



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 14, 2016 – 06:08 PM EDT

PDB ID : 4U8T  
Title : Crystal structure of YTH domain of Zygosaccharomyces rouxii MRB1 protein  
in complex with N6-Methyladenosine RNA  
Authors : Luo, S.; Tong, L.  
Deposited on : 2014-08-04  
Resolution : 2.70 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027790  
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) : rb-20027790

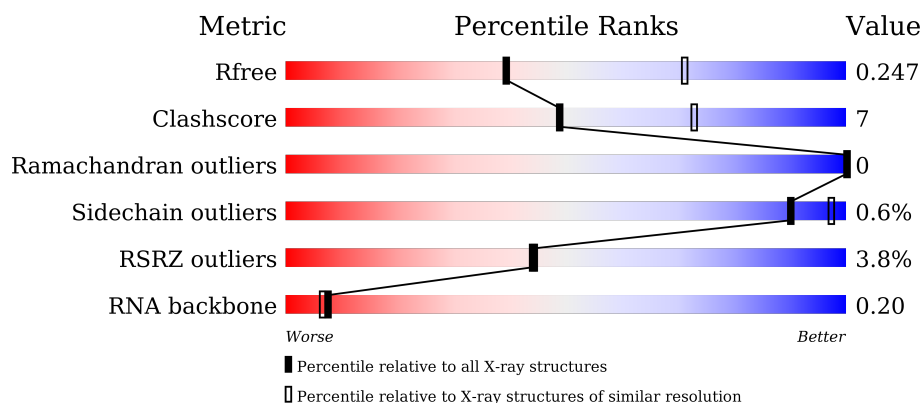
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)
RNA backbone	2183	1069 (3.10-2.30)

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	177	<div> <div>3%</div> <div>76% 12% 11%</div> </div>
1	B	177	<div> <div>2%</div> <div>76% 11% 13%</div> </div>
1	C	177	<div> <div>4%</div> <div>73% 14% 12%</div> </div>
1	D	177	<div> <div>2%</div> <div>76% 13% 11%</div> </div>

