



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:50 AM GMT

PDB ID : 2OEZ
Title : Protein of Unknown Function (DUF1342) from *Vibrio parahaemolyticus*
Authors : Kim, Y.; Volkart, L.; Abdullah, J.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2007-01-02
Resolution : 1.97 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

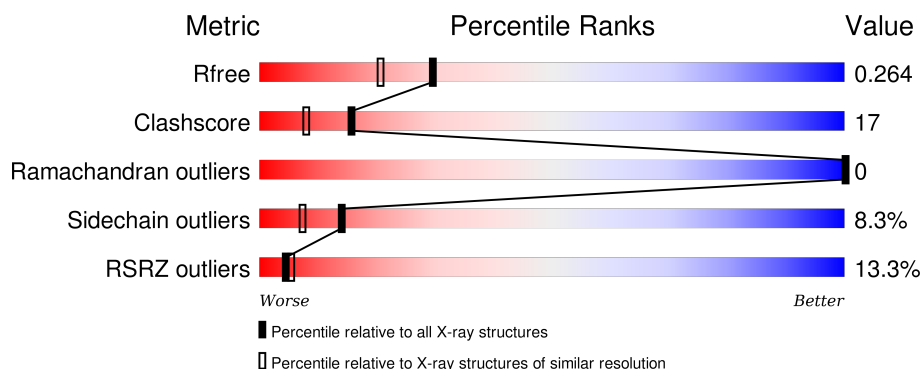
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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 $\leq 5\%$. 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	247	
1	B	247	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4932 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 UPF0289 protein VP2528.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	Se	0	29	0
			2266	1433	415	407	5	6			
1	B	243	Total	C	N	O	S	Se	0	26	0
			2242	1419	412	401	4	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	CLONING ARTIFACT	UNP Q87LT3
A	0	ASN	-	CLONING ARTIFACT	UNP Q87LT3
A	1	ALA	-	CLONING ARTIFACT	UNP Q87LT3
A	49	MSE	MET	MODIFIED RESIDUE	UNP Q87LT3
A	102	MSE	MET	MODIFIED RESIDUE	UNP Q87LT3
A	206	MSE	MET	MODIFIED RESIDUE	UNP Q87LT3
A	213	MSE	MET	MODIFIED RESIDUE	UNP Q87LT3
A	226	MSE	MET	MODIFIED RESIDUE	UNP Q87LT3
B	-1	SER	-	CLONING ARTIFACT	UNP Q87LT3
B	0	ASN	-	CLONING ARTIFACT	UNP Q87LT3
B	1	ALA	-	CLONING ARTIFACT	UNP Q87LT3
B	49	MSE	MET	MODIFIED RESIDUE	UNP Q87LT3
B	102	MSE	MET	MODIFIED RESIDUE	UNP Q87LT3
B	206	MSE	MET	MODIFIED RESIDUE	UNP Q87LT3
B	213	MSE	MET	MODIFIED RESIDUE	UNP Q87LT3
B	226	MSE	MET	MODIFIED RESIDUE	UNP Q87LT3

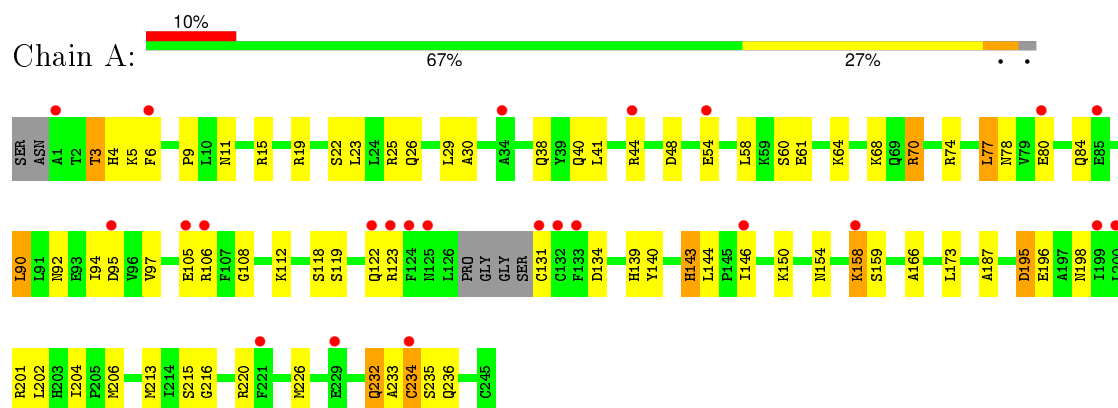
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	221	Total	O	0	0
			221	221		
2	B	203	Total	O	0	0
			203	203		

