



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:16 AM UTC

PDB ID : 4FA5 / pdb\_00004fa5  
Title : Crystal Structure of WT MauG in Complex with Pre-Methylamine Dehydrogenase Aged 20 Days  
Authors : Yukl, E.T.; Wilmot, C.M.  
Deposited on : 2012-05-21  
Resolution : 1.94 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

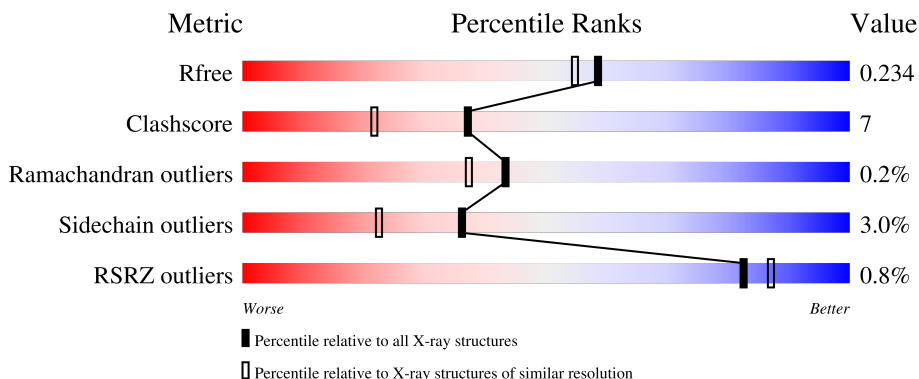
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.94 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.



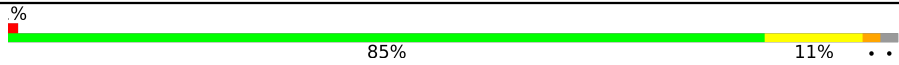
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	80% 14% • 5%
1	B	373	82% 13% • •
2	C	137	4% 77% 15% •• 6%
2	E	137	% 69% 19% • 9%
3	D	385	% 81% 15% ••

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Mol	Chain	Length	Quality of chain
3	F	385	 <p>A horizontal bar chart representing the quality of chain. The bar is primarily green, indicating a high quality score of 85%. A small portion at the end is yellow, indicating a lower quality score of 11%. The bar is labeled with a '%' symbol at the start and '85%' and '11%' at the corresponding points. There are two small black dots at the far right end of the bar.</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	0AF	E	57[B]	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15078 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	Total	C	N	O	S	0	5	0
			2779	1732	501	535	11			
1	B	357	Total	C	N	O	S	0	8	0
			2838	1765	517	544	12			

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	129	Total	C	N	O	S	0	3	0
			1026	638	177	197	14			
2	E	125	Total	C	N	O	S	0	5	0
			1002	624	167	197	14			

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
3	D	376	Total	C	N	O	S	0	3	0
			2945	1865	507	564	9			
3	F	376	Total	C	N	O	S	0	5	0
			2965	1876	512	568	9			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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>).

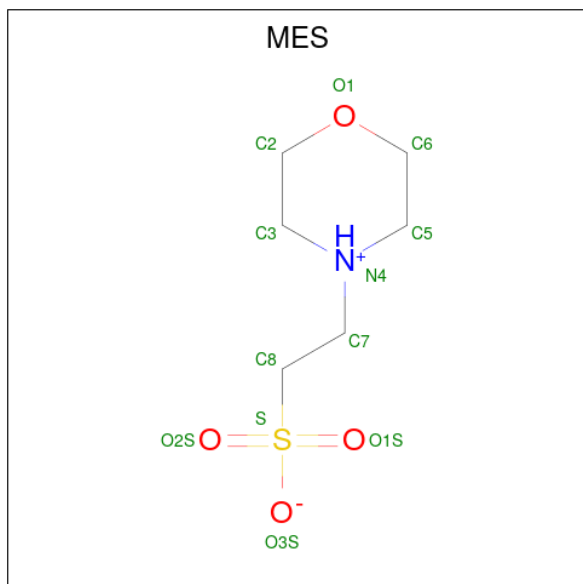


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
8	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		


- Molecule 9 is water.

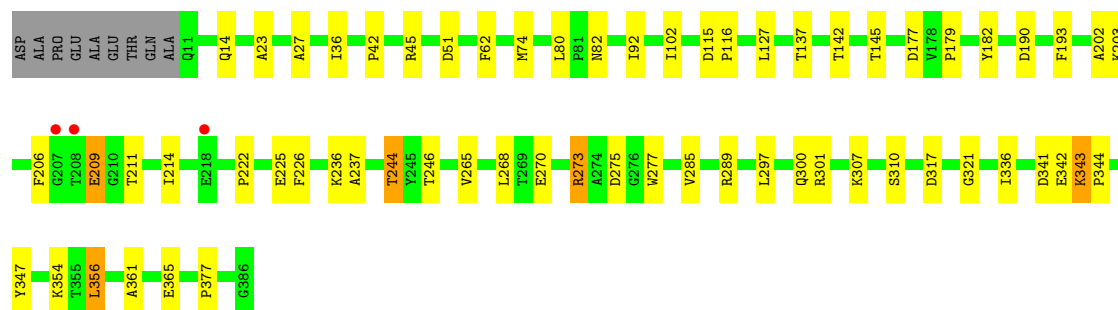
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	226	Total 228	O 228	0	2
9	B	308	Total 310	O 310	0	2
9	C	80	Total 80	O 80	0	0
9	D	235	Total 235	O 235	0	0
9	E	98	Total 98	O 98	0	0
9	F	358	Total 359	O 359	0	1




HIS  
HIS  
HIS

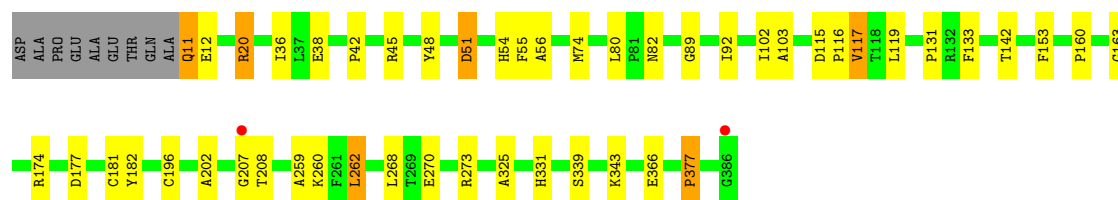
• Molecule 3: Methylamine dehydrogenase heavy chain

Chain D:  %



• Molecule 3: Methylamine dehydrogenase heavy chain

Chain F:  %



## 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 109.94° 91.54° 105.78°	Depositor
Resolution (Å)	44.49 – 1.94 44.49 – 1.94	Depositor EDS
% Data completeness (in resolution range)	97.6 (44.49-1.94) 97.6 (44.49-1.94)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 1.94Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.152 , 0.204 (Not available) , 0.234	Depositor DCC
$R_{free}$ test set	6440 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.2	Xtrriage
Anisotropy	0.045	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 33.9	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	0.97	EDS
Total number of atoms	15078	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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: MES, EDO, HEC, CA, OAF, NA

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	1.14	5/2846 (0.2%)	1.14	3/3860 (0.1%)
1	B	1.29	4/2902 (0.1%)	1.18	6/3932 (0.2%)
2	C	1.19	1/1029 (0.1%)	1.13	2/1406 (0.1%)
2	E	1.36	4/1001 (0.4%)	1.28	3/1368 (0.2%)
3	D	1.19	6/3026 (0.2%)	1.14	8/4122 (0.2%)
3	F	1.34	9/3045 (0.3%)	1.21	3/4147 (0.1%)
All	All	1.25	29/13849 (0.2%)	1.17	25/18835 (0.1%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	207	GLY	C-O	7.39	1.30	1.23
3	D	27	ALA	CA-CB	6.85	1.64	1.53
1	A	158	ALA	CA-CB	6.59	1.63	1.53
3	F	51	ASP	N-CA	-6.59	1.39	1.46
3	D	80	LEU	N-CA	6.55	1.51	1.46
2	E	112	ALA	CA-CB	6.39	1.63	1.53
1	B	101	LYS	C-O	-6.06	1.17	1.24
3	D	343	LYS	C-O	5.98	1.26	1.23
3	F	377	PRO	N-CA	-5.90	1.40	1.47
3	D	23	ALA	CA-CB	5.90	1.62	1.53
3	F	325	ALA	CA-C	-5.79	1.45	1.52
3	F	259	ALA	CA-CB	-5.72	1.45	1.53
2	E	107	ILE	CA-CB	5.71	1.59	1.53
1	A	252	ARG	C-O	-5.60	1.17	1.24
3	F	117	VAL	C-O	-5.59	1.17	1.23
3	F	103	ALA	CA-CB	5.57	1.62	1.53
3	D	80	LEU	CA-CB	5.46	1.57	1.52
2	C	86	CYS	C-O	5.42	1.26	1.23
1	B	242	ALA	CA-CB	5.36	1.62	1.53
1	A	104	ALA	CA-CB	5.33	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	112	VAL	CA-CB	5.33	1.60	1.54
3	D	356	LEU	N-CA	-5.20	1.39	1.46
2	E	120	HIS	CA-C	5.20	1.57	1.52
3	F	131	PRO	N-CA	-5.16	1.43	1.47
1	B	266	VAL	CA-C	5.08	1.58	1.52
1	B	12	ALA	CA-CB	5.04	1.61	1.53
3	F	80	LEU	N-CA	5.03	1.50	1.46
1	A	122	VAL	CA-CB	5.02	1.60	1.54
2	E	22	ALA	C-O	5.01	1.30	1.23

