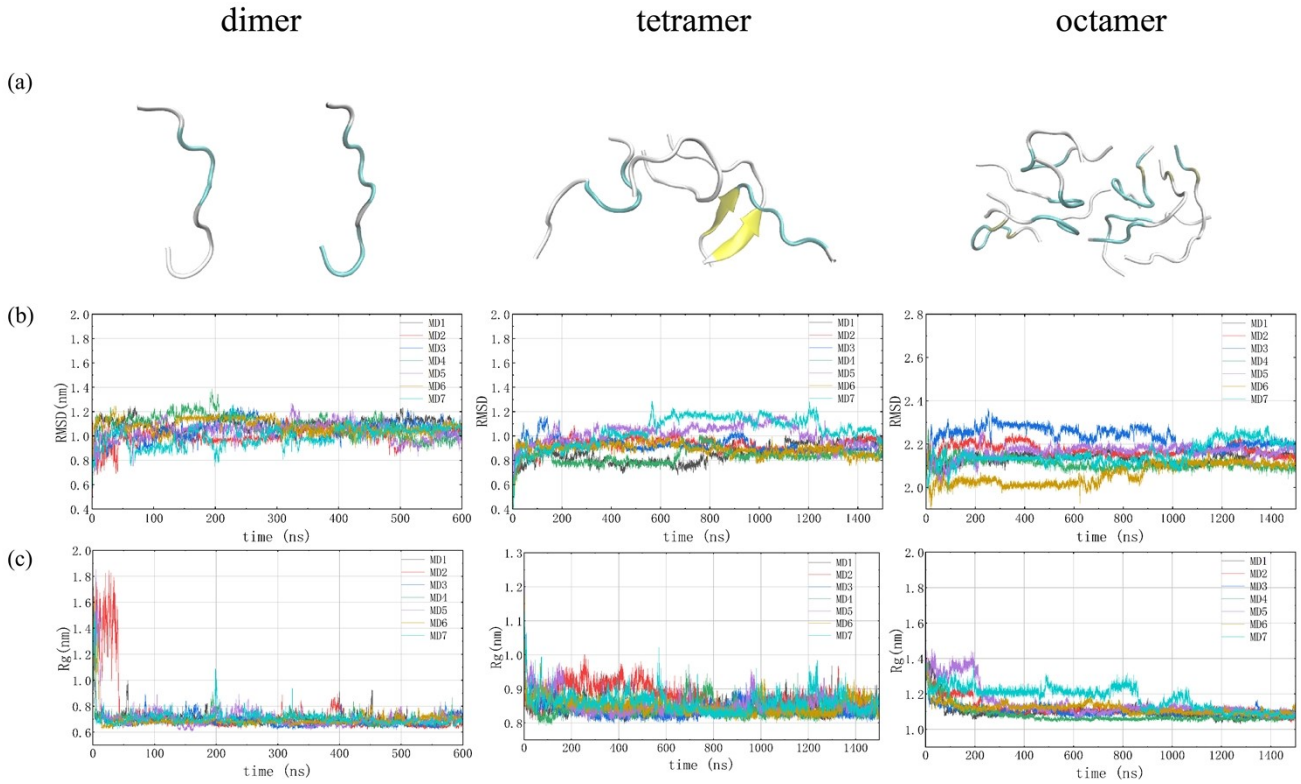

Fig. S1 RMSD, Rg and initial structure of different systems of NACore (68-78). (a) Images of RMSD over time for dimer, tetramer, and octamer. (b) Images of Rg of dimer, tetramer, and octamer as a function of time. (c) Initial structures of different systems.

