



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 09:10 PM EDT

PDB ID : 7JMS  
Title : Structure of the Hazara virus OTU bound to ubiquitin  
Authors : Dzimianski, J.V.; Pegan, S.D.  
Deposited on : 2020-08-02  
Resolution : 2.78 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

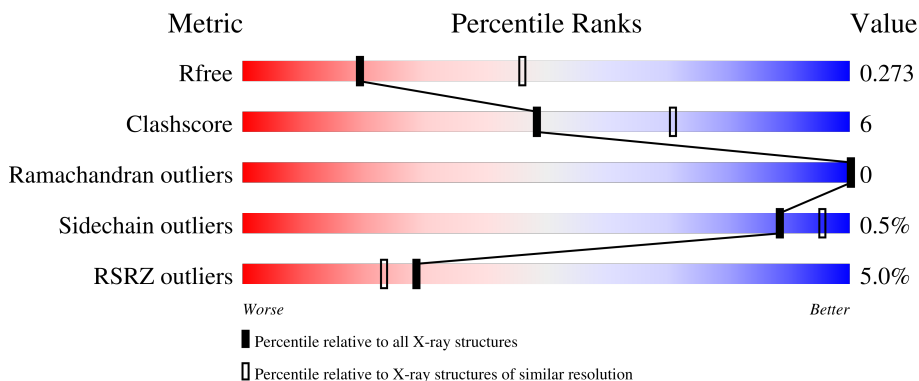
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.78 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



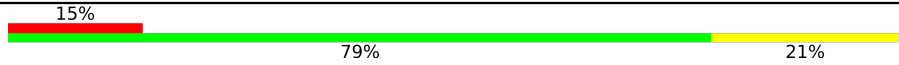
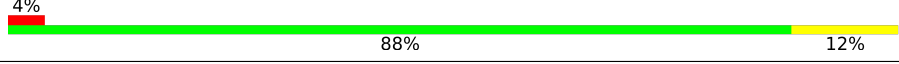
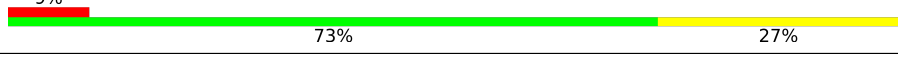
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	178	 4% 71% 17% 12%
1	C	178	 2% 81% 8% 11%
1	E	178	 3% 75% 14% 11%
1	G	178	 3% 78% 10% 12%
2	B	75	 7% 88% 12%

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Mol	Chain	Length	Quality of chain
2	D	75	 15% 79% 21%
2	F	75	 4% 88% 12%
2	H	75	 9% 73% 27%

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 7706 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 Replicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	157	1239	787	212	237	3	0	0	0
1	C	159	1259	799	217	240	3	0	1	0
1	E	158	1252	795	216	238	3	0	1	0
1	G	157	1250	793	216	238	3	0	1	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	SER	-	expression tag	UNP A6XA53
A	171	GLY	-	expression tag	UNP A6XA53
A	172	SER	-	expression tag	UNP A6XA53
A	173	HIS	-	expression tag	UNP A6XA53
A	174	HIS	-	expression tag	UNP A6XA53
A	175	HIS	-	expression tag	UNP A6XA53
A	176	HIS	-	expression tag	UNP A6XA53
A	177	HIS	-	expression tag	UNP A6XA53
A	178	HIS	-	expression tag	UNP A6XA53
C	170	SER	-	expression tag	UNP A6XA53
C	171	GLY	-	expression tag	UNP A6XA53
C	172	SER	-	expression tag	UNP A6XA53
C	173	HIS	-	expression tag	UNP A6XA53
C	174	HIS	-	expression tag	UNP A6XA53
C	175	HIS	-	expression tag	UNP A6XA53
C	176	HIS	-	expression tag	UNP A6XA53
C	177	HIS	-	expression tag	UNP A6XA53
C	178	HIS	-	expression tag	UNP A6XA53
E	170	SER	-	expression tag	UNP A6XA53
E	171	GLY	-	expression tag	UNP A6XA53
E	172	SER	-	expression tag	UNP A6XA53

