Supporting information

A Network of Conformational Transitions revealed by Molecular Dynamics simulations of the Binary Complex of Escherichia coli HPPK with MgATP

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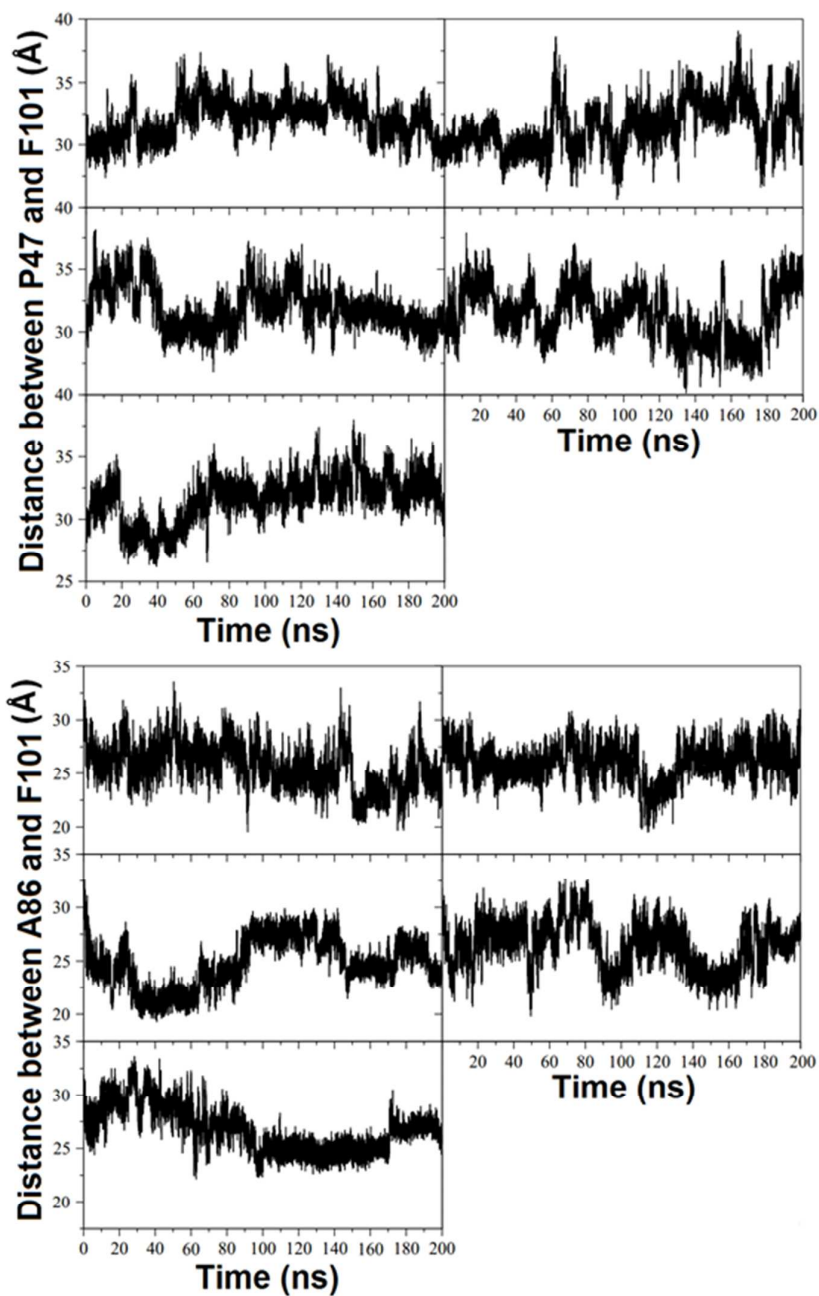
Figure S1 The C_α distances between Pro47 and Phe101 and between Ala86 and Phe101.

Principal component analysis

The PCA has been performed for all the trajectories. All C_α atoms was used to define the backbone conformation of HPPK for such analysis. This results in 474 principal components from the 158 C_α atoms in the form of 474 eigenvectors and their associated eigenvalues. It shows that, as the same as the earlier research[64], in our trajectories 20 out of 474 PCs capture about 80% of the protein's motion, especially

for the first five PCs, they have much larger eigenvalues than other PCs, and in every trajectory, they capture more than or about 50% of the motion(Figure 3). Hence, in each of them, it is sufficient to analyze the first three PCs.
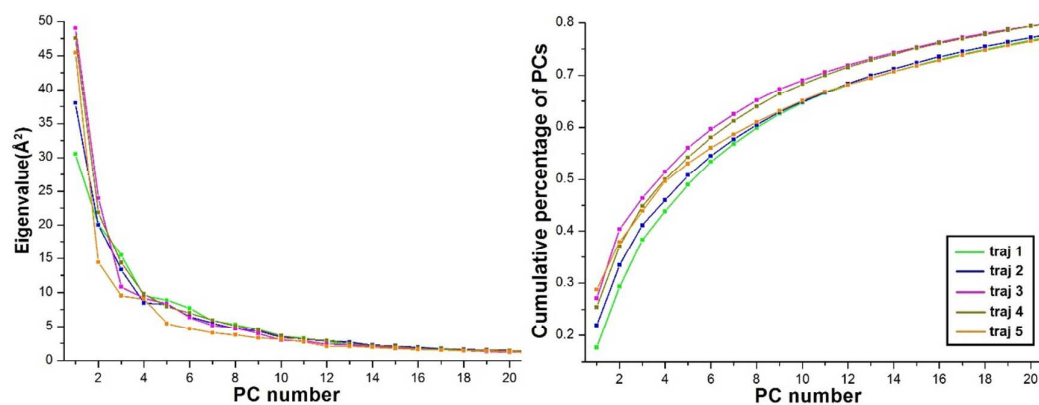

Figure S2 Magnitudes and cumulative percentage and of the first 20 PC eigenvectors for our trajectories.