



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:32 am BST

PDB ID : 3UCP
Title : Outer membrane Endecaheme cytochrome UndA from *Shewanella* sp. HRCR-6
Authors : Edwards, M.J.; Clarke, T.A.
Deposited on : 2011-10-27
Resolution : 1.76 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 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 : 2.11
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) : 2.11

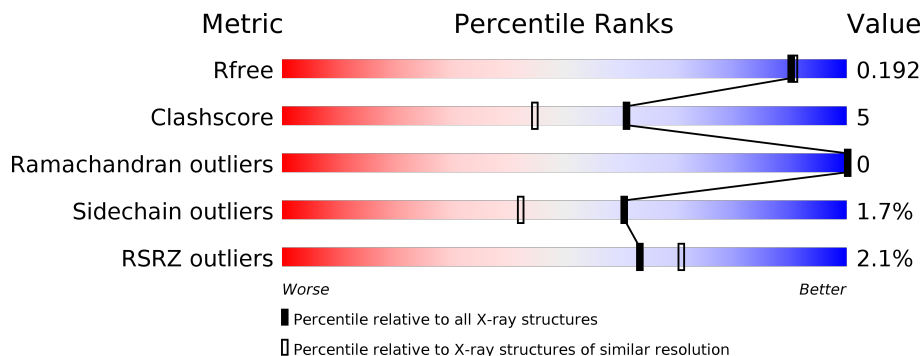
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	874	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7814 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 UndA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	800	5990	3720	1030	1205	35	0	11	0

There are 58 discrepancies between the modelled and reference sequences:

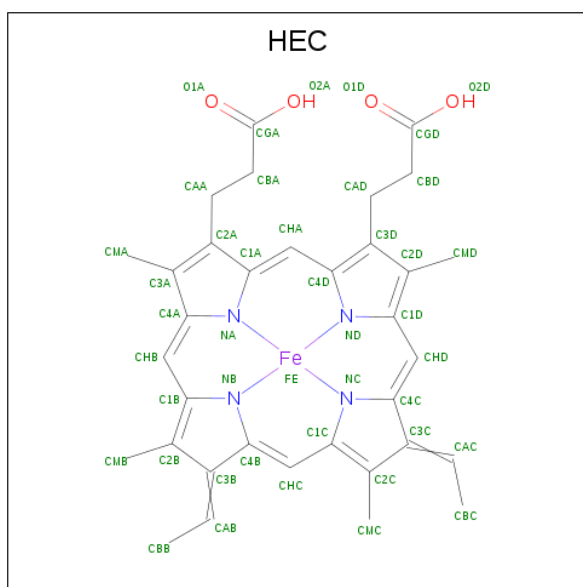
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP F8UWD6
A	1	SER	-	EXPRESSION TAG	UNP F8UWD6
A	2	LYS	-	EXPRESSION TAG	UNP F8UWD6
A	3	LYS	-	EXPRESSION TAG	UNP F8UWD6
A	4	LEU	-	EXPRESSION TAG	UNP F8UWD6
A	5	LEU	-	EXPRESSION TAG	UNP F8UWD6
A	6	SER	-	EXPRESSION TAG	UNP F8UWD6
A	7	VAL	-	EXPRESSION TAG	UNP F8UWD6
A	8	LEU	-	EXPRESSION TAG	UNP F8UWD6
A	9	PHE	-	EXPRESSION TAG	UNP F8UWD6
A	10	GLY	-	EXPRESSION TAG	UNP F8UWD6
A	11	ALA	-	EXPRESSION TAG	UNP F8UWD6
A	12	SER	-	EXPRESSION TAG	UNP F8UWD6
A	13	LEU	-	EXPRESSION TAG	UNP F8UWD6
A	14	ALA	-	EXPRESSION TAG	UNP F8UWD6
A	15	ALA	-	EXPRESSION TAG	UNP F8UWD6
A	16	LEU	-	EXPRESSION TAG	UNP F8UWD6
A	17	ALA	-	EXPRESSION TAG	UNP F8UWD6
A	18	LEU	-	EXPRESSION TAG	UNP F8UWD6
A	19	SER	-	EXPRESSION TAG	UNP F8UWD6
A	20	PRO	-	EXPRESSION TAG	UNP F8UWD6
A	21	THR	-	EXPRESSION TAG	UNP F8UWD6
A	22	ALA	-	EXPRESSION TAG	UNP F8UWD6
A	23	PHE	-	EXPRESSION TAG	UNP F8UWD6
A	24	ALA	-	EXPRESSION TAG	UNP F8UWD6
A	25	ALA	-	EXPRESSION TAG	UNP F8UWD6
A	26	ASP	-	EXPRESSION TAG	UNP F8UWD6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	27	GLN	-	EXPRESSION TAG	UNP F8UWD6
A	844	LYS	-	EXPRESSION TAG	UNP F8UWD6
A	845	GLY	-	EXPRESSION TAG	UNP F8UWD6
A	846	GLU	-	EXPRESSION TAG	UNP F8UWD6
A	847	LEU	-	EXPRESSION TAG	UNP F8UWD6
A	848	LYS	-	EXPRESSION TAG	UNP F8UWD6
A	849	LEU	-	EXPRESSION TAG	UNP F8UWD6
A	850	GLU	-	EXPRESSION TAG	UNP F8UWD6
A	851	GLY	-	EXPRESSION TAG	UNP F8UWD6
A	852	LYS	-	EXPRESSION TAG	UNP F8UWD6
A	853	PRO	-	EXPRESSION TAG	UNP F8UWD6
A	854	ILE	-	EXPRESSION TAG	UNP F8UWD6
A	855	PRO	-	EXPRESSION TAG	UNP F8UWD6
A	856	ASN	-	EXPRESSION TAG	UNP F8UWD6
A	857	PRO	-	EXPRESSION TAG	UNP F8UWD6
A	858	LEU	-	EXPRESSION TAG	UNP F8UWD6
A	859	LEU	-	EXPRESSION TAG	UNP F8UWD6
A	860	GLY	-	EXPRESSION TAG	UNP F8UWD6
A	861	LEU	-	EXPRESSION TAG	UNP F8UWD6
A	862	ASP	-	EXPRESSION TAG	UNP F8UWD6
A	863	SER	-	EXPRESSION TAG	UNP F8UWD6
A	864	THR	-	EXPRESSION TAG	UNP F8UWD6
A	865	ARG	-	EXPRESSION TAG	UNP F8UWD6
A	866	THR	-	EXPRESSION TAG	UNP F8UWD6
A	867	GLY	-	EXPRESSION TAG	UNP F8UWD6
A	868	HIS	-	EXPRESSION TAG	UNP F8UWD6
A	869	HIS	-	EXPRESSION TAG	UNP F8UWD6
A	870	HIS	-	EXPRESSION TAG	UNP F8UWD6
A	871	HIS	-	EXPRESSION TAG	UNP F8UWD6
A	872	HIS	-	EXPRESSION TAG	UNP F8UWD6
A	873	HIS	-	EXPRESSION TAG	UNP F8UWD6

- Molecule 2 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

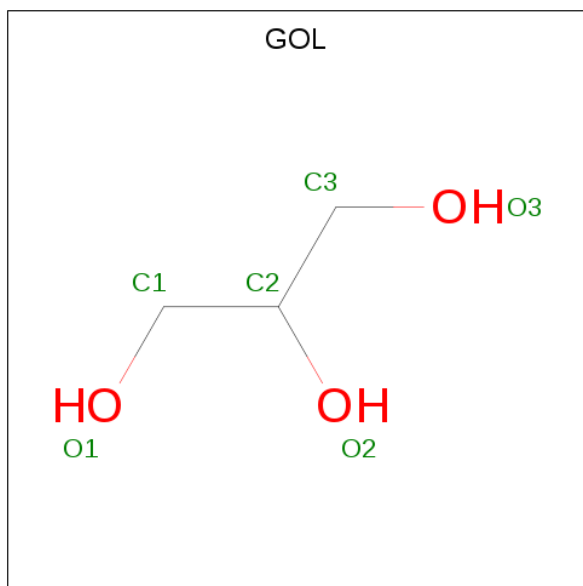
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

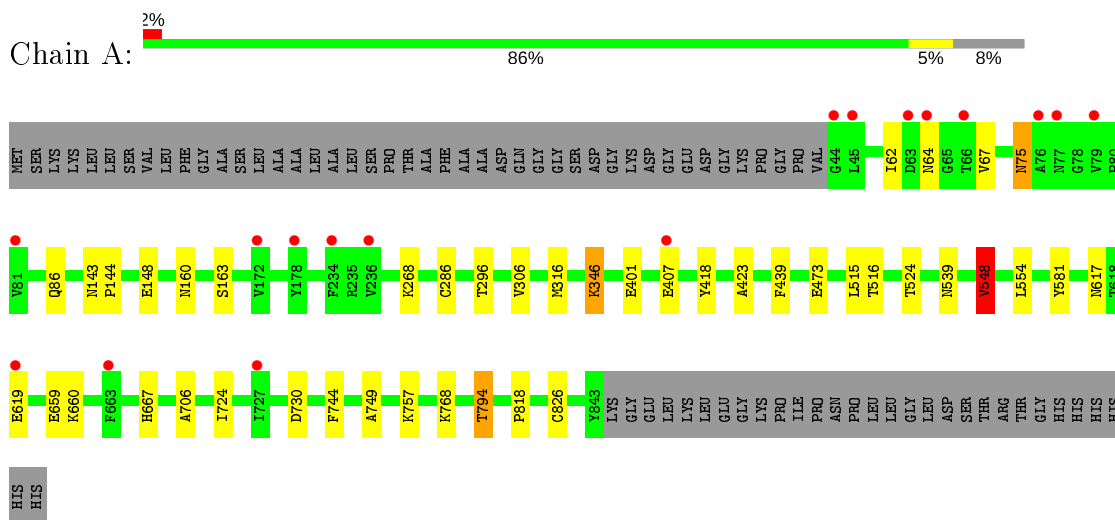
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1318	Total O 1318 1318	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: UndA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.64Å 106.09Å 151.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.91 – 1.76 40.91 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.91-1.76) 99.6 (40.91-1.76)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.144 , 0.177 0.165 , 0.192	Depositor DCC
R_{free} test set	5538 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7814	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: GOL, CA, MG, HEC

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	0.71	1/6151 (0.0%)	0.67	1/8368 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	548	VAL	CB-CG2	-5.51	1.41	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	548	VAL	CB-CA-C	-5.21	101.49	111.40

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	5990	0	5782	43	0
2	A	473	0	331	22	0
3	A	1	0	0	0	0
4	A	2	0	0	0	0
5	A	30	0	40	4	0
6	A	1318	0	0	17	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7814	0	6153	55	1

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 5.