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Chain	Residue	Modelled	Actual	Comment	Reference
E	173	HIS	-	expression tag	UNP A6XA53
E	174	HIS	-	expression tag	UNP A6XA53
E	175	HIS	-	expression tag	UNP A6XA53
E	176	HIS	-	expression tag	UNP A6XA53
E	177	HIS	-	expression tag	UNP A6XA53
E	178	HIS	-	expression tag	UNP A6XA53
G	170	SER	-	expression tag	UNP A6XA53
G	171	GLY	-	expression tag	UNP A6XA53
G	172	SER	-	expression tag	UNP A6XA53
G	173	HIS	-	expression tag	UNP A6XA53
G	174	HIS	-	expression tag	UNP A6XA53
G	175	HIS	-	expression tag	UNP A6XA53
G	176	HIS	-	expression tag	UNP A6XA53
G	177	HIS	-	expression tag	UNP A6XA53
G	178	HIS	-	expression tag	UNP A6XA53

- Molecule 2 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	75	597	376	104	116	1	0	0	0
2	D	75	608	382	108	117	1	0	1	0
2	F	75	597	376	104	116	1	0	0	0
2	H	75	597	376	104	116	1	0	0	0

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

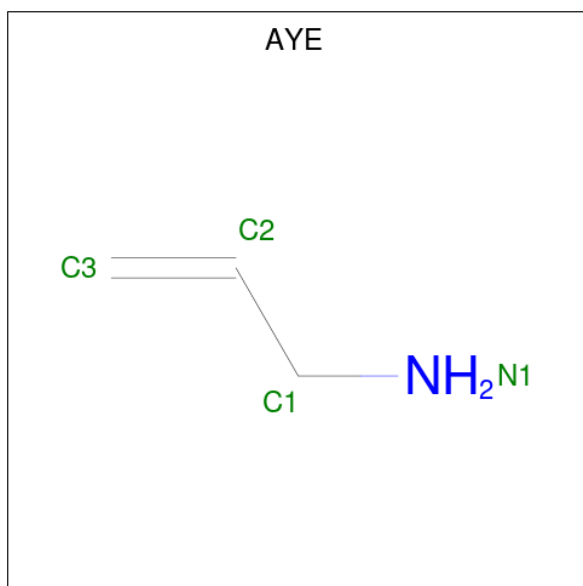
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	A	3	3	3	0	0
3	C	2	2	2	0	0
3	D	1	1	1	0	0
3	E	1	1	1	0	0
3	F	1	1	1	0	0

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

- Molecule 4 is prop-2-en-1-amine (three-letter code: AYE) (formula: C<sub>3</sub>H<sub>7</sub>N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	N	0	0
			4	3	1		
4	D	1	Total	C	N	0	0
			4	3	1		
4	F	1	Total	C	N	0	0
			4	3	1		
4	H	1	Total	C	N	0	0
			4	3	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

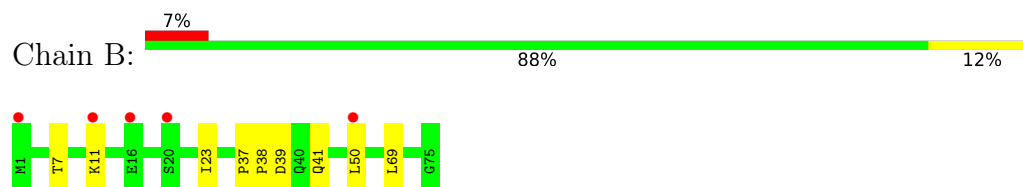
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	45	Total	O	0	0
			45	45		
6	B	25	Total	O	0	0
			25	25		
6	C	30	Total	O	0	0
			30	30		
6	D	16	Total	O	0	0
			16	16		
6	E	40	Total	O	0	0
			40	40		
6	F	31	Total	O	0	0
			31	31		
6	G	55	Total	O	0	0
			55	55		
6	H	28	Total	O	0	0
			28	28		

