



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:44 PM EDT

PDB ID : 3FUV / pdb_00003fuv
Title : Apo-form of T. thermophilus 16S rRNA A1518 and A1519 methyltransferase (KsgA) in space group P43212
Authors : Demirci, H.; Belardinelli, R.; Seri, E.; Gregory, S.T.; Gualerzi, C.; Dahlberg, A.E.; Jogl, G.
Deposited on : 2009-01-14
Resolution : 1.95 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

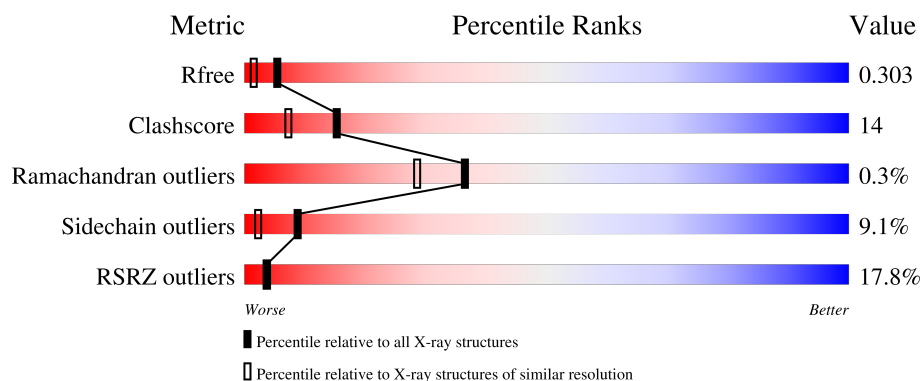
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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 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	271	
1	B	271	
1	C	271	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6657 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 Dimethyladenosine transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	2	0
			2042	1315	374	352	1			
1	B	256	Total	C	N	O	S	0	1	0
			2013	1298	369	345	1			
1	C	252	Total	C	N	O	S	0	4	0
			2008	1295	370	342	1			

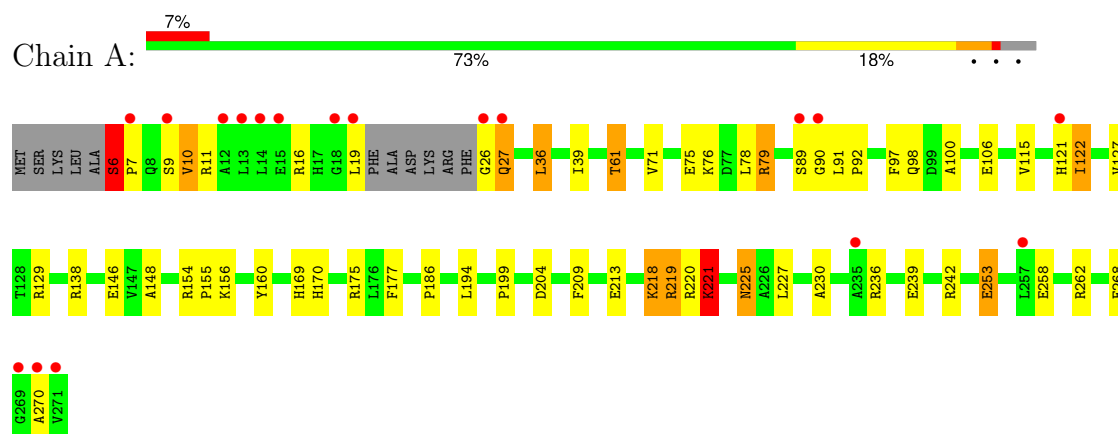
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	230	Total	O	0	10
			240	240		
2	B	177	Total	O	0	6
			183	183		
2	C	161	Total	O	0	8
			171	171		

