



wwPDB EM Model Validation Summary Report ⓘ

May 25, 2020 – 09:36 AM EDT

PDB ID : 7C2K
EMDB ID : EMD-30275
Title : COVID-19 RNA-dependent RNA polymerase pre-translocated catalytic complex
Authors : Wang, Q.; Gao, Y.; Ji, W.; Mu, A.; Rao, Z.
Deposited on : 2020-05-07
Resolution : 2.93 Å(reported)

This is a wwPDB EM Model Validation Summary Report for a publicly released PDB/EMDB 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.10.1

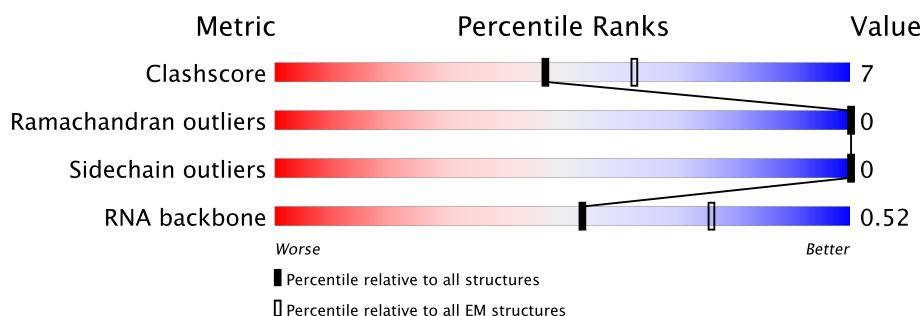
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.93 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

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 on 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	944	83% 15% .
2	B	200	52% 7% 42%
2	D	200	50% 20% 31%
3	C	85	72% 14% 14%
4	F	29	31% 31% 7% 31%
5	G	18	39% 28% 33%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10692 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	Atoms					AltConf	Trace
1	A	927	Total	C	N	O	S	0	0
			7464	4766	1252	1392	54		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P0DTD1
A	0	GLY	-	expression tag	UNP P0DTD1
A	933	HIS	-	expression tag	UNP P0DTD1
A	934	HIS	-	expression tag	UNP P0DTD1
A	935	HIS	-	expression tag	UNP P0DTD1
A	936	HIS	-	expression tag	UNP P0DTD1
A	937	HIS	-	expression tag	UNP P0DTD1
A	938	HIS	-	expression tag	UNP P0DTD1
A	939	HIS	-	expression tag	UNP P0DTD1
A	940	HIS	-	expression tag	UNP P0DTD1
A	941	HIS	-	expression tag	UNP P0DTD1
A	942	HIS	-	expression tag	UNP P0DTD1

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	117	Total	C	N	O	S	0	0
			905	569	152	177	7		
2	D	139	Total	C	N	O	S	0	0
			1080	676	186	208	10		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP P0DTD1
B	0	PRO	-	expression tag	UNP P0DTD1
D	-1	GLY	-	expression tag	UNP P0DTD1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	PRO	-	expression tag	UNP P0DTD1

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	73	Total	C	N	O	S	0	0
			554	349	92	107	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP P0DTD1
C	0	PRO	-	expression tag	UNP P0DTD1

- Molecule 4 is a RNA chain called RNA (29-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	20	Total	C	N	O	P	0	0
			423	188	70	145	20		

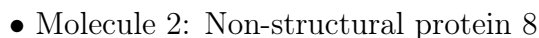
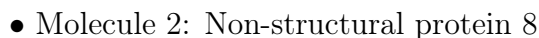
- Molecule 5 is a RNA chain called RNA (5'-R(*UP*GP*UP*UP*CP*GP*AP*CP*GP*AP*CP*AP*CP*AP*GP*G*(F86)P*G)-3').

