



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2026 – 09:06 PM UTC

PDB ID : 2V3C / pdb_00002v3c
Title : Crystal structure of the SRP54-SRP19-7S.S SRP RNA complex of M. jannaschii
Authors : Hainzl, T.; Huang, S.; Sauer-Eriksson, A.E.
Deposited on : 2007-06-15
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 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	:	FAILED
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

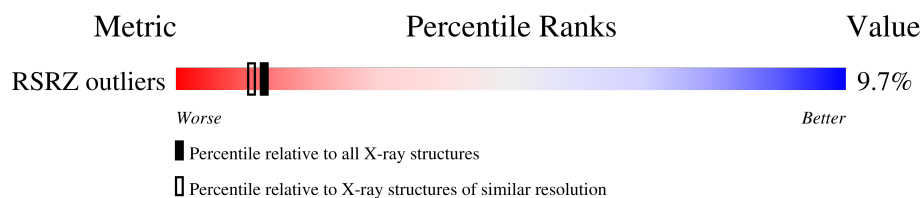
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
RSRZ outliers	180081	5833 (2.50-2.50)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12336 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 SIGNAL RECOGNITION PARTICLE 19 KDA PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	87	Total	C	N	O	S	0	0	0
			727	468	130	125	4			
1	B	87	Total	C	N	O	S	0	0	0
			727	468	130	125	4			

- Molecule 2 is a protein called SIGNAL RECOGNITION 54 KDA PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	404	Total	C	N	O	S	0	0	1
			3149	1998	541	600	10			
2	D	402	Total	C	N	O	S	0	0	1
			3133	1989	538	597	9			

- Molecule 3 is a RNA chain called 7S RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	96	Total	C	N	O	P	0	0	0
			2063	919	385	664	95			
3	N	96	Total	C	N	O	P	0	0	0
			2063	919	385	664	95			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total	O	0	0
			23	23		
4	B	26	Total	O	0	0
			26	26		
4	C	107	Total	O	0	0
			107	107		
4	D	107	Total	O	0	0
			107	107		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	92	Total 92	O 92	0	0
4	N	119	Total 119	O 119	0	0

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3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.29Å 129.40Å 163.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.50) 98.1 (20.00-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.244 , 0.294 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	57.8	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 74.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12336	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.55% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

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4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 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	87/87 (100%)	0.22	1 (1%) 78 75	27, 42, 50, 53	0
1	B	87/87 (100%)	0.23	1 (1%) 78 75	27, 42, 53, 62	0
2	C	404/432 (93%)	0.77	46 (11%) 10 8	29, 57, 77, 88	0
2	D	402/432 (93%)	1.17	66 (16%) 4 3	31, 67, 80, 89	0
3	M	96/96 (100%)	-0.44	0 100 100	18, 37, 50, 61	0
3	N	96/96 (100%)	-0.39	0 100 100	20, 37, 52, 70	0
All	All	1172/1230 (95%)	0.63	114 (9%) 13 11	18, 56, 77, 89	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	324	GLY	6.1
2	C	314	THR	4.6
2	C	310	VAL	4.1
2	D	261	ALA	4.1
2	C	30	VAL	4.0
2	D	141	PRO	3.8
2	D	19	ALA	3.7
2	D	155	HIS	3.7
2	D	34	ILE	3.7
1	B	87	ASN	3.7
2	D	280	ASP	3.7
2	C	182	ALA	3.5
2	D	95	LEU	3.5
2	D	199	LEU	3.5
2	D	251	GLY	3.5
2	D	102	VAL	3.3
2	D	142	ALA	3.2
2	D	262	VAL	3.2
2	C	203	MET	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	297	GLY	3.0
2	D	120	LEU	3.0
2	C	279	ASP	3.0
2	D	198	GLY	3.0
2	C	337	ALA	3.0
2	C	326	PHE	3.0
2	C	315	GLU	2.9
2	D	86	LEU	2.9
2	D	327	THR	2.9
2	D	97	PRO	2.9
2	D	233	ALA	2.9
1	A	87	ASN	2.8
2	C	340	ASN	2.8
2	C	302	LEU	2.8
2	C	160	GLY	2.8
2	C	318	ILE	2.8
2	C	329	ASN	2.8
2	D	337	ALA	2.7
2	D	40	GLN	2.7
2	D	206	ILE	2.7
2	C	317	SER	2.7
2	C	68	LEU	2.7
2	D	135	ALA	2.7
2	C	307	GLU	2.7
2	D	241	ILE	2.7
2	D	310	VAL	2.7
2	C	320	ALA	2.7
2	C	308	ASP	2.7
2	C	180	LYS	2.6
2	D	300	GLU	2.6
2	D	118	ALA	2.6
2	D	103	ILE	2.6
2	C	303	LEU	2.6
2	D	218	VAL	2.5
2	D	12	ALA	2.5
2	D	151	ALA	2.5
2	D	231	ALA	2.5
2	C	316	GLU	2.5
2	C	200	LEU	2.5
2	D	93	LEU	2.5
2	C	190	ALA	2.5
2	D	163	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	304	GLU	2.4
2	C	92	LYS	2.4
2	C	321	ILE	2.4
2	D	410	VAL	2.4
2	C	333	THR	2.4
2	D	42	ASP	2.4
2	D	143	ALA	2.4
2	D	156	VAL	2.4
2	D	65	PRO	2.3
2	D	157	PRO	2.3
2	D	133	LEU	2.3
2	C	181	LYS	2.3
2	D	222	THR	2.3
2	D	67	GLY	2.3
2	D	242	GLY	2.3
2	D	278	ILE	2.3
2	D	331	LEU	2.3
2	D	22	VAL	2.3
2	D	117	ALA	2.3
2	D	131	PRO	2.3
2	C	402	GLY	2.3
2	C	163	THR	2.3
2	D	160	GLY	2.3
2	C	117	ALA	2.2
2	C	338	ILE	2.2
2	D	187	ILE	2.2
2	D	301	SER	2.2
2	D	317	SER	2.2
2	C	410	VAL	2.2
2	C	323	ARG	2.2
2	D	44	ASN	2.2
2	D	258	ALA	2.2
2	C	239	GLY	2.2
2	D	31	ILE	2.2
2	C	97	PRO	2.2
2	D	78	VAL	2.1
2	D	320	ALA	2.1
2	C	290	ILE	2.1
2	C	312	GLU	2.1
2	D	318	ILE	2.1
2	D	98	LYS	2.1
2	C	331	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	101	ASN	2.1
2	C	285	ASP	2.1
2	D	18	ALA	2.0
2	D	263	ALA	2.0
2	D	316	GLU	2.0
2	C	34	ILE	2.0
2	D	159	TYR	2.0
2	C	258	ALA	2.0
2	D	121	ALA	2.0
2	C	276	GLU	2.0
2	D	209	ILE	2.0

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

There are no ligands in this entry.

5.5 Other polymers [i](#)

There are no such residues in this entry.