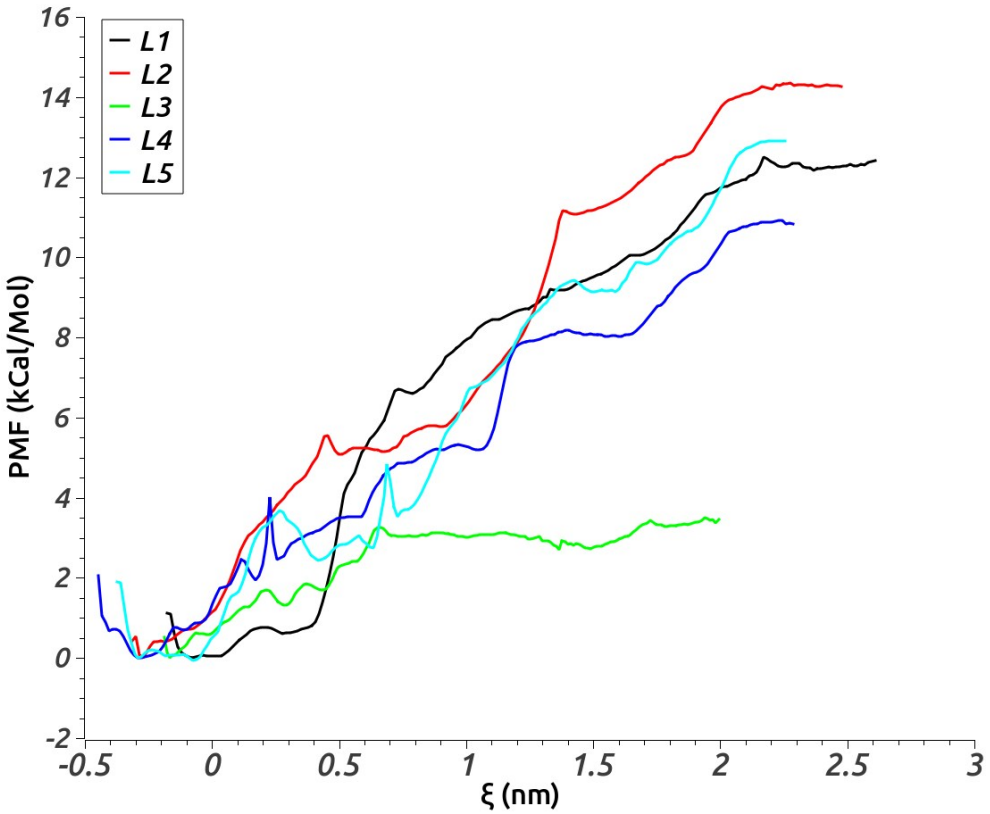
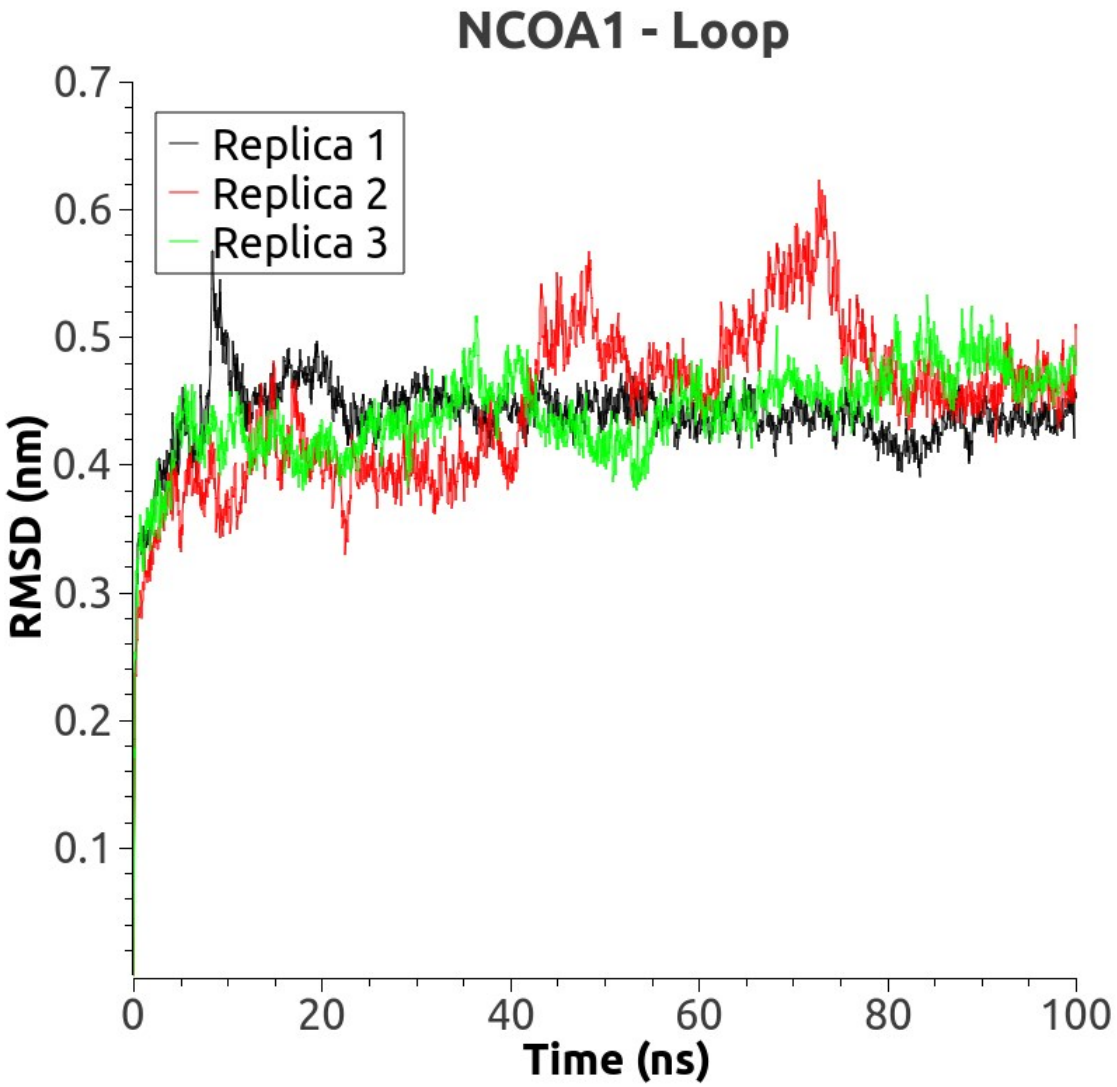
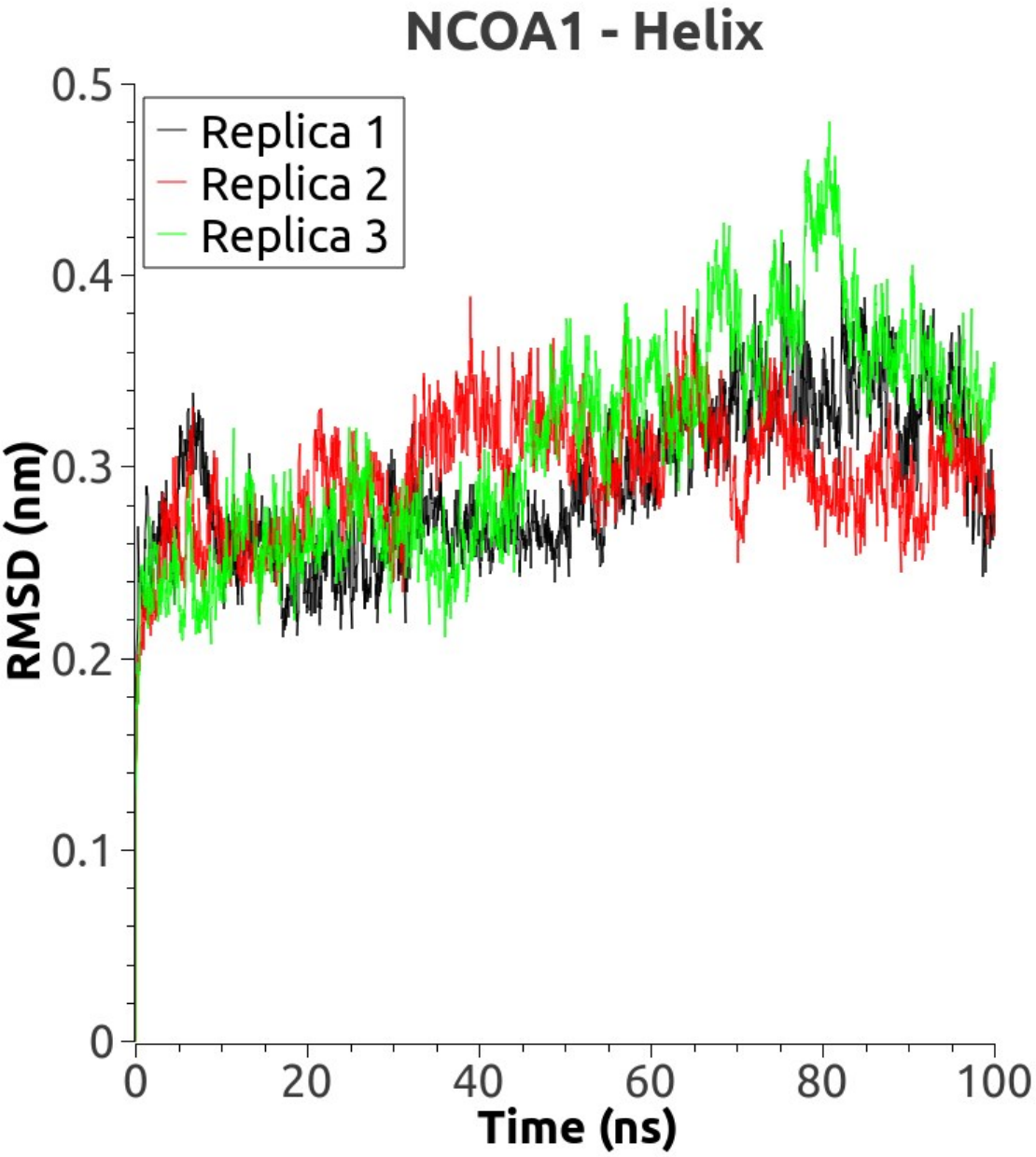
Electronic Supplementary Material (ESI) for MedChemComm.



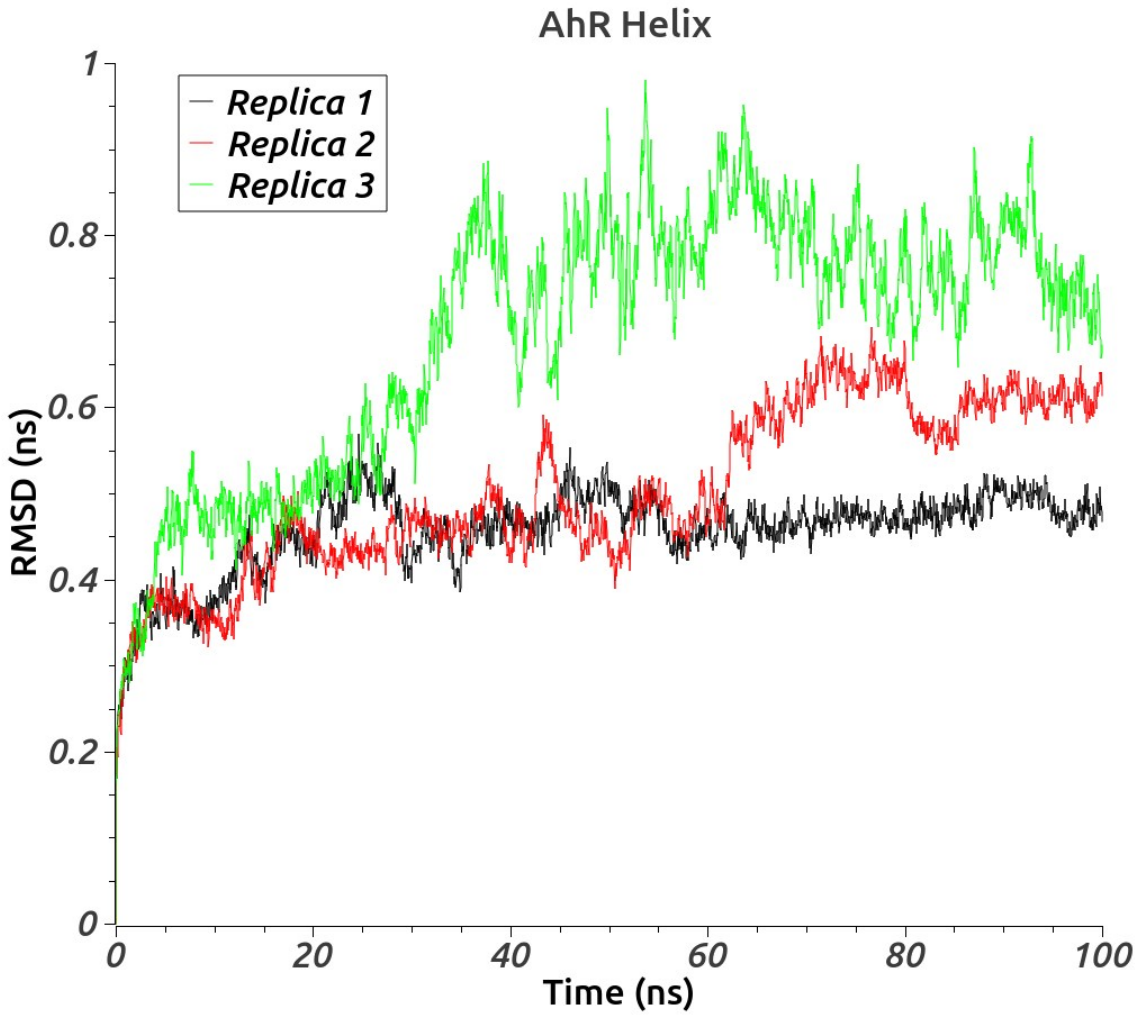
