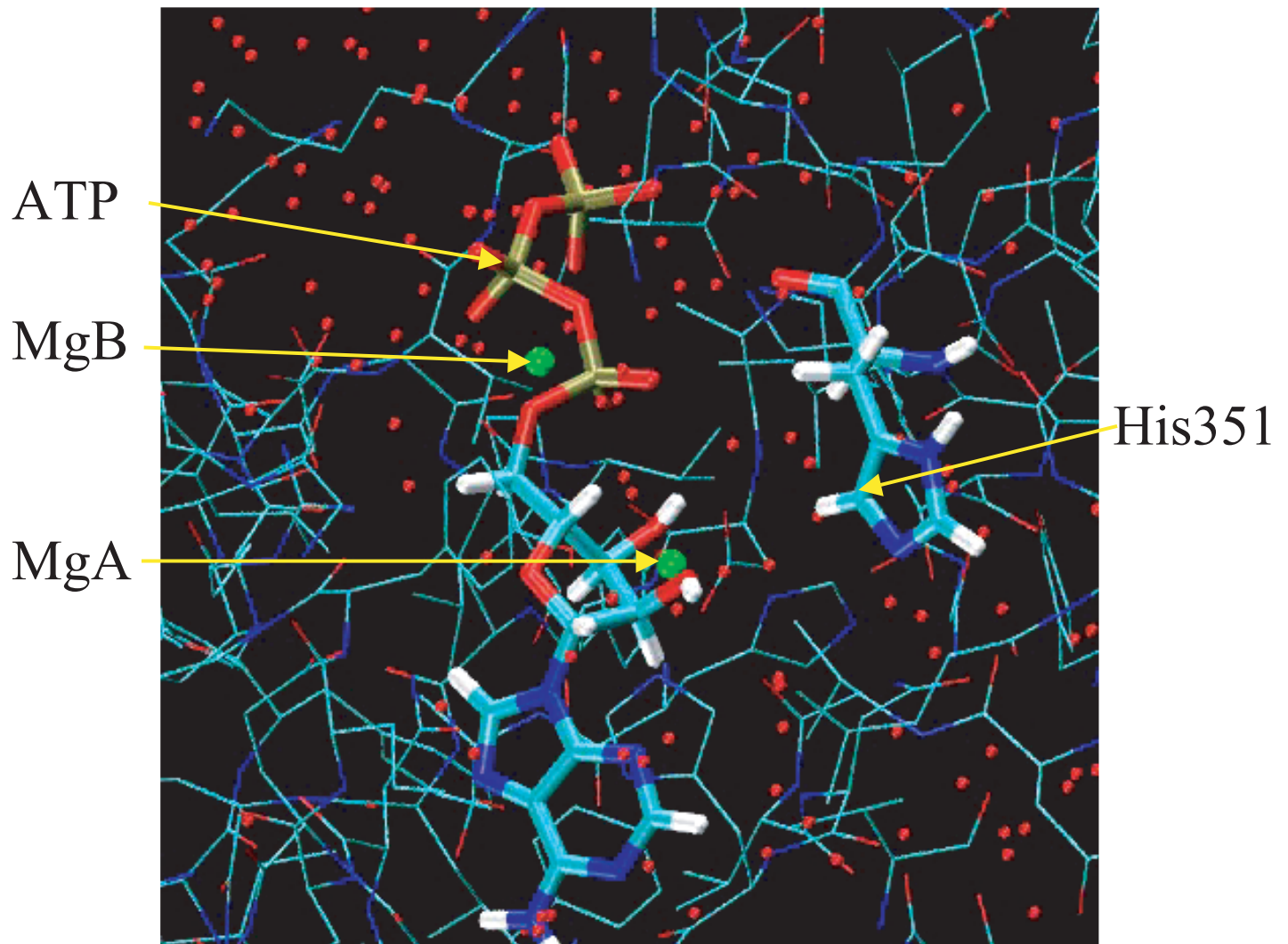


## Supplemental movie legend



**Molecular dynamic simulation of ATP at the catalytic site of EF. Oxygen, nitrogen, carbon, hydrogen, phosphorus and magnesium atoms are in red, blue, cyan, white, gold, and green, respectively. His351 is moving around during the 2 ns simulation. Positions of the ATP molecule, two magnesium ions and key residues such as Asp491, Asp493 and His577 coordinated  $Mg^{2+}$  show smaller fluctuations. Note that a fluctuation at the end of the movie brings MgA close to the  $P_{\alpha}$  non-bridging oxygen. This fluctuation also allows a close approach of the nucleophile (3'OH) to  $P_{\alpha}$  and thus establishes a presumed pre-catalytic conformation. However, the 3'OH group has to be deprotonated before a productive nucleophilic attack may proceed.**