



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:15 am BST

PDB ID : 5SVD  
Title : Nop9, a new PUF-like protein, prevents premature pre-rRNA cleavage to correctly process mature 18S rRNA  
Authors : Zhang, J.; Qiu, C.; Hall, T.  
Deposited on : 2016-08-05  
Resolution : 2.10 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](mailto: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 ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtrriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

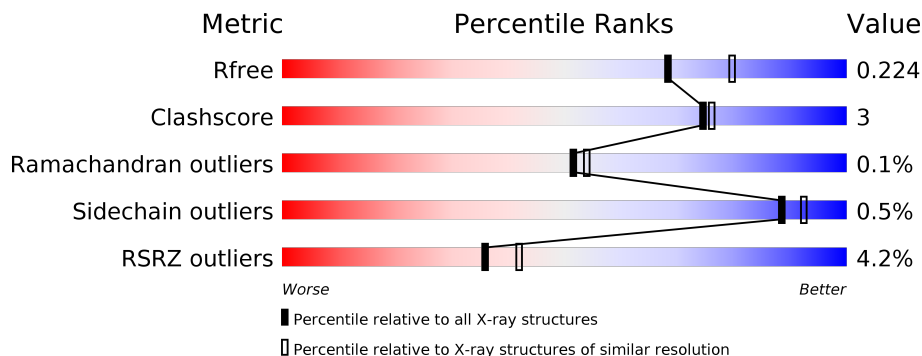
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	600	 3% 82% 8% • 10%
1	B	600	 5% 81% 8% 11%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 9186 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 Nucleolar protein 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	543	4443	2865	737	820	21	0	1	0
1	B	534	4366	2812	725	808	21	0	2	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	430	THR	ALA	engineered mutation	UNP P47077
B	430	THR	ALA	engineered mutation	UNP P47077

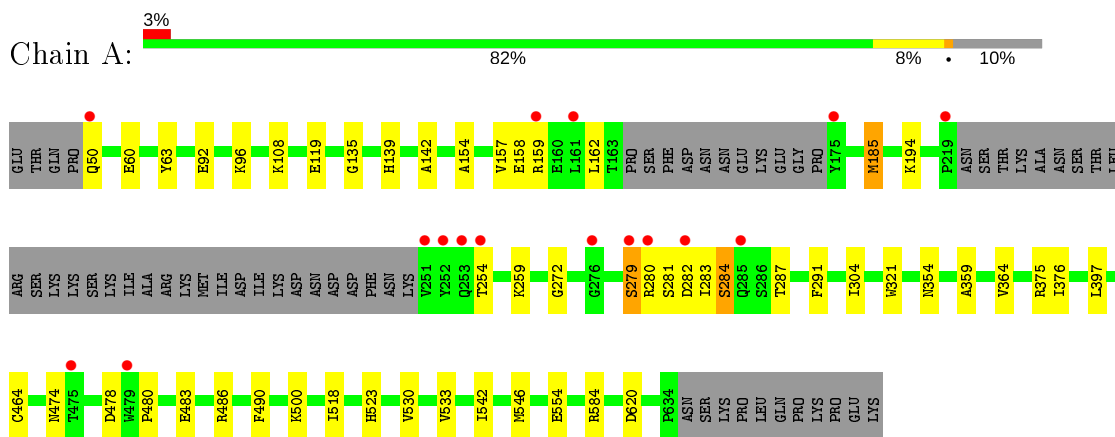
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	290	290	290	0	0
2	B	87	87	87	0	0

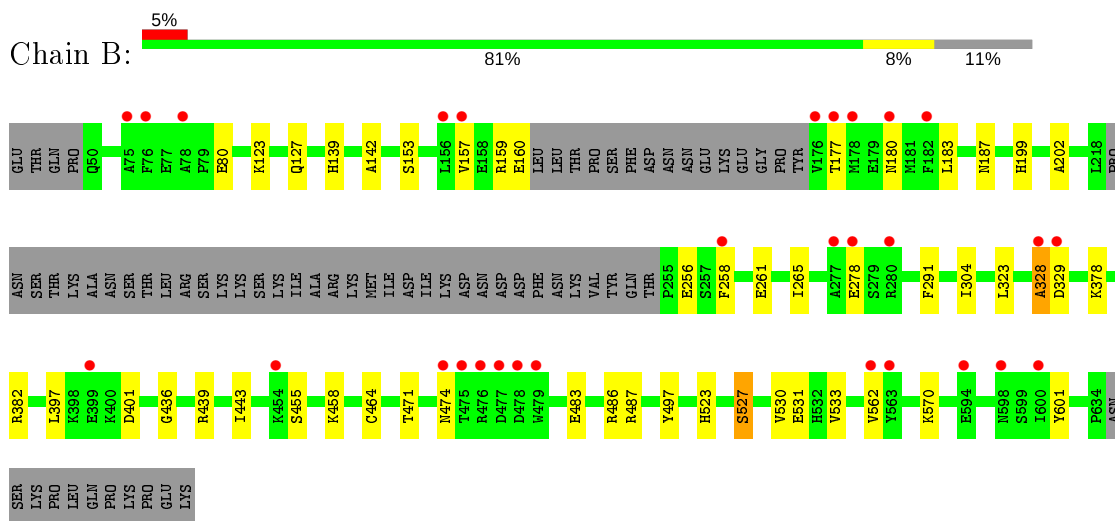
### 3 Residue-property plots [i](#)

