

Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 11:56 AM EST

PDB ID	:	4PL1
Title	:	X-ray crystal structure of C118A RlmN from Escherichia coli with S-
		adenosylmethionine
Authors	:	Boal, A.K.; Rosenzweig, A.C.
Deposited on	:	2014-05-15
Resolution	:	2.58 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:

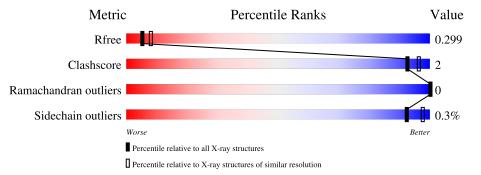
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as 541 be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.58 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	$\begin{array}{l} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)

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	Quality of chain					
1	А	359	87%	6%	8%			
1	В	359	96%		•			



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5523 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.

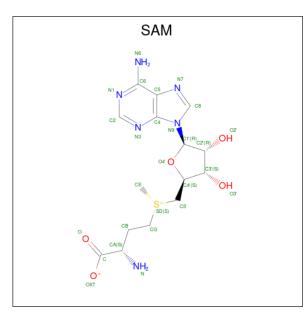
• Molecule 1 is a protein called Dual-specificity RNA methyltransferase RlmN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	В	359	Total	С	Ν	0	\mathbf{S}	0	0	0
	D	009	2832	1775	509	528	20	0	0	0
1	Λ	332	Total	С	Ν	0	S	0	0	0
	А	552	2621	1650	466	487	18	0	U	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	118	ALA	CYS	engineered mutation	UNP C9QPQ6
А	118	ALA	CYS	engineered mutation	UNP C9QPQ6

• Molecule 2 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



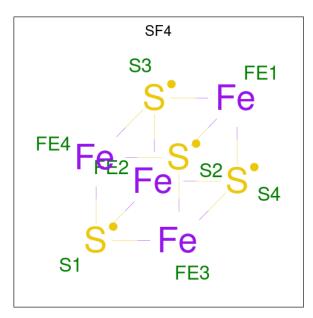
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
0	В	1	Total	С	Ν	Ο	\mathbf{S}	0	0
	D	1	27	15	6	5	1	0	0

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\mathbf{M}	ol	Chain	Residues	Atoms			ZeroOcc	AltConf		
2		А	1	Total 27	C 15	2	O 5	S 1	0	0



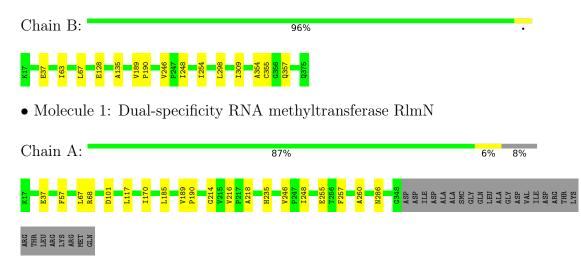
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	TotalFeS844	0	0
3	А	1	TotalFeS844	0	0



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.

• Molecule 1: Dual-specificity RNA methyltransferase RlmN





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	55.63Å 55.73 Å 254.03 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.85 - 2.58	Depositor
Resolution (A)	28.83 - 2.58	EDS
% Data completeness	94.5 (28.85-2.58)	Depositor
(in resolution range)	94.2 (28.83-2.58)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.23 (at 2.57 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
D D.	0.263 , 0.300	Depositor
R, R_{free}	0.261 , 0.299	DCC
R_{free} test set	1230 reflections (5.05%)	wwPDB-VP
Wilson B-factor $(Å^2)$	55.6	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33, 21.1	EDS
L-test for twinning ²	$< L >=0.39, < L^2>=0.22$	Xtriage
Estimated twinning fraction	0.318 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5523	wwPDB-VP
Average B, all atoms $(Å^2)$	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities 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: SF4, SMC, SAM

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	А	0.27	0/2667	0.46	0/3604	
1	В	0.27	0/2870	0.46	0/3873	
All	All	0.27	0/5537	0.46	0/7477	

There are no bond length outliers.

There are no bond angle outliers.

