WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:19 am GMT

PDB ID	:	1U04
Title	:	Crystal structure of full length Argonaute from Pyrococcus furiosus
Authors	:	Song, J.J.; Smith, S.K.; Hannon, G.J.; Joshua-Tor, L.
Deposited on	:	2004-07-12
Resolution	:	2.25 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

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 2.25 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	Percentile Ranks	Value
Rfree		0.261
Clashscore		18
Ramachandran outliers		1.9%
Sidechain outliers		4.0%
RSRZ outliers		5.6%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
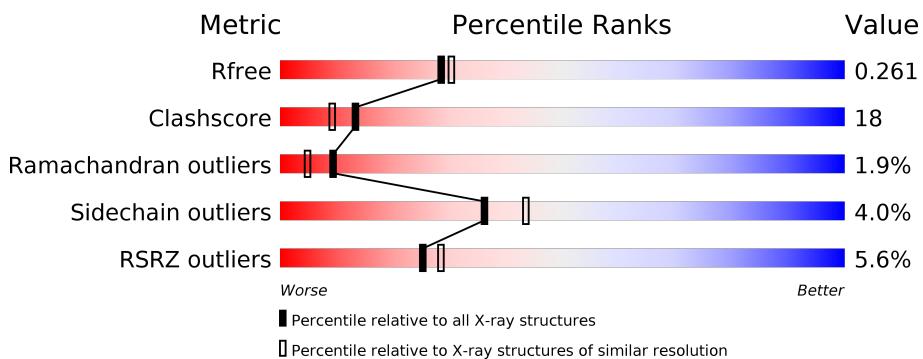
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1062 (2.26-2.26)
Clashscore	112137	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)
RSRZ outliers	101464	1066 (2.26-2.26)

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	771	5% — 61% — 28% — • — 8%
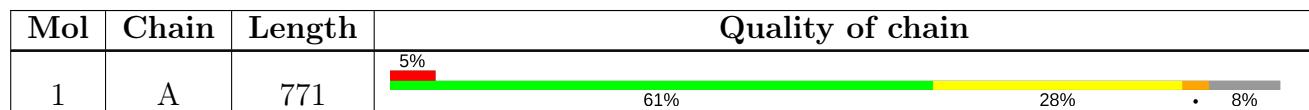
2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6112 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 hypothetical protein PF0537.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	713	Total 5920	C 3848	N 979	O 1074	S 1	Se 18	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	CLONING ARTIFACT	UNP Q8U3D2
A	4	ILE	LYS	ENGINEERED	UNP Q8U3D2

