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Supplemental Information

Histone Acetylation Regulates Chromatin Accessibility: Role of H4K16 in Inter-nucleosome Interaction

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Supporting Material

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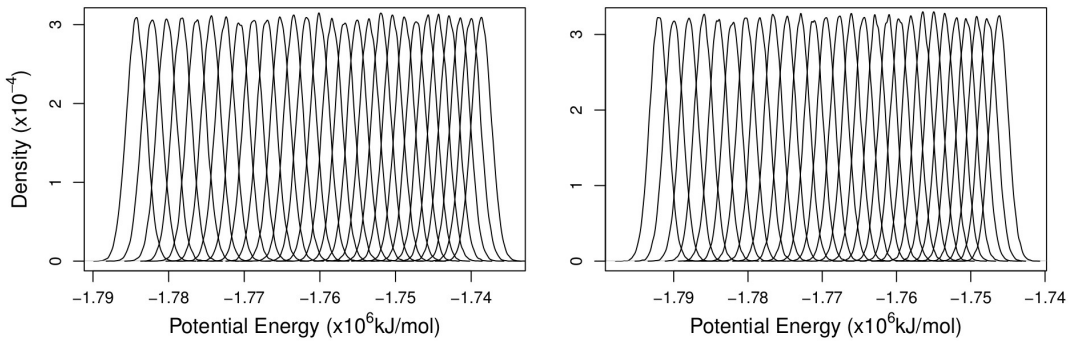

Figure S1. Probability density distribution of potential energy. For each replica of WT (left) and AC (right) system.