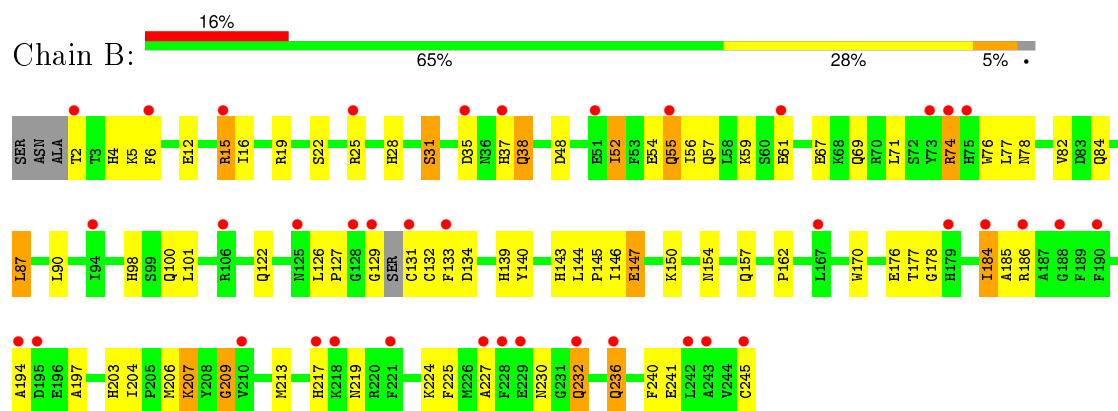
3 Residue-property plots [i](#)

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: UPF0289 protein VP2528



- Molecule 1: UPF0289 protein VP2528



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.76 Å 77.57 Å 146.17 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.25 – 1.97 49.25 – 1.95	Depositor EDS
% Data completeness (in resolution range)	93.7 (49.25-1.97) 92.0 (49.25-1.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 1.95 Å)	Xtriage
Refinement program	REFMAC 5.2.0000	Depositor
R, R_{free}	0.210 , 0.267 0.207 , 0.264	Depositor DCC
R_{free} test set	4870 reflections (11.09%)	DCC
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 49232 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4932	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.81	1/2310 (0.0%)	0.83	3/3090 (0.1%)
1	B	0.90	4/2290 (0.2%)	0.81	1/3070 (0.0%)
All	All	0.86	5/4600 (0.1%)	0.82	4/6160 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	209	GLY	C-O	13.80	1.45	1.23
1	B	209	GLY	C-N	9.45	1.55	1.34
1	B	230	ASN	C-N	6.85	1.45	1.33
1	B	227	ALA	C-O	6.32	1.35	1.23
1	A	215	SER	CB-OG	-5.30	1.35	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	A	220	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	A	220	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	48	ASP	CB-CG-OD1	5.06	122.85	118.30

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	2266	0	2200	84	0
1	B	2242	0	2153	88	1
2	A	221	0	0	29	0
2	B	203	0	0	26	0
All	All	4932	0	4353	153	1

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 17.

