Tutorial
Refinement in Phenix
with advanced (low resolution) restraints

Oleg V Sobolev

General considerations

Figure out proper restraints:

- Do I have a source of information?
- Was my map symmetrized?
- Does my model have NCS?
- Do I have good enough data to reasonably expect to see difference in NCS copies?

Tell Phenix to establish restraints:

- Click in the GUI
- Prepare (save) parameter file for later use

Make sure the restraints are established

- Check the proper locations in .log or .geo file.

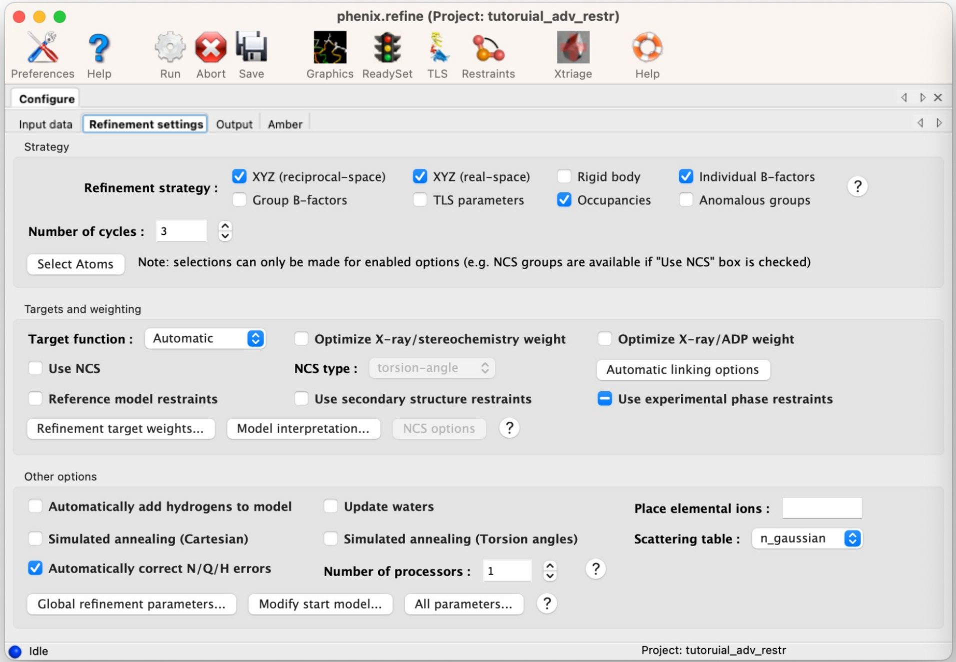
Restraints for low resolution

- Secondary structure
- NCS
  - Torsion (X-ray only)
  - Cartesian (=global) (X-ray only)
  - Constraints
- Reference model
  - Torsion
  - Coordinate (=cartesian)
- Ramachandran

Both phenix.refine and phenix.real_space_refine use (almost) the same machinery to establish restraints

Difference between phenix.refine and phenix.real_space_refine

phenix.refine



Strategy

Refinement strategy : ☑ XYZ (reciprocal-space) ☑ XYZ (real-space) ☐ Rigid body ☑ Individual B-factors ☐ Group B-factors ☐ TLS parameters ☑ Occupancies ☐ Anomalous groups ?

Number of cycles : 3

Select Atoms Note: selections can only be made for enabled options (e.g. NCS groups are available if "Use NCS" box is checked)

Targets and weighting

Target function : Automatic ☐ Optimize X-ray/stereochemistry weight ☐ Optimize X-ray/ADP weight

☐ Use NCS **NCS type :** torsion-angle Automatic linking options

☐ Reference model restraints ☐ Use secondary structure restraints ☐ Use experimental phase restraints

Refinement target weights... Model interpretation... NCS options ?

