



# Preliminary Full wwPDB X-ray Structure Validation Report ⓘ

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This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030345

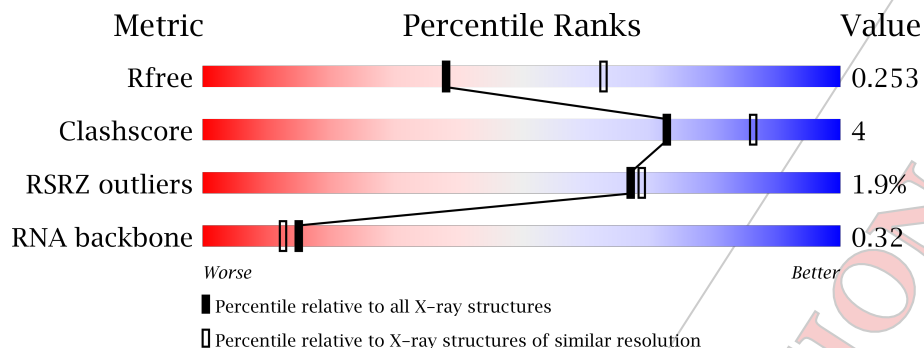
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)
RNA backbone	2435	1019 (2.90-2.10)

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	117	
1	B	117	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	D	4	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4545 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 RNA chain called PRPP riboswitch from *T. mathranii*.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	108	Total	C	N	O	P	0	0	0
			2276	1017	409	744	106			
1	B	100	Total	C	N	O	P	0	0	0
			2142	957	393	693	99			

- Molecule 2 is BARIUM ION (three-letter code: BA) (formula: Ba).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Ba	0	0
			1	1		
2	C	1	Total	Ba	0	0
			1	1		
2	C	1	Total	Ba	0	0
			1	1		
2	C	1	Total	Ba	0	0
			1	1		
2	C	1	Total	Ba	0	0
			1	1		
2	C	1	Total	Ba	0	0
			1	1		
2	C	1	Total	Ba	0	0
			1	1		
2	C	1	Total	Ba	0	0
			1	1		
2	C	1	Total	Ba	0	0
			1	1		
2	C	1	Total	Ba	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Ba	0	0
			1	1		
2	C	1	Total	Ba	0	0
			1	1		
2	C	1	Total	Ba	0	0
			1	1		
2	C	1	Total	Ba	0	0
			1	1		
2	C	1	Total	Ba	0	0
			1	1		
2	C	1	Total	Ba	0	0
			1	1		
2	C	1	Total	Ba	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

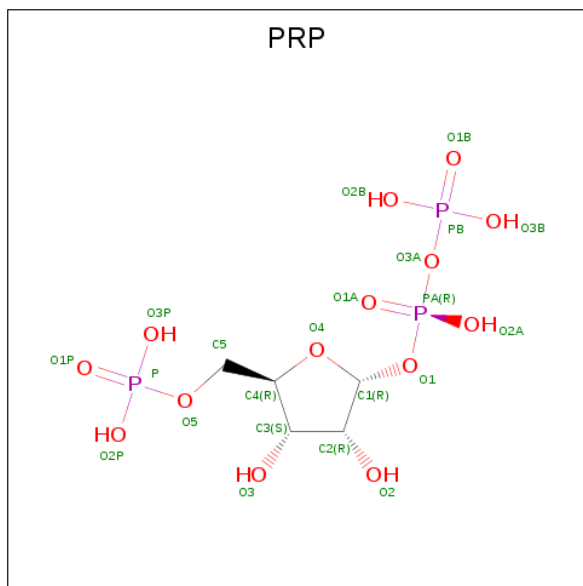
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total	K	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total K 1 1	0	0
4	E	1	Total K 1 1	0	0

- Molecule 5 is ALPHA-PHOSPHORIBOSYLPYROPHOSPHORIC ACID (three-letter code: PRP) (formula: C<sub>5</sub>H<sub>13</sub>O<sub>14</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total C O P 22 5 14 3	0	0
5	G	1	Total C O P 22 5 14 3	0	0

