Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:19 AM GMT

PDB ID	:	2Q8U
Title	:	CRYSTAL STRUCTURE OF MRE11 FROM THERMOTOGA MARITIMA MSB8 (TM1635) AT 2.20 A RESOLUTION
Authors	:	Joint Center for Structural Genomics (JCSG)
Deposited on	:	2007-06-11
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

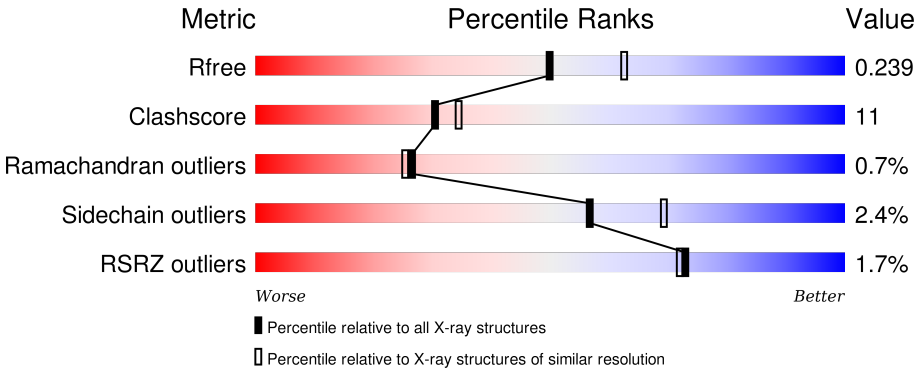
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

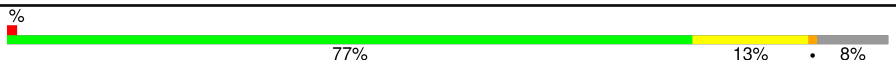
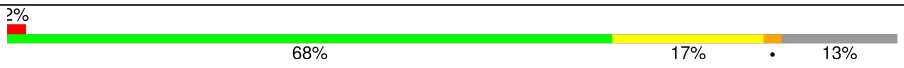
The reported resolution of this entry is 2.20 Å.

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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	336	
1	B	336	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5017 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 Exonuclease, putative.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	Se	0	7	0
			2507	1627	419	455	1	5			
1	B	294	Total	C	N	O	S	Se	0	7	0
			2351	1537	383	423	1	7			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MSE	-	LEADER SEQUENCE	UNP Q9X1X0
A	-10	GLY	-	LEADER SEQUENCE	UNP Q9X1X0
A	-9	SER	-	LEADER SEQUENCE	UNP Q9X1X0
A	-8	ASP	-	LEADER SEQUENCE	UNP Q9X1X0
A	-7	LYS	-	LEADER SEQUENCE	UNP Q9X1X0
A	-6	ILE	-	LEADER SEQUENCE	UNP Q9X1X0
A	-5	HIS	-	LEADER SEQUENCE	UNP Q9X1X0
A	-4	HIS	-	LEADER SEQUENCE	UNP Q9X1X0
A	-3	HIS	-	LEADER SEQUENCE	UNP Q9X1X0
A	-2	HIS	-	LEADER SEQUENCE	UNP Q9X1X0
A	-1	HIS	-	LEADER SEQUENCE	UNP Q9X1X0
A	0	HIS	-	LEADER SEQUENCE	UNP Q9X1X0
A	1	VAL	MET	SEE REMARK 999	UNP Q9X1X0
A	81	MSE	MET	MODIFIED RESIDUE	UNP Q9X1X0
A	82	MSE	MET	MODIFIED RESIDUE	UNP Q9X1X0
A	117	MSE	MET	MODIFIED RESIDUE	UNP Q9X1X0
A	178	MSE	MET	MODIFIED RESIDUE	UNP Q9X1X0
A	314	MSE	MET	MODIFIED RESIDUE	UNP Q9X1X0
B	-11	MSE	-	LEADER SEQUENCE	UNP Q9X1X0
B	-10	GLY	-	LEADER SEQUENCE	UNP Q9X1X0
B	-9	SER	-	LEADER SEQUENCE	UNP Q9X1X0
B	-8	ASP	-	LEADER SEQUENCE	UNP Q9X1X0
B	-7	LYS	-	LEADER SEQUENCE	UNP Q9X1X0
B	-6	ILE	-	LEADER SEQUENCE	UNP Q9X1X0
B	-5	HIS	-	LEADER SEQUENCE	UNP Q9X1X0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	LEADER SEQUENCE	UNP Q9X1X0
B	-3	HIS	-	LEADER SEQUENCE	UNP Q9X1X0
B	-2	HIS	-	LEADER SEQUENCE	UNP Q9X1X0
B	-1	HIS	-	LEADER SEQUENCE	UNP Q9X1X0
B	0	HIS	-	LEADER SEQUENCE	UNP Q9X1X0
B	1	VAL	MET	SEE REMARK 999	UNP Q9X1X0
B	81	MSE	MET	MODIFIED RESIDUE	UNP Q9X1X0
B	82	MSE	MET	MODIFIED RESIDUE	UNP Q9X1X0
B	117	MSE	MET	MODIFIED RESIDUE	UNP Q9X1X0
B	178	MSE	MET	MODIFIED RESIDUE	UNP Q9X1X0
B	314	MSE	MET	MODIFIED RESIDUE	UNP Q9X1X0

