

Supplementary Materials

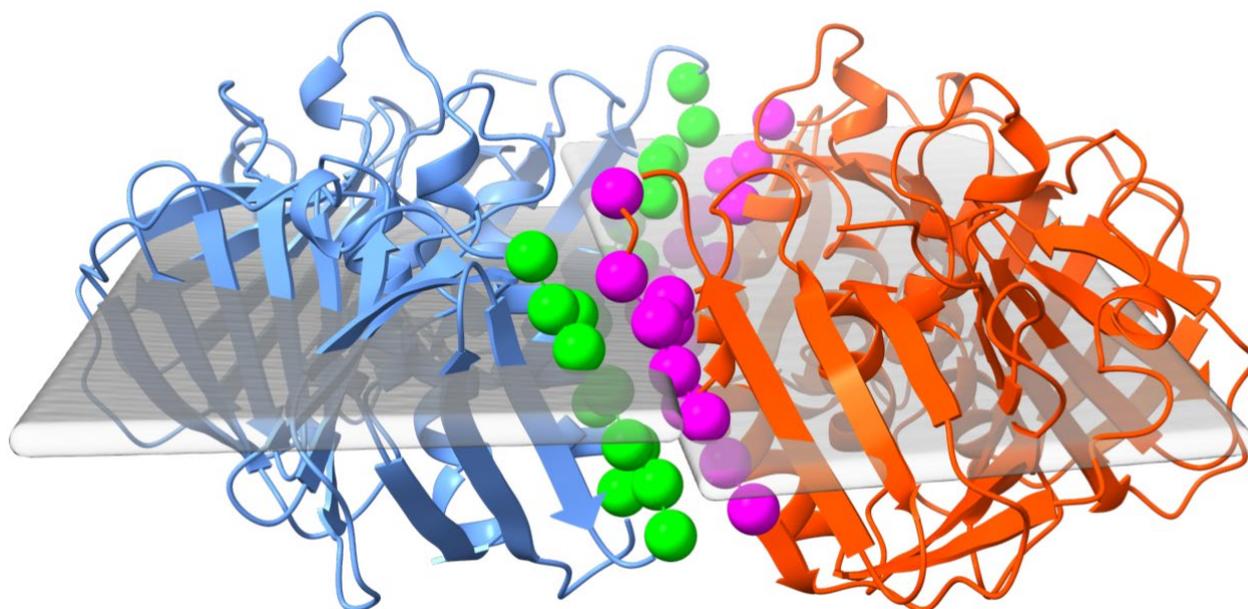


Figure S1. The two subunits of the clamp are shown in orange and blue cartoon. Groups of C atoms used to measure the distance at each interface are shown in purple and green spheres. Imaginary planes that pass through residues 75, 169, 267 and residues 441, 535, 633 are shown in gray and were used to monitor the angle between the two subunits.

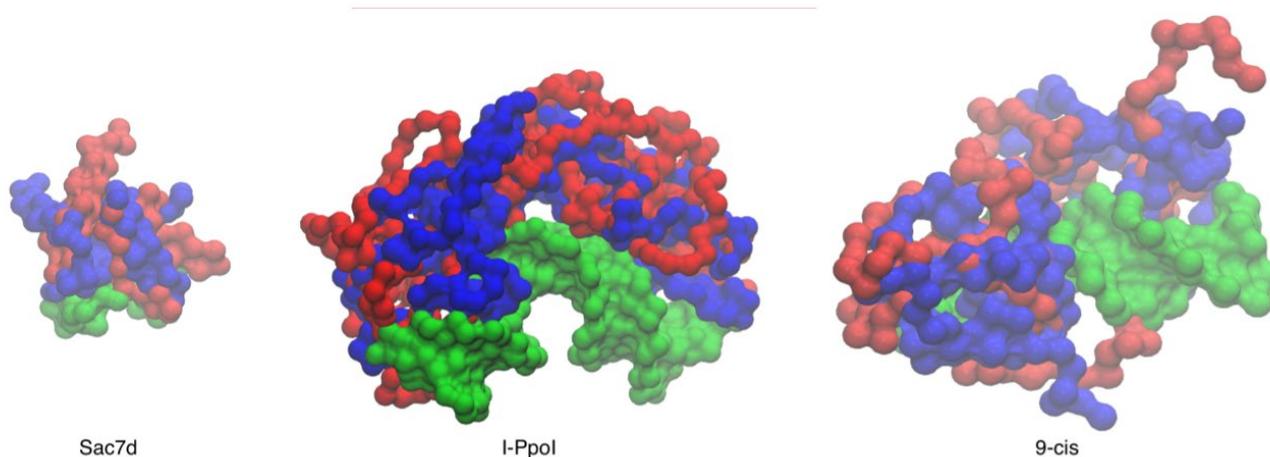


Figure S2. Three small transcription factor systems sampled for 10 μ s with SIRAH in explicit solvent and clustered on the latter half of the trajectory. Clusters are superposed on the reference structure with alignment on the C5X beads of DNA. Green shows DNA in reference conformation, blue is the reference protein. Red is the first cluster from the trajectory.

