Full wwPDB EM Validation Report ⓘ

Jun 18, 2025 – 06:24 PM JST

PDB ID	:	9IS7 / pdb_00009is7
EMDB ID	:	EMD-60833
Title	:	Paracandidimonas lactea CP group II intron 2S state
Authors	:	Wang, L.; Xie, J.H.; Zhang, C.; Zou, J.; Huang, Z.; Shang, S.; Chen, X.; Yang, Y.; Liu, J.; Dong, H.; Huang, D.; Su, Z.
Deposited on	:	2024-07-17
Resolution	:	2.87 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

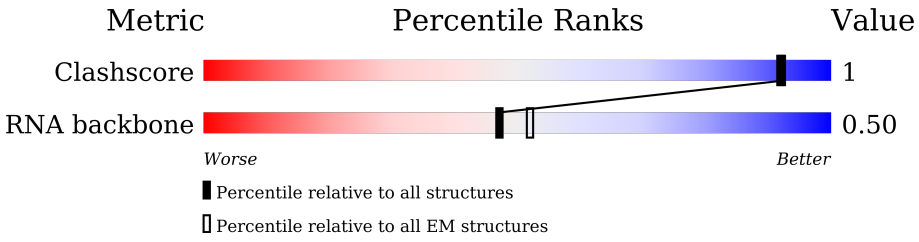
EMDB validation analysis	:	FAILED
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.87 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)	EM structures (#Entries)
Clashscore	210492	15764
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	153	57% 18% 5% 20%
2	B	582	74% 23% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15216 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 RNA chain called RNA (153-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	123	2636	1174	488	851	123	0	0

- Molecule 2 is a RNA chain called RNA (582-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	582	12547	5586	2340	4039	582	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
3	A	4	4	4	0
3	B	25	25	25	0

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

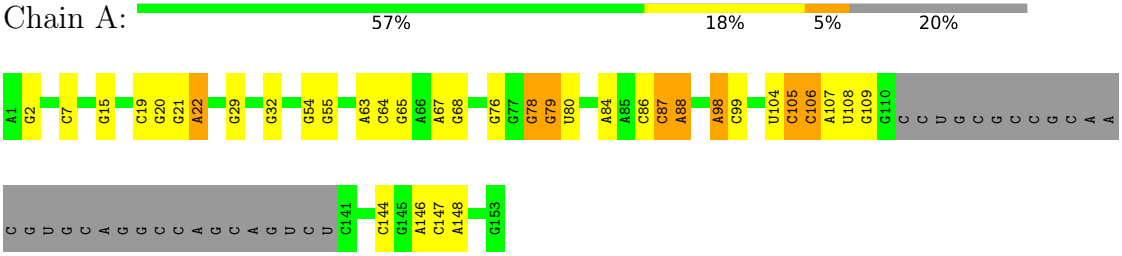
Mol	Chain	Residues	Atoms		AltConf
			Total	K	
4	A	2	2	2	0
4	B	2	2	2	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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.

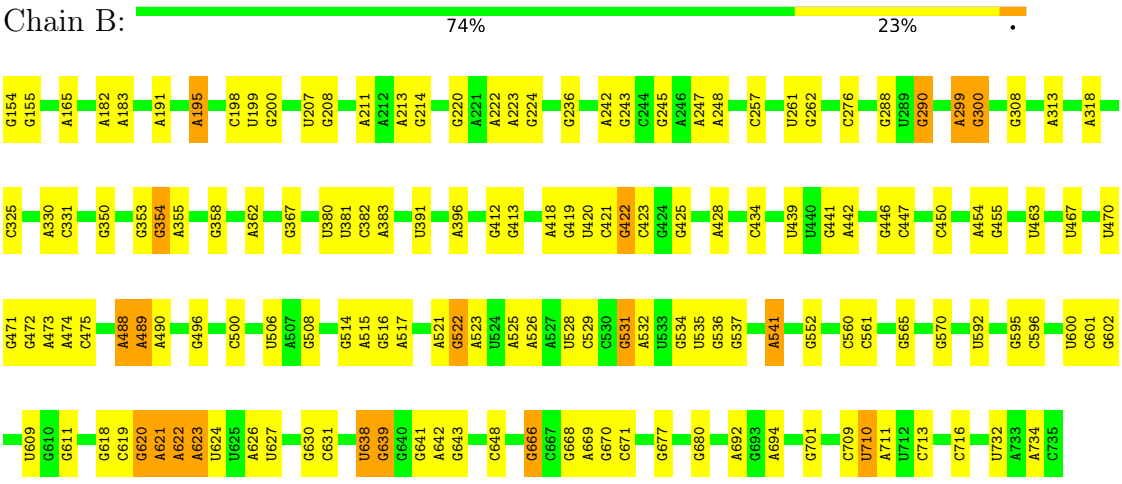
- Molecule 1: RNA (153-MER)

Chain A:



- Molecule 2: RNA (582-MER)

Chain B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33739	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	58	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, K

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	0.11	0/2947	0.26	0/4593
2	B	0.18	0/14058	0.32	0/21946
All	All	0.17	0/17005	0.31	0/26539

There are no bond length outliers.

There are no bond angle outliers.

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	2636	0	1340	6	0
2	B	12547	0	6301	23	0
3	A	4	0	0	0	0
3	B	25	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
All	All	15216	0	7641	27	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 1.