All (55) 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:346:LYS:HD2	6:A:1403:HOH:O	1.57	1.02
1:A:826:CYS:SG	2:A:911:HEC:HAC	1.94	1.01
1:A:794:THR:HG23	6:A:1242:HOH:O	1.60	1.00
1:A:730[A]:ASP:OD1	6:A:1301:HOH:O	1.83	0.97
1:A:86:GLN:HG2	6:A:1272:HOH:O	1.67	0.93
5:A:917:GOL:H11	6:A:1405:HOH:O	1.77	0.82
1:A:286:CYS:SG	2:A:902:HEC:CBC	2.78	0.71
1:A:286:CYS:SG	2:A:902:HEC:C3C	2.78	0.70
1:A:826:CYS:SG	2:A:911:HEC:C3C	2.80	0.69
1:A:794:THR:CG2	6:A:1242:HOH:O	2.28	0.66
1:A:160:ASN:OD1	5:A:918:GOL:H32	2.00	0.61
2:A:902:HEC:HMC1	2:A:902:HEC:HBC3	1.84	0.60
1:A:163[A]:SER:OG	5:A:918:GOL:H31	2.02	0.59
1:A:346:LYS:CD	6:A:1403:HOH:O	2.31	0.58
2:A:910:HEC:HMA3	2:A:910:HEC:HBA1	1.87	0.57
2:A:903:HEC:HMB1	2:A:903:HEC:HBB3	1.87	0.56
1:A:768:LYS:HG3	6:A:1280:HOH:O	2.07	0.55
1:A:757:LYS:HE2	6:A:1278:HOH:O	2.08	0.53
2:A:904:HEC:HMC1	2:A:904:HEC:HBC3	1.89	0.53
2:A:910:HEC:HBB3	2:A:910:HEC:HMB1	1.91	0.53
1:A:826:CYS:HG	2:A:911:HEC:HAC	1.71	0.53
1:A:346:LYS:CE	6:A:1403:HOH:O	2.58	0.52
1:A:659:GLU:OE2	1:A:660[B]:LYS:HE3	2.10	0.52
1:A:524[B]:THR:HG23	1:A:706:ALA:CB	2.40	0.51
1:A:524[B]:THR:HG21	6:A:2033:HOH:O	2.11	0.50
2:A:907:HEC:HBB3	2:A:907:HEC:HMB1	1.93	0.50
1:A:62:ILE:HG12	1:A:67:VAL:HG22	1.94	0.49
1:A:749:ALA:HB2	2:A:910:HEC:HMD2	1.96	0.48
1:A:401:GLU:OE1	6:A:2260:HOH:O	2.20	0.47
1:A:617:ASN:OD1	1:A:619:GLU:HG2	2.15	0.47
1:A:75:ASN:HD22	1:A:75:ASN:C	2.19	0.46
2:A:911:HEC:HBC3	2:A:911:HEC:HMC1	1.97	0.46
1:A:439:PHE:HA	2:A:905:HEC:HMC2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:GLU:OE2	6:A:2297:HOH:O	2.21	0.45
1:A:548:VAL:HG13	1:A:554:LEU:HG	1.98	0.45
1:A:160:ASN:CG	6:A:2002:HOH:O	2.54	0.45
1:A:524[B]:THR:CG2	6:A:2033:HOH:O	2.64	0.45
1:A:286:CYS:CB	2:A:902:HEC:CAC	2.93	0.45
2:A:910:HEC:CMA	2:A:910:HEC:HBA1	2.45	0.44
2:A:905:HEC:HBC3	2:A:905:HEC:HMC1	1.99	0.43
1:A:524[B]:THR:HG23	1:A:706:ALA:HB3	2.01	0.43
1:A:524[B]:THR:CG2	1:A:706:ALA:CB	2.96	0.43
1:A:524[B]:THR:HG23	1:A:706:ALA:HB2	2.01	0.42
1:A:724:ILE:HG21	2:A:909:HEC:HMD2	2.00	0.42
1:A:296:THR:HG21	1:A:316:MET:HA	2.02	0.42
1:A:306:VAL:HG11	2:A:903:HEC:HMD2	2.00	0.42
1:A:524[B]:THR:CG2	1:A:706:ALA:HB3	2.49	0.42
5:A:916:GOL:H11	6:A:2157:HOH:O	2.18	0.41
1:A:744:PHE:CE1	2:A:906:HEC:HBC2	2.56	0.41
1:A:516:THR:HA	1:A:539:ASN:O	2.21	0.41
2:A:910:HEC:HMC1	2:A:910:HEC:HBC3	2.02	0.40
1:A:143:ASN:HA	1:A:144:PRO:HD3	1.93	0.40
1:A:667:HIS:CD2	2:A:908:HEC:ND	2.89	0.40
1:A:346:LYS:NZ	6:A:1403:HOH:O	2.38	0.40
1:A:418:TYR:CE1	1:A:423:ALA:HA	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1417:HOH:O	6:A:2274:HOH:O[4_555]	2.19	0.01

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	809/874 (93%)	783 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	655/700 (94%)	644 (98%)	11 (2%)	60	42

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	75	ASN
1	A	148	GLU
1	A	268	LYS
1	A	346	LYS
1	A	407	GLU
1	A	515	LEU
1	A	548	VAL
1	A	581	TYR
1	A	794	THR
1	A	818	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	89	GLN
1	A	437	HIS
1	A	441	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 3 are monoatomic - leaving 16 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
2	HEC	A	904	1	26,50,50	2.00	4 (15%)	18,82,82	1.86	7 (38%)
2	HEC	A	908	1,4	26,50,50	2.10	6 (23%)	18,82,82	1.92	6 (33%)
5	GOL	A	916	-	5,5,5	0.46	0	5,5,5	0.45	0
2	HEC	A	905	1	26,50,50	2.27	7 (26%)	18,82,82	1.96	5 (27%)
5	GOL	A	915	-	5,5,5	0.31	0	5,5,5	0.70	0
2	HEC	A	911	1	26,50,50	2.02	5 (19%)	18,82,82	2.18	5 (27%)
2	HEC	A	902	1,3	26,50,50	2.03	5 (19%)	18,82,82	2.10	6 (33%)
2	HEC	A	910	1	26,50,50	2.22	7 (26%)	18,82,82	2.28	8 (44%)
2	HEC	A	906	1	26,50,50	2.18	4 (15%)	18,82,82	2.27	7 (38%)
2	HEC	A	901	1	26,50,50	2.43	6 (23%)	18,82,82	2.31	6 (33%)
2	HEC	A	903	1	26,50,50	2.04	6 (23%)	18,82,82	2.45	7 (38%)
2	HEC	A	907	1	26,50,50	2.34	6 (23%)	18,82,82	2.34	5 (27%)
5	GOL	A	917	-	5,5,5	0.53	0	5,5,5	0.50	0
2	HEC	A	909	1	26,50,50	2.21	6 (23%)	18,82,82	2.76	7 (38%)
5	GOL	A	919	-	5,5,5	0.51	0	5,5,5	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	A	918	-	5,5,5	0.49	0	5,5,5	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	A	904	1	-	0/6/54/54	-
2	HEC	A	908	1,4	-	3/6/54/54	-
5	GOL	A	916	-	-	2/4/4/4	-
2	HEC	A	905	1	-	0/6/54/54	-
5	GOL	A	915	-	-	4/4/4/4	-
2	HEC	A	911	1	-	0/6/54/54	-
2	HEC	A	902	1,3	-	0/6/54/54	-
2	HEC	A	910	1	-	3/6/54/54	-
2	HEC	A	906	1	-	0/6/54/54	-
2	HEC	A	901	1	-	0/6/54/54	-
2	HEC	A	903	1	-	0/6/54/54	-
2	HEC	A	907	1	-	0/6/54/54	-
5	GOL	A	917	-	-	0/4/4/4	-
2	HEC	A	909	1	-	0/6/54/54	-
5	GOL	A	919	-	-	2/4/4/4	-
5	GOL	A	918	-	-	2/4/4/4	-

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	HEC	C3B-C2B	-7.79	1.32	1.40
2	A	906	HEC	C3C-C2C	-6.39	1.34	1.40
2	A	907	HEC	C3B-C2B	-6.20	1.34	1.40
2	A	907	HEC	C3C-C2C	-6.18	1.34	1.40
2	A	908	HEC	C3C-C2C	-5.64	1.34	1.40
2	A	906	HEC	C3B-C2B	-5.53	1.35	1.40
2	A	903	HEC	C3B-C2B	-5.36	1.35	1.40
2	A	910	HEC	C3B-C2B	-5.19	1.35	1.40
2	A	909	HEC	C3B-C2B	-5.18	1.35	1.40
2	A	905	HEC	C3C-C2C	-5.13	1.35	1.40
2	A	902	HEC	C3B-C2B	-5.12	1.35	1.40
2	A	909	HEC	C3C-C2C	-5.11	1.35	1.40
2	A	904	HEC	C3B-C2B	-5.10	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	908	HEC	C3B-C2B	-5.07	1.35	1.40
2	A	911	HEC	C3D-C2D	5.04	1.52	1.37
2	A	905	HEC	C3D-C2D	5.04	1.52	1.37
2	A	901	HEC	C3C-C2C	-5.03	1.35	1.40
2	A	905	HEC	C3B-C2B	-4.97	1.35	1.40
2	A	902	HEC	C3C-C2C	-4.88	1.35	1.40
2	A	910	HEC	C3D-C2D	4.85	1.52	1.37
2	A	911	HEC	C3C-C2C	-4.75	1.35	1.40
2	A	904	HEC	C3C-C2C	-4.73	1.35	1.40
2	A	910	HEC	C3C-C2C	-4.69	1.35	1.40
2	A	903	HEC	C3D-C2D	4.52	1.51	1.37
2	A	901	HEC	C3D-C2D	4.44	1.50	1.37
2	A	909	HEC	C3D-C2D	4.40	1.50	1.37
2	A	902	HEC	C3D-C2D	4.31	1.50	1.37
2	A	911	HEC	C3B-C2B	-4.16	1.36	1.40
2	A	903	HEC	C3C-C2C	-4.15	1.36	1.40
2	A	907	HEC	C3D-C2D	3.90	1.49	1.37
2	A	904	HEC	C3D-C2D	3.87	1.49	1.37
2	A	906	HEC	C3D-C2D	3.59	1.48	1.37
2	A	908	HEC	C3D-C2D	3.29	1.47	1.37
2	A	910	HEC	C4D-ND	3.11	1.42	1.36
2	A	905	HEC	CAD-C3D	3.06	1.56	1.52
2	A	910	HEC	CAD-C3D	2.37	1.55	1.52
2	A	903	HEC	CAA-C2A	2.36	1.56	1.52
2	A	901	HEC	CMB-C2B	2.36	1.57	1.51
2	A	909	HEC	CMD-C2D	2.35	1.56	1.51
2	A	908	HEC	CAA-C2A	2.33	1.56	1.52
2	A	902	HEC	C1D-ND	2.33	1.41	1.36
2	A	902	HEC	CMD-C2D	2.31	1.56	1.51
2	A	908	HEC	CMC-C2C	2.29	1.57	1.51
2	A	908	HEC	CBB-CAB	2.28	1.58	1.49
2	A	901	HEC	CBB-CAB	2.20	1.57	1.49
2	A	903	HEC	C1D-ND	2.20	1.40	1.36
2	A	909	HEC	C3B-C4B	2.19	1.47	1.43
2	A	910	HEC	CAA-C2A	2.19	1.56	1.52
2	A	904	HEC	C1D-ND	2.19	1.40	1.36
2	A	906	HEC	CMA-C3A	2.19	1.56	1.51
2	A	909	HEC	CMB-C2B	2.17	1.56	1.51
2	A	905	HEC	CMD-C2D	2.14	1.56	1.51
2	A	911	HEC	CMD-C2D	2.12	1.56	1.51
2	A	911	HEC	C1D-ND	2.11	1.40	1.36
2	A	903	HEC	CAD-C3D	2.08	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	907	HEC	C1B-NB	2.08	1.40	1.36
2	A	907	HEC	CBB-CAB	2.07	1.57	1.49
2	A	907	HEC	C1D-ND	2.06	1.40	1.36
2	A	905	HEC	C1D-ND	2.05	1.40	1.36
2	A	901	HEC	C1D-ND	2.05	1.40	1.36
2	A	910	HEC	CMC-C2C	2.04	1.56	1.51
2	A	905	HEC	C3B-C4B	2.02	1.46	1.43

