PROBITY

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Duke Biochemistry
Duke University School of Medicine

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

We reserve the right to bar access to users who violate our usage guidelines:
In particular, users making burst submissions of large number of structures should download and install their own local instance of MolProbity for this purpose. Once again, recent abuse of our server originating from a single institution has caused downtime and denial of service to our broader community. Regrettably, we will need to bar these users if this abuse continues.

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 code: 1ct9 type: PDB coords Fetch >

Choose File No file chosen 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.

PROBITY

Uploaded PDB file as 1ct9.pdb

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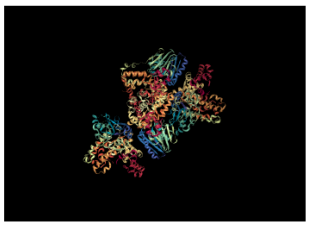
Your file from http://www.pdb.org/ was uploaded as 1ct9.pdb.

- This compound is identified as **CRYSTAL STRUCTURE OF ASPARAGINE SYNTHETASE B FROM ESCHERICHI**
- This structure was solved by X-RAY DIFFRACTION.
- This structure was solved at 2.00 Å resolution.
- 4 chain(s) is/are present [3 unique chain(s)]
- A total of 1982 residues are present.
- Protein mainchain and sidechains are present.
- No explicit hydrogen atoms are included.
- 1074 hetero group(s) is/are present.
- Refinement was carried out in TNT.
- R = 0.197; Rfree = 0.297
- 0 PDBv2.3 atoms were found. Proceeding assuming PDBv3 formatted file.



Continue >

About MolProbity | Website for the Richardson Lab | Using ecloud x-H | Internal reference 4.5.1

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SUGGESTED TOOLS (ALL TOOLS)

Due to the parameter adjustments to hydrogen bondlengths 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: **1ct9.pdb**


Add hydrogens

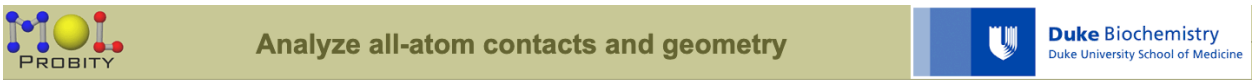

Make simple kinemages


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:

1ct9.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.

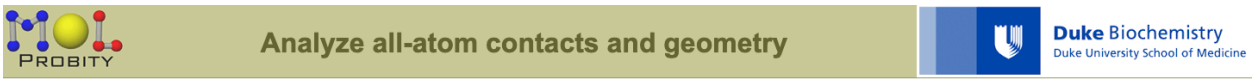
- [x] **3-D kinemage graphics**
  Universal
  - [ ] Hydrogen bonds
  - [ ] van der Waals contacts
  - [x] Geometry evaluation

  Protein
  - [x] Ramachandran plots
  - [x] Rotamer evaluation
  - [x] Cβ deviations
  - [x] 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

< uncheck this box



Select a model to work with:

1ct9.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**
- [x] **Charts, plots, and tables**
  Universal
  - [x] Geometry evaluation

  Protein
  - [x] Ramachandran plots
  - [x] Rotamer evaluation
  - [x] Cβ deviations
  - [x] Cis-Peptide evaluation
  - [ ] Show cis-nonPro and twisted peptide statistics even if the model has none
  - [ ] 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
  - [x] Create html version of multi-chart
    - [ ] List all residues in multi-chart, not just outliers
    - [x] Remove residue rows with ' ' altloc when other alternate(s) present

< uncheck these

Run programs to perform these analyses >

Cancel

Analyze all-atom contacts and geometry

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Select a model to work with:

◉	**1ct9.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
    - ☐ Cβ 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

Analysis output: geometry for 1ct9.pdb

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Summary statistics

Protein Geometry	Ramachandran outliers	15	0.77%	Goal: <0.05%
	Ramachandran favored	1831	93.80%	Goal: >98%
	Rama distribution Z-score	-2.76 ± 0.17		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 (968 bytes)

