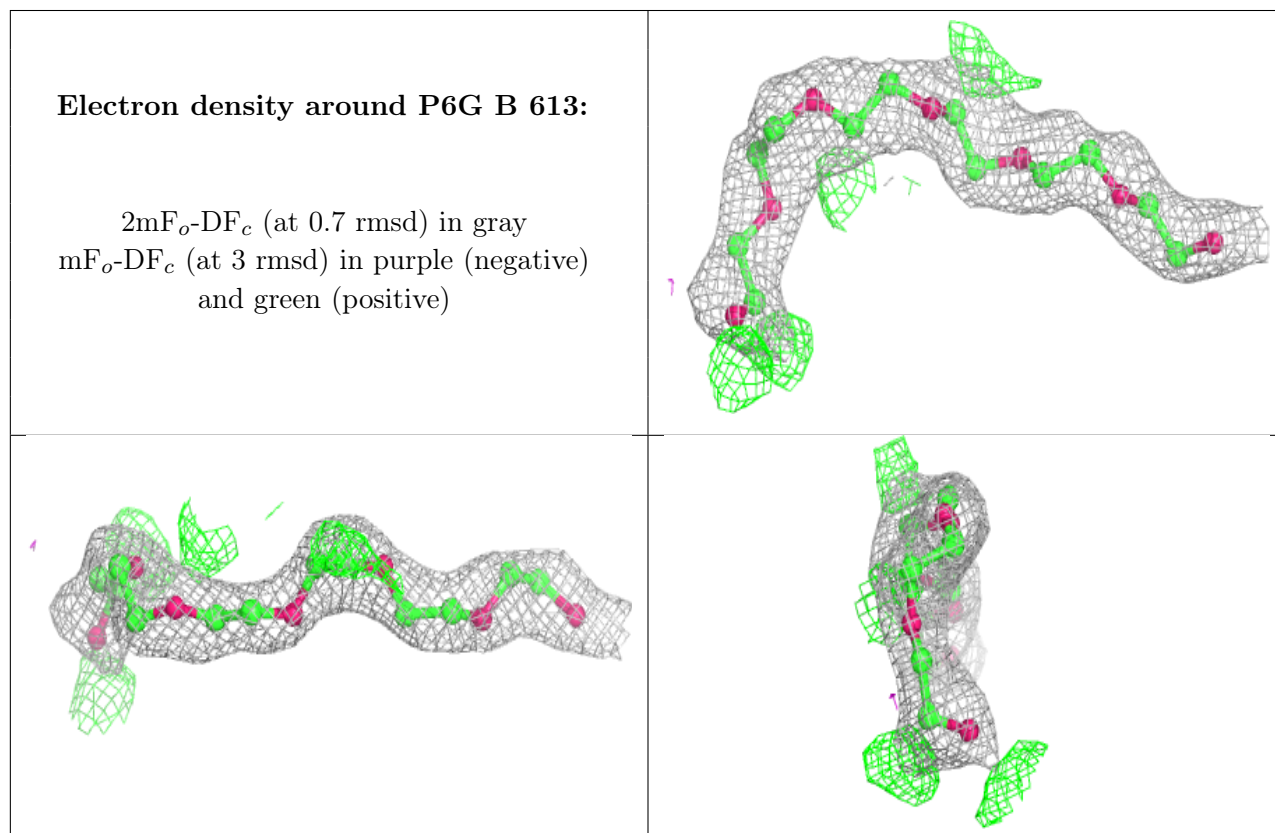
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	NO3	F	101	4/4	0.80	0.28	70,71,71,71	0
5	PEG	C	610	7/7	0.81	0.24	54,58,61,63	0
5	PEG	B	610	7/7	0.81	0.18	58,59,63,66	0
5	PEG	C	611	7/7	0.82	0.20	54,60,63,64	0
10	NO3	C	619	4/4	0.83	0.24	72,72,72,72	0
5	PEG	C	622	7/7	0.83	0.24	43,48,50,51	0
7	EDO	C	618	4/4	0.84	0.17	51,52,53,55	0
7	EDO	B	615	4/4	0.84	0.17	50,51,51,55	0
5	PEG	C	612	7/7	0.85	0.14	54,56,58,60	0
5	PEG	C	613	7/7	0.86	0.16	50,55,60,61	0
5	PEG	A	613	7/7	0.86	0.22	56,57,58,60	0
7	EDO	C	620	4/4	0.87	0.14	48,48,49,51	0
8	P6G	B	613	19/19	0.87	0.16	54,60,64,65	0
9	PG4	B	614	13/13	0.87	0.16	43,50,64,65	0
7	EDO	A	616	4/4	0.88	0.13	44,46,46,50	0
5	PEG	A	612	7/7	0.88	0.18	56,58,61,64	0
5	PEG	F	102	7/7	0.88	0.24	50,51,54,56	0
6	PGE	A	615	10/10	0.88	0.18	52,55,62,62	0
7	EDO	C	615	4/4	0.91	0.12	50,51,52,55	0
6	PGE	C	614	10/10	0.91	0.16	49,52,54,57	0
5	PEG	C	609	7/7	0.91	0.17	55,59,59,61	0
5	PEG	B	611	7/7	0.91	0.12	60,61,61,62	0
5	PEG	A	611	7/7	0.92	0.19	53,55,57,59	0
5	PEG	B	609	7/7	0.92	0.12	46,48,52,52	0
7	EDO	C	621	4/4	0.92	0.16	41,42,44,45	0
7	EDO	C	616	4/4	0.92	0.14	40,45,46,50	0
7	EDO	A	618	4/4	0.93	0.10	42,46,46,52	0
10	NO3	B	617	4/4	0.93	0.12	51,53,54,56	0
5	PEG	A	610	7/7	0.93	0.25	56,57,64,67	0
5	PEG	A	609	7/7	0.93	0.13	44,45,51,51	0
7	EDO	C	617	4/4	0.93	0.09	42,45,46,49	0
7	EDO	B	621	4/4	0.94	0.16	51,52,52,53	0
4	ISW	C	601	43/43	0.95	0.14	20,32,47,50	0
7	EDO	B	619	4/4	0.95	0.10	45,47,49,50	0
7	EDO	A	619	4/4	0.95	0.19	44,45,48,49	0
4	ISW	B	608	43/43	0.95	0.14	22,34,51,56	0
4	ISW	A	608	43/43	0.96	0.11	21,32,46,47	0
3	HEC	B	601	43/43	0.98	0.09	26,34,43,48	0
3	HEC	B	603	43/43	0.98	0.09	23,29,33,35	0
3	HEC	C	602	43/43	0.98	0.09	25,34,39,43	0
3	HEC	C	603	43/43	0.98	0.10	18,25,28,31	0
3	HEC	C	604	43/43	0.98	0.10	20,25,29,31	0

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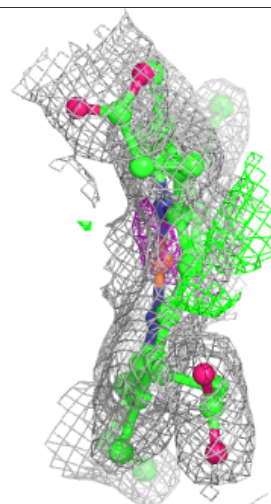
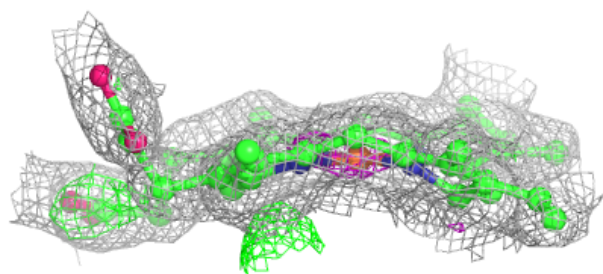
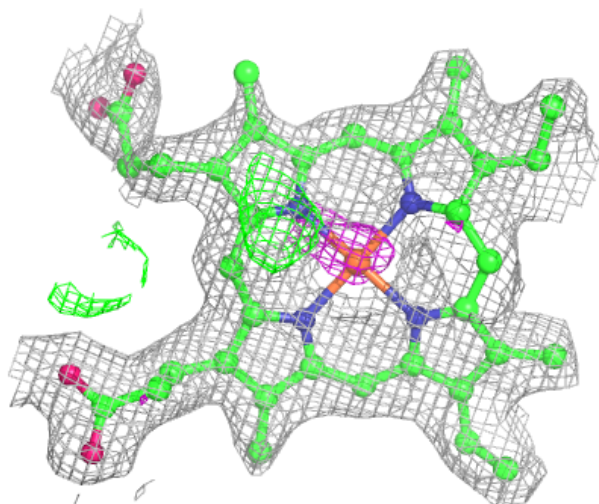
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	HEC	A	601	43/43	0.98	0.10	21,29,33,44	0
3	HEC	A	602	43/43	0.98	0.11	20,24,29,34	0
3	HEC	A	603	43/43	0.98	0.10	20,28,32,34	0
3	HEC	B	606	43/43	0.99	0.13	15,21,25,26	0
3	HEC	B	607	43/43	0.99	0.13	15,21,31,36	0
3	HEC	A	606	43/43	0.99	0.12	17,23,29,30	0
3	HEC	A	607	43/43	0.99	0.10	20,24,30,32	0
3	HEC	A	604	43/43	0.99	0.12	20,25,31,36	0
3	HEC	C	605	43/43	0.99	0.11	17,25,30,32	0
3	HEC	C	606	43/43	0.99	0.12	17,22,33,44	0
3	HEC	C	607	43/43	0.99	0.12	16,22,28,32	0
3	HEC	C	608	43/43	0.99	0.14	16,21,32,33	0
3	HEC	B	602	43/43	0.99	0.09	21,26,31,33	0
3	HEC	A	605	43/43	0.99	0.15	17,23,37,39	0
3	HEC	B	604	43/43	0.99	0.10	15,24,28,33	0
3	HEC	B	605	43/43	0.99	0.11	17,24,30,36	0

