



wwPDB EM Validation Summary Report ⓘ

Mar 19, 2026 – 11:59 PM UTC

PDB ID : 9S1F / pdb_00009s1f
EMDB ID : EMD-54448
Title : Cryo-EM structure of activated retron Eco2 (Ec67)
Authors : Skorupskaite, A.; Jasnauskaite, M.; Grigaitis, R.; Malinauskaite, L.; Pausch, P.
Deposited on : 2025-07-18
Resolution : 2.90 Å(reported)
Based on initial model : .

This is a wwPDB EM Validation Summary 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 : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

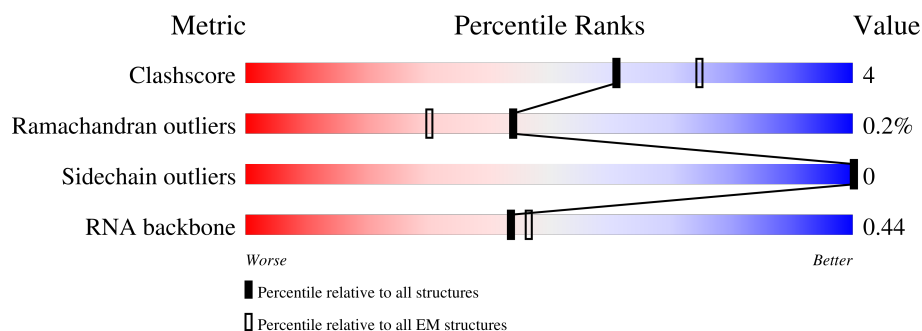
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

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	D	132	
1	E	132	
1	F	132	
2	A	596	
2	B	596	
2	C	596	
3	G	67	

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Mol	Chain	Length	Quality of chain
3	H	67	 28% 69%
3	I	67	 24% 6% 70%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 34918 atoms, of which 16504 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 (132-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
1	D	52	Total	C	H	N	O	P	0	0
			1674	498	557	202	365	52		
1	E	51	Total	C	H	N	O	P	0	0
			1640	488	546	197	358	51		
1	F	52	Total	C	H	N	O	P	0	0
			1674	498	557	202	365	52		

- Molecule 2 is a protein called Retron Ec67 protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	570	Total	C	H	N	O	S	0	0
			9328	2957	4712	791	848	20		
2	A	570	Total	C	H	N	O	S	0	0
			9328	2957	4712	791	848	20		
2	C	570	Total	C	H	N	O	S	0	0
			9328	2957	4712	791	848	20		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	587	GLY	-	expression tag	UNP P21325
B	588	SER	-	expression tag	UNP P21325
B	589	TRP	-	expression tag	UNP P21325
B	590	SER	-	expression tag	UNP P21325
B	591	HIS	-	expression tag	UNP P21325
B	592	PRO	-	expression tag	UNP P21325
B	593	GLN	-	expression tag	UNP P21325
B	594	PHE	-	expression tag	UNP P21325
B	595	GLU	-	expression tag	UNP P21325
B	596	LYS	-	expression tag	UNP P21325
A	587	GLY	-	expression tag	UNP P21325
A	588	SER	-	expression tag	UNP P21325
A	589	TRP	-	expression tag	UNP P21325

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Chain	Residue	Modelled	Actual	Comment	Reference
A	590	SER	-	expression tag	UNP P21325
A	591	HIS	-	expression tag	UNP P21325
A	592	PRO	-	expression tag	UNP P21325
A	593	GLN	-	expression tag	UNP P21325
A	594	PHE	-	expression tag	UNP P21325
A	595	GLU	-	expression tag	UNP P21325
A	596	LYS	-	expression tag	UNP P21325
C	587	GLY	-	expression tag	UNP P21325
C	588	SER	-	expression tag	UNP P21325
C	589	TRP	-	expression tag	UNP P21325
C	590	SER	-	expression tag	UNP P21325
C	591	HIS	-	expression tag	UNP P21325
C	592	PRO	-	expression tag	UNP P21325
C	593	GLN	-	expression tag	UNP P21325
C	594	PHE	-	expression tag	UNP P21325
C	595	GLU	-	expression tag	UNP P21325
C	596	LYS	-	expression tag	UNP P21325