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: Nucleolar protein 9



- Molecule 1: Nucleolar protein 9



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.50Å 110.47Å 114.85Å 90.00° 92.22° 90.00°	Depositor
Resolution (Å)	32.02 – 2.10 49.77 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.8 (32.02-2.10) 95.7 (49.77-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.99 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.185 , 0.221 0.190 , 0.224	Depositor DCC
$R_{free}$ test set	2023 reflections (2.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.1	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.001 for -h,l,k 0.011 for -h,-l,-k 0.024 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9186	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 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	0.50	0/4526	0.60	2/6104 (0.0%)
1	B	0.36	0/4449	0.49	0/5996
All	All	0.43	0/8975	0.55	2/12100 (0.0%)

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	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	MET	CG-SD-CE	-6.97	89.05	100.20
1	A	279	SER	C-N-CA	5.81	136.22	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	284	SER	Peptide
1	B	328	ALA	Peptide

## 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	4443	0	4505	31	0
1	B	4366	0	4422	26	0
2	A	290	0	0	4	0
2	B	87	0	0	0	0
All	All	9186	0	8927	57	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 3.

All (57) 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:281:SER:HB2	1:A:282:ASP:HA	1.52	0.88
1:B:378:LYS:HE3	1:B:382:ARG:HH21	1.59	0.68
1:A:483:GLU:OE1	1:A:486:ARG:NH1	2.33	0.57
1:A:50:GLN:HB2	1:A:135:GLY:HA3	1.86	0.57
1:A:375:ARG:NH1	2:A:705:HOH:O	2.29	0.55
1:A:620:ASP:OD2	2:A:701:HOH:O	2.18	0.55
1:B:139:HIS:HB3	1:B:142:ALA:HB3	1.89	0.54
1:A:279:SER:HB3	1:A:281:SER:O	2.08	0.53
1:B:199:HIS:HB3	1:B:202:ALA:HB3	1.90	0.53
1:B:183:LEU:O	1:B:187:ASN:ND2	2.35	0.53
1:B:439:ARG:O	1:B:443:ILE:HG12	2.09	0.52
1:B:123:LYS:O	1:B:127:GLN:HG3	2.10	0.52
1:A:474:ASN:ND2	1:A:478:ASP:HB2	2.25	0.51
1:A:280:ARG:HG3	1:A:283:ILE:HG13	1.92	0.51
1:B:530:VAL:O	1:B:533:VAL:HG22	2.11	0.51
1:A:518:ILE:HD12	1:A:554:GLU:HG3	1.93	0.50
1:A:280:ARG:HD3	1:A:283:ILE:HD12	1.92	0.50
1:A:254:THR:O	1:A:259:LYS:NZ	2.45	0.50
1:B:439:ARG:HA	1:B:497:TYR:OH	2.10	0.50
1:B:177:THR:HG23	1:B:180:ASN:H	1.76	0.49
1:A:194:LYS:HD2	1:A:272:GLY:HA3	1.93	0.48
1:B:328:ALA:HB1	1:B:329:ASP:CG	2.34	0.48
1:A:500:LYS:NZ	2:A:718:HOH:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLU:OE2	1:A:159:ARG:NH1	2.46	0.48
1:A:284:SER:O	1:A:287:THR:HB	2.14	0.48
1:A:281:SER:CB	1:A:282:ASP:HA	2.30	0.47
1:A:364:VAL:HG12	1:A:397:LEU:HD21	1.96	0.47
1:B:256:GLU:C	1:B:258:PHE:H	2.19	0.46
1:B:261:GLU:O	1:B:265:ILE:HG12	2.16	0.46
1:A:158:GLU:O	1:A:162:LEU:HG	2.16	0.46
1:B:291:PHE:CZ	1:B:304:ILE:HD12	2.50	0.46
1:B:455:SER:HB3	1:B:458:LYS:HB3	1.97	0.46
1:A:280:ARG:CG	1:A:281:SER:HA	2.46	0.45
1:B:523:HIS:O	1:B:527:SER:HB3	2.17	0.45
1:A:139:HIS:HB3	1:A:142:ALA:HB3	1.98	0.45
1:B:562:VAL:HG22	1:B:601:TYR:CE2	2.52	0.45
1:A:464[A]:CYS:SG	1:A:490:PHE:HD2	2.39	0.45
1:A:60:GLU:OE2	1:A:96:LYS:NZ	2.34	0.45
1:B:531:GLU:HG3	1:B:570:LYS:HD2	1.98	0.45
1:A:542:ILE:O	1:A:546:MET:HE2	2.17	0.45
1:B:159:ARG:HA	1:B:160:GLU:HA	1.75	0.44
1:A:63:TYR:CE2	1:A:92:GLU:HG2	2.52	0.44
1:A:354:ASN:ND2	2:A:722:HOH:O	2.50	0.44
1:B:464[B]:CYS:O	1:B:487:ARG:HD3	2.19	0.43
1:A:280:ARG:HG3	1:A:281:SER:HA	2.00	0.42
1:A:321:TRP:CZ3	1:A:359:ALA:HB2	2.54	0.42
1:A:154:ALA:O	1:A:157:VAL:HG22	2.18	0.42
1:B:153:SER:O	1:B:157:VAL:HG23	2.21	0.41
1:A:480:PRO:HB3	1:A:523:HIS:CE1	2.55	0.41
1:B:323:LEU:HA	1:B:323:LEU:HD23	1.83	0.41
1:A:291:PHE:CZ	1:A:304:ILE:HD12	2.55	0.41
1:B:483:GLU:OE1	1:B:486:ARG:NH1	2.54	0.41
1:A:530:VAL:O	1:A:533:VAL:HG22	2.21	0.40
1:B:471:THR:O	1:B:474:ASN:ND2	2.47	0.40
1:B:436:GLY:O	1:B:439:ARG:HB2	2.21	0.40
1:B:80:GLU:OE1	1:B:80:GLU:N	2.50	0.40
1:B:397:LEU:HD13	1:B:401:ASP:HB3	2.04	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	Percentiles	
1	A	538/600 (90%)	522 (97%)	16 (3%)	0	100	100
1	B	530/600 (88%)	513 (97%)	16 (3%)	1 (0%)	47	49
All	All	1068/1200 (89%)	1035 (97%)	32 (3%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	278	GLU

