



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:53 PM GMT

PDB ID : 4L1Q  
Title : Crystal Structure of the E113Q-MauG/pre-MethylamineDehydrogenase Complex  
Authors : Yukl, E.Y.; Wilmot, C.M.  
Deposited on : 2013-06-03  
Resolution : 1.92 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

---

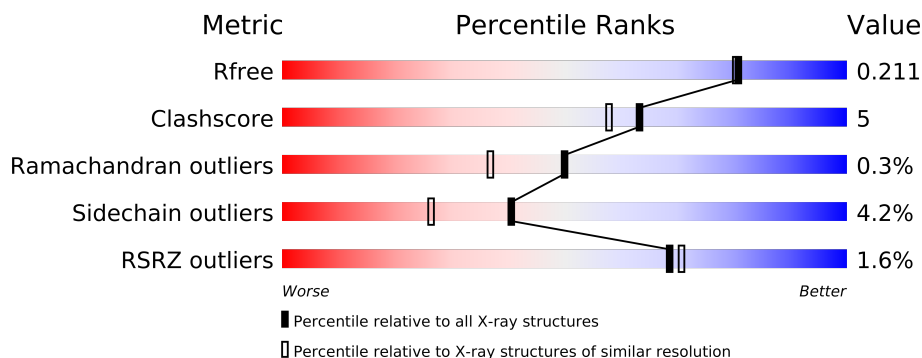
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.92 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))
$R_{free}$	66092	4387 (1.94-1.90)
Clashscore	79885	5258 (1.94-1.90)
Ramachandran outliers	78287	5193 (1.94-1.90)
Sidechain outliers	78261	5194 (1.94-1.90)
RSRZ outliers	66119	4389 (1.94-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
6	EDO	B	405	-	X
7	NA	B	406	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
7	NA	B	407	-	X
8	MES	D	401	-	X
8	MES	F	401	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15249 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	354	Total	C	N	O	S	0	6	0
			2795	1742	509	533	11			
1	B	357	Total	C	N	O	S	0	4	0
			2801	1745	510	535	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	GLN	GLU	ENGINEERED MUTATION	UNP Q51658
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	113	GLN	GLU	ENGINEERED MUTATION	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
2	C	131	Total	C	N	O	S	0	1	0
			1017	628	179	196	14			
2	E	125	Total	C	N	O	S	0	4	0
			976	604	163	194	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	132	HIS	-	EXPRESSION TAG	UNP A1BBA0
C	133	HIS	-	EXPRESSION TAG	UNP A1BBA0
C	134	HIS	-	EXPRESSION TAG	UNP A1BBA0
C	135	HIS	-	EXPRESSION TAG	UNP A1BBA0
C	136	HIS	-	EXPRESSION TAG	UNP A1BBA0
C	137	HIS	-	EXPRESSION TAG	UNP A1BBA0
E	132	HIS	-	EXPRESSION TAG	UNP A1BBA0
E	133	HIS	-	EXPRESSION TAG	UNP A1BBA0
E	134	HIS	-	EXPRESSION TAG	UNP A1BBA0
E	135	HIS	-	EXPRESSION TAG	UNP A1BBA0
E	136	HIS	-	EXPRESSION TAG	UNP A1BBA0
E	137	HIS	-	EXPRESSION TAG	UNP A1BBA0

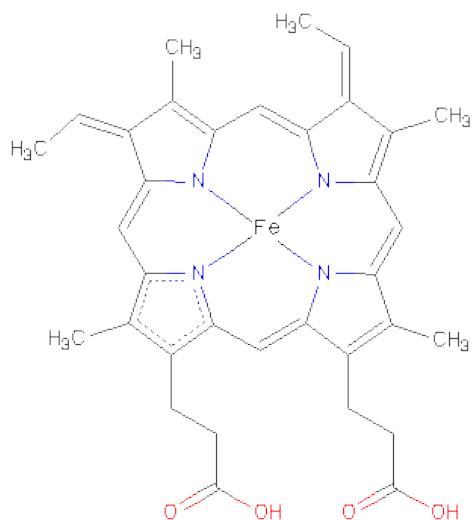
- Molecule 3 is a protein called Methylamine dehydrogenase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	376	Total	C	N	O	S	0	2	0
			2943	1864	507	564	8			
3	F	376	Total	C	N	O	S	0	5	0
			2963	1875	511	568	9			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

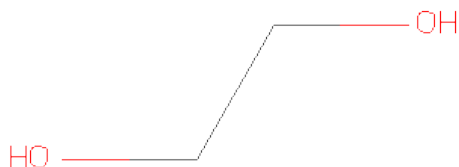
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		

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



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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).

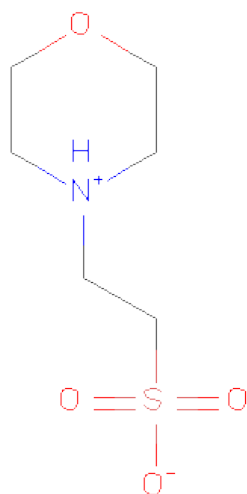


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONICACID (three-letter code: 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	270	Total 274	O 274	0	4
9	B	384	Total 390	O 390	0	6
9	C	81	Total 81	O 81	0	0
9	D	272	Total 277	O 277	0	5
9	E	125	Total 125	O 125	0	0
9	F	389	Total 394	O 394	0	5