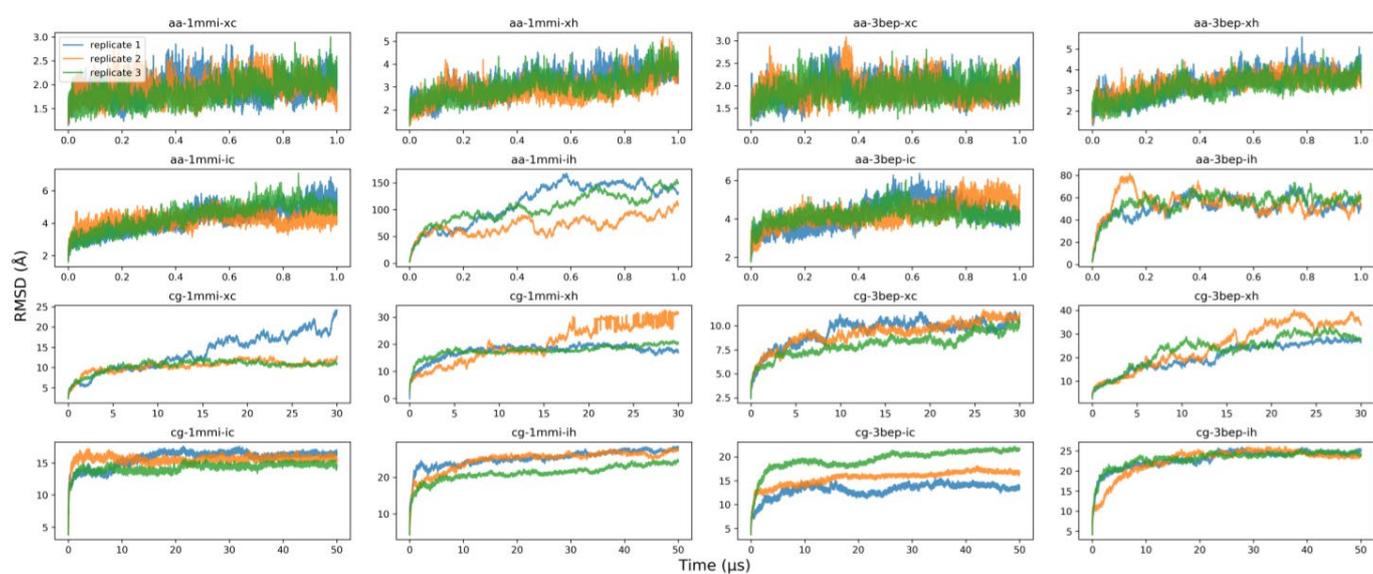


Figure S3. RMSD of the whole clamp protein. The three replicates are shown in blue, orange and green. aa = all-atom, cg = coarse grain, i = implicit solvation, x = explicit solvation, c = cold (298K), h = hot (368K), 1,2,3 = replicate number.