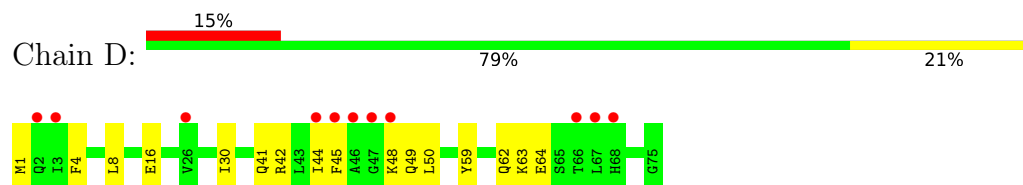




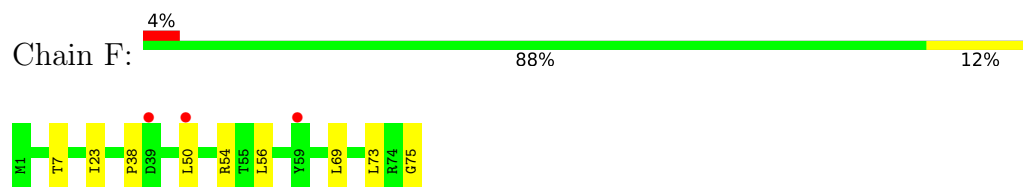
- Molecule 2: Polyubiquitin-B



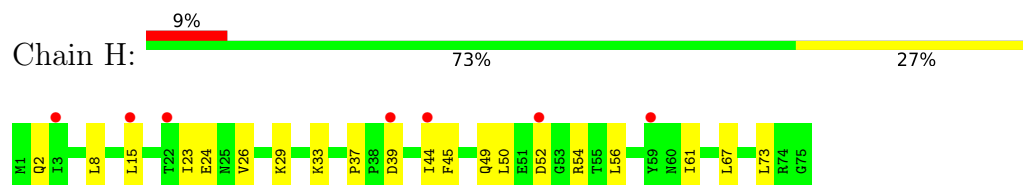
- Molecule 2: Polyubiquitin-B



- Molecule 2: Polyubiquitin-B



- Molecule 2: Polyubiquitin-B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.85Å 55.59Å 97.43Å 90.00° 97.20° 90.00°	Depositor
Resolution (Å)	41.59 – 2.78 41.59 – 2.74	Depositor EDS
% Data completeness (in resolution range)	97.0 (41.59-2.78) 95.8 (41.59-2.74)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 2.73Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.235 , 0.273 0.235 , 0.273	Depositor DCC
$R_{free}$ test set	1107 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.8	Xtrriage
Anisotropy	0.415	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 55.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7706	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.98% 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, AYE, GOL

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	0.35	0/1268	0.56	0/1723
1	C	0.39	0/1291	0.58	0/1754
1	E	0.38	0/1284	0.58	0/1744
1	G	0.34	0/1279	0.51	0/1737
2	B	0.30	0/603	0.50	0/811
2	D	0.38	0/614	0.60	0/825
2	F	0.30	0/603	0.50	0/811
2	H	0.24	0/603	0.44	0/811
All	All	0.35	0/7545	0.54	0/10216

There are no bond length outliers.

There are no bond angle outliers.

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	1239	0	1198	17	0
1	C	1259	0	1223	11	0
1	E	1252	0	1216	18	0
1	G	1250	0	1210	13	0
2	B	597	0	626	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	608	0	638	13	0
2	F	597	0	626	7	0
2	H	597	0	626	12	0
3	A	3	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
4	B	4	0	4	1	0
4	D	4	0	5	1	0
4	F	4	0	5	1	0
4	H	4	0	5	0	0
5	B	6	0	8	0	0
5	C	6	0	8	1	0
6	A	45	0	0	0	0
6	B	25	0	0	0	0
6	C	30	0	0	1	0
6	D	16	0	0	1	0
6	E	40	0	0	3	0
6	F	31	0	0	1	0
6	G	55	0	0	2	0
6	H	28	0	0	0	0
All	All	7706	0	7398	89	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 6.

