



## Full wwPDB EM Validation Report ⓘ

Oct 15, 2025 – 12:11 PM JST

PDB ID : 9M31 / pdb\_00009m31  
EMDB ID : EMD-63595  
Title : CasRx-crRNA binary complex  
Authors : Chen, X.Y.; Huang, H.D.  
Deposited on : 2025-02-28  
Resolution : 2.86 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](mailto: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>.

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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

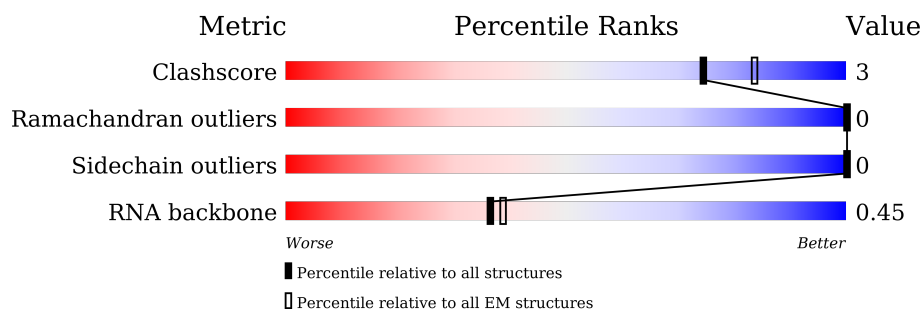
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*



The reported resolution of this entry is 2.86 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
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
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  $\geq 3$ , 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	967	 90% 8% .
2	B	51	 69% 27% .

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8744 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 protein called CasRx.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	945	Total	C	N	O	S	0	0
			7661	4874	1316	1443	28		

- Molecule 2 is a RNA chain called RNA (51-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	51	Total	C	N	O	P	0	0
			1082	486	199	347	50		

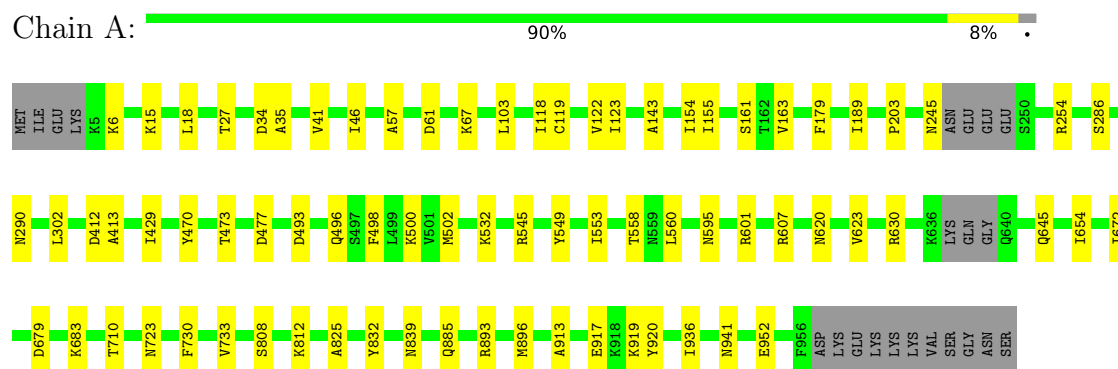
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Mg	0
			1	1	

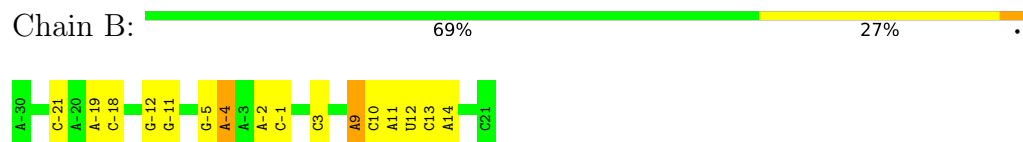
### 3 Residue-property plots [i](#)

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: CasRx



#### • Molecule 2: RNA (51-MER)



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	194460	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k 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

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	0.16	0/7800	0.29	0/10491
2	B	0.15	0/1210	0.20	0/1883
All	All	0.16	0/9010	0.28	0/12374

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	7661	0	7620	48	0
2	B	1082	0	555	7	0
3	B	1	0	0	0	0
All	All	8744	0	8175	51	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 3.

