



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 15, 2026 – 12:17 AM UTC

PDB ID : 9XYB / pdb_00009xyb
Title : Crystal structure of a ZIKV E glycoprotein DI-DIII vaccine candidate in complex with human neutralizing antibody MZ4
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Deposited on : 2025-08-25
Resolution : 2.85 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

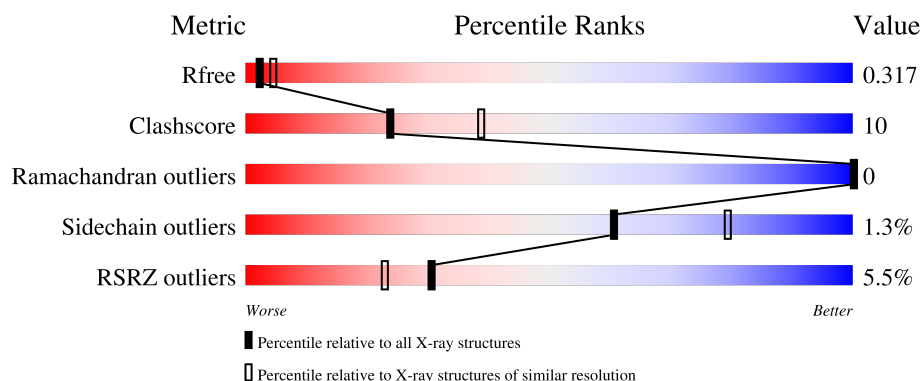
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	H	219	<div> <div>10%</div> <div> <div></div> <div>76%</div> <div>23%</div> </div> </div>
2	L	214	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>14%</div> </div> </div>
3	E	277	<div> <div>4%</div> <div> <div></div> <div>58%</div> <div>21%</div> <div>•</div> <div>20%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4937 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	219	Total	C	N	O	S	0	0	0
			1644	1035	274	329	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1604	1002	276	322	4			

- Molecule 3 is a protein called Envelope protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	221	Total	C	N	O	S	0	0	0
			1674	1045	290	324	15			

There are 43 discrepancies between the modelled and reference sequences:

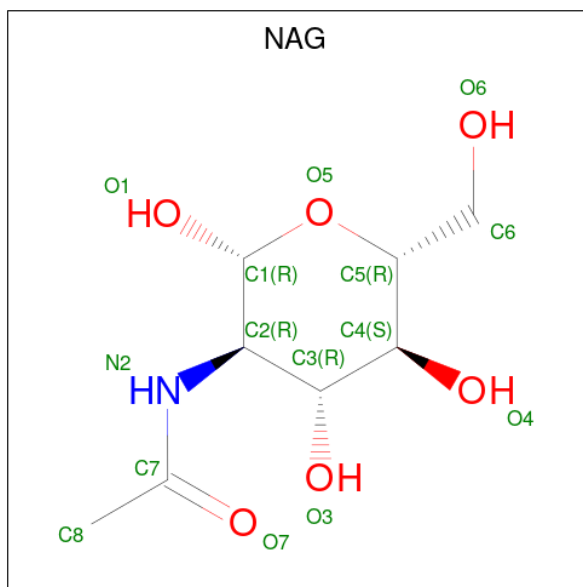
Chain	Residue	Modelled	Actual	Comment	Reference
E	127	GLY	-	linker	UNP A0A024B7W1
E	128	GLY	-	linker	UNP A0A024B7W1
E	129	GLY	-	linker	UNP A0A024B7W1
E	130	GLY	-	linker	UNP A0A024B7W1
E	131	GLY	-	linker	UNP A0A024B7W1
E	132	GLY	-	linker	UNP A0A024B7W1
E	133	GLY	-	linker	UNP A0A024B7W1
E	134	GLY	-	linker	UNP A0A024B7W1
E	278	GLY	-	linker	UNP A0A024B7W1
E	279	GLY	-	linker	UNP A0A024B7W1
E	280	GLY	-	linker	UNP A0A024B7W1
E	281	GLY	-	linker	UNP A0A024B7W1
E	282	GLY	-	linker	UNP A0A024B7W1
E	283	GLY	-	linker	UNP A0A024B7W1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	284	GLY	-	linker	UNP A0A024B7W1
E	285	GLY	-	linker	UNP A0A024B7W1
E	406	GLY	-	expression tag	UNP A0A024B7W1
E	407	GLY	-	expression tag	UNP A0A024B7W1
E	408	GLY	-	expression tag	UNP A0A024B7W1
E	409	SER	-	expression tag	UNP A0A024B7W1
E	410	GLY	-	expression tag	UNP A0A024B7W1
E	411	LEU	-	expression tag	UNP A0A024B7W1
E	412	ASN	-	expression tag	UNP A0A024B7W1
E	413	ASP	-	expression tag	UNP A0A024B7W1
E	414	ILE	-	expression tag	UNP A0A024B7W1
E	415	PHE	-	expression tag	UNP A0A024B7W1
E	416	GLU	-	expression tag	UNP A0A024B7W1
E	417	ALA	-	expression tag	UNP A0A024B7W1
E	418	GLN	-	expression tag	UNP A0A024B7W1
E	419	LYS	-	expression tag	UNP A0A024B7W1
E	420	ILE	-	expression tag	UNP A0A024B7W1
E	421	GLU	-	expression tag	UNP A0A024B7W1
E	422	TRP	-	expression tag	UNP A0A024B7W1
E	423	HIS	-	expression tag	UNP A0A024B7W1
E	424	GLU	-	expression tag	UNP A0A024B7W1
E	425	HIS	-	expression tag	UNP A0A024B7W1
E	426	HIS	-	expression tag	UNP A0A024B7W1
E	427	HIS	-	expression tag	UNP A0A024B7W1
E	428	HIS	-	expression tag	UNP A0A024B7W1
E	429	HIS	-	expression tag	UNP A0A024B7W1
E	430	HIS	-	expression tag	UNP A0A024B7W1
E	431	HIS	-	expression tag	UNP A0A024B7W1
E	432	HIS	-	expression tag	UNP A0A024B7W1

