Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:44 AM GMT

PDB ID	:	3FUV
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

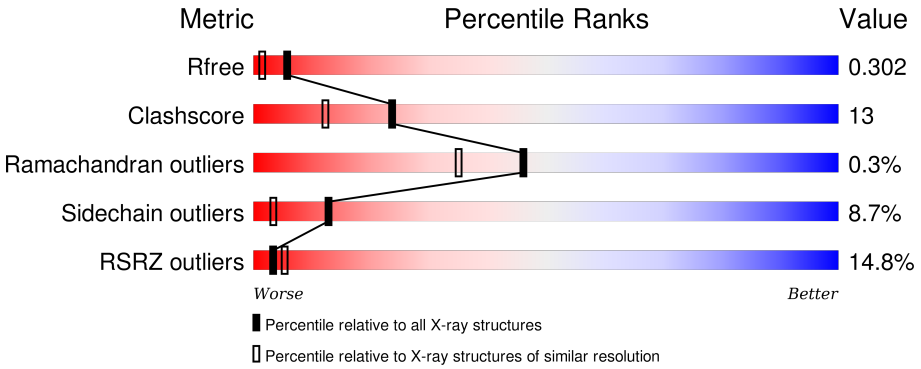
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	271	10% 75% 17% • •
1	B	271	13% 65% 24% 5% • 6%
1	C	271	19% 63% 25% 5% 7%

2 Entry composition (i)

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.

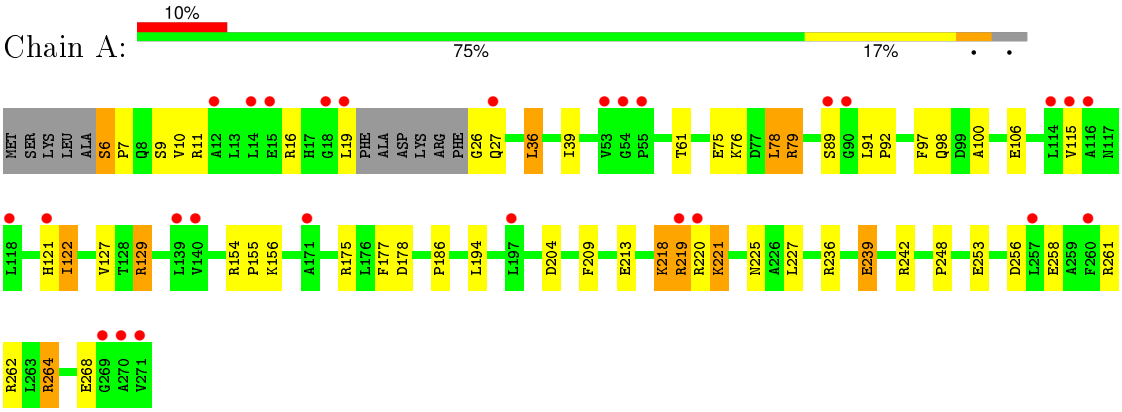
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	230	Total	O	0	10
			240	240		
2	B	177	Total	O	0	6
			183	183		
2	C	161	Total	O	0	8
			171	171		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

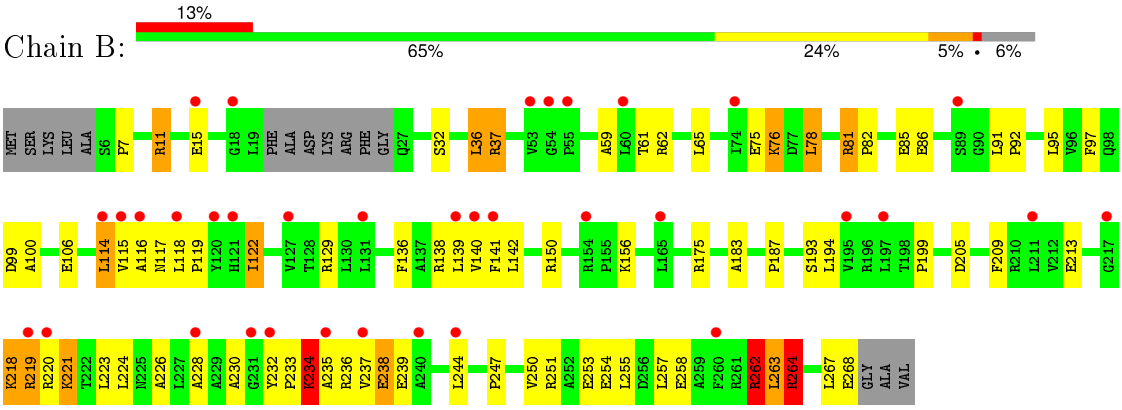
- Molecule 1: Dimethyladenosine transferase

