SUPPORTING INFORMATION

Structure and binding of the H4 histone tail and the effects of lysine 16 acetylation

Darren Yang and Gaurav Arya

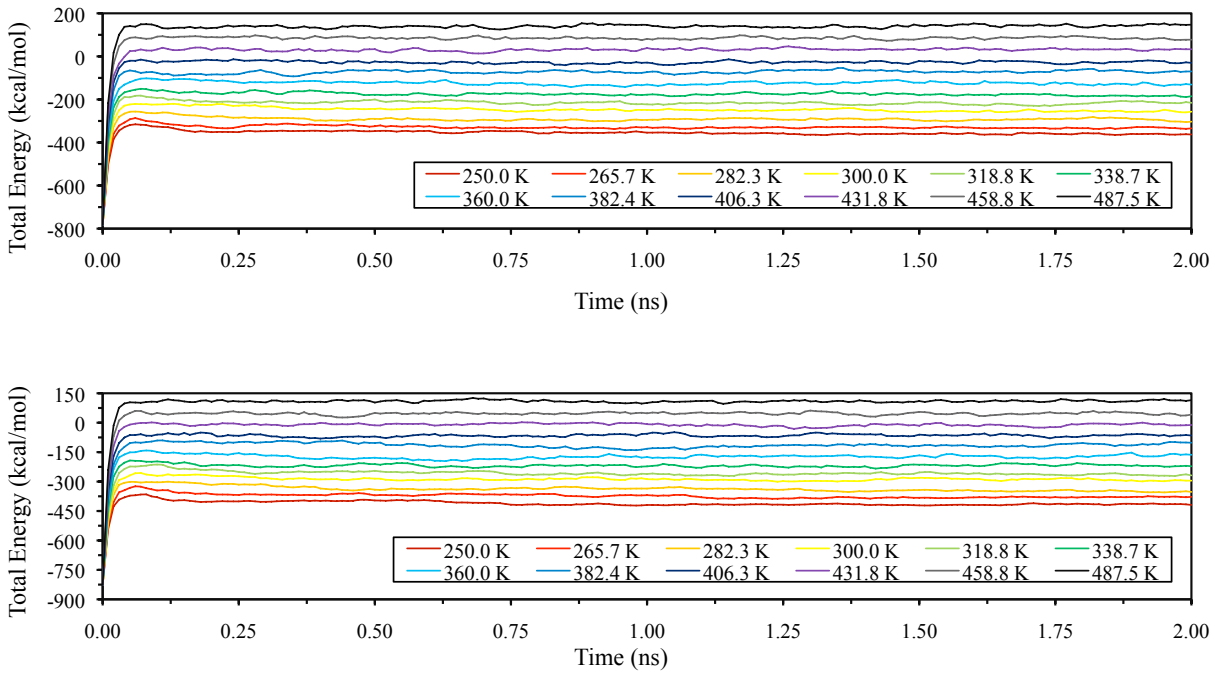

Figure S1. Total energies for the 12 replicas computed from REMD simulations during the initial 2 ns target temperature simulation without exchange of configurations across replicas. The top and bottom figures correspond to results from wild type (WT) and K16-acetylated (AcK) tail.