- Molecule 2 is water.

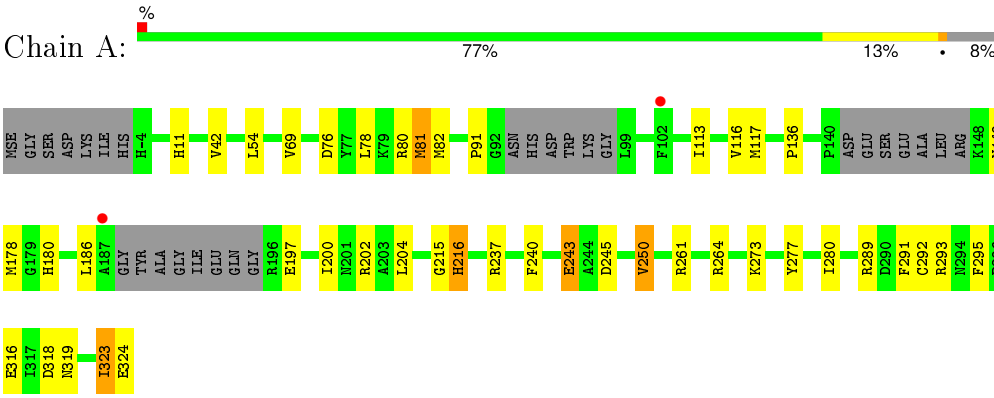
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	96	Total O 96 96	0	0
2	B	63	Total O 63 63	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

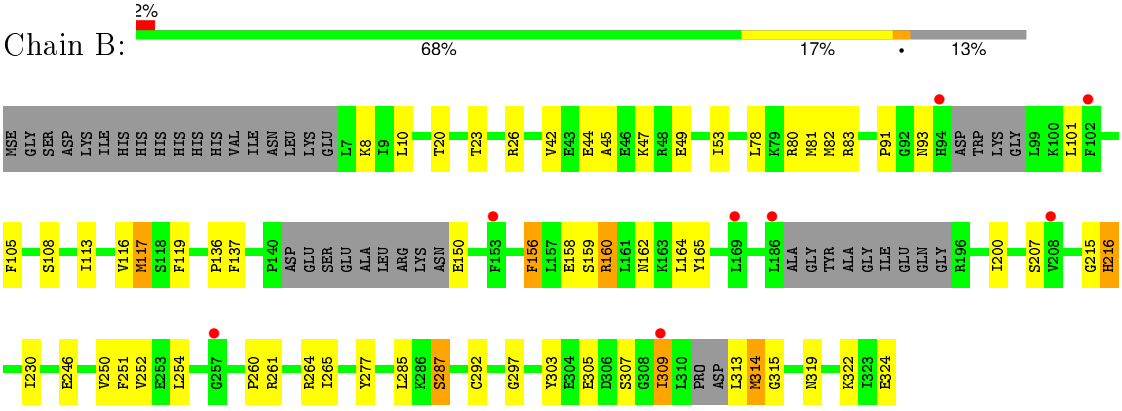
- Molecule 1: Exonuclease, putative

Chain A:



- Molecule 1: Exonuclease, putative

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	47.60Å 113.41Å 80.95Å 90.00° 101.77° 90.00°	Depositor
Resolution (Å)	37.45 – 2.20 79.25 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (37.45-2.20) 98.7 (79.25-2.20)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.198 , 0.241 0.199 , 0.239	Depositor DCC
R_{free} test set	2120 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	45.8	Xtriage
Anisotropy	0.522	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 56.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 42149 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5017	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.70	1/2579 (0.0%)	0.74	3/3480 (0.1%)
1	B	0.76	6/2416 (0.2%)	0.71	0/3258
All	All	0.73	7/4995 (0.1%)	0.73	3/6738 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	162	ASN	C-O	11.53	1.45	1.23
1	B	158	GLU	C-N	7.06	1.50	1.34
1	B	207	SER	C-O	6.36	1.35	1.23
1	B	160	ARG	C-O	6.27	1.35	1.23
1	B	164	LEU	C-O	5.69	1.34	1.23
1	B	156	PHE	C-O	5.35	1.33	1.23
1	A	81	MSE	CG-SE	-5.12	1.78	1.95

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	237	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	A	264	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	245	ASP	CB-CG-OD1	-5.39	113.45	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	323	ILE	Peptide

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	2507	0	2510	51	0
1	B	2351	0	2346	58	0
2	A	96	0	0	4	0
2	B	63	0	0	4	0
All	All	5017	0	4856	107	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 11.