All (153) 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:A:6[B]:PHE:CE1	2:B:399:HOH:O	2.12	1.01
1:B:56:ILE:HG12	2:B:442:HOH:O	1.59	1.00
1:A:4:HIS:HD2	1:A:206:MSE:HE2	1.37	0.90
1:A:232:GLN:HE21	1:A:232:GLN:HA	1.37	0.90
1:A:4:HIS:NE2	1:A:206:MSE:HG2	1.90	0.85
1:A:29:LEU:HG	2:A:463:HOH:O	1.76	0.85
1:A:4:HIS:CD2	1:A:206:MSE:HE2	2.14	0.82
1:B:4:HIS:CE1	1:B:206:MSE:HG2	2.14	0.81
1:B:2:THR:HA	1:B:206:MSE:SE	2.31	0.81
1:B:154[B]:ASN:ND2	2:B:335:HOH:O	1.96	0.80
1:A:4:HIS:CD2	1:A:206:MSE:HG2	2.17	0.80
1:B:127:PRO:HD3	2:B:433:HOH:O	1.82	0.79
1:A:139:HIS:HD2	2:A:389:HOH:O	1.71	0.73
2:A:447:HOH:O	1:B:6[B]:PHE:CE1	2.42	0.72
1:B:71:LEU:CD1	1:B:74[B]:ARG:HH11	2.02	0.72
1:A:139:HIS:CD2	2:A:389:HOH:O	2.43	0.70
1:B:194:ALA:HB1	1:B:197:ALA:HB3	1.72	0.70
1:B:61[B]:GLU:OE1	2:B:410:HOH:O	2.10	0.70
1:A:11:ASN:HD21	1:A:198:ASN:HD22	1.39	0.69
1:B:19:ARG:HD3	2:B:440:HOH:O	1.92	0.69
1:A:5:LYS:O	1:B:139:HIS:HE1	1.76	0.69
1:B:71:LEU:HD22	2:B:375:HOH:O	1.92	0.69
1:A:15[A]:ARG:HG3	1:B:133:PHE:CE1	2.29	0.68
1:A:23:LEU:HD21	1:B:129:GLY:HA3	1.74	0.67
1:A:134:ASP:HB2	2:A:449:HOH:O	1.94	0.67
1:B:28:HIS:O	1:B:31:SER:HB2	1.95	0.67
1:A:143:HIS:CE1	2:A:434:HOH:O	2.47	0.66
1:B:52:ILE:O	1:B:55[A]:GLN:HG2	1.95	0.66
1:B:4:HIS:HE1	1:B:206:MSE:HE3	1.61	0.66
1:A:97:VAL:HG11	1:A:166:ALA:HA	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158[B]:LYS:HD2	1:A:159:SER:N	2.13	0.63
1:B:35:ASP:HB3	2:B:370:HOH:O	1.96	0.63
1:A:233:ALA:HB2	2:A:446:HOH:O	1.98	0.63
2:A:339:HOH:O	1:B:6[B]:PHE:HZ	1.82	0.63
1:B:139:HIS:ND1	2:B:398:HOH:O	2.29	0.62
1:A:213[A]:MSE:SE	1:A:226:MSE:HG3	2.50	0.62
1:A:234[A]:CYS:O	1:A:234[A]:CYS:SG	2.58	0.62
1:A:97:VAL:CG1	1:A:166:ALA:HA	2.31	0.60
1:A:232:GLN:NE2	1:A:232:GLN:HA	2.13	0.60
1:A:22:SER:HB2	1:B:131:CYS:HB3	1.82	0.60
1:A:30:ALA:HA	1:A:38[B]:GLN:HG2	1.83	0.60
1:A:78:ASN:H	1:A:84:GLN:NE2	2.01	0.59
1:B:54:GLU:HG3	2:B:347:HOH:O	2.00	0.59
1:A:187:ALA:HA	1:A:235[A]:SER:O	2.01	0.59
1:B:74[B]:ARG:NH1	2:B:257:HOH:O	2.35	0.59
1:B:15[B]:ARG:NE	2:B:440:HOH:O	2.23	0.59
1:A:44[B]:ARG:NH1	2:A:452:HOH:O	2.36	0.59
1:A:92:ASN:HA	1:A:95[B]:ASP:OD1	2.04	0.58
1:A:144:LEU:HD23	2:B:402:HOH:O	2.03	0.58
1:A:4:HIS:NE2	2:A:424:HOH:O	2.32	0.57
1:B:2:THR:C	1:B:206:MSE:HG3	2.24	0.57
1:A:4:HIS:CE1	1:B:140:TYR:CE1	2.93	0.57
1:A:216:GLY:O	2:A:444:HOH:O	2.18	0.56
1:A:54:GLU:OE2	1:A:112:LYS:HE3	2.05	0.56
1:A:74[A]:ARG:HA	1:A:77:LEU:HD22	1.87	0.56
1:B:37[B]:HIS:HB2	2:B:370:HOH:O	2.05	0.55
1:A:139:HIS:HE1	1:B:5:LYS:O	1.88	0.55
1:A:22:SER:CB	1:B:131:CYS:HB3	2.37	0.55
1:A:146:ILE:HG13	1:A:150:LYS:HD2	1.88	0.55
1:B:143[B]:HIS:CE1	2:B:398:HOH:O	2.60	0.54
1:A:143:HIS:HD2	1:B:4:HIS:HA	1.73	0.54
1:B:28:HIS:HA	1:B:157:GLN:HE22	1.72	0.54
1:A:44[A]:ARG:HG2	2:A:422:HOH:O	2.06	0.54
1:B:67:GLU:OE2	1:B:98:HIS:HE1	1.91	0.54
1:B:224:LYS:HE2	2:B:424:HOH:O	2.07	0.53
1:A:213[B]:MSE:HE3	2:A:443:HOH:O	2.08	0.53
1:B:131:CYS:SG	1:B:133:PHE:CE2	3.02	0.53
1:A:68[A]:LYS:HD2	2:A:466:HOH:O	2.08	0.53
1:B:146:ILE:HG13	1:B:150:LYS:HD2	1.90	0.52
1:A:68[B]:LYS:HE2	2:A:465:HOH:O	2.10	0.52
1:A:195[B]:ASP:OD1	1:A:196[B]:GLU:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:PRO:HB2	1:B:147[A]:GLU:HG2	1.92	0.52
1:A:30:ALA:HB2	1:B:37[B]:HIS:CE1	2.45	0.52
1:A:143:HIS:ND1	2:A:434:HOH:O	2.34	0.52
2:A:447:HOH:O	1:B:6[B]:PHE:HE1	1.84	0.52
1:A:44[A]:ARG:HD2	1:A:48:ASP:OD2	2.09	0.51
1:A:131:CYS:HB3	1:B:22:SER:OG	2.11	0.51
