



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:40 PM UTC

PDB ID : 9MUK / pdb_00009muk
Title : RlmR 23S rRNA methyltransferase from *Thermus thermophilus*
Authors : Tanouti, Y.; Roovers, M.; Droogmans, L.; Van Elder, D.; Kruys, V.; Labar, G.
Deposited on : 2025-01-14
Resolution : 1.97 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

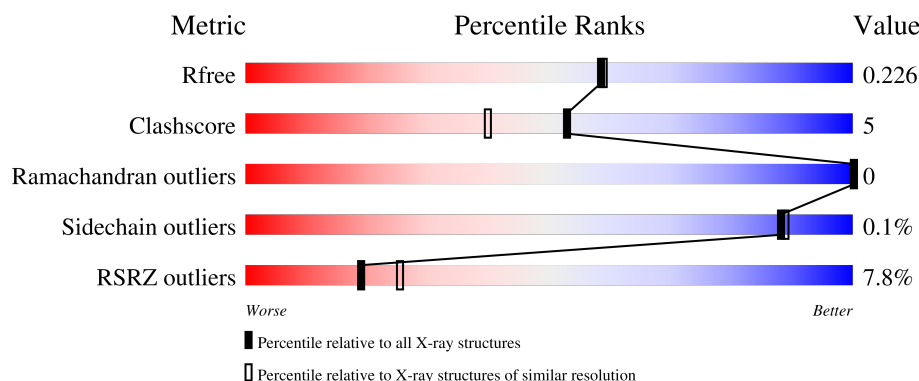
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	280	7% 84% 9% 7%
1	B	280	9% 83% 10% 7%
1	C	280	3% 82% 10% 7%
1	D	280	10% 80% 13% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8594 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 23S rRNA methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			1973	1241	370	360	2			
1	B	261	Total	C	N	O	S	0	0	0
			1974	1242	373	357	2			
1	C	260	Total	C	N	O	S	0	0	0
			1959	1232	370	356	1			
1	D	261	Total	C	N	O	S	0	0	0
			1981	1248	374	357	2			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q72GY4
A	-18	GLY	-	expression tag	UNP Q72GY4
A	-17	SER	-	expression tag	UNP Q72GY4
A	-16	SER	-	expression tag	UNP Q72GY4
A	-15	HIS	-	expression tag	UNP Q72GY4
A	-14	HIS	-	expression tag	UNP Q72GY4
A	-13	HIS	-	expression tag	UNP Q72GY4
A	-12	HIS	-	expression tag	UNP Q72GY4
A	-11	HIS	-	expression tag	UNP Q72GY4
A	-10	HIS	-	expression tag	UNP Q72GY4
A	-9	SER	-	expression tag	UNP Q72GY4
A	-8	SER	-	expression tag	UNP Q72GY4
A	-7	GLY	-	expression tag	UNP Q72GY4
A	-6	LEU	-	expression tag	UNP Q72GY4
A	-5	VAL	-	expression tag	UNP Q72GY4
A	-4	PRO	-	expression tag	UNP Q72GY4
A	-3	ARG	-	expression tag	UNP Q72GY4
A	-2	GLY	-	expression tag	UNP Q72GY4
A	-1	SER	-	expression tag	UNP Q72GY4
A	0	HIS	-	expression tag	UNP Q72GY4
B	-19	MET	-	initiating methionine	UNP Q72GY4

Continued on next page...

Continued from previous page...

