



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 06:55 pm GMT

PDB ID : 4J0X
Title : Structure of Rrp9
Authors : Zhang, L.; Lin, J.; Ye, K.
Deposited on : 2013-01-31
Resolution : 2.50 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

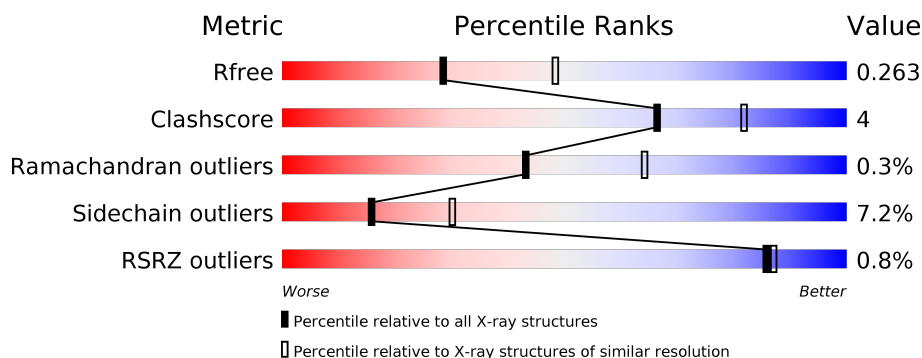
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	4155 (2.50-2.50)
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (2.50-2.50)

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. 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	451	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; left: 0; top: -10px; width: 5px; height: 5px; background-color: red;"></div> <div style="position: absolute; left: 0; top: 0; width: 68%; height: 10px; background-color: green;"></div> <div style="position: absolute; left: 68%; top: 0; width: 11%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; left: 79%; top: 0; width: 19%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; width: 100%; font-size: 0.8em;"> 68% 11% • 19% </div> </div>
1	B	451	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; left: 0; top: 0; width: 69%; height: 10px; background-color: green;"></div> <div style="position: absolute; left: 69%; top: 0; width: 11%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; left: 80%; top: 0; width: 19%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; width: 100%; font-size: 0.8em;"> 69% 11% • 19% </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5872 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 Ribosomal RNA-processing protein 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			2916	1871	506	529	10			
1	B	366	Total	C	N	O	S	0	0	0
			2924	1875	508	531	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	GLY	-	EXPRESSION TAG	UNP Q06506
A	124	PRO	-	EXPRESSION TAG	UNP Q06506
A	125	GLU	-	EXPRESSION TAG	UNP Q06506
A	126	ALA	-	EXPRESSION TAG	UNP Q06506
B	123	GLY	-	EXPRESSION TAG	UNP Q06506
B	124	PRO	-	EXPRESSION TAG	UNP Q06506
B	125	GLU	-	EXPRESSION TAG	UNP Q06506
B	126	ALA	-	EXPRESSION TAG	UNP Q06506

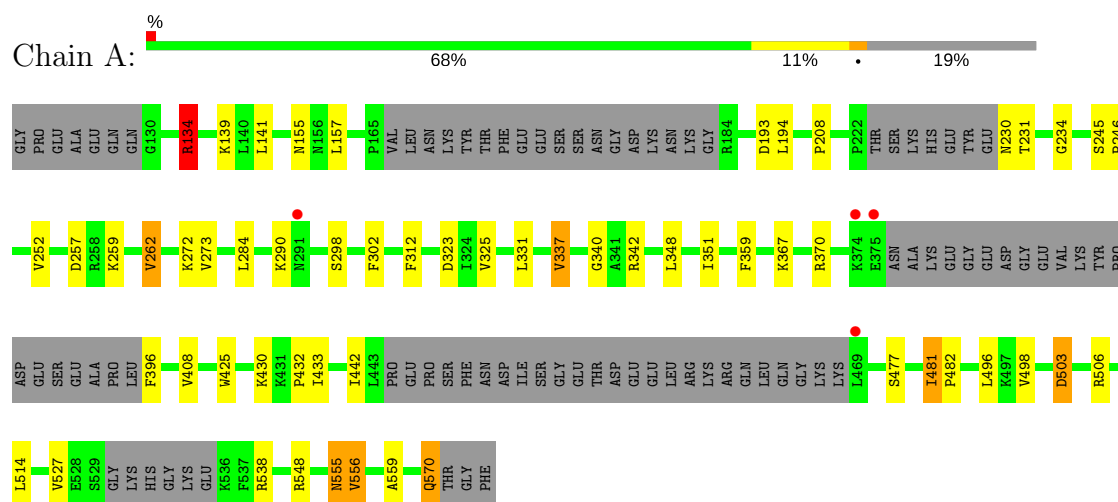
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	11	Total	O	0	0
			11	11		
2	B	21	Total	O	0	0
			21	21		

