

Supplementary Material

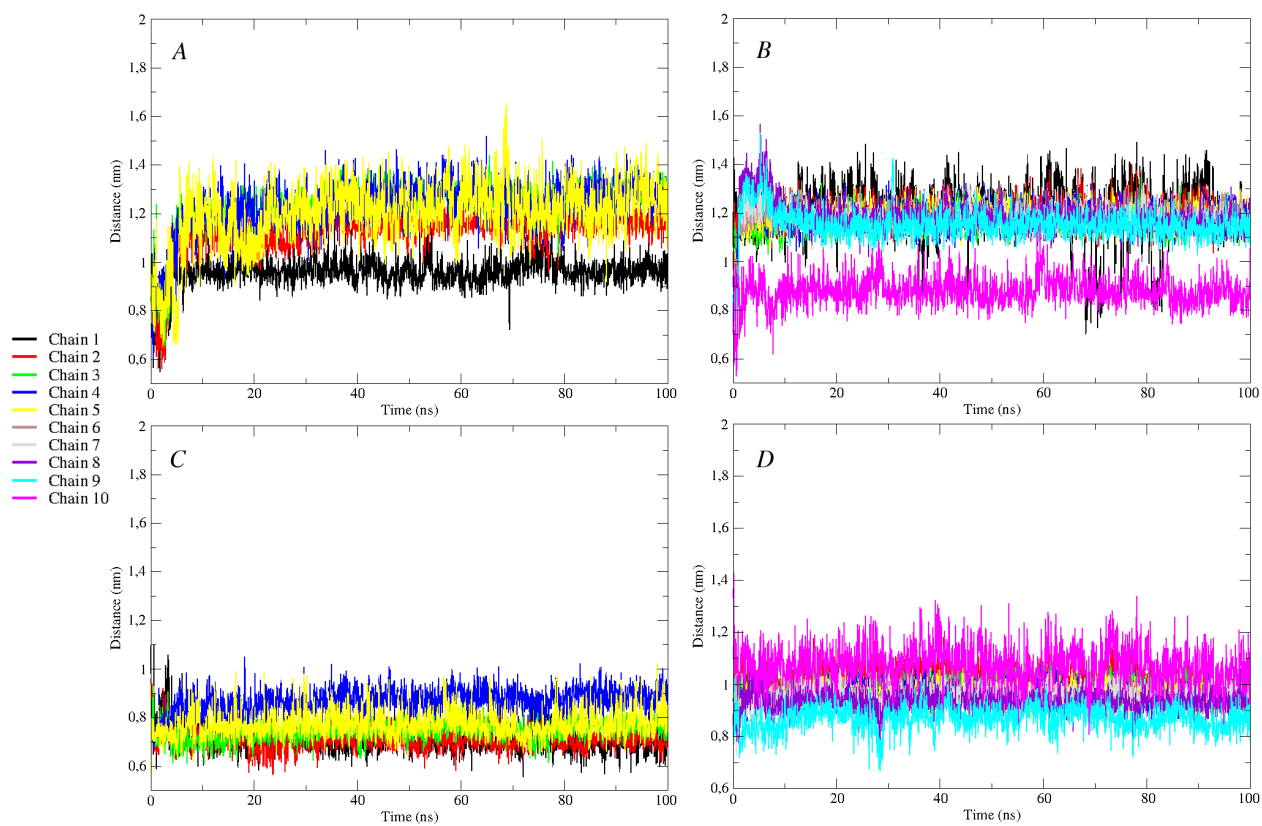


Figure S1: F19-G38 and A21-V36 intra-chain Ca distances as a function of time for the pentamer (A and C) and decamer (B and D), respectively.