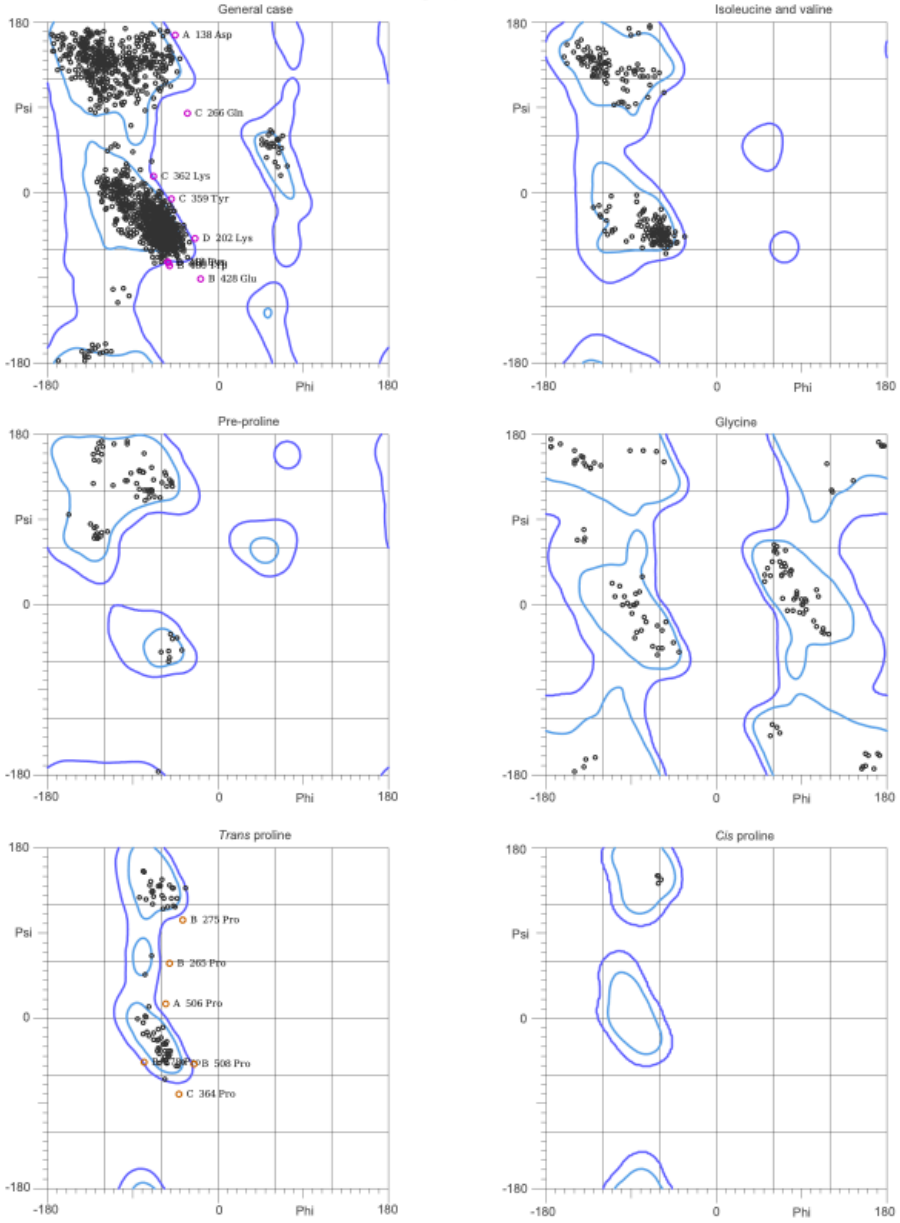
Single-criterion visualizations

- **Ramachandran plot kinemage** (521 Kb): View in KiNG | View in NGL | Download
- **Ramachandran plot PDF** (1.8 Mb): View
- **Ramachandran distribution Z-score analysis** (90 Kb): View

Continue >

MolProbity Ramachandran analysis

1ct9.pdb, model 1



93.8% (1831/1952) of all residues were in favored (98%) regions.
99.2% (1937/1952) of all residues were in allowed (>99.8%) regions.

There were 15 outliers (phi, psi):

A 138 Asp (-46.8, 168.7)	B 508 Pro (-26.7, -48.6)
A 506 Pro (-56.4, 16.1)	C 266 Gln (-33.2, 85.7)
B 248 Lys (-54.1, -74.0)	C 359 Tyr (-50.9, -6.5)
B 265 Pro (-52.6, 59.0)	C 362 Lys (-69.5, 18.5)
B 275 Pro (-38.2, 105.1)	C 364 Pro (-42.6, -80.3)
B 278 Pro (-79.5, -46.4)	D 202 Lys (-25.7, -48.5)
B 428 Glu (-19.5, -91.5)	D 460 Trp (-54.0, -74.7)
B 460 Trp (-52.4, -77.7)	

http://kinemage.biochem.duke.edu

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