

**A**



**B**



**C**

**Supplementary figure S12. Properties of target protein (H/K ATPase PDBID: 4UX2)**

Part (**A**) represents the total residues, protein chain, atoms, heavy atoms, and charged atoms. Part (**B**) shows the mean root square fluctuation (RMSF) in angstrom (Å) of the target protein. Part (**C**) represents the protein secondary structure elements (SSE), alpha-helices shown in red, and beta-strands shown in blue monitored through simulation. The plot summarizes the SSE composition for each trajectory frame over the course of simulation.