

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 unit cell

Initial model

- chimera - model from template

Rigid fitting

- powerfit_scipion - powerfit
- chimera - chimera rigid fit

Flexible fitting

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

Validation

- phenix - emringer
- phenix - molprobity
- phenix - validation_cryoem

Tools-Calculators

- phenix - superpose pdbs
- atomstructutils - operator
- atomstructutils - convert_sym
- chimera - chimera operate
- chimera - chimera restore session
- chimera - contacts

Others

- xmipp3 - 3d bionotes

Exports

- export to EMDB

Protocol Run: ProtExportEMDB

Protocol: scipion - export emdb

finished Cite Help

Run

Run name: scipion - export emdb

Run mode: Continue

Host: localhost

Use queue? No

Wait for:

Input

Volume to export: import half1.outputVolume

FSC to export: xmipp3 - resolution 3D

Atomic structure to export: import atom_struct mmCIF 5ni1.cif.output

Mask to export: xmipp3 - create 3d mask.outputMask

Export to directory: /home/Submission1_03_24_2019

Summary Methods Output Log

Input

- exportVolume (from import half1 -> outputVolume)
- exportFSC (from xmipp3 - resolution 3D)
- exportAtomStruct (from import atom_struct)
- exportMask (from xmipp3 - create 3d mask -> outputMask [outputMask])

Output

SUMMARY

Data Available at : /home/Submission1_03_24_2019

1 2 3 4 5 6