

# Electrostatics Calculations

- I ran electrostatic potential calculations with PDB2PQR and APBS (<http://www.poissonboltzmann.org>) on the PDB2PQR server ([http://nbc-222.ucsd.edu/pdb2pqr\\_2.1.1/](http://nbc-222.ucsd.edu/pdb2pqr_2.1.1/)). There were three steps:
  - Uploading the PDB file and selecting parameters. I used the defaults.
  - Running PDB2PQR by pressing “Submit”. This performs some basic structural preparation, e.g. adding missing atoms and optimizing hydrogen positions.
  - Running APBS by following “Click here to run APBS with your results”. This actually solves the PB equation.
- For TS, none of these calculations took a very long time.

The screenshot displays the PDB2PQR Server interface, which is used for performing electrostatic calculations. It shows the submission and results for two different calculations.

**PDB2PQR Server**  
Currently using PDB2PQR Version 2.1.1  
Return to the PDB2PQR homepage.

This server enables a user to convert PDB files into PQR files. PQR files are PDB files where the occupancy and B-factor columns have been replaced by per-atom charge and radius. pKa calculations are performed by PROPKA.

For more information on PDB2PQR please see the:

- Home Page
- Register (and help support PDB2PQR & APBS)
- User Guide
- Examples
- Release Notes

If you use the PDB2PQR service in a publication, please cite:

Dolinsky TJ, Nielsen JE, McCammon JA, Baker NA. PDB2PQR: an automated pipeline for the setup, execution, and analysis of Poisson-Boltzmann electrostatics calculations. *Nucleic Acids Research* 32 W665-W667 (2004). [\[Link\]](#)

**Note:** In order to distribute server load, the PDB2PQR server currently is limited to a maximum size of 10000 atoms per protein. If you are interested in using PDB2PQR for larger proteins, you are encouraged to download a command line version of PDB2PQR from the [PDB2PQR download page](#). For additional limitations, please see the [PDB2PQR user guide](#).

**Note:** This server uses automatic refreshing to update the status of your PDB2PQR submission. Do not use the back button on your browser while the server is running.

Please enter either:

- a PDB ID:
- upload a PDB file:

**Status: complete ✓**  
Run time: 0:00:34  
Current time: Mon Jan 20 13:52:26 2020

Here are the results:

- Input files
  - TS\_human.pdb
- Output files
  - TS\_human.propka
  - TS\_human.pqr
  - TS\_human.in
- Runtime and debugging information
  - Program output (stdout)
  - Program errors and warnings (stderr)

[Click here](#) to run APBS with your results.

**Status: complete ✓**  
Run time: 0:01:35  
Current time: Mon Jan 20 13:57:47 2020

Here are the results:

- Input files
  - 15795571126.pqr
  - apbsinput.in
- Output files
  - 15795571126-pot-PEO.dx.gz
  - 15795571126.cube.gz
- Runtime and debugging information
  - Program output (stdout)
  - Program errors and warnings (stderr)

Visualize your results online:

- 3Dmol
- Jmol

# **Visualizing Electrostatic Potentials with VMD**