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	7	ASP	N-CA-C	-8.73	101.67	111.71
2	E	129	LYS	N-CA-C	-7.40	99.53	110.48
1	B	186	THR	CA-C-N	-6.53	112.10	119.28
1	B	186	THR	C-N-CA	-6.53	112.10	119.28
1	A	121	ALA	N-CA-C	-6.32	104.26	112.23
3	F	262	LEU	CA-C-N	-6.11	113.65	119.76
3	F	262	LEU	C-N-CA	-6.11	113.65	119.76
3	D	244	THR	N-CA-C	-6.03	101.53	110.46
3	D	209	GLU	N-CA-C	5.99	118.18	109.07
2	C	129	LYS	N-CA-C	-5.96	101.13	110.36
3	F	339	SER	N-CA-C	-5.88	102.77	110.53
3	D	80	LEU	CA-C-N	-5.78	114.65	120.31
3	D	80	LEU	C-N-CA	-5.78	114.65	120.31
3	D	137	THR	N-CA-C	5.61	117.83	109.59
1	B	228	LEU	N-CA-C	5.51	116.83	109.83
2	E	46	CYS	CA-C-N	5.50	123.62	119.66
2	E	46	CYS	C-N-CA	5.50	123.62	119.66
1	A	33	THR	N-CA-C	-5.25	105.64	111.36
1	A	203	LEU	N-CA-C	-5.23	106.41	112.89
2	C	54	THR	N-CA-C	-5.20	107.11	113.50
3	D	285	VAL	N-CA-C	5.16	115.91	108.48
1	B	20	ASP	CA-C-N	-5.13	114.75	120.45
1	B	20	ASP	C-N-CA	-5.13	114.75	120.45
3	D	145	THR	N-CA-C	-5.03	102.84	110.39
3	D	115	ASP	N-CA-C	-5.00	103.35	109.65

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	2779	0	2648	40	0
1	B	2838	0	2708	31	0
2	C	1026	0	907	24	0
2	E	1002	0	893	32	0
3	D	2945	0	2826	48	0
3	F	2965	0	2844	29	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	86	0	60	2	0
5	B	86	0	60	1	0
6	A	8	0	12	0	0
6	B	4	0	6	0	0
7	A	1	0	0	0	0
7	B	2	0	0	0	0
8	D	12	0	12	0	0
8	F	12	0	12	0	0
9	A	228	0	0	4	0
9	B	310	0	0	4	0
9	C	80	0	0	5	0
9	D	235	0	0	2	0
9	E	98	0	0	4	0
9	F	359	0	0	4	0
All	All	15078	0	12988	189	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 7.