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	А	2621	0	2641	9	0
1	В	2832	0	2859	8	0
2	А	27	0	22	0	0
2	В	27	0	22	0	0
3	А	8	0	0	0	0
3	В	8	0	0	0	0
All	All	5523	0	5544	17	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 2.

All (17) close contacts within the same asymmetric unit are listed below, sorted by their clash



Atom-2

1:A:170:ILE:HD13

1:B:67:LEU:HD13

1:B:67:LEU:HD23

1:B:135:ALA:HB1

1:B:309:ILE:HD12

1:A:257:PHE:CE1

1:B:357:GLN:HG3

1:A:190:PRO:HD3

1:A:286:ASN:ND2

		I
1:A:248:ILE:HG22	1.71	0.72
1:A:260:ALA:HB2	1.92	0.51
1:A:218:ALA:HB1	1.95	0.48
1:B:190:PRO:HD3	1.97	0.47
1:A:67:LEU:HD13	1.98	0.46
1:B:248:ILE:HG22	1.98	0.44
1:A:68:ARG:HD2	2.18	0.44
1:B:298:LEU:HD21	2.01	0.43

Interatomic

distance (Å)

2.02

2.01

2.02

2.03

2.35

2.56

2.03

2.04

2.51

Clash

overlap (Å)

0.42

0.42

0.41

0.41

0.41

0.41

0.40

0.40

0.40

magnitude.

Atom-1

1:A:246:VAL:HG12

1:A:216:VAL:HG13

1:A:185:LEU:HD11

1:B:189:VAL:HB

1:A:37:GLU:HG3

1:B:246:VAL:HG12

1:A:57:PHE:O

1:B:254:ILE:HG21

1:A:117:LEU:HD22

1:B:37:GLU:HG3

1:B:63:ILE:HG23

1:B:128:GLU:HA

1:B:309:ILE:N

1:A:214:GLY:HA2

1:B:354:ALA:HB3

1:A:189:VAL:HB

1:A:235:HIS:O

There are no symmetry-related clashes.

Torsion angles (i) 5.3

5.3.1Protein 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	Favoured Allowed		Percentiles
1	А	330/359~(92%)	321~(97%)	9~(3%)	0	100 100
1	В	356/359~(99%)	344~(97%)	12 (3%)	0	100 100
All	All	686/718~(96%)	665~(97%)	21 (3%)	0	100 100

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		
1	А	287/308~(93%)	285~(99%)	2(1%)	84 93		
1	В	308/308~(100%)	308 (100%)	0	100 100		
All	All	595/616~(97%)	593~(100%)	2~(0%)	92 97		

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

Mol	Chain	Res	Type
1	А	101	ASP
1	А	255	GLU

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

Mol	Chain	Res	Type
1	А	184	ASN
1	А	187	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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).



ſ	Mol Typ	Tuno	Chain	Chain	Dog	Link	B	ond leng	gths	В	ond ang	gles
		туре		nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
	1	SMC	В	355	1	5,6,7	1.43	1 (20%)	$2,\!6,\!8$	3.41	1 (50%)	

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	SMC	В	355	1	-	0/3/5/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	В	355	SMC	CB-SG	-2.99	1.76	1.80

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	355	SMC	CS-SG-CB	4.62	109.80	101.30

There are no chirality outliers.

There are no torsion outliers.

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)

4 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	Type	vpe Chain	hain Res	Link	Link Bond lengths				Bond angles		
10101	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
3	SF4	В	402	1,2	0,12,12	-	-	-			
3	SF4	А	402	1,2	0,12,12	-	-	-			
2	SAM	В	401	3	24,29,29	1.20	3 (12%)	23,42,42	1.65	4 (17%)	
2	SAM	А	401	3	24,29,29	1.23	3 (12%)	23,42,42	1.64	3 (13%)	

