



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:48 PM BST

PDB ID : 3J8D
EMDB ID: : EMD-6146
Title : Cryoelectron microscopy of dengue-Fab E104 complex at pH 5.5
Authors : Zhang, X.Z.; Sheng, J.; Austin, S.K.; Hoornweg, T.; Smit, J.M.; Kuhn, R.J.;
Diamond, M.S.; Rossmann, M.G.
Deposited on : 2014-10-13
Resolution : 26.00 Å(reported)
Based on PDB ID : 1OK8, 4FFZ

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

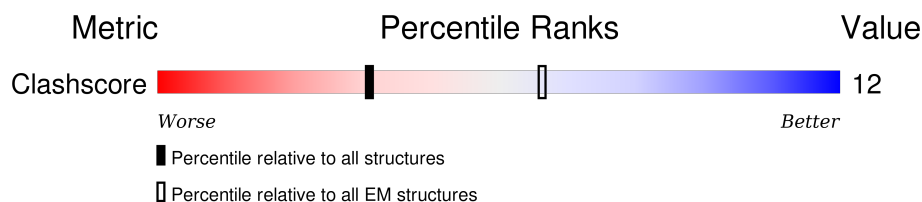
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

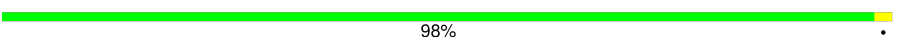
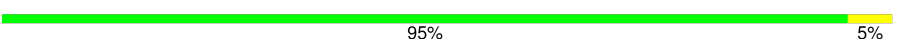
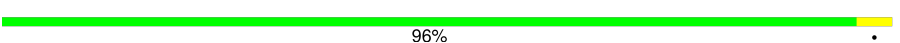
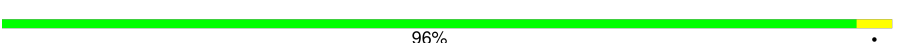
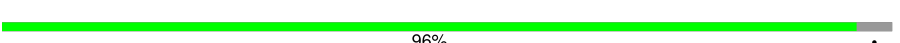


The reported resolution of this entry is 26.00 Å.

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	B	97	 98% .
1	F	97	 95% 5% .
2	A	425	 96% .
2	D	425	 96% .
3	G	394	 96% .
3	H	394	 71% . 28%
3	I	394	 71% . 28%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1990 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 glycoprotein DIII.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	B	97	Total C 97 97	0	97
1	F	97	Total C 97 97	0	97

- Molecule 2 is a protein called antibody E111 Fab fragment.

Mol	Chain	Residues	Atoms	AltConf	Trace
2	A	425	Total C 425 425	0	425
2	D	425	Total C 425 425	0	425

- Molecule 3 is a protein called Envelope protein E.

Mol	Chain	Residues	Atoms	AltConf	Trace
3	G	380	Total C 380 380	0	380
3	H	283	Total C 283 283	0	283
3	I	283	Total C 283 283	0	283

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	71	GLU	ASP	CONFLICT	UNP P12823
G	335	ILE	THR	CONFLICT	UNP P12823
G	352	ILE	THR	CONFLICT	UNP P12823
G	390	ASN	ASP	CONFLICT	UNP P12823
H	71	GLU	ASP	CONFLICT	UNP P12823
H	335	ILE	THR	CONFLICT	UNP P12823
H	352	ILE	THR	CONFLICT	UNP P12823

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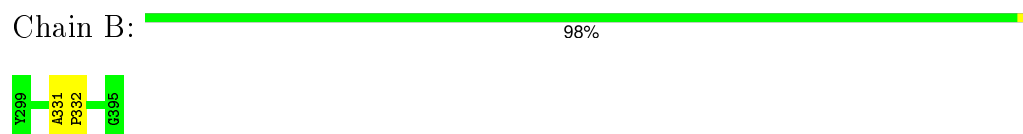
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Chain	Residue	Modelled	Actual	Comment	Reference
H	390	ASN	ASP	CONFLICT	UNP P12823
I	71	GLU	ASP	CONFLICT	UNP P12823
I	335	ILE	THR	CONFLICT	UNP P12823
I	352	ILE	THR	CONFLICT	UNP P12823
I	390	ASN	ASP	CONFLICT	UNP P12823

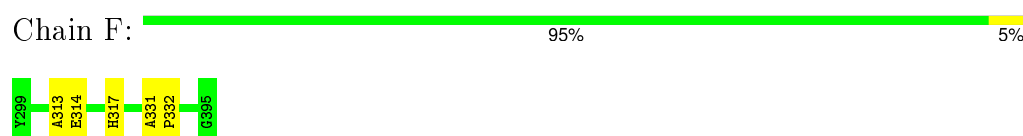
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

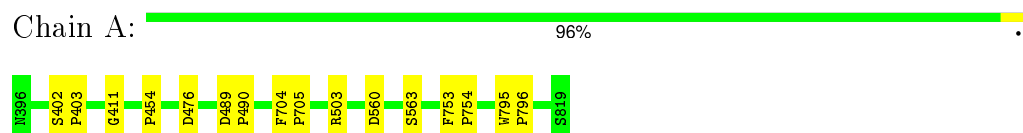
- Molecule 1: glycoprotein DIII



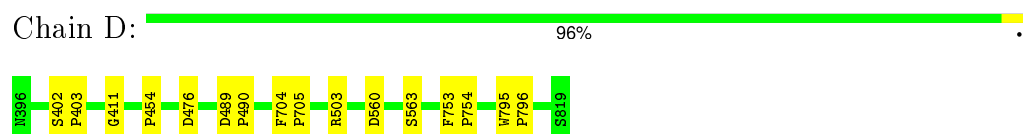
- Molecule 1: glycoprotein DIII



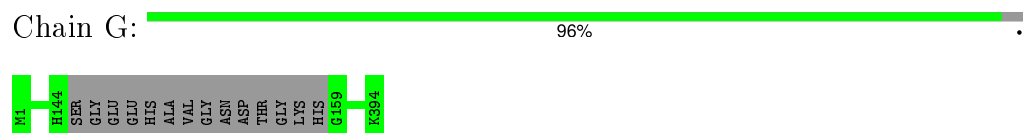
- Molecule 2: antibody E111 Fab fragment