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	909	HEC	CMC-C2C-C1C	-5.90	119.39	128.46
2	A	907	HEC	CMC-C2C-C3C	5.61	132.42	125.82
2	A	907	HEC	CMC-C2C-C1C	-5.36	120.23	128.46
2	A	903	HEC	CAD-CBD-CGD	-5.17	104.00	112.67
2	A	911	HEC	CMC-C2C-C1C	-4.97	120.83	128.46
2	A	909	HEC	CBA-CAA-C2A	-4.81	103.61	112.48
2	A	901	HEC	CMC-C2C-C1C	-4.80	121.08	128.46
2	A	901	HEC	CMC-C2C-C3C	4.72	131.37	125.82
2	A	906	HEC	CMB-C2B-C1B	-4.70	121.24	128.46
2	A	909	HEC	CMC-C2C-C3C	4.68	131.32	125.82
2	A	903	HEC	CMC-C2C-C1C	-4.65	121.31	128.46
2	A	909	HEC	CMB-C2B-C1B	-4.58	121.43	128.46
2	A	910	HEC	CBA-CAA-C2A	-4.19	104.76	112.48
2	A	906	HEC	CMB-C2B-C3B	4.14	130.69	125.82
2	A	901	HEC	CBA-CAA-C2A	-4.07	104.98	112.48
2	A	911	HEC	CBA-CAA-C2A	-3.96	105.18	112.48
2	A	903	HEC	C1D-C2D-C3D	-3.90	104.28	107.00
2	A	902	HEC	CMC-C2C-C3C	3.90	130.41	125.82
2	A	910	HEC	CAA-CBA-CGA	-3.83	106.25	112.67
2	A	902	HEC	CMB-C2B-C1B	-3.79	122.64	128.46
2	A	905	HEC	CMC-C2C-C1C	-3.77	122.67	128.46
2	A	910	HEC	CMC-C2C-C1C	-3.71	122.77	128.46
2	A	911	HEC	CMC-C2C-C3C	3.65	130.11	125.82
2	A	902	HEC	CMC-C2C-C1C	-3.63	122.88	128.46
2	A	906	HEC	CBD-CAD-C3D	-3.58	105.89	112.49
2	A	904	HEC	CBD-CAD-C3D	-3.49	106.05	112.49
2	A	906	HEC	CMC-C2C-C3C	3.46	129.88	125.82
2	A	908	HEC	CMA-C3A-C2A	3.43	131.41	124.94
2	A	901	HEC	CBD-CAD-C3D	-3.40	106.21	112.49
2	A	904	HEC	CMC-C2C-C1C	-3.34	123.33	128.46
2	A	908	HEC	CMB-C2B-C1B	-3.30	123.40	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	910	HEC	CBD-CAD-C3D	-3.27	106.45	112.49
2	A	903	HEC	CMB-C2B-C1B	-3.18	123.58	128.46
2	A	906	HEC	CMC-C2C-C1C	-3.18	123.58	128.46
2	A	905	HEC	CMB-C2B-C1B	-3.13	123.65	128.46
2	A	907	HEC	C1D-C2D-C3D	-3.11	104.83	107.00
2	A	908	HEC	C1D-C2D-C3D	-3.07	104.86	107.00
2	A	907	HEC	CMB-C2B-C1B	-3.06	123.76	128.46
2	A	909	HEC	CMB-C2B-C3B	3.06	129.42	125.82
2	A	910	HEC	CAD-CBD-CGD	-3.04	107.56	112.67
2	A	902	HEC	CBD-CAD-C3D	-2.98	106.98	112.49
2	A	903	HEC	CBA-CAA-C2A	-2.95	107.04	112.48
2	A	905	HEC	CMB-C2B-C3B	2.81	129.13	125.82
2	A	902	HEC	C1D-C2D-C3D	-2.79	105.06	107.00
2	A	903	HEC	CMC-C2C-C3C	2.77	129.08	125.82
2	A	904	HEC	CMB-C2B-C1B	-2.70	124.31	128.46
2	A	901	HEC	CMB-C2B-C1B	-2.69	124.34	128.46
2	A	911	HEC	CMB-C2B-C1B	-2.68	124.35	128.46
2	A	910	HEC	CMC-C2C-C3C	2.64	128.93	125.82
2	A	906	HEC	CAA-CBA-CGA	-2.62	108.28	112.67
2	A	905	HEC	CMC-C2C-C3C	2.58	128.85	125.82
2	A	905	HEC	CAA-CBA-CGA	-2.56	108.38	112.67
2	A	901	HEC	C1D-C2D-C3D	-2.54	105.23	107.00
2	A	902	HEC	CMB-C2B-C3B	2.53	128.79	125.82
2	A	910	HEC	CMA-C3A-C2A	2.39	129.44	124.94
2	A	907	HEC	CBD-CAD-C3D	-2.28	108.29	112.49
2	A	909	HEC	CBD-CAD-C3D	-2.27	108.29	112.49
2	A	910	HEC	C3C-C4C-NC	-2.27	106.66	110.94
2	A	911	HEC	C1D-C2D-C3D	-2.25	105.43	107.00
2	A	904	HEC	CAD-CBD-CGD	-2.25	108.90	112.67
2	A	904	HEC	C4B-C3B-C2B	2.24	108.77	106.35
2	A	908	HEC	CMB-C2B-C3B	2.21	128.41	125.82
2	A	908	HEC	CMD-C2D-C3D	2.10	128.91	124.94
2	A	904	HEC	CMB-C2B-C3B	2.06	128.24	125.82
2	A	908	HEC	CAD-CBD-CGD	2.05	116.12	112.67
2	A	909	HEC	C3B-C4B-NB	-2.05	107.08	110.94
2	A	904	HEC	C1D-C2D-C3D	-2.03	105.58	107.00
2	A	903	HEC	CMA-C3A-C2A	2.01	128.74	124.94
2	A	906	HEC	C4C-C3C-C2C	2.00	108.51	106.35

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	908	HEC	C1A-C2A-CAA-CBA
2	A	908	HEC	C3A-C2A-CAA-CBA
5	A	915	GOL	O1-C1-C2-C3
5	A	915	GOL	O2-C2-C3-O3
2	A	910	HEC	C1A-C2A-CAA-CBA
2	A	910	HEC	C3A-C2A-CAA-CBA
2	A	910	HEC	C2A-CAA-CBA-CGA
5	A	916	GOL	C1-C2-C3-O3
5	A	915	GOL	C1-C2-C3-O3
5	A	919	GOL	C1-C2-C3-O3
5	A	918	GOL	C1-C2-C3-O3
5	A	915	GOL	O1-C1-C2-O2
5	A	918	GOL	O2-C2-C3-O3
5	A	916	GOL	O2-C2-C3-O3
5	A	919	GOL	O2-C2-C3-O3
2	A	908	HEC	C2D-C3D-CAD-CBD

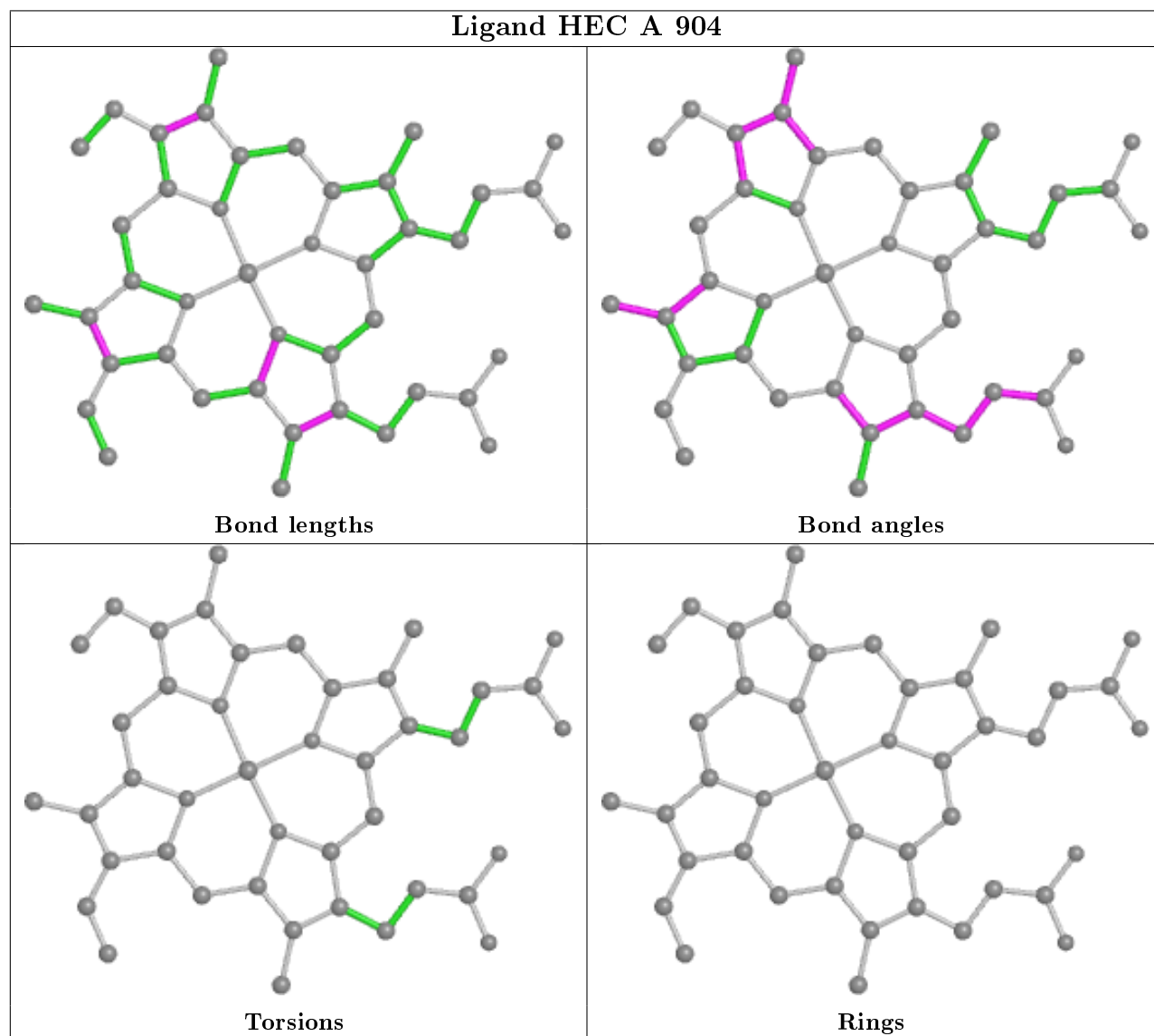
There are no ring outliers.

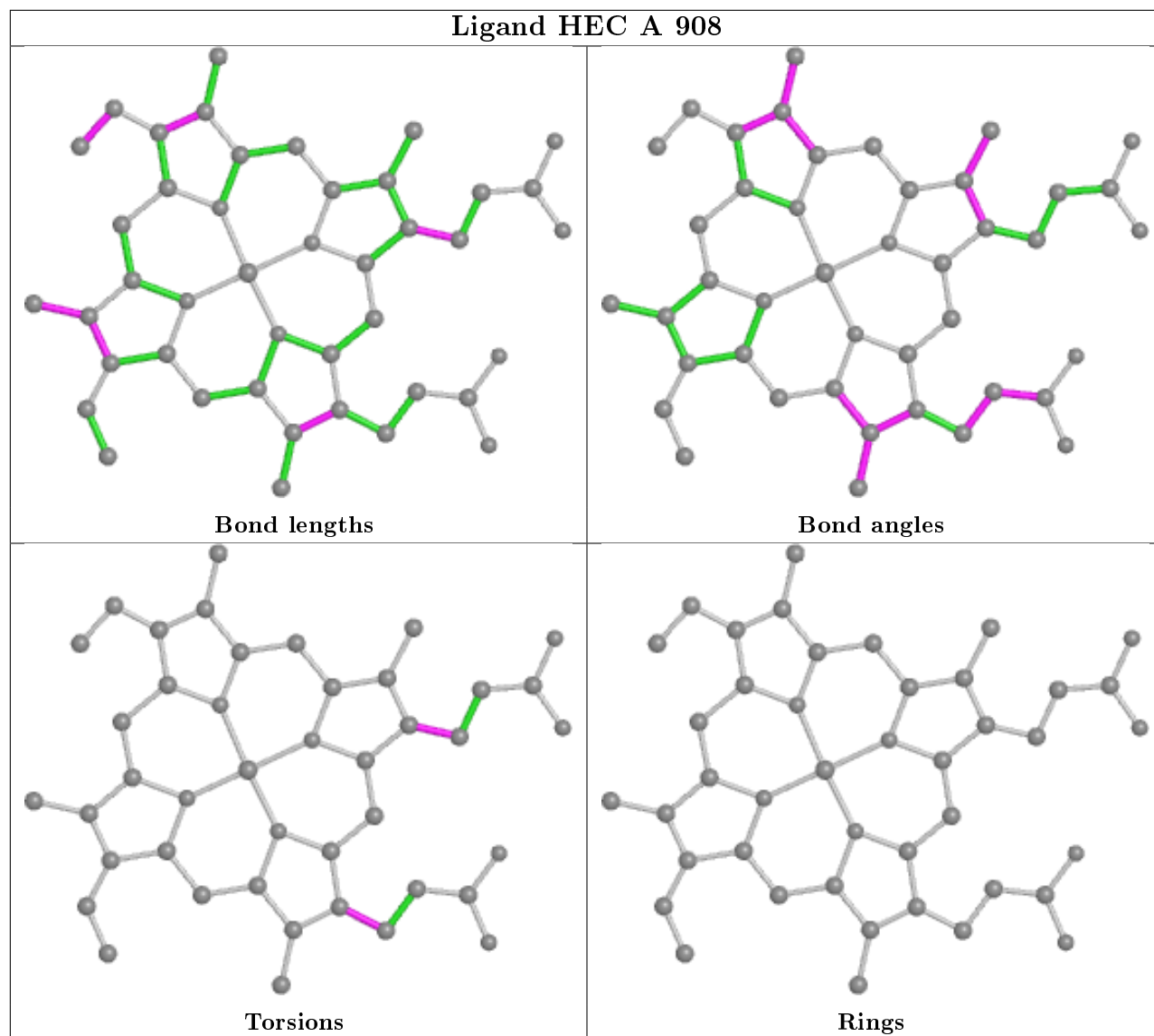
13 monomers are involved in 26 short contacts:

