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Dissociation Free-Energy Profiles of Specific and Nonspecific DNA–Protein Complexes

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In Figures S1 and S2, behavior of the Lac H1-H3 domain at the points, S_I - S_{III} (specific) and N_I - N_{III} (nonspecific), are characterized. The specific S_I shows lower RMSD (Fig. S1) and smaller orientational fluctuation (Fig. S2) than nonspecific N_I, which confirmed that specific binding is tight and nonspecific binding loose.

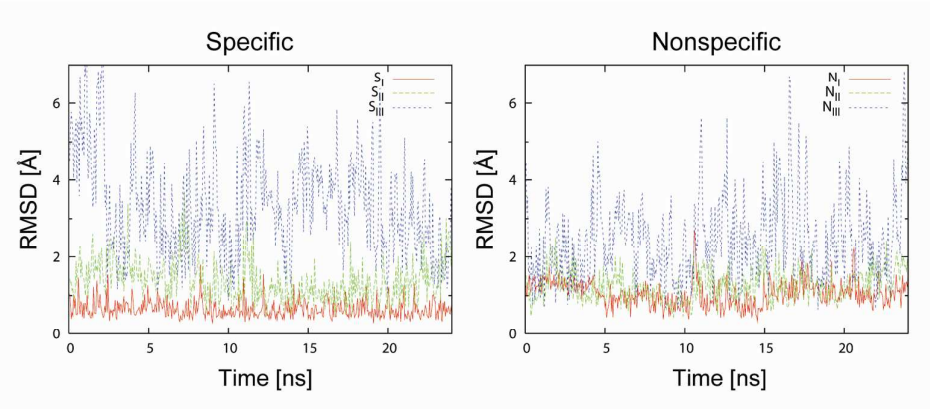

Figure S1. Root mean square deviations for main-chain atoms in the Lac H1-H3 domain (residues 6-45). Shown are the trajectories in each 1 Å window: S_I (12 - 13 Å), S_{II} (15 - 16 Å), S_{III} (25 - 26 Å), N_I (14 - 15 Å), N_{II} (16 - 17 Å), and N_{III} (25 - 26 Å). The reference structure used here was the average structure in each trajectory, which was calculated after the DNA fragment bound to the Lac H1-H3 domain was superimposed.

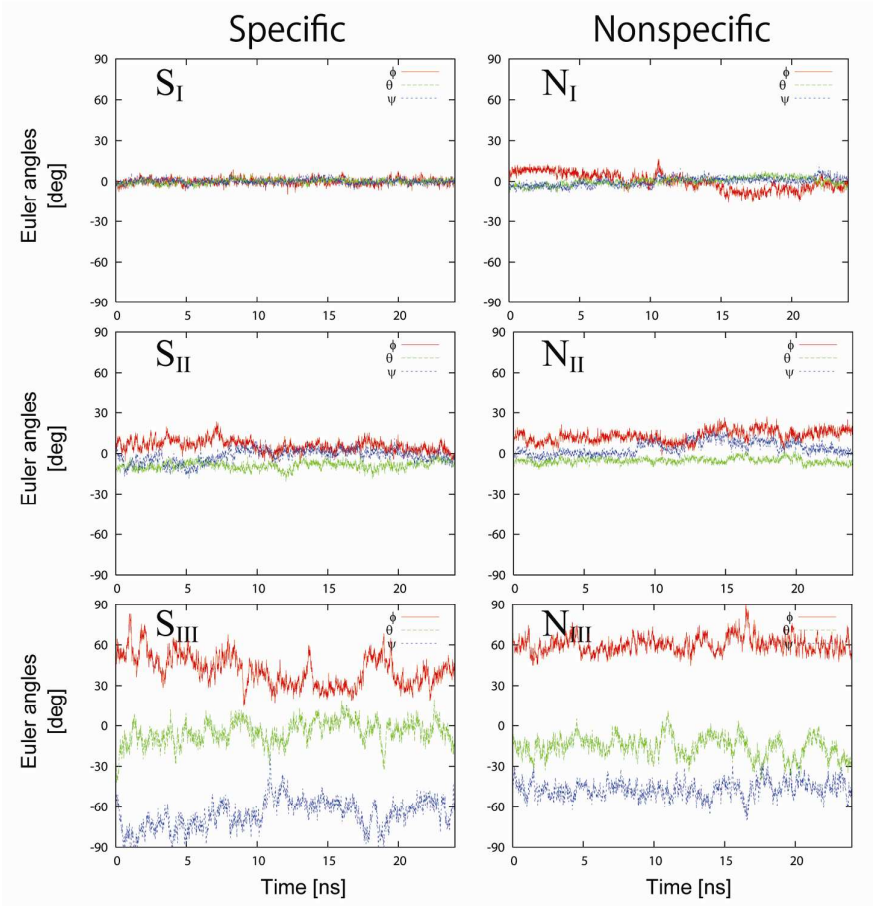

Figure S2. Orientation of the Lac H1-H3 domain. Shown are the trajectories in each 1 Å window: S_I (12 - 13 Å), S_{II} (15 - 16 Å), S_{III} (25 - 26 Å), N_I (14 - 15 Å), N_{II} (16 - 17 Å), and N_{III} (25 - 26 Å). The reference that corresponds to $\phi = \theta = \varphi = 0$ is the average structure at each bound state (i.e., S_I for specific S_I - S_{III} and N_I for nonspecific N_I - N_{III}). The average structure was calculated after the DNA fragment bound to the Lac H1-H3 domain was superimposed. Euler angles ϕ , θ , and φ denote a rotational transformation which makes the reference Lac structure best fit to the current structure. The Euler angles are according to the Tait-Bryan *xyz*-convention (see H. Goldstein, Classical Mechanics, 2nd Ed., 1980, Addison-Wesley).