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:**

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 [number of processors]

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 6

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 [number of processors]

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 6

* 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. This is so that per-atom Q-scores can be written to a PDB file in the same folder (see below).
* Multiple models can be specified on the command line; the script will iterate over all of them. Just one map should be specified however.

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

Map: emd\_20026.map, Model: 3ajo.pdb

--> avg. Q score: 0.776

* The score for the entire model is on the 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 **Occupancy** column.
* When using multiprocessing, there will be an ‘error’ output at the end, e.g. “Error processing 6: …”. Chimera is complaining that it did not know what to do with the parameter which specifies the number of processors, even though it was used by the script as intended; otherwise the script should have completed successfully.