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	192	Total 192	O 192	0	0

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 the various outlier classes 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: hypothetical protein PF0537
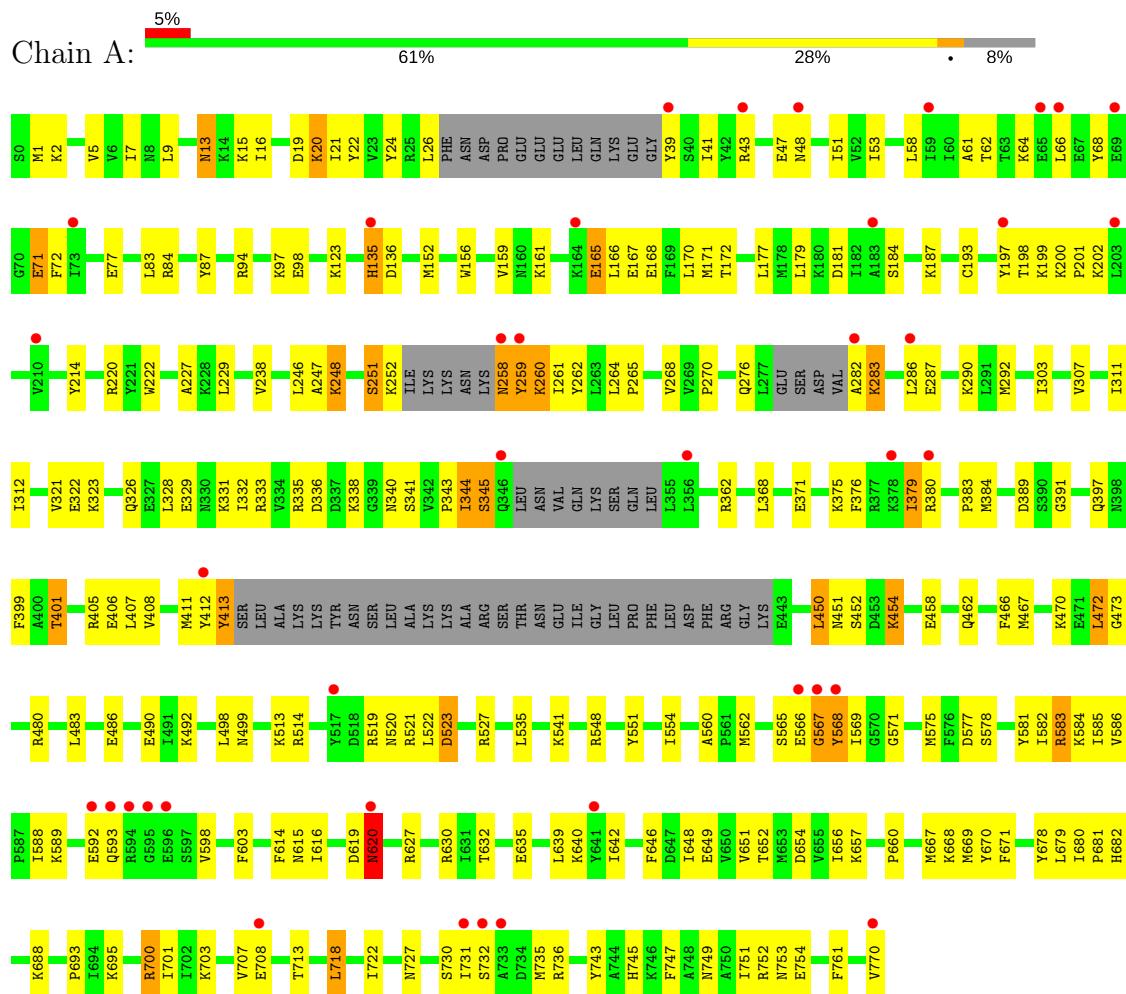
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.73Å 104.19Å 74.02Å 90.00° 102.83° 90.00°	Depositor
Resolution (Å)	38.17 – 2.25 49.39 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.17-2.25) 99.7 (49.39-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.50 (at 2.25Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.227 , 0.258 0.231 , 0.261	Depositor DCC
R_{free} test set	2528 reflections (5.18%)	DCC
Wilson B-factor (Å^2)	52.0	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 53.1	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6112	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.36	0/6018	0.59	0/8063

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 ⓘ

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	5920	0	6088	217	0
2	A	192	0	0	11	0
All	All	6112	0	6088	217	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 18.

