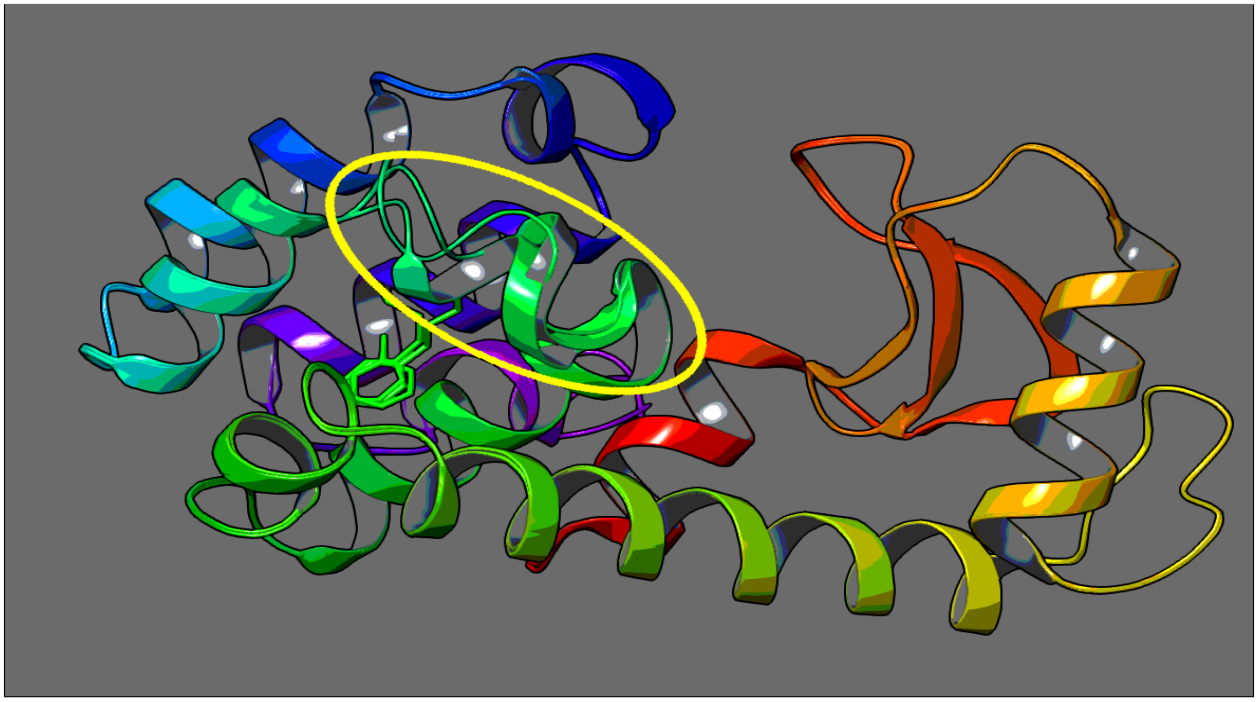
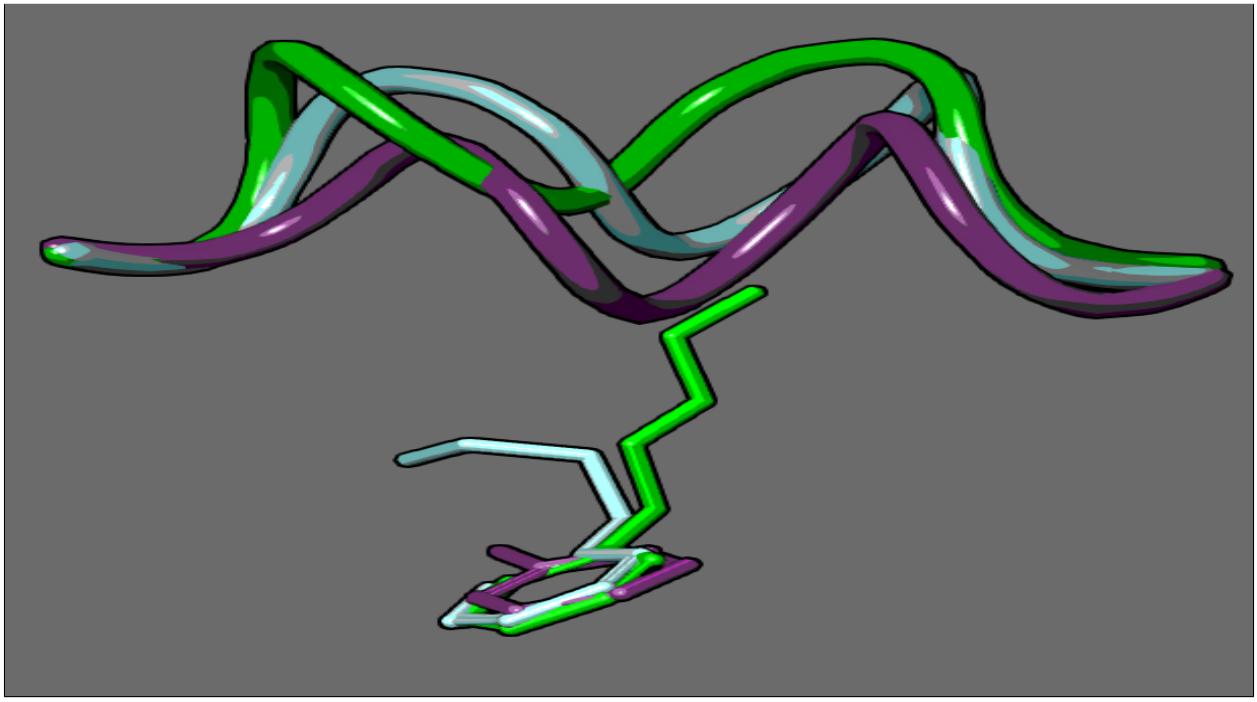


