



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:29 AM UTC

PDB ID : 4FA4 / pdb\_00004fa4  
Title : Crystal Structure of WT MauG in Complex with Pre-Methylamine Dehydrogenase Aged 10 Days  
Authors : Yukl, E.T.; Wilmot, C.M.  
Deposited on : 2012-05-21  
Resolution : 2.14 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

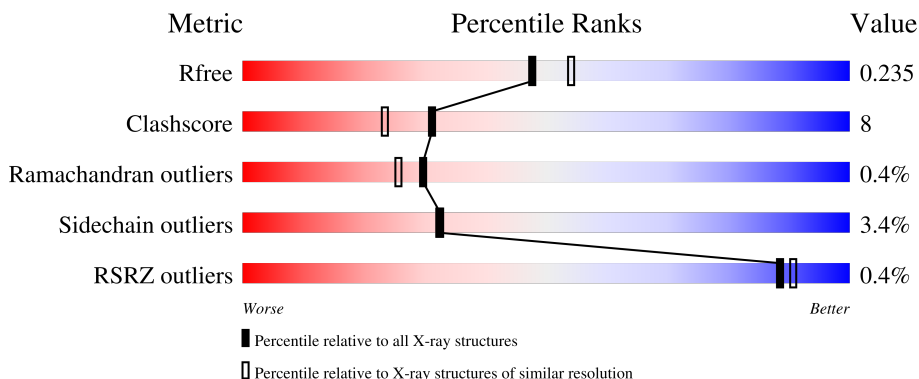
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

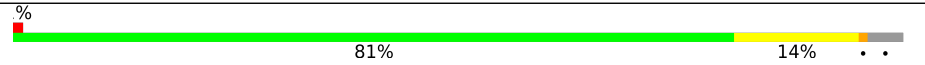
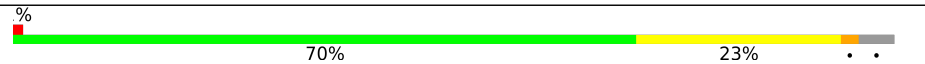
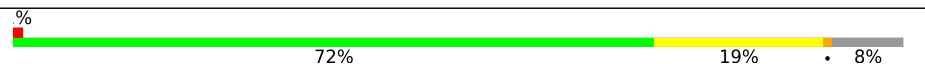
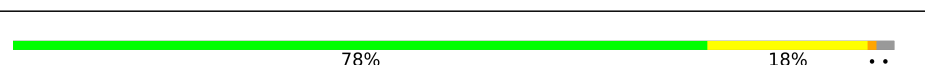
The reported resolution of this entry is 2.14 Å.

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))
$R_{free}$	180053	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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

Mol	Chain	Length	Quality of chain
1	A	373	
1	B	373	
2	C	137	
2	E	137	
3	D	385	

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Mol	Chain	Length	Quality of chain
3	F	385	 81% 15% ..

## 2 Entry composition i

There are 11 unique types of molecules in this entry. The entry contains 14775 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 Methylamine utilization protein MauG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	354	2813	1752	514	536	11	0	7	0
1	B	359	2781	1733	502	535	11	0	1	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	368	HIS	-	expression tag	UNP Q51658
A	369	HIS	-	expression tag	UNP Q51658
A	370	HIS	-	expression tag	UNP Q51658
A	371	HIS	-	expression tag	UNP Q51658
A	372	HIS	-	expression tag	UNP Q51658
A	373	HIS	-	expression tag	UNP Q51658
B	368	HIS	-	expression tag	UNP Q51658
B	369	HIS	-	expression tag	UNP Q51658
B	370	HIS	-	expression tag	UNP Q51658
B	371	HIS	-	expression tag	UNP Q51658
B	372	HIS	-	expression tag	UNP Q51658
B	373	HIS	-	expression tag	UNP Q51658

- Molecule 2 is a protein called Methylamine dehydrogenase light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	131	1017	628	179	196	14	0	1	0
2	E	126	973	601	163	194	15	0	3	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	132	HIS	-	expression tag	UNP P22619
C	133	HIS	-	expression tag	UNP P22619
C	134	HIS	-	expression tag	UNP P22619
C	135	HIS	-	expression tag	UNP P22619
C	136	HIS	-	expression tag	UNP P22619
C	137	HIS	-	expression tag	UNP P22619
E	132	HIS	-	expression tag	UNP P22619
E	133	HIS	-	expression tag	UNP P22619
E	134	HIS	-	expression tag	UNP P22619
E	135	HIS	-	expression tag	UNP P22619
E	136	HIS	-	expression tag	UNP P22619
E	137	HIS	-	expression tag	UNP P22619

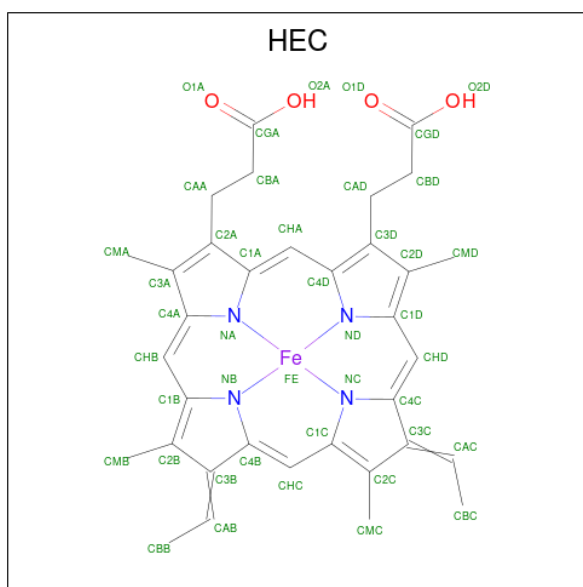
- Molecule 3 is a protein called Methylamine dehydrogenase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	376	Total	C	N	O	S	0	5	0
			2959	1874	506	570	9			
3	F	376	Total	C	N	O	S	0	4	0
			2957	1872	511	565	9			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

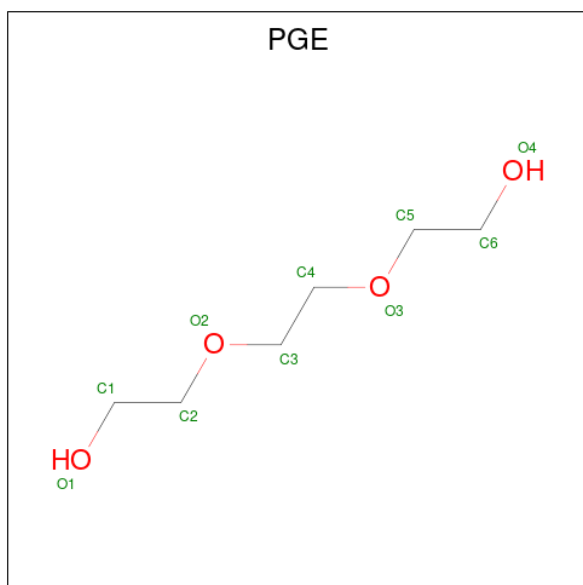
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		

- Molecule 5 is HEME C (CCD ID: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).



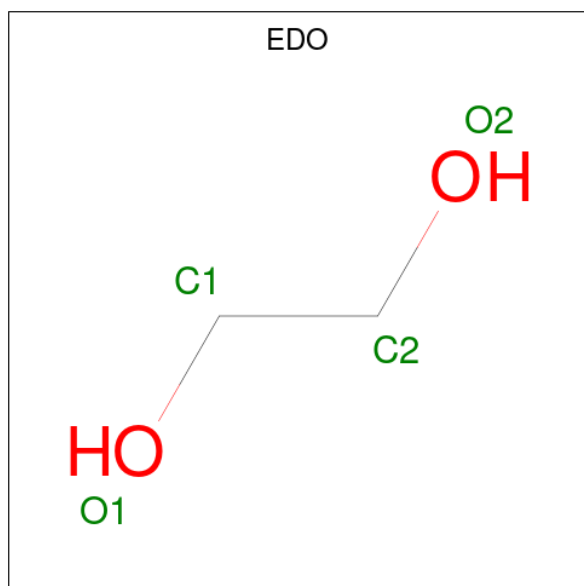
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
5	A	1	43	34	1	4	4	0	0
5	A	1	43	34	1	4	4	0	0
5	B	1	43	34	1	4	4	0	0
5	B	1	43	34	1	4	4	0	0

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula:  $C_6H_{14}O_4$ ).



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

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).

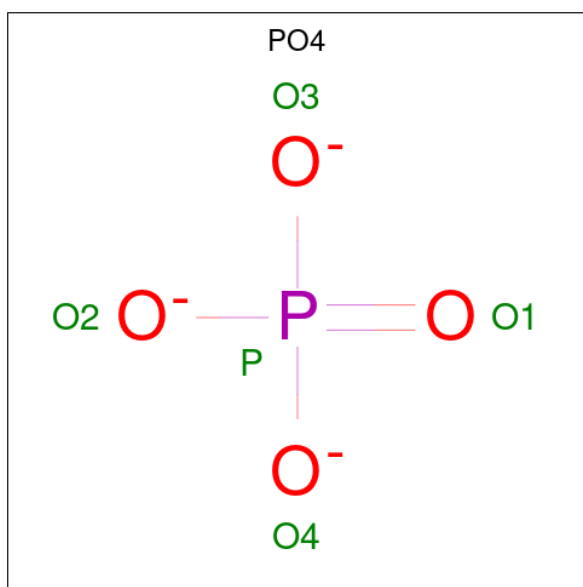


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

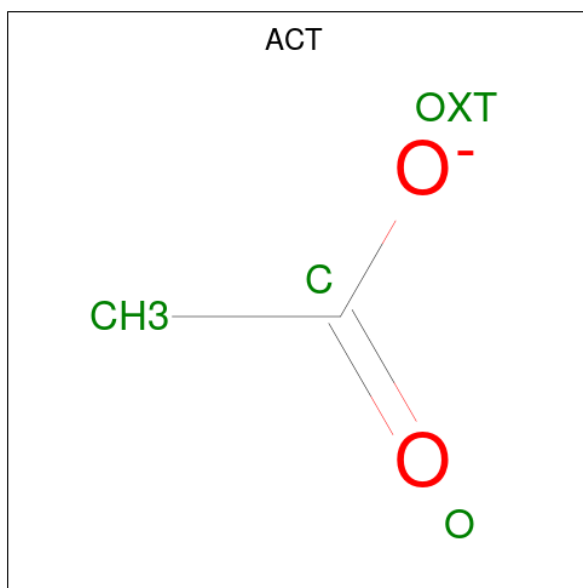
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Na	0	0
			1	1		
8	B	2	Total	Na	0	0
			2	2		

- Molecule 9 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
9	B	1	5	4	1	0	0

- Molecule 10 is ACETATE ION (CCD ID: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).

