

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

#### Aug 23, 2023 – 11:49 AM EDT

PDB ID : 3DIY

Title: Crystallization of the Thermotoga maritima lysine riboswitch bound to lysine,

Mn2+ soak

Authors : Serganov, A.A. Deposited on : 2008-06-21

Resolution : 2.71 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 : 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.35

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)

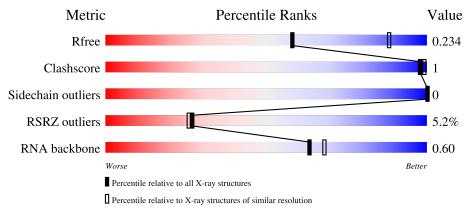
Validation Pipeline (wwPDB-VP) : 2.35

## 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 2.71 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},\ {\rm resolution\ range}({\rm \AA})) \end{array}$
$R_{free}$	130704	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)
RNA backbone	3102	1067 (3.00-2.44)

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		
			5%		
1	A	174	82%	15%	•

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
1	CCC	A	174	X	-	-	-



# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3814 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 RNA (174-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	174	Total 3756	C 1666	N 695	O 1219	P 176	0	0	0

• Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0

• Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

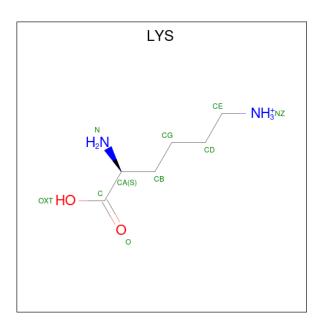
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total Na 8 8	0	0

• Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mn 2 2	0	0

• Molecule 5 is LYSINE (three-letter code: LYS) (formula:  $C_6H_{15}N_2O_2$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 10 6 2 2	0	0

• Molecule 6 is water.

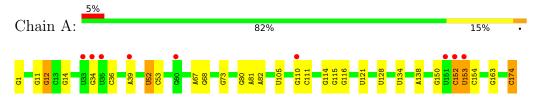
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	37	Total O 37 37	0	0



# 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: RNA (174-MER)





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	54.19Å 78.66Å 140.52Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 - 2.71	Depositor
Resolution (A)	19.67 - 2.71	EDS
% Data completeness	96.3 (20.00-2.71)	Depositor
(in resolution range)	96.3 (19.67-2.71)	EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.11 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
D D.	0.189 , 0.237	Depositor
$R, R_{free}$	0.188 , 0.234	DCC
$R_{free}$ test set	822 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.6	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.29, 41.3	EDS
L-test for twinning <sup>2</sup>	$ < L > = 0.49, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3814	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.10% 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: NA, K, MN, CCC, GDP

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  > 5	RMSZ	# Z  > 5
1	A	0.61	0/4147	1.14	8/6473 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$Ideal(^{o})$
1	A	52	U	P-O3'-C3'	6.70	127.74	119.70
1	A	153	U	O4'-C1'-N1	5.98	112.98	108.20
1	A	153	U	C1'-O4'-C4'	-5.93	105.15	109.90
1	A	12	G	O4'-C1'-N9	5.87	112.89	108.20
1	A	152	С	C2-N1-C1'	5.27	124.60	118.80
1	A	134	U	O4'-C1'-N1	5.15	112.32	108.20
1	A	105	U	O4'-C1'-N1	5.11	112.29	108.20
1	A	121	U	O4'-C1'-N1	5.10	112.28	108.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	174	CCC	C3'

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	3756	0	1884	4	0
2	A	1	0	0	0	0
3	A	8	0	0	0	0
4	A	2	0	0	0	0
5	A	10	0	12	1	0
6	A	37	0	0	0	0
All	All	3814	0	1896	4	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 1.

All (4) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} &  ext{Interatomic} \ &  ext{distance} \ &  ext{(Å)} \end{aligned}$	Clash overlap (Å)
1:A:114:G:HO2'	5:A:175:LYS:N	1.87	0.72
1:A:67:A:H2'	1:A:68:G:O4'	2.15	0.47
1:A:115:G:H2'	1:A:116:G:C8	2.55	0.41
1:A:81:A:N6	1:A:115:G:H5"	2.36	0.41

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	$172/174 \ (98\%)$	19 (11%)	6 (3%)

All (19) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	12	
1	A	14	G
1	A	34	G
1	A	36	С
1	A	52	G G C U
1	A	53	С
1	A	73	G
1	A	80	G
1	A A	82	A
1	A	110	G C
1	A	111	С
1	A	128	U
1	A	138	A
1	A	150	G C U
1	A	152	С
1	A	153	
1	A	154	С
1	A	163	G
1	A	174	CCC

