PDB ID : 6U1S
EMDB ID : EMD-20613
Title : Cryo-EM structure of a de novo designed 16-helix transmembrane nanopore, TMHC8_R.
Authors : Johnson, M.J.; Reggiano, G.; Xu, C.; Lu, P.; Hsia, Y.; Brunette, T.J.; DiMaio, F.; Baker, D.; Kollman, J.
Deposited on : 2019-08-16
Resolution : 7.60 Å (reported)

This is a Full wwPDB EM 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.

The following versions of software and data (see references) were used in the production of this report:

MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1
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 7.60 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.

<table>
<thead>
<tr>
<th>Metric</th>
<th>Whole archive (#Entries)</th>
<th>EM structures (#Entries)</th>
</tr>
</thead>
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<td>4297</td>
</tr>
<tr>
<td>Ramachandran outliers</td>
<td>154571</td>
<td>4023</td>
</tr>
<tr>
<td>Sidechain outliers</td>
<td>154315</td>
<td>3826</td>
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</tbody>
</table>

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. 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 respectively. 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%.

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Length</th>
<th>Quality of chain</th>
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<td>95% 5%</td>
</tr>
<tr>
<td>1</td>
<td>B</td>
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<td>95% 5%</td>
</tr>
<tr>
<td>1</td>
<td>H</td>
<td>310</td>
<td>95% 5%</td>
</tr>
<tr>
<td>1</td>
<td>J</td>
<td>310</td>
<td>95% 5%</td>
</tr>
<tr>
<td>1</td>
<td>L</td>
<td>310</td>
<td>95% 5%</td>
</tr>
<tr>
<td>1</td>
<td>N</td>
<td>310</td>
<td>95% 5%</td>
</tr>
</tbody>
</table>
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 40208 atoms, of which 20568 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 de novo designed 16-helix transmembrane nanopore, TMHC8_R.

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<th>Atoms</th>
<th>AltConf</th>
<th>Trace</th>
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<td></td>
<td></td>
<td>5026 1550 2571 437 460 8</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>B</td>
<td>310</td>
<td>Total C H N O S</td>
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<td>0</td>
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<td>5026 1550 2571 437 460 8</td>
<td></td>
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</tr>
<tr>
<td>1</td>
<td>D</td>
<td>310</td>
<td>Total C H N O S</td>
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<td></td>
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<tr>
<td>1</td>
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<td>310</td>
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<td>0</td>
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<td>5026 1550 2571 437 460 8</td>
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<td></td>
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<td>5026 1550 2571 437 460 8</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: de novo designed 16-helix transmembrane nanopore, TMHC8_R
  Chain A:

• Molecule 1: de novo designed 16-helix transmembrane nanopore, TMHC8_R
  Chain B:

• Molecule 1: de novo designed 16-helix transmembrane nanopore, TMHC8_R
  Chain D:

• Molecule 1: de novo designed 16-helix transmembrane nanopore, TMHC8_R
  Chain F:

• Molecule 1: de novo designed 16-helix transmembrane nanopore, TMHC8_R
  Chain H:

• Molecule 1: de novo designed 16-helix transmembrane nanopore, TMHC8_R
  Chain J:
• Molecule 1: de novo designed 16-helix transmembrane nanopore, TMHC8_R

Chain L:

• Molecule 1: de novo designed 16-helix transmembrane nanopore, TMHC8_R

Chain N:
# 4 Experimental information

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<td>Depositor</td>
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<td>CTF correction method</td>
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<td>Microscope</td>
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<td>GATAN K2 SUMMIT (4k x 4k)</td>
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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).

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<th>Bond angles</th>
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<td>All</td>
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All (16) bond length outliers are listed below:

