



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:11 PM GMT

PDB ID : 4KR7  
Title : Crystal structure of a 4-thiouridine synthetase - RNA complex with bound ATP  
Authors : Neumann, P.; Ficner, R.; Lakomek, K.  
Deposited on : 2013-05-16  
Resolution : 3.42 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (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

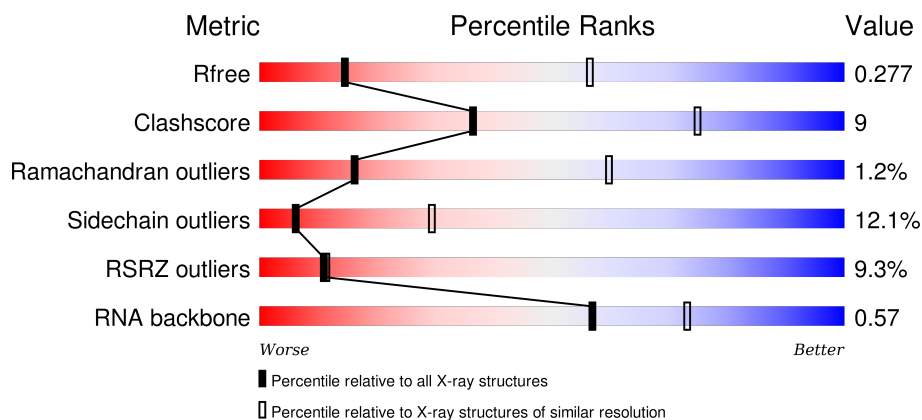
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.42 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	1049 (3.52-3.32)
Clashscore	102246	1032 (3.50-3.34)
Ramachandran outliers	100387	1002 (3.50-3.34)
Sidechain outliers	100360	1003 (3.50-3.34)
RSRZ outliers	91569	1054 (3.52-3.32)
RNA backbone	2183	1042 (4.02-2.80)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	388	<div> <div>2%</div> <div>69%</div> <div>26%</div> <div>• •</div> </div>
1	B	388	<div> <div>7%</div> <div>69%</div> <div>26%</div> <div>5%</div> <div>•</div> </div>
2	M	39	<div> <div>62%</div> <div>38%</div> <div>33%</div> <div>23%</div> <div>5%</div> </div>
2	X	39	<div> <div>59%</div> <div>44%</div> <div>33%</div> <div>13%</div> <div>10%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7924 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 Probable tRNA sulfurtransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	0	0
			3099	1996	530	568	5			
1	B	386	Total	C	N	O	S	0	0	0
			3099	1996	530	568	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLU	LYS	ENGINEERED MUTATION	UNP Q9X220
B	2	GLU	LYS	ENGINEERED MUTATION	UNP Q9X220

- Molecule 2 is a RNA chain called RNA (39-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	39	Total	C	N	O	P	0	0	0
			831	372	153	268	38			
2	X	39	Total	C	N	O	P	0	0	0
			831	372	153	268	38			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

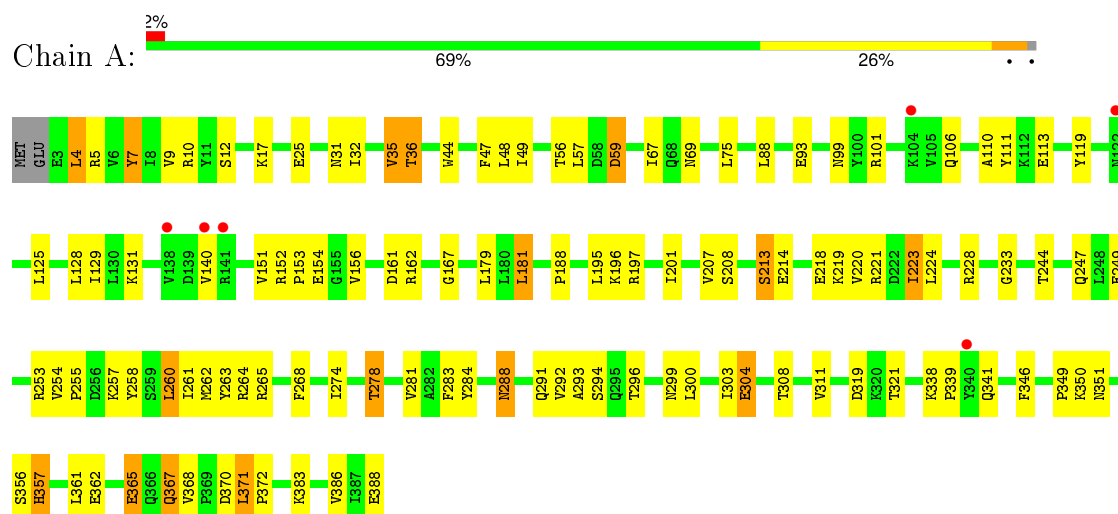
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