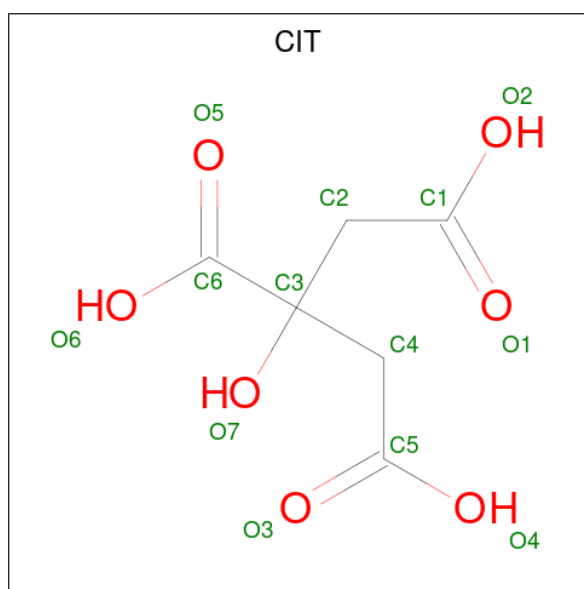
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP Q72GY4
B	-17	SER	-	expression tag	UNP Q72GY4
B	-16	SER	-	expression tag	UNP Q72GY4
B	-15	HIS	-	expression tag	UNP Q72GY4
B	-14	HIS	-	expression tag	UNP Q72GY4
B	-13	HIS	-	expression tag	UNP Q72GY4
B	-12	HIS	-	expression tag	UNP Q72GY4
B	-11	HIS	-	expression tag	UNP Q72GY4
B	-10	HIS	-	expression tag	UNP Q72GY4
B	-9	SER	-	expression tag	UNP Q72GY4
B	-8	SER	-	expression tag	UNP Q72GY4
B	-7	GLY	-	expression tag	UNP Q72GY4
B	-6	LEU	-	expression tag	UNP Q72GY4
B	-5	VAL	-	expression tag	UNP Q72GY4
B	-4	PRO	-	expression tag	UNP Q72GY4
B	-3	ARG	-	expression tag	UNP Q72GY4
B	-2	GLY	-	expression tag	UNP Q72GY4
B	-1	SER	-	expression tag	UNP Q72GY4
B	0	HIS	-	expression tag	UNP Q72GY4
C	-19	MET	-	initiating methionine	UNP Q72GY4
C	-18	GLY	-	expression tag	UNP Q72GY4
C	-17	SER	-	expression tag	UNP Q72GY4
C	-16	SER	-	expression tag	UNP Q72GY4
C	-15	HIS	-	expression tag	UNP Q72GY4
C	-14	HIS	-	expression tag	UNP Q72GY4
C	-13	HIS	-	expression tag	UNP Q72GY4
C	-12	HIS	-	expression tag	UNP Q72GY4
C	-11	HIS	-	expression tag	UNP Q72GY4
C	-10	HIS	-	expression tag	UNP Q72GY4
C	-9	SER	-	expression tag	UNP Q72GY4
C	-8	SER	-	expression tag	UNP Q72GY4
C	-7	GLY	-	expression tag	UNP Q72GY4
C	-6	LEU	-	expression tag	UNP Q72GY4
C	-5	VAL	-	expression tag	UNP Q72GY4
C	-4	PRO	-	expression tag	UNP Q72GY4
C	-3	ARG	-	expression tag	UNP Q72GY4
C	-2	GLY	-	expression tag	UNP Q72GY4
C	-1	SER	-	expression tag	UNP Q72GY4
C	0	HIS	-	expression tag	UNP Q72GY4
D	-19	MET	-	initiating methionine	UNP Q72GY4
D	-18	GLY	-	expression tag	UNP Q72GY4
D	-17	SER	-	expression tag	UNP Q72GY4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP Q72GY4
D	-15	HIS	-	expression tag	UNP Q72GY4
D	-14	HIS	-	expression tag	UNP Q72GY4
D	-13	HIS	-	expression tag	UNP Q72GY4
D	-12	HIS	-	expression tag	UNP Q72GY4
D	-11	HIS	-	expression tag	UNP Q72GY4
D	-10	HIS	-	expression tag	UNP Q72GY4
D	-9	SER	-	expression tag	UNP Q72GY4
D	-8	SER	-	expression tag	UNP Q72GY4
D	-7	GLY	-	expression tag	UNP Q72GY4
D	-6	LEU	-	expression tag	UNP Q72GY4
D	-5	VAL	-	expression tag	UNP Q72GY4
D	-4	PRO	-	expression tag	UNP Q72GY4
D	-3	ARG	-	expression tag	UNP Q72GY4
D	-2	GLY	-	expression tag	UNP Q72GY4
D	-1	SER	-	expression tag	UNP Q72GY4
D	0	HIS	-	expression tag	UNP Q72GY4

