

# Full wwPDB X-ray Structure Validation Report (i)

#### Apr 28, 2024 – 01:55 pm BST

PDB ID : 2XO1

Title : xpt-pbuX C74U Riboswitch from B. subtilis bound to N6-methyladenine Authors : Daldrop, P.; Reyes, F.E.; Robinson, D.A.; Hammond, C.M.; Lilley, D.M.J.;

Batey, R.T.; Brenk, R.

Deposited on : 2010-08-09

Resolution : 1.60 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*A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

 $Mol Probity \quad : \quad 4.02b\text{-}467$ 

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36.2

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

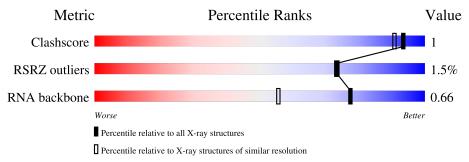
Validation Pipeline (wwPDB-VP) : 2.36.2

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
Clashscore	141614	3665 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)
RNA backbone	3102	1015 (2.36-0.86)

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 >=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 <=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			
			<u>%</u>			
1	A	67	84%	9%	٠	•



# 2 Entry composition (i)

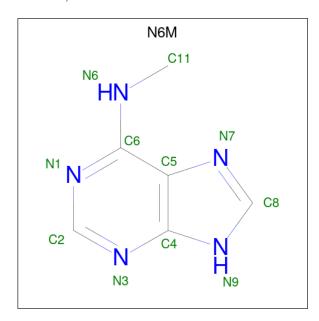
There are 6 unique types of molecules in this entry. The entry contains 1657 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Guanine riboswitch.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Δ	65	Total	С	N	О	Р	0	0	0
1	11	0.0	1364	609	241	449	65		U	U

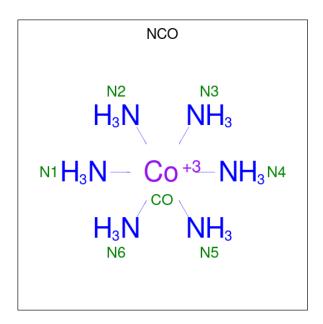
• Molecule 2 is N-METHYL-9H-PURIN-6-AMINE (three-letter code: N6M) (formula:  $C_6H_7N_5$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N 11 6 5	0	0

• Molecule 3 is COBALT HEXAMMINE(III) (three-letter code: NCO) (formula:  $CoH_{18}N_6$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Co N 7 1 6	0	0
3	A	1	Total Co N 7 1 6	0	0
3	A	1	Total Co N 7 1 6	0	0
3	A	1	Total Co N 7 1 6	1	0
3	A	1	Total Co N 7 1 6	4	0
3	A	1	Total Co N 7 1 6	3	0
3	A	1	Total Co N 7 1 6	2	0

 $\bullet$  Molecule 4 is ACETATE ION (three-letter code: ACT) (formula:  $\mathrm{C_2H_3O_2}).$ 





Mo	ol	Chain	Residues	Atoms		ZeroOcc	AltConf	
4		A	1	Total 4	C 2	O 2	0	0

• Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total K 3 3	0	0

• Molecule 6 is water.

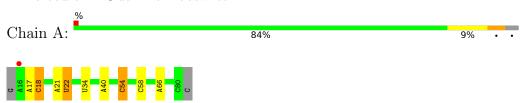
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	226	Total O 226 226	0	0



# 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: Guanine riboswitch





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	132.76Å 35.18Å 41.74Å	Donogitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.51^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	66.38 - 1.60	Depositor
Resolution (A)	19.86 - 1.59	EDS
% Data completeness	95.5 (66.38-1.60)	Depositor
(in resolution range)	95.4 (19.86-1.59)	EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.99 (at 1.59Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
D.D.	0.195 , 0.211	Depositor
$R, R_{free}$	0.194 , (Not available)	DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.6	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.39, 55.1	EDS
L-test for twinning <sup>2</sup>	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	1657	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 9.00% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 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, N6M, NCO, ACT

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).

