Protein Structure Quality Assessment and Validation — Hands-on

Go beyond simply downloading PDB files and learn how to critically assess protein structure quality before using it in docking, MD or design workflows. This module covers core validation concepts, geometry and stereochemistry checks, clash analysis, Ramachandran and rotamer statistics, plus practical QC reporting.

Protein Structure Quality Assessment and Validation

Help Desk · WhatsApp

Session Index

Session 1

Fee: Rs 8800 Apply Now

Quality Concepts & Experimental Context

From experimental data to 3D models

X ray resolution and data completeness | **NMR restraints and ensembles** | **Cryo EM maps and local resolution**

Model limitations and interpretation

disorder, missing loops and termini | **alternate**

conformations | crystal contacts vs biological interfaces

Choosing a structure for downstream use

resolution and R free thresholds | ligand and cofactor presence | mutations and engineered constructs

Session 2

Fee: Rs 11800 Apply Now

Geometry, Stereochemistry & Metrics

Backbone geometry and Ramachandran analysis

phi / psi distributions | favored, allowed and outlier regions | Gly, Pro and special cases

Side chain and covalent geometry checks

rotamer distributions | bond lengths and angles | planarity and chirality

Clashes and contact analysis

steric clash detection | hydrogen bonding and salt bridges | water networks and ion positions

Session 3

Fee: Rs 14800 Apply Now

Global Validation Scores & Reports

Electron density and fit-to-data indicators

R factor and R free | map correlation and local density | B factor interpretation

Composite quality metrics and servers

MolProbity like summaries | PDB validation reports | per residue and per chain scores

Deciding fitness for docking and MD

picking between alternative models | trade offs between resolution and completeness | documenting limitations and caveats

Session 4

Fee: Rs 18800 Apply Now

Mini Capstone: Full Structure QC

Select, validate and annotate a protein structure

Theory + Practical

Summarize issues and propose a fix strategy

geometry and clash fixes | loop rebuilding and mutational edits | selection for refinement or remodeling

Deliverables: QC report and decision memo

PDF or HTML QC summary | annotated screenshots | structure selection rationale