

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

#### Oct 11, 2021 – 05:02 AM EDT

PDB ID	:	2PXT
Title	:	Variant 15 of Ribonucleoprotein Core of the E. Coli Signal Recognition Particle
Authors	:	Keel, A.Y.; Rambo, R.P.; Batey, R.T.; Kieft, J.S.
Deposited on	:	2007-05-14
Resolution	:	2.50  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 following versions of software and data (see references (1)) were used in the production of this report:

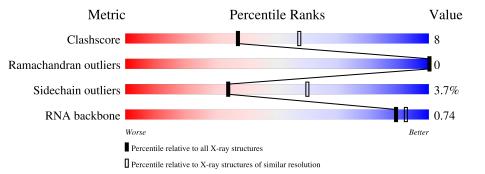
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as 541 be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.50 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	$5346 \ (2.50-2.50)$
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

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%

Mol	Chain	Length	Qual	ity of chair	1	
1	В	49	82%			18%
2	А	102	45%	22%	·	32%



#### 2PXT

## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1641 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 4.5 S RNA.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	В	49	Total 1052	C 470	N 198	O 336	Р 48	0	0	0

• Molecule 2 is a protein called Signal recognition particle protein.

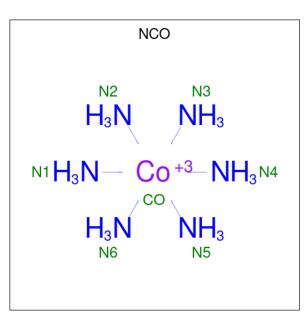
Mol	Chain	Residues		Ate	$\mathbf{oms}$			ZeroOcc	AltConf	Trace
2	А	69	Total 533	C 329	N 97	O 99	Se 8	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	9G	MSE	MET	modified residue	UNP P0AGD7
А	9J	MSE	MET	modified residue	UNP P0AGD7
А	9N	MSE	MET	modified residue	UNP P0AGD7
А	9T	MSE	MET	modified residue	UNP P0AGD7
А	10E	MSE	MET	modified residue	UNP P0AGD7
А	28	MSE	MET	modified residue	UNP P0AGD7
А	35	MSE	MET	modified residue	UNP P0AGD7
А	37	MSE	MET	modified residue	UNP P0AGD7
А	58	SER	CYS	engineered mutation	UNP P0AGD7
А	60	MSE	MET	modified residue	UNP P0AGD7
А	75	MSE	MET	modified residue	UNP P0AGD7
А	78	MSE	MET	modified residue	UNP P0AGD7
А	79	MSE	MET	modified residue	UNP P0AGD7
А	82	MSE	MET	modified residue	UNP P0AGD7

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





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	TotalCoN716	0	0
3	В	1	TotalCoN716	0	0
3	В	1	TotalCoN716	0	0
3	В	1	Total Co N 7 1 6	0	0
3	В	1	Total Co N 7 1 6	0	0
3	В	1	Total Co N 7 1 6	0	0
3	В	1	Total Co N 7 1 6	0	0
3	В	1	Total Co N 7 1 6	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. 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. 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.

 $\bullet$  Molecule 1: 4.5 S RNA

R7 M7 M7 M7 K8 K8 K8 K8

Chain B:	82%		18%	•
G130 A140 G150 U151 A156	C163 A164 C165 C166 A168 A168 C178 C178			
• Molecule	2: Signal recognition particl	e protein		
Chain A:	45%	22% •	32%	
F1 D2 L3 L3 C1 R C1 R C1 R C1 R C1 R C1 R C1 R C1	LYE ASN ASN ASN ASN ACA ACA ACA ACA ACA ACA ACA ACA ACA AC	ASP ASN VAL LYS SER GLN MSE ASP ASP ASP ASP ASP ASP ASP	S34 M35 M35 M41 F42 F43 F43 M60 M60 M60 M60 V61	Q63 N66 R67



