

molprobity.biochem.duke.edu

# Main page

**Duke Biochemistry**  
Duke University School of Medicine

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You are using 0% of your 200 Mb of disk space.

**Looking at deposited SARS-CoV-2 related structures? Check PDB for updated versions as well as new structures.**  
(Our Fetch > always returns the latest version.)  
**Solving or improving them? Look at MolProbity's CaBLAM outliers, and at sparse H-bonds.**

**FILE UPLOAD/RETRIEVAL (MORE OPTIONS)**

PDB/NDB COD: **1EVE** type: PDB coords **Fetch >**

Browse... No file selected. type: PDB coords Upload >

**Molprobity sites:**  
Duke (US) | Manchester (UK)

**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:**

molprobity.biochem.duke.edu/index.php/MolProbity-1e1401a4q220e1a701u0029k0k0e1e1d-13

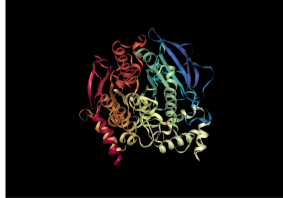
# Uploaded PDB file as 1eve.pdb

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Your file from <http://www.pdb.org/> was uploaded as 1eve.pdb.

- This compound is identified as **THREE DIMENSIONAL STRUCTURE OF THE ANTI-ALZHEIMER DRUG, E202 (ARICEPT), 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) is/are present [1 unique chain(s)]
- A total of 534 residues are present.
- Protein mainchain and sidechains are present.
- No explicit hydrogen atoms are included.
- 402 hetero group(s) is/are present.
- Refinement was carried out in X-PLOR 3.851.
- R = 0.188; Rfree = 0.228
- 0 PDBv2.3 atoms were found. Proceeding assuming PDBv3 formatted file.

**Continue >**



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**SUGGESTED TOOLS (ALL TOOLS)**

Due to the parameter adjustments to hydrogen bond lengths and van der Waals radii, the current default behavior for MolProbity is to remove hydrogens, if they are present, before analysis. Please re-add hydrogens using the "Add hydrogens" option below, where you will have the option to choose either the default electron-cloud position hydrogens (i.e. for crystal structures) or nuclear-position hydrogens (i.e. for neutron-diffraction structures or for NMR structures).

Currently working on: **1eve.pdb**

**Add hydrogens**

**Make simple kinemages**

**Edit PDB file**

**Downgrade file to PDBv2.3 format (for download only)**

**Fill gaps in protein backbone with JiffiLoop (beta test)**

**Analyze geometry without all-atom contacts**

Select a model to work with: 1eve.pdb Original file downloaded from web

Choose the outputs you want: Default options have been selected based on the content of the submitted file. Follow the ? symbols for more information on the validation options.

- 3-D kinemage graphics
  - Universal**
    - Clashes
    - Hydrogen bonds
    - van der Waals contacts
    - Geometry evaluation
  - Protein**
    - Ramachandran plots
    - Rotamer evaluation
    - C $\beta$  deviations
    - Cis-Peptide evaluation
    - CaBLAM backbone markup
  - RNA**
    - RNA sugar pucker analysis
    - RNA backbone conformations
  - Other options**
    - Make views of trouble spots even if it takes longer
    - Alternate conformations
    - Model colored by B-factors
    - Model colored by occupancy
    - Ribbons
  - Charts, plots, and tables
    - Universal**
      - Clashes & clashscore
      - Geometry evaluation
    - Protein**
      - Ramachandran plots
      - Rotamer evaluation
      - C $\beta$  deviations
      - Cis-Peptide evaluation
      - Show cis-*nonPro* and twisted peptide statistics even if the model has none
      - CaBLAM backbone evaluation
    - RNA**

Select a model to work with: 1eve.pdb Original file downloaded from web

Choose the outputs you want: Default options have been selected based on the content of the submitted file. Follow the ? symbols for more information on the validation options.

- 3-D kinemage graphics
- Charts, plots, and tables
  - Universal**
    - Clashes & clashscore
    - Geometry evaluation
  - Protein**
    - Ramachandran plots
    - Rotamer evaluation
    - C $\beta$  deviations
    - Cis-Peptide evaluation
    - CaBLAM backbone evaluation
  - RNA**
    - RNA sugar pucker analysis
    - RNA backbone conformations
  - Other options**
    - Horizontal chart with real-space correlation data
    - Chart for use with Coot (may take a long time, but should take less than 1 hour)
    - Suggest / report on automatic structure fix-ups
    - Create html version of multi-chart

Run programs to perform these analyses >

Cancel

Summary statistics

Protein Geometry	Ramachdran outliers	0	0.00%	Goal: <0.05%
	Ramachdran favored	501	94.17%	Goal: >98%
	Rama distribution Z-score	-2.20 ± 0.31		Goal: abs(Z score) < 2

In the two column results, the left column gives the raw count, right column gives the percentage.  
Key to table colors and cutoffs here: ?

