

# Immunoproteasome and non-covalent inhibition: exploration by advanced molecular dynamics and docking methods

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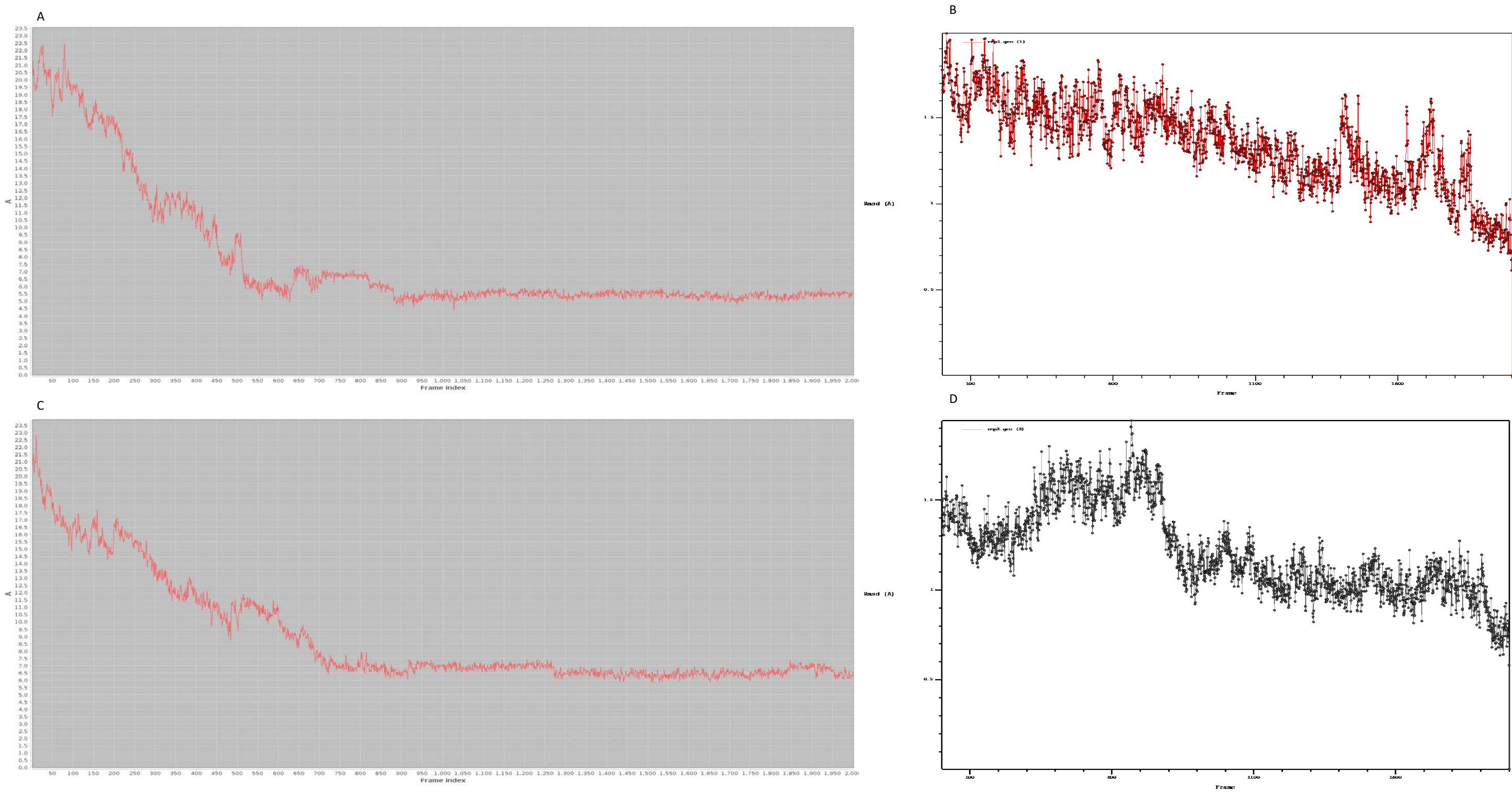


Figure S1. MD-binding: Ligand RMSD calculated from the centroid of binding pocket and protein backbone RMSD (20ns) for Replica 1 (A-B) and Replica 2 (C-D).