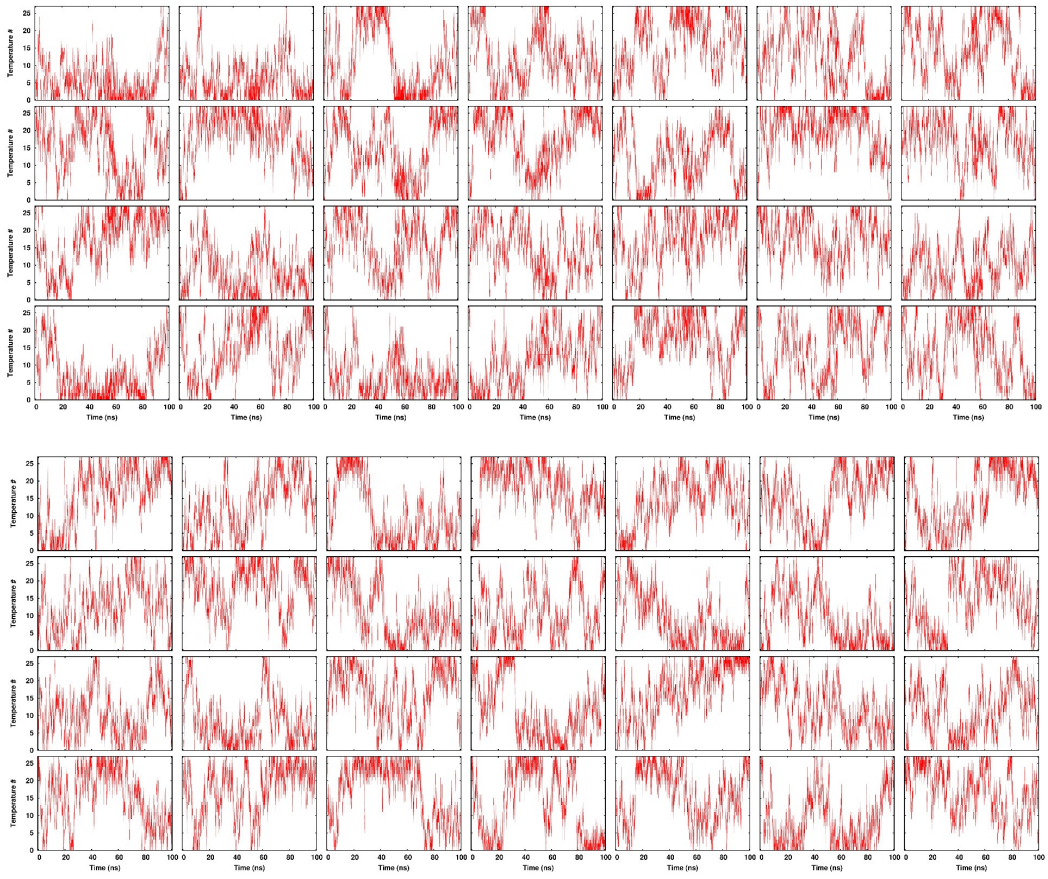

Figure S2. Replica exchange through temperature space. Upper panel: WT, lower panel: AC. Plots in each panel are in order of replica number, from left to right and up to down. Y axis is the index of temperature, the X axis is the simulation time in ns.

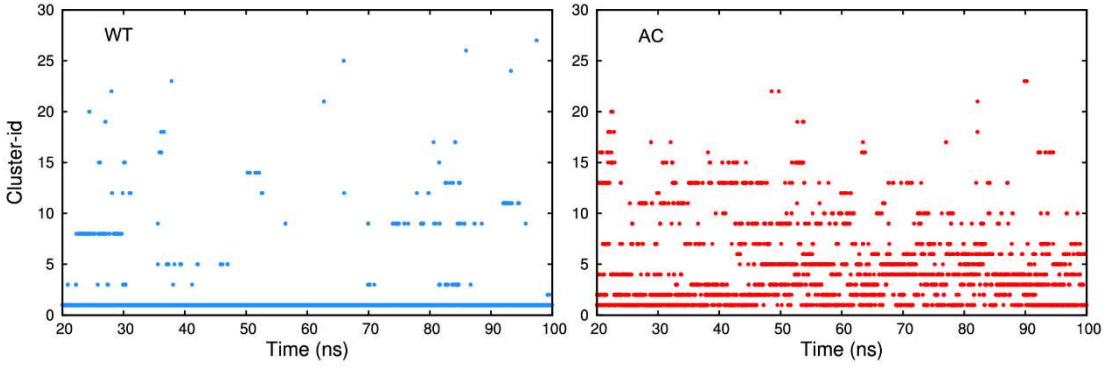

Figure S3. Evolution of the structure clusters in REST simulation (20-100ns)

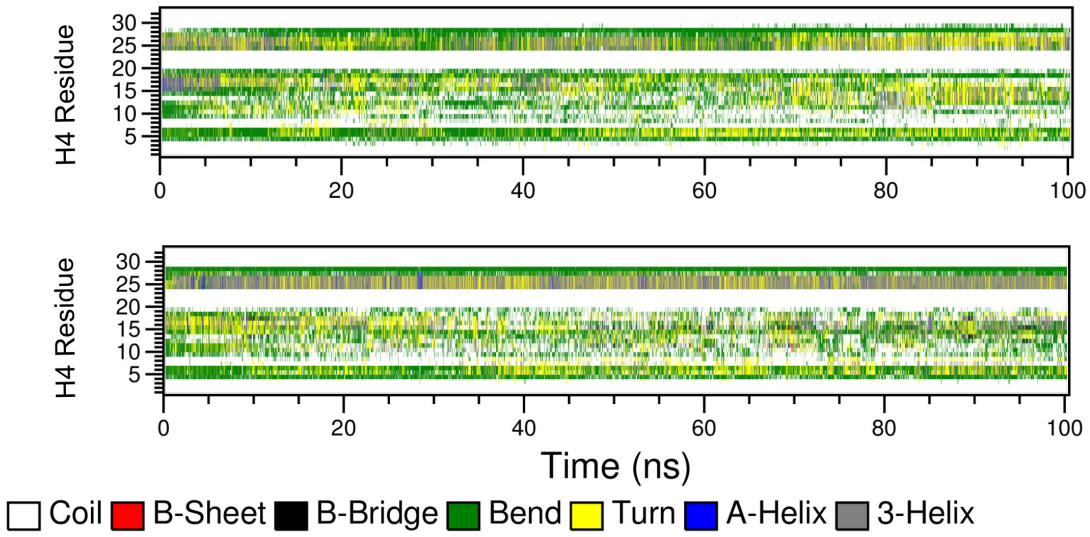

Figure S4. Secondary structure of H4 tail. Upper panel: WT, lower panel: AC.