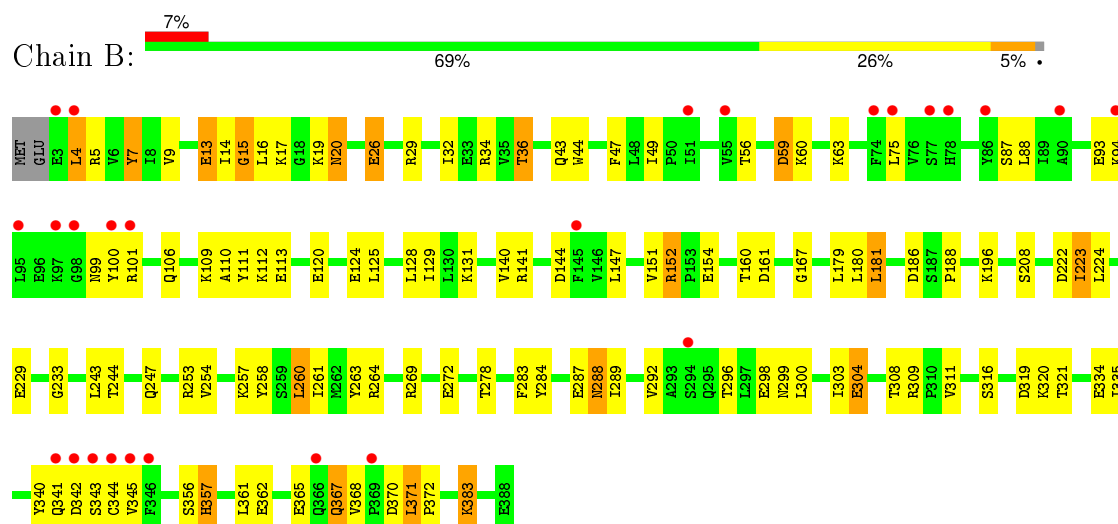
### 3 Residue-property plots

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: Probable tRNA sulfurtransferase

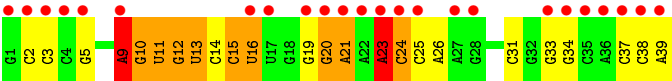


- Molecule 1: Probable tRNA sulfurtransferase

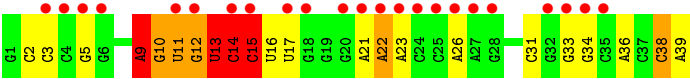


- Molecule 2: RNA (39-MER)





• Molecule 2: RNA (39-MER)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.17Å 113.22Å 133.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.39 – 3.42 48.10 – 3.42	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.39-3.42) 98.0 (48.10-3.42)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.00	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.14 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.230 , 0.274 0.240 , 0.277	Depositor DCC
$R_{free}$ test set	1062 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	98.1	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 81.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 21271 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	7924	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.33	0/3158	0.48	0/4254
1	B	0.33	0/3158	0.49	1/4254 (0.0%)
2	M	0.39	0/929	0.99	3/1447 (0.2%)
2	X	0.37	0/929	1.14	13/1447 (0.9%)
All	All	0.34	0/8174	0.68	17/11402 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	23	A	O4'-C1'-N9	16.46	121.37	108.20
2	X	14	C	C2-N1-C1'	10.88	130.76	118.80
2	X	14	C	C6-N1-C1'	-7.78	111.47	120.80
2	X	13	U	C2-N1-C1'	7.21	126.35	117.70
2	X	13	U	N1-C2-O2	7.17	127.82	122.80
2	X	15	C	C2-N1-C1'	6.68	126.15	118.80
2	X	13	U	N3-C2-O2	-6.67	117.53	122.20
2	X	15	C	N1-C2-O2	6.58	122.84	118.90
2	X	14	C	C6-N1-C2	-6.39	117.74	120.30
2	X	14	C	C5-C6-N1	6.33	124.16	121.00
1	B	181	LEU	CA-CB-CG	6.28	129.75	115.30
2	M	23	A	C1'-O4'-C4'	-6.21	104.93	109.90
2	X	9	A	OP2-P-O3'	5.52	117.34	105.20
2	M	9	A	P-O3'-C3'	5.48	126.27	119.70
2	X	14	C	N1-C2-O2	5.38	122.13	118.90
2	X	9	A	P-O3'-C3'	5.17	125.91	119.70
2	X	15	C	C6-N1-C1'	-5.10	114.68	120.80

