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Model building, validation, and visualization

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ABSTRACT

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Model building

- 1 Generate a model by
 - [1] existing model in PDB
 - [2] creating a homology model by SWISS-MODEL
 - [3] creating a ab-initial model by AlphaFold
- 2 Do the flexible model fitting by [ISOLDE] Roughly fit the secodary structures into the map
- 3 Do model fitting manually in [Coot] or automatically in [Phenix] Repeat the model fitting until the coordinates fit the map resonably

Validation

4 Validate the quality of the models by using the validation tools in Phenix and the online validation service provided by wwPDB (https://www.wwpdb.org/validation/validation-reports)

Make sure the statistics, particularly the Ramachandran plot, Rotamers, R.m.s. deviations and B-factors are resonable.

Visualization

Visualize the models and maps by [ChimeraX]
Create figures by [Adobe Illustrator]
Create movies by [iMovie]