(a) T4-L99A



(b) T4-L99A

Figure 1: T4-L99A

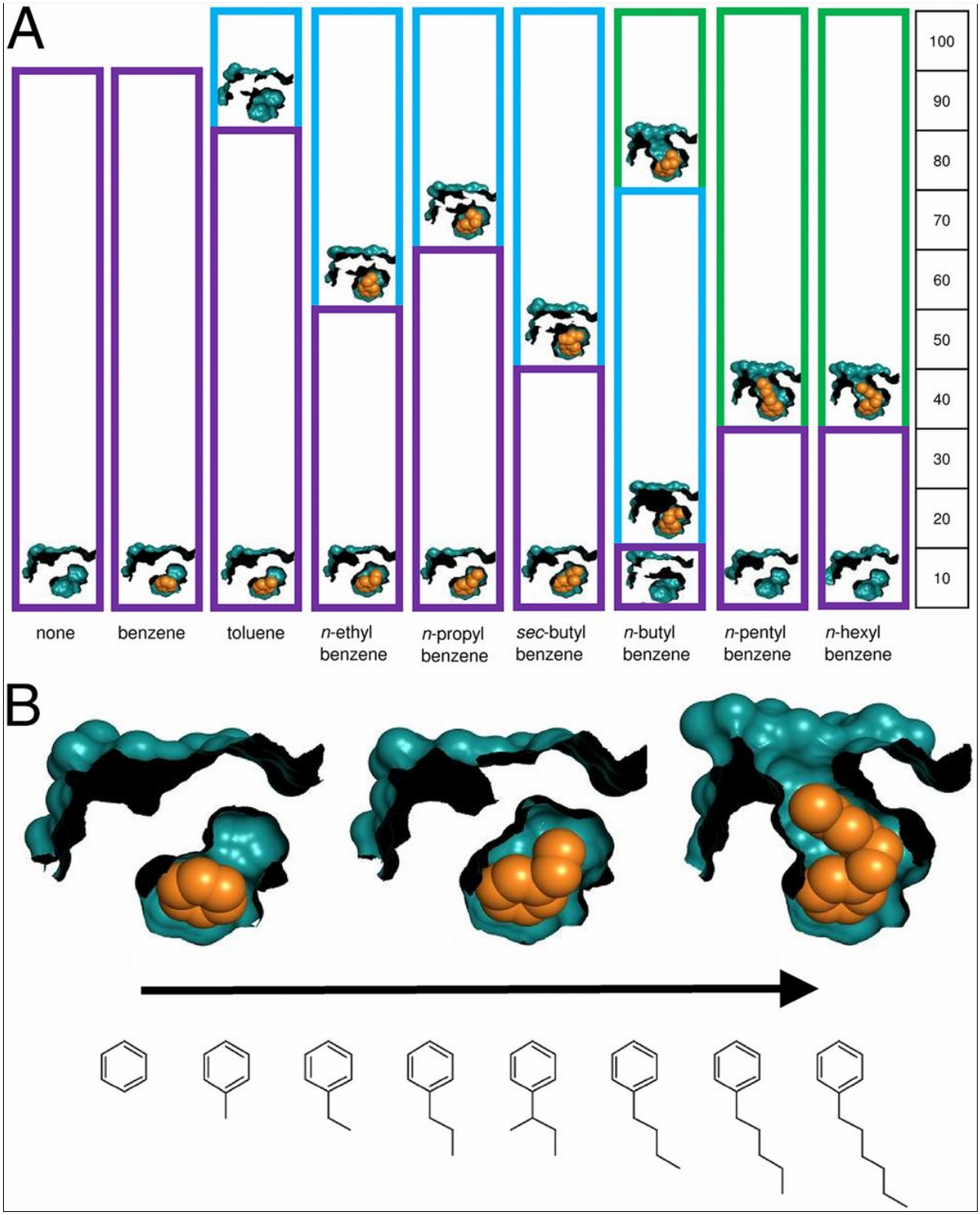