All (189) 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)
2:E:57[B]:0AF:CA	2:E:57[B]:0AF:CB	1.76	1.61
3:D:273[B]:ARG:HH11	3:D:273[B]:ARG:CG	1.66	1.08
3:D:270:GLU:HA	3:D:273[A]:ARG:HH12	1.11	1.08
3:D:273[B]:ARG:HG2	3:D:273[B]:ARG:NH1	1.55	1.05
1:A:206:MET:HA	1:A:206:MET:HE2	1.46	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:273[A]:ARG:HB2	3:D:273[A]:ARG:HH11	1.29	0.97
3:D:265:VAL:HG21	3:D:321:GLY:HA3	1.53	0.89
3:F:11:GLN:HB3	9:F:853:HOH:O	1.74	0.87
3:D:273[A]:ARG:HH11	3:D:273[A]:ARG:CB	1.85	0.87
3:D:273[B]:ARG:HH11	3:D:273[B]:ARG:HG2	0.74	0.87
9:B:797:HOH:O	2:E:127:VAL:HG12	1.74	0.86
1:A:206:MET:HE1	1:A:218:PHE:CD2	2.10	0.85
3:D:237:ALA:HB2	3:D:289:ARG:HG3	1.58	0.85
3:D:14:GLN:HE21	2:E:21:GLN:HE22	1.25	0.84
1:B:197:ILE:O	1:B:202[B]:ARG:HD2	1.75	0.84
1:A:127[A]:ARG:HD2	9:A:708:HOH:O	1.77	0.83
2:C:57[B]:OAF:HBC1	2:C:108[B]:TRP:NE1	1.95	0.82
1:B:210:GLN:HE22	2:E:44:THR:HG21	1.43	0.82
3:D:265:VAL:HG21	3:D:321:GLY:CA	2.10	0.81
3:D:342:GLU:HA	9:D:733:HOH:O	1.81	0.80
3:D:273[A]:ARG:HH11	3:D:273[A]:ARG:CG	1.92	0.80
1:B:197:ILE:HG22	1:B:206[A]:MET:HE1	1.67	0.75
9:C:273:HOH:O	3:F:36:ILE:HD11	1.87	0.74
1:A:107:PRO:HG3	9:A:661[B]:HOH:O	1.88	0.73
3:F:11:GLN:HA	3:F:11:GLN:NE2	2.06	0.71
3:D:265:VAL:CG2	3:D:321:GLY:HA3	2.20	0.70
1:A:210:GLN:HE22	2:C:44:THR:HG21	1.56	0.70
3:D:273[B]:ARG:CG	3:D:273[B]:ARG:NH1	2.36	0.68
2:E:58[A]:VAL:HG12	2:E:73:ALA:HA	1.74	0.68
1:B:285:THR:HG22	1:B:286:ASP:OD1	1.93	0.68
1:A:206:MET:CE	1:A:218:PHE:CD2	2.77	0.68
3:F:11:GLN:HA	3:F:11:GLN:HE21	1.59	0.67
1:A:205:HIS:O	1:A:206:MET:HE3	1.93	0.67
2:E:57[A]:OAF:CE3	2:E:108[A]:TRP:CD1	2.79	0.66
3:D:270:GLU:HA	3:D:273[A]:ARG:NH1	1.97	0.66
2:E:57[B]:OAF:HBC1	2:E:108[B]:TRP:NE1	2.11	0.66
3:D:273[A]:ARG:CG	3:D:273[A]:ARG:NH1	2.54	0.66
1:B:301:ARG:NH2	3:F:177[B]:ASP:OD1	2.30	0.65
2:C:129:LYS:O	2:C:130:ALA:CB	2.45	0.65
3:D:273[A]:ARG:NH1	3:D:273[A]:ARG:HG3	2.12	0.64
3:D:270:GLU:CA	3:D:273[A]:ARG:HH12	1.99	0.64
1:A:133:ARG:HB2	1:A:133:ARG:NH1	2.14	0.62
1:A:68:PRO:HG2	5:A:402:HEC:HBA1	1.82	0.62
1:A:110:ASN:OD1	1:A:112:VAL:HG13	2.00	0.62
1:A:133:ARG:HB2	1:A:133:ARG:CZ	2.29	0.61
2:E:23:CYS:SG	2:E:88[B]:CYS:HB2	2.40	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180[B]:ARG:HD3	1:A:182:GLU:CD	2.26	0.61
2:E:57[B]:0AF:CB	2:E:57[B]:0AF:HA	2.16	0.61
1:B:300[A]:ARG:HG2	1:B:300[A]:ARG:O	1.98	0.61
1:A:206:MET:HA	1:A:206:MET:CE	2.28	0.60
3:F:12:GLU:OE1	3:F:20:ARG:HD3	2.02	0.60
3:F:270[B]:GLU:HB2	3:F:273[B]:ARG:NH2	2.17	0.59
1:A:206:MET:HE1	1:A:218:PHE:CE2	2.37	0.59
3:D:51:ASP:HA	3:D:377:PRO:HA	1.85	0.58
2:E:57[B]:0AF:CA	2:E:57[B]:0AF:CG	2.73	0.58
3:D:343:LYS:HE3	3:D:343:LYS:HA	1.85	0.58
2:E:57[B]:0AF:CB	2:E:57[B]:0AF:N	2.62	0.57
3:D:273[A]:ARG:HB2	3:D:273[A]:ARG:NH1	2.10	0.57
2:C:57[A]:0AF:CE3	2:C:108[A]:TRP:CD1	2.88	0.57
1:A:48:LYS:H	1:A:62:HIS:HE1	1.52	0.56
1:A:243[A]:ASP:OD2	1:A:243[A]:ASP:N	2.37	0.56
1:B:202[A]:ARG:HG2	1:B:206[A]:MET:HE2	1.88	0.56
1:B:210:GLN:NE2	2:E:44:THR:HG21	2.19	0.56
3:F:82:ASN:HB3	3:F:142:THR:HB	1.88	0.56
2:C:129:LYS:NZ	9:C:247:HOH:O	2.39	0.55
3:F:51:ASP:HA	3:F:377:PRO:HA	1.89	0.55
1:B:198:THR:HG22	2:E:58[A]:VAL:HG13	1.87	0.55
1:B:299:SER:HB2	1:B:333:MET:HG3	1.88	0.54
1:B:300[A]:ARG:NH1	9:F:855:HOH:O	2.40	0.54
3:D:246:THR:O	3:D:273[A]:ARG:HD3	2.08	0.53
1:B:197:ILE:HA	1:B:202[A]:ARG:HG3	1.91	0.53
1:B:296:LYS:NZ	9:B:570:HOH:O	2.37	0.53
3:D:236:LYS:HD3	3:D:289:ARG:NH1	2.24	0.53
2:C:57[B]:0AF:HZ3	9:C:225:HOH:O	2.08	0.53
3:D:265:VAL:HG21	3:D:321:GLY:HA2	1.89	0.53
2:E:19:ASP:O	2:E:25:TYR:HB2	2.09	0.53
1:B:197:ILE:O	1:B:202[B]:ARG:CD	2.55	0.51
1:A:21:PRO:O	1:A:27:ALA:HA	2.11	0.51
1:A:205:HIS:O	1:A:206:MET:CE	2.59	0.51
2:C:57[B]:0AF:HBC1	2:C:108[B]:TRP:HE1	1.71	0.51
1:A:9:ALA:HB3	1:A:139:LEU:HD21	1.93	0.50
3:D:179:PRO:HD3	3:D:214:ILE:HD13	1.94	0.50
3:D:347:TYR:HB3	3:D:356:LEU:HD11	1.94	0.50
3:F:331:HIS:HE1	3:F:366:GLU:OE1	1.95	0.49
1:A:243[B]:ASP:HB3	9:A:629:HOH:O	2.12	0.49
3:F:54:HIS:HE1	9:F:706:HOH:O	1.94	0.49
3:D:297:LEU:HD22	3:D:310:SER:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:56:SER:CB	2:E:74:TYR:O	2.60	0.49
2:E:57[A]:OAF:HE3	2:E:108[A]:TRP:CD1	2.47	0.49
9:E:242:HOH:O	3:F:54:HIS:HD2	1.95	0.49
2:E:56:SER:HB2	2:E:74:TYR:O	2.12	0.49
2:C:129:LYS:O	2:C:130:ALA:HB3	2.12	0.49
1:A:120:ALA:HA	1:A:148:PRO:HB3	1.94	0.49
1:B:52:ALA:O	1:B:66:ASN:HA	2.13	0.49
3:D:336:ILE:HA	3:D:347:TYR:O	2.12	0.49
1:A:82:ASP:C	1:A:82:ASP:OD2	2.55	0.48
1:B:194:THR:HG21	2:E:101[B]:GLU:HG3	1.95	0.48
3:F:268:LEU:O	3:F:273[B]:ARG:NH1	2.46	0.48
3:D:36:ILE:HD13	2:E:46:CYS:HB2	1.95	0.48
2:E:75:ARG:HA	9:E:289:HOH:O	2.12	0.48
2:C:75:ARG:HD2	9:C:279:HOH:O	2.12	0.48
2:E:71:LEU:HD22	2:E:129:LYS:O	2.14	0.48
1:A:177:ARG:HG2	1:A:180[B]:ARG:HH11	1.78	0.47
2:E:76:ASP:HB2	2:E:108[B]:TRP:O	2.14	0.47
3:D:222:PRO:HG2	3:D:225:GLU:HB2	1.96	0.47
2:E:58[B]:VAL:O	2:E:102:PHE:HD1	1.98	0.47
1:B:243[B]:ASP:OD2	9:B:635[B]:HOH:O	2.21	0.47
3:D:62:PHE:CE2	3:D:74:MET:HE3	2.49	0.47
3:F:45:ARG:NH2	3:F:343:LYS:O	2.47	0.47
3:D:275:ASP:HB2	9:D:715:HOH:O	2.13	0.46
3:D:344:PRO:HG2	3:D:361:ALA:HB3	1.97	0.46
1:A:60:GLN:O	1:A:62:HIS:HD2	1.98	0.46
2:E:57[B]:OAF:HBC1	2:E:108[B]:TRP:HE1	1.80	0.46
3:F:153:PHE:CZ	3:F:163:GLY:HA3	2.50	0.46
3:D:45:ARG:NH2	3:D:343:LYS:O	2.49	0.46
1:B:202[A]:ARG:HH22	1:B:209:LYS:HA	1.81	0.46
2:C:25:TYR:HB3	2:C:28:HIS:CD2	2.51	0.45
3:D:82:ASN:HB3	3:D:142:THR:HB	1.97	0.45
3:D:226:PHE:O	3:D:244:THR:HA	2.16	0.45
2:C:23:CYS:SG	2:C:88[B]:CYS:HB2	2.56	0.45
3:D:341:ASP:OD1	3:D:341:ASP:N	2.40	0.45
1:B:355:GLU:O	1:B:358:LEU:HB2	2.16	0.45
3:D:277:TRP:CE2	3:D:300:GLN:HG3	2.51	0.45
2:E:53:ALA:HB2	2:E:109:CYS:HA	1.98	0.45
1:A:180[B]:ARG:HD3	1:A:182:GLU:OE1	2.17	0.45
3:D:36:ILE:CD1	2:E:46:CYS:HB2	2.46	0.45
1:A:299:SER:HB2	1:A:333:MET:HG3	1.99	0.45
3:D:190:ASP:HB2	3:D:206:PHE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:75:ARG:HA	9:C:272:HOH:O	2.17	0.44
2:E:75:ARG:HD2	9:E:269:HOH:O	2.17	0.44
1:A:147:ASP:OD1	1:A:147:ASP:C	2.60	0.44
1:B:81:ARG:HB2	1:B:87:TYR:CE2	2.53	0.44
2:C:23:CYS:SG	2:C:88[B]:CYS:SG	3.15	0.44
3:F:115:ASP:O	3:F:119:LEU:HA	2.17	0.44
2:C:105:ASP:OD1	3:D:307:LYS:NZ	2.47	0.44
3:F:89:GLY:HA2	9:F:571:HOH:O	2.17	0.43
1:B:81:ARG:NH1	1:B:85:GLY:HA2	2.32	0.43
2:E:101[B]:GLU:HG2	2:E:102:PHE:CD2	2.53	0.43
1:B:202[A]:ARG:NH2	9:B:699:HOH:O	2.51	0.43
1:A:210:GLN:NE2	2:C:44:THR:HG21	2.28	0.43
1:A:65:ARG:HH12	1:A:94:ASP:CG	2.27	0.43
2:C:63:ASN:OD1	2:C:63:ASN:C	2.62	0.43
2:C:23:CYS:HB3	2:C:88[B]:CYS:SG	2.59	0.43
1:B:21:PRO:O	1:B:27:ALA:HA	2.19	0.43
1:A:81:ARG:CZ	1:A:85:GLY:HA2	2.48	0.43
1:A:40:ALA:HA	1:A:354:TYR:CZ	2.54	0.42
1:A:206:MET:CE	1:A:218:PHE:HD2	2.27	0.42
3:D:42:PRO:HG3	3:D:116:PRO:HB2	2.01	0.42
2:E:130:ALA:HB3	9:E:287:HOH:O	2.19	0.42
1:B:39:ARG:HD2	1:B:44:PRO:HB3	2.00	0.42
1:A:91:GLN:O	1:A:92:PHE:HB2	2.18	0.42
2:C:10:ARG:HB3	3:D:301:ARG:HB3	2.02	0.42
2:E:107:ILE:HD12	2:E:119:TYR:HB2	2.01	0.42
1:A:48:LYS:HD2	1:A:62:HIS:NE2	2.34	0.42
1:A:95:GLY:HA3	1:A:223:TYR:OH	2.19	0.42
1:A:133:ARG:NH1	1:A:133:ARG:CB	2.81	0.42
3:F:48:TYR:CZ	3:F:92:ILE:HG21	2.55	0.42
1:A:267:PRO:HD3	5:A:403:HEC:CAD	2.50	0.42
1:A:197:ILE:HA	1:A:202:ARG:HB3	2.02	0.41
2:E:82:VAL:HG12	3:F:56:ALA:HA	2.02	0.41
1:B:278:TYR:O	1:B:279:MET:HB2	2.21	0.41
3:D:268:LEU:HD22	3:D:277:TRP:HB3	2.01	0.41
3:F:38:GLU:HB3	3:F:117:VAL:CG1	2.49	0.41
1:A:186:THR:O	1:A:187:PRO:C	2.61	0.41
2:C:57[A]:OAF:HE3	2:C:108[A]:TRP:CD1	2.55	0.41
3:D:203:LYS:O	3:D:214:ILE:HA	2.21	0.41
1:A:202:ARG:NE	9:A:697:HOH:O	2.47	0.41
2:C:23:CYS:CB	2:C:88[B]:CYS:SG	3.08	0.41
3:F:38:GLU:HB3	3:F:117:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:98:TYR:HA	3:D:182:TYR:CE1	2.56	0.41
3:F:42:PRO:HG3	3:F:116:PRO:HB2	2.02	0.41
1:B:88[A]:LYS:HE2	1:B:88[A]:LYS:HB3	1.97	0.41
1:B:113:GLU:HG2	5:B:402:HEC:HBC2	2.03	0.41
3:D:236:LYS:HD3	3:D:289:ARG:HH12	1.86	0.41
3:F:174[B]:ARG:CZ	3:F:208:THR:HA	2.51	0.41
1:B:197:ILE:HG22	1:B:206[A]:MET:CE	2.46	0.41
2:C:56:SER:CB	2:C:74:TYR:O	2.69	0.41
1:B:96:ARG:HA	1:B:252[B]:ARG:HG3	2.02	0.40
1:B:223:TYR:HB3	1:B:263:ARG:HB3	2.03	0.40
3:F:54:HIS:O	3:F:55:PHE:HB2	2.21	0.40
1:B:299:SER:HB3	1:B:304:ALA:CB	2.51	0.40
2:E:106:ILE:HG12	3:F:133:PHE:CZ	2.57	0.40
3:F:74:MET:HE2	3:F:74:MET:HB3	1.92	0.40
3:F:181[B]:CYS:HA	3:F:196:CYS:HA	2.03	0.40
3:F:196:CYS:SG	3:F:202:ALA:HB2	2.61	0.40
2:C:57[B]:OAF:HBC1	2:C:108[B]:TRP:CE2	2.56	0.40
2:C:102:PHE:HE1	2:C:132:HIS:CE1	2.39	0.40
3:D:193:PHE:HA	3:D:202:ALA:O	2.22	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	357/373 (96%)	348 (98%)	9 (2%)	0	100	100
1	B	363/373 (97%)	351 (97%)	12 (3%)	0	100	100
2	C	128/137 (93%)	123 (96%)	4 (3%)	1 (1%)	16	7
2	E	126/137 (92%)	124 (98%)	2 (2%)	0	100	100
3	D	377/385 (98%)	359 (95%)	17 (4%)	1 (0%)	36	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	379/385 (98%)	366 (97%)	12 (3%)	1 (0%)	36	30
All	All	1730/1790 (97%)	1671 (97%)	56 (3%)	3 (0%)	43	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	130	ALA
3	F	102	ILE
3	D	102	ILE

### 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	281/292 (96%)	269 (96%)	12 (4%)	26	13
1	B	287/292 (98%)	274 (96%)	13 (4%)	24	11
2	C	110/112 (98%)	106 (96%)	4 (4%)	31	17
2	E	108/112 (96%)	106 (98%)	2 (2%)	50	40
3	D	307/310 (99%)	297 (97%)	10 (3%)	33	20
3	F	309/310 (100%)	304 (98%)	5 (2%)	55	46
All	All	1402/1428 (98%)	1356 (97%)	46 (3%)	36	20

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	51	LEU
1	A	84	ASN
1	A	112	VAL
1	A	142	LYS
1	A	197	ILE
1	A	206	MET
1	A	243[A]	ASP

