



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:30 AM UTC

PDB ID : 1WWR / pdb_00001wvr
Title : Crystal structure of tRNA adenosine deaminase TadA from Aquifex aeolicus
Authors : Kuratani, M.; Ishii, R.; Bessho, Y.; Fukunaga, R.; Sengoku, T.; Sekine, S.;
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Deposited on : 2005-01-12
Resolution : 1.80 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
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

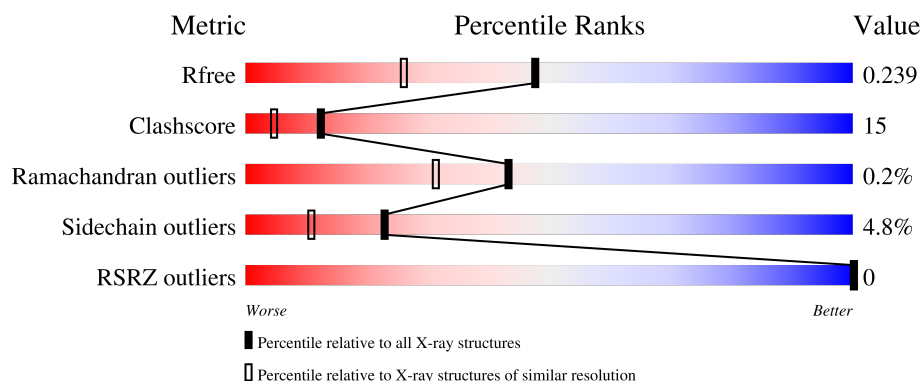
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

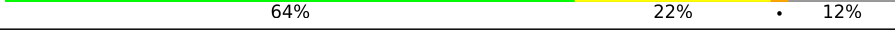
The reported resolution of this entry is 1.80 Å.

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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	171	
1	B	171	
1	C	171	
1	D	171	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5495 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 tRNA adenosine deaminase TadA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	154	Total	C	N	O	S	0	0	0
			1232	792	207	226	7			
1	B	157	Total	C	N	O	S	0	0	0
			1252	804	213	228	7			
1	C	160	Total	C	N	O	S	0	0	0
			1275	819	216	233	7			
1	D	151	Total	C	N	O	S	0	0	0
			1212	781	202	222	7			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP O67050
A	-19	GLY	-	expression tag	UNP O67050
A	-18	SER	-	expression tag	UNP O67050
A	-17	SER	-	expression tag	UNP O67050
A	-16	HIS	-	expression tag	UNP O67050
A	-15	HIS	-	expression tag	UNP O67050
A	-14	HIS	-	expression tag	UNP O67050
A	-13	HIS	-	expression tag	UNP O67050
A	-12	HIS	-	expression tag	UNP O67050
A	-11	HIS	-	expression tag	UNP O67050
A	-10	SER	-	expression tag	UNP O67050
A	-9	SER	-	expression tag	UNP O67050
A	-8	GLY	-	expression tag	UNP O67050
A	-7	LEU	-	expression tag	UNP O67050
A	-6	VAL	-	expression tag	UNP O67050
A	-5	PRO	-	expression tag	UNP O67050
A	-4	ARG	-	expression tag	UNP O67050
A	-3	GLY	-	expression tag	UNP O67050
A	-2	SER	-	expression tag	UNP O67050
A	-1	HIS	-	expression tag	UNP O67050
B	-20	MET	-	expression tag	UNP O67050

