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Uncovering the microscopic mechanism of strand exchange during RecA mediated homologous recombination using all-atom molecular dynamics simulations[1] MANISH SHANKLA, JEJOONG YOO, ALEKSEI AKSIMENTIEV, University of Illinois at Urbana-Champaign — Homologous recombination (HR) is a key step during the repair process of double-stranded DNA (dsDNA) breakage. RecA is a protein that mediates HR in bacteria. RecA monomers polymerize on a single-stranded DNA (ssDNA) separated from the broken dsDNA to form a helical filament, thus allowing strand exchange to occur. Recent crystal structures depict each RecA monomer in contact with three contiguous nucleotides called DNA triplets. Surprisingly, the conformation of each triplet is similar to that of a triplet in B-form DNA. However, in the filament the neighboring triplets are separated by loops of the RecA proteins. Single molecule experiments demonstrated that strand exchange propagation occurs in 3 base-pair increments. However, the temporal resolution of the experiments was insufficient to determine the exact molecular mechanism of the triplet propagation. Using all-atom molecular dynamics simulations, we investigated the effect of both the RecA protein and the conformation of the bound ssDNA fragment on the stability of the duplex DNA intermediate formed during the strand-exchange process. Specifically, we report simulations of force-induced unzipping of duplex DNA in the presence and absence of the RecA filament that explored the effect of the triplet ladder conformation.

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