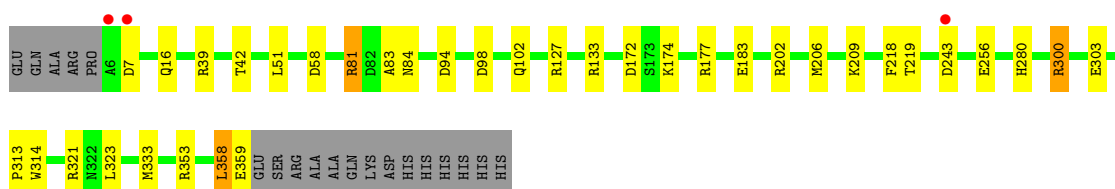


### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

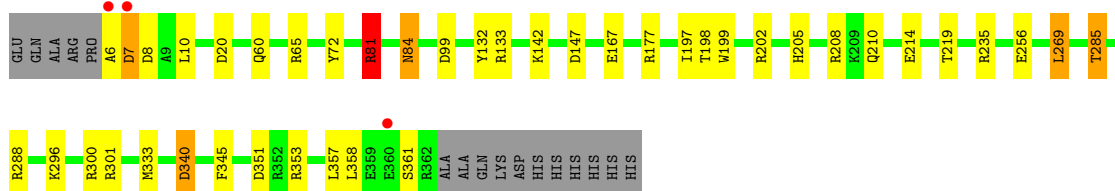
- Molecule 1: Methylamine utilization protein MauG

Chain A: 



- Molecule 1: Methylamine utilization protein MauG

Chain B: 



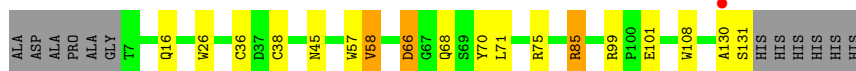
- Molecule 2: Methylamine dehydrogenase light chain

Chain C: 



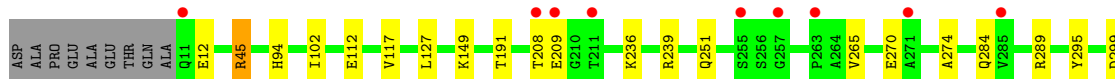
- Molecule 2: Methylamine dehydrogenase light chain

Chain E: 



- 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)	24.35 – 1.92 24.34 – 1.92	Depositor EDS
% Data completeness (in resolution range)	97.3 (24.35-1.92) 97.4 (24.34-1.92)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.49 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.160 , 0.207 0.169 , 0.211	Depositor DCC
$R_{free}$ test set	6447 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.6	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 35.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 129055 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15249	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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: 0AF, NA, CA, EDO, MES, HEC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.91	0/2859	0.94	2/3876 (0.1%)
1	B	1.06	1/2865 (0.0%)	1.02	11/3884 (0.3%)
2	C	0.95	0/1035	0.96	2/1413 (0.1%)
2	E	1.20	3/991 (0.3%)	1.06	3/1353 (0.2%)
3	D	0.89	0/3020	0.93	1/4114 (0.0%)
3	F	1.08	1/3043 (0.0%)	1.06	3/4145 (0.1%)
All	All	1.00	5/13813 (0.0%)	0.99	22/18785 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	26	TRP	CB-CG	-5.96	1.39	1.50
2	E	101[A]	GLU	CD-OE1	-5.52	1.19	1.25
2	E	101[B]	GLU	CD-OE1	-5.52	1.19	1.25
1	B	345	PHE	CB-CG	-5.42	1.42	1.51
3	F	303	GLU	CD-OE2	-5.18	1.20	1.25

