



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2021 – 02:04 PM EDT

PDB ID : 3BT7  
Title : Structure of E. coli 5-Methyluridine Methyltransferase TrmA in complex with 19 nucleotide T-arm analogue  
Authors : Alian, A.; Stroud, R.M.; Finer-Moore, J.  
Deposited on : 2007-12-27  
Resolution : 2.43 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

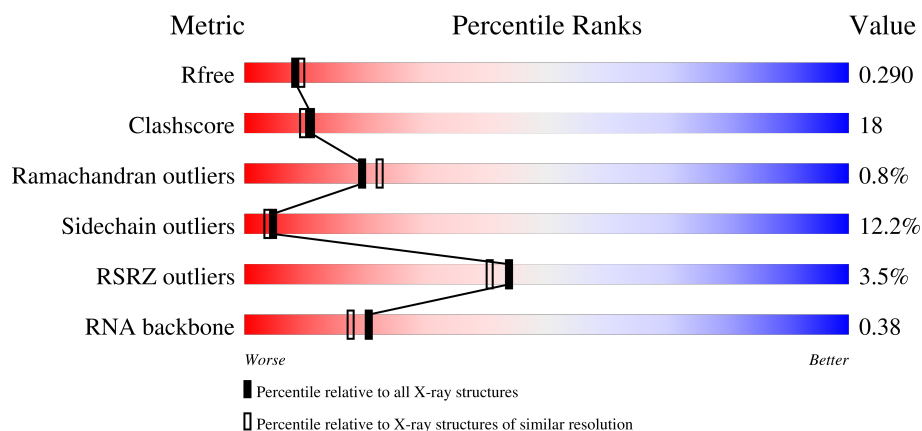
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.43 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))
$R_{free}$	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)
RNA backbone	3102	1062 (2.80-2.08)

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	369	<div> <div>6%</div> <div>62%</div> <div>33%</div> <div>5%</div> </div>
1	B	369	<div> <div>%</div> <div>66%</div> <div>28%</div> <div>6%</div> </div>
2	C	19	<div> <div>5%</div> <div>16%</div> <div>37%</div> <div>32%</div> <div>16%</div> </div>
2	D	19	<div> <div>11%</div> <div>53%</div> <div>32%</div> <div>5%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6982 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called tRNA (uracil-5-)-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	1	0
			2958	1862	520	558	18			
1	B	369	Total	C	N	O	S	0	0	0
			2959	1864	521	556	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P23003
A	-1	SER	-	expression tag	UNP P23003
A	0	HIS	-	expression tag	UNP P23003
A	358	GLN	GLU	engineered mutation	UNP P23003
B	-2	GLY	-	expression tag	UNP P23003
B	-1	SER	-	expression tag	UNP P23003
B	0	HIS	-	expression tag	UNP P23003
B	358	GLN	GLU	engineered mutation	UNP P23003

- Molecule 2 is a RNA chain called RNA (5'-D(P\*GP\*CP\*UP\*GP\*UP\*GP\*(5MU)P\*UP\*C P\*GP\*AP\*UP\*CP\*CP\*AP\*CP\*AP\*GP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	19	Total	C	N	O	P	0	0	0
			402	180	68	135	19			
2	D	19	Total	C	N	O	P	0	0	0
			402	180	68	135	19			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	80	Total	O	0	0
			80	80		

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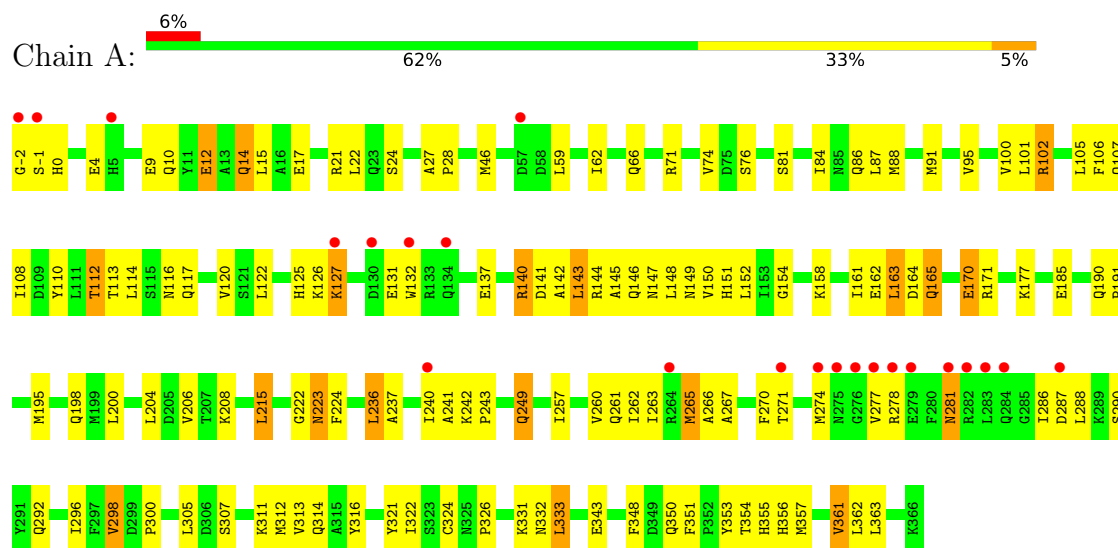
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	137	Total 137	O 137	0	0
3	C	12	Total 12	O 12	0	0
3	D	32	Total 32	O 32	0	0