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



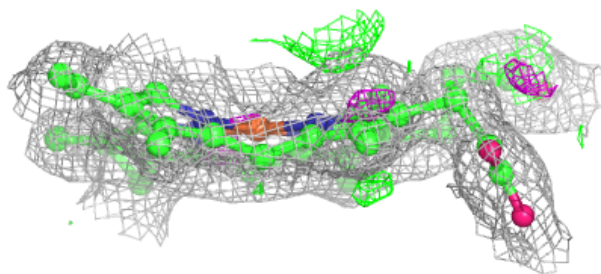
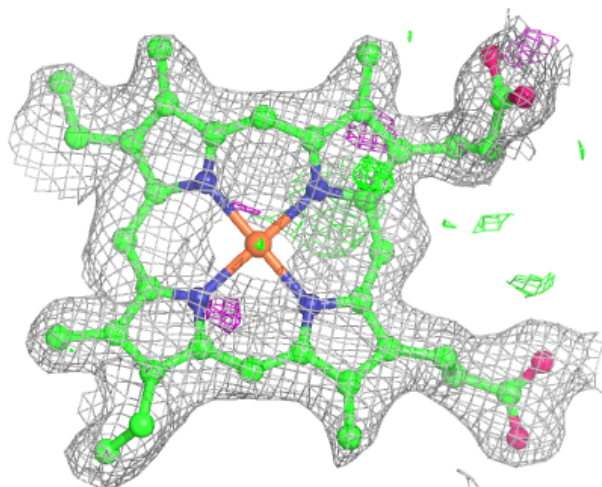
Electron density around ISW C 601:

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



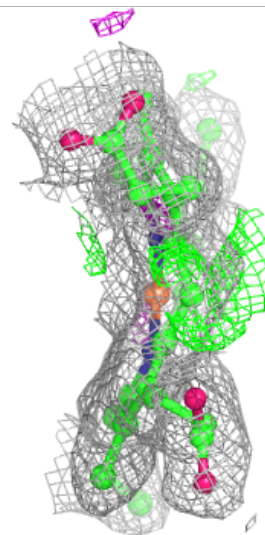
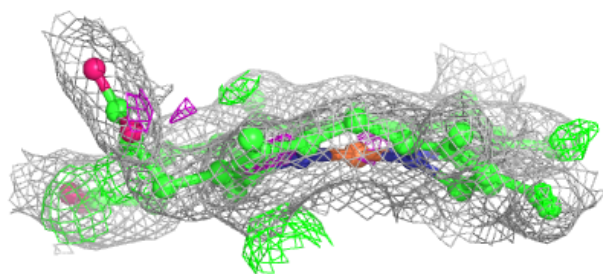
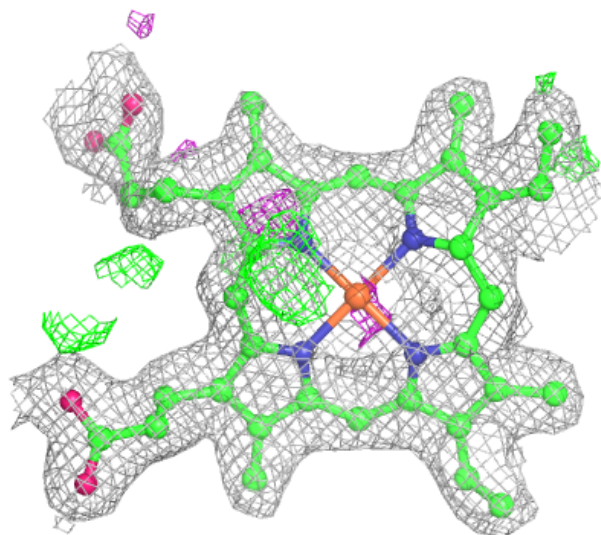
Electron density around ISW B 608:

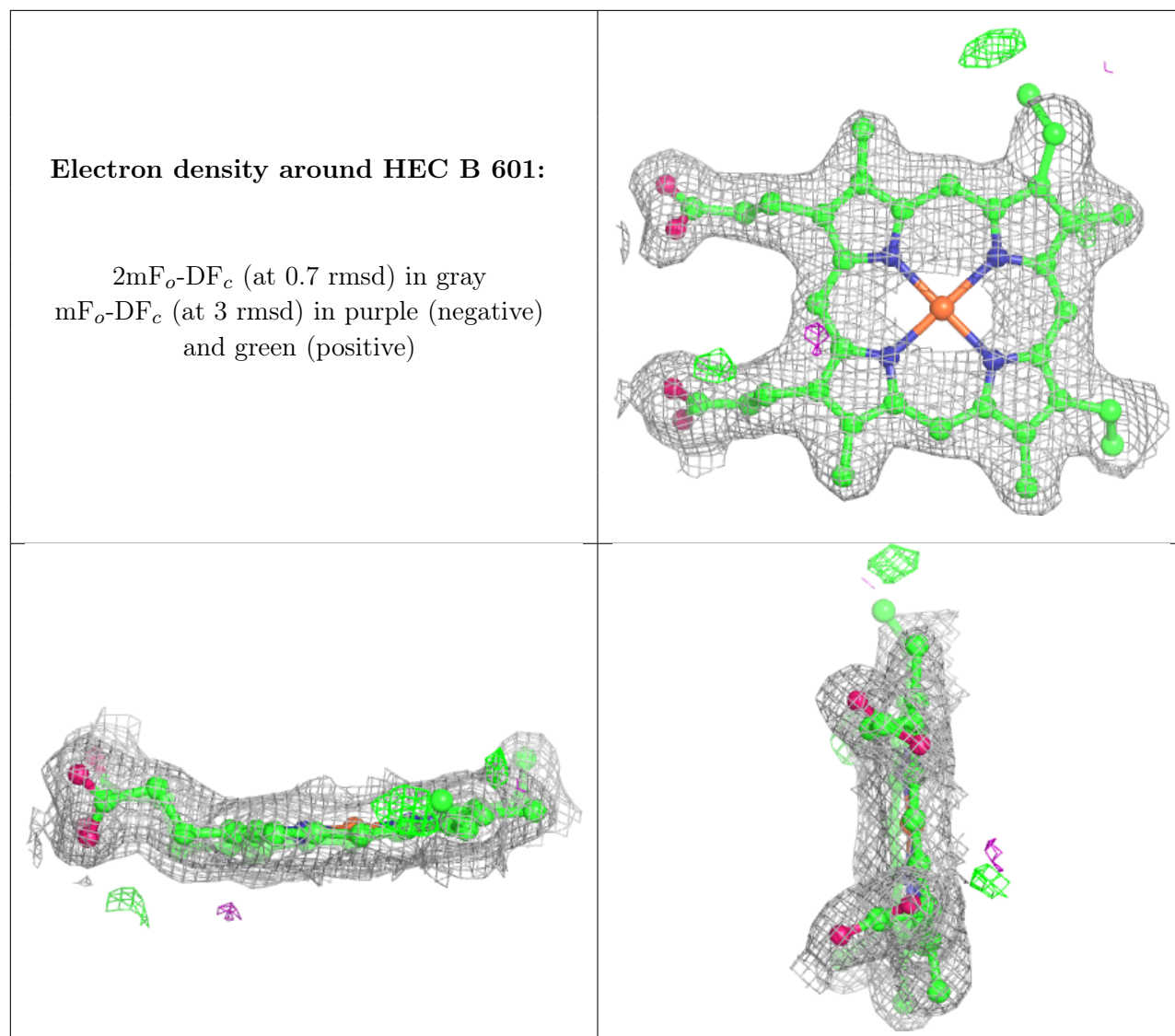
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