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	177	ARG	NE-CZ-NH1	5.97	123.29	120.30
2	C	75	ARG	NE-CZ-NH1	-5.85	117.38	120.30
3	F	35	ARG	NE-CZ-NH1	5.75	123.17	120.30
2	E	85	ARG	NE-CZ-NH1	5.68	123.14	120.30
3	F	305	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	B	99	ASP	CB-CG-OD1	5.68	123.41	118.30
1	B	235	ARG	NE-CZ-NH1	5.65	123.13	120.30
2	E	99	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	B	208	ARG	NE-CZ-NH1	-5.47	117.56	120.30
1	A	98	ASP	CB-CG-OD2	-5.30	113.53	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	341	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	285	THR	N-CA-CB	-5.29	100.26	110.30
1	B	65	ARG	NE-CZ-NH1	-5.25	117.68	120.30
1	B	81	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	94	ASP	CB-CG-OD1	5.22	123.00	118.30
1	B	81	ARG	NE-CZ-NH1	5.21	122.91	120.30
2	C	132	HIS	N-CA-C	5.12	124.84	111.00
1	B	333	MET	CG-SD-CE	-5.11	92.02	100.20
3	D	239	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	340	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	B	142	LYS	CD-CE-NZ	-5.07	100.05	111.70
2	E	66	ASP	CB-CG-OD1	5.00	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2795	0	0	18	0
1	B	2801	0	0	21	0
2	C	1017	0	0	7	0
2	E	976	0	0	8	0
3	D	2943	0	0	10	0
3	F	2963	0	0	14	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	86	0	0	1	0
5	B	86	0	0	0	0
6	A	4	0	6	0	0
6	B	8	0	12	0	0
7	A	1	0	0	0	0
7	B	2	0	0	0	0
8	D	12	0	13	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	12	0	13	0	0
9	A	274	0	0	10	0
9	B	390	0	0	7	0
9	C	81	0	0	4	0
9	D	277	0	0	3	0
9	E	125	0	0	2	0
9	F	394	0	0	4	0
All	All	15249	0	44	75	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (75) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:131:SER:N	2:C:132:HIS:CA	2.39	0.86
2:E:36[B]:CYS:SG	2:E:45:ASN:O	2.44	0.76
1:A:133[A]:ARG:NH1	9:A:764:HOH:O	2.20	0.71
3:F:12:GLU:OE1	3:F:20:ARG:NH1	2.25	0.69
1:B:198:THR:CG2	2:E:58[B]:VAL:CG2	2.70	0.69
2:C:57:0AF:CE3	2:C:108:TRP:CD1	2.76	0.69
1:A:127[A]:ARG:NH2	9:A:761:HOH:O	2.27	0.67
1:B:301:ARG:NH2	3:F:177[B]:ASP:OD1	2.30	0.65
1:B:269[B]:LEU:N	1:B:269[B]:LEU:CD1	2.61	0.64
3:F:236:LYS:NZ	9:F:789:HOH:O	2.31	0.64
1:A:206:MET:CE	1:A:218:PHE:CD1	2.81	0.64
3:D:341:ASP:OD1	3:D:341:ASP:N	2.32	0.62
1:B:81:ARG:NH2	9:B:821:HOH:O	2.34	0.61
1:A:303[A]:GLU:OE1	1:A:303[A]:GLU:N	2.33	0.61
2:C:131:SER:CA	2:C:132:HIS:CB	2.77	0.61
2:E:130:ALA:CB	9:E:293:HOH:O	2.52	0.57
3:D:332:GLU:N	9:D:673:HOH:O	2.39	0.56
2:E:57:0AF:CE3	2:E:108:TRP:CD1	2.90	0.54
2:C:129:LYS:N	9:C:237:HOH:O	2.41	0.54
1:B:210:GLN:NE2	9:B:559:HOH:O	2.40	0.54
1:B:288:ARG:NH1	1:B:340:ASP:OD1	2.43	0.51
1:A:177:ARG:NE	1:A:183:GLU:OE1	2.43	0.51
3:D:299:ASP:OD2	3:D:311[B]:ARG:CD	2.58	0.51
1:A:58:ASP:C	1:A:58:ASP:OD1	2.49	0.50
1:A:39:ARG:O	1:A:42:THR:OG1	2.30	0.50
1:B:296:LYS:NZ	9:B:661:HOH:O	2.44	0.50
3:F:45:ARG:NH2	3:F:343:LYS:O	2.45	0.50
1:A:81:ARG:NH2	9:A:734:HOH:O	2.44	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:174[B]:ARG:NH1	3:F:207:GLY:O	2.45	0.49
1:A:313:PRO:O	1:A:314:TRP:C	2.50	0.49
3:D:251:GLN:N	9:D:745:HOH:O	2.45	0.49
3:D:295:TYR:CD1	3:D:295:TYR:N	2.80	0.48
1:B:197:ILE:O	1:B:202:ARG:CD	2.61	0.48
1:A:300[A]:ARG:N	9:A:715:HOH:O	2.47	0.48
1:B:256:GLU:N	9:B:719:HOH:O	2.47	0.47
1:B:6:ALA:O	1:B:10:LEU:N	2.47	0.47
3:D:112:GLU:OE2	3:F:104:ARG:NH2	2.47	0.47
1:B:81:ARG:NH2	9:B:700:HOH:O	2.48	0.47
2:E:75:ARG:NH2	9:E:314:HOH:O	2.47	0.47
3:F:236:LYS:NZ	3:F:384:ASP:O	2.48	0.46
1:B:147:ASP:OD1	1:B:147:ASP:C	2.54	0.46
1:B:205:HIS:ND1	1:B:269[B]:LEU:CD1	2.79	0.46
3:D:284:GLN:NE2	9:D:688:HOH:O	2.47	0.46
1:A:174:LYS:NZ	9:A:682:HOH:O	2.48	0.46
1:A:83:ALA:N	9:A:767:HOH:O	2.49	0.46
1:B:72:TYR:OH	1:B:351:ASP:OD1	2.35	0.45
9:C:262:HOH:O	3:F:36:ILE:CD1	2.64	0.45
2:E:66:ASP:OD2	2:E:70:TYR:OH	2.35	0.45
1:B:300:ARG:NH1	9:F:543:HOH:O	2.51	0.44
3:F:326:LYS:NZ	9:F:724:HOH:O	2.50	0.44
1:B:84:ASN:OD1	1:B:84:ASN:N	2.50	0.44
1:A:172:ASP:O	1:A:177:ARG:NH1	2.51	0.43
3:F:174[A]:ARG:NH1	3:F:210:GLY:O	2.52	0.43
1:B:214:GLU:N	9:B:835:HOH:O	2.51	0.43
1:B:20:ASP:OD2	1:B:132:TYR:OH	2.37	0.43
3:D:45:ARG:NH1	3:D:343:LYS:O	2.51	0.43
2:C:23:CYS:SG	2:C:88[B]:CYS:SG	3.16	0.43
1:A:280:HIS:N	5:A:403:HEC:O1D	2.52	0.42
3:D:236:LYS:NZ	3:D:384:ASP:O	2.53	0.42
1:B:353:ARG:NE	9:B:822:HOH:O	2.53	0.42
3:D:270:GLU:O	3:D:274:ALA:N	2.53	0.42
2:C:23:CYS:SG	2:C:88[B]:CYS:CB	3.08	0.41
3:F:181[B]:CYS:CB	3:F:196:CYS:SG	3.08	0.41
1:A:300[A]:ARG:CD	9:A:715:HOH:O	2.69	0.41
3:F:366:GLU:OE2	9:F:743:HOH:O	2.22	0.41
9:C:275:HOH:O	3:F:36:ILE:CD1	2.69	0.40
1:B:7:ASP:N	1:B:7:ASP:OD1	2.54	0.40
2:E:130:ALA:O	2:E:131:SER:OG	2.39	0.40
2:E:38:CYS:O	2:E:85:ARG:NH1	2.54	0.40
2:C:27:ARG:NH2	9:C:279:HOH:O	2.54	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:300[B]:ARG:N	9:A:715:HOH:O	2.55	0.40
1:A:353:ARG:NE	9:A:547:HOH:O	2.54	0.40
1:A:209:LYS:NZ	9:A:525:HOH:O	2.54	0.40
1:B:199:TRP:CD1	1:B:199:TRP:N	2.89	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	358/373 (96%)	345 (96%)	12 (3%)	1 (0%)	50	37
1	B	359/373 (96%)	350 (98%)	9 (2%)	0	100	100
2	C	129/137 (94%)	119 (92%)	8 (6%)	2 (2%)	14	3
2	E	126/137 (92%)	124 (98%)	2 (2%)	0	100	100
3	D	376/385 (98%)	360 (96%)	15 (4%)	1 (0%)	50	37
3	F	379/385 (98%)	366 (97%)	12 (3%)	1 (0%)	50	37
All	All	1727/1790 (96%)	1664 (96%)	58 (3%)	5 (0%)	50	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	130	ALA
2	C	131	SER
1	A	358	LEU
3	F	102	ILE
3	D	102	ILE