- Molecule 2 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			13	6	7		

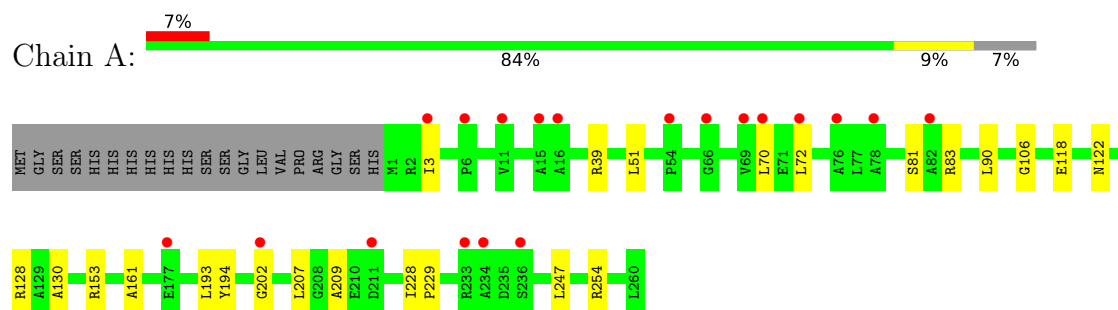
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	195	Total 195	O 195	0	0
3	B	155	Total 155	O 155	0	0
3	C	205	Total 205	O 205	0	0
3	D	139	Total 139	O 139	0	0

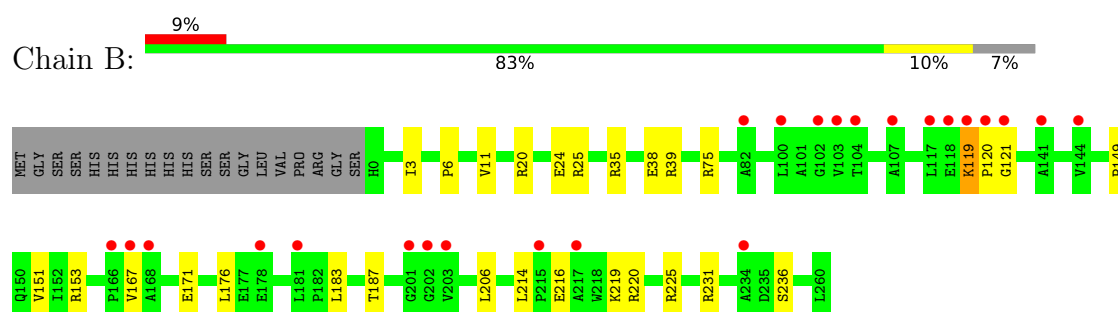
3 Residue-property plots [i](#)

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.

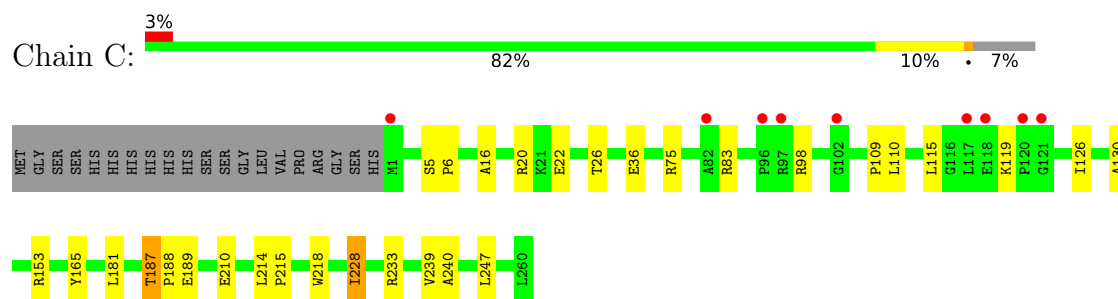
- Molecule 1: 23S rRNA methyltransferase