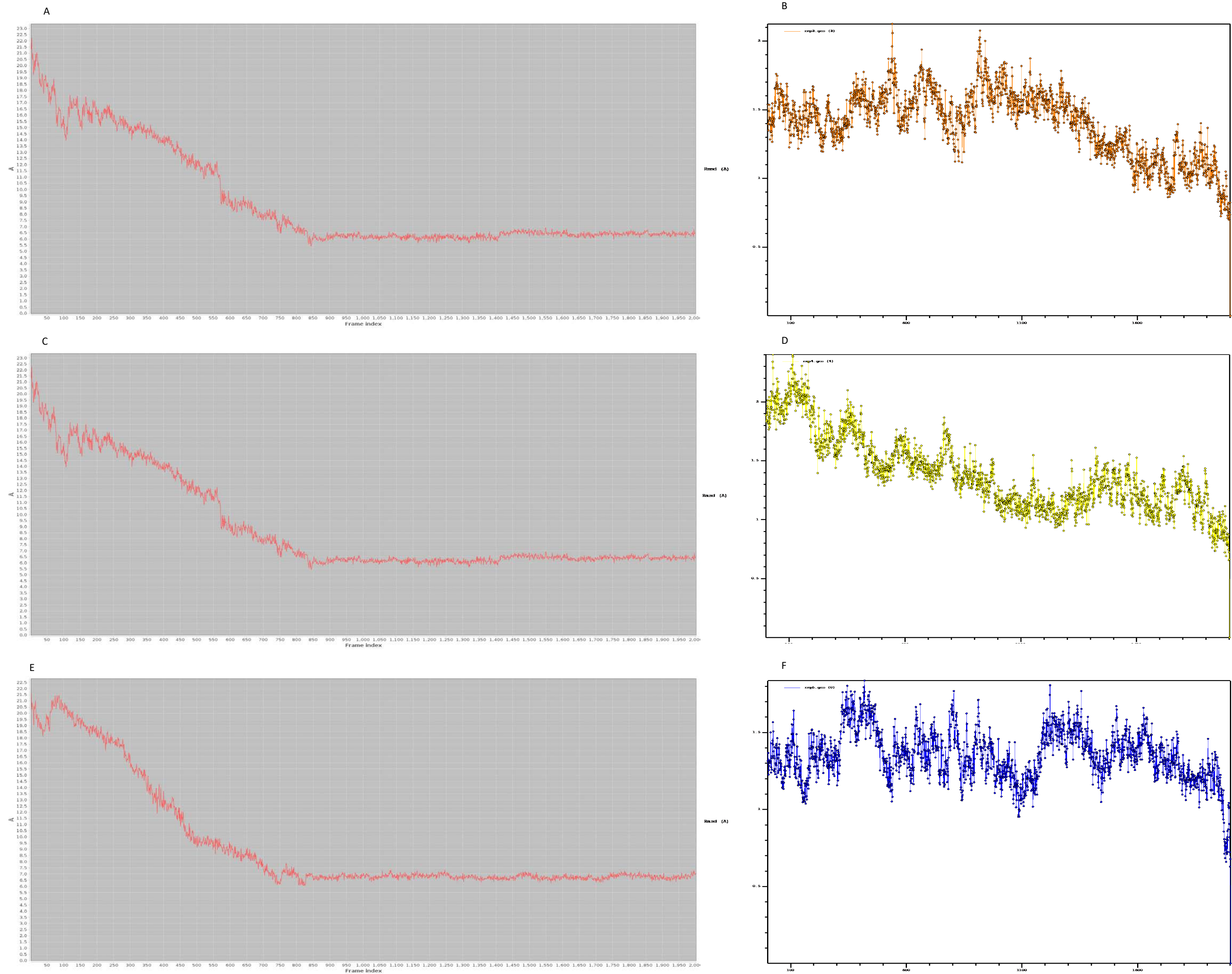


Figure S2. MD-binding: Ligand RMSD calculated from the centroid of