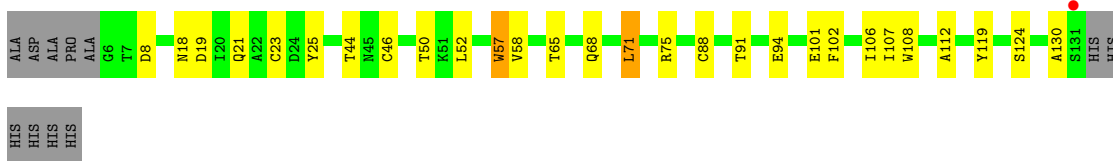


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	D	1	4	2	2	0	0
10	F	1	4	2	2	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	179	Total O 181 181	0	2
11	B	258	Total O 260 260	0	2
11	C	61	Total O 61 61	0	0
11	D	184	Total O 184 184	0	0
11	E	87	Total O 87 87	0	0
11	F	293	Total O 294 294	0	1





- Molecule 3: Methylamine dehydrogenase heavy chain

Chain D: 78% 18% ..



- Molecule 3: Methylamine dehydrogenase heavy chain

Chain F: 81% 15% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.53Å 83.52Å 107.78Å 109.92° 91.52° 105.78°	Depositor
Resolution (Å)	43.46 – 2.14 43.46 – 2.14	Depositor EDS
% Data completeness (in resolution range)	97.4 (43.46-2.14) 97.4 (43.46-2.14)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 2.14Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.163 , 0.227 0.172 , 0.235	Depositor DCC
$R_{free}$ test set	4829 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.0	Xtrriage
Anisotropy	0.043	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 36.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14775	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ACT, PGE, PO4, HEC, NA, EDO, 0AF

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	1.06	3/2880 (0.1%)	1.12	7/3902 (0.2%)
1	B	1.26	6/2845 (0.2%)	1.21	6/3859 (0.2%)
2	C	1.17	1/1035 (0.1%)	1.18	5/1413 (0.4%)
2	E	1.25	1/988 (0.1%)	1.21	3/1348 (0.2%)
3	D	1.08	3/3040 (0.1%)	1.14	9/4142 (0.2%)
3	F	1.27	6/3037 (0.2%)	1.19	10/4136 (0.2%)
All	All	1.18	20/13825 (0.1%)	1.17	40/18800 (0.2%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	80	LEU	CA-C	-6.73	1.49	1.53
3	F	117	VAL	C-O	-6.67	1.17	1.23
3	D	378	GLN	CA-C	-6.48	1.45	1.52
1	B	68	PRO	CA-C	6.08	1.60	1.52
3	F	207	GLY	C-O	5.88	1.30	1.23
3	D	24	ALA	CA-CB	5.79	1.62	1.53
1	A	112	VAL	CA-CB	5.69	1.61	1.54
3	F	306	HIS	N-CA	-5.68	1.38	1.46
1	A	156	ALA	CA-CB	5.60	1.62	1.53
2	C	31	ILE	CA-CB	-5.42	1.48	1.54
1	B	320	ALA	CA-CB	5.38	1.62	1.53
3	D	117	VAL	C-O	-5.38	1.18	1.23
1	A	291	ILE	CA-CB	-5.38	1.47	1.54
1	B	98	ASP	CA-C	-5.34	1.45	1.52
3	F	188	ALA	CA-CB	5.32	1.60	1.53
2	E	112	ALA	CA-CB	5.30	1.62	1.53
1	B	290	ALA	CA-CB	5.20	1.61	1.53
3	F	142	THR	CA-CB	5.16	1.62	1.53
1	B	112	VAL	C-O	-5.10	1.18	1.24
1	B	268	SER	CA-C	-5.07	1.46	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	244	THR	N-CA-C	-7.60	98.75	109.69
3	F	262	LEU	CA-C-N	-6.89	112.86	119.76
3	F	262	LEU	C-N-CA	-6.89	112.86	119.76
1	A	200	ASN	N-CA-C	6.79	120.66	112.38
3	D	337	ASN	N-CA-C	-6.56	98.63	107.88
1	A	43	ASP	CA-C-N	6.09	126.20	119.87
1	A	43	ASP	C-N-CA	6.09	126.20	119.87
3	F	117	VAL	N-CA-C	5.85	116.64	111.90
3	F	95	ALA	N-CA-C	-5.72	99.86	109.07
1	B	76	VAL	CA-C-N	-5.71	113.81	119.92
1	B	76	VAL	C-N-CA	-5.71	113.81	119.92
2	C	104	ASN	N-CA-C	5.70	122.16	113.61
3	F	335	SER	CA-C-N	-5.66	114.77	122.92
3	F	335	SER	C-N-CA	-5.66	114.77	122.92
3	D	281	GLY	N-CA-C	-5.62	103.10	110.29
2	C	47	PRO	CA-C-N	5.62	125.55	119.76
2	C	47	PRO	C-N-CA	5.62	125.55	119.76
1	A	29	GLN	N-CA-C	5.55	117.83	109.23
3	D	118	THR	N-CA-C	-5.54	106.36	113.23
1	B	192	GLY	N-CA-C	-5.51	106.11	112.50
1	B	76	VAL	CB-CA-C	-5.48	105.84	110.94
3	D	211	THR	CA-C-N	-5.48	115.10	120.52
3	D	211	THR	C-N-CA	-5.48	115.10	120.52
2	C	49	GLY	N-CA-C	-5.44	108.22	114.69
3	D	228	ILE	N-CA-C	5.42	116.33	110.21
3	D	343	LYS	CB-CA-C	5.31	115.62	111.00
1	B	169	SER	CA-C-N	-5.29	114.32	120.04
1	B	169	SER	C-N-CA	-5.29	114.32	120.04
3	F	57	ALA	N-CA-C	-5.25	105.61	112.23
1	A	164	ALA	N-CA-C	-5.25	106.56	113.17
2	C	54	THR	N-CA-C	-5.20	107.06	113.41
3	F	339	SER	N-CA-C	-5.15	103.73	110.53
3	F	232	ALA	N-CA-C	-5.14	101.32	109.96
2	E	50	THR	N-CA-C	-5.14	102.55	109.95
3	F	71	VAL	N-CA-C	-5.11	100.97	108.54
3	D	245	TYR	N-CA-C	5.07	117.54	111.71
2	E	124	SER	CA-C-N	-5.07	114.77	120.14
2	E	124	SER	C-N-CA	-5.07	114.77	120.14
1	A	19	VAL	CB-CA-C	-5.01	106.43	112.19
1	A	108	MET	N-CA-C	5.01	116.74	111.28

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	2813	0	2695	70	0
1	B	2781	0	2655	35	0
2	C	1017	0	906	32	0
2	E	973	0	876	17	0
3	D	2959	0	2831	45	0
3	F	2957	0	2841	35	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	86	0	61	5	0
5	B	86	0	62	9	0
6	A	10	0	14	1	0
7	A	4	0	6	0	0
7	B	4	0	6	0	0
8	A	1	0	0	0	0
8	B	2	0	0	0	0
9	B	5	0	0	0	0
10	D	4	0	3	0	0
10	F	4	0	3	0	0
11	A	181	0	0	6	0
11	B	260	0	0	3	0
11	C	61	0	0	2	0
11	D	184	0	0	8	0
11	E	87	0	0	1	0
11	F	294	0	0	2	0
All	All	14775	0	12959	214	0

