Parallel simulation 1:

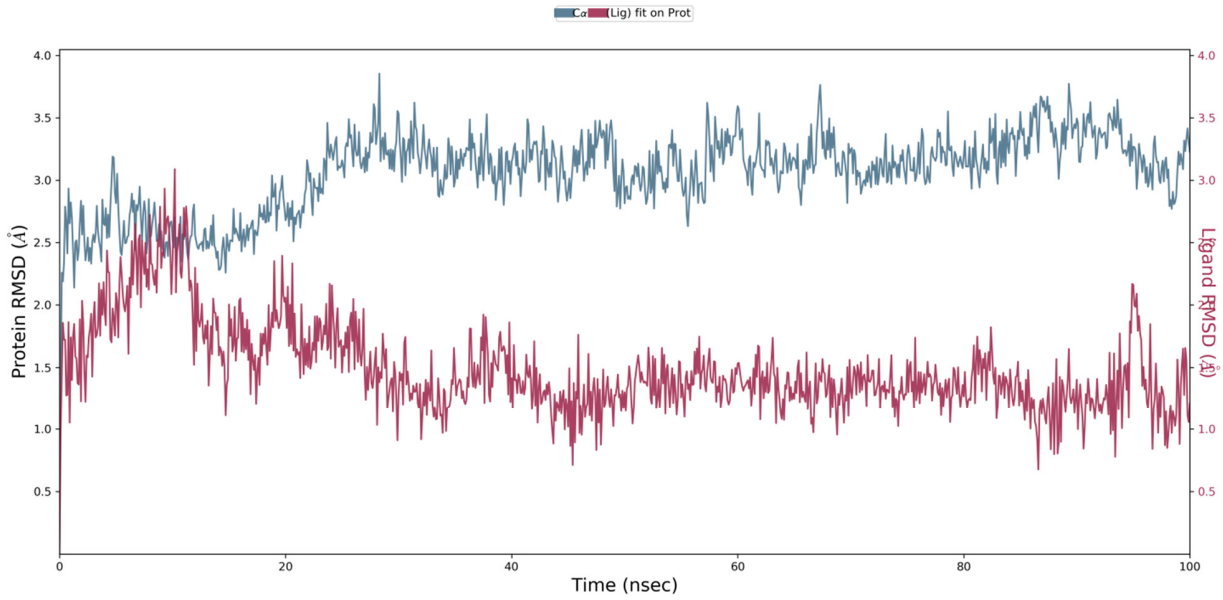

Figure S1. Root mean square deviation of Piperbetol with dimeric GRB2 during 100ns molecular dynamics simulation