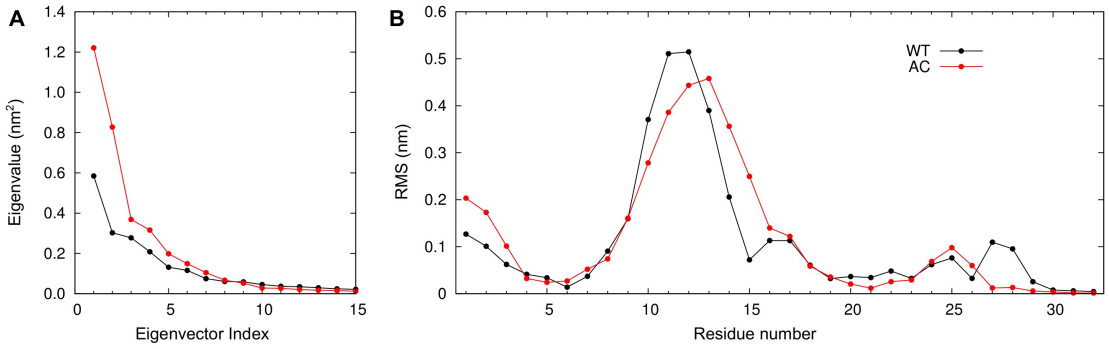

Figure S5. Eigenvalue of the top 15 eigenvectors of REST simulation (A) and the RMS fluctuation of H4 tail Cα atoms of eigenvector 1 (B).

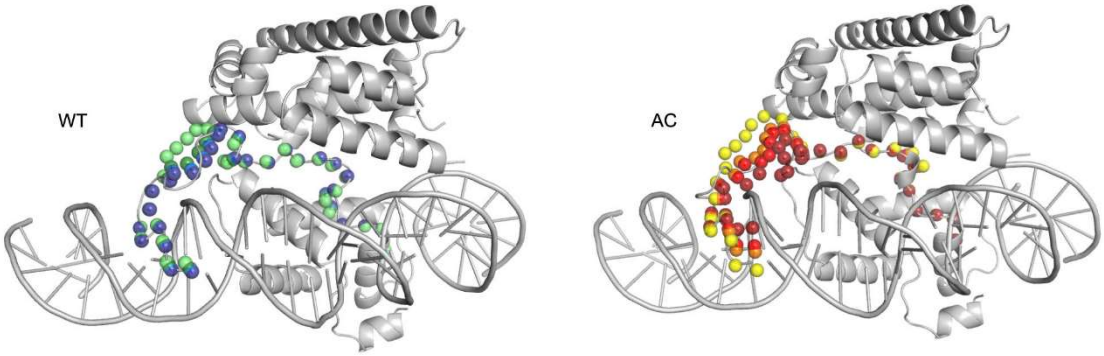

Fig S6. Motion along the first principle component (PC). Representative snapshots of the Cα of H4 tail were shown in spheres.

