



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:07 AM UTC

PDB ID : 1U04 / pdb_00001u04
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

<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>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

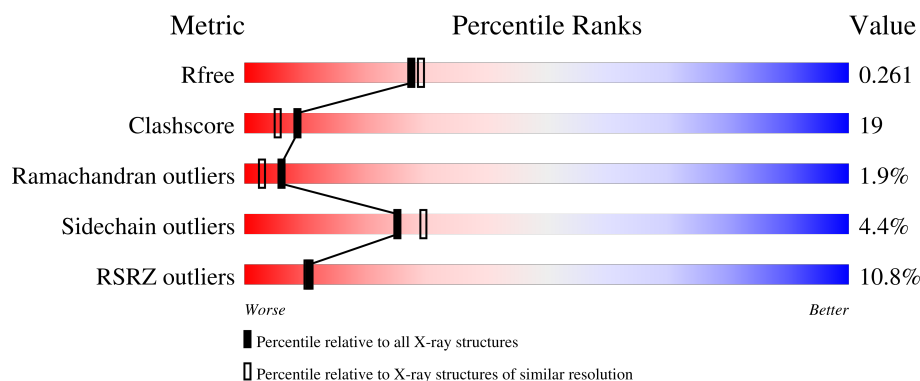
1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	771	10% 58% 30% 8%

2 Entry composition

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	C	N	O	S	Se	0	0	0
			5920	3848	979	1074	1	18			

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 mutation	UNP Q8U3D2

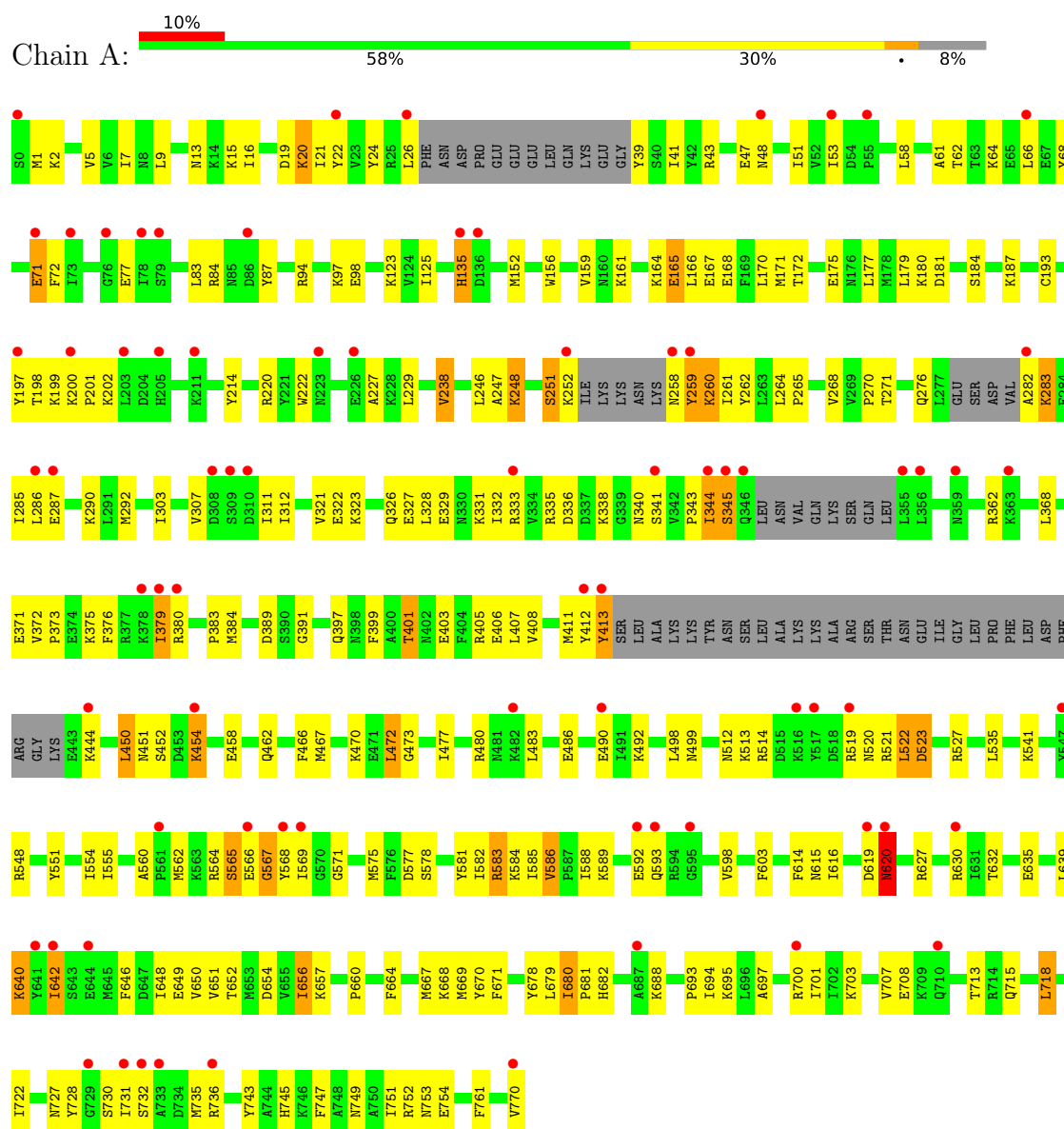
- Molecule 2 is water.