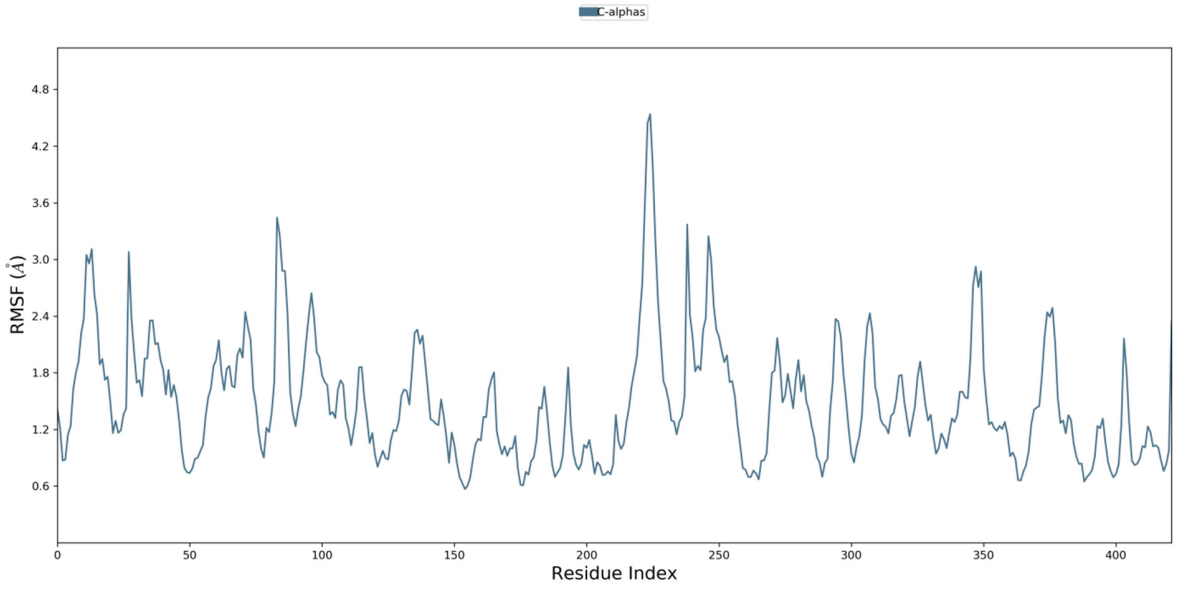

Figure S2. Root mean square fluctuation of Piperbetol with dimeric GRB2 during 100ns molecular dynamics simulation

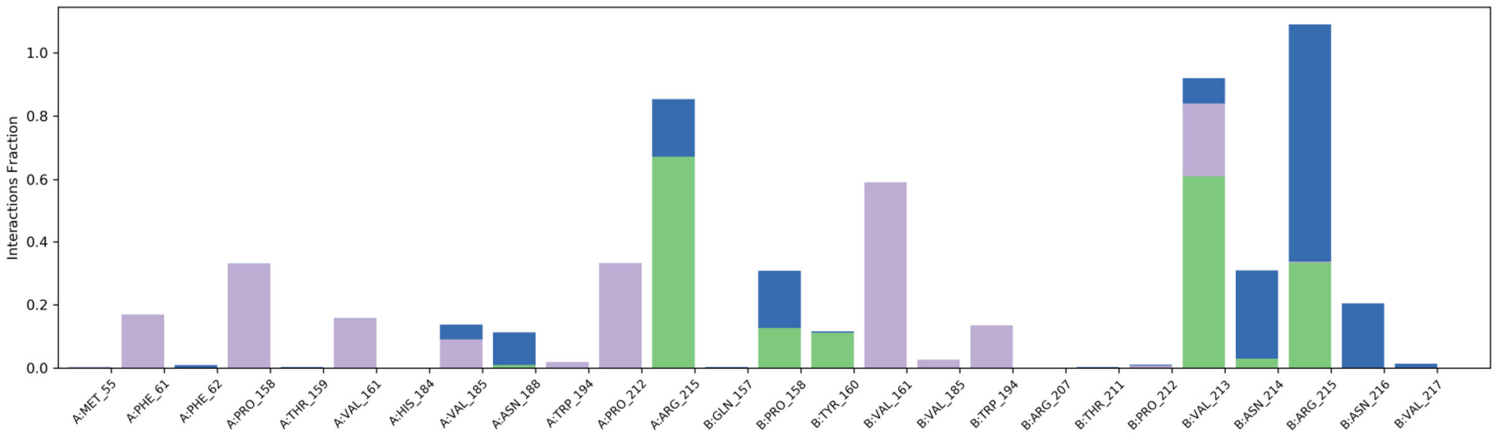

Figure S3. Protein-ligand contacts of Piperbetol with dimeric GRB2 during 100ns molecular dynamics simulation

