Supporting information

Mechanism for the Autophosphorylation of CheA Histidine Kinase: QM/MM Calculations

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Figure S1. The constructed 3D model of P1-P4-ATP complex

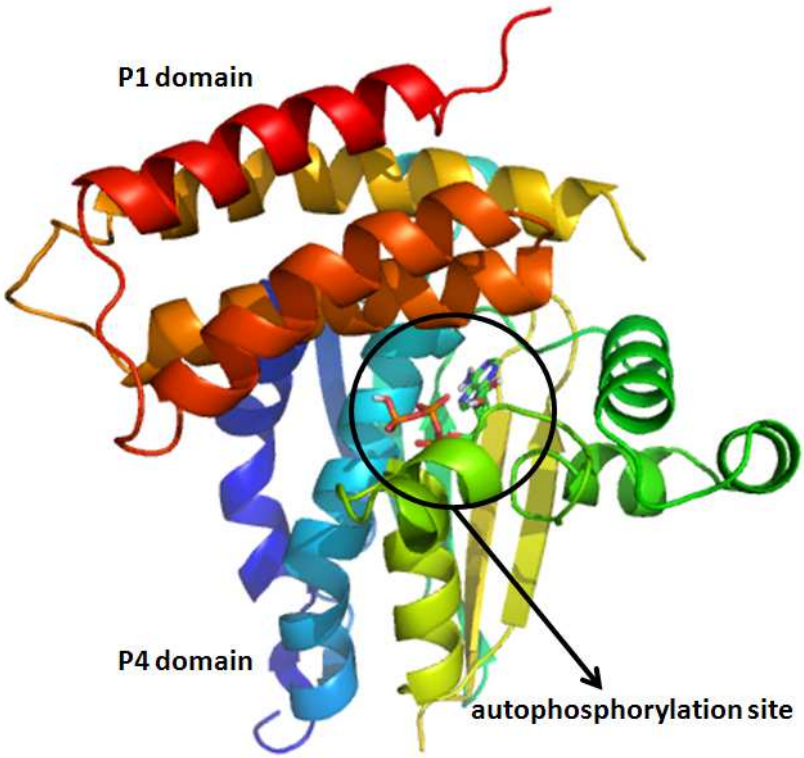

Figure S2. Key residues around the active site of P1-P4-ATP complex including His45, Thr46, Leu47, Lys48, Gly49, His64, Glu67, Arg160, Asn161, Ala162, His165, Gly166, Gly255 and Val256. Complex is shown in green; ATP in yellow and key residues in mauve.

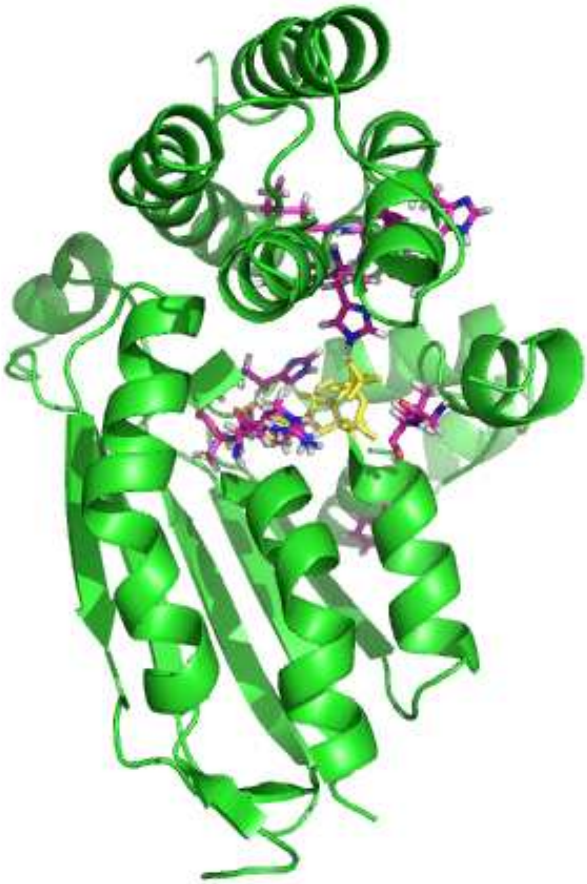

Figure S3. RMSD of C^{α} atoms in P1-P4-ATP complex (A) and RMSD of heavy atoms of the key residues (shown in the Supplementary **Figure S2**) and ATP around the active site in P1-P4-ATP complex (B) relative to the initial structure versus simulation time.