Other options

☐ Automatically add hydrogens to model ☐ Update waters **Place elemental ions :**

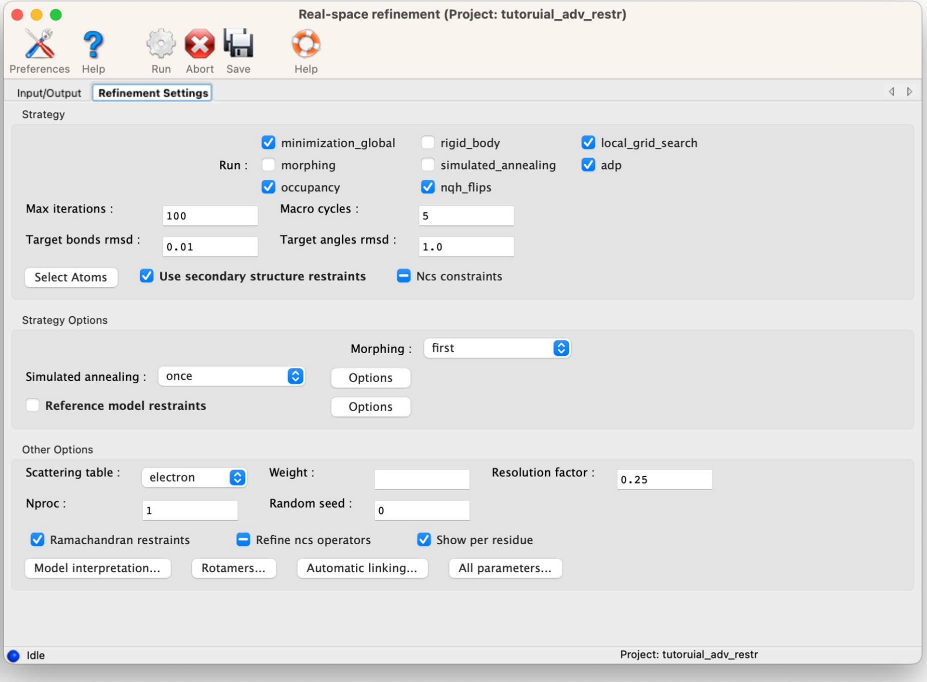
☐ Simulated annealing (Cartesian) ☐ Simulated annealing (Torsion angles) **Scattering table :** n_gaussian

☑ Automatically correct N/Q/H errors **Number of processors :** 1 ?

Global refinement parameters... Modify start model... All parameters... ?

Idle Project: tutoruial_adv_restr

phenix.real_space_refine



Strategy

Run : ☑ minimization_global ☐ rigid_body ☑ local_grid_search ☐ morphing ☐ simulated_annealing ☑ adp ☑ occupancy ☑ nqh_flips

Max iterations : 100 Macro cycles : 5

Target bonds rmsd : 0.01 Target angles rmsd : 1.0

Select Atoms ☑ Use secondary structure restraints ☐ Ncs constraints

Strategy Options

Morphing : first

Simulated annealing : once Options

☐ Reference model restraints Options

Other Options

Scattering table : electron Weight : Resolution factor : 0.25

Nproc : 1 Random seed : 0

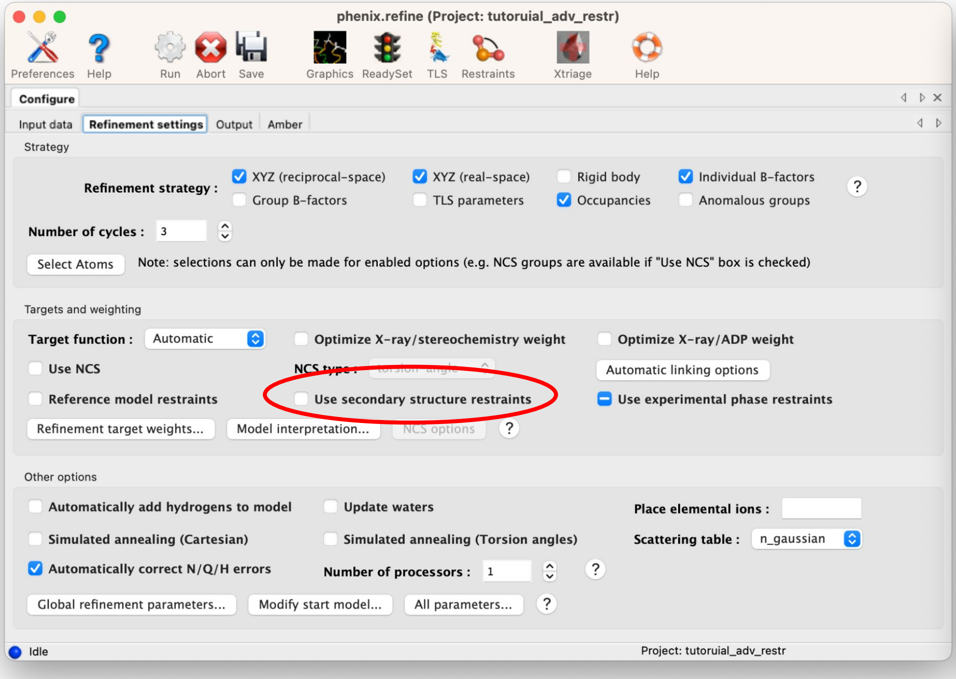
☑ Ramachandran restraints ☐ Refine ncs operators ☑ Show per residue

Model interpretation... Rotamers... Automatic linking... All parameters...