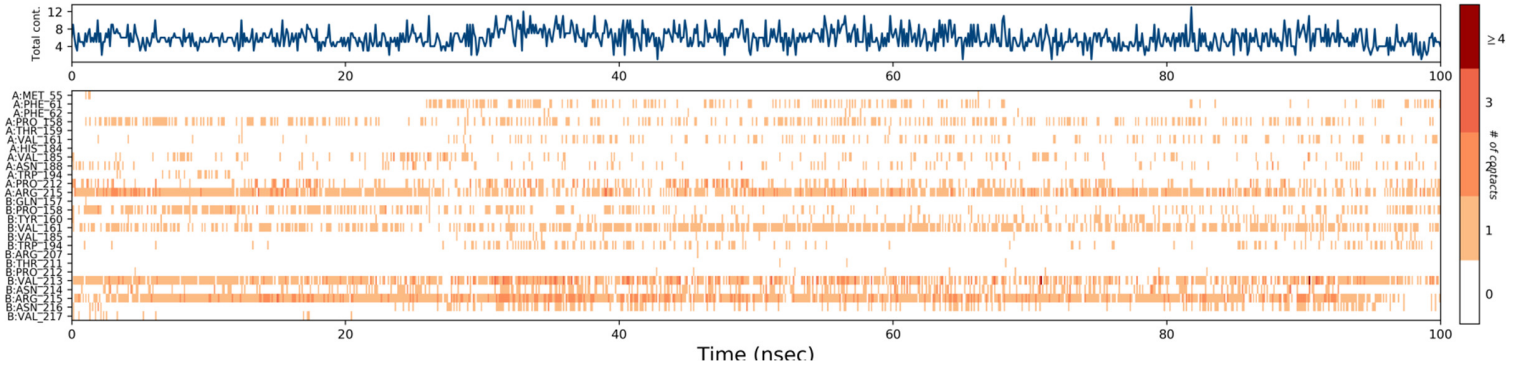

Figure S4. Timeline representation of Piperbetol with dimeric GRB2 contacts during 100ns molecular dynamics simulation

Parallel simulation 2:

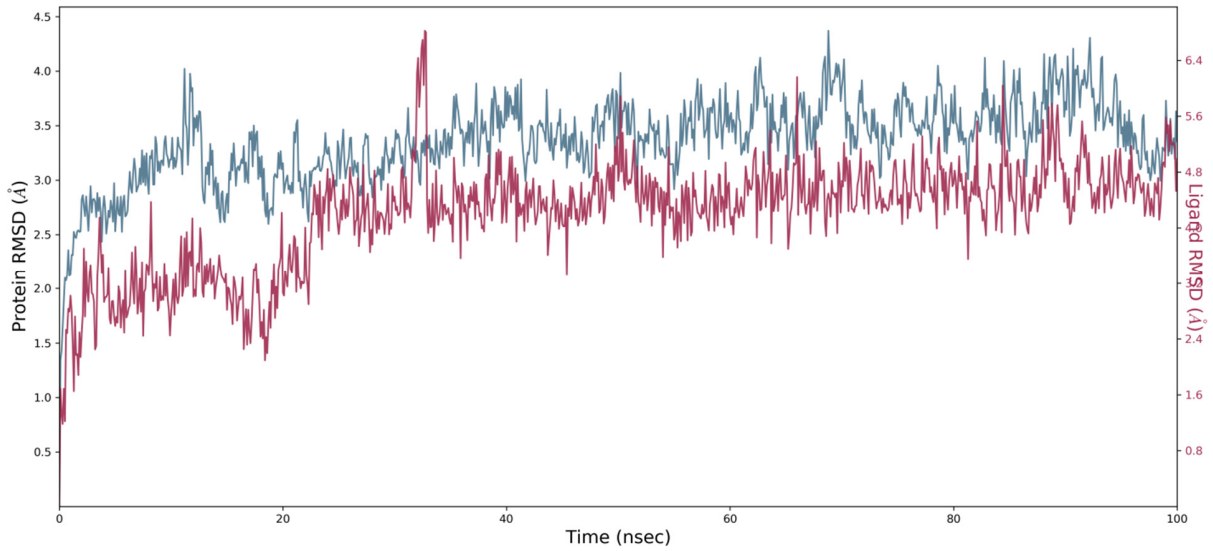

Figure S5. Root mean square deviation of Piperbetol with dimeric GRB2 during 100ns molecular dynamics simulation