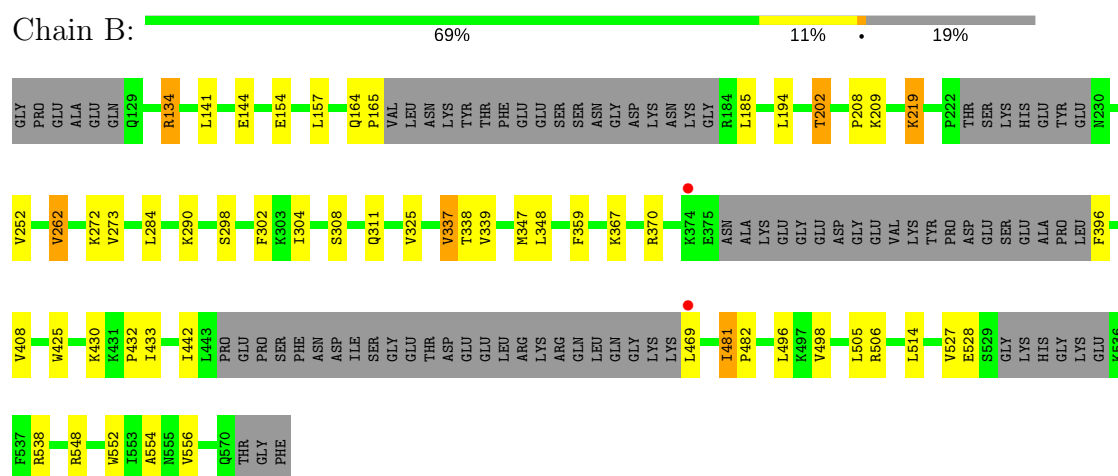
3 Residue-property plots

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: Ribosomal RNA-processing protein 9



• Molecule 1: Ribosomal RNA-processing protein 9



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	48.45Å 78.56Å 80.03Å 61.77° 86.44° 71.99°	Depositor
Resolution (Å)	19.96 – 2.50 19.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.3 (19.96-2.50) 95.3 (19.96-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.50Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.218 , 0.262 0.219 , 0.263	Depositor DCC
R_{free} test set	1642 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5872	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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.*

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	0.25	0/2975	0.51	1/4008 (0.0%)
1	B	0.25	0/2983	0.48	0/4018
All	All	0.25	0/5958	0.49	1/8026 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	ARG	NE-CZ-NH1	5.76	123.18	120.30

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	A	2916	0	2947	26	0
1	B	2924	0	2951	24	0
2	A	11	0	0	0	0
2	B	21	0	0	0	0
All	All	5872	0	5898	50	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 4.