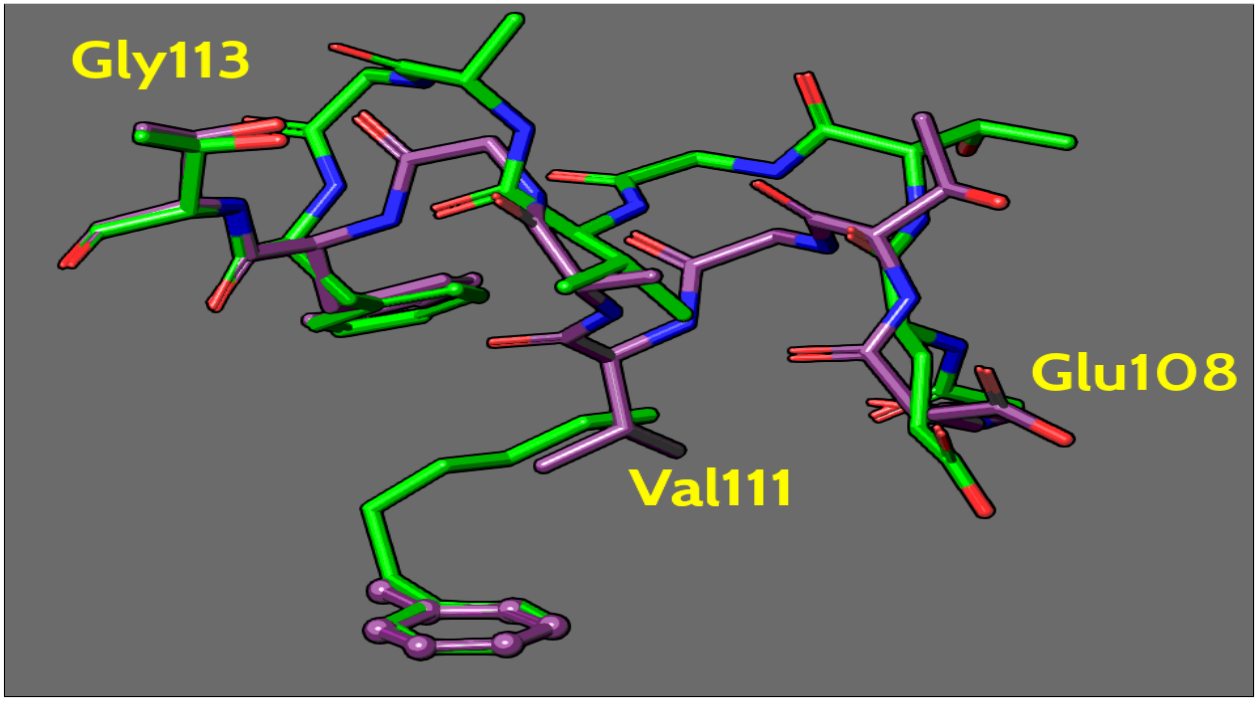
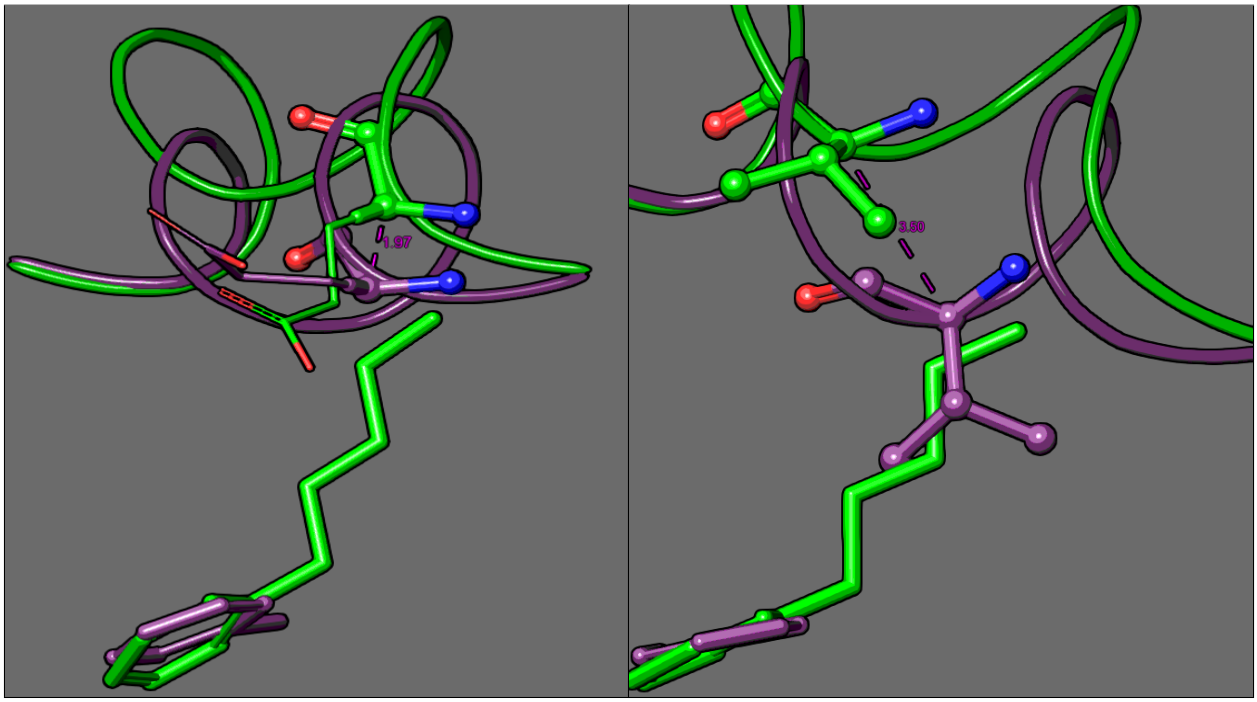


