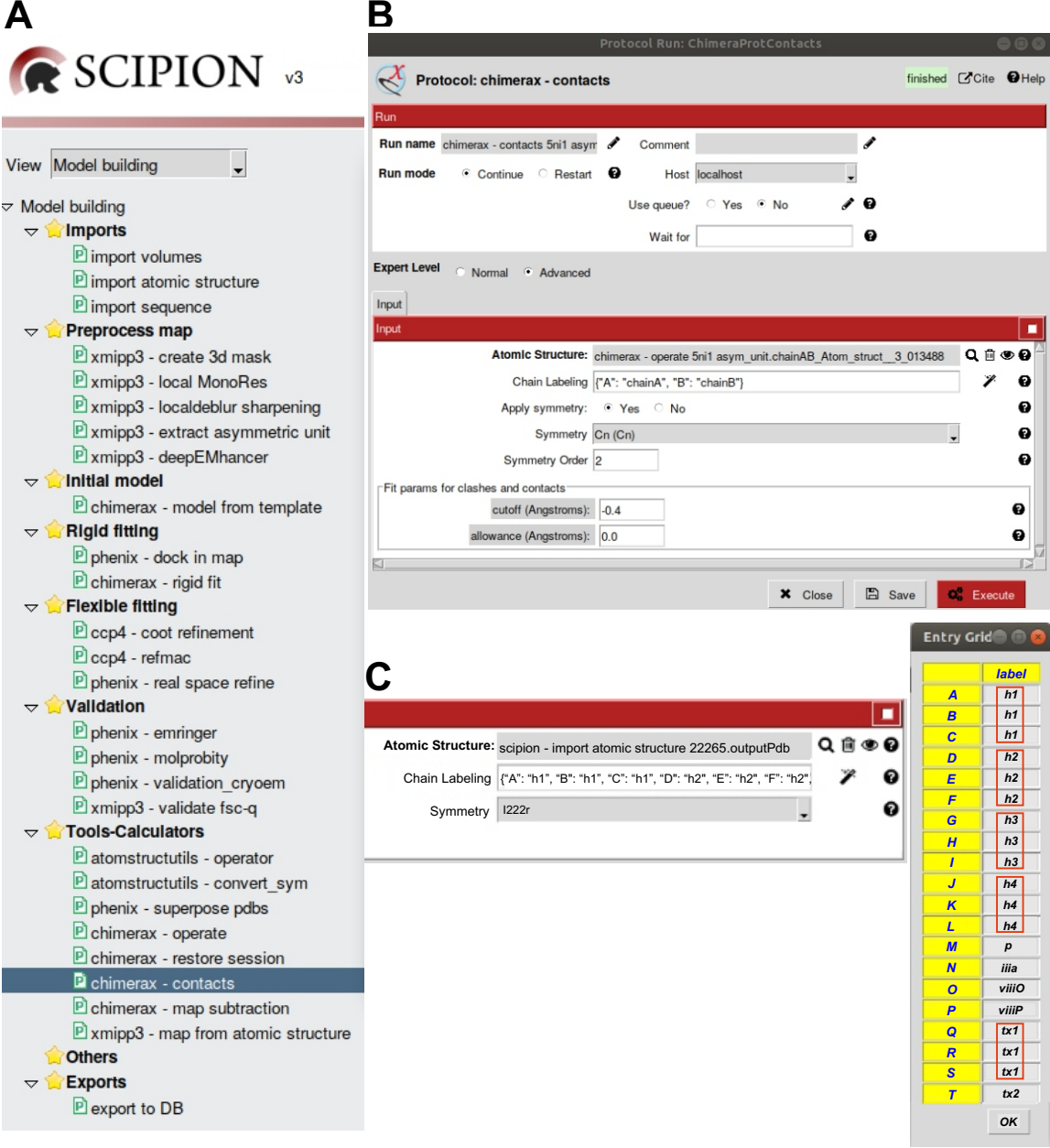
A
SCIPION v3
View Model building
Model building
Imports
import volumes
import atomic structure
import sequence
Preprocess map
xmipp3 - create 3d mask
xmipp3 - local MonoRes
xmipp3 - localdeblur sharpening
xmipp3 - extract asymmetric unit
xmipp3 - deepEMhancer
Initial model
chimerax - model from template
Rigid fitting
phenix - dock in map
chimerax - rigid fit
Flexible fitting
ccp4 - coot refinement
ccp4 - refmac
phenix - real space refine
Validation
phenix - emringer
phenix - molprobity
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
B
Protocol Run: ChimeraProtContacts
Protocol: chimerax - contacts
finished
Cite
Help
Run
Run name
chimerax - contacts 5ni1 asym
Comment
Run mode
Continue
Restart
Host
localhost
Use queue?
Yes
No
Wait for
Expert Level
Normal
Advanced
Input
Input
Atomic Structure:
chimerax - operate 5ni1 asym_unit.chainAB_Atom_struct__3_013488
Chain Labeling
{"A": "chainA", "B": "chainB"}
Apply symmetry:
Yes
No
Symmetry
Cn (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