



wwPDB X-ray Structure Validation Summary Report i

Oct 2, 2023 – 12:30 PM EDT

PDB ID : 6NIU
Title : Crystal structure of a human anti-ZIKV-DENV neutralizing antibody MZ4 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 : 4.30 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
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
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 4.30 Å.

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

MolProbit 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 19232 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 Human MZ4 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	120	Total	C	N	O	S	0	0	0
			930	584	157	185	4			
1	F	120	Total	C	N	O	S	0	0	0
			930	584	157	185	4			
1	I	120	Total	C	N	O	S	0	0	0
			930	584	157	185	4			
1	M	120	Total	C	N	O	S	0	0	0
			930	584	157	185	4			

- Molecule 2 is a protein called Human MZ4 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	111	Total	C	N	O	S	0	0	0
			825	513	145	165	2			
2	G	111	Total	C	N	O	S	0	0	0
			825	513	145	165	2			
2	J	111	Total	C	N	O	S	0	0	0
			825	513	145	165	2			
2	N	111	Total	C	N	O	S	0	0	0
			825	513	145	165	2			

- Molecule 3 is a protein called Envelope protein E.

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

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	406	GLY	-	expression tag	UNP A0A024B7W1
B	407	PRO	-	expression tag	UNP A0A024B7W1
B	408	LEU	-	expression tag	UNP A0A024B7W1
B	409	GLU	-	expression tag	UNP A0A024B7W1
B	410	VAL	-	expression tag	UNP A0A024B7W1
B	411	LEU	-	expression tag	UNP A0A024B7W1
B	412	PHE	-	expression tag	UNP A0A024B7W1
B	413	GLN	-	expression tag	UNP A0A024B7W1
B	414	GLY	-	expression tag	UNP A0A024B7W1
B	415	PRO	-	expression tag	UNP A0A024B7W1
B	416	GLY	-	expression tag	UNP A0A024B7W1
B	417	SER	-	expression tag	UNP A0A024B7W1
B	418	ALA	-	expression tag	UNP A0A024B7W1
B	419	TRP	-	expression tag	UNP A0A024B7W1
B	420	SER	-	expression tag	UNP A0A024B7W1
B	421	HIS	-	expression tag	UNP A0A024B7W1
B	422	PRO	-	expression tag	UNP A0A024B7W1
B	423	GLN	-	expression tag	UNP A0A024B7W1
B	424	PHE	-	expression tag	UNP A0A024B7W1
B	425	GLU	-	expression tag	UNP A0A024B7W1
B	426	LYS	-	expression tag	UNP A0A024B7W1
B	427	GLY	-	expression tag	UNP A0A024B7W1
B	428	GLY	-	expression tag	UNP A0A024B7W1
B	429	GLY	-	expression tag	UNP A0A024B7W1
B	430	SER	-	expression tag	UNP A0A024B7W1
B	431	GLY	-	expression tag	UNP A0A024B7W1
B	432	GLY	-	expression tag	UNP A0A024B7W1
B	433	GLY	-	expression tag	UNP A0A024B7W1
B	434	SER	-	expression tag	UNP A0A024B7W1
B	435	GLY	-	expression tag	UNP A0A024B7W1
B	436	GLY	-	expression tag	UNP A0A024B7W1
B	437	GLY	-	expression tag	UNP A0A024B7W1
B	438	SER	-	expression tag	UNP A0A024B7W1
B	439	ALA	-	expression tag	UNP A0A024B7W1
B	440	TRP	-	expression tag	UNP A0A024B7W1
B	441	SER	-	expression tag	UNP A0A024B7W1
B	442	HIS	-	expression tag	UNP A0A024B7W1
B	443	PRO	-	expression tag	UNP A0A024B7W1
B	444	GLN	-	expression tag	UNP A0A024B7W1
B	445	PHE	-	expression tag	UNP A0A024B7W1
B	446	GLU	-	expression tag	UNP A0A024B7W1
B	447	LYS	-	expression tag	UNP A0A024B7W1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	406	GLY	-	expression tag	UNP A0A024B7W1
