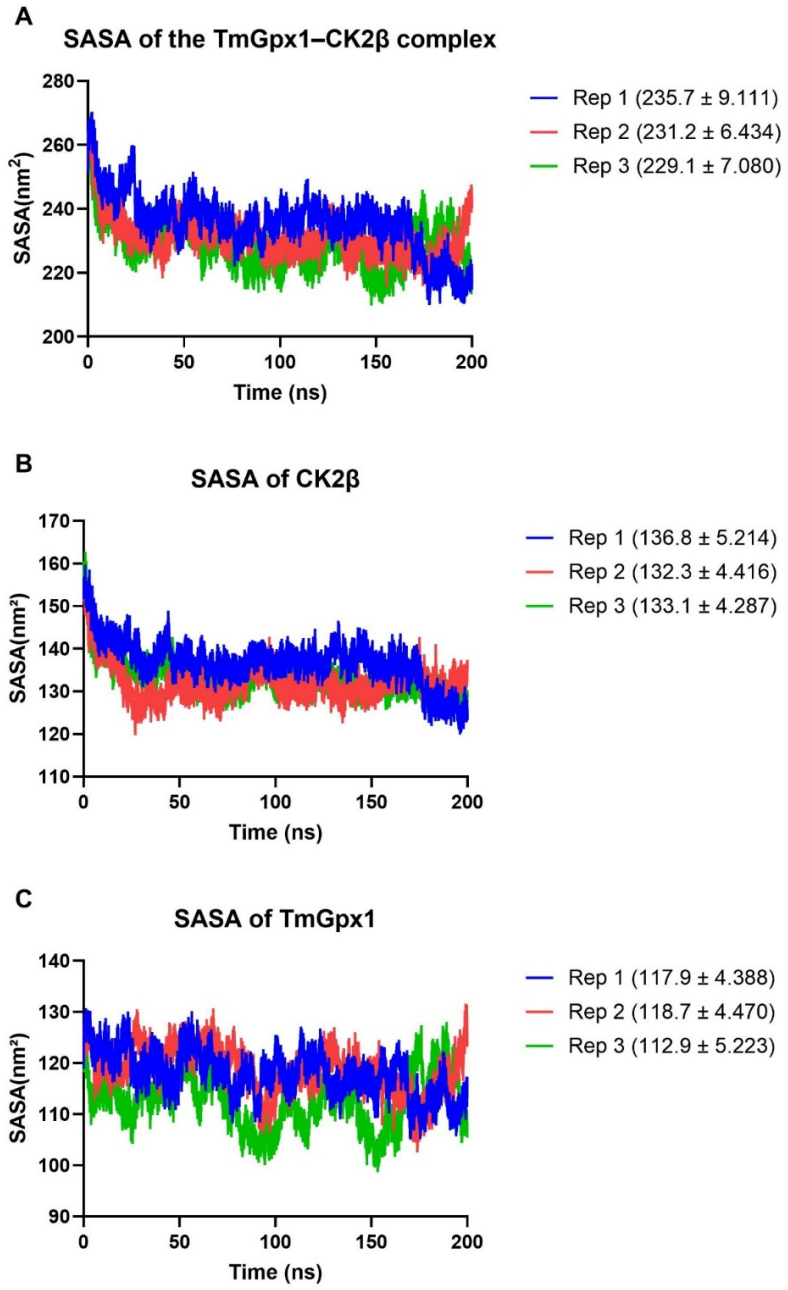
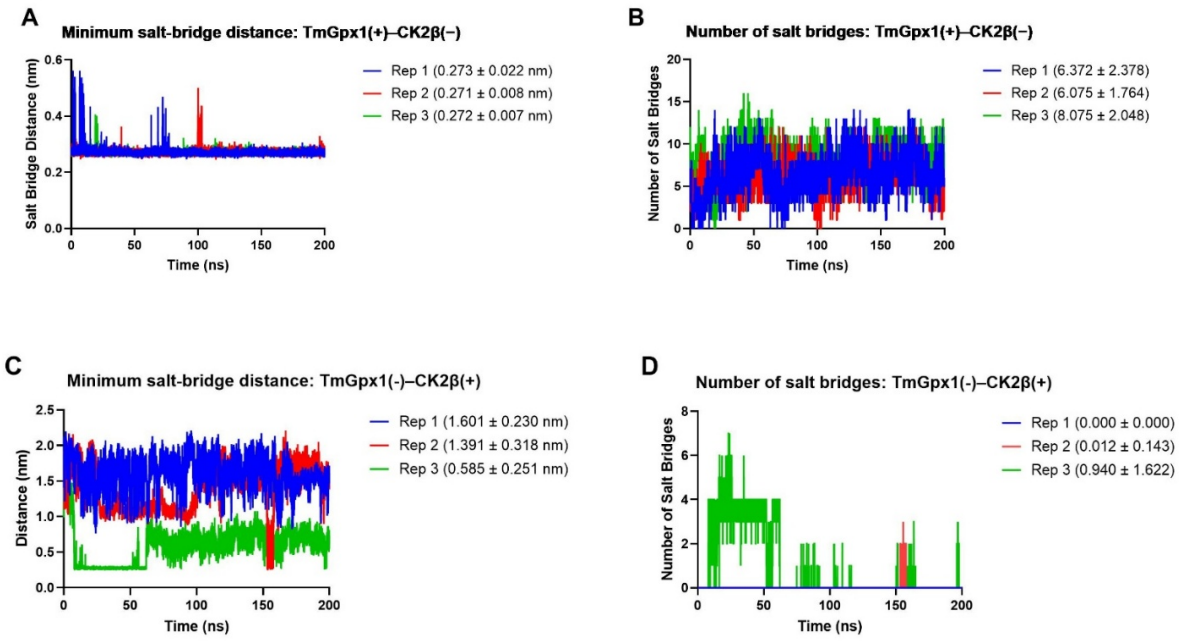