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	3099	0	3202	61	1
1	B	3099	0	3202	58	0
2	M	831	0	425	15	0
2	X	831	0	425	17	1
3	A	31	0	12	1	0
3	B	31	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	7924	0	7278	143	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 9.

All (143) 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)
2:X:10:G:H3'	2:X:11:U:H5''	1.62	0.82
1:A:181:LEU:HD11	1:A:220:VAL:HG13	1.63	0.78
1:A:371:LEU:HD23	1:A:372:PRO:HD3	1.68	0.76
1:A:283:PHE:HB2	1:A:311:VAL:HG12	1.65	0.75
1:B:188:PRO:HG3	1:B:223:ILE:HD12	1.67	0.75
2:M:13:U:O2'	2:M:15:C:N3	2.20	0.74
1:B:371:LEU:HD23	1:B:372:PRO:HD3	1.68	0.74
2:X:12:G:H3'	2:X:13:U:C5'	2.17	0.73
1:B:283:PHE:HB2	1:B:311:VAL:HG12	1.72	0.72
1:B:243:LEU:HB3	1:B:247:GLN:HE21	1.54	0.72
1:A:288:ASN:ND2	1:A:291:GLN:OE1	2.22	0.72
1:A:188:PRO:HG3	1:A:223:ILE:HD12	1.72	0.71
1:A:10:ARG:HD2	1:A:69:ASN:HD21	1.53	0.71
1:A:350:LYS:HD3	2:X:12:G:H8	1.57	0.70
1:A:196:LYS:NZ	1:B:319:ASP:OD1	2.24	0.70
1:A:181:LEU:HD13	1:A:223:ILE:HD11	1.75	0.69
2:X:10:G:H3'	2:X:11:U:C5'	2.22	0.69
2:M:3:C:H42	2:M:33:G:H1	1.37	0.68
1:A:319:ASP:OD1	1:B:196:LYS:NZ	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:9:A:O4'	2:X:10:G:N2	2.26	0.68
2:X:12:G:H1	2:X:15:C:H41	1.40	0.67
2:X:3:C:H42	2:X:33:G:H1	1.43	0.67
1:B:94:LYS:NZ	1:B:161:ASP:OD1	2.27	0.65
2:M:23:A:O2'	2:M:24:C:O5'	2.09	0.65
1:B:343:SER:H	1:B:345:VAL:HG23	1.62	0.65
1:B:288:ASN:HD21	1:B:320:LYS:NZ	1.95	0.64
1:B:180:LEU:O	3:B:401:ATP:O2'	2.08	0.64
1:A:32:ILE:O	1:A:36:THR:OG1	2.16	0.63
1:B:88:LEU:HD21	1:B:128:LEU:HG	1.79	0.63
1:A:288:ASN:N	1:A:288:ASN:OD1	2.32	0.63
1:A:195:LEU:HD21	1:A:201:ILE:HG12	1.81	0.62
1:B:356:SER:OG	1:B:357:HIS:N	2.33	0.61
1:B:288:ASN:N	1:B:288:ASN:OD1	2.33	0.61
1:B:9:VAL:HB	1:B:47:PHE:HB2	1.83	0.61
1:A:257:LYS:HG3	1:A:258:TYR:HD1	1.66	0.61
1:A:356:SER:OG	1:A:357:HIS:N	2.33	0.60
1:B:32:ILE:O	1:B:36:THR:OG1	2.18	0.60
1:B:186:ASP:OD1	1:B:320:LYS:NZ	2.35	0.59
1:A:265:ARG:NH2	1:A:365:GLU:OE2	2.36	0.59
1:A:338:LYS:N	1:A:339:PRO:HD2	2.19	0.57
1:A:350:LYS:HD3	2:X:12:G:C8	2.37	0.57
1:A:88:LEU:HD21	1:A:128:LEU:HG	1.86	0.57
1:B:288:ASN:HD21	1:B:320:LYS:HZ3	1.53	0.56
