Supporting Information: Histone H3 N-terminal tail: a computational analysis of free energy landscape and kinetics

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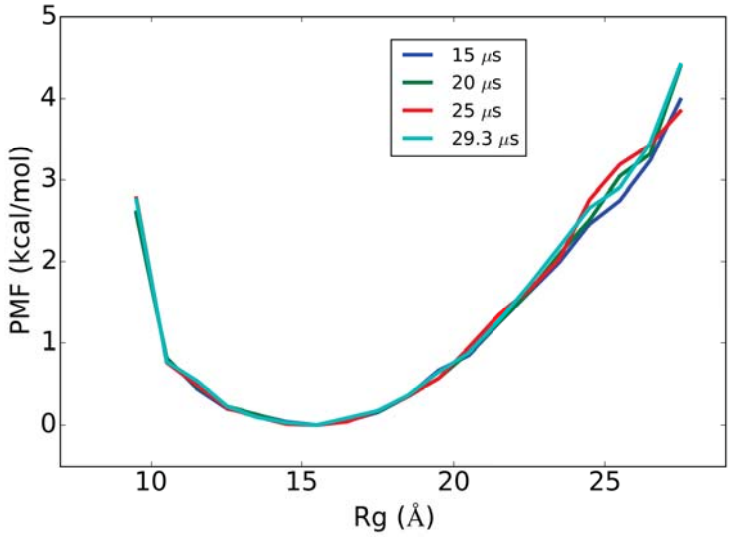

Figure S1: Distribution of R_g when different subsets of sampled trajectories are used.

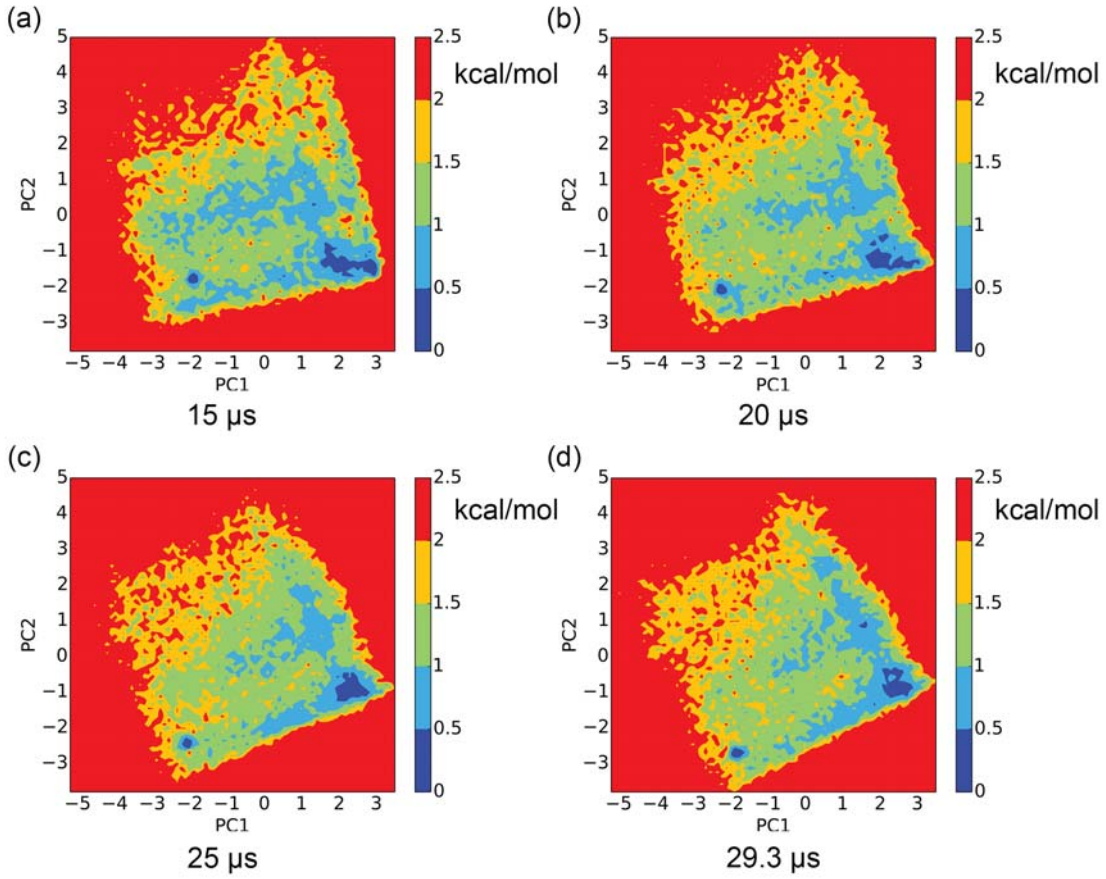

Figure S2: Free energy landscape analyzed with dPCA when different subsets of sampled trajectories are used.

