



Full wwPDB EM Validation Report ⓘ

Oct 19, 2025 – 12:15 AM JST

PDB ID : 9LE5 / pdb_00009le5
EMDB ID : EMD-63015
Title : Focused asymmetric unit of UCC118 Rool RNA
Authors : Zhang, K.; Li, S.
Deposited on : 2025-01-07
Resolution : 2.58 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 Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

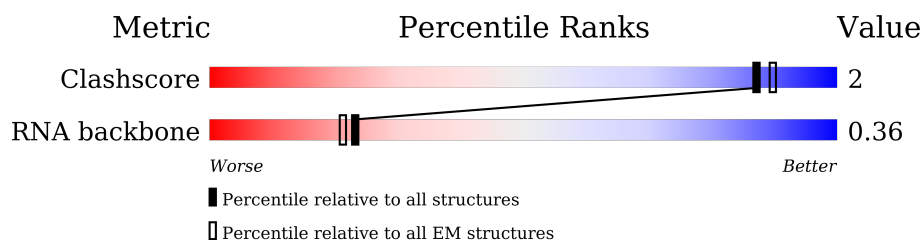
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY


The reported resolution of this entry is 2.58 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	520	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10633 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 UCC118 Rool RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	498	Total	C	N	O	P	0	0
			10633	4760	1919	3456	498		

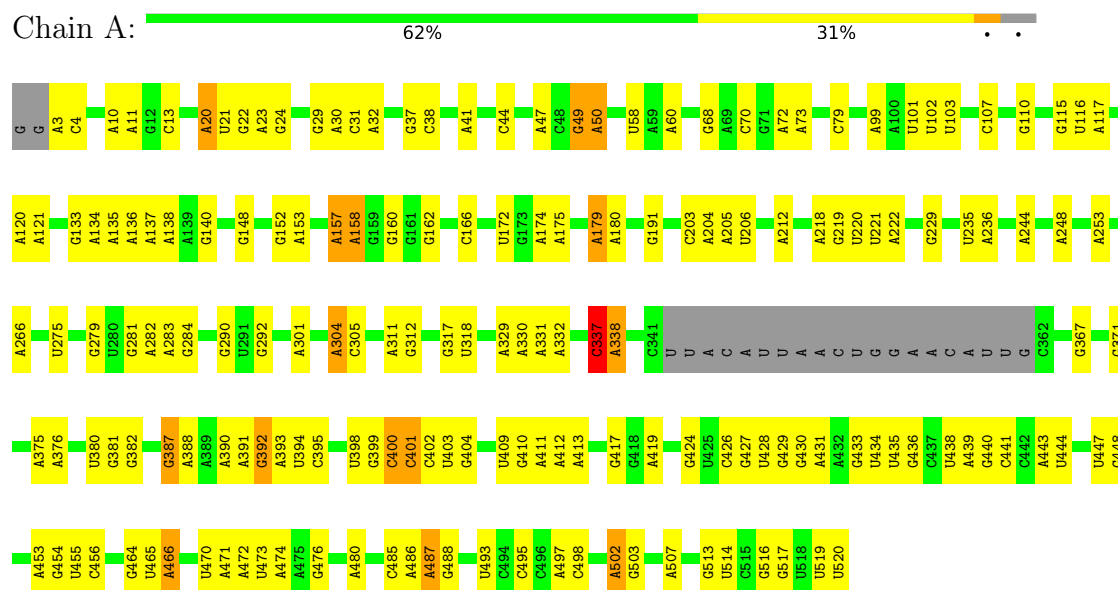
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	G	U	conflict	GB 90821902

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: UCC118 Rool RNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	3025782	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 ($e^-/\text{\AA}^2$)	46	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

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	0.36	0/11905	0.52	2/18548 (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	A	304	A	P-O3'-C3'	5.66	128.69	120.20
1	A	337	C	O4'-C1'-N1	5.08	115.81	108.20

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	10633	0	5349	25	0
All	All	10633	0	5349	25	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 2.