All (89) 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:B:41:GLN:HB2	2:B:69:LEU:HD11	1.58	0.85
2:D:42:ARG:HG3	2:D:49:GLN:HG3	1.66	0.75
1:G:70:GLU:HG2	1:G:86:LEU:HD21	1.70	0.72
1:G:114:LEU:HD22	6:G:336:HOH:O	1.91	0.70
1:A:38:GLY:H	4:B:101:AYE:H3	1.59	0.66
1:A:40:CYS:HA	1:A:43:HIS:HB2	1.79	0.65
1:C:117:VAL:HG22	1:C:132:ARG:HG3	1.79	0.64
2:F:23:ILE:CD1	2:F:56:LEU:HD23	2.28	0.63
2:D:4:PHE:CE2	2:D:64:GLU:HA	2.34	0.63
2:B:7:THR:HG21	2:B:11:LYS:HE3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:GLY:O	5:C:203:GOL:H12	2.00	0.62
1:G:40:CYS:HA	1:G:43:HIS:HB2	1.84	0.60
1:E:54:SER:HB3	1:E:57:ALA:HB2	1.84	0.60
2:D:4:PHE:HE2	2:D:64:GLU:HA	1.66	0.59
2:F:54:ARG:NH2	6:F:202:HOH:O	2.34	0.59
1:A:42:TYR:HE1	1:A:65:LEU:HD13	1.68	0.59
2:D:62:GLN:HG2	2:D:63:LYS:H	1.69	0.57
1:E:117:VAL:HG22	1:E:132[A]:ARG:HG3	1.86	0.56
2:F:7:THR:HG22	2:F:69:LEU:HB3	1.87	0.55
2:D:1:MET:HG3	2:D:63:LYS:HA	1.88	0.55
1:E:93:ALA:HA	1:E:98:GLU:HG2	1.90	0.54
1:A:9:TRP:HB3	1:A:17:SER:HB3	1.90	0.53
1:A:13:SER:HB3	1:A:16:GLN:HB3	1.91	0.53
2:D:48:LYS:HE2	2:D:59:TYR:HD1	1.74	0.53
2:D:62:GLN:HG2	2:D:63:LYS:N	2.25	0.52
1:C:85:ARG:NH2	6:C:303:HOH:O	2.41	0.52
1:E:70:GLU:HA	1:E:86:LEU:HD21	1.92	0.52
1:G:32:VAL:HB	1:G:154:ALA:HB3	1.92	0.51
2:H:45:PHE:HB3	2:H:50:LEU:HD21	1.93	0.51
1:A:26:THR:HG21	1:A:125:ASN:ND2	2.26	0.51
2:D:45:PHE:O	2:D:48:LYS:NZ	2.41	0.51
2:D:16:GLU:HG2	6:D:204:HOH:O	2.10	0.51
1:E:78:GLU:OE1	6:E:301:HOH:O	2.20	0.50
1:E:25:ILE:HG22	1:E:125:ASN:HB3	1.93	0.50
2:F:23:ILE:HD12	2:F:50:LEU:HD13	1.94	0.49
1:G:135:LYS:HA	6:G:326:HOH:O	2.12	0.49
1:A:92:THR:O	1:A:98:GLU:HG2	2.12	0.49
2:B:23:ILE:HG12	2:B:50:LEU:HB3	1.93	0.49
1:A:124:SER:O	1:A:125:ASN:HB2	2.11	0.49
1:G:117:VAL:HG22	1:G:132:ARG:HG3	1.95	0.49
1:A:64:GLU:HG2	1:A:112:LEU:HD21	1.93	0.49
2:D:42:ARG:HG2	2:D:44:ILE:HD11	1.95	0.49
1:G:82:THR:HG23	1:G:84:MET:H	1.77	0.48
2:B:37:PRO:HB2	2:B:39:ASP:OD1	2.14	0.48
2:B:38:PRO:HA	2:B:41:GLN:HG2	1.96	0.48
1:G:145:LEU:HD13	1:G:155:LEU:HD11	1.96	0.47
2:H:24:GLU:HB2	2:H:52:ASP:HB3	1.97	0.47
1:C:131:THR:HB	2:D:8:LEU:HD21	1.97	0.47
1:A:87:ASP:OD1	1:A:87:ASP:N	2.48	0.47
2:D:30:ILE:HB	2:D:41:GLN:HE22	1.79	0.47
1:C:76:GLU:HG3	1:C:107:MET:HG2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:158:LEU:N	6:E:305:HOH:O	2.48	0.46
1:A:45:LEU:HD21	1:A:144:LEU:HD11	1.98	0.46
1:E:9:TRP:HB3	1:E:17:SER:HB3	1.98	0.45
1:C:145:LEU:HD13	1:C:155:LEU:HD11	1.97	0.45
1:G:49:TYR:CE2	1:G:114:LEU:HD21	2.52	0.45
1:G:131:THR:OG1	2:H:8:LEU:HD21	2.17	0.45
2:F:23:ILE:HD13	2:F:56:LEU:HD23	1.99	0.44
1:C:14:ASP:OD1	1:C:14:ASP:N	2.49	0.44
1:C:146:HIS:NE2	1:C:149:LEU:HA	2.33	0.44
1:A:70:GLU:HA	1:A:86:LEU:HD21	1.99	0.44
1:E:44:SER:HB3	1:E:154:ALA:HB2	2.00	0.44
1:E:56:HIS:HB2	1:E:59:ARG:HD2	1.99	0.44
1:E:40:CYS:HB3	4:F:102:AYE:H3A	1.63	0.44
1:C:40:CYS:HB3	4:D:102:AYE:H3A	1.67	0.44
1:E:71:LYS:O	1:G:66:ARG:NH1	2.51	0.44
2:H:23:ILE:HB	2:H:52:ASP:HA	1.99	0.43
1:E:74:PRO:HB2	1:G:66:ARG:NH2	2.33	0.43
1:A:30:GLU:HB2	1:A:158:LEU:HD21	2.01	0.43
1:A:65:LEU:HD11	1:A:104:GLU:HB3	2.00	0.43
2:H:26:VAL:HG21	2:H:56:LEU:HD21	2.00	0.43
2:H:61:ILE:HG21	2:H:67:LEU:HD11	2.00	0.43
2:H:29:LYS:O	2:H:33:LYS:HG3	2.19	0.42
2:H:2:GLN:HA	2:H:15:LEU:O	2.19	0.42
2:H:37:PRO:HB2	2:H:39:ASP:OD1	2.19	0.42
2:D:45:PHE:HB3	2:D:50:LEU:HD21	2.01	0.42
2:H:23:ILE:HG12	2:H:54:ARG:O	2.19	0.42
1:A:76:GLU:HG3	1:A:107:MET:HG2	2.02	0.42
1:A:139:LYS:HB2	1:A:139:LYS:HE2	1.78	0.42
1:E:59:ARG:NE	6:E:307:HOH:O	2.53	0.42
1:E:152:PHE:CD2	2:F:75:GLY:HA3	2.55	0.42
1:G:101:GLY:HA3	2:H:73:LEU:O	2.19	0.41
1:E:135:LYS:HA	1:E:135:LYS:HD3	1.80	0.41
1:C:40:CYS:HA	1:C:43:HIS:HB2	2.02	0.41
2:H:44:ILE:HD13	2:H:49:GLN:HA	2.02	0.41
1:E:101:GLY:HA3	2:F:73:LEU:O	2.20	0.41
1:E:73:PHE:HB3	1:E:74:PRO:HD3	2.03	0.41
1:C:25:ILE:HG12	1:C:145:LEU:HD13	2.03	0.40
1:A:73:PHE:N	1:A:74:PRO:HD2	2.37	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	155/178 (87%)	154 (99%)	1 (1%)	0	100	100
1	C	158/178 (89%)	153 (97%)	5 (3%)	0	100	100
1	E	157/178 (88%)	151 (96%)	6 (4%)	0	100	100
1	G	156/178 (88%)	154 (99%)	2 (1%)	0	100	100
2	B	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
2	D	74/75 (99%)	74 (100%)	0	0	100	100
2	F	73/75 (97%)	73 (100%)	0	0	100	100
2	H	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
All	All	919/1012 (91%)	903 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	132/151 (87%)	131 (99%)	1 (1%)	81	93
1	C	134/151 (89%)	134 (100%)	0	100	100
1	E	133/151 (88%)	133 (100%)	0	100	100
1	G	133/151 (88%)	131 (98%)	2 (2%)	65	87
2	B	68/68 (100%)	68 (100%)	0	100	100
2	D	69/68 (102%)	69 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	68/68 (100%)	67 (98%)	1 (2%)	65	87
2	H	68/68 (100%)	68 (100%)	0	100	100
All	All	805/876 (92%)	801 (100%)	4 (0%)	88	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	VAL
2	F	38	PRO
1	G	85	ARG
1	G	135	LYS

