



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:41 PM UTC

PDB ID : 4XD9 / pdb_00004xd9
Title : Structure of Rpf2-Rrs1 complex involved in ribosome biogenesis
Authors : Asano, N.; Kato, K.; Yao, M.
Deposited on : 2014-12-19
Resolution : 2.35 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 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

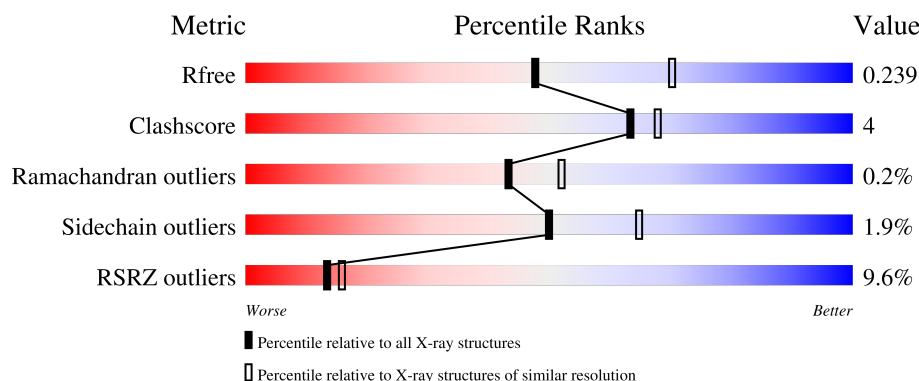
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

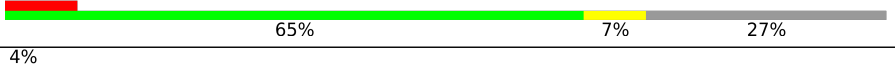
The reported resolution of this entry is 2.35 Å.

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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	323	
1	C	323	
2	B	221	
2	D	221	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5165 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 Ribosome biogenesis protein, putative (AFU_orthologue AFUA_8G04790).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	236	Total	C	N	O	S	0	0	0
			1846	1176	320	337	13			
1	C	236	Total	C	N	O	S	0	0	0
			1846	1176	320	337	13			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP C8VMF9
A	-19	ASN	-	expression tag	UNP C8VMF9
A	-18	HIS	-	expression tag	UNP C8VMF9
A	-17	LYS	-	expression tag	UNP C8VMF9
A	-16	HIS	-	expression tag	UNP C8VMF9
A	-15	HIS	-	expression tag	UNP C8VMF9
A	-14	HIS	-	expression tag	UNP C8VMF9
A	-13	HIS	-	expression tag	UNP C8VMF9
A	-12	HIS	-	expression tag	UNP C8VMF9
A	-11	HIS	-	expression tag	UNP C8VMF9
A	-10	SER	-	expression tag	UNP C8VMF9
A	-9	SER	-	expression tag	UNP C8VMF9
A	-8	GLY	-	expression tag	UNP C8VMF9
A	-7	GLU	-	expression tag	UNP C8VMF9
A	-6	ASN	-	expression tag	UNP C8VMF9
A	-5	LEU	-	expression tag	UNP C8VMF9
A	-4	TYR	-	expression tag	UNP C8VMF9
A	-3	PHE	-	expression tag	UNP C8VMF9
A	-2	GLN	-	expression tag	UNP C8VMF9
A	-1	GLY	-	expression tag	UNP C8VMF9
A	0	HIS	-	expression tag	UNP C8VMF9
C	-20	MET	-	expression tag	UNP C8VMF9
C	-19	ASN	-	expression tag	UNP C8VMF9
C	-18	HIS	-	expression tag	UNP C8VMF9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	LYS	-	expression tag	UNP C8VMF9
C	-16	HIS	-	expression tag	UNP C8VMF9
C	-15	HIS	-	expression tag	UNP C8VMF9
C	-14	HIS	-	expression tag	UNP C8VMF9
C	-13	HIS	-	expression tag	UNP C8VMF9
C	-12	HIS	-	expression tag	UNP C8VMF9
C	-11	HIS	-	expression tag	UNP C8VMF9
C	-10	SER	-	expression tag	UNP C8VMF9
C	-9	SER	-	expression tag	UNP C8VMF9
C	-8	GLY	-	expression tag	UNP C8VMF9
C	-7	GLU	-	expression tag	UNP C8VMF9
C	-6	ASN	-	expression tag	UNP C8VMF9
C	-5	LEU	-	expression tag	UNP C8VMF9
C	-4	TYR	-	expression tag	UNP C8VMF9
C	-3	PHE	-	expression tag	UNP C8VMF9
C	-2	GLN	-	expression tag	UNP C8VMF9
C	-1	GLY	-	expression tag	UNP C8VMF9
C	0	HIS	-	expression tag	UNP C8VMF9