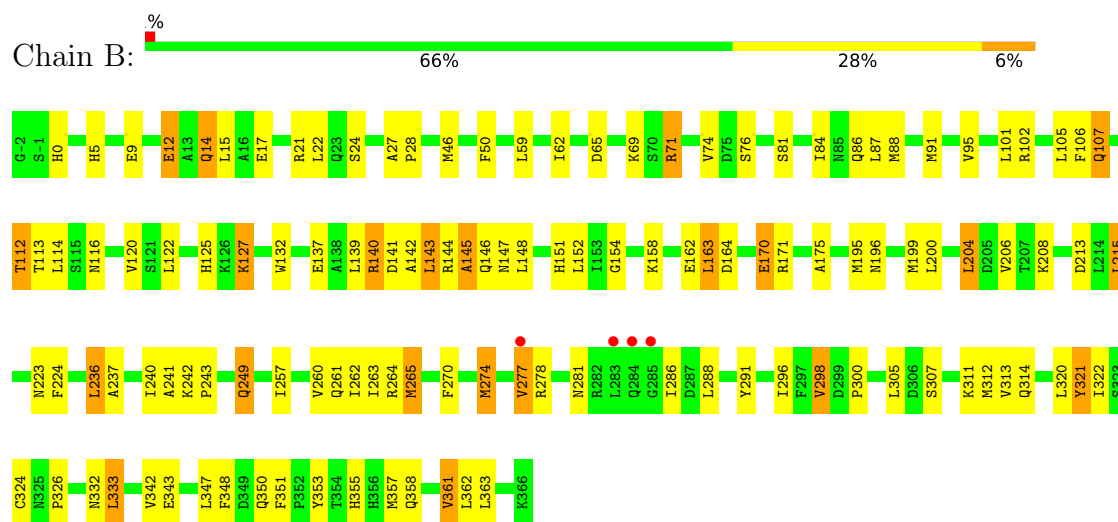
### 3 Residue-property plots [i](#)

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: tRNA (uracil-5-)-methyltransferase

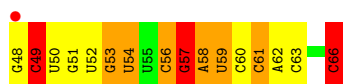


#### • Molecule 1: tRNA (uracil-5-)-methyltransferase



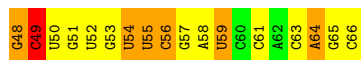
#### • Molecule 2: RNA (5'-D(P\*GP\*CP\*UP\*GP\*UP\*GP\*(5MU)P\*UP\*CP\*GP\*AP\*UP\*CP\*CP\*A P\*CP\*AP\*GP\*C)-3')





● Molecule 2: RNA (5'-D(P\*GP\*CP\*UP\*GP\*UP\*GP\*(5MU)P\*UP\*CP\*GP\*AP\*UP\*CP\*CP\*AP\*CP\*AP\*GP\*C)-3')

Chain D: 11% 53% 32% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	184.41Å 70.13Å 107.95Å 90.00° 120.88° 90.00°	Depositor
Resolution (Å)	35.07 – 2.43 35.07 – 2.43	Depositor EDS
% Data completeness (in resolution range)	93.6 (35.07-2.43) 93.6 (35.07-2.43)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.225 , 0.286 0.227 , 0.290	Depositor DCC
$R_{free}$ test set	3230 reflections (7.69%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.1	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 57.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6982	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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: 5MU

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	0.77	0/3023	0.82	0/4098
1	B	0.77	0/3018	0.83	0/4090
2	C	1.46	2/424 (0.5%)	2.33	33/658 (5.0%)
2	D	1.80	9/424 (2.1%)	2.50	31/658 (4.7%)
All	All	0.92	11/6889 (0.2%)	1.18	64/9504 (0.7%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	53	G	P-O5'	8.13	1.67	1.59
2	D	58	A	N7-C5	-7.11	1.34	1.39
2	D	55	U	P-O5'	6.98	1.66	1.59
2	D	57	G	C5-C4	-6.65	1.33	1.38
2	C	49	C	C1'-N1	6.24	1.58	1.48
2	C	61	C	N3-C4	-6.19	1.29	1.33
2	D	53	G	N3-C4	-5.88	1.31	1.35
2	D	61	C	O3'-P	-5.79	1.54	1.61
2	D	57	G	C2-N3	5.29	1.36	1.32
2	D	52	U	N3-C4	5.16	1.43	1.38
2	D	63	C	C4-C5	5.01	1.47	1.43