- Molecule 3 is a DNA chain called msDNA (67-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
3	G	21	Total	C	H	N	O	P	0	0
			657	201	240	63	132	21		
3	I	20	Total	C	H	N	O	P	0	0
			625	191	228	61	125	20		
3	H	21	Total	C	H	N	O	P	0	0
			657	201	240	63	132	21		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	D	1	Total	Mg	0
			1	1	
4	F	1	Total	Mg	0
			1	1	
4	B	2	Total	Mg	0
			2	2	
4	I	1	Total	Mg	0
			1	1	
4	A	1	Total	Mg	0
			1	1	

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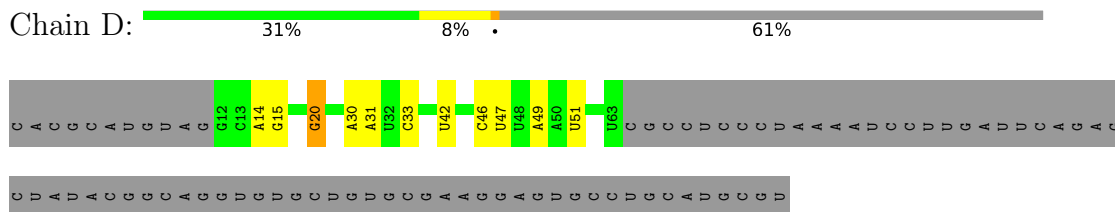
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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	C	1	1	1	0

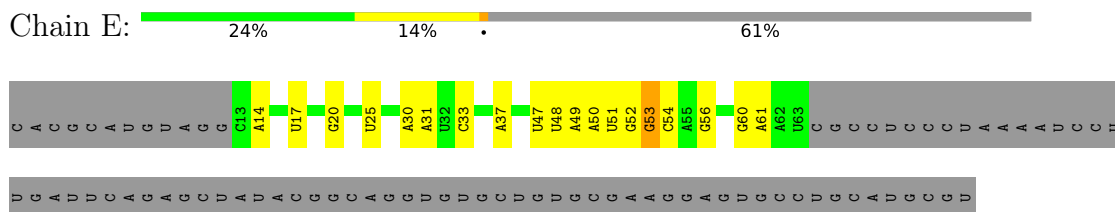
3 Residue-property plots [i](#)

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.

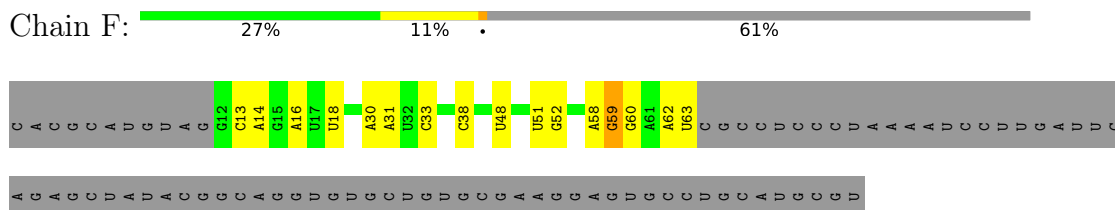
- Molecule 1: RNA (132-MER)



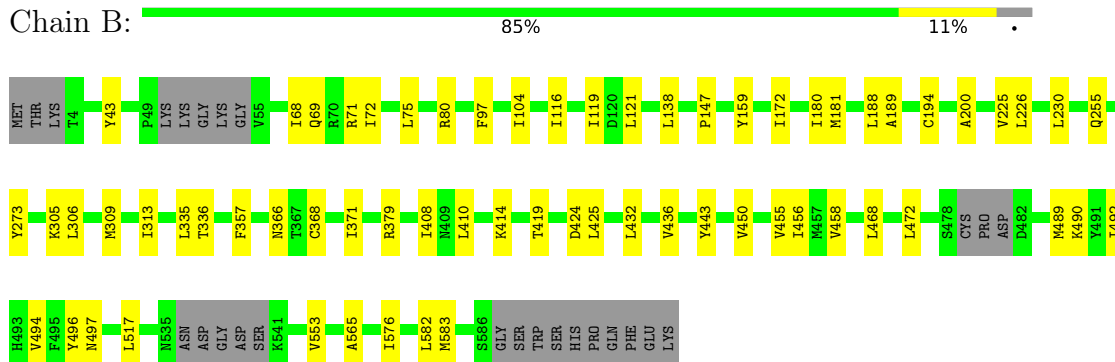
- Molecule 1: RNA (132-MER)