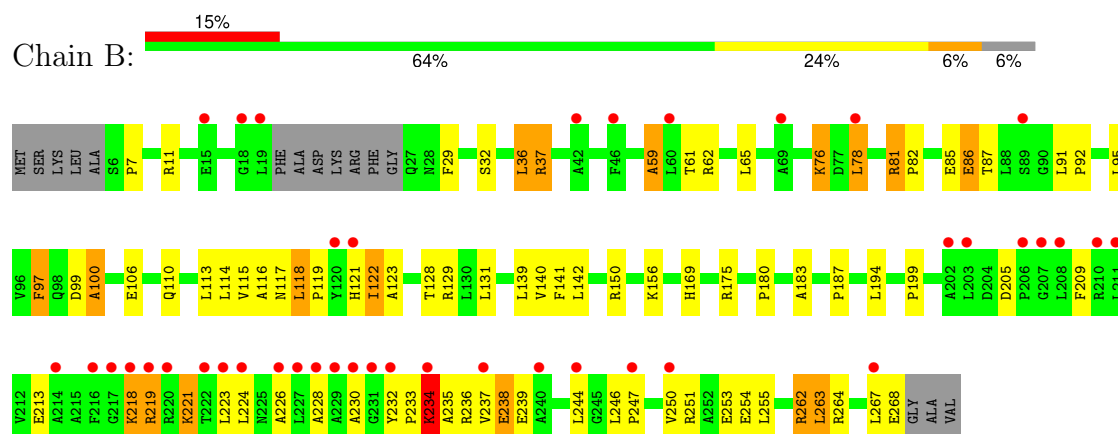
3 Residue-property plots [i](#)

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.

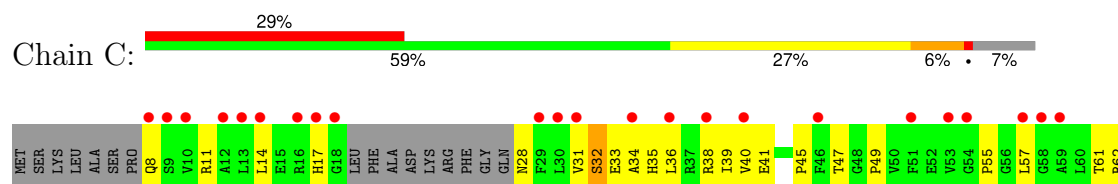
• Molecule 1: Dimethyladenosine transferase

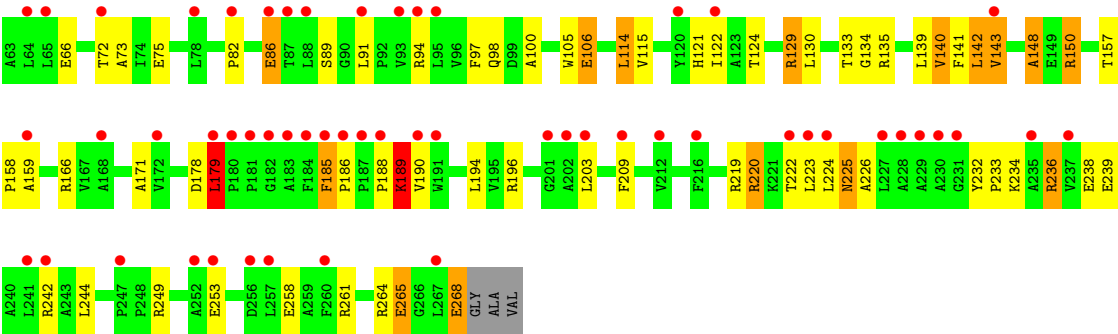


• Molecule 1: Dimethyladenosine transferase



• Molecule 1: Dimethyladenosine transferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	85.11Å 85.11Å 215.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.95 25.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (25.00-1.95) 99.9 (25.00-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.229 , 0.309 0.228 , 0.303	Depositor DCC
R_{free} test set	2986 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.2	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	0.94	EDS
Total number of atoms	6657	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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 70.55 % 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 3.0619e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	1.46	9/2087 (0.4%)	1.32	10/2838 (0.4%)
1	B	1.38	13/2058 (0.6%)	1.28	9/2798 (0.3%)
1	C	1.38	9/2052 (0.4%)	1.29	10/2788 (0.4%)
All	All	1.41	31/6197 (0.5%)	1.30	29/8424 (0.3%)