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	57	G	C5-C6-O6	-11.94	121.44	128.60
2	D	53	G	N9-C4-C5	9.55	109.22	105.40
2	C	57	G	C3'-C2'-C1'	-9.48	93.91	101.50
2	D	53	G	O4'-C1'-N9	9.02	115.42	108.20
2	D	57	G	C5-C6-N1	8.96	115.98	111.50
2	D	54	5MU	P-O3'-C3'	8.94	130.43	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	48	G	C3'-C2'-C1'	-8.93	94.36	101.50
2	D	53	G	C4-C5-N7	-8.89	107.24	110.80
2	C	61	C	C4-C5-C6	8.75	121.77	117.40
2	D	57	G	C6-N1-C2	-8.63	119.92	125.10
2	D	50	U	C5-C4-O4	-8.21	120.97	125.90
2	D	52	U	N3-C4-O4	7.97	124.98	119.40
2	C	49	C	C6-N1-C2	-7.86	117.16	120.30
2	C	49	C	O5'-P-OP1	7.68	119.91	110.70
2	C	61	C	C5-C6-N1	-7.61	117.20	121.00
2	D	55	U	OP1-P-OP2	7.48	130.81	119.60
2	D	52	U	C5-C4-O4	-7.29	121.53	125.90
2	C	53	G	O4'-C1'-N9	7.17	113.94	108.20
2	C	49	C	N3-C4-N4	6.98	122.89	118.00
2	C	57	G	C4'-C3'-C2'	-6.78	95.82	102.60
2	D	56	C	O5'-P-OP2	-6.72	99.66	105.70
2	D	53	G	C5-N7-C8	6.62	107.61	104.30
2	D	50	U	O4'-C4'-C3'	-6.57	97.43	104.00
2	C	49	C	C2-N1-C1'	6.42	125.86	118.80
2	C	48	G	O3'-P-O5'	-6.39	91.87	104.00
2	C	49	C	O4'-C4'-C3'	-6.37	97.63	104.00
2	C	57	G	N3-C2-N2	6.25	124.27	119.90
2	D	58	A	N1-C6-N6	6.23	122.34	118.60
2	C	52	U	P-O3'-C3'	6.20	127.14	119.70
2	C	61	C	OP1-P-OP2	6.18	128.88	119.60
2	C	59	U	C5-C4-O4	-6.18	122.19	125.90
2	C	58	A	O4'-C1'-N9	5.81	112.84	108.20
2	C	53	G	O5'-P-OP2	-5.80	100.48	105.70
2	D	65	G	C8-N9-C4	-5.71	104.11	106.40
2	D	55	U	OP2-P-O3'	5.70	117.75	105.20
2	C	61	C	C2-N3-C4	-5.66	117.07	119.90
2	C	56	C	OP2-P-O3'	5.62	117.58	105.20
2	C	60	C	C5-C4-N4	-5.59	116.29	120.20
2	C	54	5MU	P-O3'-C3'	5.52	126.32	119.70
2	D	58	A	P-O3'-C3'	5.45	126.24	119.70
2	D	49	C	O4'-C4'-C3'	-5.44	98.56	104.00
2	D	53	G	C8-N9-C4	-5.44	104.22	106.40
2	C	57	G	OP1-P-OP2	-5.40	111.50	119.60
2	D	52	U	N1-C1'-C2'	5.39	121.01	114.00
2	C	49	C	O5'-P-OP2	-5.36	100.88	105.70
2	D	66	C	C5-C4-N4	5.35	123.94	120.20
2	C	51	G	C2-N3-C4	-5.33	109.24	111.90
2	D	53	G	N3-C4-N9	-5.30	122.82	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	64	A	O5'-P-OP2	-5.27	100.95	105.70
2	D	58	A	C4'-C3'-C2'	-5.25	97.35	102.60
2	C	59	U	N3-C4-O4	5.24	123.07	119.40
2	C	57	G	P-O3'-C3'	5.23	125.98	119.70
2	C	49	C	N3-C4-C5	-5.22	119.81	121.90
2	D	53	G	C5'-C4'-C3'	-5.22	107.65	116.00
2	C	56	C	C4'-C3'-C2'	-5.21	97.39	102.60
2	C	61	C	C5-C4-N4	5.20	123.84	120.20
2	D	49	C	C2-N3-C4	5.20	122.50	119.90
2	D	55	U	N3-C4-O4	5.17	123.02	119.40
2	D	57	G	N7-C8-N9	-5.09	110.56	113.10
2	C	50	U	O4'-C1'-N1	5.09	112.27	108.20
2	C	66	C	C3'-C2'-C1'	5.09	105.57	101.50
2	C	61	C	N3-C2-O2	-5.05	118.37	121.90
2	D	63	C	OP2-P-O3'	5.00	116.21	105.20
2	D	48	G	N9-C1'-C2'	5.00	120.50	114.00

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	2958	0	2906	121	1
1	B	2959	0	2918	95	0
2	C	402	0	207	16	0
2	D	402	0	206	7	0
3	A	80	0	0	9	2
3	B	137	0	0	8	1
3	C	12	0	0	1	0
3	D	32	0	0	2	0
All	All	6982	0	6237	232	2

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 18.

