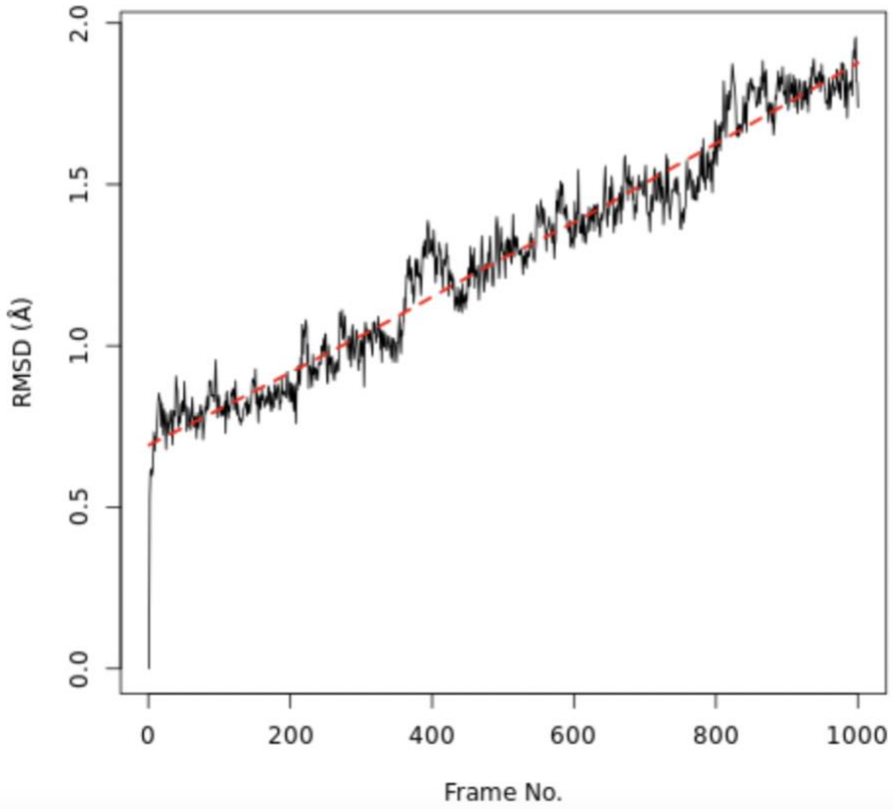
RMSD

RMSD, or root-mean-square deviation, is a standard measure of structural distance between coordinates. It measures the average distance between a group of atoms (e.g. backbone atoms of a protein). If we calculate RMSD between two sets of atomic coordinates - for example, two time points from the trajectory - the value is a measure of how much the protein conformation has changed. Wikipedia provides more information.



Question

What do the features in the RMSD plot tell us?

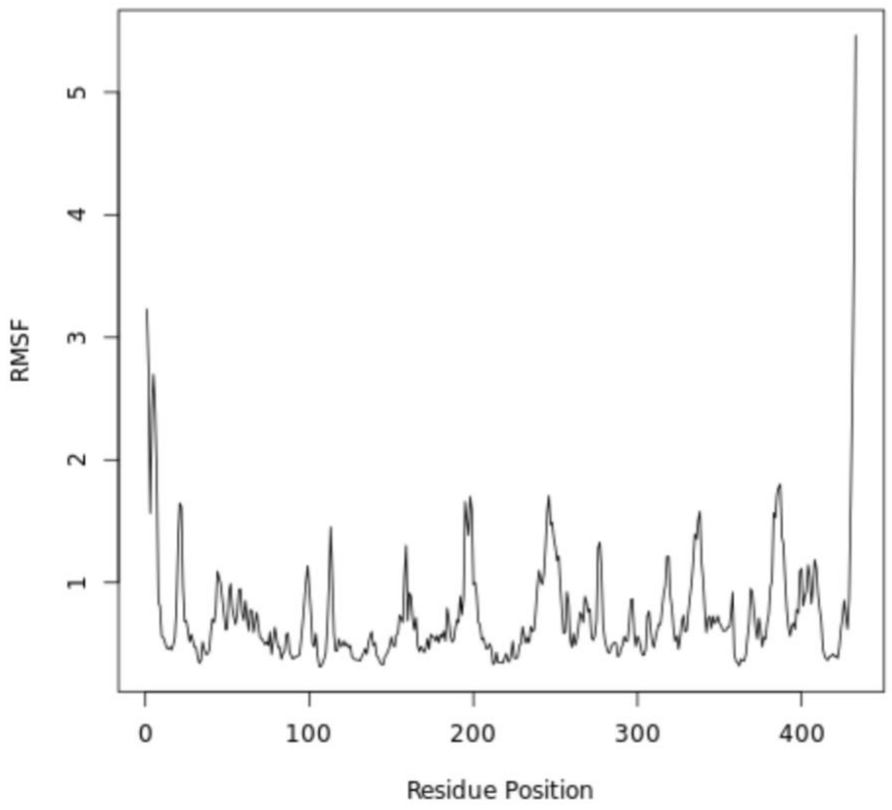
Solution

The increase in the RMSD plot with time shows the protein steadily deviates from its original conformation.

The three peaks visible in the histogram suggests the presence of three main conformations which are accessed during the trajectory.

RMSF

The root-mean-square fluctuation (RMSF) measures the average deviation of a particle (e.g. a protein residue) over time from a reference position (typically the time-averaged position of the particle). Thus, RMSF analyzes the portions of structure that are fluctuating from their mean structure the most (or least).



Question

What can we learn from the features in the RMSF plot?

Solution

Higher RMSF values most likely are loop regions with more conformational flexibility, where the structure is not as well defined.

This allows a link with experimental spectroscopic techniques which detect the secondary structure of a protein.