Supplementary Figure 1. *Potential of mean forces calculated by umbrella sampling simulations for five different ligands, with NCOA1 PASB in the loop-helix-loop canonical conformation. L3 (green) has considerably lower binding energy in comparison to the other four ligands.*



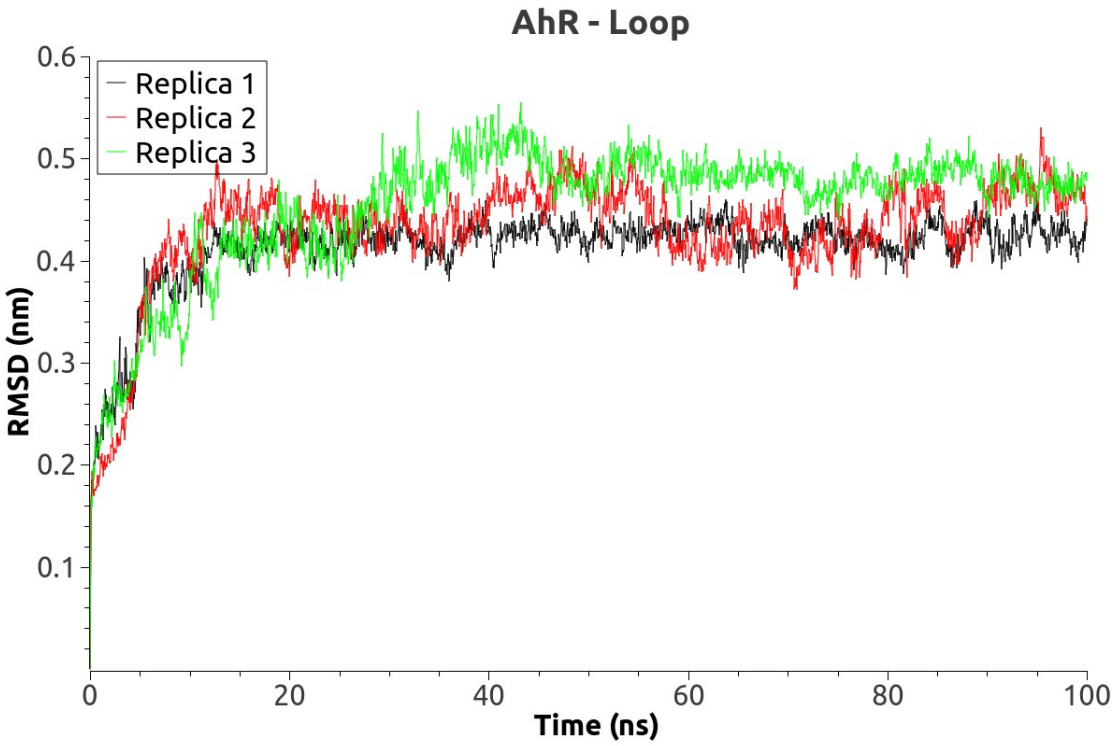
Supplementary Figure 2. *RMSD plot for the three replicas on the partially disordered loop conformation of the PASB-NCOA1.*