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	141	PHE	C-O	7.99	1.33	1.23
1	A	169	HIS	C-O	-7.17	1.15	1.24
1	B	100	ALA	CA-CB	-6.61	1.42	1.53
1	A	127	VAL	N-CA	6.18	1.53	1.46
1	C	253	GLU	N-CA	6.14	1.54	1.46
1	C	171	ALA	CA-CB	6.13	1.64	1.53
1	B	128	THR	N-CA	6.08	1.53	1.46
1	C	150	ARG	C-O	6.01	1.31	1.24
1	B	131	LEU	C-O	6.00	1.31	1.24
1	C	124	THR	CA-C	5.96	1.59	1.52
1	B	169	HIS	C-O	-5.83	1.17	1.24
1	A	221	LYS	C-O	-5.70	1.16	1.23
1	B	128	THR	CA-C	5.68	1.60	1.52
1	B	29	PHE	CA-C	-5.60	1.45	1.52
1	C	148	ALA	CA-CB	-5.56	1.44	1.53
1	A	253	GLU	N-CA	5.43	1.53	1.46
1	B	59	ALA	CA-CB	5.39	1.61	1.53
1	B	118	LEU	CA-C	5.34	1.59	1.52
1	C	72	THR	C-O	5.31	1.30	1.24
1	B	97	PHE	C-O	-5.24	1.17	1.24
1	A	115	VAL	CB-CG2	5.21	1.69	1.52
1	B	113	LEU	CA-C	-5.19	1.46	1.52
1	C	140	VAL	CA-CB	5.17	1.61	1.54
1	A	61	THR	N-CA	5.16	1.52	1.46
1	A	10	VAL	CA-CB	5.14	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	180	PRO	CA-C	5.11	1.56	1.52
1	A	225	ASN	C-O	-5.11	1.17	1.24
1	B	110	GLN	C-O	-5.03	1.17	1.23
1	C	49	PRO	CA-C	5.02	1.58	1.52
1	A	138	ARG	CD-NE	5.02	1.53	1.46
1	B	121	HIS	N-CA	5.00	1.52	1.46

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	157	THR	CA-C-N	-9.51	110.04	119.64
1	C	157	THR	C-N-CA	-9.51	110.04	119.64
1	A	170	HIS	N-CA-C	7.58	122.30	112.89
1	B	123	ALA	N-CA-C	7.55	120.23	111.02
1	A	270	ALA	N-CA-C	7.34	120.21	111.33
1	B	118	LEU	CA-C-N	6.96	127.00	119.90
1	B	118	LEU	C-N-CA	6.96	127.00	119.90
1	C	189	LYS	N-CA-C	-6.80	104.56	112.92
1	C	105	TRP	N-CA-C	6.79	119.55	111.33
1	A	90	GLY	N-CA-C	-6.79	106.40	114.48
1	A	204	ASP	N-CA-C	6.70	118.95	110.24
1	A	148	ALA	N-CA-C	6.67	118.55	111.28
1	C	179	LEU	CA-C-N	-6.61	113.57	120.38
1	C	179	LEU	C-N-CA	-6.61	113.57	120.38
1	C	222	THR	N-CA-C	-6.48	102.44	110.41
1	B	246	LEU	CA-C-N	-5.99	114.22	120.38
1	B	246	LEU	C-N-CA	-5.99	114.22	120.38
1	A	230	ALA	N-CA-C	-5.82	105.84	113.17
1	C	225	ASN	N-CA-C	5.55	119.22	112.23
1	B	128	THR	CA-C-N	5.53	127.62	120.44
1	B	128	THR	C-N-CA	5.53	127.62	120.44
1	C	219	ARG	N-CA-C	5.50	119.09	112.38
1	C	234	LYS	N-CA-C	5.47	116.94	110.97
1	A	6	SER	CA-C-N	-5.25	114.20	119.56
1	A	6	SER	C-N-CA	-5.25	114.20	119.56
1	A	160	TYR	N-CA-C	5.18	117.73	109.96
1	A	71	VAL	N-CA-C	5.05	115.24	108.17
1	B	59	ALA	N-CA-C	5.04	116.46	111.07
1	B	86	GLU	N-CA-C	5.03	117.54	111.40

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	2042	0	2128	36	0
1	B	2013	0	2102	69	0
1	C	2008	0	2097	64	0
2	A	240	0	0	10	0
2	B	183	0	0	9	1
2	C	171	0	0	10	1
All	All	6657	0	6327	168	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 14.

