

**Supplementary Information –**

**Allosteric Conformational Transition in Adenylate Kinase:  
Dynamic Correlations and Implication for Allostery**

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Figure S1:

Distance-difference matrix between the Open state (i.e. PDB:4AKE) and the Closed state (i.e. PDB:1AKE) of AdK: Major structural re-arrangements and inter domain motions occur during this conformational transition. The color-coded dots indicate the distance difference in unit of Å as globally aligned by the backbone carbons (with RMSD of 7.92 Å), and secondary structures of the whole domain are also depicted.

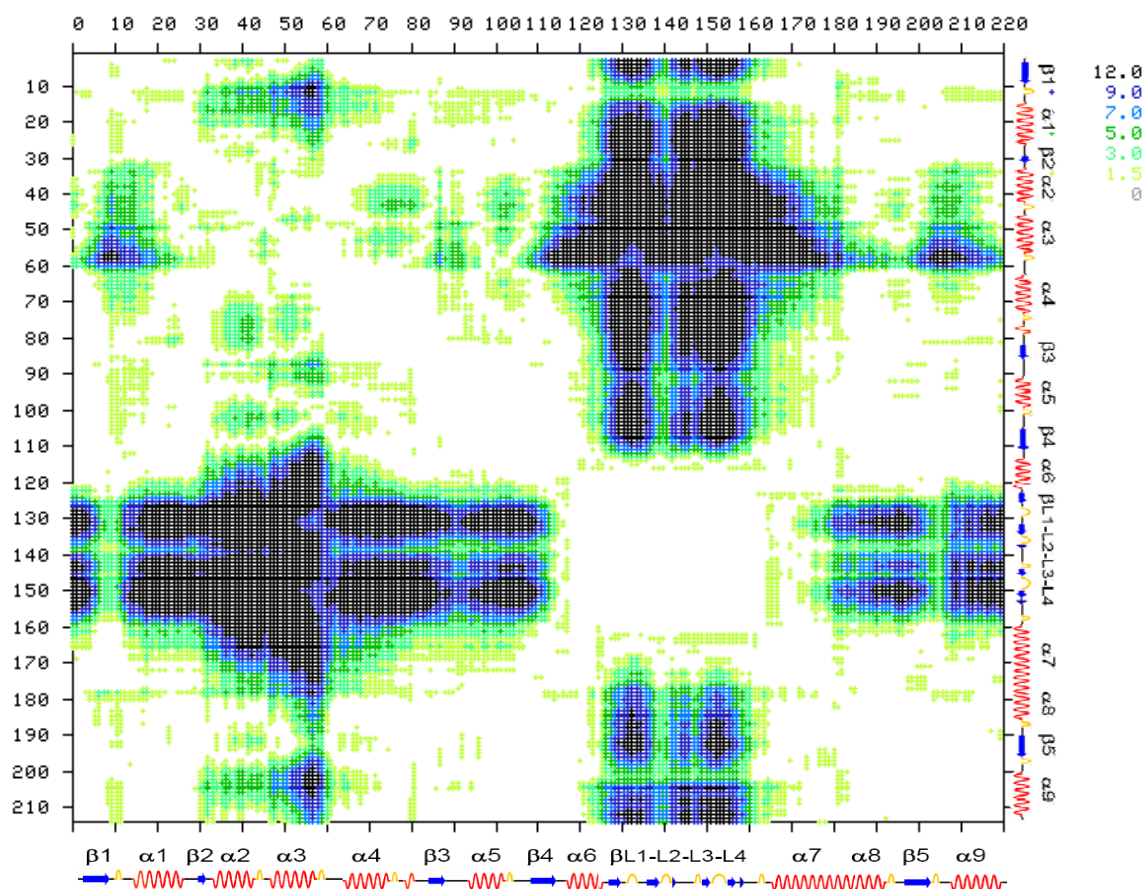


Figure S2:

Residue temperature factors ( $B$ -factors) of the Open and Closed states of AdK as predicted by the elastic network model using the GNM algorithm (a cutoff value for the harmonic potential energy was set at  $r_c = 10 \text{ \AA}$ ). Major dynamics fluctuation during the conformational transitions differ at the NMP lid (NMP domain) and ATP lid (LID domain), with LID and NMP domain much more flexible in the Open state.

