



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 11:58 AM UTC

PDB ID : 5WTY / pdb_00005wtY
Title : Structure of Nop9 RNA complex
Authors : Ye, K.; Wang, B.
Deposited on : 2016-12-15
Resolution : 2.79 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

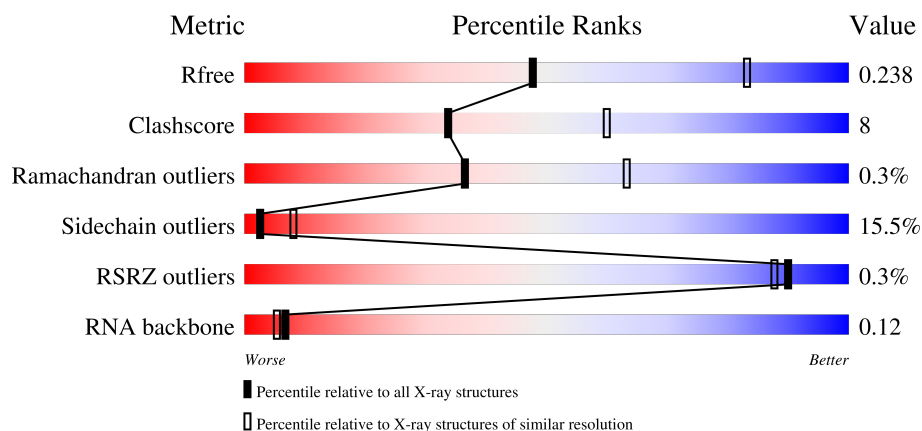
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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}	180053	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)
RNA backbone	3983	1133 (3.00-2.56)

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 $\leq 5\%$. 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	587	 64% 25% • 7%
1	B	587	 66% 24% • 7%
2	C	18	 28% 22% 11% 39%
2	D	18	 11% 50% 39%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9520 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
1	B	547	Total	C	N	O	S	0	0	0
			4477	2877	748	833	19			
1	A	544	Total	C	N	O	S	0	0	0
			4457	2865	745	828	19			

There are 10 discrepancies between the modelled and reference sequences:

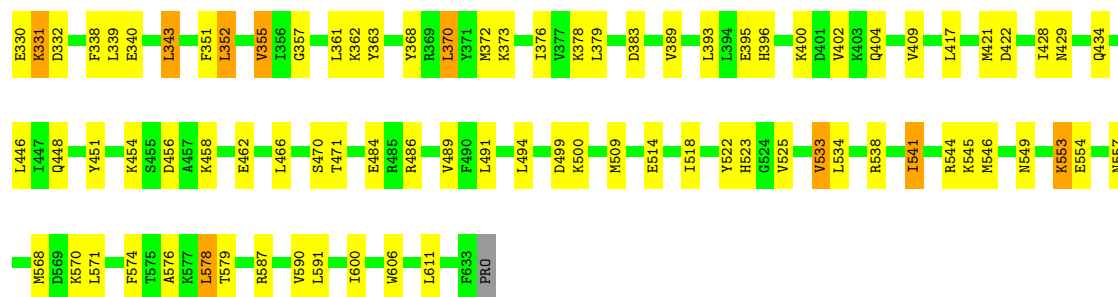
Chain	Residue	Modelled	Actual	Comment	Reference
B	48	GLY	-	expression tag	UNP P47077
B	49	PRO	-	expression tag	UNP P47077
B	50	GLU	-	expression tag	UNP P47077
B	51	ALA	-	expression tag	UNP P47077
B	52	SER	-	expression tag	UNP P47077
A	48	GLY	-	expression tag	UNP P47077
A	49	PRO	-	expression tag	UNP P47077
A	50	GLU	-	expression tag	UNP P47077
A	51	ALA	-	expression tag	UNP P47077
A	52	SER	-	expression tag	UNP P47077

- Molecule 2 is a RNA chain called RNA (5'-R(*AP*AP*AP*GP*GP*AP*AP*UP*UP*GP*AP*CP*GP*GP*AP*AP*GP*G)-3').