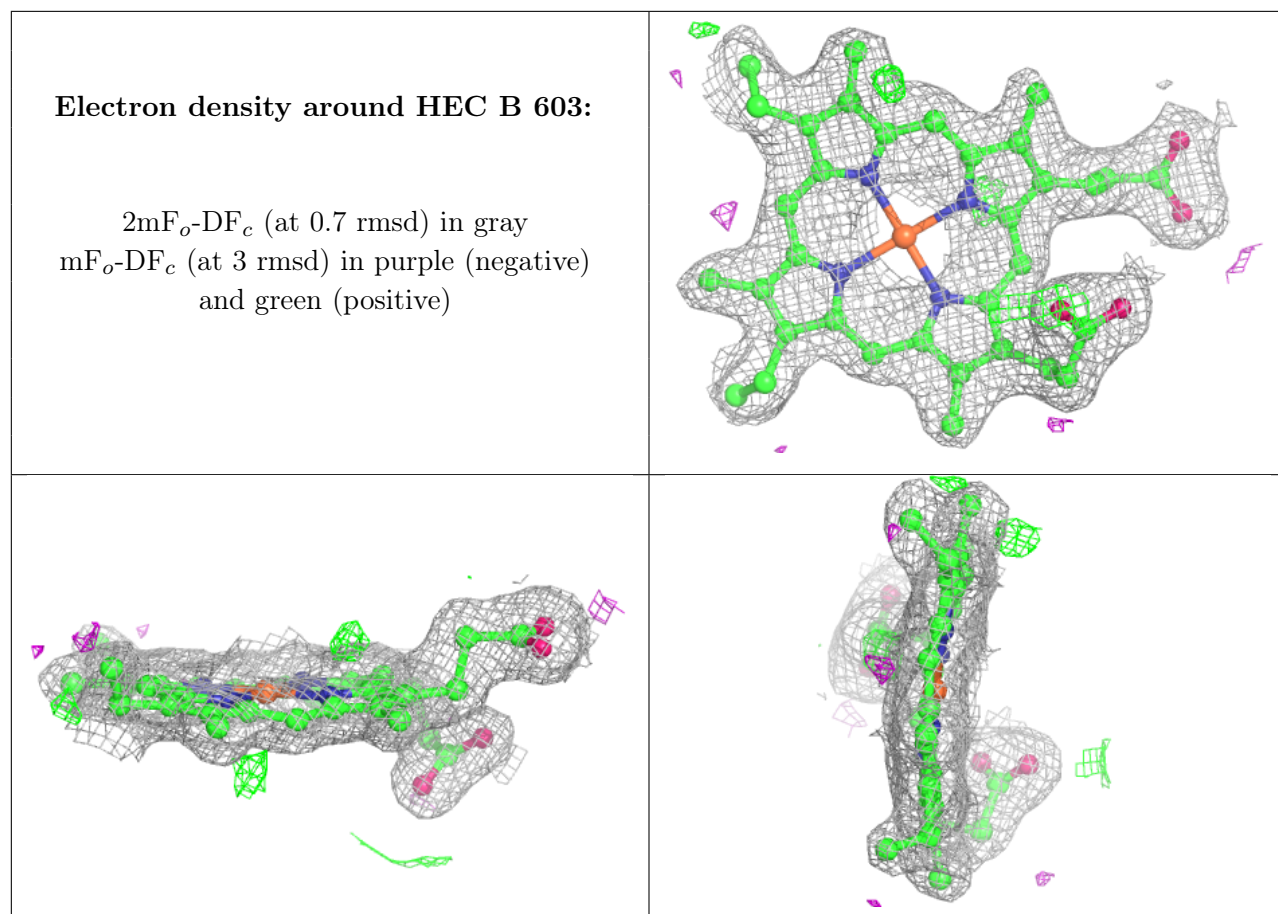


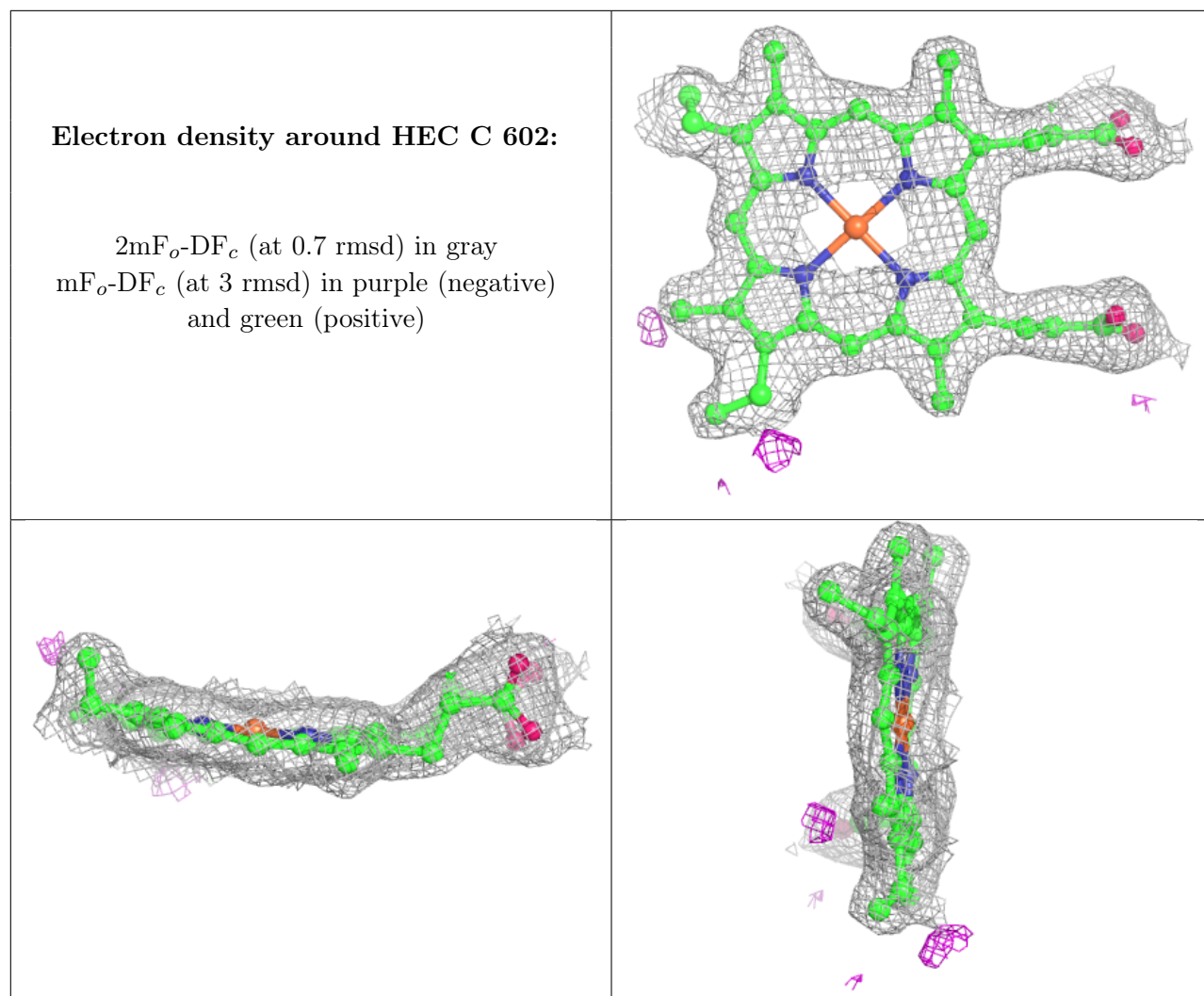
Electron density around ISW A 608:

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



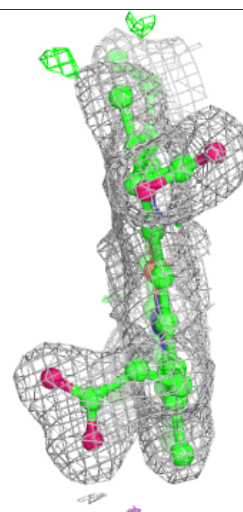
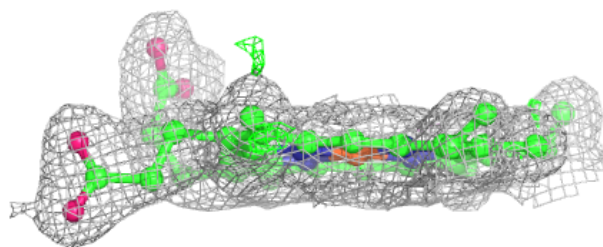
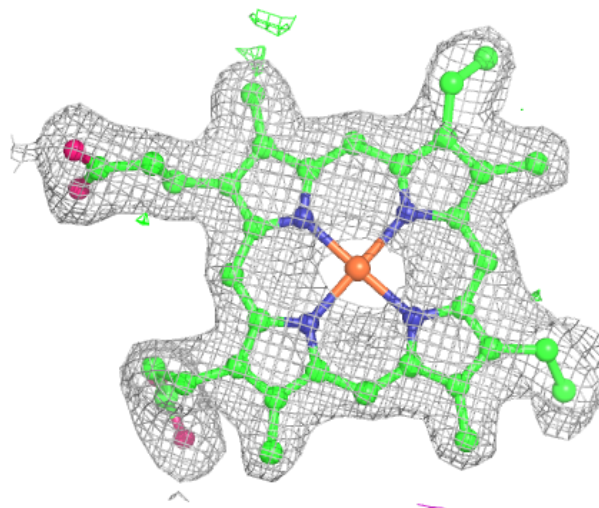