Idle Project: tutoruial_adv_restr

phenix.refine vs phenix.real_space_refine: secondary structure

phenix.refine



phenix.refine (Project: tutoruial_adv_restr)

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Number of cycles : 3

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Targets and weighting

Target function : Automatic
☐ Optimize X-ray/stereochemistry weight
☐ Optimize X-ray/ADP weight
☐ Use NCS
NCS type : torsion angle
☐ Reference model restraints
☐ Use secondary structure restraints
⊟ Use experimental phase restraints

Other options

☐ Automatically add hydrogens to model
☐ Update waters
Place elemental ions :
☐ Simulated annealing (Cartesian)
☐ Simulated annealing (Torsion angles)
Scattering table : n_gaussian
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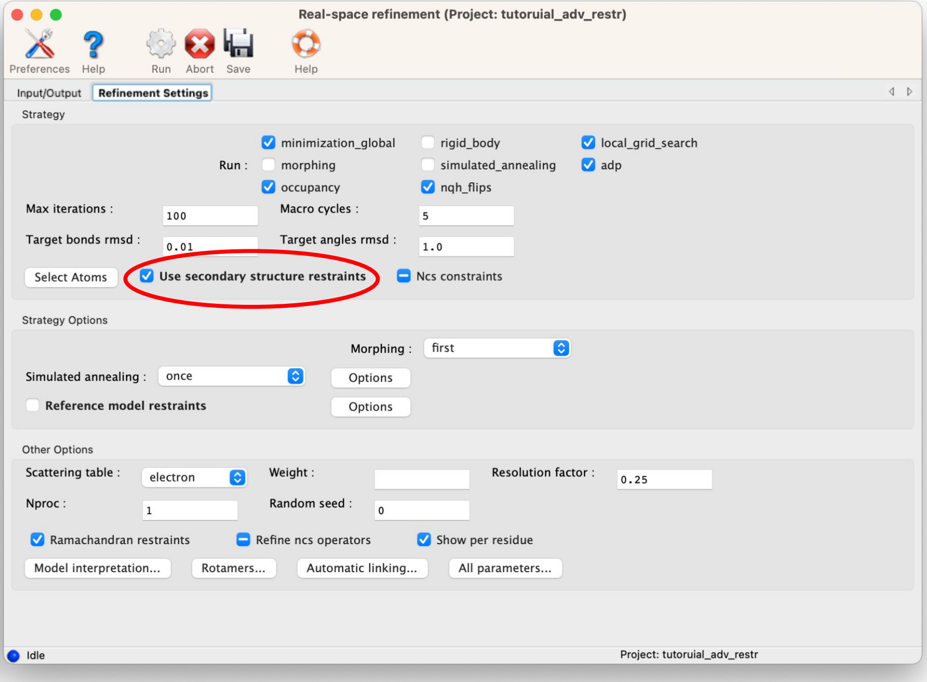
Idle
Project: tutoruial_adv_restr

phenix.real_space_refine



Real-space refinement (Project: tutoruial_adv_restr)

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Max iterations : 100
Macro cycles : 5
Target bonds rmsd : 0.01
Target angles rmsd : 1.0
☑ Use secondary structure restraints
⊟ Ncs constraints

