

PDB Structures — Quality Metrics & Remediation — Hands-on

Learn how to read, assess, and remediate macromolecular structures from the PDB so that they are fit for downstream docking, simulation and design workflows. You will work end-to-end from raw PDB/mmCIF inspection to validation, repair, and deposition-ready curated models.

PDB Structures — Quality Metrics & Remediation

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Session 1

Fee: Rs 11800 [Apply Now](#)

PDB/mmCIF Formats & Structure Anatomy

PDB/mmCIF basics and coordinate models

[RCSB / PDBe / PDBj](#) [AlphaFold DB links](#) [biological vs asymmetric unit](#)

Structure anatomy and annotations

[chains / residues / ligands](#) [altLoc / occupancy](#) [waters / ions / cofactors](#)

Toolchain for inspection

PyMOL **UCSF ChimeraX** **pdb-tools / Biopython**

Session 2

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Quality Metrics & Validation Dashboards

Geometric quality checks

bond lengths / angles **Ramachandran & rotamers**
chiral centers & planarity

Global and local validation statistics

R / R_{free} **B-factor profiles** **clashscore / MolProbity**

Density & map-based validation (X-ray / cryo-EM)

RSCC / RSR **FSC curves** **validation reports & dashboards**

Session 3

Fee: Rs 19800 Apply Now

Structure Remediation & Optimization

Fixing common structural issues

missing sidechains / loops **altLoc clean-up** **chain IDs & residue numbering**

Protonation, hydrogens & local refinement

hydrogen placement **pK_a-aware protonation** **H-bond & salt-bridge networks**

Automated re-refinement workflows

pdb-redo **Phenix / REFMAC** **before-after metric comparison**

Session 4

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Deposition-Ready Models & Case Study

Preparing curated structures for downstream use

docking-ready clean PDB **biological assemblies**
ligand & cofactor handling

Building a QC & remediation checklist

standard operating steps **automation via scripts**
integration with MD / docking pipelines

Deliverables: curated model & validation dossier

clean PDB/mmCIF **validation report (PDF/HTML)**
before/after comparison slides