Mal	Chain	Bond	lengths	Bo	nd angles
IVIOI	Chain	RMSZ   #  Z		RMSZ	# Z  > 5
1	A	0.80	0/1524	1.32	6/2371 (0.3%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	34	U	N1-C1'-C2'	-6.33	105.04	112.00
1	A	54	С	C4'-C3'-C2'	-5.96	96.64	102.60
1	A	40	A	C3'-C2'-C1'	-5.49	97.11	101.50
1	A	58	С	N3-C2-O2	5.24	125.57	121.90
1	A	66	A	N9-C1'-C2'	-5.13	106.36	112.00
1	A	66	A	C4'-C3'-C2'	-5.09	97.51	102.60

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	1364	0	687	2	0
2	A	11	0	7	0	0
3	A	49	0	0	0	0
4	A	4	0	3	0	0
5	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	226	0	0	0	1
All	All	1657	0	697	2	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 1.

All (2) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:17:A:H2'	1:A:18:C:O4'	2.17	0.44
1:A:21:A:H2'	1:A:22:U:H2'	2.00	0.42

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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
6:A:2087:HOH:O	6:A:2140:HOH:O[4_454]	2.03	0.17

### 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	63/67 (94%)	3 (4%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	18	С

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Mol	Chain	Res	Type
1	A	22	U
1	A	54	С

There are no RNA pucker outliers to report.

#### 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 monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 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	В	ond leng	$_{ m gths}$	H	Bond an	gles
WIOI	Type	Chain	nes	es Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NCO	A	1084	-	6,6,6	0.67	0	-		
3	NCO	A	1083	-	6,6,6	0.58	0	-		
3	NCO	A	1088	_	6,6,6	0.75	0	-		
3	NCO	A	1086	-	6,6,6	0.57	0	ı		
3	NCO	A	1085	_	6,6,6	0.58	0	-		
3	NCO	A	1087	-	6,6,6	0.58	0	ı		
4	ACT	A	1089	-	3,3,3	0.83	0	3,3,3	0.86	0
3	NCO	A	1082	-	6,6,6	0.53	0	-		
2	N6M	A	1081	-	9,12,12	1.16	0	5,16,16	3.66	5 (100%)

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.



$\mathbf{Mol}$	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	N6M	A	1081	-	-	0/2/2/2	0/2/2/2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	A	1081	N6M	C2-N1-C6	4.77	120.68	116.59
2	A	1081	N6M	N3-C2-N1	-4.23	122.06	128.68
2	A	1081	N6M	C2-N3-C4	3.07	120.64	113.45
2	A	1081	N6M	C4-C5-N7	-2.97	106.31	109.40
2	A	1081	N6M	C11-N6-C6	2.86	125.33	122.87

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.



### 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,  $95^{th}$  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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	$65/67 \ (97\%)$	-0.28	1 (1%) 73 73	11, 21, 49, 77	0

#### All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	16	A	4.9

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

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

### 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

### 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
5	K	A	1091	1/1	0.92	0.25	46,46,46,46	0
5	K	A	1090	1/1	0.94	0.16	43,43,43,43	0
3	NCO	A	1088	7/7	0.96	0.12	29,30,30,31	2
2	N6M	A	1081	11/11	0.96	0.15	17,17,19,19	0
3	NCO	A	1087	7/7	0.96	0.17	35,35,38,38	3
3	NCO	A	1086	7/7	0.97	0.10	35,39,40,40	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B-factors}({f \AA}^2)$	Q<0.9
3	NCO	A	1085	7/7	0.98	0.10	17,19,21,21	1
5	K	A	1092	1/1	0.98	0.11	30,30,30,30	0
4	ACT	A	1089	4/4	0.99	0.09	12,12,13,13	0
3	NCO	A	1083	7/7	0.99	0.09	17,19,21,22	0
3	NCO	A	1084	7/7	0.99	0.07	13,15,17,17	0
3	NCO	A	1082	7/7	0.99	0.08	16,17,19,20	0

# 6.5 Other polymers (i)

There are no such residues in this entry.