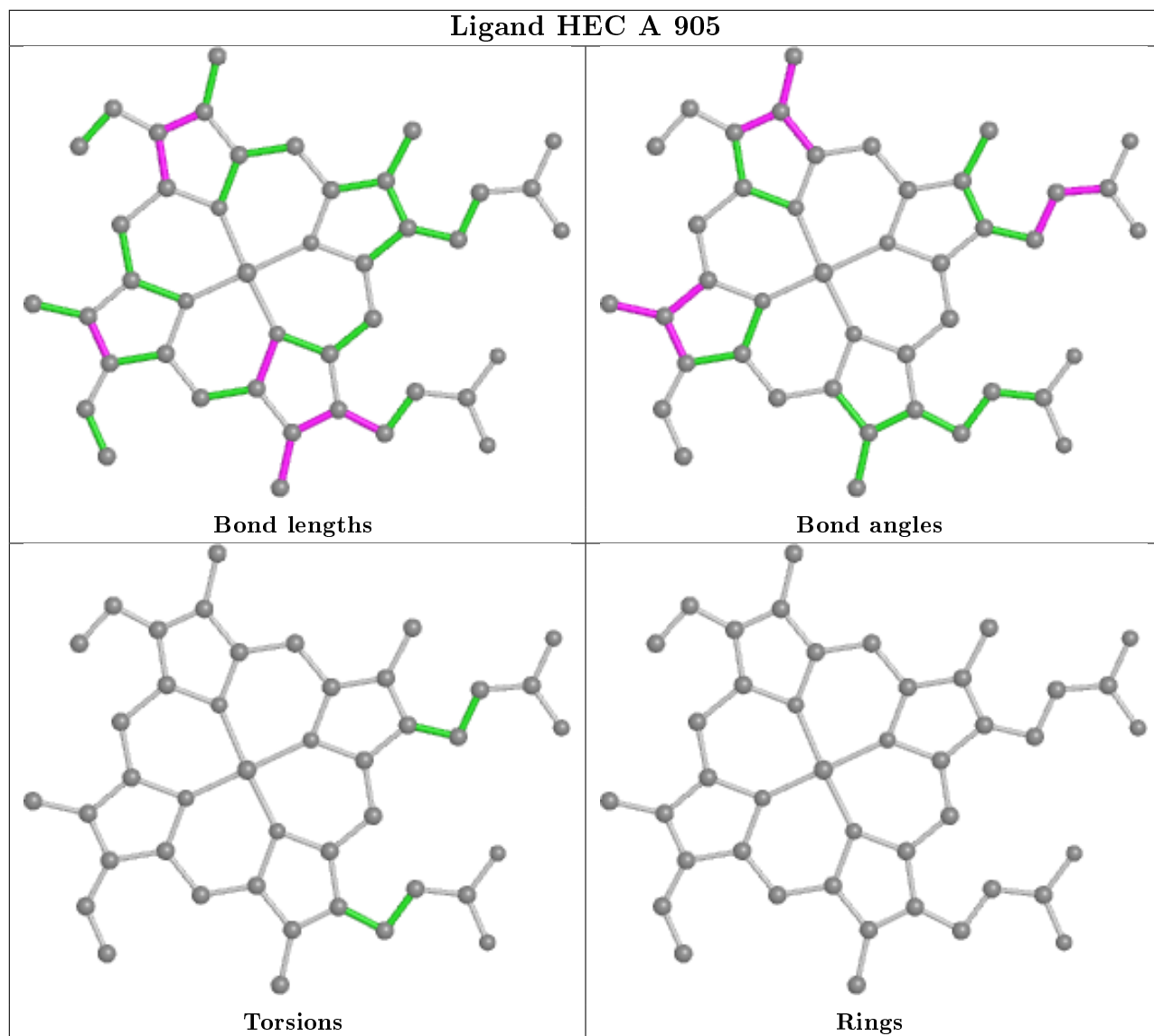
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	904	HEC	1	0
2	A	908	HEC	1	0
5	A	916	GOL	1	0
2	A	905	HEC	2	0
2	A	911	HEC	4	0
2	A	902	HEC	4	0
2	A	910	HEC	5	0
2	A	906	HEC	1	0
2	A	903	HEC	2	0
2	A	907	HEC	1	0
5	A	917	GOL	1	0
2	A	909	HEC	1	0
5	A	918	GOL	2	0

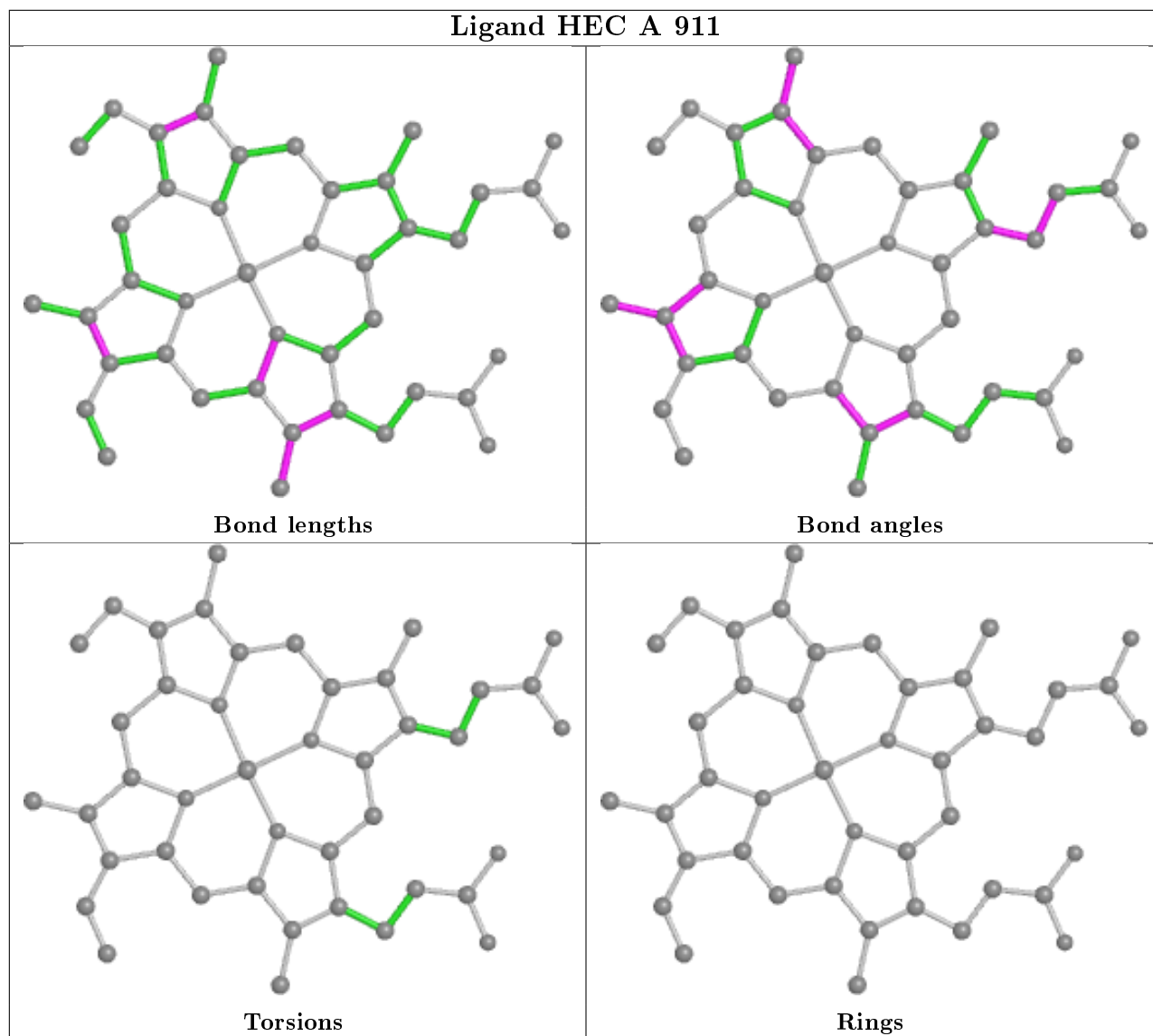
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

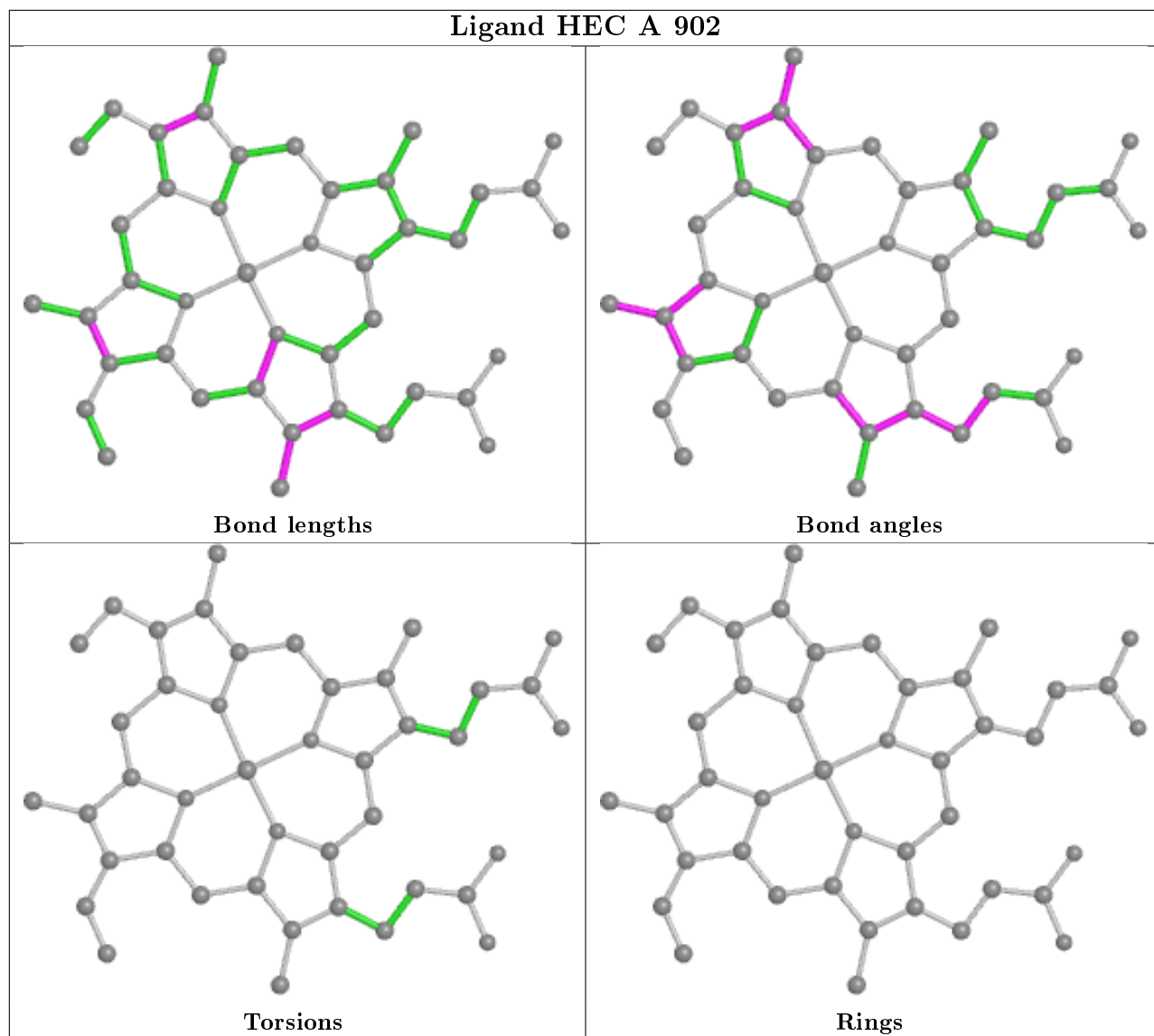
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

