

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

#### Aug 23, 2023 – 02:06 PM EDT

:	8EED
:	Crystal structure of a NHP anti-ZIKV neutralizing antibody rhMZ107-B in
	complex with ZIKV E glycoprotein
:	Sankhala, R.S.; Joyce, M.G.
:	2022-09-07
:	3.49  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
$\mathrm{EDS}$	:	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 3.49 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 <sub>free</sub>	130704	1379(3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

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			
1	А	405	70%	24%	•••	
1	В	405	% • 67%	28%	•	
1	С	405	% 64%	29%	•••	
1	D	405	61%	27%	5% 6%	
2	Е	226	4% 38% 15% •	46%		

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Mol	Chain	Length	(	Quality of chain	
2	Н	226	2% <b>3</b> 9%	12% •	44%
2	Ι	226	34%	18% •	45%
2	М	226	33%	17% •	46%
3	F	220	3% 41%	11%	48%
3	J	220	40%	12%	48%
3	L	220	34%	18% •	47%
3	Ν	220	% <b>4</b> 1%	11%	47%



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 19188 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		At	oms			ZeroOcc	AltConf	Trace
1	Δ	400	Total	С	Ν	0	$\mathbf{S}$	0	0 0	0
	A	400	3030	1896	524	584	26	0	0	0
1	C	201	Total	С	Ν	0	S	0	0	0
		591	2969	1857	517	570	25	0	0	U
1	. D	280	Total	С	Ν	0	S	0	0	0
		D 380	2841	1774	492	551	24	0	0	0
1	1 B	402	Total	С	Ν	0	S	0	0	0
		403	3069	1916	534	593	26	0	0	0

• Molecule 1 is a protein called Envelope protein E.

• Molecule 2 is a protein called rhMZ107-B antibody heavy chain.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
0	и	196	Total	С	Ν	0	$\mathbf{S}$	0	0	0
	п	120	962	612	157	191	2	0	0	0
0	м	199	Total	С	Ν	0	S	0	0	0
	1/1	122	939	600	153	184	2	0	0	0
0	F	192	Total	С	Ν	0	S	0	0	0
	Ľ	123	945	603	154	186	2	0	0	0
0	2 I	195	Total	С	Ν	0	S	0	0	0
		120	956	609	156	189	2	0		U

• Molecule 3 is a protein called rhMZ107-B antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
2	т	117	Total	С	Ν	0	S	0	0	0	
5		111	878	551	143	181	3	0	0	0	
2	N	116	Total	С	Ν	0	S	0	0	0	
5	IN	110	869	546	141	179	3	0	0	0	
9	F	115	Total	С	Ν	0	S	0	0	0	
0		Г	Г	110	865	544	140	178	3	0	0
2	т	J 115	Total	С	Ν	0	S	0	0	0	
5	J		865	544	140	178	3	U	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





Chain M: 33% 17% · 46%





• Molecule 3: rhMZ1	07-B antibody lig	ght chain		
Chain N:	41%	11%	47%	
GLN 82 83 83 84 82 829 829 829 829 829 829 829 829 829	Q40 P46 R47 L48 Y51 Y51 Y53 Y53 S56	L60 V 64 V 64 V 65 R67 K72 E73 E73 E73 E73 E73 E73 E73 E73 E73	A92 495 0105 0105 0113 0117 0117 0117 0117 0117 0117	ALA PRO
SER VAL THR LEU PHC PHC PRO SER SER SER SER SER SER SER SER SER SER	LTS THR THR LEU VAL CYS CYS CYS CYS LEU TLE SER SER TYR PHE TYR	GLY ALA VAL VAL GLU VAL CVAL ALA ALA SER ASP SER SER VAL	ASN ALA ALA GLY VAL THR THR THR TYS FRO SER CLYS SER ASN ASN ASN	TYR
ALA SER SER TTRR TTR LEU LEU TRR ASP ASP ASP TRP TRP TRP TRP TRP	LTS SER SER SER CYS GLN VAL HTS GLU GLU SER STHR	VAL GLU LYS LYS THR VAL ALA ALA ALA GLU		
• Molecule 3: rhMZ1	07-B antibody lig	ght chain		
Chain F:	41%	11%	48%	
GLN S2 14 15 15 46 12 46 12 46 12 46 12 46 12 41 8 12 41 8 12 41 8 12 41 8 12 41 8 12 41 8 12 14 12 12 14 12 12 14 14 15 15 14 14 15 15 14 14 15 15 14 15 15 14 15 15 15 15 15 15 15 15 15 15 15 15 15	A45 R47 L48 Y51 Y52 Y53 S54 B55 K58 K58	K72 E73 T74 S75 S76 S76 C96 C96 C96 C96 C97 C97 C98	D100 M104 M104 M104 M105 F107 F106 G108 G11 G12 G12 G12 G12 M14 M14	ALA PRO
SER VAL THR LEU PHE PRO PRO SER SER SER SER SER SER SER SER SER SER	LTS ALA THR LEU VAL CYS CYS CYS CYS LEU TLE SER ASP PHE TYR	GLY ALA ALA ALA GLU VAL ALA ALA ALA ALA GLY SER ALA VAL	ASN ALA ALA GLY VAL THR THR THR LVS PRO SER CLN SER ASN ASN	TYR
ALA SER SER TTR TTR LEU LEU TRP ASP ASP TRP TRP TRP TRP TRP	LTS TYR SER SER SER CYS GLN HIS GLN GLU SER THR	VAL GLU LYS LYS THR VAL ALA ALA ALA GLU		
• Molecule 3: rhMZ1	07-B antibody lig	ght chain		
Chain J:	40%	12%	48%	
6 6 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8	S25 226 D27 D27 039 Q39 Q40 K41 K41 L48 K41 L48 F48	L50 Y51 Y52 V52 D55 V68 T74 T74 L81 L81 L82	D90 V 98 V 98 C 101 C 100 C 101 C 111 C 111 C 101 C 101	PRO
VAL THR LEU PHE PRO PRO SER SER GLU GLU GLU GLU GLU ASN ASN CLYS	ALA THR LEU VAL CYS CYS CYS LEU LEU LEU LEU TLE SER ASP PHE TYR PHE TYR	ALA VAL GLU CAL CALA TRP TRP TRP TRP TRP CIV SER ASP SER ASP VAL ASN	ALA GLY VAL GLU THR THR LYS PRO SER LYS SER ASN SER ASN LYS TYS	ALA
SER SER LLEU LLEU THR LLEU THR ASP ASP ASP ASP ASP ASP ALM CLM CLM	SER SER CYS GLN VAL HIS GLV GLV GLV SER THR VAL VAL	GLU LYS THR VAL ALA ALA ALA GLU GLU		



