



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:58 PM BST

PDB ID : 4UIH
EMDB ID: : EMD-2968
Title : Cryo-EM structure of Dengue virus serotype 2 strain New Guinea-C complexed with human antibody 2D22 Fab at 37 degree C. The Fab molecules were added to the virus before 37 degree C incubation.
Authors : Fibriansah, G.; Ibarra, K.D.; Ng, T.-S.; Smith, S.A.; Tan, J.L.; Lim, X.N.; Ooi, J.S.G.; Kostyuchenko, V.A.; Wang, J.; deSilva, A.M.; Harris, E.; Crowe, J.E.; Lok, S.-M.
Deposited on : 2015-03-30
Resolution : 20.00 Å(reported)
Based on PDB ID : 4UIF

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

For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

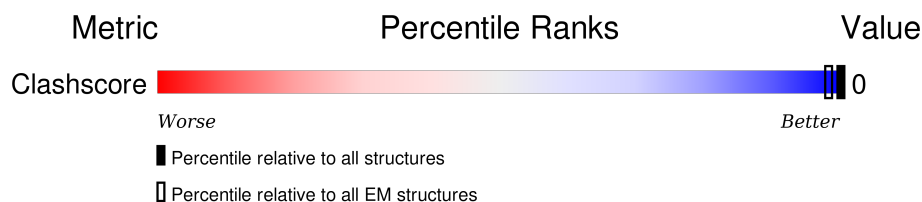
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY



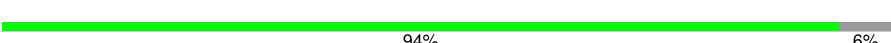


The reported resolution of this entry is 20.00 Å.

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)	EM structures (#Entries)
Clashscore	114402	924

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 ≥ 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	495	 80% 20%
1	B	495	 80% 20%
1	C	495	 80% 20%
2	D	128	 94% 6%
2	F	128	 94% 6%
3	E	115	 97% .
3	G	115	 97% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1647 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 DENGUE VIRUS SEROTYPE 2 STRAIN NEW GUINEA-C E PROTEIN ECTODOMAIN.

Mol	Chain	Residues	Atoms		AltConf	Trace
1	A	395	Total	C	0	395
			395	395		
1	B	395	Total	C	0	395
			395	395		
1	C	395	Total	C	0	395
			395	395		

- Molecule 2 is a protein called ANTIGEN-BINDING FRAGMENT OF HUMAN ANTIBODY 2D22 -HEAVY CHAIN.

Mol	Chain	Residues	Atoms		AltConf	Trace
2	D	120	Total	C	0	120
			120	120		
2	F	120	Total	C	0	120
			120	120		

- Molecule 3 is a protein called ANTIGEN-BINDING FRAGMENT OF HUMAN ANTIBODY 2D22 -LIGHT CHAIN.

Mol	Chain	Residues	Atoms		AltConf	Trace
3	E	111	Total	C	0	111
			111	111		
3	G	111	Total	C	0	111
			111	111		

● Molecule 1: DENGUE VIRUS SEROTYPE 2 STRAIN NEW GUINEA-C E PROTEIN ECTODOMAIN

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- Molecule 2: ANTIGEN-BINDING FRAGMENT OF HUMAN ANTIBODY 2D22 -HEAVY CHAIN

- Molecule 2: ANTIGEN-BINDING FRAGMENT OF HUMAN ANTIBODY 2D22 -HEAVY CHAIN

WORLDWIDE
PDB
PROTEIN DATA BANK

 **EMDataBank**
Unified Data Resource for 3DEM



- Molecule 3: ANTIGEN-BINDING FRAGMENT OF HUMAN ANTIBODY 2D22 -LIGHT CHAIN

Chain E:  97% .



- Molecule 3: ANTIGEN-BINDING FRAGMENT OF HUMAN ANTIBODY 2D22 -LIGHT CHAIN

Chain G:  97% .



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE, Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1.0	Depositor
Maximum defocus (nm)	3.6	Depositor
Magnification	47000	Depositor
Image detector	FEI FALCON II (4K X 4K)	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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	395	0	0	0	0
1	B	395	0	0	0	0
1	C	395	0	0	0	0
2	D	120	0	0	0	0
2	F	120	0	0	0	0
3	E	111	0	0	0	0
3	G	111	0	0	0	0
All	All	1647	0	0	0	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 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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.