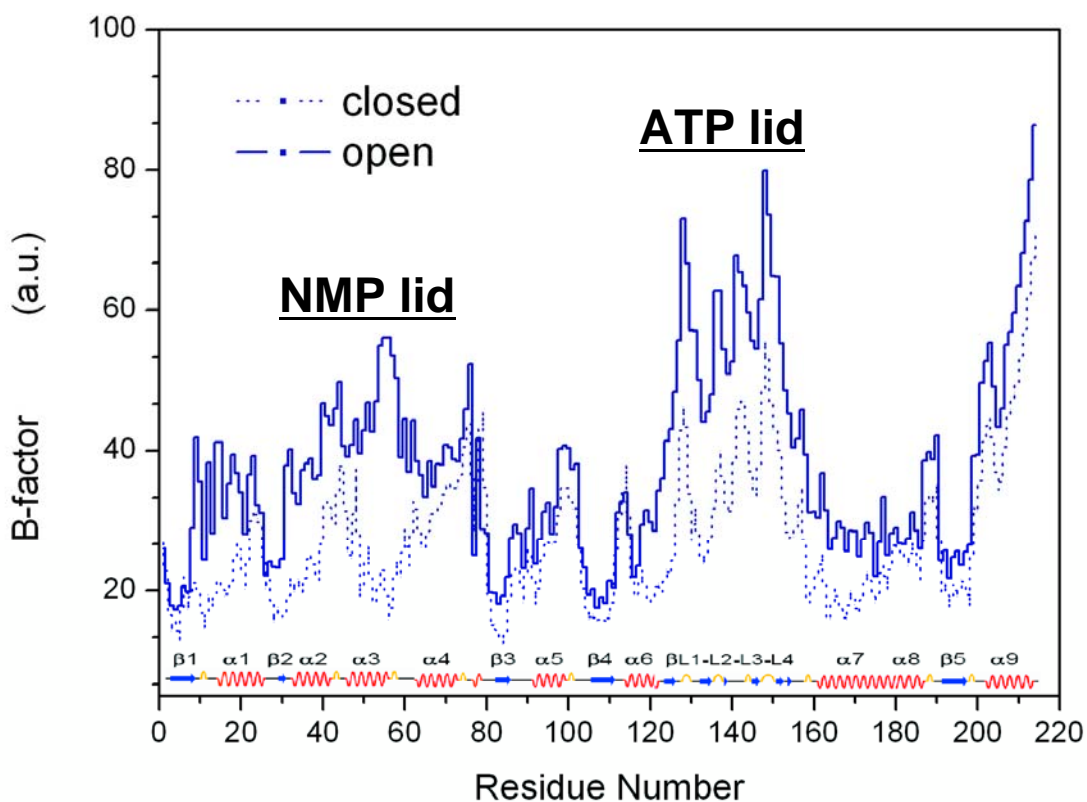


Figure S3:

Dynamics fluctuation correlation in the Closed or Open states of AdK as predicted by the elastic network mode of GNM. The correlation varies between -1 and 1, corresponding to anti-correlated (two residues move in opposite directions, colored in blue) and correlated (two residue move in the same direction, colored in red), respectively.