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	92.03Å 105.63Å 132.38Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$82.52^{\circ}$ $70.48^{\circ}$ $81.04^{\circ}$	Depositor
Bosolution (Å)	48.84 - 3.49	Depositor
	48.84 - 3.49	EDS
% Data completeness	80.6 (48.84-3.49)	Depositor
(in resolution range)	66.3(48.84-3.49)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.99 (at 3.48 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
B B.	0.289 , $0.331$	Depositor
II, II, <i>free</i>	0.289 , $0.331$	DCC
$R_{free}$ test set	1996 reflections $(4.20\%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.5	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.27 , -10.6	EDS
L-test for $twinning^2$	$ < L >=0.46, < L^2>=0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.76	EDS
Total number of atoms	19188	wwPDB-VP
Average B, all atoms $(Å^2)$	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.18% 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.

# 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	Bo	nd lengths	Bo	ond angles	
	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.25	0/3094	0.51	2/4194~(0.0%)	
1	В	0.24	0/3134	0.49	0/4248	
1	С	0.29	1/3032~(0.0%)	0.50	0/4110	
1	D	0.26	0/2898	0.53	1/3934~(0.0%)	
2	Ε	0.24	0/970	0.46	0/1320	
2	Н	0.26	0/987	0.49	0/1343	
2	Ι	0.25	0/981	0.48	0/1335	
2	М	0.26	0/964	0.50	0/1312	
3	F	0.24	0/886	0.43	0/1207	
3	J	0.25	0/886	0.43	0/1207	
3	L	0.26	0/899	0.45	0/1224	
3	Ν	0.24	0/890	0.43	0/1212	
All	All	0.26	1/19621~(0.0%)	0.49	3/26646~(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	В	0	1
1	С	0	1
1	D	0	2
2	М	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	С	131	GLN	C-N	8.43	1.50	1.34

All (3) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	D	352	LEU	CA-CB-CG	6.36	129.93	115.30
1	А	280	ALA	CB-CA-C	-5.24	102.24	110.10
1	А	161	ASP	CB-CG-OD2	5.18	122.97	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	В	152	ILE	Peptide
1	С	130	ILE	Mainchain
1	D	191	GLU	Peptide
1	D	351	THR	Peptide
2	М	106	TYR	Peptide

#### 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	3030	0	2947	63	0
1	В	3069	0	2991	70	0
1	С	2969	0	2891	81	0
1	D	2841	0	2730	71	0
2	Е	945	0	917	20	0
2	Н	962	0	932	27	0
2	Ι	956	0	927	29	0
2	М	939	0	912	32	0
3	F	865	0	829	16	0
3	J	865	0	829	16	0
3	L	878	0	843	29	0
3	N	869	0	832	16	0
All	All	19188	0	18580	444	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 12.