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

Mol	Chain	Res	Type
2	D	41	GLN
1	E	63	ASN
2	F	49	GLN
1	G	43	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](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 9 are monoatomic - leaving 6 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
4	AYE	H	101	2,1	3,3,3	0.74	0	1,2,2	1.27	0
4	AYE	F	102	2,1	3,3,3	0.73	0	1,2,2	1.32	0
4	AYE	B	101	2,1	3,3,3	0.76	0	1,2,2	1.27	0
4	AYE	D	102	2,1	3,3,3	0.71	0	1,2,2	1.27	0
5	GOL	B	102	-	5,5,5	0.09	0	5,5,5	0.34	0
5	GOL	C	203	-	5,5,5	0.08	0	5,5,5	0.27	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
4	AYE	H	101	2,1	-	0/1/1/1	-
4	AYE	F	102	2,1	-	1/1/1/1	-
4	AYE	B	101	2,1	-	1/1/1/1	-
4	AYE	D	102	2,1	-	1/1/1/1	-
5	GOL	B	102	-	-	0/4/4/4	-
5	GOL	C	203	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	102	AYE	N1-C1-C2-C3
5	C	203	GOL	O2-C2-C3-O3
4	B	101	AYE	N1-C1-C2-C3
4	D	102	AYE	N1-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	102	AYE	1	0
4	B	101	AYE	1	0
4	D	102	AYE	1	0
5	C	203	GOL	1	0