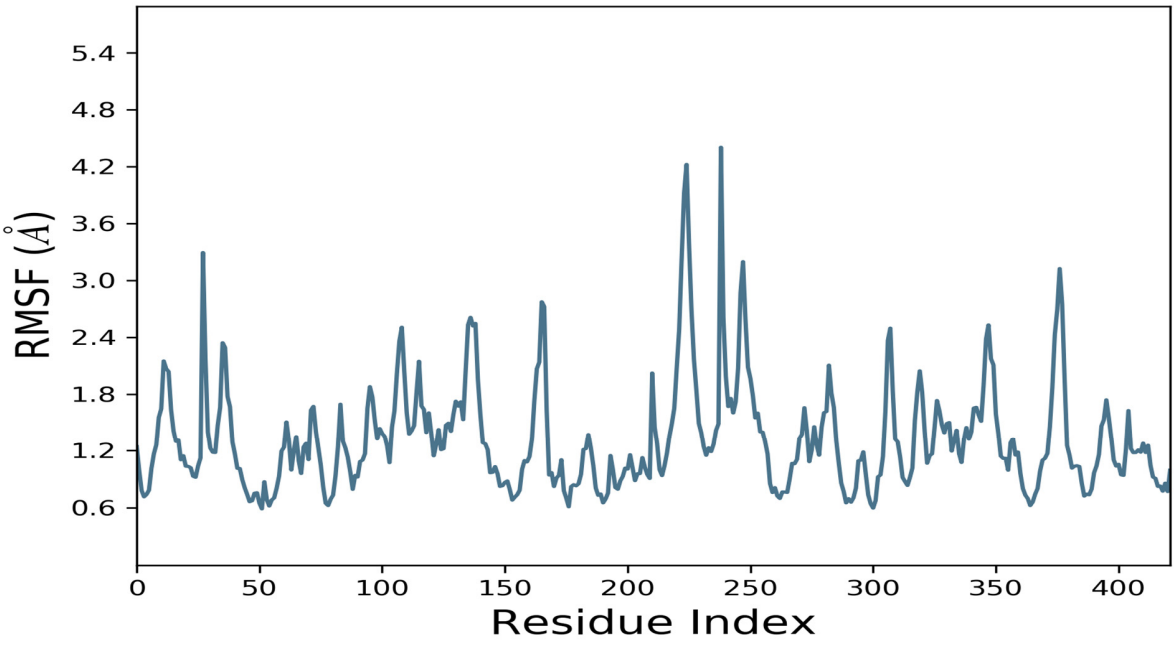

Figure S6. Root mean square fluctuation of Piperbetol with dimeric GRB2 during 100ns molecular dynamics simulation.

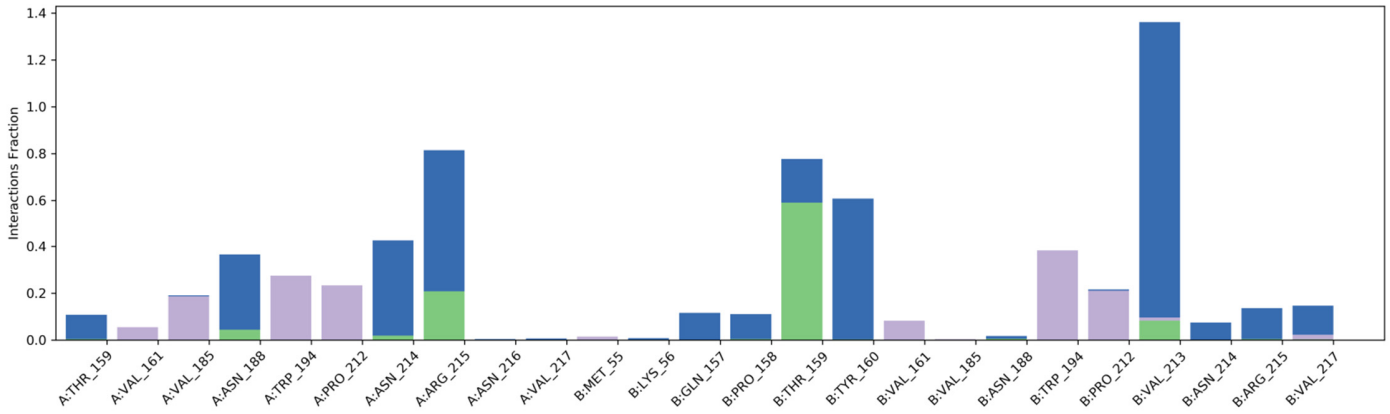

Figure S7. Protein-ligand contacts of Piperbetol with dimeric GRB2 during 100ns molecular dynamics simulation

