



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 - molprobity
- phenix - validation_cryoem
- xmipp3 - validate fsc-q

Tools-Calculators

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

Protocol Run: ChimeraModelFromTemplate

Protocol: chimera - model from template

finished Cite Help

Run

Run name: chimera - model from template Comment

Run mode: ☒ Continue ☐ Restart Host: localhost

Use queue? ☐ Yes ☒ No

Wait for

Input Help

Input

Do you already have a template? ☒ Yes ☐ No

Atomic structure used as template: pwem - import atomic structure 1PBX.outputPdb

Chain: {"model": 0, "chain": "A", "residues": 142}

Target sequence: pwem - import sequence HBA_HUMAN.outputSequence

Options to improve the alignment: Additional sequences to align

Other sequences to align

Object	Info
pwem - import sequence HBA_TURTLE.o	Sequence (name = HBA_
pwem - import sequence HBA_TURKEY.c	Sequence (name = HBA_
pwem - import sequence HBA_RABBIT.o	Sequence (name = HBA_
pwem - import sequence HBA_HORSE.o	Sequence (name = HBA_

Multiple alignment tool: Clustal Omega

Additional target sequence to include? ☐ Yes ☒ No

Close Save Execute

rem - import sequer
finish

Analyze Results