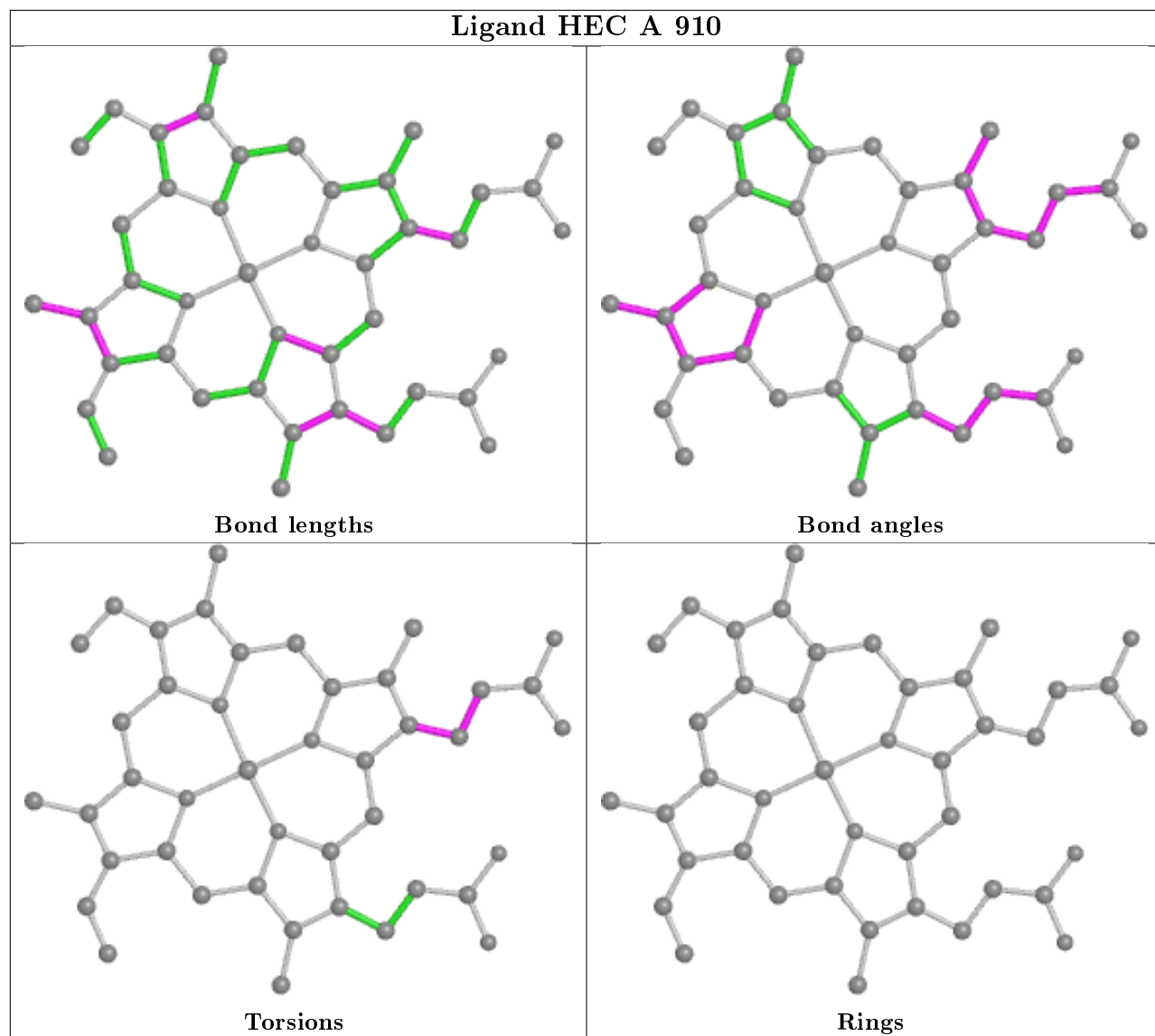


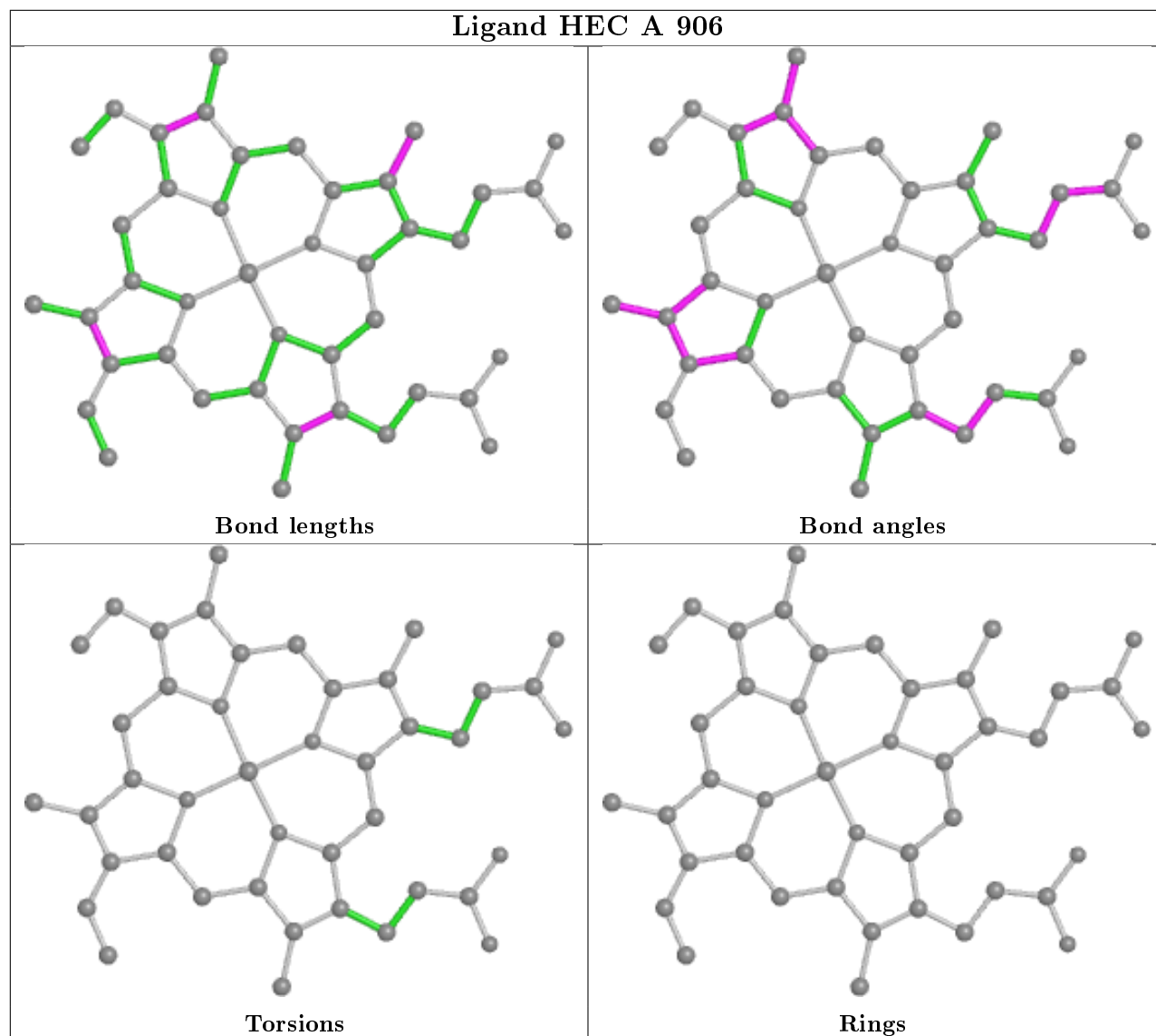


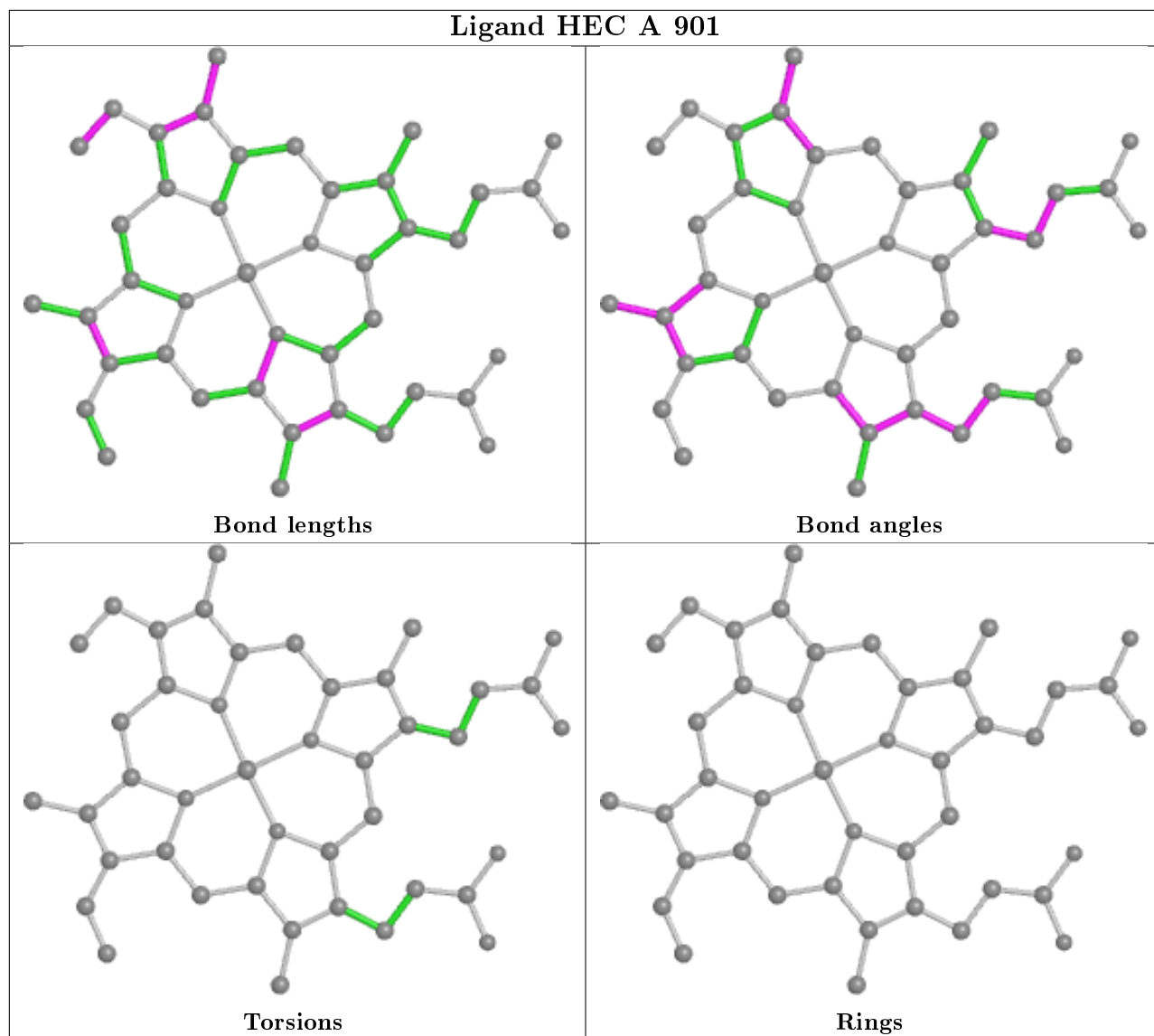


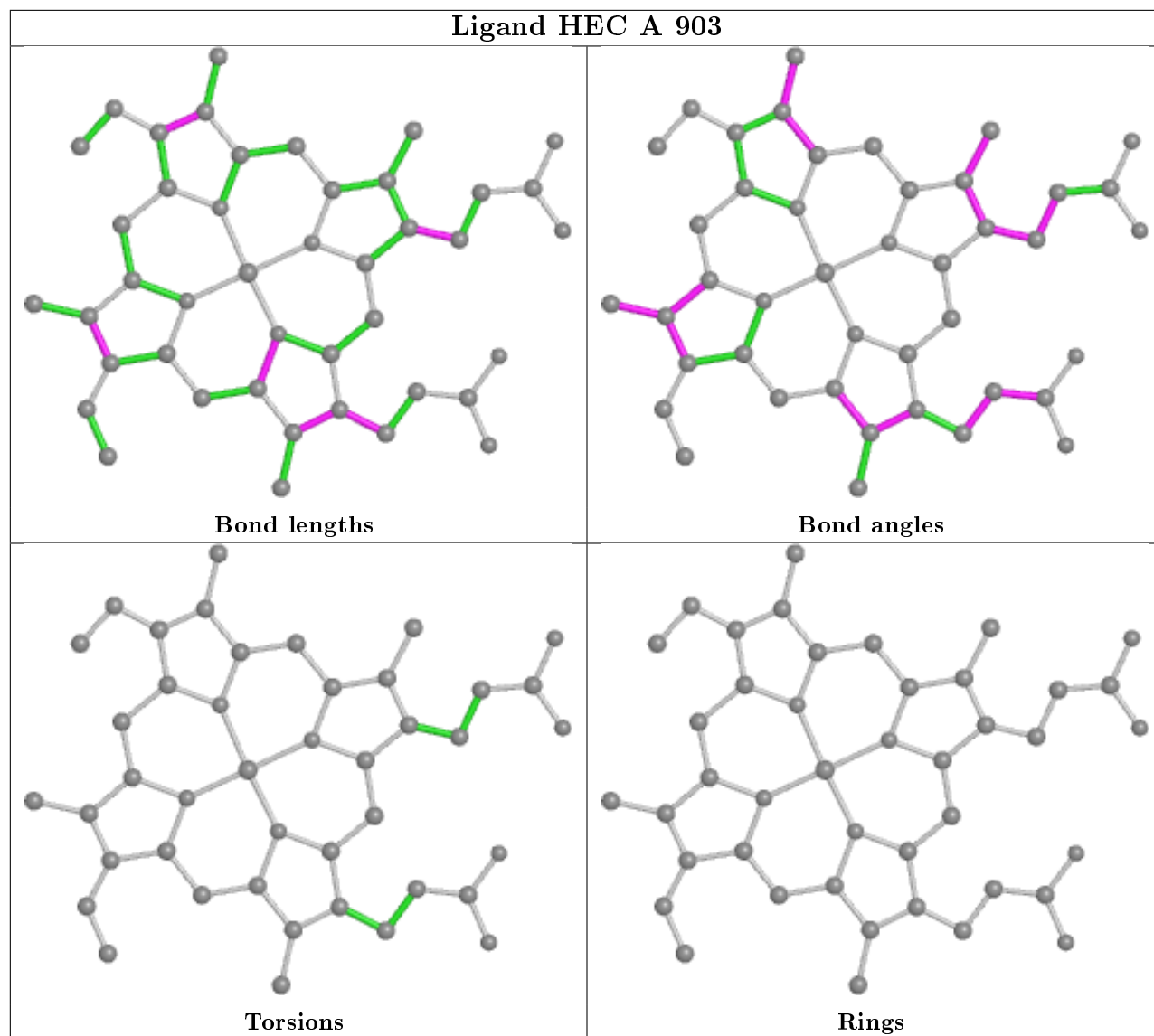


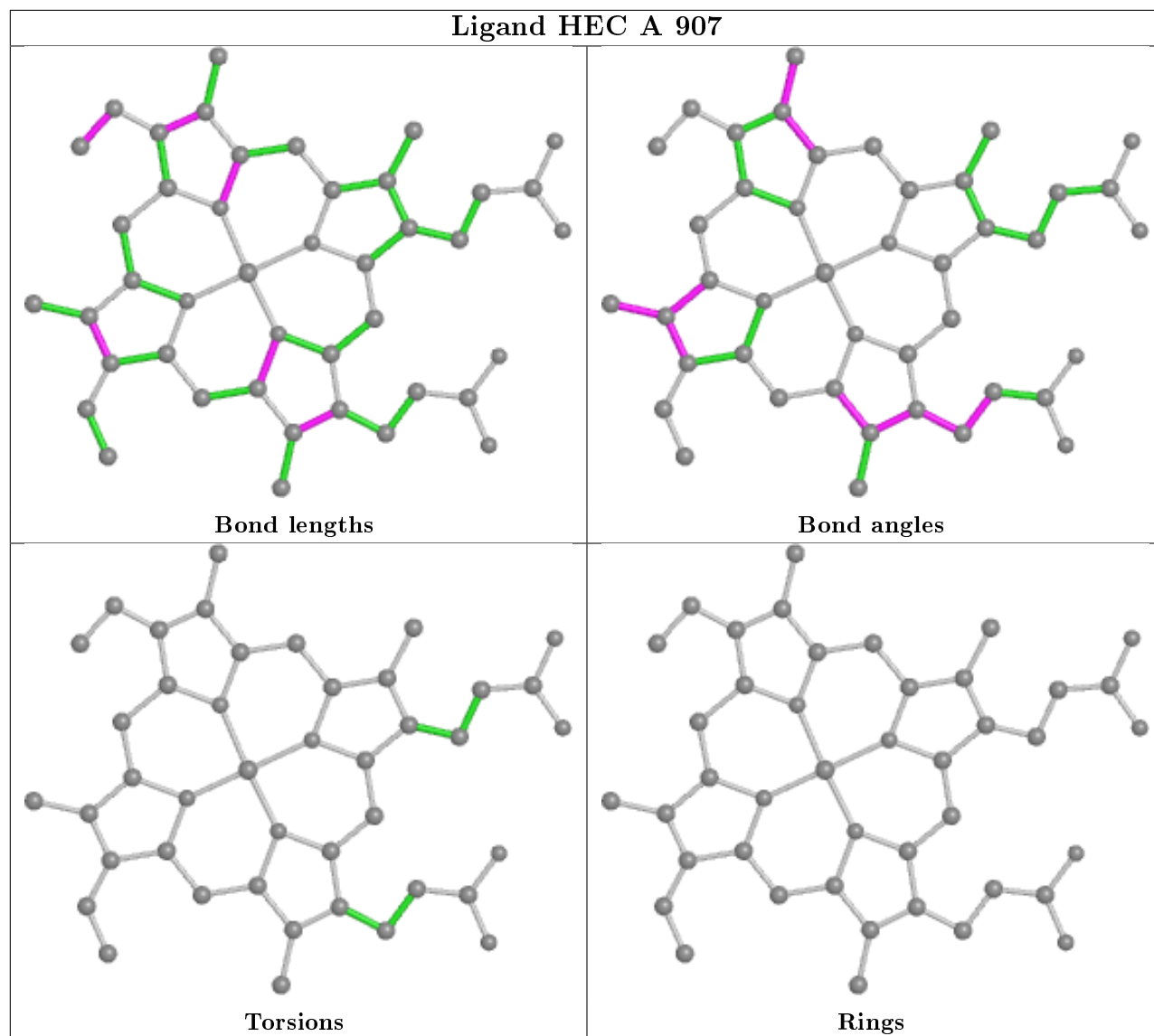


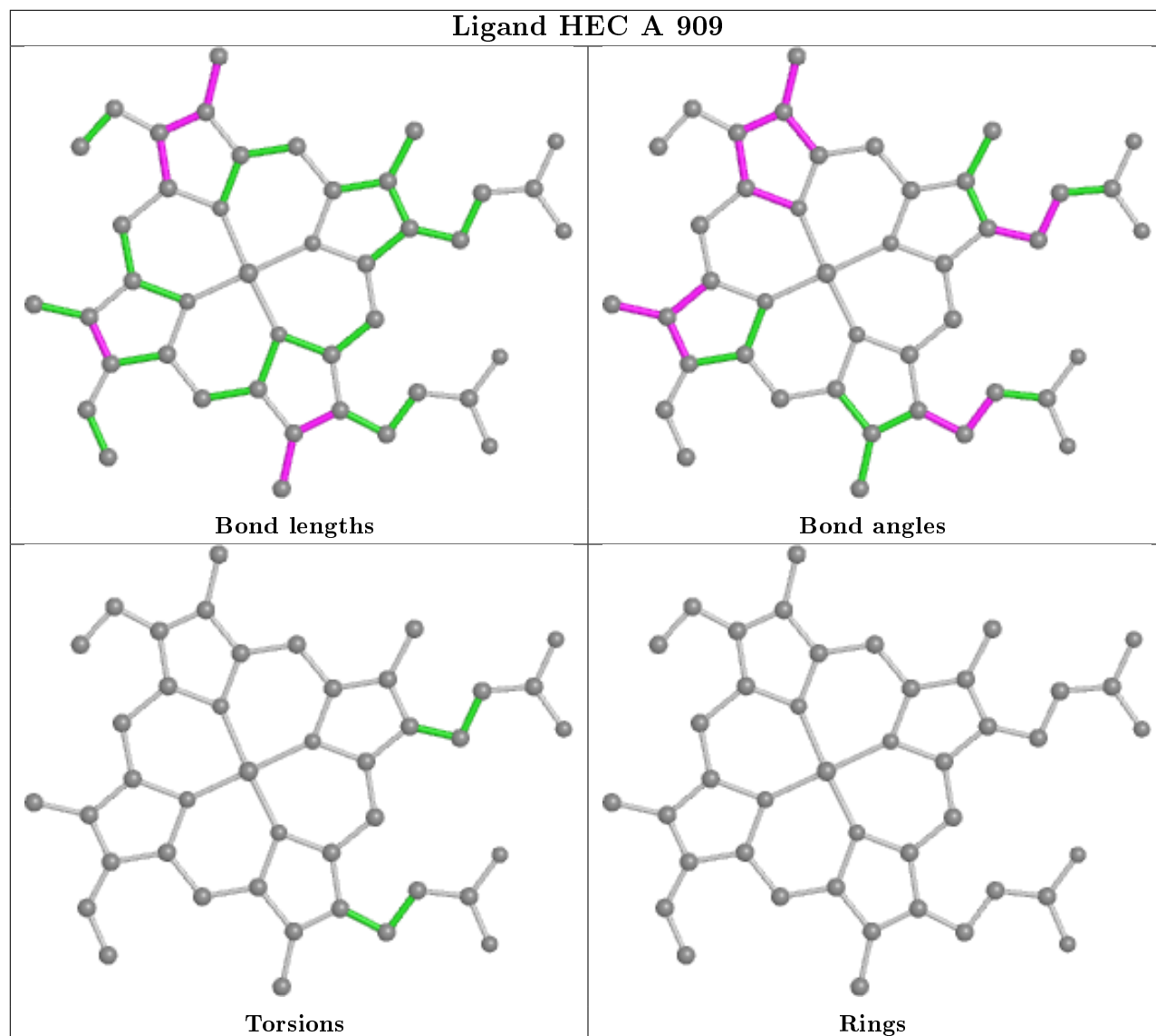












5.7 Other polymers [\(i\)](#)

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, 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	800/874 (91%)	0.11	17 (2%) 63 71	7, 19, 39, 58	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	77	ASN	3.3
1	A	79	VAL	3.0
1	A	64	ASN	2.8
1	A	236	VAL	2.7
1	A	76	ALA	2.6
1	A	81	VAL	2.5
1	A	663	PHE	2.5
1	A	44	GLY	2.5
1	A	172	VAL	2.4
1	A	63	ASP	2.4
1	A	407	GLU	2.2
1	A	234	PHE	2.1
1	A	727	ILE	2.1
1	A	178	TYR	2.1
1	A	66	THR	2.0
1	A	619	GLU	2.0
1	A	45	LEU	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 carbohydrates in this entry.

6.4 Ligands

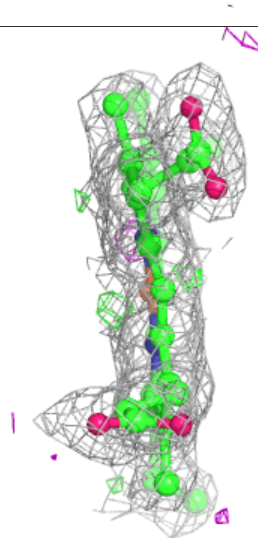
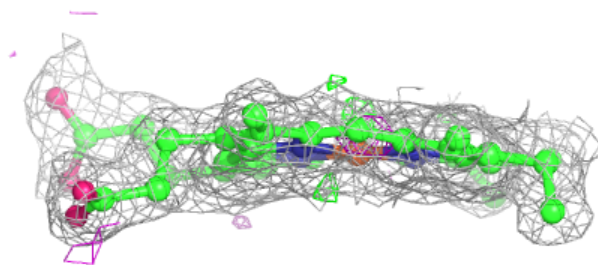