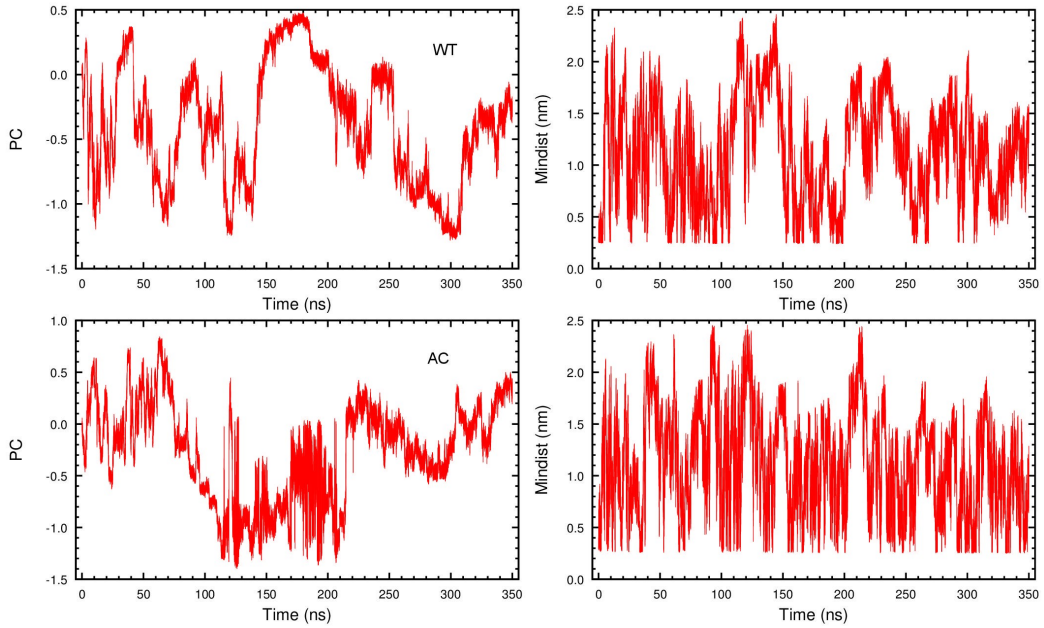

Fig S7. The exploration of the two CVs: PC (left) and Mindist (right)

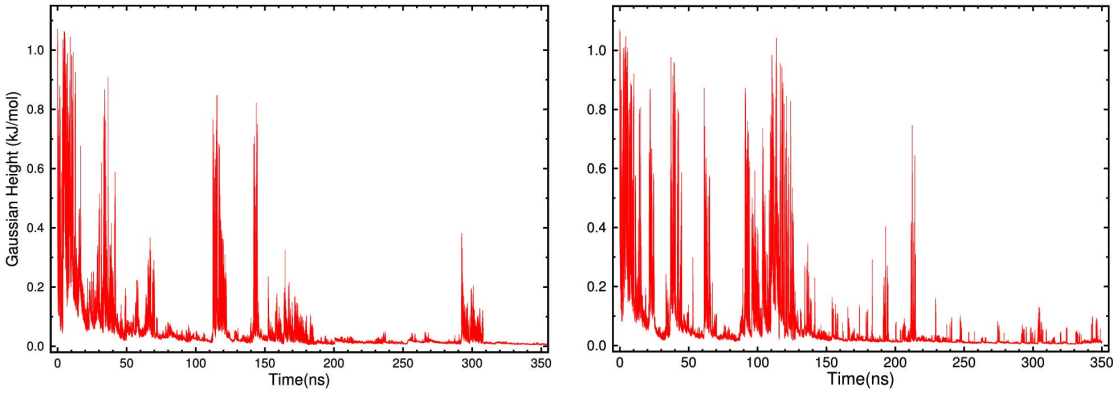

Fig S8. The height of Gaussian during Metadynamics: WT (left), AC (right).