Strategy Options

Morphing : first
Simulated annealing : once
☐ Reference model restraints

Other Options

Scattering table : electron
Weight :
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Nproc : 1
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☑ Ramachandran restraints
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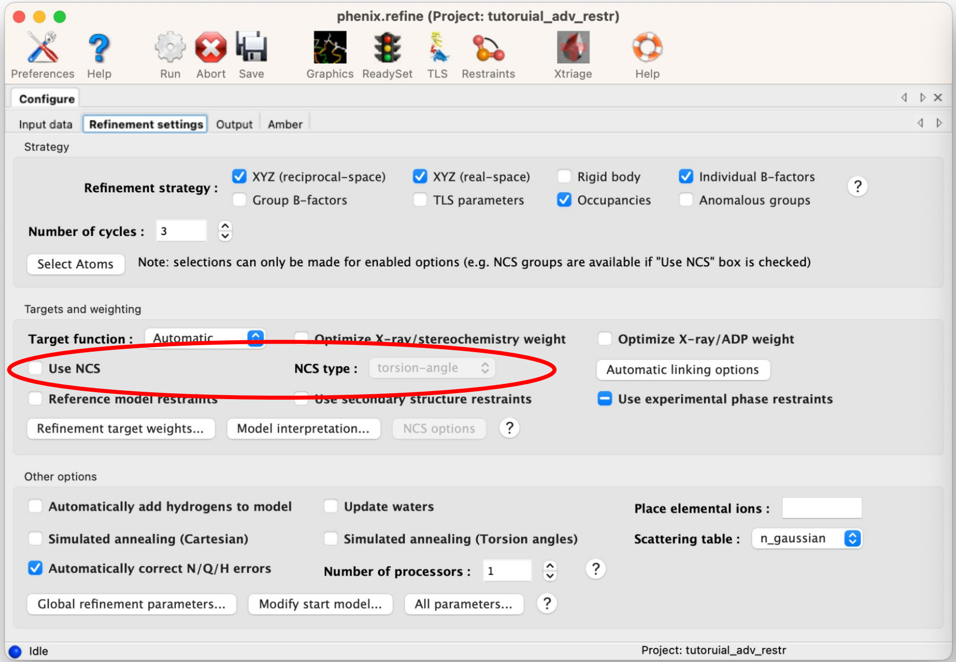
☑ Show per residue

Idle
Project: tutoruial_adv_restr

phenix.refine vs phenix.real_space_refine: NCS

phenix.refine



phenix.refine (Project: tutoruial_adv_restr)

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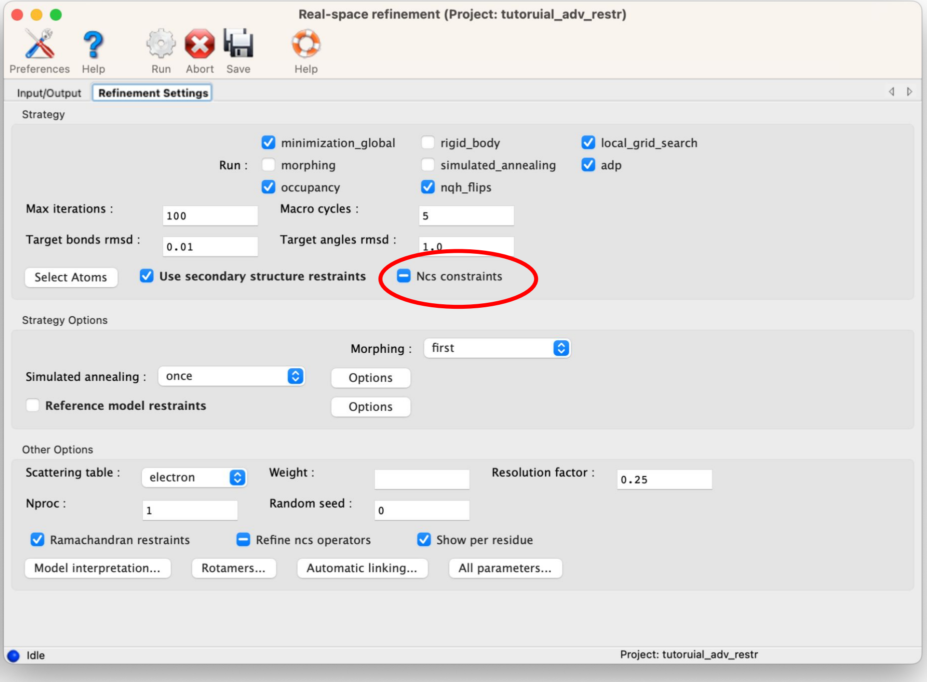