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

All (214) 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:B:34:CYS:SG	5:B:402:HEC:HAC	1.71	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:CYS:SG	5:A:403:HEC:HAC	1.81	1.16
1:A:133[B]:ARG:HB3	1:A:133[B]:ARG:NH1	1.64	1.12
1:B:204:CYS:SG	5:B:403:HEC:HAC	1.90	1.07
1:A:202[A]:ARG:HH22	2:C:127:VAL:HG11	1.31	0.96
1:A:202[A]:ARG:HB2	1:A:202[A]:ARG:HH11	1.33	0.94
2:C:57:0AF:CE3	2:C:108:TRP:CD1	2.54	0.90
1:B:285:THR:HG22	1:B:286:ASP:OD1	1.71	0.89
1:B:204:CYS:SG	5:B:403:HEC:C3C	2.65	0.85
1:A:204:CYS:HG	5:A:403:HEC:HAC	1.43	0.82
1:A:133[B]:ARG:CB	1:A:133[B]:ARG:HH11	1.92	0.81
1:B:210:GLN:HE22	2:E:44:THR:HG21	1.43	0.81
1:A:133[B]:ARG:HB3	1:A:133[B]:ARG:HH11	1.42	0.81
1:A:210:GLN:HE22	2:C:44:THR:HG21	1.45	0.80
1:B:34:CYS:SG	5:B:402:HEC:C3C	2.69	0.79
1:A:301:ARG:CZ	1:A:333:MET:HE1	2.12	0.79
2:C:57:0AF:HE3	2:C:108:TRP:CD1	2.17	0.79
1:B:364:ALA:HB2	11:B:620:HOH:O	1.82	0.79
1:B:113:GLU:HG2	5:B:402:HEC:HBC2	1.67	0.77
1:A:204:CYS:SG	5:A:403:HEC:C3C	2.74	0.76
2:C:23:CYS:HB3	2:C:88[B]:CYS:SG	2.26	0.76
1:A:133[B]:ARG:NH1	1:A:133[B]:ARG:CB	2.44	0.75
1:B:197:ILE:HG22	1:B:206:MET:CE	2.17	0.74
1:A:333:MET:HE2	3:D:159:ALA:HB2	1.70	0.74
1:A:97:ALA:HA	1:A:102[B]:GLN:HE21	1.52	0.73
2:C:106:ILE:HG12	3:D:133:PHE:HZ	1.53	0.72
2:E:57:0AF:CE3	2:E:108:TRP:CD1	2.71	0.72
1:A:202[A]:ARG:HB2	1:A:202[A]:ARG:NH1	2.05	0.72
2:C:106:ILE:HG12	3:D:133:PHE:CZ	2.24	0.71
1:A:48:LYS:H	1:A:62:HIS:HE1	1.39	0.71
3:D:14:GLN:HE21	2:E:21:GLN:HE22	1.40	0.70
3:D:275:ASP:HB2	11:D:636:HOH:O	1.91	0.69
2:C:23:CYS:CB	2:C:88[B]:CYS:SG	2.80	0.69
1:A:133[B]:ARG:HB3	1:A:133[B]:ARG:CZ	2.22	0.69
3:D:333:ILE:HD12	3:D:348:ALA:HB1	1.74	0.68
3:F:174[B]:ARG:CZ	3:F:208:THR:HA	2.24	0.68
3:D:51:ASP:HA	3:D:377:PRO:HA	1.77	0.67
1:A:333:MET:HE2	3:D:159:ALA:CB	2.26	0.65
1:A:133[B]:ARG:HH11	1:A:133[B]:ARG:CA	2.09	0.65
2:C:57:0AF:CE3	2:C:108:TRP:HD1	2.09	0.64
1:A:68:PRO:HG2	5:A:402:HEC:HBA1	1.79	0.64
3:D:342[A]:GLU:HA	11:D:653:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:268:LEU:HD22	3:D:277:TRP:HB3	1.81	0.63
1:A:9:ALA:HB3	1:A:139:LEU:HD21	1.81	0.62
3:D:342[B]:GLU:HA	11:D:653:HOH:O	2.00	0.61
1:B:91:GLN:O	1:B:92:PHE:HB2	1.99	0.60
1:A:202[A]:ARG:NH2	2:C:127:VAL:HG11	2.10	0.60
3:F:54:HIS:O	3:F:55:PHE:HB2	2.00	0.59
1:B:197:ILE:HG22	1:B:206:MET:HE2	1.83	0.59
1:A:45:ARG:NH1	11:A:564:HOH:O	2.36	0.58
1:A:39[A]:ARG:O	1:A:39[A]:ARG:HG2	2.03	0.58
3:D:276:GLY:O	3:D:300:GLN:HA	2.03	0.58
1:A:209:LYS:HG2	3:F:33:GLU:HG3	1.85	0.58
3:D:193:PHE:CE2	3:D:203:LYS:HB2	2.39	0.58
3:F:82:ASN:HB3	3:F:142:THR:HB	1.85	0.57
3:D:275:ASP:CB	11:D:636:HOH:O	2.50	0.56
1:A:206:MET:HE2	1:A:216:GLU:CD	2.31	0.56
2:E:71:LEU:HD13	2:E:130:ALA:HB2	1.87	0.56
2:C:58:VAL:HG22	2:C:59:ALA:N	2.20	0.56
1:A:359:GLU:HA	11:A:647:HOH:O	2.06	0.56
1:A:199:TRP:O	1:A:202[A]:ARG:HG3	2.07	0.55
2:C:35:ILE:HD11	2:C:88[A]:CYS:SG	2.47	0.55
1:B:210:GLN:NE2	2:E:44:THR:HG21	2.19	0.55
3:F:12:GLU:OE1	3:F:20:ARG:NH1	2.39	0.55
3:F:174[B]:ARG:NH2	3:F:208:THR:HA	2.22	0.55
1:A:210:GLN:NE2	2:C:44:THR:HG21	2.21	0.54
2:C:62:TYR:CE1	2:C:67:GLY:HA2	2.43	0.54
1:A:176:ASP:OD2	6:A:404:PGE:H6	2.08	0.54
1:A:359:GLU:CA	11:A:647:HOH:O	2.56	0.54
1:B:197:ILE:HG22	1:B:206:MET:HE1	1.89	0.54
1:A:127:ARG:HG2	1:A:133[C]:ARG:NH2	2.23	0.54
1:A:21:PRO:O	1:A:27:ALA:HA	2.08	0.53
1:A:172:ASP:O	1:A:177:ARG:NH1	2.41	0.53
2:C:62:TYR:CZ	2:C:67:GLY:HA2	2.43	0.53
1:B:208:ARG:HD2	11:B:687:HOH:O	2.08	0.53
3:D:45:ARG:NH2	3:D:343:LYS:O	2.42	0.53
1:A:70:LEU:HD13	1:A:163:GLN:NE2	2.24	0.52
1:A:208:ARG:NH2	3:F:29:GLY:O	2.36	0.52
2:C:12:LYS:NZ	11:C:219:HOH:O	2.40	0.52
3:D:297:LEU:HD11	3:D:333:ILE:HG22	1.92	0.52
1:A:303[B]:GLU:CD	1:A:303[B]:GLU:H	2.14	0.52
1:A:178:VAL:HG12	1:A:179:MET:HE2	1.92	0.52
1:A:127:ARG:HG2	1:A:133[C]:ARG:HH21	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:331:HIS:HE1	3:F:366:GLU:OE1	1.93	0.51
3:D:336:ILE:HA	3:D:347:TYR:O	2.11	0.51
1:B:84:ASN:HD22	1:B:86:LYS:NZ	2.08	0.51
3:F:42:PRO:HG3	3:F:116:PRO:HB2	1.92	0.50
3:F:297:LEU:HD22	3:F:310:SER:HB2	1.92	0.50
3:D:20:ARG:NH1	11:D:562:HOH:O	2.42	0.50
3:D:96:SER:HB3	3:D:110:TYR:CZ	2.46	0.50
3:D:244:THR:HG23	3:D:248:LYS:O	2.12	0.50
1:B:299:SER:HB2	1:B:333:MET:HG3	1.94	0.49
3:D:344:PRO:HG2	3:D:361:ALA:HB3	1.94	0.49
1:B:226:ILE:O	1:B:297:TYR:OH	2.25	0.49
1:B:229:PRO:HG3	1:B:314:TRP:O	2.13	0.49
3:F:115:ASP:O	3:F:119:LEU:HA	2.11	0.49
1:A:48:LYS:H	1:A:62:HIS:CE1	2.26	0.49
1:A:230:VAL:CG2	1:A:318:GLU:HG3	2.43	0.49
3:D:239:ARG:HG3	3:D:241:VAL:HG23	1.95	0.48
2:E:46:CYS:SG	2:E:52:LEU:HD13	2.53	0.48
2:C:95:LEU:HD12	2:C:102:PHE:CD2	2.48	0.48
1:A:71:GLY:O	1:A:72:TYR:HB2	2.14	0.48
3:D:265:VAL:CG2	3:D:321:GLY:HA3	2.44	0.48
1:A:103:GLN:C	1:A:103:GLN:CD	2.82	0.47
3:D:186:PRO:HB2	3:D:235:GLN:NE2	2.28	0.47
1:A:204:CYS:HA	1:A:220:ASN:ND2	2.29	0.47
3:D:155:GLN:NE2	11:D:621:HOH:O	2.28	0.47
3:F:80:LEU:N	3:F:81:PRO:CD	2.77	0.47
3:D:82:ASN:HB3	11:D:608:HOH:O	2.13	0.47
1:A:91:GLN:O	1:A:92:PHE:HB2	2.14	0.47
3:D:265:VAL:HG21	3:D:321:GLY:CA	2.45	0.47
1:A:353:ARG:NE	11:A:606:HOH:O	2.42	0.47
3:F:147:ASP:OD1	3:F:147:ASP:C	2.58	0.47
3:F:51:ASP:HA	3:F:377:PRO:HA	1.96	0.47
1:A:264:PHE:CE1	1:A:280:HIS:CE1	3.03	0.46
2:E:8:ASP:OD2	11:E:284:HOH:O	2.21	0.46
3:F:38:GLU:HB3	3:F:117:VAL:HG23	1.97	0.46
3:F:214:ILE:HD12	11:F:780:HOH:O	2.15	0.46
3:D:42:PRO:HD3	3:D:117:VAL:HG12	1.98	0.46
3:D:331:HIS:HE1	3:D:366:GLU:OE1	1.98	0.46
3:D:92:ILE:HG13	3:D:114:PHE:HB2	1.96	0.46
2:E:19:ASP:O	2:E:25:TYR:HB2	2.15	0.46
1:A:197:ILE:HA	1:A:202[A]:ARG:HB3	1.98	0.46
2:C:23:CYS:SG	2:C:88[B]:CYS:CB	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:350:SER:HB3	3:F:353:ASP:HB2	1.98	0.46
1:B:107:PRO:HG2	5:B:402:HEC:HBB2	1.97	0.46
1:A:102[A]:GLN:HG2	11:A:666:HOH:O	2.17	0.45
1:A:209:LYS:HE3	3:F:33:GLU:HG3	1.97	0.45
1:A:65:ARG:HH12	1:A:94:ASP:CG	2.24	0.45
1:B:300[A]:ARG:NH1	11:B:511:HOH:O	2.36	0.45
1:B:52:ALA:O	1:B:66:ASN:HA	2.16	0.45
1:A:120:ALA:HA	1:A:148:PRO:HB3	1.97	0.45
2:E:91:THR:HG21	3:F:307:LYS:HD2	1.97	0.45
3:F:286:ALA:HB3	3:F:295:TYR:HB2	1.98	0.45
2:C:94:GLU:HG2	2:C:102:PHE:O	2.16	0.45
1:A:29:GLN:HE22	5:A:402:HEC:HBC3	1.81	0.45
1:B:61:SER:HB3	1:B:112:VAL:HB	1.98	0.45
1:B:76:VAL:HG12	1:B:77:PRO:O	2.17	0.45
1:B:247:HIS:HB3	1:B:250:LEU:HB3	1.99	0.45
2:C:18:ASN:O	3:F:16:GLN:HA	2.16	0.45
3:F:237:ALA:HB2	3:F:289:ARG:HG3	1.98	0.45
3:F:354:LYS:HG2	3:F:374:GLY:O	2.17	0.45
1:A:103:GLN:C	1:A:103:GLN:OE1	2.59	0.45
1:B:110:ASN:HB3	1:B:113:GLU:HB2	1.99	0.45
3:D:299:ASP:OD1	3:D:300:GLN:N	2.45	0.45
2:E:57:0AF:HE3	2:E:108:TRP:CD1	2.50	0.45
1:B:34:CYS:CB	5:B:402:HEC:C3C	2.95	0.44
2:C:57:0AF:HE3	2:C:108:TRP:CG	2.52	0.44
2:C:23:CYS:SG	2:C:88[B]:CYS:HB2	2.57	0.44
2:E:23:CYS:CB	2:E:88[B]:CYS:SG	3.06	0.44
2:E:23:CYS:SG	2:E:88[B]:CYS:SG	3.15	0.44
1:B:91:GLN:HB3	5:B:402:HEC:HAA1	1.98	0.44
1:B:202:ARG:HH21	2:E:75:ARG:HD2	1.83	0.44
3:D:82:ASN:HB3	3:D:142:THR:HB	2.00	0.44
3:D:333:ILE:HD12	3:D:348:ALA:CB	2.46	0.44
1:A:289:THR:HG23	1:A:308:PRO:HD2	1.98	0.44
1:A:60:GLN:O	1:A:62:HIS:HD2	2.01	0.44
3:D:262:LEU:HB3	3:D:263:PRO:HD2	2.00	0.44
1:B:204:CYS:SG	5:B:403:HEC:CBC	2.97	0.44
3:F:260:LYS:NZ	3:F:260:LYS:HB3	2.33	0.43
1:A:82:ASP:OD2	1:A:82:ASP:C	2.60	0.43
3:F:174[A]:ARG:NH2	3:F:207:GLY:O	2.50	0.43
1:A:223:TYR:CG	1:A:249:LEU:HD22	2.53	0.43
2:C:25:TYR:HB3	2:C:28:HIS:CD2	2.53	0.43
2:E:106:ILE:HA	3:F:135:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:151:LEU:C	3:F:151:LEU:HD23	2.43	0.43
1:A:112:VAL:HG23	1:A:112:VAL:O	2.17	0.43
3:F:347:TYR:HB3	3:F:356:LEU:HD11	2.01	0.43
1:A:40:ALA:HA	1:A:354:TYR:CZ	2.54	0.43
2:E:107:ILE:HD12	2:E:119:TYR:HB2	2.00	0.42
1:A:170:PRO:HG3	1:A:353:ARG:HH12	1.83	0.42
3:D:54:HIS:HD2	11:D:625:HOH:O	2.01	0.42
2:C:83:SER:HB3	2:C:120:HIS:CE1	2.53	0.42
1:A:43:ASP:HA	1:A:44:PRO:HD2	1.85	0.42
3:D:191:THR:HA	3:D:204:VAL:O	2.19	0.42
3:F:173:LYS:HB3	3:F:174[B]:ARG:NH2	2.34	0.42
2:C:57:0AF:HBC1	2:C:108:TRP:NE1	2.34	0.42
1:B:74:ALA:HA	1:B:100:LEU:HD11	2.01	0.42
2:C:85:ARG:O	2:C:86:CYS:C	2.63	0.42
1:A:15:ALA:HB2	1:A:162:TYR:CE1	2.54	0.42
2:C:19:ASP:OD1	3:F:15:GLY:HA3	2.20	0.42
1:A:21:PRO:HA	1:A:29:GLN:O	2.20	0.41
3:F:107:ARG:NE	3:F:130:ALA:HB1	2.35	0.41
3:D:297:LEU:HD22	3:D:310:SER:HB2	2.02	0.41
1:A:186:THR:O	1:A:187:PRO:C	2.60	0.41
1:A:302:PRO:O	1:A:305:LYS:HG2	2.20	0.41
2:C:20:ILE:HG22	2:C:25:TYR:CZ	2.55	0.41
2:C:75:ARG:HA	11:C:251:HOH:O	2.20	0.41
2:C:104:ASN:OD1	2:C:104:ASN:C	2.64	0.41
3:D:323:ARG:HE	3:D:323:ARG:HB2	1.73	0.41
1:B:277:PRO:HB3	1:B:285:THR:HA	2.02	0.41
2:C:58:VAL:HA	2:C:72:ILE:O	2.20	0.41
2:E:94:GLU:HG2	2:E:102:PHE:O	2.20	0.41
3:F:11:GLN:HA	11:F:739:HOH:O	2.20	0.41
1:A:188:LEU:HD23	1:A:344:ALA:HB2	2.03	0.41
3:D:277:TRP:CE2	3:D:300:GLN:HG3	2.55	0.41
3:F:78:GLY:O	3:F:81:PRO:HD3	2.21	0.41
1:A:88:LYS:HA	1:A:221:PHE:O	2.20	0.41
1:A:202[A]:ARG:HG3	1:A:202[A]:ARG:H	1.65	0.41
1:B:193:TYR:O	1:B:197:ILE:HG12	2.20	0.41
2:C:13:TRP:NE1	2:C:24:ASP:HA	2.36	0.41
3:D:16:GLN:HA	2:E:18:ASN:O	2.21	0.41
3:D:53:ALA:HB3	3:D:56:ALA:HB3	2.03	0.41
3:D:249:ILE:HB	3:D:265:VAL:HG12	2.03	0.41
3:D:272:GLU:HB3	3:D:277:TRP:HB2	2.03	0.41
1:B:40:ALA:HA	1:B:354:TYR:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:SER:O	1:B:363:ALA:N	2.54	0.40
3:F:150:THR:HA	3:F:165:VAL:O	2.22	0.40
1:B:355:GLU:O	1:B:358:LEU:HB2	2.21	0.40
3:D:152:LEU:HA	3:D:163:GLY:O	2.21	0.40
1:A:19:VAL:HG13	11:A:537:HOH:O	2.21	0.40
1:A:206:MET:HE3	1:A:218:PHE:CD2	2.56	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	360/373 (96%)	342 (95%)	18 (5%)	0	100	100
1	B	358/373 (96%)	344 (96%)	13 (4%)	1 (0%)	36	33
2	C	129/137 (94%)	123 (95%)	5 (4%)	1 (1%)	16	9
2	E	126/137 (92%)	123 (98%)	3 (2%)	0	100	100
3	D	379/385 (98%)	360 (95%)	16 (4%)	3 (1%)	16	9
3	F	378/385 (98%)	363 (96%)	13 (3%)	2 (0%)	24	19
All	All	1730/1790 (97%)	1655 (96%)	68 (4%)	7 (0%)	30	26

