

Model Evaluation, Refinement & Validation — Hands-on

Turn draft structures into reliable models. Learn systematic evaluation of geometry and stereochemistry, density fit and map correlation, targeted refinement, and final validation bundles suitable for peer review and deposition.

Model Evaluation, Refinement & Validation (Ramachandran, RMSD, etc.)

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Session 1

Fee: Rs 6300 [Apply Now](#)

Geometry & Stereochemistry Checks

Fundamentals of model quality and common pathologies

Theory

Backbone and side chain diagnostics

Ramachandran **rotamer outliers** **bond lengths/angles**
clashscore **CaBLAM**

Global and local QA metrics

RMSD/RMSF **Verify3D** **ProSA/ERRAT** **WHAT_CHECK**

Session 2

Fee: Rs 8400 Apply Now

Map Fit & Density Validation

X-ray and cryo EM validation concepts and metrics

Rwork/Rfree map model CC FSC

Cryo EM focused checks and tools

EMRinger Q score local resolution

Practical map inspection and model building fixes

Coot ChimeraX ISOLDE

Session 3

Fee: Rs 11200 Apply Now

Refinement Strategies

Real space and reciprocal space refinement workflows

Phenix refine/real space refine REFMAC5 overview
PDB REDO concepts

Energy guided fixes and side chain repacking

Rosetta Relax/FastRelax SCWRL minimization basics

Water, ligands and alternate conformations

validation of occupancy and B factors chemistry
checks

Session 4

Fee: Rs 14000 Apply Now

Mini Capstone: Validate → Refine → Report

Diagnose a model, apply targeted fixes, and re validate

Theory + Practical

Assemble depositor ready validation bundle

MolProbity summary **map model metrics** **figures and tables**

Deliverables: figures, tables, README & manifest

PDF **CSV/TSV** **checksums**