



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:49 PM UTC

PDB ID : 1YVU / pdb_00001yvu
Title : Crystal structure of A. aeolicus Argonaute
Authors : Yuan, Y.R.; Pei, Y.; Ma, J.B.; Kuryavyi, V.; Zhadina, M.; Meister, G.; Chen, H.Y.; Dauter, Z.; Tuschl, T.; Patel, D.J.
Deposited on : 2005-02-16
Resolution : 2.90 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

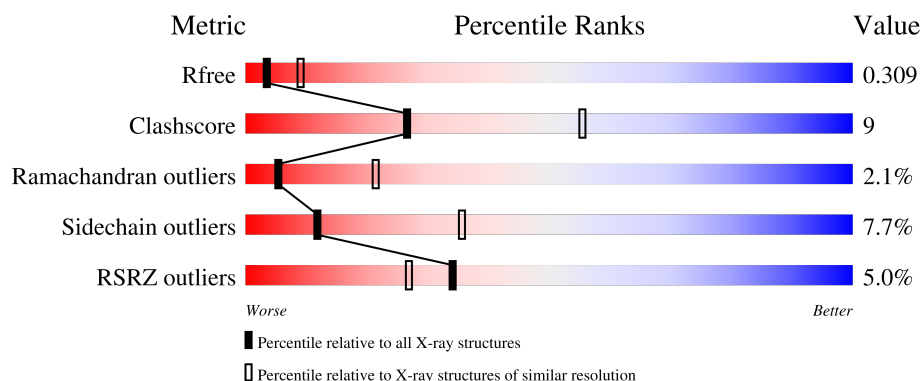
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	706	5% 65% 25% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5740 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 aq_1447.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	682	Total	C	N	O	S	Se	0	0	0
			5670	3694	965	1000	5	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	214	MSE	MET	modified residue	UNP O67434
A	278	MSE	MET	modified residue	UNP O67434
A	450	MSE	MET	modified residue	UNP O67434
A	665	MSE	MET	modified residue	UNP O67434
A	689	MSE	MET	modified residue	UNP O67434
A	703	MSE	MET	modified residue	UNP O67434

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

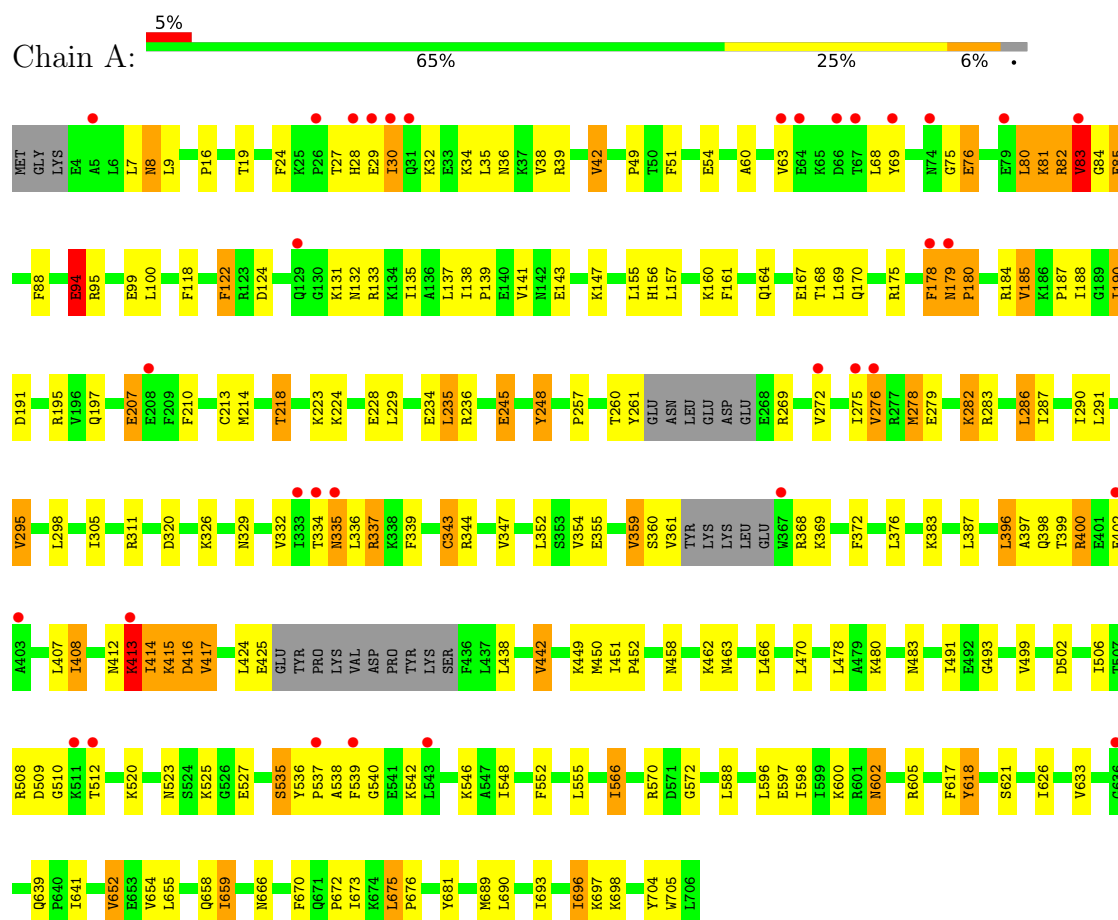
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	69	Total	O	0	0
			69	69		

