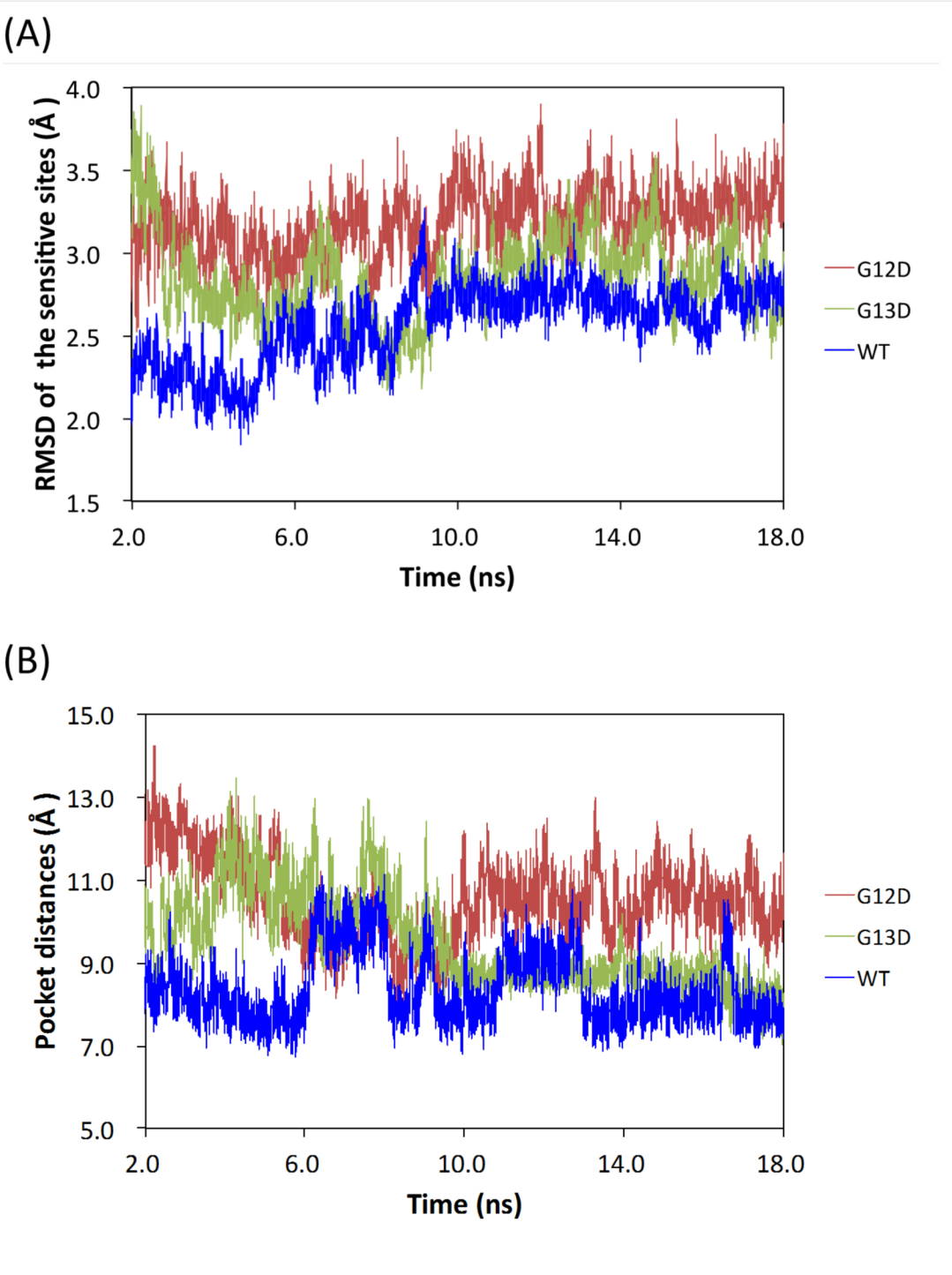

Figure S5 – The third repeated molecular dynamics trajectories for:

(A) Comparison of the RMSD plots of the sensitive sites (P-loop, switch I and II regions) of WT, G12D and G13D structures with respect to the initial conformation during the course of the simulation; (B) the pocket distances between the mass center of residues 12-13 and the mass center of residues 32-34 for WT, G12D, and G13D, respectively.