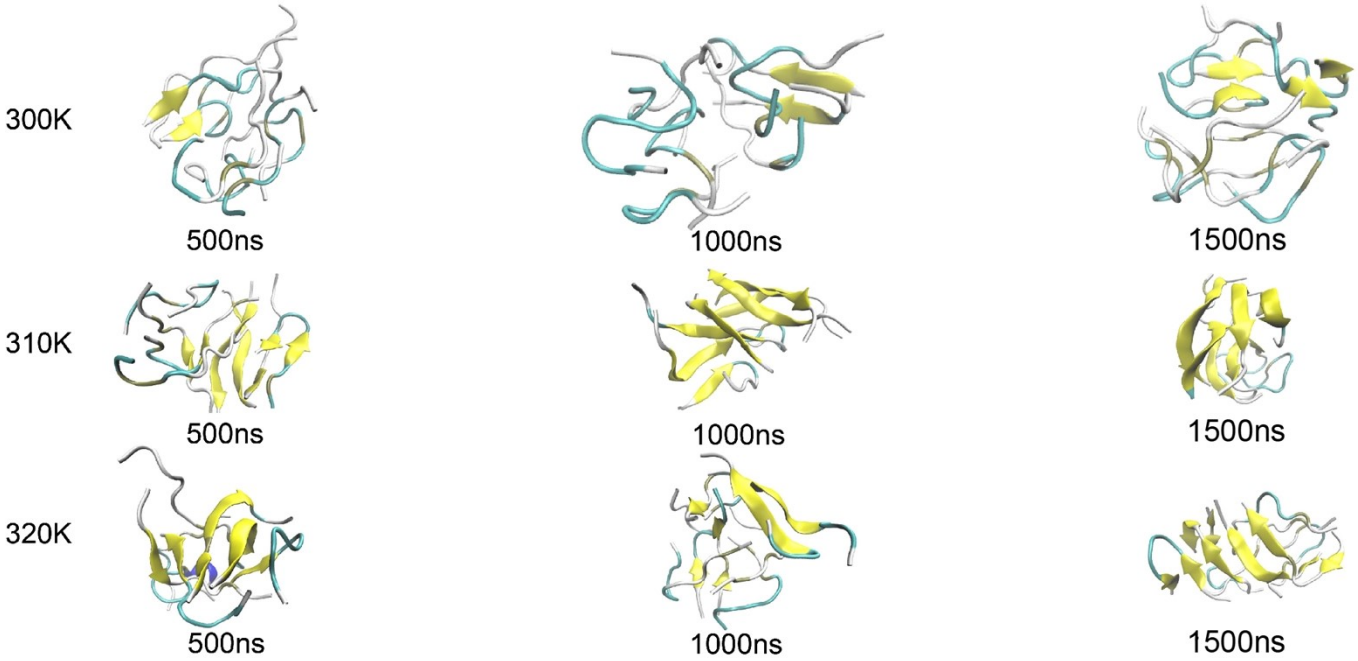

Fig. S2 Snapshots of oligomeric assemblies were captured at intervals of five hundred nanoseconds across temperatures of 300K, 310K, and 320K.