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	362	ARG
3	D	102[A]	ILE
3	D	102[B]	ILE
3	F	55	PHE
2	C	67	GLY
3	F	102	ILE
3	D	179	PRO

### 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	284/292 (97%)	271 (95%)	13 (5%)	24	20
1	B	280/292 (96%)	267 (95%)	13 (5%)	24	20
2	C	111/112 (99%)	110 (99%)	1 (1%)	70	77
2	E	107/112 (96%)	101 (94%)	6 (6%)	19	14
3	D	309/310 (100%)	300 (97%)	9 (3%)	37	38
3	F	308/310 (99%)	301 (98%)	7 (2%)	44	47
All	All	1399/1428 (98%)	1350 (96%)	49 (4%)	32	31

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	23	LEU
1	A	51	LEU
1	A	75	LEU
1	A	84	ASN
1	A	112	VAL
1	A	167	GLU
1	A	202[A]	ARG
1	A	202[B]	ARG
1	A	206	MET
1	A	232	GLU
1	A	321	ARG
1	A	358	LEU
1	B	68	PRO
1	B	75	LEU
1	B	84	ASN
1	B	112	VAL
1	B	167	GLU
1	B	219	THR
1	B	269	LEU
1	B	285	THR
1	B	303	GLU

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Mol	Chain	Res	Type
1	B	323	LEU
1	B	357	LEU
1	B	358	LEU
1	B	360	GLU
2	C	71	LEU
3	D	75	ILE
3	D	117	VAL
3	D	127	LEU
3	D	173	LYS
3	D	209	GLU
3	D	215	THR
3	D	265	VAL
3	D	316	LEU
3	D	354	LYS
2	E	58	VAL
2	E	65	THR
2	E	68	GLN
2	E	71	LEU
2	E	101[A]	GLU
2	E	101[B]	GLU
3	F	75	ILE
3	F	117	VAL
3	F	160	PRO
3	F	218	GLU
3	F	260	LYS
3	F	262	LEU
3	F	343	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	60	GLN
1	A	62	HIS
1	A	91	GLN
1	A	163	GLN
1	A	210	GLN
1	B	29	GLN
1	B	60	GLN
1	B	84	ASN
1	B	91	GLN
1	B	163	GLN

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Mol	Chain	Res	Type
1	B	210	GLN
2	C	134	HIS
2	C	135	HIS
3	D	14	GLN
3	D	235	GLN
2	E	68	GLN
3	F	30	GLN
3	F	50	ASN
3	F	61	GLN
3	F	235	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
2	0AF	C	57	2	15,16,17	1.39	2 (13%)	14,22,24	1.54	2 (14%)
2	0AF	E	57	2	15,16,17	1.21	1 (6%)	14,22,24	1.04	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	0AF	C	57	2	-	1/5/6/8	0/2/2/2
2	0AF	E	57	2	-	1/5/6/8	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	57	0AF	CD2-CE2	-3.76	1.36	1.41
2	E	57	0AF	CD2-CE2	-2.50	1.38	1.41
2	C	57	0AF	CE2-NE1	-2.22	1.34	1.37

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	57	0AF	CE2-NE1-CD1	3.40	111.86	108.93
2	C	57	0AF	CG-CD1-NE1	-3.28	106.70	110.31

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	57	0AF	C-CA-CB-CG
2	C	57	0AF	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	57	0AF	5	0
2	E	57	0AF	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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
10	ACT	D	401	-	3,3,3	0.83	0	3,3,3	1.04	0
5	HEC	A	403	1	46,50,50	2.71	24 (52%)	58,82,82	2.40	19 (32%)
5	HEC	B	403	1	46,50,50	2.54	19 (41%)	58,82,82	2.61	19 (32%)
7	EDO	A	405	-	3,3,3	0.44	0	2,2,2	0.42	0
9	PO4	B	404	-	4,4,4	0.76	0	6,6,6	0.75	0
6	PGE	A	404	-	9,9,9	0.64	0	8,8,8	0.46	0
7	EDO	B	405	-	3,3,3	0.44	0	2,2,2	0.19	0
5	HEC	A	402	1,11	46,50,50	2.66	22 (47%)	58,82,82	2.37	20 (34%)
5	HEC	B	402	1,11	46,50,50	2.62	20 (43%)	58,82,82	2.42	19 (32%)
10	ACT	F	401	-	3,3,3	1.00	0	3,3,3	1.44	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
5	HEC	A	403	1	-	6/14/54/54	-
5	HEC	B	403	1	-	6/14/54/54	-
7	EDO	A	405	-	-	1/1/1/1	-
6	PGE	A	404	-	-	3/7/7/7	-
7	EDO	B	405	-	-	1/1/1/1	-
5	HEC	A	402	1,11	-	6/14/54/54	-
5	HEC	B	402	1,11	-	4/14/54/54	-