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Mol	Chain	Length	Quality of chain
1	E	177	<div><div></div><div>2%</div><div>73%</div><div>13%</div><div>14%</div></div>
1	F	177	<div><div></div><div>5%</div><div>72%</div><div>15%</div><div>14%</div></div>
2	O	7	<div><div></div><div>86%</div><div>14%</div></div>
2	P	7	<div><div></div><div>14%</div><div>57%</div><div>14%</div><div>14%</div><div>14%</div></div>
2	Q	7	<div><div></div><div>43%</div><div>29%</div><div>14%</div><div>14%</div></div>
2	R	7	<div><div></div><div>14%</div><div>14%</div><div>57%</div><div>29%</div></div>
2	S	7	<div><div></div><div>14%</div><div>43%</div><div>43%</div><div>14%</div></div>
2	T	7	<div><div></div><div>71%</div><div>14%</div><div>14%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8572 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 ZYRO0G01672p.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	Se	0	0	0
			1278	823	223	229	1	2			
1	B	154	Total	C	N	O	S	Se	0	0	0
			1253	810	217	223	1	2			
1	C	155	Total	C	N	O	S	Se	0	0	0
			1262	815	221	223	1	2			
1	D	157	Total	C	N	O	S	Se	0	0	0
			1278	824	221	230	1	2			
1	E	153	Total	C	N	O	S	Se	0	0	0
			1245	806	216	220	1	2			
1	F	153	Total	C	N	O	S	Se	0	0	0
			1245	806	216	220	1	2			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	MSE	-	initiating methionine	UNP C5E1V0
A	154	GLY	-	expression tag	UNP C5E1V0
A	155	SER	-	expression tag	UNP C5E1V0
A	156	SER	-	expression tag	UNP C5E1V0
A	157	HIS	-	expression tag	UNP C5E1V0
A	158	HIS	-	expression tag	UNP C5E1V0
A	159	HIS	-	expression tag	UNP C5E1V0
A	160	HIS	-	expression tag	UNP C5E1V0
A	161	HIS	-	expression tag	UNP C5E1V0
A	162	HIS	-	expression tag	UNP C5E1V0
A	163	SER	-	expression tag	UNP C5E1V0
A	164	SER	-	expression tag	UNP C5E1V0
A	165	GLY	-	expression tag	UNP C5E1V0
B	153	MSE	-	initiating methionine	UNP C5E1V0
B	154	GLY	-	expression tag	UNP C5E1V0
B	155	SER	-	expression tag	UNP C5E1V0
B	156	SER	-	expression tag	UNP C5E1V0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	157	HIS	-	expression tag	UNP C5E1V0
B	158	HIS	-	expression tag	UNP C5E1V0
B	159	HIS	-	expression tag	UNP C5E1V0
B	160	HIS	-	expression tag	UNP C5E1V0
B	161	HIS	-	expression tag	UNP C5E1V0
B	162	HIS	-	expression tag	UNP C5E1V0
B	163	SER	-	expression tag	UNP C5E1V0
B	164	SER	-	expression tag	UNP C5E1V0
B	165	GLY	-	expression tag	UNP C5E1V0
C	153	MSE	-	initiating methionine	UNP C5E1V0
C	154	GLY	-	expression tag	UNP C5E1V0
C	155	SER	-	expression tag	UNP C5E1V0
C	156	SER	-	expression tag	UNP C5E1V0
C	157	HIS	-	expression tag	UNP C5E1V0
C	158	HIS	-	expression tag	UNP C5E1V0
C	159	HIS	-	expression tag	UNP C5E1V0
C	160	HIS	-	expression tag	UNP C5E1V0
C	161	HIS	-	expression tag	UNP C5E1V0
C	162	HIS	-	expression tag	UNP C5E1V0
C	163	SER	-	expression tag	UNP C5E1V0
C	164	SER	-	expression tag	UNP C5E1V0
C	165	GLY	-	expression tag	UNP C5E1V0
D	153	MSE	-	initiating methionine	UNP C5E1V0
D	154	GLY	-	expression tag	UNP C5E1V0
D	155	SER	-	expression tag	UNP C5E1V0
D	156	SER	-	expression tag	UNP C5E1V0
D	157	HIS	-	expression tag	UNP C5E1V0
D	158	HIS	-	expression tag	UNP C5E1V0
D	159	HIS	-	expression tag	UNP C5E1V0
D	160	HIS	-	expression tag	UNP C5E1V0
D	161	HIS	-	expression tag	UNP C5E1V0
D	162	HIS	-	expression tag	UNP C5E1V0
D	163	SER	-	expression tag	UNP C5E1V0
D	164	SER	-	expression tag	UNP C5E1V0
D	165	GLY	-	expression tag	UNP C5E1V0
E	153	MSE	-	initiating methionine	UNP C5E1V0
E	154	GLY	-	expression tag	UNP C5E1V0
E	155	SER	-	expression tag	UNP C5E1V0
E	156	SER	-	expression tag	UNP C5E1V0
E	157	HIS	-	expression tag	UNP C5E1V0
E	158	HIS	-	expression tag	UNP C5E1V0
E	159	HIS	-	expression tag	UNP C5E1V0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	160	HIS	-	expression tag	UNP C5E1V0
E	161	HIS	-	expression tag	UNP C5E1V0
E	162	HIS	-	expression tag	UNP C5E1V0
E	163	SER	-	expression tag	UNP C5E1V0
E	164	SER	-	expression tag	UNP C5E1V0
E	165	GLY	-	expression tag	UNP C5E1V0
F	153	MSE	-	initiating methionine	UNP C5E1V0
F	154	GLY	-	expression tag	UNP C5E1V0
F	155	SER	-	expression tag	UNP C5E1V0
F	156	SER	-	expression tag	UNP C5E1V0
F	157	HIS	-	expression tag	UNP C5E1V0
F	158	HIS	-	expression tag	UNP C5E1V0
F	159	HIS	-	expression tag	UNP C5E1V0
F	160	HIS	-	expression tag	UNP C5E1V0
F	161	HIS	-	expression tag	UNP C5E1V0
F	162	HIS	-	expression tag	UNP C5E1V0
F	163	SER	-	expression tag	UNP C5E1V0
F	164	SER	-	expression tag	UNP C5E1V0
F	165	GLY	-	expression tag	UNP C5E1V0