1:B:59:ASP:OD2	1:B:59:ASP:N	2.36	0.56
1:A:257:LYS:HE2	1:A:258:TYR:HE1	1.70	0.56
2:X:13:U:H2'	2:X:13:U:O2	2.05	0.56
1:A:257:LYS:HG3	1:A:258:TYR:CD1	2.42	0.55
1:B:14:ILE:HG23	1:B:15:GLY:H	1.72	0.54
1:A:218:GLU:OE2	1:A:221:ARG:NH1	2.41	0.54
1:B:264:ARG:NH2	1:B:287:GLU:OE1	2.40	0.54
1:B:63:LYS:HD2	1:B:229:GLU:HB3	1.89	0.54
1:B:88:LEU:HD23	1:B:129:ILE:HD13	1.90	0.53
1:A:264:ARG:NH2	3:A:401:ATP:O2A	2.38	0.53
2:X:14:C:H4'	2:X:15:C:C2	2.44	0.52
2:X:10:G:C8	2:X:11:U:H5''	2.44	0.52
1:A:293:ALA:HB2	1:B:19:LYS:HD2	1.92	0.52
1:A:59:ASP:OD2	1:A:59:ASP:N	2.42	0.51
1:B:370:ASP:N	1:B:370:ASP:OD1	2.34	0.51
1:A:197:ARG:HB3	1:B:289:ILE:O	2.11	0.51
1:B:26:GLU:OE1	1:B:29:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:9:A:H4'	2:M:10:G:O4'	2.10	0.51
1:A:9:VAL:HB	1:A:47:PHE:HB2	1.93	0.50
1:B:257:LYS:HG3	1:B:258:TYR:HD1	1.77	0.50
1:B:111:TYR:CE2	1:B:113:GLU:HB3	2.47	0.50
1:B:208:SER:OG	1:B:247:GLN:NE2	2.45	0.49
2:M:15:C:H3'	2:M:16:U:C5'	2.41	0.49
1:B:257:LYS:HE2	1:B:258:TYR:HE1	1.77	0.49
1:A:370:ASP:OD1	1:A:370:ASP:N	2.36	0.49
2:X:5:G:H1	2:X:31:C:H42	1.60	0.49
2:X:12:G:H3'	2:X:13:U:H5'	1.95	0.49
1:A:213:SER:HB2	1:A:341:GLN:HB3	1.94	0.49
2:M:25:C:H2'	2:M:26:A:C8	2.48	0.49
1:B:299:ASN:O	1:B:303:ILE:HG13	2.12	0.49
1:A:111:TYR:HD1	1:A:153:PRO:HD3	1.78	0.49
1:A:299:ASN:O	1:A:303:ILE:HG13	2.13	0.49
1:A:228:ARG:NH1	1:A:233:GLY:O	2.45	0.49
1:A:274:ILE:O	1:A:278:THR:OG1	2.25	0.48
1:B:257:LYS:HG3	1:B:258:TYR:CD1	2.48	0.48
1:A:386:VAL:HG12	1:A:388:GLU:HG2	1.96	0.48
1:A:7:TYR:HB2	1:A:49:ILE:HB	1.95	0.48
2:X:14:C:H4'	2:X:15:C:N3	2.29	0.47
2:M:5:G:H1	2:M:31:C:H42	1.61	0.47
1:A:110:ALA:HB3	1:A:152:ARG:HA	1.96	0.47
1:A:253:ARG:HB3	1:A:367:GLN:HB3	1.97	0.47
1:A:44:TRP:CZ3	1:A:48:LEU:HD11	2.49	0.47
1:B:7:TYR:HB2	1:B:49:ILE:HB	1.97	0.47
1:A:125:LEU:O	1:A:129:ILE:HG12	2.15	0.47
1:B:179:LEU:HD12	1:B:284:TYR:O	2.15	0.47
1:B:13:GLU:H	1:B:13:GLU:HG2	1.35	0.46
1:B:125:LEU:O	1:B:129:ILE:HG12	2.16	0.46
1:A:4:LEU:HD12	1:A:75:LEU:HB3	1.98	0.46
2:M:12:G:O2'	2:M:13:U:P	2.74	0.46
2:X:12:G:H1	2:X:15:C:N4	2.12	0.45
1:B:60:LYS:H	1:B:60:LYS:HD2	1.81	0.45
1:B:222:ASP:HB3	1:B:335:ILE:HD13	1.97	0.45