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Mol	Chain	Res	Type
1	A	243[B]	ASP
1	A	323	LEU
1	A	357	LEU
1	A	358	LEU
1	B	84	ASN
1	B	167	GLU
1	B	183	GLU
1	B	202[A]	ARG
1	B	202[B]	ARG
1	B	219	THR
1	B	300[A]	ARG
1	B	300[B]	ARG
1	B	321[A]	ARG
1	B	321[B]	ARG
1	B	357	LEU
1	B	358	LEU
1	B	361	SER
2	C	7	THR
2	C	71	LEU
2	C	129	LYS
2	C	131	SER
3	D	92	ILE
3	D	127	LEU
3	D	177	ASP
3	D	209	GLU
3	D	211	THR
3	D	273[A]	ARG
3	D	273[B]	ARG
3	D	317	ASP
3	D	354	LYS
3	D	365	GLU
2	E	68	GLN
2	E	71	LEU
3	F	11	GLN
3	F	20	ARG
3	F	160	PRO
3	F	260	LYS
3	F	262	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	62	HIS
1	A	91	GLN
1	A	210	GLN
1	B	60	GLN
1	B	91	GLN
1	B	163	GLN
1	B	210	GLN
2	C	21	GLN
2	C	132	HIS
2	E	21	GLN
2	E	68	GLN
3	F	11	GLN
3	F	30	GLN
3	F	50	ASN
3	F	54	HIS
3	F	61	GLN
3	F	300	GLN
3	F	331	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 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	E	57[A]	2	15,16,17	1.57	3 (20%)	14,22,24	1.54	4 (28%)
2	0AF	C	57[A]	2	15,16,17	1.41	2 (13%)	14,22,24	1.06	0
2	0AF	C	57[B]	2	15,16,17	2.27	6 (40%)	14,22,24	1.66	4 (28%)
2	0AF	E	57[B]	2	15,16,17	3.63	5 (33%)	14,22,24	2.19	6 (42%)

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	E	57[A]	2	-	1/5/6/8	0/2/2/2
2	0AF	C	57[A]	2	-	1/5/6/8	0/2/2/2
2	0AF	C	57[B]	2	-	0/5/6/8	0/2/2/2
2	0AF	E	57[B]	2	-	0/5/6/8	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	57[B]	0AF	CB-CA	11.03	1.76	1.53
2	C	57[B]	0AF	CE2-NE1	-5.23	1.29	1.37
2	E	57[B]	0AF	CE2-NE1	-5.14	1.29	1.37
2	E	57[B]	0AF	CD1-NE1	-4.78	1.29	1.37
2	C	57[B]	0AF	CD1-NE1	-4.19	1.30	1.37
2	E	57[B]	0AF	CE3-CD2	3.07	1.44	1.39
2	C	57[A]	0AF	CD2-CE2	-2.79	1.38	1.41
2	E	57[A]	0AF	CD1-CG	2.76	1.40	1.36
2	C	57[B]	0AF	CD2-CE2	-2.57	1.38	1.41
2	E	57[B]	0AF	CE2-CZ2	-2.56	1.34	1.40
2	E	57[A]	0AF	CD2-CE2	-2.45	1.38	1.41
2	C	57[A]	0AF	CD2-CG	-2.43	1.40	1.44
2	E	57[A]	0AF	CD2-CG	-2.39	1.40	1.44
2	C	57[B]	0AF	CE3-CD2	2.35	1.43	1.39
2	C	57[B]	0AF	CD2-CG	-2.25	1.40	1.44
2	C	57[B]	0AF	CE2-CZ2	-2.13	1.35	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	57[B]	0AF	CB-CG-CD1	-4.07	119.03	126.97
2	E	57[B]	0AF	CD2-CE2-NE1	3.34	112.29	107.54
2	E	57[B]	0AF	CB-CG-CD2	3.08	132.62	126.70
2	C	57[B]	0AF	CD2-CE2-NE1	2.94	111.72	107.54
2	C	57[B]	0AF	CB-CG-CD1	-2.85	121.41	126.97
2	E	57[B]	0AF	CE3-CD2-CG	2.80	138.02	133.85
2	E	57[A]	0AF	CG-CD1-NE1	-2.45	107.62	110.31
2	E	57[B]	0AF	CZ3-CE3-CD2	-2.39	115.48	119.80
2	C	57[B]	0AF	CZ3-CE3-CD2	-2.29	115.66	119.80
2	E	57[B]	0AF	CD2-CG-CD1	2.15	108.35	106.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	57[A]	0AF	CH2-CZ2-CE2	2.11	122.33	118.69
2	E	57[A]	0AF	O1-CZ2-CH2	2.10	125.01	119.36
2	C	57[B]	0AF	CB-CG-CD2	2.07	130.67	126.70
2	E	57[A]	0AF	CD2-CE2-NE1	2.03	110.42	107.54

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	57[A]	0AF	2	0
2	C	57[A]	0AF	2	0
2	C	57[B]	0AF	4	0
2	E	57[B]	0AF	6	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 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
8	MES	F	401	-	12,12,12	2.09	1 (8%)	15,16,16	3.72	8 (53%)
6	EDO	B	404	-	3,3,3	0.41	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	HEC	B	403	1	46,50,50	2.46	21 (45%)	58,82,82	2.76	21 (36%)
5	HEC	A	402	9,1	46,50,50	2.60	25 (54%)	58,82,82	2.42	23 (39%)
6	EDO	A	406	-	3,3,3	0.51	0	2,2,2	0.42	0
5	HEC	A	403	1	46,50,50	2.54	21 (45%)	58,82,82	2.83	19 (32%)
6	EDO	A	404	-	3,3,3	0.48	0	2,2,2	0.47	0
5	HEC	B	402	9,1	46,50,50	2.48	19 (41%)	58,82,82	2.61	24 (41%)
8	MES	D	401	-	12,12,12	1.73	1 (8%)	15,16,16	2.72	6 (40%)

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
8	MES	F	401	-	-	5/6/14/14	0/1/1/1
6	EDO	B	404	-	-	1/1/1/1	-
5	HEC	B	403	1	-	6/14/54/54	-
5	HEC	A	402	9,1	-	6/14/54/54	-
6	EDO	A	406	-	-	1/1/1/1	-
5	HEC	A	403	1	-	6/14/54/54	-
6	EDO	A	404	-	-	1/1/1/1	-
5	HEC	B	402	9,1	-	5/14/54/54	-
8	MES	D	401	-	-	6/6/14/14	0/1/1/1

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	401	MES	C8-S	-6.82	1.68	1.77
5	A	402	HEC	CAB-C3B	5.56	1.53	1.35
8	D	401	MES	C8-S	-5.53	1.69	1.77
5	A	402	HEC	CAC-C3C	5.49	1.52	1.35
5	B	402	HEC	CAB-C3B	5.33	1.52	1.35
5	B	403	HEC	C4D-ND	-5.17	1.29	1.39
5	A	403	HEC	CAC-C3C	5.16	1.51	1.35
5	A	403	HEC	CHB-C4A	5.12	1.48	1.38
5	B	403	HEC	CAC-C3C	5.05	1.51	1.35
5	B	402	HEC	CHB-C4A	4.93	1.48	1.38
5	B	403	HEC	C4A-NA	-4.86	1.30	1.39
5	B	402	HEC	CAC-C3C	4.85	1.50	1.35
5	B	403	HEC	CAB-C3B	4.85	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	403	HEC	CAB-C3B	4.74	1.50	1.35
5	A	402	HEC	CHC-C4B	4.73	1.47	1.38
5	B	402	HEC	C4B-NB	-4.43	1.31	1.39
5	A	402	HEC	CHD-C4C	4.30	1.46	1.38
5	A	403	HEC	CHC-C4B	4.28	1.46	1.38
5	A	403	HEC	C1B-NB	-4.27	1.31	1.39
5	A	403	HEC	C4A-NA	-4.24	1.31	1.39
5	A	403	HEC	C4C-NC	-4.14	1.31	1.39
5	B	402	HEC	CHD-C4C	4.11	1.46	1.38
5	A	402	HEC	CHA-C1A	4.10	1.46	1.38
5	B	402	HEC	CHC-C4B	4.07	1.46	1.38
5	A	402	HEC	C1D-ND	-4.04	1.32	1.39
5	A	402	HEC	CHB-C4A	3.98	1.46	1.38
5	A	402	HEC	C4D-ND	-3.98	1.32	1.39
5	B	402	HEC	C4A-NA	-3.97	1.32	1.39
5	B	403	HEC	CHD-C4C	3.93	1.46	1.38
5	B	403	HEC	C4B-NB	-3.79	1.32	1.39
5	A	403	HEC	C4D-ND	-3.78	1.32	1.39
5	B	403	HEC	CHB-C4A	3.75	1.45	1.38
5	B	403	HEC	CHD-C1D	3.72	1.47	1.39
5	B	403	HEC	C1B-NB	-3.70	1.32	1.39
5	A	402	HEC	CHD-C1D	3.69	1.47	1.39
5	B	402	HEC	CHA-C1A	3.67	1.45	1.38
5	B	403	HEC	C4C-NC	-3.61	1.32	1.39
5	A	403	HEC	CHD-C1D	3.60	1.47	1.39
5	A	402	HEC	CHA-C4D	3.55	1.47	1.39
5	A	403	HEC	CHD-C4C	3.52	1.45	1.38
5	B	402	HEC	C4C-NC	-3.50	1.33	1.39
5	B	402	HEC	C1D-ND	-3.41	1.33	1.39
5	B	403	HEC	CHC-C1C	3.41	1.47	1.39
5	A	403	HEC	CHA-C1A	3.36	1.45	1.38
5	B	402	HEC	C1C-NC	-3.33	1.33	1.39
5	B	402	HEC	C1B-NB	-3.32	1.33	1.39
5	A	402	HEC	CHB-C1B	3.31	1.46	1.39
5	A	403	HEC	CHB-C1B	3.29	1.46	1.39
5	A	402	HEC	C4A-NA	-3.28	1.33	1.39
5	A	403	HEC	C1A-NA	-3.25	1.33	1.39
5	A	402	HEC	CHC-C1C	3.21	1.46	1.39
5	A	403	HEC	C4B-NB	-3.19	1.33	1.39
5	B	402	HEC	CHD-C1D	3.16	1.46	1.39
5	A	403	HEC	CHA-C4D	3.10	1.46	1.39
5	B	402	HEC	CHB-C1B	3.07	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	402	HEC	C4C-NC	-3.02	1.33	1.39
5	B	403	HEC	CHC-C4B	3.00	1.44	1.38
5	A	402	HEC	C1A-NA	-3.00	1.34	1.39
5	A	403	HEC	C1C-NC	-2.96	1.34	1.39
5	B	403	HEC	CHA-C4D	2.90	1.45	1.39
5	B	402	HEC	CHA-C4D	2.53	1.45	1.39
5	A	402	HEC	C1B-NB	-2.53	1.34	1.39
5	A	402	HEC	C1C-C2C	2.53	1.49	1.43
5	A	402	HEC	C4B-NB	-2.52	1.34	1.39
5	B	403	HEC	C1C-NC	-2.49	1.34	1.39
5	A	402	HEC	C1C-NC	-2.48	1.34	1.39
5	A	403	HEC	C1D-ND	-2.48	1.34	1.39
5	B	403	HEC	C1A-NA	-2.48	1.34	1.39
5	B	403	HEC	CBD-CAD	2.47	1.60	1.51
5	A	402	HEC	C4A-C3A	2.47	1.50	1.45
5	A	402	HEC	O2A-CGA	-2.47	1.22	1.30
5	B	403	HEC	C4A-C3A	2.44	1.50	1.45
5	A	403	HEC	C4A-C3A	2.42	1.50	1.45
5	A	402	HEC	C1D-C2D	2.41	1.48	1.43
5	B	402	HEC	CHC-C1C	2.39	1.44	1.39
5	B	402	HEC	C1D-C2D	2.37	1.48	1.43
5	A	403	HEC	CHC-C1C	2.35	1.44	1.39
5	B	403	HEC	C4D-C3D	2.34	1.49	1.44
5	B	403	HEC	O1A-CGA	2.30	1.29	1.22
5	A	403	HEC	O2D-CGD	-2.30	1.23	1.30
5	B	402	HEC	C4D-ND	-2.29	1.35	1.39
5	B	403	HEC	O2A-CGA	-2.21	1.23	1.30
5	A	402	HEC	C3C-C4C	2.20	1.49	1.46
5	A	402	HEC	C1A-C2A	2.17	1.49	1.45
5	B	402	HEC	C1B-C2B	2.10	1.48	1.43
5	A	403	HEC	C1B-C2B	2.10	1.48	1.43
5	A	402	HEC	C1B-C2B	2.04	1.47	1.43
5	B	403	HEC	CHA-C1A	2.04	1.42	1.38