binding pocket and protein backbone RMSD (20ns) for Replica 3 (A-B), Replica 4 (C-D), Replica 5 (E-F).



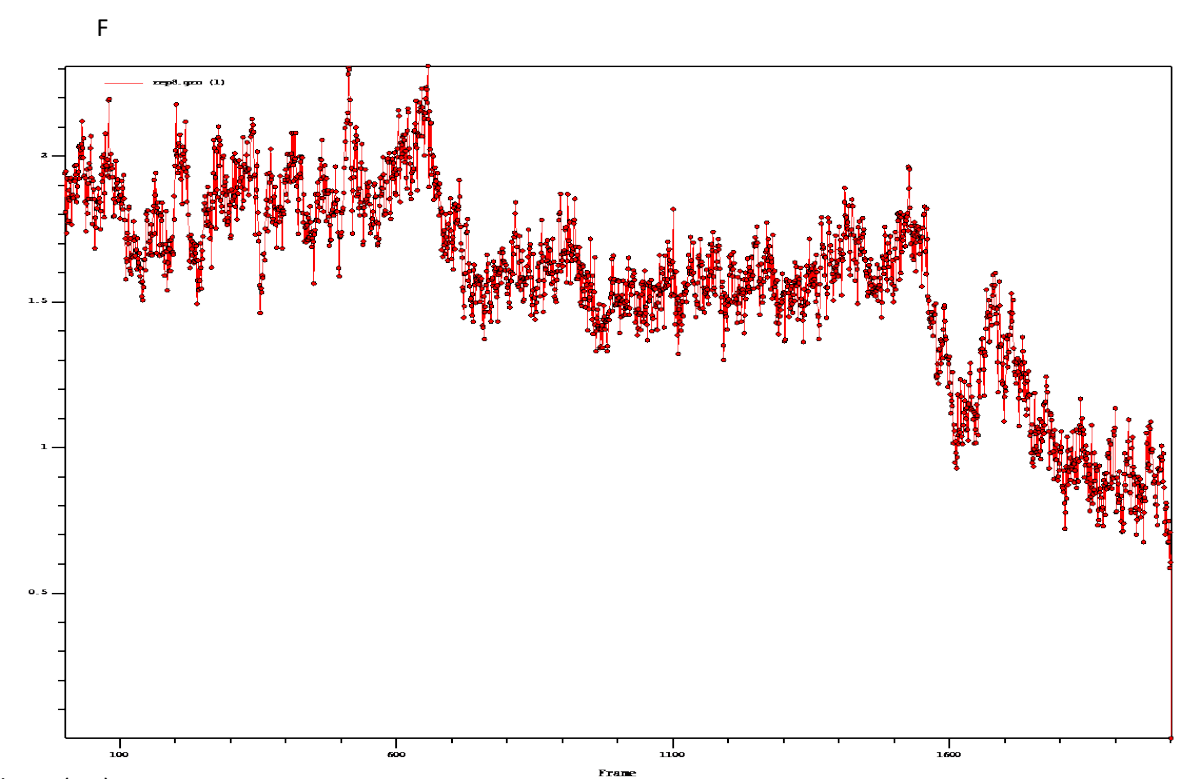
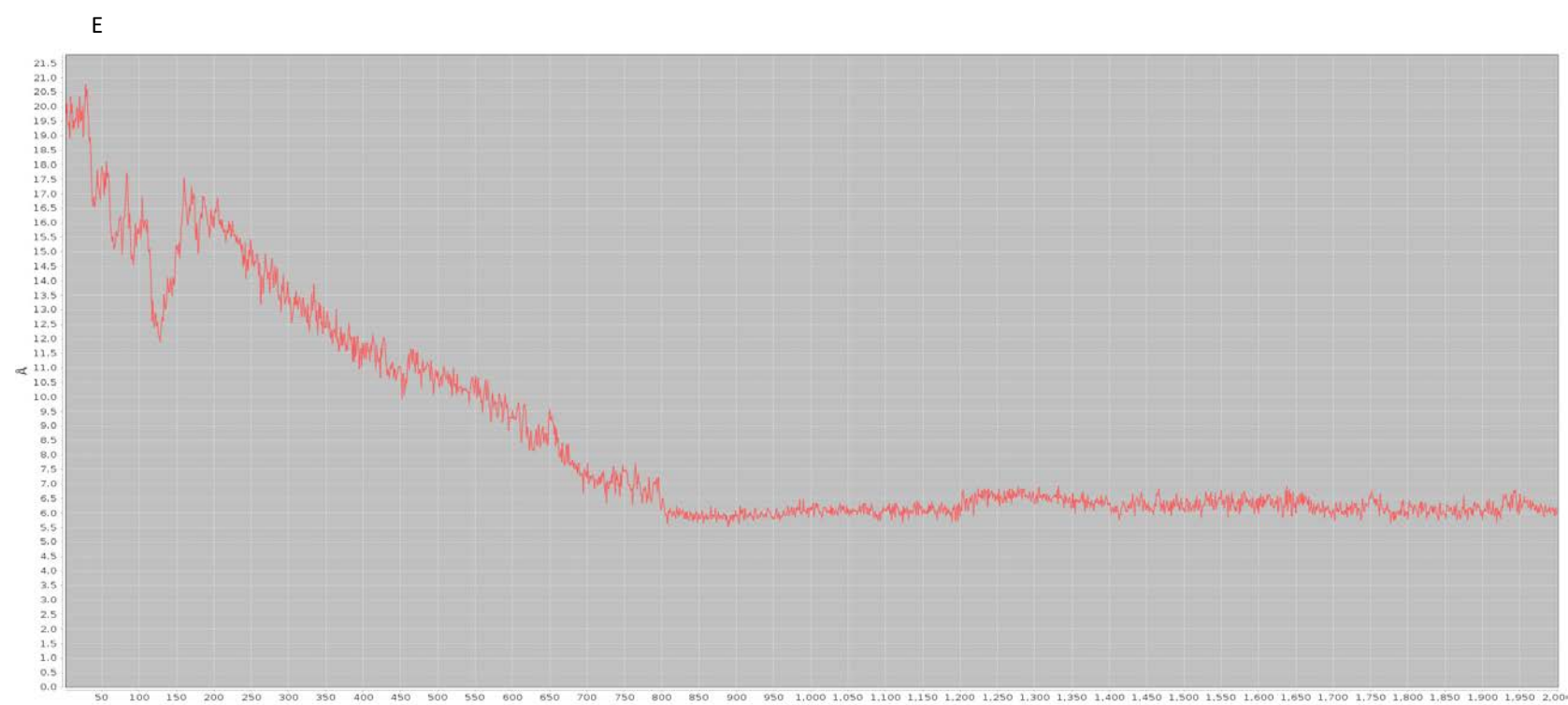
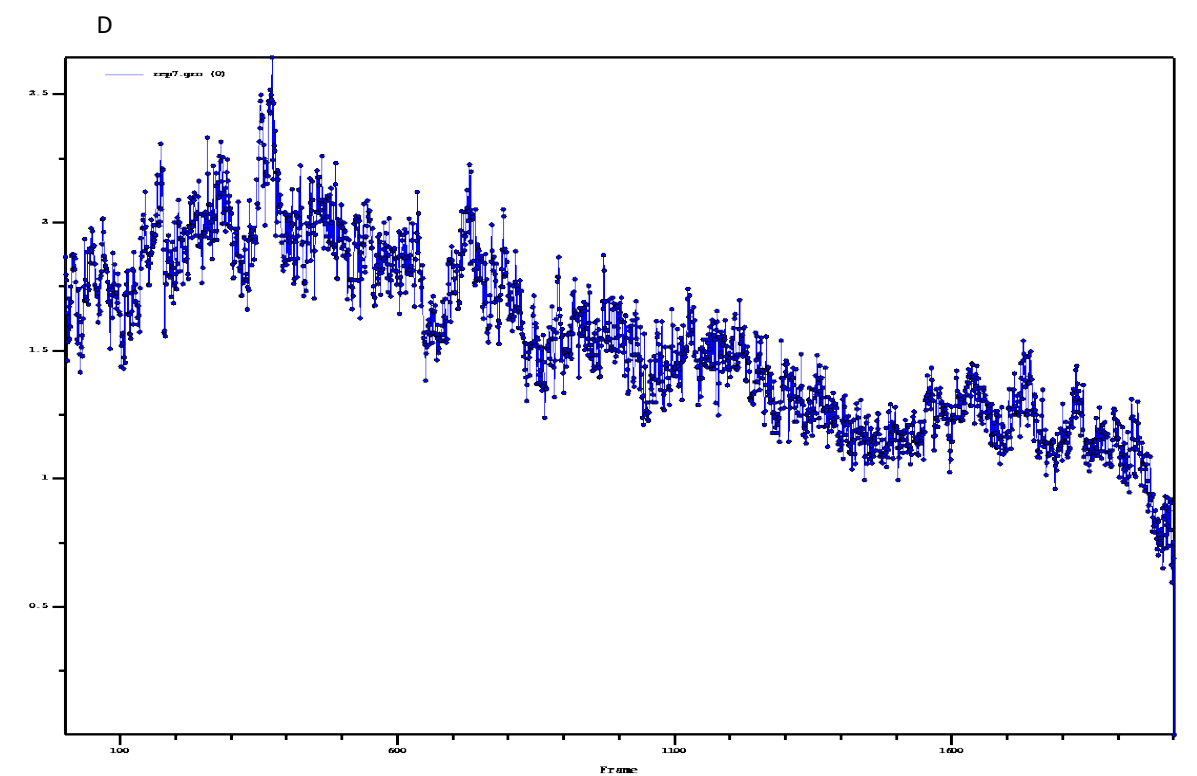