1:B:341:GLN:HG3	1:B:342:ASP:N	2.31	0.45
1:B:253:ARG:HB3	1:B:367:GLN:HB3	1.98	0.45
1:B:272:GLU:HG3	1:B:309:ARG:HD2	1.97	0.45
1:B:87:SER:HB3	1:B:147:LEU:HD21	1.99	0.45
1:B:304:GLU:HG3	1:B:304:GLU:O	2.17	0.45
1:A:5:ARG:HH22	1:A:93:GLU:CD	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LEU:HB2	1:A:349:PRO:HG3	1.98	0.44
2:M:10:G:H2'	2:M:11:U:H5'	2.00	0.44
2:M:19:G:H1	2:M:24:C:H42	1.65	0.44
1:B:109:LYS:HA	1:B:151:VAL:HG13	2.00	0.44
1:B:110:ALA:HB3	1:B:152:ARG:HG3	1.99	0.43
1:B:261:ILE:HB	1:B:361:LEU:HD21	1.99	0.43
1:B:224:LEU:HA	1:B:224:LEU:HD12	1.82	0.43
1:A:88:LEU:HD23	1:A:129:ILE:HD13	2.01	0.43
1:A:179:LEU:HD12	1:A:284:TYR:O	2.18	0.43
1:A:208:SER:OG	1:A:247:GLN:OE1	2.37	0.43
1:A:304:GLU:O	1:A:304:GLU:HG3	2.17	0.43
1:B:383:LYS:HB2	1:B:383:LYS:HE3	1.81	0.43
1:A:224:LEU:HA	1:A:224:LEU:HD12	1.81	0.43
1:B:100:TYR:HB3	1:B:144:ASP:HB3	2.01	0.42
1:B:4:LEU:HD12	1:B:75:LEU:HB3	2.01	0.42
2:X:2:C:H42	2:X:34:G:H1	1.65	0.42
1:A:268:PHE:CD2	1:A:303:ILE:HG22	2.54	0.42
1:B:5:ARG:HH22	1:B:93:GLU:CD	2.23	0.42
1:A:260:LEU:HA	1:A:263:TYR:CD2	2.55	0.42
1:A:281:VAL:HG11	1:B:298:GLU:HG2	2.01	0.42
2:M:20:G:H1	2:M:21:A:HO2'	1.61	0.42
1:A:151:VAL:HG13	1:A:156:VAL:HG22	2.02	0.42
2:M:20:G:C2	2:M:21:A:H4'	2.54	0.42
1:B:260:LEU:HA	1:B:263:TYR:CD2	2.55	0.42
1:A:161:ASP:OD2	1:A:161:ASP:N	2.52	0.42
2:M:2:C:H42	2:M:34:G:H1	1.68	0.41
2:M:19:G:H1	2:M:24:C:N4	2.18	0.41
1:A:36:THR:HG21	1:A:57:LEU:HD13	2.03	0.41
1:B:34:ARG:HD2	1:B:233:GLY:HA3	2.02	0.41
1:A:262:MET:SD	1:A:361:LEU:HD23	2.60	0.41
1:B:43:GLN:HG2	1:B:44:TRP:CD2	2.56	0.41
1:A:31:ASN:O	1:A:35:VAL:HG13	2.21	0.41
2:X:22:A:H2'	2:X:22:A:N3	2.36	0.41
1:B:120:GLU:O	1:B:124:GLU:HG3	2.21	0.41
1:B:269:ARG:NH2	1:B:365:GLU:OE1	2.49	0.41
1:A:219:LYS:HD2	1:A:339:PRO:HB3	2.02	0.41
1:A:261:ILE:HB	1:A:361:LEU:HD21	2.03	0.41
1:A:249:GLU:O	1:A:253:ARG:HD3	2.21	0.40
1:A:5:ARG:NH2	1:A:93:GLU:OE2	2.54	0.40
1:B:264:ARG:HH22	1:B:287:GLU:CD	2.24	0.40
1:A:9:VAL:HG13	1:A:67:ILE:HG23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:TYR:CE2	2:M:37:C:H4'	2.56	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)
1:A:350:LYS:NZ	2:X:38:C:O2'[3_544]	2.08	0.12

