Calculation of Q-scores from Command Line

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

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

Using only a single processor:

Mac Command:

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

Unix Command:

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

Using multi-processing (the number of processors/cores will be automatically detected and used – this may be set as an option in the future):

Mac Command:

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

Unix Command:

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

* Please note that [path to model] is required when using the multi-processing script, and should be an absolute path, even if the script is run from the directory where the model is located.

The output should be something like this (will vary slightly depending on whether multi-processing was used or not):

Q Scores:

- 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

[...]

- done, time: 70.172916

- done, time: 1 min, 10.2 sec

Saving pdb with Q-scores: /Users/greg/\_data/mmetrics/emd\_20026/3ajo\_\_Q\_\_emd\_20026.pdb

Q for 413 res...

Model Q-score: 0.776

Chain Avg.Q-score Est.Res.(A)

chain A (hoh) 0.506 3.45

chain A (mg) 0.510 3.42

chain A (protein) 0.820 1.69

Type Avg.Q-score Est.Res.(A)

Protein 0.820 1.69

MG 0.510 3.42

HOH 0.506 3.45

Avg. Q score: 0.776

* The score for the entire model is on the third last line (0.776).
* The other few last lines summarize the scores by atom type: protein, nucleic acids, and other, e.g. Mg, Hoh (water atoms).
* Per-atom Q-scores are stored in the pdb file [model name]\_\_Q\_\_[map name] in the B-factor column.