- Molecule 2 is a protein called Ribosome biogenesis protein (Rrs1), putative (AFU_orthologue AFUA_7G04430).

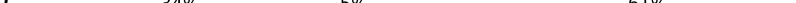
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	88	Total	C	N	O	S	0	0	0
			665	425	113	126	1			
2	D	86	Total	C	N	O	S	0	0	0
			645	414	108	122	1			

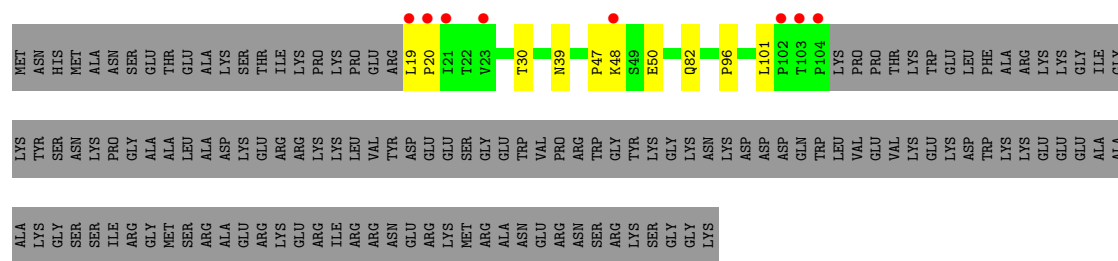
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	MET	-	expression tag	UNP Q5B6T5
B	-1	ASN	-	expression tag	UNP Q5B6T5
B	0	HIS	-	expression tag	UNP Q5B6T5
D	-2	MET	-	expression tag	UNP Q5B6T5
D	-1	ASN	-	expression tag	UNP Q5B6T5
D	0	HIS	-	expression tag	UNP Q5B6T5

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	55	Total 55	O 55	0	0
3	B	14	Total 14	O 14	0	0
3	C	76	Total 76	O 76	0	0
3	D	18	Total 18	O 18	0	0

- Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.16Å 123.59Å 133.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.10 – 2.35 42.10 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.4 (42.10-2.35) 99.6 (42.10-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.192 , 0.235 0.201 , 0.239	Depositor DCC
R_{free} test set	1910 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5165	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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

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	0.30	0/1884	0.76	2/2542 (0.1%)
1	C	0.30	0/1884	0.80	4/2542 (0.2%)
2	B	0.29	0/682	0.81	2/940 (0.2%)
2	D	0.29	0/662	0.84	2/914 (0.2%)
All	All	0.30	0/5112	0.79	10/6938 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	101	LEU	CA-C-N	7.90	128.37	119.92
2	D	101	LEU	C-N-CA	7.90	128.37	119.92
1	C	195	GLU	CA-C-N	6.54	126.72	120.31
1	C	195	GLU	C-N-CA	6.54	126.72	120.31
1	C	68	HIS	CA-C-N	5.99	126.14	119.32
1	C	68	HIS	C-N-CA	5.99	126.14	119.32
1	A	38	CYS	CA-C-N	5.96	126.30	119.92
1	A	38	CYS	C-N-CA	5.96	126.30	119.92
2	B	19	LEU	CA-C-N	5.76	125.95	119.90
2	B	19	LEU	C-N-CA	5.76	125.95	119.90