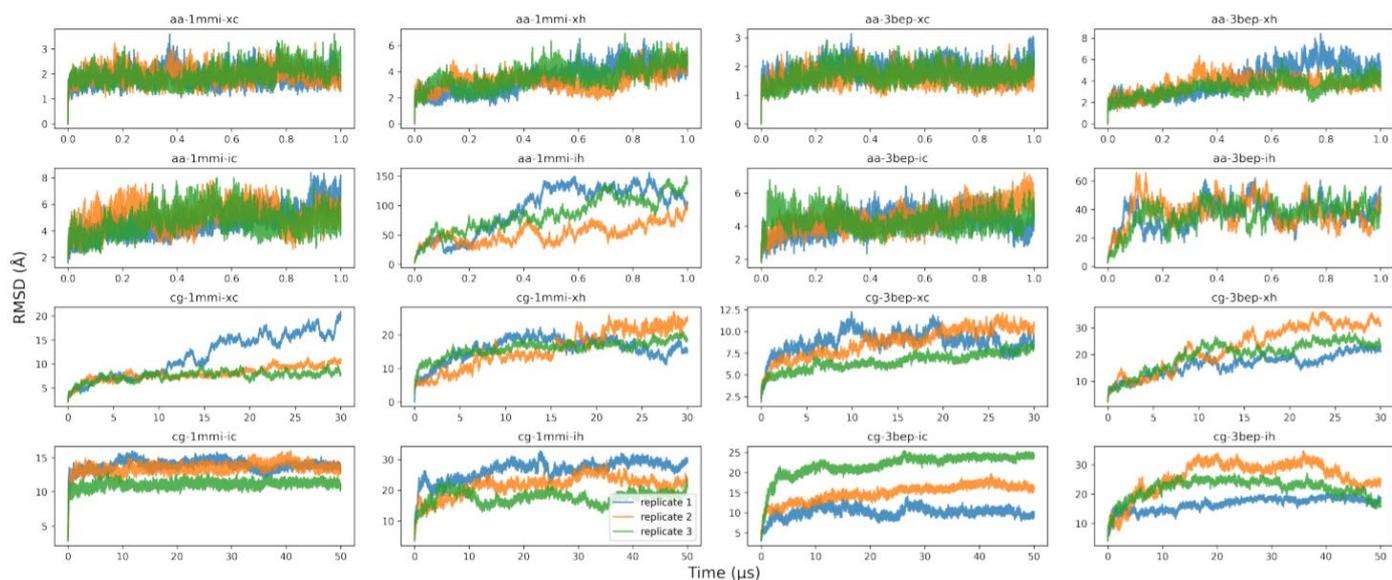


Figure S4. RMSD of the loop region in non-MELD systems. Notice the increased values at room temperature in all-atom implicit systems compared with explicit systems.

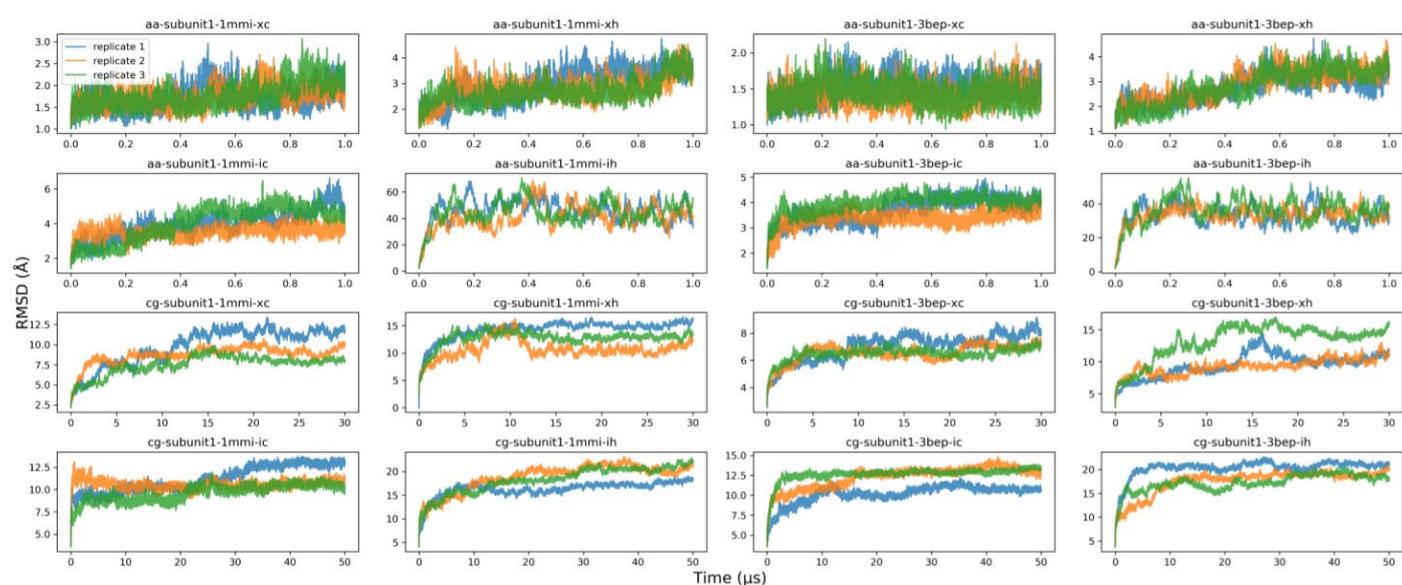


Figure S5. RMSD of the first subunit of the clamp. The three replicates are shown in blue, orange and green. aa = all-atom, cg = coarse grain, i = implicit solvation, x = explicit solvation, c = cold (298K), h = hot (368K), 1,2,3 = replicate number.