3 Residue-property plots

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 aq_1447



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.15Å 100.68Å 115.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.90 – 2.90 23.90 – 2.90	Depositor EDS
% Data completeness (in resolution range)	89.3 (23.90-2.90) 97.2 (23.90-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 2.89Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.208 , 0.298 0.225 , 0.309	Depositor DCC
R_{free} test set	806 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5740	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
CA

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	0.90	3/5771 (0.1%)	1.33	51/7734 (0.7%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	408	ILE	CA-CB	13.04	1.60	1.54
1	A	83	VAL	CA-CB	5.79	1.62	1.54
1	A	334	THR	CA-CB	5.39	1.62	1.53

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	GLU	N-CA-C	8.68	129.28	110.80
1	A	337	ARG	N-CA-C	-8.61	101.83	111.82
1	A	493	GLY	N-CA-C	8.25	132.74	113.18
1	A	617	PHE	N-CA-C	8.22	121.89	108.99
1	A	347	VAL	N-CA-C	8.09	119.84	108.93
1	A	175	ARG	N-CA-C	7.01	118.61	110.97
1	A	122	PHE	N-CA-C	6.82	121.77	113.17
1	A	88	PHE	N-CA-C	6.82	119.61	109.59
1	A	275	ILE	N-CA-C	-6.77	105.02	112.80
1	A	60	ALA	N-CA-C	6.75	120.86	108.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	GLN	N-CA-C	-6.72	96.50	110.80
1	A	675	LEU	N-CA-C	6.71	119.11	110.39
1	A	207	GLU	N-CA-C	6.54	122.16	111.37
1	A	602	ASN	N-CA-C	6.51	120.53	111.74
1	A	223	LYS	N-CA-C	-6.48	104.14	111.07
1	A	413	LYS	N-CA-C	6.37	120.53	113.21
1	A	94	GLU	N-CA-C	-6.27	104.33	112.23
1	A	234	GLU	N-CA-C	-6.26	104.38	111.14
1	A	218	THR	N-CA-C	6.19	118.03	111.28
1	A	652	VAL	CB-CA-C	-6.08	103.93	112.14
1	A	491	ILE	N-CA-C	-6.06	99.62	108.11
1	A	512	THR	N-CA-C	6.04	119.37	110.30
1	A	463	ASN	N-CA-C	6.03	120.83	112.45
1	A	245	GLU	N-CA-C	5.94	121.11	111.37
1	A	298	LEU	N-CA-C	5.94	122.37	114.12
1	A	282	LYS	N-CA-C	5.89	117.78	111.36
1	A	343	CYS	N-CA-C	5.82	118.90	110.28
1	A	29	GLU	N-CA-C	5.82	119.15	109.96
1	A	16	PRO	N-CA-C	5.74	120.33	111.21
1	A	466	LEU	N-CA-C	5.73	119.08	111.75
1	A	32	LYS	N-CA-C	5.69	122.91	110.80
1	A	697	LYS	N-CA-C	-5.68	97.35	107.28
1	A	538	ALA	N-CA-C	5.61	118.18	107.75
1	A	179	ASN	CA-C-N	5.56	125.40	119.28
1	A	179	ASN	C-N-CA	5.56	125.40	119.28
1	A	626	ILE	N-CA-C	-5.56	99.72	108.23
1	A	502	ASP	N-CA-C	-5.50	99.71	109.06
1	A	618	TYR	N-CA-C	-5.50	99.47	108.76
1	A	188	ILE	N-CA-C	5.49	120.76	109.34
1	A	417	VAL	N-CA-C	5.44	117.47	109.63
1	A	42	VAL	CB-CA-C	-5.44	104.72	112.22
1	A	352	LEU	N-CA-C	5.43	118.41	109.72
1	A	704	TYR	N-CA-C	5.38	119.47	113.01
1	A	287	ILE	N-CA-C	-5.38	105.13	110.62
1	A	190	ILE	N-CA-C	5.30	115.53	108.11
1	A	566	ILE	N-CA-C	5.29	115.48	107.75
1	A	180	PRO	N-CA-C	5.29	120.79	113.65
1	A	535	SER	N-CA-C	-5.23	101.18	109.76
1	A	396	LEU	N-CA-C	5.21	117.20	107.99
1	A	442	VAL	N-CA-C	5.06	115.78	110.62
1	A	597	GLU	N-CA-C	-5.05	101.48	109.76