### 5.3.2 Protein sidechains ⓘ

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	282/292 (97%)	265 (94%)	17 (6%)	27	13
1	B	283/292 (97%)	268 (95%)	15 (5%)	32	17
2	C	111/112 (99%)	109 (98%)	2 (2%)	71	65
2	E	108/112 (96%)	103 (95%)	5 (5%)	37	22
3	D	306/310 (99%)	291 (95%)	15 (5%)	35	20
3	F	309/310 (100%)	300 (97%)	9 (3%)	55	43
All	All	1399/1428 (98%)	1336 (96%)	63 (4%)	40	23

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	16	GLN
1	A	51	LEU
1	A	81	ARG
1	A	84	ASN
1	A	102	GLN
1	A	202	ARG
1	A	219	THR
1	A	243	ASP
1	A	256	GLU
1	A	300[A]	ARG
1	A	300[B]	ARG
1	A	321	ARG
1	A	323	LEU
1	A	333	MET
1	A	358	LEU
1	A	359	GLU
1	B	7	ASP
1	B	8	ASP
1	B	60	GLN
1	B	81	ARG
1	B	84	ASN
1	B	133[A]	ARG
1	B	133[B]	ARG
1	B	167	GLU
1	B	219	THR
1	B	269[A]	LEU
1	B	269[B]	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	285	THR
1	B	357	LEU
1	B	358	LEU
1	B	361	SER
2	C	16	GLN
2	C	71	LEU
3	D	12	GLU
3	D	45	ARG
3	D	94	HIS
3	D	117	VAL
3	D	127	LEU
3	D	149	LYS
3	D	191	THR
3	D	208	THR
3	D	209	GLU
3	D	265	VAL
3	D	289	ARG
3	D	311[A]	ARG
3	D	311[B]	ARG
3	D	316	LEU
3	D	319	LYS
2	E	16	GLN
2	E	58[A]	VAL
2	E	58[B]	VAL
2	E	68	GLN
2	E	71	LEU
3	F	11	GLN
3	F	20	ARG
3	F	94	HIS
3	F	104	ARG
3	F	117	VAL
3	F	262	LEU
3	F	293	ARG
3	F	316	LEU
3	F	354	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	16,16,17	5.15	4 (25%)	19,22,24	2.68	5 (26%)
2	0AF	E	57	2	16,16,17	4.45	5 (31%)	19,22,24	3.04	6 (31%)

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	-	0/4/6/8	0/0/2/2
2	0AF	E	57	2	-	0/4/6/8	0/0/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	57	0AF	O-C	19.80	1.25	1.11
2	E	57	0AF	O-C	16.80	1.23	1.11
2	C	57	0AF	CD2-CE2	-3.04	1.35	1.41
2	E	57	0AF	CD1-NE1	-2.70	1.32	1.37
2	E	57	0AF	CD2-CE2	-2.55	1.36	1.41
2	E	57	0AF	CB-CA	-2.15	1.48	1.53
2	C	57	0AF	CA-C	2.15	1.52	1.48
2	C	57	0AF	CZ2-CE2	-2.13	1.37	1.41
2	E	57	0AF	CZ3-CE3	2.06	1.41	1.36

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	57	0AF	C-CA-N	-11.12	102.73	113.83
2	C	57	0AF	C-CA-N	-9.64	104.20	113.83

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	57	0AF	CH2-CZ2-CE2	4.24	121.81	118.40
2	C	57	0AF	CH2-CZ2-CE2	3.53	121.23	118.40
2	E	57	0AF	CZ2-CE2-CD2	-2.71	118.16	121.47
2	C	57	0AF	CE3-CD2-CE2	2.61	122.03	117.08
2	C	57	0AF	CD1-NE1-CE2	2.59	112.20	107.66
2	E	57	0AF	CE3-CD2-CE2	2.56	121.94	117.08
2	E	57	0AF	CD1-NE1-CE2	2.38	111.83	107.66
2	E	57	0AF	CG-CB-CA	2.18	119.66	114.16
2	C	57	0AF	CG-CB-CA	2.03	119.29	114.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates i