All (232) 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:B:163:LEU:HD12	1:B:164:ASP:N	1.55	1.21
1:B:163:LEU:CD1	1:B:164:ASP:N	2.13	1.11
1:A:296:ILE:HD13	1:A:313:VAL:HG12	1.23	1.08
1:B:296:ILE:HD13	1:B:313:VAL:HG12	1.36	1.06
1:A:163:LEU:HD12	1:A:164:ASP:H	1.01	1.05
1:A:163:LEU:HD12	1:A:164:ASP:N	1.76	1.00
1:B:163:LEU:HD12	1:B:164:ASP:H	0.87	1.00
1:B:5:HIS:HE1	3:B:462:HOH:O	1.45	0.99
1:A:163:LEU:CD1	1:A:164:ASP:N	2.25	0.99
1:A:163:LEU:CD1	1:A:164:ASP:H	1.76	0.96
1:A:117:GLN:HG2	1:A:149:ASN:ND2	1.83	0.93
1:B:206:VAL:HG13	1:B:362:LEU:HD22	1.48	0.93
1:B:163:LEU:CD1	1:B:164:ASP:H	1.72	0.92
1:A:206:VAL:HG13	1:A:362:LEU:HD22	1.51	0.91
1:B:206:VAL:CG1	1:B:362:LEU:HD22	2.01	0.91
1:B:281:ASN:OD1	3:B:507:HOH:O	1.92	0.88
2:C:53:G:H1	2:C:61:C:H5	1.22	0.88
1:A:324:CYS:SG	2:C:54:5MU:H6	1.95	0.86
1:B:213:ASP:O	3:B:465:HOH:O	1.94	0.83
1:A:142:ALA:O	1:A:145:ALA:HB3	1.80	0.81
1:A:66:GLN:NE2	3:A:432:HOH:O	2.06	0.80
1:B:5:HIS:CE1	3:B:462:HOH:O	2.27	0.79
1:A:151:HIS:CD2	1:A:163:LEU:HD11	2.20	0.77
1:A:206:VAL:CG1	1:A:362:LEU:HD22	2.15	0.76
1:B:163:LEU:HD13	1:B:164:ASP:N	2.00	0.75
1:A:86:GLN:NE2	1:A:148:LEU:HD21	2.01	0.75
1:B:151:HIS:HD2	1:B:163:LEU:HD11	1.53	0.74
1:B:152:LEU:H	1:B:163:LEU:HG	1.52	0.74
1:B:151:HIS:CD2	1:B:163:LEU:HD11	2.24	0.73
1:A:163:LEU:HD13	1:A:164:ASP:N	2.02	0.73
1:A:152:LEU:H	1:A:163:LEU:HG	1.52	0.73
1:A:117:GLN:CG	1:A:149:ASN:ND2	2.55	0.70
1:A:95:VAL:HG22	1:A:101:LEU:HB3	1.75	0.69
1:A:151:HIS:HD2	1:A:163:LEU:HD11	1.55	0.69
1:A:-2:GLY:HA3	1:A:355:HIS:CD2	2.28	0.69
1:A:91:MET:CE	1:A:122:LEU:HD21	2.22	0.68
1:A:74:VAL:HG13	1:A:76:SER:O	1.94	0.68
1:A:46:MET:HE3	1:A:112:THR:HG22	1.75	0.68
1:B:249:GLN:HE22	1:B:262:ILE:HB	1.58	0.68
1:A:324:CYS:SG	2:C:54:5MU:C5	2.86	0.67
1:A:257:ILE:CG2	1:A:260:VAL:HG12	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ASP:O	1:A:145:ALA:HB2	1.96	0.65
1:A:240:ILE:HD12	1:A:241:ALA:N	2.11	0.65
2:C:57:G:C8	2:C:57:G:H3'	2.31	0.65
1:A:148:LEU:O	1:A:150:VAL:HG12	1.97	0.65
1:A:113:THR:HG22	1:A:170:GLU:HG2	1.78	0.64
1:A:296:ILE:CD1	1:A:313:VAL:HG12	2.15	0.64
1:A:298:VAL:CG1	1:A:305:LEU:HD21	2.27	0.64
1:A:257:ILE:HG22	1:A:260:VAL:HG12	1.80	0.64
1:B:240:ILE:HD12	1:B:241:ALA:N	2.13	0.64
1:B:95:VAL:HG22	1:B:101:LEU:HB3	1.81	0.63
1:B:257:ILE:CG2	1:B:260:VAL:HG12	2.29	0.63
1:B:265:MET:HE2	1:B:270:PHE:HA	1.80	0.63
1:A:81:SER:OG	1:A:112:THR:HG21	1.97	0.63
1:B:86:GLN:NE2	1:B:148:LEU:HD21	2.13	0.63
1:B:163:LEU:HD13	1:B:164:ASP:CG	2.20	0.63
1:B:274:MET:HE1	3:B:521:HOH:O	1.99	0.63
1:A:249:GLN:HE22	1:A:262:ILE:HB	1.64	0.62
1:B:81:SER:OG	1:B:112:THR:HG21	1.98	0.62
1:A:-1:SER:HA	1:A:356:HIS:NE2	2.15	0.61
1:B:12:GLU:HG3	3:B:454:HOH:O	2.00	0.61
1:A:324:CYS:SG	2:C:54:5MU:N1	2.72	0.61
1:B:264:ARG:HB3	3:B:489:HOH:O	2.00	0.60
1:B:298:VAL:HG11	1:B:305:LEU:HD21	1.82	0.60
1:B:257:ILE:HG22	1:B:260:VAL:HG12	1.84	0.60
1:A:266:ALA:HB3	3:A:407:HOH:O	2.01	0.60
1:B:326:PRO:HG2	1:B:357:MET:CE	2.33	0.59
1:A:14:GLN:HB3	3:A:423:HOH:O	2.03	0.59
1:A:298:VAL:HG11	1:A:305:LEU:HD21	1.84	0.59
1:A:277:VAL:HG22	1:A:278:ARG:H	1.69	0.58
1:B:237:ALA:HB3	1:B:262:ILE:HD13	1.85	0.58
1:B:298:VAL:CG1	1:B:305:LEU:HD21	2.33	0.58
1:B:326:PRO:HG2	1:B:357:MET:HE2	1.84	0.58
1:A:14:GLN:HE21	1:A:353:TYR:HA	1.69	0.58
1:A:144:ARG:C	1:A:146:GLN:H	2.07	0.57
1:B:215:LEU:HD13	1:B:296:ILE:HG13	1.86	0.57