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	618	TYR	Sidechain

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	5670	0	5939	108	0
2	A	1	0	0	0	0
3	A	69	0	0	2	0
All	All	5740	0	5939	108	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 9.

All (108) 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:133:ARG:HB3	1:A:269:ARG:HH22	1.31	0.95
1:A:399:THR:HG22	1:A:400:ARG:H	1.40	0.84
1:A:260:THR:HG22	1:A:261:TYR:H	1.50	0.77
1:A:376:LEU:HD12	1:A:470:LEU:HD12	1.68	0.75
1:A:42:VAL:HG22	1:A:81:LYS:HE2	1.74	0.68
1:A:278:MSE:HE3	1:A:283:ARG:HG2	1.76	0.68
1:A:184:ARG:HE	1:A:195:ARG:HE	1.43	0.67
1:A:326:LYS:HG3	1:A:344:ARG:HH11	1.60	0.67
1:A:596:LEU:HD21	1:A:655:LEU:HD13	1.76	0.66
1:A:291:LEU:O	1:A:295:VAL:HG23	1.95	0.66
1:A:8:ASN:ND2	1:A:605:ARG:H	1.95	0.65
1:A:83:VAL:HG12	1:A:84:GLY:H	1.61	0.65
1:A:168:THR:HG22	1:A:170:GLN:H	1.60	0.65
1:A:83:VAL:HG12	1:A:84:GLY:N	2.14	0.62
1:A:94:GLU:HG2	1:A:147:LYS:HB2	1.80	0.62
1:A:245:GLU:HB3	3:A:860:HOH:O	2.00	0.61
1:A:368:ARG:HH12	1:A:462:LYS:HD3	1.66	0.61
1:A:161:PHE:HE1	1:A:278:MSE:HE2	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:LEU:O	1:A:442:VAL:HG23	2.04	0.58
1:A:548:ILE:O	1:A:552:PHE:HD1	1.87	0.56
1:A:184:ARG:HG2	1:A:195:ARG:HG2	1.88	0.56
1:A:24:PHE:HA	1:A:82:ARG:O	2.05	0.56
1:A:478:LEU:HB3	1:A:483:ASN:O	2.07	0.55
1:A:337:ARG:HE	1:A:670:PHE:HE2	1.52	0.55
1:A:260:THR:HG22	1:A:261:TYR:N	2.20	0.54
1:A:415:LYS:O	1:A:416:ASP:HB2	2.07	0.54
1:A:248:TYR:H	1:A:248:TYR:HD1	1.56	0.54
1:A:570:ARG:NH1	1:A:572:GLY:H	2.06	0.54
1:A:542:LYS:O	1:A:546:LYS:HB2	2.08	0.53
1:A:286:LEU:O	1:A:290:ILE:HG13	2.09	0.53
1:A:34:LYS:O	1:A:38:VAL:HG23	2.10	0.52
1:A:397:ALA:HB2	1:A:402:GLU:OE2	2.09	0.52
1:A:354:VAL:HG21	1:A:387:LEU:HD13	1.92	0.52
1:A:83:VAL:CG1	1:A:84:GLY:H	2.23	0.51
1:A:143:GLU:HB3	1:A:155:LEU:HD11	1.92	0.51
1:A:399:THR:HG22	1:A:400:ARG:N	2.19	0.51
1:A:414:ILE:O	1:A:416:ASP:N	2.44	0.51
1:A:450:MSE:SE	1:A:698:LYS:HD2	2.60	0.51
1:A:207:GLU:HG2	1:A:236:ARG:HH22	1.75	0.50
1:A:38:VAL:O	1:A:42:VAL:HG23	2.12	0.50
1:A:400:ARG:C	1:A:402:GLU:H	2.20	0.50
1:A:424:LEU:C	1:A:458:ASN:HD22	2.19	0.50
1:A:654:VAL:O	1:A:658:GLN:HG3	2.11	0.50
1:A:143:GLU:HG3	1:A:157:LEU:HD13	1.94	0.50
1:A:160:LYS:NZ	1:A:602:ASN:HA	2.26	0.49
1:A:30:ILE:HG22	1:A:35:LEU:HD11	1.94	0.49
1:A:95:ARG:O	1:A:99:GLU:HG3	2.12	0.49
1:A:68:LEU:HD22	1:A:80:LEU:HD12	1.94	0.49
1:A:178:PHE:H	1:A:178:PHE:HD2	1.59	0.49
1:A:133:ARG:HB3	1:A:269:ARG:NH2	2.14	0.49
1:A:570:ARG:HH11	1:A:572:GLY:H	1.60	0.49
1:A:336:LEU:HB2	1:A:339:PHE:H	1.78	0.48
