

# wwPDB X-ray Structure Validation Summary Report (i)

#### Oct 3, 2023 – 04:54 AM EDT

PDB ID :	ID : 6PZQ
Title :	itle : Structure of the human respiratory syncytial virus M2-1 protein in complex
	with a short positive-sense gene-end RNA
Authors :	nors : Gao, Y.; Cao, D.; Liang, B.
eposited on :	l on : 2019-08-01
Resolution :	tion : $2.70 \text{ Å}(\text{reported})$
Authors : eposited on :	with a short positive-sense gene-end RNA nors : Gao, Y.; Cao, D.; Liang, B. l on : 2019-08-01

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp 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 (1)) were used in the production of this report:

MolProbity	:	FAILED
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.70 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.



#### 6PZQ

# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10653 atoms, of which 5324 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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.

Mol	Chain	Residues		Atoms						AltConf	Trace
1	Δ	157	Total	С	Η	Ν	0	S	0	0	0
	A	157	2589	802	1314	234	231	8	0	0	0
1	В	155	Total	С	Η	Ν	0	S	0	0	0
	D	155	2558	794	1297	232	228	$\overline{7}$	0	0	0
1	С	150	Total	С	Η	Ν	0	S	0	0	0
		152	2505	779	1271	226	222	$\overline{7}$		0	0
1	D	156	Total	С	Н	Ν	0	S	0	0	0
	D	100	2572	798	1303	234	230	7	0	0	U

• Molecule 1 is a protein called Matrix M2-1.

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	179	LEU	SER	conflict	UNP P04545
В	179	LEU	SER	conflict	UNP P04545
С	179	LEU	SER	conflict	UNP P04545
D	179	LEU	SER	conflict	UNP P04545

• Molecule 2 is a RNA chain called RNA (5'-R(P\*GP\*UP\*UP\*AP\*AP\*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
2	т	6	Total	С	Η	Ν	0	Р	0	0	0
	1	0	189	57	64	21	41	6			
2	т	7	Total	С	Η	Ν	Ο	Р	0	0	0
	J	1	222	67	75	26	47	7	0	0	0

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Zn 1 1	0	0
3	В	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	С	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	2	Total O 2 2	0	0
4	В	8	Total O 8 8	0	0
4	С	3	Total O 3 3	0	0
4	Ι	1	Total O 1 1	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.



# 3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants	94.75Å 94.75Å 199.63Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	63.52 - 2.70	Depositor
% Data completeness	99.6 (63.52-2.70)	Depositor
(in resolution range)		-
R <sub>merge</sub>	0.13	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.73 (at 2.69 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
$R, R_{free}$	0.225 , $0.288$	Depositor
Wilson B-factor $(Å^2)$	85.8	Xtriage
Anisotropy	0.188	Xtriage
L-test for twinning <sup>2</sup>	$ < L >=0.48, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10653	wwPDB-VP
Average B, all atoms $(Å^2)$	104.0	wwPDB-VP

EDS failed to run properly - this section is therefore incomplete.

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.93% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 4 Model quality (i)

### 4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3 Torsion angles (i)

#### 4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

#### 4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 4.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 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.

### 4.7 Other polymers (i)

There are no such residues in this entry.

## 4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



## 5 Fit of model and data (i)

## 5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

## 5.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

## 5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

## 5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

### 5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

