



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 17, 2025 – 02:05 PM EDT

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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

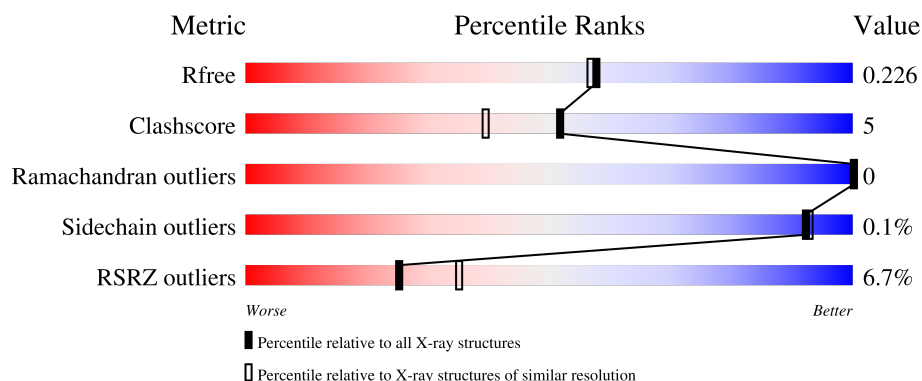
# 1 Overall quality at a glance

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))
$R_{free}$	164625	1356 (1.98-1.98)
Clashscore	180529	1437 (1.98-1.98)
Ramachandran outliers	177936	1426 (1.98-1.98)
Sidechain outliers	177891	1426 (1.98-1.98)
RSRZ outliers	164620	1356 (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  $\geq 3$ , 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	<div> <div>5%</div> <div>86%</div> <div>7%</div> <div>7%</div> </div>
1	B	280	<div> <div>8%</div> <div>85%</div> <div>8%</div> <div>7%</div> </div>
1	C	280	<div> <div>3%</div> <div>83%</div> <div>10%</div> <div>7%</div> </div>
1	D	280	<div> <div>9%</div> <div>81%</div> <div>12%</div> <div>7%</div> </div>

## 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

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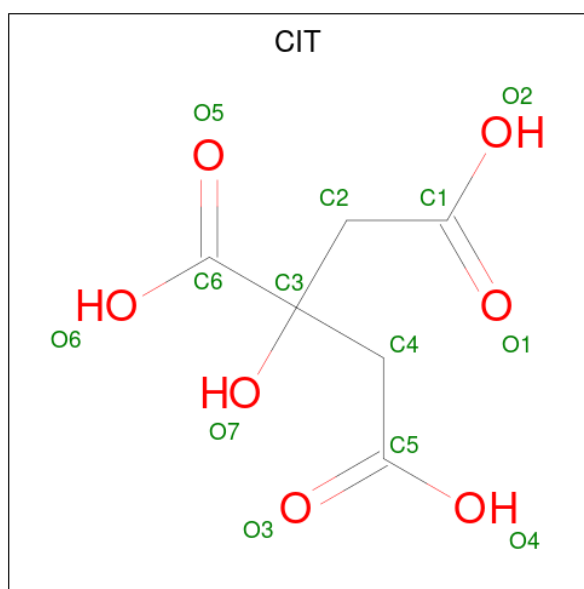
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP Q72GY4
B	-17	SER	-	expression tag	UNP Q72GY4
B	-16	SER	-	expression tag	UNP Q72GY4
B	-15	HIS	-	expression tag	UNP Q72GY4
B	-14	HIS	-	expression tag	UNP Q72GY4
B	-13	HIS	-	expression tag	UNP Q72GY4
B	-12	HIS	-	expression tag	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

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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		

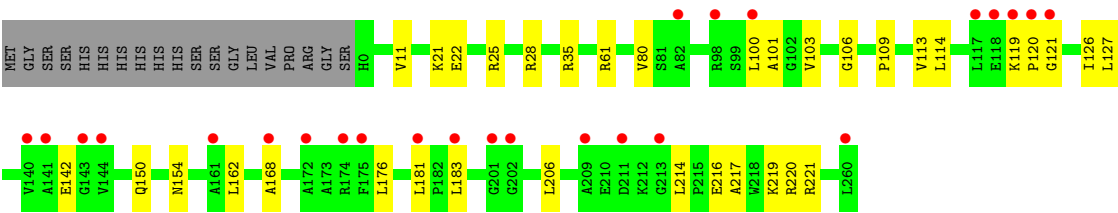
- Molecule 3 is water.