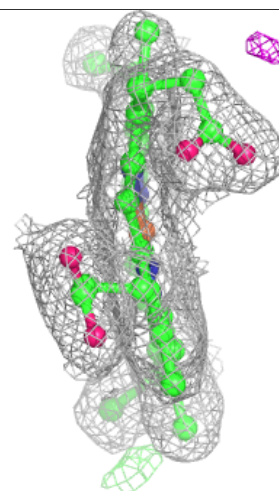
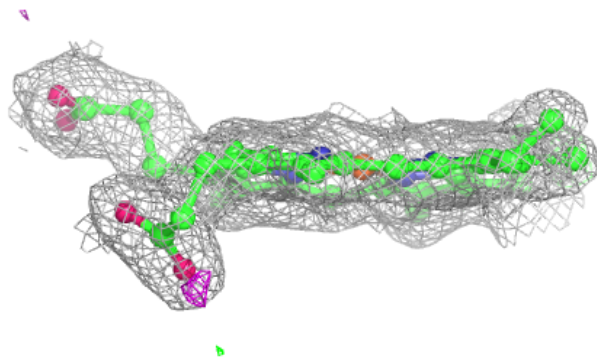
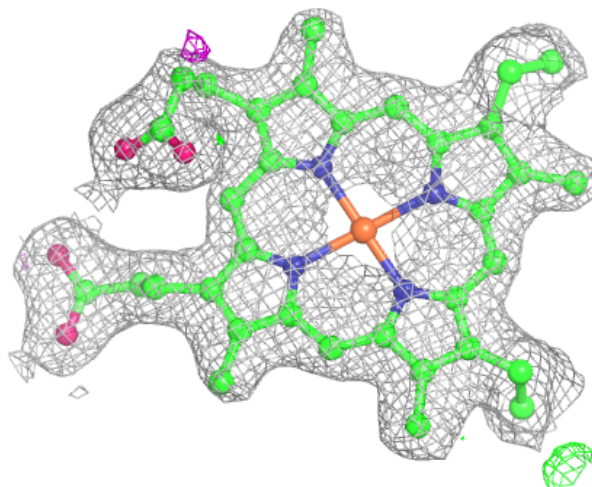
Electron density around HEC C 603:

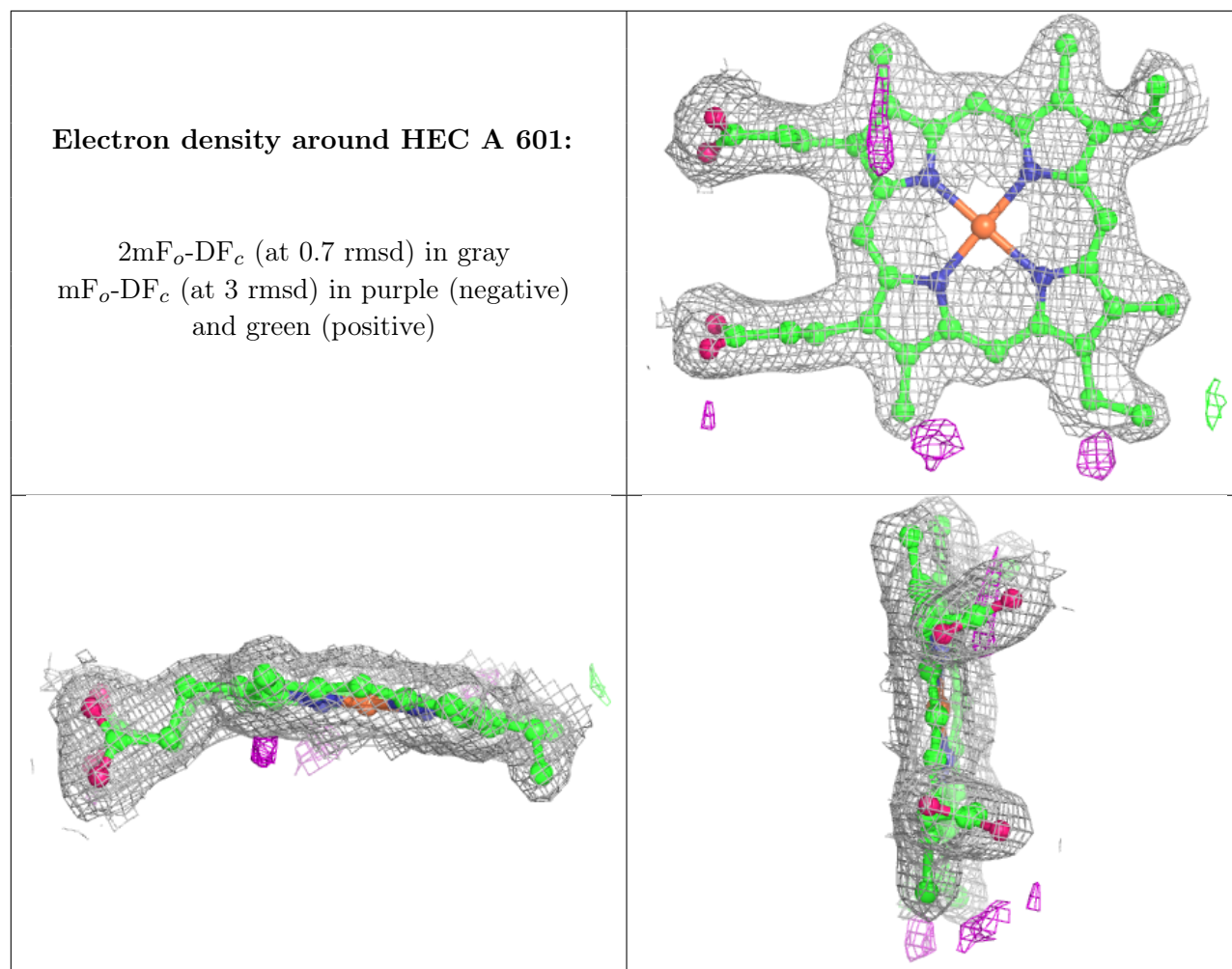
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC C 604:

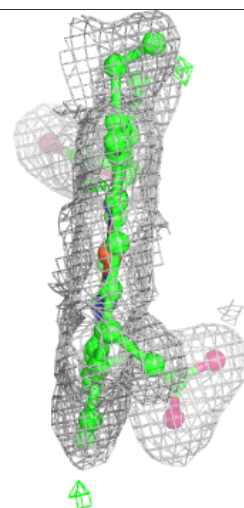
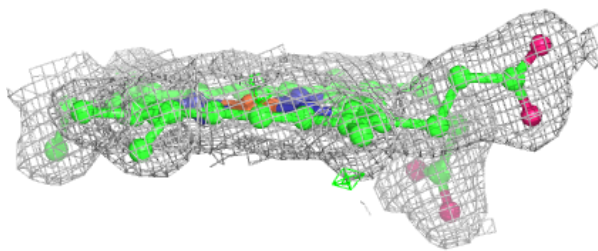
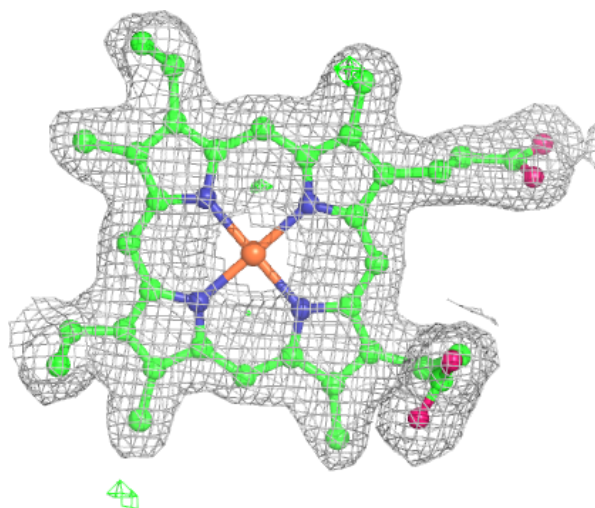
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





