Looking at deposited SARS-CoV-2 related structures! Check PDB for updated versions as well as new structures.

Usage Guidelines:
These web services are provided for analysis of individual structures.
For batch runs, please download and install your own copy of MolProbity.

Walkthroughs, tutorials, and usage FAQs:

Citations, science, and technical FAQs:

Uploaded PDB file as 1eve.pdb

- This compound is identified as THREE DIMENSIONAL STRUCTURE OF THE ANTI-ALZHEIMER DRUG, E202 (ACIEPT), COMPLEXED WITH ITS TARGET ACETYLCHOLINESTERASE.
- This structure was solved by X-RAY DIFFRACTION.
- This structure was solved at 2.50 Å resolution.
- 1 chain(s) (on file)
- A total of 234 residues are present.
- Protein mainchain and sidechains are present.
- No explicit hydrogen atoms are included.
- 402 hetero groups are present.
- Refinement was carried out in X-PLOR 3.81.
- R = 0.188; Rfree = 0.228
- 4 PDBx2 files were found. Proceeding assuming PDBx3 formatted file.

Main page

- Add hydrogen
- Make simple kinematics
- Edit PDB file
- Downgrade file to PDBx2.3 format (for download only)
- Fill gaps in protein backbone with fill loop beta turn
- Analyze geometry without all-atom contacts
Summary statistics

<table>
<thead>
<tr>
<th>Protein</th>
<th>Ramachandran outlier</th>
<th>0.00%</th>
<th>Goal &lt;0.05%</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Ramachandran favored</td>
<td>501</td>
<td>Goal &lt;98%</td>
</tr>
<tr>
<td></td>
<td>Ramachandran Z-score</td>
<td>-2.20 ± 0.31</td>
<td>Goal dhZ score &lt; 3</td>
</tr>
</tbody>
</table>

In the two column results, the left column gives the row count; right column gives the percentage.

Key to table values and colors:

Multi-criterion visualizations

Single-criterion visualizations

[Additional links and options for visualization and download]
MolProbity Ramachandran analysis

leve.pdb, model 1

94.2% (353/378) of all residues were in favored (99.9%) regions.
100% (378/378) of all residues were in allowed (99.9%) regions.
There were no outliers.

http://kinemage.biochem.duke.edu