



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 1, 2023 – 10:04 PM EDT

PDB ID : 6NIP  
Title : Crystal structure of a human anti-ZIKV-DENV neutralizing antibody MZ1 in complex with ZIKV E glycoprotein  
Authors : Sankhala, R.S.; Dussupt, V.; Donofrio, G.; Choe, M.; Modjarrad, K.; Michael, N.L.; Krebs, S.J.; Joyce, M.G.  
Deposited on : 2018-12-31  
Resolution : 4.16 Å(reported)

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](mailto: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 ⓘ 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:

MolProbity : **FAILED**  
Xtrriage (Phenix) : 1.13  
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

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.16 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.

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12632 atoms, of which 0 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.

- Molecule 1 is a protein called MZ1 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	221	Total 1663	C 1049	N 273	O 332	S 9	0	2	0
1	H	221	Total 1663	C 1049	N 273	O 332	S 9	0	2	0

- Molecule 2 is a protein called MZ1 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	214	Total 1600	C 997	N 274	O 325	S 4	0	0	0
2	L	214	Total 1600	C 997	N 274	O 325	S 4	0	0	0

- Molecule 3 is a protein called Envelope protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	Z	399	Total 3053	C 1907	N 534	O 586	S 26	0	0	0
3	E	399	Total 3053	C 1907	N 534	O 586	S 26	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	406	GLY	-	expression tag	UNP A0A024B7W1
Z	407	PRO	-	expression tag	UNP A0A024B7W1
Z	408	LEU	-	expression tag	UNP A0A024B7W1
Z	409	GLU	-	expression tag	UNP A0A024B7W1
Z	410	VAL	-	expression tag	UNP A0A024B7W1
Z	411	LEU	-	expression tag	UNP A0A024B7W1
Z	412	PHE	-	expression tag	UNP A0A024B7W1
Z	413	GLN	-	expression tag	UNP A0A024B7W1

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	414	GLY	-	expression tag	UNP A0A024B7W1
Z	415	PRO	-	expression tag	UNP A0A024B7W1
Z	416	GLY	-	expression tag	UNP A0A024B7W1
Z	417	SER	-	expression tag	UNP A0A024B7W1
Z	418	ALA	-	expression tag	UNP A0A024B7W1
Z	419	TRP	-	expression tag	UNP A0A024B7W1
Z	420	SER	-	expression tag	UNP A0A024B7W1
Z	421	HIS	-	expression tag	UNP A0A024B7W1
Z	422	PRO	-	expression tag	UNP A0A024B7W1
Z	423	GLN	-	expression tag	UNP A0A024B7W1
Z	424	PHE	-	expression tag	UNP A0A024B7W1
Z	425	GLU	-	expression tag	UNP A0A024B7W1
Z	426	LYS	-	expression tag	UNP A0A024B7W1
Z	427	GLY	-	expression tag	UNP A0A024B7W1
Z	428	GLY	-	expression tag	UNP A0A024B7W1
Z	429	GLY	-	expression tag	UNP A0A024B7W1
Z	430	SER	-	expression tag	UNP A0A024B7W1
Z	431	GLY	-	expression tag	UNP A0A024B7W1
Z	432	GLY	-	expression tag	UNP A0A024B7W1
Z	433	GLY	-	expression tag	UNP A0A024B7W1
Z	434	SER	-	expression tag	UNP A0A024B7W1
Z	435	GLY	-	expression tag	UNP A0A024B7W1
Z	436	GLY	-	expression tag	UNP A0A024B7W1
Z	437	GLY	-	expression tag	UNP A0A024B7W1
Z	438	SER	-	expression tag	UNP A0A024B7W1
Z	439	ALA	-	expression tag	UNP A0A024B7W1
Z	440	TRP	-	expression tag	UNP A0A024B7W1
Z	441	SER	-	expression tag	UNP A0A024B7W1
Z	442	HIS	-	expression tag	UNP A0A024B7W1
Z	443	PRO	-	expression tag	UNP A0A024B7W1
Z	444	GLN	-	expression tag	UNP A0A024B7W1
Z	445	PHE	-	expression tag	UNP A0A024B7W1
Z	446	GLU	-	expression tag	UNP A0A024B7W1
Z	447	LYS	-	expression tag	UNP A0A024B7W1
E	406	GLY	-	expression tag	UNP A0A024B7W1
E	407	PRO	-	expression tag	UNP A0A024B7W1
E	408	LEU	-	expression tag	UNP A0A024B7W1
E	409	GLU	-	expression tag	UNP A0A024B7W1
E	410	VAL	-	expression tag	UNP A0A024B7W1
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E	414	GLY	-	expression tag	UNP A0A024B7W1
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E	416	GLY	-	expression tag	UNP A0A024B7W1
E	417	SER	-	expression tag	UNP A0A024B7W1
E	418	ALA	-	expression tag	UNP A0A024B7W1
E	419	TRP	-	expression tag	UNP A0A024B7W1
E	420	SER	-	expression tag	UNP A0A024B7W1
E	421	HIS	-	expression tag	UNP A0A024B7W1
E	422	PRO	-	expression tag	UNP A0A024B7W1
E	423	GLN	-	expression tag	UNP A0A024B7W1
E	424	PHE	-	expression tag	UNP A0A024B7W1
E	425	GLU	-	expression tag	UNP A0A024B7W1
E	426	LYS	-	expression tag	UNP A0A024B7W1
E	427	GLY	-	expression tag	UNP A0A024B7W1
E	428	GLY	-	expression tag	UNP A0A024B7W1
E	429	GLY	-	expression tag	UNP A0A024B7W1
E	430	SER	-	expression tag	UNP A0A024B7W1
E	431	GLY	-	expression tag	UNP A0A024B7W1
E	432	GLY	-	expression tag	UNP A0A024B7W1
E	433	GLY	-	expression tag	UNP A0A024B7W1
E	434	SER	-	expression tag	UNP A0A024B7W1
E	435	GLY	-	expression tag	UNP A0A024B7W1
E	436	GLY	-	expression tag	UNP A0A024B7W1
E	437	GLY	-	expression tag	UNP A0A024B7W1
E	438	SER	-	expression tag	UNP A0A024B7W1
E	439	ALA	-	expression tag	UNP A0A024B7W1
E	440	TRP	-	expression tag	UNP A0A024B7W1
E	441	SER	-	expression tag	UNP A0A024B7W1
E	442	HIS	-	expression tag	UNP A0A024B7W1
E	443	PRO	-	expression tag	UNP A0A024B7W1
E	444	GLN	-	expression tag	UNP A0A024B7W1
E	445	PHE	-	expression tag	UNP A0A024B7W1
E	446	GLU	-	expression tag	UNP A0A024B7W1
E	447	LYS	-	expression tag	UNP A0A024B7W1

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

### 3 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	417.33Å 69.30Å 212.58Å 90.00° 112.96° 90.00°	Depositor
Resolution (Å)	14.99 – 4.16	Depositor
% Data completeness (in resolution range)	70.1 (14.99-4.16)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.27	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.15 (at 4.14Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.188 , 0.237	Depositor
Wilson B-factor (Å <sup>2</sup> )	63.5	Xtrriage
Anisotropy	0.062	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	12632	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.76% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 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](#)

There are no ligands in this entry.

### 4.7 Other polymers [i](#)

There are no such residues in this entry.

## 4.8 Polymer linkage issues

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.