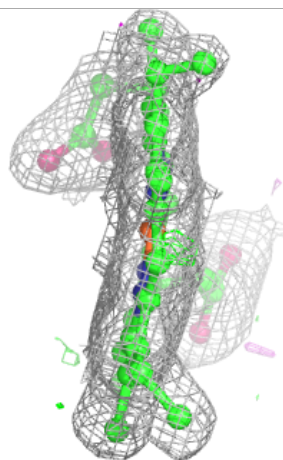
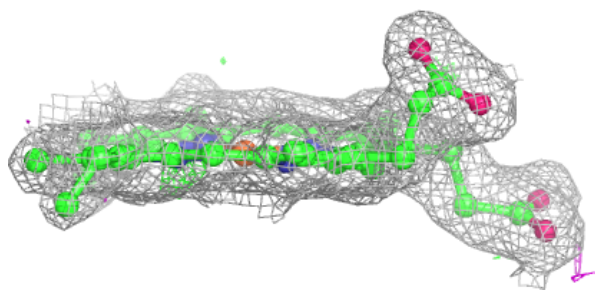
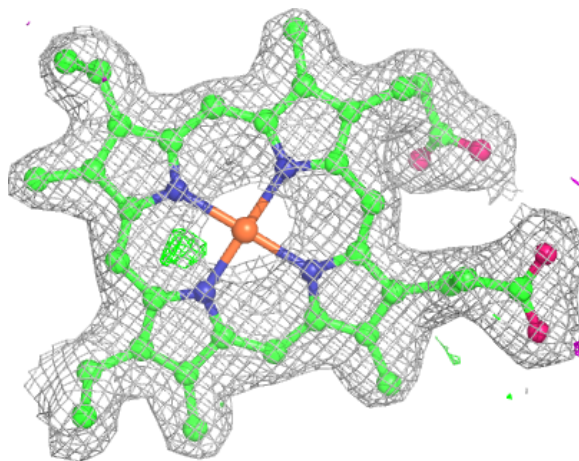
Electron density around HEC A 602:

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



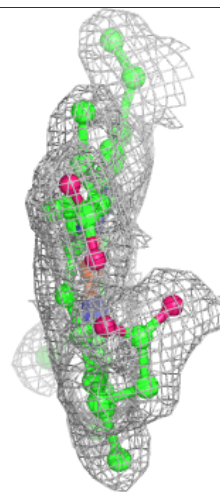
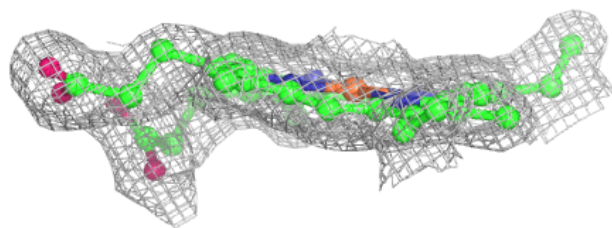
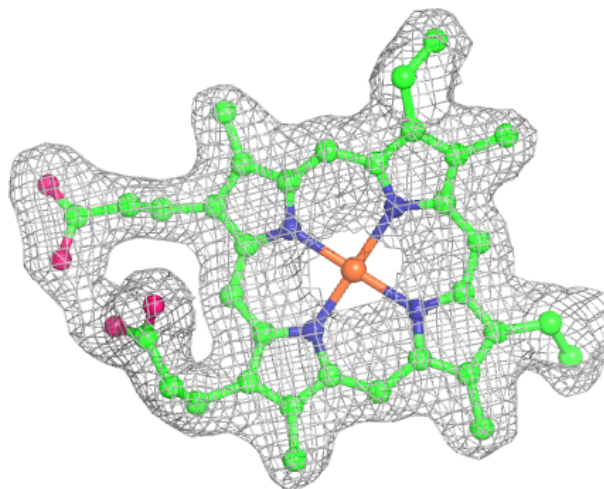
Electron density around HEC A 603:

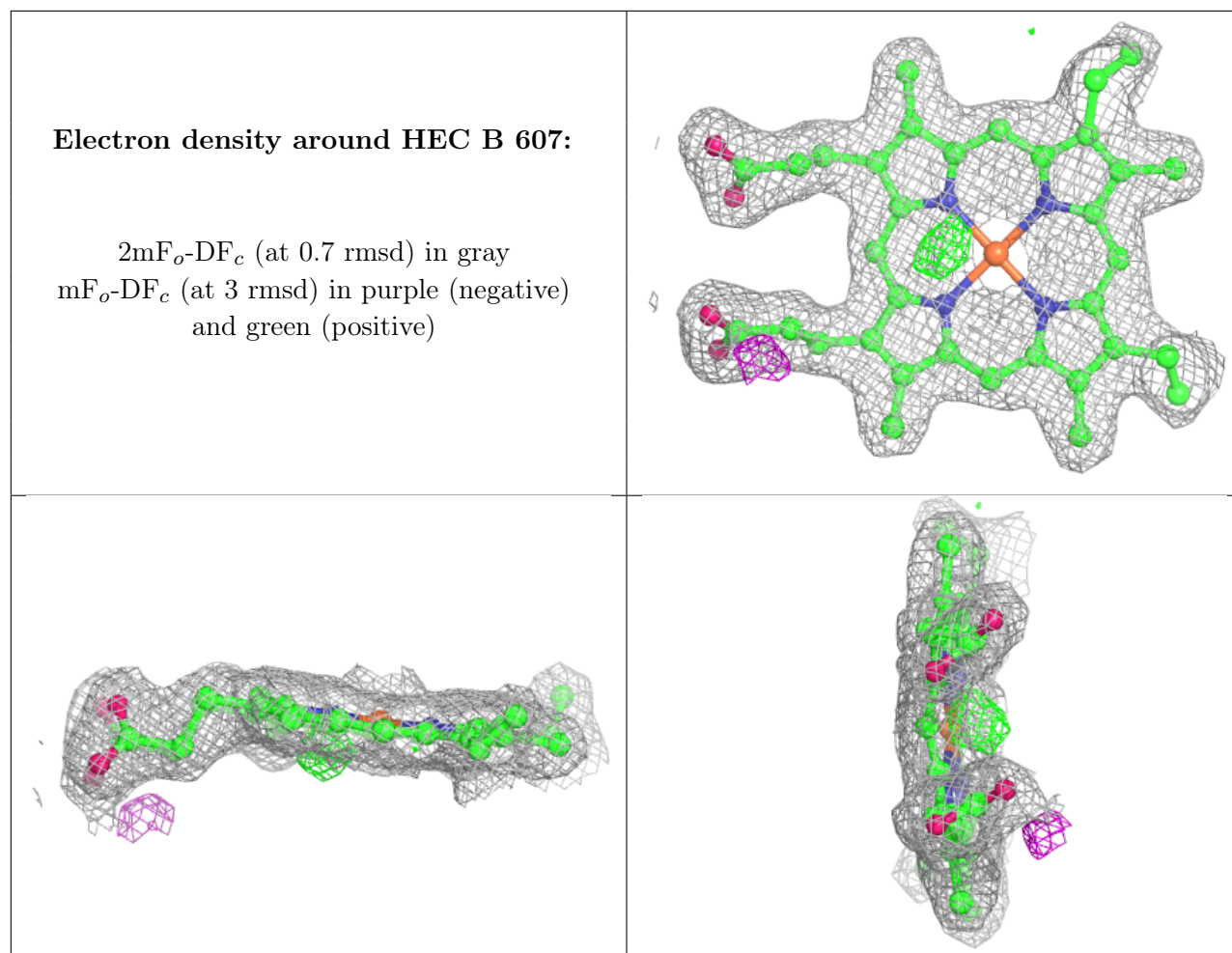
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