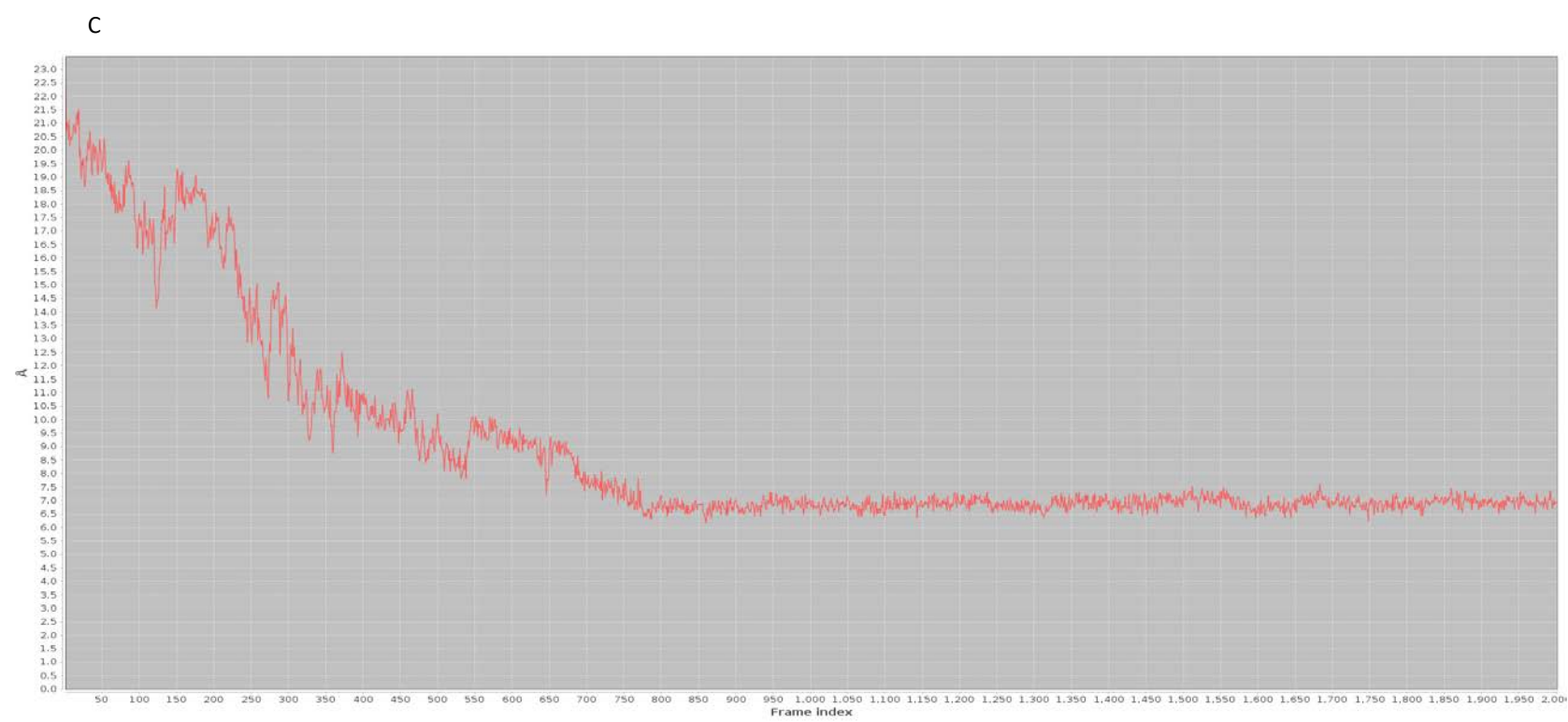
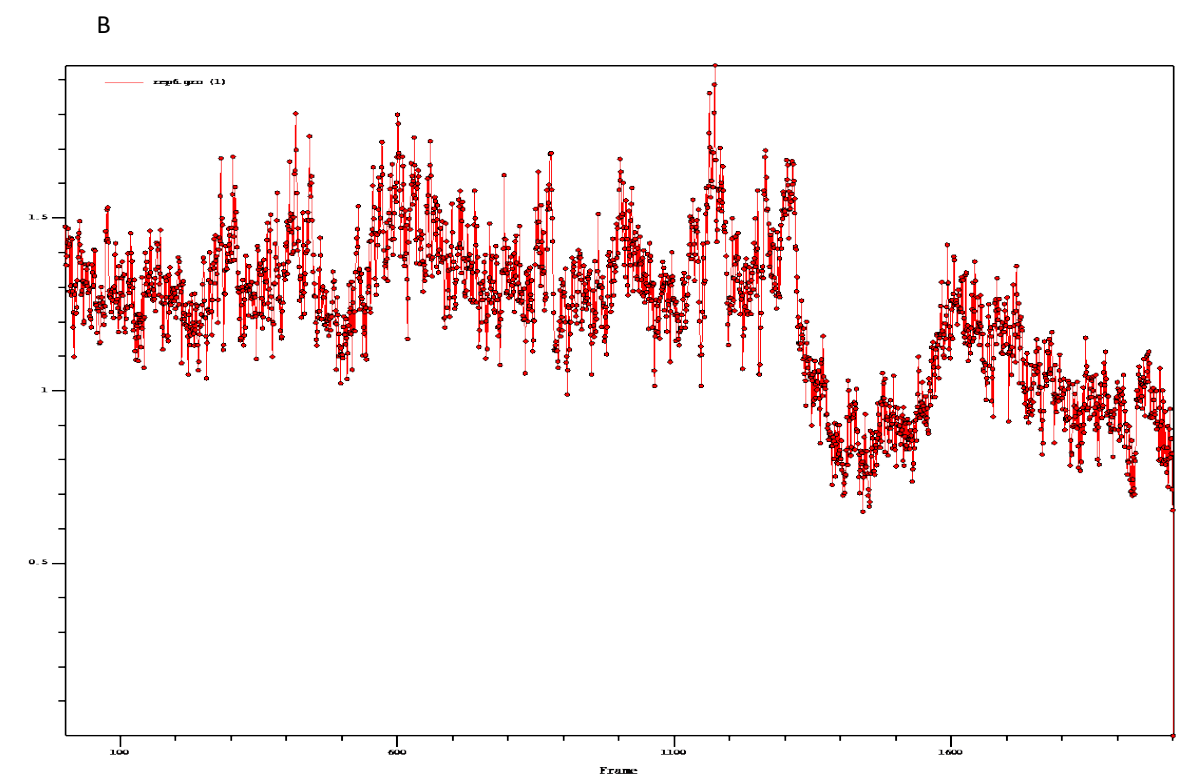
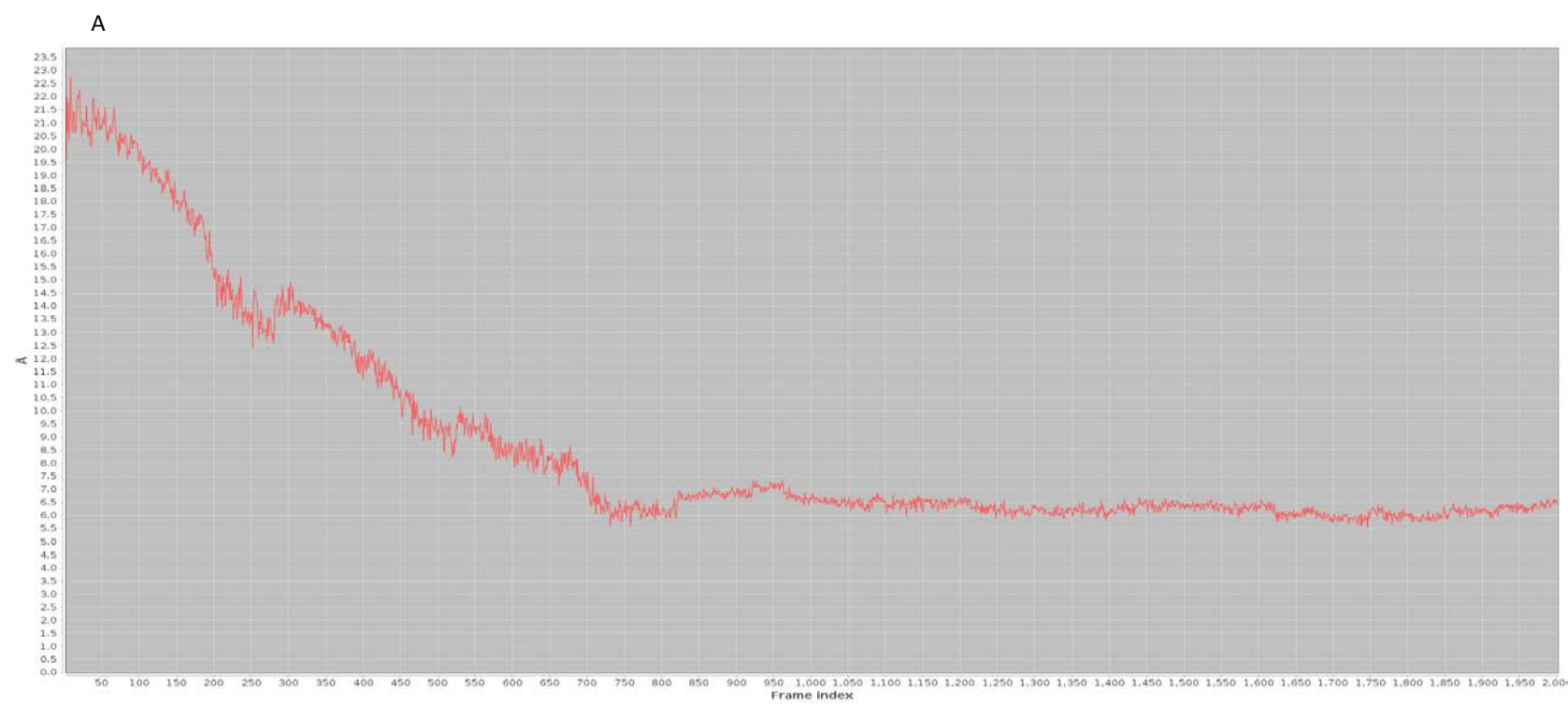


