

The network of the 70% most relevant folding pathways for PinWW. The numbers on the left indicate the committor probabilities, the thickness of the arrow indicates the flux of folding trajecto-

traps:

ries between each pair of conformations. For each conformation, a representative mean structure is shown in color along with an overlay of equilibrium-distributed structures from that conformation indicating the structural flexibility (gray cloud). The numbers next to the arrows give the normalized net flux (large number) and the 80% confidence-interval limits (small numbers) in percentages. The blue numbers next to the structures indicate whether the first/second hairpin has the native register (0), is register-shifted by one or two residues (1,2) or is not formed at all (-). (Lower Right) Register-shifted trap states that do not carry significant folding flux but reduce the folding speed by nearly a factor of 2.

Fig. 3. PinWW folding flux. (Left)