All (217) 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:593:GLN:HE22	1:A:598:VAL:HG22	1.18	1.08
1:A:13:ASN:HD22	1:A:15:LYS:H	1.10	0.99
1:A:454:LYS:H	1:A:454:LYS:HD2	1.29	0.95
1:A:62:THR:HG22	1:A:64:LYS:H	1.27	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:GLN:NE2	1:A:598:VAL:HG22	1.90	0.87
1:A:619:ASP:HB3	1:A:646:PHE:HB3	1.58	0.86
1:A:575:MSE:HE1	1:A:616:ILE:HG13	1.58	0.85
1:A:391:GLY:HA3	1:A:480:ARG:NH1	1.93	0.83
1:A:384:MSE:HE3	1:A:408:VAL:HB	1.61	0.82
1:A:620:ASN:HB3	2:A:844:HOH:O	1.80	0.81
1:A:48:ASN:O	1:A:62:THR:HG23	1.82	0.78
1:A:13:ASN:ND2	1:A:15:LYS:H	1.82	0.77
1:A:26:LEU:HD23	1:A:72:PHE:HB3	1.66	0.77
1:A:371:GLU:HB2	1:A:541:LYS:HB2	1.67	0.77
1:A:700:ARG:HG2	1:A:700:ARG:HH11	1.53	0.74
1:A:198:THR:HG22	1:A:199:LYS:H	1.52	0.73
1:A:375:LYS:HE3	1:A:379:ILE:HD11	1.70	0.73
1:A:333:ARG:NH1	1:A:341:SER:HB3	2.03	0.73
1:A:562:MSE:SE	1:A:752:ARG:HG2	2.39	0.73
1:A:26:LEU:HD23	1:A:72:PHE:CB	2.21	0.70
1:A:397:GLN:O	1:A:401:THR:HG23	1.91	0.70
1:A:53:ILE:HD11	1:A:61:ALA:HB2	1.72	0.70
1:A:198:THR:HG22	1:A:199:LYS:N	2.06	0.70
1:A:642:ILE:HG12	1:A:648:ILE:HD12	1.75	0.69
1:A:336:ASP:OD2	1:A:340:ASN:HB2	1.93	0.69
1:A:408:VAL:O	1:A:411:MSE:HB2	1.92	0.69
1:A:214:TYR:CD2	1:A:238:VAL:HG22	2.29	0.68
1:A:577:ASP:OD2	1:A:583:ARG:HD2	1.93	0.68
1:A:389:ASP:OD2	1:A:480:ARG:HG3	1.94	0.68
1:A:1:MSE:HE3	1:A:2:LYS:HB2	1.75	0.67
1:A:165:GLU:N	2:A:798:HOH:O	2.28	0.67
1:A:657:LYS:HB2	1:A:736:ARG:HD2	1.76	0.67
1:A:26:LEU:CD2	1:A:72:PHE:HB3	2.24	0.66
1:A:332:ILE:HG22	1:A:344:ILE:HD13	1.78	0.65
1:A:222:TRP:HB3	1:A:227:ALA:HB1	1.79	0.64
1:A:19:ASP:HB2	1:A:20:LYS:HD3	1.79	0.63
1:A:16:ILE:HB	1:A:311:ILE:HD11	1.80	0.63
1:A:214:TYR:CE2	1:A:238:VAL:HG22	2.34	0.63
1:A:238:VAL:HG23	2:A:869:HOH:O	1.98	0.62
1:A:375:LYS:HE2	1:A:761:PHE:CE1	2.34	0.62
1:A:651:VAL:HG22	1:A:701:ILE:HD13	1.82	0.62
1:A:575:MSE:SE	1:A:616:ILE:HG21	2.50	0.61
1:A:62:THR:HG22	1:A:64:LYS:N	2.09	0.61
1:A:167:GLU:O	1:A:171:MSE:HG3	2.00	0.60
1:A:177:LEU:HD11	1:A:270:PRO:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ILE:HD12	1:A:261:ILE:N	2.15	0.60
1:A:335:ARG:CZ	1:A:368:LEU:HD12	2.31	0.60
1:A:652:THR:HG23	1:A:700:ARG:HH11	1.67	0.60
1:A:97:LYS:HE2	2:A:839:HOH:O	2.00	0.59
1:A:328:LEU:HD23	1:A:331:LYS:HE2	1.85	0.59
1:A:7:ILE:HD12	1:A:9:LEU:HD13	1.85	0.59
1:A:13:ASN:ND2	1:A:15:LYS:HG2	2.17	0.59
1:A:259:TYR:HD2	1:A:261:ILE:HD11	1.67	0.59
