Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Imprints of Function on the Folding Landscape: Functional Role for an Intermediate in a Conserved Eukaryotic Binding Protein

Sneha Munshi & Athi N. Naganathan*

*Department of Biotechnology, Bhupat & Jyoti Mehta School of Biosciences, Indian Institute of Technology Madras, Chennai 600036, India.

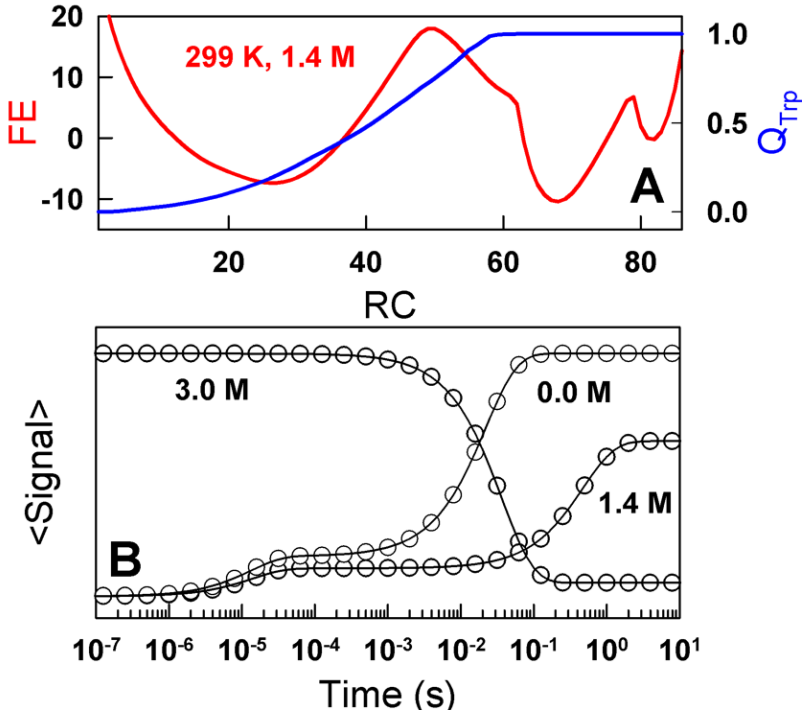

Fig. S1 (A) 1D free energy profile (red in kJ mol^{-1}) and the normalized tryptophan contact probabilities (blue; Q_{Trp}) as a function of the reaction coordinate (RC) the number of structured residues. (B) Simulated kinetic phases from the 1D free energy profile at the indicated final GuHCl concentrations (circles) and the fit to single- (3 M) or double-exponential functions (0 M and 1.4 M).

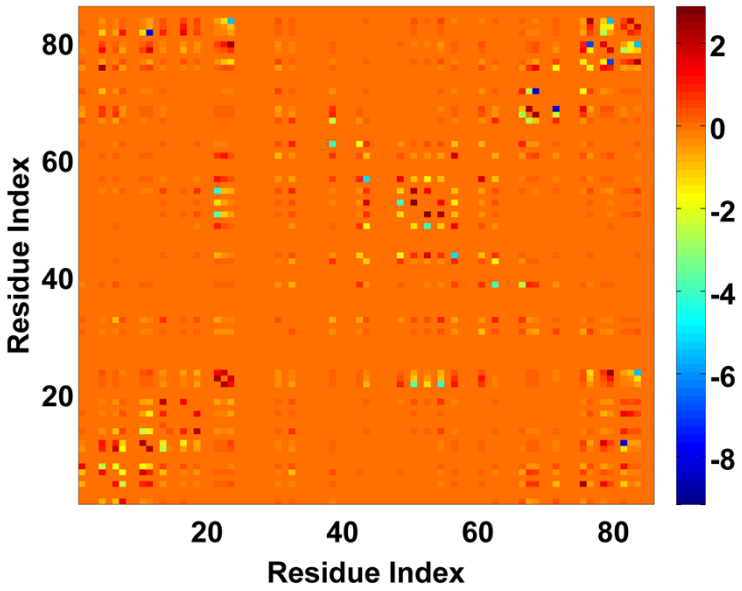

Fig. S2 Symmetric 2D map of the apo-ACBP charge-charge interaction energy (in kJ mol^{-1}) as estimated from the Tanford-Kirkwood (TK) algorithm.

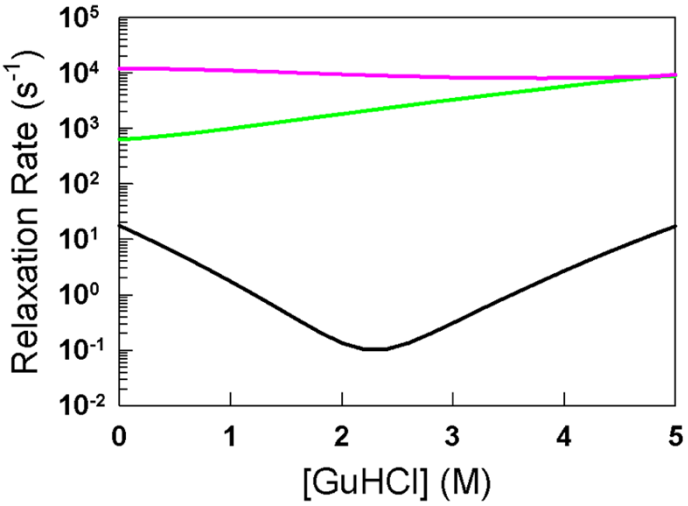

Fig. S3 The chemical denaturant dependence of the three rates (shown in black, green and magenta following the color code in Figure 4B) predicted from the Eigen values of the rate matrix at 278 K.