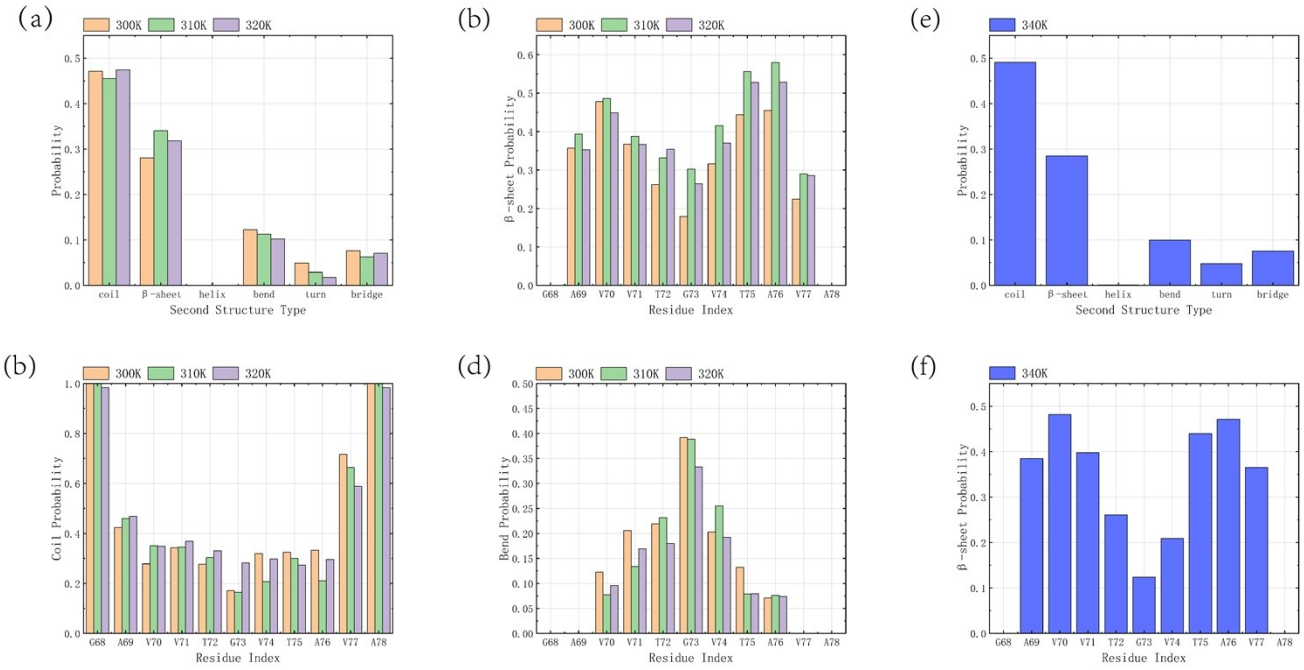

Fig. S3 Secondary structure analysis of NACore (68-78) at different temperatures.

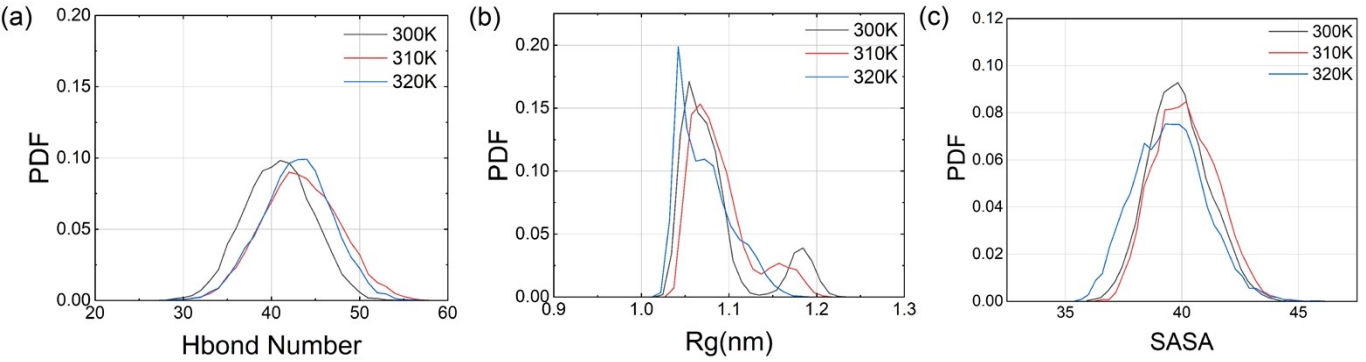

Fig. S4 The probability distribution function of the number of hydrogen bonds, the radius of gyration and SASA in each system.