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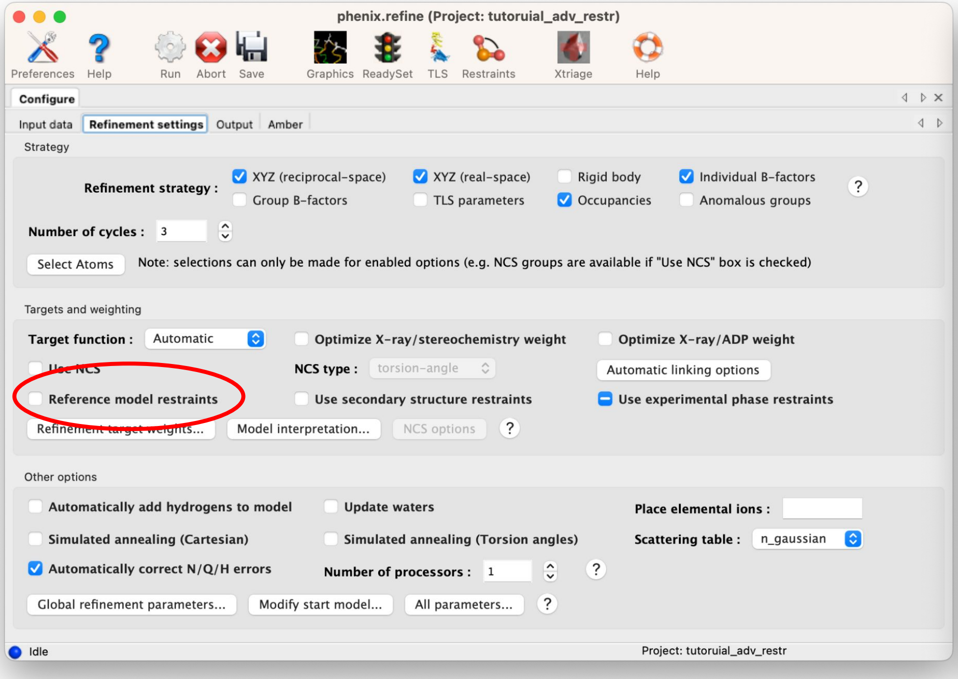
NCS - only constraints in RSR

phenix.refine vs phenix.real_space_refine: reference model

phenix.refine



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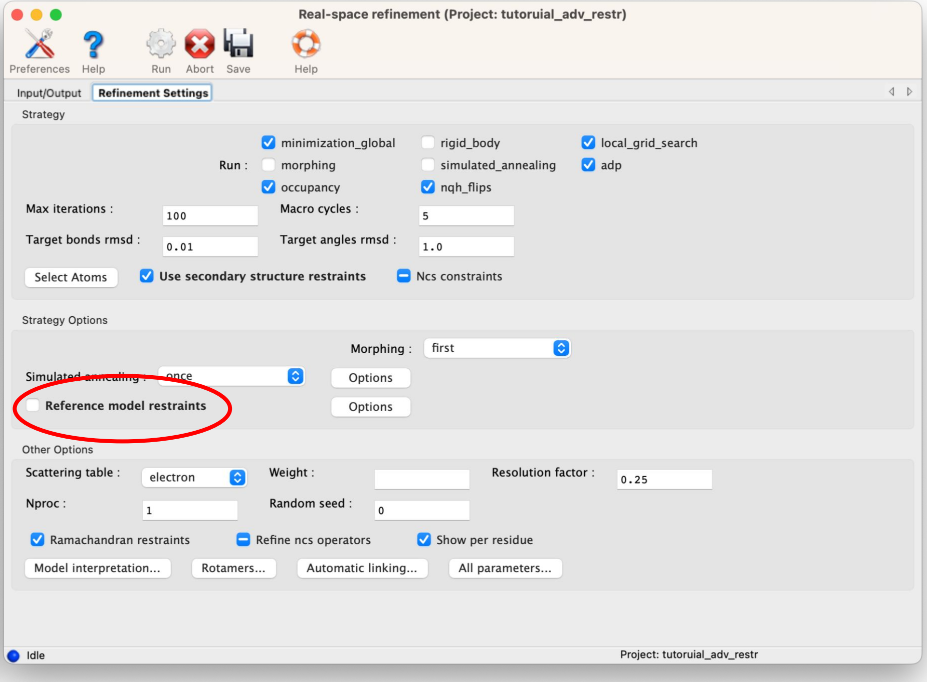