There are no carbohydrates 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
5	HEC	A	402	1	50,50,50	3.23	22 (44%)	56,82,82	3.58	28 (50%)
5	HEC	A	403	1	50,50,50	2.78	21 (42%)	56,82,82	3.57	29 (51%)
6	EDO	A	404	-	3,3,3	0.63	0	2,2,2	0.22	0
5	HEC	B	402	1	50,50,50	2.80	22 (44%)	56,82,82	3.22	28 (50%)
5	HEC	B	403	1	50,50,50	2.33	14 (28%)	56,82,82	3.37	28 (50%)
6	EDO	B	404	-	3,3,3	0.53	0	2,2,2	0.13	0
6	EDO	B	405	-	3,3,3	0.55	0	2,2,2	0.58	0
8	MES	D	401	-	12,12,12	1.52	3 (25%)	16,16,16	5.26	8 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	MES	F	401	-	12,12,12	1.38	1 (8%)	16,16,16	4.73	9 (56%)

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	402	1	-	0/10/54/54	0/0/8/8
5	HEC	A	403	1	-	0/10/54/54	0/0/8/8
6	EDO	A	404	-	-	0/1/1/1	0/0/0/0
5	HEC	B	402	1	-	0/10/54/54	0/0/8/8
5	HEC	B	403	1	-	0/10/54/54	0/0/8/8
6	EDO	B	404	-	-	0/1/1/1	0/0/0/0
6	EDO	B	405	-	-	0/1/1/1	0/0/0/0
8	MES	D	401	-	-	0/6/14/14	0/1/1/1
8	MES	F	401	-	-	0/6/14/14	1/1/1/1

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	402	HEC	C3B-CAB	8.78	1.53	1.35
5	A	402	HEC	C3C-CAC	8.37	1.52	1.35
5	A	402	HEC	C1C-C2C	8.04	1.50	1.40
5	A	402	HEC	C3C-C4C	7.66	1.51	1.41
5	B	402	HEC	C3B-CAB	7.63	1.51	1.35
5	B	403	HEC	C3B-CAB	7.56	1.51	1.35
5	B	402	HEC	C3C-CAC	6.89	1.49	1.35
5	B	403	HEC	C3C-CAC	6.64	1.49	1.35
5	A	402	HEC	C4C-NC	-6.60	1.27	1.37
5	B	402	HEC	C1D-C2D	6.42	1.48	1.40
5	A	403	HEC	C3B-CAB	6.34	1.48	1.35
5	A	403	HEC	C1B-C2B	6.24	1.48	1.40
5	A	403	HEC	C3C-CAC	6.17	1.48	1.35
5	B	402	HEC	C1B-C2B	6.12	1.47	1.40
5	A	402	HEC	C1B-C2B	5.57	1.47	1.40
5	A	403	HEC	C1A-NA	-5.37	1.29	1.37
5	B	402	HEC	C3B-C4B	5.28	1.48	1.41
5	A	403	HEC	C4A-NA	-5.04	1.29	1.37
5	B	403	HEC	C3C-C4C	4.90	1.47	1.41
5	A	402	HEC	C1A-NA	-4.88	1.30	1.37
5	A	403	HEC	C1C-C2C	4.80	1.46	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	403	HEC	C3C-C4C	4.54	1.47	1.41
5	A	403	HEC	FE-NA	4.32	2.11	1.92
5	A	403	HEC	C1D-C2D	4.22	1.45	1.40
5	A	402	HEC	C3B-C4B	4.05	1.46	1.41
5	B	402	HEC	C4A-NA	-4.02	1.31	1.37
8	F	401	MES	C8-S	-3.98	1.71	1.78
5	A	402	HEC	FE-NA	3.96	2.09	1.92
5	B	403	HEC	C1C-C2C	3.95	1.45	1.40
5	A	403	HEC	C3B-C4B	3.88	1.46	1.41
5	A	402	HEC	C1D-C2D	3.76	1.44	1.40
5	A	402	HEC	FE-NC	3.68	2.08	1.92
5	B	403	HEC	C1B-C2B	3.62	1.44	1.40
5	B	403	HEC	C4C-NC	-3.62	1.31	1.37
5	B	402	HEC	C4D-C3D	3.61	1.49	1.43
5	B	402	HEC	C4B-NB	-3.55	1.32	1.37
5	A	403	HEC	C4C-NC	-3.55	1.32	1.37
5	B	402	HEC	C4C-NC	-3.49	1.32	1.37
5	B	402	HEC	C3C-C4C	3.49	1.46	1.41
5	A	403	HEC	C4B-NB	-3.32	1.32	1.37
8	D	401	MES	C8-S	-3.28	1.72	1.78
5	B	402	HEC	C1B-NB	-3.22	1.30	1.36
8	D	401	MES	O2S-S	3.19	1.53	1.45
5	B	402	HEC	FE-ND	3.13	2.05	1.92
5	B	402	HEC	FE-NB	3.03	2.05	1.92
5	A	403	HEC	C4A-CHB	2.98	1.47	1.38
5	A	403	HEC	FE-NC	2.91	2.04	1.92
5	B	402	HEC	FE-NA	2.90	2.04	1.92
5	B	403	HEC	C4B-NB	-2.90	1.32	1.37
5	A	402	HEC	C4A-NA	-2.88	1.32	1.37
5	B	402	HEC	C1C-NC	-2.71	1.31	1.36
5	B	403	HEC	C4B-CHC	2.69	1.46	1.38
5	A	402	HEC	C1B-CHB	2.67	1.47	1.39
5	B	402	HEC	C1C-C2C	2.66	1.43	1.40
5	A	403	HEC	C4B-CHC	2.64	1.46	1.38
5	B	403	HEC	C4D-ND	-2.59	1.31	1.36
5	A	402	HEC	C4B-CHC	2.53	1.46	1.38
5	B	403	HEC	C3C-C2C	-2.51	1.36	1.41
5	B	402	HEC	FE-NC	2.49	2.03	1.92
5	A	402	HEC	O2A-CGA	-2.47	1.21	1.30
5	B	402	HEC	C4B-CHC	2.41	1.45	1.38
5	A	402	HEC	C4D-CHA	2.40	1.46	1.39
5	B	403	HEC	FE-NA	2.40	2.02	1.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	403	HEC	C1C-NC	-2.35	1.32	1.36
5	B	403	HEC	CMD-C2D	-2.30	1.46	1.51
5	A	403	HEC	FE-NB	2.29	2.02	1.92
5	A	402	HEC	C1A-C2A	2.29	1.51	1.43
5	B	403	HEC	C4C-CHD	2.28	1.45	1.38
5	B	402	HEC	C1A-NA	-2.26	1.33	1.37
5	A	402	HEC	FE-NB	2.26	2.02	1.92
5	B	403	HEC	C4A-NA	-2.24	1.33	1.37
5	A	403	HEC	C3C-C2C	-2.24	1.36	1.41
5	B	402	HEC	C4A-CHB	2.22	1.45	1.38
5	A	403	HEC	C1C-CHC	2.19	1.45	1.39
5	A	402	HEC	FE-ND	2.17	2.01	1.92
5	A	403	HEC	C1B-CHB	2.17	1.45	1.39
5	B	402	HEC	C1D-ND	-2.16	1.32	1.36
5	A	403	HEC	O2D-CGD	-2.15	1.22	1.30
5	A	402	HEC	C4A-CHB	2.14	1.44	1.38
5	B	402	HEC	C1D-CHD	2.14	1.45	1.39
5	A	402	HEC	C3C-C2C	-2.10	1.37	1.41
8	D	401	MES	O3S-S	2.06	1.50	1.45
5	A	402	HEC	C1D-CHD	2.04	1.45	1.39