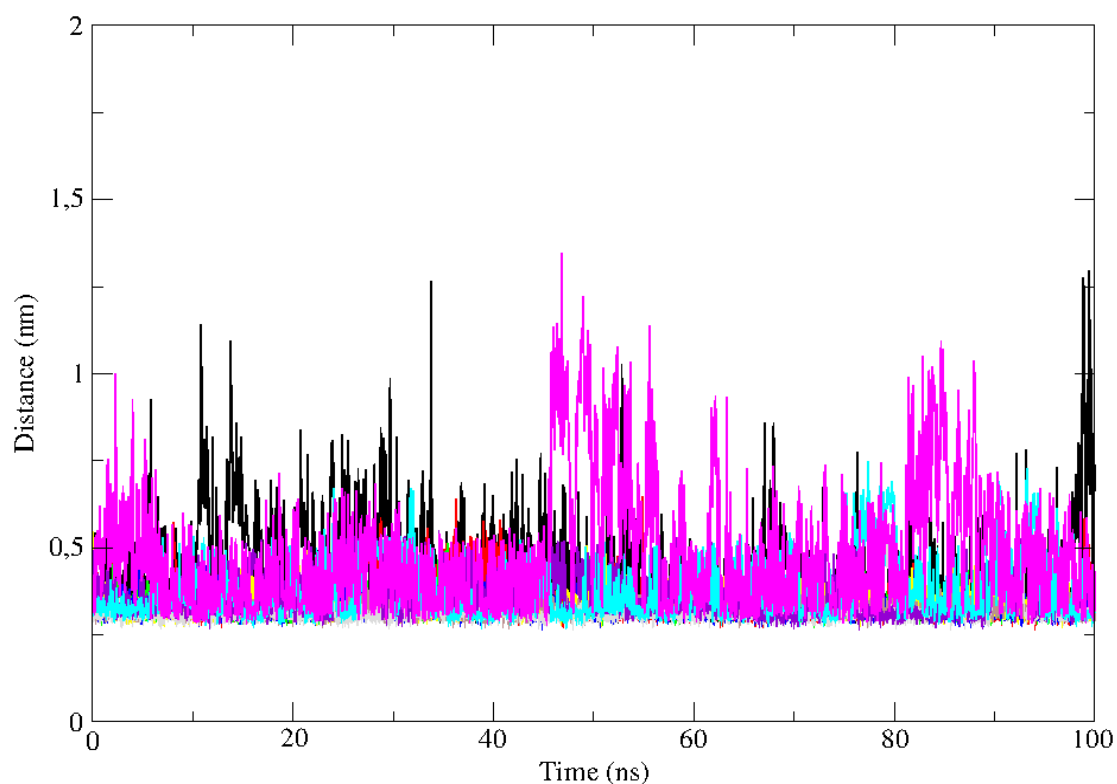
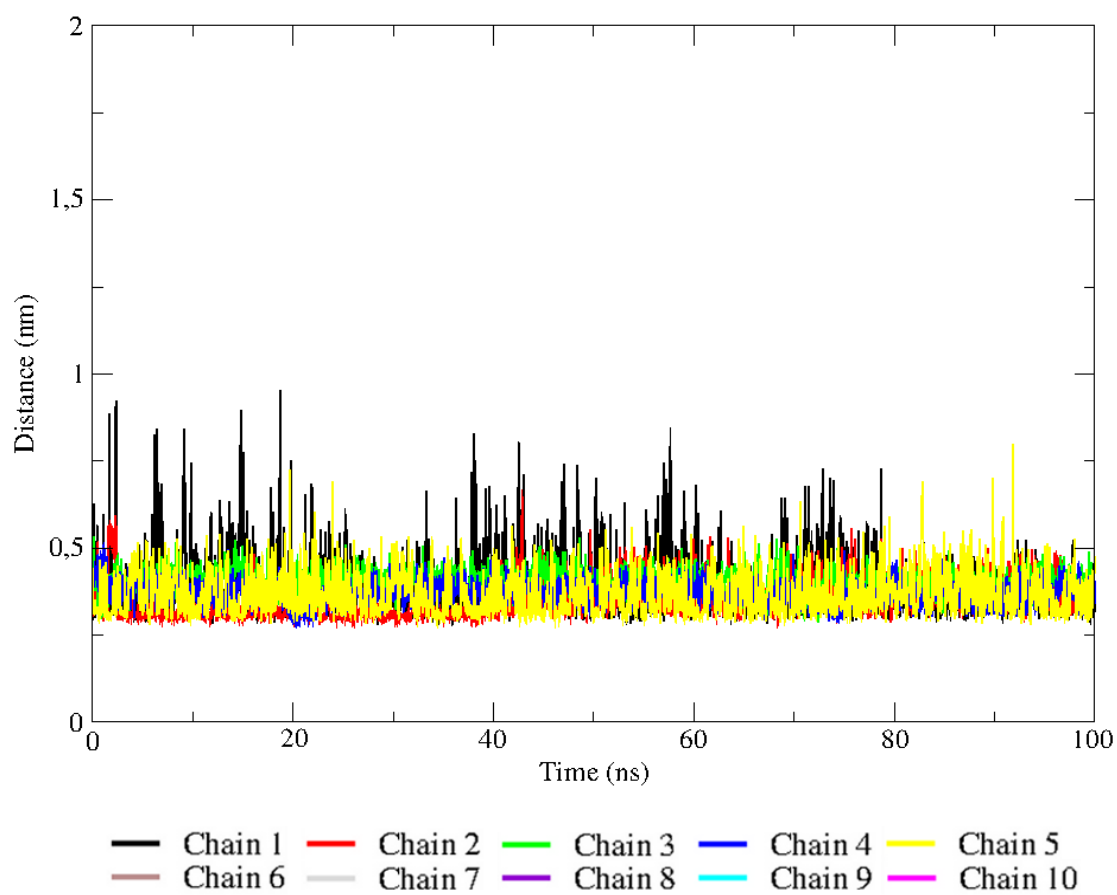


