Calculation of Q-scores from Command Line – NEW (Simpler method)

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 python script that is in the zip file downloaded when installing the MapQ plugin. The command has the following format:

python mapq\_cmd.py [path to Chimera] [path to map] [path to model 1] [path to model 2] [path to model …] np=N res=N.N bfactor=N sigma=N.N

Example:

python mapq\_cmd.py ~/\_mol/Chimera/bin/chimera ~/Dropbox/\_data/Ferritin/k175/k175\_fi.mrc ~/Dropbox/\_data/Ferritin/k175/3ajo\_f.pdb np=4 res=3.0 bfactor=200

Notes:

* np=N (e.g. np=4) – optional – default is 1 - it specifies number of processes to use
* res=N.N (e.g. res=3.2) – optional - default is 3.0 - specifies resolution of map; it is used to output per-residue statistics along with expected Q-score at this resolution
* bfactor=N (suggested bfactor=200) – optional - if specified, a separate pdb file will be written where bfactor=N\*(1-Qscore) for each atom
* sigma=N.N (e.g. sigma=0.6) – optional – default is 0.6 – specifies width of reference Gaussian (for sigma=0.6, the higest Q-score of 1 occurs at ~1.5Å resolution, for sigma=0.4, highest is at ~1.1Å)
* [path to Chimera] - the path where Chimera is installed (note, not to the binary file)

The output should be something like this (will vary slightly depending on whether multi-processing was used or not, and whether more than one model was specified):

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

Saving per-chain & per-residue Q-scores:

-> res= 1.75

-> file: /Users/greg/\_data/maps2/FerritinT/3ajo\_\_Q\_\_emd\_20026\_All.txt

* 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 B-factor column. Note that the full path to the model must be given in the command for this file to be put in the same folder as this model.