Supporting Information

Liu et al. 10.1073/pnas.0900532106

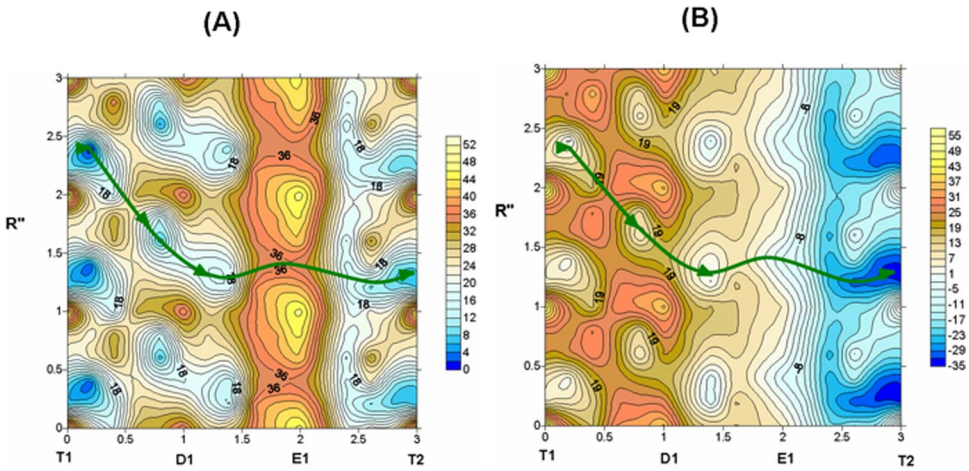


Fig. S1. The effective free energy surface (in kcal/mol) for the translocation process in LTag. (*A*) The PDLD/S −LRA for the interactions of DNA and the LTag helicase . The indexes T1 and T2 designate the same T state but with translated DNA. R″ represents DNA coordinates (see text for details) and Q″ (Q″ = Q/λ_Q; $\lambda_Q = (\hbar/2)\omega_Q\delta_Q^2$) represents the protein structural changes. (*B*) The surface after the adjustment that considers the internal energy of the protein (see text).

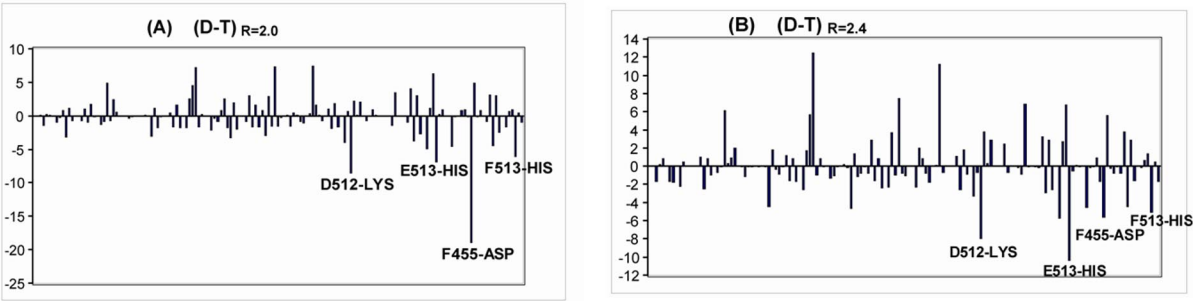


Fig. S2. The effect of different residues on the translocation potential. The bars in each figures shows the difference in the contribution of each residue to the total free energy of the system. (*A*) The different between the residue contributions at R″ = 2.4 and R″ = 2.0, when LTag is in ATP bound state (residues with negative contributions help the translocation process) (*B*) The different in the residue contributions at R″ = 2.4 and R″ = 2.0, when LTag is in ADP bound state (positive contributions help the translocation).

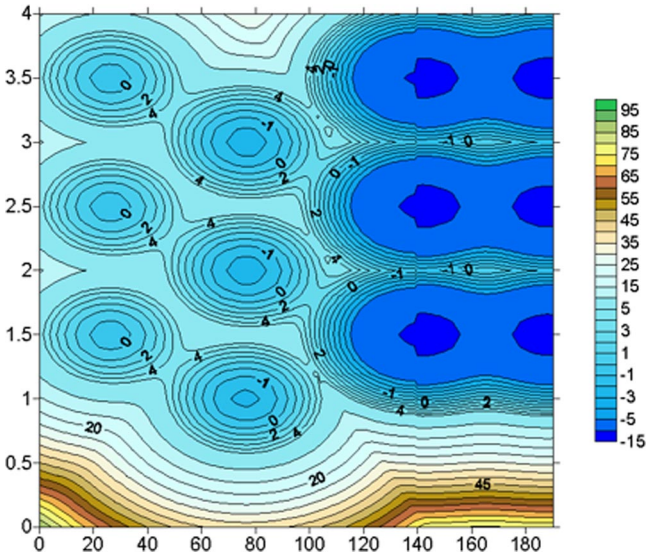


Fig. S3. The simplified surface used in Langevin dynamics simulations. The energies are in the unit of kcal/mol. In the specific example here we have a barrier of 4 kacl/mol for the T to D transition . As stated in the text we examined the effect of different barriers and consider the case with a barrier of 18 kacl/mol as the actual barrier in the system.