Multi-criterion visualizations



[View](#) (966 bytes)

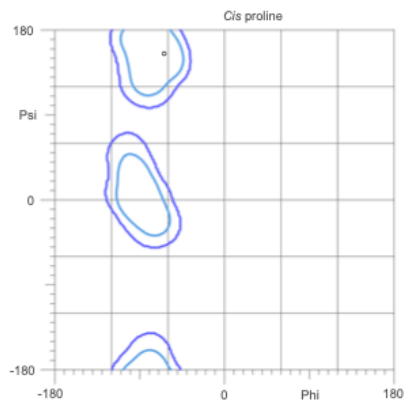
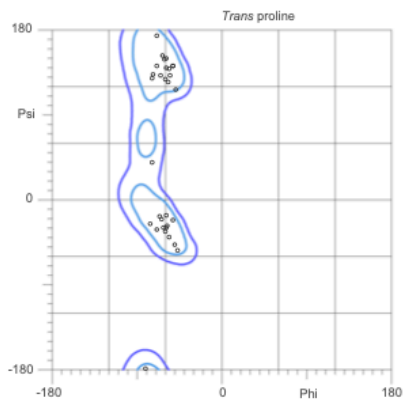
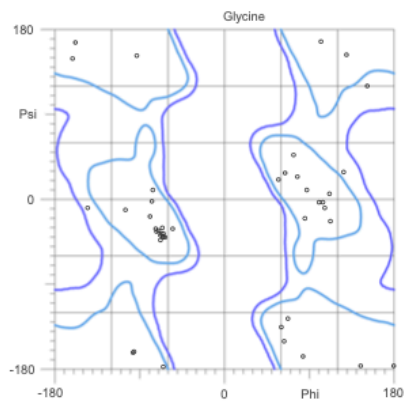
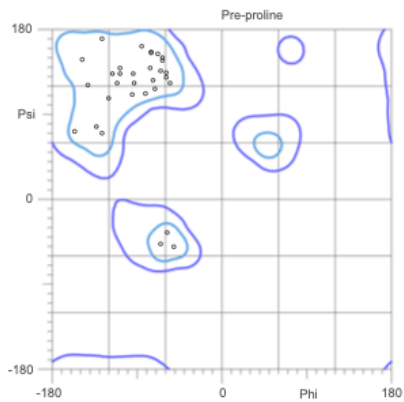
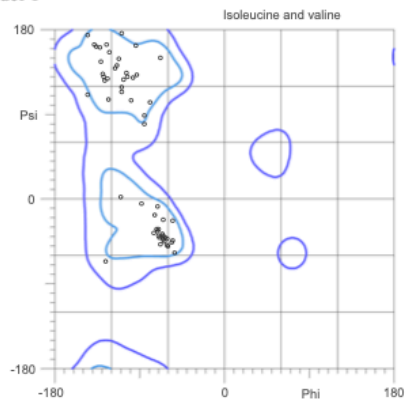
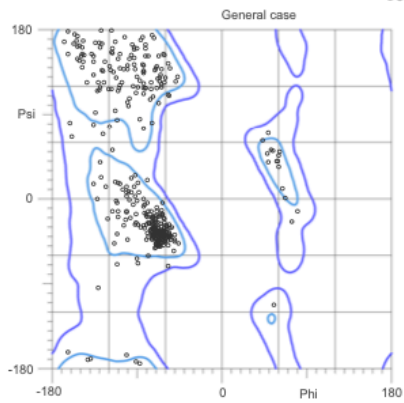
Single-criterion visualizations

- [Ramachdran plot Message](#) (435 Kb): [View in KING](#) | [View in NGL](#) | [Download](#)
- [Ramachdran plot PDF](#) (1.7 Mb): [View](#)
- [Ramachdran distribution Z-score analysis](#) (26 Kb): [View](#)

[Continue >](#)

# MolProbity Ramachandran analysis

1eve.pdb, model 1



94.2% (501/532) of all residues were in favored (98%) regions.  
100.0% (532/532) of all residues were in allowed (>99.8%) regions.

There were no outliers.

<http://kinemage.biochem.duke.edu>

Lovell, Davis, et al. Proteins 50:437 (2003)