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	402	HEC	CAC-C3C	5.84	1.54	1.35
5	A	402	HEC	CAC-C3C	5.69	1.53	1.35
5	A	403	HEC	CAB-C3B	5.51	1.52	1.35
5	B	403	HEC	C4D-ND	-5.23	1.29	1.39
5	A	403	HEC	CAC-C3C	5.19	1.51	1.35
5	B	403	HEC	CAB-C3B	5.14	1.51	1.35
5	B	403	HEC	CAC-C3C	5.11	1.51	1.35
5	B	402	HEC	CHB-C4A	5.09	1.48	1.38
5	A	403	HEC	CHC-C4B	5.08	1.48	1.38
5	B	402	HEC	CAB-C3B	5.00	1.51	1.35
5	B	402	HEC	CHD-C1D	4.99	1.50	1.39
5	A	402	HEC	CHC-C4B	4.94	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	403	HEC	CHC-C4B	4.88	1.47	1.38
5	A	402	HEC	CAB-C3B	4.81	1.50	1.35
5	A	403	HEC	CHA-C1A	4.79	1.47	1.38
5	A	402	HEC	CHA-C1A	4.65	1.47	1.38
5	A	402	HEC	C1D-ND	-4.63	1.30	1.39
5	B	402	HEC	CHD-C4C	4.57	1.47	1.38
5	B	403	HEC	C4A-NA	-4.50	1.31	1.39
5	A	403	HEC	CHB-C4A	4.50	1.47	1.38
5	B	403	HEC	CHB-C4A	4.50	1.47	1.38
5	A	402	HEC	CHC-C1C	4.48	1.49	1.39
5	A	403	HEC	C4B-NB	-4.40	1.31	1.39
5	A	402	HEC	CHD-C4C	4.31	1.46	1.38
5	B	403	HEC	CHD-C4C	4.26	1.46	1.38
5	B	402	HEC	CHA-C1A	4.15	1.46	1.38
5	A	402	HEC	C4D-ND	-4.11	1.31	1.39
5	B	402	HEC	CHC-C1C	4.06	1.48	1.39
5	A	403	HEC	C4A-NA	-4.03	1.32	1.39
5	B	402	HEC	C1C-NC	-4.02	1.32	1.39
5	A	403	HEC	CHA-C4D	3.99	1.48	1.39
5	A	403	HEC	C4D-ND	-3.99	1.32	1.39
5	A	402	HEC	CHB-C4A	3.95	1.46	1.38
5	B	402	HEC	CHC-C4B	3.92	1.46	1.38
5	B	402	HEC	CHB-C1B	3.85	1.48	1.39
5	A	403	HEC	C4C-NC	-3.82	1.32	1.39
5	B	403	HEC	C4C-NC	-3.80	1.32	1.39
5	B	402	HEC	C1D-ND	-3.80	1.32	1.39
5	A	402	HEC	C4C-NC	-3.62	1.32	1.39
5	B	402	HEC	C1B-NB	-3.61	1.32	1.39
5	A	402	HEC	CHD-C1D	3.60	1.47	1.39
5	A	403	HEC	CHD-C1D	3.59	1.47	1.39
5	B	403	HEC	C4B-NB	-3.57	1.32	1.39
5	A	402	HEC	CHA-C4D	3.49	1.47	1.39
5	A	403	HEC	CHD-C4C	3.48	1.45	1.38
5	A	403	HEC	CHC-C1C	3.40	1.47	1.39
5	A	403	HEC	C4A-C3A	3.37	1.52	1.45
5	A	402	HEC	C4A-NA	-3.30	1.33	1.39
5	B	403	HEC	CHC-C1C	3.27	1.46	1.39
5	A	402	HEC	CHB-C1B	3.12	1.46	1.39
5	B	403	HEC	CHA-C1A	3.10	1.44	1.38
5	A	403	HEC	C1D-ND	-3.09	1.33	1.39
5	A	402	HEC	C1A-NA	-3.05	1.33	1.39
5	B	402	HEC	C1A-NA	-2.99	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	403	HEC	C1B-NB	-2.97	1.34	1.39
5	B	403	HEC	CHA-C4D	2.88	1.45	1.39
5	B	402	HEC	CHA-C4D	2.87	1.45	1.39
5	A	402	HEC	C1C-NC	-2.79	1.34	1.39
5	B	403	HEC	C1A-NA	-2.78	1.34	1.39
5	B	403	HEC	C1C-NC	-2.76	1.34	1.39
5	B	402	HEC	C4B-NB	-2.67	1.34	1.39
5	B	403	HEC	C4A-C3A	2.65	1.50	1.45
5	A	403	HEC	CHB-C1B	2.59	1.45	1.39
5	B	403	HEC	CHD-C1D	2.57	1.45	1.39
5	A	403	HEC	C1A-C2A	2.56	1.49	1.45
5	B	403	HEC	C1B-NB	-2.55	1.34	1.39
5	A	403	HEC	C1C-NC	-2.51	1.34	1.39
5	B	402	HEC	C4A-NA	-2.50	1.34	1.39
5	A	402	HEC	C1B-NB	-2.48	1.34	1.39
5	A	402	HEC	C1D-C2D	2.45	1.48	1.43
5	B	403	HEC	C3C-C4C	2.43	1.50	1.46
5	B	403	HEC	C1A-C2A	2.42	1.49	1.45
5	A	402	HEC	C1A-C2A	2.35	1.49	1.45
5	A	403	HEC	C1A-NA	-2.34	1.35	1.39
5	B	402	HEC	O2A-CGA	-2.33	1.23	1.30
5	A	402	HEC	C1B-C2B	2.28	1.48	1.43
5	A	402	HEC	C1C-C2C	2.23	1.48	1.43
5	A	402	HEC	C4B-NB	-2.20	1.35	1.39
5	A	403	HEC	C1B-C2B	2.13	1.48	1.43
5	A	403	HEC	O2D-CGD	-2.11	1.23	1.30
5	A	403	HEC	C3C-C4C	2.10	1.49	1.46
5	A	403	HEC	C1C-C2C	2.10	1.48	1.43
5	B	402	HEC	C1D-C2D	2.09	1.48	1.43
5	B	402	HEC	C1C-C2C	2.05	1.47	1.43
5	B	402	HEC	C1B-C2B	2.02	1.47	1.43

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	403	HEC	CBB-CAB-C3B	-11.07	105.31	127.43
5	B	402	HEC	CBB-CAB-C3B	-10.88	105.68	127.43
5	A	403	HEC	CBB-CAB-C3B	-9.57	108.31	127.43
5	A	402	HEC	CBB-CAB-C3B	-7.98	111.49	127.43
5	B	403	HEC	CBC-CAC-C3C	-7.40	112.63	127.43
5	A	403	HEC	CBC-CAC-C3C	-7.34	112.75	127.43
5	A	402	HEC	CBC-CAC-C3C	-7.19	113.07	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	402	HEC	C3D-C4D-ND	5.12	115.83	110.15
5	B	403	HEC	C2A-C1A-NA	5.04	115.18	110.32
5	B	402	HEC	CBC-CAC-C3C	-4.68	118.07	127.43
5	B	402	HEC	C2A-C1A-NA	4.47	114.63	110.32
5	B	402	HEC	C3D-C4D-ND	4.27	114.89	110.15
5	A	403	HEC	C2A-C1A-NA	4.01	114.19	110.32
5	A	403	HEC	CBD-CAD-C3D	-3.93	101.67	112.53
5	A	403	HEC	CHB-C4A-NA	-3.77	120.35	124.45
5	A	403	HEC	C1D-C2D-C3D	-3.75	102.52	106.82
5	B	403	HEC	C1D-C2D-C3D	-3.74	102.54	106.82
5	B	403	HEC	CBD-CAD-C3D	-3.72	102.25	112.53
5	A	402	HEC	C2A-C1A-NA	3.61	113.81	110.32
5	B	403	HEC	C1A-C2A-C3A	-3.59	102.38	107.11
5	B	402	HEC	CMB-C2B-C3B	3.59	134.99	126.55
5	A	402	HEC	C1D-C2D-C3D	-3.56	102.74	106.82
5	B	402	HEC	C4D-C3D-C2D	-3.55	101.38	106.87
5	A	402	HEC	C2B-C1B-NB	3.50	115.76	110.14
5	B	403	HEC	CHC-C1C-C2C	-3.46	117.38	127.43
5	A	402	HEC	C2D-C1D-ND	3.45	115.67	110.14
5	A	402	HEC	CBD-CAD-C3D	-3.27	103.49	112.53
5	B	403	HEC	C2C-C1C-NC	3.21	115.29	110.14
5	B	403	HEC	CMC-C2C-C3C	3.16	133.99	126.55
5	B	402	HEC	CAA-C2A-C1A	3.02	130.99	124.85
5	A	402	HEC	C1A-C2A-C3A	-2.99	103.17	107.11
5	A	403	HEC	CHD-C4C-NC	-2.93	121.27	124.45
5	B	403	HEC	C2B-C1B-NB	2.92	114.82	110.14
5	B	402	HEC	CHA-C1A-NA	-2.91	121.28	124.45
5	A	403	HEC	C2B-C1B-NB	2.90	114.78	110.14
5	A	402	HEC	CHC-C4B-NB	-2.89	121.31	124.45
5	B	403	HEC	C2D-C1D-ND	2.87	114.75	110.14
5	B	402	HEC	CMB-C2B-C1B	-2.87	121.04	125.42
5	A	403	HEC	C1A-C2A-C3A	-2.83	103.38	107.11
5	A	403	HEC	CMA-C3A-C4A	2.82	129.70	124.73
5	B	402	HEC	C2C-C1C-NC	2.82	114.66	110.14
5	A	403	HEC	C3D-C4D-ND	2.81	113.27	110.15
5	A	403	HEC	O2A-CGA-CBA	2.79	122.81	114.00
5	B	402	HEC	C1A-C2A-C3A	-2.74	103.50	107.11
5	A	402	HEC	CAA-CBA-CGA	-2.73	106.42	113.67
5	B	403	HEC	CMA-C3A-C4A	2.70	129.48	124.73
5	A	402	HEC	CHD-C4C-NC	-2.65	121.56	124.45
5	A	403	HEC	C2D-C1D-ND	2.63	114.36	110.14
5	A	403	HEC	CBA-CAA-C2A	-2.60	105.35	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	403	HEC	CBA-CAA-C2A	-2.55	105.48	112.53
5	B	402	HEC	CAD-C3D-C4D	2.54	129.90	124.94
5	B	402	HEC	O1D-CGD-CBD	-2.54	115.04	123.09
5	A	402	HEC	CMB-C2B-C3B	2.53	132.51	126.55
5	B	402	HEC	O2D-CGD-CBD	2.52	121.98	114.00
5	B	403	HEC	C3A-C4A-NA	2.52	114.30	109.64
5	A	403	HEC	CHC-C4B-NB	-2.49	121.75	124.45
5	B	403	HEC	CHD-C1D-C2D	-2.42	120.40	127.43
5	B	402	HEC	CHC-C4B-C3B	-2.41	121.15	125.21
5	A	402	HEC	CHA-C1A-NA	-2.41	121.83	124.45
5	B	402	HEC	C2B-C1B-NB	2.31	113.84	110.14
5	A	402	HEC	CBA-CAA-C2A	-2.30	106.17	112.53
5	B	403	HEC	CAA-C2A-C1A	2.28	129.48	124.85
5	A	402	HEC	C4D-ND-C1D	-2.24	102.16	105.82
5	A	403	HEC	CMB-C2B-C3B	2.24	131.81	126.55
5	B	403	HEC	C3D-C4D-ND	2.24	112.64	110.15
5	B	402	HEC	C3A-C4A-NA	2.23	113.76	109.64
5	A	402	HEC	O2D-CGD-CBD	2.21	120.98	114.00
5	A	402	HEC	CMD-C2D-C3D	2.19	130.27	125.62
5	A	403	HEC	O1A-CGA-CBA	-2.18	116.19	123.09
5	A	402	HEC	C4D-C3D-C2D	-2.13	103.57	106.87
5	B	402	HEC	CMC-C2C-C3C	2.10	131.48	126.55
5	A	403	HEC	C3A-C4A-NA	2.08	113.48	109.64
5	B	402	HEC	C4C-NC-C1C	-2.06	102.47	105.82
5	A	403	HEC	CHA-C1A-C2A	-2.03	121.66	124.86
5	A	402	HEC	CAA-C2A-C1A	2.02	128.96	124.85
5	B	403	HEC	CAD-C3D-C4D	2.01	128.86	124.94
5	B	403	HEC	CHB-C1B-C2B	-2.00	121.61	127.43

