Electronic supplementary information

Topological frustration leading to backtracking in a coupled folding-binding process

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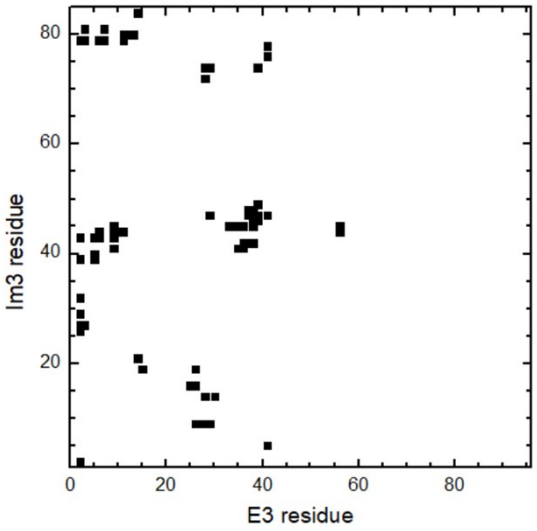

Figure S1　Intermolecular native contacts between E3 and Im3 in the native bound state. The N-terminal segment (residues 1−15) and the central segment (residues 25−41) of E3 form 32 and 35 native contacts with Im3, respectively.

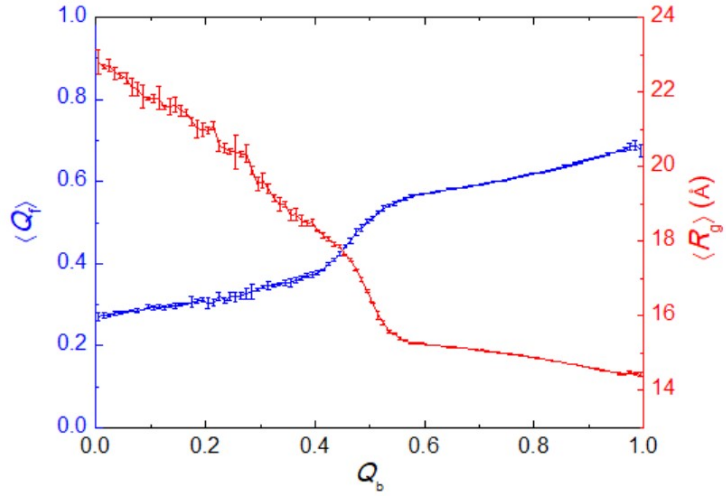

Figure S2. Average fraction of intramolecular native contacts within E3 ($\langle Q_f \rangle$) and radius of gyration of E3 ($\langle R_g \rangle$) at various fraction of intermolecular native contacts between E3 and Im3 (Q_b) for simulation at 0.10 M salt. Errors are standard deviations of five independent simulations.

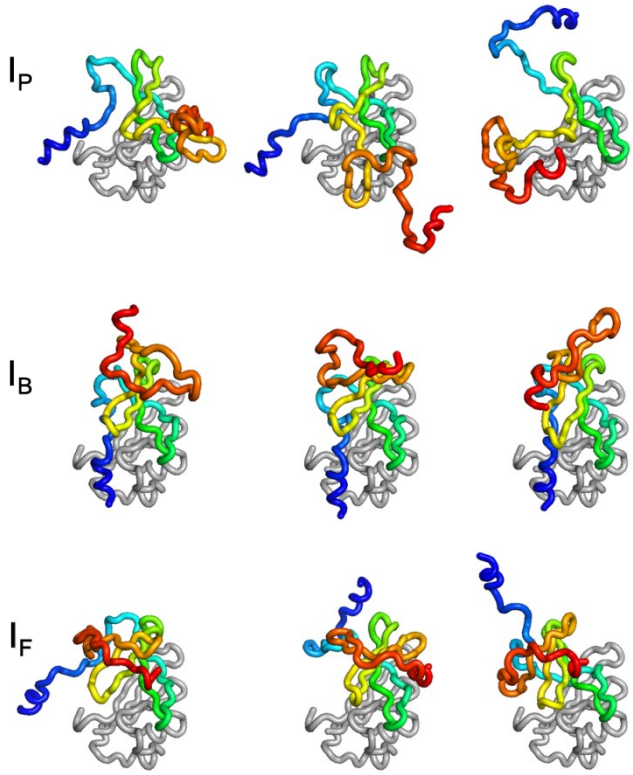

Figure S3. Representative conformations of I_P, I_B, and I_F intermediate states for simulation at 0.10 M salt. E3 is shown in rainbow color and Im3 is shown in gray.

