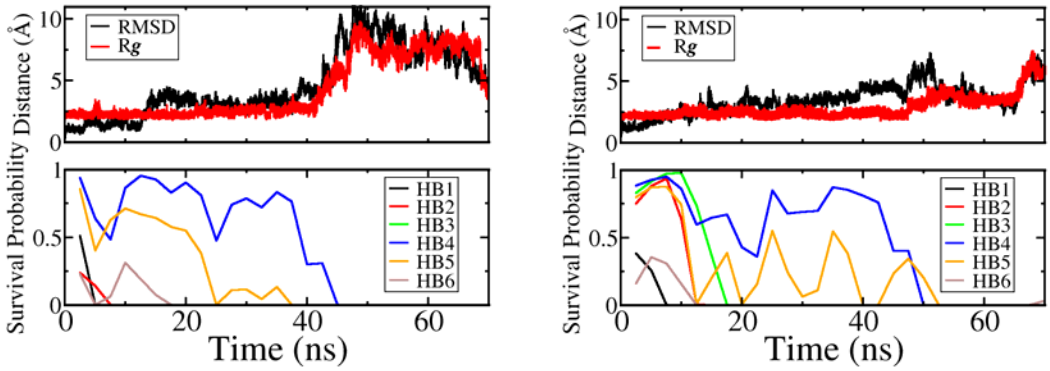
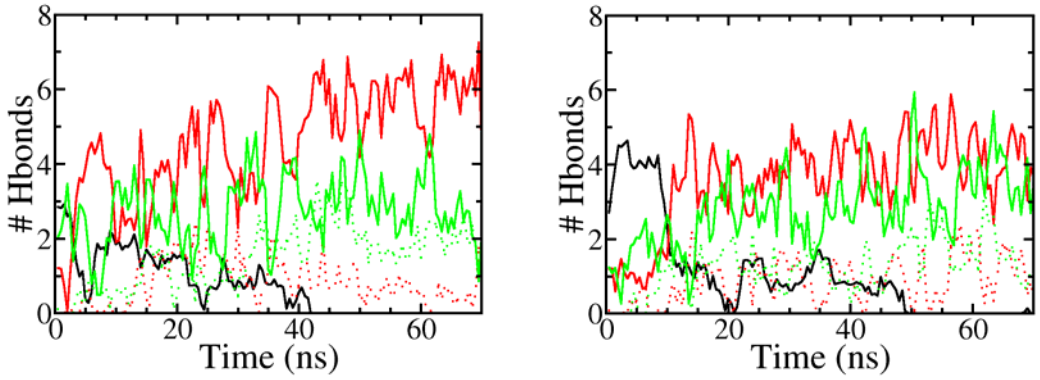


(a) (b)

Fig. S1 (a) and (b) (Two additional trajectories showing the hydrogen bond breaking for peptide 1) Top panel: the RMSDs of the backbone heavy atoms ((N, C and C_α) and radius of gyration (R_g) of the hydrophobic residue: Ile5 and Trp11 in peptide 1 with reference to the starting structure during the two other simulations; bottom panel: the survival probability of individual native hydrogen bonds;



(a) (b)

Fig. S2 (a) and (b) Additional trajectories: The breaking and formation of all native backbone hydrogen bonds: black (the number of backbone hydrogen bonds); red (the number of hydrogen bonds formed with water); green (the number of hydrogen bonds formed with urea). The solid lines represent hydrogen bonds in which water or urea serve as the hydrogen donors and the dashed ones are for hydrogen bonds in which water or urea are proton acceptors.