

Full wwPDB X-ray Structure Validation Report (i)

May 27, 2020 - 12:54 am BST

PDB ID	:	109G
Title	:	rRNA methyltransferase aviRa from Streptomyces viridochromogenes at 1.5A
Authors	:	Mosbacher, T.G.; Schulz, G.E.
Deposited on		
Resolution	:	1.50 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:

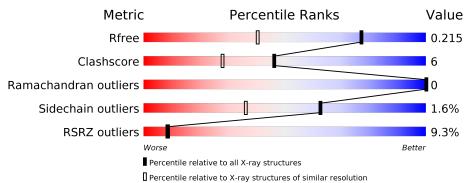
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\rm CCP4$:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.50 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$		
R_{free}	130704	2936 (1.50-1.50)		
Clashscore	141614	3144 (1.50-1.50)		
Ramachandran outliers	138981	3066 (1.50-1.50)		
Sidechain outliers	138945	3064 (1.50-1.50)		
RSRZ outliers	127900	2884 (1.50-1.50)		

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 >=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		
			9%		
1	A	250	86%	13%	•



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2201 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 RRNA METHYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	A	249	Total 1867	C 1173	N 348	O 340	$\frac{S}{4}$	${ m Se} 2$	0	0	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	11	MSE	ILE	engineered mutation	UNP Q9F5K5
A	180	GLU	SER	$\operatorname{conflict}$	UNP Q9F5K5
A	181	ARG	ALA	$\operatorname{conflict}$	UNP Q9F5K5
A	182	THR	ARG	$\operatorname{conflict}$	UNP Q9F5K5
A	183	HIS	THR	$\operatorname{conflict}$	UNP Q9F5K5
A	184	TRP	GLY	$\operatorname{conflict}$	UNP Q9F5K5
A	185	GLU	LYS	$\operatorname{conflict}$	UNP Q9F5K5
A	187	GLN	ARG	$\operatorname{conflict}$	UNP Q9F5K5
A	188	VAL	CYS	$\operatorname{conflict}$	UNP Q9F5K5
A	190	GLY	ARG	engineered mutation	UNP Q9F5K5
A	191	GLN	SER	$\operatorname{conflict}$	UNP Q9F5K5
A	192	PRO	ARG	$\operatorname{conflict}$	UNP Q9F5K5
A	193	VAL	TRP	$\operatorname{conflict}$	UNP Q9F5K5
A	194	ALA	ARG	$\operatorname{conflict}$	UNP Q9F5K5
A	195	GLY	ALA	$\operatorname{conflict}$	UNP Q9F5K5
А	239	MSE	LEU	engineered mutation	UNP Q9F5K5

There are 16 discrepancies between the modelled and reference sequences:

• Molecule 2 is water.

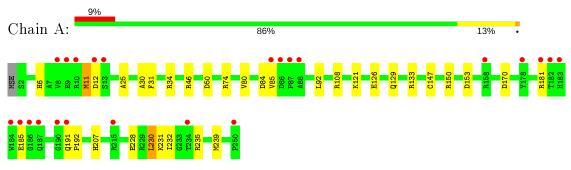
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	334	Total O 334 334	0	0



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: RRNA METHYLTRANSFERASE





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	36.36Å 47.32 Å 63.38 Å	Depositor
a, b, c, α , β , γ	90.00° 99.44° 90.00°	Depositor
Resolution (Å)	37.80 - 1.50	Depositor
Resolution (A)	14.85 - 1.50	EDS
% Data completeness	96.5 (37.80-1.50)	Depositor
(in resolution range)	96.6(14.85 - 1.50)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	0.03	Depositor
$< I/\sigma(I) > 1$	$9.37 (at 1.50 \text{\AA})$	Xtriage
Refinement program	REFMAC	Depositor
D D.	0.169 , 0.202	Depositor
R, R_{free}	0.180 , 0.215	DCC
R_{free} test set	1288 reflections (3.91%)	wwPDB-VP
Wilson B-factor $(Å^2)$	17.8	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.36 , 50.6	EDS
L-test for twinning ²	$ \langle L \rangle = 0.50, \langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2201	wwPDB-VP
Average B, all atoms $(Å^2)$	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.68% 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.