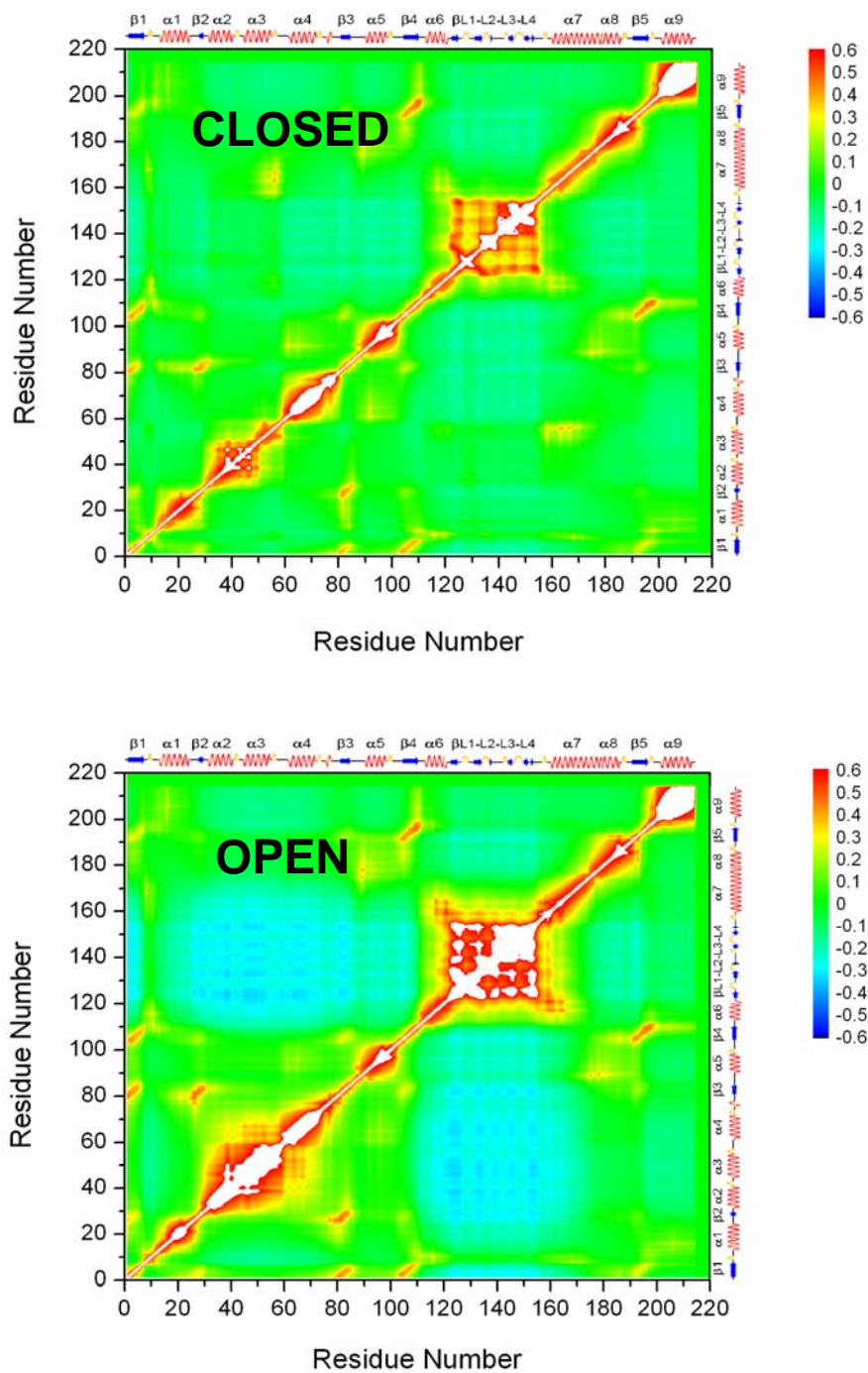


Figure S4:

Residue RMSD of the dominant normal modes of motions (mode 7, mode 9 and mode 10, in a trajectory from the closed state) responsible for the Closed  $\rightarrow$  Open transition of AdK.