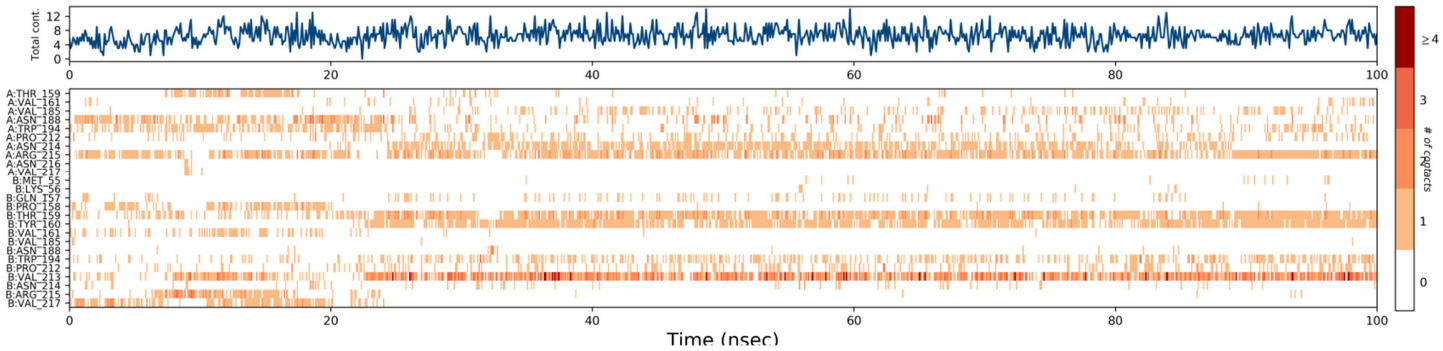

Figure S8. Timeline representation of Piperbetol with dimeric GRB2 contacts during 100ns molecular dynamics simulation

Comparative Assessment of Primary & Parallel simulations

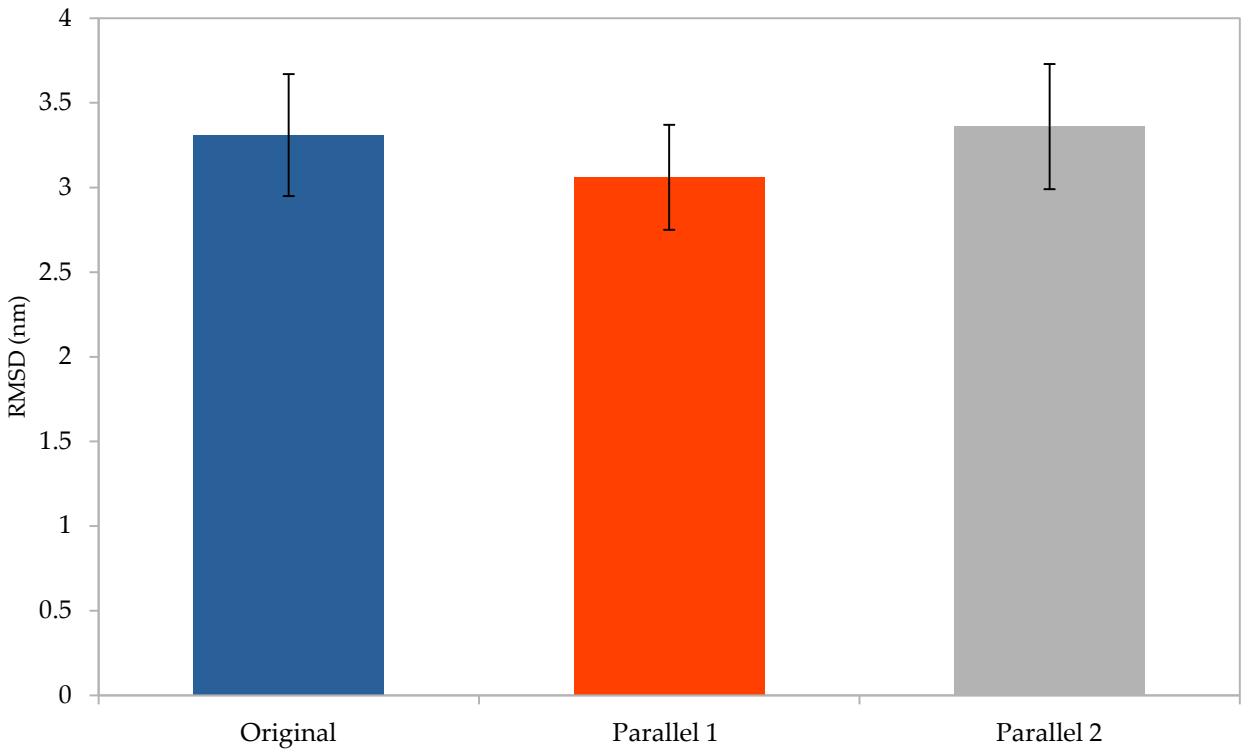

Figure S9. Bar graph showing the RMSD (C-α) average and standard deviation for the dimer GRB2 with piperbetol presenting no differences in the trajectories in both primary and parallel simulation during 100 ns.