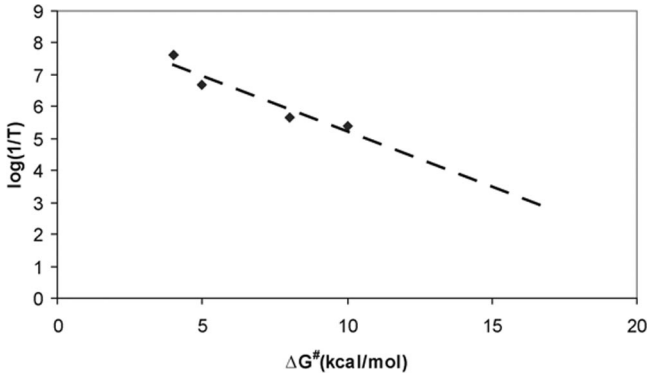
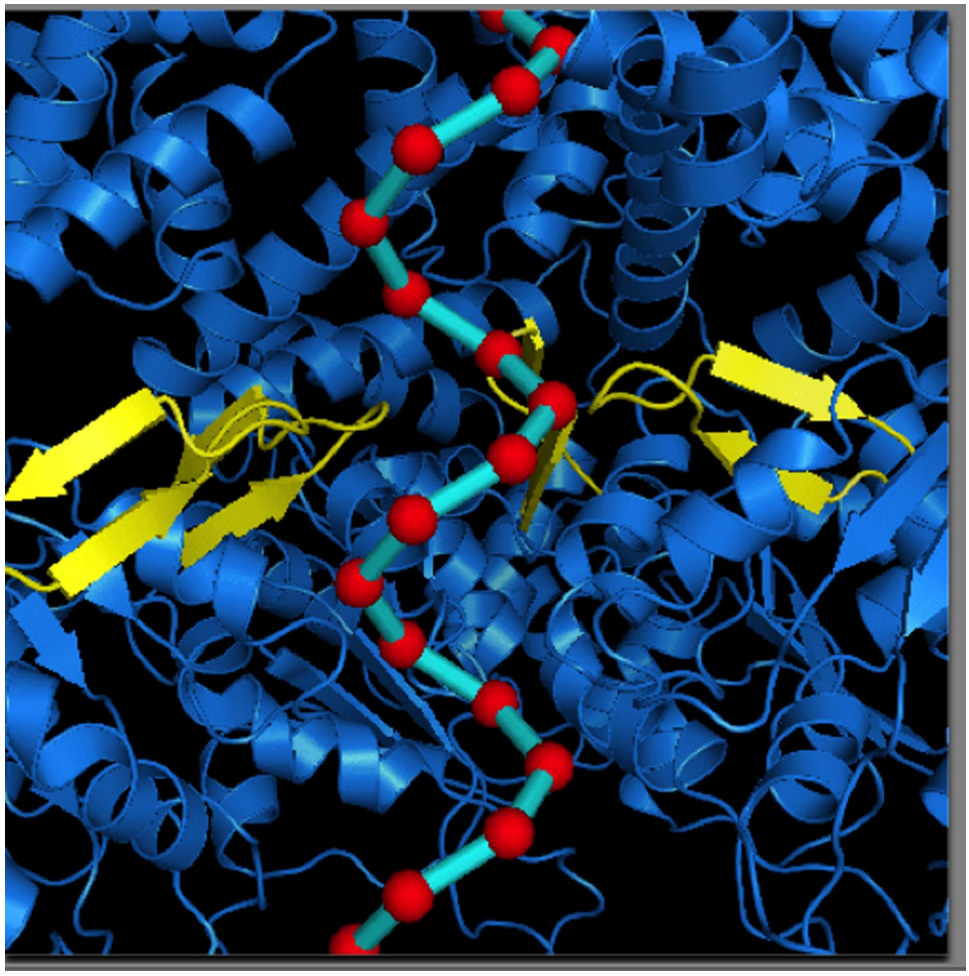


Fig. S4. The correlation between the trajectory time and the activation free energy. The time, T (in seconds) corresponds to the time of translocating a distance of one nucleotide. Interpolating this curve to ≈18 kcal/mol gives a translocation time of ≈0.004 s per nucleotide in a qualitative agreement with the observed trend. The time for a small barrier does not interpolate to picoseconds because the barrier in the R direction is not eliminated.



Movie S1. The simulated translocation of ssDNA in LTag. The LTag hexamer structure is shown in ribbon style, with 2 subunits in the front of the hexamer taken away to reveal the central channel. The beta-hairpins in the channel are in yellow. The DNA strand in the central channel is shown in cyan, with each nucleotide represented by a red sphere. The conformational changes of LTag powered by ATP binding and hydrolysis translocate the DNA unidirectionally.

Movie S1 (MPG)

Other Supporting Information Files

SI Appendix