Targeting Electrostatic Interactions in Accelerated Molecular Dynamics with Application to Protein Partial Unfolding

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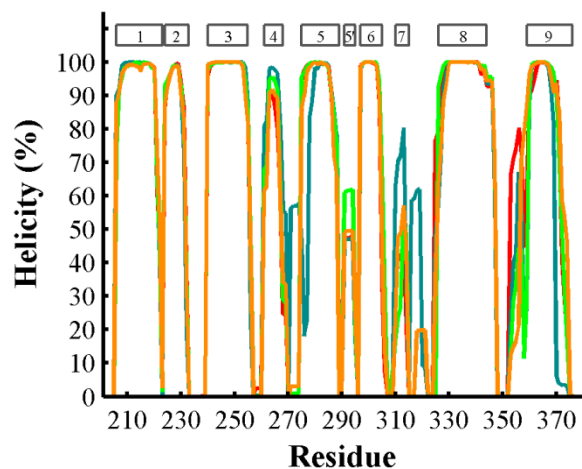
Figure S1. Average helicity content per residue shown as a percentage. Four independent trajectories generated by dual-boost aMD are represented by orange, dark cyan, green and red lines. Helices TH1-9, TH5' are represented by rectangles on the top of the figure. Simulation lengths of all trajectories vary within 140 – 150 ns.