Direct folding simulation of helical proteins using an effective polarizable bond force field

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Figure S1 The radius of gyration (Rg) as a function of MD simulation time using AMBER03/EPB03 (A), AMBER12SB/EPB12SB (B) for 2I9M, Trpcage, 1WN8, C34, N36, 2KES, and 2KHK respectively. Blue lines denote those experimental values.

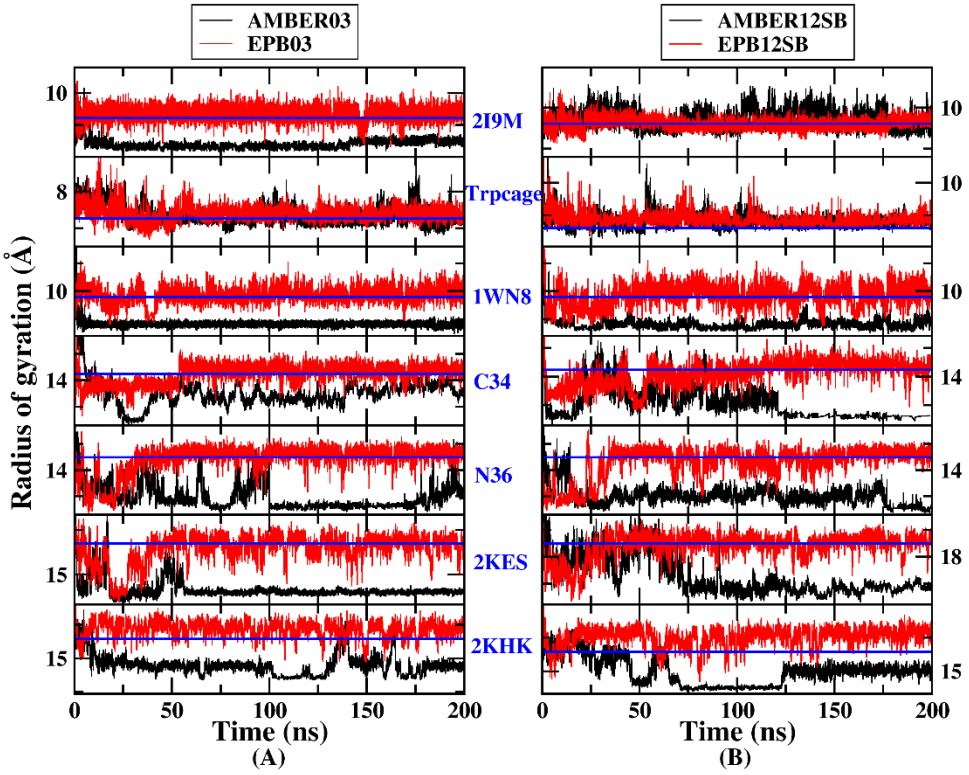

Figure S2 Fractional native helix content averaged every 100 snapshots during MD simulation as a function of time using AMBER03/EPB03 (A), AMBER12SB/EPB12SB (B) for 2I9M, Trpcage, 1WN8, C34, N36, 2KES, and 2KHK respectively.

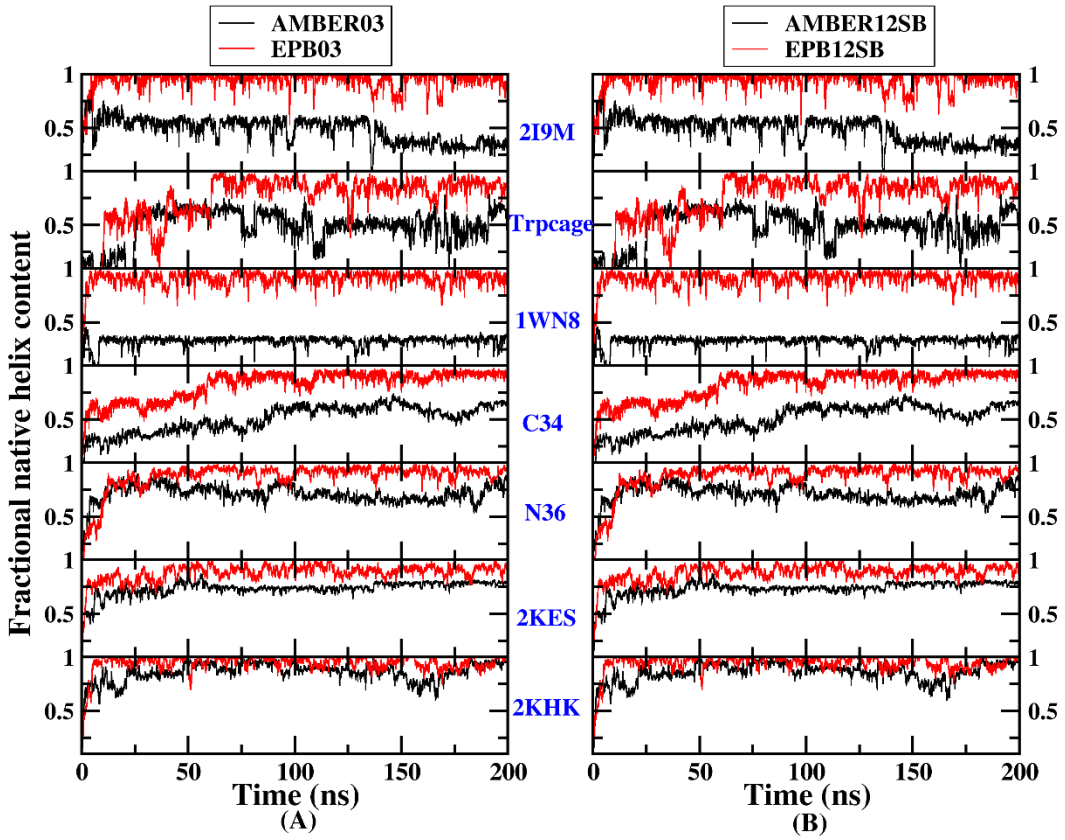

Figure S3 RMSD of backbone atoms as a function of another MD simulation time using AMBER03/EPB03 (A), AMBER12SB/EPB12SB (B) under implicit solvent model for 2I9M, Trpcage, 1WN8, C34, N36, 2KES, and 2KHK respectively.