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	1846	0	1898	20	0
1	C	1846	0	1898	12	0
2	B	665	0	697	7	0
2	D	645	0	678	6	0
3	A	55	0	0	2	0
3	B	14	0	0	0	0
3	C	76	0	0	0	0
3	D	18	0	0	0	0
All	All	5165	0	5171	41	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 (41) 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:19:LEU:HD23	2:B:20:PRO:HD2	1.76	0.67
1:A:122:ASP:OD2	1:A:127:GLY:N	2.30	0.63
1:A:19:LYS:NZ	3:A:402:HOH:O	2.24	0.63
1:A:123:ALA:O	1:A:124:ASN:HB2	2.00	0.61
2:D:19:LEU:HD23	2:D:20:PRO:HD2	1.83	0.61
1:C:62:LYS:NZ	1:C:65:GLU:O	2.36	0.57
1:C:222:ARG:HG2	2:D:19:LEU:HD13	1.86	0.56
1:A:34:HIS:ND1	3:A:403:HOH:O	2.33	0.55
1:C:122:ASP:OD1	1:C:123:ALA:N	2.44	0.50
2:B:82:GLN:OE1	2:B:82:GLN:N	2.44	0.49
1:C:202:PRO:HG2	1:C:236:VAL:HB	1.95	0.49
1:A:99:ASN:HB3	1:A:119:LEU:HB3	1.95	0.48
1:A:189:LEU:HD13	1:A:208:TRP:CE2	2.48	0.48
1:C:189:LEU:HD13	1:C:208:TRP:CE2	2.49	0.48
1:A:247:MET:HE2	1:A:251:MET:HG2	1.94	0.48
1:A:122:ASP:OD1	1:A:123:ALA:N	2.39	0.47
1:C:114:MET:HB2	1:C:240:GLN:HB3	1.98	0.46
1:A:19:LYS:N	1:A:19:LYS:HD3	2.30	0.46
2:B:21:ILE:O	2:B:69:ASN:ND2	2.40	0.45
2:D:82:GLN:N	2:D:82:GLN:OE1	2.49	0.45
2:B:101:LEU:HA	2:B:102:PRO:HD3	1.91	0.44
1:A:145:LEU:HD11	1:A:185:LEU:HD22	1.98	0.44
1:A:247:MET:HE1	2:B:96:PRO:HB3	1.99	0.44
1:C:200:LEU:HD12	1:C:200:LEU:O	2.18	0.43
1:C:34:HIS:HB2	1:C:38:CYS:HB2	2.01	0.43
1:A:131:MET:HE1	1:A:229:GLY:HA2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:GLY:HA3	1:C:200:LEU:HA	1.58	0.42
1:A:87:MET:HE2	1:A:87:MET:HB3	1.82	0.42
1:A:220:LEU:O	2:B:21:ILE:HG21	2.19	0.42
2:B:30:THR:OG1	2:B:39:ASN:HB2	2.19	0.42
2:D:47:PRO:HG2	2:D:50:GLU:HB2	2.01	0.42
1:A:248:LYS:HA	1:A:248:LYS:HD3	1.49	0.41
1:A:202:PRO:HG2	1:A:236:VAL:HB	2.02	0.41
1:A:42:LEU:HD22	1:A:101:LEU:HD13	2.03	0.41
1:C:247:MET:HE1	2:D:96:PRO:HB3	2.03	0.41
2:D:30:THR:OG1	2:D:39:ASN:HB2	2.21	0.41
1:A:76:LEU:HD22	1:A:76:LEU:HA	1.96	0.41
1:A:214:LYS:HE2	1:A:214:LYS:HB2	1.90	0.41
1:C:209:TYR:HB3	1:C:225:LEU:HB3	2.03	0.41
1:A:42:LEU:HD23	1:A:42:LEU:HA	1.88	0.40
1:C:61:HIS:CD2	1:C:61:HIS:C	3.00	0.40