- Molecule 2: antibody E111 Fab fragment



- Molecule 3: Envelope protein E



- Molecule 3: Envelope protein E



H1	S7	R8	R9	H144	SER	GLY	GLU	GLU	HIS	ALA	VAL	GLY	ASN	ASP	THR	GLY	LYS	HIS	G159	G159	H297	SER	TYR	SER	GLU	TYR	GLU	LYS	MET	CYS	THR	GLY	LYS	PHE	LYS	VAL	VAL	LYS	LYS	GLU	ILE	ALA	GLU	THR	GLN	HIS	GLY	THR	ILE	VAL	ILE	ARG	VAL	GLN	TYR	GLU	GLY	ASP	GLY	TRP	PHE	PRO	CYS
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LYS	ILE	PRO	PHE	GLU	ILE	MET	ASP	LEU	GLU	LYS	ARG	HIS	ALA	VAL	GLY	LEU	GLY	ASN	ARG	LEU	ILE	THR	VAL	ASN	PRO	ILE	VAL	THR	GLU	SER	LYS	ASP	SER	PRO	VAL	ASN	PHE	ILE	GLU	VAL	ALA	GLU	PRO	PHE	ILE	GLY	ASP	SER	GLN	TYR	ILE	ILE	THR	ILE	GLY	VAL	ILE	ARG	PRO	GLY	GLN	TYR	GLU	LEU	LYS	LEU	ASN	GLY	TRP	PHE	PRO	LYS
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- Molecule 3: Envelope protein E



H1	H144	GLY	GLU	GLU	HIS	ALA	VAL	GLY	ASN	ASP	THR	GLY	LYS	PHE	LYS	VAL	VAL	LYS	GLU	ILE	ALA	GLU	THR	GLN	HIS	GLY	THR	ILE	VAL	ILE	ARG	VAL	GLN	TYR	GLU	GLY	ASP	GLY	TRP	PHE	PRO
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CYS	LYS	ILE	PRO	PHE	GLU	ILE	MET	ASP	LEU	GLU	LYS	ARG	HIS	VAL	GLY	LEU	GLY	ASN	ARG	LEU	ILE	THR	VAL	ASN	PRO	ILE	VAL	THR	GLU	SER	LYS	ASP	SER	PRO	VAL	ASN	PHE	ILE	GLU	VAL	ALA	GLU	PRO	PHE	ILE	GLY	ASP	SER	GLN	TYR	ILE	ILE	THR	ILE	GLY	VAL	ILE	ARG	PRO	GLY	GLN	TYR	GLU	LEU	LYS	LEU	ASN	GLY	TRP	PHE
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LYS
LYS

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	528	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	24	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor

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).

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 ⓘ

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	B	97	0	0	1	0
1	F	97	0	0	6	0
2	A	425	0	0	8	0
2	D	425	0	0	8	0
3	G	380	0	0	0	0
3	H	283	0	0	2	0
3	I	283	0	0	3	0
All	All	1990	0	0	23	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 12.

All (23) 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)
2:D:411:GLY:CA	2:D:503:ARG:CA	2.21	1.19
2:A:411:GLY:CA	2:A:503:ARG:CA	2.21	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:314:GLU:CA	3:I:182:THR:CA	2.55	0.84
2:A:454:PRO:CA	2:A:563:SER:CA	2.57	0.82
2:D:454:PRO:CA	2:D:563:SER:CA	2.57	0.82
1:F:313:ALA:CA	3:I:171:THR:CA	2.61	0.77
1:F:317:HIS:CA	3:H:9:ARG:CA	2.65	0.74
2:A:476:ASP:CA	2:A:560:ASP:CA	2.69	0.70
2:D:476:ASP:CA	2:D:560:ASP:CA	2.69	0.70
1:F:317:HIS:CA	3:H:7:SER:CA	2.80	0.59
2:A:704:PHE:CA	2:A:705:PRO:CA	2.87	0.53
2:D:402:SER:CA	2:D:403:PRO:CA	2.87	0.52
2:A:402:SER:CA	2:A:403:PRO:CA	2.87	0.52
2:D:704:PHE:CA	2:D:705:PRO:CA	2.87	0.52
2:D:489:ASP:CA	2:D:490:PRO:CA	2.89	0.51
1:F:314:GLU:CA	3:I:172:GLU:CA	2.89	0.51
2:A:489:ASP:CA	2:A:490:PRO:CA	2.88	0.50
1:B:331:ALA:CA	1:B:332:PRO:CA	2.90	0.49
1:F:331:ALA:CA	1:F:332:PRO:CA	2.90	0.49
2:A:795:TRP:CA	2:A:796:PRO:CA	2.95	0.44
2:D:795:TRP:CA	2:D:796:PRO:CA	2.95	0.44
2:A:753:PHE:CA	2:A:754:PRO:CA	2.96	0.44
2:D:753:PHE:CA	2:D:754:PRO:CA	2.96	0.44

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.