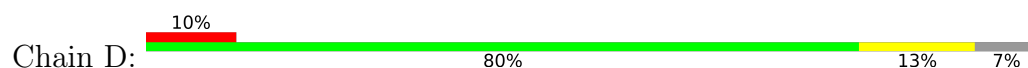
- Molecule 1: 23S rRNA methyltransferase

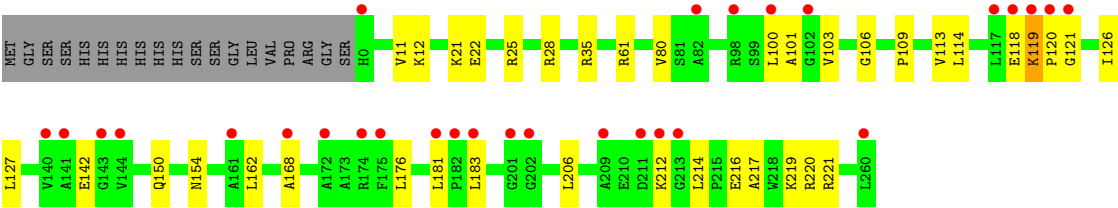


- Molecule 1: 23S rRNA methyltransferase



- Molecule 1: 23S rRNA methyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	221.84Å 62.15Å 98.04Å 90.00° 114.21° 90.00°	Depositor
Resolution (Å)	101.17 – 1.97 101.16 – 1.97	Depositor EDS
% Data completeness (in resolution range)	100.0 (101.17-1.97) 100.0 (101.16-1.97)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 1.97Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.205 , 0.225 0.206 , 0.226	Depositor DCC
R_{free} test set	4414 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.057 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8594	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.79	2/2002 (0.1%)	0.86	3/2710 (0.1%)
1	B	0.76	4/2004 (0.2%)	0.84	4/2713 (0.1%)
1	C	0.69	0/1988	0.84	8/2692 (0.3%)
1	D	0.67	1/2011 (0.0%)	0.70	2/2721 (0.1%)
All	All	0.73	7/8005 (0.1%)	0.81	17/10836 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	ARG	C-O	-6.82	1.16	1.24
1	B	187	THR	C-O	-6.14	1.17	1.24
1	B	151	VAL	C-O	-5.58	1.17	1.24
1	A	153	ARG	C-O	-5.51	1.17	1.24
1	D	12	LYS	C-O	-5.51	1.17	1.24
1	B	149	PRO	C-O	-5.45	1.17	1.24
1	B	153	ARG	C-O	-5.37	1.17	1.24

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	LYS	CA-C-N	8.94	128.67	119.19
1	B	119	LYS	C-N-CA	8.94	128.67	119.19
1	C	210	GLU	N-CA-C	7.68	119.65	111.28
1	D	212	LYS	N-CA-C	6.91	118.81	111.28
1	C	228	ILE	N-CA-C	-6.76	100.20	107.77
1	C	83	ARG	N-CA-C	6.11	119.50	109.85
1	C	26	THR	N-CA-C	6.02	117.92	111.36
1	C	187	THR	CA-C-N	5.98	125.69	119.05
1	C	187	THR	C-N-CA	5.98	125.69	119.05
1	A	81	SER	N-CA-C	5.87	118.74	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	ARG	N-CA-C	5.74	120.28	113.28
1	D	119	LYS	N-CA-C	-5.70	100.28	109.40
1	A	83	ARG	N-CA-C	5.66	118.79	109.85
1	C	5	SER	CA-C-N	5.46	125.07	119.56
1	C	5	SER	C-N-CA	5.46	125.07	119.56
1	A	161	ALA	N-CA-C	5.26	118.80	112.38
1	B	236	SER	N-CA-C	5.07	117.08	109.23

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	1973	0	2045	14	0
1	B	1974	0	2039	21	0
1	C	1959	0	2022	18	0
1	D	1981	0	2059	28	0
2	B	13	0	5	1	0
3	A	195	0	0	2	0
3	B	155	0	0	2	0
3	C	205	0	0	3	0
3	D	139	0	0	7	0
All	All	8594	0	8170	81	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 5.