All (107) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82[A]:MSE:HE2	1:B:113:ILE:CD1	1.80	1.12
1:A:82:MSE:HE2	1:A:113:ILE:CD1	1.79	1.12
1:B:91:PRO:HG3	1:B:117:MSE:CE	1.80	1.09
1:B:91:PRO:HG3	1:B:117:MSE:HE1	1.07	1.05
1:A:82:MSE:HE2	1:A:113:ILE:HD12	1.38	1.03
1:B:82[A]:MSE:HE2	1:B:113:ILE:HD12	1.47	0.94
1:A:91:PRO:HG3	1:A:117:MSE:CE	2.02	0.88
1:A:91:PRO:HG3	1:A:117:MSE:HE2	1.53	0.88
1:B:42:VAL:HG22	1:B:81[B]:MSE:HE3	1.56	0.87
1:A:69:VAL:HG23	2:A:407:HOH:O	1.74	0.86
1:B:10:LEU:HD22	1:B:45:ALA:HB2	1.59	0.85
1:B:82[A]:MSE:CE	1:B:113:ILE:CD1	2.54	0.85
1:A:82:MSE:HE2	1:A:113:ILE:HD13	1.57	0.85
1:B:82[A]:MSE:HE2	1:B:113:ILE:HD13	1.57	0.84
1:A:82:MSE:HE1	1:B:105:PHE:HZ	1.42	0.82
1:B:309:ILE:H	1:B:309:ILE:HD12	1.45	0.81
1:B:82[A]:MSE:CE	1:B:113:ILE:HD13	2.11	0.80
1:B:150:GLU:N	1:B:150:GLU:OE1	2.18	0.76
1:B:78:LEU:HB3	1:B:82[A]:MSE:HE3	1.67	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82[A]:MSE:CE	1:B:113:ILE:HD12	2.16	0.73
1:B:81[B]:MSE:HE2	1:B:81[B]:MSE:HA	1.70	0.73
1:A:150:GLU:N	1:A:150:GLU:OE1	2.22	0.72
1:A:82:MSE:CE	1:A:113:ILE:HD13	2.20	0.71
1:A:82:MSE:CE	1:A:113:ILE:CD1	2.66	0.70
1:A:78:LEU:HB3	1:A:82:MSE:HE3	1.77	0.67
1:B:20:THR:HG22	1:B:23:THR:HG22	1.76	0.66
1:B:117:MSE:HA	1:B:117:MSE:HE2	1.79	0.65
1:A:116:VAL:HG11	1:A:136:PRO:HB3	1.79	0.64
1:B:91:PRO:CG	1:B:117:MSE:CE	2.70	0.64
1:A:297:GLY:O	1:A:319[A]:ASN:ND2	2.32	0.62
1:A:91:PRO:CG	1:A:117:MSE:CE	2.78	0.61
1:B:322:LYS:HE3	1:B:324:GLU:OE2	2.00	0.61
1:A:91:PRO:HG3	1:A:117:MSE:HE1	1.80	0.61
1:A:273:LYS:HG2	1:A:291:PHE:CZ	2.36	0.60
1:B:215:GLY:O	1:B:216:HIS:CB	2.50	0.60
1:B:307:SER:N	2:B:356:HOH:O	2.35	0.59
1:A:197:GLU:HG3	2:A:416:HOH:O	2.00	0.59
1:A:116:VAL:HG11	1:A:136:PRO:CB	2.32	0.59
1:A:323:ILE:O	1:A:324:GLU:CB	2.50	0.59
1:B:277:TYR:HH	1:B:287:SER:HG	1.52	0.58
1:A:280:ILE:HG22	1:A:280:ILE:O	2.03	0.58
1:B:254:LEU:HD23	1:B:260:PRO:HB3	1.86	0.58
1:B:42:VAL:HG22	1:B:81[B]:MSE:CE	2.31	0.58
1:B:215:GLY:O	1:B:216:HIS:HB3	2.02	0.57
1:B:26:ARG:NH2	1:B:314:MSE:O	2.38	0.56
1:B:137:PHE:CE1	1:B:200:ILE:HD11	2.40	0.56
1:B:250:VAL:HG12	1:B:252:VAL:HG23	1.88	0.56
1:B:309:ILE:CD1	1:B:309:ILE:H	2.14	0.55
1:A:277:TYR:O	1:A:303:TYR:HA	2.07	0.55
1:A:323:ILE:O	1:A:324:GLU:CG	2.55	0.54
1:B:116:VAL:CG1	1:B:136:PRO:HG3	2.37	0.54
1:B:116:VAL:HG11	1:B:136:PRO:HG3	1.88	0.54
1:A:314:MSE:HE2	1:A:323:ILE:HG13	1.91	0.53
1:A:180:HIS:HB2	2:A:419:HOH:O	2.08	0.53
1:B:53:ILE:HD13	1:B:81[A]:MSE:HG2	1.91	0.53
1:A:116:VAL:HG11	1:A:136:PRO:HG3	1.90	0.53
1:B:285:LEU:HD23	1:B:313:LEU:HD21	1.90	0.52
1:A:215:GLY:O	1:A:216:HIS:HB3	2.10	0.52
1:A:323:ILE:O	1:A:324:GLU:HB3	2.10	0.51
1:A:82:MSE:HE1	1:B:105:PHE:CZ	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:THR:CG2	1:B:23:THR:HG22	2.41	0.51
1:B:82[A]:MSE:HE2	1:B:113:ILE:HB	1.93	0.50
1:A:91:PRO:CG	1:A:117:MSE:HE1	2.41	0.49
1:B:20:THR:HG22	1:B:23:THR:CG2	2.41	0.49
1:A:197:GLU:CG	2:A:416:HOH:O	2.57	0.49
1:B:42:VAL:CG2	1:B:81[A]:MSE:HE3	2.44	0.48
