

IMPORTANCE OF LOCAL INTERACTIONS FOR THE STABILITY OF INHIBITORY HELIX 1 OF ETS-1 IN THE APO STATE. Aleksandra Karolak, Arjan van der Vaart, Department of Chemistry, University of South Florida, 4202 E. Fowler Ave CHE205, Tampa, FL 33620.

DNA binding induces the unfolding of inhibitory helix 1 (HI-1) in the Ets-1 human transcription factor. To investigate the local interactions that stabilize HI-1 in the apo state, we performed simulations of various Ets-1 constructs. Our results show that the HI-2 and H4 helices stabilize the helical state of HI-1 through specific residue-residue contacts and macrodipolar interactions. The importance of these contacts was verified by simulations on Ets-1 mutants. Our calculations indicate the importance of local interactions for the stability of the HI-1 helix in the apo protein.