W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 05:22 pm GMT

PDB ID	:	3NVM
Title	:	Structural basis for substrate placement by an archaeal box C/D ribonucleo-protein particle
Authors	:	Xue, S.; Wang, R.; Li, H.
Deposited on	:	2010-07-08
Resolution	:	3.41 Å(reported)

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

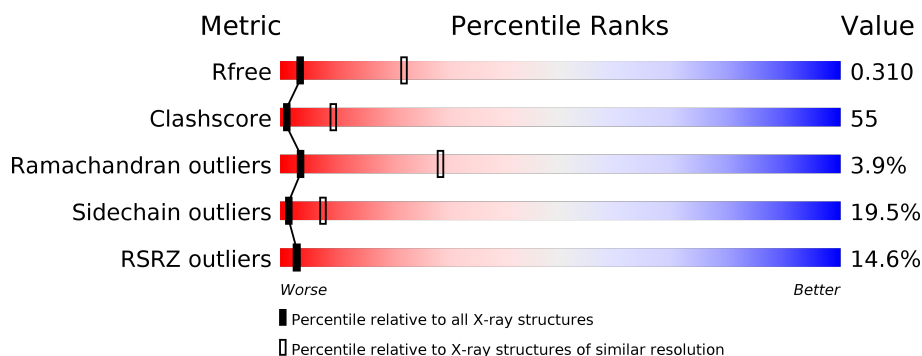|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

1   Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.41 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	Percentile Ranks	Value
Rfree		0.310
Clashscore		55
Ramachandran outliers		3.9%
Sidechain outliers		19.5%
RSRZ outliers		14.6%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)

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. 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
1	A	371	13% / 33% / 44% / 14% · 8%
2	B	234	15% / 30% / 51% / 14% · ·

2   Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 4597 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 NOP5/NOP56 related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total 2775	C 1770	N 479	O 519	S 7	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	EXPRESSION TAG	UNP Q8U4M1
A	-4	HIS	-	EXPRESSION TAG	UNP Q8U4M1
A	-3	HIS	-	EXPRESSION TAG	UNP Q8U4M1
A	-2	HIS	-	EXPRESSION TAG	UNP Q8U4M1
A	-1	HIS	-	EXPRESSION TAG	UNP Q8U4M1
A	0	HIS	-	EXPRESSION TAG	UNP Q8U4M1
A	1	HIS	-	EXPRESSION TAG	UNP Q8U4M1
A	2	VAL	-	EXPRESSION TAG	UNP Q8U4M1
A	3	MET	-	EXPRESSION TAG	UNP Q8U4M1
A	4	ILE	-	EXPRESSION TAG	UNP Q8U4M1
A	?	-	VAL	DELETION	UNP Q8U4M1
A	?	-	ASP	DELETION	UNP Q8U4M1
A	?	-	LYS	DELETION	UNP Q8U4M1
A	?	-	VAL	DELETION	UNP Q8U4M1
A	?	-	ASP	DELETION	UNP Q8U4M1
A	?	-	ARG	DELETION	UNP Q8U4M1
A	?	-	LEU	DELETION	UNP Q8U4M1
A	?	-	TYR	DELETION	UNP Q8U4M1

- Molecule 2 is a protein called Fibrillarin-like rRNA/tRNA 2'-O-methyltransferase.

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total 1822	C 1174	N 312	O 334	S 2	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	MET	-	EXPRESSION TAG	UNP Q8U4M2
B	-5	HIS	-	EXPRESSION TAG	UNP Q8U4M2
B	-4	HIS	-	EXPRESSION TAG	UNP Q8U4M2
B	-3	HIS	-	EXPRESSION TAG	UNP Q8U4M2
B	-2	HIS	-	EXPRESSION TAG	UNP Q8U4M2
B	-1	HIS	-	EXPRESSION TAG	UNP Q8U4M2
B	0	HIS	-	EXPRESSION TAG	UNP Q8U4M2

3 Residue-property plots ⓘ

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: NOP5/NOP56 related protein