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

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 38.17 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.17-2.25) 99.7 (38.17-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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%)	wwPDB-VP
Wilson B-factor (Å ²)	52.0	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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](#)

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	0.41	0/6018	0.88	15/8063 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	586	VAL	N-CA-C	12.04	119.06	109.19
1	A	477	ILE	N-CA-C	6.34	116.99	108.11
1	A	650	VAL	N-CA-C	6.15	116.96	107.99
1	A	125	ILE	N-CA-C	6.00	114.02	107.60
1	A	680	ILE	CA-C-N	5.82	125.68	119.28
1	A	680	ILE	C-N-CA	5.82	125.68	119.28
1	A	555	ILE	N-CA-C	5.81	116.25	108.11
1	A	512	ASN	N-CA-C	5.38	120.50	113.30
1	A	728	TYR	N-CA-C	5.35	118.78	111.39
1	A	697	ALA	N-CA-C	5.33	116.38	108.60
1	A	640	LYS	N-CA-C	-5.27	105.61	111.36
1	A	664	PHE	N-CA-C	5.17	117.61	109.39
1	A	656	ILE	N-CA-C	5.15	115.26	107.80
1	A	175	GLU	N-CA-C	5.11	117.58	111.71
1	A	694	ILE	N-CA-C	-5.07	101.12	108.36

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	5920	0	6088	224	0
2	A	192	0	0	11	0
All	All	6112	0	6088	224	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 19.

All (224) 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:62:THR:HG22	1:A:64:LYS:H	1.27	0.95
1:A:454:LYS:HD2	1:A:454:LYS:H	1.29	0.95
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:HH11	1:A:700:ARG:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:630:ARG:HG3	1:A:654:ASP:CG	2.32	0.55
1:A:43:ARG:O	1:A:47:GLU:HG3	2.05	0.55
1:A:66:LEU:HD13	1:A:66:LEU:C	2.32	0.55
1:A:492:LYS:HD2	2:A:917:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD23	1:A:407:LEU:O	2.07	0.54
1:A:344:ILE:O	1:A:345:SER:OG	2.26	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:1:MSE:HG3	1:A:2:LYS:N	2.23	0.53
1:A:198:THR:CG2	1:A:199:LYS:H	2.21	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
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:NZ	1:A:248:LYS:HB3	2.26	0.51
1:A:407:LEU:HD23	1:A:407:LEU:C	2.36	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:562:MSE:SE	1:A:751:ILE:CG2	3.09	0.50
1:A:282:ALA:C	1:A:283:LYS:HG2	2.36	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:362:ARG:NH2	1:A:520:ASN:HB2	2.28	0.49
1:A:405:ARG:O	1:A:408:VAL:HG22	2.13	0.49
1:A:389:ASP:CG	1:A:480:ARG:NH1	2.71	0.49
1:A:753:ASN:O	1:A:754:GLU:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LYS:HD3	1:A:20:LYS:N	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:84:ARG:HH12	1:A:87:TYR:HE2	1.59	0.48
1:A:450:LEU:HB3	1:A:483:LEU:HD21	1.95	0.48
1:A:452:SER:HB2	1:A:454:LYS:CD	2.44	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:247:ALA:O	1:A:260:LYS:HA	2.14	0.48
1:A:166:LEU:C	1:A:166:LEU:HD23	2.38	0.48
1:A:376:PHE:HA	1:A:379:ILE:HD12	1.95	0.48
1:A:51:ILE:C	1:A:51:ILE:HD12	2.39	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
1:A:179:LEU:HD23	1:A:270:PRO:HA	1.96	0.47
1:A:260:LYS:C	1:A:261:ILE:HD12	2.39	0.47
1:A:292:MSE:SE	1:A:688:LYS:HG3	2.64	0.47
1:A:135:HIS:O	2:A:812:HOH:O	2.21	0.47
1:A:258:ASN:O	1:A:258:ASN:ND2	2.48	0.47
1:A:323:LYS:HG2	1:A:667:MSE:CE	2.45	0.47
1:A:326:GLN:O	1:A:329:GLU:HB2	2.14	0.47
1:A:412:TYR:O	1:A:413:TYR:C	2.58	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:454:LYS:H	1:A:454:LYS:CD	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:GLU:CD	1:A:522:LEU:HB2	2.42	0.44
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: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:285:ILE:O	1:A:286:LEU:C	2.61	0.44
1:A:372:VAL:O	1:A:373:PRO:C	2.61	0.44
1:A:197:TYR:CD1	1:A:562:MSE:HA	2.53	0.43
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: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: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:564:ARG:O	1:A:565:SER:C	2.62	0.43
1:A:5:VAL:HG21	1:A:669:MSE:HE1	2.01	0.43
1:A:181:ASP:HA	1:A:268:VAL:HG12	2.01	0.43
1:A:193:CYS:HB3	1:A:202:LYS:HE3	2.01	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: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: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:22:TYR:CD1	1:A:77:GLU:HG2	2.55	0.42
1:A:276:GLN:O	1:A:276:GLN:HG2	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:41:ILE:HD12	1:A:58:LEU:CD2	2.50	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:327:GLU:C	1:A:329:GLU:H	2.29	0.41
1:A:408:VAL:C	1:A:411:MSE:HB2	2.46	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
1:A:632:THR:OG1	1:A:635:GLU:HG3	2.21	0.40
1:A:1:MSE:CE	1:A:2:LYS:H	2.34	0.40
1:A:214:TYR:CD2	1:A:214:TYR:C	2.98	0.40
1:A:264:LEU:HA	1:A:265:PRO:HD2	1.92	0.40
1:A:554:ILE:HD12	1:A:554:ILE:N	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 [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	701/771 (91%)	648 (92%)	40 (6%)	13 (2%)	6 3