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	11	G
1	A	12	G
1	A	39	A
1	A	52	U
1	A	53	С
1	A	153	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	Trmo	Chain	Dag	Link	Вс	Bond lengths		Bond angles		
IVIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
1	GDP	A	1	1	24,30,30	0.99	2 (8%)	30,47,47	0.83	0
1	CCC	A	174	1	20,25,26	1.09	1 (5%)	28,38,41	2.04	7 (25%)

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
1	CCC	A	174	1	1/1/6/6	2/7/35/36	0/3/3/3
1	GDP	A	1	1	-	5/12/32/32	0/3/3/3

#### All (3) bond length outliers are listed below:

$\mathbf{Mol}$	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(A)
1	A	1	GDP	C8-N7	-2.56	1.30	1.35
1	A	1	GDP	C5-C6	-2.51	1.42	1.47
1	A	174	CCC	C6-C5	2.02	1.39	1.35

#### All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	174	CCC	O3'-C3'-C2'	6.63	117.23	105.08
1	A	174	CCC	O4'-C4'-C3'	-3.86	96.59	104.87
1	A	174	CCC	O2'-C2'-C1'	3.65	121.88	111.43
1	A	174	CCC	C3'-C2'-C1'	-2.81	96.62	103.56
1	A	174	CCC	O2'-PC-O1C	-2.68	108.69	115.76
1	A	174	CCC	C2'-C1'-N1	-2.59	109.19	114.22
1	A	174	CCC	O2-C2-N3	-2.17	118.80	122.33

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

Mol	Chain	Res	Type	Atom
1	A	174	CCC	C3'

#### All (7) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
1	A	1	GDP	PA-O3A-PB-O2B
1	A	174	CCC	C3'-C4'-C5'-O5'
1	A	1	GDP	O4'-C4'-C5'-O5'
1	A	1	GDP	PB-O3A-PA-O1A
1	A	174	CCC	C4'-C5'-O5'-P
1	A	1	GDP	C3'-C4'-C5'-O5'
1	A	1	GDP	PB-O3A-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 11 are monoatomic - leaving 1 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	oe Chain	Chain	Chain	Chain	Chain	Pog	Link	B	ond leng	gths	В	ond ang	gles
			nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2				
5	LYS	A	175	2	8,9,9	0.79	1 (12%)	9,10,10	1.31	2 (22%)				

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	LYS	A	175	2	-	0/9/9/9	-

All (1) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
5	A	175	LYS	OXT-C	-2.02	1.23	1.30

#### All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
5	A	175	LYS	OXT-C-O	-3.15	116.94	124.09
5	A	175	LYS	OXT-C-CA	2.23	121.00	113.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	175	LYS	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 (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 $>$	#RSR	Z>2	$OWAB(Å^2)$	Q < 0.9
1	A	172/174 (98%)	-0.36	9 (5%) 2	7 26	19, 31, 67, 73	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	152	С	5.8
1	A	34	G	3.3
1	A	33	U	3.2
1	A	151	U	2.8
1	A	110	G	2.5
1	A	35	U	2.4
1	A	60	G	2.3
1	A	39	A	2.1
1	A	153	U	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,  $95^{th}$  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
1	GDP	A	1	28/28	0.85	0.23	41,43,77,77	0
1	CCC	A	174	23/24	0.92	0.23	39,42,43,43	0

## 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
3	NA	A	205	1/1	0.77	0.16	44,44,44,44	0
3	NA	A	204	1/1	0.80	0.22	51,51,51,51	0
3	NA	A	201	1/1	0.85	0.14	23,23,23,23	0
3	NA	A	208	1/1	0.86	0.41	50,50,50,50	0
4	MN	A	251	1/1	0.91	0.11	51,51,51,51	1
3	NA	A	202	1/1	0.93	0.20	33,33,33,33	0
4	MN	A	250	1/1	0.94	0.26	46,46,46,46	1
3	NA	A	207	1/1	0.94	0.13	35,35,35,35	0
3	NA	A	206	1/1	0.95	0.22	44,44,44,44	0
2	K	A	200	1/1	0.96	0.30	41,41,41,41	1
5	LYS	A	175	10/10	0.96	0.19	23,25,25,25	0
3	NA	A	203	1/1	0.97	0.29	28,28,28,28	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