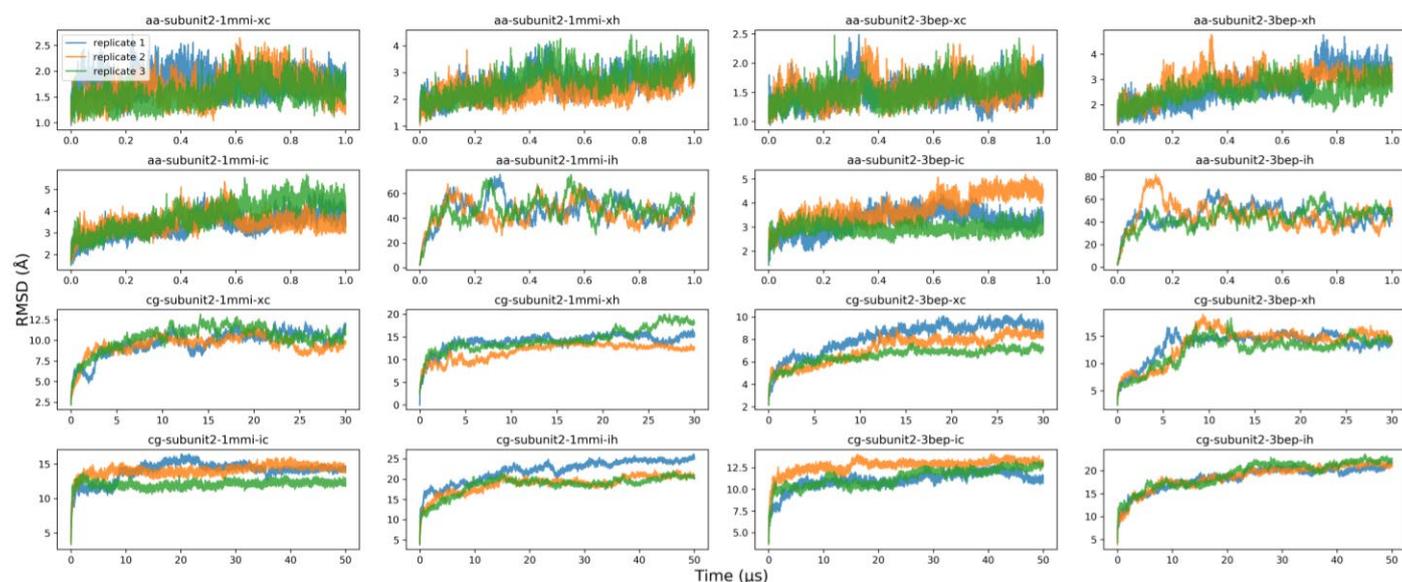


Figure S6. RMSD of the second subunit of the clamp. The three replicates are shown in blue, orange and green. aa = all-atom, cg = coarse grain, i = implicit solvation, x = explicit solvation, c = cold (298K), h = hot (368K), 1,2,3 = replicate number.

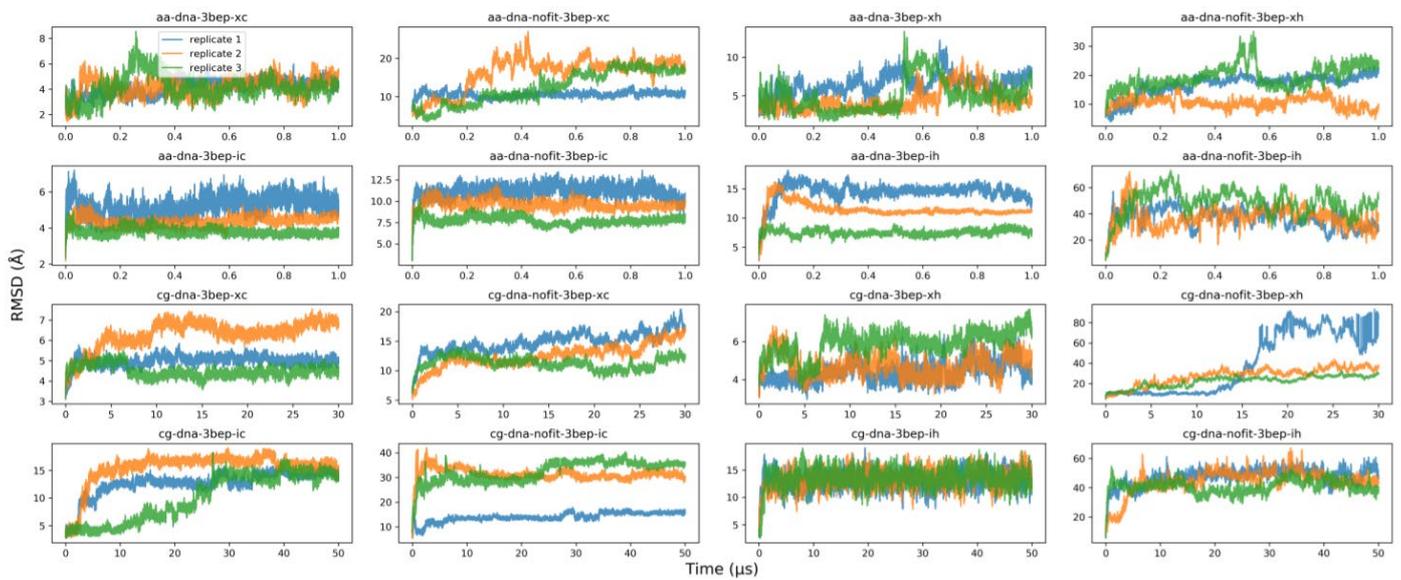


Figure S7. RMSD of the DNA in the bound systems. "fit" panels show internal RMSD of the DNA while "nofit" panels show it's relative RMSD with regards to the clamp. The three replicates are shown in blue, orange and green. aa = all-atom, cg = coarse grain, i = implicit solvation, x = explicit solvation, c = cold (298K), h = hot (368K), 1,2,3 = replicate number.