1:A:168:GLU:HA	1:A:171:MSE:HE3	1.84	0.59
1:A:652:THR:HG23	1:A:700:ARG:NH1	2.18	0.59
1:A:321:VAL:HG11	1:A:669:MSE:HE3	1.84	0.58
1:A:1:MSE:HE3	1:A:2:LYS:CB	2.33	0.57
1:A:375:LYS:HG2	1:A:379:ILE:HD11	1.87	0.57
1:A:619:ASP:CB	1:A:646:PHE:HB3	2.32	0.57
1:A:568:TYR:CE1	1:A:592:GLU:HA	2.39	0.57
1:A:1:MSE:HE3	1:A:2:LYS:H	1.70	0.56
1:A:514:ARG:HD3	1:A:519:ARG:O	2.05	0.56
1:A:718:LEU:O	1:A:722:ILE:HG12	2.05	0.56
1:A:700:ARG:HG2	1:A:700:ARG:NH1	2.17	0.56
1:A:567:GLY:HA2	1:A:589:LYS:HE2	1.88	0.56
1:A:321:VAL:HG11	1:A:669:MSE:CE	2.36	0.56
1:A:41:ILE:HD12	1:A:58:LEU:HD22	1.87	0.56
1:A:670:TYR:HA	1:A:678:TYR:O	2.06	0.55
1:A:168:GLU:HA	1:A:171:MSE:CE	2.36	0.55
1:A:43:ARG:O	1:A:47:GLU:HG3	2.05	0.55
1:A:492:LYS:HD2	2:A:917:HOH:O	2.06	0.55
1:A:668:LYS:HG2	1:A:682:HIS:HA	1.89	0.55
1:A:171:MSE:HG2	1:A:199:LYS:O	2.07	0.54
1:A:407:LEU:O	1:A:407:LEU:HD23	2.07	0.54
1:A:614:PHE:O	1:A:615:ASN:HB2	2.07	0.54
1:A:640:LYS:HD3	1:A:707:VAL:HG23	1.90	0.53
1:A:619:ASP:HB2	1:A:646:PHE:O	2.08	0.53
1:A:24:TYR:CE2	1:A:66:LEU:HB2	2.43	0.53
1:A:620:ASN:HB2	2:A:850:HOH:O	2.07	0.53
1:A:94:ARG:NH1	1:A:98:GLU:HG2	2.23	0.53
1:A:251:SER:O	1:A:252:LYS:HB2	2.08	0.53
1:A:198:THR:CG2	1:A:199:LYS:H	2.21	0.53
1:A:1:MSE:HG3	1:A:2:LYS:N	2.23	0.53
1:A:727:ASN:HA	1:A:735:MSE:HE1	1.90	0.53
1:A:747:PHE:CE2	1:A:751:ILE:HD11	2.44	0.52
1:A:159:VAL:HG11	1:A:166:LEU:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:MSE:SE	1:A:751:ILE:HG22	2.60	0.52
1:A:2:LYS:HG2	1:A:322:GLU:OE2	2.09	0.52
1:A:384:MSE:HE3	1:A:408:VAL:CB	2.36	0.52
1:A:168:GLU:O	1:A:172:THR:HG23	2.10	0.52
1:A:588:ILE:HD12	1:A:603:PHE:CE2	2.45	0.52
1:A:156:TRP:NE1	1:A:161:LYS:HG2	2.25	0.51
1:A:486:GLU:O	1:A:490:GLU:HG3	2.10	0.51
1:A:639:LEU:HA	1:A:642:ILE:HG22	1.92	0.51
1:A:383:PRO:HD2	1:A:472:LEU:O	2.11	0.51
1:A:248:LYS:HB3	1:A:248:LYS:NZ	2.26	0.51
1:A:39:TYR:HA	1:A:43:ARG:HD2	1.93	0.51
1:A:303:ILE:O	1:A:307:VAL:HG23	2.12	0.50
1:A:630:ARG:HG3	1:A:654:ASP:CG	2.32	0.50
1:A:66:LEU:HD13	1:A:66:LEU:C	2.32	0.50
1:A:562:MSE:SE	1:A:751:ILE:CG2	3.09	0.50
1:A:635:GLU:O	1:A:639:LEU:HG	2.12	0.50
1:A:548:ARG:HG2	1:A:548:ARG:HH11	1.76	0.50
1:A:743:TYR:HE1	1:A:770:VAL:HG11	1.76	0.50
1:A:71:GLU:O	1:A:72:PHE:HB3	2.13	0.49
1:A:1:MSE:HG3	1:A:2:LYS:H	1.76	0.49
1:A:198:THR:CG2	1:A:199:LYS:N	2.75	0.49
1:A:405:ARG:O	1:A:408:VAL:HG22	2.13	0.49
1:A:362:ARG:NH2	1:A:520:ASN:HB2	2.28	0.49