A	407	PRO	-	expression tag	UNP A0A024B7W1
A	408	LEU	-	expression tag	UNP A0A024B7W1
A	409	GLU	-	expression tag	UNP A0A024B7W1
A	410	VAL	-	expression tag	UNP A0A024B7W1
A	411	LEU	-	expression tag	UNP A0A024B7W1
A	412	PHE	-	expression tag	UNP A0A024B7W1
A	413	GLN	-	expression tag	UNP A0A024B7W1
A	414	GLY	-	expression tag	UNP A0A024B7W1
A	415	PRO	-	expression tag	UNP A0A024B7W1
A	416	GLY	-	expression tag	UNP A0A024B7W1
A	417	SER	-	expression tag	UNP A0A024B7W1
A	418	ALA	-	expression tag	UNP A0A024B7W1
A	419	TRP	-	expression tag	UNP A0A024B7W1
A	420	SER	-	expression tag	UNP A0A024B7W1
A	421	HIS	-	expression tag	UNP A0A024B7W1
A	422	PRO	-	expression tag	UNP A0A024B7W1
A	423	GLN	-	expression tag	UNP A0A024B7W1
A	424	PHE	-	expression tag	UNP A0A024B7W1
A	425	GLU	-	expression tag	UNP A0A024B7W1
A	426	LYS	-	expression tag	UNP A0A024B7W1
A	427	GLY	-	expression tag	UNP A0A024B7W1
A	428	GLY	-	expression tag	UNP A0A024B7W1
A	429	GLY	-	expression tag	UNP A0A024B7W1
A	430	SER	-	expression tag	UNP A0A024B7W1
A	431	GLY	-	expression tag	UNP A0A024B7W1
A	432	GLY	-	expression tag	UNP A0A024B7W1
A	433	GLY	-	expression tag	UNP A0A024B7W1
A	434	SER	-	expression tag	UNP A0A024B7W1
A	435	GLY	-	expression tag	UNP A0A024B7W1
A	436	GLY	-	expression tag	UNP A0A024B7W1
A	437	GLY	-	expression tag	UNP A0A024B7W1
A	438	SER	-	expression tag	UNP A0A024B7W1
A	439	ALA	-	expression tag	UNP A0A024B7W1
A	440	TRP	-	expression tag	UNP A0A024B7W1
A	441	SER	-	expression tag	UNP A0A024B7W1
A	442	HIS	-	expression tag	UNP A0A024B7W1
A	443	PRO	-	expression tag	UNP A0A024B7W1
A	444	GLN	-	expression tag	UNP A0A024B7W1
A	445	PHE	-	expression tag	UNP A0A024B7W1
A	446	GLU	-	expression tag	UNP A0A024B7W1
A	447	LYS	-	expression tag	UNP A0A024B7W1

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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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
E	411	LEU	-	expression tag	UNP A0A024B7W1
E	412	PHE	-	expression tag	UNP A0A024B7W1
E	413	GLN	-	expression tag	UNP A0A024B7W1
E	414	GLY	-	expression tag	UNP A0A024B7W1
E	415	PRO	-	expression tag	UNP A0A024B7W1
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 i

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	113.53 Å 137.26 Å 136.79 Å 80.12° 65.74° 65.75°	Depositor
Resolution (Å)	10.00 – 4.30	Depositor
% Data completeness (in resolution range)	29.6 (10.00-4.30)	Depositor
R _{merge}	(Not available)	Depositor
R _{sym}	0.23	Depositor
$< I/\sigma(I) >$ ¹	2.59 (at 4.29 Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R _{free}	0.264, 0.359	Depositor
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.210	Xtriage
L-test for twinning ²	$< L > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.045 for h,h-l,k 0.045 for h,l,h-k 0.358 for h,h-k,h-l 0.048 for -h,-k,-h+l 0.053 for -h,-h+k,-l 0.350 for -h,-l,-k 0.356 for -h,-h+l,-h+k	Xtriage
Total number of atoms	19232	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $< |L| >$, $< L^2 >$ 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 [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.