All (50) 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:134:ARG:HH11	1:A:134:ARG:HG2	1.31	0.92
1:A:272:LYS:HG2	1:A:312:PHE:HB3	1.59	0.83
1:B:337:VAL:HG13	1:B:348:LEU:HD23	1.75	0.68
1:B:262:VAL:HG13	1:B:272:LYS:HB3	1.78	0.64
1:A:337:VAL:HG13	1:A:348:LEU:HD23	1.79	0.64
1:A:234:GLY:O	1:A:259:LYS:NZ	2.34	0.58
1:B:185:LEU:HD12	1:B:202:THR:HA	1.84	0.57
1:B:308:SER:HB3	1:B:311:GLN:HB2	1.87	0.56
1:A:262:VAL:HG13	1:A:272:LYS:HB3	1.88	0.54
1:B:165:PRO:HD2	1:B:185:LEU:HD23	1.90	0.54
1:B:185:LEU:H	1:B:202:THR:HG22	1.74	0.53
1:A:284:LEU:O	1:A:548:ARG:NH2	2.41	0.52
1:B:367:LYS:HE3	1:B:370:ARG:HH21	1.75	0.51
1:B:433:ILE:HD11	1:B:506:ARG:HG2	1.93	0.50
1:A:359:PHE:HB3	1:A:425:TRP:CZ3	2.46	0.50
1:B:134:ARG:NH2	1:B:481:ILE:HD11	2.27	0.49
1:A:134:ARG:HG2	1:A:134:ARG:NH1	2.06	0.49
1:B:284:LEU:O	1:B:548:ARG:NH2	2.45	0.49
1:B:164:GLN:NE2	1:B:528:GLU:O	2.47	0.48
1:A:323:ASP:HB3	1:A:340:GLY:O	2.14	0.48
1:A:433:ILE:HD11	1:A:506:ARG:HG2	1.95	0.48
1:A:367:LYS:HE3	1:A:370:ARG:HH21	1.77	0.48
1:B:304:ILE:HG12	1:B:338:THR:HG21	1.95	0.48
1:B:209:LYS:HB2	1:B:209:LYS:HE3	1.67	0.47
1:B:359:PHE:HB3	1:B:425:TRP:CZ3	2.49	0.47
1:B:290:LYS:HE3	1:B:290:LYS:HB3	1.74	0.47
1:A:503:ASP:OD1	1:A:503:ASP:N	2.32	0.47
1:B:425:TRP:CH2	1:B:432:PRO:HG3	2.50	0.47
1:A:139:LYS:O	1:A:570:GLN:HB3	2.15	0.46
1:A:290:LYS:HD3	1:A:331:LEU:HA	1.96	0.46
1:B:298:SER:HB2	1:B:325:VAL:HB	1.96	0.46
1:A:298:SER:HB2	1:A:325:VAL:HB	1.98	0.45
1:A:556:VAL:HG13	1:A:559:ALA:HB2	1.97	0.45
1:B:552:TRP:CH2	1:B:554:ALA:HA	2.52	0.45
1:A:481:ILE:HA	1:A:482:PRO:HD3	1.84	0.44
1:A:323:ASP:OD2	1:A:342:ARG:HB2	2.18	0.44
1:A:230:ASN:ND2	1:A:259:LYS:HG3	2.33	0.43
1:A:302:PHE:N	1:A:302:PHE:CD1	2.86	0.43
1:A:425:TRP:CZ2	1:A:432:PRO:HG3	2.53	0.43
1:A:230:ASN:ND2	1:A:257:ASP:O	2.52	0.43
1:B:481:ILE:HA	1:B:482:PRO:HD3	1.83	0.42
1:A:155:ASN:HB2	1:A:193:ASP:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:TRP:CZ2	1:B:432:PRO:HG3	2.55	0.41
1:B:302:PHE:CD1	1:B:302:PHE:N	2.87	0.41
1:A:351:ILE:HG12	1:A:351:ILE:H	1.71	0.41
1:A:208:PRO:HD3	1:A:538:ARG:NH2	2.36	0.40
1:A:245:SER:HA	1:A:246:PRO:HD3	1.88	0.40
1:B:141:LEU:HB3	1:B:144:GLU:HG2	2.03	0.40
1:B:469:LEU:HD23	1:B:469:LEU:HA	1.94	0.40
1:B:208:PRO:HD3	1:B:538:ARG:NH2	2.37	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	353/451 (78%)	341 (97%)	11 (3%)	1 (0%)	43	64
1	B	354/451 (78%)	343 (97%)	10 (3%)	1 (0%)	43	64
All	All	707/902 (78%)	684 (97%)	21 (3%)	2 (0%)	43	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	555	ASN
1	B	219	LYS

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	317/390 (81%)	294 (93%)	23 (7%)	15	29
1	B	318/390 (82%)	295 (93%)	23 (7%)	16	30
All	All	635/780 (81%)	589 (93%)	46 (7%)	16	30

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	ARG
1	A	141	LEU
1	A	157	LEU
1	A	194	LEU
1	A	231	THR
1	A	252	VAL
1	A	262	VAL
1	A	273	VAL
1	A	337	VAL
1	A	396	PHE
1	A	408	VAL
1	A	430	LYS
1	A	442	ILE
1	A	477	SER
1	A	481	ILE
1	A	496	LEU
1	A	498	VAL
1	A	503	ASP
1	A	514	LEU
1	A	527	VAL
1	A	555	ASN
1	A	556	VAL
1	A	570	GLN
1	B	134	ARG
1	B	154	GLU
1	B	157	LEU
1	B	194	LEU
1	B	202	THR
1	B	219	LYS
1	B	252	VAL
1	B	262	VAL
1	B	273	VAL
1	B	337	VAL
1	B	339	VAL

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Mol	Chain	Res	Type
1	B	347	MET
1	B	396	PHE
1	B	408	VAL
1	B	430	LYS
1	B	442	ILE
1	B	481	ILE
1	B	496	LEU
1	B	498	VAL
1	B	505	LEU
1	B	514	LEU
1	B	527	VAL
1	B	556	VAL

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 [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	365/451 (80%)	-0.24	4 (1%) 80 82	13, 31, 53, 80	0
1	B	366/451 (81%)	-0.26	2 (0%) 90 91	11, 30, 53, 79	0
All	All	731/902 (81%)	-0.25	6 (0%) 86 87	11, 30, 53, 80	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	374	LYS	3.7
1	B	469	LEU	3.2
1	A	375	GLU	2.9
1	A	291	ASN	2.6
1	A	469	LEU	2.6
1	A	374	LYS	2.2

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.