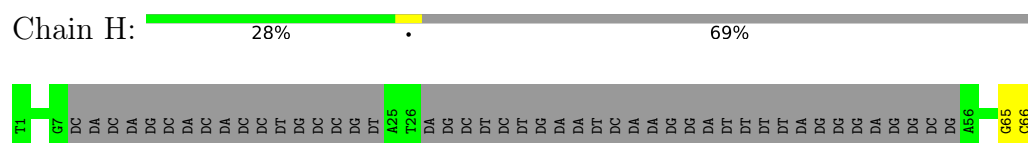


- Molecule 1: RNA (132-MER)



- Molecule 2: Retron Ec67 protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	617364	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	29	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	92000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	D	0.12	0/1250	0.21	0/1948
1	E	0.11	0/1224	0.22	0/1907
1	F	0.14	0/1250	0.26	0/1948
2	A	0.14	0/4700	0.32	0/6318
2	B	0.13	0/4700	0.31	0/6318
2	C	0.13	0/4700	0.33	0/6318
3	G	0.17	0/460	0.44	0/700
3	H	0.17	0/460	0.43	0/700
3	I	0.16	0/438	0.46	0/666
All	All	0.13	0/19182	0.31	0/26823

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 [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	D	1117	557	558	2	0
1	E	1094	546	547	3	0
1	F	1117	557	558	1	0
2	A	4616	4712	4723	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4616	4712	4723	46	0
2	C	4616	4712	4723	47	0
3	G	417	240	242	1	0
3	H	417	240	242	1	0
3	I	397	228	230	2	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	I	1	0	0	0	0
All	All	18414	16504	16546	153	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.

The worst 5 of 153 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:C:408:ILE:HG22	2:C:410:LEU:H	1.54	0.73
2:B:436:VAL:HG11	2:B:468:LEU:HD11	1.71	0.71
2:C:489:MET:HE3	2:C:490:LYS:H	1.54	0.70
2:C:472:LEU:HD22	2:C:486:MET:SD	2.33	0.69
2:C:432:LEU:O	2:C:436:VAL:HG23	1.94	0.67

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 PDB entries followed by that with respect to all EM entries.

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
2	A	562/596 (94%)	558 (99%)	2 (0%)	2 (0%)	30 59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	562/596 (94%)	559 (100%)	2 (0%)	1 (0%)	43	72
2	C	562/596 (94%)	558 (99%)	4 (1%)	0	100	100
All	All	1686/1788 (94%)	1675 (99%)	8 (0%)	3 (0%)	44	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	463	THR
2	B	497	ASN
2	A	497	ASN

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 PDB entries followed by that with respect to all EM entries.

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	
2	A	514/536 (96%)	514 (100%)	0	100	100
2	B	514/536 (96%)	514 (100%)	0	100	100
2	C	514/536 (96%)	514 (100%)	0	100	100
All	All	1542/1608 (96%)	1542 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	341	HIS
2	C	45	GLN
2	A	106	ASN
2	B	442	ASN
2	A	146	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	D	51/132 (38%)	8 (15%)	0
1	E	50/132 (37%)	15 (30%)	1 (2%)
1	F	51/132 (38%)	15 (29%)	0
All	All	152/396 (38%)	38 (25%)	1 (0%)

5 of 38 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	D	14	A
1	D	15	G
1	D	20	G
1	D	30	A
1	D	31	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	E	48	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 7 ligands modelled in this entry, 7 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.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-54448. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.