1:B:100[A]:GLN:HG2	1:B:162:PRO:HB3	1.93	0.51
1:A:5:LYS:H	1:B:143[B]:HIS:CE1	2.28	0.51
1:B:131:CYS:O	2:B:438:HOH:O	2.20	0.51
1:A:23:LEU:CD2	1:B:129:GLY:HA3	2.40	0.51
1:A:4:HIS:NE2	1:A:206:MSE:CG	2.70	0.51
1:B:16:ILE:HD13	1:B:56:ILE:HG21	1.93	0.50
1:B:194:ALA:HB1	1:B:197:ALA:CB	2.42	0.50
1:B:71:LEU:CD1	1:B:74[B]:ARG:NH1	2.72	0.50
1:B:131:CYS:SG	1:B:133:PHE:CD2	3.05	0.50
1:B:35:ASP:C	1:B:37[B]:HIS:H	2.14	0.50
1:A:74[B]:ARG:HA	1:A:77:LEU:HD22	1.92	0.50
1:A:64[B]:LYS:HE3	2:A:466:HOH:O	2.12	0.49
1:B:69[A]:GLN:HE22	1:B:170:TRP:HA	1.77	0.49
1:A:90:LEU:HD21	1:A:173:LEU:HD21	1.94	0.49
1:A:140:TYR:OH	1:B:209:GLY:HA2	2.12	0.49
1:A:4:HIS:HE1	1:B:140:TYR:CE1	2.31	0.48
1:A:202:LEU:HD12	1:A:202:LEU:N	2.28	0.48
1:A:15[B]:ARG:NH1	2:A:387:HOH:O	2.47	0.48
1:A:44[A]:ARG:HD3	2:A:453:HOH:O	2.12	0.48
1:A:70[A]:ARG:NE	1:A:95[A]:ASP:OD1	2.46	0.48
1:A:158[B]:LYS:C	1:A:158[B]:LYS:HD2	2.34	0.48
1:A:122:GLN:HB3	2:A:331:HOH:O	2.14	0.48
1:B:132:CYS:HB2	2:B:422:HOH:O	2.14	0.47
1:B:59:LYS:HE3	1:B:101:LEU:O	2.14	0.47
1:B:147[A]:GLU:CD	1:B:147[A]:GLU:H	2.17	0.47
1:B:178:GLY:HA3	1:B:245:CYS:SG	2.55	0.47
1:B:224:LYS:CB	1:B:224:LYS:NZ	2.78	0.47
1:A:213[A]:MSE:SE	2:A:369:HOH:O	2.83	0.47
1:B:77:LEU:HD23	1:B:87:LEU:HD13	1.95	0.47
2:A:428:HOH:O	1:B:127:PRO:HB2	2.15	0.47
1:A:25[A]:ARG:HD2	2:A:308:HOH:O	2.15	0.46
1:B:139:HIS:HD2	2:B:422:HOH:O	1.97	0.46
1:A:4:HIS:CE1	1:A:206:MSE:HG2	2.50	0.46
1:A:30:ALA:HB2	1:B:37[B]:HIS:HE1	1.81	0.46
1:B:122[A]:GLN:HG2	2:B:334:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:GLU:OE1	2:B:443:HOH:O	2.21	0.46
1:A:6[A]:PHE:CE1	1:A:204:ILE:HD12	2.51	0.46
1:B:126:LEU:HB3	1:B:127:PRO:HD2	1.98	0.45
1:B:232:GLN:HA	1:B:232:GLN:HE21	1.80	0.45
1:A:154:ASN:CG	2:A:416:HOH:O	2.53	0.45
1:B:25[B]:ARG:HG2	2:B:341:HOH:O	2.16	0.45
1:A:70[A]:ARG:O	1:A:74[A]:ARG:HG3	2.16	0.45
1:B:150:LYS:NZ	2:B:309:HOH:O	2.50	0.45
1:A:154:ASN:OD1	2:A:416:HOH:O	2.21	0.45
1:B:176[B]:GLU:HA	1:B:176[B]:GLU:OE2	2.17	0.45
1:A:119:SER:O	1:A:123:ARG:NH2	2.49	0.44
2:A:424:HOH:O	1:B:144:LEU:HD23	2.16	0.44
1:B:204:ILE:HD13	1:B:225:PHE:HE1	1.82	0.44
1:B:184:ILE:HD13	1:B:185:ALA:N	2.33	0.43
1:A:108:GLY:O	1:A:112:LYS:HG3	2.17	0.43
1:B:35:ASP:HB2	1:B:38:GLN:HG2	2.01	0.43
1:A:143:HIS:CD2	1:B:4:HIS:HA	2.54	0.43
1:B:194:ALA:N	1:B:219:ASN:O	2.52	0.43
1:A:26:GLN:HE22	1:A:44[A]:ARG:CZ	2.31	0.43
1:B:224:LYS:HB3	1:B:224:LYS:HZ3	1.83	0.43
1:B:236[A]:GLN:HE21	1:B:236[A]:GLN:HB3	1.54	0.43
1:A:5:LYS:O	1:B:139:HIS:CE1	2.65	0.43
2:A:357:HOH:O	1:B:213[B]:MSE:SE	2.86	0.43
1:A:70[A]:ARG:CZ	1:A:95[A]:ASP:OD1	2.67	0.42
1:B:203:HIS:O	1:B:240:PHE:HB2	2.19	0.42
1:A:105[B]:GLU:O	1:A:106[B]:ARG:C	2.57	0.42
1:B:56:ILE:HG13	1:B:57:GLN:N	2.35	0.42
1:A:4:HIS:CD2	1:A:206:MSE:CE	2.94	0.42
1:B:31:SER:HB3	2:B:446:HOH:O	2.20	0.42
1:A:15[A]:ARG:O	1:A:19:ARG:HG3	2.20	0.41
1:A:29:LEU:HD13	2:B:370:HOH:O	2.19	0.41
1:B:78:ASN:H	1:B:84:GLN:NE2	2.18	0.41
1:A:29:LEU:HD12	1:B:37[A]:HIS:CE1	2.56	0.41
1:A:9:PRO:HG2	1:A:15[A]:ARG:CZ	2.50	0.41
1:A:15[A]:ARG:HG3	1:B:133:PHE:HE1	1.82	0.41
1:A:70[B]:ARG:HB2	1:A:94:ILE:HG21	2.02	0.41
1:B:35:ASP:HB3	1:B:37[B]:HIS:HB2	2.03	0.41
1:B:224:LYS:HB3	1:B:224:LYS:NZ	2.35	0.41
1:B:25[B]:ARG:HG3	2:B:324:HOH:O	2.20	0.41
1:B:76:TRP:HE3	1:B:82:VAL:HG21	1.86	0.41
1:A:3:THR:CG2	2:A:399:HOH:O	2.68	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74[B]:ARG:NH2	1:B:207:LYS:O[4_556]	2.10	0.10