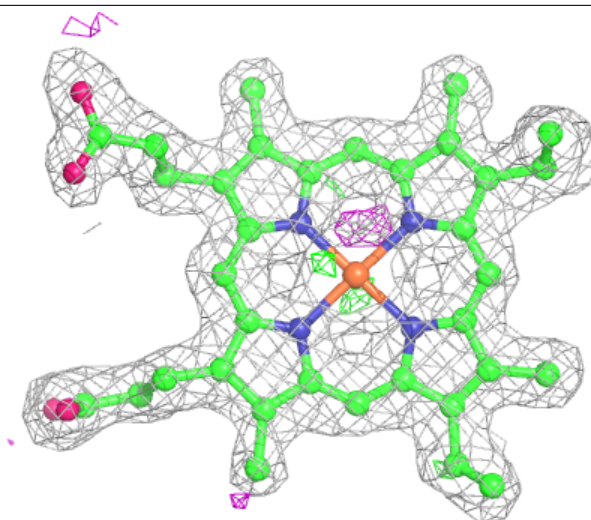
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	A	916	6/6	0.79	0.21	37,41,43,49	0
5	GOL	A	918	6/6	0.82	0.16	49,53,56,60	0
5	GOL	A	917	6/6	0.92	0.17	39,45,46,47	0
5	GOL	A	915	6/6	0.93	0.13	33,36,42,43	0
2	HEC	A	911	43/43	0.96	0.13	19,25,40,50	0
5	GOL	A	919	6/6	0.96	0.12	30,41,42,45	0
2	HEC	A	910	43/43	0.96	0.11	12,20,47,56	0
2	HEC	A	905	43/43	0.97	0.10	14,18,24,26	0
2	HEC	A	902	43/43	0.98	0.14	13,16,24,34	0
2	HEC	A	909	43/43	0.98	0.10	9,12,15,19	0
2	HEC	A	904	43/43	0.98	0.09	9,13,18,24	0
2	HEC	A	903	43/43	0.98	0.11	10,13,16,23	0
4	MG	A	914	1/1	0.99	0.06	13,13,13,13	0
2	HEC	A	907	43/43	0.99	0.11	5,9,12,13	0
2	HEC	A	908	43/43	0.99	0.14	5,8,10,15	0
2	HEC	A	906	43/43	0.99	0.15	7,9,12,14	0
2	HEC	A	901	43/43	0.99	0.13	8,12,27,32	0
3	CA	A	912	1/1	0.99	0.12	20,20,20,20	0
4	MG	A	913	1/1	1.00	0.12	10,10,10,10	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.