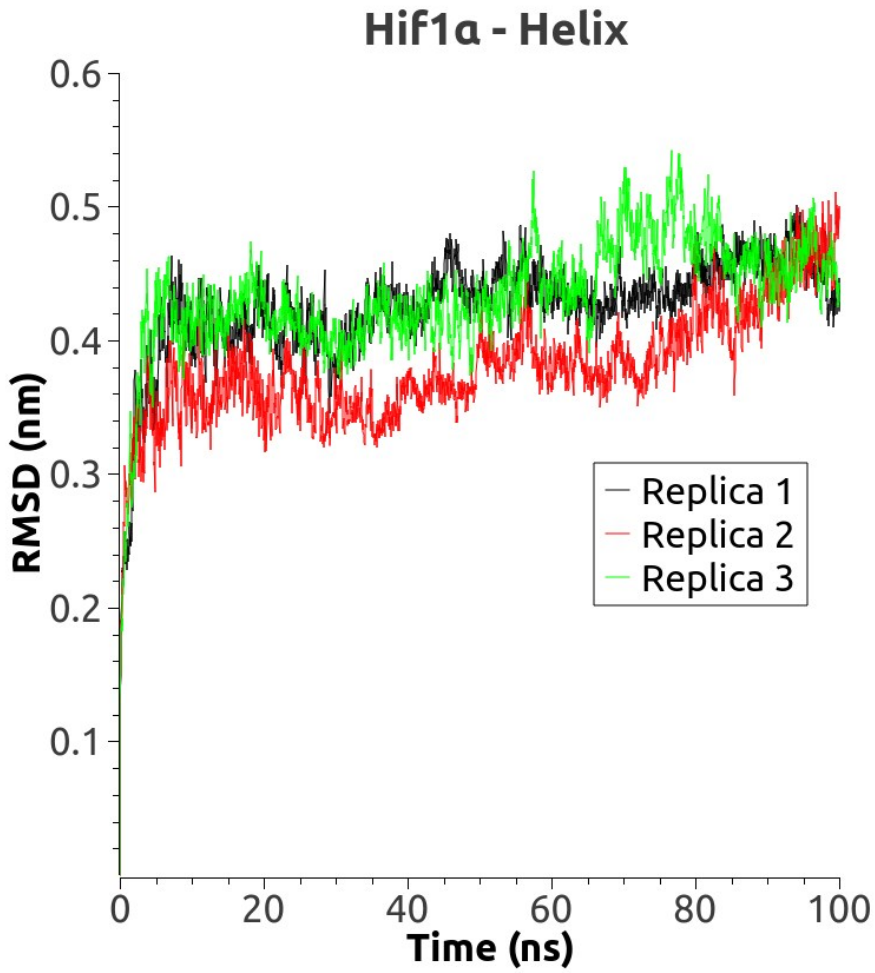
Supplementary Figure 3. *RMSD plot for the three replicas of the helix conformation of the PASB-NCOA1.*



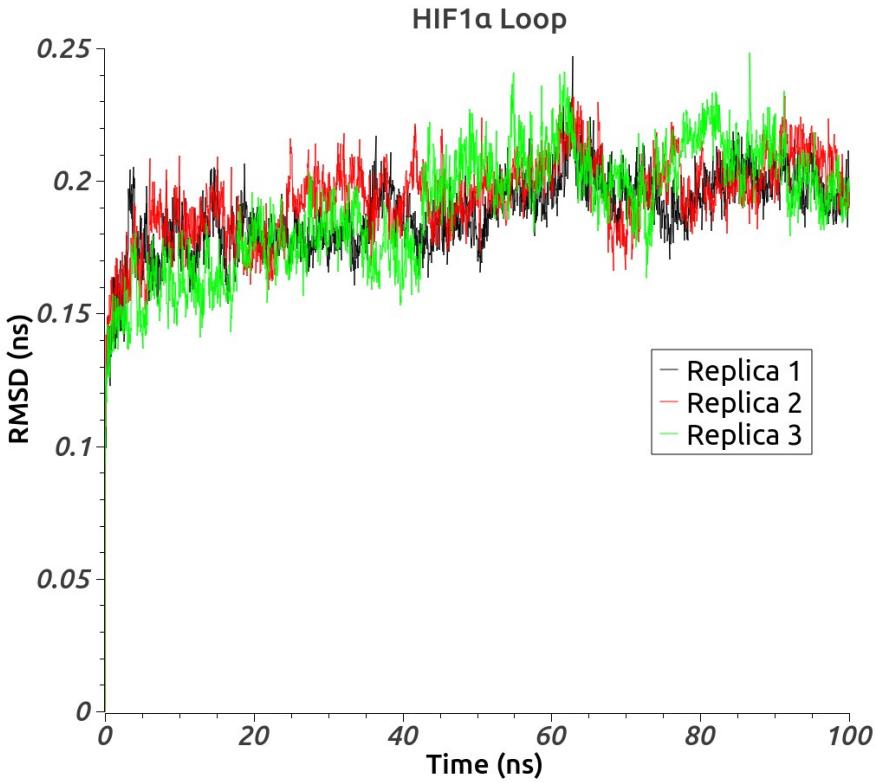
Supplementary Figure 4*. RMSD plot for the