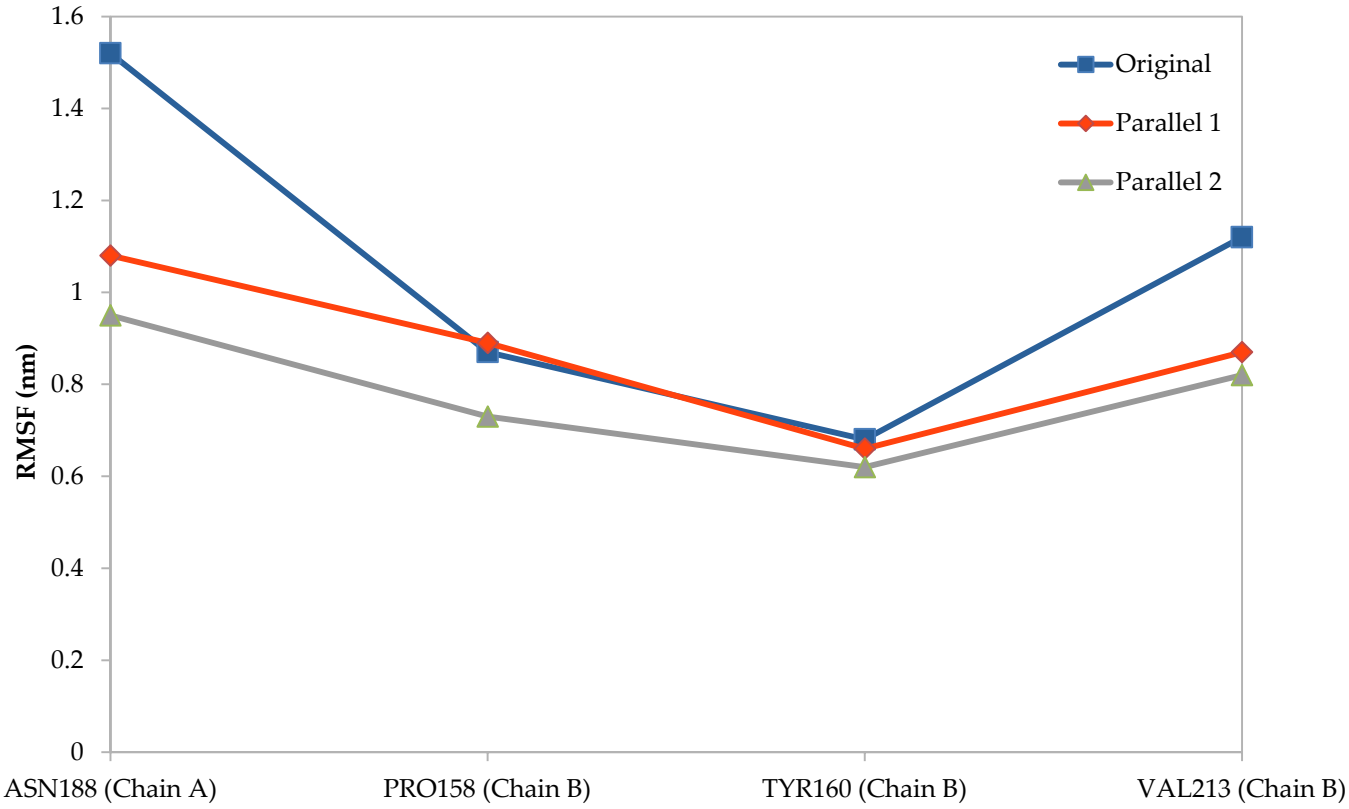

Figure S10. The Line graph present RMSF value of amino acids at piperbetol binding sites with dimeric GRB2. Both the primary and parallel simulations shows similar pattern of fluctuation confirming the consistency in simulation results.