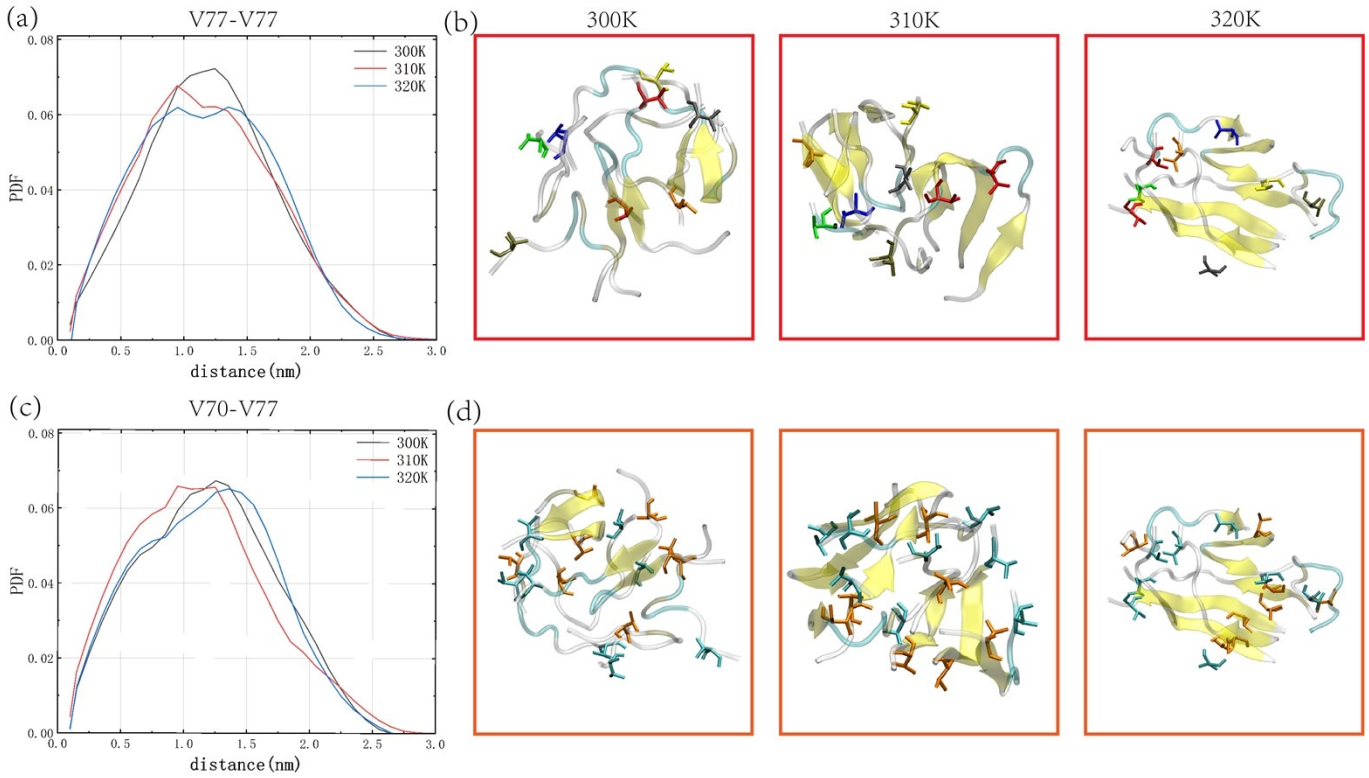

Fig. S5 Distance transformations between two residues that may affect β-sheet formation at different temperatures. (a,c) The PDF curve of the V77-V77 and V70-V77 distance. (b,d) Representative snapshots of NACore octamers at different temperatures. It is shown that both V70-V77 and V77-V77 are more compact at 310K.