All (168) 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:79:ARG:HD2	2:A:652:HOH:O	1.34	1.24
1:B:37:ARG:HH11	1:B:37:ARG:HG3	1.08	1.11
1:A:100:ALA:HB3	1:A:122:ILE:HD11	1.37	1.05
1:B:100:ALA:HB3	1:B:122:ILE:HD11	1.50	0.94
1:C:28:ASN:HB2	1:C:186:PRO:HD2	1.54	0.89
1:A:92:PRO:HD2	2:A:316:HOH:O	1.72	0.88
1:B:205:ASP:OD1	1:B:264[A]:ARG:NH2	2.08	0.87
1:A:154[B]:ARG:HD3	1:A:155:PRO:HD2	1.54	0.86
1:B:37:ARG:HG3	1:B:37:ARG:NH1	1.86	0.86
1:A:209:PHE:O	1:A:213:GLU:HG3	1.77	0.84
1:C:31:VAL:HG22	2:C:519:HOH:O	1.78	0.84
1:C:224:LEU:HD11	1:C:238:GLU:HG3	1.61	0.83
1:B:221:LYS:HE3	1:B:221:LYS:HA	1.63	0.81
1:B:219:ARG:HG2	1:B:219:ARG:HH11	1.47	0.79
1:B:205:ASP:CG	1:B:264[A]:ARG:HH22	1.94	0.75
1:B:233:PRO:O	1:B:235:ALA:N	2.16	0.75
1:A:100:ALA:CB	1:A:122:ILE:HD11	2.15	0.75
1:C:258:GLU:HG3	2:C:312:HOH:O	1.84	0.75
1:C:268:GLU:HA	1:C:268:GLU:OE1	1.85	0.75
1:A:218:LYS:HZ2	1:A:220:ARG:H	1.33	0.74
1:C:122:ILE:O	1:C:122:ILE:HG13	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:ARG:HH11	1:B:219:ARG:CG	2.02	0.73
1:C:98:GLN:HG3	2:C:604:HOH:O	1.88	0.71
1:B:262:ARG:HG2	1:B:262:ARG:HH11	1.54	0.71
1:C:28:ASN:HB2	1:C:186:PRO:CD	2.21	0.71
1:B:37:ARG:HH11	1:B:37:ARG:CG	1.97	0.70
1:C:226:ALA:O	2:C:300:HOH:O	2.10	0.70
1:C:17:HIS:CE1	1:C:82:PRO:HB2	2.28	0.69
1:C:34:ALA:O	1:C:38[B]:ARG:HG3	1.93	0.69
1:B:7:PRO:O	1:B:11:ARG:HG3	1.92	0.68
1:A:7:PRO:O	1:A:11:ARG:HG3	1.94	0.68
1:C:158:PRO:HD2	2:C:515:HOH:O	1.94	0.67
1:B:81:ARG:CB	1:B:82:PRO:HD3	2.25	0.66
1:C:106:GLU:OE2	1:C:129[A]:ARG:NH1	2.30	0.65
1:C:224:LEU:CD1	1:C:238:GLU:HG3	2.27	0.64
1:A:154[B]:ARG:HD3	1:A:155:PRO:CD	2.27	0.64
1:C:185:PHE:CD2	1:C:185:PHE:C	2.76	0.64
1:C:32:SER:OG	1:C:35:HIS:ND1	2.14	0.63
1:C:33:GLU:HA	1:C:36:LEU:HD13	1.79	0.63
1:B:236:ARG:HD2	1:B:267:LEU:HA	1.81	0.62
1:B:268:GLU:HG3	2:B:374[B]:HOH:O	2.00	0.62
1:B:156:LYS:HD3	1:B:254:GLU:HG2	1.82	0.61
1:C:14:LEU:HD21	1:C:57:LEU:HD21	1.83	0.59
1:A:175:ARG:NH1	2:A:651:HOH:O	2.36	0.59
1:C:39:ILE:HG12	1:C:194:LEU:HD13	1.82	0.58
1:A:221:LYS:HE3	1:A:225:ASN:HB2	1.84	0.58
1:B:233:PRO:C	1:B:235:ALA:H	2.06	0.58
1:C:121:HIS:H	1:C:121:HIS:CD2	2.20	0.58
1:B:224:LEU:HD11	1:B:238:GLU:HG2	1.86	0.58
1:B:228:ALA:HB1	1:B:234:LYS:HG2	1.87	0.57
1:C:236:ARG:HH11	1:C:236:ARG:HG3	1.69	0.57
1:C:189:LYS:HD2	1:C:189:LYS:N	2.17	0.57
1:B:106:GLU:H	1:B:106:GLU:CD	2.12	0.56
1:C:8:GLN:O	1:C:11:ARG:HB2	2.05	0.56
1:A:121:HIS:H	1:A:121:HIS:CD2	2.22	0.56
1:B:76:LYS:HE2	1:B:99:ASP:HA	1.87	0.56
