

Supplementary Data

Research Article

Unraveling the molecular basis for GTP preference of unique histidine kinase BA2291 from *Bacillus anthracis* using a multilevel *in silico* approach

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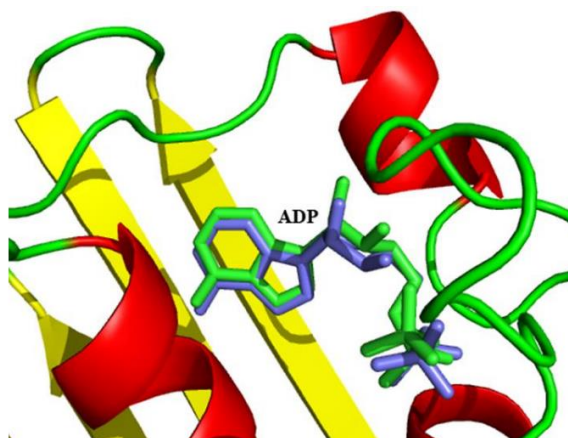


Figure S1: Crystallographic position of ADP from 3D36 (green) and docked position of ADP (blue)

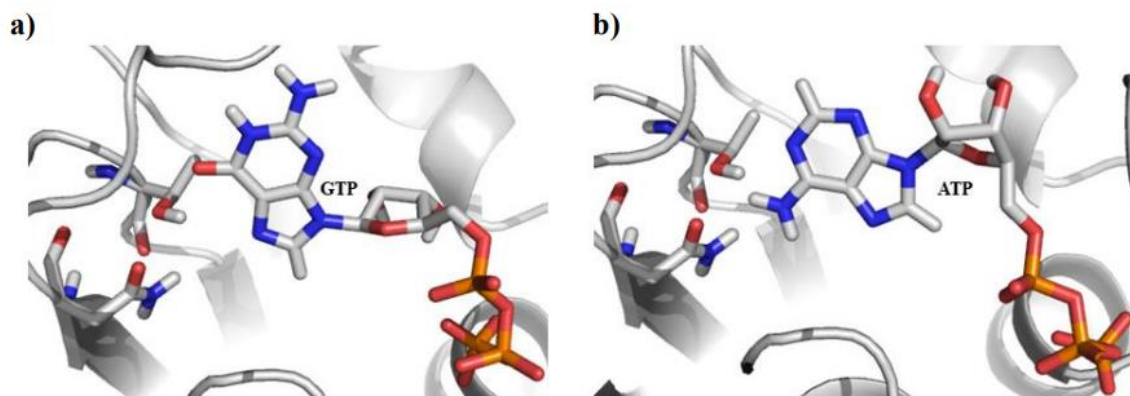


