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分子动力学研究 F_1-ATP 合酶对三磷酸腺苷的稳定和定位作用

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F_1-ATPase Stabilizes and Positions Adenosine Triphosphate Revealed by Molecular Dynamics Simulations

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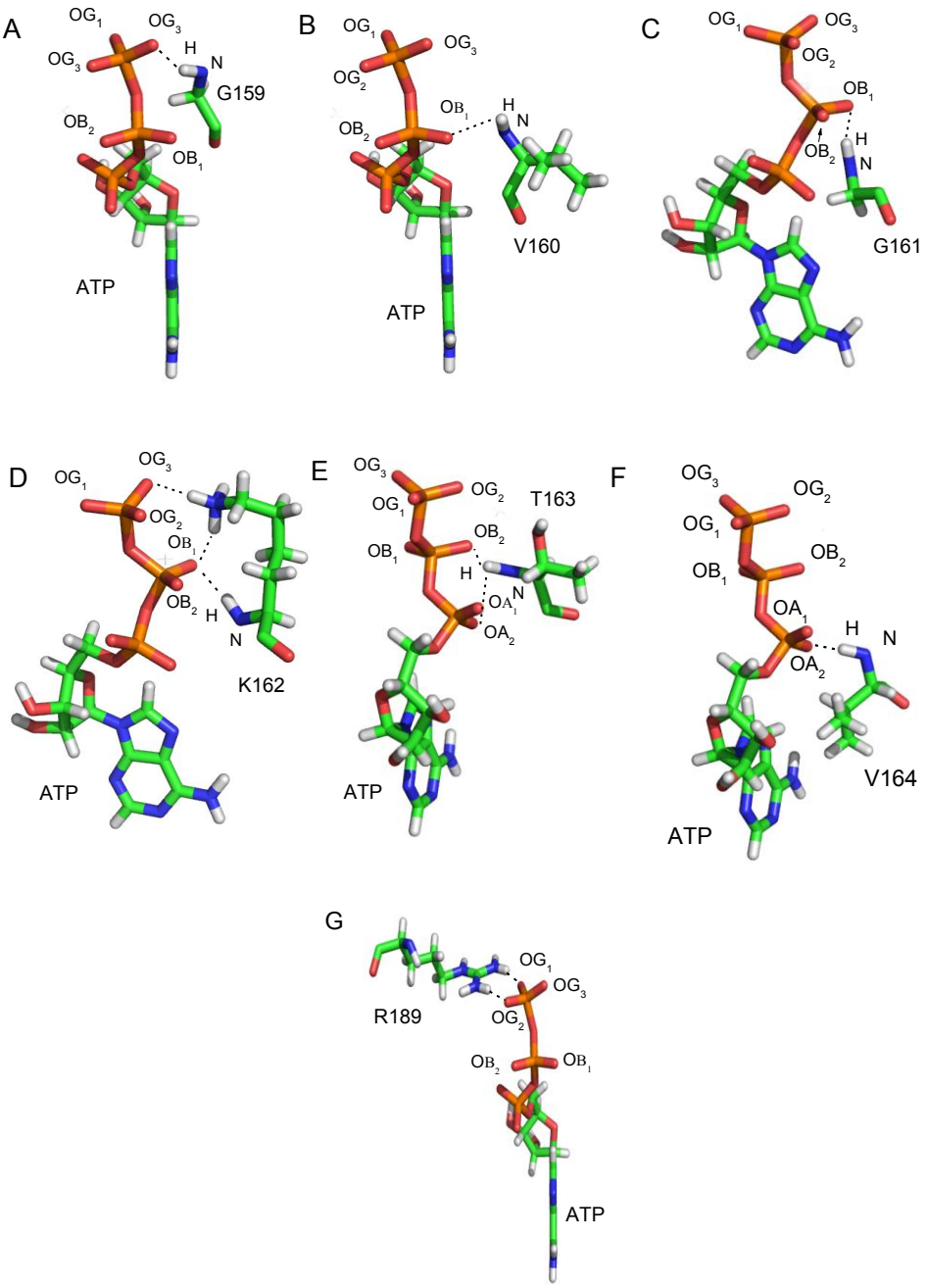

Fig.S1 Snapshots of the hydrogen bonds between ATP triphosphate and F_1-ATPase. These involved residues include (A) G159, (B) V160, (C) G161, (D) K162, (E) T163, (F) V164, (G) R189

These hydrogen bonds form an interaction network to constraint the motion of ATP triphosphate.