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	402	HEC	C2B-C3B-CAB-CBB
5	A	402	HEC	C4B-C3B-CAB-CBB
5	A	402	HEC	C2C-C3C-CAC-CBC
5	A	402	HEC	C4C-C3C-CAC-CBC
5	A	403	HEC	C2B-C3B-CAB-CBB
5	A	403	HEC	C4B-C3B-CAB-CBB
5	A	403	HEC	C2C-C3C-CAC-CBC
5	A	403	HEC	C4C-C3C-CAC-CBC
5	B	402	HEC	C2B-C3B-CAB-CBB

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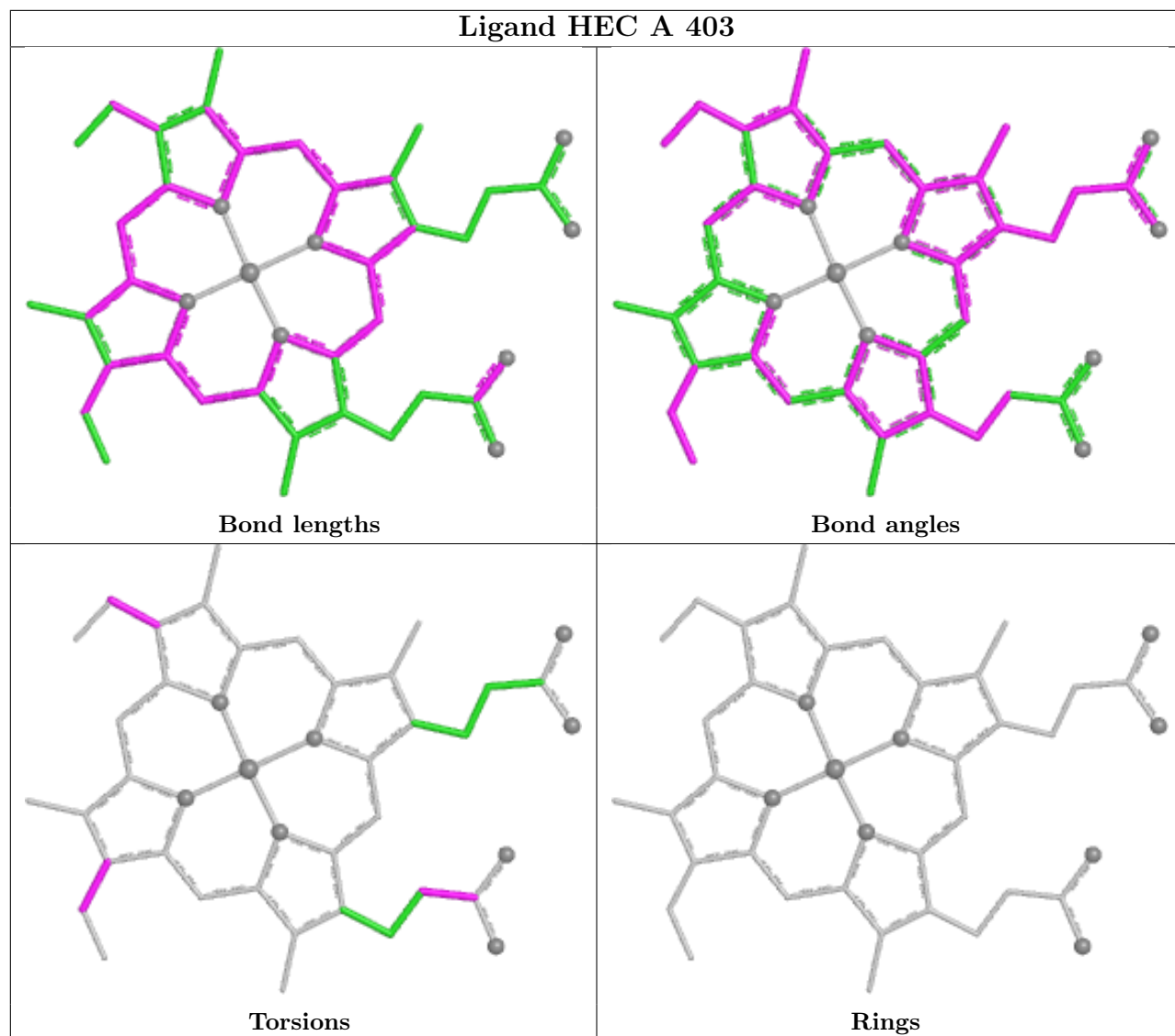
Mol	Chain	Res	Type	Atoms
5	B	402	HEC	C4B-C3B-CAB-CBB
5	B	402	HEC	C2C-C3C-CAC-CBC
5	B	402	HEC	C4C-C3C-CAC-CBC
5	B	403	HEC	C2B-C3B-CAB-CBB
5	B	403	HEC	C4B-C3B-CAB-CBB
5	B	403	HEC	C2C-C3C-CAC-CBC
5	B	403	HEC	C4C-C3C-CAC-CBC
6	A	404	PGE	O1-C1-C2-O2
7	B	405	EDO	O1-C1-C2-O2
7	A	405	EDO	O1-C1-C2-O2
6	A	404	PGE	C1-C2-O2-C3
5	A	402	HEC	CAD-CBD-CGD-O2D
5	A	402	HEC	CAD-CBD-CGD-O1D
5	A	403	HEC	CAD-CBD-CGD-O2D
5	B	403	HEC	CAD-CBD-CGD-O2D
5	B	403	HEC	CAD-CBD-CGD-O1D
5	A	403	HEC	CAD-CBD-CGD-O1D
6	A	404	PGE	O2-C3-C4-O3

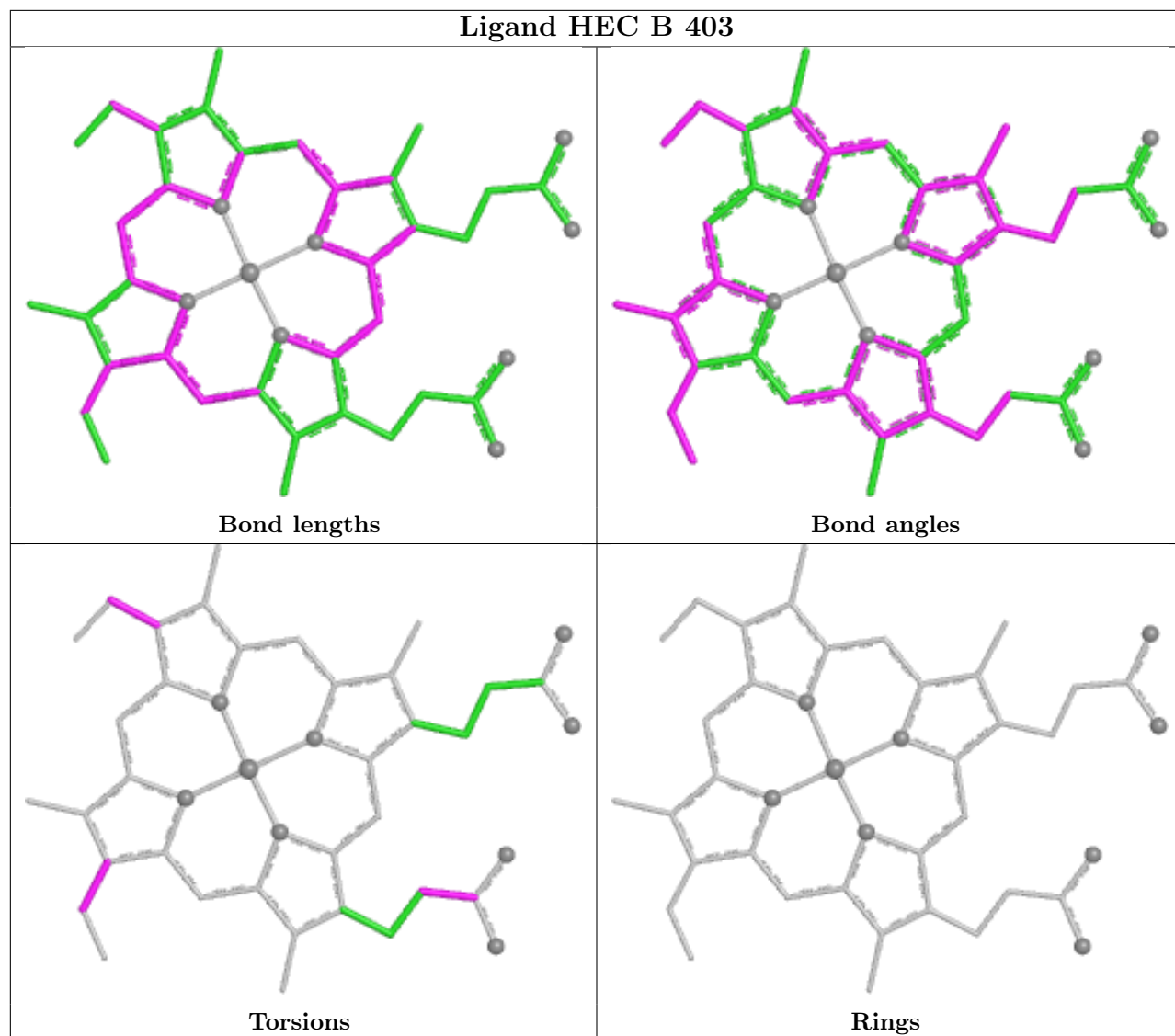
There are no ring outliers.