- Molecule 2: Fibrillarin-like rRNA/tRNA 2'-O-methyltransferase
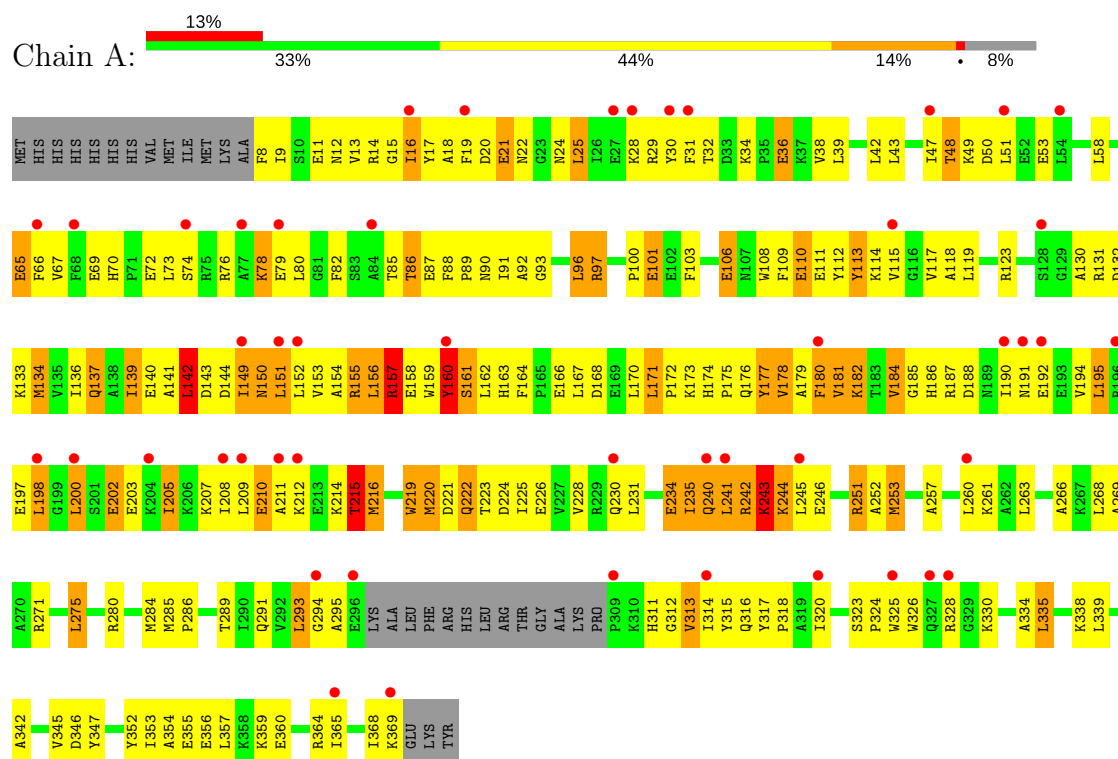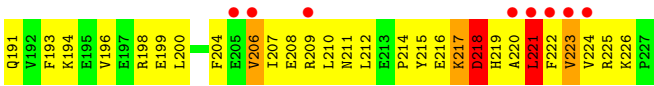
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α, β, γ	100.62Å 100.62Å 265.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.43 – 3.41 49.43 – 3.41	Depositor EDS
% Data completeness (in resolution range)	76.7 (49.43-3.41) 83.3 (49.43-3.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.66 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.242 , 0.316 0.241 , 0.310	Depositor DCC
R_{free} test set	901 reflections (5.07%)	DCC
Wilson B-factor (Å^2)	126.8	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 180.3	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.063 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4597	wwPDB-VP
Average B, all atoms (Å^2)	209.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.42	0/2824	0.60	0/3800
2	B	0.43	0/1861	0.67	1/2515 (0.0%)
All	All	0.42	0/4685	0.63	1/6315 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	221	LEU	CA-CB-CG	6.13	129.41	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	2775	0	2805	300	0
2	B	1822	0	1869	232	0
All	All	4597	0	4674	514	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 55.

The worst 5 of 514 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)
2:B:109:ARG:HH11	2:B:109:ARG:HG2	0.98	1.08
2:B:4:VAL:HG23	2:B:15:VAL:HG12	1.46	0.97
2:B:43:TRP:HD1	2:B:44:GLU:HG3	1.30	0.96
1:A:173:LYS:O	1:A:176:GLN:HG2	1.63	0.95
1:A:167:LEU:HD23	1:A:177:TYR:CE2	2.01	0.95

There are no symmetry-related clashes.

5.3   Torsion angles ⓘ

5.3.1   Protein backbone ⓘ

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	Percentiles	
1	A	338/371 (91%)	281 (83%)	44 (13%)	13 (4%)	4	29
2	B	225/234 (96%)	175 (78%)	41 (18%)	9 (4%)	3	28
All	All	563/605 (93%)	456 (81%)	85 (15%)	22 (4%)	3	28

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	ARG
1	A	160	TYR
2	B	82	ILE
2	B	83	ALA
2	B	218	ASP

5.3.2   Protein sidechains ⓘ

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	A	291/316 (92%)	234 (80%)	57 (20%)	1	7
2	B	197/204 (97%)	159 (81%)	38 (19%)	1	8
All	All	488/520 (94%)	393 (80%)	95 (20%)	1	7

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	222	GLN
1	A	293	LEU
2	B	181	ARG
1	A	234	GLU
1	A	242	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	240	GLN
1	A	291	GLN
2	B	64	ASN
1	A	230	GLN
2	B	7	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Fit of model and data ⓘ

6.1   Protein, DNA and RNA chains ⓘ

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>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	342/371 (92%)	0.72	48 (14%)	3	4	131, 206, 298, 351	0
2	B	227/234 (97%)	0.85	35 (15%)	2	2	145, 197, 268, 338	0
All	All	569/605 (94%)	0.77	83 (14%)	3	3	131, 203, 291, 351	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	174	GLY	8.6
1	A	208	ILE	7.7
1	A	325	TRP	5.9
1	A	296	GLU	5.2
2	B	224	VAL	5.1

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

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

6.3   Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4   Ligands ⓘ

There are no ligands in this entry.

6.5   Other polymers ⓘ

There are no such residues in this entry.