1:A:221:LYS:HE3	1:A:225:ASN:CB	2.36	0.56
1:C:100:ALA:HB3	1:C:122:ILE:CD1	2.36	0.56
1:B:218:LYS:HB2	1:B:218:LYS:NZ	2.23	0.54
1:C:133:THR:HB	1:C:135:ARG:HG3	1.89	0.54
1:C:188:PRO:C	1:C:189:LYS:HD2	2.33	0.54
1:C:261:ARG:O	1:C:265:GLU:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:PRO:HB2	1:C:47:THR:HG23	1.89	0.54
1:C:122:ILE:O	1:C:122:ILE:CG1	2.55	0.53
1:B:81:ARG:HG2	1:B:97:PHE:CZ	2.43	0.53
1:C:98:GLN:CG	2:C:604:HOH:O	2.50	0.53
1:B:219:ARG:CG	1:B:219:ARG:NH1	2.68	0.53
1:B:244:LEU:HD11	1:B:263:LEU:HA	1.91	0.53
1:B:224:LEU:HD13	1:B:237:VAL:HG12	1.90	0.52
2:A:492[A]:HOH:O	1:B:187:PRO:HB3	2.09	0.52
1:B:263:LEU:HD22	1:B:267:LEU:CD2	2.39	0.52
1:B:117:ASN:HA	1:B:142:LEU:HB2	1.91	0.52
1:B:116:ALA:O	1:B:141:PHE:HA	2.11	0.51
1:B:81:ARG:HB2	1:B:82:PRO:HD3	1.91	0.51
1:C:134:GLY:HA3	1:C:203:LEU:HD23	1.91	0.51
1:C:66:GLU:OE2	1:C:91:LEU:HD11	2.09	0.51
1:A:6:SER:HA	1:A:9:SER:OG	2.10	0.51
1:B:86:GLU:HG2	2:B:281:HOH:O	2.10	0.51
1:C:268:GLU:HB3	2:C:522:HOH:O	2.10	0.51
1:C:226:ALA:HB1	2:C:300:HOH:O	2.11	0.50
1:B:139:LEU:HD12	1:B:139:LEU:N	2.27	0.50
1:A:75:GLU:O	1:A:97:PHE:HA	2.11	0.49
1:B:78:LEU:O	1:B:81:ARG:HB2	2.11	0.49
1:B:253:GLU:CG	2:B:543:HOH:O	2.60	0.49
1:A:98:GLN:OE1	2:A:588:HOH:O	2.19	0.49
1:A:39:ILE:HG12	1:A:194:LEU:HD13	1.93	0.49
1:B:264[B]:ARG:HE	1:B:268:GLU:CD	2.17	0.49
1:B:263:LEU:HD22	1:B:267:LEU:HD23	1.93	0.49
1:C:115:VAL:HA	1:C:140:VAL:O	2.13	0.49
1:B:81:ARG:CB	1:B:82:PRO:CD	2.90	0.49
1:B:129:ARG:HD3	2:B:627:HOH:O	2.12	0.48
1:B:228:ALA:CB	1:B:234:LYS:HG2	2.43	0.48
1:A:76:LYS:HD2	2:A:511:HOH:O	2.11	0.48
1:C:75:GLU:O	1:C:97:PHE:HA	2.14	0.48
1:C:220:ARG:N	1:C:220:ARG:HD2	2.29	0.48
1:B:175:ARG:NH2	2:B:315:HOH:O	2.41	0.48
1:B:81:ARG:HB3	1:B:82:PRO:HD3	1.93	0.48
1:B:223:LEU:HD22	1:B:255:LEU:CD1	2.44	0.48
1:C:179:LEU:HD12	1:C:179:LEU:N	2.29	0.47
1:C:185:PHE:O	1:C:185:PHE:HD2	1.97	0.47
1:A:7:PRO:HB2	1:C:41:GLU:OE1	2.15	0.47
1:A:26:GLY:CA	2:A:490:HOH:O	2.62	0.47
1:B:218:LYS:HB2	1:B:218:LYS:HZ2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:PRO:HG3	1:C:73:ALA:HB1	1.97	0.47
1:C:225:ASN:HB2	2:C:603:HOH:O	2.14	0.47
1:A:78:LEU:HD23	1:A:97:PHE:CG	2.51	0.46
1:A:177:PHE:CZ	1:A:194:LEU:HD22	2.50	0.46
1:C:114:LEU:HG	1:C:130:LEU:HD12	1.98	0.46
1:C:143:VAL:HG23	1:C:148:ALA:HB2	1.98	0.46
1:A:239:GLU:HG3	2:A:573:HOH:O	2.15	0.45
1:B:76:LYS:HE3	1:B:76:LYS:HB3	1.69	0.45
1:C:106:GLU:CD	1:C:129[A]:ARG:NH1	2.74	0.45
1:C:114:LEU:HG	1:C:130:LEU:CD1	2.46	0.45