The worst 5 of 444 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:B:53:MET:SD	1:B:130:ILE:HG22	1.36	1.65
1:B:53:MET:SD	1:B:130:ILE:CG2	2.25	1.24
1:C:53:MET:HE2	1:C:130:ILE:HB	1.52	0.91
1:C:131:GLN:OE1	1:B:77:GLN:NE2	2.12	0.83
1:C:342:PRO:HG2	1:C:391:VAL:HG22	1.63	0.80

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	Perce	ntiles
1	А	396/405~(98%)	358~(90%)	38 (10%)	0	100	100
1	В	401/405~(99%)	369 (92%)	31 (8%)	1 (0%)	47	80
1	С	387/405~(96%)	351 (91%)	35~(9%)	1 (0%)	41	75
1	D	372/405~(92%)	338 (91%)	29 (8%)	5 (1%)	12	45
2	Е	121/226~(54%)	113 (93%)	8 (7%)	0	100	100
2	Н	124/226~(55%)	113 (91%)	9 (7%)	2 (2%)	9	41
2	Ι	123/226~(54%)	114 (93%)	8 (6%)	1 (1%)	19	57
2	М	120/226~(53%)	108 (90%)	12 (10%)	0	100	100
3	F	113/220~(51%)	108 (96%)	5(4%)	0	100	100
3	J	113/220~(51%)	109 (96%)	4 (4%)	0	100	100
3	L	115/220~(52%)	107~(93%)	8 (7%)	0	100	100
3	N	114/220~(52%)	109 (96%)	5 (4%)	0	100	100
All	All	2499/3404 (73%)	2297 (92%)	192 (8%)	10 (0%)	34	70

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	192	PRO
	<i>a</i>	-	

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		1	1 0
Mol	Chain	$\mathbf{Res}$	Type
1	В	153	VAL
1	D	193	ARG
2	Н	42	PRO
2	H	41	PRO

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perc	entiles
1	А	329/338~(97%)	292~(89%)	37 (11%)	6	25
1	В	335/338~(99%)	294 (88%)	41 (12%)	5	22
1	С	322/338~(95%)	284 (88%)	38 (12%)	5	23
1	D	304/338~(90%)	260 (86%)	44 (14%)	3	16
2	Ε	104/196~(53%)	95~(91%)	9~(9%)	10	36
2	Н	106/196~(54%)	92~(87%)	14 (13%)	4	19
2	Ι	105/196~(54%)	92~(88%)	13~(12%)	4	21
2	М	103/196~(53%)	91~(88%)	12 (12%)	5	24
3	F	98/185~(53%)	97~(99%)	1 (1%)	76	89
3	J	98/185~(53%)	95~(97%)	3 (3%)	40	70
3	L	99/185~(54%)	95~(96%)	4 (4%)	31	62
3	Ν	98/185~(53%)	94 (96%)	4 (4%)	30	62
All	All	2101/2876 (73%)	1881 (90%)	220 (10%)	7	29

5 of 220 residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	D	369	THR
1	В	198	PHE
3	J	41	LYS
3	Ν	47	ARG
1	В	9	ARG



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	$\operatorname{Res}$	Type
3	J	34	ASN
3	F	6	GLN
1	В	131	GLN
1	D	77	GLN
3	Ν	39	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)

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,  $95^{th}$  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	<RSRZ $>$	# RSRZ > 2	$OWAB(Å^2)$	Q<0.9
1	А	400/405~(98%)	0.10	2 (0%) 91 88	16, 40, 70, 93	0
1	В	403/405~(99%)	0.11	4 (0%) 82 78	20, 41, 75, 101	0
1	С	391/405~(96%)	0.12	3 (0%) 86 82	20, 43, 72, 108	0
1	D	380/405~(93%)	0.11	2 (0%) 91 88	18, 40, 78, 104	0
2	Ε	123/226~(54%)	0.46	10 (8%) 12 14	38, 69, 85, 96	0
2	Н	126/226~(55%)	0.18	4 (3%) 47 45	24, 59, 75, 84	0
2	Ι	125/226~(55%)	0.51	12 (9%) 8 10	39, 82, 102, 116	0
2	М	122/226~(53%)	0.21	0 100 100	33, 60, 79, 96	0
3	F	115/220~(52%)	0.31	6 (5%) 27 26	29, 53, 72, 98	0
3	J	115/220~(52%)	0.11	1 (0%) 84 80	34, 52, 79, 88	0
3	L	117/220~(53%)	-0.04	0 100 100	22, 41, 58, 67	0
3	Ν	116/220~(52%)	0.11	2 (1%) 70 66	23, 42, 62, 71	0
All	All	2533/3404 (74%)	0.16	46 (1%) 68 64	16, 47, 81, 116	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	390	GLY	5.4
1	С	391	VAL	5.0
2	Е	120	LEU	3.8
2	Е	123	VAL	3.8
2	Е	11	LEU	3.5

## 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.

