Phenix

BERKELEY LAB

phenix.polder – short tutorial

A tool for calculating omit maps around atom selections by excluding the bulk solvent mask

Dorothee Liebschner

Example 1: Ligand density

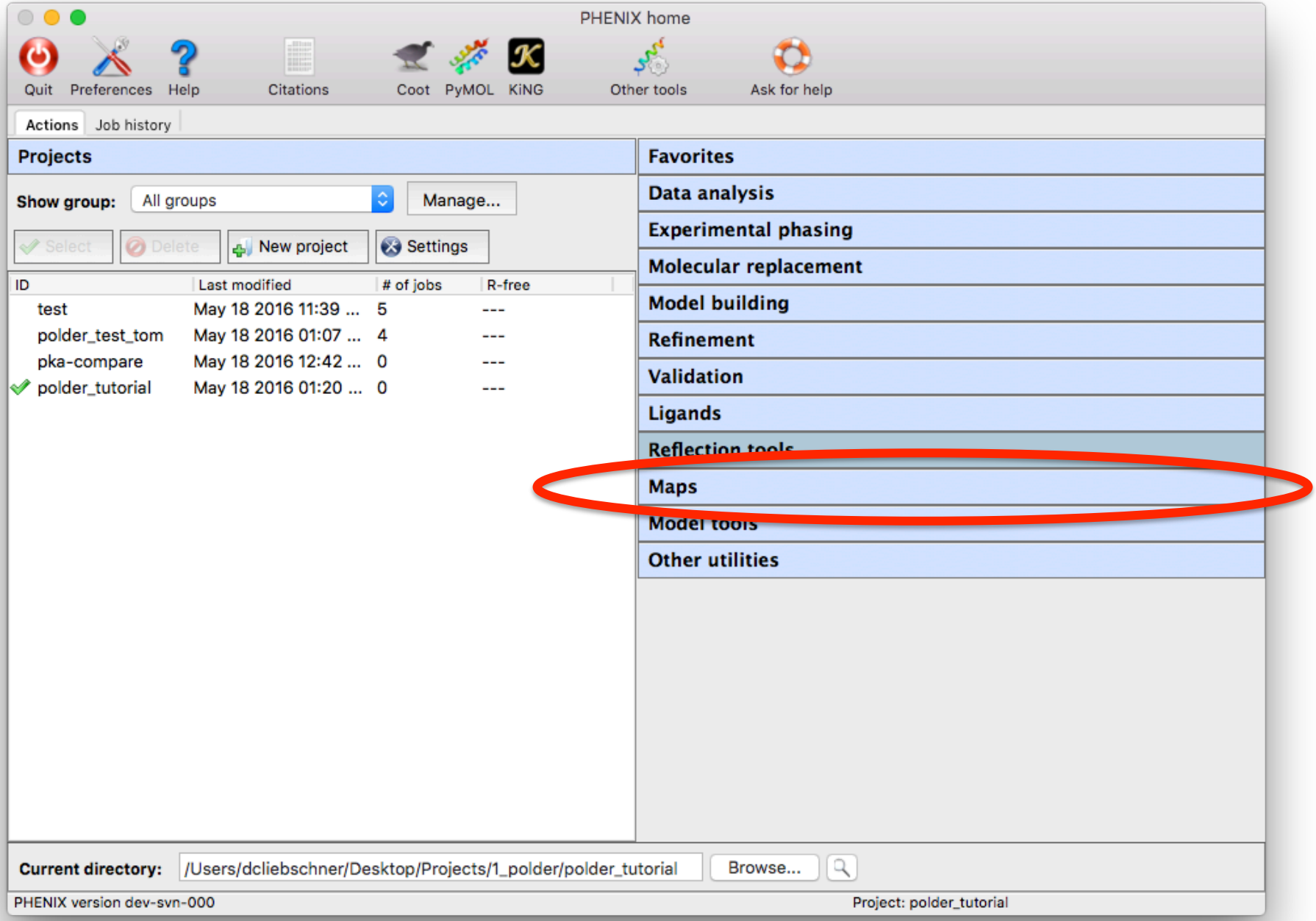
Goal: Learn how to calculate a polder map with the Phenix GUI

The first example of this tutorial shows how to compute a polder map
It shows improved density of a MES molecule in structure 1ABA.

