Calculation of Q-scores from Command Line

First, download and install UCSF Chimera and the ModelZ plugin: <https://github.com/gregdp/mapq>

Then, Q-scores can be calculated from the command line using a command which varies slightly by platform:

Mac Command:

[path to Chimera]/Contents/MacOS/chimera --nogui --silent --nostatus [path to map] [path to model] [path to Chimera]/Contents/Resources/share/modelz/mapq\_run.py

Mac Example:

~/Desktop/Chimera.app/Contents/MacOS/chimera --nogui --silent --nostatus ~/\_data/mmetrics/emd\_20026/emd\_20026.map ~/\_data/mmetrics/emd\_20026/3ajo.pdb ~/Desktop/Chimera.app/Contents/Resources/share/modelz/mapq\_run.py

Unix Command:

[path to Chimera]/bin/chimera --nogui --silent --nostatus [path to map] [path to model] [path to Chimera]/share/modelz/mapq\_run.py

Unix Example:

~/\_mol/Chimera/bin/chimera --nogui --silent --nostatus ~/Dropbox/\_data/Ferritin/k175/k175\_fi.mrc ~/Dropbox/\_data/Ferritin/k175/3ajo\_f.pdb ~/\_mol/Chimera/share/modelz/mapq\_run.py

In all cases, the output should be something like this:

Q Scores - using 6 processors

- map: emd\_20026.map

- mol: 3ajo.pdb, chain: \_all\_

- sigma: 0.50

- mind: -0.061, maxd: 0.109

- atoms to do: 1714

- path: /Users/greg/Desktop/Chimera.app/Contents/Resources/share/mapqp.py

- on mac

Starting parallel processes...

- 1/6, 5-37

- 2/6, 37-68

- 3/6, 68-101

- 4/6, 101-135

- 5/6, 136-171

- 6/6, 171-423

Waiting...

0 1 2 3 4 5

Getting...

0 1 2 3 4 5

- done, time: 67.532019

- done, time: 1 min, 7.5 sec

Saving pdb with Q-scores in B-factor column:

- /Users/greg/\_data/mmetrics/emd\_20026/3ajo\_\_Q\_\_emd\_20026.pdb

Average atom Q-score for entire model: 0.73471

- Protein: 0.77718

- Other: 0.47512

* The score for the entire model is on the third last line (0.73471).
* The last lines summarize the scores by atom type: protein, nucleic acids, and other (e.g. ligands, water molecules).
* Per-atom Q-scores are stored in the pdb file [model name]\_\_Q\_\_[map name] in the B-factor column.