

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 - re mac
 - phenix - real space refine
- Validation
 - phenix - emringer**
 - phenix - molprobtity
 - 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: PhenixProtRunEMRinger

Phenix Protocol: phenix - emringer finished [Cite](#) [Help](#)

Run

Run name phenix - emringer Comment

Run mode Continue Restart Host localhost

Use queue? Yes No

Wait for

Input

Input Volume ccp4 - coot refinement.output3DMap_0003

Input atomic structure ccp4 - re mac.outputPdb

Execute

Input

inputVolume (from ccp4 - coot refinement -> output3DMap 000 Volume (81 x 81 x 81, 1.05 Å/px))

inputStructure (from ccp4 - re mac -> outputPdb [outputPdb]) AtomStruct (pseudoatoms=False, volume=False)

Output

SUMMARY

Optimal Threshold: 0.40 Rotamer-Ratio: 0.89

Max Zscore: 2.09 Model Length: 85

EMRinger Score: 2.27

Workflow Diagram:

```

graph TD
    A[ccp4 - re mac finished] --> B[phenix - emringer finished]
    B --> C[Analyze Results]
  
```

Annotations:

- 1: Arrow pointing to "phenix - emringer" in the left sidebar.
- 2: Arrow pointing to the "Input" tab.
- 3: Arrow pointing to the "Input Volume" field.
- 4: Arrow pointing to the "Execute" button.
- 5: Arrow pointing to the "phenix - emringer finished" box in the workflow diagram.
- 6: Arrow pointing to the "SUMMARY" section.