Figure S2: Intra-chain distances of the atom involved into the D23-K28 salt-bridge (O and N), as a function of time, for the pentamer (A and C) and decamer (B and D), respectively.

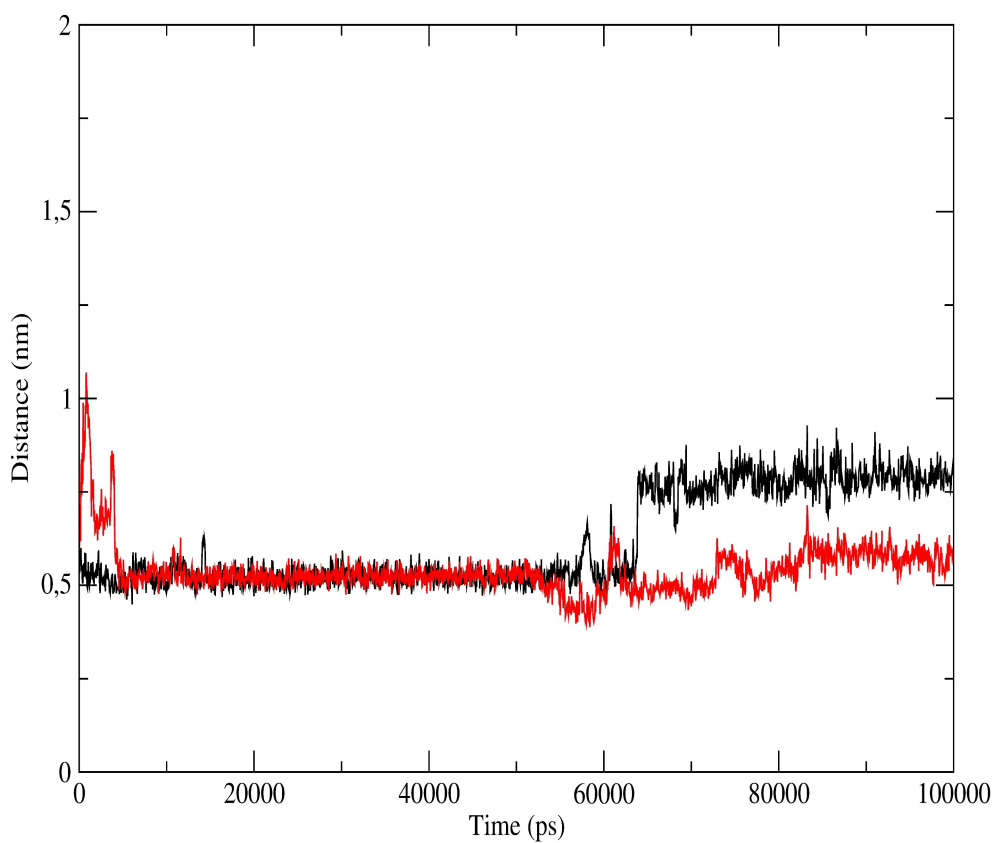


Figure S3: Center of mass distances as a function of time between the peptidic portion of the ligand (LPFFD) and the initial binding site (residues 17-21 of Chain 1), in the complex of CT with the pentamer (black) and the decamer (red).