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	401	MES	O3S-S-O1S	-13.00	79.04	112.48
8	D	401	MES	O3S-S-O2S	-10.54	85.38	112.48
8	F	401	MES	O3S-S-O1S	-10.53	85.39	112.48
5	A	402	HEC	C2D-C1D-ND	9.89	116.88	109.41
8	F	401	MES	O3S-S-O2S	-9.56	87.90	112.48
5	A	403	HEC	CBB-CAB-C3B	-9.41	101.94	128.44
8	F	401	MES	O3S-S-C8	-8.89	83.06	105.99
8	D	401	MES	O2S-S-O1S	8.62	129.05	112.44
5	B	402	HEC	C2D-C1D-ND	8.26	115.65	109.41
5	B	403	HEC	CBB-CAB-C3B	-8.10	105.62	128.44
5	A	402	HEC	CBB-CAB-C3B	-7.87	106.28	128.44
5	A	403	HEC	C3B-C2B-C1B	-7.47	102.10	107.07
5	A	402	HEC	C4C-C3C-C2C	-7.45	101.92	106.68
5	B	403	HEC	C2C-C1C-NC	7.29	114.92	109.41
5	A	403	HEC	C4A-C3A-C2A	-7.27	102.27	106.89
5	A	402	HEC	C2B-C1B-NB	7.15	114.81	109.41
5	B	402	HEC	C2B-C1B-NB	7.07	114.75	109.41
5	A	402	HEC	CMC-C2C-C3C	6.83	133.26	125.72