1:B:140:ARG:HD3	1:B:163:LEU:HD22	1.86	0.57
1:A:292:GLN:OE1	3:A:406:HOH:O	2.17	0.57
1:A:326:PRO:HG2	1:A:357:MET:CE	2.35	0.57
1:B:286:ILE:CD1	1:B:288:LEU:HD23	2.34	0.56
1:A:237:ALA:HB3	1:A:262:ILE:HD13	1.87	0.56
1:A:84:ILE:HG22	1:A:88:MET:HE2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:LEU:HD12	1:B:261:GLN:HB3	1.86	0.56
1:B:137:GLU:O	1:B:140:ARG:HG3	2.05	0.55
2:C:53:G:N1	2:C:61:C:H5	1.98	0.55
1:A:86:GLN:HE22	1:A:148:LEU:HD21	1.71	0.55
1:A:91:MET:HE1	1:A:122:LEU:HD21	1.88	0.55
1:A:195:MET:SD	1:A:348:PHE:HB3	2.47	0.55
1:B:286:ILE:HD11	1:B:288:LEU:HD23	1.88	0.55
2:D:48:G:H2'	2:D:49:C:O4'	2.07	0.55
1:B:84:ILE:HG22	1:B:88:MET:CE	2.36	0.55
1:A:236:LEU:HD12	1:A:261:GLN:HB3	1.89	0.55
1:B:74:VAL:HG13	1:B:76:SER:O	2.06	0.55
1:A:151:HIS:HD2	1:A:163:LEU:CD1	2.20	0.54
1:A:-1:SER:O	1:A:66:GLN:NE2	2.41	0.54
1:A:286:ILE:CD1	1:A:288:LEU:HD23	2.37	0.54
1:A:12:GLU:HB2	3:A:398:HOH:O	2.08	0.54
1:A:326:PRO:HG2	1:A:357:MET:HE3	1.90	0.54
1:A:163:LEU:HD13	1:A:164:ASP:CG	2.28	0.54
1:A:144:ARG:C	1:A:146:GLN:N	2.59	0.53
1:B:142:ALA:O	1:B:145:ALA:HB3	2.08	0.53
1:A:140:ARG:HD3	1:A:163:LEU:HD22	1.91	0.53
1:A:286:ILE:HD11	1:A:288:LEU:HD23	1.89	0.53
1:A:117:GLN:CG	1:A:149:ASN:HD22	2.19	0.53
1:A:265:MET:HE2	1:A:270:PHE:HA	1.90	0.53
1:A:144:ARG:O	1:A:146:GLN:N	2.41	0.53
1:B:163:LEU:CD1	1:B:163:LEU:C	2.77	0.53
2:C:66:C:H3'	3:C:145:HOH:O	2.09	0.53
2:C:62:A:H2'	2:C:63:C:H6	1.74	0.53
1:A:84:ILE:HG22	1:A:88:MET:CE	2.39	0.52
1:B:91:MET:CE	1:B:122:LEU:HD21	2.39	0.52
1:B:277:VAL:HG22	1:B:278:ARG:H	1.74	0.52
1:B:311:LYS:HA	1:B:314:GLN:HE21	1.75	0.52
1:B:46:MET:HE3	1:B:112:THR:HG22	1.92	0.52
1:B:50:PHE:O	1:B:107:GLN:HB2	2.10	0.52
1:B:347:LEU:HD12	1:B:358:GLN:O	2.09	0.52
2:C:49:C:OP2	2:C:49:C:C6	2.63	0.52
1:B:120:VAL:HB	1:B:152:LEU:HD23	1.91	0.52
1:A:146:GLN:O	1:A:147:ASN:CB	2.58	0.52
1:A:87:LEU:O	1:A:91:MET:HG2	2.10	0.51
1:B:87:LEU:O	1:B:91:MET:HG2	2.10	0.51
1:B:195:MET:SD	1:B:348:PHE:HB3	2.50	0.51
1:A:120:VAL:HB	1:A:152:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ILE:HD12	1:A:286:ILE:C	2.31	0.50
1:B:84:ILE:HG22	1:B:88:MET:HE2	1.92	0.50
1:A:298:VAL:HG13	1:A:305:LEU:HD21	1.93	0.50
1:B:139:LEU:O	1:B:143:LEU:HD22	2.12	0.50
1:B:249:GLN:NE2	1:B:262:ILE:HB	2.26	0.50
1:B:113:THR:HG22	1:B:170:GLU:HG2	1.93	0.50
2:C:66:C:H2'	2:D:48:G:C4'	2.41	0.50
1:A:263:ILE:HG22	1:A:265:MET:HB2	1.93	0.49
1:B:286:ILE:C	1:B:286:ILE:HD12	2.33	0.49
1:B:296:ILE:CD1	1:B:313:VAL:HG12	2.24	0.49
2:C:49:C:OP2	2:C:49:C:H6	1.95	0.48
1:A:198:GLN:NE2	3:A:383:HOH:O	2.33	0.48
1:A:137:GLU:O	1:A:140:ARG:HG3	2.13	0.48
1:A:-1:SER:HA	1:A:356:HIS:HE2	1.78	0.48
1:A:-2:GLY:HA3	1:A:355:HIS:CG	2.49	0.48
1:A:27:ALA:HB3	1:A:28:PRO:HD3	1.96	0.48
1:B:27:ALA:HB3	1:B:28:PRO:HD3	1.96	0.48
1:B:305:LEU:H	1:B:332:ASN:HD21	1.62	0.48
2:D:55:U:H3'	3:D:70:HOH:O	2.14	0.48
1:A:222:GLY:O	1:A:223:ASN:C	2.52	0.47
1:B:62:ILE:HD12	1:B:71:ARG:HB2	1.95	0.47
1:A:242:LYS:N	1:A:243:PRO:HD2	2.29	0.47
1:A:311:LYS:HA	1:A:314:GLN:HE21	1.80	0.47
1:B:46:MET:CE	1:B:112:THR:HG22	2.44	0.47
1:B:106:PHE:CG	1:B:125:HIS:CE1	3.03	0.47
1:B:291:TYR:OH	3:B:537:HOH:O	2.19	0.47
1:A:257:ILE:HG21	1:A:260:VAL:HG12	1.95	0.46
1:A:161:ILE:N	1:A:161:ILE:HD13	2.30	0.46
1:B:324:CYS:HB3	2:D:54:5MU:C4	2.50	0.46
1:A:249:GLN:NE2	1:A:262:ILE:HB	2.29	0.46
1:A:106:PHE:CG	1:A:125:HIS:CE1	3.03	0.46