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
3	SF4	В	402	1,2	-	-	0/6/5/5
3	SF4	А	402	1,2	-	-	0/6/5/5
2	SAM	В	401	3	-	0/12/33/33	0/3/3/3
2	SAM	А	401	3	-	1/12/33/33	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	А	401	SAM	C2-N3	4.07	1.38	1.32
2	В	401	SAM	C2-N3	3.92	1.38	1.32
2	А	401	SAM	C2-N1	2.68	1.38	1.33
2	В	401	SAM	C2-N1	2.67	1.38	1.33
2	В	401	SAM	OXT-C	-2.09	1.23	1.30
2	А	401	SAM	OXT-C	-2.06	1.23	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	А	401	SAM	N3-C2-N1	-5.77	119.65	128.68
2	В	401	SAM	N3-C2-N1	-5.56	119.99	128.68
2	В	401	SAM	C3'-C2'-C1'	2.61	104.91	100.98
2	А	401	SAM	OXT-C-O	-2.53	118.35	124.09
2	В	401	SAM	OXT-C-O	-2.49	118.44	124.09
2	А	401	SAM	OXT-C-CA	2.42	121.64	113.38
2	В	401	SAM	OXT-C-CA	2.38	121.47	113.38

There are no chirality outliers.

All (1) torsion outliers are listed below:

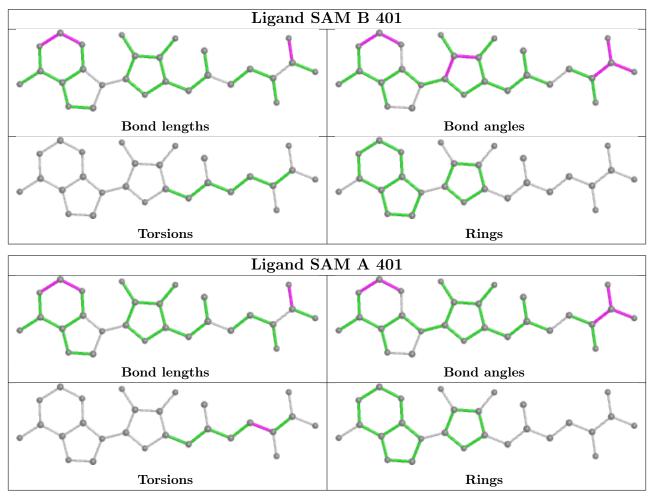


Mol	Chain	Res	Type	Atoms
2	А	401	SAM	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

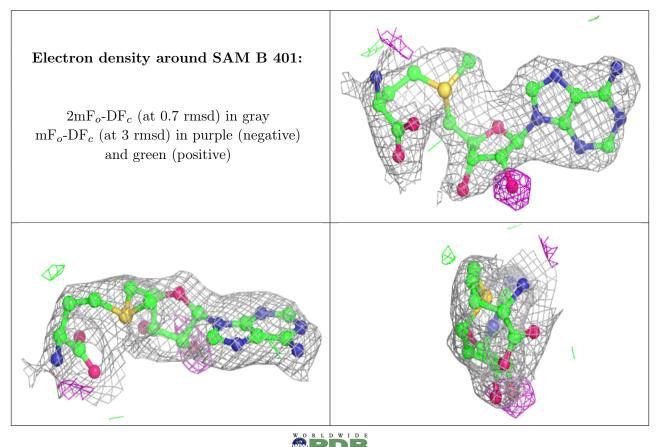
6.3 Carbohydrates (i)

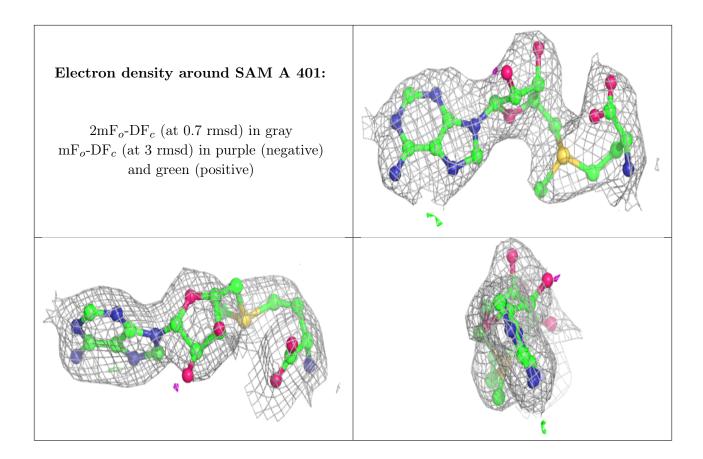
Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

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

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers (i)

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