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	403	HEC	CMB-C2B-C3B	6.83	133.26	125.72
5	A	403	HEC	CBD-CAD-C3D	-6.82	100.67	112.69
5	B	403	HEC	CMC-C2C-C3C	6.71	133.12	125.72
5	B	402	HEC	C2C-C1C-NC	6.63	114.42	109.41
5	A	403	HEC	C2A-C1A-NA	6.59	114.58	109.64
5	B	402	HEC	CBB-CAB-C3B	-6.41	110.41	128.44
5	A	403	HEC	C2B-C1B-NB	6.39	114.24	109.41
5	A	402	HEC	C1D-C2D-C3D	-6.33	102.59	107.00
5	B	403	HEC	CBD-CAD-C3D	-6.29	101.60	112.69
5	A	403	HEC	CBC-CAC-C3C	-6.09	111.29	128.44
5	B	403	HEC	C3C-C2C-C1C	-6.00	103.08	107.07
5	A	402	HEC	C4B-C3B-C2B	-5.97	102.87	106.68
5	B	402	HEC	C4B-C3B-C2B	-5.82	102.96	106.68
8	D	401	MES	O3S-S-C8	-5.70	91.29	105.99
5	B	402	HEC	C4C-C3C-C2C	-5.68	103.05	106.68
5	A	402	HEC	CBD-CAD-C3D	-5.61	102.81	112.69
5	B	403	HEC	C4B-CHC-C1C	-5.54	120.18	127.47
5	B	402	HEC	C1D-C2D-C3D	-5.44	103.21	107.00
5	B	403	HEC	C3A-C4A-NA	5.36	113.46	109.41
5	A	403	HEC	C3A-C4A-NA	5.34	113.44	109.41
5	B	403	HEC	C3B-C2B-C1B	-5.34	103.52	107.07
5	B	403	HEC	C4A-C3A-C2A	-5.31	103.52	106.89
5	B	402	HEC	C3B-C2B-C1B	-5.30	103.54	107.07
5	A	402	HEC	CBC-CAC-C3C	-5.25	113.66	128.44
5	A	402	HEC	C4D-ND-C1D	-5.19	99.92	106.76
5	A	402	HEC	C3D-C4D-ND	5.19	116.95	109.73
5	A	403	HEC	CMC-C2C-C3C	5.10	131.35	125.72
5	A	403	HEC	C2D-C1D-ND	5.08	113.25	109.41
5	B	403	HEC	C2A-C1A-NA	5.03	113.41	109.64
5	B	402	HEC	C2A-C1A-NA	5.01	113.40	109.64
5	B	402	HEC	C3C-C2C-C1C	-4.94	103.78	107.07
5	A	402	HEC	C4B-NB-C1B	-4.86	100.36	106.76
5	A	402	HEC	CMC-C2C-C1C	-4.83	121.19	128.62
5	B	403	HEC	C2D-C1D-ND	4.79	113.03	109.41
5	B	403	HEC	C2C-C1C-CHC	-4.79	116.91	126.00
5	B	402	HEC	C1A-C2A-C3A	-4.63	103.03	106.69
5	B	403	HEC	CBC-CAC-C3C	-4.62	115.43	128.44
5	A	403	HEC	C2C-C1C-NC	4.58	112.87	109.41
5	B	403	HEC	C4D-C3D-C2D	-4.51	102.25	106.92
8	F	401	MES	O1S-S-C8	4.32	119.68	106.36
5	B	403	HEC	C2B-C1B-NB	4.26	112.63	109.41
8	F	401	MES	O2S-S-C8	4.18	119.26	106.36

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	403	HEC	C3D-C4D-ND	4.16	115.51	109.73
5	A	402	HEC	C1A-C2A-C3A	-4.15	103.41	106.69
8	D	401	MES	C2-C3-N4	4.04	115.14	109.96
5	A	403	HEC	C3C-C2C-C1C	-4.04	104.38	107.07
5	A	402	HEC	C2A-C1A-NA	3.87	112.53	109.64
5	A	403	HEC	C3D-C4D-ND	3.84	115.07	109.73
5	B	402	HEC	C3A-C4A-NA	3.81	112.29	109.41
5	A	403	HEC	C4D-C3D-C2D	-3.79	102.99	106.92
5	B	402	HEC	CBD-CAD-C3D	-3.71	106.16	112.69
5	A	402	HEC	CHD-C1D-ND	-3.70	118.40	124.58
5	B	402	HEC	CMB-C2B-C3B	3.67	129.77	125.72
5	A	403	HEC	CMA-C3A-C2A	3.66	131.84	124.94
5	A	403	HEC	C4C-C3C-C2C	-3.66	104.34	106.68
5	B	403	HEC	C4D-ND-C1D	-3.61	102.00	106.76
5	A	403	HEC	C4B-CHC-C1C	-3.58	122.76	127.47
8	F	401	MES	O2S-S-O1S	3.50	119.18	112.44
5	A	403	HEC	C1A-CHA-C4D	-3.43	122.96	127.47
5	B	402	HEC	CBC-CAC-C3C	-3.39	118.89	128.44
8	D	401	MES	O2S-S-C8	3.36	116.72	106.36
5	B	402	HEC	C4D-C3D-C2D	-3.32	103.48	106.92
5	B	403	HEC	C4B-C3B-C2B	-3.29	104.58	106.68
5	A	402	HEC	C4D-C3D-C2D	-3.27	103.53	106.92
5	A	403	HEC	C1A-C2A-C3A	-3.27	104.11	106.69
5	B	403	HEC	C4C-CHD-C1D	-3.26	123.18	127.47
5	B	403	HEC	CMC-C2C-C1C	-3.21	123.68	128.62
5	A	402	HEC	C3B-C4B-NB	3.19	116.14	111.52
8	F	401	MES	O1-C6-C5	-3.18	107.55	111.34
5	A	402	HEC	CMA-C3A-C2A	3.18	130.93	124.94
5	A	403	HEC	CMC-C2C-C1C	-3.18	123.74	128.62
5	A	403	HEC	CBA-CAA-C2A	-3.17	106.42	112.35
8	F	401	MES	C2-C3-N4	-3.15	105.91	109.96
5	B	403	HEC	C4C-NC-C1C	-3.07	102.71	106.76
5	B	402	HEC	C3D-C4D-ND	3.07	114.00	109.73
5	A	403	HEC	C4D-ND-C1D	-3.03	102.77	106.76
5	B	402	HEC	CMC-C2C-C3C	3.01	129.04	125.72
5	B	402	HEC	C4D-ND-C1D	-2.94	102.89	106.76
5	B	402	HEC	C4C-NC-C1C	-2.92	102.92	106.76
8	D	401	MES	C8-C7-N4	2.87	117.35	112.44
5	A	402	HEC	C4A-C3A-C2A	-2.85	105.08	106.89
5	B	402	HEC	CAA-C2A-C1A	2.84	129.80	124.67
5	B	403	HEC	C1A-CHA-C4D	-2.83	123.75	127.47
5	B	403	HEC	CMB-C2B-C3B	2.81	128.82	125.72