- Molecule 2 is a RNA chain called RNA (5'-R(\*AP\*GP\*GP\*(6MZ)P\*CP\*AP\*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	7	Total	C	N	O	P	0	0	0
			150	69	30	45	6			
2	P	7	Total	C	N	O	P	0	0	0
			150	69	30	45	6			
2	Q	7	Total	C	N	O	P	0	0	0
			150	69	30	45	6			
2	R	7	Total	C	N	O	P	0	0	0
			150	69	30	45	6			
2	S	7	Total	C	N	O	P	0	0	0
			150	69	30	45	6			
2	T	7	Total	C	N	O	P	0	0	0
			150	69	30	45	6			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total	O	0	0
			21	21		
3	B	10	Total	O	0	0
			10	10		

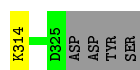
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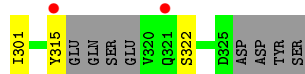
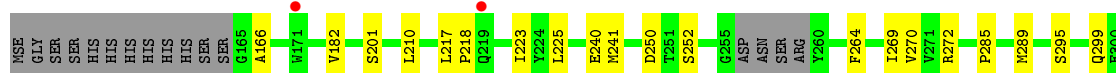
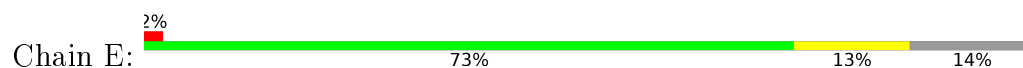
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	10	Total 10	O 10	0	0
3	D	16	Total 16	O 16	0	0
3	E	10	Total 10	O 10	0	0
3	F	15	Total 15	O 15	0	0
3	O	5	Total 5	O 5	0	0
3	P	4	Total 4	O 4	0	0
3	Q	6	Total 6	O 6	0	0
3	R	2	Total 2	O 2	0	0
3	S	5	Total 5	O 5	0	0
3	T	7	Total 7	O 7	0	0



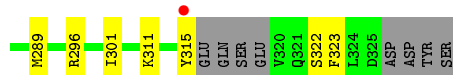




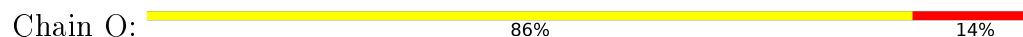
- Molecule 1: ZYRO0G01672p



- Molecule 1: ZYRO0G01672p



- Molecule 2: RNA (5'-R(\*AP\*GP\*GP\*(6MZ)P\*CP\*AP\*U)-3')



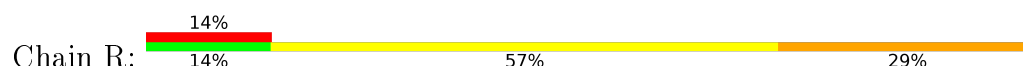
- Molecule 2: RNA (5'-R(\*AP\*GP\*GP\*(6MZ)P\*CP\*AP\*U)-3')



- Molecule 2: RNA (5'-R(\*AP\*GP\*GP\*(6MZ)P\*CP\*AP\*U)-3')

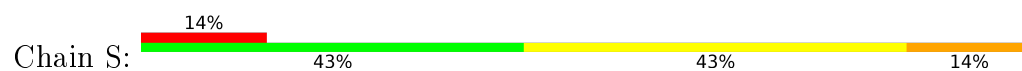


- Molecule 2: RNA (5'-R(\*AP\*GP\*GP\*(6MZ)P\*CP\*AP\*U)-3')





- Molecule 2: RNA (5'-R(\*AP\*GP\*GP\*(6MZ)P\*CP\*AP\*U)-3')



- Molecule 2: RNA (5'-R(\*AP\*GP\*GP\*(6MZ)P\*CP\*AP\*U)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.39Å 117.39Å 380.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.92 – 2.70 24.92 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.2 (24.92-2.70) 88.2 (24.92-2.70)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 2.72Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1675)	Depositor
R, $R_{free}$	0.199 , 0.245 0.203 , 0.247	Depositor DCC
$R_{free}$ test set	1773 reflections (4.44%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.5	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 43.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8572	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6MZ