All (81) 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:153:ARG:HD3	3:C:312:HOH:O	1.93	0.69
1:B:25:ARG:NH1	3:B:403:HOH:O	2.29	0.64
1:A:193:LEU:HD22	1:A:229:PRO:HG3	1.82	0.62
1:D:120:PRO:HB2	1:D:150:GLN:HB2	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:PRO:HD3	1:B:75:ARG:HG3	1.83	0.60
1:B:167:VAL:CG2	1:B:171:GLU:HG3	2.32	0.59
1:B:183:LEU:HB3	1:B:206:LEU:HD11	1.84	0.59
1:C:187:THR:OG1	1:C:188:PRO:HD2	2.02	0.58
1:A:70:LEU:HD22	1:A:72:LEU:CD2	2.33	0.58
1:C:233:ARG:HA	1:C:233:ARG:HE	1.70	0.56
1:A:3:ILE:HD12	1:A:70:LEU:HD11	1.88	0.56
1:D:21:LYS:HG2	3:D:389:HOH:O	2.06	0.55
1:D:106:GLY:HA3	3:D:408:HOH:O	2.07	0.54
1:D:216:GLU:O	1:D:220:ARG:HG2	2.07	0.54
1:A:70:LEU:CD2	1:A:72:LEU:HD23	2.39	0.53
1:C:189:GLU:OE1	1:C:189:GLU:N	2.38	0.53
1:C:215:PRO:HG2	1:C:218:TRP:HD1	1.74	0.52
1:C:130:ALA:HA	1:C:247:LEU:HD13	1.90	0.52
1:B:220:ARG:CZ	1:B:220:ARG:HA	2.40	0.52
1:D:28:ARG:NH1	3:D:307:HOH:O	2.43	0.52
1:C:233:ARG:HA	1:C:233:ARG:NE	2.24	0.52
1:B:216:GLU:O	1:B:220:ARG:HG2	2.10	0.52
1:B:20:ARG:O	1:B:24:GLU:HG2	2.09	0.52
1:C:20:ARG:NH1	3:C:302:HOH:O	2.25	0.51
1:D:119:LYS:HD2	1:D:119:LYS:N	2.26	0.51
1:D:119:LYS:N	1:D:119:LYS:CD	2.73	0.51
1:D:150:GLN:HG2	3:D:425:HOH:O	2.11	0.51
1:C:6:PRO:HG3	1:C:75:ARG:HB3	1.94	0.50
1:D:217:ALA:C	1:D:221:ARG:HH21	2.20	0.50
1:D:28:ARG:NH2	3:D:308:HOH:O	2.45	0.50
1:A:70:LEU:HD22	1:A:72:LEU:HD23	1.92	0.49
1:B:171:GLU:OE2	1:B:171:GLU:HA	2.12	0.49
1:B:176:LEU:HD13	1:B:183:LEU:HD21	1.95	0.49
1:D:142:GLU:HG2	1:D:168:ALA:HA	1.93	0.49
1:C:119:LYS:O	3:C:301:HOH:O	2.20	0.48
1:A:106:GLY:O	3:A:301:HOH:O	2.20	0.48
1:A:194:TYR:CD2	1:A:228:ILE:HD13	2.50	0.47
1:D:120:PRO:HG2	3:D:425:HOH:O	2.14	0.47
1:D:121:GLY:HA2	1:D:154:ASN:OD1	2.15	0.47
1:D:214:LEU:HB3	1:D:219:LYS:HE2	1.97	0.47
1:C:126:ILE:HD11	1:C:239:VAL:HG12	1.96	0.46
1:B:119:LYS:HG3	1:B:121:GLY:H	1.81	0.46
1:D:35:ARG:N	1:D:35:ARG:HD3	2.30	0.46
1:B:176:LEU:HD13	1:B:183:LEU:CD2	2.45	0.46
1:D:101:ALA:C	1:D:103:VAL:H	2.24	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:ILE:HG12	1:C:240:ALA:HA	1.98	0.45
1:B:220:ARG:HH22	1:B:225:ARG:HH12	1.65	0.44