## 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	384/388 (99%)	362 (94%)	17 (4%)	5 (1%)	15	58
1	B	384/388 (99%)	362 (94%)	18 (5%)	4 (1%)	19	64
All	All	768/776 (99%)	724 (94%)	35 (5%)	9 (1%)	16	60

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	GLU
1	A	346	PHE
1	A	12	SER
1	B	17	LYS
1	A	167	GLY
1	B	15	GLY
1	B	20	ASN
1	B	167	GLY
1	A	255	PRO

### 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	340/342 (99%)	300 (88%)	40 (12%)	6	30
1	B	340/342 (99%)	298 (88%)	42 (12%)	6	28
All	All	680/684 (99%)	598 (88%)	82 (12%)	6	29

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	7	TYR
1	A	17	LYS
1	A	25	GLU
1	A	35	VAL
1	A	36	THR
1	A	56	THR
1	A	59	ASP
1	A	99	ASN
1	A	101	ARG
1	A	106	GLN
1	A	113	GLU
1	A	131	LYS
1	A	140	VAL
1	A	154	GLU
1	A	162	ARG
1	A	181	LEU
1	A	207	VAL
1	A	213	SER
1	A	223	ILE
1	A	244	THR
1	A	254	VAL
1	A	260	LEU
1	A	278	THR
1	A	288	ASN
1	A	292	VAL
1	A	294	SER

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Mol	Chain	Res	Type
1	A	296	THR
1	A	300	LEU
1	A	304	GLU
1	A	308	THR
1	A	321	THR
1	A	351	ASN
1	A	357	HIS
1	A	362	GLU
1	A	365	GLU
1	A	367	GLN
1	A	368	VAL
1	A	371	LEU
1	A	383	LYS
1	B	4	LEU
1	B	7	TYR
1	B	13	GLU
1	B	16	LEU
1	B	20	ASN
1	B	26	GLU
1	B	36	THR
1	B	56	THR
1	B	59	ASP
1	B	99	ASN
1	B	101	ARG
1	B	106	GLN
1	B	112	LYS
1	B	131	LYS
1	B	140	VAL
1	B	141	ARG
1	B	152	ARG
1	B	154	GLU
1	B	160	THR
1	B	181	LEU
1	B	223	ILE
1	B	244	THR
1	B	254	VAL
1	B	260	LEU
1	B	278	THR
1	B	288	ASN
1	B	292	VAL
1	B	296	THR
1	B	300	LEU

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Mol	Chain	Res	Type
1	B	304	GLU
1	B	308	THR
1	B	316	SER
1	B	321	THR
1	B	334	GLU
1	B	340	TYR
1	B	344	CYS
1	B	357	HIS
1	B	362	GLU
1	B	367	GLN
1	B	368	VAL
1	B	371	LEU
1	B	383	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	247	GLN
1	B	288	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	M	38/39 (97%)	13 (34%)	3 (7%)
2	X	38/39 (97%)	15 (39%)	4 (10%)
All	All	76/78 (97%)	28 (36%)	7 (9%)

All (28) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	M	9	A
2	M	10	G
2	M	11	U
2	M	12	G
2	M	13	U
2	M	14	C
2	M	15	C
2	M	16	U
2	M	20	G
2	M	21	A

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Mol	Chain	Res	Type
2	M	23	A
2	M	24	C
2	M	39	A
2	X	9	A
2	X	10	G
2	X	11	U
2	X	12	G
2	X	13	U
2	X	14	C
2	X	15	C
2	X	16	U
2	X	17	U
2	X	21	A
2	X	22	A
2	X	23	A
2	X	26	A
2	X	36	A
2	X	39	A

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	M	9	A
2	M	12	G
2	M	38	C
2	X	9	A
2	X	13	U
2	X	21	A
2	X	38	C

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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$
3	ATP	A	401	4	24,33,33	0.94	1 (4%)	31,52,52	2.21	5 (16%)
3	ATP	B	401	4	24,33,33	0.93	1 (4%)	31,52,52	1.94	5 (16%)