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	GLY	-	expression tag	UNP O67050
B	-18	SER	-	expression tag	UNP O67050
B	-17	SER	-	expression tag	UNP O67050
B	-16	HIS	-	expression tag	UNP O67050
B	-15	HIS	-	expression tag	UNP O67050
B	-14	HIS	-	expression tag	UNP O67050
B	-13	HIS	-	expression tag	UNP O67050
B	-12	HIS	-	expression tag	UNP O67050
B	-11	HIS	-	expression tag	UNP O67050
B	-10	SER	-	expression tag	UNP O67050
B	-9	SER	-	expression tag	UNP O67050
B	-8	GLY	-	expression tag	UNP O67050
B	-7	LEU	-	expression tag	UNP O67050
B	-6	VAL	-	expression tag	UNP O67050
B	-5	PRO	-	expression tag	UNP O67050
B	-4	ARG	-	expression tag	UNP O67050
B	-3	GLY	-	expression tag	UNP O67050
B	-2	SER	-	expression tag	UNP O67050
B	-1	HIS	-	expression tag	UNP O67050
C	-20	MET	-	expression tag	UNP O67050
C	-19	GLY	-	expression tag	UNP O67050
C	-18	SER	-	expression tag	UNP O67050
C	-17	SER	-	expression tag	UNP O67050
C	-16	HIS	-	expression tag	UNP O67050
C	-15	HIS	-	expression tag	UNP O67050
C	-14	HIS	-	expression tag	UNP O67050
C	-13	HIS	-	expression tag	UNP O67050
C	-12	HIS	-	expression tag	UNP O67050
C	-11	HIS	-	expression tag	UNP O67050
C	-10	SER	-	expression tag	UNP O67050
C	-9	SER	-	expression tag	UNP O67050
C	-8	GLY	-	expression tag	UNP O67050
C	-7	LEU	-	expression tag	UNP O67050
C	-6	VAL	-	expression tag	UNP O67050
C	-5	PRO	-	expression tag	UNP O67050
C	-4	ARG	-	expression tag	UNP O67050
C	-3	GLY	-	expression tag	UNP O67050
C	-2	SER	-	expression tag	UNP O67050
C	-1	HIS	-	expression tag	UNP O67050
D	-20	MET	-	expression tag	UNP O67050
D	-19	GLY	-	expression tag	UNP O67050
D	-18	SER	-	expression tag	UNP O67050

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	SER	-	expression tag	UNP O67050
D	-16	HIS	-	expression tag	UNP O67050
D	-15	HIS	-	expression tag	UNP O67050
D	-14	HIS	-	expression tag	UNP O67050
D	-13	HIS	-	expression tag	UNP O67050
D	-12	HIS	-	expression tag	UNP O67050
D	-11	HIS	-	expression tag	UNP O67050
D	-10	SER	-	expression tag	UNP O67050
D	-9	SER	-	expression tag	UNP O67050
D	-8	GLY	-	expression tag	UNP O67050
D	-7	LEU	-	expression tag	UNP O67050
D	-6	VAL	-	expression tag	UNP O67050
D	-5	PRO	-	expression tag	UNP O67050
D	-4	ARG	-	expression tag	UNP O67050
D	-3	GLY	-	expression tag	UNP O67050
D	-2	SER	-	expression tag	UNP O67050
D	-1	HIS	-	expression tag	UNP O67050

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is water.

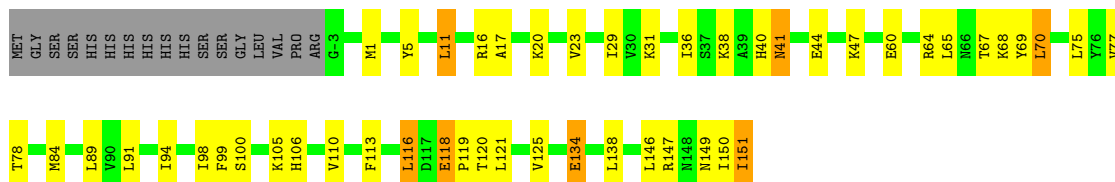
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	123	Total O 123 123	0	0
3	B	131	Total O 131 131	0	0
3	C	153	Total O 153 153	0	0
3	D	113	Total O 113 113	0	0

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: tRNA adenosine deaminase TadA

Chain A: 



V110	L116	D117	E118	L121	N122	H123	R124	V125	K126	W127	E128	Y129	Y130	P131	L132	E133	E134	F143	R147	N148	N149	I150	I151
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.18Å 151.95Å 54.13Å 90.00° 113.42° 90.00°	Depositor
Resolution (Å)	35.47 – 1.80 35.47 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.4 (35.47-1.80) 48.2 (35.47-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 1.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.198 , 0.248 0.199 , 0.239	Depositor DCC
R_{free} test set	518 reflections (1.82%)	wwPDB-VP
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.298 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5495	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 96.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.2521e-10.*