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	403	HEC	CBB-CAB-C3B	-12.59	102.26	127.43
5	B	402	HEC	CBB-CAB-C3B	-12.17	103.12	127.43
5	B	403	HEC	CBB-CAB-C3B	-11.78	103.89	127.43
5	A	402	HEC	CBB-CAB-C3B	-9.27	108.90	127.43
5	A	403	HEC	CBC-CAC-C3C	-8.64	110.16	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	401	MES	C2-C3-N4	-7.82	98.23	110.12
5	B	403	HEC	CBC-CAC-C3C	-7.57	112.31	127.43
8	F	401	MES	C6-C5-N4	-7.44	98.82	110.12
5	B	403	HEC	C2A-C1A-NA	6.30	116.40	110.32
5	B	402	HEC	CBC-CAC-C3C	-6.25	114.94	127.43
5	A	403	HEC	C2A-C1A-NA	6.20	116.30	110.32
5	A	402	HEC	CBC-CAC-C3C	-5.65	116.14	127.43
8	D	401	MES	C2-C3-N4	-5.36	101.97	110.12
5	A	403	HEC	CBD-CAD-C3D	-4.98	98.77	112.53
5	A	402	HEC	C3D-C4D-ND	4.96	115.66	110.15
5	A	402	HEC	CHD-C4C-NC	-4.80	119.23	124.45
5	B	403	HEC	CBD-CAD-C3D	-4.75	99.39	112.53
8	F	401	MES	O2S-S-C8	4.65	113.75	106.73
8	F	401	MES	C5-N4-C3	4.58	118.71	108.84
5	A	402	HEC	C2A-C1A-NA	4.54	114.70	110.32
8	F	401	MES	C7-N4-C3	4.50	123.23	111.24
8	D	401	MES	C5-N4-C3	4.37	118.26	108.84
8	D	401	MES	C6-C5-N4	-4.28	103.61	110.12
5	A	403	HEC	CHB-C4A-NA	-4.21	119.87	124.45
8	D	401	MES	C7-N4-C5	4.16	122.32	111.24
5	B	403	HEC	C1A-C2A-C3A	-4.10	101.71	107.11
5	B	402	HEC	CMB-C2B-C3B	3.95	135.84	126.55
5	B	402	HEC	C2A-C1A-NA	3.89	114.07	110.32
5	A	403	HEC	CHA-C1A-NA	-3.66	120.47	124.45
5	B	402	HEC	C3D-C4D-ND	3.51	114.05	110.15
5	A	403	HEC	C1A-C2A-C3A	-3.44	102.58	107.11
5	B	402	HEC	C2C-C1C-NC	3.32	115.47	110.14
5	B	403	HEC	CBA-CAA-C2A	-3.31	103.37	112.53
5	B	403	HEC	C1D-C2D-C3D	-3.25	103.09	106.82
5	B	403	HEC	CHB-C4A-NA	-3.24	120.92	124.45
5	A	403	HEC	CBA-CAA-C2A	-3.21	103.67	112.53
5	B	402	HEC	CHC-C4B-NB	-3.16	121.01	124.45
5	B	402	HEC	C1A-C2A-C3A	-3.16	102.95	107.11
5	B	403	HEC	C2B-C1B-NB	3.15	115.20	110.14
5	B	402	HEC	C2B-C1B-NB	3.11	115.14	110.14
5	A	403	HEC	C1D-C2D-C3D	-3.10	103.27	106.82
5	B	403	HEC	CHA-C1A-NA	-3.08	121.10	124.45
8	D	401	MES	C7-N4-C3	3.06	119.39	111.24
5	A	403	HEC	CHD-C4C-NC	-3.01	121.17	124.45
5	A	403	HEC	CMD-C2D-C1D	2.99	129.97	125.42
5	B	403	HEC	CAD-CBD-CGD	-2.99	105.73	113.67
5	A	402	HEC	CBA-CAA-C2A	-2.93	104.44	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	403	HEC	CMB-C2B-C3B	2.89	133.35	126.55
5	B	403	HEC	C3A-C4A-NA	2.86	114.92	109.64
5	A	402	HEC	C2C-C1C-NC	2.84	114.69	110.14
5	B	402	HEC	CMB-C2B-C1B	-2.83	121.11	125.42
5	A	402	HEC	C1A-C2A-C3A	-2.71	103.54	107.11
5	A	403	HEC	C3A-C4A-NA	2.68	114.59	109.64
5	A	402	HEC	CHA-C1A-NA	-2.67	121.55	124.45
5	A	402	HEC	CHB-C4A-NA	-2.65	121.56	124.45
5	B	402	HEC	CHB-C4A-NA	-2.64	121.58	124.45
5	A	402	HEC	C4D-C3D-C2D	-2.63	102.80	106.87
5	A	402	HEC	CMB-C2B-C3B	2.63	132.72	126.55
5	B	402	HEC	CAA-C2A-C1A	2.61	130.16	124.85
5	B	403	HEC	C2C-C1C-NC	2.57	114.27	110.14
5	A	403	HEC	C2B-C1B-NB	2.57	114.26	110.14
5	A	403	HEC	C3D-C4D-ND	2.57	113.00	110.15
5	B	403	HEC	C3D-C4D-ND	2.55	112.98	110.15
8	F	401	MES	C7-N4-C5	2.53	117.97	111.24
5	B	403	HEC	C2D-C1D-ND	2.52	114.19	110.14
5	B	402	HEC	CHA-C1A-C2A	-2.51	120.90	124.86
5	B	403	HEC	CHC-C1C-C2C	-2.49	120.20	127.43
5	A	402	HEC	O1D-CGD-CBD	-2.48	115.23	123.09
8	F	401	MES	O1-C6-C5	-2.48	106.43	111.77
5	B	403	HEC	CHD-C1D-C2D	-2.46	120.28	127.43
5	A	402	HEC	CHC-C4B-NB	-2.44	121.79	124.45
5	A	403	HEC	C2C-C1C-NC	2.43	114.04	110.14
5	A	403	HEC	CMB-C2B-C3B	2.43	132.25	126.55
5	B	402	HEC	CBD-CAD-C3D	-2.40	105.90	112.53
5	B	402	HEC	CHD-C4C-NC	-2.38	121.87	124.45
5	B	402	HEC	CMC-C2C-C3C	2.37	132.13	126.55
5	B	402	HEC	CBA-CAA-C2A	-2.36	106.01	112.53
5	A	402	HEC	C2D-C1D-ND	2.33	113.87	110.14
5	A	402	HEC	CMD-C2D-C3D	2.32	130.55	125.62
5	A	402	HEC	CMC-C2C-C3C	2.30	131.97	126.55
5	B	402	HEC	CMA-C3A-C4A	2.29	128.77	124.73
5	B	402	HEC	C4D-C3D-C2D	-2.29	103.32	106.87
5	A	402	HEC	O2A-CGA-O1A	-2.29	117.45	123.33
5	A	402	HEC	C1D-C2D-C3D	-2.28	104.20	106.82
5	B	402	HEC	CHC-C1C-C2C	-2.27	120.83	127.43
8	D	401	MES	O3S-S-C8	2.26	110.43	106.00
5	A	402	HEC	O2D-CGD-CBD	2.25	121.11	114.00
5	B	403	HEC	C4A-NA-C1A	-2.21	102.21	105.82
5	A	402	HEC	C2B-C1B-NB	2.21	113.68	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	402	HEC	O2A-CGA-CBA	2.20	120.96	114.00
5	B	402	HEC	CAD-C3D-C4D	2.19	129.21	124.94
5	A	402	HEC	C3A-C4A-NA	2.17	113.66	109.64
5	B	402	HEC	C2D-C1D-ND	2.13	113.56	110.14
5	B	402	HEC	C1D-C2D-C3D	-2.11	104.41	106.82
5	B	403	HEC	CHB-C1B-C2B	-2.10	121.32	127.43
5	B	403	HEC	CAA-CBA-CGA	-2.10	108.10	113.67
5	A	403	HEC	CAA-C2A-C3A	2.09	131.78	127.87
8	F	401	MES	O1S-S-C8	-2.06	103.61	106.73
5	A	403	HEC	C4A-NA-C1A	-2.06	102.46	105.82
5	A	403	HEC	CHB-C1B-C2B	-2.04	121.50	127.43
5	A	402	HEC	CBD-CAD-C3D	-2.00	106.99	112.53

There are no chirality outliers.