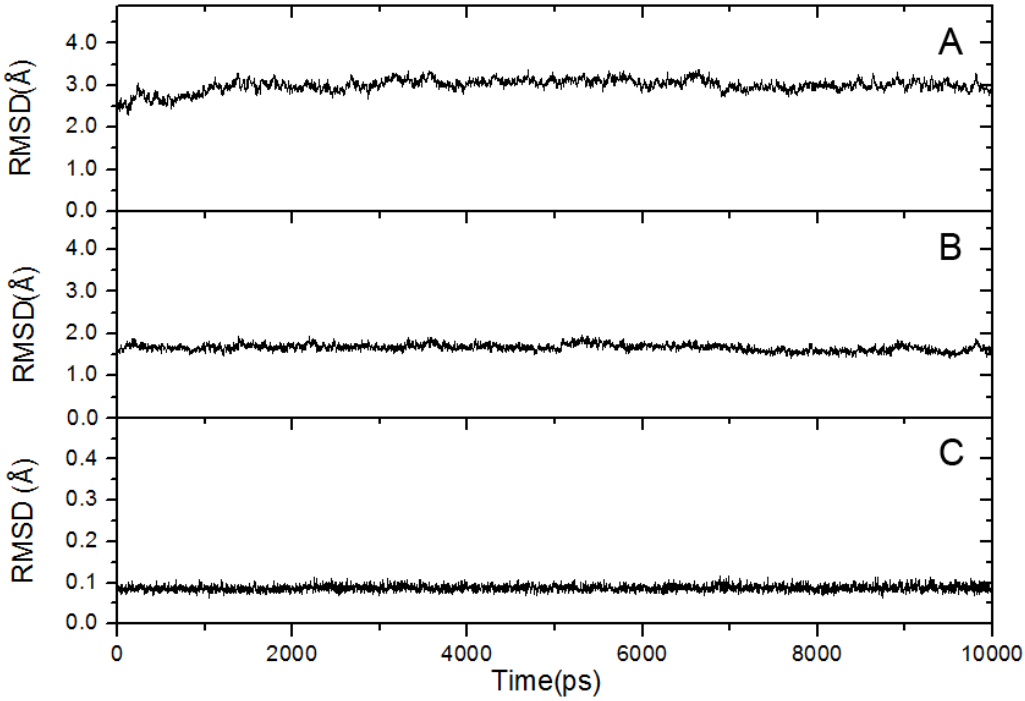

Figure S4. (A) The binding environment of O^{β} and O^{γ} atoms of ATP binding to Mg^{2+} ion in AMP-activated protein kinase (PDB ID code: 2V9J). (B) The binding environment of O^{α}, O^{β} and O^{γ} atoms of ATP binding to Mg^{2+} ion in P_{II} signal transduction protein (PDB ID code: 2ZXW). Yellow dished lines represent the bond lengths between Mg^{2+} and O atoms of ATP.

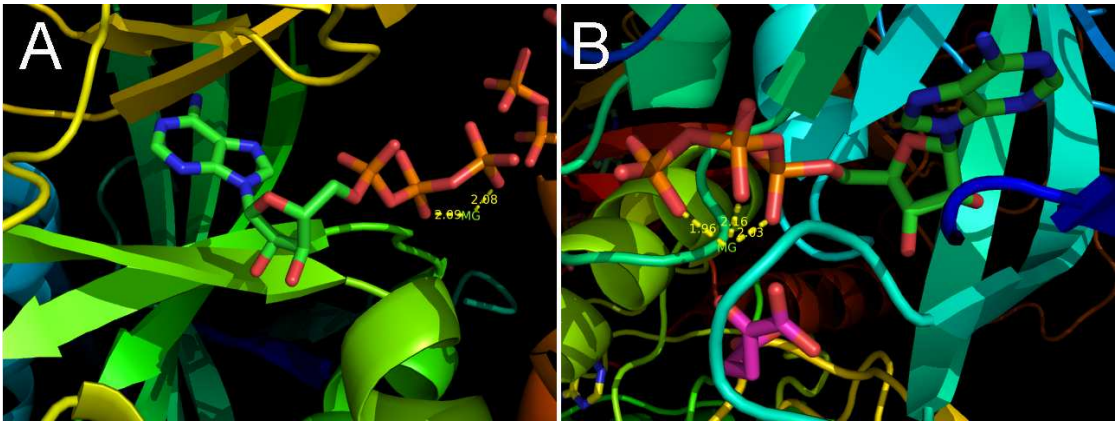

Figure S5. (A) The comparative view of catalytic environments between the R conformation and the M conformation in the P1-P4-ATP complex. ATP, Mg^{2+} and carbon atoms in the R conformation are colored in green and in the M conformation are colored in yellow. All side chains of crucial residues in the binding site are shown as stick and labeled. (B) The energy difference between the R conformation and the M conformation.