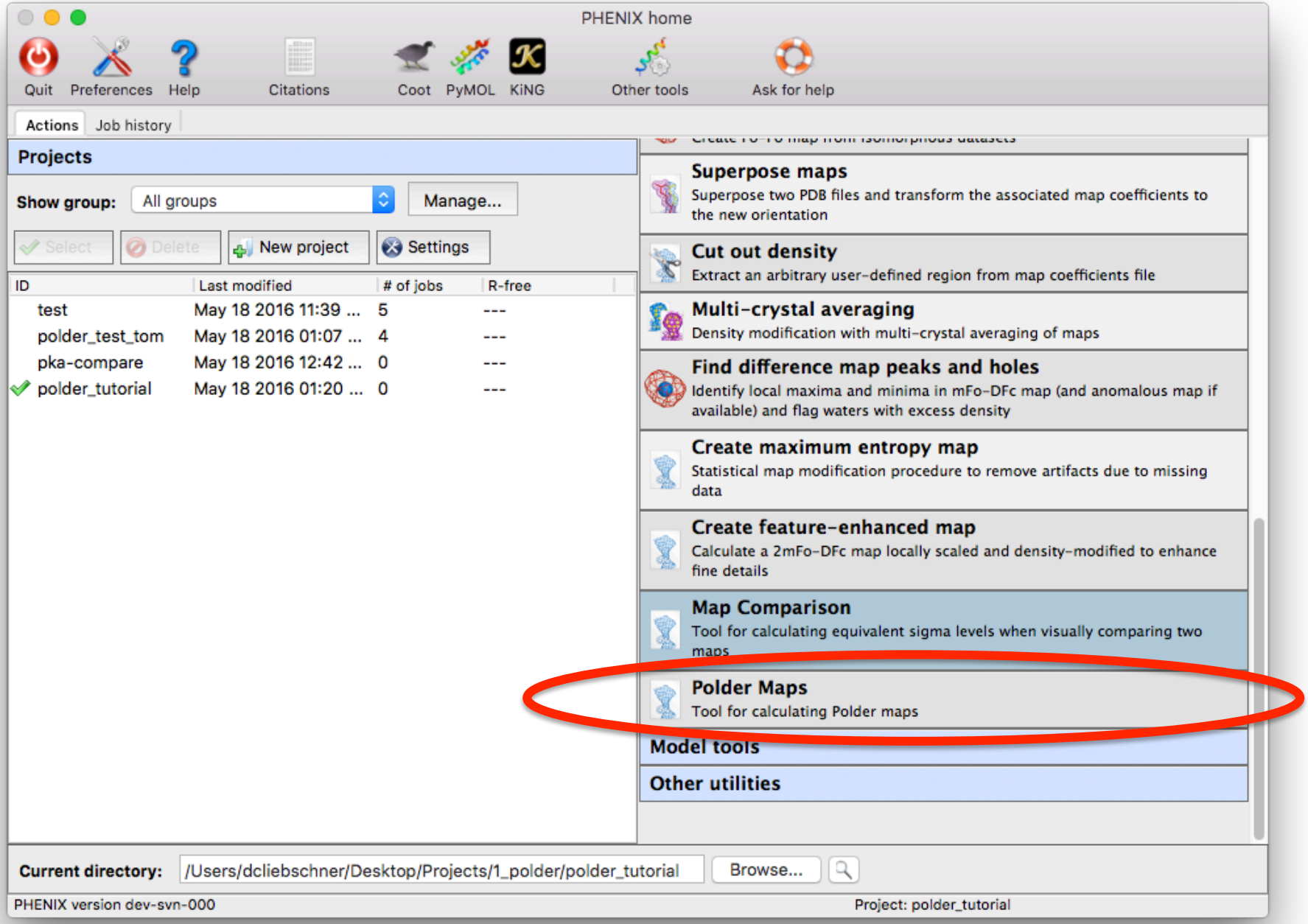
To reduce file size of the data, the resolution is limited to 2.5 Å.
As a practice, it can be useful to download the original data and to recalculate the examples from this tutorial.

Easy way to get data from the PDB via command line:

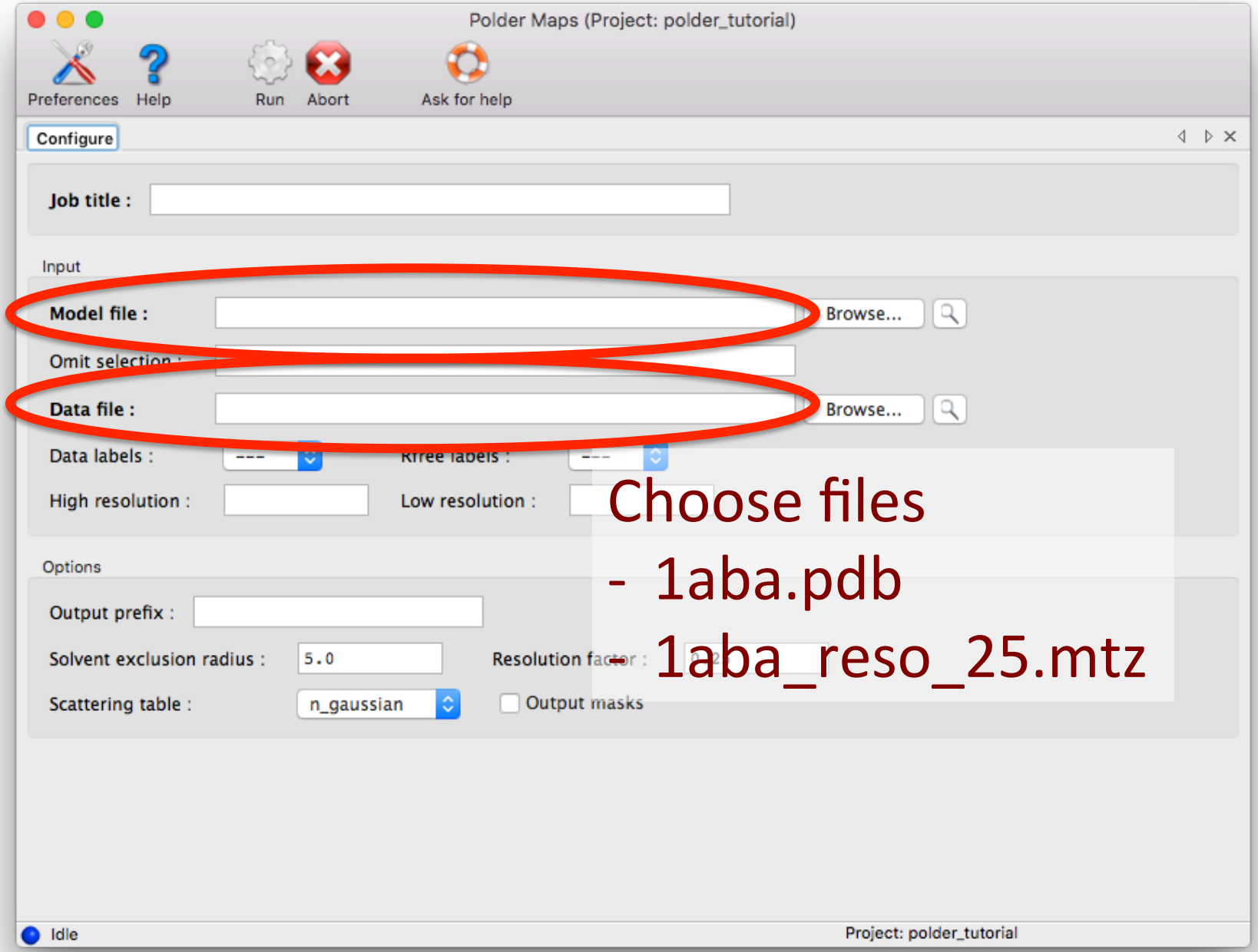
```
phenix.fetch_pdb --mtz 1aba
```


PHENIX home
Quit
Preferences
Help
Citations
Coot
PyMOL
KiNG
Other tools
Ask for help
Actions
Job history
Projects
Show group:
All groups
Manage...
Select
Delete
New project
Settings
ID
Last modified
# of jobs
R-free
test
May 18 2016 11:39 ...
5
---
polder_test_tom
May 18 2016 01:07 ...
4
---
pka-compare
May 18 2016 12:42 ...
0
---
polder_tutorial
May 18 2016 01:20 ...
0