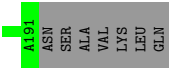
Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	12	Total	C	N	O	P	0	0
			264	119	54	79	12		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

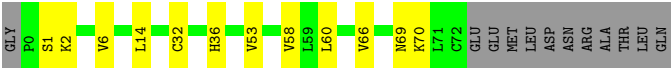
Mol	Chain	Residues	Atoms		AltConf
6	A	2	Total	Zn	0
			2	2	

- Molecule 1: RNA-directed RNA polymerase

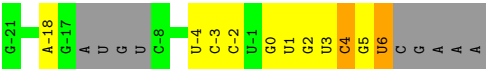
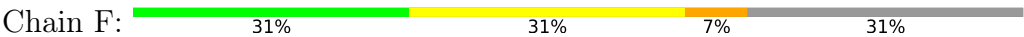




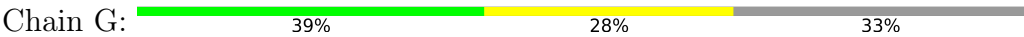
- Molecule 3: Non-structural protein 7



- Molecule 4: RNA (29-MER)



- Molecule 5: RNA (5'-R(*UP*GP*UP*UP*CP*GP*AP*CP*GP*AP*CP*AP*CP*AP*GP*G*(F86)P*G)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	214419	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60, 60	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k), 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: ZN, F86

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	0.33	1/7652 (0.0%)	0.44	0/10382
2	B	0.27	0/918	0.45	0/1252
2	D	0.25	0/1094	0.46	0/1484
3	C	0.26	0/558	0.42	0/752
4	F	0.88	3/469 (0.6%)	0.92	1/726 (0.1%)
5	G	0.29	0/268	0.78	0/414
All	All	0.36	4/10959 (0.0%)	0.49	1/15010 (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
2	D	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	-4	U	O3'-P	-9.49	1.49	1.61
1	A	682	SER	C-N	7.39	1.46	1.33
4	F	-2	C	O3'-P	-7.39	1.52	1.61
4	F	-3	C	O3'-P	-6.34	1.53	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	-2	C	C1'-C2'-O2'	-9.51	82.08	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	182	TRP	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	A	7464	0	7204	92	0
2	B	905	0	917	9	0
2	D	1080	0	1099	30	0
3	C	554	0	585	10	0
4	F	423	0	216	9	0
5	G	264	0	122	3	0
6	A	2	0	0	0	0
All	All	10692	0	10143	144	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 7.

The worst 5 of 144 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:312:ASN:HD21	1:A:464:CYS:H	1.29	0.80
2:D:147:PHE:HB3	2:D:154:TRP:HB2	1.64	0.77
1:A:758:LEU:HD23	1:A:759:SER:H	1.51	0.76
2:D:162:ALA:HB2	2:D:183:PRO:HD2	1.68	0.76
1:A:170:ASP:OD2	1:A:173:ARG:NH2	2.26	0.69

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	923/944 (98%)	877 (95%)	46 (5%)	0	100	100
2	B	115/200 (58%)	113 (98%)	2 (2%)	0	100	100
2	D	137/200 (68%)	130 (95%)	7 (5%)	0	100	100
3	C	71/85 (84%)	70 (99%)	1 (1%)	0	100	100
All	All	1246/1429 (87%)	1190 (96%)	56 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	817/834 (98%)	817 (100%)	0	100	100
2	B	103/168 (61%)	103 (100%)	0	100	100
2	D	119/168 (71%)	119 (100%)	0	100	100
3	C	67/78 (86%)	67 (100%)	0	100	100
All	All	1106/1248 (89%)	1106 (100%)	0	100	100

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	613	HIS
1	A	725	HIS
2	D	109	ASN
1	A	642	HIS
1	A	705	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	F	18/29 (62%)	3 (16%)	0
5	G	9/18 (50%)	2 (22%)	0
All	All	27/47 (57%)	5 (18%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	F	2	G
4	F	4	C
4	F	6	U
5	G	-5	C
5	G	-4	G

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 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.