

Figure S7: Umbrella sampling data and biased statistics. Individual pmfs associated to 4 independently conducted umbrella sampling simulations and the biased probability distributions (histograms) obtained from individual windows that stratify the  $\xi$  space, for TadA\*0.1-RNA (A), TadA\*1.1-RNA (B), TadA\*0.1(L84F)-RNA (C), and, TadA\*1.1(L84F)-RNA (D) complex. In each pmf profile the shaded region indicated the standard deviation of the individual pmfs and the error bars are the error calculated using block averaging method for individual windows.