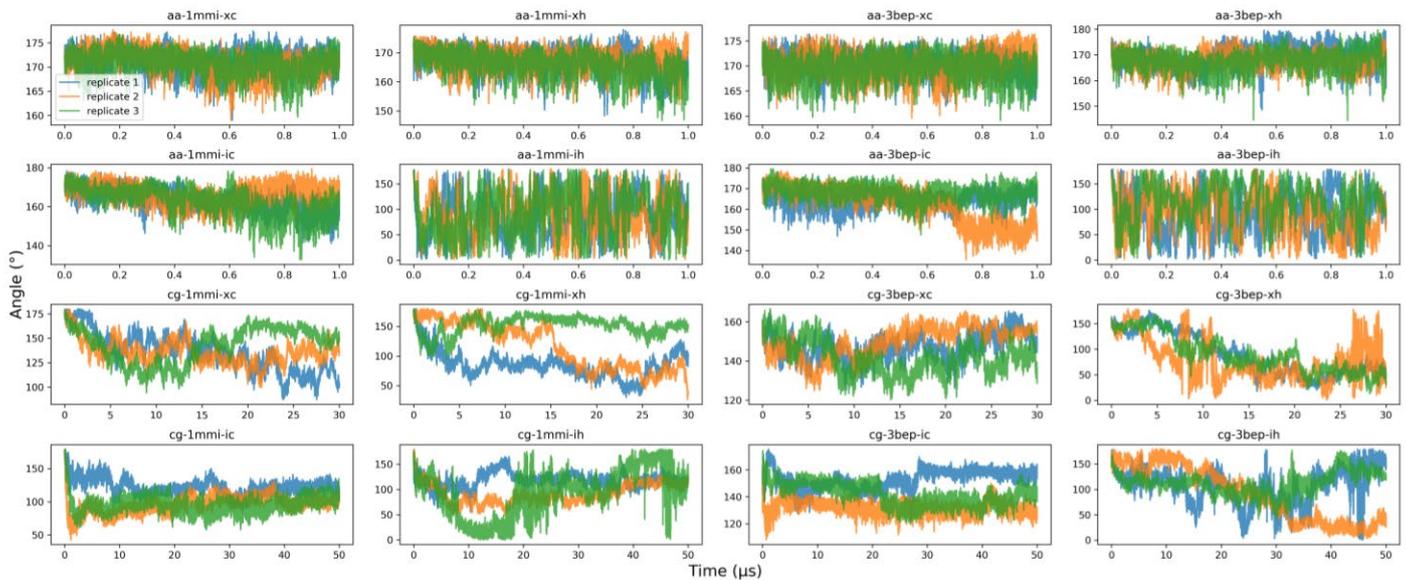


Figure S8. Angle between the planes of the two subunits. The three replicates are shown in blue, orange and green. aa = all-atom, cg = coarse grain, i = implicit solvation, x = explicit solvation, c = cold (298K), h = hot (368K), 1,2,3 = replicate number.

