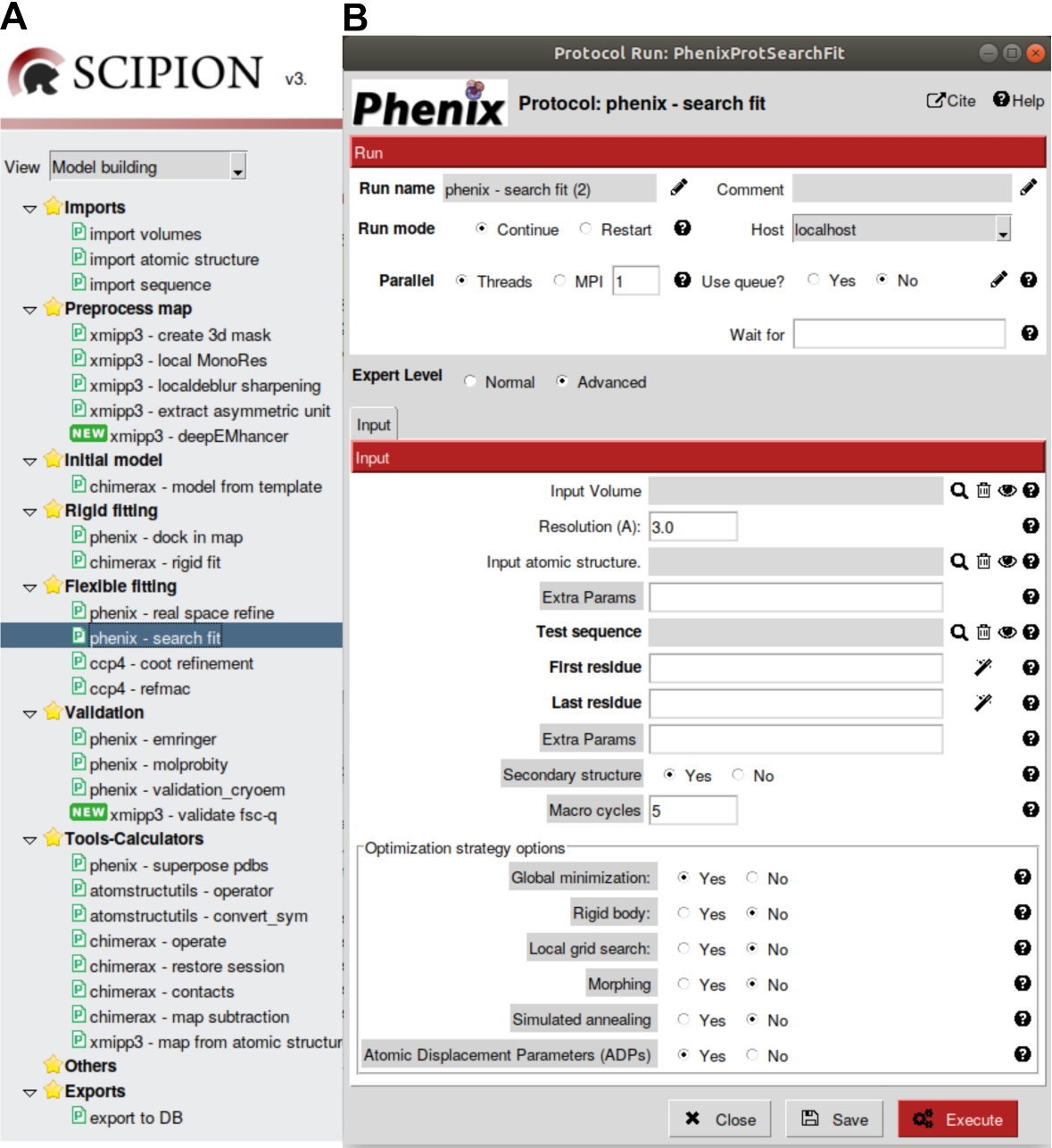
A
SCIPION v3.
View Model building
Imports
import volumes
import atomic structure
import sequence
Preprocess map
xmipp3 - create 3d mask
xmipp3 - local MonoRes
xmipp3 - localdeblur sharpening
xmipp3 - extract asymmetric unit
NEW xmipp3 - deepEMhancer
Initial model
chimerax - model from template
Rigid fitting
phenix - dock in map
chimerax - rigid fit
Flexible fitting
phenix - real space refine
phenix - search fit
ccp4 - coot refinement
ccp4 - refmac
Validation
phenix - emringer
phenix - molprobity
phenix - validation_cryoem
NEW xmipp3 - validate fsc-q
Tools-Calculators
phenix - superpose pdbs
atomstructutils - operator
atomstructutils - convert_sym
chimerax - operate
chimerax - restore session
chimerax - contacts
chimerax - map subtraction
xmipp3 - map from atomic structur
Others
Exports
export to DB
B
Protocol Run: PhenixProtSearchFit
Phenix
Protocol: phenix - search fit
Cite
Help
Run
Run name phenix - search fit (2)
Comment
Run mode Continue Restart
Host localhost
Parallel Threads MPI 1
Use queue? Yes No
Wait for
Expert Level Normal Advanced
Input
Input
Input Volume
Resolution (A): 3.0
Input atomic structure.
Extra Params
Test sequence
First residue
Last residue
Extra Params
Secondary structure Yes No
Macro cycles 5
Optimization strategy options
Global minimization: Yes No
Rigid body: Yes No
Local grid search: Yes No
Morphing Yes No
Simulated annealing Yes No
Atomic Displacement Parameters (ADPs) Yes No
Close
Save
Execute