All (27) 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:78:G:O2'	1:A:79:G:O5'	2.06	0.73
2:B:353:G:OP1	2:B:354:G:N2	2.24	0.70
2:B:450:C:H42	2:B:531:G:H1	1.40	0.69
1:A:87:C:O2'	1:A:88:A:OP1	2.11	0.66
2:B:257:C:O2'	2:B:488:A:N3	2.32	0.63
2:B:380:U:N3	2:B:383:A:OP2	2.39	0.56
1:A:98:A:O2'	2:B:154:G:OP2	2.20	0.55
2:B:198:C:OP2	2:B:199:U:O2'	2.21	0.53
1:A:105:C:O2'	1:A:106:C:O5'	2.24	0.53
2:B:536:G:H2'	2:B:537:G:H8	1.74	0.52
2:B:521:A:O2'	2:B:522:G:N2	2.38	0.51
2:B:709:C:O2'	2:B:710:U:O5'	2.27	0.51
2:B:620:G:C2	2:B:621:A:H1'	2.46	0.51
2:B:439:U:O4'	2:B:541:A:N6	2.45	0.50
2:B:299:A:O2'	2:B:300:G:OP1	2.23	0.49
2:B:666:G:N2	2:B:669:A:OP2	2.45	0.47
2:B:245:G:N2	2:B:248:A:OP2	2.48	0.46
2:B:421:C:H2'	2:B:422:G:O4'	2.16	0.46
1:A:22:A:H61	2:B:734:A:H2	1.64	0.45
2:B:236:G:H21	2:B:489:A:H2	1.65	0.45
1:A:78:G:HO2'	1:A:79:G:P	2.37	0.44
2:B:290:G:N3	2:B:592:U:O2'	2.51	0.43
2:B:534:G:H2'	2:B:535:U:C6	2.54	0.42
2:B:622:A:H3'	2:B:623:A:H8	1.84	0.42
2:B:638:U:O2'	2:B:639:G:OP1	2.36	0.41
2:B:412:G:O2'	2:B:434:C:OP2	2.25	0.40
2:B:195:A:N3	2:B:570:G:O2'	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein molecules in this entry.

5.3.2 Protein sidechains (i)

There are no protein molecules in this entry.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	121/153 (79%)	35 (28%)	1 (0%)
2	B	581/582 (99%)	123 (21%)	5 (0%)
All	All	702/735 (95%)	158 (22%)	6 (0%)

All (158) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	G
1	A	7	C
1	A	15	G
1	A	19	C
1	A	20	G
1	A	21	G
1	A	22	A
1	A	29	G
1	A	32	G
1	A	54	G
1	A	55	G
1	A	63	A
1	A	64	C
1	A	65	G
1	A	67	A
1	A	68	G
1	A	76	G
1	A	78	G
1	A	79	G
1	A	80	U
1	A	84	A
1	A	86	C
1	A	88	A
1	A	98	A
1	A	99	C
1	A	104	U
1	A	105	C
1	A	106	C
1	A	107	A
1	A	108	U
1	A	109	G
1	A	144	C
1	A	146	A
1	A	147	C

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Mol	Chain	Res	Type
1	A	148	A
2	B	155	G
2	B	165	A
2	B	182	A
2	B	183	A
2	B	191	A
2	B	195	A
2	B	200	G
2	B	207	U
2	B	208	G
2	B	211	A
2	B	213	A
2	B	214	G
2	B	220	G
2	B	222	A
2	B	223	A
2	B	224	G
2	B	242	A
2	B	243	G
2	B	247	A
2	B	261	U
2	B	262	G
2	B	276	C
2	B	288	G
2	B	290	G
2	B	300	G
2	B	308	G
2	B	313	A
2	B	318	A
2	B	325	C
2	B	330	A
2	B	331	C
2	B	350	G
2	B	354	G
2	B	355	A
2	B	358	G
2	B	362	A
2	B	367	G
2	B	381	U
2	B	382	C
2	B	391	U
2	B	396	A

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Mol	Chain	Res	Type
2	B	413	G
2	B	418	A
2	B	419	G
2	B	420	U
2	B	422	G
2	B	423	C
2	B	425	G
2	B	428	A
2	B	441	G
2	B	442	A
2	B	446	G
2	B	447	C
2	B	454	A
2	B	455	G
2	B	463	U
2	B	467	U
2	B	470	U
2	B	471	G
2	B	472	G
2	B	473	A
2	B	474	A
2	B	475	C
2	B	488	A
2	B	489	A
2	B	490	A
2	B	496	G
2	B	500	C
2	B	506	U
2	B	508	G
2	B	514	G
2	B	515	A
2	B	516	G
2	B	517	A
2	B	522	G
2	B	523	A
2	B	525	A
2	B	526	A
2	B	528	U
2	B	529	C
2	B	531	G
2	B	532	A
2	B	541	A

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Mol	Chain	Res	Type
2	B	552	G
2	B	561	C
2	B	565	G
2	B	595	G
2	B	596	C
2	B	600	U
2	B	601	C
2	B	602	G
2	B	609	U
2	B	611	G
2	B	618	G
2	B	619	C
2	B	620	G
2	B	621	A
2	B	622	A
2	B	623	A
2	B	624	U
2	B	626	A
2	B	627	U
2	B	630	G
2	B	631	C
2	B	639	G
2	B	641	G
2	B	642	A
2	B	643	G
2	B	648	C
2	B	666	G
2	B	668	G
2	B	670	G
2	B	671	C
2	B	677	G
2	B	680	G
2	B	692	A
2	B	694	A
2	B	701	G
2	B	710	U
2	B	711	A
2	B	713	C
2	B	716	C
2	B	732	U

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	87	C
2	B	299	A
2	B	381	U
2	B	418	A
2	B	560	C
2	B	638	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)

Of 33 ligands modelled in this entry, 33 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.