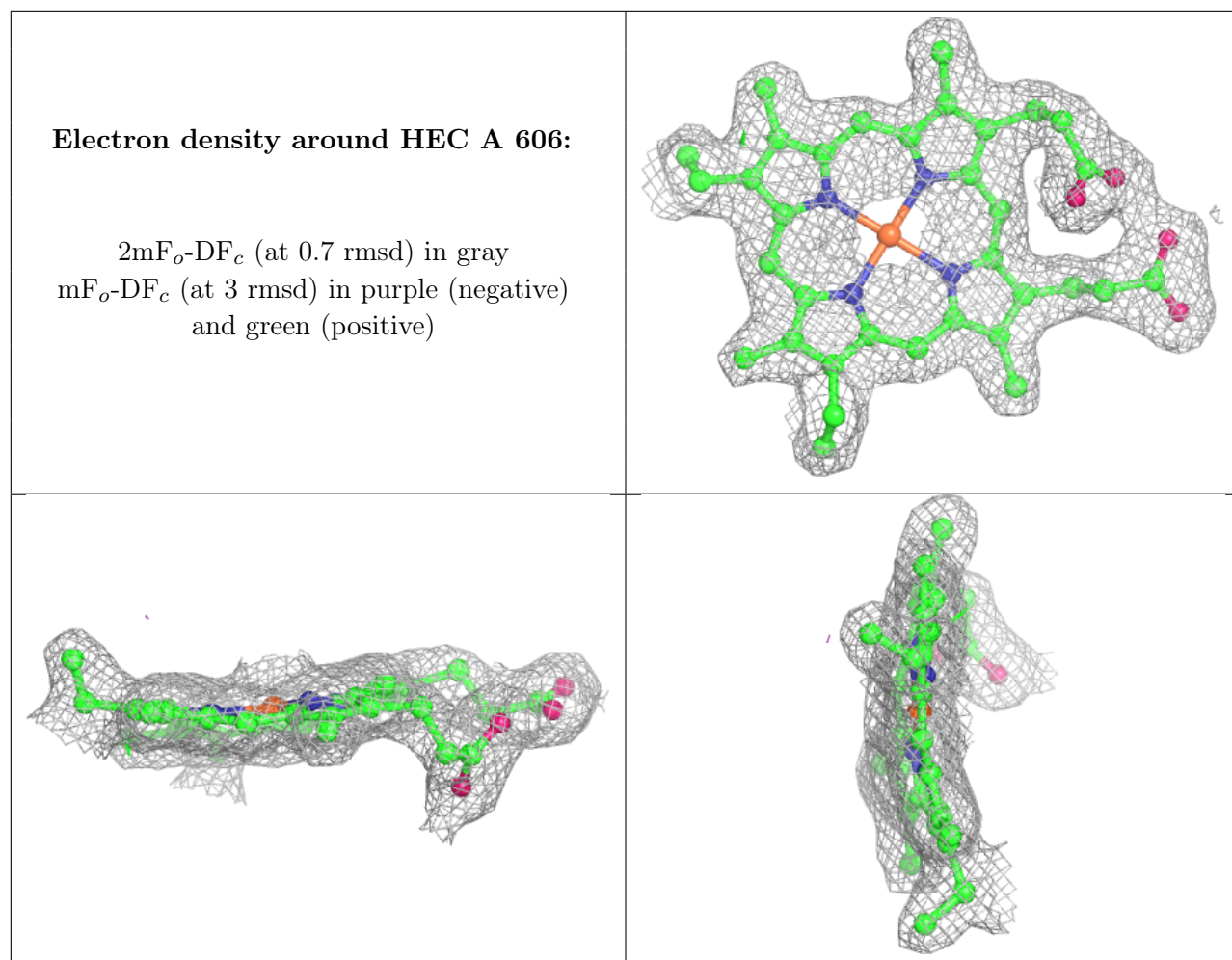


Electron density around HEC B 606:

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

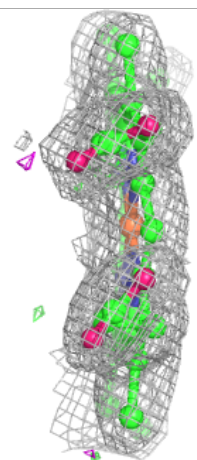
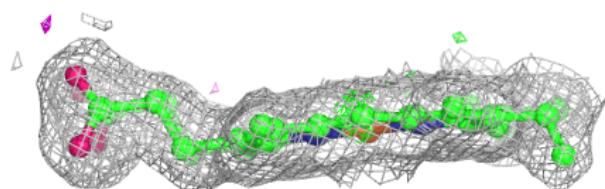
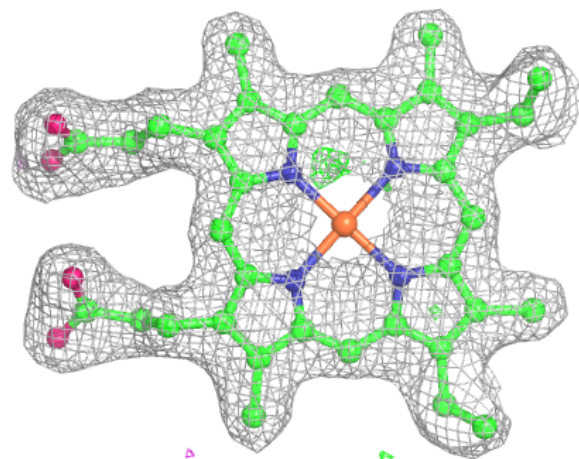






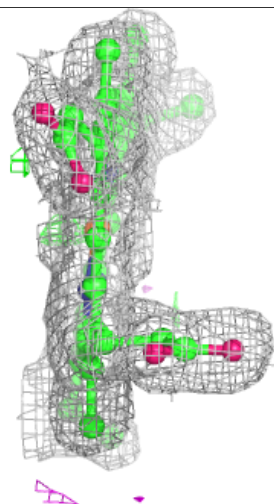
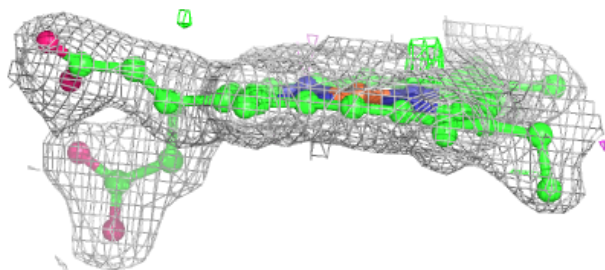
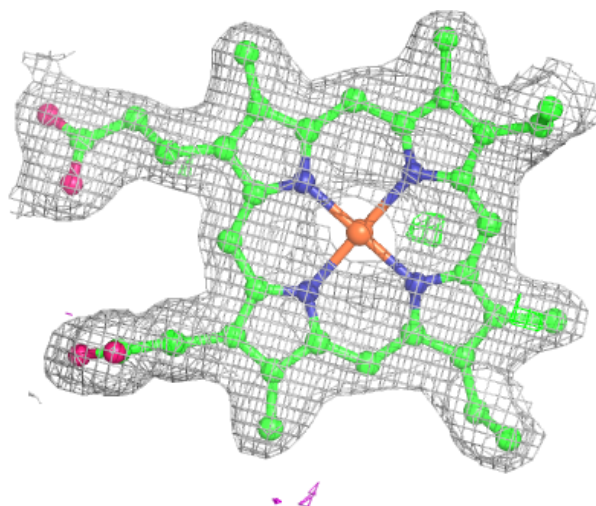
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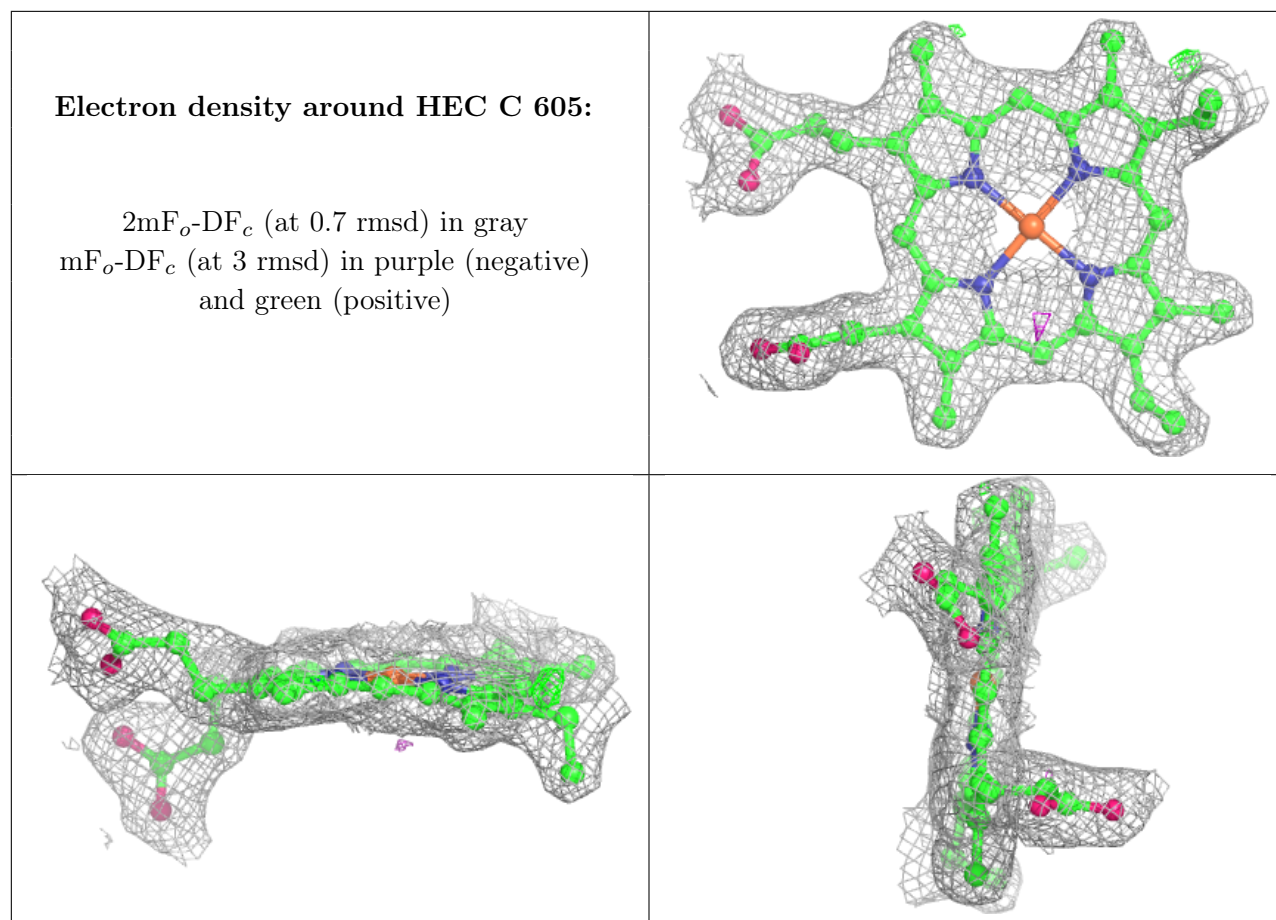
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC A 604:

