



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:48 AM UTC

PDB ID : 8EF3 / pdb_00008ef3
Title : Crystal structure of a NHP anti-ZIKV neutralizing antibody rhMZ119-D
Authors : Sankhala, R.S.; Joyce, M.G.
Deposited on : 2022-09-07
Resolution : 1.67 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
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

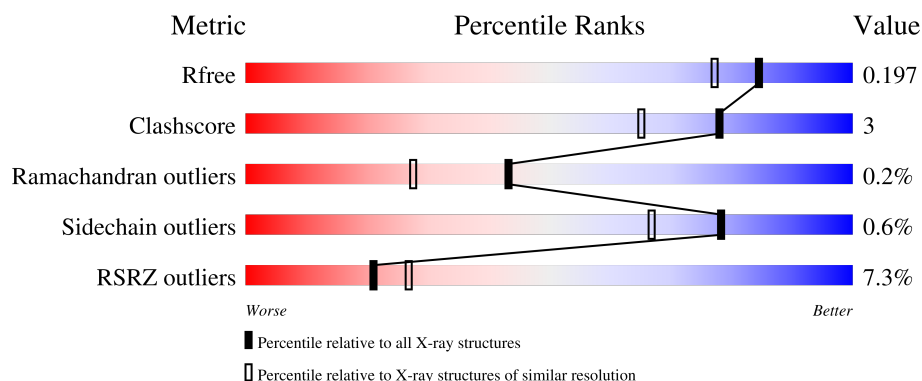
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.67 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	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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	A	220	8% 94% • •
1	C	220	10% 93% 5% •
2	B	212	6% 89% 10%
2	D	212	5% 88% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7390 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 rhMZ119-D antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1600	1012	262	320	6			
1	C	215	Total	C	N	O	S	0	0	0
			1604	1014	262	322	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	1	0
			1587	997	263	323	4			
2	D	211	Total	C	N	O	S	0	1	0
			1587	997	263	323	4			

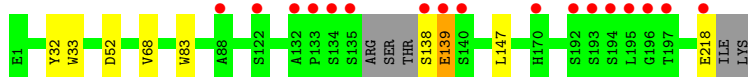
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	294	Total	O	0	0
			294	294		
3	B	250	Total	O	0	0
			250	250		
3	C	222	Total	O	0	0
			222	222		
3	D	246	Total	O	0	0
			246	246		

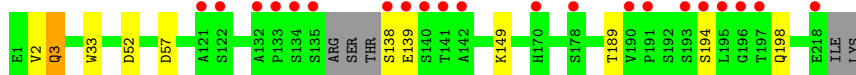
3 Residue-property plots [i](#)

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.

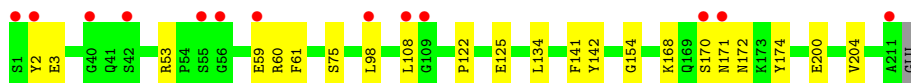
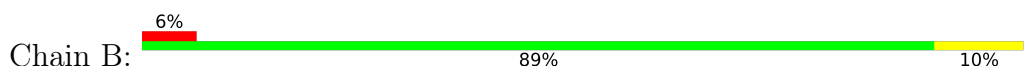
- Molecule 1: rhMZ119-D antibody heavy chain



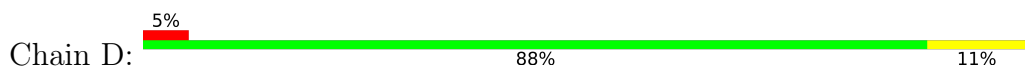
- Molecule 1: rhMZ119-D antibody heavy chain



- Molecule 2: rhMZ119-D antibody light chain



- Molecule 2: rhMZ119-D antibody light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.24Å 71.02Å 103.74Å 90.00° 102.38° 90.00°	Depositor
Resolution (Å)	34.30 – 1.67 34.30 – 1.67	Depositor EDS
% Data completeness (in resolution range)	91.9 (34.30-1.67) 92.0 (34.30-1.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 1.67Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.182 , 0.198 0.182 , 0.197	Depositor DCC
R_{free} test set	2000 reflections (1.73%)	wwPDB-VP
Wilson B-factor (Å ²)	14.8	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 57.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7390	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.44% 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