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%)	626 (96%)	29 (4%)	25 29

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	71	GLU
1	A	164	LYS
1	A	170	LEU
1	A	180	LYS
1	A	220	ARG
1	A	229	LEU
1	A	238	VAL

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Mol	Chain	Res	Type
1	A	248	LYS
1	A	271	THR
1	A	283	LYS
1	A	401	THR
1	A	413	TYR
1	A	444	LYS
1	A	450	LEU
1	A	454	LYS
1	A	458	GLU
1	A	472	LEU
1	A	522	LEU
1	A	523	ASP
1	A	535	LEU
1	A	566	GLU
1	A	583	ARG
1	A	620	ASN
1	A	627	ARG
1	A	642	ILE
1	A	660	PRO
1	A	715	GLN
1	A	718	LEU

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

Mol	Chain	Res	Type
1	A	13	ASN
1	A	99	ASN
1	A	148	GLN
1	A	176	ASN
1	A	258	ASN
1	A	276	GLN
1	A	359	ASN
1	A	550	ASN
1	A	579	GLN
1	A	593	GLN
1	A	658	ASN
1	A	742	HIS
1	A	745	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 oligosaccharides 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	695/771 (90%)	0.71	75 (10%)	11 10	33, 57, 112, 167	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	282	ALA	6.1
1	A	355	LEU	4.8
1	A	568	TYR	4.6
1	A	733	ALA	4.4
1	A	620	ASN	4.2
1	A	412	TYR	4.2
1	A	286	LEU	4.2
1	A	413	TYR	3.8
1	A	346	GLN	3.6
1	A	619	ASP	3.6
1	A	593	GLN	3.6
1	A	258	ASN	3.6
1	A	76	GLY	3.5
1	A	22	TYR	3.5
1	A	309	SER	3.4
1	A	66	LEU	3.4
1	A	770	VAL	3.3
1	A	345	SER	3.2
1	A	136	ASP	3.2
1	A	252	LYS	3.2
1	A	26	LEU	3.2
1	A	363	LYS	3.1
1	A	308	ASP	3.0
1	A	287	GLU	3.0
1	A	0	SER	3.0
1	A	731	ILE	2.9
1	A	197	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	344	ILE	2.9
1	A	223	ASN	2.9
1	A	211	LYS	2.9
1	A	379	ILE	2.8
1	A	517	TYR	2.8
1	A	71	GLU	2.7
1	A	378	LYS	2.7
1	A	482	LYS	2.7
1	A	444	LYS	2.7
1	A	642	ILE	2.6
1	A	644	GLU	2.6
1	A	259	TYR	2.6
1	A	78	ILE	2.6
1	A	359	ASN	2.6
1	A	55	PRO	2.6
1	A	547	TYR	2.6
1	A	135	HIS	2.6
1	A	341	SER	2.5
1	A	203	LEU	2.5
1	A	380	ARG	2.4
1	A	205	HIS	2.4
1	A	200	LYS	2.3
1	A	516	LYS	2.3
1	A	630	ARG	2.3
1	A	310	ASP	2.3
1	A	732	SER	2.3
1	A	687	ALA	2.3
1	A	566	GLU	2.3
1	A	48	ASN	2.2
1	A	356	LEU	2.2
1	A	86	ASP	2.2
1	A	595	GLY	2.2
1	A	333	ARG	2.1
1	A	226	GLU	2.1
1	A	454	LYS	2.1
1	A	710	GLN	2.1
1	A	53	ILE	2.1
1	A	519	ARG	2.1
1	A	490	GLU	2.1
1	A	592	GLU	2.1
1	A	561	PRO	2.1
1	A	729	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	73	ILE	2.1
1	A	569	ILE	2.1
1	A	641	TYR	2.1
1	A	700	ARG	2.0
1	A	736	ARG	2.0
1	A	79	SER	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 oligosaccharides 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.