

How to create a properly weighted map... generate structure factors with phenix.fmodel and then compute the map from the structure factors with phenix.mtz2map.

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```
Phenix.fmodel
```

A tool to compute structure factors.

Documentation: <https://www.phenix-online.org/documentation/reference/fmodel.html>

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```
phenix.mtz2map [mtz_file] [pdb_file] [param_file] [--show_maps]
```

If you already have map coefficients in an MTZ file and just want to run an FFT to produce X-plor or CCP4 map files, use phenix.fft or phenix.mtz2map (these are synonyms for the same program).

Documentation: <https://www.phenix-online.org/documentation/reference/mtz2map.html>

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In our example from the T20S\_validate folder, run the following commands:

```
bash-3.2$ phenix.fmodel 1yar_fit_rsr_combined_rsr.pdb high_res=2.4  
scattering_table=electron
```

Typically, I use a resolution better than the stated resolution of the EM map. Technically, the resolution of the experimental map is 2.8Å at FSC of 0.143, but the curve FSC curves has a resolution of ~2.4Å when the FSC is 0. Thus, there is data out to ~2.4Å which is why I use that value.

Once complete I run the following to obtain a ccp4, properly weighted map.

```
bash-3.2$ phenix.mtz2map 1yar_fit_rsr_combined_rsr.pdb.mtz  
1yar_fit_rsr_combined_rsr.pdb high_res=2.4  
scattering_table=electron include_fmodel=true
```

These can then be opened up in Chimera for comparison and manipulation, and then FSC curves can be computed. It should be noted that B-factor values must be refined to generate the proper weights.