5.1 Standard geometry

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	A	0.14	0/1638	0.42	0/2234
1	C	0.28	1/1642 (0.1%)	0.42	0/2239
2	B	0.57	6/1630 (0.4%)	0.46	0/2223
2	D	0.61	6/1630 (0.4%)	0.50	1/2223 (0.0%)
All	All	0.45	13/6540 (0.2%)	0.45	1/8919 (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	A	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	138	ILE	C-O	-7.11	1.16	1.24
2	B	141	PHE	C-O	-7.05	1.15	1.23
2	B	168	LYS	C-O	-6.80	1.15	1.23
1	C	3	GLN	C-O	-6.59	1.15	1.23
2	B	171	ASN	C-O	-6.47	1.15	1.24
2	D	139	SER	C-O	-6.40	1.15	1.23
2	B	142	TYR	C-O	-6.11	1.16	1.24
2	B	170	SER	C-O	-6.09	1.16	1.24
2	D	142	TYR	C-O	-5.97	1.16	1.24
2	B	174	TYR	C-O	-5.86	1.16	1.23
2	D	145	ALA	C-O	-5.86	1.17	1.23
2	D	146	VAL	C-O	-5.52	1.16	1.23
2	D	144	GLY	C-O	-5.39	1.16	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	139	SER	N-CA-C	5.59	117.47	109.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	GLU	Peptide

5.2 Too-close contacts

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	A	1600	0	1547	7	0
1	C	1604	0	1551	7	0
2	B	1587	0	1532	11	0
2	D	1587	0	1532	12	0
3	A	294	0	0	4	5
3	B	250	0	0	6	4
3	C	222	0	0	2	1
3	D	246	0	0	4	2
All	All	7390	0	6162	35	6

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 3.

All (35) 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:C:189:THR:O	3:C:301:HOH:O	1.91	0.87
1:C:57:ASP:OD1	3:C:302:HOH:O	1.98	0.80
1:A:139:GLU:O	3:A:301:HOH:O	1.99	0.79
2:B:172:ASN:HD21	2:D:1:SER:HA	1.50	0.76
2:B:125:GLU:HG3	3:B:408:HOH:O	1.86	0.75
2:D:110:GLN:O	3:D:301:HOH:O	2.04	0.75
2:B:200:GLU:OE2	3:B:301:HOH:O	2.03	0.75
1:A:32:TYR:OH	3:A:302:HOH:O	2.05	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:125:GLU:OE1	3:D:302:HOH:O	2.07	0.71
2:B:204:VAL:HG21	3:B:342:HOH:O	1.89	0.71
2:D:53[B]:ARG:NH1	2:D:57:ILE:O	2.26	0.68
2:B:125:GLU:OE1	3:B:302:HOH:O	2.12	0.68
1:A:139:GLU:OE1	3:A:303:HOH:O	2.12	0.67
1:C:149:LYS:HZ3	2:D:131:LYS:HD3	1.63	0.64
2:D:165:LYS:HD3	3:D:505:HOH:O	1.99	0.62
2:D:60:ARG:HB2	2:D:75:SER:O	2.05	0.56
2:B:59:GLU:O	3:B:303:HOH:O	2.18	0.54
1:A:139:GLU:HB3	3:A:544:HOH:O	2.08	0.52
2:D:30:LYS:NZ	3:D:305:HOH:O	2.41	0.51
2:D:2:TYR:CD2	2:D:98:LEU:HD13	2.46	0.51
2:B:2:TYR:CD2	2:B:98:LEU:HD13	2.46	0.51
1:C:2:VAL:C	1:C:3:GLN:HG3	2.37	0.48
2:B:154:GLY:N	3:B:304:HOH:O	2.21	0.48
1:A:138:SER:C	1:A:139:GLU:HG2	2.39	0.48
2:B:122:PRO:HD3	2:B:134:LEU:CD2	2.44	0.47
1:C:33:TRP:CE2	1:C:52:ASP:HB2	2.50	0.46
2:B:60:ARG:HB2	2:B:75:SER:O	2.16	0.45
1:C:138:SER:C	1:C:139:GLU:HG2	2.42	0.45
2:D:151:LYS:HE2	2:D:196:GLN:OE1	2.19	0.43
2:D:131:LYS:HE2	2:D:131:LYS:HB3	1.81	0.43
2:B:53[A]:ARG:HD3	2:B:61:PHE:O	2.18	0.42
2:D:194:SER:OG	2:D:207:THR:HG22	2.19	0.42
1:A:33:TRP:CE2	1:A:52:ASP:HB2	2.55	0.41
1:A:68:VAL:HG12	1:A:83:TRP:CD1	2.55	0.41
1:C:194:SER:HB2	1:C:198:GLN:HB3	2.03	0.41