All (37) 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
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
8	D	401	MES	C8-C7-N4-C5
8	D	401	MES	C7-C8-S-O1S
8	D	401	MES	C7-C8-S-O2S
8	D	401	MES	C7-C8-S-O3S
8	F	401	MES	C7-C8-S-O3S
6	A	404	EDO	O1-C1-C2-O2
8	D	401	MES	C8-C7-N4-C3
8	F	401	MES	C8-C7-N4-C5
6	B	404	EDO	O1-C1-C2-O2

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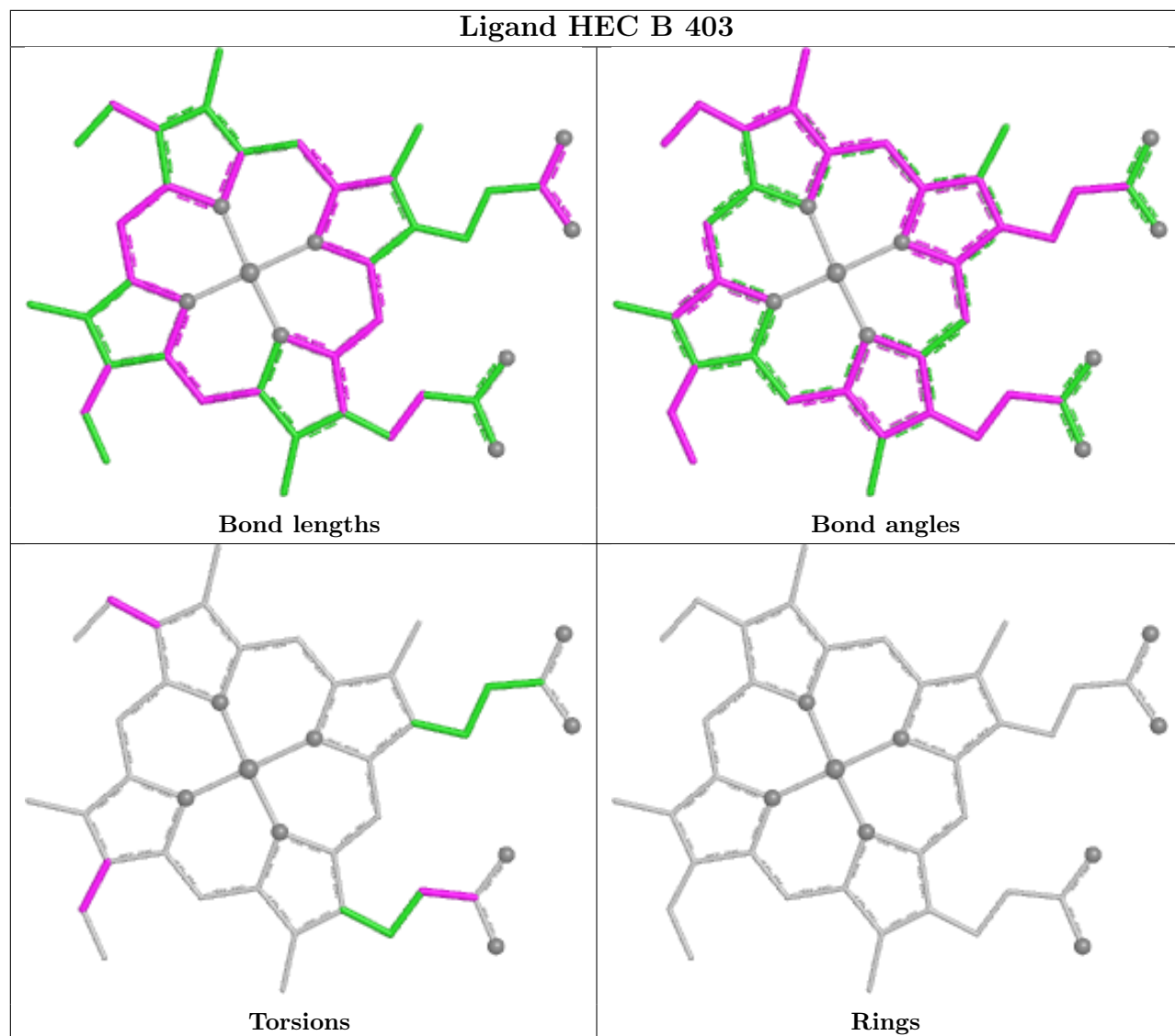
Mol	Chain	Res	Type	Atoms
8	F	401	MES	C7-C8-S-O1S
8	F	401	MES	C7-C8-S-O2S
8	D	401	MES	N4-C7-C8-S
8	F	401	MES	N4-C7-C8-S
6	A	406	EDO	O1-C1-C2-O2
5	A	403	HEC	CAD-CBD-CGD-O2D
5	B	403	HEC	CAD-CBD-CGD-O2D
5	A	403	HEC	CAD-CBD-CGD-O1D
5	B	403	HEC	CAD-CBD-CGD-O1D
5	B	402	HEC	CAD-CBD-CGD-O2D
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5	A	402	HEC	CAA-CBA-CGA-O2A

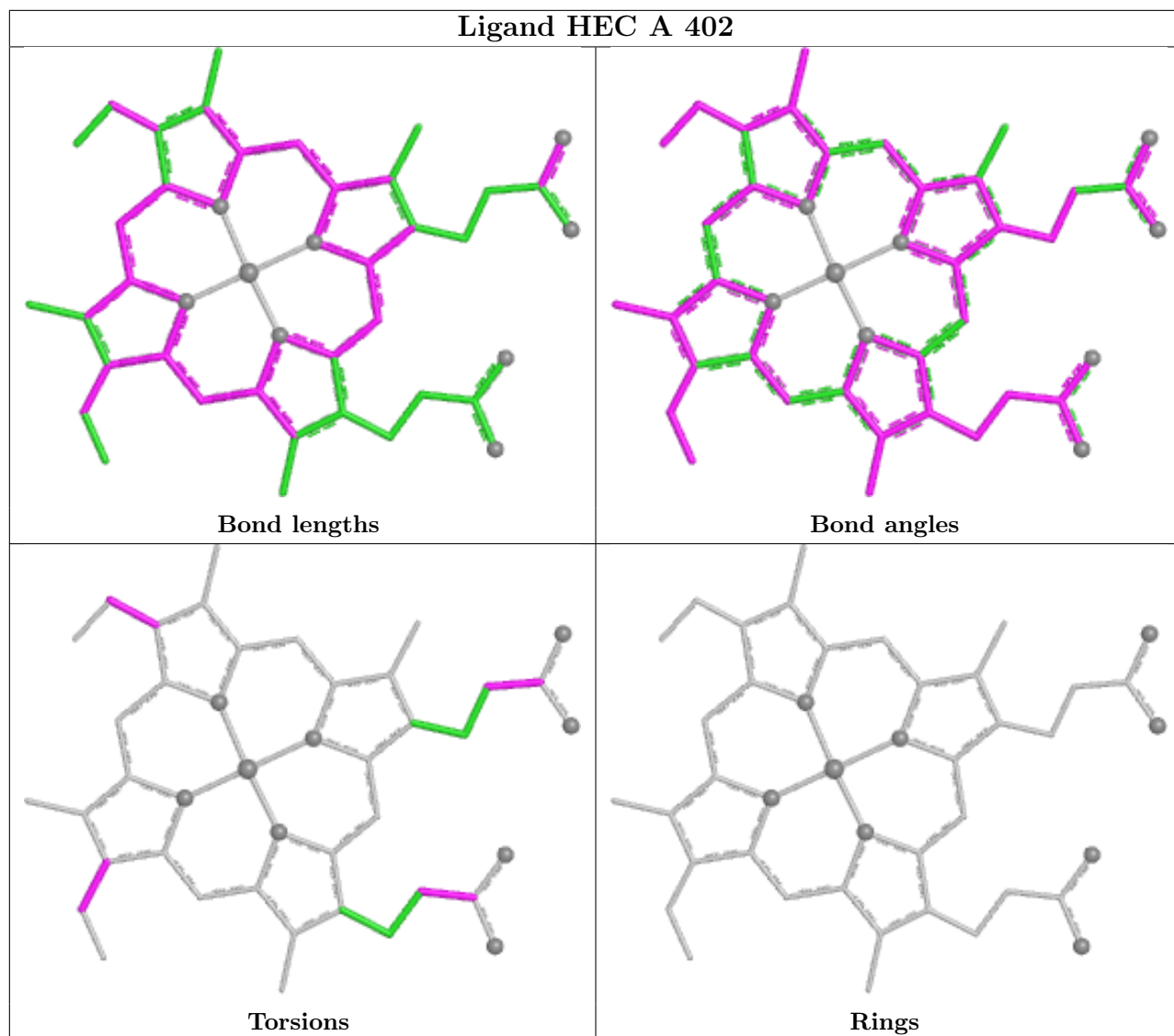
There are no ring outliers.