**Supplementary Figure S1. Radius of gyration of CK2β and TmGpx1 during molecular dynamics simulations.** (A) Time evolution of the radius of gyration (Rg) of CK2β over 200 ns. (B) Time evolution of the Rg of TmGpx1 over 200 ns. Replicates 1, 2, and 3 are shown in blue, red, and green, respectively. Values shown in the plot legends represent the mean ± standard deviation calculated over the full trajectory for each replicate. CK2β exhibited a gradual decrease in Rg followed by stabilization, whereas TmGpx1 showed greater fluctuations, indicating comparatively higher conformational flexibility.




**Supplementary Figure S2. Solvent-accessible surface area of the TmGpx1–CK2β complex and its individual components during molecular dynamics simulations.** (A) Time evolution of the solvent-accessible surface area (SASA) of the complete TmGpx1–CK2β complex over 200 ns. (B) SASA of CK2β calculated from the complex trajectories. (C) SASA of TmGpx1 calculated from the complex trajectories. Replicates 1, 2, and 3 are shown in blue, red, and green, respectively. Values presented in the plot legends indicate the mean ± standard deviation calculated over the full 200-ns trajectory for each replicate. The SASA of the complete complex and CK2β decreased during the initial simulation period and subsequently fluctuated within relatively stable ranges, whereas TmGpx1 showed greater replicate-dependent fluctuations in solvent exposure.




**Supplementary Figure S3. Salt-bridge interactions between TmGpx1 and CK2β during molecular dynamics simulations.** (A) Time evolution of the minimum charged-atom distance between positively charged TmGpx1 residues (Arg and Lys) and negatively charged CK2β residues (Asp and Glu). (B) Number of salt-bridge contacts per frame between positively charged TmGpx1 residues and negatively charged CK2β residues. (C) Time evolution of the minimum charged-atom distance between negatively charged TmGpx1 residues (Asp and Glu) and positively charged CK2β residues (Arg and Lys). (D) Number of salt-bridge contacts per frame between negatively charged TmGpx1 residues and positively charged CK2β residues. Salt bridges were defined using a charged heavy-atom distance cutoff of 0.40 nm. Replicates 1, 2, and 3 are shown in blue, red, and green, respectively. Values in the plot legends represent the mean ± standard deviation calculated over the full 200-ns trajectory for each replicate.