Figure 2: "Congeneric ligands are accommodated in L99A with conformational changes. (A) In the L99A cavity, the ligand poses were assigned to their respective protein conformations by matching the ligand occupancy with that of the F-helix conformation, which was typically unambiguous. (B) Molecular surface of the cavity, cut away to reveal the ligand (orange space-filling model), in examples of the closed (benzene complex), intermediate (ethylbenzene complex), and open (n-hexylbenzene complex) conformations. The full congeneric series is shown." Adapted figure[?]



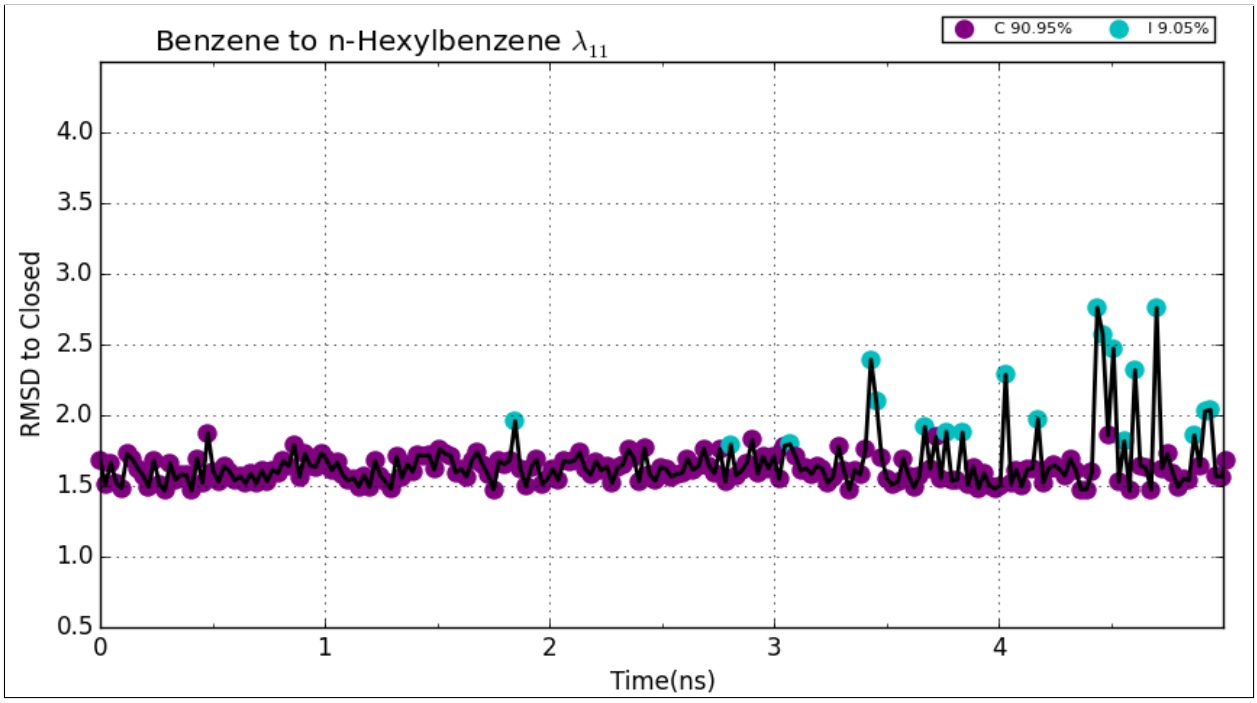
(a) Selected pREST residues



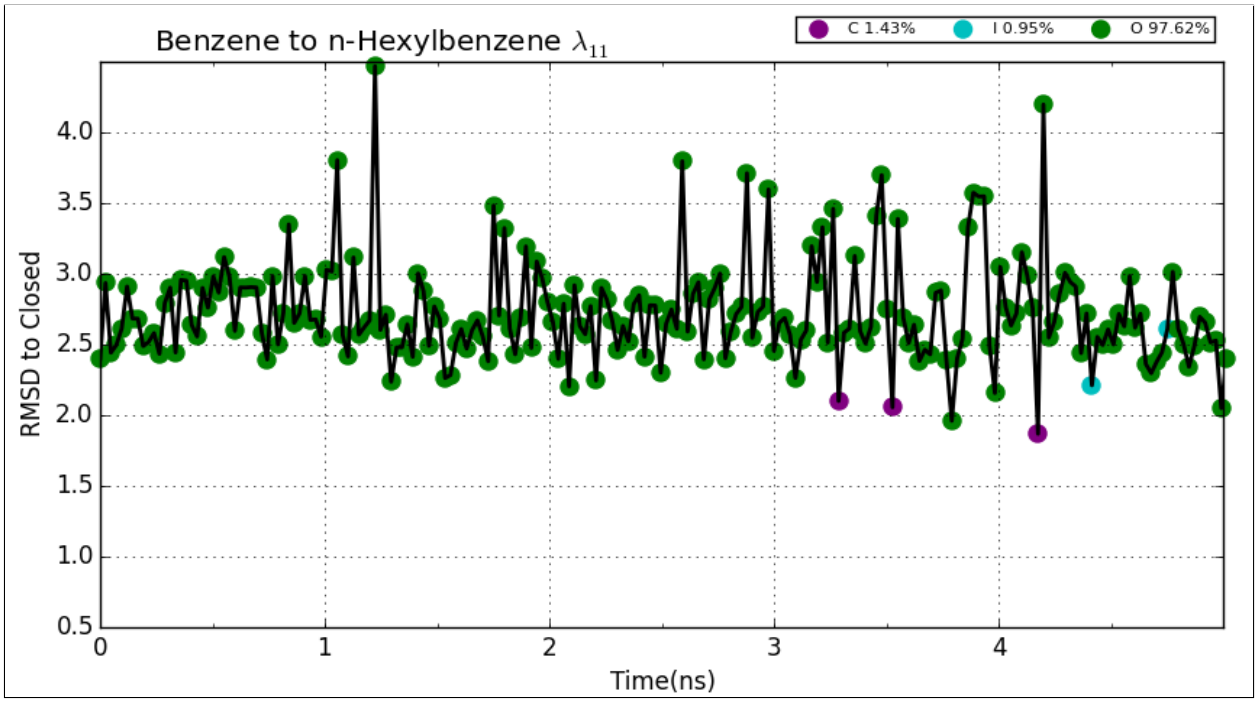
(b) Residue Glu108

(c) Residue Val111

Figure 3: pREST residues

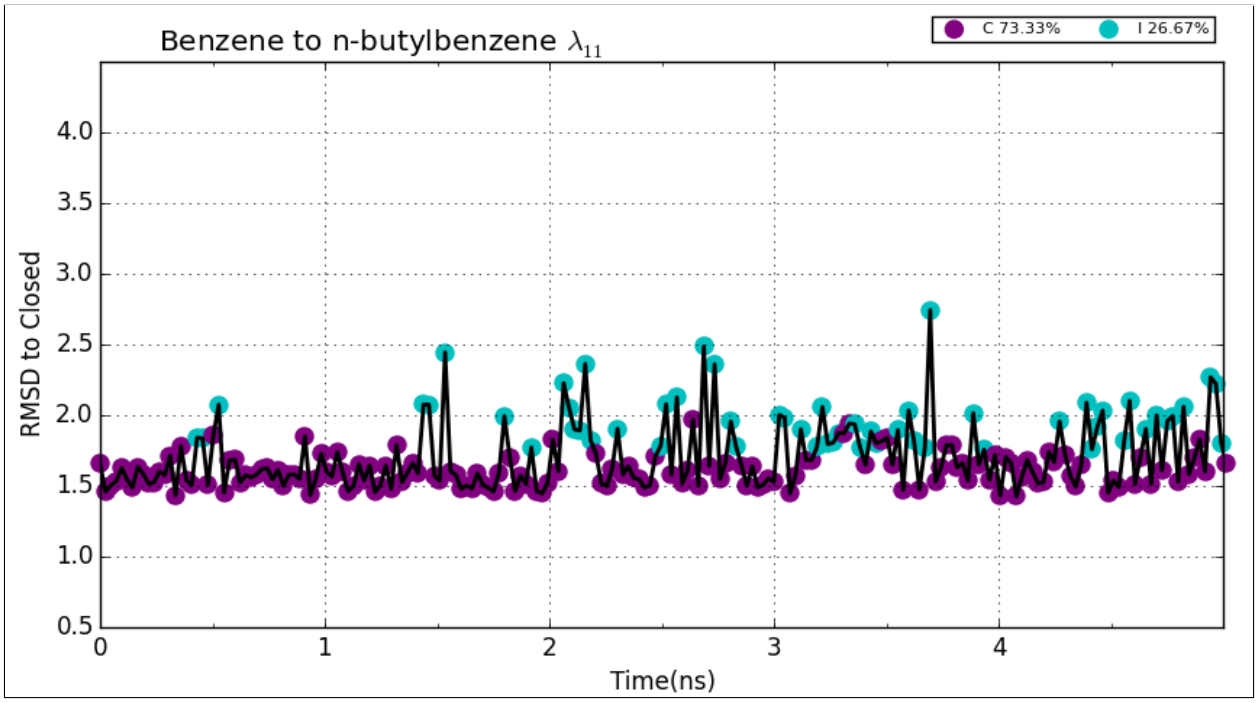


(a) Closed - Benzene to n-Hexylbenzene 0-5ns RMSD Replica11

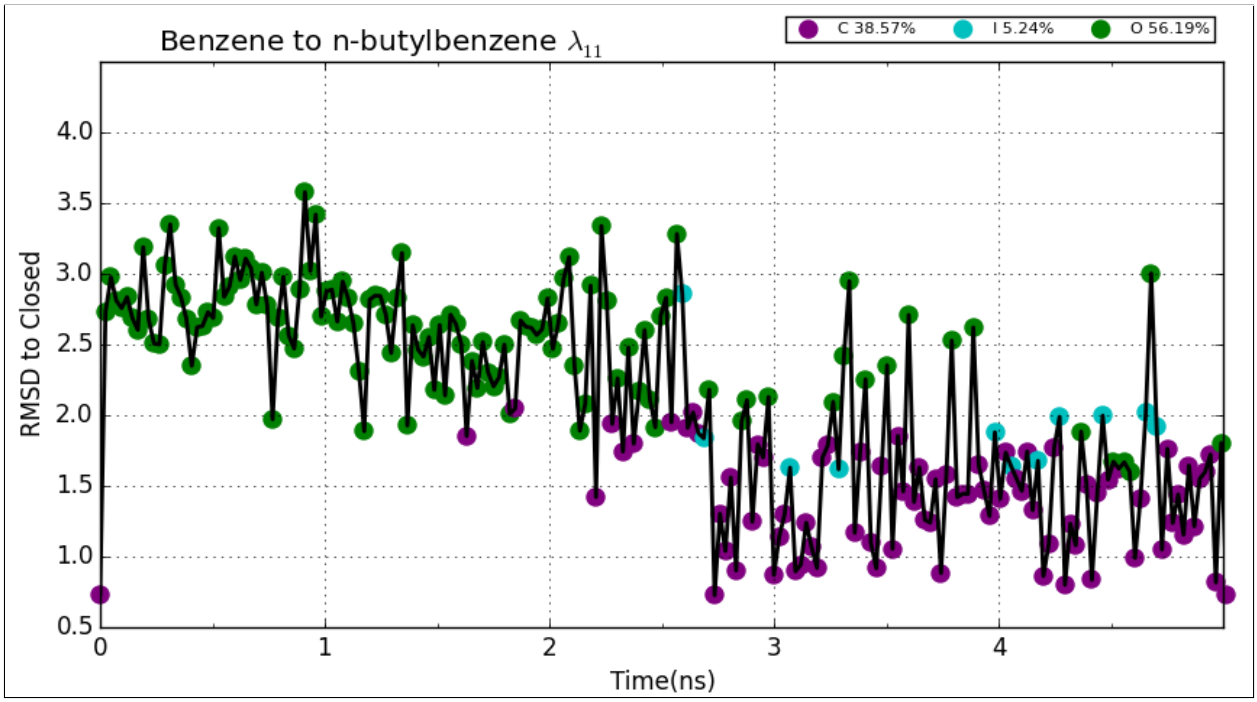


(b) Open - Benzene to n-Hexylbenzene 0-5ns RMSD Replica11

Figure 4: Benzene To n-Hexylbenzene (Default)

