

## wwPDB EM Validation Summary Report (i)

#### Jul 20, 2023 – 12:19 PM JST

DDB ID		7517
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EMDB ID	:	EMD-31146
Title	:	Coupling of N7-methyltransferase and 3'-5' exoribonuclease with SARS-CoV-2
		polymerase reveals mechanisms for capping and proofreading
Authors	:	Yan, L.; Yang, Y.X.; Li, M.Y.; Zhang, Y.; Zheng, L.T.; Ge, J.; Huang, Y.C.;
		Liu, Z.Y.; Wang, T.; Gao, S.; Zhang, R.; Huang, Y.Y.; Guddat, L.W.; Gao,
		Y.; Rao, Z.H.; Lou, Z.Y.
Deposited on	:	2021-04-01
Resolution	:	Not provided

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 (i) 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 (i)) were used in the production of this report:

EMDB validation analysis	:	0.0.1. dev 50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

## 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 unknown.

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM\ structures}\ (\#{f Entries})$		
Clashscore	158937	4297		
Ramachandran outliers	154571	4023		
Sidechain outliers	154315	3826		
RNA backbone	4643	859		

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	Qual	ity of chain	
1	А	929	47%	50%	•
2	В	198	46%	47%	• 6%
2	D	198	41%	51%	• 6%
3	С	83	40%	47%	13%
4	G	113	48%	51%	•
5	Н	139	39%	55%	6%
6	Ι	25	• 56%	40%	
7	J	27	15% 52%	30%	·



Mol	Chain	Length	(	Quality of chain						
8	K	527	58%	41%	••					
9	Е	601	26%	70%	••					
9	F	601	37%	60%	••					



## 2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 27083 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 RNA-directed RNA polymerase.

Mol	Chain	Residues		А	AltConf	Trace			
1	А	926	Total 7458	C 4763	N 1251	O 1390	S 54	0	0

• Molecule 2 is a protein called Non-structural protein 8.

Mol	Chain	Residues		$\mathbf{A}$	toms	AltConf	Trace		
2	B	187	Total	С	Ν	0	$\mathbf{S}$	0	0
	D	107	1396	872	240	273	11		0
2	D	186	Total	С	Ν	0	S	0	0
		100	1414	889	242	272	11	0	0

• Molecule 3 is a protein called Non-structural protein 7.

Mol	Chain	Residues		Ate	oms	AltConf	Trace		
3	С	72	Total 553	C 349	N 91	O 107	S 6	0	0

• Molecule 4 is a protein called Non-structural protein 9.

Mol	Chain	Residues		At	oms	AltConf	Trace		
4	G	113	Total 868	$\begin{array}{c} \mathrm{C} \\ 549 \end{array}$	N 150	0 164	${ m S}{ m 5}$	0	0

• Molecule 5 is a protein called Non-structural protein 10.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	AltConf	Trace			
5	Н	131	Total 955	C 593	N 160	0 186	S 16	0	0

• Molecule 6 is a RNA chain called primer.



Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms	AltConf	Trace		
6	Ι	25	Total 545	C 242	N 105	O 173	Р 25	0	0

• Molecule 7 is a RNA chain called template.

Mol	Chain	Residues		At	oms	AltConf	Trace		
7	J	27	Total 565	C 253	N 94	0 191	Р 27	0	0

• Molecule 8 is a protein called Proofreading exoribonuclease.

Mol	Chain	Residues	Atoms				AltConf	Trace	
8	K	523	Total 4169	C 2674	N 710	O 749	S 36	0	0

• Molecule 9 is a protein called Helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace			
9	Е	E	E	587	Total	С	Ν	0	$\mathbf{S}$	1	0
5		001	4544	2893	765	851	35	1	0		
0	Б	500	Total	С	Ν	Ο	$\mathbf{S}$	0	0		
9	Г	F 590	4602	2926	781	861	34	0	0		

• Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
10	А	2	Total Zn 2 2	0
10	Н	2	Total Zn 2 2	0
10	K	3	Total Zn 3 3	0
10	Е	3	Total Zn 3 3	0
10	F	3	Total Zn 3 3	0

• Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
11	K	1	Total Mg 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-directed RNA polymerase





• Molecule 2: Non-structural protein 8











# 8513 8613 8514 744 7514 1446 8517 1446 8517 1446 8517 1446 8527 845 8517 1446 8526 845 8517 1446 8526 8457 8527 8466 8528 8456 8454 8456 8456 8466 8535 8466 8535 8466 8536 8466 8536 8472 8536 8472 8535 8472 8535 8486 8536 8486 8536 8486 8536 8486 8536 8486 8536 8486 8536 8486 8536 8486 8536 8486 8536 8486 8536 8486 8546



# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80256	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (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: ZN, 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).

Mal	Chain	Bo	ond lengths	B	ond angles
MIOI	Unain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.98	1/7647~(0.0%)	0.73	10/10379~(0.1%)
2	В	0.63	0/1414	0.63	0/1922
2	D	0.58	0/1433	0.64	1/1944~(0.1%)
3	С	0.79	0/556	0.76	1/749~(0.1%)
4	G	0.30	0/884	0.55	1/1200~(0.1%)
5	Н	0.31	0/976	0.54	0/1327
6	Ι	1.49	5/611~(0.8%)	1.29	1/953~(0.1%)
7	J	1.46	2/628~(0.3%)	1.23	3/974~(0.3%)
8	Κ	0.29	0/4288	0.49	0/5831
9	Е	0.45	0/4647	0.58	0/6329
9	F	0.42	0/4706	0.56	0/6402
All	All	0.70	8/27790~(0.0%)	0.66	17/38010~(0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	2
2	В	0	1
8	Κ	0	1
9	Е	0	1
9	F	0	2
All	All	0	7