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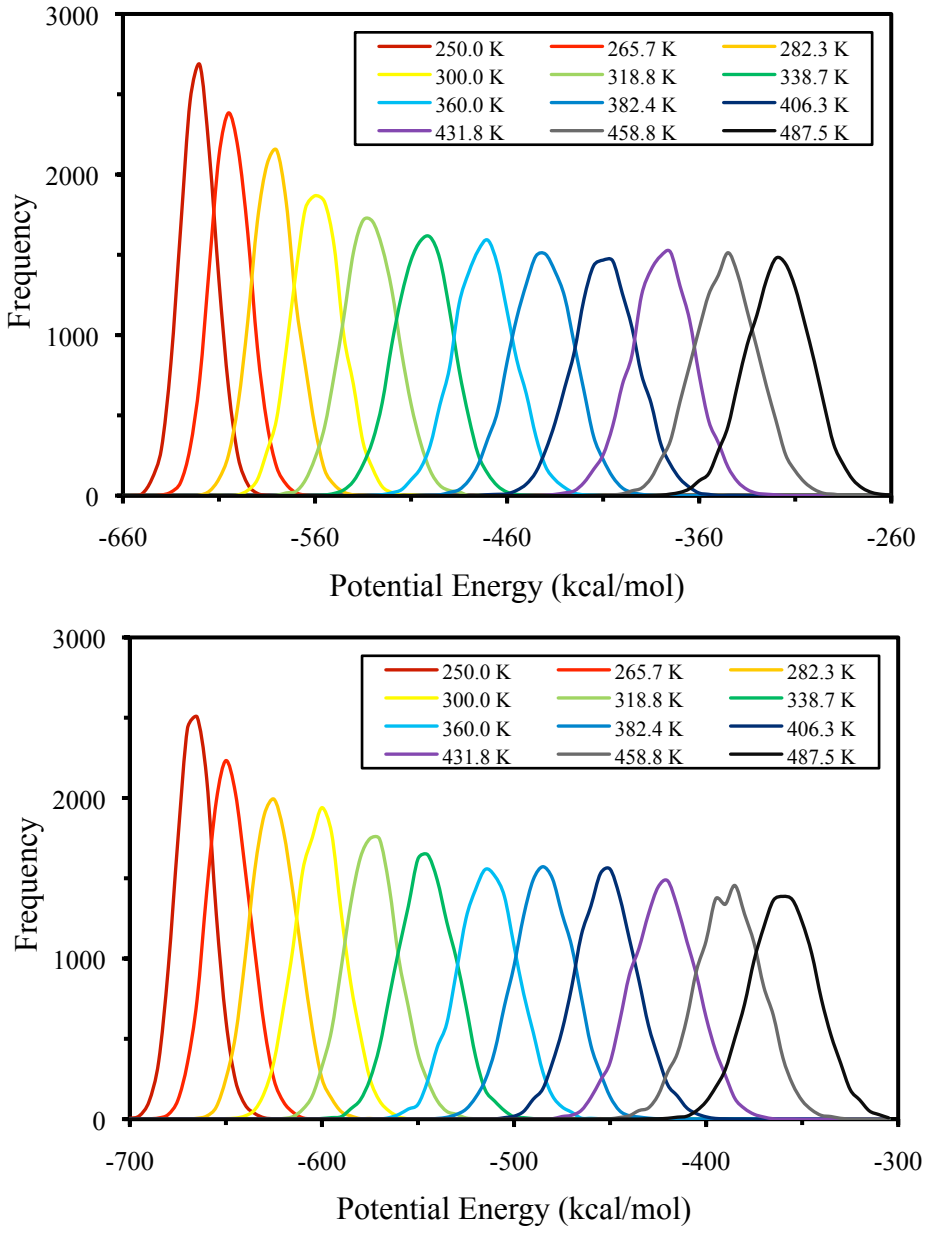

Figure S2. Distribution of total potential energy values computed from the 10 ns equilibrium REMD simulation for the 12 replicas. The figure shows overlapping of potential energy, suggesting that the replicas are able to exchange with each other.

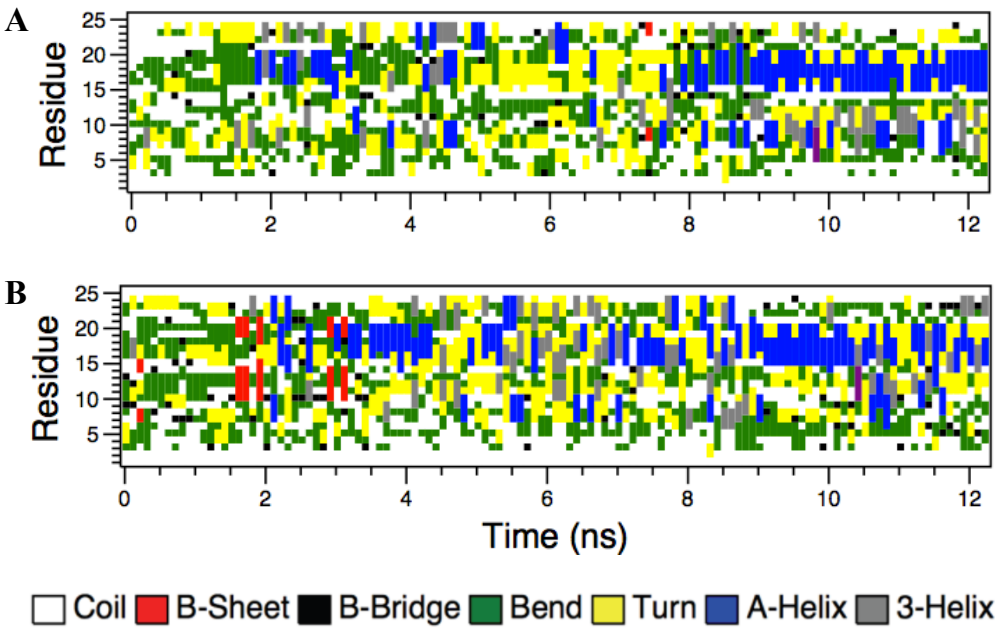

Figure S3. Time evolution of the secondary structures of the wild type (A) and acetylated-K16 H4 tail (B) during the ~12 ns long equilibration step (before production) starting from an extended (unfolded) H4 tail structure.

