Full wwPDB/EMDataBank EM Map/Model Validation Report

Jul 11, 2018 – 05:38 PM EDT

PDB ID : 3IXX
EMDB ID: : EMD-5103
Title : The pseudo-atomic structure of West Nile immature virus in complex with Fab fragments of the anti-fusion loop antibody E53
Deposited on : 2009-02-26
Resolution : 15.00 Å(reported)
Based on PDB ID : 2OF6, 3C5X

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
with specific help available everywhere you see the symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031172
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 15.00 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.

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%
2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2308 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.

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Residues</th>
<th>Atoms</th>
<th>AltConf</th>
<th>Trace</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>A</td>
<td>400</td>
<td>Total C 400</td>
<td>0</td>
<td>400</td>
</tr>
<tr>
<td>1</td>
<td>B</td>
<td>400</td>
<td>Total C 400</td>
<td>0</td>
<td>400</td>
</tr>
<tr>
<td>1</td>
<td>C</td>
<td>400</td>
<td>Total C 400</td>
<td>0</td>
<td>400</td>
</tr>
</tbody>
</table>

- Molecule 2 is a protein called Peptide pr.

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Residues</th>
<th>Atoms</th>
<th>AltConf</th>
<th>Trace</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>D</td>
<td>80</td>
<td>Total C 80</td>
<td>0</td>
<td>80</td>
</tr>
<tr>
<td>2</td>
<td>E</td>
<td>80</td>
<td>Total C 80</td>
<td>0</td>
<td>80</td>
</tr>
<tr>
<td>2</td>
<td>F</td>
<td>80</td>
<td>Total C 80</td>
<td>0</td>
<td>80</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Residues</th>
<th>Atoms</th>
<th>AltConf</th>
<th>Trace</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>G</td>
<td>221</td>
<td>Total C 221</td>
<td>0</td>
<td>221</td>
</tr>
<tr>
<td>3</td>
<td>I</td>
<td>221</td>
<td>Total C 221</td>
<td>0</td>
<td>221</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Residues</th>
<th>Atoms</th>
<th>AltConf</th>
<th>Trace</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>H</td>
<td>213</td>
<td>Total C 213</td>
<td>0</td>
<td>213</td>
</tr>
<tr>
<td>4</td>
<td>J</td>
<td>213</td>
<td>Total C 213</td>
<td>0</td>
<td>213</td>
</tr>
</tbody>
</table>
3 Residue-property plots

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: Envelope protein E

Chain A:
[Graphic]

• Molecule 1: Envelope protein E

Chain B:
[Graphic]

There are no outlier residues recorded for this chain.

• Molecule 1: Envelope protein E

Chain C:
[Graphic]

• Molecule 2: Peptide pr

Chain D:
[Graphic]

• Molecule 2: Peptide pr

Chain E:
[Graphic]

• Molecule 2: Peptide pr

Chain F:
[Graphic]

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:

- Molecule 4: E53 Fab Fragment (chain L)
## 4 Experimental information

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reconstruction method</td>
<td>SINGLE PARTICLE</td>
<td>Depositor</td>
</tr>
<tr>
<td>Imposed symmetry</td>
<td>POINT, I</td>
<td>Depositor</td>
</tr>
<tr>
<td>Number of particles used</td>
<td>3927</td>
<td>Depositor</td>
</tr>
<tr>
<td>Resolution determination method</td>
<td>FSC 0.5 CUT-OFF</td>
<td>Depositor</td>
</tr>
<tr>
<td>CTF correction method</td>
<td>Each particle</td>
<td>Depositor</td>
</tr>
<tr>
<td>Microscope</td>
<td>FEI/PHILIPS CM300FEG/T</td>
<td>Depositor</td>
</tr>
<tr>
<td>Voltage (kV)</td>
<td>300</td>
<td>Depositor</td>
</tr>
<tr>
<td>Electron dose (e⁻/Å²)</td>
<td>12.0</td>
<td>Depositor</td>
</tr>
<tr>
<td>Minimum defocus (nm)</td>
<td>1193</td>
<td>Depositor</td>
</tr>
<tr>
<td>Maximum defocus (nm)</td>
<td>2859</td>
<td>Depositor</td>
</tr>
<tr>
<td>Magnification</td>
<td>47244</td>
<td>Depositor</td>
</tr>
<tr>
<td>Image detector</td>
<td>KODAK SO-163 FILM</td>
<td>Depositor</td>
</tr>
</tbody>
</table>
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.

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Non-H</th>
<th>H(model)</th>
<th>H(added)</th>
<th>Clashes</th>
<th>Symm-Clashes</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>A</td>
<td>400</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>B</td>
<td>400</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>C</td>
<td>400</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>D</td>
<td>80</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>E</td>
<td>80</td>
<td>0</td>
<td>0</td>
<td>3</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>F</td>
<td>80</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>G</td>
<td>221</td>
<td>0</td>
<td>0</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>I</td>
<td>221</td>
<td>0</td>
<td>0</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>H</td>
<td>213</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>J</td>
<td>213</td>
<td>0</td>
<td>0</td>
<td>4</td>
<td>0</td>
</tr>
<tr>
<td>All</td>
<td>All</td>
<td>2308</td>
<td>0</td>
<td>0</td>
<td>11</td>
<td>0</td>
</tr>
</tbody>
</table>

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 5.

All (11) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.
<table>
<thead>
<tr>
<th>Atom-1</th>
<th>Atom-2</th>
<th>Interatomic distance (Å)</th>
<th>Clash overlap (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2:E:56:ALA:CA</td>
<td>4:J:30:SER:CA</td>
<td>2.05</td>
<td>1.33</td>
</tr>
<tr>
<td>1:C:51:ALA:CA</td>
<td>1:C:52:ASN:CA</td>
<td>2.41</td>
<td>0.97</td>
</tr>
<tr>
<td>2:E:26:ALA:CA</td>
<td>4:J:59:VAL:CA</td>
<td>2.72</td>
<td>0.68</td>
</tr>
<tr>
<td>4:H:7:SER:CA</td>
<td>4:H:8:PRO:CA</td>
<td>2.87</td>
<td>0.53</td>
</tr>
<tr>
<td>4:J:7:SER:CA</td>
<td>4:J:8:PRO:CA</td>
<td>2.87</td>
<td>0.52</td>
</tr>
<tr>
<td>1:A:69:SER:CA</td>
<td>2:D:48:THR:CA</td>
<td>2.90</td>
<td>0.50</td>
</tr>
<tr>
<td>3:G:196:TRP:CA</td>
<td>3:G:197:PRO:CA</td>
<td>2.97</td>
<td>0.42</td>
</tr>
<tr>
<td>3:I:196:TRP:CA</td>
<td>3:I:197:PRO:CA</td>
<td>2.97</td>
<td>0.42</td>
</tr>
<tr>
<td>3:I:156:GLU:CA</td>
<td>3:I:157:PRO:CA</td>
<td>3.00</td>
<td>0.40</td>
</tr>
</tbody>
</table>

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

5.3.2 Protein sidechains

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

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.
5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.