1:B:160:ARG:HD2	2:B:325:HOH:O	2.13	0.48
1:A:117:MSE:HE2	1:A:117:MSE:HA	1.96	0.48
1:A:215:GLY:O	1:A:216:HIS:CB	2.61	0.48
1:B:81[B]:MSE:CE	1:B:81[B]:MSE:HA	2.42	0.48
1:B:264:ARG:NH2	2:B:366:HOH:O	2.47	0.48
1:B:251:PHE:HB2	1:B:265:ILE:HD11	1.96	0.48
1:B:156:PHE:O	1:B:159:SER:OG	2.25	0.47
1:B:230:ILE:HG21	1:B:250:VAL:HG21	1.97	0.47
1:A:240:PHE:O	1:A:243:GLU:HG2	2.15	0.47
1:A:323:ILE:O	1:A:324:GLU:CD	2.53	0.47
1:B:254:LEU:CD2	1:B:260:PRO:HB3	2.43	0.47
1:A:54:LEU:HB3	1:A:178:MSE:HE3	1.97	0.47
1:A:116:VAL:CG1	1:A:136:PRO:HG3	2.46	0.46
1:B:292:CYS:O	1:B:319:ASN:ND2	2.47	0.46
1:A:297:GLY:O	1:A:319[A]:ASN:CG	2.55	0.46
1:B:165:TYR:CD1	1:B:165:TYR:C	2.89	0.46
1:A:149:ASN:HB3	1:A:153:PHE:HB2	1.99	0.45
1:A:116:VAL:HG11	1:A:136:PRO:CG	2.46	0.45
1:A:314:MSE:CE	1:A:323:ILE:HG13	2.46	0.45
1:B:80:ARG:HG2	1:B:83:ARG:HH12	1.82	0.45
1:A:11:HIS:HB3	1:A:250:VAL:HG12	1.99	0.45
1:B:119[B]:PHE:HE1	1:B:137:PHE:CD2	2.35	0.44
1:A:149:ASN:CB	1:A:153:PHE:HB2	2.48	0.43
1:A:292:CYS:O	1:A:293:ARG:C	2.57	0.43
1:B:78:LEU:HB3	1:B:82[A]:MSE:CE	2.41	0.43
1:A:161:LEU:HD13	1:A:204:LEU:HB3	2.01	0.43
1:B:8:LYS:HE3	1:B:49:GLU:O	2.19	0.43
1:B:277:TYR:O	1:B:303:TYR:HA	2.18	0.42
1:B:44:GLU:OE2	1:B:47:LYS:CD	2.68	0.42
1:A:78:LEU:O	1:A:82:MSE:HG3	2.19	0.42
1:B:42:VAL:HA	1:B:81[B]:MSE:HE1	2.02	0.42
1:A:76:ASP:O	1:A:80:ARG:HG3	2.20	0.42
1:B:101:LEU:HA	1:B:101:LEU:HD23	1.86	0.42
1:B:297:GLY:O	1:B:319:ASN:OD1	2.38	0.41
1:A:91:PRO:CG	1:A:117:MSE:HE2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:GLU:CG	2:B:336:HOH:O	2.68	0.41
1:B:313:LEU:O	1:B:315:GLY:N	2.52	0.41
1:A:42:VAL:HG22	1:A:81:MSE:HE3	2.02	0.41
1:A:186:LEU:HA	1:A:186:LEU:HD23	1.89	0.41
1:A:295:PHE:O	1:A:319[A]:ASN:ND2	2.54	0.40
1:A:289:ARG:NE	1:A:316:GLU:OE2	2.54	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	307/336 (91%)	292 (95%)	14 (5%)	1 (0%)	46	50
1	B	291/336 (87%)	272 (94%)	16 (6%)	3 (1%)	19	16
All	All	598/672 (89%)	564 (94%)	30 (5%)	4 (1%)	26	25

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	314	MSE
1	A	216	HIS
1	B	216	HIS
1	B	93	ASN

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	272/292 (93%)	266 (98%)	6 (2%)	60 72
1	B	249/292 (85%)	243 (98%)	6 (2%)	57 69
All	All	521/584 (89%)	509 (98%)	12 (2%)	57 71

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	ILE
1	A	202	ARG
1	A	243	GLU
1	A	250	VAL
1	A	261	ARG
1	A	318	ASP
1	B	108	SER
1	B	117	MSE
1	B	261	ARG
1	B	287	SER
1	B	305	GLU
1	B	309	ILE

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 molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	303/336 (90%)	0.06	2 (0%)	89 88	38, 48, 72, 114	0
1	B	289/336 (86%)	0.23	8 (2%)	56 55	35, 48, 70, 114	0
All	All	592/672 (88%)	0.14	10 (1%)	73 72	35, 48, 71, 114	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	208	VAL	3.4
1	B	309	ILE	2.8
1	B	94	HIS	2.8
1	B	186	LEU	2.7
1	B	169	LEU	2.6
1	B	153	PHE	2.5
1	B	102[A]	PHE	2.5
1	A	187	ALA	2.4
1	B	257	GLY	2.2
1	A	102[A]	PHE	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.