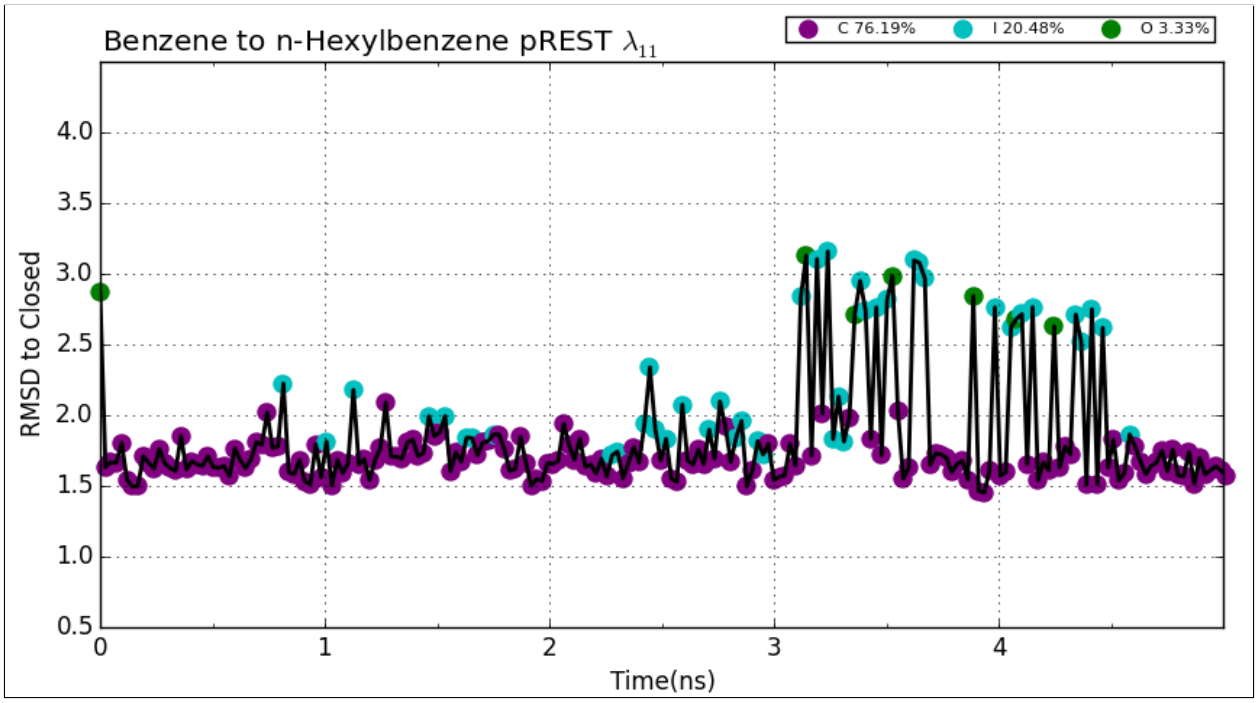


(a) Closed - Benzene to n-butylbenzene 0-5ns RMSD Replica11

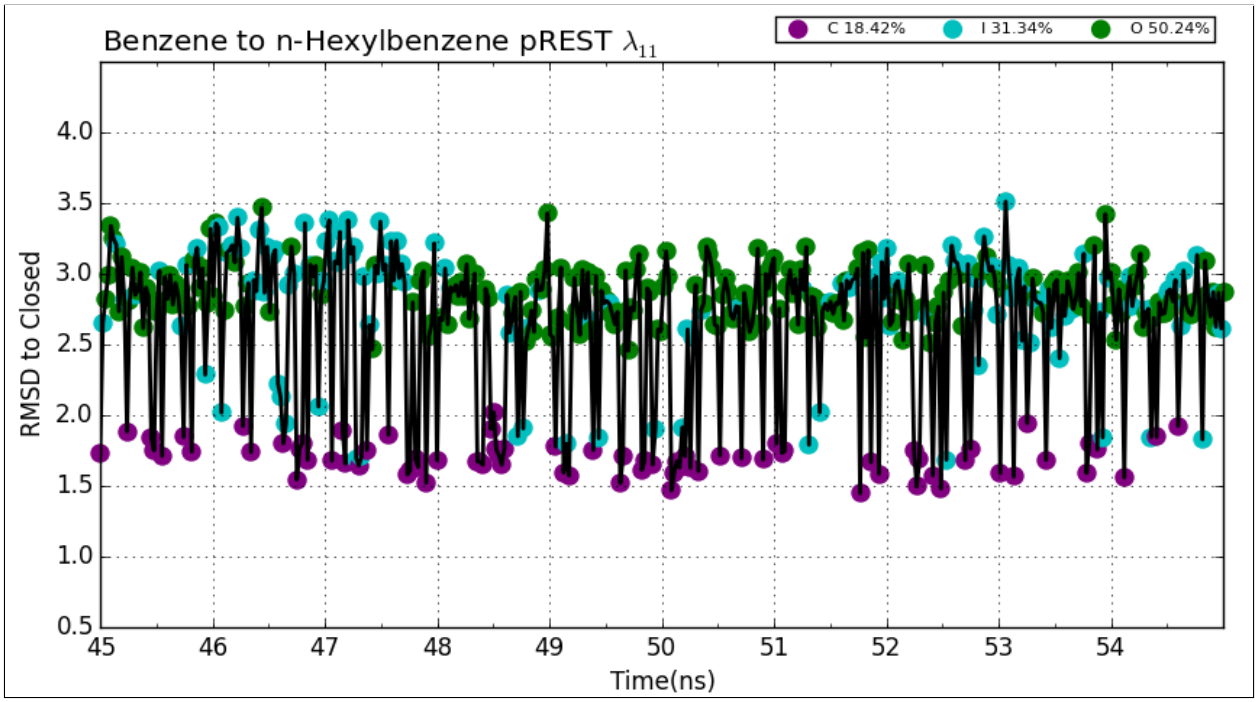


(b) Open - Benzene to n-butylbenzene 0-5ns RMSD Replica11

Figure 5: Benzene To n-Butylbenzenebenzene (Default)

