

wwPDB X-ray Structure Validation Summary Report (i)

Aug 23, 2023 – 02:11 PM EDT

PDB ID : 8EE5

Title: Crystal structure of a NHP anti-ZIKV neutralizing antibody rhMZ119-D in

complex with ZIKV E glycoprotein

Authors : Sankhala, R.S.; Joyce, M.G.

Deposited on : 2022-09-06

Resolution : 3.58 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:

Mol Probity : 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.35

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

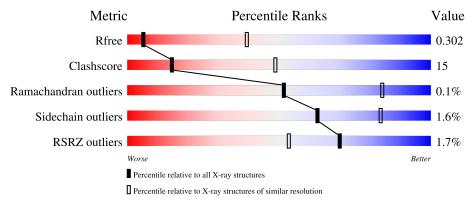
Validation Pipeline (wwPDB-VP) : 2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 3.58 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
R_{free}	130704	1094 (3.66-3.50)
Clashscore	141614	1181 (3.66-3.50)
Ramachandran outliers	138981	1143 (3.66-3.50)
Sidechain outliers	138945	1143 (3.66-3.50)
RSRZ outliers	127900	1012 (3.66-3.50)

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	Z	405	67% 30%		•			
2	Н	218	81%	17%				
3	L	212	83%	17%				
4	A	2	100%					

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard



residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	1	-	-	X	-



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6300 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 Envelope protein E.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	7	403	Total	С	N	О	S	0	0	0
1	L	403	3079	1921	538	594	26	0	U	

• Molecule 2 is a protein called rhMZ119-D antibody heavy chain.

Mo	l Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	Н	215	Total 1613	C 1016	N 267	O 324	S 6	0	0	0

• Molecule 3 is a protein called rhMZ119-D antibody light chain.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	L	211	Total 1580	C 992	N 260	O 324	S 4	0	0	0

• Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



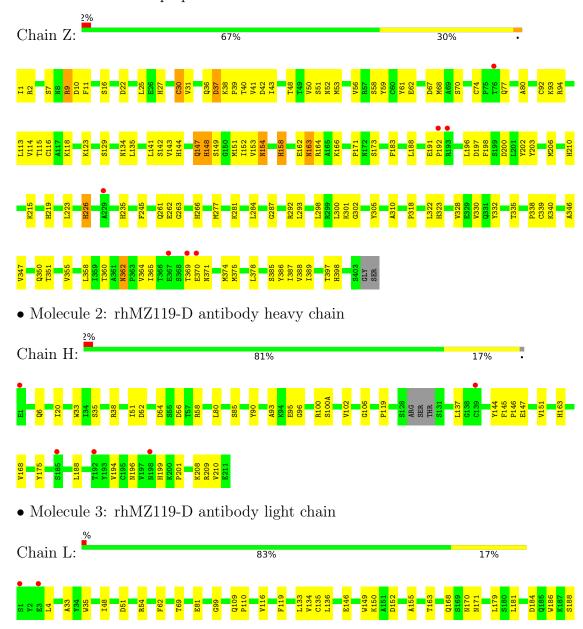
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	A	2	Total 28	C 16	N 2	O 10	0	0	0



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 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A: 100%





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants	51.68Å 103.67Å 196.70Å	Donositon
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.99 - 3.58	Depositor
Resolution (A)	29.36 - 3.57	EDS
% Data completeness	99.6 (14.99-3.58)	Depositor
(in resolution range)	90.8 (29.36-3.57)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$< I/\sigma(I) > 1$	0.51 (at 3.55Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
D D	0.249 , 0.296	Depositor
R, R_{free}	0.272 , 0.302	DCC
R_{free} test set	654 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	91.6	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.30 , 46.1	EDS
L-test for twinning ²	$ < L > = 0.46, < L^2> = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	6300	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.73% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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	Boı	nd lengths	Bond angles		
Moi Chain		RMSZ	# Z > 5	RMSZ	# Z >5	
1	Z	0.34	1/3144 (0.0%)	0.56	0/4260	
2	Н	0.25	0/1651	0.45	0/2249	
3	L	0.26	0/1620	0.46	0/2209	
All	All	0.30	1/6415 (0.0%)	0.51	0/8718	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
1	Z	362	ASN	C-N	7.75	1.49	1.34

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	Z	3079	0	3007	135	0
2	Н	1613	0	1580	23	0
3	L	1580	0	1522	27	0
4	A	28	0	25	15	0
All	All	6300	0	6134	190	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 15.

The worst 5 of 190 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	Clash overlap (Å)
1:Z:305:TYR:CE1	1:Z:338:PRO:HB2	1.38	1.53
1:Z:305:TYR:HE1	1:Z:338:PRO:CB	1.43	1.31
1:Z:151:MET:O	4:A:1:NAG:H82	1.43	1.18
3:L:109:GLN:HG2	3:L:110:PRO:HD2	1.21	1.16
1:Z:305:TYR:CE1	1:Z:338:PRO:CB	2.20	1.14

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	Z	401/405 (99%)	369 (92%)	31 (8%)	1 (0%)	47	80
2	Н	211/218 (97%)	204 (97%)	7 (3%)	0	100	100
3	L	209/212 (99%)	204 (98%)	5 (2%)	0	100	100
All	All	821/835 (98%)	777 (95%)	43 (5%)	1 (0%)	51	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Z	37	ASP

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 o	of residues	for	which	the	${\rm sidechain}$	conformation	was
analysed, and the total number of residues.								