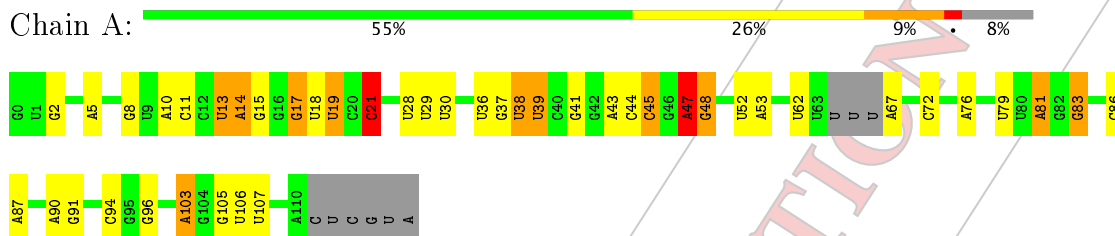
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	52	Total O 52 52	0	0

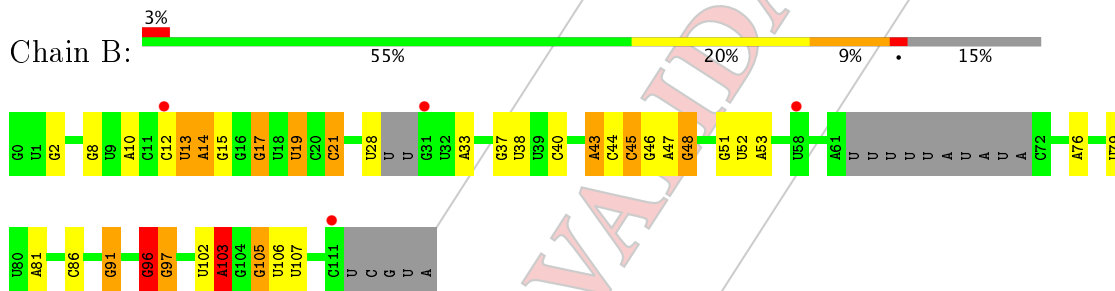
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: PRPP riboswitch from *T. mathranii*



- Molecule 1: PRPP riboswitch from *T. mathranii*



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	33.98Å 89.58Å 136.37Å 90.00° 96.90° 90.00°	Depositor
Resolution (Å)	37.35 – 2.49 37.35 – 2.49	Depositor EDS
% Data completeness (in resolution range)	97.0 (37.35-2.49) 97.0 (37.35-2.49)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.21 (at 2.48Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.214 , 0.253 0.216 , 0.253	Depositor DCC
$R_{free}$ test set	1368 reflections (5.15%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.9	Xtrriage
Anisotropy	0.711	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.00 , -89.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.137 for h,-k,-h-l	Xtrriage
Reported twinning fraction	0.798 for H, K, L 0.202 for -H, -K, H+L	Depositor
Outliers	1 of 27945 reflections (0.004%)	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4545	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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: K, MG, PRP, BA

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	0.71	6/2545 (0.2%)	1.04	13/3963 (0.3%)
1	B	0.61	1/2396 (0.0%)	0.97	8/3731 (0.2%)
All	All	0.66	7/4941 (0.1%)	1.01	21/7694 (0.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	C	O3'-P	-8.39	1.51	1.61
1	B	45	C	O3'-P	-7.53	1.52	1.61
1	A	90	A	O3'-P	-6.71	1.53	1.61
1	A	47	A	O3'-P	-6.61	1.53	1.61
1	A	11	C	O3'-P	-5.45	1.54	1.61
1	A	96	G	O3'-P	-5.37	1.54	1.61
1	A	83	G	O3'-P	-5.08	1.55	1.61

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	G	O5'-P-OP2	-16.82	90.52	110.70
1	B	17	G	O5'-P-OP2	-13.82	93.27	105.70
1	A	14	A	O5'-P-OP1	-9.03	97.57	105.70
1	A	13	U	C2'-C3'-O3'	8.30	127.77	109.50
1	B	13	U	C2'-C3'-O3'	7.48	125.95	109.50
1	A	19	U	O5'-P-OP1	-7.35	99.09	105.70
1	B	19	U	O5'-P-OP1	-6.63	99.73	105.70
1	B	96	G	C2'-C3'-O3'	6.44	124.00	113.70
1	A	14	A	O5'-P-OP2	5.99	117.89	110.70
1	A	39	U	O5'-P-OP1	-5.90	100.39	105.70
1	A	103	A	N9-C1'-C2'	5.88	121.65	114.00
1	B	43	A	O4'-C4'-C3'	-5.87	98.13	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	U	O5'-P-OP2	-5.80	100.48	105.70
1	B	14	A	O5'-P-OP1	-5.64	100.62	105.70
1	A	47	A	N9-C1'-C2'	-5.48	105.98	112.00
1	A	28	U	C2'-C3'-O3'	5.38	122.31	113.70
1	A	90	A	C2'-C3'-O3'	5.36	122.27	113.70
1	A	21	C	O5'-P-OP2	5.25	117.00	110.70
1	A	81	A	O5'-P-OP1	-5.20	101.02	105.70
1	B	103	A	N9-C1'-C2'	5.16	120.71	114.00
1	B	17	G	O5'-P-OP1	5.04	116.75	110.70