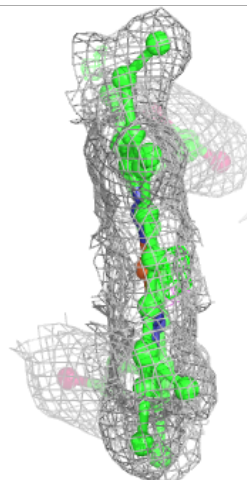
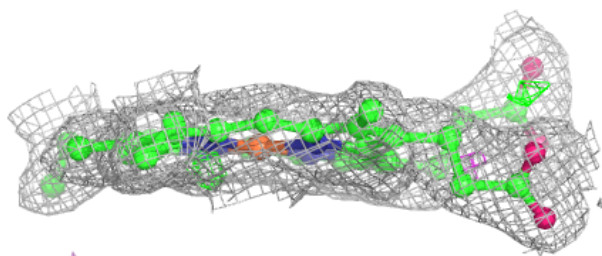
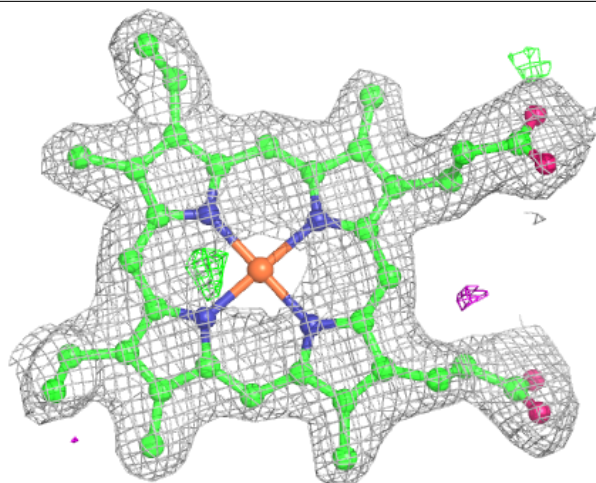
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





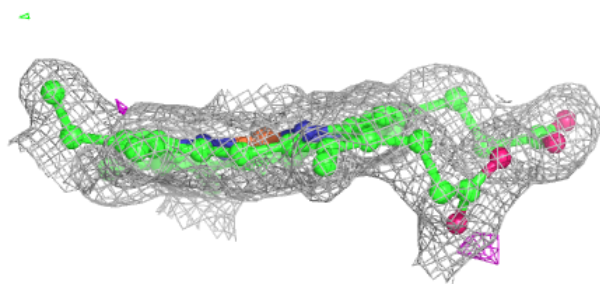
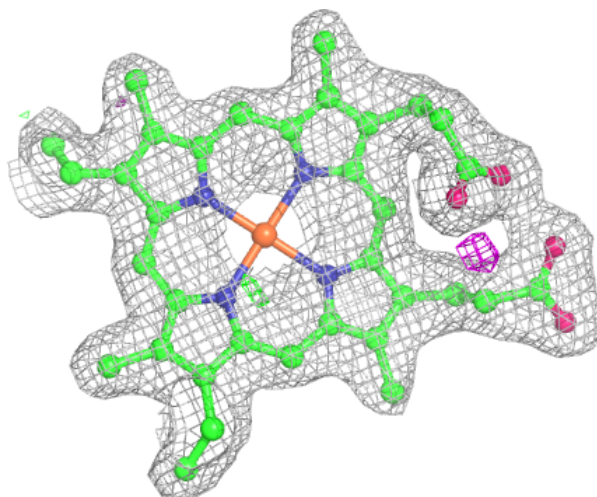
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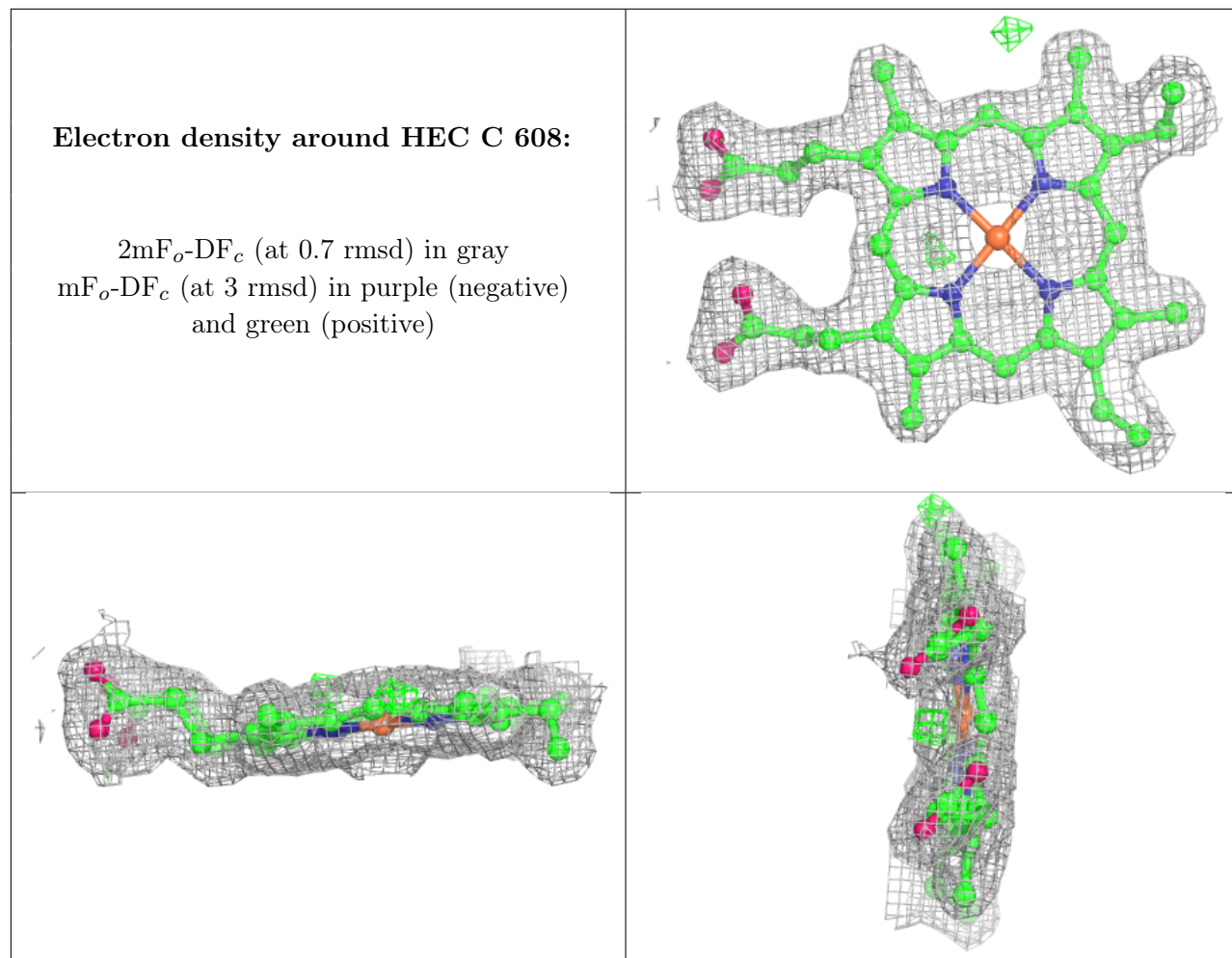
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC C 607:

