

View Protocols SPA

- ▷ Preprocess
- ▷ Filter
- ▷ Mask

2D

- ▷ Align
- ▷ Classify

3D

- ▷ Initial volume
- ▷ Preprocess
- ▷ Classify
- ▷ Refine
- ▷ Analysis
- ▷ Reconstruct

Tools

Model Building

- ▷ xmipp3 - extract unit cell
- ▷ chimera - chimera rigid fit
- ▷ chimera - model from template
- ▷ powerfit_scipion - powerfit
- ▷ ccp4 - coot refinement
- ▷ **ccp4 - refmac**
- ▷ phenix - emringer
- ▷ phenix - real space refine
- ▷ phenix - molprobtity
- ▷ xmipp3 - 3d bionotes



Run

Run name **ccp4 - refmac HBA_HUMAN**

Comment

Run mode ☒ Continue ☐ Restart

Host localhost

Use queue? ☐ Yes ☒ No

Wait for

Expert Level

☐ Normal ☒ Advanced

Input

Input

Input Volume **ccp4 - coot refinement.output**Atomic structure to be refined **phenix - real space refine HBA_HUM**

Max. Resolution (A): 3.2

Min. Resolution (A): 200.0

Generate masked volume ☒ Yes ☐ No

SFCALC mapradius: 3.0

SFCALC mradius: 3.0

Number of refinement iterations: 30

Matrix refinement weight: 0.0

B Factor: 40.0

Close

Save

Execute

018 Protocols | Data

Refresh

emringer (copy)
ished

p

Analyze Results

(px)

lume=False)

lume=True)