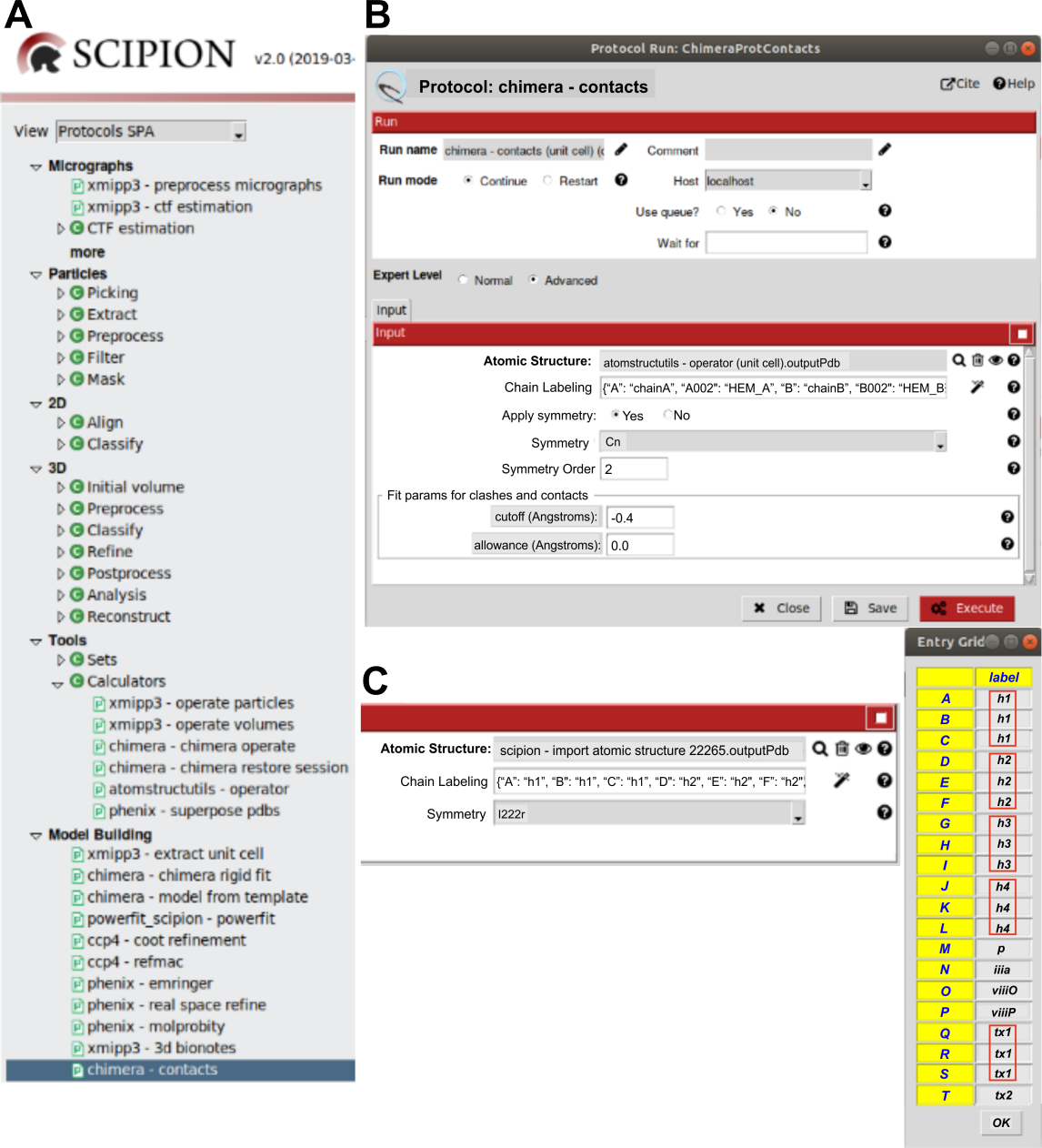
A
SCIPION
v2.0 (2019-03-
View
Protocols SPA
Micrographs
xmipp3 - preprocess micrographs
xmipp3 - ctf estimation
CTF estimation
more
Particles
Picking
Extract
Preprocess
Filter
Mask
2D
Align
Classify
3D
Initial volume
Preprocess
Classify
Refine
Postprocess
Analysis
Reconstruct
Tools
Sets
Calculators
xmipp3 - 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
B
Protocol Run: ChimeraProtContacts
Protocol: chimera - contacts
Cite
Help
Run
Run name
chimera - contacts (unit cell) (
Comment
Run mode
Continue
Restart
Host
localhost
Use queue?
Yes
No
Wait for
Expert Level
Normal
Advanced
Input
Input
Atomic Structure:
atomstructutils - operator (unit cell).outputPdb
Chain Labeling
{"A": "chainA", "A002": "HEM_A", "B": "chainB", "B002": "HEM_B
Apply symmetry:
Yes
No
Symmetry
Cn
Symmetry Order
2
Fit params for clashes and contacts
cutoff (Angstroms):
-0.4
allowance (Angstroms):
0.0
Close
Save
Execute
C
Atomic Structure:
scipion - import atomic structure 22265.outputPdb
Chain Labeling
{"A": "h1", "B": "h1", "C": "h1", "D": "h2", "E": "h2", "F": "h2",
Symmetry
I222r
Entry Grid
label
A h1
B h1
C h1
D h2
E h2
F h2
G h3
H h3
I h3
J h4
K h4
L h4
M p
N iiia
O viiiO
P viiiP
Q tx1
R tx1
S tx1
T tx2
OK