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



- 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	4415 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.9	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.59	0/2002	0.69	0/2710
1	B	0.59	0/2004	0.69	1/2713 (0.0%)
1	C	0.53	0/1988	0.68	1/2692 (0.0%)
1	D	0.55	0/2011	0.65	0/2721
All	All	0.56	0/8005	0.67	2/10836 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	83	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	B	233	ARG	NE-CZ-NH1	5.23	122.91	120.30

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	1973	0	2045	14	0
1	B	1974	0	2039	21	0
1	C	1959	0	2022	18	0
1	D	1981	0	2059	27	0
2	B	13	0	5	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	80	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 (80) 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
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:28:ARG:NH2	3:D:308:HOH:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:217:ALA:C	1:D:221:ARG:HH21	2.20	0.45
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:ALA:C	1:D:103:VAL:H	2.24	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%)	192 (100%)	1 (0%)	86	86
1	C	191/213 (90%)	191 (100%)	0	100	100
1	D	195/213 (92%)	195 (100%)	0	100	100
All	All	774/852 (91%)	773 (100%)	1 (0%)	92	93

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

Mol	Chain	Res	Type
1	B	225	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	260/280 (92%)	0.43	14 (5%)	32 43	25, 40, 63, 79	0
1	B	261/280 (93%)	0.58	22 (8%)	18 27	26, 42, 68, 76	0
1	C	260/280 (92%)	0.30	9 (3%)	47 58	24, 38, 62, 71	0
1	D	261/280 (93%)	0.67	25 (9%)	15 22	27, 44, 70, 79	0
All	All	1042/1120 (93%)	0.50	70 (6%)	25 35	24, 41, 68, 79	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	121	GLY	4.4
1	B	120	PRO	4.1
1	D	144	VAL	3.6
1	D	120	PRO	3.5
1	B	144	VAL	3.5
1	A	6	PRO	3.4
1	C	1	MET	3.4
1	B	202	GLY	3.4
1	D	202	GLY	3.4
1	A	3	ILE	3.4
1	A	11	VAL	3.3
1	D	172	ALA	3.2
1	D	181	LEU	3.1
1	D	143	GLY	3.1
1	D	201	GLY	3.1
1	D	118	GLU	3.0
1	A	76	ALA	3.0
1	D	117	LEU	3.0
1	B	104	THR	2.9
1	D	209	ALA	2.8
1	C	82	ALA	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	121	GLY	2.8
1	D	183	LEU	2.7
1	B	119	LYS	2.7
1	C	120	PRO	2.7
1	B	100	LEU	2.7
1	D	82	ALA	2.6
1	C	102	GLY	2.6
1	C	97	ARG	2.6
1	D	168	ALA	2.6
1	D	175	PHE	2.6
1	A	211	ASP	2.6
1	D	119	LYS	2.6
1	B	166	PRO	2.6
1	B	82	ALA	2.6
1	C	96	PRO	2.5
1	A	236	SER	2.5
1	B	201	GLY	2.5
1	B	178	GLU	2.4
1	D	141	ALA	2.4
1	D	174	ARG	2.4
1	A	82	ALA	2.3
1	D	213	GLY	2.3
1	A	70	LEU	2.3
1	B	102	GLY	2.3
1	B	167	VAL	2.3
1	B	181	LEU	2.3
1	D	100	LEU	2.3
1	A	233	ARG	2.3
1	B	117	LEU	2.3
1	B	107	ALA	2.2
1	B	103	VAL	2.2
1	B	217	ALA	2.2
1	B	118	GLU	2.2
1	C	118	GLU	2.2
1	A	66	GLY	2.1
1	C	121	GLY	2.1
1	B	168	ALA	2.1
1	D	140	VAL	2.1
1	A	72	LEU	2.1
1	D	98	ARG	2.1
1	D	211	ASP	2.0
1	A	69	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	234	ALA	2.0
1	C	117	LEU	2.0
1	D	260	LEU	2.0
1	A	54	PRO	2.0
1	B	141	ALA	2.0
1	B	203	VAL	2.0
1	D	161	ALA	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 monosaccharides 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, 95<sup>th</sup> 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.