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: ZN

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	0.43	0/1255	0.91	4/1687 (0.2%)
1	B	0.42	0/1276	0.81	2/1717 (0.1%)
1	C	0.42	0/1299	0.88	4/1747 (0.2%)
1	D	0.44	0/1234	0.87	2/1659 (0.1%)
All	All	0.43	0/5064	0.87	12/6810 (0.2%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	VAL	N-CA-C	-10.96	98.21	108.95
1	D	23	VAL	N-CA-C	-9.77	98.32	108.96
1	C	23	VAL	N-CA-C	-8.44	99.76	108.96
1	D	100	SER	N-CA-C	6.13	120.45	112.92
1	C	9	VAL	N-CA-C	-5.90	104.76	110.72
1	A	118	GLU	CA-C-N	5.88	125.36	119.24
1	A	118	GLU	C-N-CA	5.88	125.36	119.24
1	B	-6	VAL	N-CA-C	5.69	114.15	107.84
1	C	131	PRO	N-CA-C	5.58	119.61	111.03
1	C	-6	VAL	N-CA-C	5.27	114.78	108.45
1	A	100	SER	N-CA-C	5.24	119.64	112.88
1	B	131	PRO	N-CA-C	5.13	119.63	111.26

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	1232	0	1262	49	0
1	B	1252	0	1283	46	0
1	C	1275	0	1310	34	0
1	D	1212	0	1247	42	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	123	0	0	6	0
3	B	131	0	0	3	0
3	C	153	0	0	5	0
3	D	113	0	0	5	0
All	All	5495	0	5102	155	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 15.

