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.