1:C:236:ARG:HG3	1:C:236:ARG:NH1	2.32	0.45
1:A:268:GLU:CG	2:A:301:HOH:O	2.65	0.45
1:B:92:PRO:HG2	2:B:333:HOH:O	2.15	0.45
1:B:253:GLU:CD	2:B:543:HOH:O	2.59	0.45
1:B:209:PHE:O	1:B:213:GLU:HG2	2.16	0.45
1:B:267:LEU:HD12	2:B:374[B]:HOH:O	2.16	0.45
1:A:258:GLU:O	1:A:262:ARG:HG3	2.17	0.45
1:B:247:PRO:O	1:B:250:VAL:HB	2.16	0.45
1:B:122:ILE:HD13	1:B:122:ILE:HG21	1.63	0.44
1:A:218:LYS:HD2	1:A:221:LYS:HG2	1.98	0.44
1:B:232:TYR:HA	1:B:233:PRO:HD3	1.84	0.44
1:A:227:LEU:HD23	1:A:227:LEU:HA	1.82	0.44
1:C:36:LEU:O	1:C:40:VAL:HG23	2.18	0.43
1:C:106:GLU:OE1	1:C:129[A]:ARG:NH1	2.51	0.43
1:B:262:ARG:HG2	1:B:262:ARG:NH1	2.30	0.43
1:C:166:ARG:HA	1:C:209:PHE:CZ	2.53	0.43
1:A:219:ARG:H	1:A:219:ARG:HG3	1.39	0.43
1:B:32:SER:HB2	1:B:183:ALA:HA	2.00	0.43
1:B:156:LYS:CD	1:B:254:GLU:HG2	2.47	0.43
1:B:236:ARG:HH12	1:B:268:GLU:C	2.26	0.43
1:A:129:ARG:HH11	1:A:129:ARG:HD3	1.53	0.43
1:C:139:LEU:O	1:C:196:ARG:HA	2.18	0.43
1:A:221:LYS:HD2	1:A:221:LYS:HA	1.31	0.43
1:A:106:GLU:H	1:A:106:GLU:CD	2.27	0.43
1:B:142:LEU:HD23	1:B:194:LEU:HD12	2.01	0.42
1:B:150:ARG:HD3	2:B:322:HOH:O	2.18	0.42
1:C:129[A]:ARG:O	1:C:133:THR:HG23	2.19	0.42
1:C:150:ARG:HA	1:C:159:ALA:HB1	2.01	0.42
1:C:223:LEU:O	1:C:224:LEU:C	2.61	0.42
1:A:26:GLY:HA3	2:A:490:HOH:O	2.19	0.42
1:B:115:VAL:HA	1:B:140:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:ALA:O	1:B:230:ALA:HB2	2.20	0.42
1:A:36:LEU:HD12	1:A:36:LEU:HA	1.69	0.42
1:B:81:ARG:HH11	1:B:95:LEU:HD12	1.85	0.42
1:B:118:LEU:HA	1:B:119:PRO:HD3	1.83	0.42
1:B:36:LEU:HD21	1:B:59:ALA:HB1	2.02	0.41
1:C:232:TYR:HA	1:C:233:PRO:HD3	1.92	0.41
1:B:62:ARG:HG3	1:B:91:LEU:HD11	2.00	0.41
1:B:236:ARG:O	1:B:239:GLU:N	2.49	0.41
1:C:100:ALA:HB3	1:C:122:ILE:HD12	2.03	0.41
1:B:238:GLU:H	1:B:238:GLU:HG3	1.56	0.41
1:A:155:PRO:O	1:A:156:LYS:HB2	2.20	0.41
1:B:219:ARG:O	1:B:251:ARG:NH2	2.53	0.41
1:C:86:GLU:H	1:C:86:GLU:HG2	1.68	0.41
1:C:225:ASN:HB3	2:C:575:HOH:O	2.21	0.41
1:A:6:SER:O	1:A:10:VAL:HG23	2.21	0.41
1:A:27:GLN:O	1:A:186:PRO:HD2	2.21	0.41
1:C:142:LEU:HD13	1:C:194:LEU:CD1	2.51	0.41
1:C:178:ASP:C	1:C:179:LEU:HD12	2.46	0.41
1:C:264:ARG:HD3	1:C:264:ARG:C	2.46	0.41
1:C:239:GLU:HG3	1:C:242:ARG:HH21	1.85	0.41
1:C:239:GLU:HG3	1:C:242:ARG:NH2	2.36	0.40
1:B:65:LEU:HD22	1:B:92:PRO:O	2.20	0.40
1:B:223:LEU:HD22	1:B:255:LEU:HD13	2.02	0.40
1:C:185:PHE:HA	1:C:186:PRO:HA	1.74	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)
2:B:605:HOH:O	2:C:604:HOH:O[8_565]	2.11	0.09