All (155) 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:C:144:LYS:HA	1:C:144:LYS:HE2	1.39	1.01
1:A:84:MET:HE3	1:B:91:LEU:HD22	1.47	0.94
1:A:41:ASN:HB3	3:A:264:HOH:O	1.77	0.84
1:C:11:LEU:HD22	1:C:78:THR:HG22	1.58	0.83
1:A:84:MET:HE2	1:B:88:ALA:HA	1.59	0.83
1:D:105:LYS:HE3	1:D:105:LYS:HA	1.61	0.83
1:D:7:LEU:O	1:D:11:LEU:HD23	1.79	0.82
1:D:11:LEU:HD22	1:D:78:THR:HG22	1.68	0.74
1:A:84:MET:CE	1:B:91:LEU:HD22	2.18	0.74
1:B:41:ASN:HD21	1:B:43:VAL:HG22	1.50	0.74
1:A:118:GLU:HG3	1:A:120:THR:HG22	1.70	0.73
1:A:84:MET:HE2	1:B:88:ALA:CA	2.19	0.72
1:D:151:ILE:HG12	3:D:288:HOH:O	1.90	0.72
1:D:134:GLU:H	1:D:134:GLU:CD	1.98	0.71
1:A:149:ASN:HA	1:C:122:ASN:ND2	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:LYS:HD2	1:C:104:LYS:H	1.57	0.69
1:A:29:ILE:HD11	1:A:75:LEU:HD12	1.76	0.68
1:A:31:LYS:CB	1:A:36:ILE:HD11	2.25	0.67
1:A:84:MET:CE	1:B:88:ALA:HA	2.25	0.67
1:D:4:GLU:O	1:D:8:LYS:HE3	1.97	0.65
1:D:116:LEU:HG	1:D:125:VAL:HB	1.79	0.65
1:C:68:LYS:HE3	1:C:69:TYR:CE2	2.33	0.63
1:B:104:LYS:O	1:B:104:LYS:HD3	1.98	0.62
1:C:144:LYS:HE2	1:C:144:LYS:CA	2.21	0.62
1:A:31:LYS:HB2	1:A:36:ILE:HD11	1.82	0.62
1:B:143:PHE:O	1:B:146:LEU:HB3	2.00	0.61
1:D:64:ARG:HD3	3:D:240:HOH:O	2.00	0.61
1:B:87:TYR:CE2	1:B:91:LEU:HD11	2.36	0.60
1:A:134:GLU:H	1:A:134:GLU:CD	2.10	0.60
1:B:118:GLU:O	1:B:121:LEU:HG	2.02	0.60
1:C:68:LYS:HE3	1:C:69:TYR:CZ	2.36	0.60
1:C:32:GLU:HG2	3:C:291:HOH:O	2.02	0.59
1:B:41:ASN:ND2	1:B:43:VAL:HG22	2.18	0.58
1:A:118:GLU:CG	1:A:120:THR:HG22	2.33	0.58
3:A:248:HOH:O	1:D:151:ILE:HG22	2.03	0.58
1:B:68:LYS:HE3	1:B:69:TYR:CZ	2.39	0.58
1:D:7:LEU:O	1:D:11:LEU:CD2	2.51	0.57
3:A:304:HOH:O	1:B:59:LYS:HD3	2.05	0.57
1:C:7:LEU:O	1:C:11:LEU:HD23	2.04	0.56
1:B:147:ARG:NH1	1:B:147:ARG:HB3	2.20	0.56
1:B:116:LEU:HG	1:B:125:VAL:HB	1.87	0.56
1:D:132:LEU:HB3	1:D:134:GLU:OE1	2.06	0.55
1:B:43:VAL:HG22	3:B:206:HOH:O	2.07	0.55
1:A:151:ILE:N	1:A:151:ILE:HD13	2.22	0.55
1:D:1:MET:HE2	1:D:5:TYR:CZ	2.42	0.55
1:D:1:MET:HA	3:D:306:HOH:O	2.06	0.54
1:A:116:LEU:HG	1:A:125:VAL:HB	1.90	0.54
1:A:147:ARG:HD3	1:D:143:PHE:CE1	2.43	0.53
1:B:-4:ARG:HH11	1:B:-4:ARG:HG2	1.74	0.53
1:C:87:TYR:CE2	1:C:91:LEU:HD11	2.44	0.53
1:C:123:HIS:HB2	3:C:243:HOH:O	2.07	0.53
1:C:83:ILE:HG13	3:C:276:HOH:O	2.08	0.53
1:B:93:ARG:HA	1:B:123:HIS:CD2	2.44	0.53
1:A:31:LYS:HB3	1:A:36:ILE:HD11	1.90	0.53
1:B:122:ASN:HD22	1:D:149:ASN:ND2	2.07	0.53
1:B:41:ASN:ND2	1:B:43:VAL:H	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HE3	1:A:5:TYR:CE1	2.44	0.52
3:C:253:HOH:O	1:D:59:LYS:HD2	2.08	0.52
1:A:118:GLU:OE2	1:A:120:THR:HG22	2.10	0.52
1:C:17:ALA:HB2	1:C:40:HIS:HB2	1.90	0.52
1:A:16:ARG:HG2	1:A:20:LYS:HZ2	1.75	0.52
1:D:41:ASN:C	1:D:41:ASN:HD22	2.18	0.52
1:C:41:ASN:C	1:C:41:ASN:HD22	2.18	0.51
1:A:105:LYS:HB3	3:D:244:HOH:O	2.10	0.51
1:C:139:LEU:HG	1:C:143:PHE:CE2	2.45	0.51
1:B:68:LYS:HE3	1:B:69:TYR:CE2	2.46	0.51
1:B:122:ASN:HB3	1:D:149:ASN:ND2	2.24	0.51
1:C:103:ASP:OD1	1:C:105:LYS:HG3	2.10	0.51
1:C:65:LEU:HB3	1:C:67:THR:HG22	1.91	0.51
1:C:133:GLU:O	1:C:137:GLU:HG3	2.10	0.51
1:C:129:TYR:CZ	1:C:131:PRO:HB3	2.46	0.51
1:A:84:MET:HE3	1:B:91:LEU:CD2	2.32	0.51
1:A:36:ILE:HD13	1:A:65:LEU:HD11	1.93	0.50
1:C:12:ARG:NH1	1:C:15:LYS:HD2	2.27	0.50
1:B:72:GLY:H	1:B:95:GLU:CG	2.24	0.50
1:C:77:VAL:O	1:C:99:PHE:HA	2.12	0.49
1:A:68:LYS:HE3	1:A:69:TYR:CZ	2.47	0.49
1:A:44:GLU:O	1:A:47:LYS:NZ	2.46	0.48
1:B:22:GLU:HG2	3:B:206:HOH:O	2.14	0.48
1:D:77:VAL:O	1:D:99:PHE:HA	2.14	0.48
1:A:40:HIS:HE1	3:A:206:HOH:O	1.95	0.47
1:C:41:ASN:ND2	1:C:43:VAL:H	2.12	0.47
1:C:11:LEU:HD22	1:C:78:THR:CG2	2.37	0.47
1:D:68:LYS:HE3	1:D:69:TYR:CE2	2.50	0.47
1:B:72:GLY:H	1:B:95:GLU:HG2	1.79	0.47