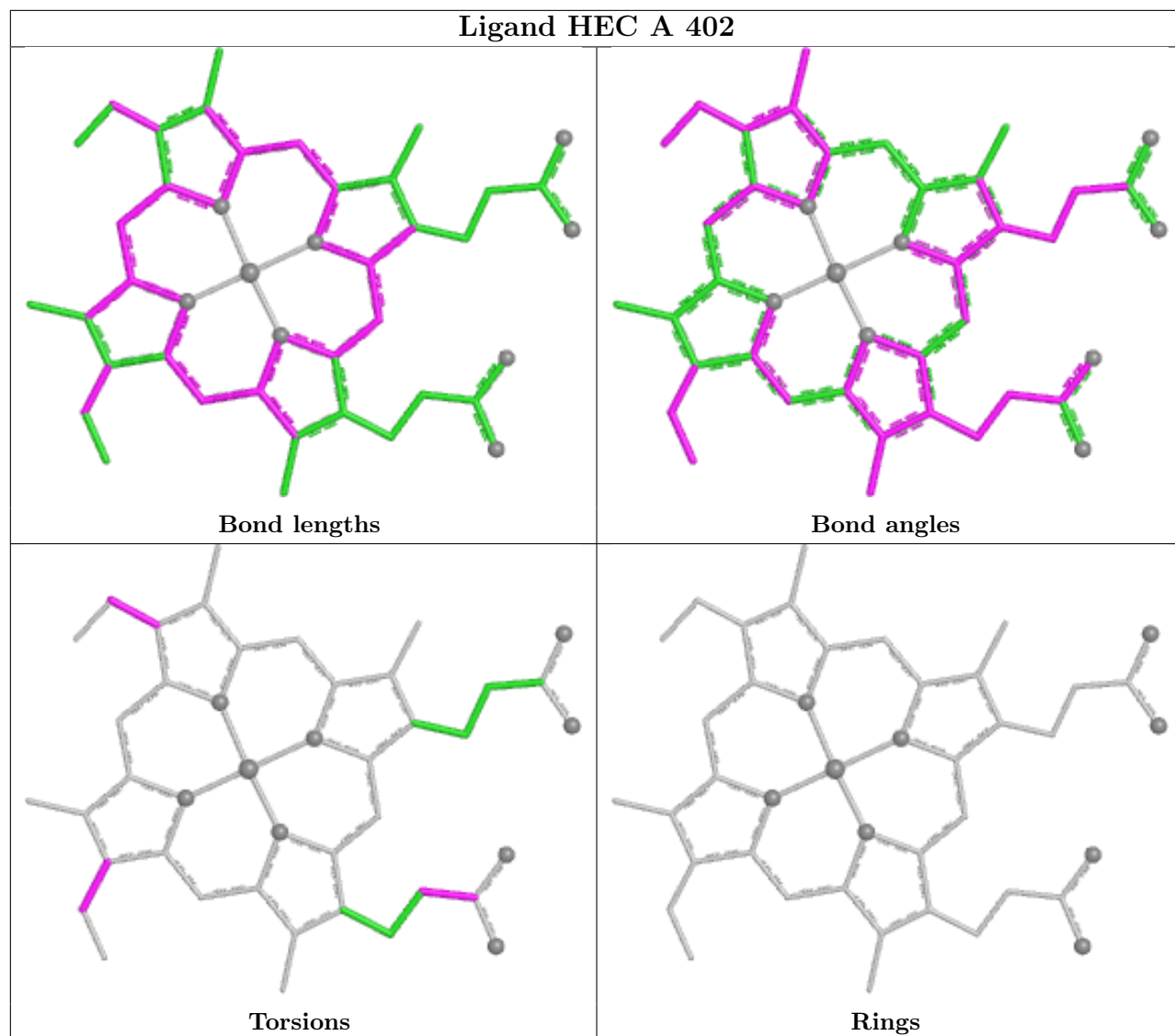
5 monomers are involved in 15 short contacts:

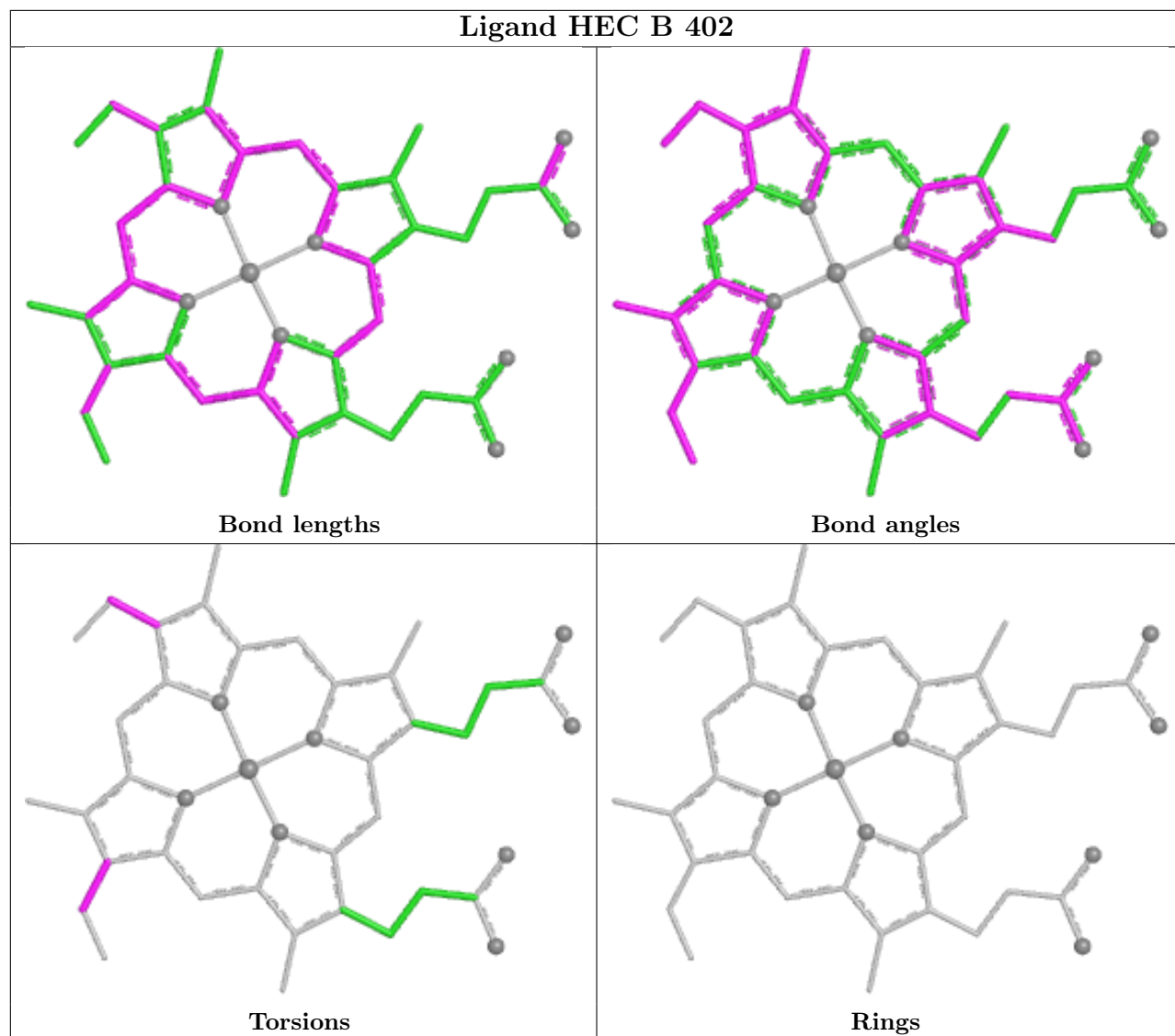
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	403	HEC	3	0
5	B	403	HEC	3	0
6	A	404	PGE	1	0
5	A	402	HEC	2	0
5	B	402	HEC	6	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	354/373 (94%)	-0.19	2 (0%) 85 88	13, 39, 55, 71	7 (1%)
1	B	359/373 (96%)	-0.39	2 (0%) 85 88	18, 33, 51, 87	1 (0%)
2	C	130/137 (94%)	-0.14	1 (0%) 82 85	22, 36, 65, 82	1 (0%)
2	E	125/137 (91%)	-0.45	1 (0%) 82 85	14, 29, 42, 69	3 (2%)
3	D	376/385 (97%)	-0.17	0 100 100	13, 42, 67, 77	5 (1%)
3	F	376/385 (97%)	-0.51	1 (0%) 90 92	15, 30, 47, 61	4 (1%)
All	All	1720/1790 (96%)	-0.31	7 (0%) 88 91	13, 35, 58, 87	21 (1%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	131	SER	3.4
1	B	364	ALA	3.0
1	A	133[A]	ARG	2.7
2	C	137	HIS	2.6
1	A	6	ALA	2.6
3	F	207	GLY	2.5
1	B	6	ALA	2.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	0AF	C	57	15/16	0.90	0.10	39,43,47,49	0
2	0AF	E	57	15/16	0.94	0.07	31,34,38,40	0

### 6.3 Carbohydrates [i](#)

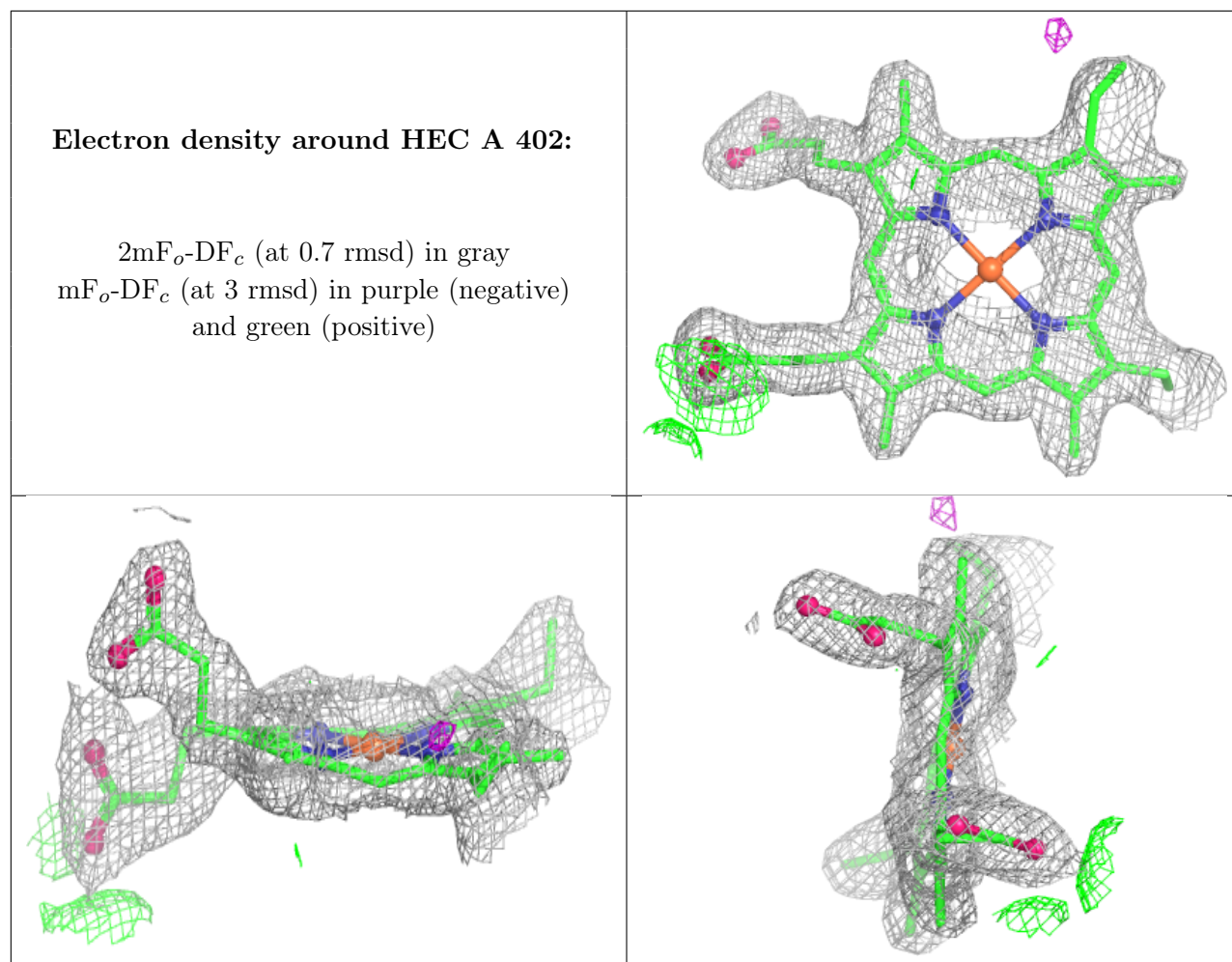
There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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