Chain A:



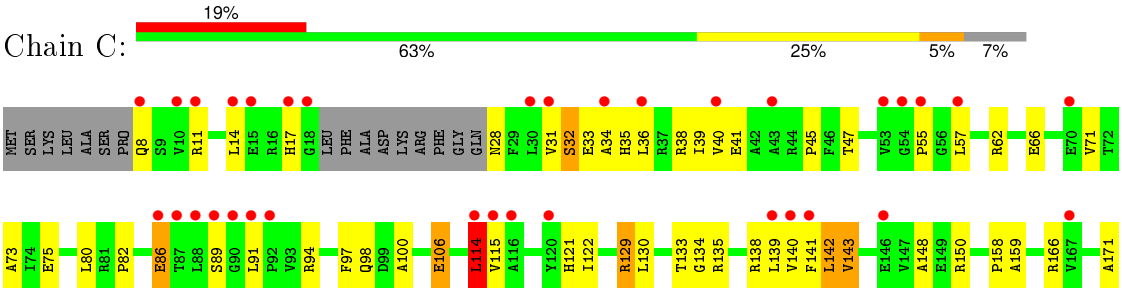
- Molecule 1: Dimethyladenosine transferase

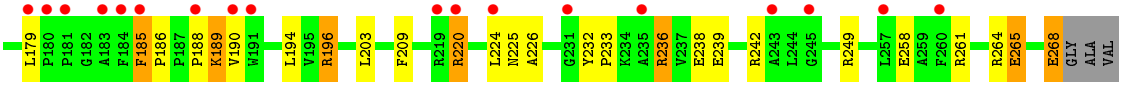
Chain B:



- Molecule 1: Dimethyladenosine transferase

Chain C:




L179
P180
P181
G182
A183
F184
F185
P186
P187
P188
K189
V190
W191
L194
Y195
R196
L203
F209
R219
R220
L224
N225
A226
G231
Y232
P233
K234
A235
R236
Y237
E238
E239
R242
A243
L244
G245
R249
L257
E258
A259
F260
R261
R264
E265
E268
GLY
ALA
VAL

4 Data and refinement statistics (i)

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 24.97 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (25.00-1.95) 99.9 (24.97-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.229 , 0.309 0.228 , 0.302	Depositor DCC
R_{free} test set	2968 reflections (5.32%)	DCC
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 , 62.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	2 of 58998 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.95	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.20	4/2087 (0.2%)	1.10	7/2838 (0.2%)
1	B	1.13	5/2058 (0.2%)	1.07	7/2798 (0.3%)
1	C	1.12	3/2052 (0.1%)	1.01	4/2788 (0.1%)
All	All	1.15	12/6197 (0.2%)	1.06	18/8424 (0.2%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	VAL	CB-CG2	8.05	1.69	1.52
1	A	106	GLU	CD-OE1	7.44	1.33	1.25
1	A	239	GLU	CG-CD	7.38	1.63	1.51
1	C	71	VAL	CB-CG1	6.18	1.65	1.52
1	B	258	GLU	CG-CD	6.16	1.61	1.51
1	C	171	ALA	CA-CB	5.79	1.64	1.52
1	A	127	VAL	CB-CG1	5.62	1.64	1.52
1	B	75	GLU	CB-CG	5.61	1.62	1.52
1	B	136	PHE	CE1-CZ	5.49	1.47	1.37
1	B	193	SER	CB-OG	-5.40	1.35	1.42
1	C	141	PHE	C-O	5.39	1.33	1.23
1	B	15	GLU	CG-CD	5.15	1.59	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	129	ARG	NE-CZ-NH1	-7.11	116.75	120.30
1	B	257	LEU	CB-CG-CD2	-7.02	99.06	111.00
1	B	11	ARG	NE-CZ-NH1	-6.94	116.83	120.30
1	C	138	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	B	138	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	B	264[A]	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	B	264[B]	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	B	262	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	C	80	LEU	CB-CG-CD2	-5.83	101.09	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	261	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	C	114	LEU	CA-CB-CG	5.74	128.50	115.30
1	A	204	ASP	CB-CG-OD1	5.70	123.43	118.30
1	B	114	LEU	CB-CG-CD2	5.58	120.49	111.00
1	A	178	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	264	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	C	196	ARG	NE-CZ-NH1	-5.19	117.71	120.30
1	A	78	LEU	CA-CB-CG	5.17	127.20	115.30
1	A	256	ASP	CB-CG-OD1	5.03	122.83	118.30