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	267/247 (108%)	257 (96%)	10 (4%)	0	100	100
1	B	265/247 (107%)	255 (96%)	10 (4%)	0	100	100
All	All	532/494 (108%)	512 (96%)	20 (4%)	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	240/209 (115%)	218 (91%)	22 (9%)	11	5
1	B	237/209 (113%)	212 (90%)	25 (10%)	8	4
All	All	477/418 (114%)	430 (90%)	47 (10%)	14	4

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	40	GLN
1	A	41	LEU
1	A	58	LEU
1	A	60	SER
1	A	61	GLU
1	A	70[A]	ARG
1	A	70[B]	ARG
1	A	77	LEU
1	A	80[A]	GLU
1	A	80[B]	GLU
1	A	90	LEU
1	A	118	SER
1	A	143	HIS
1	A	158[A]	LYS
1	A	158[B]	LYS
1	A	195[A]	ASP
1	A	195[B]	ASP
1	A	232	GLN
1	A	234[A]	CYS
1	A	234[B]	CYS
1	A	236	GLN
1	B	12[A]	GLU
1	B	12[B]	GLU
1	B	15[A]	ARG
1	B	15[B]	ARG
1	B	31	SER
1	B	38	GLN
1	B	52	ILE
1	B	55[A]	GLN
1	B	55[B]	GLN
1	B	74[A]	ARG
1	B	74[B]	ARG
1	B	87	LEU
1	B	90	LEU
1	B	134[A]	ASP
1	B	134[B]	ASP
1	B	147[A]	GLU
1	B	147[B]	GLU
1	B	177	THR
1	B	184	ILE
1	B	186	ARG
1	B	207	LYS

