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Supplemental information

Single-molecule biophysics experiments *in silico*: Toward a physical model of a replisome

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Supplementary Figures

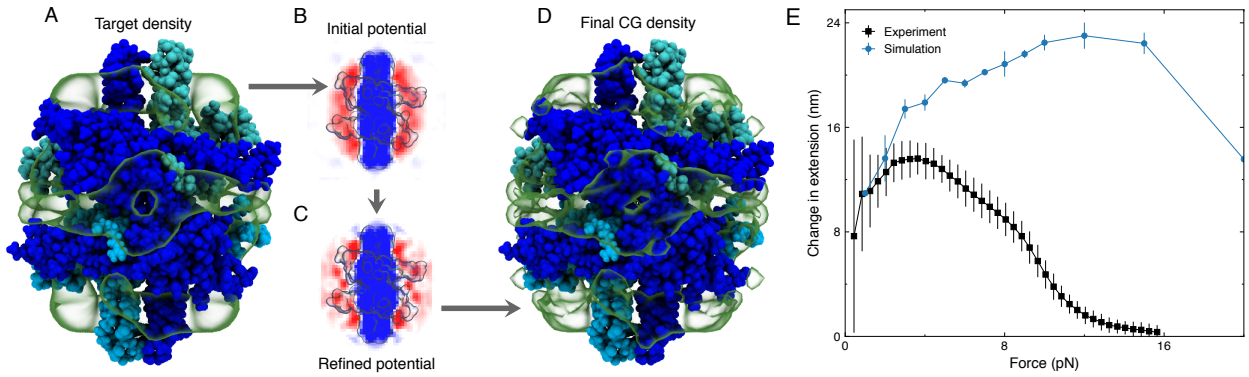

Figure S1: Parametrization of the CG model of single-stranded DNA binding (SSB) protein with naïve application of the IBI protocol, related to Figure 2. (A) Target density of each CG ssDNA bead type was extracted from the mapped trajectory. (B-D) Iterative Boltzmann inversion of the target density. Boltzmann inversion provided an initial estimate for the CG SSB–ssDNA interaction potential (D). Each CG potential was refined until they produced a CG density that matched the target density. The potentials and densities shown are for the P ssDNA beads. (E) Force-extension dependence of an ssDNA–SSB complex. Average change in dT_{70} extension upon SSB dissociation experimentally measured [76] *in vitro* (black) and *in silico* (blue) as a function of applied tension. Each simulated data point was obtained by time-averaging DNA extension and taking the difference between the values obtained with and without SSB, using the potential resulting from the naïve application of IBI.

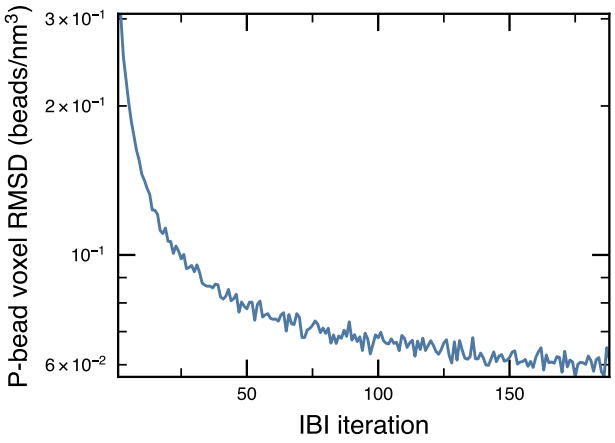

Figure S2: Convergence of the iterative Boltzmann inversion (IBI) protocol, related to Figure 2. The convergence was characterized by the root-mean-square difference between time-averaged target P bead density and bead density obtained from the coarse-grained (CG) simulations performed in accordance with the IBI protocol. The average in the root-mean-square was performed over grid voxels that had values $> 10^{-5}$ beads/nm^3.

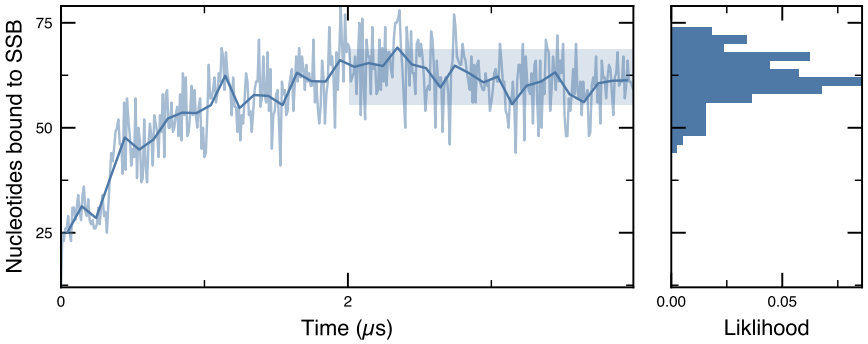

Figure S3: SSB binding a long DNA strand, related to Figure 2. Number of nucleotides from a dT_{150} strand that bind a single-stranded DNA binding (SSB) protein in a CG simulation. The left panel depicts a time series (light blue) of the number of bound nucleotides ant its block average (blue; 100 ns blocks). The shaded region shows the mean and standard deviation after 2 μs of simulation. The right panel depicts a histogram of the data in the left panel after 2 μs (average 62.0 nt). A nucleotide is considered bound to the SSB when its P bead is within 6 Å of any non-hydrogen SSB protein atom. For this analysis, the rigid body transformation for the SSB was applied to the PDB coordinates at each frame of the trajectory.