Structure Validation — Ramachandran, Geometry & Energetics — Hands-on

Learn how to rigorously validate protein structures using Ramachandran statistics, backbone and sidechain geometry, steric clashes and energy-based metrics. This module takes you from raw PDB models to fully checked, documented, and simulation-ready structures with clear validation reports suitable for publications and downstream design.

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Session Index

Session 1

Fee: Rs 14800 Apply Now

Ramachandran Plots & Backbone Geometry

Backbone torsion angles and secondary structure

ϕ/ψ angles **α-helix / β-sheet / loop regions** **cis/trans peptide bonds**

Reading and interpreting Ramachandran plots

favored / allowed / disallowed regions **Gly / Pro / pre-Pro special cases** **outlier classification**

Backbone geometry validation toolkit

MolProbity / PROCHECK **Phenix validation integration with PyMOL / ChimeraX**

Session 2
Fee: Rs 18800 Apply Now

Sidechains, Rotamers & Steric Clashes

Sidechain geometry and rotamer preferences

rotamer libraries **outlier sidechains** **environment-dependence**

Steric clashes and packing defects

clashscore and bump analysis **van der Waals overlaps** **core vs surface packing issues**

Hydrogen bond and salt-bridge networks

donor/acceptor geometry **electrostatic contacts** **water-mediated interactions**

Session 3
Fee: Rs 22800 Apply Now

Energetics, Force Fields & Stability Checks

Energy functions and scoring terms

bonded vs non-bonded terms **electrostatics / van der Waals** **implicit solvent models**

Force-field based structure checks

AMBER / CHARMM / OPLS **restrained minimization** **strain and hotspot identification**

Stability and suitability for MD/docking

energy profiles and outliers **interface vs core**

stability screening models before simulation

Session 4

Fee: Rs 25800 Apply Now

Integrated Validation Workflow & Reporting

Designing a structure validation checklist

backbone & sidechain geometry clashes & packing energy and stability metrics

Automation and batch validation

command-line validation tools Python / shell scripting integration with modelling pipelines

Deliverables: validation dossier & simulation-ready structure

clean PDB with annotations validation report (PDF/HTML) before/after comparison figures