

Model building

Imports

- import volumes
- import atomic structure
- import sequence

Preprocess map

- xmipp3 - create 3d mask
- xmipp3 - local MonoRes
- xmipp3 - localdeblur sharp
- xmipp3 - extract asymmet
- xmipp3 - deepEMhancer

Initial model

- chimeraX - model from template

Rigid fitting

- phenix - dock in map
- chimeraX - rigid fit

Flexible fitting

- ccp4 - coot refinement
- ccp4 - reformat
- phenix - real space refine

Validation

- phenix - emringer
- phenix - molprobability
- phenix - validation cryoem
- xmipp3 - validate fsc-q

Tools-Calculators

- atomstructutils - operator
- atomstructutils - convert
- phenix - superpose pdbs
- chimeraX - operate

import atomic structure
finished

chimeraX - model from template
finished

phenix - dock in map
finished

chimeraX - rigid fit
finished

ccp4 - coot refinement
running (done 1/2)

Summary Methods C

Browsing: Runs/007193_CootRefine

Refresh
 Home
 Launch folder
 Working dir
 Up

Path /home/marta/OLD/marta/ScipionUserData/projects/Demo_Modeling_2020/Runs

File	Size	Time
.	4 kB	06-11-2020 20:33
coot.ini	80 bytes	06-11-2020 20:33
cootScript.py	8 kB	06-11-2020 20:33
deepPostProcess_output_volume.mrc	2.0 MB	06-11-2020 20:33
import_emd_3488_output_volume.mrc	2.0 MB	06-11-2020 20:33
outputDataBaseNameWithLabels.sqlite	12 kB	06-11-2020 20:33
sharpenedMap_2_output_volume.mrc	2.0 MB	06-11-2020 20:33

Open *coot.ini Save

~/OLD/marta/ScipionUserData...

```
[myvars]
imol: 0
aa_main_chain: A
aa_auxiliary_chain: AA
aaNumber: 4
step: 10
```

.ini Tab Width: 8 Ln 5, Col 12 INS