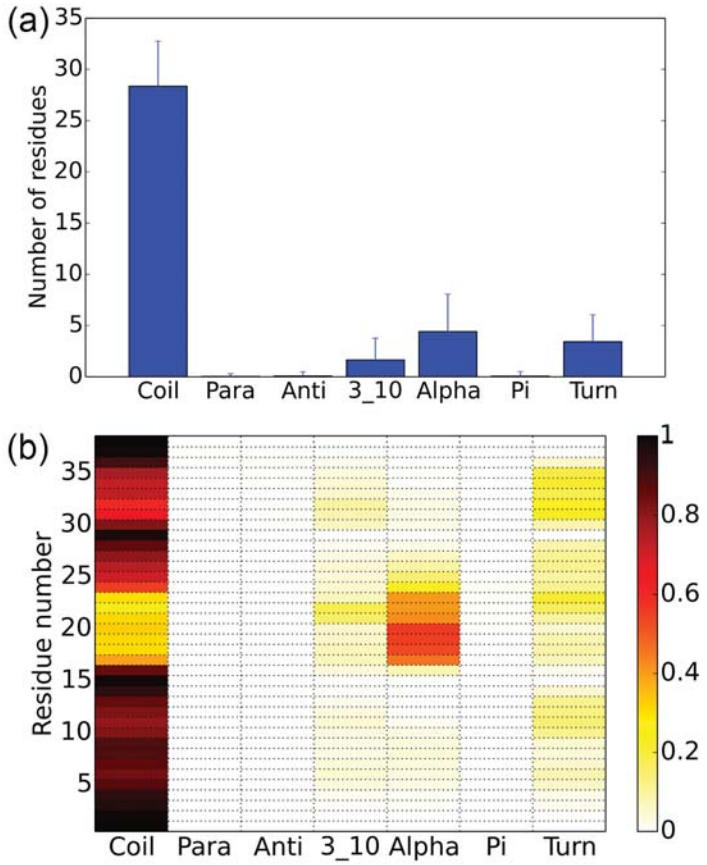

Figure S3: Secondary structure of histone H3 tail in implicit solvent simulations. (a) The average number of residues having a specific type of secondary structure. The error bars show the standard deviation. (b) The probability for each residue to have each type of secondary structure.

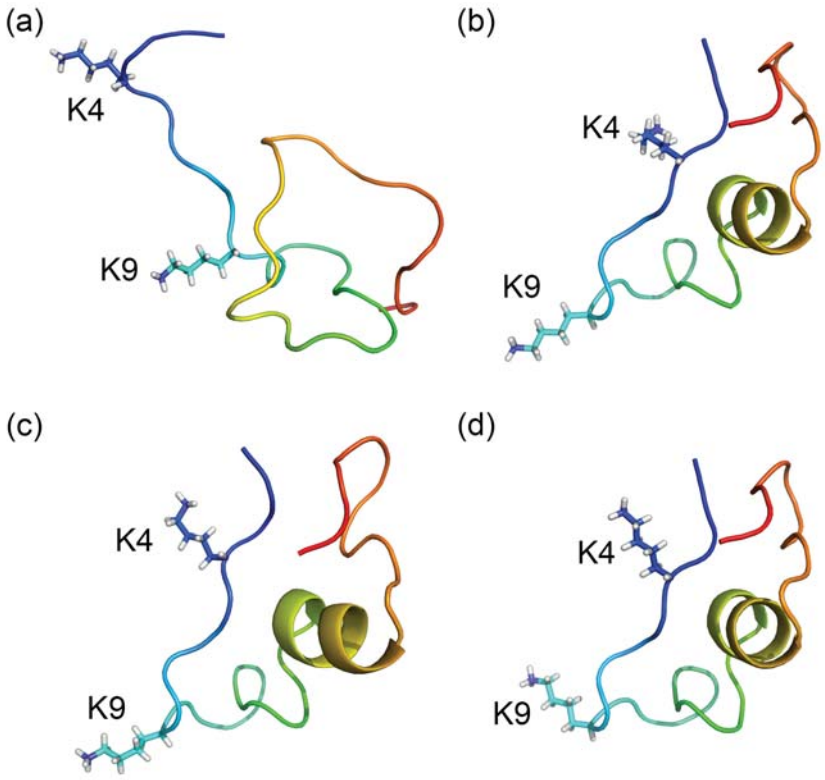

Figure S4: Secondary structure and K4, K9 side chain orientations. The structures are shown in rainbow colors, with blue denoting the N-terminus and red for C-terminus. (a) Representative structure of the 122^{nd} most populated macrostate. (b) Representative structure of the 9^{th} most populated macrostate. (c) Representative structure of basin 'i' on the free energy surface analyzed with dPCA. (d) Representative structure of basin 'i' on the free energy surface analyzed with LSDMap.