1:C:109:PRO:HG2	1:C:181:LEU:HD21	1.99	0.44
1:C:110:LEU:HD11	1:C:247:LEU:HD23	2.00	0.44
1:D:114:LEU:HD11	1:D:126:ILE:HG21	1.99	0.44
1:C:98:ARG:HB2	1:C:165:TYR:CE1	2.53	0.43
1:B:35:ARG:HD2	1:B:39:ARG:NH2	2.34	0.43
1:B:220:ARG:HA	1:B:220:ARG:NH2	2.32	0.43
1:A:130:ALA:HA	1:A:247:LEU:HD13	1.99	0.43
1:D:118:GLU:C	1:D:119:LYS:HD2	2.42	0.43
1:D:113:VAL:HG21	1:D:176:LEU:HD11	2.01	0.43
1:B:24:GLU:OE2	3:B:401:HOH:O	2.22	0.43
1:D:183:LEU:HB3	1:D:206:LEU:HD11	2.00	0.42
1:A:202:GLY:HA2	1:A:254:ARG:NH2	2.34	0.42
1:D:61:ARG:HB2	1:D:61:ARG:NH1	2.35	0.42
1:A:118:GLU:CG	1:A:122:ASN:HD22	2.33	0.42
1:B:119:LYS:HA	1:B:120:PRO:HD3	1.83	0.42
1:B:167:VAL:CG2	1:B:171:GLU:CG	2.98	0.42
1:A:51:LEU:HB2	1:A:90:LEU:HB2	2.02	0.41
1:C:36:GLU:HA	1:C:36:GLU:OE1	2.20	0.41
1:B:38:GLU:OE2	2:B:301:CIT:O5	2.37	0.41
1:A:118:GLU:OE1	1:A:209:ALA:HA	2.21	0.41
1:A:207:LEU:HD12	1:A:207:LEU:HA	1.86	0.41
1:D:11:VAL:HG13	1:D:80:VAL:HG23	2.03	0.41
1:D:61:ARG:NH1	3:D:311:HOH:O	2.48	0.41
1:D:109:PRO:HG2	1:D:181:LEU:HD21	2.03	0.41
1:B:214:LEU:HB3	1:B:219:LYS:HE2	2.03	0.41
1:D:127:LEU:HD22	1:D:162:LEU:HD23	2.01	0.41
1:A:39:ARG:NH2	3:A:311:HOH:O	2.53	0.41
1:B:3:ILE:HG21	1:B:11:VAL:HG23	2.02	0.41
1:B:220:ARG:HH22	1:B:225:ARG:NH1	2.19	0.41
1:C:16:ALA:HB1	1:C:22:GLU:HG2	2.03	0.41
1:D:217:ALA:HB1	1:D:221:ARG:NH2	2.36	0.40
1:D:22:GLU:OE1	1:D:25:ARG:NH1	2.55	0.40
1:D:100:LEU:O	1:D:103:VAL:HB	2.22	0.40
1:C:115:LEU:HD12	1:C:214:LEU:HD11	2.02	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	258/280 (92%)	255 (99%)	3 (1%)	0	100	100
1	B	259/280 (92%)	253 (98%)	6 (2%)	0	100	100
1	C	258/280 (92%)	256 (99%)	2 (1%)	0	100	100
1	D	259/280 (92%)	253 (98%)	6 (2%)	0	100	100
All	All	1034/1120 (92%)	1017 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	195/213 (92%)	195 (100%)	0	100	100
1	B	193/213 (91%)	193 (100%)	0	100	100
1	C	191/213 (90%)	190 (100%)	1 (0%)	81	79
1	D	195/213 (92%)	195 (100%)	0	100	100
All	All	774/852 (91%)	773 (100%)	1 (0%)	88	89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	228	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	D	179	GLN