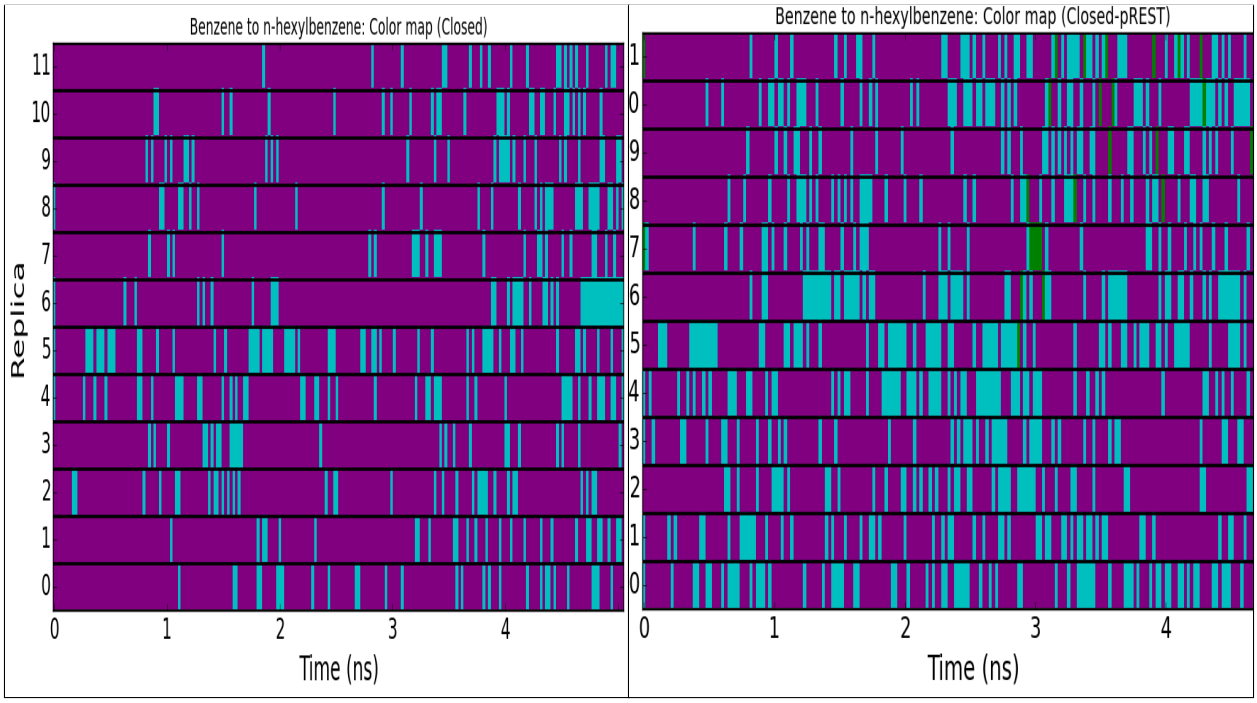


(a) Closed - Benzene to n-Hexylbenzene 0-5ns RMSD Replica11 pREST

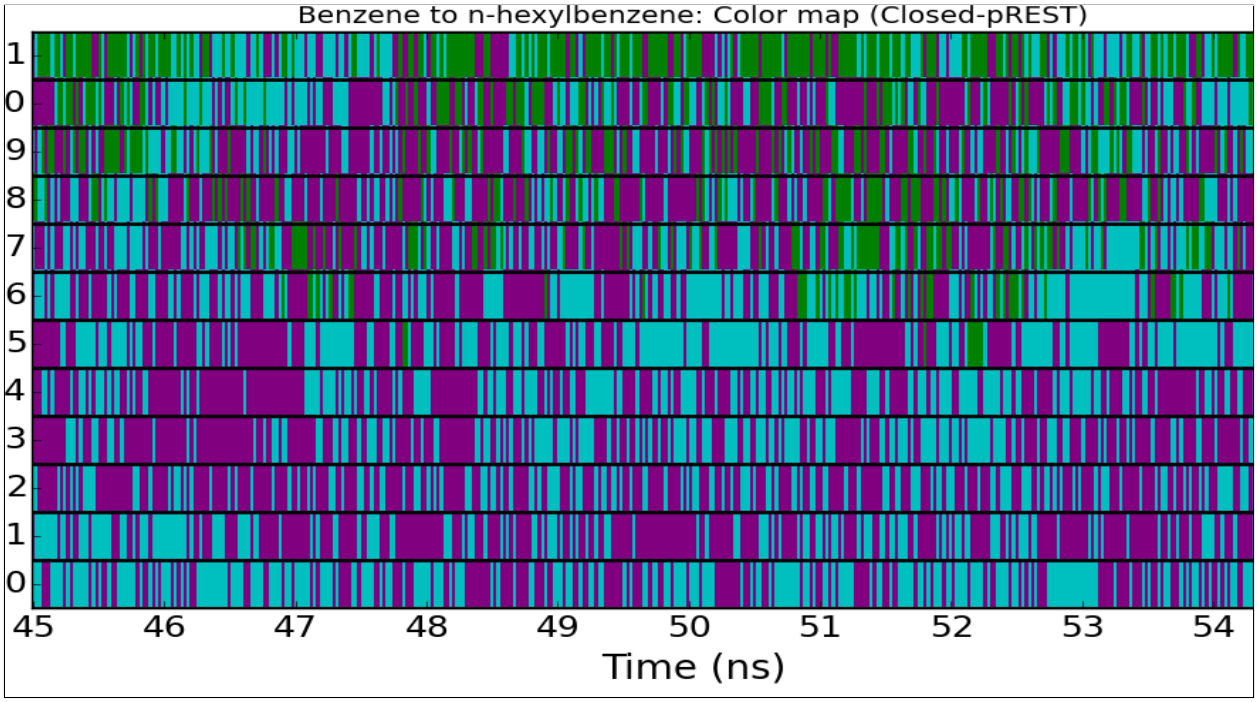


(b) Closed - Benzene to n-Hexylbenzene 45-55ns RMSD Replica11 pREST

Figure 6: Benzene To n-Hexylbenzene (pREST)