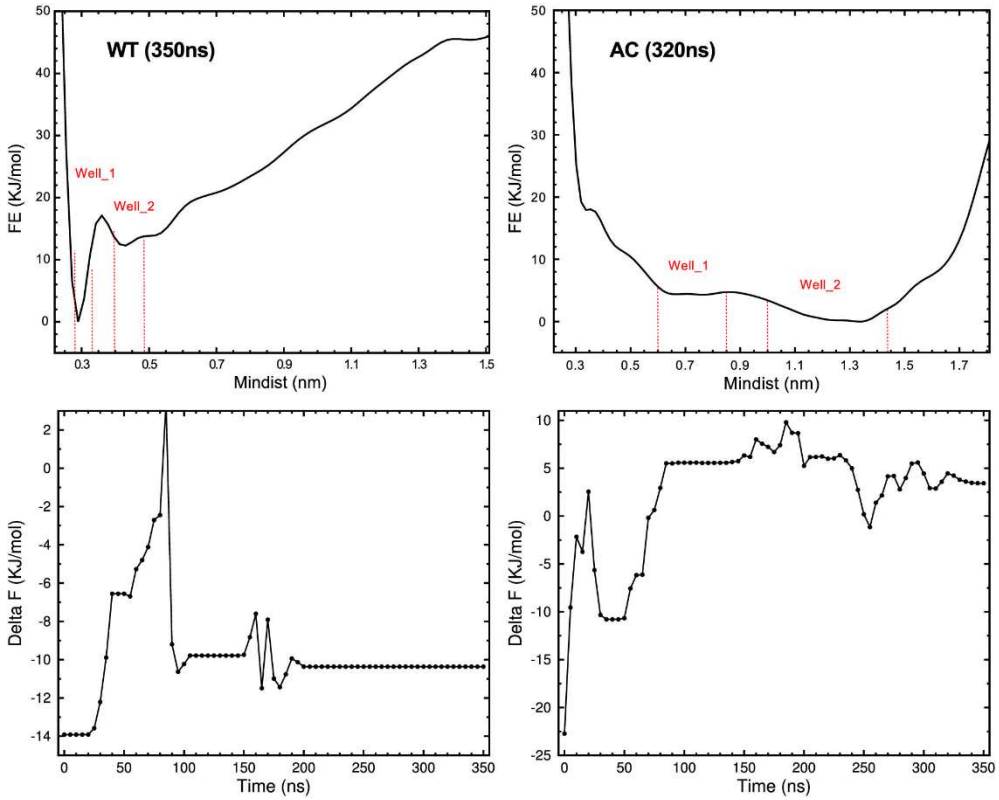

Fig S9. The difference of free energy wells. The free energy difference between two wells (defined in the upper panel) against the metadynamics simulation time is plotted in the lower panel. The data point is calculated every 5ns. For the AC system, there is no disdinguishable well in the free energy landscape, especially in 350ns, as shown in Fig.5. Here we use the profile at 320ns to define two shallow wells.

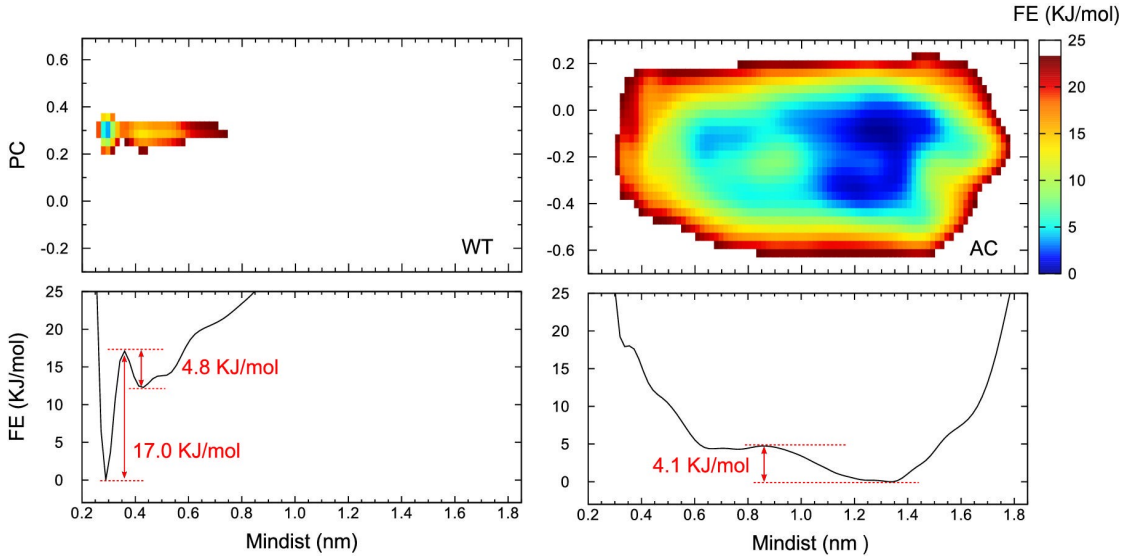

Fig S10. 2-D Free energy (FE) surface after 280ns (for WT) and 300ns (for AC) metadynamics (upper panel), and the projection of free energy on the Mindist dimension (lower panel).