Figure S3. MD-binding: Ligand RMSD calculated from the centroid of binding pocket and protein backbone RMSD (20ns) for Replica 6 (A-B), Replica 7 (C-D), Replica 8 (E-F).

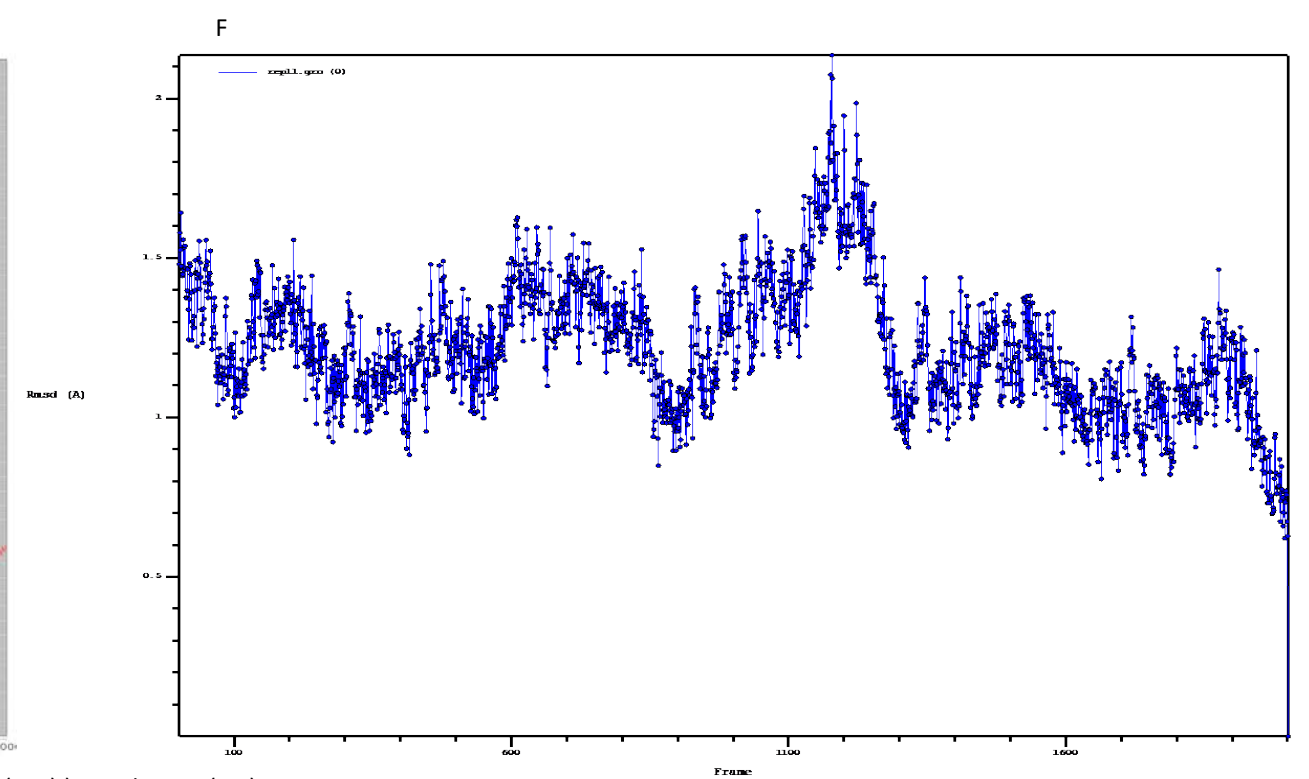