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	134.38Å 78.52Å 32.60Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $94.99^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	50.00 - 2.50	Depositor
Resolution (A)	39.26 - 1.65	EDS
% Data completeness	99.8 (50.00-2.50)	Depositor
(in resolution range)	73.5(39.26-1.65)	EDS
R <sub>merge</sub>	0.09	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.50 (at 1.65 \text{\AA})$	Xtriage
Refinement program	CNS	Depositor
D D.	0.223 , $0.245$	Depositor
$R, R_{free}$	0.227 , (Not available)	DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor $(Å^2)$	24.2	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.31,61.9	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.46, \langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	1641	wwPDB-VP
Average B, all atoms $(Å^2)$	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.05% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<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: NCO

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		
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	В	0.40	0/1178	0.66	0/1837	
2	А	0.38	0/527	0.56	0/682	
All	All	0.39	0/1705	0.64	0/2519	

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 mainchain group or atoms of a sidechain that are expected to be planar.

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group	
1	В	156	А	Sidechain	

### 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	В	1052	0	534	5	0
2	А	533	0	528	18	0
3	В	56	0	0	0	0
All	All	1641	0	1062	21	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 8.

All (21) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:A:61:GLN:HB3	2:A:63:GLN:HG2	1.79	0.64
2:A:59:GLY:O	2:A:60:MSE:HE2	2.00	0.62
2:A:62:VAL:HG12	2:A:66:ASN:ND2	2.17	0.60
2:A:75:MSE:O	2:A:79:MSE:HG2	2.02	0.60
2:A:62:VAL:HG12	2:A:66:ASN:HD21	1.67	0.59
2:A:82:MSE:OXT	2:A:82:MSE:HG3	2.05	0.56
2:A:35:MSE:HE2	2:A:54:ILE:HD13	1.90	0.54
2:A:81:LYS:O	2:A:82:MSE:HB3	2.09	0.53
2:A:60:MSE:HE2	2:A:60:MSE:HA	1.91	0.53
1:B:163:C:H1'	2:A:34:SER:OG	2.09	0.52
1:B:163:C:H1'	2:A:34:SER:HG	1.75	0.51
2:A:67:ARG:O	2:A:71:GLN:HG3	2.11	0.51
2:A:3:LEU:HD12	2:A:43:PRO:HG3	1.96	0.47
1:B:150:G:O2'	1:B:151:U:H5'	2.15	0.46
1:B:165:G:H2'	1:B:166:C:O4'	2.19	0.43
2:A:28:MSE:HE3	2:A:68:LEU:CD2	2.50	0.42
2:A:79:MSE:C	2:A:81:LYS:H	2.23	0.42
2:A:1:PHE:CD2	2:A:79:MSE:HG3	2.54	0.42
1:B:167:C:H2'	1:B:168:A:O4'	2.20	0.41
2:A:41:ALA:C	2:A:43:PRO:HD3	2.41	0.41
2:A:77:ARG:HH11	2:A:77:ARG:HG2	1.86	0.40

There are no symmetry-related clashes.

### 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	Percentil	es
2	А	65/102~(64%)	59 (91%)	6 (9%)	0	100 10	0

There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains (i)

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	
2	А	54/76~(71%)	52~(96%)	2(4%)	34 60	

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	А	61	GLN
2	А	78	MSE

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

Mol	Chain	Res	Type
2	А	9	GLN
2	А	63	GLN

#### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	В	48/49~(97%)	1 (2%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	В	140	A



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)

8 ligands 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	Turne	Chain	Res	Link	B	ond leng	gths	В	ond angles
INIOI	Type	Unam	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ   #  Z  > 2
3	NCO	В	202	-	6,6,6	0.05	0	-	
3	NCO	В	207	-	6,6,6	0.09	0	-	
3	NCO	В	208	-	6,6,6	0.19	0	-	
3	NCO	В	201	-	6,6,6	0.11	0	-	
3	NCO	В	204	-	6,6,6	0.08	0	-	
3	NCO	В	206	-	6,6,6	0.05	0	-	
3	NCO	В	203	-	$6,\!6,\!6$	0.07	0	-	
3	NCO	В	205	-	6,6,6	0.04	0	-	

There are no bond length outliers.

There are no bond angle outliers.

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

#### 6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

#### 6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

#### 6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