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Mol	Chain	Res	Type
1	B	217	HIS
1	B	232	GLN
1	B	236[A]	GLN
1	B	236[B]	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	HIS
1	A	26	GLN
1	A	78	ASN
1	A	84	GLN
1	A	139	HIS
1	A	198	ASN
1	A	232	GLN
1	B	4	HIS
1	B	84	GLN
1	B	98	HIS
1	B	139	HIS
1	B	157	GLN
1	B	232	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 95th 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	236/247 (95%)	1.12	24 (10%) 9 11	45, 56, 75, 85	0
1	B	238/247 (96%)	1.32	39 (16%) 2 3	43, 57, 79, 92	0
All	All	474/494 (95%)	1.22	63 (13%) 4 5	43, 57, 78, 92	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	131	CYS	7.5
1	B	6[A]	PHE	4.9
1	B	128	GLY	4.9
1	B	184	ILE	4.6
1	B	129	GLY	4.6
1	B	133	PHE	4.5
1	B	217	HIS	4.5
1	B	194	ALA	4.2
1	B	186	ARG	3.8
1	B	131	CYS	3.7
1	B	188	GLY	3.6
1	B	218	LYS	3.6
1	A	125	ASN	3.6
1	B	232	GLN	3.5
1	B	55[A]	GLN	3.5
1	A	133	PHE	3.4
1	A	6[A]	PHE	3.2
1	B	2	THR	3.0
1	B	74[A]	ARG	3.0
1	A	158[A]	LYS	2.9
1	B	245	CYS	2.9
1	B	227	ALA	2.9
1	A	54	GLU	2.9
1	A	34	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	190	PHE	2.8
1	A	122	GLN	2.8
1	B	125[A]	ASN	2.8
1	A	80[A]	GLU	2.7
1	B	106[A]	ARG	2.7
1	A	95[A]	ASP	2.6
1	B	179[A]	HIS	2.6
1	B	195[A]	ASP	2.6
1	A	200	LEU	2.5
1	B	75[A]	HIS	2.5
1	A	44[A]	ARG	2.5
1	A	106[A]	ARG	2.5
1	B	61[A]	GLU	2.5
1	B	243	ALA	2.5
1	B	210	VAL	2.5
1	A	221	PHE	2.4
1	B	94	ILE	2.4
1	B	73	TYR	2.4
1	A	234[A]	CYS	2.3
1	B	37[A]	HIS	2.3
1	A	199	ILE	2.3
1	A	132	CYS	2.3
1	B	242	LEU	2.2
1	A	146	ILE	2.2
1	A	85	GLU	2.2
1	B	35	ASP	2.1
1	A	123	ARG	2.1
1	B	221	PHE	2.1
1	A	229[A]	GLU	2.1
1	B	229	GLU	2.1
1	A	105[A]	GLU	2.1
1	A	124	PHE	2.1
1	B	228	PHE	2.1
1	B	167	LEU	2.1
1	B	51[A]	GLU	2.0
1	B	15[A]	ARG	2.0
1	B	25[A]	ARG	2.0
1	A	1	ALA	2.0
1	B	236[A]	GLN	2.0

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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.