Favorites
Data analysis
Experimental phasing
Molecular replacement
Model building
Refinement
Validation
Ligands
Reflection tools
Maps
Model tools
Other utilities
Current directory:
/Users/dcliebschner/Desktop/Projects/1_polder/polder_tutorial
Browse...
PHENIX version dev-svn-000
Project: polder_tutorial

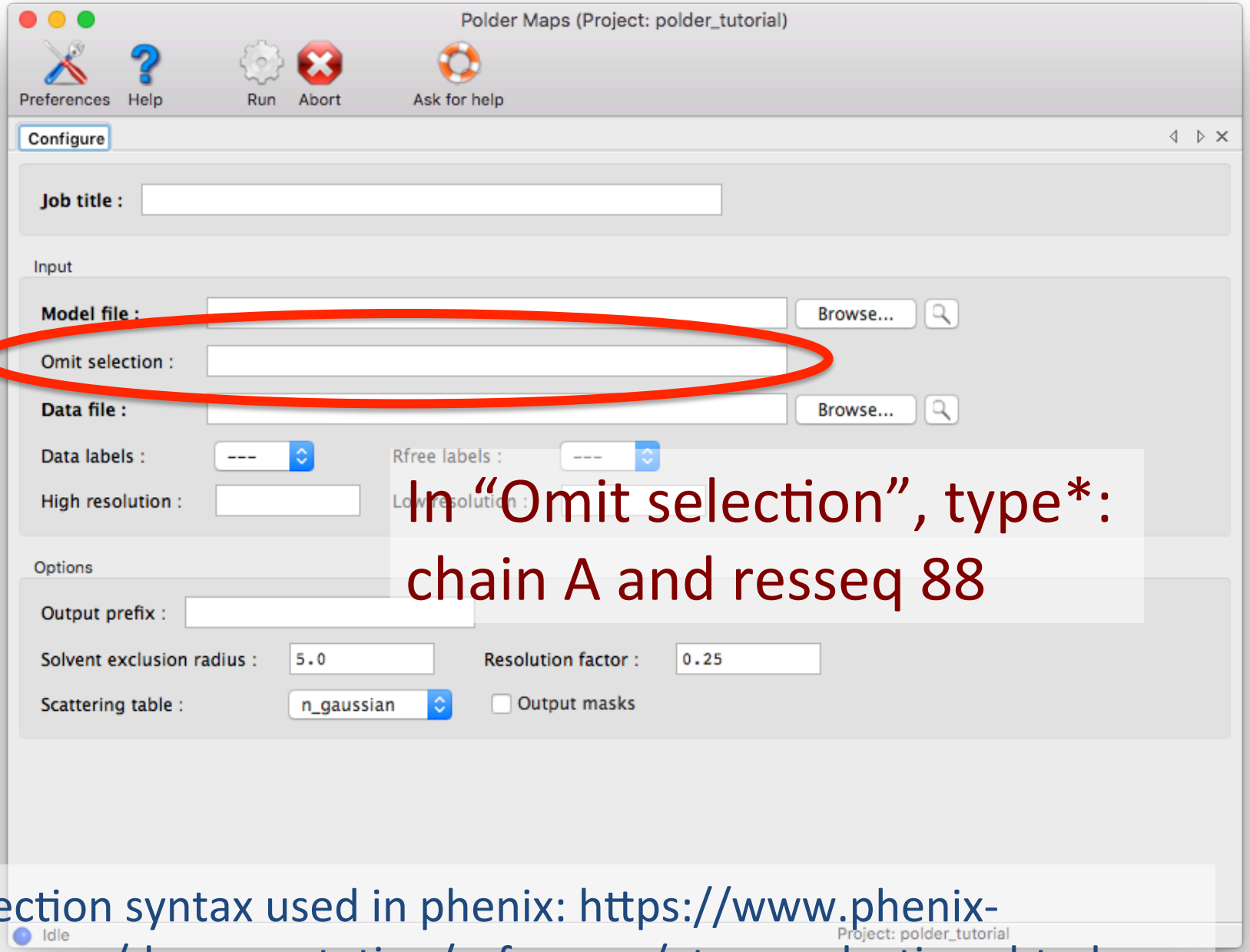

PHENIX home
Quit
Preferences
Help
Citations
Coot
PyMOL
KiNG
Other tools
Ask for help
Actions
Job history
Projects
Show group:
All groups
Manage...
Select
Delete
New project
Settings
ID
Last modified
# of jobs
R-free
test
May 18 2016 11:39 ...
5
---
polder_test_tom
May 18 2016 01:07 ...
4
---
pka-compare
May 18 2016 12:42 ...
0
---
polder_tutorial
May 18 2016 01:20 ...
0

Superpose maps
Superpose two PDB files and transform the associated map coefficients to the new orientation
Cut out density
Extract an arbitrary user-defined region from map coefficients file
Multi-crystal averaging
Density modification with multi-crystal averaging of maps
Find difference map peaks and holes
Identify local maxima and minima in mFo-DFc map (and anomalous map if available) and flag waters with excess density
Create maximum entropy map
Statistical map modification procedure to remove artifacts due to missing data
Create feature-enhanced map
Calculate a 2mFo-DFc map locally scaled and density-modified to enhance fine details
Map Comparison
Tool for calculating equivalent sigma levels when visually comparing two maps
Polder Maps
Tool for calculating Polder maps
Model tools
Other utilities
Current directory:
/Users/dcliebschner/Desktop/Projects/1_polder/polder_tutorial
Browse...
PHENIX version dev-svn-000
Project: polder_tutorial


