

wwPDB X-ray Structure Validation Summary Report (i)

Aug 23, 2023 – 02:13 PM EDT

PDB ID	:	8EE8
Title	:	Crystal structure of a NHP anti-ZIKV neutralizing antibody rhMZ100-C in
		complex with ZIKV E glycoprotein
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Deposited on	:	2022-09-06
Resolution	:	2.80 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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.80 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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		
			26%		
1	А	405	66%	27%	6%
			5%		
1	В	405	74%	22%	• •
			9%		
1	Ε	405	68%	30%	•
			7%		
1	Z	405	69%	30%	•
			30%		
2	D	222	76%	21%	••

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Mol	Chain	Length	Quality of chain		
2	Н	222	73%	24%	·
3	С	219	2% 77%	21%	·
3	L	219	77%	21%	



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 18906 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	7	402	Total	С	Ν	0	\mathbf{S}	0	0	0
		402	3068	1913	537	593	25	0	0	0
1	F	402	Total	С	Ν	0	S	0	0	0
1		403	3079	1921	538	594	26	0	0	0
1	р	402	Total	С	Ν	0	S	0	0	0
1	D	402	3071	1915	537	593	26	0	0	0
1	Δ	403	Total	С	Ν	0	S	0	0	0
1		403	3079	1921	538	594	26		0	0

• Molecule 1 is a protein called Envelope protein E.

• Molecule 2 is a protein called rhMZ100-C antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	ц	218	Total	С	Ν	0	S	0	0	0
	11	210	1599	996	274	323	6	0	0	0
0	П	917	Total	С	Ν	0	S	0	0	0
	D	217	1592	991	273	322	6		0	0

• Molecule 3 is a protein called rhMZ100-C antibody light chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	т	217	Total	С	Ν	0	S	0	0	0
0		211	1632	1024	272	331	5	0	0	0
2	С	217	Total	С	Ν	Ο	S	0	0	0
3		211	1632	1024	272	331	5	0	0	

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Z	13	Total O 13 13	0	0
4	Н	23	Total O 23 23	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	20	TotalO2020	0	0
4	Е	18	Total O 18 18	0	0
4	В	19	Total O 19 19	0	0
4	С	27	TotalO2727	0	0
4	А	13	Total O 13 13	0	0
4	D	21	$\begin{array}{ccc} \text{Total} & \text{O} \\ 21 & 21 \end{array}$	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: Envelope protein E

 \bullet Molecule 1: Envelope protein E







• Molecule 2: rhMZ100-C antibody heavy chain







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	101.84Å 126.68Å 140.48Å	Denesitor
a, b, c, α , β , γ	90.00° 89.97° 90.00°	Depositor
$\mathbf{Posolution}(\mathbf{\hat{A}})$	14.98 - 2.80	Depositor
Resolution (A)	47.88 - 2.80	EDS
% Data completeness	61.2 (14.98-2.80)	Depositor
(in resolution range)	61.2(47.88-2.80)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$5.55 (at 2.81 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
P. P.	0.241 , 0.295	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.244 , 0.297	DCC
R_{free} test set	2026 reflections $(3.78%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	51.4	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.31, 19.8	EDS
L-test for $twinning^2$	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.438 for h,-k,-l	Xtriage
Reported twinning fraction	0.490 for h,-k,-l	Depositor
Outliers	0 of 53569 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	18906	wwPDB-VP
Average B, all atoms $(Å^2)$	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.41% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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		
	Ullaili	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.28	0/3143	0.53	0/4257	
1	В	0.27	0/3136	0.54	1/4249~(0.0%)	
1	Е	0.38	0/3144	0.60	2/4260~(0.0%)	
1	Ζ	0.28	0/3133	0.53	0/4246	
2	D	0.30	0/1626	0.57	2/2214~(0.1%)	
2	Н	0.30	0/1633	0.57	0/2224	
3	С	0.28	0/1672	0.51	0/2281	
3	L	0.32	0/1672	0.51	0/2281	
All	All	0.31	0/19159	0.55	5/26012~(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
1	А	0	4
1	В	0	1
1	Е	0	1
3	С	0	1
All	All	0	7

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	196	LEU	CA-CB-CG	7.73	133.08	115.30
2	D	154	PHE	N-CA-C	6.40	128.28	111.00
1	Е	346	ALA	N-CA-C	6.33	128.08	111.00
1	Е	351	THR	CA-C-N	-5.98	104.05	117.20
2	D	154	PHE	C-N-CD	-5.61	108.26	120.60

There are no chirality outliers.