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	0/1309	0.69	0/1764
1	B	0.73	0/1284	0.64	0/1731
1	C	0.68	0/1293	0.65	0/1742
1	D	0.71	0/1310	0.62	1/1767 (0.1%)
1	E	0.69	0/1276	0.64	0/1720
1	F	0.65	0/1276	0.60	0/1720
2	O	1.55	0/141	1.55	4/216 (1.9%)
2	P	1.40	0/141	1.48	4/216 (1.9%)
2	Q	1.30	0/141	1.68	6/216 (2.8%)
2	R	1.35	0/141	1.28	1/216 (0.5%)
2	S	1.35	0/141	1.44	1/216 (0.5%)
2	T	1.46	0/141	1.63	4/216 (1.9%)
All	All	0.80	0/8594	0.79	21/11740 (0.2%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	1	C	N3-C4-C5	7.87	125.05	121.90
2	Q	1	C	C5-C6-N1	-7.23	117.38	121.00
2	S	1	C	N3-C2-O2	-6.73	117.19	121.90
2	O	1	C	C5-C6-N1	-6.68	117.66	121.00
2	T	1	C	N3-C4-N4	-6.66	113.34	118.00
2	Q	1	C	N3-C4-N4	-6.43	113.50	118.00
2	T	1	C	C6-N1-C2	6.24	122.80	120.30
2	Q	1	C	N3-C2-O2	-6.20	117.56	121.90
2	P	-1	G	O5'-P-OP1	-6.07	100.24	105.70
2	P	1	C	N1-C2-O2	5.91	122.44	118.90
2	O	1	C	C2-N1-C1'	-5.86	112.36	118.80
2	O	-3	A	C8-N9-C4	5.75	108.10	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	1	C	N1-C2-O2	5.61	122.27	118.90
2	P	1	C	N3-C2-O2	-5.44	118.09	121.90
2	O	-3	A	N9-C4-C5	-5.27	103.69	105.80
2	R	-1	G	O5'-P-OP1	-5.26	100.96	105.70
2	Q	-2	G	O5'-P-OP2	-5.26	100.97	105.70
2	Q	1	C	C2-N1-C1'	-5.16	113.12	118.80
1	D	284	ILE	CG1-CB-CG2	-5.10	100.19	111.40
2	Q	1	C	C2-N3-C4	-5.04	117.38	119.90
2	P	1	C	N3-C4-N4	-5.04	114.47	118.00

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	1278	0	1266	18	1
1	B	1253	0	1244	12	1
1	C	1262	0	1258	29	0
1	D	1278	0	1266	17	0
1	E	1245	0	1240	20	0
1	F	1245	0	1240	23	0
2	O	150	0	80	7	0
2	P	150	0	80	2	0
2	Q	150	0	80	4	0
2	R	150	0	80	5	0
2	S	150	0	80	3	0
2	T	150	0	80	3	0
3	A	21	0	0	1	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	16	0	0	0	0
3	E	10	0	0	0	0
3	F	15	0	0	0	0
3	O	5	0	0	0	0
3	P	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Q	6	0	0	0	0
3	R	2	0	0	0	0
3	S	5	0	0	0	0
3	T	7	0	0	0	0
All	All	8572	0	7994	119	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 7.