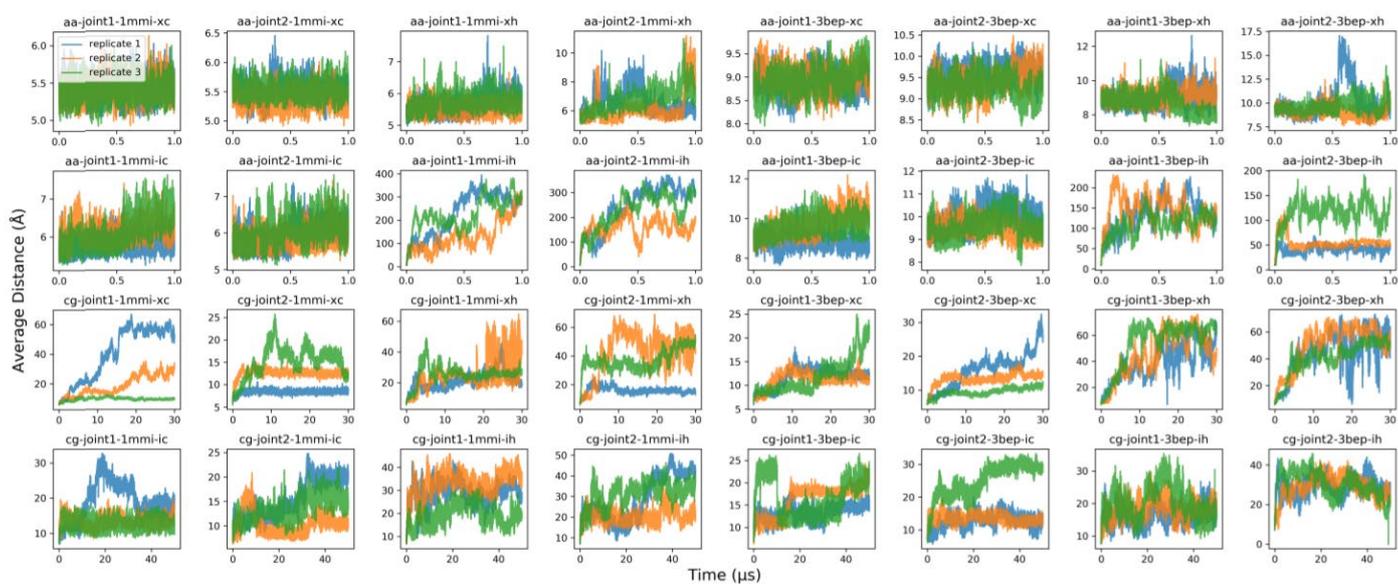
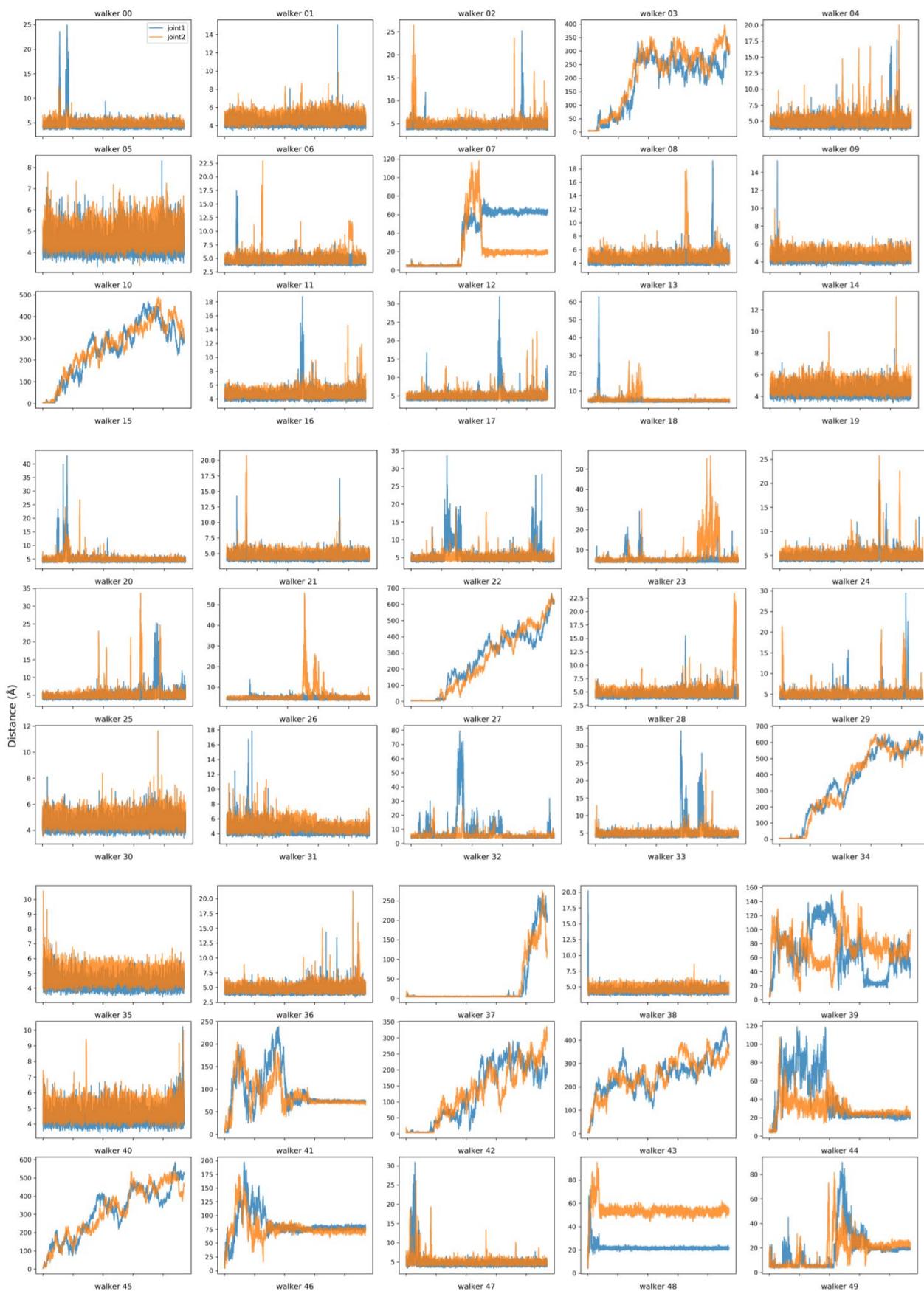


Figure S9. Distance between two groups of residues at each interface (interface 1 and interface 2). The three replicates are shown in blue, orange and green. aa = all-atom, cg = coarse grain, i = implicit solvation, x = explicit solvation, c = cold (298K), h = hot (368K), 1,2,3 = replicate number.