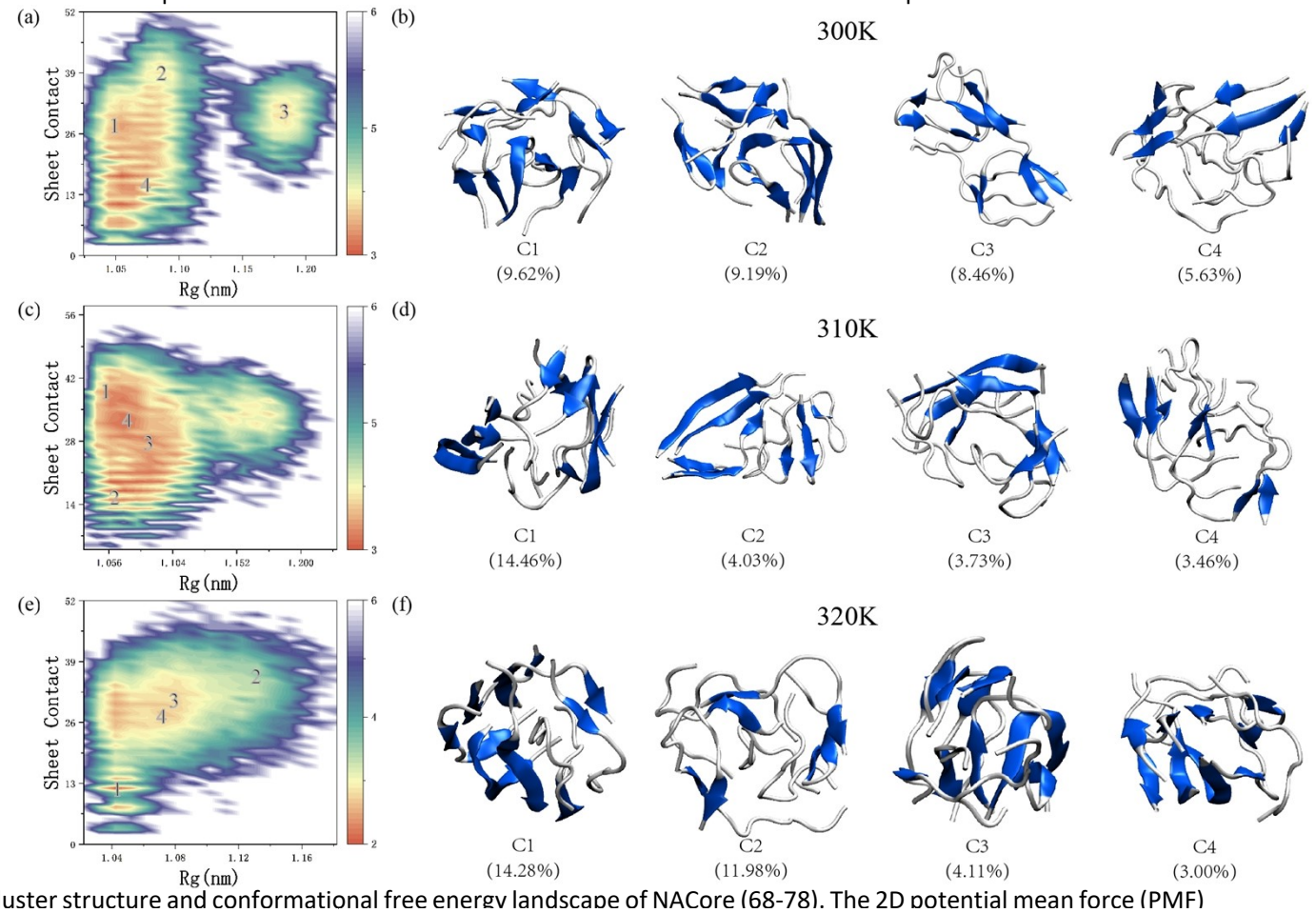

Fig. S6 Cluster structure and conformational free energy landscape of NACore (68-78). The 2D potential mean force (PMF) as a function of radius of gyration (Rg) and β-Sheet contact at 300K (a), 310K (c) and 320K (e). (b, d, f) Representative conformations of the top four most populated clusters for 300K, 310K and 320K systems.