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	1	Total	O	0	0
			1	1		

- Molecule 1: Human MZ4 Fab heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	135.55Å 57.26Å 88.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.90 – 2.85 32.90 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (32.90-2.85) 99.7 (32.90-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.85Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.235 , 0.316 0.242 , 0.317	Depositor DCC
R_{free} test set	857 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	65.0	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 66.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4937	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

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: NAG

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	H	0.56	0/1687	0.85	0/2305
2	L	0.54	0/1644	0.83	0/2245
3	E	0.54	0/1704	0.81	0/2308
All	All	0.55	0/5035	0.83	0/6858

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	H	1644	0	1596	41	0
2	L	1604	0	1568	19	0
3	E	1674	0	1658	46	0
4	E	14	0	13	0	0
5	E	1	0	0	0	0
All	All	4937	0	4835	99	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 10.

The worst 5 of 99 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:H:126:PRO:HD2	1:H:211:VAL:HG22	1.30	1.07
3:E:43:ILE:HG22	3:E:141:LEU:HD22	1.39	1.02
1:H:125:ALA:HB1	1:H:211:VAL:HG21	1.44	0.98
3:E:43:ILE:HG22	3:E:141:LEU:CD2	2.00	0.90
3:E:43:ILE:CG2	3:E:141:LEU:HD22	2.03	0.88

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 X-ray entries followed by that with respect to entries of similar resolution.

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	H	217/219 (99%)	212 (98%)	5 (2%)	0	100	100
2	L	212/214 (99%)	201 (95%)	11 (5%)	0	100	100
3	E	215/277 (78%)	210 (98%)	5 (2%)	0	100	100
All	All	644/710 (91%)	623 (97%)	21 (3%)	0	100	100

There are no Ramachandran outliers to report.

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 X-ray entries followed by that with respect to entries of similar resolution.

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	H	189/189 (100%)	188 (100%)	1 (0%)	81	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	181/181 (100%)	180 (99%)	1 (1%)	78	89
3	E	188/221 (85%)	183 (97%)	5 (3%)	39	63
All	All	558/591 (94%)	551 (99%)	7 (1%)	61	79

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	357	ARG
3	E	362	ASN
3	E	403	SER
3	E	378	LEU
3	E	174	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	E	362	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	E	501	3	14,14,15	1.13	2 (14%)	17,19,21	2.33	4 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	501	3	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	501	NAG	C1-C2	2.73	1.56	1.52
4	E	501	NAG	C4-C5	2.11	1.57	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	501	NAG	C1-O5-C5	7.54	122.30	112.19
4	E	501	NAG	C2-N2-C7	2.83	126.70	122.90
4	E	501	NAG	O5-C5-C6	2.28	112.10	107.66
4	E	501	NAG	C4-C3-C2	-2.15	107.87	111.02

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	501	NAG	C8-C7-N2-C2
4	E	501	NAG	O7-C7-N2-C2

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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	H	219/219 (100%)	0.70	21 (9%) 13 11	40, 84, 155, 215	0
2	L	214/214 (100%)	0.11	5 (2%) 61 52	37, 58, 103, 133	0
3	E	221/277 (79%)	0.43	10 (4%) 38 29	49, 73, 121, 168	0
All	All	654/710 (92%)	0.42	36 (5%) 30 23	37, 70, 137, 215	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	194	TYR	6.5
1	H	211	VAL	4.1
2	L	97	VAL	3.8
1	H	189	LEU	3.7
1	H	165	THR	3.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	E	501	14/15	0.43	0.19	94,113,120,121	0

6.5 Other polymers [i](#)

There are no such residues in this entry.