



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:28 am GMT

PDB ID : 3J2Y  
EMDB ID: : EMD-5578  
Title : Electron Cryo-microscopy of Chikungunya VLP in complex with neutralizing antibody Fab 9.8B  
Authors : Sun, S.; Xiang, Y.; Rossmann, M.G.  
Deposited on : 2013-01-28  
Resolution : 14.90 Å(reported)  
Based on PDB ID : 4GQ9

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc29047

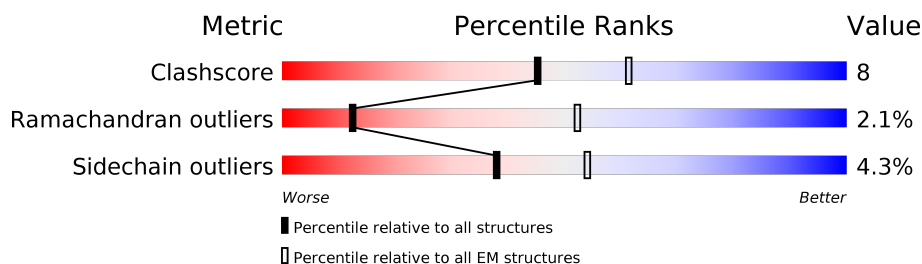
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 14.90 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	212	83% 16% .
1	C	212	83% 15% .
1	E	212	85% 13% .
1	G	212	85% 14% .
2	B	218	78% 19% .
2	D	218	79% 18% .
2	F	218	79% 17% .
2	H	218	77% 20% .

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13120 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 9.8B light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	212	Total	C	N	O	S	0	0
			1633	1015	273	336	9		
1	C	212	Total	C	N	O	S	0	0
			1633	1015	273	336	9		
1	E	212	Total	C	N	O	S	0	0
			1633	1015	273	336	9		
1	G	212	Total	C	N	O	S	0	0
			1633	1015	273	336	9		

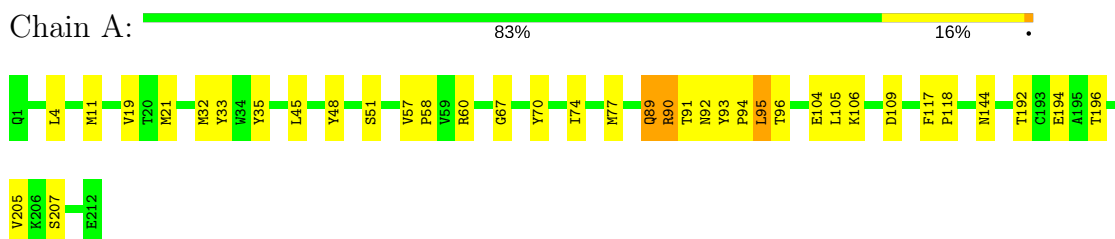
- Molecule 2 is a protein called 9.8B heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	218	Total	C	N	O	S	0	0
			1647	1039	275	326	7		
2	D	218	Total	C	N	O	S	0	0
			1647	1039	275	326	7		
2	F	218	Total	C	N	O	S	0	0
			1647	1039	275	326	7		
2	H	218	Total	C	N	O	S	0	0
			1647	1039	275	326	7		

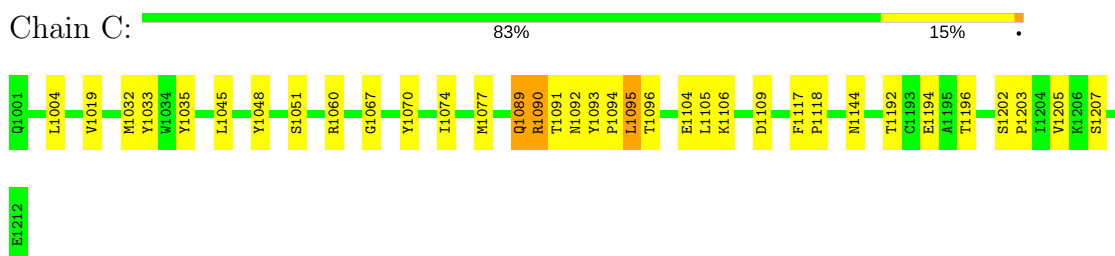
### 3 Residue-property plots [i](#)

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. 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. 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.