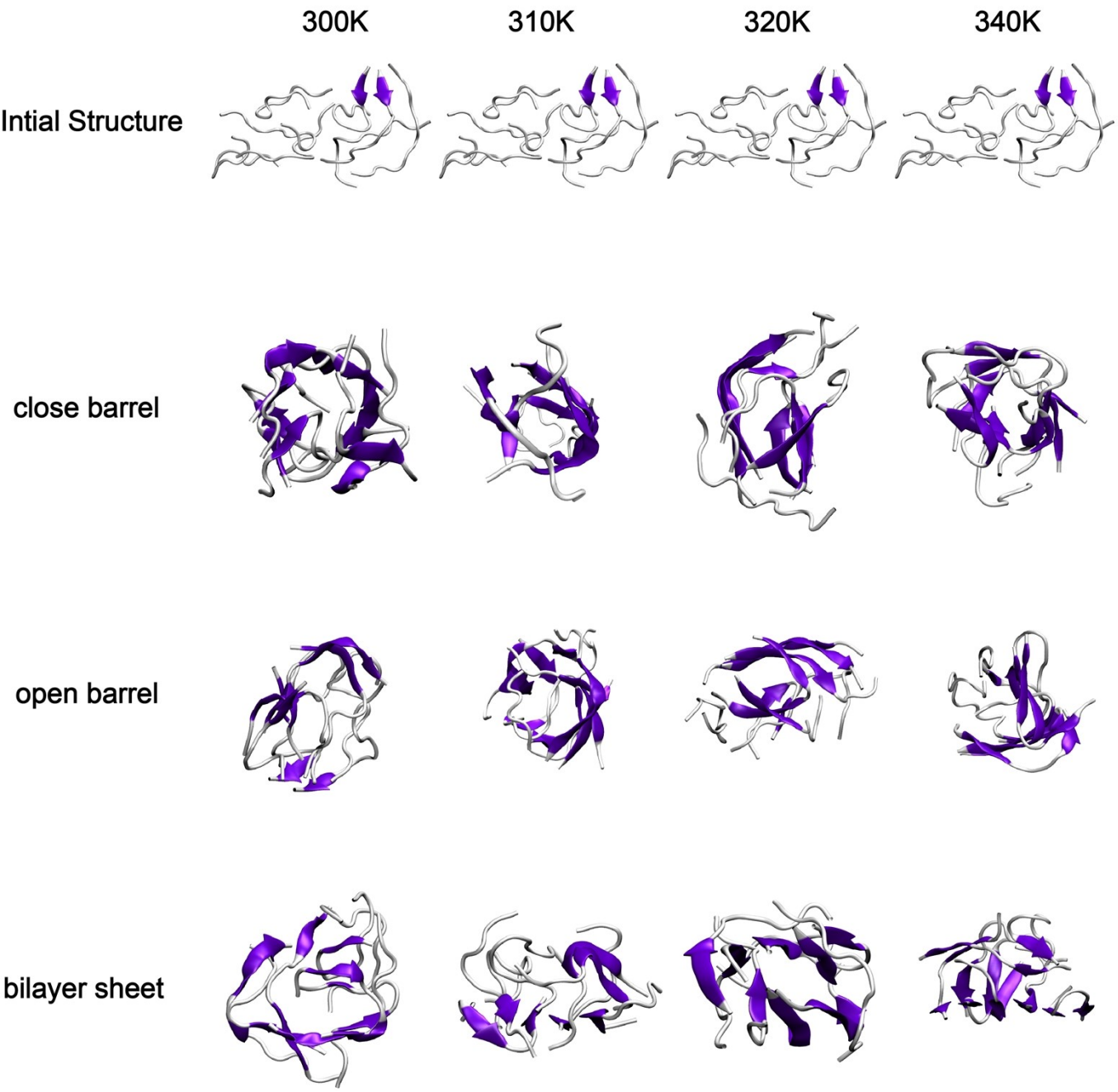

Fig. S7 Snapshots of representative structures of different reaction coordinate in 300K, 310K, 320K and 340K systems.

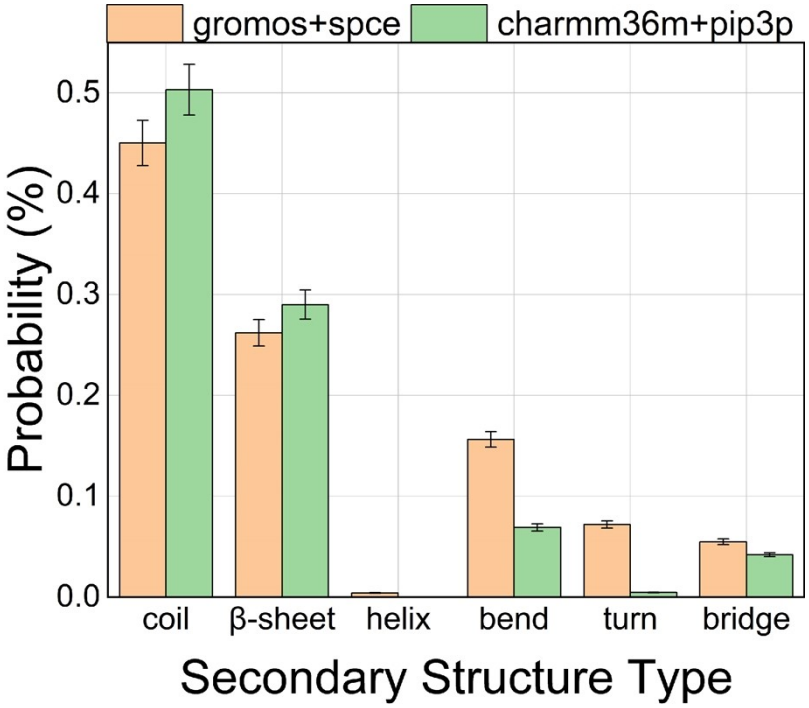

Fig. S8 At 310K, the average distribution of the secondary structure of the NACore octamer under two different force fields and different water models.

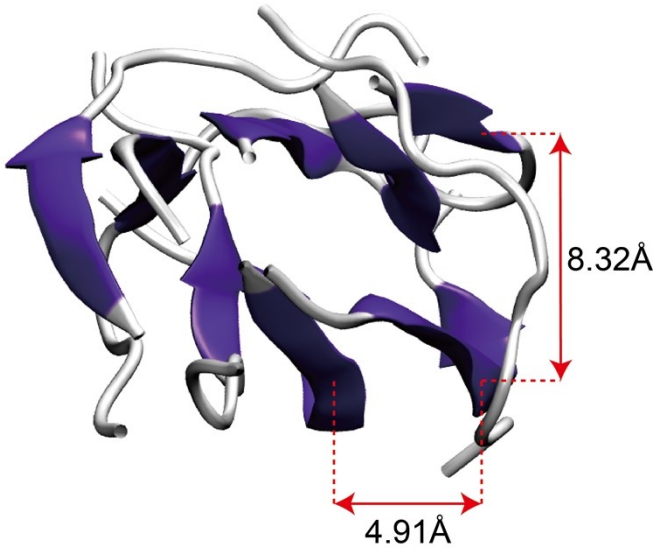

Fig. S9 Representative structures of NACore. The intermolecular distances between the β-strands and between the β-sheets are 8.32 Å and 4.91 Å, respectively.