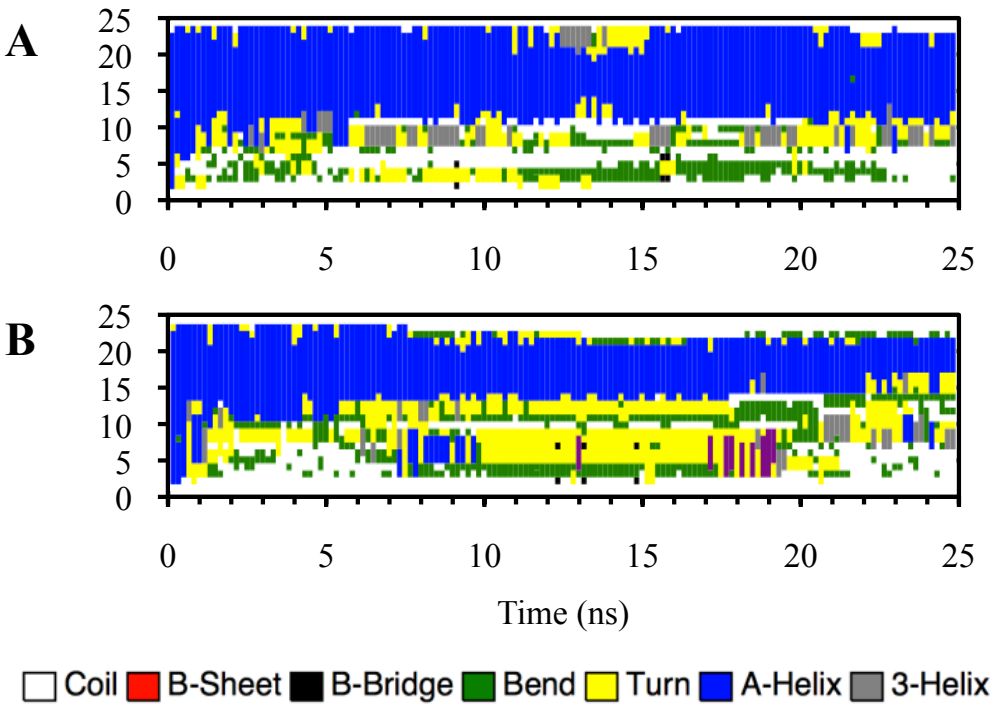

Figure S4. Time evolution of the secondary structures of the wild type (A) and acetylated-K16 H4 tail (B), computed from 25 ns-long explicit-solvent MD simulations using the DSSP method.