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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	CIT	B	301	-	12,12,12	1.22	1 (8%)	17,17,17	1.20	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIT	B	301	-	-	0/16/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	CIT	C3-C6	-2.23	1.51	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	CIT	O6-C6-C3	3.41	119.67	113.14
2	B	301	CIT	O5-C6-C3	-2.11	118.01	122.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	CIT	1	0

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	260/280 (92%)	0.54	19 (7%) 21 28	25, 40, 63, 79	0
1	B	261/280 (93%)	0.69	24 (9%) 14 20	26, 42, 68, 76	0
1	C	260/280 (92%)	0.41	9 (3%) 47 57	24, 38, 62, 71	0
1	D	261/280 (93%)	0.79	29 (11%) 10 14	27, 44, 70, 79	0
All	All	1042/1120 (93%)	0.61	81 (7%) 19 25	24, 41, 68, 79	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	121	GLY	4.6
1	B	120	PRO	4.3
1	D	144	VAL	3.8
1	D	120	PRO	3.7
1	B	144	VAL	3.7
1	A	6	PRO	3.6
1	B	202	GLY	3.6
1	D	202	GLY	3.6
1	C	1	MET	3.5
1	A	3	ILE	3.5
1	A	11	VAL	3.5
1	D	172	ALA	3.4
1	D	181	LEU	3.3
1	D	143	GLY	3.3
1	D	201	GLY	3.3
1	A	76	ALA	3.2
1	D	117	LEU	3.1
1	D	118	GLU	3.1
1	B	104	THR	3.1
1	D	209	ALA	3.0
1	C	82	ALA	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	121	GLY	2.9
1	D	183	LEU	2.9
1	D	82	ALA	2.8
1	B	100	LEU	2.8
1	C	102	GLY	2.8
1	B	119	LYS	2.8
1	C	120	PRO	2.8
1	D	168	ALA	2.8
1	D	175	PHE	2.8
1	B	166	PRO	2.8
1	B	82	ALA	2.7
1	A	211	ASP	2.7
1	C	97	ARG	2.7
1	C	96	PRO	2.7
1	D	119	LYS	2.7
1	B	201	GLY	2.6
1	A	236	SER	2.6
1	D	141	ALA	2.6
1	A	82	ALA	2.5
1	B	178	GLU	2.5
1	D	213	GLY	2.5
1	A	70	LEU	2.5
1	B	102	GLY	2.5
1	D	174	ARG	2.5
1	B	167	VAL	2.5
1	B	181	LEU	2.4
1	D	100	LEU	2.4
1	B	117	LEU	2.4
1	A	233	ARG	2.4
1	B	107	ALA	2.4
1	B	217	ALA	2.3
1	B	103	VAL	2.3
1	B	168	ALA	2.3
1	A	66	GLY	2.3
1	C	121	GLY	2.3
1	D	140	VAL	2.3
1	A	72	LEU	2.3
1	B	118	GLU	2.2
1	C	118	GLU	2.2
1	A	234	ALA	2.2
1	A	69	VAL	2.2
1	C	117	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	260	LEU	2.2
1	B	141	ALA	2.2
1	D	161	ALA	2.2
1	B	203	VAL	2.2
1	D	211	ASP	2.2
1	A	54	PRO	2.2
1	A	15	ALA	2.2
1	D	98	ARG	2.2
1	A	202	GLY	2.1
1	D	102	GLY	2.1
1	A	16	ALA	2.1
1	A	78	ALA	2.1
1	B	215	PRO	2.1
1	D	182	PRO	2.1
1	D	212	LYS	2.1
1	B	234	ALA	2.0
1	A	177	GLU	2.0
1	D	0	HIS	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	CIT	B	301	13/13	0.91	0.08	43,50,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.