three replicas on the helix conformation of the PASB-AhR.*



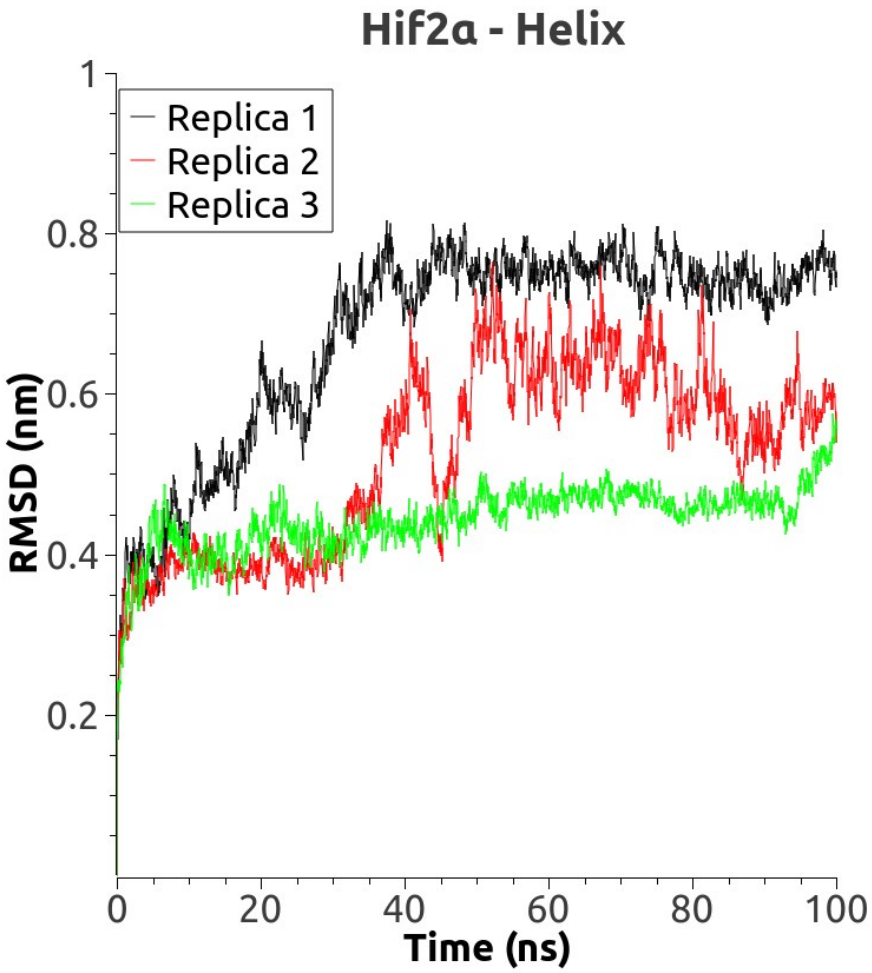
Supplementary Figure 5. *RMSD plot for the three replicas on the loop conformation of the PASB-AhR.*