1:D:40:HIS:HE1	3:D:205:HOH:O	1.96	0.47
1:A:113:PHE:CE2	1:B:118:GLU:HG3	2.50	0.47
1:B:117:ASP:HA	1:B:124:ARG:HH11	1.78	0.47
1:B:11:LEU:O	1:B:11:LEU:HD13	2.15	0.47
1:A:151:ILE:HD13	1:A:151:ILE:H	1.80	0.46
1:B:69:TYR:CD1	1:B:93:ARG:HD3	2.50	0.46
1:A:150:ILE:O	1:A:150:ILE:HG23	2.15	0.46
1:B:79:LEU:CD2	1:B:103:ASP:HB2	2.47	0.45
1:C:142:PHE:CZ	1:C:146:LEU:HD11	2.50	0.45
1:A:118:GLU:HB3	1:A:121:LEU:HD13	1.99	0.45
1:B:118:GLU:HG2	3:B:303:HOH:O	2.16	0.45
1:A:11:LEU:HD13	1:A:78:THR:CG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:LEU:HD12	1:C:116:LEU:N	2.32	0.45
1:A:65:LEU:HB2	1:A:67:THR:HG22	1.98	0.45
1:B:122:ASN:HB3	1:D:149:ASN:HD21	1.82	0.45
1:D:134:GLU:CD	1:D:134:GLU:N	2.72	0.45
1:A:106:HIS:ND1	1:D:151:ILE:HG21	2.32	0.45
1:D:93:ARG:HA	1:D:123:HIS:CD2	2.52	0.44
1:D:151:ILE:HG13	1:D:151:ILE:OXT	2.17	0.44
1:A:98:ILE:HD12	1:A:98:ILE:N	2.32	0.44
1:B:149:ASN:C	1:B:149:ASN:HD22	2.26	0.44
1:C:4:GLU:HG2	1:C:8:LYS:HE2	2.00	0.44
1:C:114:ASN:HB3	1:C:117:ASP:HB2	2.00	0.44
1:B:144:LYS:HG2	1:B:148:ASN:ND2	2.33	0.44
1:A:41:ASN:CB	3:A:264:HOH:O	2.50	0.44
1:A:106:HIS:CG	1:D:151:ILE:HG21	2.53	0.44
1:C:144:LYS:O	1:C:147:ARG:HB3	2.18	0.44
1:A:75:LEU:HD13	1:A:89:LEU:HD21	2.00	0.43
1:D:149:ASN:N	1:D:149:ASN:HD22	2.17	0.43
1:A:29:ILE:CD1	1:A:75:LEU:HD12	2.48	0.43
1:A:118:GLU:HG3	1:A:120:THR:CG2	2.44	0.43
1:B:38:LYS:HZ2	1:B:38:LYS:HB2	1.82	0.43
1:C:16:ARG:HA	1:C:19:GLU:OE1	2.19	0.43
1:B:41:ASN:HD22	1:B:41:ASN:C	2.26	0.43
1:A:147:ARG:NH1	1:D:143:PHE:HB3	2.34	0.43
1:B:43:VAL:HG23	1:B:44:GLU:N	2.33	0.43
1:C:104:LYS:HD2	1:C:104:LYS:N	2.29	0.43
1:B:93:ARG:HG2	1:B:93:ARG:HH11	1.83	0.42
1:D:105:LYS:HE3	1:D:105:LYS:CA	2.41	0.42
1:A:38:LYS:NZ	3:A:272:HOH:O	2.52	0.42
1:A:77:VAL:O	1:A:99:PHE:HA	2.20	0.42
1:D:148:ASN:C	1:D:149:ASN:HD22	2.28	0.42
1:D:29:ILE:CD1	1:D:75:LEU:HD23	2.50	0.42
1:A:16:ARG:HG2	1:A:20:LYS:NZ	2.34	0.42
1:B:72:GLY:N	1:B:95:GLU:HG2	2.35	0.42
1:B:13:GLU:OE2	1:B:38:LYS:NZ	2.53	0.42
1:B:122:ASN:ND2	1:D:149:ASN:ND2	2.66	0.42
1:D:98:ILE:HD12	1:D:98:ILE:N	2.34	0.42
1:C:60:GLU:OE2	1:C:64:ARG:NE	2.53	0.41
1:C:116:LEU:N	1:C:116:LEU:CD1	2.83	0.41
1:D:28:ILE:O	1:D:75:LEU:HD22	2.20	0.41
1:D:110:VAL:CG1	1:D:127:TRP:CH2	3.03	0.41
1:B:11:LEU:HD12	1:B:15:LYS:HE3	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:TYR:CZ	1:D:131:PRO:HB3	2.55	0.41
1:D:150:ILE:O	1:D:150:ILE:HG23	2.21	0.41
1:B:93:ARG:HG2	1:B:93:ARG:NH1	2.36	0.41
1:A:110:VAL:HG22	1:A:110:VAL:O	2.19	0.41
1:A:60:GLU:HG3	1:A:64:ARG:NH1	2.36	0.41
1:C:25:VAL:HG22	3:C:242:HOH:O	2.20	0.41
1:D:110:VAL:HG12	1:D:127:TRP:CH2	2.55	0.41
1:B:11:LEU:O	1:B:15:LYS:HG3	2.20	0.41
1:A:17:ALA:HB2	1:A:40:HIS:HB2	2.03	0.41
1:A:47:LYS:HD3	1:A:47:LYS:HA	1.82	0.41
1:B:38:LYS:NZ	1:B:38:LYS:CB	2.84	0.41
1:D:4:GLU:HG2	1:D:8:LYS:CE	2.51	0.41
1:D:75:LEU:HD12	1:D:97:VAL:HG23	2.03	0.41
1:A:70:LEU:HD23	1:A:94:ILE:HD11	2.03	0.40
1:A:118:GLU:HA	1:A:119:PRO:HD3	1.95	0.40
1:D:118:GLU:HB3	1:D:121:LEU:HD13	2.03	0.40
1:C:104:LYS:H	1:C:104:LYS:CD	2.29	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	152/171 (89%)	146 (96%)	6 (4%)	0	100	100
1	B	155/171 (91%)	148 (96%)	7 (4%)	0	100	100
1	C	158/171 (92%)	152 (96%)	5 (3%)	1 (1%)	21	11
1	D	149/171 (87%)	145 (97%)	4 (3%)	0	100	100
All	All	614/684 (90%)	591 (96%)	22 (4%)	1 (0%)	43	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	-8	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	134/149 (90%)	125 (93%)	9 (7%)	15	5
1	B	136/149 (91%)	129 (95%)	7 (5%)	21	9
1	C	139/149 (93%)	135 (97%)	4 (3%)	37	25
1	D	132/149 (89%)	126 (96%)	6 (4%)	24	12
All	All	541/596 (91%)	515 (95%)	26 (5%)	23	11

