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 ($Q_{\text{inter}}^{1-15}$), fraction of intermolecular native contacts between E3$^{25-41}$ and Im3 ($Q_{\text{inter}}^{25-41}$), 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\textsuperscript{1–15} and E3\textsuperscript{25–41} are shown in red and blue, respectively.