Polder Maps (Project: polder_tutorial)
Preferences
Help
Run
Abort
Ask for help
Configure
Job title :
Input
Model file :
Browse...
Omit selection :
Data file :
Browse...
Data labels :

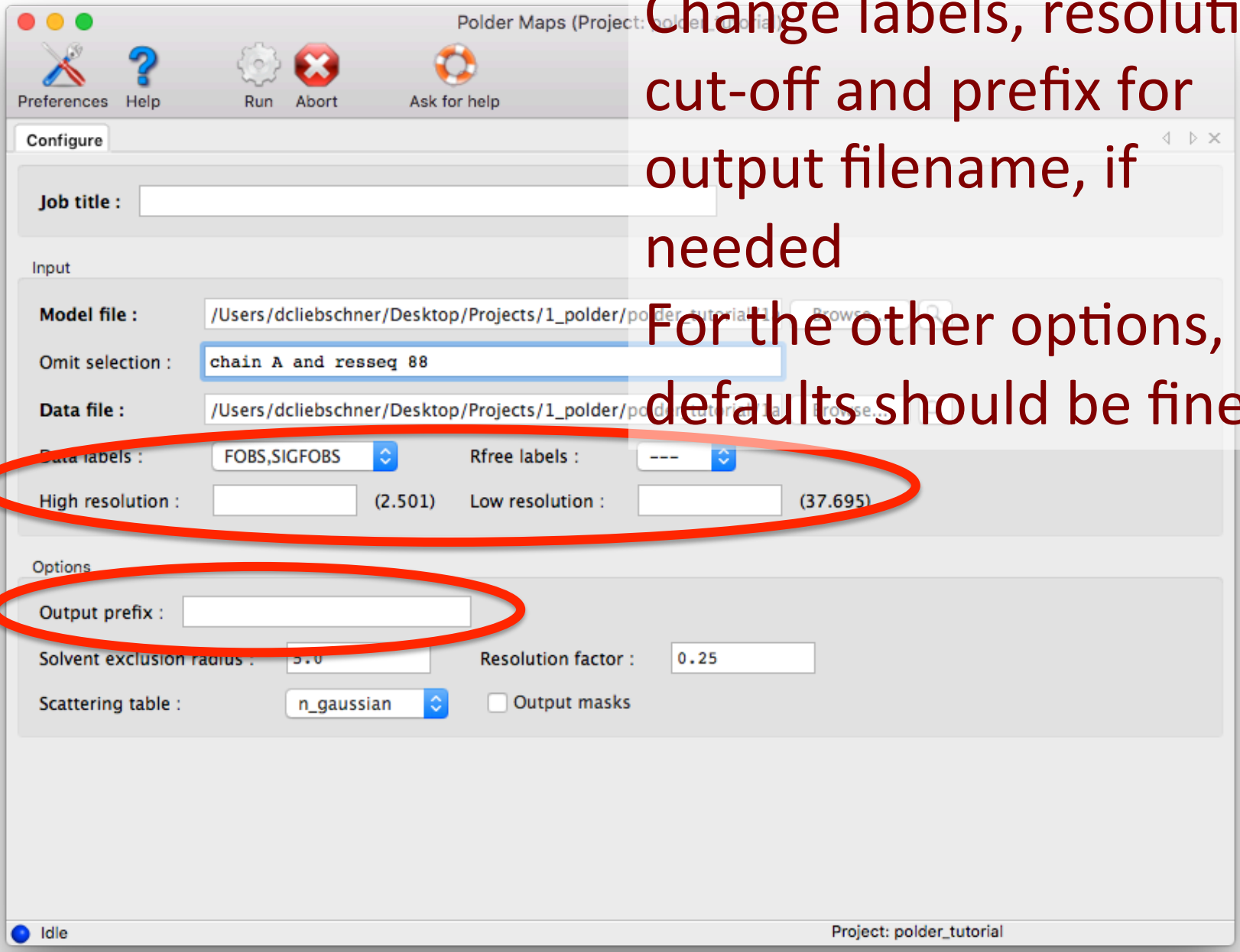
Rfree labels :

High resolution :
Low resolution :
Options
Output prefix :
Solvent exclusion radius :
5.0
Resolution factor :
Scattering table :
n_gaussian
Output masks
Idle
Project: polder_tutorial
Choose files
- 1aba.pdb
1aba_reso_25.mtz