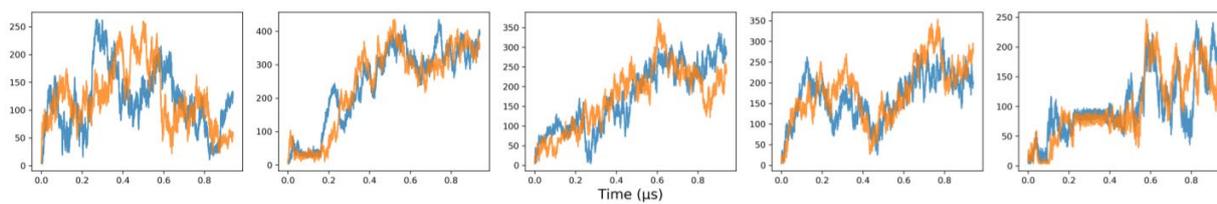


Figure S10. Distance between two groups of residues at each interface (interface 1 and interface 2) for the unbound clamp with no restraints on any of the interfaces. Each plot represents a different walker as they sample through different conditions of temperature and hamiltonian.

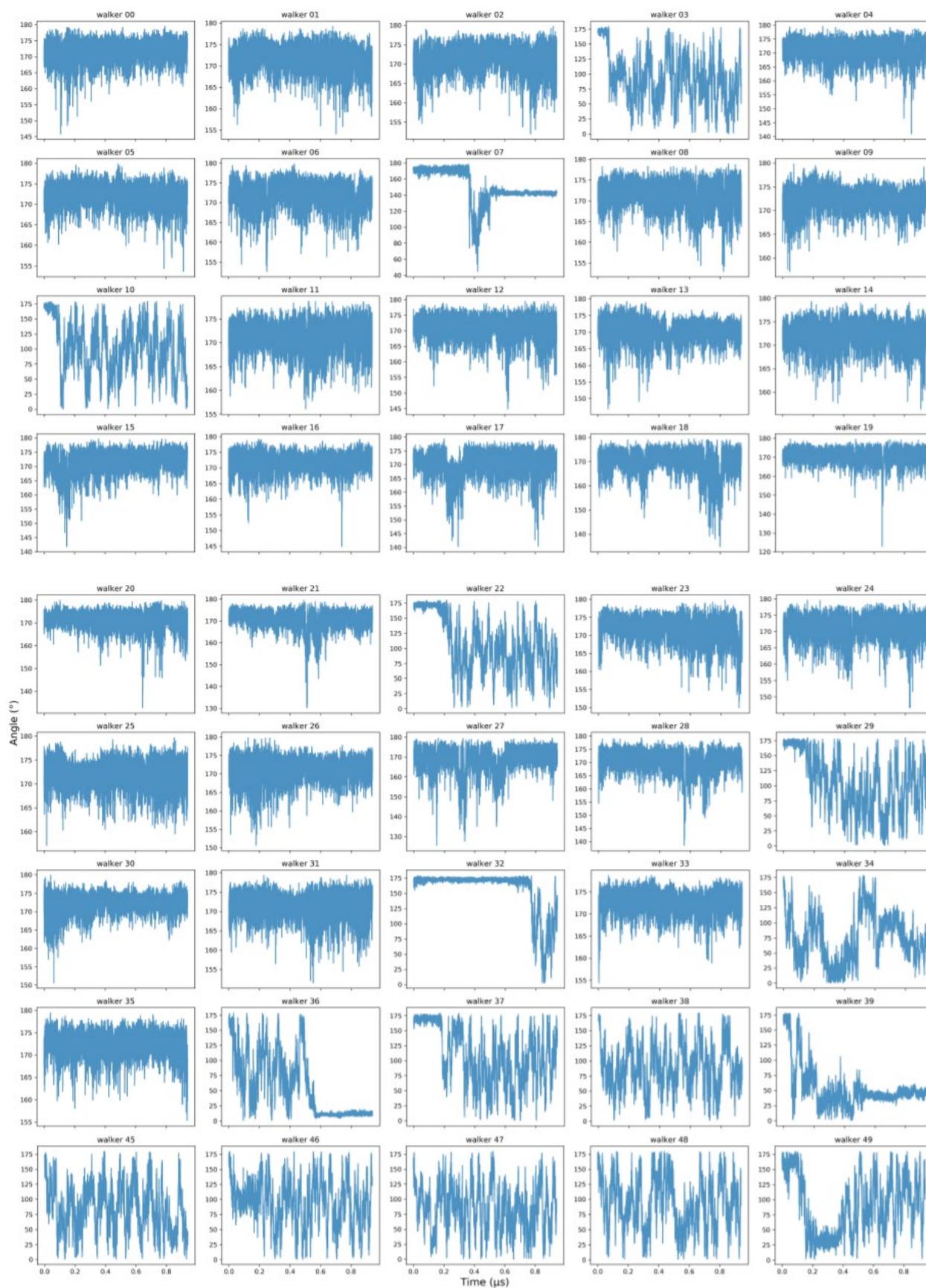