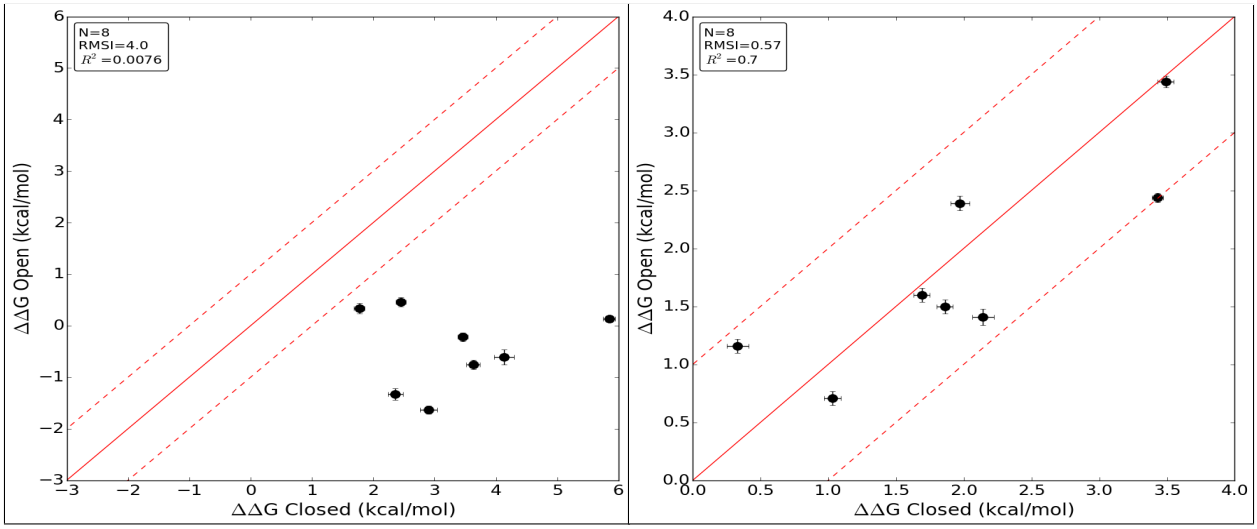


(a) Default (b) pREST



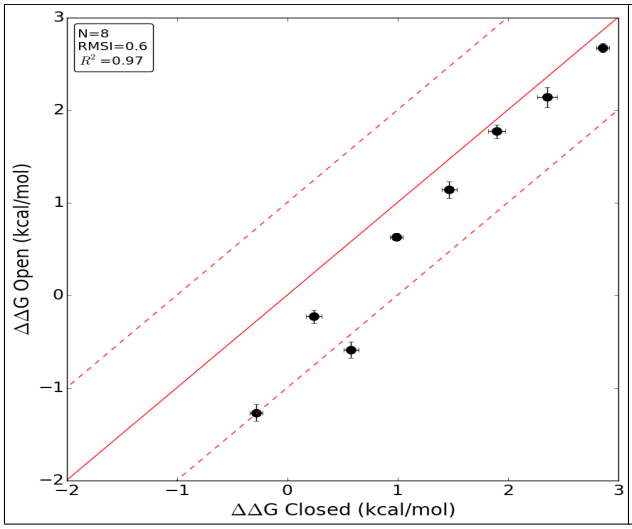
(c) Closed - Benzene to n-Hexylbenzene 45-55ns Colormap pREST

Figure 7: Benzene To n-Hexylbenzene (pREST) Colormap

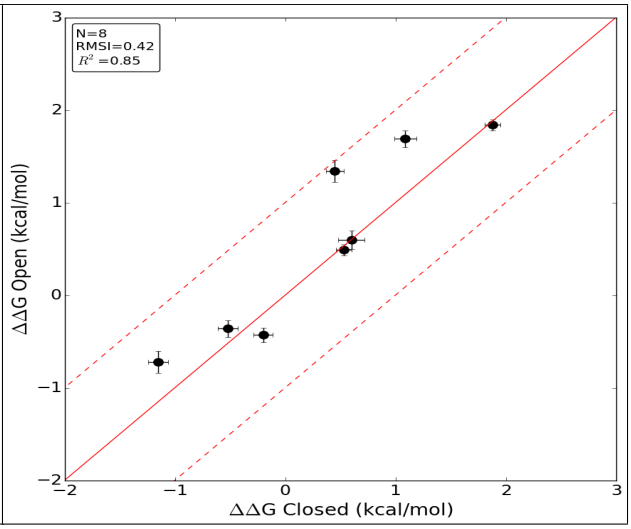


(a) Closed-Open XYplot (Default)

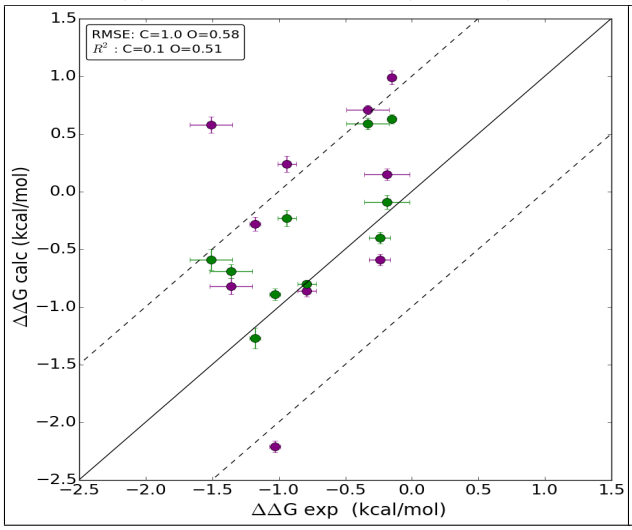
(b) Closed-Open XYplot (pREST)



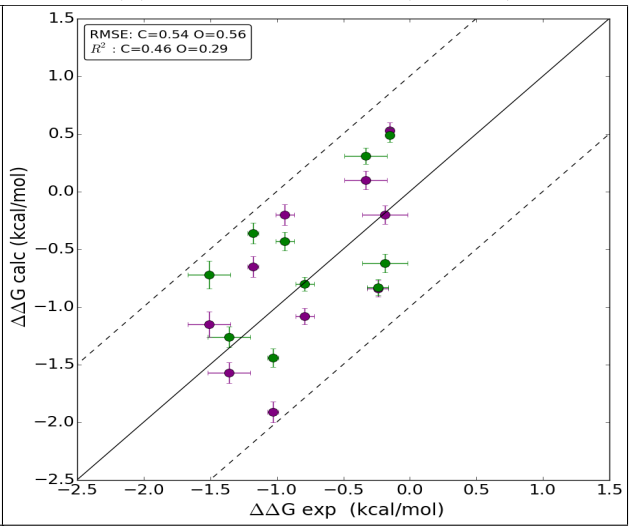
(c) Closed-Int XYplot (Default)



(d) Closed-Int XYplot (pREST)



(e) Exp XYplot (Default)



(f) Closed-Int XYplot (pREST)

Figure 8: Conf-XY