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	258/271 (95%)	249 (96%)	9 (4%)	0	100	100
1	B	253/271 (93%)	239 (94%)	13 (5%)	1 (0%)	30	21
1	C	252/271 (93%)	243 (96%)	8 (3%)	1 (0%)	30	21
All	All	763/813 (94%)	731 (96%)	30 (4%)	2 (0%)	36	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	234	LYS
1	C	32	SER

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	210/217 (97%)	192 (91%)	18 (9%)	10	2
1	B	208/217 (96%)	190 (91%)	18 (9%)	9	2
1	C	207/217 (95%)	186 (90%)	21 (10%)	7	1
All	All	625/651 (96%)	568 (91%)	57 (9%)	9	2

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	16	ARG
1	A	19	LEU
1	A	27	GLN
1	A	36	LEU
1	A	61	THR
1	A	79	ARG
1	A	89	SER
1	A	91	LEU

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Mol	Chain	Res	Type
1	A	122	ILE
1	A	146	GLU
1	A	199	PRO
1	A	218	LYS
1	A	219	ARG
1	A	221	LYS
1	A	236	ARG
1	A	242	ARG
1	A	253	GLU
1	B	36	LEU
1	B	37	ARG
1	B	61	THR
1	B	76	LYS
1	B	78	LEU
1	B	81	ARG
1	B	85	GLU
1	B	87	THR
1	B	114	LEU
1	B	122	ILE
1	B	199	PRO
1	B	218	LYS
1	B	219	ARG
1	B	221	LYS
1	B	234	LYS
1	B	238	GLU
1	B	262	ARG
1	B	263	LEU
1	C	61	THR
1	C	62	ARG
1	C	86	GLU
1	C	89	SER
1	C	94	ARG
1	C	106	GLU
1	C	114	LEU
1	C	129[A]	ARG
1	C	129[B]	ARG
1	C	142	LEU
1	C	143	VAL
1	C	179	LEU
1	C	185	PHE
1	C	189	LYS
1	C	190	VAL

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Mol	Chain	Res	Type
1	C	220	ARG
1	C	236	ARG
1	C	244	LEU
1	C	249	ARG
1	C	265	GLU
1	C	268	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	27	GLN
1	C	17	HIS
1	C	98	GLN
1	C	117	ASN
1	C	121	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 ⓘ

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	260/271 (95%)	0.46	18 (6%)	23 26	15, 31, 49, 59	2 (0%)
1	B	256/271 (94%)	1.10	41 (16%)	5 5	18, 34, 60, 67	1 (0%)
1	C	252/271 (92%)	1.61	78 (30%)	1 1	15, 40, 60, 76	4 (1%)
All	All	768/813 (94%)	1.05	137 (17%)	4 4	15, 35, 57, 76	7 (0%)