All (119) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ARG:NH2	2:O:0:6MZ:O1P	2.05	0.90
1:D:217:LEU:HD11	1:D:223:ILE:HG13	1.58	0.86
1:B:210:LEU:HB3	1:B:241:MSE:HE1	1.64	0.80
1:E:225:LEU:HD21	1:E:241:MSE:HE3	1.62	0.79
1:C:182:VAL:HG23	1:C:301:ILE:HD11	1.64	0.79
1:E:250:ASP:OD1	1:E:252:SER:OG	2.00	0.79
1:E:217:LEU:HD11	1:E:223:ILE:HG13	1.68	0.76
1:B:217:LEU:HD11	1:B:223:ILE:HG13	1.67	0.75
2:P:1:C:N4	2:S:0:6MZ:O1P	2.19	0.74
1:E:272:ARG:HH22	1:E:315:TYR:HB2	1.54	0.71
1:F:182:VAL:HG23	1:F:301:ILE:HD11	1.75	0.69
2:O:0:6MZ:O1P	2:T:1:C:N4	2.26	0.69
1:F:214:TYR:HD1	1:F:241:MSE:HE3	1.58	0.68
1:F:223:ILE:HB	1:F:241:MSE:HE2	1.75	0.68
1:C:170:PRO:O	1:C:314:LYS:NZ	2.26	0.68
1:C:217:LEU:HD11	1:C:223:ILE:HG13	1.76	0.66
2:Q:1:C:H41	2:R:0:6MZ:P	2.18	0.66
1:D:210:LEU:HD22	1:D:241:MSE:HE1	1.77	0.65
1:F:189:GLU:OE2	1:F:193:LYS:HE2	1.98	0.63
1:A:172:ILE:HG13	1:A:314:LYS:HD3	1.80	0.63
1:E:182:VAL:HG23	1:E:301:ILE:HD11	1.80	0.63
1:F:217:LEU:HD11	1:F:223:ILE:HG13	1.79	0.63
1:C:245:LEU:HD23	1:E:289:MSE:HE3	1.81	0.62
1:D:289:MSE:HG2	1:F:247:GLU:HB2	1.81	0.61
1:E:285:PRO:HA	1:E:289:MSE:CE	2.31	0.61
1:E:285:PRO:HA	1:E:289:MSE:HE1	1.84	0.60
1:C:189:GLU:OE2	1:C:193:LYS:HE3	2.01	0.60
1:C:240:GLU:OE2	1:C:269:ILE:HD11	2.00	0.60
1:C:272:ARG:HH22	1:C:315:TYR:C	2.06	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ILE:HG22	1:B:270:VAL:HG23	1.83	0.58
1:E:295:SER:HB3	1:E:299:GLN:HG2	1.85	0.58
1:F:214:TYR:HB2	1:F:241:MSE:HE1	1.85	0.58
1:C:225:LEU:HD21	1:C:241:MSE:HE3	1.84	0.58
1:B:225:LEU:HD21	1:B:241:MSE:HE3	1.85	0.57
1:C:314:LYS:HG3	1:C:314:LYS:O	2.05	0.57
1:F:214:TYR:CD1	1:F:241:MSE:HE3	2.38	0.57
1:D:225:LEU:HD21	1:D:241:MSE:HE3	1.85	0.57
1:B:210:LEU:HD22	1:B:241:MSE:HE1	1.87	0.56
1:A:258:SER:N	1:A:261:ARG:HH12	2.04	0.56
1:C:245:LEU:HB3	1:E:289:MSE:HE1	1.87	0.56
2:P:1:C:H41	2:S:0:6MZ:P	2.29	0.56
2:Q:1:C:N4	2:R:0:6MZ:O1P	2.35	0.56
1:A:184:LYS:HE2	3:A:421:HOH:O	2.05	0.55
1:E:210:LEU:HD13	1:E:241:MSE:HE1	1.88	0.55
1:D:250:ASP:OD1	1:D:252:SER:OG	2.25	0.55
1:B:182:VAL:HG23	1:B:301:ILE:HD11	1.88	0.55
1:A:308:SER:HA	1:A:311:LYS:HD2	1.89	0.53
1:B:240:GLU:OE2	1:B:269:ILE:HD11	2.09	0.53
1:D:225:LEU:HD21	1:D:241:MSE:CE	2.40	0.52
1:F:166:ALA:HB2	1:F:322:SER:HB3	1.92	0.52
1:F:246:ARG:NH2	1:F:248:ASP:OD2	2.41	0.52
1:A:245:LEU:HG	1:C:289:MSE:HE1	1.92	0.51
2:Q:0:6MZ:O1P	2:R:1:C:N4	2.35	0.51
1:A:269:ILE:HG22	1:A:270:VAL:HG23	1.93	0.51
1:E:240:GLU:OE2	1:E:269:ILE:HD11	2.11	0.51
1:E:241:MSE:HE2	1:E:264:PHE:CE2	2.47	0.50
1:E:269:ILE:HG22	1:E:270:VAL:HG23	1.92	0.50
1:C:247:GLU:OE1	1:C:247:GLU:N	2.39	0.49
1:A:247:GLU:HB2	1:C:289:MSE:HG2	1.94	0.49
1:A:296:ARG:HH11	1:A:296:ARG:HG2	1.78	0.49