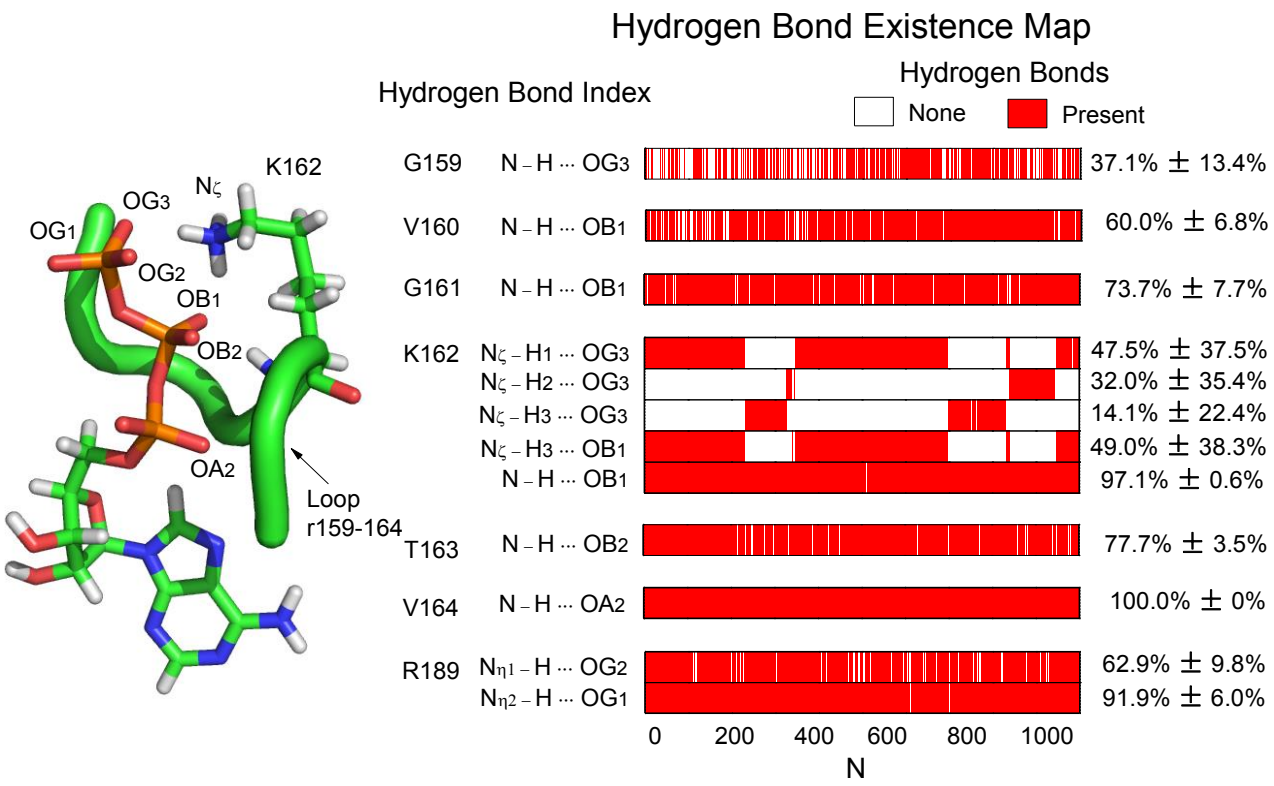

Fig.S2 Mapping of the existence of hydrogen bonds

Conformations were sampled every 20 ps and a total number of 1000 conformations were taken from each trajectory. The average occupancies and corresponding standard deviations are calculated from 12 independent trajectories of 20 ns.