Molecular Dynamics Simulation Report: RMSF and RMSD Analyses

RMSF Analysis

Plot Overview: The RMSF plot shows the fluctuation of each residue in the protein structure over the entire simulation.

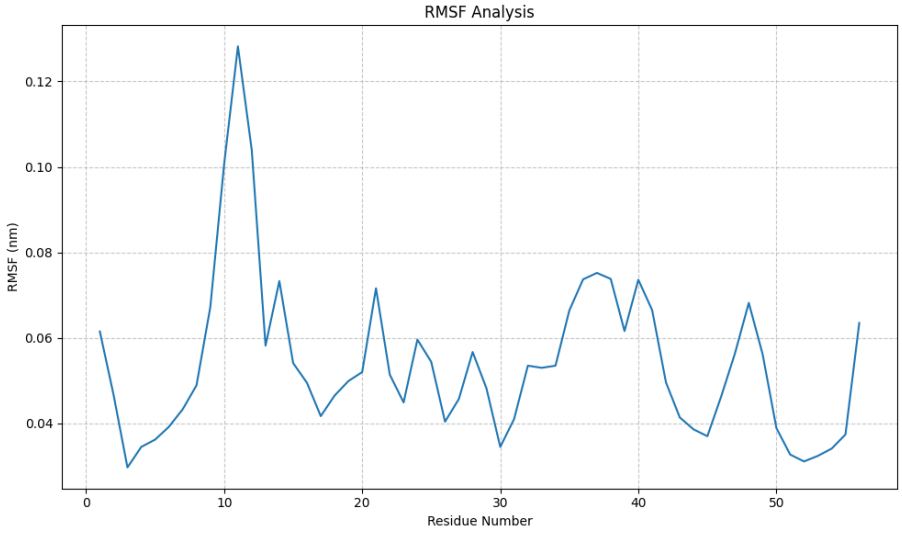

Figure 1: Residue RMSF

Interpretation: - RMSF values indicate how much each residue fluctuates around its average position during the simulation. - High RMSF values suggest that the residues are flexible or part of loop regions, which often show higher mobility. - Low RMSF values indicate stable regions, often associated with secondary structures like -helices and -sheets. - Analyzing RMSF helps identify which parts of the protein undergo significant conformational changes and may be involved in binding or active sites.

RMSD Analysis

Plot Overview: The RMSD plot provides insights into the overall structural stability of the protein over time.

Interpretation: - RMSD values show the deviation of the protein structure from a reference structure, usually the initial structure, over the simulation time. - A rising RMSD value indicates structural changes or unfolding, while a stable RMSD suggests structural stability. - Initial fluctuations might be observed as the system equilibrates, but consistent trends depict the overall conformational changes. - A significant change in RMSD could imply binding interactions or

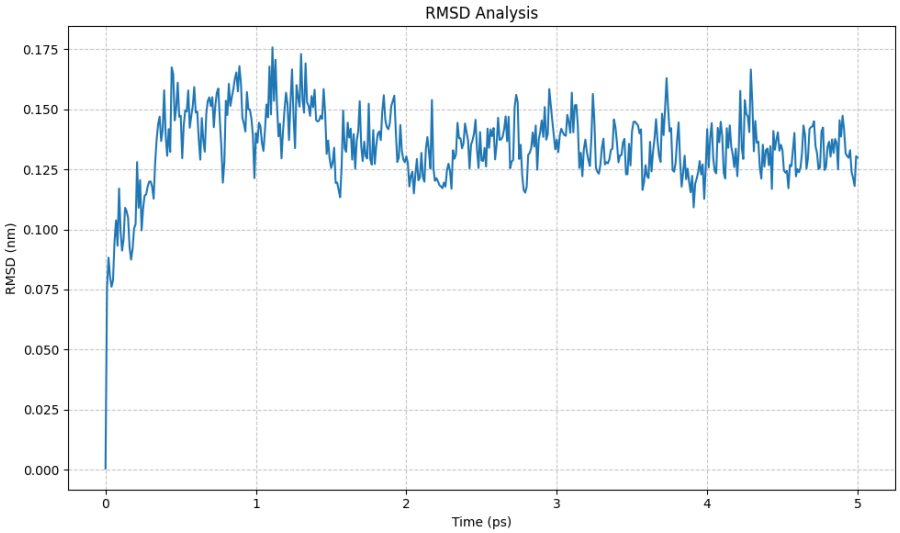

Figure 2: RMSD Plot

conformational shifts.

Summary

The RMSF and RMSD analyses combined provide a comprehensive view of residue-specific fluctuations and overall structural changes during the MD simulation. Understanding these patterns is crucial, especially when interpreting the biological significance of the conformational dynamics in molecular interactions and function.