Mol	Chain	Res	Type	Group
1	А	195	GLY	Peptide
1	А	345	MET	Peptide
1	В	190	CYS	Peptide
3	С	148	TYR	Peptide
1	Е	351	THR	Mainchain

5 of 7 planarity outliers are listed below:

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	А	3079	0	3009	96	0
1	В	3071	0	2994	65	0
1	Ε	3079	0	3007	125	0
1	Ζ	3068	0	2987	115	4
2	D	1592	0	1558	45	3
2	Н	1599	0	1565	57	0
3	С	1632	0	1582	35	0
3	L	1632	0	1581	76	1
4	А	13	0	0	0	0
4	В	19	0	0	6	0
4	С	27	0	0	4	0
4	D	21	0	0	1	0
4	Е	18	0	0	3	0
4	Н	23	0	0	0	0
4	L	20	0	0	3	0
4	Z	13	0	0	2	0
All	All	18906	0	18283	595	4

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 16.

The worst 5 of 595 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:E:149:SER:HB3	1:E:375:MET:SD	1.42	1.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:SER:CB	1:E:375:MET:SD	2.21	1.28
3:L:124:THR:OG1	3:L:143:LEU:HD11	1.33	1.23
2:H:192:VAL:HG11	2:H:202:TYR:OH	1.42	1.17
1:Z:17:GLY:HA2	1:Z:36:GLN:OE1	1.49	1.12

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All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:197:ASP:OD2	2:D:13:GLN:NE2[1_455]	1.94	0.26
1:Z:197:ASP:OD1	2:D:13:GLN:NE2[1_455]	2.00	0.20
1:Z:197:ASP:CG	2:D:13:GLN:NE2[1_455]	2.11	0.09
1:Z:317:ILE:CD1	3:L:83:SER:OG[2_445]	2.18	0.02

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	Perce	entiles
1	А	399/405~(98%)	359~(90%)	40 (10%)	0	100	100
1	В	400/405~(99%)	367~(92%)	33 (8%)	0	100	100
1	Е	401/405~(99%)	368 (92%)	33 (8%)	0	100	100
1	Z	400/405~(99%)	361 (90%)	39 (10%)	0	100	100
2	D	215/222~(97%)	202 (94%)	12 (6%)	1 (0%)	29	61
2	Н	216/222~(97%)	204 (94%)	12 (6%)	0	100	100
3	С	215/219~(98%)	201 (94%)	14 (6%)	0	100	100
3	L	215/219~(98%)	201 (94%)	14 (6%)	0	100	100
All	All	2461/2502~(98%)	2263 (92%)	197 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
2	D	134	PRO

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	А	337/338~(100%)	294~(87%)	43 (13%)	4 13
1	В	336/338~(99%)	308~(92%)	28~(8%)	11 32
1	Ε	337/338~(100%)	335~(99%)	2(1%)	86 96
1	Ζ	335/338~(99%)	333~(99%)	2(1%)	86 96
2	D	181/186~(97%)	175~(97%)	6 (3%)	38 72
2	Н	182/186~(98%)	181 (100%)	1 (0%)	88 96
3	\mathbf{C}	182/184~(99%)	175~(96%)	7 (4%)	33 67
3	L	182/184~(99%)	181 (100%)	1 (0%)	88 96
All	All	2072/2092~(99%)	1982 (96%)	90~(4%)	29 62

5 of 90 residues with a non-rotameric side chain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	179	THR
1	А	316	LYS
1	А	191	GLU
1	А	293	LEU
1	А	357	ARG

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such side chains are listed below:

Mol	Chain	Res	Type
1	А	27	HIS
1	А	36	GLN
1	А	207	ASN
2	Н	179	GLN
3	L	116	GLN



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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	А	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	163:ASN	C	164:ARG	N	3.09



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, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	А	403/405~(99%)	1.40	107 (26%) 0 0	18, 88, 137, 177	0
1	В	402/405~(99%)	0.36	21 (5%) 27 18	25, 53, 97, 116	0
1	Ε	403/405~(99%)	0.56	36 (8%) 9 5	16,63,102,129	0
1	Z	402/405~(99%)	0.53	28 (6%) 16 9	32, 61, 104, 132	0
2	D	217/222~(97%)	1.87	66 (30%) 0 0	37, 94, 161, 178	0
2	Η	218/222~(98%)	0.10	3 (1%) 75 70	20, 42, 79, 124	0
3	С	217/219~(99%)	0.21	5 (2%) 60 51	22, 46, 87, 105	0
3	L	217/219~(99%)	0.22	7 (3%) 47 37	$19, 45, \overline{87, 109}$	0
All	All	2479/2502 (99%)	0.67	273 (11%) 5 3	16, 59, 126, 178	0

The worst 5 of 273 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	182	GLY	11.3
1	А	195	GLY	10.9
2	D	198	GLY	10.9
2	D	133	ALA	10.9
1	А	386	TYR	10.8

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 monosaccharides in this entry.



6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

