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Figure S-1. Displacements between C $\alpha$  atoms of the transient structures and the structure averaged over the structures observed during the molecular dynamics simulations of wild-type SNase in vacuo (a) and in water (b). (c) The *B* factors of C $\alpha$  atoms of SNase in the monomeric structure without Ca $^{2+}$  and pdTp (solid line) and in the ternary complex with Ca $^{2+}$  and pdTp (dashed line) determined by the X-ray crystallographic studies (Hynes & Fox, 1991; Loll & Lattman, 1989). At the bottom of each panel, the continuous segments represent  $\beta$ -strands, the dotted segments  $\alpha$ -helices, and the crosses Pro positions.