All (6) 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)
3:B:473:HOH:O	3:D:509:HOH:O[1_655]	1.94	0.26
3:A:494:HOH:O	3:B:486:HOH:O[2_654]	2.02	0.18
3:A:579:HOH:O	3:D:458:HOH:O[2_655]	2.02	0.18
3:A:472:HOH:O	3:B:464:HOH:O[2_654]	2.06	0.14
3:A:554:HOH:O	3:B:518:HOH:O[2_654]	2.11	0.09
3:A:411:HOH:O	3:C:449:HOH:O[2_554]	2.16	0.04

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	A	211/220 (96%)	205 (97%)	6 (3%)	0	100	100
1	C	211/220 (96%)	204 (97%)	7 (3%)	0	100	100
2	B	210/212 (99%)	205 (98%)	4 (2%)	1 (0%)	24	8
2	D	210/212 (99%)	205 (98%)	4 (2%)	1 (0%)	24	8
All	All	842/864 (98%)	819 (97%)	21 (2%)	2 (0%)	43	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	108	LEU
2	B	108	LEU

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	A	178/190 (94%)	176 (99%)	2 (1%)	65	47
1	C	179/190 (94%)	179 (100%)	0	100	100
2	B	175/176 (99%)	174 (99%)	1 (1%)	78	67
2	D	175/176 (99%)	174 (99%)	1 (1%)	78	67
All	All	707/732 (97%)	703 (99%)	4 (1%)	78	67

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	LEU
1	A	218	GLU
2	B	3	GLU
2	D	3	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	GLN
2	B	78	GLN
2	B	172	ASN
2	B	199	HIS
1	C	82	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 oligosaccharides 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	A	215/220 (97%)	0.03	17 (7%) 18 24	8, 17, 43, 75	0
1	C	215/220 (97%)	0.27	21 (9%) 13 16	11, 18, 50, 89	0
2	B	211/212 (99%)	0.11	13 (6%) 26 34	6, 18, 40, 68	1 (0%)
2	D	211/212 (99%)	0.08	11 (5%) 33 41	10, 19, 38, 86	1 (0%)
All	All	852/864 (98%)	0.12	62 (7%) 21 27	6, 18, 43, 89	2 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	138	SER	7.8
2	B	2	TYR	7.3
1	C	138	SER	7.1
1	C	133	PRO	6.1
2	D	2	TYR	5.9
2	B	211	ALA	5.9
2	B	1	SER	5.9
2	B	109	GLY	5.5
1	A	195	LEU	5.4
1	C	132	ALA	5.2
1	A	139	GLU	5.1
2	D	211	ALA	4.9
2	B	40	GLY	4.5
1	C	135	SER	4.5
1	A	194	SER	4.4
1	A	140	SER	4.3
2	D	1	SER	4.3
1	C	140	SER	4.2
1	C	195	LEU	3.9
1	C	134	SER	3.9
2	D	109	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	139	GLU	3.8
1	C	196	GLY	3.7
1	C	141	THR	3.5
1	A	134	SER	3.4
2	B	171	ASN	3.4
1	C	142	ALA	3.4
2	B	108	LEU	3.4
2	D	170	SER	3.2
1	A	196	GLY	3.2
1	A	193	SER	3.2
1	A	197	THR	3.1
1	C	197	THR	3.1
2	D	171	ASN	3.1
1	A	133	PRO	3.0
1	C	193	SER	3.0
1	C	121	ALA	3.0
2	D	108	LEU	3.0
2	B	170	SER	2.8
2	B	98	LEU	2.7
2	B	56	GLY	2.7
1	A	218	GLU	2.6
1	A	135	SER	2.6
1	C	178	SER	2.6
1	C	170	HIS	2.5
2	B	42	SER	2.5
1	C	191	PRO	2.4
1	A	122	SER	2.3
2	B	59	GLU	2.3
1	A	88	ALA	2.3
1	A	192	SER	2.3
2	D	98	LEU	2.3
1	C	190	VAL	2.3
2	D	40	GLY	2.2
2	D	158	ASN	2.2
1	A	132	ALA	2.2
2	B	55	SER	2.2
1	C	218	GLU	2.2
1	A	170	HIS	2.1
1	C	194	SER	2.1
1	C	122	SER	2.0
2	D	143	PRO	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.