ABSTRACT

Studying protein intramolecular motion gives an important knowledge about its function. In this work, the convergence of the conformational sampling space was performed on a 30ns long molecular dynamics simulation of Bovine Pancreatic Trypsin Inhibitor (BPTI). The overlap between the principle component vectors for different time windows of the simulation time were calculated using two methods. The first method measures the total overlap between covariance matrices of different time segments. It shows a lack of convergence with steady values throughout the simulation. The second method examines the subspace overlap between eigenvectors of different time windows of simulation. This method shows high convergence between 4ns long time fragments. The most of atomic fluctuations of BPTI C_α atoms can be seen in 4ns time intervals. The B-factor and RMSD were calculated in water to check the validity of the simulation results. They give good agreement with the experiment.