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	181	PRO	6.1
1	B	232	TYR	5.3
1	C	8	GLN	4.8
1	C	18	GLY	4.7
1	C	31	VAL	4.5
1	B	18	GLY	3.7
1	C	257	LEU	3.7
1	B	237	VAL	3.7
1	C	190	VAL	3.7
1	C	184	PHE	3.7
1	C	30	LEU	3.6
1	C	201	GLY	3.6
1	C	203	LEU	3.6
1	B	217	GLY	3.5
1	C	36	LEU	3.5
1	C	65	LEU	3.5
1	A	271	VAL	3.5
1	A	270	ALA	3.4
1	C	191	TRP	3.4
1	B	203	LEU	3.3
1	C	180	PRO	3.3
1	C	186	PRO	3.3
1	A	18	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	207	GLY	3.3
1	C	183	ALA	3.3
1	C	224	LEU	3.3
1	B	226	ALA	3.2
1	C	231	GLY	3.2
1	B	19	LEU	3.2
1	A	90	GLY	3.2
1	B	240	ALA	3.1
1	C	212[A]	VAL	3.1
1	C	17	HIS	3.1
1	C	209	PHE	3.1
1	C	228	ALA	3.1
1	B	219	ARG	3.1
1	C	9	SER	3.1
1	B	228	ALA	3.0
1	C	78	LEU	3.0
1	A	12	ALA	3.0
1	B	202	ALA	3.0
1	C	202	ALA	3.0
1	B	224	LEU	3.0
1	B	89	SER	3.0
1	C	185	PHE	3.0
1	A	19	LEU	2.9
1	A	269	GLY	2.9
1	B	15	GLU	2.9
1	B	230	ALA	2.9
1	C	10	VAL	2.9
1	B	46	PHE	2.9
1	C	120	TYR	2.9
1	C	222	THR	2.9
1	B	247	PRO	2.9
1	C	252	ALA	2.9
1	C	88[A]	LEU	2.9
1	C	179	LEU	2.9
1	B	121	HIS	2.8
1	C	29	PHE	2.8
1	B	231	GLY	2.8
1	B	222	THR	2.8
1	C	235	ALA	2.8
1	C	38[A]	ARG	2.8
1	C	242	ARG	2.8
1	C	188	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	244	LEU	2.7
1	B	267	LEU	2.7
1	C	14	LEU	2.7
1	B	214	ALA	2.7
1	C	34	ALA	2.7
1	C	91	LEU	2.7
1	B	211	LEU	2.6
1	C	12	ALA	2.6
1	C	229	ALA	2.6
1	C	13	LEU	2.6
1	C	95	LEU	2.6
1	C	87	THR	2.6
1	A	27	GLN	2.5
1	C	51	PHE	2.5
1	A	26	GLY	2.5
1	C	122	ILE	2.5
1	C	237	VAL	2.5
1	B	206	PRO	2.5
1	B	227	LEU	2.5
1	C	241	LEU	2.5
1	B	69	ALA	2.5
1	C	59	ALA	2.5
1	C	40	VAL	2.5
1	C	86	GLU	2.5
1	C	260	PHE	2.4
1	C	93	VAL	2.4
1	C	58	GLY	2.4
1	B	208	LEU	2.4
1	C	46	PHE	2.4
1	A	13	LEU	2.4
1	C	57	LEU	2.4
1	A	235	ALA	2.4
1	C	82	PRO	2.4
1	A	121	HIS	2.4
1	C	64	LEU	2.3
1	B	229	ALA	2.3
1	B	250	VAL	2.3
1	C	172	VAL	2.3
1	B	60	LEU	2.3
1	C	267	LEU	2.3
1	C	216	PHE	2.3
1	C	94	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	143	VAL	2.3
1	C	168	ALA	2.2
1	B	220	ARG	2.2
1	C	72	THR	2.2
1	C	223	LEU	2.2
1	C	182	GLY	2.2
1	A	15	GLU	2.2
1	C	230	ALA	2.2
1	B	223	LEU	2.2
1	B	218	LYS	2.2
1	A	9	SER	2.1
1	A	7	PRO	2.1
1	B	120	TYR	2.1
1	C	53	VAL	2.1
1	A	257	LEU	2.1
1	B	78	LEU	2.1
1	B	42	ALA	2.1
1	C	256	ASP	2.1
1	C	54	GLY	2.1
1	C	187	PRO	2.1
1	A	14	LEU	2.1
1	C	159	ALA	2.1
1	B	234	LYS	2.0
1	C	227	LEU	2.0
1	C	253	GLU	2.0
1	A	89	SER	2.0
1	B	216	PHE	2.0
1	C	247	PRO	2.0
1	B	210	ARG	2.0
1	C	16	ARG	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 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.