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.