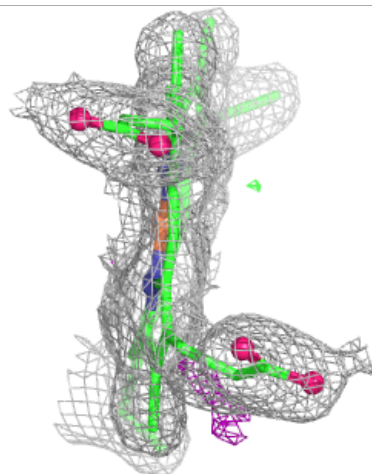
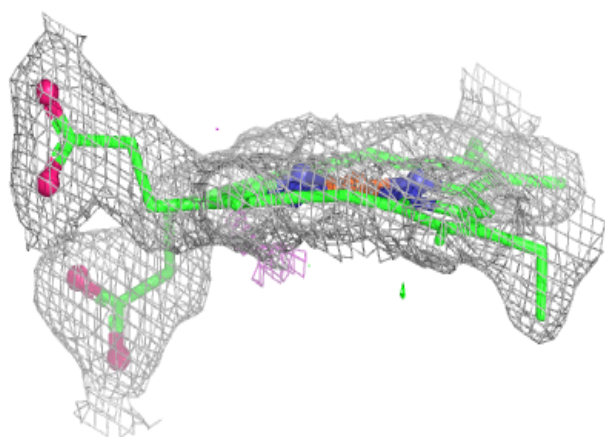
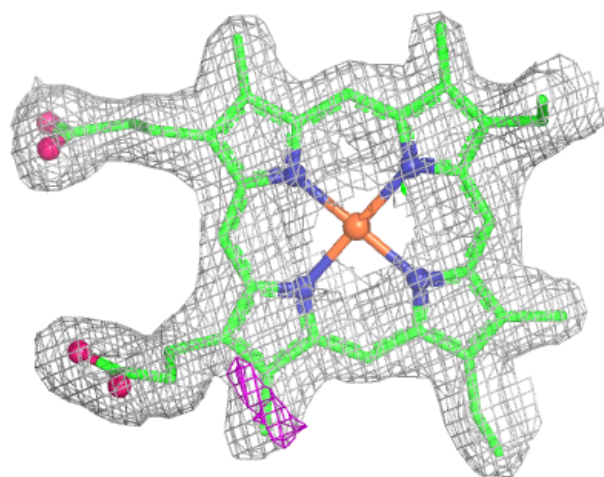
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	PGE	A	404	10/10	0.73	0.17	78,86,90,90	0
9	PO4	B	404	5/5	0.82	0.10	83,84,84,85	0
8	NA	A	406	1/1	0.84	0.10	61,61,61,61	0
7	EDO	A	405	4/4	0.86	0.10	59,59,60,60	0
10	ACT	D	401	4/4	0.92	0.12	46,47,47,48	0
7	EDO	B	405	4/4	0.94	0.10	44,46,47,48	0
10	ACT	F	401	4/4	0.95	0.12	42,44,46,46	0
8	NA	B	406	1/1	0.96	0.04	38,38,38,38	0
5	HEC	A	402	43/43	0.97	0.07	27,35,38,40	0
5	HEC	B	402	43/43	0.98	0.06	20,27,31,31	0
5	HEC	A	403	43/43	0.98	0.06	27,31,35,38	0
8	NA	B	407	1/1	0.98	0.03	42,42,42,42	0
4	CA	B	401	1/1	0.99	0.03	26,26,26,26	0
4	CA	A	401	1/1	0.99	0.03	33,33,33,33	0
5	HEC	B	403	43/43	0.99	0.05	16,22,26,29	0

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



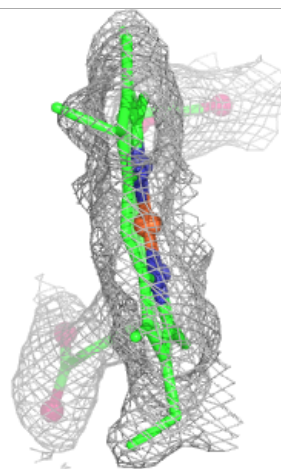
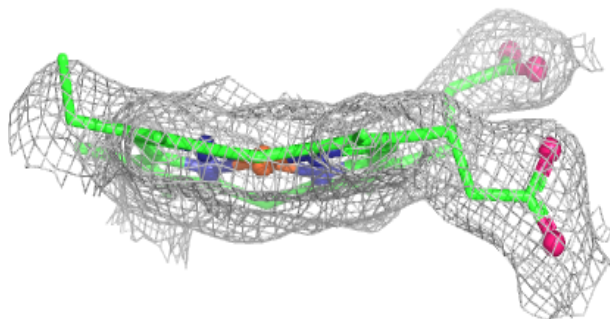
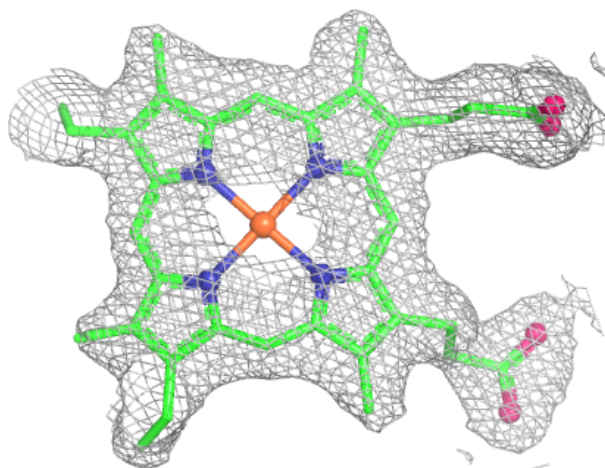
**Electron density around HEC B 402:**

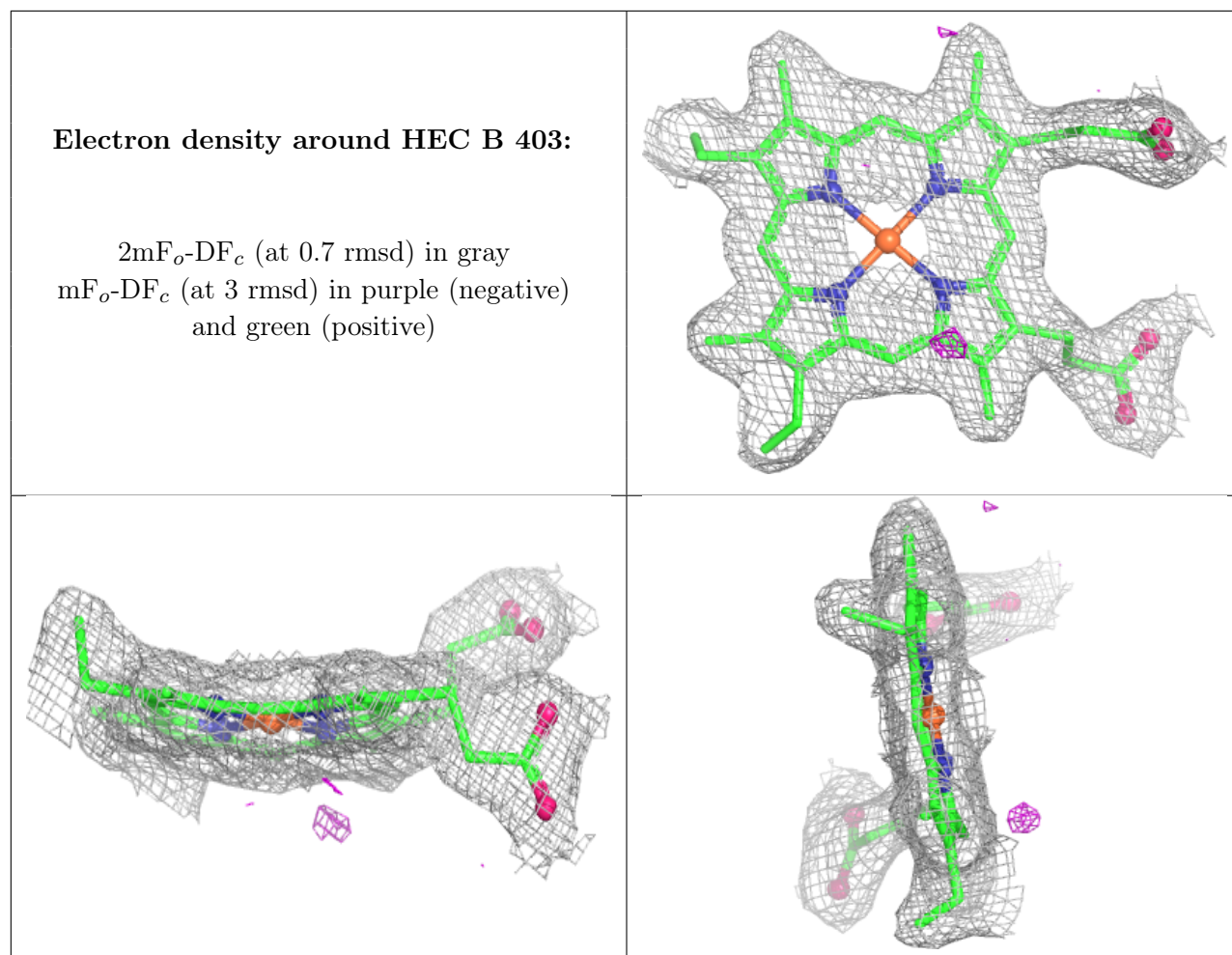
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC A 403:**

$2mF_o-DF_c$  (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.