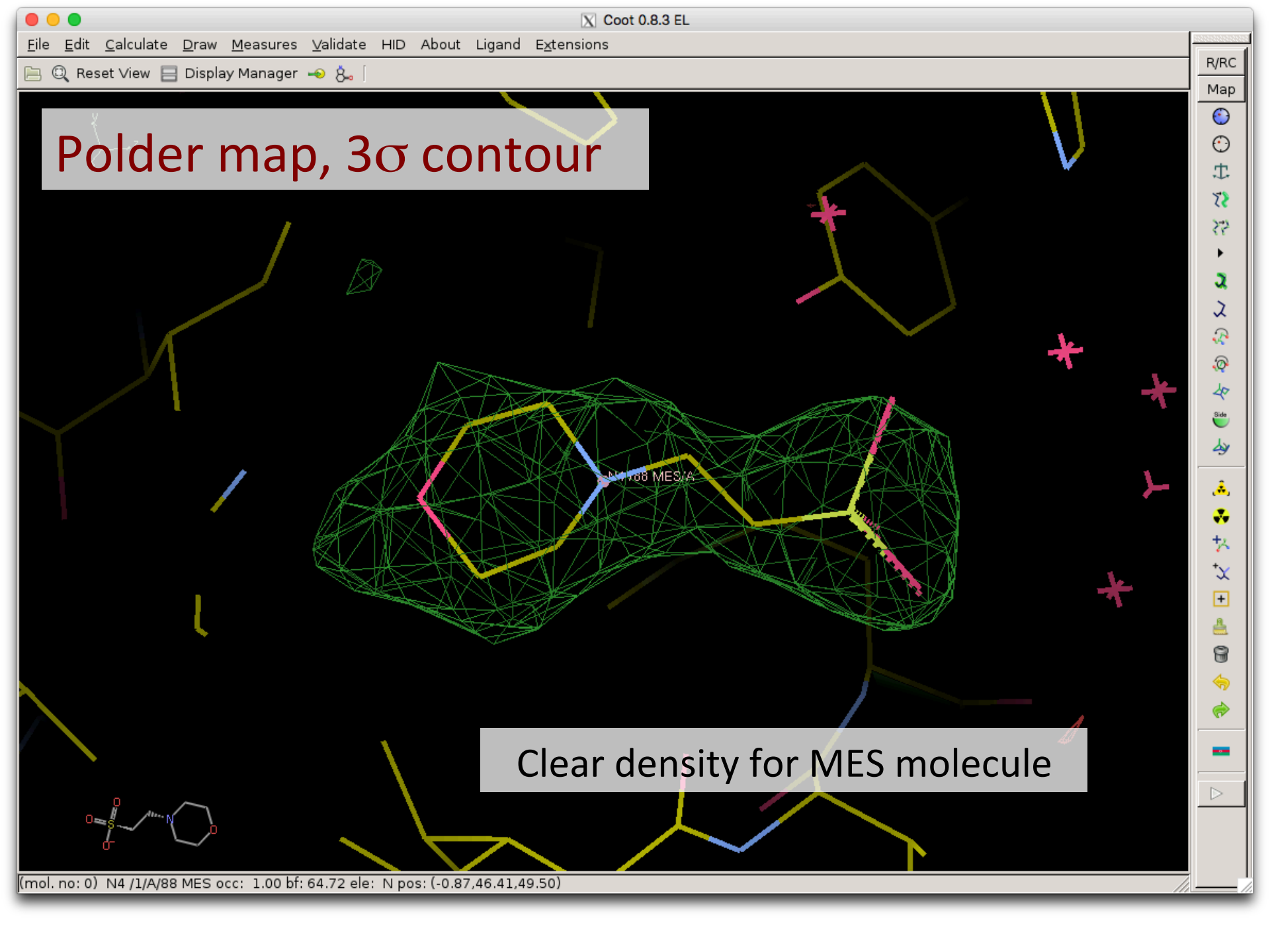
In "Omit selection", type*: chain A and resseq 88

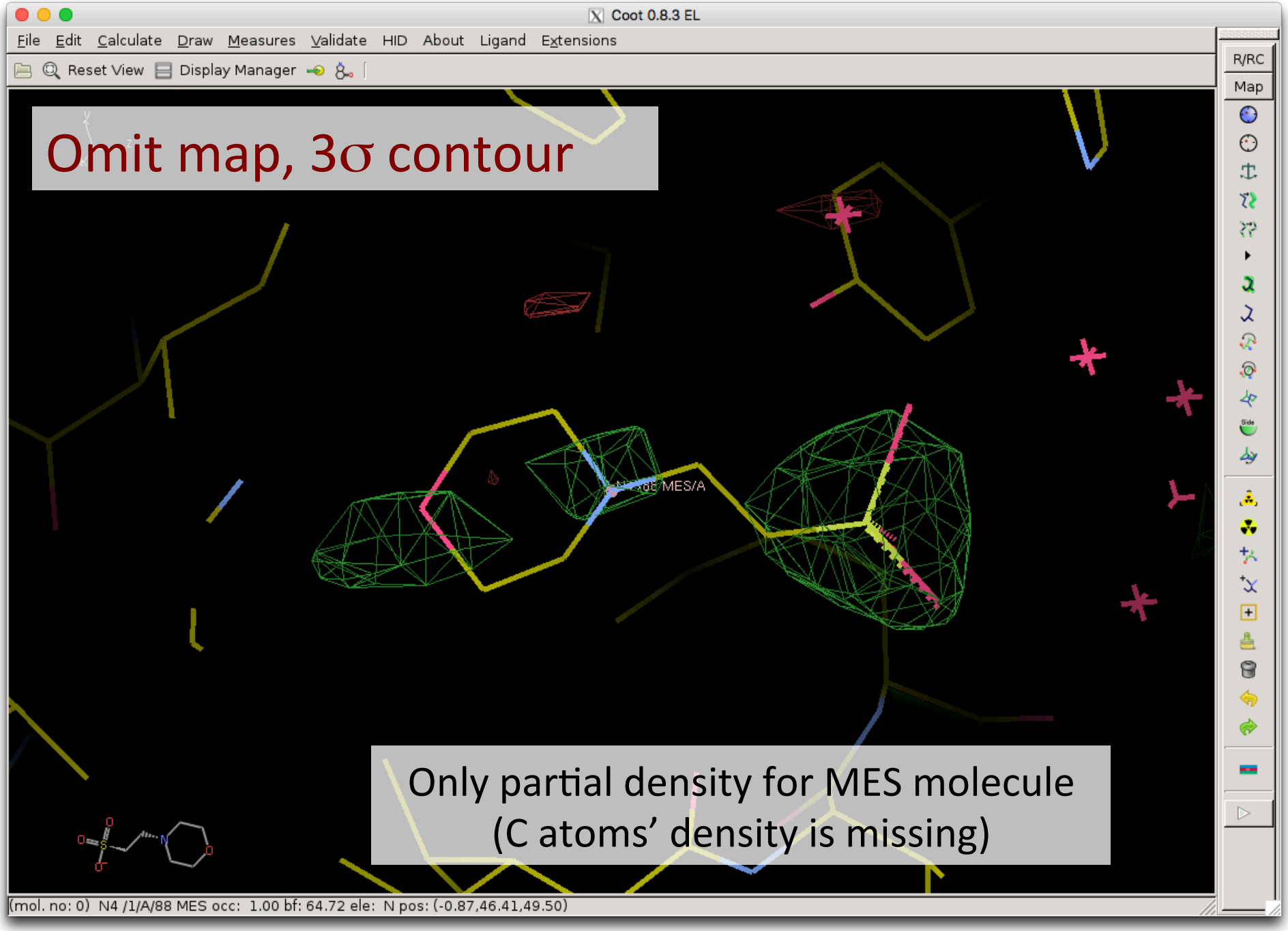
*Selection syntax used in phenix: https://www.phenix-online.org/documentation/reference/atom_selections.html



Change labels, resolution cut-off and prefix for output filename, if needed

For the other options, defaults should be fine.