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	234/323 (72%)	230 (98%)	3 (1%)	1 (0%)	30	34
1	C	234/323 (72%)	228 (97%)	6 (3%)	0	100	100
2	B	86/221 (39%)	85 (99%)	1 (1%)	0	100	100
2	D	84/221 (38%)	82 (98%)	2 (2%)	0	100	100
All	All	638/1088 (59%)	625 (98%)	12 (2%)	1 (0%)	43	52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	ASN

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	207/281 (74%)	202 (98%)	5 (2%)	43	57
1	C	207/281 (74%)	202 (98%)	5 (2%)	43	57
2	B	80/192 (42%)	80 (100%)	0	100	100
2	D	78/192 (41%)	77 (99%)	1 (1%)	61	76
All	All	572/946 (60%)	561 (98%)	11 (2%)	50	65

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	76	LEU
1	A	183	GLU
1	A	212	VAL
1	A	248	LYS
1	C	33	LEU
1	C	76	LEU
1	C	126	GLU
1	C	200	LEU
1	C	248	LYS
2	D	48	LYS

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

Mol	Chain	Res	Type
1	A	34	HIS
1	C	22	GLN
1	C	43	HIS
1	C	218	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 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 ⓘ

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(Å ²)	Q<0.9
1	A	236/323 (73%)	0.57	20 (8%) 16 18	37, 55, 94, 116	0
1	C	236/323 (73%)	0.49	26 (11%) 10 12	34, 51, 93, 115	0
2	B	88/221 (39%)	0.63	8 (9%) 15 17	42, 55, 89, 116	0
2	D	86/221 (38%)	0.48	8 (9%) 14 17	36, 49, 85, 124	0
All	All	646/1088 (59%)	0.54	62 (9%) 13 16	34, 53, 93, 124	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	198	ALA	6.4
1	A	123	ALA	6.0
2	D	103	THR	5.9
1	C	200	LEU	5.8
1	A	125	GLY	5.2
2	B	19	LEU	5.0
2	D	19	LEU	5.0
1	C	199	GLY	4.9
2	B	104	PRO	4.9
2	D	104	PRO	4.2
1	C	125	GLY	4.2
1	C	124	ASN	4.2
2	B	103	THR	3.9
1	C	66	ASN	3.5
1	A	127	GLY	3.5
1	C	21	PRO	3.4
1	C	197	THR	3.4
1	A	38	CYS	3.4
2	D	102	PRO	3.3
1	C	35	GLY	3.3
1	A	124	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	64	ASN	3.3
1	A	254	GLY	3.2
1	C	219	LYS	3.1
1	C	122	ASP	3.1
2	D	21	ILE	3.0
2	D	20	PRO	3.0
1	C	254	GLY	2.7
1	A	63	LYS	2.7
1	A	121	PRO	2.7
1	C	196	PRO	2.7
1	A	197	THR	2.7
1	C	218	HIS	2.6
1	A	19	LYS	2.6
1	A	141	GLY	2.6
1	A	128	ILE	2.6
1	A	216	SER	2.6
1	C	217	GLY	2.6
1	A	66	ASN	2.5
1	C	137	HIS	2.5
2	B	23	VAL	2.4
2	D	23	VAL	2.4
1	A	200	LEU	2.4
1	C	61	HIS	2.3
1	C	216	SER	2.3
1	C	33	LEU	2.3
1	A	60	PHE	2.2
1	C	60	PHE	2.2
1	C	39	PRO	2.2
1	A	214	LYS	2.2
1	C	123	ALA	2.2
2	D	48	LYS	2.2
1	A	248	LYS	2.2
1	C	37	LYS	2.2
1	A	201	ALA	2.1
1	A	39	PRO	2.1
2	B	102	PRO	2.1
2	B	18	ARG	2.1
1	C	34	HIS	2.1
2	B	22	THR	2.0
2	B	48	LYS	2.0
1	C	65	GLU	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 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.