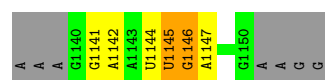
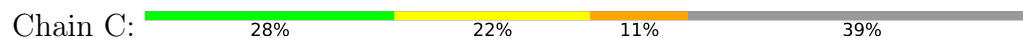
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	P	0	0	0
			241	107	47	76	11			
2	D	11	Total	C	N	O	P	0	0	0
			241	107	47	76	11			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	43	Total 43	O 43	0	0
3	A	55	Total 55	O 55	0	0
3	C	4	Total 4	O 4	0	0
3	D	2	Total 2	O 2	0	0



- Molecule 2: RNA (5'-R(*AP*AP*AP*GP*GP*AP*AP*UP*UP*GP*AP*CP*GP*GP*AP*AP*GP*G)-3')



- Molecule 2: RNA (5'-R(*AP*AP*AP*GP*GP*AP*AP*UP*UP*GP*AP*CP*GP*GP*AP*AP*GP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.50Å 102.74Å 114.71Å 90.00° 95.51° 90.00°	Depositor
Resolution (Å)	19.96 – 2.79 19.96 – 2.79	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.96-2.79) 97.7 (19.96-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.83 (at 2.79Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.176 , 0.237 0.180 , 0.238	Depositor DCC
R_{free} test set	1974 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9520	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.58	0/4538	0.88	0/6117
1	B	0.55	0/4559	0.86	2/6146 (0.0%)
2	C	0.36	0/270	0.59	0/420
2	D	0.33	0/270	0.59	0/420
All	All	0.56	0/9637	0.85	2/13103 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	190	LYS	CA-C-N	-5.24	114.42	119.87
1	B	190	LYS	C-N-CA	-5.24	114.42	119.87

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	A	4457	0	4533	73	0
1	B	4477	0	4549	69	0
2	C	241	0	120	2	0
2	D	241	0	120	1	0
3	A	55	0	0	1	0
3	B	43	0	0	2	0
3	C	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	2	0	0	0	0
All	All	9520	0	9322	145	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.

The worst 5 of 145 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:73:LEU:HD13	1:A:75:ALA:H	1.35	0.88
1:B:499:ASP:OD1	1:B:538:ARG:NH1	2.13	0.81
1:B:362:LYS:HD2	1:B:362:LYS:H	1.53	0.73
1:B:71:LEU:HD12	1:B:112:ARG:HD3	1.71	0.72
1:B:114:ILE:HD11	1:B:125:ILE:HG21	1.72	0.71

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	538/587 (92%)	519 (96%)	18 (3%)	1 (0%)	43	70
1	B	541/587 (92%)	514 (95%)	25 (5%)	2 (0%)	30	57
All	All	1079/1174 (92%)	1033 (96%)	43 (4%)	3 (0%)	36	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	278	GLU
1	A	276	GLY
1	B	280	ARG

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	499/538 (93%)	421 (84%)	78 (16%)	2	8
1	B	501/538 (93%)	424 (85%)	77 (15%)	2	8
All	All	1000/1076 (93%)	845 (84%)	155 (16%)	2	8

5 of 155 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	330	GLU
1	A	500	LYS
1	A	340	GLU
1	A	409	VAL
1	A	578	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	503	ASN
1	A	434	GLN
1	A	121	GLN
1	B	404	GLN
1	A	420	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	10/18 (55%)	6 (60%)	0
2	D	10/18 (55%)	7 (70%)	1 (10%)
All	All	20/36 (55%)	13 (65%)	1 (5%)

5 of 13 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	1141	G
2	C	1142	A
2	C	1144	U
2	C	1145	U
2	C	1146	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	D	1144	U

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 oligosaccharides 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>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	544/587 (92%)	-0.46	1 (0%) 91 89	15, 32, 60, 78	0
1	B	547/587 (93%)	-0.34	2 (0%) 88 85	16, 37, 69, 91	0
2	C	11/18 (61%)	0.09	0 100 100	33, 44, 92, 103	0
2	D	11/18 (61%)	0.24	0 100 100	44, 53, 114, 121	0
All	All	1113/1210 (91%)	-0.39	3 (0%) 90 88	15, 35, 67, 121	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	48	GLY	4.0
1	A	51	ALA	3.4
1	B	280	ARG	3.1

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 oligosaccharides 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.