1:B:245:LEU:HD23	1:F:289:MSE:HE1	1.94	0.49
1:C:296:ARG:HG3	2:Q:1:C:O2	2.13	0.49
1:F:223:ILE:CB	1:F:241:MSE:HE2	2.42	0.49
1:D:246:ARG:HH21	1:D:248:ASP:CG	2.16	0.48
1:C:188:LEU:HG	1:C:192:LYS:HE2	1.96	0.48
1:C:182:VAL:CG2	1:C:301:ILE:HD11	2.39	0.48
1:A:259:ARG:HH22	2:O:0:6MZ:P	2.36	0.47
1:F:189:GLU:HA	1:F:192:LYS:HE2	1.96	0.47
1:F:271:VAL:HG13	1:F:323:PHE:CE2	2.49	0.47
1:C:289:MSE:HE2	1:C:289:MSE:HB2	1.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:VAL:HG23	1:D:301:ILE:HD11	1.97	0.47
2:R:2:A:N6	2:R:3:U:O4	2.48	0.47
1:D:269:ILE:HG22	1:D:270:VAL:HG23	1.97	0.46
1:A:182:VAL:HG23	1:A:301:ILE:HD11	1.96	0.46
1:A:250:ASP:OD1	1:A:252:SER:OG	2.26	0.46
1:A:245:LEU:CG	1:C:289:MSE:HE1	2.46	0.46
1:F:272:ARG:NH2	1:F:315:TYR:H	2.13	0.46
1:C:296:ARG:HB2	1:C:296:ARG:HE	1.48	0.46
1:F:184:LYS:NZ	1:F:228:SER:OG	2.40	0.46
2:O:0:6MZ:P	2:T:1:C:N4	2.88	0.46
1:C:210:LEU:HD13	1:C:241:MSE:HE1	1.97	0.45
1:D:172:ILE:HG13	1:D:314:LYS:HD3	1.98	0.45
1:F:280:LYS:O	1:F:280:LYS:HG3	2.15	0.45
1:C:245:LEU:HB3	1:E:289:MSE:CE	2.46	0.45
1:C:295:SER:HB3	1:C:299:GLN:HG2	1.98	0.45
1:B:210:LEU:HD22	1:B:241:MSE:CE	2.47	0.45
1:A:217:LEU:HD11	1:A:223:ILE:HG13	1.98	0.45
1:A:258:SER:O	1:A:261:ARG:NH2	2.49	0.45
1:C:314:LYS:O	1:C:314:LYS:CG	2.65	0.45
1:C:225:LEU:HD21	1:C:241:MSE:CE	2.47	0.45
1:E:166:ALA:HB2	1:E:322:SER:HB3	1.99	0.45
1:E:269:ILE:HG21	1:E:269:ILE:HD13	1.76	0.44
1:F:296:ARG:HG3	2:R:1:C:O2	2.17	0.44
1:B:173:HIS:O	1:B:175:PRO:HD3	2.17	0.44
1:F:182:VAL:CG2	1:F:301:ILE:HD11	2.44	0.44
1:C:272:ARG:NH2	1:C:315:TYR:H	2.15	0.44
1:F:223:ILE:CG2	1:F:241:MSE:HE2	2.48	0.44
1:E:201:SER:O	2:S:0:6MZ:N6	2.42	0.43
1:D:289:MSE:HE1	1:F:245:LEU:HD23	1.99	0.43
2:O:2:A:C6	2:O:3:U:C4	3.06	0.43
1:B:247:GLU:OE2	1:B:261:ARG:NH2	2.52	0.43
1:C:189:GLU:OE2	1:C:193:LYS:HG2	2.18	0.43
1:C:223:ILE:HB	1:C:241:MSE:HG2	2.01	0.43
1:A:296:ARG:HG3	2:O:1:C:O2	2.19	0.42
1:D:219:GLN:HG3	1:D:220:GLY:N	2.34	0.42
1:D:217:LEU:HA	1:D:218:PRO:HD2	1.91	0.42
1:E:217:LEU:HA	1:E:218:PRO:HD2	1.83	0.42
1:A:312:LEU:HD23	1:A:312:LEU:HA	1.79	0.41
1:C:193:LYS:HD3	1:C:193:LYS:HA	1.88	0.41
1:C:269:ILE:HG22	1:C:270:VAL:HG23	2.03	0.41
1:E:182:VAL:CG2	1:E:301:ILE:HD11	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:LEU:HA	1:A:218:PRO:HD2	1.91	0.41
1:D:289:MSE:HE2	1:D:289:MSE:HB2	1.65	0.41
1:B:247:GLU:HB2	1:F:289:MSE:HG2	2.03	0.40
1:F:311:LYS:HD3	1:F:311:LYS:HA	1.86	0.40
1:D:290:LYS:HA	1:D:291:PRO:HD3	1.93	0.40
1:D:246:ARG:NH2	1:D:248:ASP:OD2	2.40	0.40
2:O:0:6MZ:P	2:T:1:C:H41	2.44	0.40
1:D:240:GLU:OE2	1:D:269:ILE:HD11	2.22	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:189:GLU:OE2	1:B:196:TYR:OH[5_554]	2.01	0.19