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
3	ATP	A	401	4	-	0/18/38/38	0/3/3/3
3	ATP	B	401	4	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	ATP	C5-C4	2.97	1.47	1.40
3	B	401	ATP	C5-C4	3.03	1.47	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	ATP	N3-C2-N1	-7.21	123.37	128.89
3	A	401	ATP	C2'-C1'-N9	-7.13	103.40	114.29
3	B	401	ATP	N3-C2-N1	-6.26	124.10	128.89
3	B	401	ATP	C2'-C1'-N9	-5.31	106.18	114.29
3	B	401	ATP	PA-O3A-PB	-3.68	122.39	132.73
3	A	401	ATP	C4-C5-N7	-3.10	106.63	109.48
3	B	401	ATP	C4-C5-N7	-2.96	106.76	109.48
3	A	401	ATP	PA-O3A-PB	-2.90	124.59	132.73
3	A	401	ATP	C2-N1-C6	2.00	122.34	118.77
3	B	401	ATP	C4'-O4'-C1'	2.17	112.10	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	ATP	1	0
3	B	401	ATP	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	386/388 (99%)	0.31	6 (1%) 74 69	42, 83, 141, 195	0
1	B	386/388 (99%)	0.49	26 (6%) 21 19	43, 87, 143, 198	0
2	M	39/39 (100%)	2.60	24 (61%) 0 0	79, 120, 216, 257	0
2	X	39/39 (100%)	2.42	23 (58%) 0 0	106, 152, 223, 229	0
All	All	850/854 (99%)	0.59	79 (9%) 11 11	42, 88, 157, 257	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	22	A	10.4
2	M	21	A	7.7
2	X	22	A	5.7
1	B	97	LYS	5.1
2	X	5	G	5.0
2	M	23	A	4.7
1	B	94	LYS	4.2
2	M	3	C	4.2
2	X	32	G	4.1
1	B	3	GLU	4.1
2	X	27	A	3.8
2	X	23	A	3.8
2	X	26	A	3.8
1	B	4	LEU	3.7
2	X	3	C	3.7
2	M	39	A	3.6
1	B	90	ALA	3.6
2	M	38	C	3.6
2	M	34	G	3.6
2	X	4	C	3.5
2	X	34	G	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	341	GLN	3.4
1	B	77	SER	3.3
2	X	12	G	3.3
2	X	21	A	3.3
2	M	37	C	3.2
1	B	345	VAL	3.2
2	X	25	C	3.2
1	B	98	GLY	3.2
2	X	33	G	3.2
1	A	141	ARG	3.2
1	B	346	PHE	3.1
2	M	20	G	3.1
2	M	36	A	3.1
2	X	15	C	3.1
1	A	340	TYR	3.1
1	A	140	VAL	3.1
2	M	35	C	3.0
2	X	14	C	3.0
1	B	342	ASP	2.9
2	M	28	G	2.9
1	B	369	PRO	2.8
2	X	6	G	2.8
2	M	17	U	2.8
1	B	100	TYR	2.7
2	X	11	U	2.7
1	A	104	LYS	2.7
2	M	5	G	2.6
2	M	33	G	2.6
2	X	35	C	2.6
1	B	95	LEU	2.6
1	B	86	TYR	2.6
1	B	75	LEU	2.5
2	M	2	C	2.5
2	X	24	C	2.5
2	X	18	G	2.5
1	B	101	ARG	2.5
2	M	16	U	2.5
1	B	145	PHE	2.5
2	X	20	G	2.5
2	M	4	C	2.4
2	M	19	G	2.4
2	X	28	G	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	343	SER	2.4
1	B	74	PHE	2.4
2	M	25	C	2.3
2	M	1	G	2.3
1	B	344	CYS	2.3
1	B	55	VAL	2.2
2	M	9	A	2.2
1	B	294	SER	2.2
2	M	27	A	2.2
1	B	366	GLN	2.1
1	A	122	ASN	2.1
2	X	17	U	2.1
1	A	138	VAL	2.1
1	B	78	HIS	2.1
1	B	51	ILE	2.0
2	M	24	C	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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ATP	B	401	31/31	0.93	0.31	0.30	85,88,90,92	0
3	ATP	A	401	31/31	0.93	0.26	0.02	99,102,106,107	0
4	MG	B	402	1/1	0.42	1.37	-	65,65,65,65	0
4	MG	A	402	1/1	0.83	0.58	-	71,71,71,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.