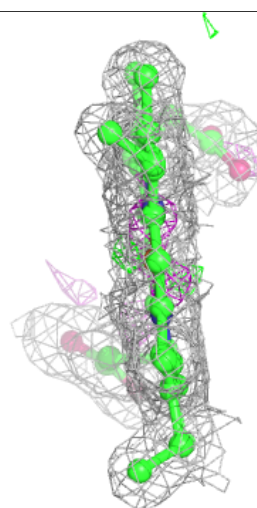
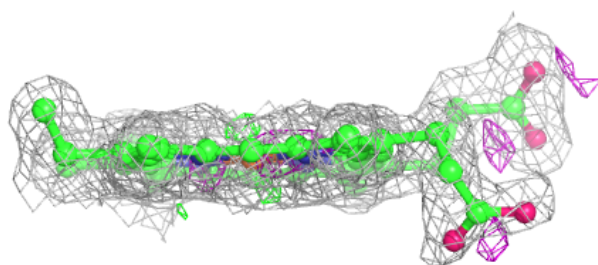
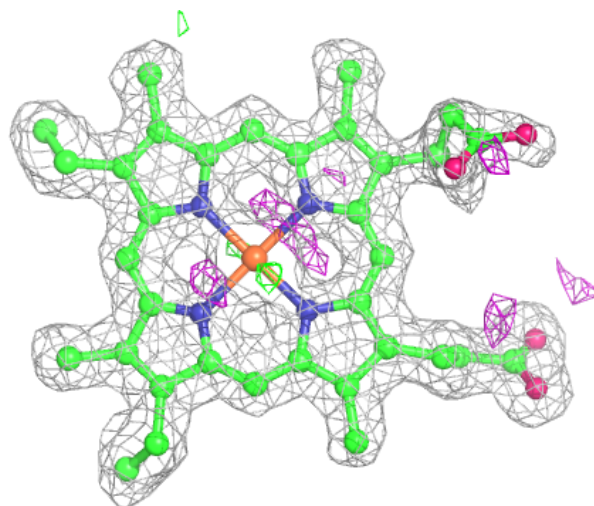
Electron density around HEC A 911:

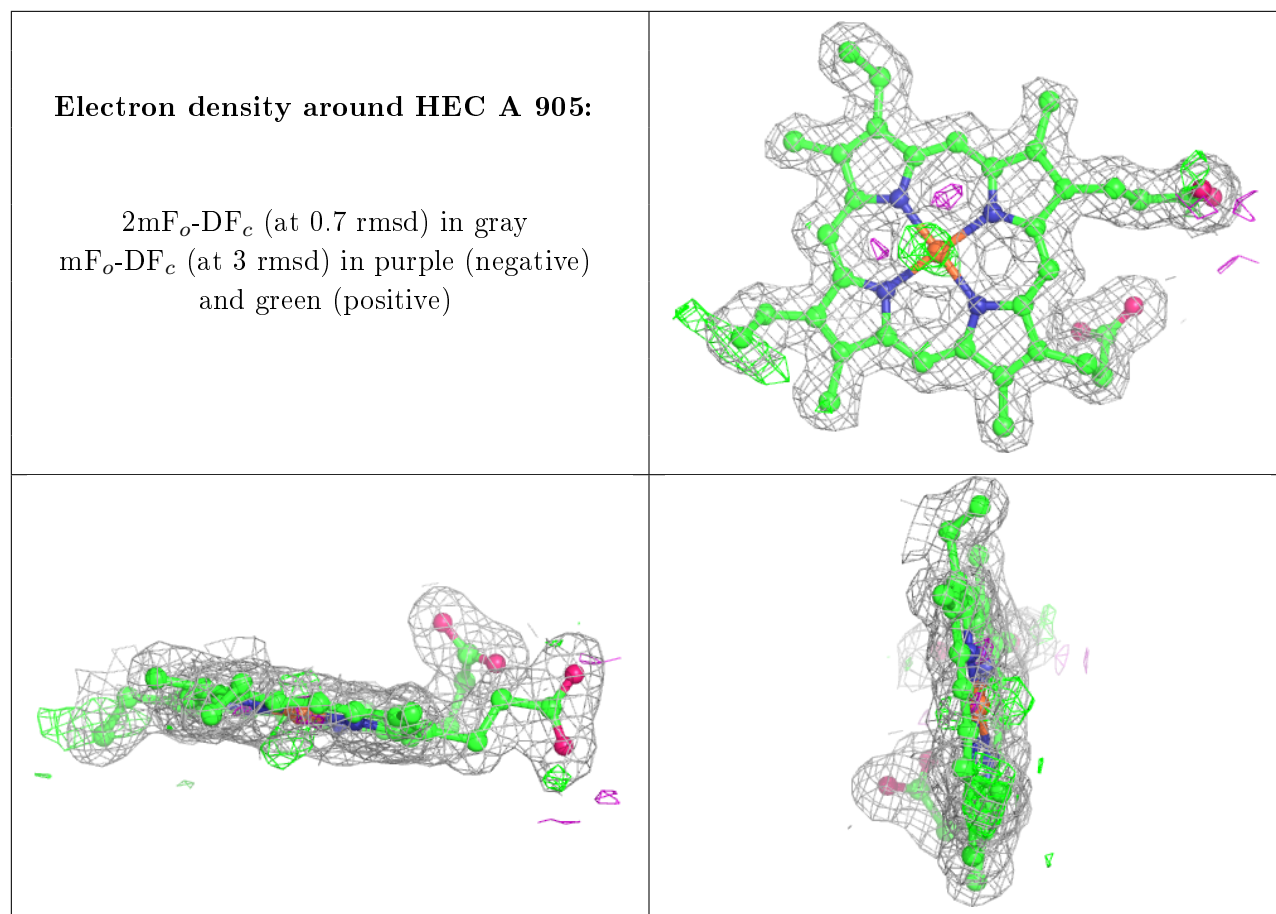
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC A 910:

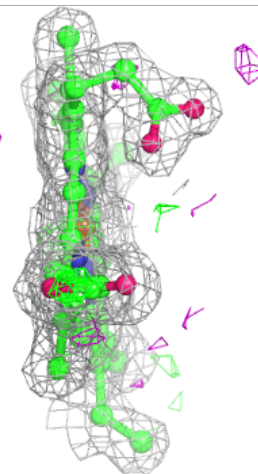
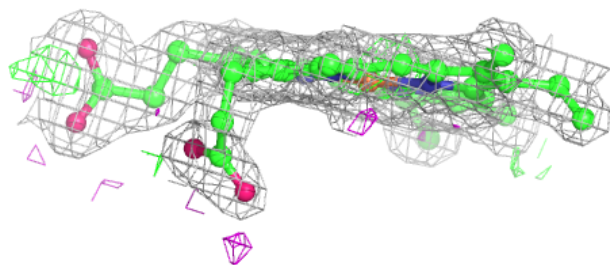
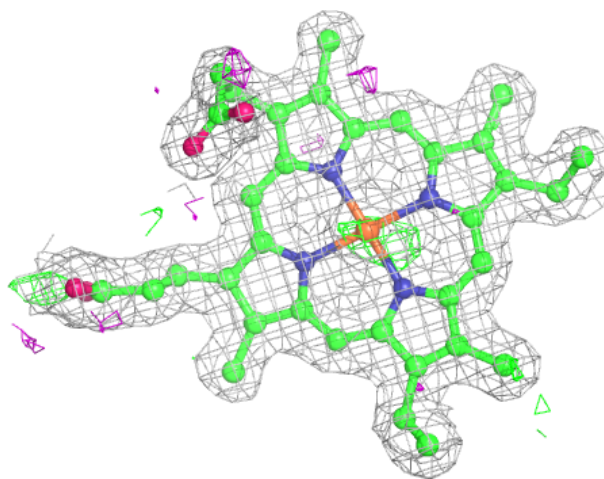
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

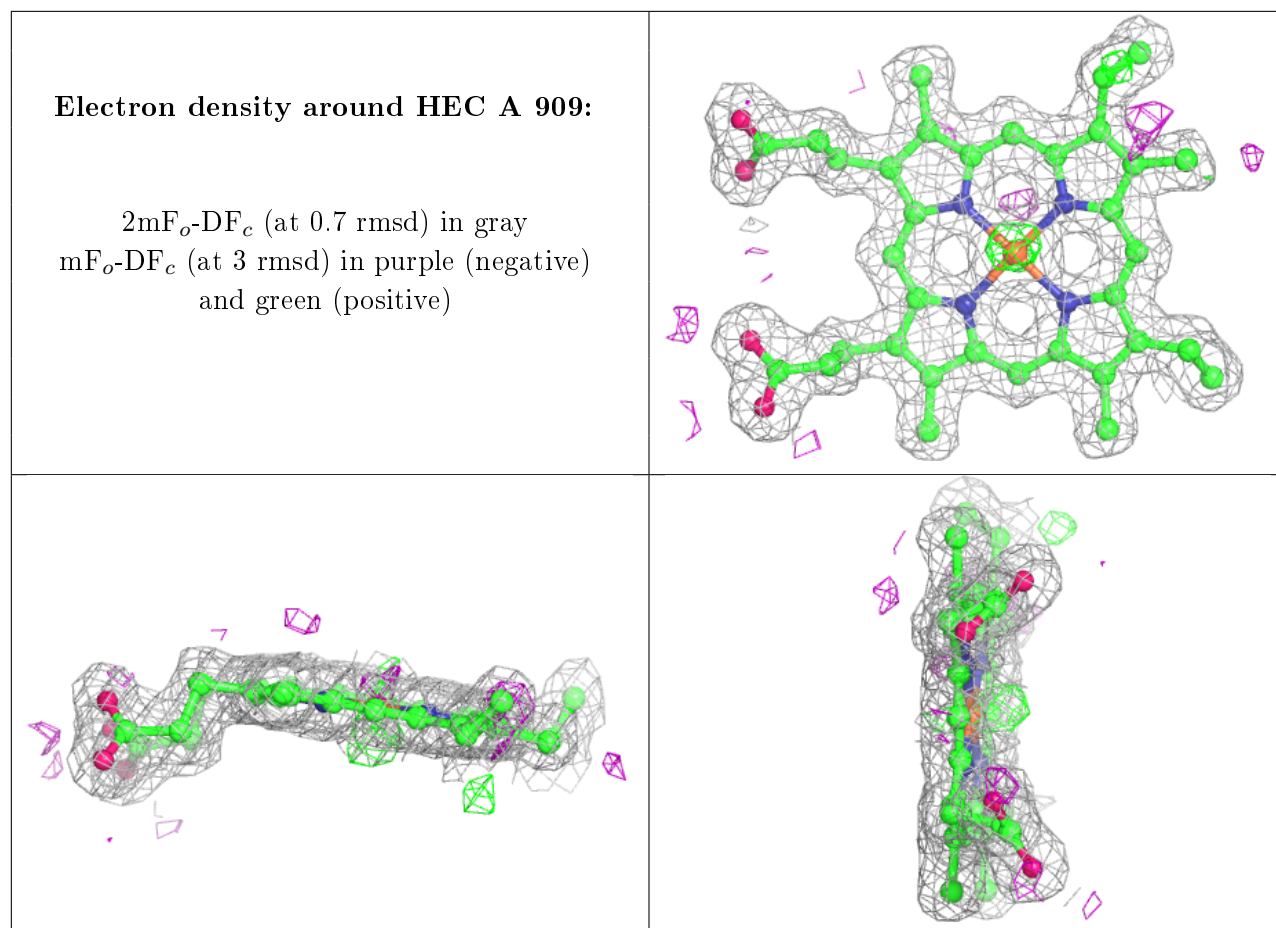




Electron density around HEC A 902:

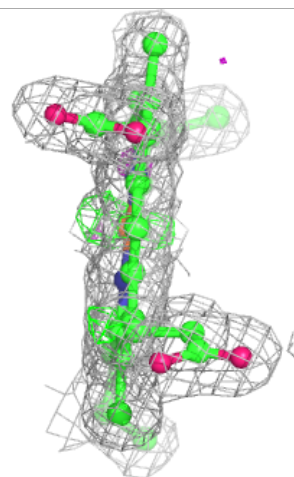
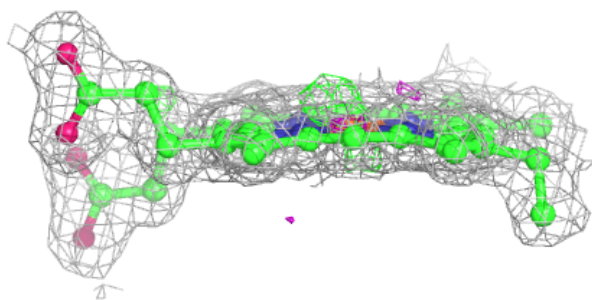
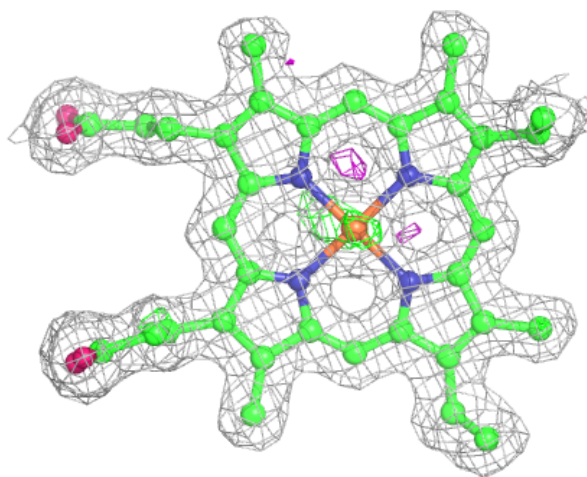
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





