



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 12:44 pm BST

PDB ID : 6DFJ
Title : Crystal structure of anti-Zika antibody Z021 bound to DENV-1 envelope protein DIII
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Deposited on : 2018-05-14
Resolution : 2.07 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 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 : 2.11
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) : 2.11

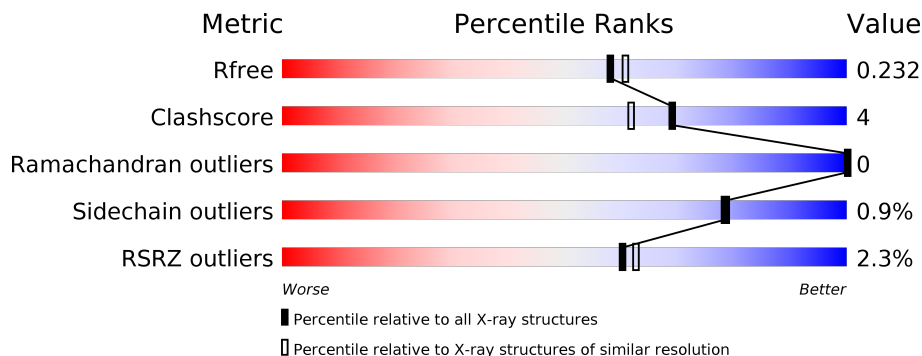
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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 on 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	H	230	
2	L	216	
3	E	99	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4191 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 anti-Zika antibody Z021, Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	219	1647	1041	272	327	7	0	0	0

- Molecule 2 is a protein called anti-Zika antibody Z021, Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	214	1661	1044	282	331	4	0	0	0

- Molecule 3 is a protein called Dengue 1 Envelope DIII domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	99	757	482	123	149	3	0	0	0

- Molecule 4 is water.

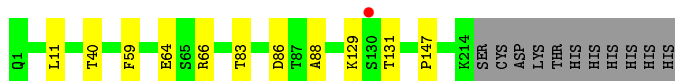
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	68	Total 68 O 68	0	0
4	L	49	Total 49 O 49	0	0
4	E	9	Total 9 O 9	0	0

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA 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: anti-Zika antibody Z021, Heavy Chain

Chain H: 




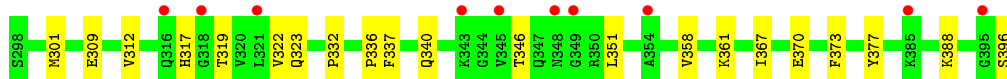
- Molecule 2: anti-Zika antibody Z021, Light Chain

Chain L: 



- Molecule 3: Dengue 1 Envelope DIII domain

Chain E: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	60.54Å 91.60Å 187.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.51 – 2.07 50.51 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.51-2.07) 99.5 (50.51-2.07)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.07Å)	Xtrriage
Refinement program	PHENIX 1.13_2998, PHENIX 1.13_2998	Depositor
R, R_{free}	0.184 , 0.232 0.184 , 0.232	Depositor DCC
R_{free} test set	1566 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	50.3	Xtrriage
Anisotropy	0.199	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4191	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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	H	0.32	0/1691	0.55	0/2311
2	L	0.32	0/1700	0.52	0/2313
3	E	0.28	0/772	0.48	0/1043
All	All	0.31	0/4163	0.53	0/5667

There are no bond length outliers.

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	H	1647	0	1605	5	0
2	L	1661	0	1616	14	0
3	E	757	0	757	13	0
4	E	9	0	0	0	0
4	H	68	0	0	0	0
4	L	49	0	0	1	0
All	All	4191	0	3978	30	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 4.

