



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 - reffmac

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: XmippProtExtractUnit



Protocol: xmipp3 - extract unit cell

finished Cite Help

Run

Run name xmipp3 - extract unit cell sym

Comment

Run mode

Continue Restart

Host localhost

Use queue?

Yes No

Wait for

Input

Input

Input volume scipion - import volumes HEMOGLOBIN.outputVolume

Symmetry Cn (Cn)

Symmetry Order 2

offset -45.0

Inner Radius (px) 0.0

Outer Radius (px) 40.0

Expand Factor 0.2

Close

Save

Execute

Summary

Methods

Output Log

Input

inputVolumes (from scipion - import volumes HEMOGLOBIN -> outputVolume [alpha Volume (100 x 100 x 100, 1.05 Å/px)

Output

xmipp3 - extract unit cell sym C2 -> outputVolume

Volume (81 x 81 x 81, 1.05 Å/px)

Protocols | Data

View: Tree

create 3d mask (2)
finishedlocal MonoRes (2)
finishedlocaldeblur sharpening (2)
finishedphenix - real space refine (copy 2)
finished

Analyze Results