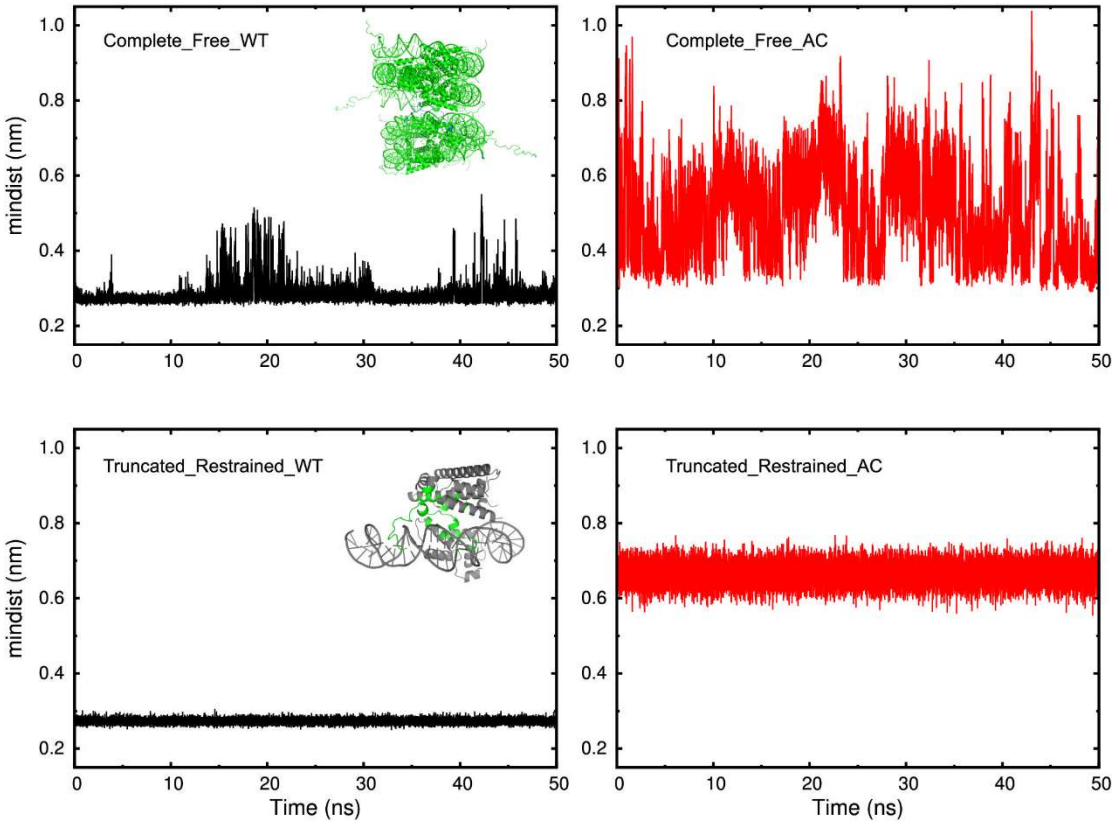

Fig S11. Comparison of the free two-nucleosome system and the restrained truncated system. MD simulations with water and 200mM NaCl were performed for the two-nucleosome system (PDB ID: 1KX5) (Complete_Free_WT/AC), and the model used for REST and metadynamics simulation (Truncated_Restrained_WT/AC). Green part is flexible, gray part is subjected to position restraint. The starting configuration of H4 tail is the representing structure of the WT-1 and AC-1, obtained from the cluster analysis of the REST trajectories. The minimum distance (mindist) between the H4(Ac)K16 and the acidic patch were calculated. The "top" atom of H4(Ac)K16 sidechain (N_ζ of K16, C_θ of AcK16) and the non-hydrogen atoms on H2A-H2B fragment were selected for measurement. WT: black, AC: red. In the free two-nucleosome system, the fluctuation of mindist is larger than that in the restrained system. Nevertheless the K16 is still attached to the acidic patch of the neighboring nucleosome after 50ns, whereas the AcK16 has very unstable binding position, same as the conclusion of the REST simulation.