1:A:452:PRO:HB3	1:A:480:LYS:HB3	1.95	0.48
1:A:372:PHE:O	1:A:376:LEU:HD13	2.14	0.48
1:A:7:LEU:C	1:A:9:LEU:H	2.21	0.48
1:A:51:PHE:HD2	1:A:100:LEU:HD13	1.79	0.48
1:A:169:LEU:HD22	1:A:185:VAL:HG11	1.96	0.48
1:A:414:ILE:HA	1:A:451:ILE:HD11	1.95	0.47
1:A:555:LEU:HD13	1:A:566:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:THR:CG2	1:A:400:ARG:H	2.20	0.47
1:A:675:LEU:HD12	3:A:821:HOH:O	2.14	0.47
1:A:184:ARG:NH2	1:A:195:ARG:HH21	2.12	0.47
1:A:197:GLN:NE2	1:A:508:ARG:HA	2.28	0.47
1:A:343:CYS:O	1:A:383:LYS:HE2	2.15	0.47
1:A:332:VAL:HG13	1:A:335:ASN:OD1	2.16	0.46
1:A:282:LYS:O	1:A:286:LEU:HB2	2.16	0.46
1:A:400:ARG:C	1:A:402:GLU:N	2.73	0.46
1:A:135:ILE:HD11	1:A:269:ARG:HH11	1.81	0.45
1:A:187:PRO:HB2	1:A:190:ILE:HB	1.98	0.45
1:A:137:LEU:HD22	1:A:276:VAL:HG21	1.98	0.45
1:A:197:GLN:HE22	1:A:508:ARG:HA	1.81	0.45
1:A:291:LEU:HD22	1:A:305:ILE:HG21	1.98	0.45
1:A:184:ARG:HH21	1:A:195:ARG:NH2	2.15	0.45
1:A:523:ASN:HD22	1:A:527:GLU:HG2	1.82	0.45
1:A:83:VAL:CG1	1:A:84:GLY:N	2.79	0.45
1:A:168:THR:HG22	1:A:169:LEU:N	2.32	0.44
1:A:224:LYS:O	1:A:228:GLU:HG2	2.16	0.44
1:A:326:LYS:HG3	1:A:344:ARG:NH1	2.29	0.44
1:A:689:MSE:HB3	1:A:696:ILE:HD11	1.99	0.44
1:A:69:TYR:O	1:A:80:LEU:HA	2.18	0.44
1:A:260:THR:CG2	1:A:261:TYR:H	2.24	0.43
1:A:506:ILE:HG13	1:A:690:LEU:HD13	2.00	0.43
1:A:184:ARG:HH21	1:A:195:ARG:HH21	1.65	0.43
1:A:229:LEU:HD23	1:A:235:LEU:HD13	1.99	0.43
1:A:179:ASN:HA	1:A:180:PRO:HD2	1.92	0.43
1:A:659:ILE:HG23	1:A:676:PRO:HG3	2.00	0.43
1:A:413:LYS:HE3	1:A:413:LYS:HB2	1.72	0.42
1:A:535:SER:HB2	1:A:696:ILE:HD12	2.00	0.42
1:A:359:VAL:HG12	1:A:425:GLU:H	1.83	0.42
1:A:525:LYS:HA	1:A:525:LYS:HD3	1.92	0.42
1:A:633:VAL:HG21	1:A:672:PRO:HG3	2.01	0.42
1:A:520:LYS:HD3	1:A:705:TRP:CZ2	2.54	0.42
1:A:131:LYS:HE2	1:A:132:ASN:HD21	1.84	0.41
1:A:369:LYS:HE2	1:A:458:ASN:OD1	2.19	0.41
1:A:75:GLY:O	1:A:76:GLU:HB2	2.19	0.41
1:A:138:ILE:HA	1:A:139:PRO:HD3	1.87	0.41
1:A:408:ILE:O	1:A:412:ASN:ND2	2.52	0.41
1:A:260:THR:O	1:A:261:TYR:HB2	2.19	0.41
1:A:666:ASN:HB3	1:A:673:ILE:HD12	2.01	0.41
1:A:210:PHE:O	1:A:214:MSE:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:ILE:HG23	1:A:641:ILE:HD12	2.03	0.41
1:A:164:GLN:HG2	1:A:257:PRO:O	2.20	0.41
1:A:414:ILE:HD11	1:A:449:LYS:HZ3	1.85	0.41
1:A:361:VAL:HG23	1:A:425:GLU:HG2	2.01	0.41
1:A:118:PHE:O	1:A:122:PHE:HB2	2.20	0.40
1:A:279:GLU:H	1:A:282:LYS:HD2	1.86	0.40
1:A:536:TYR:HA	1:A:537:PRO:HD3	1.93	0.40
1:A:376:LEU:CD1	1:A:470:LEU:HD12	2.46	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	674/706 (96%)	617 (92%)	43 (6%)	14 (2%)	5	21

