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

Alexey V. Shvetsov, Dmitry V. Lebedev, Daria B. Chervyakova, Irina V. Bakhlanova, Igor A. Yung, Aurel Radulescu, Aleksandr I. Kuklin, Dmitry M. Baitin, Vladimir V. Isaev-Ivanov

PII: S0014-5793(14)00095-7
DOI: http://dx.doi.org/10.1016/j.febslet.2014.01.053
Reference: FEBS 36417

To appear in: *FEBS Letters*

Please cite this article as: Shvetsov, A.V., Lebedev, D.V., Chervyakova, D.B., Bakhlanova, I.V., Yung, I.A., Radulescu, A., Kuklin, A.I., Baitin, D.M., Isaev-Ivanov, V.V., Structure of RecX protein complex with the presynaptic RecA filament: molecular dynamics simulations and small angle neutron scattering, *FEBS Letters* (2014), doi: http://dx.doi.org/10.1016/j.febslet.2014.01.053

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

Alexey V. Shvetsov[a,c], Dmitry V. Lebedev[a], Daria B. Chervyakova[a,b], Irina V. Bakhlanova[a], Igor A. Yung[a,c], Aurel Radulescu[e], Aleksandr I. Kuklin[d], Dmitry M. Baitin[a,c], Vladimir V. Isaev-Ivanov[a]

[a] *Petersburg Nuclear Physics Institute, NRC Kurchatov Institute, Gatchina, Russia*
[b] *Saint-Petersburg State University, Saint-Petersburg, Russia*
[c] *St.Petersburg State Polytechnical University, St.Petersburg, Russia*
[d] *Joint Centre for Nuclear Research, Dubna, Russia*
[e] *Jülich Centre for Neutron Science outstation at FRM II, Garching, Germany*

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 grove 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

Email addresses: alexxy@omrb.pnpi.spb.ru (Alexey V. Shvetsov), dtry@omrb.pnpi.spb.ru (Dmitry V. Lebedev)