## 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

### 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	157/178 (88%)	0.30	7 (4%) 33 27	27, 40, 63, 80	0
1	C	159/178 (89%)	0.19	4 (2%) 57 52	22, 39, 58, 70	0
1	E	158/178 (88%)	0.21	5 (3%) 47 42	26, 42, 59, 83	0
1	G	157/178 (88%)	0.23	5 (3%) 47 42	31, 42, 60, 72	0
2	B	75/75 (100%)	0.35	5 (6%) 17 13	24, 40, 54, 56	0
2	D	75/75 (100%)	0.75	11 (14%) 2 1	31, 49, 61, 70	0
2	F	75/75 (100%)	0.43	3 (4%) 38 33	28, 44, 56, 58	0
2	H	75/75 (100%)	0.54	7 (9%) 8 6	35, 46, 59, 62	0
All	All	931/1012 (91%)	0.32	47 (5%) 28 23	22, 42, 59, 83	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	83	GLY	5.0
1	A	158	LEU	3.9
1	G	12	VAL	3.8
2	D	67	LEU	3.6
1	C	83	GLY	3.6
1	E	60	LEU	3.6
1	C	15	ILE	3.4
2	B	1	MET	3.1
2	H	39	ASP	3.0
1	A	125	ASN	3.0
1	A	84	MET	3.0
2	D	46	ALA	2.9
2	D	48	LYS	2.9
1	C	82	THR	2.8
1	G	114	LEU	2.8
2	B	20	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	16	GLU	2.6
2	D	44	ILE	2.6
2	H	44	ILE	2.6
1	G	11	SER	2.5
2	D	45	PHE	2.5
1	G	81	ALA	2.5
2	D	3	ILE	2.5
2	F	39	ASP	2.4
2	D	68	HIS	2.4
1	A	123	GLY	2.3
1	C	2	ASP	2.3
2	H	22	THR	2.3
2	H	52	ASP	2.3
2	D	47	GLY	2.3
1	E	87	ASP	2.3
2	H	59	TYR	2.3
2	D	66	THR	2.3
2	B	11	LYS	2.3
1	A	85	ARG	2.2
2	F	59	TYR	2.2
1	A	51	PRO	2.2
2	D	26	VAL	2.2
1	G	5	GLU	2.2
1	E	123	GLY	2.2
2	H	3	ILE	2.2
2	B	50	LEU	2.2
2	H	15	LEU	2.1
1	E	59	ARG	2.1
2	D	2	GLN	2.1
2	F	50	LEU	2.1
1	E	51	PRO	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	CA	D	101	1/1	0.69	0.14	63,63,63,63	0
5	GOL	C	203	6/6	0.72	0.24	38,43,52,54	0
5	GOL	B	102	6/6	0.73	0.26	49,56,60,66	0
3	CA	F	101	1/1	0.81	0.12	54,54,54,54	0
3	CA	A	202	1/1	0.82	0.09	58,58,58,58	0
4	AYE	F	102	4/4	0.88	0.33	41,41,44,46	0
3	CA	A	203	1/1	0.89	0.12	79,79,79,79	0
3	CA	G	201	1/1	0.90	0.18	42,42,42,42	0
3	CA	A	201	1/1	0.91	0.07	50,50,50,50	0
4	AYE	H	101	4/4	0.94	0.15	31,33,41,42	0
4	AYE	D	102	4/4	0.94	0.19	34,35,42,42	0
3	CA	C	202	1/1	0.94	0.11	66,66,66,66	0
4	AYE	B	101	4/4	0.97	0.14	32,33,34,38	0
3	CA	C	201	1/1	0.97	0.07	39,39,39,39	0
3	CA	E	201	1/1	0.97	0.10	44,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.