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Structure of RecX protein complex with the presynaptic RecA filament: molecular dynamics simulations and small angle neutron scattering

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Abstract

Using molecular modeling techniques we have built the full atomic structure and performed molecular dynamics simulations for the complexes formed by *E.coli* RecX protein with a single-stranded oligonucleotide and with RecA presynaptic filament. Based on the modeling and SANS experimental data a sandwich-like filament structure formed two chains of RecX monomers bound to the opposite sides of the single stranded DNA is proposed for *RecX::ssDNA* complex. The model for *RecX::RecA::ssDNA* include RecX binding into the groove of *RecA::ssDNA* filament that occurs mainly via Coulomb interactions between RecX and ssDNA. Formation of *RecX::RecA::ssDNA* filaments in solution was confirmed by SANS measurements which were in agreement with the spectra computed from the molecular dynamics simulations.

Keywords: RecX, RecA, Molecular Dynamics, GROMACS, Small Angle Neutron Scattering

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