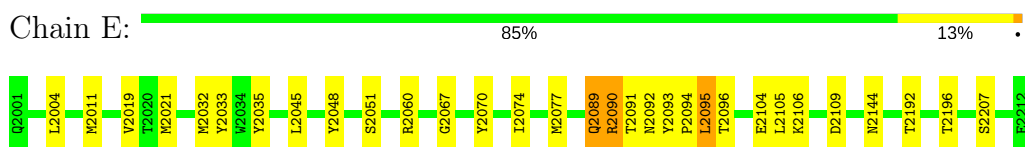
- Molecule 1: 9.8B light chain



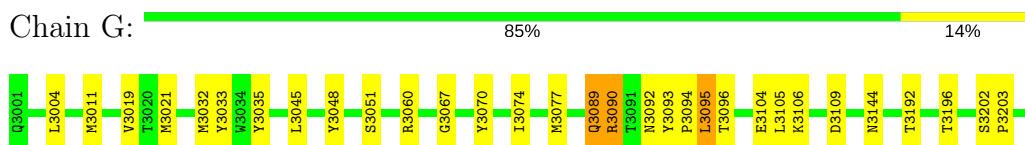
- Molecule 1: 9.8B light chain



- Molecule 1: 9.8B light chain

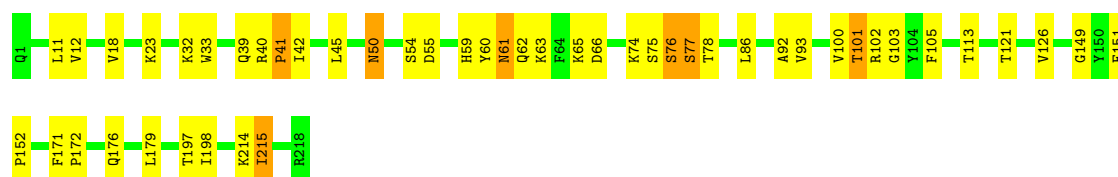


- Molecule 1: 9.8B light chain



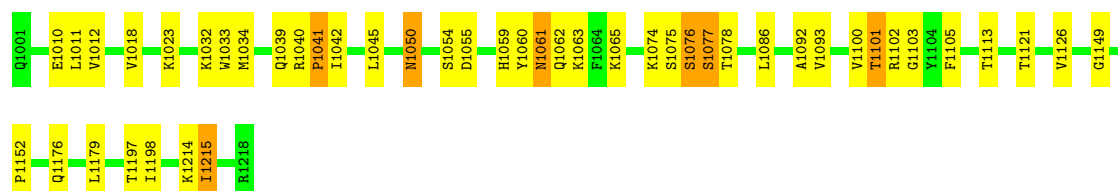
- Molecule 2: 9.8B heavy chain





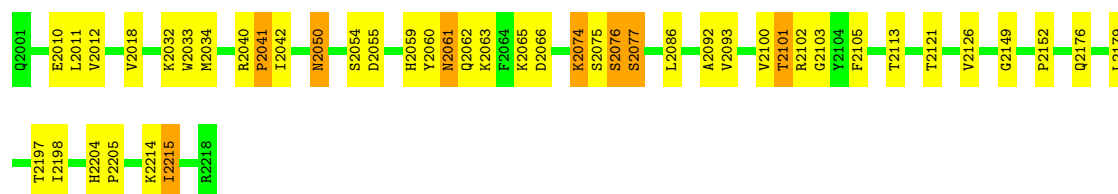
- Molecule 2: 9.8B heavy chain

Chain D: 79% 18% •



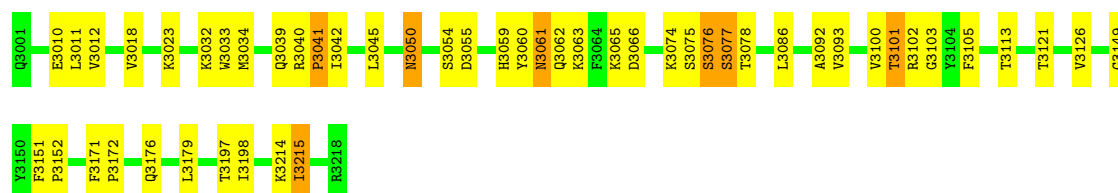
- Molecule 2: 9.8B heavy chain

Chain F: 79% 17% •



- Molecule 2: 9.8B heavy chain

Chain H: 77% 20% •



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	1820	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	Each Micrograph	Depositor
Microscope	FEI/PHILIPS CM300FEG/HE	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	39190	Depositor
Image detector	Not provided	Depositor

## 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  >2	RMSZ	# Z  >2
1	A	0.34	0/1669	0.48	0/2268
1	C	0.34	0/1669	0.48	0/2268
1	E	0.33	0/1669	0.48	0/2268
1	G	0.33	0/1669	0.48	0/2268
2	B	0.33	0/1689	0.50	0/2308
2	D	0.33	0/1689	0.50	0/2308
2	F	0.33	0/1689	0.50	0/2308
2	H	0.33	0/1689	0.50	0/2308
All	All	0.33	0/13432	0.49	0/18304

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	A	1633	0	1567	20	0
1	C	1633	0	1564	18	0
1	E	1633	0	1564	16	0
1	G	1633	0	1564	17	0
2	B	1647	0	1620	32	0
2	D	1647	0	1617	30	0
2	F	1647	0	1617	32	0
2	H	1647	0	1617	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13120	0	12730	199	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 8.