1:B:14:GLN:HE21	1:B:353:TYR:HA	1.81	0.46
1:B:132:TRP:CH2	1:B:154:GLY:HA3	2.51	0.46
1:B:151:HIS:HD2	1:B:163:LEU:CD1	2.27	0.46
1:B:350:GLN:HG2	1:B:351:PHE:CE1	2.51	0.46
1:A:286:ILE:HD11	1:A:288:LEU:CD2	2.46	0.45
1:B:21:ARG:NH2	1:B:355:HIS:O	2.49	0.45
1:A:113:THR:CG2	1:A:170:GLU:HG2	2.46	0.45
1:A:21:ARG:NH2	1:A:355:HIS:O	2.49	0.45
1:B:286:ILE:HD11	1:B:288:LEU:CD2	2.46	0.45
1:A:265:MET:CE	1:A:270:PHE:HA	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ASP:O	1:A:290:SER:HB3	2.16	0.45
1:A:95:VAL:HG22	1:A:101:LEU:CB	2.45	0.45
1:B:265:MET:CE	1:B:270:PHE:HA	2.44	0.45
1:A:100:VAL:HG11	1:A:131:GLU:OE2	2.17	0.45
1:B:257:ILE:HG21	1:B:260:VAL:HG12	1.97	0.45
1:A:0:HIS:HB2	1:A:355:HIS:H	1.82	0.45
1:A:74:VAL:HG12	1:A:74:VAL:O	2.16	0.45
1:A:305:LEU:H	1:A:332:ASN:HD21	1.64	0.45
1:A:46:MET:CE	1:A:112:THR:HG22	2.44	0.44
2:C:62:A:H2'	2:C:63:C:C6	2.52	0.44
1:B:263:ILE:HG22	1:B:265:MET:HB2	2.00	0.44
1:B:151:HIS:HA	1:B:163:LEU:HD21	2.00	0.44
1:B:321:TYR:OH	1:B:332:ASN:ND2	2.50	0.44
1:B:298:VAL:HG13	1:B:300:PRO:HD3	1.99	0.44
1:A:224:PHE:CZ	1:A:322:ILE:HD12	2.52	0.44
1:B:140:ARG:HD2	1:B:144:ARG:NH1	2.33	0.44
1:B:206:VAL:HG11	1:B:362:LEU:HB2	2.00	0.44
1:A:-2:GLY:CA	1:A:355:HIS:CD2	3.00	0.43
2:D:59:U:O2	2:D:59:U:C2'	2.66	0.43
1:A:10:GLN:O	1:A:14:GLN:HB2	2.17	0.43
1:A:215:LEU:HD13	1:A:296:ILE:HG13	2.01	0.43
1:B:65:ASP:O	1:B:69:LYS:HA	2.18	0.43
1:B:162:GLU:O	1:B:163:LEU:C	2.54	0.43
1:B:127:LYS:HA	1:B:127:LYS:HE3	2.01	0.43
1:B:224:PHE:CZ	1:B:322:ILE:HD12	2.53	0.43
1:A:95:VAL:O	1:A:102:ARG:HB2	2.19	0.43
1:B:163:LEU:HD13	1:B:164:ASP:CB	2.49	0.43
1:A:151:HIS:CD2	1:A:165:GLN:HG2	2.54	0.43
1:A:242:LYS:N	1:A:243:PRO:CD	2.82	0.43
1:B:91:MET:HE1	1:B:122:LEU:HD21	2.01	0.43
1:B:361:VAL:HG13	1:B:363:LEU:HG	2.01	0.42
1:A:132:TRP:CH2	1:A:154:GLY:HA3	2.54	0.42
1:A:281:ASN:OD1	1:A:281:ASN:N	2.52	0.42
2:C:57:G:C8	2:C:57:G:C3'	3.00	0.42
1:A:326:PRO:HG2	1:A:357:MET:HE2	2.02	0.42
1:B:342:VAL:HA	1:B:363:LEU:HD23	2.01	0.42
2:C:66:C:H2'	2:D:48:G:H4'	2.01	0.42
1:A:102:ARG:NH2	3:A:414:HOH:O	2.53	0.42
1:A:46:MET:HE3	1:A:112:THR:CG2	2.48	0.42
1:B:196:ASN:HA	1:B:199:MET:HE2	2.02	0.42
1:B:320:LEU:HD13	1:B:362:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ARG:HB3	1:A:152:LEU:HD12	2.00	0.42
1:A:146:GLN:O	1:A:147:ASN:HB2	2.20	0.42
1:B:333:LEU:HD12	1:B:333:LEU:HA	1.93	0.42
1:A:108:ILE:HG22	1:A:110:TYR:CE2	2.55	0.42
1:B:141:ASP:O	1:B:145:ALA:HB2	2.20	0.42
1:A:298:VAL:HG13	1:A:300:PRO:HD3	2.02	0.41
1:B:140:ARG:HB3	1:B:152:LEU:HD12	2.01	0.41
1:A:162:GLU:O	1:A:163:LEU:C	2.58	0.41
1:A:333:LEU:HD12	1:A:333:LEU:HA	1.91	0.41
1:B:242:LYS:N	1:B:243:PRO:HD2	2.34	0.41
1:A:62:ILE:HD12	1:A:71:ARG:HG2	2.02	0.41
1:A:215:LEU:HD23	1:A:236:LEU:O	2.20	0.41
1:A:100:VAL:O	1:A:126:LYS:NZ	2.40	0.41
1:A:267:ALA:O	1:A:271:THR:HG22	2.20	0.41
1:A:350:GLN:HG2	1:A:351:PHE:CE1	2.55	0.41
1:A:127:LYS:HE3	1:A:127:LYS:HA	2.02	0.41
1:A:300:PRO:O	2:C:54:5MU:H71	2.20	0.41
1:A:143:LEU:HB3	1:A:150:VAL:HG11	2.02	0.41
1:A:190:GLN:HA	1:A:191:PRO:HD3	1.83	0.41
1:A:177:LYS:NZ	3:A:416:HOH:O	2.54	0.41
1:B:204:LEU:HD12	1:B:204:LEU:HA	1.98	0.40
2:D:64:A:N3	3:D:86:HOH:O	2.37	0.40
1:A:4:GLU:OE2	3:A:445:HOH:O	2.22	0.40
1:A:361:VAL:HG13	1:A:363:LEU:HG	2.02	0.40
1:B:144:ARG:C	1:B:146:GLN:N	2.72	0.40
2:C:61:C:O2	2:C:61:C:O4'	2.39	0.40
1:B:146:GLN:O	1:B:147:ASN:CB	2.68	0.40