## 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	151/177 (85%)	145 (96%)	6 (4%)	0	100	100
1	B	148/177 (84%)	143 (97%)	5 (3%)	0	100	100
1	C	149/177 (84%)	144 (97%)	5 (3%)	0	100	100
1	D	153/177 (86%)	148 (97%)	5 (3%)	0	100	100
1	E	147/177 (83%)	142 (97%)	5 (3%)	0	100	100
1	F	147/177 (83%)	142 (97%)	5 (3%)	0	100	100
All	All	895/1062 (84%)	864 (96%)	31 (4%)	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	142/158 (90%)	142 (100%)	0	100	100
1	B	139/158 (88%)	136 (98%)	3 (2%)	60	86
1	C	140/158 (89%)	139 (99%)	1 (1%)	88	96
1	D	142/158 (90%)	142 (100%)	0	100	100
1	E	138/158 (87%)	138 (100%)	0	100	100
1	F	138/158 (87%)	137 (99%)	1 (1%)	88	96
All	All	839/948 (88%)	834 (99%)	5 (1%)	90	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	168	ILE
1	B	242	SER
1	B	281	GLN
1	C	259	ARG
1	F	261	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	ASN
1	B	230	ASN
1	C	230	ASN
1	D	230	ASN
1	D	281	GLN
1	E	230	ASN
1	F	230	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	O	5/7 (71%)	3 (60%)	0
2	P	5/7 (71%)	3 (60%)	0
2	Q	5/7 (71%)	3 (60%)	0
2	R	5/7 (71%)	3 (60%)	0
2	S	5/7 (71%)	3 (60%)	0
2	T	5/7 (71%)	2 (40%)	0
All	All	30/42 (71%)	17 (56%)	0