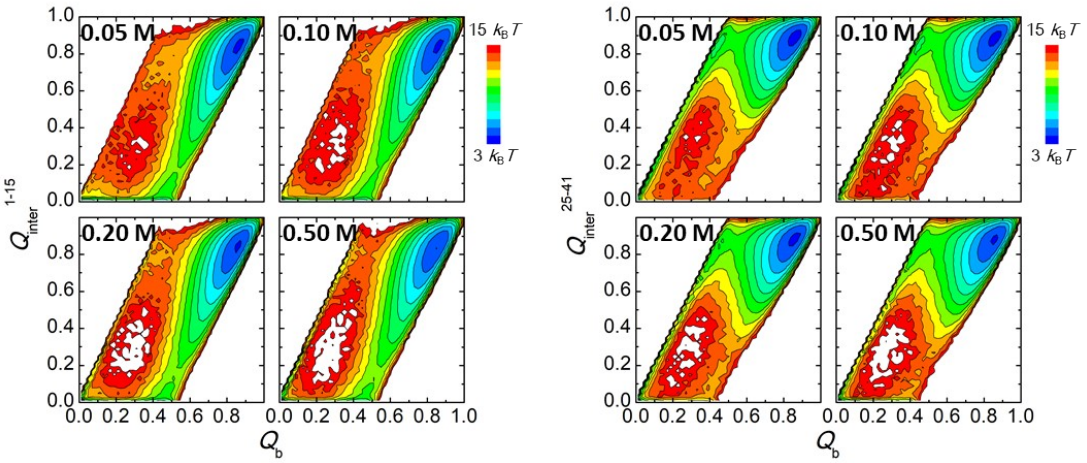

Figure S4 Two dimensional free energy landscapes using the fraction of intermolecular native contacts between E3$^{1-15}$ and Im3 (Q_{inter}^{1-15}), fraction of intermolecular native contacts between E3$^{25-41}$ and Im3 (Q_{inter}^{25-41}), and fraction of intermolecular native contacts between E3 and Im3 (Q_b) as reaction coordinates for simulations at various salt concentrations.

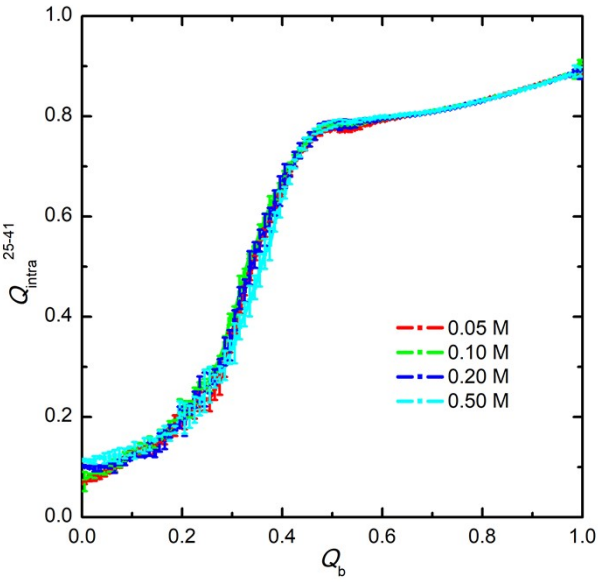

Figure S5 Formation of intramolecular native contacts within $E3^{25-41}$ along the binding process at various salt concentrations. Errors are standard deviations of five independent simulations.

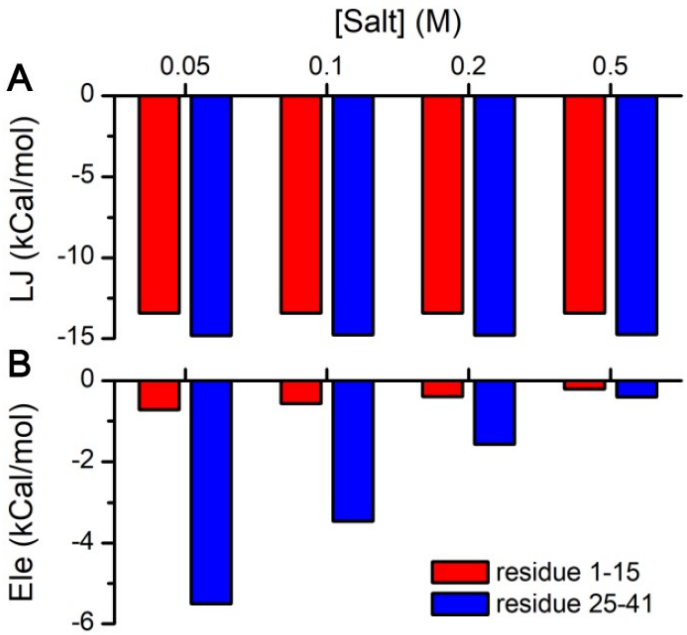

Figure S6 Energetic analysis for the native bound E3/Im3 complex at various salt concentrations. (A) Intermolecular native contact interactions between the two E3 segments and Im3. (B) Intermolecular electrostatic interactions between the two E3 segments and Im3. $E3^{1-15}$ and $E3^{25-41}$ are shown in red and blue, respectively.