All (30) 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)
3:E:340:GLN:HA	3:E:346:THR:HA	1.82	0.60
3:E:312:VAL:HG22	3:E:322:VAL:HG12	1.83	0.60
1:H:59:PHE:HB2	1:H:64:GLU:HG2	1.85	0.59
2:L:132:VAL:HG22	2:L:179:LEU:HB3	1.84	0.58
1:H:40:THR:HG22	1:H:88:ALA:HB2	1.86	0.56
2:L:185:ASP:HA	2:L:188:LYS:HE2	1.88	0.56
3:E:340:GLN:HG2	3:E:346:THR:HG22	1.89	0.54
1:H:11:LEU:HD13	1:H:147:PRO:HG3	1.93	0.50
1:H:66:ARG:NH2	1:H:86:ASP:OD2	2.44	0.50
3:E:309:GLU:HB3	3:E:323:GLN:HG2	1.93	0.50
2:L:67:SER:OG	2:L:68:GLY:N	2.44	0.49
2:L:145:LYS:HB3	2:L:197:THR:OG1	2.13	0.49
3:E:322:VAL:HG23	3:E:367:ILE:HB	1.95	0.47
2:L:48:ILE:HD13	2:L:54:ARG:HA	1.96	0.46
2:L:70:ASP:N	2:L:70:ASP:OD1	2.49	0.46
2:L:21:LEU:HD23	2:L:102:THR:HB	1.98	0.46
1:H:129:LYS:HG3	2:L:209:PHE:HB3	1.98	0.46
2:L:197:THR:HG22	2:L:204:PRO:HB3	1.97	0.45
3:E:373:PHE:HB3	3:E:396:SER:HB3	1.98	0.45
2:L:132:VAL:CG2	2:L:179:LEU:HB3	2.47	0.44
2:L:32:TYR:OH	3:E:361:LYS:NZ	2.51	0.44
3:E:332:PRO:HA	3:E:358:VAL:O	2.18	0.43
2:L:142:ARG:NH1	4:L:304:HOH:O	2.50	0.43
2:L:120:PRO:HD3	2:L:132:VAL:HG12	2.00	0.43
3:E:301:MET:HG2	3:E:336:PRO:HG3	2.01	0.42
3:E:309:GLU:HG2	3:E:323:GLN:HE21	1.84	0.42
3:E:319:THR:HG22	3:E:370:GLU:HG3	2.01	0.42
3:E:377:TYR:CD2	3:E:388:LYS:HG2	2.55	0.42
2:L:121:SER:O	2:L:125:LEU:HG	2.20	0.42
3:E:337:PHE:CD2	3:E:351:LEU:HD13	2.56	0.40

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	Percentiles	
1	H	217/230 (94%)	209 (96%)	8 (4%)	0	100	100
2	L	212/216 (98%)	203 (96%)	9 (4%)	0	100	100
3	E	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
All	All	526/545 (96%)	504 (96%)	22 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	H	190/201 (94%)	188 (99%)	2 (1%)	73	72
2	L	187/189 (99%)	186 (100%)	1 (0%)	88	89
3	E	84/84 (100%)	83 (99%)	1 (1%)	71	69
All	All	461/474 (97%)	457 (99%)	4 (1%)	78	78

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

Mol	Chain	Res	Type
1	H	83	THR
1	H	131	THR
2	L	203	SER
3	E	317	HIS

Some 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](#)

There are no carbohydrates 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	H	219/230 (95%)	-0.39	1 (0%) 91 91	37, 56, 92, 115	0
2	L	214/216 (99%)	-0.30	1 (0%) 91 91	37, 62, 108, 139	0
3	E	99/99 (100%)	0.48	10 (10%) 7 7	56, 79, 140, 151	0
All	All	532/545 (97%)	-0.19	12 (2%) 60 63	37, 63, 114, 151	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	316	GLN	3.8
3	E	345	VAL	3.8
3	E	348	ASN	3.5
3	E	343	LYS	3.4
3	E	321	LEU	3.4
3	E	349	GLY	3.1
3	E	354	ALA	3.1
3	E	385	LYS	2.9
3	E	318	GLY	2.7
2	L	1	GLU	2.4
3	E	395	GLY	2.3
1	H	130	SER	2.1

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 carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.