# Tutorial Refinement in Phenix with advanced (low resolution) restraints

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## **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

phenix.refine (Project: tutoruial_adv_restr)	Real-space refinement (Project: tutoruial_adv_restr)
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Input data Refinement settings Output Amber	d b Strategy
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## phenix.refine vs phenix.real\_space\_refine: secondary structure

phenix.refine

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Idle     Project: tutoruial_adv_restr	Idle     Project: tutoruial_adv_restr		

## phenix.refine vs phenix.real\_space\_refine: NCS

#### phenix.refine

#### phenix.real\_space\_refine

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Refinement strategy :	i body 💟 Individual B-factors upancies Anomalous groups ?	Run :       morphing       simulated_annealing       Q adp         Q occupancy       Q nqh_flips         Max iterations :       100       Macro cycles :       5         Target bonds rmsd :       0.01       Target angles rmsd :       1.0         Select Atoms       V Use secondary structure restraints       Ncs constraints
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NCS - only constraints in RSR

## phenix.refine vs phenix.real\_space\_refine: reference model

#### phenix.refine

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## phenix.refine vs phenix.real\_space\_refine: ramachandran

#### phenix.refine

phenix.refine (Project: tutoruial_adv_restr)		Real-space refinement (Project: tutoruial_adv_restr)
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Automatically add hydrogens to model Update waters Pla	ce elemental ions :	Nproc : 1 Random seed : 0
Simulated annealing (Cartesian) Simulated annealing (Torsion angles) Sca	attering table : n_gaussian 📀	🛛 🖉 Ramachandran restraints 🔪 🚍 Refine ncs operators 🗳 Show per residue
Automatically correct N/Q/H errors Number of processors:		Model Interpretation Rotamers Automatic linking All parameters
Global refinement parameters Modify start model All parameters ?		
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Thank you.