

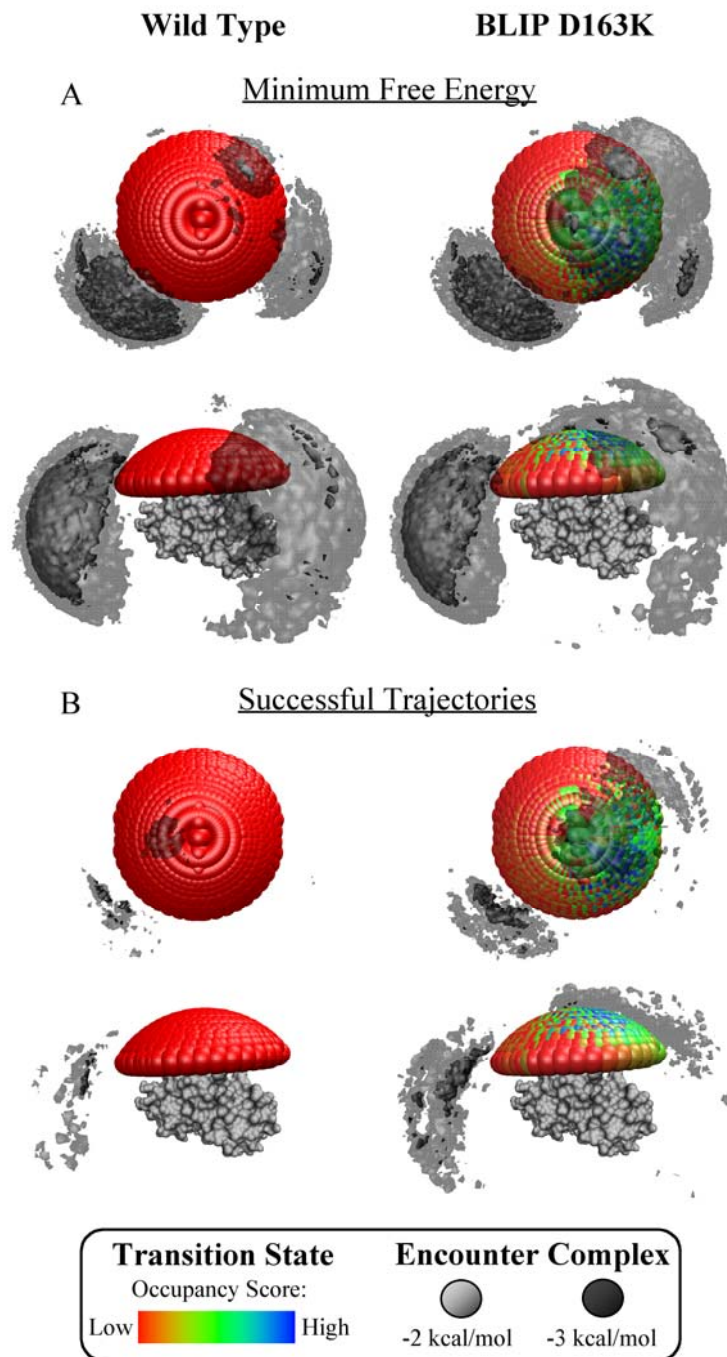
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Supporting Material

Fruitful and futile encounters along the association reaction between proteins

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Supplementary Figure S1



SUPPLEMENTARY FIGURE S1. Superimposition of the transition state occupancy maps and the encounter complex regions of the TEM1-BLIP complex. The cap represents the area of search for the transition state (each orb is the center of mass of one

conformation that was examined), with colder colors representing structures that passed a more stringent cutoff filter. The gray area represents the encounter complex regions, as was examined by Brownian dynamics simulations ($\Delta G < -2$ kcal/mol in light gray, $\Delta G < -3$ kcal/mol in dark gray). (A) Minimal free energy of the encounter complex. (B) Successful trajectories of the encounter complex.