Figure S2: Best docked pose obtained from vina. a) GTP and b) ATP

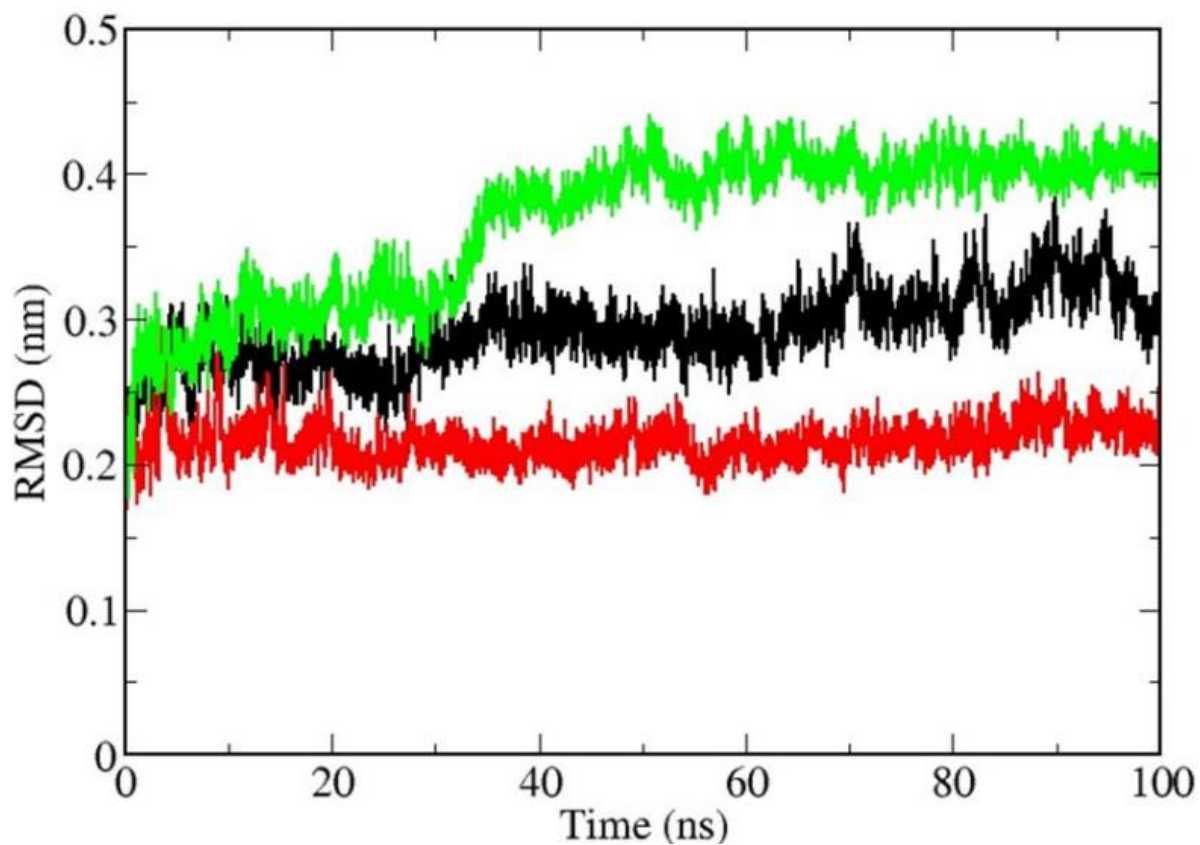
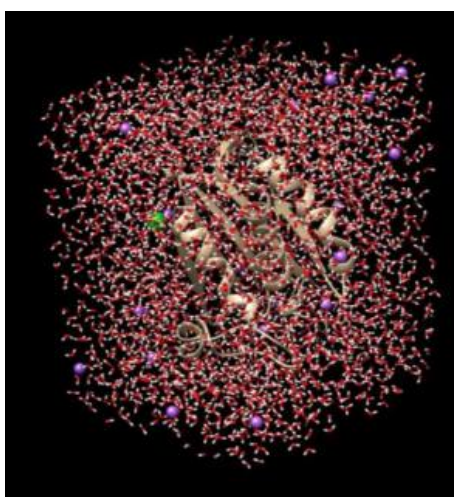
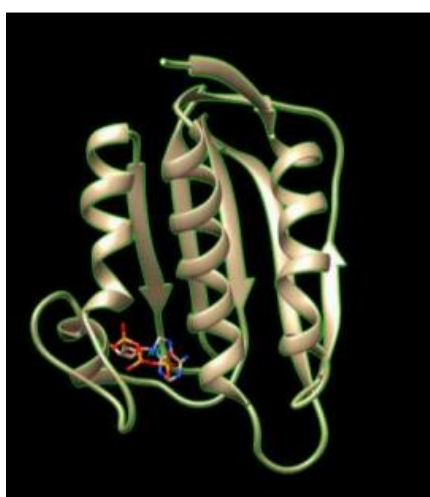


Figure S3: Root mean square deviation (RMSD) of the C α atoms of the BA2291 a) apo form (green), complexed with b) GTP (red) and c) ATP (black)



Movie S1: Simulation movie of apo BA2291



Movie S2: Simulation movie of BA2291 with ATP



Movie S3: Simulation movie of BA2291 with GTP