Coot 0.8.3 EL
File Edit Calculate Draw Measures Validate HID About Ligand Extensions
Reset View
Display Manager
R/RC
Map
Polder map, 3σ contour
Clear density for MES molecule
(mol. no: 0) N4 /1/A/88 MES occ: 1.00 bf: 64.72 ele: N pos: (-0.87,46.41,49.50)


Coot 0.8.3 EL
File Edit Calculate Draw Measures Validate HID About Ligand Extensions
Reset View
Display Manager
R/RC
Map
Omit map, 3σ contour
MES/A
Only partial density for MES molecule
(C atoms' density is missing)
(mol. no: 0) N4 /1/A/88 MES occ: 1.00 bf: 64.72 ele: N pos: (-0.87,46.41,49.50)

Example 1: Side chain density

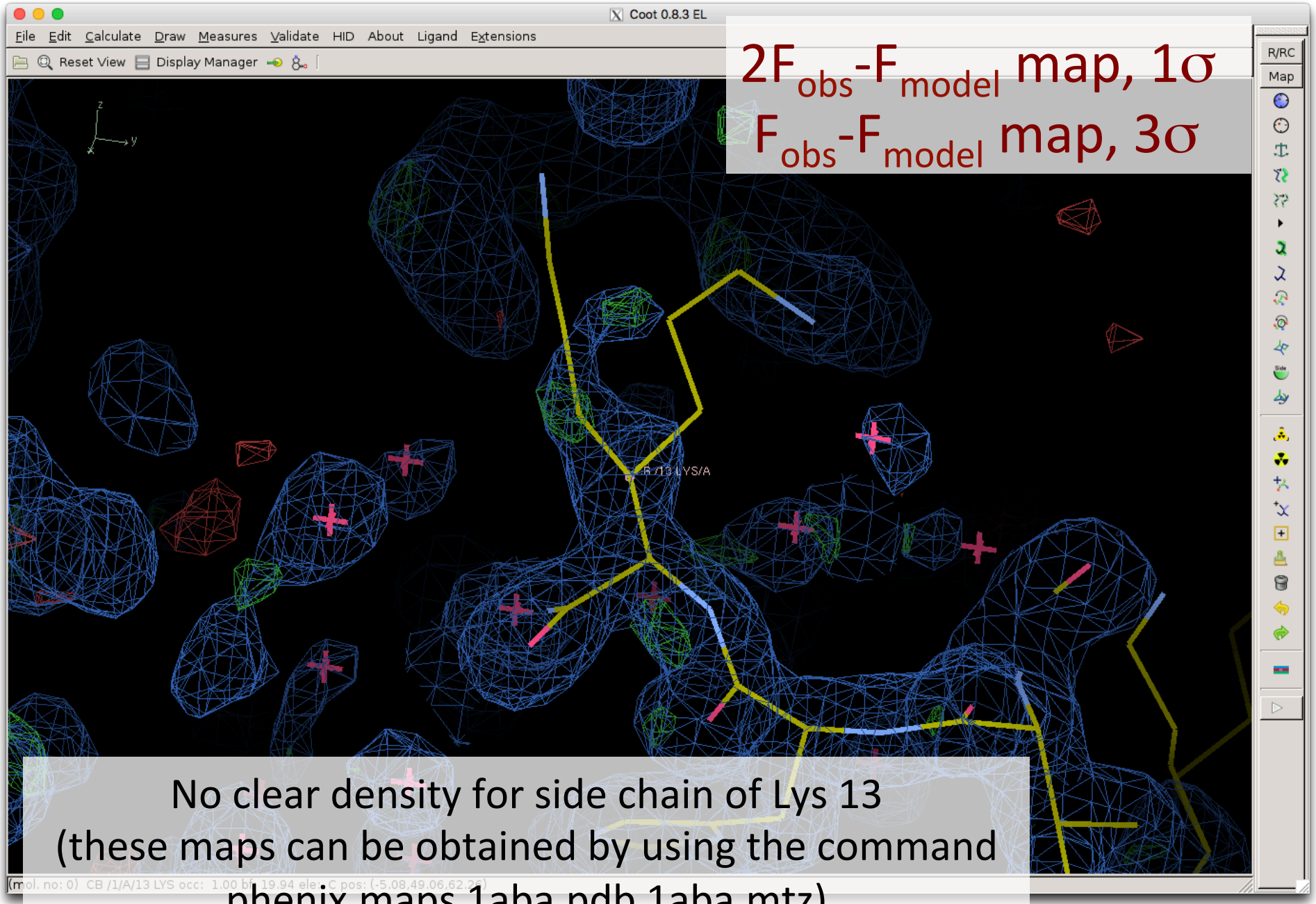
Goal: Calculate polder map for a residue

