wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:40 PM BST

PDB ID	:	3IXY
EMDB ID:	:	EMD-5102
Title	:	The pseudo-atomic structure of dengue immature virus in complex with Fab fragments of the anti-fusion loop antibody E53
Authors	:	Cherrier, M.V.; Kaufmann, B.; Nybakken, G.E.; Lok, S.M.; Warren, J.T.; Nelson, C.A.; Kostyuchenko, V.A.; Holdaway, H.A.; Chipman, P.R.; Kuhn, R.J.; Diamond, M.S.; Rossmann, M.G.; Fremont, D.H.
Deposited on	:	2009-02-26
Resolution	:	23.00 Å(reported)
Based on PDB ID	:	3C6D, 3C5X

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

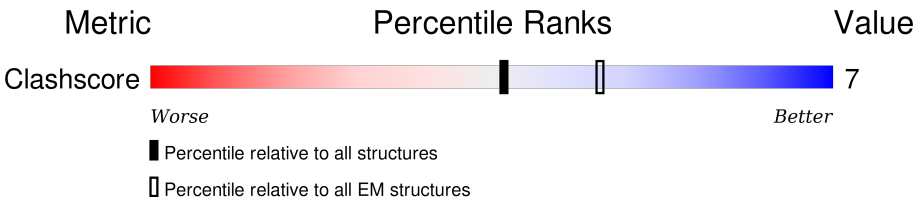
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 23.00 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	395	98% ··
1	B	395	98% ··
1	C	395	98% ··
2	D	81	99% ·
2	E	81	100%
2	F	81	100%
3	G	221	98% ·
3	I	221	95% 5%
4	H	215	98% ··
4	J	215	97% ··

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2281 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 Envelope protein E.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
1	A	390	390	390	0	390
1	B	390	390	390	0	390
1	C	390	390	390	0	390

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ILE	MET	CONFLICT	UNP O11875
A	139	VAL	ILE	CONFLICT	UNP O11875
A	162	VAL	ILE	CONFLICT	UNP O11875
A	390	ASP	ASN	CONFLICT	UNP O11875
B	6	ILE	MET	CONFLICT	UNP O11875
B	139	VAL	ILE	CONFLICT	UNP O11875
B	162	VAL	ILE	CONFLICT	UNP O11875
B	390	ASP	ASN	CONFLICT	UNP O11875
C	6	ILE	MET	CONFLICT	UNP O11875
C	139	VAL	ILE	CONFLICT	UNP O11875
C	162	VAL	ILE	CONFLICT	UNP O11875
C	390	ASP	ASN	CONFLICT	UNP O11875

- Molecule 2 is a protein called Peptide pr.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
2	D	81	81	81	0	81
2	E	81	81	81	0	81
2	F	81	81	81	0	81

- Molecule 3 is a protein called E53 Fab Fragment (chain H).

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
3	G	221	221	221	0	221
			Total	C		
3	I	221	221	221	0	221

- Molecule 4 is a protein called E53 Fab Fragment (chain L).

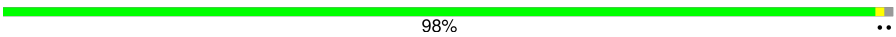
Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
4	H	213	213	213	0	213
			Total	C		
4	J	213	213	213	0	213

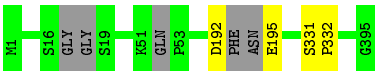
3 Residue-property plots (i)

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: Envelope protein E

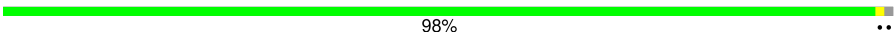
Chain A:

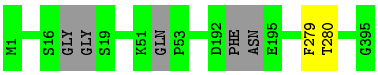




- Molecule 1: Envelope protein E

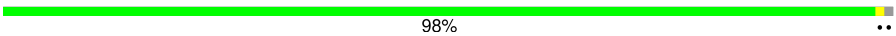
Chain B:

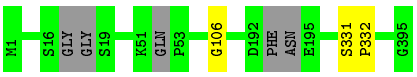




- Molecule 1: Envelope protein E

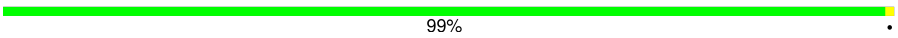
Chain C:





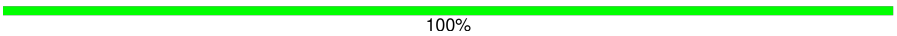
- Molecule 2: Peptide pr

Chain D:



- Molecule 2: Peptide pr

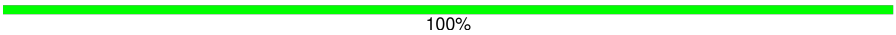
Chain E:



There are no outlier residues recorded for this chain.

- Molecule 2: Peptide pr

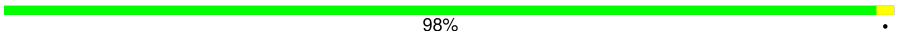
Chain F:

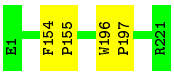


There are no outlier residues recorded for this chain.

- Molecule 3: E53 Fab Fragment (chain H)

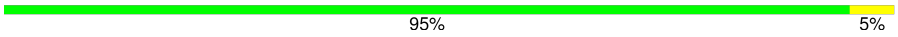
Chain G:

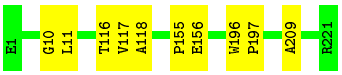




- Molecule 3: E53 Fab Fragment (chain H)

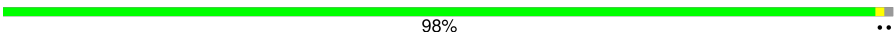
Chain I:

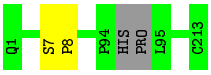




- Molecule 4: E53 Fab Fragment (chain L)

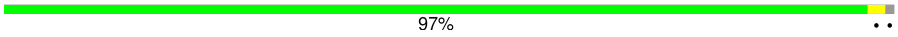
Chain H:

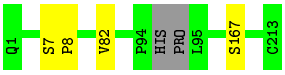




- Molecule 4: E53 Fab Fragment (chain L)

Chain J:





4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	2741	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI/PHILIPS CM300FEG/T	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	15.0	Depositor
Minimum defocus (nm)	1876	Depositor
Maximum defocus (nm)	2728	Depositor
Magnification	45000	Depositor
Image detector	Kodak SO163	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	390	0	0	2	0
1	B	390	0	0	1	0
1	C	390	0	0	2	0
2	D	81	0	0	1	0
2	E	81	0	0	0	0
2	F	81	0	0	0	0
3	G	221	0	0	2	0
3	I	221	0	0	6	0
4	H	213	0	0	1	0
4	J	213	0	0	2	0
All	All	2281	0	0	16	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 7.

The worst 5 of 16 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:I:118:ALA:CA	3:I:155:PRO:CA	1.79	1.57
3:I:116:THR:CA	3:I:156:GLU:CA	2.19	1.20
1:C:106:GLY:CA	2:D:63:ASP:CA	2.20	1.18
1:B:279:PHE:CA	1:B:280:THR:CA	2.39	1.00
3:I:10:GLY:CA	3:I:209:ALA:CA	2.42	0.97

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.