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Interaction and dynamics of homologous pairing protein 2 (HOP2) and DNA studied by MD simulation HEM MOKTAN, Oklahoma State University, ROBERTO PEZZA, Oklahoma Medical Research Foundation, DONGHUA ZHOU, Oklahoma State University — The homologous pairing protein 2 (Hop2) plays an important role in meiosis and DNA repair. Together with protein Mnd1, Hop2 enhances the strand invasion activity of recombinase Dmc1 by over 30 times, facilitating proper synapsis of homologous chromosomes. We recently determined the NMR structure of the N-terminal domain of Hop2 and proposed a model of Protein-DNA complex based on NMR chemical shift perturbations and mutagenesis studies (Moktan, J Biol Chem 2014 10.1074/jbc.M114.548180). However structure and dynamics of the complex have not been studied at the atomic level yet. Here, we used classical MD simulations to study the interactions between the N-terminal HOP2 and DNA. The simulated results indicate that helix3 (H3) interacts with DNA in major groove and wing1 (W1) interacts mostly in minor groove mainly via direct hydrogen bonds. Also it is found that binding leads to reduced fluctuations in both protein and DNA. Several water bridge interactions have been identified. The residue-wise contributions to the interaction energy were evaluated. Also the functional motion of the protein is analyzed using principal component analysis. The results confirmed the importance of H3 and W1 for the stability of the complex, which is consistent with our previous experimental studies.

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