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<th>Atoms</th>
<th>Z</th>
<th>Observed(Å)</th>
<th>Ideal(Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>001</td>
<td>H</td>
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<td>GLU</td>
<td>CD-OE2</td>
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<td>CD-OE2</td>
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<td>1.20</td>
<td>1.25</td>
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<td>1.25</td>
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<td>CD-OE2</td>
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<td>1.25</td>
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All (73) bond angle outliers are listed below:
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<td>-6.27</td>
<td>117.16</td>
<td>120.30</td>
</tr>
<tr>
<td>1</td>
<td>D</td>
<td>189</td>
<td>ARG</td>
<td>NE-CZ-NH2</td>
<td>-6.25</td>
<td>117.17</td>
<td>120.30</td>
</tr>
<tr>
<td>1</td>
<td>H</td>
<td>189</td>
<td>ARG</td>
<td>NE-CZ-NH2</td>
<td>-6.25</td>
<td>117.17</td>
<td>120.30</td>
</tr>
<tr>
<td>1</td>
<td>N</td>
<td>189</td>
<td>ARG</td>
<td>NE-CZ-NH2</td>
<td>-6.20</td>
<td>117.20</td>
<td>120.30</td>
</tr>
<tr>
<td>1</td>
<td>L</td>
<td>189</td>
<td>ARG</td>
<td>NE-CZ-NH2</td>
<td>-6.17</td>
<td>117.21</td>
<td>120.30</td>
</tr>
<tr>
<td>1</td>
<td>B</td>
<td>189</td>
<td>ARG</td>
<td>NE-CZ-NH2</td>
<td>-6.17</td>
<td>117.22</td>
<td>120.30</td>
</tr>
<tr>
<td>1</td>
<td>A</td>
<td>189</td>
<td>ARG</td>
<td>NE-CZ-NH2</td>
<td>-6.14</td>
<td>117.23</td>
<td>120.30</td>
</tr>
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<td>1</td>
<td>L</td>
<td>160</td>
<td>ARG</td>
<td>NE-CZ-NH1</td>
<td>6.02</td>
<td>123.31</td>
<td>120.30</td>
</tr>
<tr>
<td>1</td>
<td>B</td>
<td>160</td>
<td>ARG</td>
<td>NE-CZ-NH1</td>
<td>6.00</td>
<td>123.30</td>
<td>120.30</td>
</tr>
<tr>
<td>1</td>
<td>A</td>
<td>160</td>
<td>ARG</td>
<td>NE-CZ-NH1</td>
<td>5.94</td>
<td>123.27</td>
<td>120.30</td>
</tr>
<tr>
<td>1</td>
<td>D</td>
<td>160</td>
<td>ARG</td>
<td>NE-CZ-NH1</td>
<td>5.94</td>
<td>123.27</td>
<td>120.30</td>
</tr>
<tr>
<td>1</td>
<td>N</td>
<td>160</td>
<td>ARG</td>
<td>NE-CZ-NH1</td>
<td>5.94</td>
<td>123.27</td>
<td>120.30</td>
</tr>
<tr>
<td>1</td>
<td>H</td>
<td>160</td>
<td>ARG</td>
<td>NE-CZ-NH1</td>
<td>5.89</td>
<td>123.25</td>
<td>120.30</td>
</tr>
<tr>
<td>1</td>
<td>F</td>
<td>160</td>
<td>ARG</td>
<td>NE-CZ-NH1</td>
<td>5.83</td>
<td>123.21</td>
<td>120.30</td>
</tr>
<tr>
<td>1</td>
<td>J</td>
<td>160</td>
<td>ARG</td>
<td>NE-CZ-NH1</td>
<td>5.83</td>
<td>123.21</td>
<td>120.30</td>
</tr>
<tr>
<td>1</td>
<td>D</td>
<td>158</td>
<td>TYR</td>
<td>CB-CG-CD1</td>
<td>-5.54</td>
<td>117.67</td>
<td>121.00</td>
</tr>
<tr>
<td>1</td>
<td>B</td>
<td>158</td>
<td>TYR</td>
<td>CB-CG-CD1</td>
<td>-5.53</td>
<td>117.68</td>
<td>121.00</td>
</tr>
<tr>
<td>1</td>
<td>F</td>
<td>158</td>
<td>TYR</td>
<td>CB-CG-CD1</td>
<td>-5.51</td>
<td>117.69</td>
<td>121.00</td>
</tr>
</tbody>
</table>

Continued on next page...
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.
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.

