

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
```

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) is optional, it specifies number of processes to use; if left out, a single process will be used.
- res=N.N (e.g. res=3.2) is 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) is optional; if specified, a separate pdb file will be written where bfactor=N*(1-Qscore) for each atom
- [map to Chimera] is just the path where Chimera is installed, not the actual binary itself

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/mapq.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 **Occupancy** 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.