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	2042	0	2128	37	0
1	B	2013	0	2102	67	0
1	C	2008	0	2097	61	0
2	A	240	0	0	10	0
2	B	183	0	0	8	1
2	C	171	0	0	10	1
All	All	6657	0	6327	164	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 13.

All (164) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NH1	1:B:37:ARG:HG3	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:HA	1:B:221:LYS:HE3	1.63	0.81
1:B:219:ARG:HG2	1:B:219:ARG:HH11	1.47	0.79
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:C:122:ILE:HG13	1:C:122:ILE:O	1.86	0.73
1:B:219:ARG:CG	1:B:219:ARG:HH11	2.02	0.73
1:C:98:GLN:HG3	2:C:604:HOH:O	1.88	0.71
1:B:262:ARG:HH11	1:B:262:ARG:HG2	1.54	0.71
1:B:205:ASP:CG	1:B:264[A]:ARG:HH22	1.94	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:218:LYS:HZ2	1:A:220:ARG:H	1.41	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: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:C:185:PHE:C	1:C:185:PHE:CD2	2.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:C:189:LYS:HD2	2.17	0.57
1:C:8:GLN:O	1:C:11:ARG:HB2	2.05	0.56
1:A:121:HIS:CD2	1:A:121:HIS:H	2.22	0.56
1:B:76:LYS:HE2	1:B:99:ASP:HA	1.87	0.56
1:C:100:ALA:HB3	1:C:122:ILE:CD1	2.36	0.56
1:A:221:LYS:HE3	1:A:225:ASN:CB	2.36	0.56
1:C:133:THR:HB	1:C:135:ARG:HG3	1.89	0.54
1:B:218:LYS:HB2	1:B:218:LYS:NZ	2.23	0.54
1:C:261:ARG:O	1:C:265:GLU:HG2	2.08	0.54
1:C:45:PRO:HB2	1:C:47:THR:HG23	1.89	0.54
1:B:233:PRO:C	1:B:235:ALA:H	2.06	0.54
1:C:122:ILE:O	1:C:122:ILE:CG1	2.55	0.53
1:C:98:GLN:CG	2:C:604:HOH:O	2.50	0.53
1:B:81:ARG:HG2	1:B:97:PHE:CZ	2.43	0.53
1:B:244:LEU:HD11	1:B:263:LEU:HA	1.91	0.53
1:B:219:ARG:CG	1:B:219:ARG:NH1	2.68	0.53
1:B:224:LEU:HD13	1:B:237:VAL:HG12	1.90	0.52
1:B:106:GLU:H	1:B:106:GLU:CD	2.12	0.52
1:B:263:LEU:HD22	1:B:267:LEU:CD2	2.39	0.52
2:A:492[A]:HOH:O	1:B:187:PRO:HB3	2.09	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:N	1:B:139:LEU:HD12	2.27	0.50
1:B:78:LEU:O	1:B:81:ARG:HB2	2.11	0.49
1:A:75:GLU:O	1:A:97:PHE:HA	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:C:188:PRO:C	1:C:189:LYS:HD2	2.33	0.49
1:A:39:ILE:HG12	1:A:194:LEU:HD13	1.93	0.49
1:B:263:LEU:HD22	1:B:267:LEU:HD23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:228:ALA:CB	1:B:234:LYS:HG2	2.43	0.48
