Lysozyme adsorption on polyethylene surfaces: why are long time simulations needed?

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Supporting Information

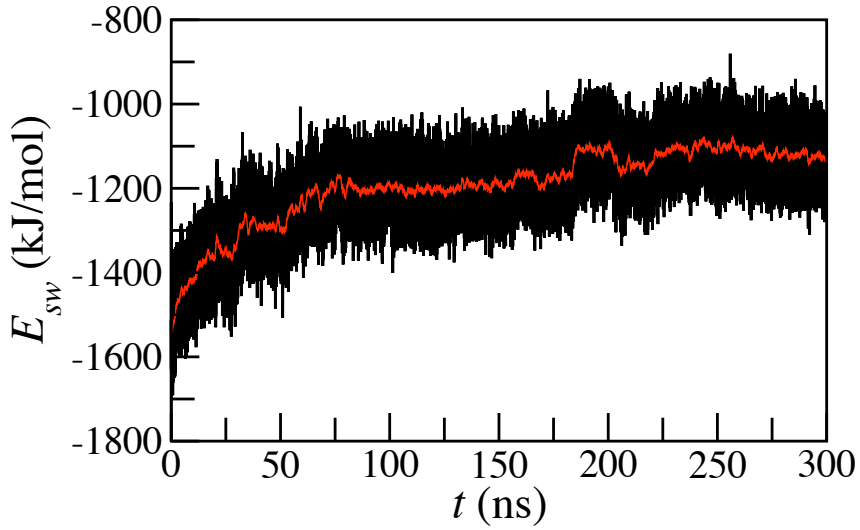

Figure 1: Interaction energy between water and the PE surface as a function of time.

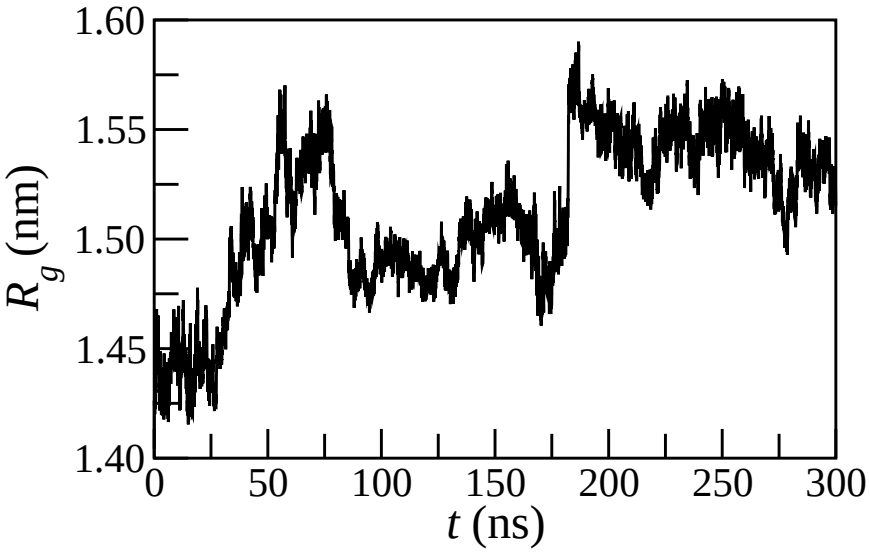

Figure 2: Protein radius of gyration as a function of time.

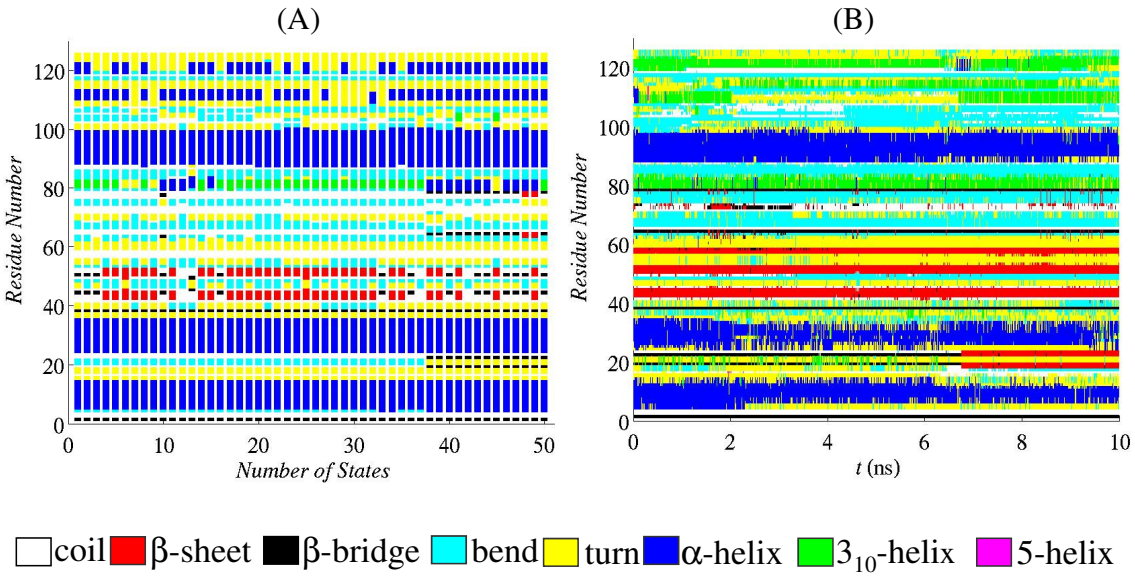

Figure 3: A: Secondary structure of 50 lysozyme as measured by NMR experiments (PDB code: 1E8LA). B: , Secondary structure from the first 10 ns of simulation.