The worst 5 of 199 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:G:3033:TYR:OH	1:G:3090:ARG:NH1	1.58	1.36
1:E:2033:TYR:OH	1:E:2090:ARG:NH1	1.58	1.36
1:C:1033:TYR:OH	1:C:1090:ARG:NH1	1.58	1.34
1:A:33:TYR:OH	1:A:90:ARG:NH1	1.58	1.31
2:D:1076:SER:HA	2:D:1077:SER:HB3	1.16	1.14

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	210/212 (99%)	195 (93%)	12 (6%)	3 (1%)	13	54
1	C	210/212 (99%)	195 (93%)	12 (6%)	3 (1%)	13	54
1	E	210/212 (99%)	195 (93%)	12 (6%)	3 (1%)	13	54
1	G	210/212 (99%)	195 (93%)	12 (6%)	3 (1%)	13	54
2	B	216/218 (99%)	188 (87%)	22 (10%)	6 (3%)	6	39
2	D	216/218 (99%)	188 (87%)	22 (10%)	6 (3%)	6	39
2	F	216/218 (99%)	188 (87%)	22 (10%)	6 (3%)	6	39
2	H	216/218 (99%)	188 (87%)	22 (10%)	6 (3%)	6	39
All	All	1704/1720 (99%)	1532 (90%)	136 (8%)	36 (2%)	12	45



5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	77	SER
2	D	1077	SER
2	F	2077	SER
2	H	3077	SER
1	A	93	TYR

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	187/187 (100%)	178 (95%)	9 (5%)	30	61
1	C	187/187 (100%)	178 (95%)	9 (5%)	30	61
1	E	187/187 (100%)	178 (95%)	9 (5%)	30	61
1	G	187/187 (100%)	178 (95%)	9 (5%)	30	61
2	B	189/189 (100%)	182 (96%)	7 (4%)	39	68
2	D	189/189 (100%)	182 (96%)	7 (4%)	39	68
2	F	189/189 (100%)	182 (96%)	7 (4%)	39	68
2	H	189/189 (100%)	182 (96%)	7 (4%)	39	68
All	All	1504/1504 (100%)	1440 (96%)	64 (4%)	38	64

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	3077	MET
1	G	3109	ASP
2	H	3061	ASN
1	G	3089	GLN
1	G	3104	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	50	ASN
2	D	1039	GLN
2	H	3050	ASN
2	B	61	ASN
2	D	1035	HIS

### 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.