All (16) 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>1:J:206:ASP:OD1</td>
<td>1:J:210:LYS:NZ</td>
<td>2.46</td>
<td>0.48</td>
</tr>
<tr>
<td>1:H:206:ASP:OD1</td>
<td>1:H:210:LYS:NZ</td>
<td>2.46</td>
<td>0.48</td>
</tr>
<tr>
<td>1:L:206:ASP:OD1</td>
<td>1:L:210:LYS:NZ</td>
<td>2.46</td>
<td>0.48</td>
</tr>
<tr>
<td>1:D:206:ASP:OD1</td>
<td>1:D:210:LYS:NZ</td>
<td>2.46</td>
<td>0.48</td>
</tr>
<tr>
<td>1:B:206:ASP:OD1</td>
<td>1:B:210:LYS:NZ</td>
<td>2.46</td>
<td>0.48</td>
</tr>
<tr>
<td>1:F:206:ASP:OD1</td>
<td>1:F:210:LYS:NZ</td>
<td>2.46</td>
<td>0.48</td>
</tr>
<tr>
<td>1:A:206:ASP:OD1</td>
<td>1:A:210:LYS:NZ</td>
<td>2.46</td>
<td>0.48</td>
</tr>
<tr>
<td>1:N:206:ASP:OD1</td>
<td>1:N:210:LYS:NZ</td>
<td>2.46</td>
<td>0.48</td>
</tr>
<tr>
<td>1:J:310:HIS:OXT</td>
<td>1:J:310:HIS:ND1</td>
<td>2.49</td>
<td>0.46</td>
</tr>
<tr>
<td>1:B:310:HIS:ND1</td>
<td>1:B:310:HIS:OXT</td>
<td>2.49</td>
<td>0.46</td>
</tr>
<tr>
<td>1:L:310:HIS:OXT</td>
<td>1:L:310:HIS:ND1</td>
<td>2.49</td>
<td>0.45</td>
</tr>
<tr>
<td>1:D:310:HIS:OXT</td>
<td>1:D:310:HIS:ND1</td>
<td>2.49</td>
<td>0.45</td>
</tr>
<tr>
<td>1:A:310:HIS:OXT</td>
<td>1:A:310:HIS:ND1</td>
<td>2.49</td>
<td>0.45</td>
</tr>
<tr>
<td>1:F:310:HIS:OXT</td>
<td>1:F:310:HIS:ND1</td>
<td>2.49</td>
<td>0.45</td>
</tr>
<tr>
<td>1:H:310:HIS:OXT</td>
<td>1:H:310:HIS:ND1</td>
<td>2.49</td>
<td>0.45</td>
</tr>
<tr>
<td>1:N:310:HIS:ND1</td>
<td>1:N:310:HIS:OXT</td>
<td>2.49</td>
<td>0.44</td>
</tr>
</tbody>
</table>

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.
The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Analysed</th>
<th>Favoured</th>
<th>Allowed</th>
<th>Outliers</th>
<th>Percentiles</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>A</td>
<td>308/310 (99%)</td>
<td>307 (100%)</td>
<td>0</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>B</td>
<td>308/310 (99%)</td>
<td>307 (100%)</td>
<td>0</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>D</td>
<td>308/310 (99%)</td>
<td>307 (100%)</td>
<td>0</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>F</td>
<td>308/310 (99%)</td>
<td>307 (100%)</td>
<td>0</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>H</td>
<td>308/310 (99%)</td>
<td>307 (100%)</td>
<td>0</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>J</td>
<td>308/310 (99%)</td>
<td>307 (100%)</td>
<td>0</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>L</td>
<td>308/310 (99%)</td>
<td>307 (100%)</td>
<td>0</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>N</td>
<td>308/310 (99%)</td>
<td>307 (100%)</td>
<td>0</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>All</td>
<td>All</td>
<td>2464/2480 (99%)</td>
<td>2456 (100%)</td>
<td>8 (0%)</td>
<td>0</td>
<td>100 100</td>
</tr>
</tbody>
</table>

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Analysed</th>
<th>Rotameric</th>
<th>Outliers</th>
<th>Percentiles</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>A</td>
<td>246/246 (100%)</td>
<td>246 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>B</td>
<td>246/246 (100%)</td>
<td>246 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>D</td>
<td>246/246 (100%)</td>
<td>246 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>F</td>
<td>246/246 (100%)</td>
<td>246 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>H</td>
<td>246/246 (100%)</td>
<td>246 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>J</td>
<td>246/246 (100%)</td>
<td>246 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>L</td>
<td>246/246 (100%)</td>
<td>246 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>N</td>
<td>246/246 (100%)</td>
<td>246 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>All</td>
<td>All</td>
<td>1968/1968 (100%)</td>
<td>1968 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
</tbody>
</table>

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such
sidechains are listed below:

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Res</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>J</td>
<td>302</td>
<td>ASN</td>
</tr>
</tbody>
</table>

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 monosaccharides 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.