 $^{^1 {\}rm Intensities}$ estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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	Mol Chain		lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.58	0/1902	0.80	5/2587~(0.2%)	

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	50	ASP	CB-CG-OD2	6.62	124.25	118.30
1	А	150	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	А	74	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	А	84	ASP	CB-CG-OD2	5.41	123.17	118.30
1	А	12	ASP	CB-CG-OD2	5.15	122.93	118.30

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	1867	0	1917	24	0
2	А	334	0	0	11	2
All	All	2201	0	1917	24	2

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 6.

All (24) 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)
1:A:46:ARG:HG3	1:A:239:MSE:HE1	1.58	0.85
1:A:85:VAL:HG12	1:A:153:ASP:HA	1.58	0.83
1:A:129:GLN:HE21	1:A:133:ARG:HH12	1.34	0.76
1:A:25:ALA:HB2	1:A:92:LEU:CD2	2.23	0.68
1:A:108:ARG:NH2	2:A:2173:HOH:O	2.30	0.64
1:A:30:ALA:C	2:A:2062:HOH:O	2.40	0.60
1:A:170:ASP:OD1	1:A:207:HIS:HE1	1.90	0.55
1:A:231:LYS:NZ	2:A:2314:HOH:O	2.36	0.54
1:A:6:HIS:HE1	2:A:2013:HOH:O	1.90	0.54
1:A:230:LEU:C	1:A:230:LEU:HD12	2.27	0.54
1:A:25:ALA:HB2	1:A:92:LEU:HD22	1.89	0.54
1:A:121:LYS:HB2	2:A:2085:HOH:O	2.08	0.52
1:A:228:GLU:HB3	1:A:239:MSE:HE2	1.92	0.51
1:A:126:GLU:CD	2:A:2205:HOH:O	2.49	0.50
1:A:181:ARG:NE	2:A:2276:HOH:O	2.45	0.49
1:A:85:VAL:HG11	2:A:2244:HOH:O	2.13	0.48
1:A:207:HIS:HD2	2:A:2298:HOH:O	1.97	0.47
1:A:46:ARG:HG3	1:A:239:MSE:CE	2.38	0.46
1:A:31:PHE:N	2:A:2062:HOH:O	2.49	0.46
1:A:191:GLN:HB2	1:A:192:PRO:HD3	2.01	0.42
1:A:235:ARG:HD3	2:A:2267:HOH:O	2.19	0.42
1:A:80:VAL:O	1:A:147:CYS:HA	2.21	0.41
1:A:11:MSE:HE1	1:A:34:ARG:HG3	2.01	0.40
1:A:230:LEU:HD13	1:A:232:ILE:HG12	2.03	0.40

All (2) 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	Interatomic distance (Å)	Clash overlap (Å)
2:A:2098:HOH:O	2:A:2258:HOH:O[2_647]	1.69	0.51
2:A:2213:HOH:O	2:A:2258:HOH:O[2_647]	2.15	0.05

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	247/250~(99%)	243~(98%)	4 (2%)	0	100 100

analysed, and the total number of residues.

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	192/190~(101%)	189~(98%)	3(2%)	62 36	

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	11	MSE
1	А	185	GLU
1	А	230	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	6	HIS
1	А	23	HIS
1	А	129	GLN
1	А	207	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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)

There are no ligands in this entry.

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, 95th 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 >	#RSF	RZ>	2	$\mathbf{OWAB}(\mathbf{A}^2)$	Q<0.9
1	А	247/250 (98%)	0.30	23~(9%)	8	9	11, 21, 51, 98	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	184	TRP	8.2
1	А	185	GLU	6.8
1	А	10	ARG	5.2
1	А	8	VAL	4.8
1	А	183	HIS	4.4
1	А	234	THR	4.1
1	А	12	ASP	3.5
1	А	178	TYR	3.3
1	А	158	ARG	3.3
1	А	85	VAL	3.2
1	А	86	ASP	3.2
1	А	9	GLU	3.0
1	А	87	PRO	3.0
1	А	191	GLN	2.7
1	А	215	ARG	2.6
1	А	182	THR	2.6
1	А	181	ARG	2.6
1	А	190	GLY	2.5
1	А	13	SER	2.5
1	А	250	PRO	2.3
1	А	186	GLY	2.3
1	А	187	GLN	2.2
1	А	88	ALA	2.1



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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