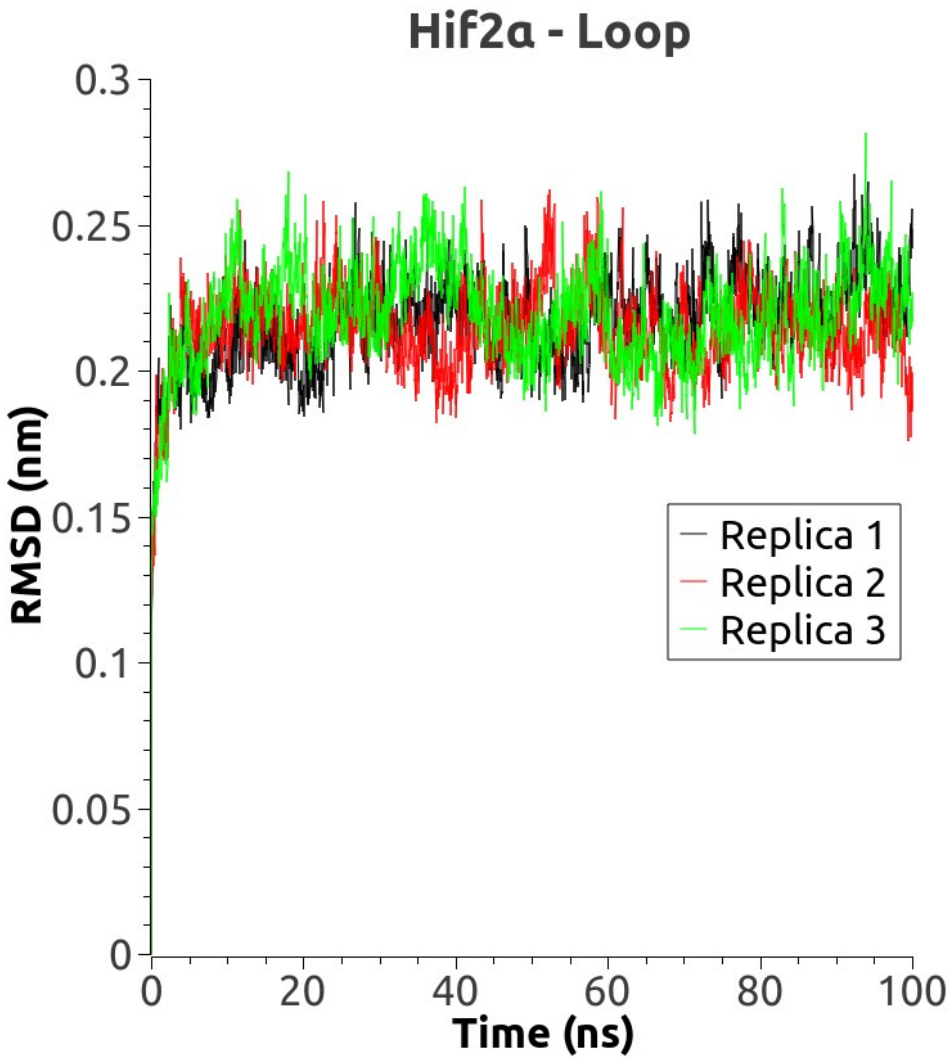
Supplementary Figure 6. *RMSD plot for the three replicas on the Helix conformation of the PASB-HIF1α.*



Supplementary Figure 7*. RMSD plot for the three replicas on the loop conformation of the PASB-HIF1α.*



Supplementary Figure 8. *RMSD plot for the three replicas on the helix conformation of the PASB-HIF2α.*



***Supplementary Figure 9**. RMSD plot for the three replicas on the loop conformation of the PASB-HIF2α.*