All (17) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	O	-2	G
2	O	-1	G
2	O	1	C
2	P	-2	G
2	P	-1	G
2	P	1	C
2	Q	-2	G
2	Q	-1	G
2	Q	1	C
2	R	-2	G
2	R	-1	G
2	R	1	C
2	S	-2	G
2	S	-1	G
2	S	1	C
2	T	-1	G
2	T	1	C

There are no RNA pucker outliers to report.

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

6 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	6MZ	O	0	2	17,25,26	0.86	1 (5%)	15,36,39	3.09	2 (13%)
2	6MZ	P	0	2	17,25,26	0.91	1 (5%)	15,36,39	3.23	3 (20%)
2	6MZ	Q	0	2	17,25,26	0.91	1 (5%)	15,36,39	3.47	3 (20%)
2	6MZ	R	0	2	17,25,26	0.96	1 (5%)	15,36,39	2.89	2 (13%)
2	6MZ	S	0	2	17,25,26	0.90	1 (5%)	15,36,39	3.12	3 (20%)
2	6MZ	T	0	2	17,25,26	0.94	0	15,36,39	3.35	3 (20%)

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	6MZ	O	0	2	-	0/5/27/28	0/3/3/3
2	6MZ	P	0	2	-	0/5/27/28	0/3/3/3
2	6MZ	Q	0	2	-	0/5/27/28	0/3/3/3
2	6MZ	R	0	2	-	0/5/27/28	0/3/3/3
2	6MZ	S	0	2	-	0/5/27/28	0/3/3/3
2	6MZ	T	0	2	-	0/5/27/28	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	0	6MZ	C5-C4	2.23	1.45	1.40
2	Q	0	6MZ	C5-C4	2.39	1.45	1.40
2	S	0	6MZ	C5-C4	2.51	1.46	1.40
2	P	0	6MZ	C5-C4	2.56	1.46	1.40
2	R	0	6MZ	C5-C4	2.63	1.46	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	0	6MZ	N3-C2-N1	-8.42	122.26	128.87
2	O	0	6MZ	N3-C2-N1	-8.01	122.58	128.87
2	Q	0	6MZ	N3-C2-N1	-7.67	122.84	128.87
2	S	0	6MZ	N3-C2-N1	-7.53	122.96	128.87
2	R	0	6MZ	N3-C2-N1	-7.12	123.28	128.87
2	P	0	6MZ	N3-C2-N1	-7.02	123.35	128.87
2	Q	0	6MZ	C1'-N9-C4	-5.18	121.02	126.81
2	S	0	6MZ	C1'-N9-C4	-4.46	121.83	126.81
2	T	0	6MZ	C1'-N9-C4	-3.40	123.01	126.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	0	6MZ	C1'-N9-C4	-3.09	123.36	126.81
2	S	0	6MZ	C2-N1-C6	8.05	122.26	116.47
2	R	0	6MZ	C2-N1-C6	8.35	122.47	116.47
2	O	0	6MZ	C2-N1-C6	8.42	122.53	116.47
2	T	0	6MZ	C2-N1-C6	9.00	122.94	116.47
2	Q	0	6MZ	C2-N1-C6	9.55	123.34	116.47
2	P	0	6MZ	C2-N1-C6	9.68	123.43	116.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	0	6MZ	5	0
2	Q	0	6MZ	1	0
2	R	0	6MZ	2	0
2	S	0	6MZ	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [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	155/177 (87%)	-0.23	5 (3%) 51 51	13, 25, 53, 67	0
1	B	152/177 (85%)	-0.14	4 (2%) 59 59	19, 30, 55, 84	0
1	C	153/177 (86%)	-0.05	7 (4%) 36 35	20, 32, 58, 86	0
1	D	155/177 (87%)	-0.17	4 (2%) 59 59	17, 31, 48, 69	0
1	E	151/177 (85%)	-0.19	4 (2%) 59 59	17, 32, 59, 76	0
1	F	151/177 (85%)	0.03	9 (5%) 25 24	23, 39, 58, 73	0
2	O	6/7 (85%)	-0.39	0 100 100	22, 26, 38, 56	0
2	P	6/7 (85%)	-0.10	1 (16%) 2 2	23, 35, 47, 66	0
2	Q	6/7 (85%)	-0.19	0 100 100	24, 37, 43, 63	0
2	R	6/7 (85%)	0.03	1 (16%) 2 2	27, 38, 54, 73	0
2	S	6/7 (85%)	0.10	1 (16%) 2 2	22, 34, 51, 69	0
2	T	6/7 (85%)	-0.18	0 100 100	22, 31, 43, 56	0
All	All	953/1104 (86%)	-0.13	36 (3%) 44 44	13, 32, 56, 86	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	171	TRP	3.6
1	C	171	TRP	3.4
1	F	219	GLN	3.4
1	A	171	TRP	3.3
1	E	315	TYR	3.3
1	C	315	TYR	3.2
1	E	171	TRP	3.1
1	F	315	TYR	3.1
1	E	219	GLN	3.1
1	C	225	LEU	3.1
1	F	171	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	183	ILE	3.0
1	A	261	ARG	2.9
1	C	219	GLN	2.9
1	A	315	TYR	2.9
1	B	261	ARG	2.7
1	D	225	LEU	2.7
2	R	3	U	2.7
1	B	173	HIS	2.7
1	D	226	LEU	2.5
1	C	226	LEU	2.5
1	A	258	SER	2.5
1	D	219	GLN	2.4
1	F	183	ILE	2.4
1	B	219	GLN	2.4
1	F	261	ARG	2.4
1	F	255	GLY	2.3
1	F	176	ASP	2.3
1	A	219	GLN	2.3
1	C	237	GLY	2.2
2	S	3	U	2.2
1	F	220	GLY	2.1
2	P	3	U	2.1
1	C	170	PRO	2.1
1	E	321	GLN	2.1
1	F	226	LEU	2.0

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

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
2	6MZ	P	0	23/24	0.98	0.10	-	18,21,28,34	0
2	6MZ	Q	0	23/24	0.98	0.11	-	21,25,27,36	0
2	6MZ	R	0	23/24	0.97	0.12	-	26,31,35,36	0
2	6MZ	T	0	23/24	0.98	0.10	-	17,20,23,30	0
2	6MZ	S	0	23/24	0.98	0.11	-	17,26,31,32	0
2	6MZ	O	0	23/24	0.98	0.11	-	17,20,23,31	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.