1:A:753:ASN:O	1:A:754:GLU:HB2	2.13	0.49
1:A:20:LYS:N	1:A:20:LYS:HD3	2.27	0.49
1:A:1:MSE:CG	1:A:2:LYS:H	2.25	0.49
1:A:21:ILE:HD13	1:A:83:LEU:HD11	1.94	0.49
1:A:214:TYR:CG	1:A:238:VAL:HG22	2.48	0.49
1:A:283:LYS:O	1:A:287:GLU:HG3	2.13	0.49
1:A:452:SER:HB2	1:A:454:LYS:CD	2.44	0.48
1:A:450:LEU:HB3	1:A:483:LEU:HD21	1.95	0.48
1:A:588:ILE:HD12	1:A:603:PHE:CZ	2.48	0.48
1:A:669:MSE:HE2	1:A:671:PHE:CE2	2.48	0.48
1:A:84:ARG:HH12	1:A:87:TYR:HE2	1.59	0.48
1:A:247:ALA:O	1:A:260:LYS:HA	2.14	0.48
1:A:376:PHE:HA	1:A:379:ILE:HD12	1.95	0.48
1:A:193:CYS:HB3	1:A:202:LYS:CE	2.44	0.47
1:A:311:ILE:HG23	1:A:312:ILE:HG23	1.96	0.47
1:A:389:ASP:OD2	1:A:480:ARG:NH1	2.47	0.47
1:A:498:LEU:O	1:A:499:ASN:HB2	2.14	0.47
1:A:575:MSE:HE2	1:A:584:LYS:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:LEU:HD23	1:A:270:PRO:HA	1.96	0.47
1:A:292:MSE:SE	1:A:688:LYS:HG3	2.64	0.47
1:A:344:ILE:O	1:A:345:SER:OG	2.26	0.47
1:A:326:GLN:O	1:A:329:GLU:HB2	2.14	0.47
1:A:323:LYS:HG2	1:A:667:MSE:CE	2.45	0.47
1:A:135:HIS:O	2:A:812:HOH:O	2.21	0.47
1:A:258:ASN:ND2	1:A:258:ASN:O	2.48	0.47
1:A:198:THR:HG22	1:A:200:LYS:H	1.80	0.47
1:A:619:ASP:O	1:A:620:ASN:OD1	2.33	0.47
1:A:1:MSE:CG	1:A:2:LYS:N	2.78	0.47
1:A:286:LEU:O	1:A:290:LYS:HG2	2.15	0.46
1:A:462:GLN:O	1:A:466:PHE:HD1	1.97	0.46
1:A:333:ARG:HG2	1:A:343:PRO:HA	1.98	0.46
1:A:407:LEU:HD23	1:A:407:LEU:C	2.36	0.46
1:A:454:LYS:H	1:A:454:LYS:CD	2.04	0.46
1:A:282:ALA:C	1:A:283:LYS:HG2	2.36	0.46
1:A:375:LYS:HE2	1:A:761:PHE:HE1	1.80	0.46
1:A:454:LYS:HD2	1:A:454:LYS:N	2.12	0.45
1:A:630:ARG:HG3	1:A:654:ASP:OD2	2.16	0.45
1:A:391:GLY:HA3	1:A:480:ARG:HH11	1.74	0.45
1:A:389:ASP:OD1	1:A:480:ARG:NH1	2.50	0.45
1:A:569:ILE:HG22	1:A:571:GLY:H	1.82	0.45
1:A:639:LEU:HA	1:A:642:ILE:CG2	2.47	0.45
1:A:586:VAL:HG12	1:A:614:PHE:CE1	2.52	0.44
1:A:184:SER:O	1:A:187:LYS:HD2	2.17	0.44
1:A:389:ASP:CG	1:A:480:ARG:NH1	2.71	0.44
1:A:66:LEU:HD12	1:A:72:PHE:CZ	2.53	0.44
1:A:680:ILE:HD11	1:A:693:PRO:HG3	1.99	0.44
1:A:451:ASN:HB2	1:A:480:ARG:NH2	2.33	0.44
1:A:48:ASN:HB3	1:A:62:THR:HG21	1.98	0.44
1:A:333:ARG:HG2	1:A:343:PRO:CA	2.47	0.43
1:A:408:VAL:HA	1:A:411:MSE:HB2	2.00	0.43
1:A:197:TYR:CD1	1:A:562:MSE:HA	2.53	0.43
1:A:649:GLU:HG2	1:A:701:ILE:HD11	2.00	0.43
1:A:651:VAL:HG22	1:A:701:ILE:CD1	2.46	0.43
1:A:656:ILE:HB	1:A:695:LYS:HB3	2.00	0.43
1:A:246:LEU:HD21	1:A:260:LYS:HD2	1.99	0.43