All (2) 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)
1:A:316:TYR:OH	3:A:442:HOH:O[4_556]	2.13	0.07
3:A:398:HOH:O	3:B:457:HOH:O[3_545]	2.18	0.02



## 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	368/369 (100%)	350 (95%)	16 (4%)	2 (0%)	29	34
1	B	367/369 (100%)	347 (95%)	16 (4%)	4 (1%)	14	15
All	All	735/738 (100%)	697 (95%)	32 (4%)	6 (1%)	19	22

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	MET
1	B	274	MET
1	A	223	ASN
1	B	175	ALA
1	B	223	ASN
1	B	145	ALA

### 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	321/323 (99%)	281 (88%)	40 (12%)	4	3
1	B	321/323 (99%)	283 (88%)	38 (12%)	5	4
All	All	642/646 (99%)	564 (88%)	78 (12%)	5	4

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLU
1	A	12	GLU
1	A	14	GLN
1	A	15	LEU
1	A	17	GLU
1	A	22	LEU
1	A	24	SER
1	A	59	LEU
1	A	102	ARG
1	A	105	LEU
1	A	107	GLN
1	A	112	THR
1	A	114	LEU
1	A	116	ASN
1	A	127	LYS
1	A	140	ARG
1	A	143	LEU
1	A	158	LYS
1	A	163	LEU
1	A	165	GLN
1	A	170	GLU
1	A	171	ARG
1	A	185	GLU
1	A	200	LEU
1	A	204	LEU
1	A	208	LYS
1	A	215	LEU
1	A	236	LEU
1	A	249	GLN
1	A	265	MET
1	A	281	ASN
1	A	298	VAL
1	A	307	SER
1	A	312	MET
1	A	321	TYR
1	A	331	LYS
1	A	333	LEU
1	A	343	GLU
1	A	354	THR
1	A	361	VAL
1	B	0	HIS
1	B	9	GLU
1	B	12	GLU

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Mol	Chain	Res	Type
1	B	14	GLN
1	B	15	LEU
1	B	17	GLU
1	B	22	LEU
1	B	24	SER
1	B	59	LEU
1	B	71	ARG
1	B	102	ARG
1	B	105	LEU
1	B	107	GLN
1	B	112	THR
1	B	114	LEU
1	B	116	ASN
1	B	127	LYS
1	B	140	ARG
1	B	143	LEU
1	B	158	LYS
1	B	163	LEU
1	B	170	GLU
1	B	171	ARG
1	B	200	LEU
1	B	204	LEU
1	B	208	LYS
1	B	215	LEU
1	B	236	LEU
1	B	249	GLN
1	B	265	MET
1	B	277	VAL
1	B	298	VAL
1	B	307	SER
1	B	312	MET
1	B	321	TYR
1	B	333	LEU
1	B	343	GLU
1	B	361	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	14	GLN
1	A	86	GLN