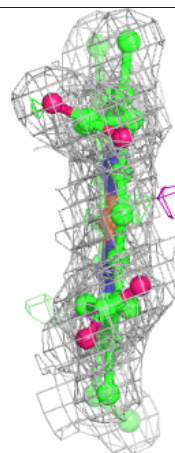
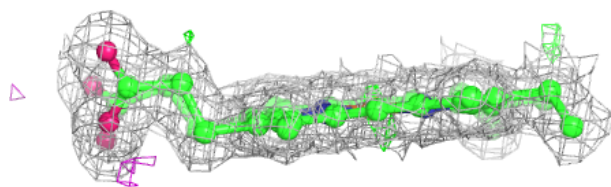
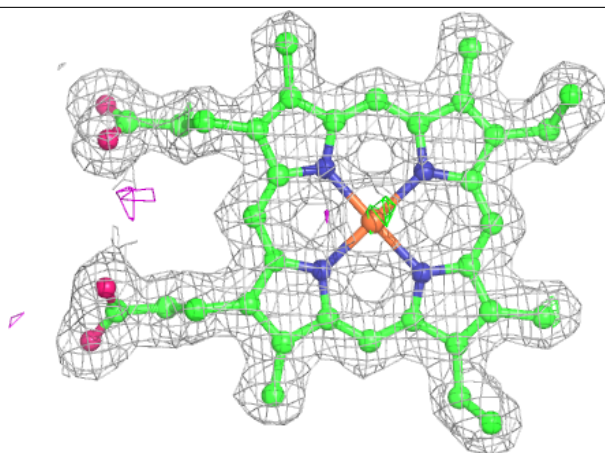
Electron density around HEC A 904:

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



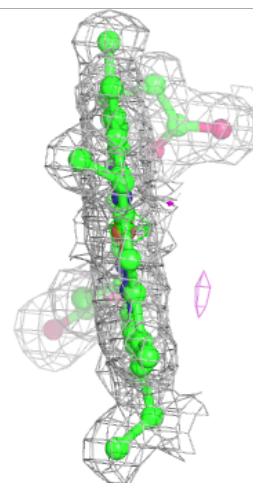
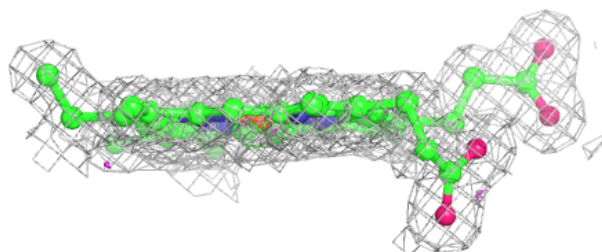
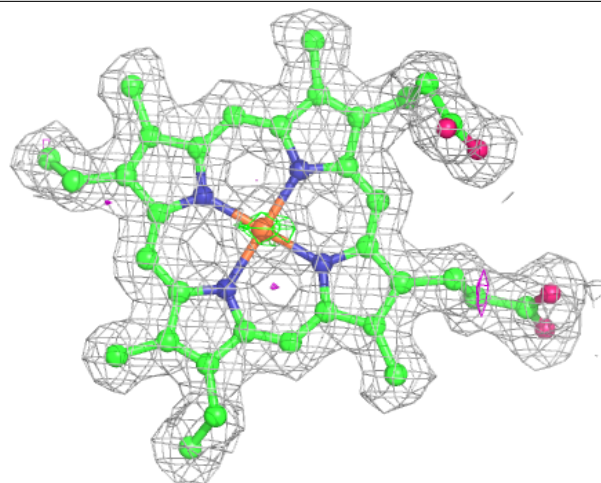
Electron density around HEC A 903:

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



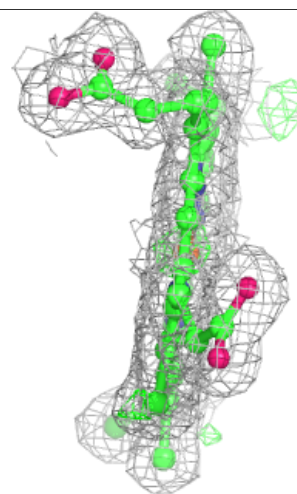
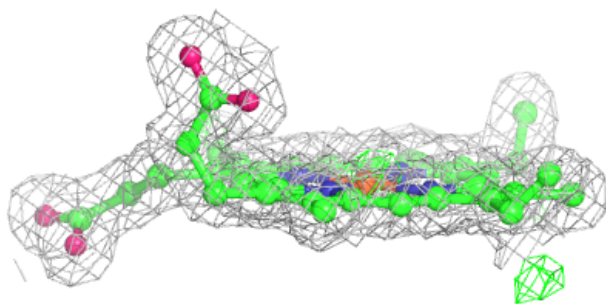
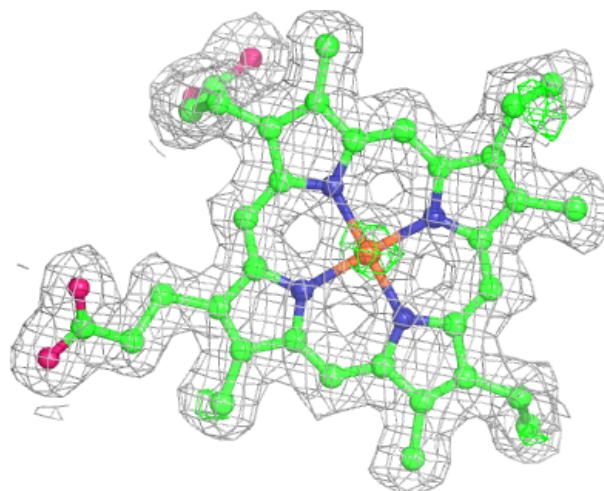
Electron density around HEC A 907:

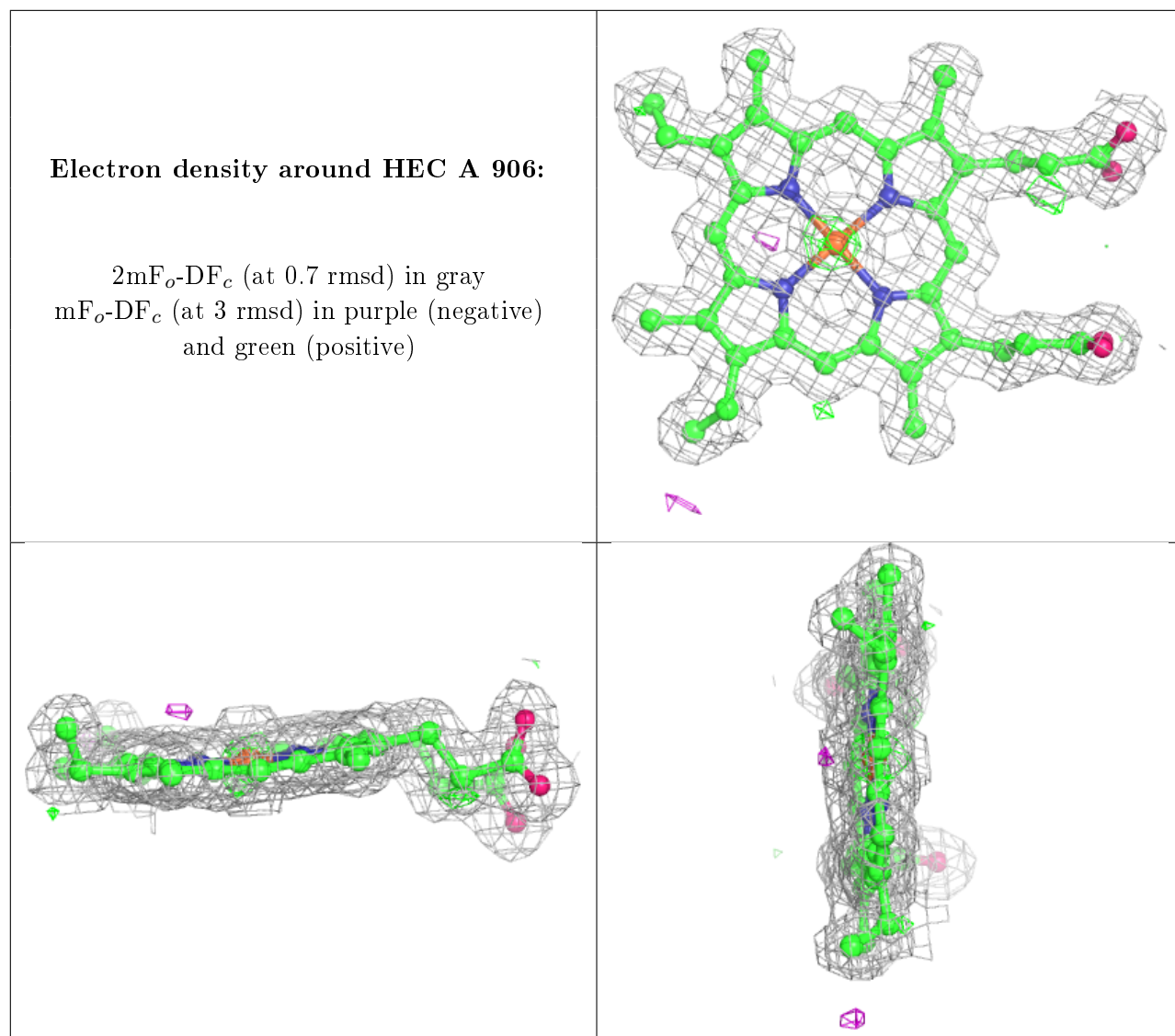
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

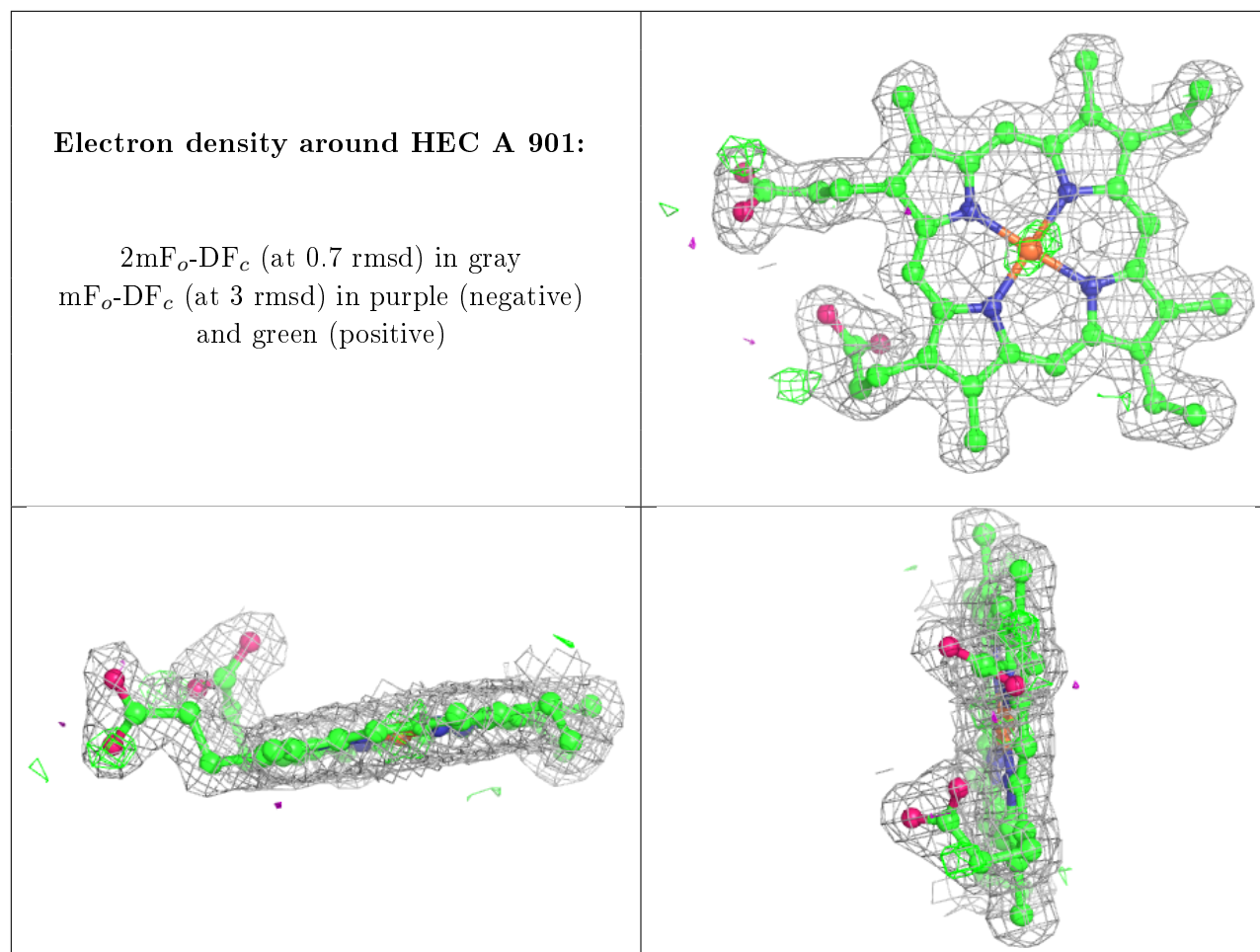


Electron density around HEC A 908:

$2mF_o-DF_c$ (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.