1:A:345:SER:HB2	2:A:936:HOH:O	2.17	0.43
1:A:575:MSE:HE2	1:A:583:ARG:HB2	2.00	0.43
1:A:344:ILE:N	1:A:344:ILE:HD12	2.33	0.43
1:A:51:ILE:HD12	1:A:51:ILE:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:ILE:HD11	1:A:585:ILE:HD11	1.99	0.43
1:A:336:ASP:OD1	1:A:338:LYS:HB2	2.18	0.43
1:A:470:LYS:NZ	2:A:872:HOH:O	2.51	0.43
1:A:472:LEU:HD23	1:A:473:GLY:H	1.84	0.43
1:A:181:ASP:HA	1:A:268:VAL:HG12	2.01	0.43
1:A:5:VAL:HG21	1:A:669:MSE:HE1	2.01	0.43
1:A:193:CYS:HB3	1:A:202:LYS:HE3	2.01	0.43
1:A:260:LYS:C	1:A:261:ILE:HD12	2.39	0.43
1:A:548:ARG:HG2	1:A:548:ARG:NH1	2.34	0.43
1:A:649:GLU:HG3	1:A:703:LYS:HG2	1.99	0.43
1:A:731:ILE:O	1:A:732:SER:HB2	2.19	0.43
1:A:166:LEU:C	1:A:166:LEU:HD23	2.38	0.42
1:A:13:ASN:HD22	1:A:15:LYS:N	1.94	0.42
1:A:541:LYS:HG3	1:A:581:TYR:CD1	2.54	0.42
1:A:679:LEU:O	1:A:681:PRO:HD3	2.19	0.42
1:A:156:TRP:CD1	1:A:161:LYS:HG2	2.54	0.42
1:A:412:TYR:O	1:A:413:TYR:C	2.58	0.42
1:A:521:ARG:HG3	1:A:527:ARG:NH2	2.34	0.42
1:A:735:MSE:SE	2:A:959:HOH:O	2.88	0.42
1:A:276:GLN:O	1:A:276:GLN:HG2	2.19	0.42
1:A:22:TYR:CD1	1:A:77:GLU:HG2	2.55	0.42
1:A:362:ARG:O	1:A:406:GLU:HG3	2.20	0.42
1:A:560:ALA:O	1:A:562:MSE:HE2	2.19	0.42
1:A:259:TYR:HD2	1:A:261:ILE:CD1	2.31	0.42
1:A:375:LYS:O	1:A:379:ILE:HG13	2.20	0.42
1:A:214:TYR:HB2	1:A:264:LEU:HD21	2.02	0.42
1:A:713:THR:HB	2:A:899:HOH:O	2.20	0.42
1:A:66:LEU:HD11	1:A:68:TYR:HB3	2.01	0.41
1:A:167:GLU:HG3	1:A:201:PRO:CG	2.50	0.41
1:A:551:TYR:O	1:A:578:SER:HB3	2.20	0.41
1:A:513:LYS:O	1:A:523:ASP:HB2	2.19	0.41
1:A:701:ILE:CG2	1:A:708:GLU:HB2	2.51	0.41
1:A:335:ARG:NE	1:A:368:LEU:HD12	2.36	0.41
1:A:745:HIS:CE1	1:A:749:ASN:HD21	2.37	0.41
1:A:467:MSE:O	1:A:470:LYS:HB2	2.21	0.41
1:A:123:LYS:HE3	1:A:152:MSE:SE	2.70	0.41
1:A:261:ILE:HG22	1:A:262:TYR:N	2.35	0.41
1:A:41:ILE:HD12	1:A:58:LEU:CD2	2.50	0.41
1:A:619:ASP:O	1:A:620:ASN:CB	2.68	0.41
1:A:562:MSE:SE	1:A:751:ILE:HB	2.70	0.41
1:A:407:LEU:HD23	1:A:411:MSE:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:THR:OG1	1:A:635:GLU:HG3	2.21	0.40
1:A:264:LEU:HA	1:A:265:PRO:HD2	1.92	0.40
1:A:1:MSE:CE	1:A:2:LYS:H	2.34	0.40
1:A:554:ILE:N	1:A:554:ILE:HD12	2.37	0.40
1:A:753:ASN:O	1:A:754:GLU:CB	2.69	0.40
1:A:399:PHE:CE2	1:A:522:LEU:HD13	2.57	0.40
1:A:323:LYS:HG2	1:A:667:MSE:HE1	2.03	0.40
1:A:577:ASP:OD2	1:A:583:ARG:NH1	2.45	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	701/771 (91%)	648 (92%)	40 (6%)	13 (2%)	9	5

