



Figure S8. Effect of sampling interval and perturbation frequency on the frequency response of residues in TMD₁. (A) Power spectral density of all residues except $\alpha 7$ sampled at 0.5, 1, 2 and 5 ps intervals. Vertical green dotted lines intersecting the frequency axis at ~ 6 ns⁻¹ represent the upper frequency limit of power spectrum which is assumed to obey $1/f^n$ distribution. (B) Percent of perturbed C _{α} atoms identified using different number of TMD simulation cycles ranging from one to 16.