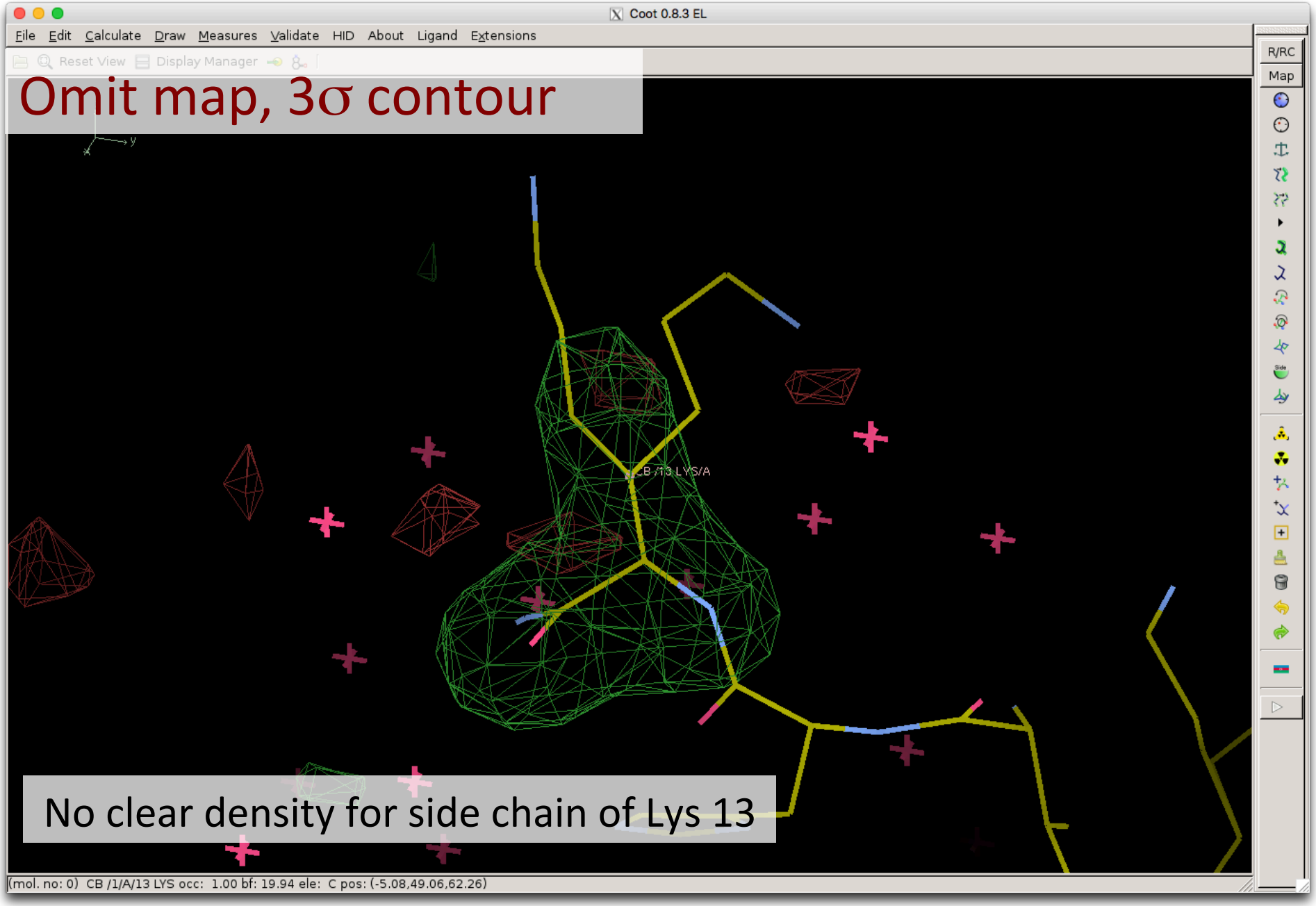
Side chains density of residues located at the surface of the protein (i.e. which are exposed to solvent), are often disordered. It can be therefore difficult to model their orientation.

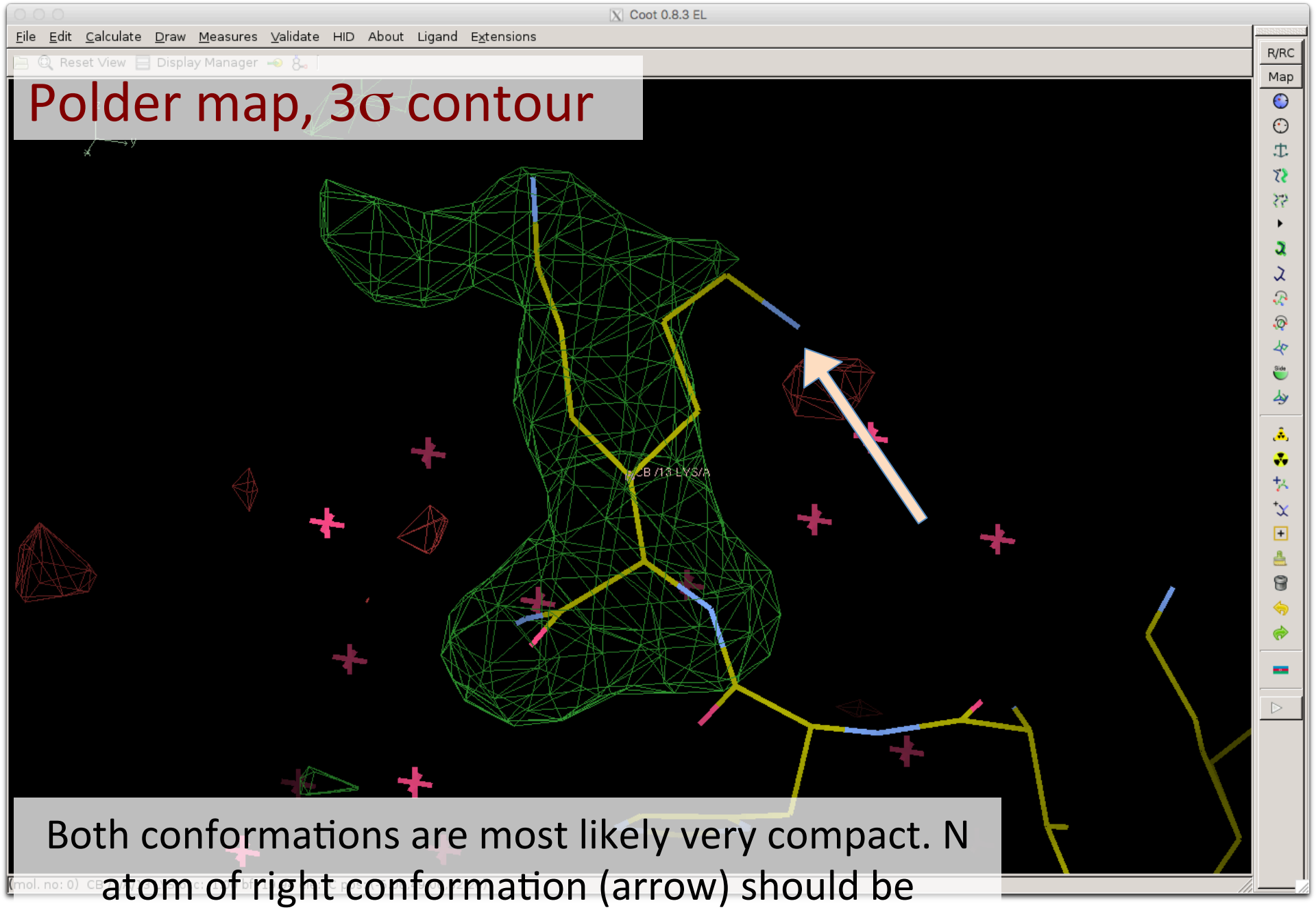
With the same files (i.e. structure + data from 1ABA), calculate a polder map using the following selection:

chain A and resseq 13

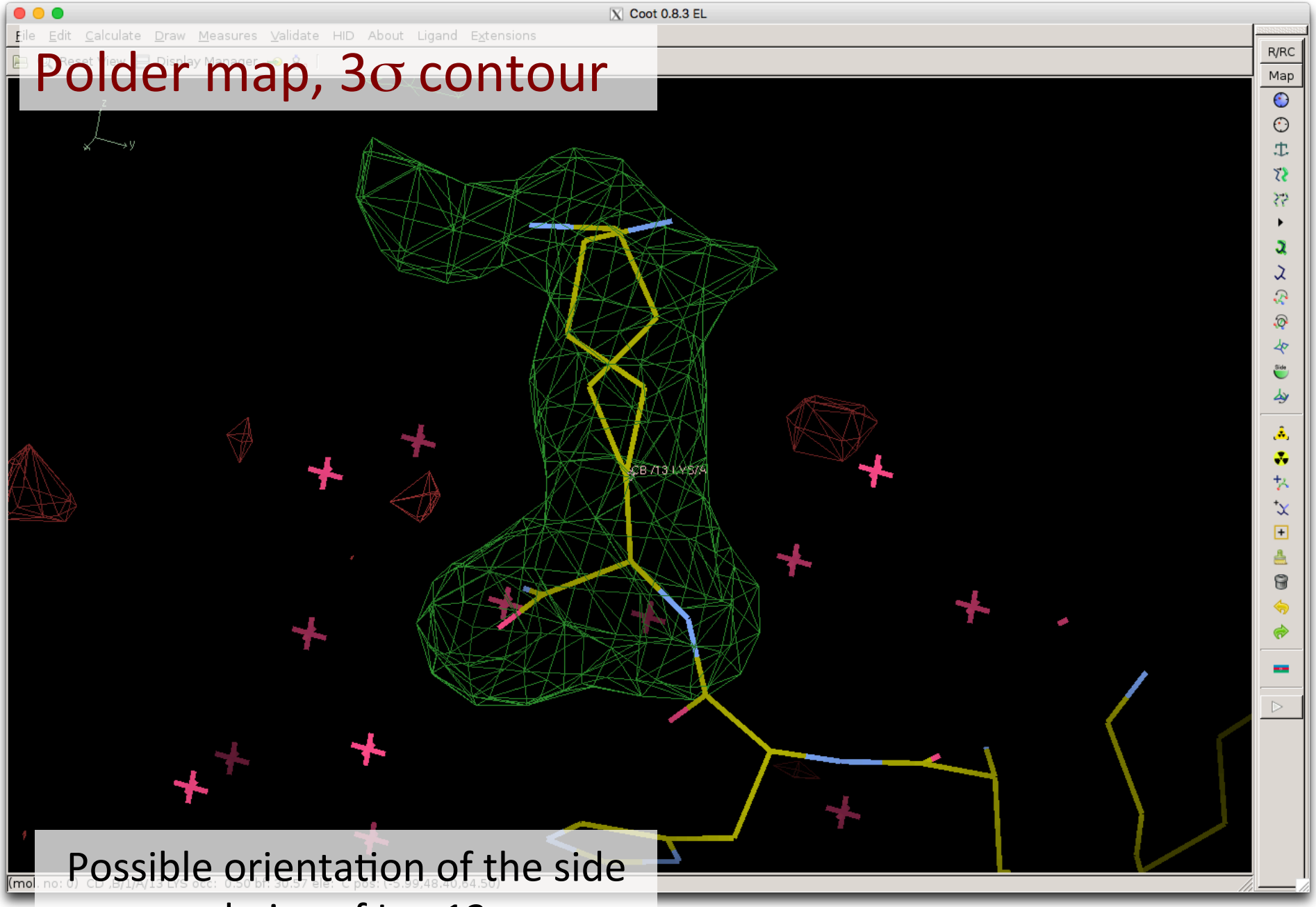
Then open the polder and the omit maps in COOT.


Coot 0.8.3 EL
File Edit Calculate Draw Measures Validate HID About Ligand Extensions
Reset View
Display Manager
R/RC
Map
$2F_{obs}$-F_{model} map, 1σ
F_{obs}-F_{model} map, 3σ
B/13 LYS/A
No clear density for side chain of Lys 13
(these maps can be obtained by using the command
phenix.maps 1aba.pdb 1aba.mtz)


Coot 0.8.3 EL
File Edit Calculate Draw Measures Validate HID About Ligand Extensions
Reset View
Display Manager
R/RC
Map
Omit map, 3σ contour
CB /13 LYS/A
No clear density for side chain of Lys 13
(mol. no: 0) CB /1/A/13 LYS occ: 1.00 bf: 19.94 ele: C pos: (-5.08,49.06,62.26)



Both conformations are most likely very compact. N atom of right conformation (arrow) should be modeled inside the difference density.


Coot 0.8.3 EL
File Edit Calculate Draw Measures Validate HID About Ligand Extensions
R/RC
Map
Polder map, 3σ contour
Possible orientation of the side chains of Lys 13