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

Mol	Chain	Res	Type
1	A	11	LEU
1	A	41	ASN
1	A	70	LEU
1	A	91	LEU
1	A	116	LEU
1	A	134	GLU
1	A	138	LEU
1	A	146	LEU
1	A	151	ILE
1	B	11	LEU
1	B	22	GLU
1	B	38	LYS
1	B	41	ASN
1	B	79	LEU
1	B	116	LEU
1	B	121	LEU
1	C	41	ASN
1	C	89	LEU
1	C	91	LEU
1	C	138	LEU
1	D	8	LYS

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Mol	Chain	Res	Type
1	D	41	ASN
1	D	91	LEU
1	D	105	LYS
1	D	116	LEU
1	D	147	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-1	HIS
1	A	66	ASN
1	A	114	ASN
1	B	41	ASN
1	B	66	ASN
1	B	106	HIS
1	B	122	ASN
1	B	148	ASN
1	B	149	ASN
1	C	41	ASN
1	C	106	HIS
1	C	114	ASN
1	C	123	HIS
1	D	40	HIS
1	D	41	ASN
1	D	114	ASN
1	D	148	ASN
1	D	149	ASN

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

Of 4 ligands modelled in this entry, 4 are 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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	154/171 (90%)	-1.06	0 100 100	12, 22, 47, 57	0
1	B	157/171 (91%)	-1.01	0 100 100	13, 21, 57, 84	0
1	C	160/171 (93%)	-1.01	0 100 100	12, 20, 57, 90	0
1	D	151/171 (88%)	-1.07	0 100 100	10, 20, 47, 56	0
All	All	622/684 (90%)	-1.04	0 100 100	10, 21, 52, 90	0

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	ZN	B	202	1/1	0.99	0.05	33,33,33,33	0
2	ZN	C	203	1/1	0.99	0.07	33,33,33,33	0
2	ZN	A	201	1/1	1.00	0.07	24,24,24,24	0
2	ZN	D	204	1/1	1.00	0.03	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.