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	Z	337/338 (100%)	328 (97%)	9 (3%)	44	74	
2	Н	185/188 (98%)	183 (99%)	2 (1%)	73	88	
3	L	175/176 (99%)	175 (100%)	0	100	100	
All	All	697/702 (99%)	686 (98%)	11 (2%)	62	83	

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Z	226	HIS
1	Z	235	HIS
2	Н	188	LEU
2	Н	38	ARG
1	Z	154	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

2 monosaccharides are 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	Т	Chain	Dag	Link	Bond lengths			Bond angles		
IVIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
4	NAG	A	1	4,1	14,14,15	0.38	0	17,19,21	1.44	3 (17%)
4	NAG	A	2	4	14,14,15	0.46	0	17,19,21	1.22	3 (17%)

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	A	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	A	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\mathbf{Ideal}(^{o})$
4	A	1	NAG	O4-C4-C3	3.23	117.81	110.35
4	A	2	NAG	C1-C2-N2	2.89	115.43	110.49
4	A	1	NAG	O5-C1-C2	-2.62	107.16	111.29
4	A	2	NAG	C1-O5-C5	2.48	115.55	112.19
4	A	1	NAG	C1-O5-C5	2.35	115.38	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2	NAG	C8-C7-N2-C2
4	A	2	NAG	O7-C7-N2-C2
4	A	1	NAG	C8-C7-N2-C2
4	A	1	NAG	O7-C7-N2-C2
4	A	1	NAG	C3-C2-N2-C7

There are no ring outliers.

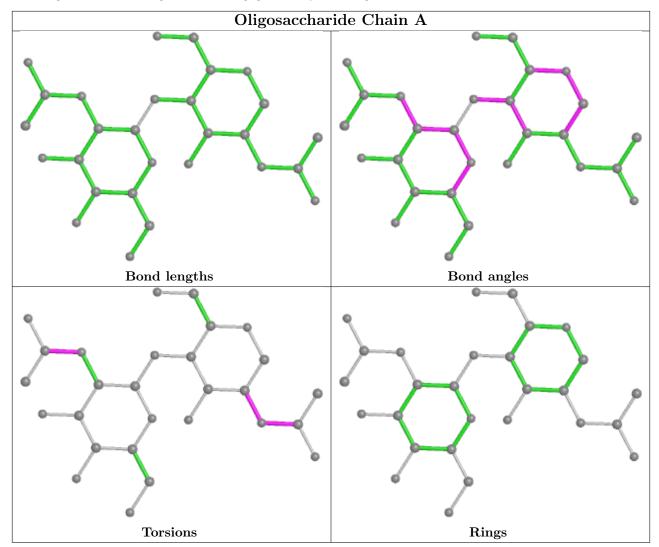
2 monomers are involved in $15\ \mathrm{short}$ contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	NAG	15	0
4	A	2	NAG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,



bond angles, torsion angles, and ring geometry for oligosaccharide.



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>	#RS	# RSRZ > 2		$\mathrm{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	Z	403/405 (99%)	0.09	7 (1%)	70	53	58, 101, 130, 165	0
2	Н	215/218 (98%)	0.08	5 (2%)	60	42	47, 105, 162, 188	0
3	L	211/212 (99%)	-0.00	2 (0%)	84	71	70, 103, 133, 219	0
All	All	829/835 (99%)	0.06	14 (1%)	70	53	47, 102, 139, 219	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Н	192	THR	2.7
3	L	3	GLU	2.6
3	L	1	SER	2.5
1	Z	193	ARG	2.5
1	Z	367	GLU	2.3

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)

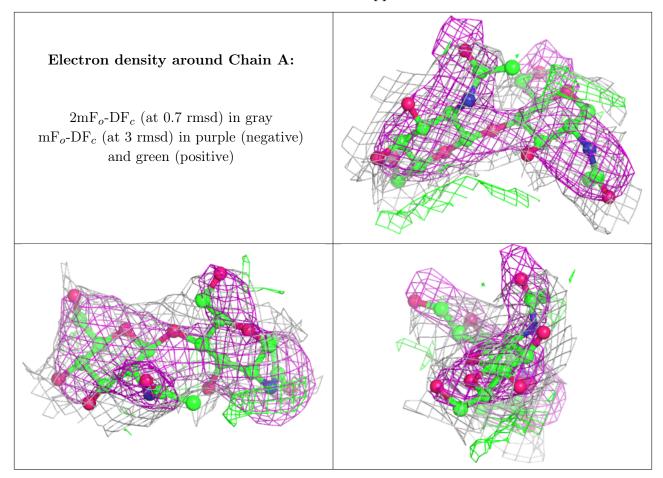
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
4	NAG	A	1	14/15	0.79	0.39	30,30,30,30	0
4	NAG	A	2	14/15	0.83	0.42	30,30,30,30	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-



charide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