All (25) 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:427:G:H1	1:A:444:U:H3	1.29	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:A:H8	1:A:471:A:H61	1.40	0.68
1:A:23:A:H2	1:A:37:G:H21	1.44	0.64
1:A:427:G:N2	1:A:444:U:O2	2.32	0.61
1:A:381:G:H1	1:A:401:C:H5	1.49	0.60
1:A:329:A:H5''	1:A:330:A:H5'	1.84	0.60
1:A:502:A:H8	1:A:507:A:H62	1.49	0.60
1:A:20:A:H2	1:A:497:A:H61	1.53	0.57
1:A:172:U:H3	1:A:480:A:H62	1.53	0.57
1:A:179:A:H2'	1:A:466:A:H61	1.74	0.53
1:A:157:A:H1'	1:A:158:A:H5''	1.97	0.47
1:A:382:G:H1	1:A:400:C:H41	1.62	0.47
1:A:431:A:N6	1:A:441:C:N3	2.63	0.46
1:A:382:G:H22	1:A:400:C:H5	1.64	0.46
1:A:133:G:N2	1:A:140:G:O6	2.49	0.45
1:A:387:G:H22	1:A:392:G:H1	1.66	0.44
1:A:3:A:H2'	1:A:4:C:C6	2.53	0.44
1:A:392:G:O2'	1:A:394:U:OP2	2.35	0.43
1:A:152:G:H2'	1:A:153:A:C8	2.54	0.42
1:A:426:C:H2'	1:A:427:G:H8	1.84	0.42
1:A:337:C:HO2'	1:A:338:A:H8	1.68	0.42
1:A:79:C:O2'	1:A:266:A:H8	2.03	0.41
1:A:49:G:H2'	1:A:50:A:C8	2.57	0.40
1:A:486:A:O2'	1:A:487:A:O4'	2.39	0.40
1:A:393:A:N6	1:A:472:A:H2'	2.37	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	496/520 (95%)	146 (29%)	8 (1%)

All (146) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	11	A
1	A	13	C
1	A	20	A
1	A	21	U
1	A	22	G
1	A	24	G
1	A	29	G
1	A	30	A
1	A	31	C
1	A	32	A
1	A	38	C
1	A	41	A
1	A	44	C
1	A	47	A
1	A	49	G
1	A	50	A
1	A	58	U
1	A	60	A
1	A	68	G
1	A	70	C
1	A	72	A
1	A	73	A
1	A	99	A
1	A	101	U
1	A	102	U
1	A	103	U
1	A	107	C
1	A	110	G
1	A	116	U
1	A	117	A
1	A	120	A
1	A	121	A
1	A	134	A
1	A	135	A
1	A	136	A
1	A	137	A
1	A	138	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	148	G
1	A	157	A
1	A	158	A
1	A	160	G
1	A	162	G
1	A	166	C
1	A	174	A
1	A	175	A
1	A	179	A
1	A	180	A
1	A	191	G
1	A	203	C
1	A	204	A
1	A	205	A
1	A	206	U
1	A	212	A
1	A	218	A
1	A	219	G
1	A	220	U
1	A	221	U
1	A	222	A
1	A	229	G
1	A	235	U
1	A	236	A
1	A	244	A
1	A	248	A
1	A	253	A
1	A	275	U
1	A	279	G
1	A	281	G
1	A	282	A
1	A	283	A
1	A	284	G
1	A	290	G
1	A	292	G
1	A	301	A
1	A	305	C
1	A	311	A
1	A	312	G
1	A	317	G
1	A	318	U
1	A	331	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	332	A
1	A	337	C
1	A	338	A
1	A	367	G
1	A	371	G
1	A	375	A
1	A	376	A
1	A	380	U
1	A	387	G
1	A	388	A
1	A	390	A
1	A	391	A
1	A	392	G
1	A	395	C
1	A	398	U
1	A	399	G
1	A	400	C
1	A	401	C
1	A	402	C
1	A	403	U
1	A	404	G
1	A	409	U
1	A	410	G
1	A	411	A
1	A	412	A
1	A	413	A
1	A	417	G
1	A	419	A
1	A	424	G
1	A	428	U
1	A	429	G
1	A	430	G
1	A	433	G
1	A	434	U
1	A	435	U
1	A	436	G
1	A	438	U
1	A	439	A
1	A	440	G
1	A	443	A
1	A	447	U
1	A	448	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	453	A
1	A	454	G
1	A	455	U
1	A	456	C
1	A	464	G
1	A	465	U
1	A	466	A
1	A	470	U
1	A	473	U
1	A	474	A
1	A	476	G
1	A	485	C
1	A	487	A
1	A	488	G
1	A	493	U
1	A	495	C
1	A	498	C
1	A	502	A
1	A	503	G
1	A	514	U
1	A	516	G
1	A	517	G
1	A	519	U
1	A	520	U

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	115	G
1	A	203	C
1	A	204	A
1	A	218	A
1	A	304	A
1	A	399	G
1	A	412	A
1	A	513	G

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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.