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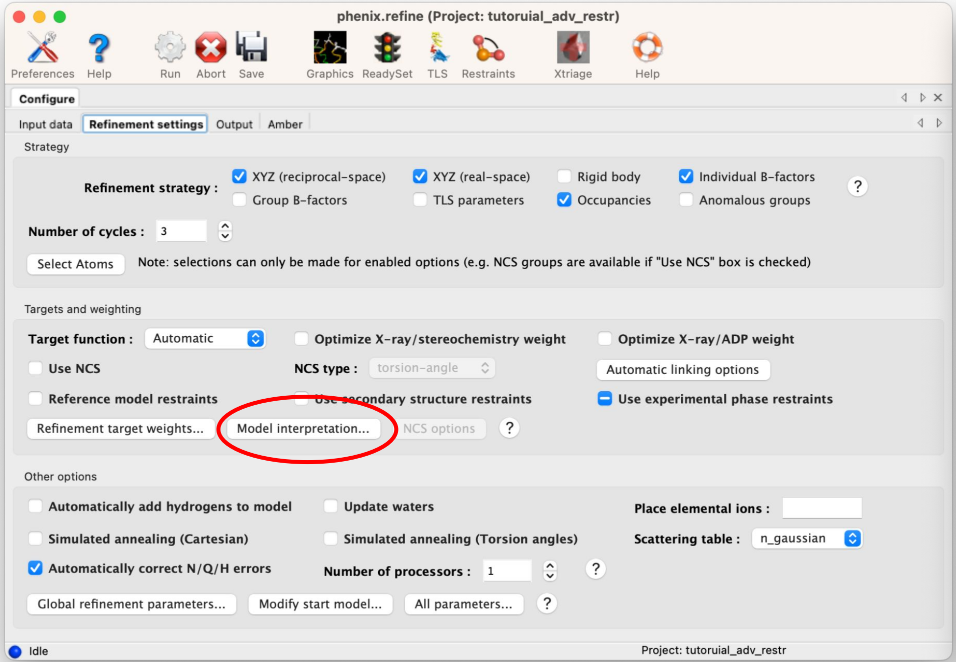
Project: tutoruial_adv_restr

phenix.refine vs phenix.real_space_refine: ramachandran

phenix.refine



phenix.refine (Project: tutoruial_adv_restr)

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Other options

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Place elemental ions :

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☐ **Simulated annealing (Torsion angles)**

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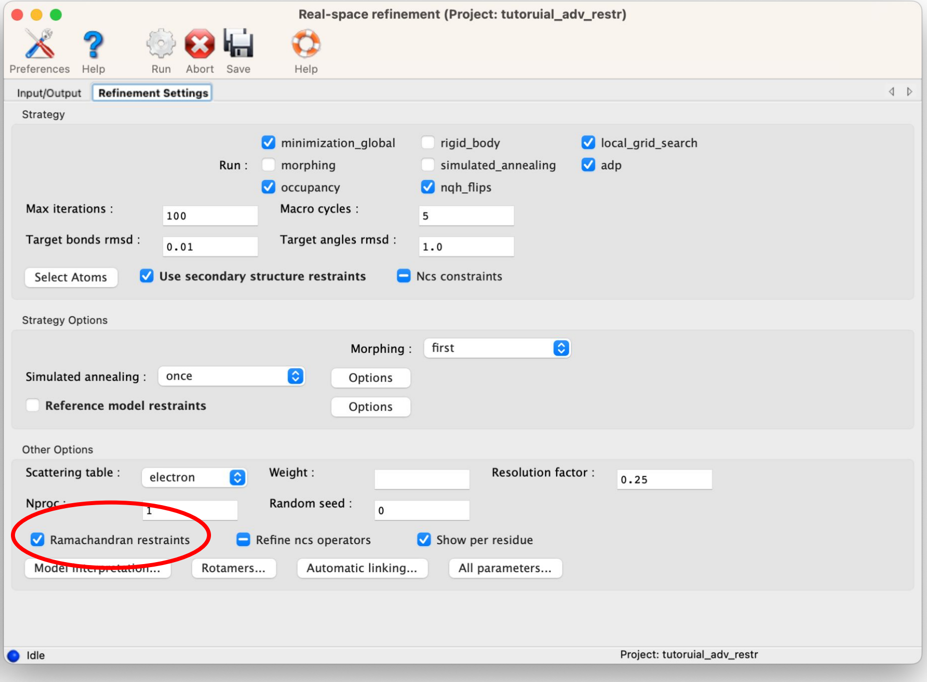
Project: tutoruial_adv_restr

phenix.real_space_refine



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☑ Ramachandran restraints

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Thank you.