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Ι	32	А	N9-C4	-7.70	1.33	1.37
6	Ι	29	А	N3-C4	-5.83	1.31	1.34



Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
6	Ι	29	А	N9-C4	-5.71	1.34	1.37
6	Ι	31	С	N1-C6	-5.60	1.33	1.37
7	J	26	А	N9-C4	-5.43	1.34	1.37

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	885	LEU	CA-CB-CG	-7.54	97.97	115.30
7	J	34	С	N1-C2-O2	-6.39	115.06	118.90
1	А	187	LEU	CA-CB-CG	-6.31	100.79	115.30
4	G	4	LEU	CA-CB-CG	5.79	128.62	115.30
1	А	503	GLY	C-N-CA	-5.69	107.48	121.70

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Group
1	А	246	THR	Peptide
1	А	848	VAL	Peptide
2	В	182	TRP	Peptide
9	Ε	406	PRO	Peptide
8	Κ	195	MET	Peptide

#### 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	А	7458	0	7191	430	0
2	В	1396	0	1365	95	0
2	D	1414	0	1416	103	0
3	С	553	0	585	38	0
4	G	868	0	880	59	0
5	Н	955	0	911	72	0
6	Ι	545	0	272	67	0
7	J	565	0	291	64	0
8	K	4169	0	4050	196	0
9	Е	4544	0	4480	524	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	F	4602	0	4577	390	0
10	А	2	0	0	0	0
10	Ε	3	0	0	0	0
10	F	3	0	0	0	0
10	Н	2	0	0	0	0
10	Κ	3	0	0	0	0
11	Κ	1	0	0	0	0
All	All	27083	0	26018	1952	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 37.

The worst 5 of 1952 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)
9:F:55:CYS:SG	9:F:75:HIS:HE1	1.60	1.24
9:E:214:THR:HG1	9:E:342:CYS:N	1.45	1.14
9:E:471:CYS:HA	9:E:572:ILE:O	1.49	1.11
9:E:561:PHE:O	9:E:565:ILE:HB	1.55	1.07
9:F:8:CYS:SG	9:F:26:CYS:HB3	1.97	1.04

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	Perce	ntiles
1	А	924/929~(100%)	690 (75%)	226 (24%)	8 (1%)	17	17
2	В	185/198~(93%)	163 (88%)	21 (11%)	1 (0%)	29	29
2	D	184/198~(93%)	152 (83%)	32 (17%)	0	100	100
3	С	70/83~(84%)	48 (69%)	22 (31%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
4	G	111/113~(98%)	94~(85%)	17~(15%)	0	100	100
5	Η	129/139~(93%)	105~(81%)	24 (19%)	0	100	100
8	Κ	521/527~(99%)	424 (81%)	96~(18%)	1 (0%)	47	47
9	Е	584/601~(97%)	429~(74%)	149 (26%)	6 (1%)	15	15
9	F	588/601~(98%)	460 (78%)	124 (21%)	4 (1%)	22	22
All	All	3296/3389~(97%)	2565 (78%)	711 (22%)	20 (1%)	29	25

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	264	PRO
1	А	296	PRO
1	А	905	VAL
1	А	928	HIS
2	В	183	PRO

#### 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	А	817/820~(100%)	801~(98%)	16 (2%)	55 55
2	В	144/167~(86%)	141 (98%)	3(2%)	53 53
2	D	149/167~(89%)	147 (99%)	2(1%)	69 69
3	С	67/77~(87%)	66~(98%)	1 (2%)	65 65
4	G	94/94~(100%)	94 (100%)	0	100 100
5	Н	105/113~(93%)	104 (99%)	1 (1%)	76 76
8	Κ	458/462~(99%)	454 (99%)	4 (1%)	78 78
9	Ε	503/523~(96%)	499 (99%)	4 (1%)	81 81
9	F	513/523~(98%)	510 (99%)	3 (1%)	86 86
All	All	2850/2946~(97%)	2816 (99%)	34 (1%)	72 71



5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	Ε	218	LYS
9	Ε	474[A]	MET
9	F	73	LYS
1	А	770	TYR
1	А	684	ASP

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such side chains are listed below:

Mol	Chain	$\mathbf{Res}$	Type
9	F	354	GLN
9	F	489	ASN
3	С	19	GLN
2	В	108	ASN
9	F	518	GLN

#### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	Ι	24/25~(96%)	6~(25%)	1 (4%)
7	J	26/27~(96%)	8~(30%)	0
All	All	50/52~(96%)	14 (28%)	1 (2%)

5 of 14 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	Ι	10	С
6	Ι	11	G
6	Ι	15	G
6	Ι	16	U
6	Ι	23	С

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	Ι	22	G

#### 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 monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 14 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 (i)

This section contains visualisations of the EMDB entry EMD-31146. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

#### 6.1 Orthogonal projections (i)

This section was not generated.

#### 6.2 Central slices (i)

This section was not generated.

#### 6.3 Largest variance slices (i)

This section was not generated.

#### 6.4 Orthogonal standard-deviation projections (False-color) (i)

This section was not generated.

#### 6.5 Orthogonal surface views (i)

This section was not generated.

#### 6.6 Mask visualisation (i)

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



## 7 Map analysis (i)

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

#### 7.1 Map-value distribution (i)

This section was not generated.

#### 7.2 Volume estimate versus contour level (i)

This section was not generated.

#### 7.3 Rotationally averaged power spectrum (i)

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



## 8 Fourier-Shell correlation (i)

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



# 9 Map-model fit (i)

This section was not generated.

