



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 - reftmac
- phenix - real space refine

Validation

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

Tools-Calculators

- atomstructutils - operator
- atomstructutils - convert swm
- phenix - superpose pdbs
- chimerax - operate
- chimerax - restore session
- chimerax - contacts
- chimerax - map subtraction
- xmipp3 - map from atomic structure

Others

Protocol Run: PhenixProtRunSuperposePDBs

Phenix

Protocol: phenix - superpose pdbs

finished Cite Help

Run

Run name phenix - superpose pdbs

Comment

Run mode

☒ Continue ☐ Restart

Host localhost

Use queue?

☐ Yes ☒ No

Wait for

Input

Input

Fixed atomic structure chimera - rigid fit (2).5ni1_chainA_fitted_Atom_struct_3_00809

Moving atomic structure phenix - real space refine.outputPdb

Close

Save

Execute

Summary

Methods

Output Log

Input

inputStructureFixed (from chimera - rigid fit (2) -> 5ni1_chainA_fitted_Atom_AtomStruct (pseudoatoms=False, volume=False))
inputStructureMoving (from phenix - real space refine -> outputPdb [outputPd AtomStruct (pseudoatoms=False, volume=True))

Output

phenix - superpose pdbs -> outputPdb AtomStruct (pseudoatoms=False, volume=False)

SUMMARY

RMSD between fixed and moving atoms (start): 0.523
RMSD between fixed and moving atoms (final): 0.474
http://www.phenix-online.org/documentation/superpose_pdb.html
Peter Zwart, Pavel Aforine, Ralf W. Grosse-Kunstleve

phenix - dock in map (2)
finishedchimerax - rigid fit (2)
finishedphenix - superpose pdbs
finished

Analyze Results