All (51) 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:885:GLN:HG2	1:A:920:TYR:HE1	1.45	0.81
1:A:245:ASN:O	1:A:254:ARG:NH2	2.27	0.67
1:A:532:LYS:NZ	2:B:3:C:O2'	2.29	0.65
1:A:885:GLN:HG2	1:A:920:TYR:CE1	2.30	0.64
1:A:41:VAL:HG22	1:A:46:ILE:HG12	1.82	0.61
1:A:601:ARG:NH1	1:A:710:THR:OG1	2.34	0.60
2:B:12:U:O2'	2:B:14:A:OP2	2.17	0.57
1:A:825:ALA:HA	1:A:839:ASN:HD22	1.72	0.54
1:A:493:ASP:O	1:A:496:GLN:HG3	2.08	0.53
1:A:154:ILE:HG23	1:A:155:ILE:HG13	1.91	0.52
1:A:470:TYR:O	1:A:473:THR:OG1	2.29	0.50
1:A:6:LYS:HD2	2:B:-1:C:H4'	1.93	0.50
1:A:119:CYS:O	1:A:123:ILE:HG12	2.12	0.49
1:A:143:ALA:HB1	1:A:607:ARG:HG2	1.94	0.49
1:A:161:SER:O	1:A:163:VAL:HG23	2.13	0.48
1:A:412:ASP:OD1	1:A:413:ALA:N	2.47	0.48
1:A:620:ASN:HB3	1:A:623:VAL:HG12	1.96	0.48
1:A:498:PHE:O	1:A:502:MET:HG3	2.14	0.47
1:A:893:ARG:HD2	1:A:896:MET:HE3	1.96	0.47
1:A:645:GLN:NE2	2:B:9:A:N7	2.58	0.47
1:A:808:SER:O	1:A:812:LYS:HG2	2.15	0.47
1:A:654:ILE:HD11	1:A:672:ILE:HG13	1.97	0.47
1:A:917:GLU:HG3	1:A:919:LYS:HG2	1.96	0.46
1:A:730:PHE:O	1:A:733:VAL:HG12	2.16	0.46
1:A:679:ASP:HB3	1:A:683:LYS:NZ	2.31	0.45
1:A:913:ALA:O	1:A:917:GLU:HG2	2.16	0.45
1:A:723:ASN:HD22	1:A:723:ASN:C	2.25	0.44
1:A:730:PHE:HA	1:A:733:VAL:HG12	2.00	0.44
1:A:549:TYR:O	1:A:553:ILE:HG12	2.18	0.44
2:B:9:A:N3	2:B:9:A:H2'	2.32	0.44
1:A:61:ASP:OD1	1:A:61:ASP:N	2.51	0.43
1:A:18:LEU:HD13	1:A:118:ILE:HD12	1.99	0.43
1:A:558:THR:HB	1:A:560:LEU:HD13	2.01	0.43
1:A:15:LYS:HE2	1:A:35:ALA:HB2	2.01	0.42
1:A:27:THR:HG21	1:A:35:ALA:HB1	2.01	0.42
1:A:27:THR:CG2	1:A:35:ALA:HB1	2.48	0.42
1:A:57:ALA:HA	1:A:67:LYS:O	2.19	0.42
1:A:119:CYS:O	1:A:122:VAL:HG22	2.20	0.42
1:A:203:PRO:HA	1:A:545:ARG:HH11	1.85	0.42
1:A:34:ASP:OD1	1:A:500:LYS:NZ	2.35	0.42
1:A:179:PHE:CE2	1:A:189:ILE:HG13	2.54	0.41
1:A:286:SER:O	1:A:290:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:ASP:OD2	1:A:607:ARG:NH2	2.52	0.41
1:A:15:LYS:HB3	1:A:27:THR:O	2.20	0.41
1:A:103:LEU:HB3	1:A:123:ILE:HG21	2.03	0.41
1:A:832:TYR:HB3	1:A:936:ILE:HG12	2.01	0.41
1:A:941:ASN:ND2	2:B:-5:G:O2'	2.43	0.41
1:A:302:LEU:HD23	1:A:429:ILE:HD12	2.03	0.41
2:B:-4:A:N3	2:B:-4:A:H2'	2.35	0.41
1:A:595:ASN:HD22	1:A:595:ASN:N	2.18	0.41
1:A:630:ARG:NH2	1:A:952:GLU:OE2	2.54	0.40

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	
1	A	939/967 (97%)	916 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	
1	A	817/842 (97%)	817 (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. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	181	ASN
1	A	263	ASN
1	A	294	ASN
1	A	420	ASN
1	A	431	HIS
1	A	595	ASN
1	A	677	ASN
1	A	680	GLN
1	A	738	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	50/51 (98%)	11 (22%)	0

All (11) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	-21	C
2	B	-19	A
2	B	-18	C
2	B	-12	G
2	B	-11	G
2	B	-4	A
2	B	-2	A
2	B	9	A
2	B	10	C
2	B	11	A
2	B	13	C

There are no RNA pucker outliers to report.

## 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](#)

Of 1 ligands modelled in this entry, 1 is 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.