

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 - refmac
- 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
- chimerax - map subtraction
- xmipp3 - map from atomic structure

## Others

## Exports

- export to DB

Protocol Run: PhenixProtRunDockInMap

# Phenix

Protocol: phenix - dock in map finished [Cite](#) [Help](#)

**Run**

Run name  Comment

Run mode ☒ Continue ☐ Restart ? Host

Parallel Threads  ? Use queue? ☐ Yes ☒ No ? Wait for  ?

Expert Level ☒ Normal ☐ Advanced

**Input**

Input map  ?

Resolution (Å):  ?

Input atom structure  ?

Atom structure number of copies  ?

Close Save Execute

**Summary** **Methods** **Output Log**

**Input**

inputVolume1 (from xmipp3 - extract asymmetric unit HEMOGLOBIN -> output Volume (81 x 81 x 81, 1.05 Å/px))

inputStructure (from chimerax - model from template -> Atom struct 6\_001702 AtomStruct (pseudoatoms=False, volume=False))

**Output**

phenix - dock in map -> outputPdb AtomStruct (pseudoatoms=False, volume=True)

**SUMMARY**

No summary information.

**Analyze Results**

Tree

HORSE

pwem - import s

nerax - model from template finished

phenix - dock in map finished