1:B:129:ARG:HD3	2:B:627:HOH:O	2.12	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:HD2	1:C:220:ARG:N	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:N	1:C:179:LEU:HD12	2.29	0.47
1:C:185:PHE:HD2	1:C:185:PHE:O	1.97	0.47
1:A:7:PRO:HB2	1:C:41:GLU:OE1	2.15	0.47
1:B:218:LYS:HZ2	1:B:218:LYS:HB2	1.79	0.47
1:A:26:GLY:CA	2:A:490:HOH:O	2.62	0.47
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:218:LYS:NZ	1:A:220:ARG:H	2.12	0.46
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:B:76:LYS:HE3	1:B:76:LYS:HB3	1.69	0.45
1:A:239:GLU:HG3	2:A:573:HOH:O	2.15	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: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:218:LYS:HZ2	1:A:220:ARG:HB2	1.81	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:B:264[B]:ARG:HE	1:B:268:GLU:CD	2.17	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:106:GLU:OE1	1:C:129[A]:ARG:NH1	2.51	0.43
1:C:36:LEU:O	1:C:40:VAL:HG23	2.18	0.43
1:B:262:ARG:NH1	1:B:262:ARG:HG2	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:ARG:HA	1:C:209:PHE:CZ	2.53	0.43
1:B:156:LYS:CD	1:B:254:GLU:HG2	2.47	0.43
1:B:32:SER:HB2	1:B:183:ALA:HA	2.00	0.43
1:A:219:ARG:HG3	1:A:219:ARG:H	1.39	0.43
1:C:139:LEU:O	1:C:196:ARG:HA	2.18	0.43
1:A:129:ARG:HH11	1:A:129:ARG:HD3	1.53	0.43
1:A:221:LYS:HD2	1:A:221:LYS:HA	1.31	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: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
1:B:226:ALA:O	1:B:230:ALA:HB2	2.20	0.42
1:B:81:ARG:HH11	1:B:95:LEU:HD12	1.85	0.42
1:A:36:LEU:HA	1:A:36:LEU:HD12	1.69	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:236:ARG:O	1:B:239:GLU:N	2.49	0.41
1:B:62:ARG:HG3	1:B:91:LEU:HD11	2.00	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:225:ASN:HB3	2:C:575:HOH:O	2.21	0.41
1:C:86:GLU:H	1:C:86:GLU:HG2	1.68	0.41
1:C:106:GLU:CD	1:C:129[A]:ARG:NH1	2.74	0.41
1:C:142:LEU:HD13	1:C:194:LEU:CD1	2.51	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: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:C:185:PHE:HA	1:C:186:PRO:HA	1.74	0.40
1:B:223:LEU:HD22	1:B:255:LEU:HD13	2.02	0.40
1:B:65:LEU:HD22	1:B:92:PRO:O	2.20	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%)	39	27
1	C	252/271 (93%)	243 (96%)	8 (3%)	1 (0%)	39	27
All	All	763/813 (94%)	731 (96%)	30 (4%)	2 (0%)	46	35

