



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 5JHL
Title : Crystal structure of zika virus envelope protein in complex with a flavivirus broadly-protective antibody
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Deposited on : 2016-04-21
Resolution : 3.00 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

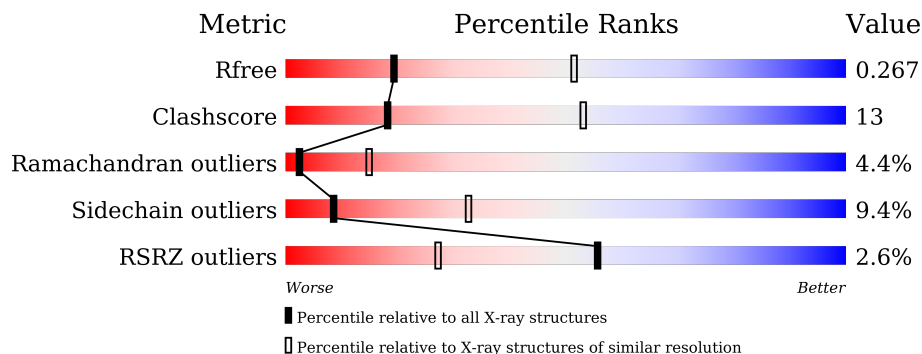
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	416	 3% (poor fit) 57% (0 outliers) 28% (1 outlier) 6% (2 outliers) 7% (3+ outliers) 0% (not modelled)
2	H	231	 3% (poor fit) 68% (0 outliers) 24% (1 outlier) 6% (2 outliers) 0% (3+ outliers) 0% (not modelled)
3	L	216	 0% (poor fit) 75% (0 outliers) 22% (1 outlier) 0% (2 outliers) 0% (3+ outliers) 0% (not modelled)

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6087 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	385	2853	1789	482	558	24	0	0	0

- Molecule 2 is a protein called Antibody Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	216	1624	1022	269	326	7	0	0	0

- Molecule 3 is a protein called antibody Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	211	1610	1000	269	334	7	0	0	0

K148	W149	T165	D166	Q167	M176	T183	K184	D185	E186	Y187	Y193	E196	A197	T198	H199	P205	I206	V207	K208	S209	F210	N211	R212	ASN	GLU	CYS	SER
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.60Å 104.86Å 81.86Å 90.00° 102.70° 90.00°	Depositor
Resolution (Å)	30.69 – 3.00 30.69 – 2.99	Depositor EDS
% Data completeness (in resolution range)	97.7 (30.69-3.00) 88.6 (30.69-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 3.00Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.228 , 0.269 0.228 , 0.267	Depositor DCC
R_{free} test set	820 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	60.9	Xtrriage
Anisotropy	0.725	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 34.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6087	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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](#)

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	0.34	0/2914	0.52	2/3966 (0.1%)
2	H	0.29	0/1666	0.46	0/2279
3	L	0.31	0/1647	0.47	1/2243 (0.0%)
All	All	0.32	0/6227	0.49	3/8488 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	53	ALA	CB-CA-C	-5.99	101.12	110.10
1	A	233	THR	C-N-CD	5.93	140.86	128.40
1	A	250	ALA	CB-CA-C	5.72	118.68	110.10

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	A	2853	0	2706	106	1
2	H	1624	0	1564	28	1
3	L	1610	0	1491	28	0
All	All	6087	0	5761	159	1

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 13.

The worst 5 of 159 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:A:331:GLN:CG	1:A:371:ASN:OD1	1.89	1.20
1:A:331:GLN:HG2	1:A:371:ASN:OD1	1.42	1.20
1:A:351:THR:HG22	1:A:352:LEU:HB2	1.12	1.09
1:A:50:VAL:HG12	1:A:135:LEU:HD23	1.41	1.01
1:A:231:THR:HG23	1:A:232:GLY:H	1.23	1.01

All (1) 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:A:279:GLY:O	2:H:212:SER:OG[2_444]	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	Percentiles	
1	A	381/416 (92%)	311 (82%)	41 (11%)	29 (8%)	1	5
2	H	214/231 (93%)	195 (91%)	13 (6%)	6 (3%)	5	25
3	L	209/216 (97%)	197 (94%)	12 (6%)	0	100	100
All	All	804/863 (93%)	703 (87%)	66 (8%)	35 (4%)	2	15

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	ALA
1	A	231	THR
1	A	247	ASP
1	A	288	HIS
2	H	64	ASN

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	302/348 (87%)	260 (86%)	42 (14%)	3	16
2	H	184/200 (92%)	173 (94%)	11 (6%)	19	53
3	L	181/192 (94%)	171 (94%)	10 (6%)	21	57
All	All	667/740 (90%)	604 (91%)	63 (9%)	8	32

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	278	ASP
3	L	84	ASP
1	A	301	LYS
3	L	58	THR
3	L	147	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	226	HIS
3	L	30	HIS
3	L	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, 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	385/416 (92%)	-0.07	13 (3%) 45 19	46, 75, 114, 166	0
2	H	216/231 (93%)	-0.22	7 (3%) 47 20	39, 63, 108, 155	0
3	L	211/216 (97%)	-0.32	1 (0%) 91 75	38, 68, 85, 107	0
All	All	812/863 (94%)	-0.18	21 (2%) 56 27	38, 69, 108, 166	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	31	GLU	8.0
1	A	18	GLY	5.0
2	H	137	SER	4.9
1	A	16	SER	4.8
1	A	22	ASP	4.5

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.