Figure S11. Angle between the planes of the two subunits for the unbound clamp with no restraints on any of the interfaces. Each plot represents a different walker as they sample through different conditions of temperature and hamiltonian.

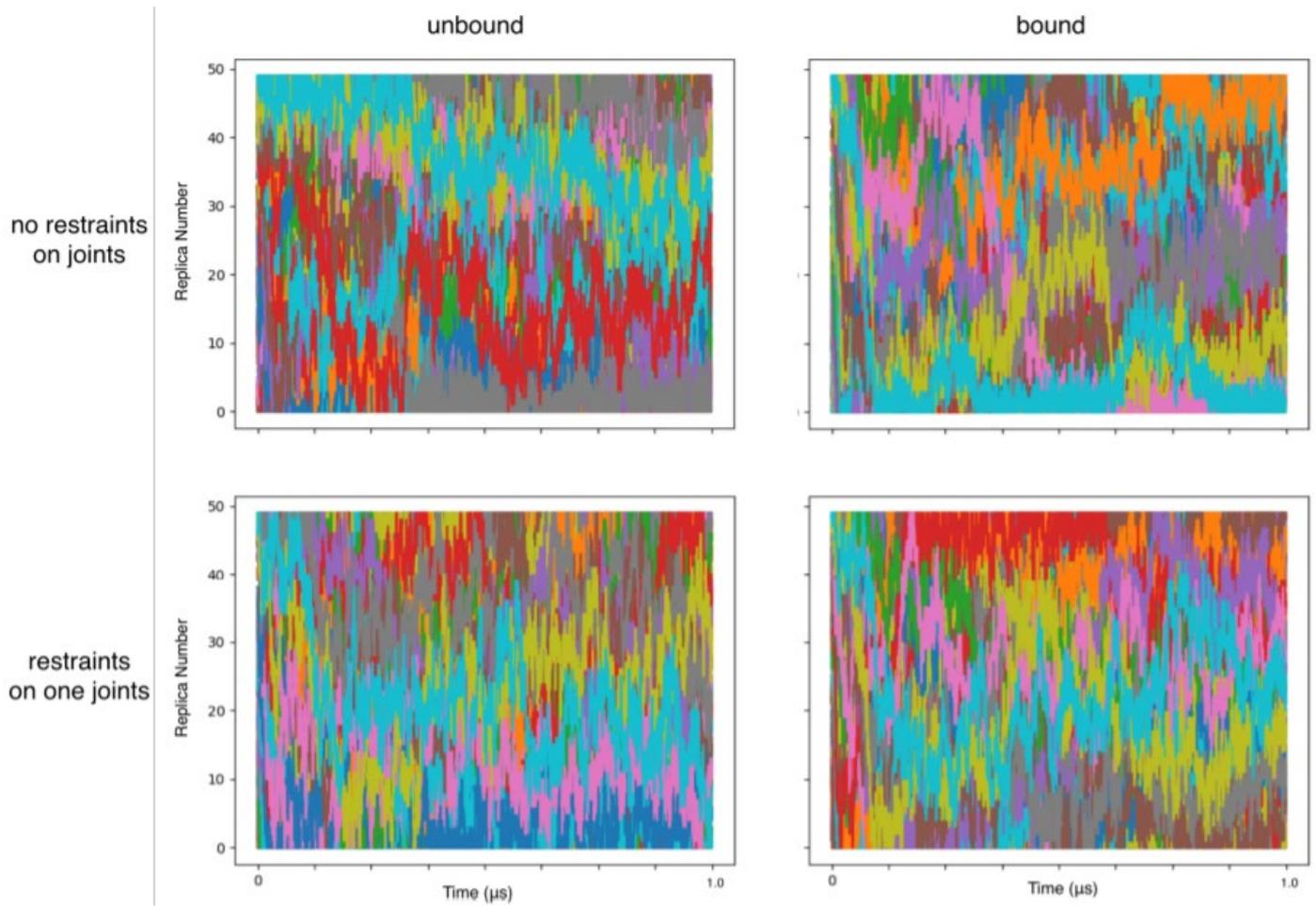


Figure S12. Replica trace for meld simulations. Each replica is represented by a color.