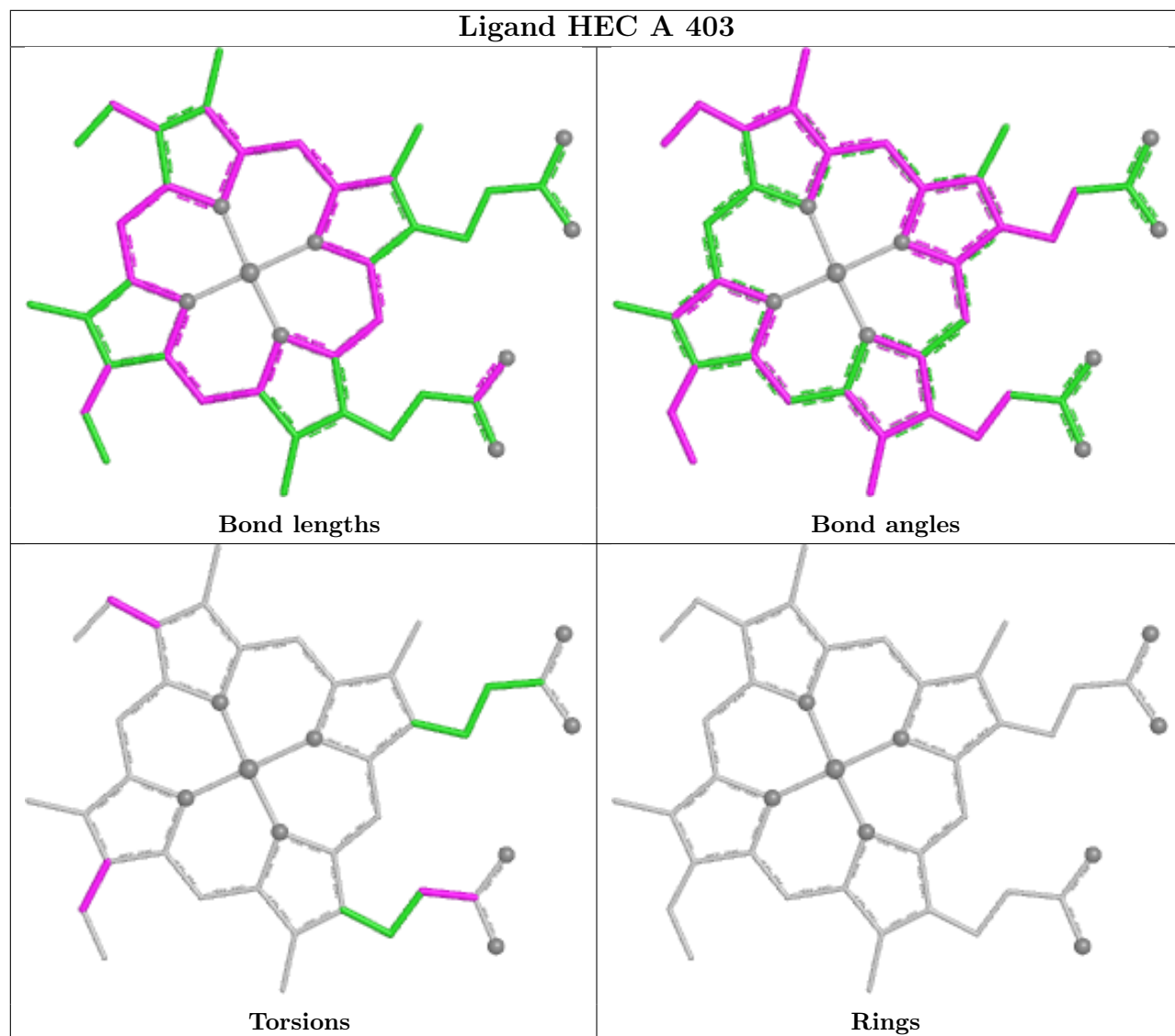
3 monomers are involved in 3 short contacts:

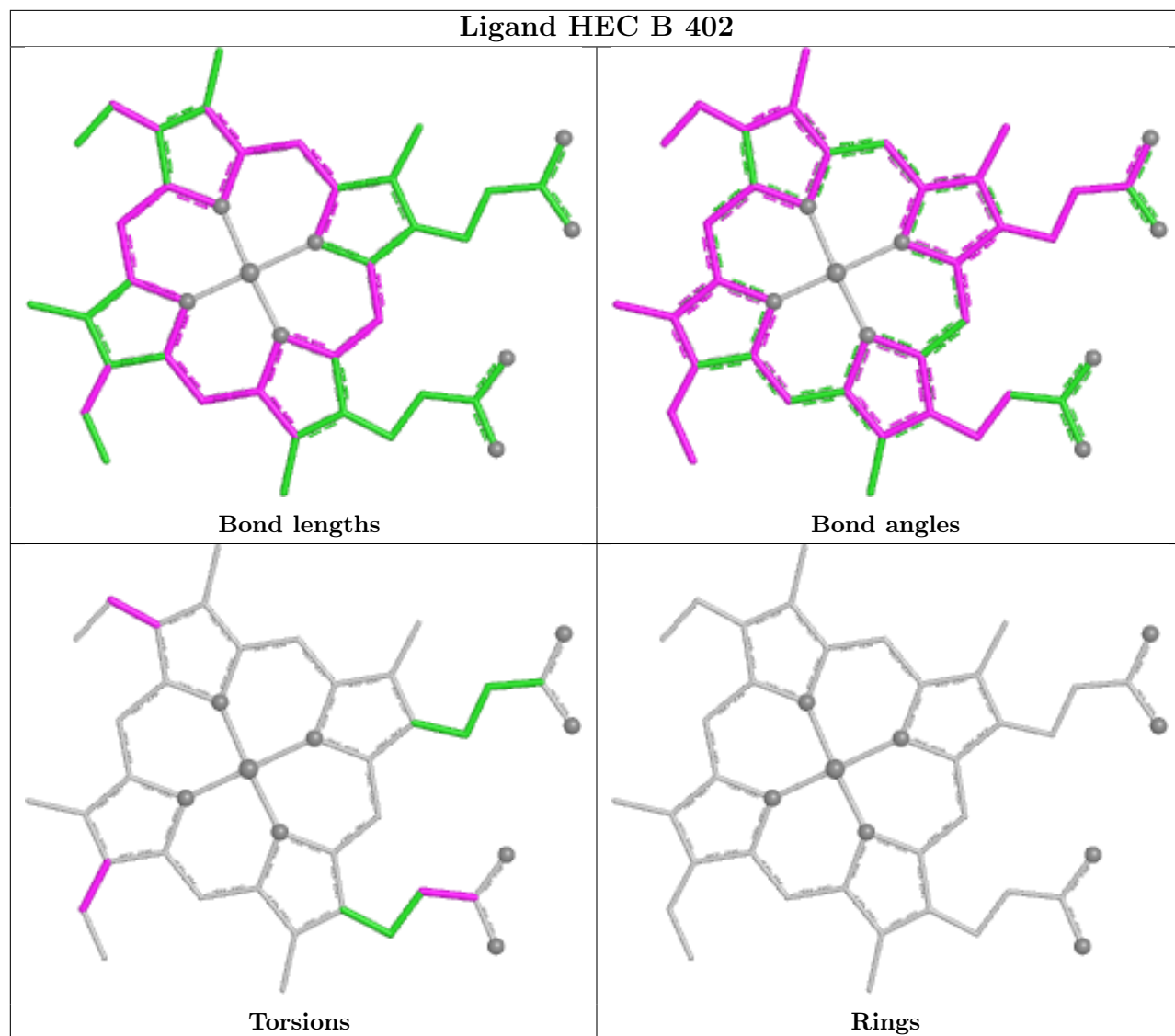
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	402	HEC	1	0
5	A	403	HEC	1	0
5	B	402	HEC	1	0

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	1 (0%) 90 93	18, 36, 53, 68	5 (1%)
1	B	357/373 (95%)	-0.40	1 (0%) 90 93	13, 29, 47, 69	8 (2%)
2	C	128/137 (93%)	-0.15	5 (3%) 43 49	17, 33, 56, 75	2 (1%)
2	E	124/137 (90%)	-0.55	1 (0%) 82 87	11, 24, 37, 63	4 (3%)
3	D	376/385 (97%)	-0.07	3 (0%) 82 87	22, 38, 64, 76	3 (0%)
3	F	376/385 (97%)	-0.56	2 (0%) 87 91	13, 26, 42, 63	5 (1%)
All	All	1715/1790 (95%)	-0.31	13 (0%) 82 87	11, 31, 55, 76	27 (1%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	ALA	3.6
1	A	6	ALA	3.3
3	D	207	GLY	2.9
3	F	386	GLY	2.7
2	C	133	HIS	2.6
2	C	131	SER	2.5
2	C	7	THR	2.4
2	E	130	ALA	2.4
3	F	207	GLY	2.4
3	D	218[A]	GLU	2.3
3	D	208	THR	2.3
2	C	127	VAL	2.2
2	C	132	HIS	2.1

### 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[A]	15/16	0.93	0.10	34,35,36,39	15
2	0AF	C	57[B]	15/16	0.93	0.10	36,42,44,44	15
2	0AF	E	57[A]	15/16	0.94	0.07	25,27,29,30	15
2	0AF	E	57[B]	15/16	0.94	0.07	23,33,36,37	15

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

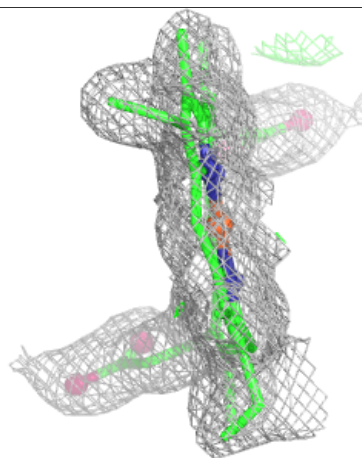
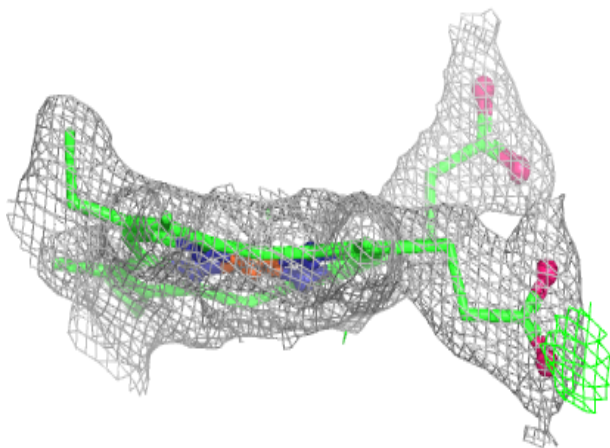
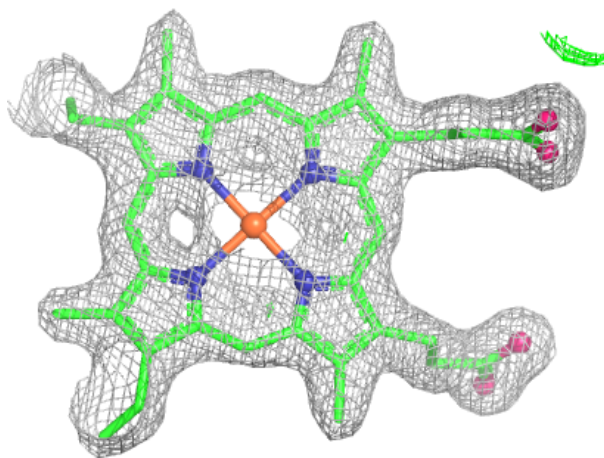
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	EDO	A	406	4/4	0.82	0.15	62,63,64,66	0
8	MES	F	401	12/12	0.88	0.17	33,53,59,60	12
6	EDO	B	404	4/4	0.90	0.12	49,50,51,53	0
6	EDO	A	404	4/4	0.91	0.08	58,59,59,60	0
8	MES	D	401	12/12	0.93	0.13	31,50,56,57	12
7	NA	A	405	1/1	0.96	0.05	49,49,49,49	0
7	NA	B	405	1/1	0.96	0.04	33,33,33,33	0
5	HEC	A	402	43/43	0.98	0.06	22,31,33,34	0
7	NA	B	406	1/1	0.98	0.05	34,34,34,34	0
4	CA	A	401	1/1	0.99	0.03	31,31,31,31	0
5	HEC	A	403	43/43	0.99	0.05	25,29,31,33	0
5	HEC	B	402	43/43	0.99	0.05	20,24,27,28	0
5	HEC	B	403	43/43	0.99	0.04	13,19,22,24	0
4	CA	B	401	1/1	1.00	0.03	22,22,22,22	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.

