

A

SCIPION

v2.0 (2019-03-20) D

B

Protocol Run: ProtAtomStrucOperate

 Cite HelpView **Protocols SPA**

Micrographs

- xmipp3 - preprocess micrographs
- xmipp3 - ctf estimation

↳ CTF estimation

more

Particles

- Picking
- Extract
- Preprocess
- Filter
- Mask

2D

- Align
- Classify

3D

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

Tools

- Sets
- Calculators

- xmipp3 - operate particles
- xmipp3 - operate volumes
- chimera - chimera operate
- chimera - chimera restore session
- atomstructutils - operator
- phenix - superpose pdbs

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 - molprobity
- xmipp3 - 3d bionotes
- chimera - contacts



Protocol: atomstructutils - operator

Run

Run name **atomstructutils - operator (2)** Run mode Continue Restart Host **localhost** Use queue? Yes No Wait for

Input

Input

Atomic Structure 1: scipion - import atomic structure 5NI1.outputPdb Operation: **extractChain** Chain **{"model": 0, "chain": "A", "residues": 141}** Start at residue # **-1** End at residue # **-1**

C

Input

Input

Atomic Structure 1: scipion - import atomic structure 5NI1.outputPdb Operation: **addChain**

Atomic Structure 2:

atomstructutils - operator (chain D) AtomStruct (pseudoa)