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	251	SER
1	A	344	ILE
1	A	380	ARG
1	A	567	GLY
1	A	730	SER
1	A	135	HIS
1	A	165	GLU
1	A	259	TYR
1	A	260	LYS
1	A	345	SER
1	A	379	ILE
1	A	565	SER
1	A	620	ASN

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	655/689 (95%)	629 (96%)	26 (4%)	36	43

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	20	LYS
1	A	71	GLU
1	A	136	ASP
1	A	170	LEU
1	A	220	ARG
1	A	229	LEU
1	A	248	LYS
1	A	258	ASN
1	A	283	LYS
1	A	401	THR
1	A	413	TYR
1	A	450	LEU
1	A	454	LYS
1	A	458	GLU
1	A	472	LEU
1	A	523	ASP
1	A	535	LEU
1	A	566	GLU
1	A	568	TYR
1	A	583	ARG
1	A	620	ASN
1	A	627	ARG
1	A	660	PRO
1	A	700	ARG
1	A	718	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	223	ASN
1	A	258	ASN
1	A	579	GLN
1	A	593	GLN
1	A	742	HIS
1	A	745	HIS

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, 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(Å²)	Q<0.9
1	A	695/771 (90%)	0.42	39 (5%)	25	28	33, 57, 112, 167	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	733	ALA	8.5
1	A	732	SER	8.5
1	A	378	LYS	5.4
1	A	282	ALA	5.0
1	A	65	GLU	5.0
1	A	380	ARG	5.0
1	A	770	VAL	4.0
1	A	594	ARG	3.9
1	A	593	GLN	3.9
1	A	567	GLY	3.9
1	A	286	LEU	3.8
1	A	259	TYR	3.8
1	A	73	ILE	3.7
1	A	197	TYR	3.7
1	A	203	LEU	3.7
1	A	258	ASN	3.4
1	A	39	TYR	3.3
1	A	164	LYS	3.3
1	A	566	GLU	3.2
1	A	731	ILE	2.9
1	A	412	TYR	2.8
1	A	620	ASN	2.8
1	A	592	GLU	2.6
1	A	66	LEU	2.6
1	A	596	GLU	2.6
1	A	346	GLN	2.5
1	A	595	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	48	ASN	2.3
1	A	43	ARG	2.3
1	A	568	TYR	2.3
1	A	517	TYR	2.2
1	A	641	TYR	2.2
1	A	135	HIS	2.2
1	A	59	ILE	2.2
1	A	210	VAL	2.1
1	A	356	LEU	2.0
1	A	708	GLU	2.0
1	A	69	GLU	2.0
1	A	183	ALA	2.0

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 ⓘ

There are no such residues in this entry.