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	2276	0	1144	14	0
1	B	2142	0	1082	12	0
2	C	21	0	0	2	0
3	D	7	0	0	0	0
4	E	3	0	0	0	0
5	G	44	0	16	0	0
6	F	52	0	0	1	0
All	All	4545	0	2242	26	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 4.

All (26) 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:C:21:BA:BA	2:C:23:BA:BA	1.67	0.89
2:C:22:BA:BA	2:C:25:BA:BA	1.89	0.69
1:A:47:A:H2'	6:F:6:HOH:O	1.99	0.62
1:A:43:A:H2'	1:A:44:C:H5'	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:U:H2'	1:B:107:U:C6	2.44	0.52
1:B:15:G:O2'	1:B:91:G:N7	2.43	0.52
1:A:15:G:O2'	1:A:91:G:N7	2.43	0.51
1:A:106:U:H2'	1:A:107:U:C6	2.46	0.50
1:A:37:G:H4'	1:A:38:U:H3'	1.93	0.49
1:A:43:A:H2'	1:A:44:C:C5'	2.43	0.49
1:A:43:A:C2'	1:A:44:C:H5'	2.45	0.46
1:B:10:A:C2	1:B:53:A:C2	3.03	0.46
1:B:43:A:C2'	1:B:44:C:H5'	2.46	0.45
1:A:10:A:C2	1:A:53:A:C2	3.04	0.45
1:A:38:U:OP1	1:A:38:U:H3'	2.17	0.45
1:B:43:A:H2'	1:B:44:C:H5'	1.98	0.45
1:A:21:C:O2'	1:B:21:C:H1'	2.18	0.44
1:A:36:U:O5'	1:A:36:U:H6	2.03	0.41
1:B:48:G:O2'	1:B:76:A:N1	2.47	0.41
1:B:103:A:C2	1:B:105:G:O6	2.73	0.41
1:B:43:A:H2'	1:B:44:C:C5'	2.50	0.41
1:B:12:C:O2	1:B:51:G:C2	2.73	0.41
1:A:83:G:N2	1:A:94:C:C2	2.89	0.41
1:A:21:C:H1'	1:B:21:C:O2'	2.21	0.40
1:A:48:G:O2'	1:A:76:A:N1	2.47	0.40
1:B:96:G:HO2'	1:B:97:G:P	2.45	0.40

There are no symmetry-related clashes.

### 5.3 Torsion angles [i](#)

#### 5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

#### 5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

#### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	105/117 (89%)	23 (21%)	5 (4%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	97/117 (82%)	23 (23%)	4 (4%)
All	All	202/234 (86%)	46 (22%)	9 (4%)

All (46) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	G
1	A	5	A
1	A	8	G
1	A	14	A
1	A	17	G
1	A	19	U
1	A	21	C
1	A	29	U
1	A	30	U
1	A	38	U
1	A	39	U
1	A	41	G
1	A	45	C
1	A	47	A
1	A	48	G
1	A	52	U
1	A	62	U
1	A	79	U
1	A	81	A
1	A	86	C
1	A	87	A
1	A	103	A
1	A	105	G
1	B	2	G
1	B	8	G
1	B	14	A
1	B	17	G
1	B	19	U
1	B	21	C
1	B	28	U
1	B	33	A
1	B	37	G
1	B	38	U
1	B	40	C
1	B	45	C
1	B	46	G

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Mol	Chain	Res	Type
1	B	47	A
1	B	48	G
1	B	52	U
1	B	79	U
1	B	81	A
1	B	86	C
1	B	97	G
1	B	102	U
1	B	103	A
1	B	105	G

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	13	U
1	A	29	U
1	A	38	U
1	A	67	A
1	A	72	C
1	B	13	U
1	B	91	G
1	B	96	G
1	B	102	U

#### 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 carbohydrates in this entry.

#### 5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 31 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
5	PRP	G	1	2	20,22,22	0.64	0	30,35,35	1.48	4 (13%)
5	PRP	G	2	3,2	20,22,22	0.78	1 (5%)	30,35,35	1.55	7 (23%)