All (2) Ramachandran outliers are listed below:

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

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	210/217 (97%)	193 (92%)	17 (8%)	15	4
1	B	208/217 (96%)	188 (90%)	20 (10%)	10	2
1	C	207/217 (95%)	188 (91%)	19 (9%)	11	3
All	All	625/651 (96%)	569 (91%)	56 (9%)	13	3

All (56) 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	36	LEU
1	A	61	THR
1	A	79	ARG
1	A	89	SER
1	A	91	LEU
1	A	122	ILE
1	A	218	LYS
1	A	219	ARG
1	A	221	LYS
1	A	236	ARG
1	A	242	ARG
1	A	248	PRO
1	A	253	GLU
1	A	264	ARG
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	114	LEU
1	B	122	ILE
1	B	199	PRO
1	B	218	LYS
1	B	219	ARG
1	B	220	ARG
1	B	221	LYS
1	B	234	LYS
1	B	238	GLU
1	B	262	ARG
1	B	263	LEU
1	B	264[A]	ARG
1	B	264[B]	ARG
1	C	62	ARG
1	C	86	GLU
1	C	89	SER
1	C	94	ARG
1	C	106	GLU

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Mol	Chain	Res	Type
1	C	114	LEU
1	C	129[A]	ARG
1	C	129[B]	ARG
1	C	142	LEU
1	C	143	VAL
1	C	185	PHE
1	C	189	LYS
1	C	190	VAL
1	C	220	ARG
1	C	236	ARG
1	C	249	ARG
1	C	264	ARG
1	C	265	GLU
1	C	268	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	HIS
1	C	17	HIS
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 carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.61	27 (10%) 8 13	19, 31, 49, 59	0
1	B	256/271 (94%)	0.91	35 (13%) 4 7	22, 35, 60, 67	0
1	C	252/271 (92%)	1.16	52 (20%) 1 1	23, 41, 60, 76	0
All	All	768/813 (94%)	0.89	114 (14%) 3 5	19, 35, 57, 76	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	219	ARG	6.2
1	C	8	GLN	5.8
1	C	120	TYR	5.7
1	C	181	PRO	5.1
1	B	232	TYR	4.9
1	A	19	LEU	4.9
1	B	53	VAL	4.8
1	C	34	ALA	4.7
1	C	91	LEU	4.6
1	B	120	TYR	4.4
1	B	60	LEU	4.4
1	B	231	GLY	4.3
1	B	114	LEU	4.2
1	B	18	GLY	4.0
1	A	220	ARG	4.0
1	B	89	SER	4.0
1	C	14	LEU	3.9
1	C	10	VAL	3.8
1	C	15	GLU	3.7
1	C	87	THR	3.7
1	C	89	SER	3.7
1	C	140	VAL	3.6
1	C	18	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	40	VAL	3.5
1	A	270	ALA	3.5
1	B	116	ALA	3.5
1	B	115	VAL	3.4
1	B	217	GLY	3.4
1	A	140	VAL	3.4
1	C	17	HIS	3.4
1	A	114	LEU	3.4
1	C	90	GLY	3.3
1	A	15	GLU	3.3
1	B	118	LEU	3.2
1	A	90	GLY	3.2
1	A	219	ARG	3.2
1	C	191	TRP	3.2
1	C	180	PRO	3.2
1	C	88[A]	LEU	3.1
1	B	237	VAL	3.1
1	C	219	ARG	3.1
1	C	114	LEU	3.1
1	B	55	PRO	3.1
1	C	31	VAL	3.0
1	C	115	VAL	3.0
1	A	27	GLN	3.0
1	C	53	VAL	3.0
1	B	165	LEU	2.9
1	C	257	LEU	2.9
1	A	116	ALA	2.9
1	C	260	PHE	2.9
1	C	183	ALA	2.9
1	B	244	LEU	2.9
1	A	115	VAL	2.9
1	A	271	VAL	2.9
1	C	188	PRO	2.8
1	A	53	VAL	2.8
1	B	197	LEU	2.8
1	B	228	ALA	2.8
1	B	220	ARG	2.8
1	B	139	LEU	2.8
1	C	54	GLY	2.8
1	B	121	HIS	2.7
1	A	139	LEU	2.7
1	B	240	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	54	GLY	2.7
1	C	184	PHE	2.7
1	C	235	ALA	2.6
1	C	141	PHE	2.6
1	C	57	LEU	2.6
1	B	140	VAL	2.6
1	B	141	PHE	2.5
1	C	30	LEU	2.5
1	C	185	PHE	2.5
1	C	231	GLY	2.5
1	B	131	LEU	2.5
1	C	92	PRO	2.5
1	C	36	LEU	2.5
1	C	139	LEU	2.5
1	C	190	VAL	2.5
1	A	257	LEU	2.5
1	B	195	VAL	2.4
1	C	179	LEU	2.4
1	B	235	ALA	2.4
1	A	54	GLY	2.3
1	C	245	GLY	2.3
1	C	86	GLU	2.3
1	B	127	VAL	2.3
1	A	18	GLY	2.3
1	C	11	ARG	2.3
1	A	197	LEU	2.3
1	A	260	PHE	2.3
1	C	167	VAL	2.2
1	A	269	GLY	2.2
1	A	55	PRO	2.2
1	B	74	ILE	2.2
1	A	12	ALA	2.2
1	A	171	ALA	2.2
1	B	154	ARG	2.2
1	A	14	LEU	2.2
1	C	116	ALA	2.1
1	B	260	PHE	2.1
1	A	121	HIS	2.1
1	C	220	ARG	2.1
1	B	15	GLU	2.1
1	C	224	LEU	2.1
1	A	89	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	146	GLU	2.1
1	C	243	ALA	2.1
1	A	118	LEU	2.1
1	C	43	ALA	2.1
1	C	70	GLU	2.0
1	B	211	LEU	2.0
1	C	55	PRO	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 carbohydrates 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.