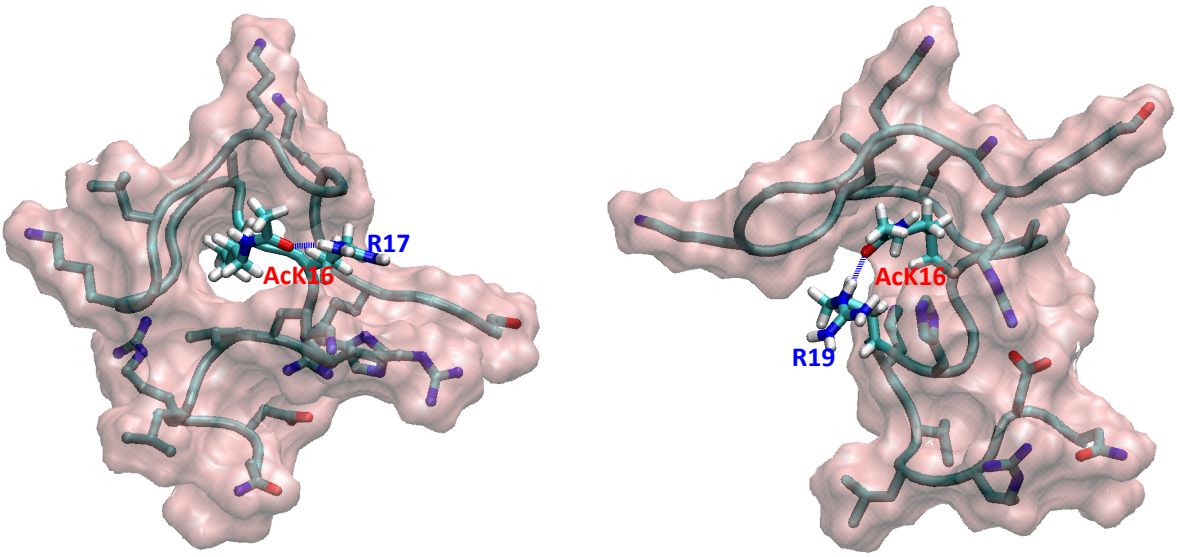

Figure S5. Two snapshots of H4-AcK taken from the REMD simulations showing intermittent hydrogen bonding between AcK16 and R17 (left) and R19 (right).

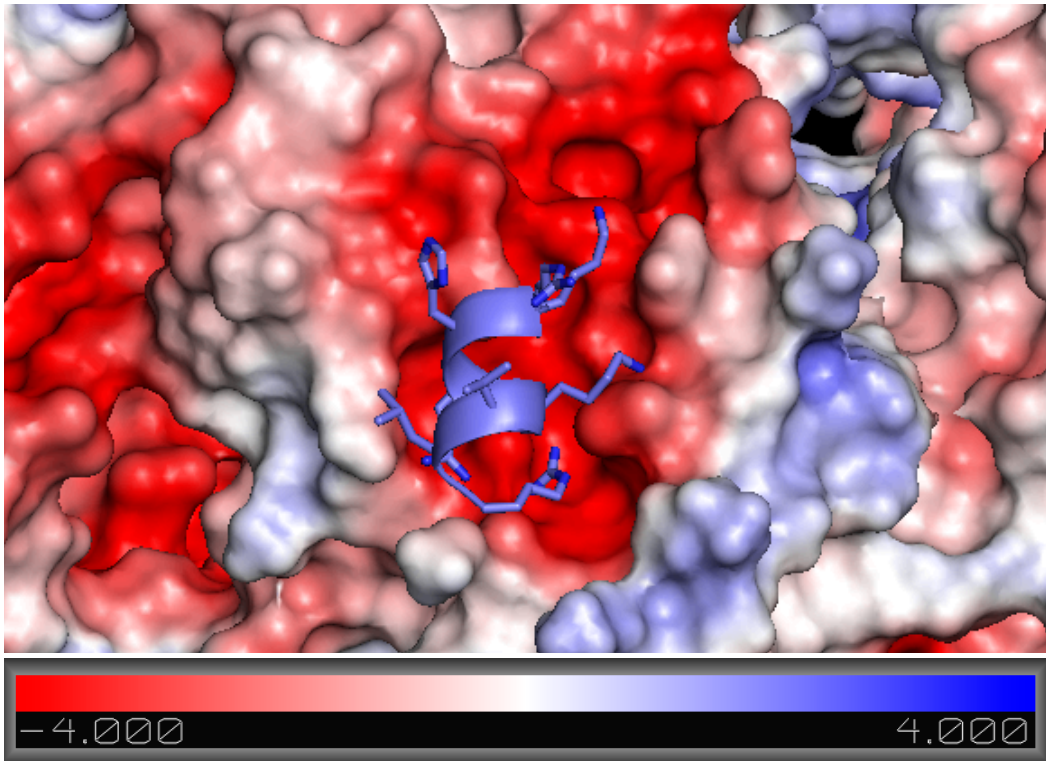

Figure S6. Electrostatic map of the nucleosomal acidic patch on its solvent accessible surface, demonstrating the glove-like fit between the acidic patch and the α-helical H4 tail fragment (K16-R23). The electrostatic map, produced by PyMol and APBS, is color-coded according to the potential in the range −4 to +4 k_BT/e.