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	GLU
1	A	83	VAL
1	A	85	GLU
1	A	335	ASN
1	A	400	ARG
1	A	415	LYS
1	A	416	ASP
1	A	8	ASN
1	A	540	GLY
1	A	54	GLU
1	A	278	MSE
1	A	509	ASP
1	A	621	SER

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Mol	Chain	Res	Type
1	A	510	GLY

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	624/641 (97%)	576 (92%)	48 (8%)	12	35

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	27	THR
1	A	28	HIS
1	A	30	ILE
1	A	36	ASN
1	A	39	ARG
1	A	49	PRO
1	A	63	VAL
1	A	80	LEU
1	A	81	LYS
1	A	82	ARG
1	A	94	GLU
1	A	124	ASP
1	A	141	VAL
1	A	156	HIS
1	A	167	GLU
1	A	178	PHE
1	A	185	VAL
1	A	191	ASP
1	A	213	CYS
1	A	218	THR
1	A	235	LEU
1	A	248	TYR
1	A	272	VAL
1	A	276	VAL

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Mol	Chain	Res	Type
1	A	286	LEU
1	A	295	VAL
1	A	311	ARG
1	A	320	ASP
1	A	329	ASN
1	A	355	GLU
1	A	359	VAL
1	A	360	SER
1	A	396	LEU
1	A	407	LEU
1	A	413	LYS
1	A	414	ILE
1	A	417	VAL
1	A	499	VAL
1	A	539	PHE
1	A	588	LEU
1	A	600	LYS
1	A	639	GLN
1	A	652	VAL
1	A	659	ILE
1	A	681	TYR
1	A	693	ILE
1	A	696	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	93	ASN
1	A	132	ASN
1	A	197	GLN
1	A	285	ASN
1	A	378	ASN
1	A	412	ASN
1	A	476	GLN
1	A	631	ASN
1	A	632	GLN

5.3.3 RNA ⓘ

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	676/706 (95%)	0.25	34 (5%) 34 27	7, 43, 96, 125	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	TYR	4.8
1	A	334	THR	4.4
1	A	335	ASN	4.0
1	A	333	ILE	3.4
1	A	402	GLU	3.4
1	A	367	TRP	3.2
1	A	543	LEU	3.1
1	A	29	GLU	2.9
1	A	66	ASP	2.8
1	A	636	GLY	2.8
1	A	63	VAL	2.7
1	A	5	ALA	2.7
1	A	79	GLU	2.6
1	A	275	ILE	2.6
1	A	30	ILE	2.6
1	A	413	LYS	2.6
1	A	178	PHE	2.6
1	A	129	GLN	2.5
1	A	67	THR	2.5
1	A	276	VAL	2.4
1	A	537	PRO	2.3
1	A	74	ASN	2.3
1	A	403	ALA	2.2
1	A	512	THR	2.2
1	A	179	ASN	2.2
1	A	83	VAL	2.2
1	A	539	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	26	PRO	2.1
1	A	64	GLU	2.1
1	A	31	GLN	2.1
1	A	28	HIS	2.1
1	A	208	GLU	2.1
1	A	511	LYS	2.0
1	A	272	VAL	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](#)

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, 95th 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($\text{\AA}^2$)	Q<0.9
2	CA	A	901	1/1	0.37	0.30	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.