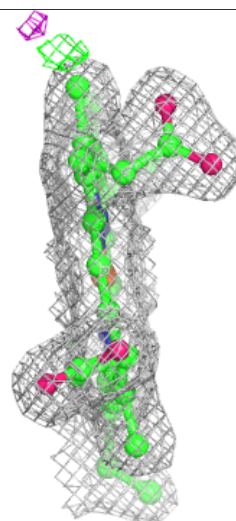
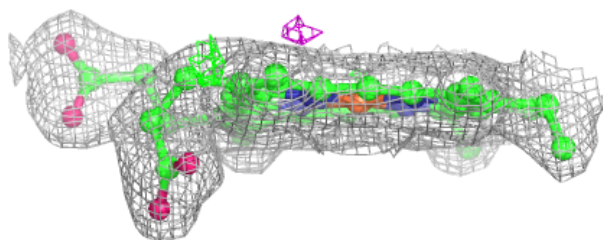
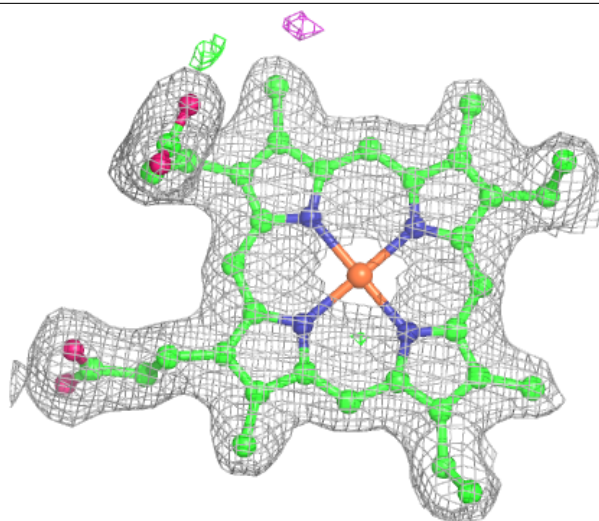
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





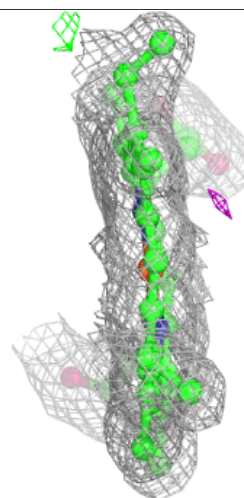
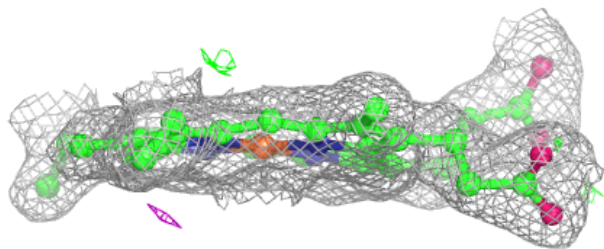
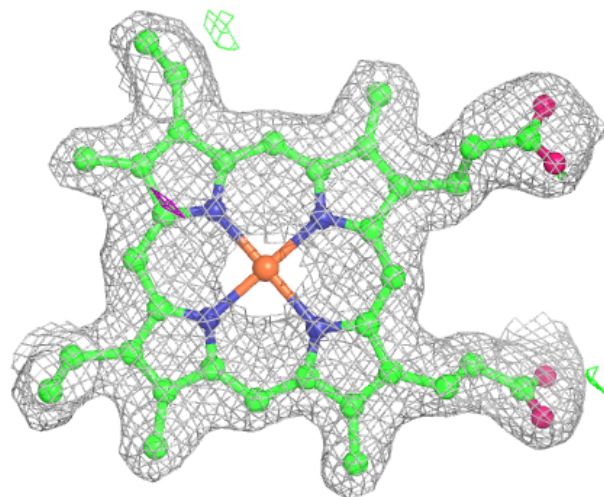
Electron density around HEC B 602:

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



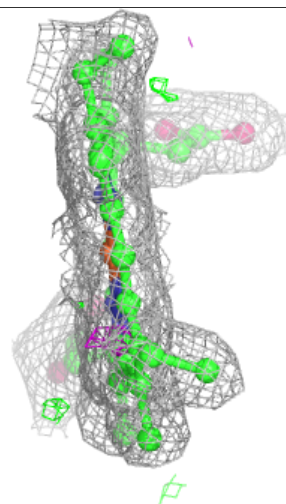
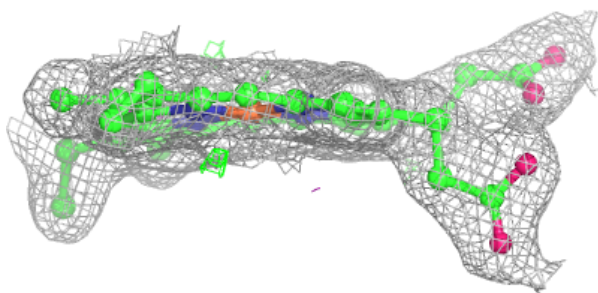
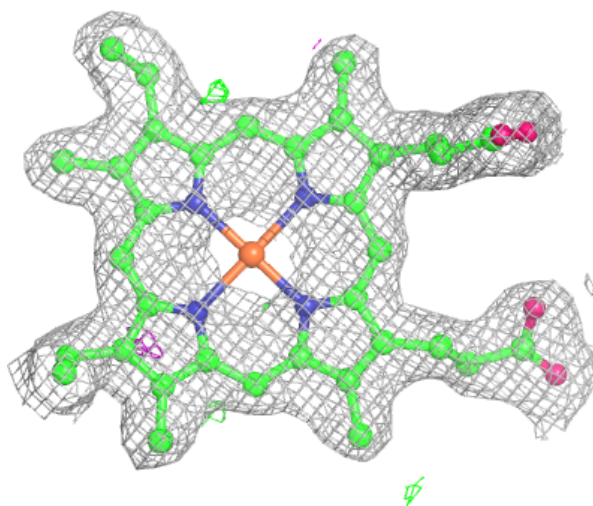
Electron density around HEC A 605:

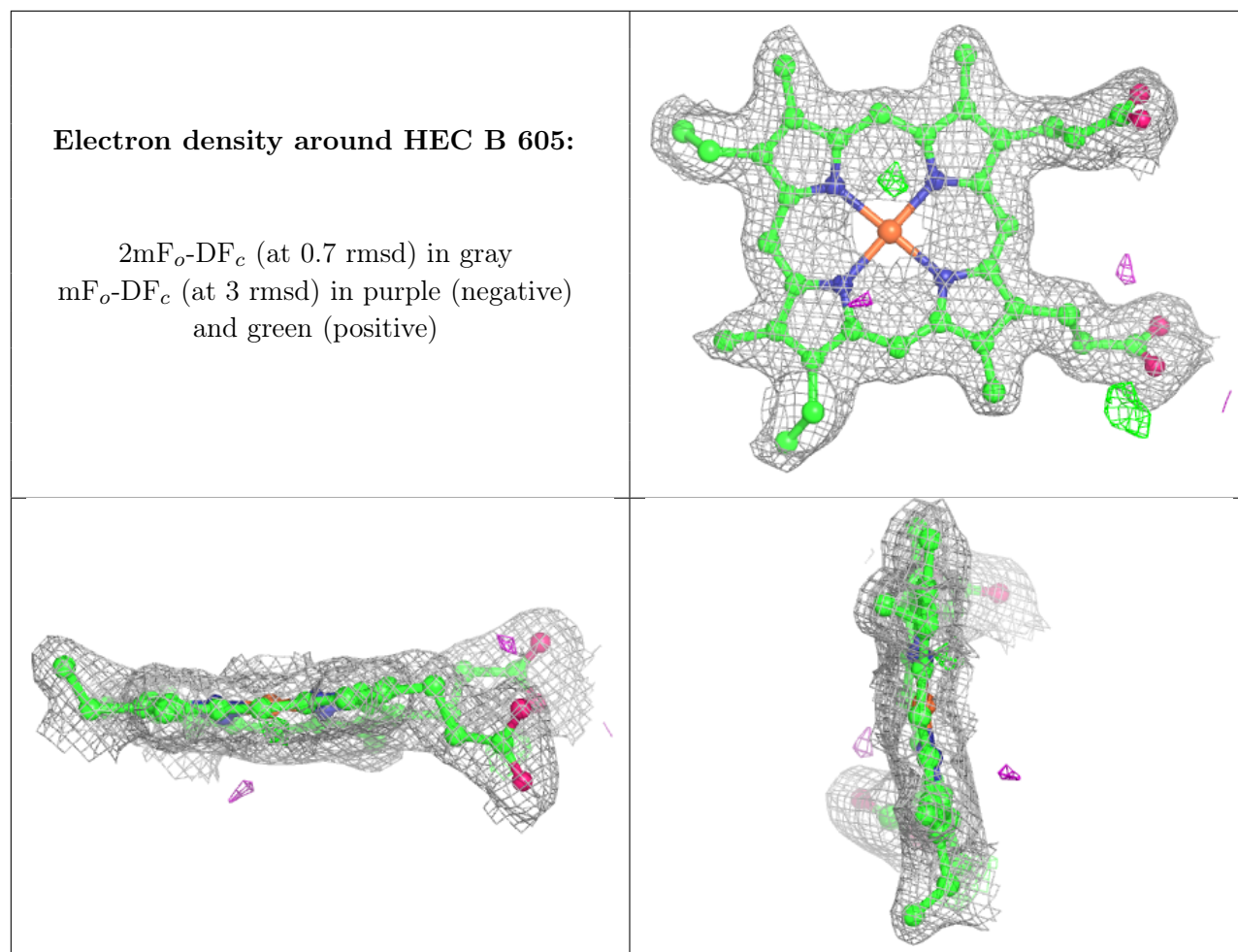
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC B 604:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.