

View Model building

Model building

Imports

- import volumes
- import atomic structure
- import sequence

Preprocess map

- xmipp3 - create 3d mask
- xmipp3 - local MonoRes
- xmipp3 - localdeblur sharpening
- xmipp3 - extract asymmetric unit
- xmipp3 - deepEMhancer

Initial model

- chimerax - model from template

Rigid fitting

- phenix - dock in map
- chimerax - rigid fit

Flexible fitting

- ccp4 - coot refinement**
- ccp4 - refrac
- phenix - real space refine

Validation

- phenix - emringer
- phenix - molprobtity
- phenix - validation_cryoem
- xmipp3 - validate fsc-q

Tools-Calculators

- atomstructutils - operator
- atomstructutils - convert_sym
- phenix - superpose pdbs
- chimerax - operate
- chimerax - restore session

Edit Copy Delete Browse Collapse Labels

ccp4 - coot refinement whole (copy)
interactive

Summary Methods Output

Input

001 (from xmipp3 - de
pdbFileToBeRefined

Output

- ccp4 - coot refine
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Browsing: Runs/0

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Path /home/marta/OLD/marta/ScipionUserData/projects/Demo_Mo

File	Size	
..	4 kB	1
coot.ini	80 bytes	1
cootScript.py	8 kB	1
coot_013799_1mol_0000_version_0001.pdb	363 kB	1
coot_013799_1mol_0000_version_0002.pdb	363 kB	1
coot_013799_1mol_0000_version_0003.pdb	363 kB	1
coot_013799_1mol_0000_version_0004.pdb	363 kB	1
coot_013799_1mol_0000_version_0005.pdb	363 kB	1
coot_013799_1mol_0000_version_0006.pdb	363 kB	1
coot_013799_1mol_0000_version_0007.pdb	363 kB	1
coot_013799_1mol_0000_version_0008.pdb	363 kB	1
deepPostProcess.mrc	3.8 MB	1
outputDataBaseNameWithLabels.sqlite	12 kB	1

SUMMARY

coot_013799_1mol_0000_version_0001:

coot_013799_1mol_0000_version_0002:

Close