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	402	HEC	C2C-C1C-CHC	-2.75	120.78	126.00
5	B	403	HEC	C2B-C1B-CHB	-2.71	120.86	126.00
5	B	403	HEC	C2D-C1D-CHD	-2.67	120.94	126.00
5	A	403	HEC	C1D-C2D-C3D	-2.66	105.14	107.00
5	A	403	HEC	CMB-C2B-C1B	-2.63	124.57	128.62
5	A	403	HEC	C3D-C4D-CHA	-2.60	121.07	126.00
5	B	402	HEC	CHD-C1D-ND	-2.58	120.26	124.58
5	A	403	HEC	C2B-C1B-CHB	-2.52	121.22	126.00
5	B	403	HEC	C3B-C4B-NB	2.49	115.12	111.52
5	A	402	HEC	CHB-C1B-NB	-2.47	120.46	124.58
5	A	402	HEC	C4B-CHC-C1C	-2.41	124.30	127.47
5	B	403	HEC	C4C-C3C-C2C	-2.38	105.16	106.68
5	A	402	HEC	C3A-C4A-NA	2.37	111.20	109.41
5	B	402	HEC	C3D-C4D-CHA	-2.37	121.51	126.00
5	A	402	HEC	CHA-C4D-ND	-2.36	120.64	124.58
5	A	402	HEC	C3C-C2C-C1C	-2.30	105.54	107.07
8	D	401	MES	O1-C6-C5	-2.27	108.64	111.34
5	B	402	HEC	CMD-C2D-C3D	2.26	129.20	124.94
5	B	402	HEC	O1A-CGA-CBA	-2.23	115.35	123.03
5	A	402	HEC	O2A-CGA-O1A	-2.19	117.72	123.30
5	A	402	HEC	CBA-CAA-C2A	-2.19	108.26	112.35
5	A	403	HEC	O2A-CGA-CBA	2.17	121.88	114.22
5	B	403	HEC	C3D-C4D-CHA	-2.16	121.91	126.00
5	B	402	HEC	C4A-C3A-C2A	-2.13	105.54	106.89
5	A	402	HEC	O2A-CGA-CBA	2.13	121.74	114.22
5	A	403	HEC	C4B-C3B-C2B	-2.12	105.32	106.68
5	B	402	HEC	CMA-C3A-C2A	2.06	128.82	124.94
8	F	401	MES	C6-O1-C2	2.03	116.83	109.90

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	401	MES	C2-C3-C5-C6-N4-O1

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.14	3 (0%)	83 85	26, 38, 56, 73	0
1	B	357/373 (95%)	-0.34	3 (0%)	83 85	16, 29, 47, 76	0
2	C	131/137 (95%)	0.10	4 (3%)	47 48	23, 36, 64, 90	2 (1%)
2	E	125/137 (91%)	-0.38	1 (0%)	83 85	20, 26, 38, 71	0
3	D	376/385 (97%)	0.07	11 (2%)	49 50	24, 41, 66, 85	0
3	F	376/385 (97%)	-0.27	5 (1%)	74 76	18, 28, 47, 68	0
All	All	1719/1790 (96%)	-0.16	27 (1%)	68 71	16, 33, 59, 90	2 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	131	SER	6.2
1	B	6	ALA	5.2
1	A	6	ALA	4.8
3	D	386	GLY	4.4
3	F	386	GLY	4.2
1	B	7	ASP	3.7
3	D	11	GLN	3.5
2	C	134	HIS	3.5
2	C	132	HIS	3.3
3	D	208	THR	3.1
2	C	7	THR	3.1
3	D	257	GLY	3.0
3	D	271	ALA	2.9
3	D	263	PRO	2.9
3	D	209	GLU	2.7
3	F	207	GLY	2.6
3	D	255	SER	2.6
1	A	243	ASP	2.6
3	D	285	VAL	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	7	ASP	2.3
3	F	211	THR	2.2
3	D	320	THR	2.2
2	E	130	ALA	2.1
3	F	336	ILE	2.1
3	D	211	THR	2.1
3	F	297	LEU	2.1
1	B	360	GLU	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	0AF	E	57	15/16	0.10	0.07	24,27,32,33	0
2	0AF	C	57	15/16	0.10	0.02	37,40,45,46	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	NA	B	406	1/1	0.13	7.13	30,30,30,30	0
8	MES	D	401	12/12	0.19	6.87	29,54,60,61	12
8	MES	F	401	12/12	0.17	5.38	44,66,68,70	0
6	EDO	B	405	4/4	0.17	4.20	37,50,50,60	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	NA	B	407	1/1	0.16	3.58	31,31,31,31	0
7	NA	A	405	1/1	0.15	0.96	47,47,47,47	0
5	HEC	A	403	43/43	0.13	0.72	26,29,32,32	0
5	HEC	A	402	43/43	0.10	0.35	28,31,34,36	0
5	HEC	B	403	43/43	0.10	-0.11	15,17,20,21	0
6	EDO	B	404	4/4	0.08	-0.23	46,47,50,53	0
5	HEC	B	402	43/43	0.08	-0.39	19,23,26,29	0
6	EDO	A	404	4/4	0.10	-0.63	57,57,59,59	0
4	CA	B	401	1/1	0.06	-1.41	20,20,20,20	0
4	CA	A	401	1/1	0.02	-4.06	30,30,30,30	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.