Unfolding transition state and intermediates of the tumor suppressor $p16^{INK4a}$ investigated by molecular dynamics simulations

Supplementary Material

Gianluca Interlandi, Giovanni Settanni and Amedeo Caflisch

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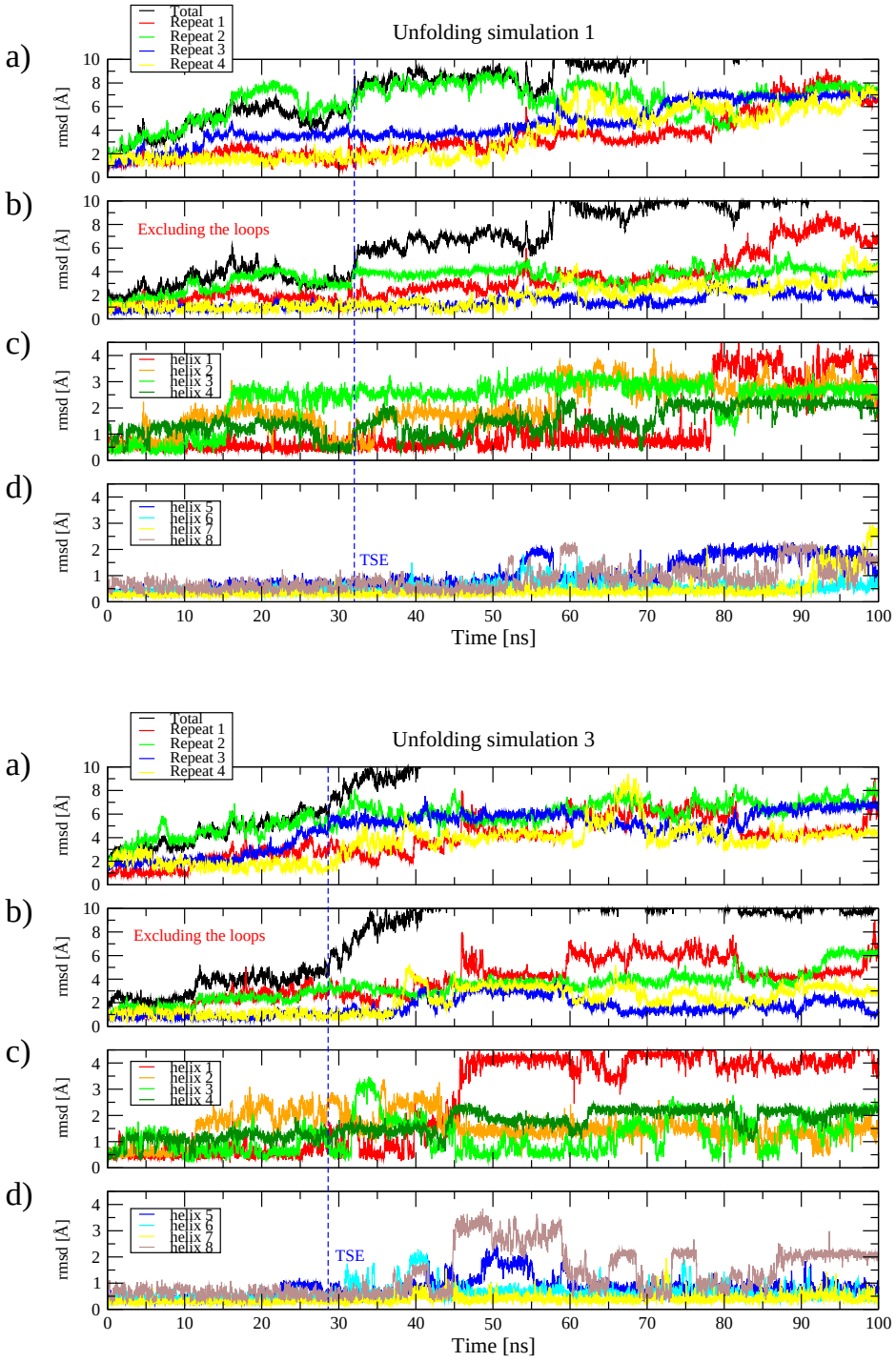

Figure 1: Time series of the C_α rmsd values with respect to the NMR native conformation in US1 and US3. The vertical blue dashed line marks the timepoint in the simulation when the TSE is reached. (a) Total, i. e., all C_α rmsd (black) and C_α rmsd of individual repeats (colored lines). (b) Same as (a) but without loop segments. (c-d) C_α rmsd of individual helices.