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Mol	Chain	Res	Type
1	A	146	GLN
1	A	149	ASN
1	A	151	HIS
1	A	196	ASN
1	A	223	ASN
1	A	249	GLN
1	A	275	ASN
1	A	314	GLN
1	A	332	ASN
1	A	355	HIS
1	B	10	GLN
1	B	14	GLN
1	B	86	GLN
1	B	146	GLN
1	B	151	HIS
1	B	196	ASN
1	B	223	ASN
1	B	249	GLN
1	B	314	GLN
1	B	332	ASN
1	B	355	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	18/19 (94%)	6 (33%)	2 (11%)
2	D	18/19 (94%)	4 (22%)	2 (11%)
All	All	36/38 (94%)	10 (27%)	4 (11%)

All (10) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	49	C
2	C	56	C
2	C	57	G
2	C	58	A
2	C	59	U
2	C	66	C
2	D	49	C
2	D	51	G
2	D	56	C

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Mol	Chain	Res	Type
2	D	59	U

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	57	G
2	C	59	U
2	D	49	C
2	D	59	U

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

2 non-standard protein/DNA/RNA residues are 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	5MU	D	54	2,1	15,22,23	1.89	3 (20%)	16,32,35	4.05	8 (50%)
2	5MU	C	54	2,1	15,22,23	2.37	3 (20%)	16,32,35	3.44	5 (31%)

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	5MU	D	54	2,1	-	3/5/25/26	0/2/2/2
2	5MU	C	54	2,1	-	4/5/25/26	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	54	5MU	C6-C5	5.45	1.55	1.40
2	C	54	5MU	O4'-C1'	5.10	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	54	5MU	C6-C5	4.57	1.52	1.40
2	C	54	5MU	C4-N3	3.50	1.39	1.33
2	D	54	5MU	C4-N3	2.97	1.38	1.33
2	D	54	5MU	C4-C5	-2.48	1.36	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	54	5MU	C4-N3-C2	10.16	123.72	115.14
2	D	54	5MU	C5-C6-N1	-9.86	111.57	122.19
2	C	54	5MU	C5-C6-N1	-8.83	112.67	122.19
2	C	54	5MU	C4-N3-C2	8.80	122.57	115.14
2	D	54	5MU	O4'-C4'-C3'	-4.86	95.49	105.11
2	D	54	5MU	C5'-C4'-C3'	-3.38	102.50	115.18
2	C	54	5MU	C5M-C5-C4	-3.37	115.33	121.37
2	D	54	5MU	C5M-C5-C4	-2.61	116.70	121.37
2	C	54	5MU	C2'-C3'-C4'	-2.36	98.05	102.64
2	C	54	5MU	C3'-C2'-C1'	2.33	104.48	100.98
2	D	54	5MU	O4'-C1'-C2'	-2.28	103.59	106.93
2	D	54	5MU	O4'-C4'-C5'	-2.18	102.19	109.37
2	D	54	5MU	C5M-C5-C6	-2.06	114.34	118.68

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	54	5MU	C2'-C1'-N1-C6
2	C	54	5MU	O4'-C1'-N1-C6
2	D	54	5MU	C2'-C1'-N1-C6
2	D	54	5MU	O4'-C1'-N1-C6
2	D	54	5MU	C3'-C4'-C5'-O5'
2	C	54	5MU	C3'-C4'-C5'-O5'
2	C	54	5MU	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	54	5MU	1	0
2	C	54	5MU	4	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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 [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	369/369 (100%)	0.17	22 (5%) 21 18	34, 58, 93, 105	0
1	B	369/369 (100%)	0.07	4 (1%) 80 79	30, 55, 86, 100	0
2	C	18/19 (94%)	-0.48	1 (5%) 24 20	37, 61, 64, 82	0
2	D	18/19 (94%)	-0.86	0 100 100	31, 45, 64, 69	0
All	All	774/776 (99%)	0.09	27 (3%) 44 40	30, 57, 89, 105	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	GLU	6.4
1	A	275	ASN	5.8
1	A	-2	GLY	5.0
1	A	276	GLY	4.0
1	B	277	VAL	4.0
1	A	264	ARG	3.7
1	A	283	LEU	3.4
1	A	277	VAL	3.4
1	A	284	GLN	3.3
1	A	132	TRP	3.3
1	A	-1	SER	2.9
1	A	281	ASN	2.8
1	B	284	GLN	2.6
1	A	278	ARG	2.4
1	A	127	LYS	2.4
1	A	240	ILE	2.4
1	A	271	THR	2.4
1	A	274	MET	2.4
1	B	283	LEU	2.3
1	A	130	ASP	2.3
1	B	285	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	5	HIS	2.2
1	A	282	ARG	2.1
1	A	134	GLN	2.1
1	A	57	ASP	2.1
2	C	48	G	2.1
1	A	287	ASP	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [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	5MU	C	54	21/22	0.97	0.16	30,35,41,44	0
2	5MU	D	54	21/22	0.99	0.15	26,31,36,39	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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.