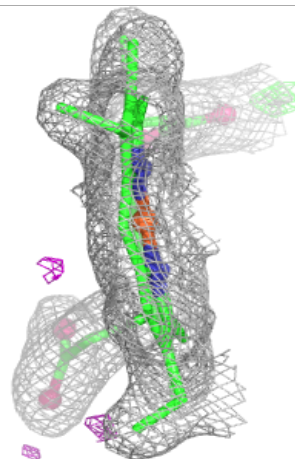
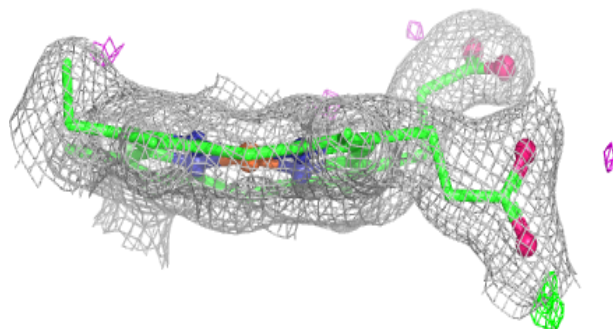
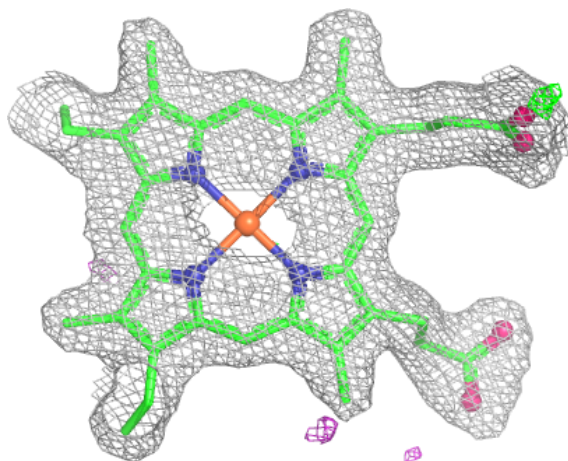
**Electron density around HEC A 402:**

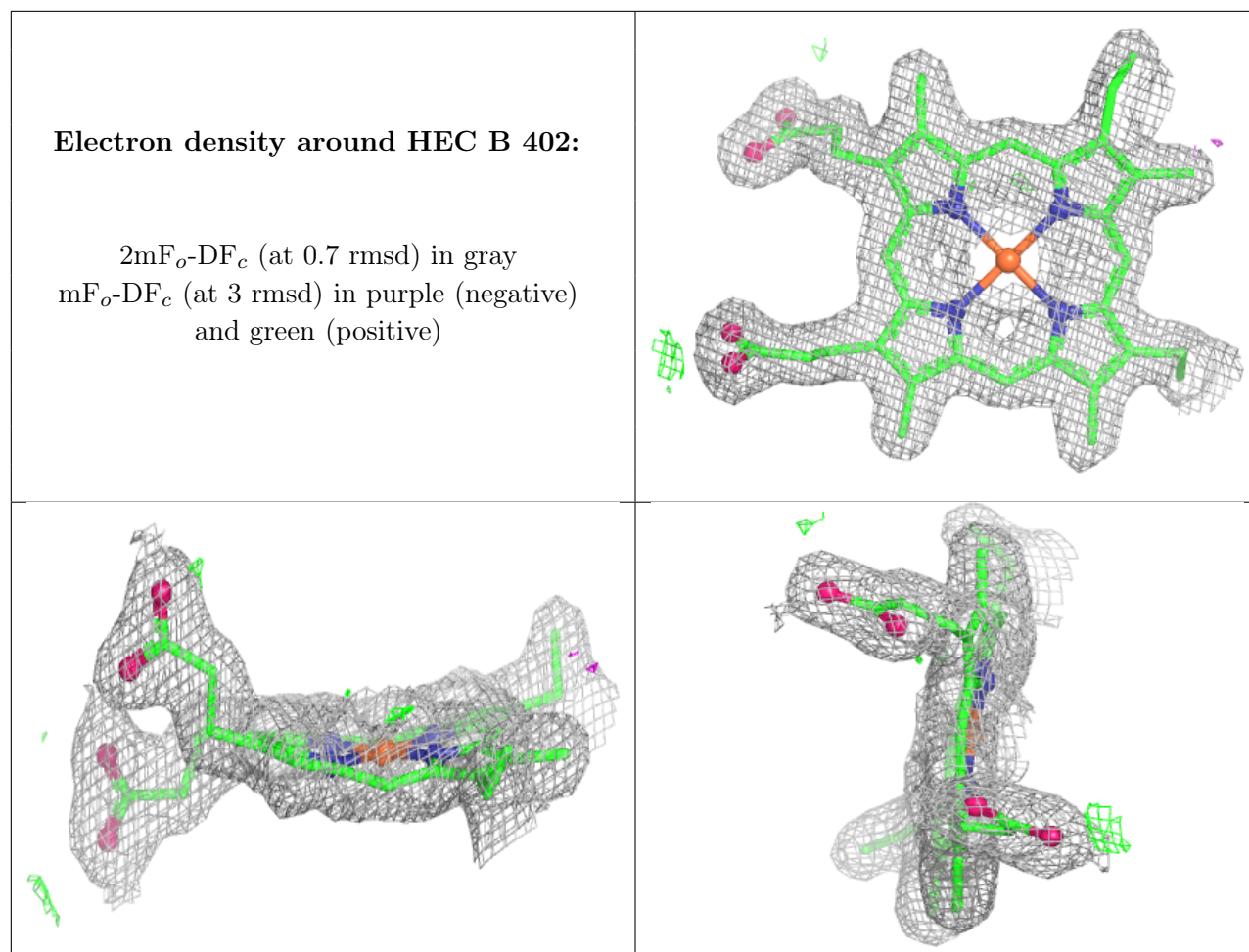
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

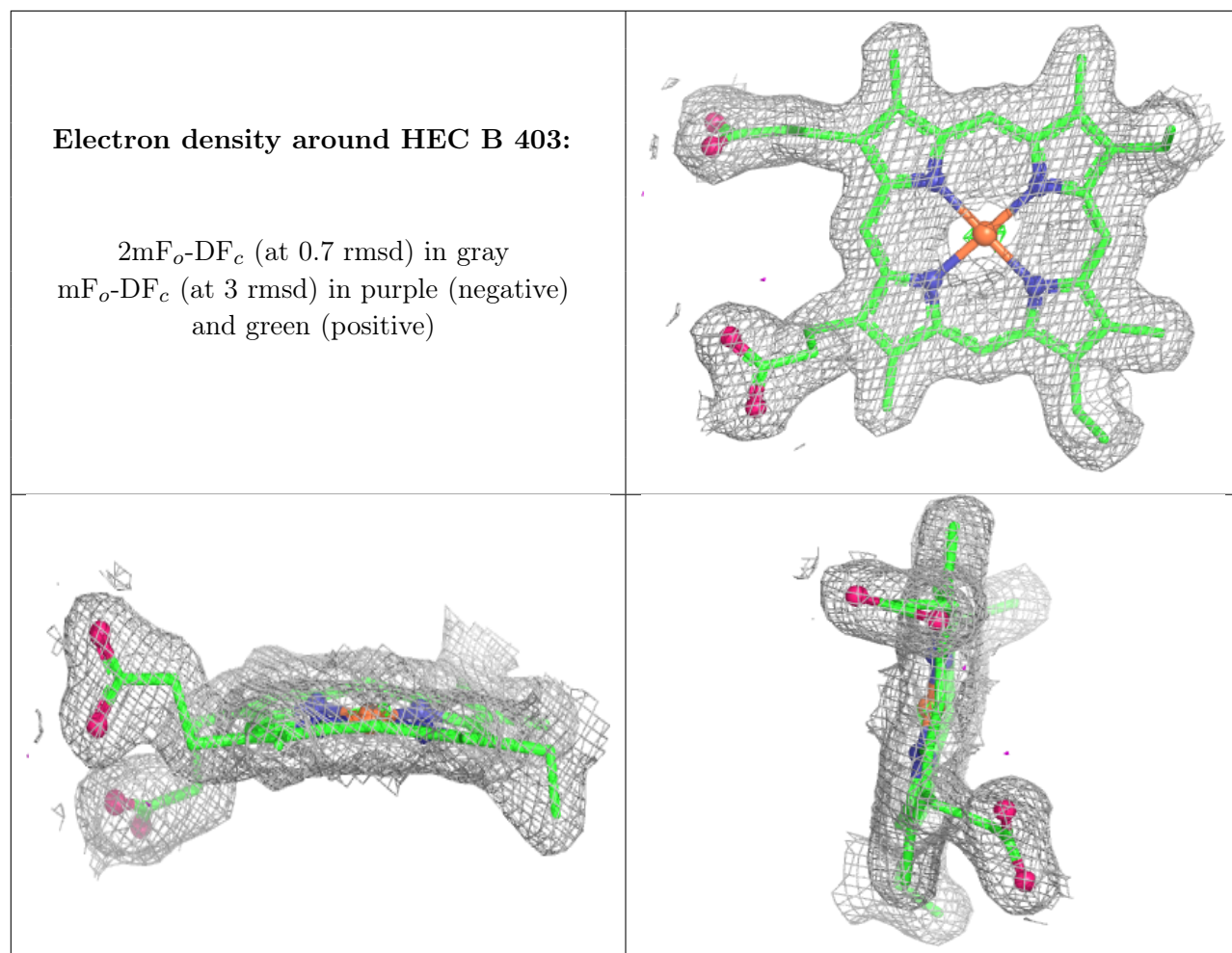


**Electron density around HEC A 403:**

$2mF_o-DF_c$  (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.