### 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	A	495/554 (89%)	491 (99%)	4 (1%)	81	86
1	B	486/554 (88%)	485 (100%)	1 (0%)	93	96
All	All	981/1108 (88%)	976 (100%)	5 (0%)	88	92

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	LYS
1	A	185	MET
1	A	376	ILE
1	A	584	ARG
1	B	527	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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

### 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
1	A	543/600 (90%)	0.14	16 (2%) 51 57	27, 44, 91, 127	0
1	B	534/600 (89%)	0.29	29 (5%) 25 31	37, 64, 101, 149	0
All	All	1077/1200 (89%)	0.21	45 (4%) 36 42	27, 56, 95, 149	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	175	TYR	7.4
1	B	479	TRP	4.9
1	B	477	ASP	4.7
1	B	277	ALA	4.7
1	A	251	VAL	4.7
1	A	479	TRP	4.4
1	B	176	VAL	4.3
1	B	156	LEU	4.0
1	B	600	ILE	4.0
1	B	178	MET	3.8
1	A	252	TYR	3.8
1	A	254	THR	3.4
1	A	280	ARG	3.3
1	B	280	ARG	3.3
1	B	478	ASP	3.2
1	B	278	GLU	3.2
1	A	276	GLY	3.0
1	A	161	LEU	3.0
1	A	159	ARG	3.0
1	A	279	SER	3.0
1	B	454	LYS	2.9
1	B	474	ASN	2.9
1	A	285	GLN	2.9
1	B	157	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	475	THR	2.8
1	B	399	GLU	2.7
1	A	253	GLN	2.7
1	B	476	ARG	2.7
1	A	50	GLN	2.5
1	B	177	THR	2.4
1	B	75	ALA	2.4
1	B	76	PHE	2.3
1	A	219	PRO	2.3
1	B	182	PHE	2.3
1	B	78	ALA	2.3
1	B	328	ALA	2.2
1	B	598	ASN	2.2
1	B	180	ASN	2.1
1	A	282	ASP	2.1
1	B	594	GLU	2.1
1	B	562	VAL	2.1
1	B	563	TYR	2.1
1	B	329	ASP	2.0
1	A	475	THR	2.0
1	B	258	PHE	2.0

## 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.