

SCIPION v2.0 (2019-0

Protocol Run: PhenixProtRunRSRefine

Protocol: phenix - real space refine

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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 - refmac
- 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

Run

Run name: phenix - real space refine

Run mode: Continue

Host: localhost

Parallel Threads: 1

Use queue? No

Expert Level: Normal

Input Volume: ccp4 - coot refinement.output3DMap_001

Resolution (A): 3.2

Input atomic structure: chimera - rigid fit HBA_HUMAN.outputPdb

Execute

1

2

3

4

5

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Analyze Results

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AtomStruct (pseudoatoms=False, volume=True)

SUMMARY

MolProbity statistics:

Ramachandran outliers: 0.00 % (Goal: < 0.2%) Ramachandran favored: 95.71 % (Goal: > 98%)

Rotamer outliers: 1.75 % (Goal: < 1%) C-beta outliers: 0 (Goal: 0)

Clashscore: 5.82 Overall score: 1.80