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
5	PRP	G	1	2	-	0/16/33/33	0/1/1/1
5	PRP	G	2	3,2	-	0/16/33/33	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	2	PRP	PB-O3A	2.08	1.63	1.60

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	2	PRP	O3P-P-O5	-3.77	96.70	106.73
5	G	1	PRP	O3P-P-O5	-2.72	99.48	106.73
5	G	2	PRP	O4-C4-C5	-2.10	102.30	109.40
5	G	2	PRP	O4-C1-O1	-2.05	104.88	108.97
5	G	1	PRP	O3P-P-O2P	2.24	116.65	107.61
5	G	2	PRP	O2-C2-C3	2.25	119.04	111.83
5	G	2	PRP	O3B-PB-O2B	2.45	117.51	107.61
5	G	2	PRP	P-O5-C5	2.68	125.67	118.30
5	G	2	PRP	O1-C1-C2	2.95	111.80	106.70
5	G	1	PRP	O1-C1-C2	3.39	112.57	106.70
5	G	1	PRP	PA-O1-C1	3.51	133.66	119.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

PRELIMINARY VALIDATION REPORT

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	108/117 (92%)	-0.77	0 <b>100</b> <b>100</b>	37, 72, 139, 168	0
1	B	100/117 (85%)	-0.40	4 (4%) 39 41	45, 84, 145, 166	0
All	All	208/234 (88%)	-0.59	4 (1%) <b>67</b> <b>69</b>	37, 81, 141, 168	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	12	C	4.4
1	B	111	C	4.3
1	B	58	U	3.2
1	B	31	G	2.5

### 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	MG	D	4	1/?	0.99	0.13	2.14	54,54,54,54	0
5	PRP	G	1	22/?	0.94	0.17	0.90	46,59,73,82	0
5	PRP	G	2	22/?	0.88	0.12	-0.69	67,87,100,109	0
2	BA	C	15	1/?	0.93	0.10	-0.72	156,156,156,156	0
2	BA	C	3	1/?	0.99	0.07	-1.71	84,84,84,84	0
2	BA	C	4	1/?	0.93	0.03	-2.60	117,117,117,117	0
2	BA	C	5	1/?	0.98	0.04	-2.60	122,122,122,122	0
2	BA	C	28	1/?	0.98	0.03	-	124,124,124,124	0
2	BA	C	21	1/?	0.99	0.06	-	132,132,132,132	0
2	BA	C	18	1/?	0.96	0.11	-	162,162,162,162	0
4	K	E	5	1/?	0.98	0.03	-	60,60,60,60	0
3	MG	D	13	1/?	0.91	0.05	-	72,72,72,72	0
3	MG	D	8	1/?	0.93	0.08	-	65,65,65,65	0
3	MG	D	12	1/?	0.96	0.05	-	60,60,60,60	0
2	BA	C	12	1/?	0.82	0.11	-	178,178,178,178	0
3	MG	D	10	1/?	0.93	0.13	-	82,82,82,82	0
2	BA	C	9	1/?	0.96	0.09	-	139,139,139,139	0
2	BA	C	17	1/?	0.93	0.08	-	170,170,170,170	0
2	BA	C	16	1/?	0.82	0.05	-	170,170,170,170	0
3	MG	D	1	1/?	0.95	0.07	-	70,70,70,70	0
2	BA	C	23	1/?	1.00	0.06	-	70,70,70,70	0
4	K	E	4	1/?	0.98	0.10	-	81,81,81,81	0
2	BA	C	8	1/?	0.95	0.05	-	157,157,157,157	0
2	BA	C	20	1/?	0.83	0.04	-	171,171,171,171	0
2	BA	C	19	1/?	0.91	0.07	-	199,199,199,199	0
3	MG	D	11	1/?	0.70	0.09	-	90,90,90,90	0
2	BA	C	14	1/?	0.89	0.18	-	165,165,165,165	0
4	K	E	3	1/?	0.89	0.17	-	96,96,96,96	0
2	BA	C	22	1/?	0.99	0.02	-	112,112,112,112	0
2	BA	C	11	1/?	0.92	0.05	-	144,144,144,144	0
2	BA	C	25	1/?	0.99	0.03	-	77,77,77,77	0
2	BA	C	27	1/?	0.97	0.09	-	140,140,140,140	0
2	BA	C	7	1/?	0.94	0.04	-	123,123,123,123	0

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

There are no such residues in this entry.