



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 13, 2017 – 01:02 PM EST

PDB ID : 3JBM
EMDB ID: : EMD-6453
Title : Electron cryo-microscopy of a virus-like particle of orange-spotted grouper nervous necrosis virus
Authors : Xie, J.; Li, K.; Gao, Y.; Huang, R.; Lai, Y.; Shi, Y.; Yang, S.; Zhu, G.; Zhang, Q.; He, J.
Deposited on : 2015-09-06
Resolution : 3.90 Å(reported)
Based on PDB ID : 4NWW

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

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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) : rb-20028442

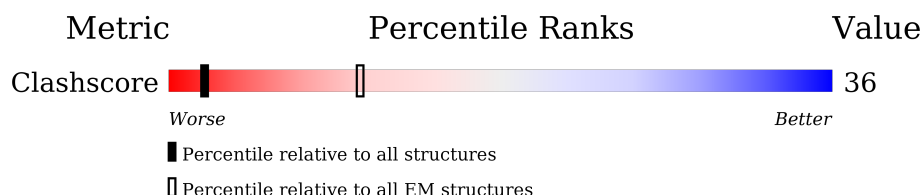
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY




The reported resolution of this entry is 3.90 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 | 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 | 338 |  47% . 50% |
| 1 | B | 338 |  47% . 50% |
| 1 | C | 338 |  51% . 45% |

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 526 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 virus-like particle of orange-spotted grouper nervous necrosis virus.

| Mol | Chain | Residues | Atoms | | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|-------|
| 1 | A | 170 | Total 170 | C 170 | 0 | 170 |
| 1 | B | 170 | Total 170 | C 170 | 0 | 170 |
| 1 | C | 186 | Total 186 | C 186 | 0 | 186 |

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- Molecule 1: virus-like particle of orange-spotted grouper nervous necrosis virus



| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| LYS | PHE | ALA | GLY | ASN | ALA | GLY | THR | PRO | ALA | GLY | TRP | PHE | ARG | TRP | GLY | ILE | TRP | ASP | ASN | PHE | ASN | LYS | THR | PHE | THR | ASP | GLY | VAL | ALA | TYR | TYR | SER | ASP | GLU | GLN | PRO | ARG | GLN | ILE | LEU | LEU | PRO | VAL | GLY | THR | VAL | CYS | THR | ARG | VAL | ASP | SER | GLU | ASN |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

4 Experimental information

| Property | Value | Source |
|--------------------------------------|--------------------------------|-----------|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, I | Depositor |
| Number of particles used | 32000 | 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 ($e^-/\text{\AA}^2$) | 20 | Depositor |
| Minimum defocus (nm) | 1000 | Depositor |
| Maximum defocus (nm) | 2910 | Depositor |
| Magnification | 96000 | 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 | A | 170 | 0 | 0 | 5 | 0 |
| 1 | B | 170 | 0 | 0 | 6 | 0 |
| 1 | C | 186 | 0 | 0 | 8 | 0 |
| All | All | 526 | 0 | 0 | 19 | 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 36.

All (19) 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:C:189:GLY:CA | 1:C:190:ASN:CA | 2.79 | 0.60 |
| 1:B:189:GLY:CA | 1:B:190:ASN:CA | 2.79 | 0.60 |
| 1:C:46:THR:CA | 1:C:47:GLY:CA | 2.79 | 0.60 |
| 1:A:51:GLY:CA | 1:A:52:THR:CA | 2.81 | 0.59 |
| 1:A:189:GLY:CA | 1:A:190:ASN:CA | 2.81 | 0.58 |
| 1:B:51:GLY:CA | 1:B:52:THR:CA | 2.84 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:A:70:ALA:CA | 1:A:71:GLY:CA | 2.84 | 0.56 |
| 1:C:121:GLY:CA | 1:C:122:GLY:CA | 2.85 | 0.55 |
| 1:C:51:GLY:CA | 1:C:52:THR:CA | 2.85 | 0.54 |
| 1:C:50:ARG:CA | 1:C:51:GLY:CA | 2.85 | 0.54 |
| 1:B:70:ALA:CA | 1:B:71:GLY:CA | 2.85 | 0.54 |
| 1:C:70:ALA:CA | 1:C:71:GLY:CA | 2.86 | 0.54 |
| 1:A:121:GLY:CA | 1:A:122:GLY:CA | 2.86 | 0.53 |
| 1:B:121:GLY:CA | 1:B:122:GLY:CA | 2.86 | 0.53 |
| 1:A:117:ALA:CA | 1:A:118:ASN:CA | 2.87 | 0.53 |
| 1:B:117:ALA:CA | 1:B:118:ASN:CA | 2.90 | 0.50 |
| 1:C:117:ALA:CA | 1:C:118:ASN:CA | 2.91 | 0.48 |
| 1:C:190:ASN:CA | 1:C:191:ASN:CA | 2.93 | 0.47 |
| 1:B:190:ASN:CA | 1:B:191:ASN:CA | 2.97 | 0.43 |

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

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.