



Figure S1. Convergence of the data with increasing simulation time for the hairpin as a function of different order parameters (NN and NH on the left and Rg and NH on the right). NN is the number of non-native hydrogen bonds, NH the number of native hydrogen bonds and Rg the radius of gyration. The data for the hairpin converges after 40 ns, with consistent PMF for the time intervals 20-40 ns, 20-60 ns and 20-80 ns. (A) PMF calculated using data between 20-40 ns. (B) PMF calculated using data between 20-60 ns. (C) PMF calculated on data between 20-80 ns.