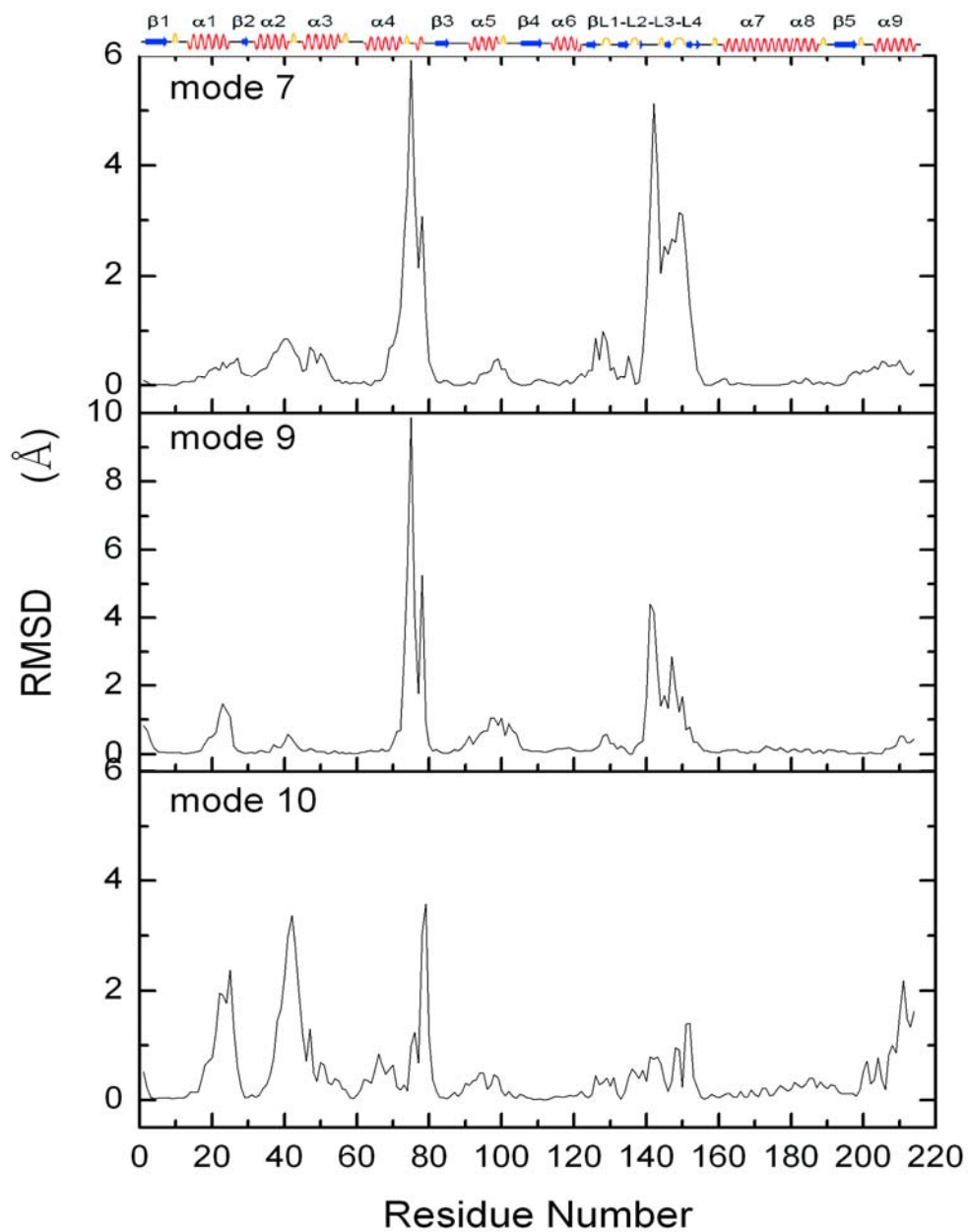


Figure S5:

Contour map of the difference cross correlation in the Closed or Open states of *Aquifex* AdK (based on PDB:2RGX\_ChainA vs PDB:2RH5\_ChainA). They show strikingly same dynamics as the *E. Coli* AdK (presented in Fig.6 of the main text).