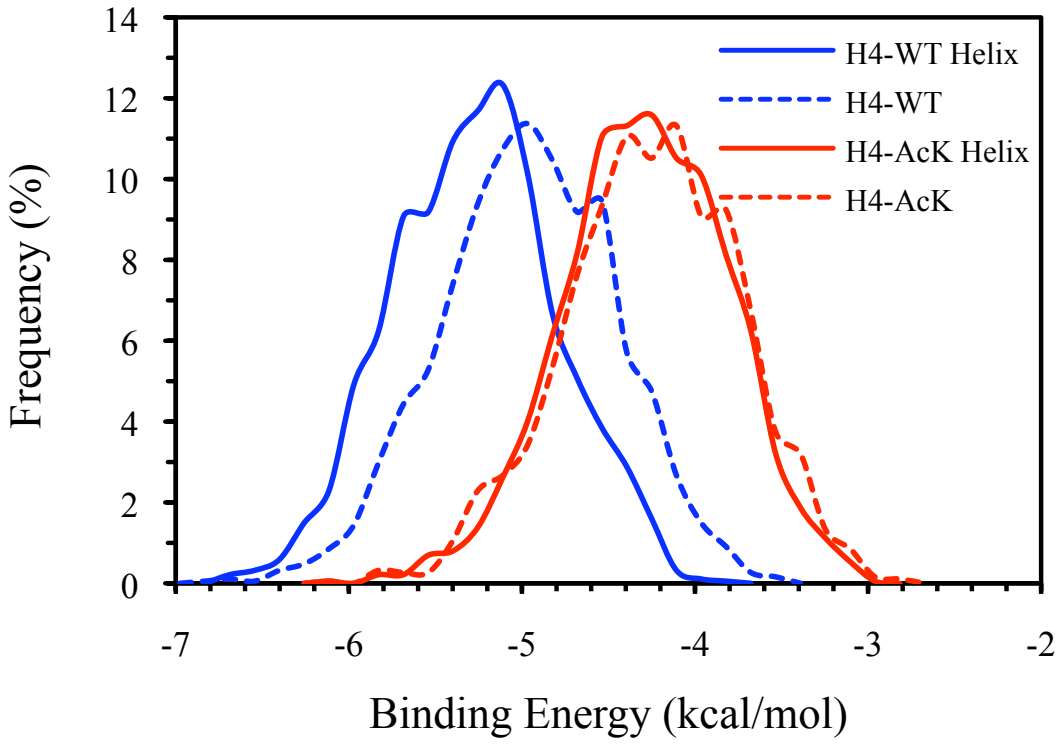

Figure S7. Distribution of binding free energy of 1000 docking runs calculated from AutoDock Vina 1.0. Results from four types of H4 tail fragments considered in the study are shown.

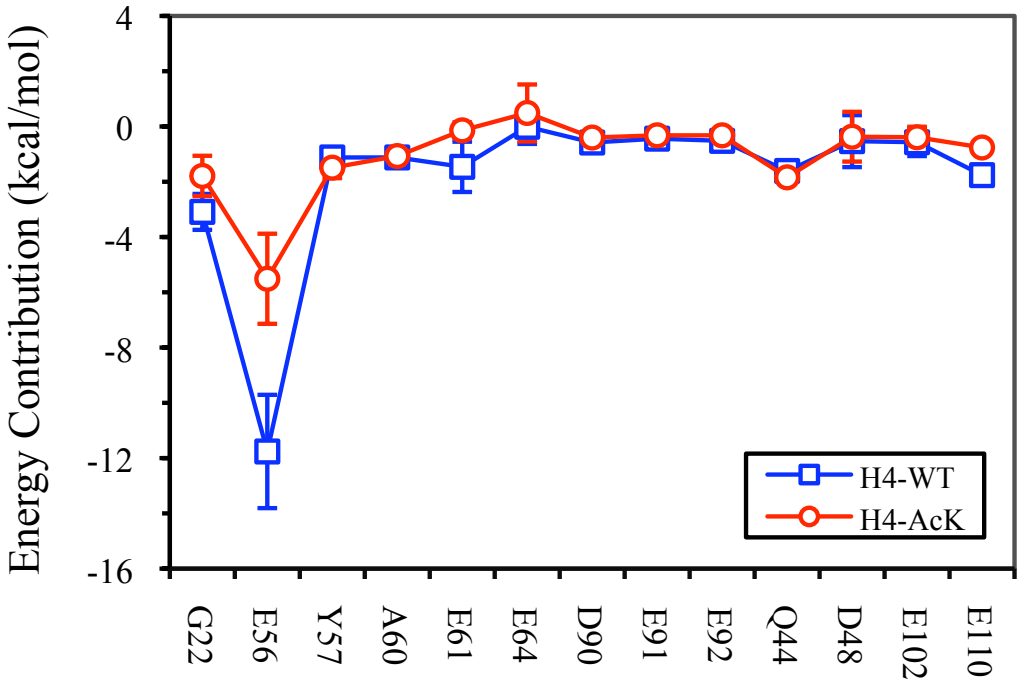

Figure S8. Individual contributions of the acidic patch residues to the net free energy of H4 tail binding at the acidic patch, as obtained from MM-GBSA calculations.