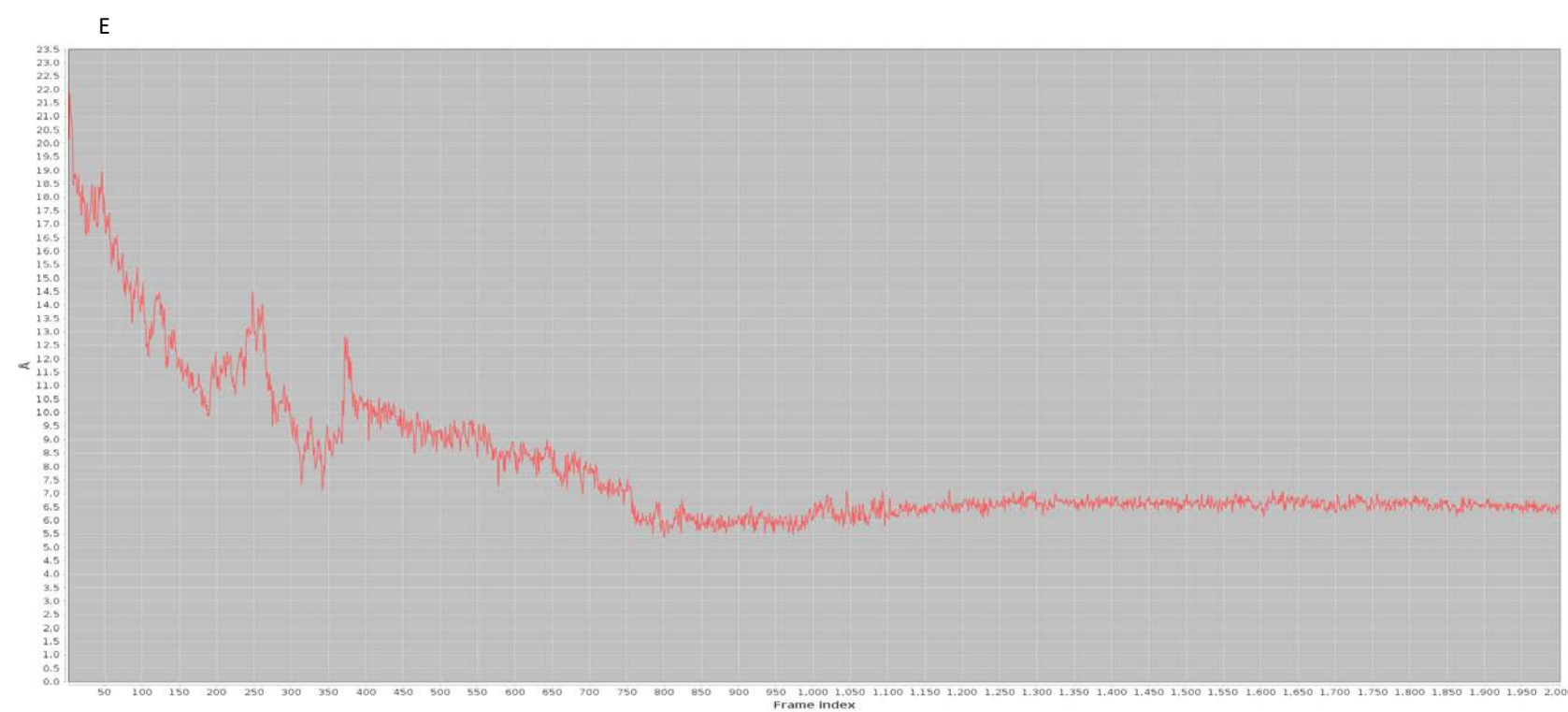
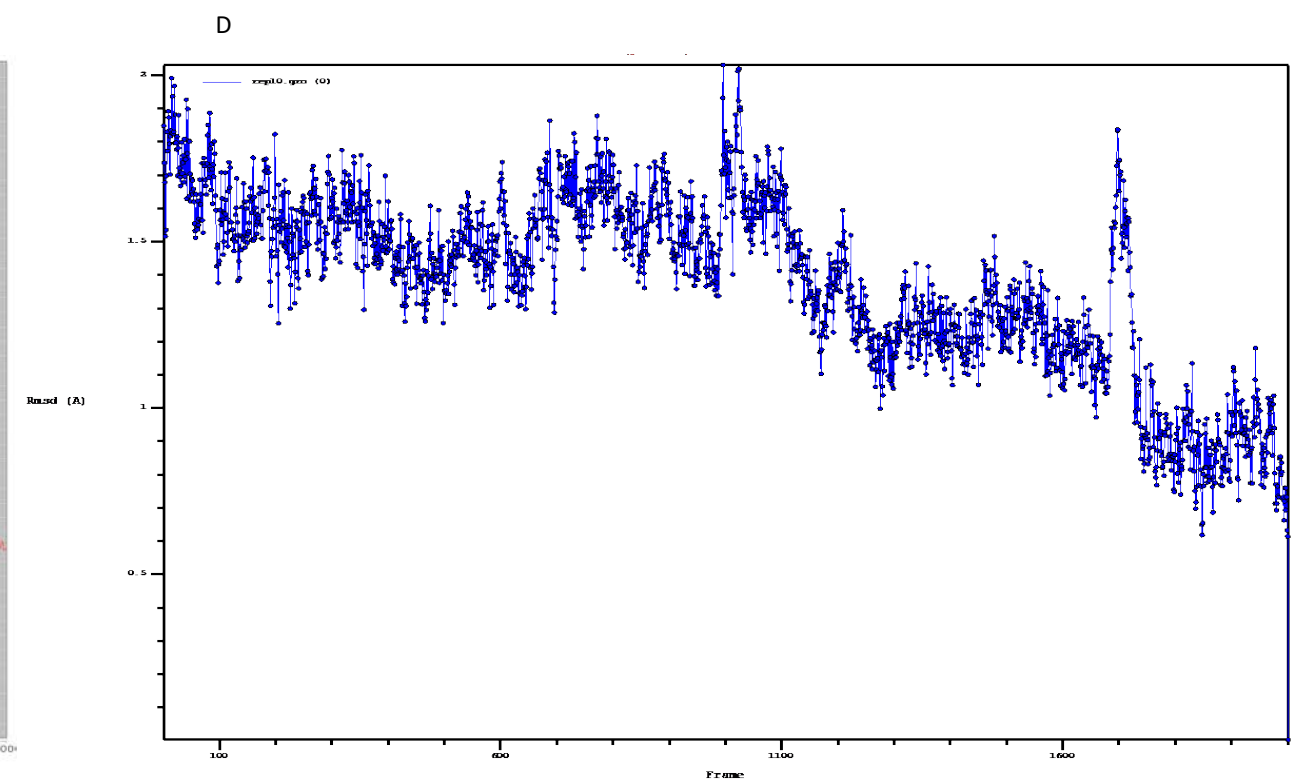
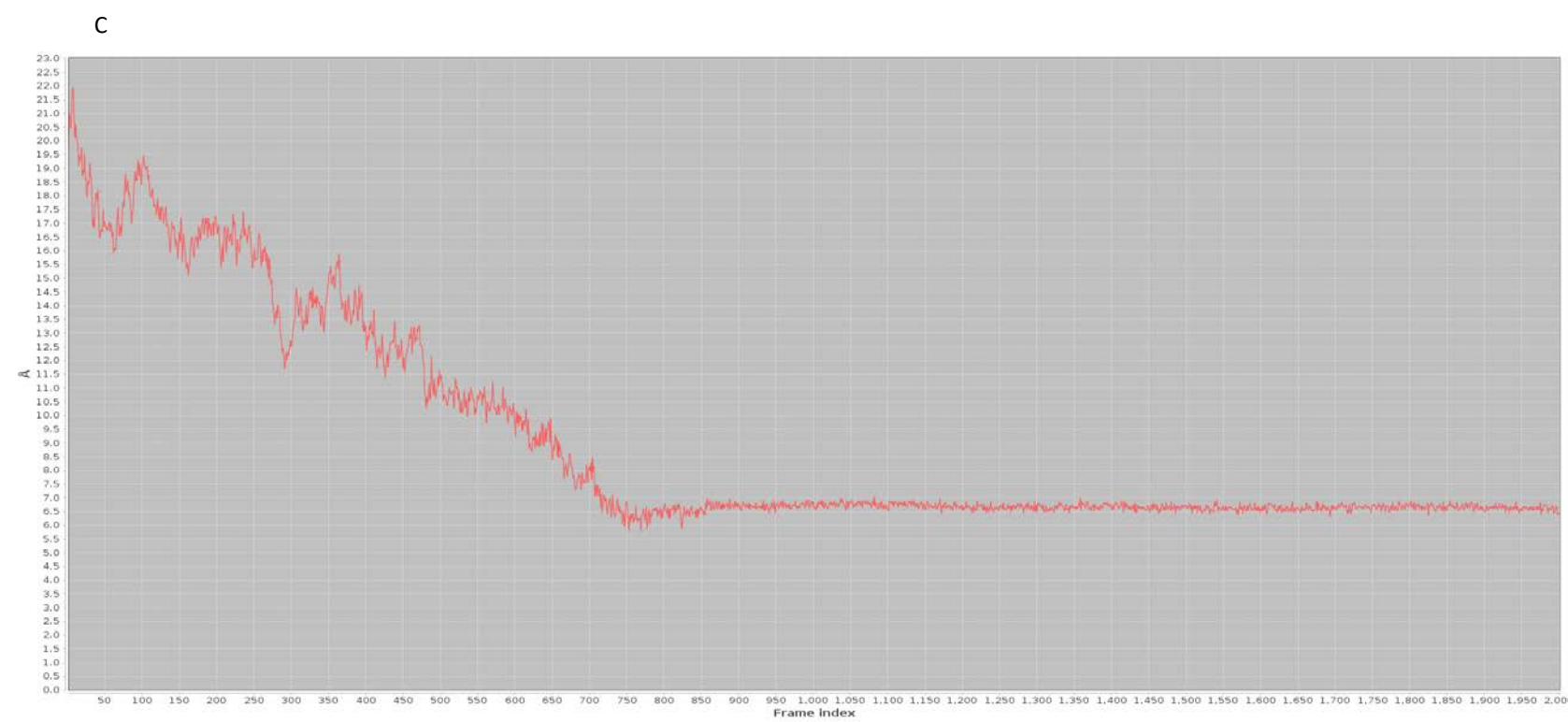
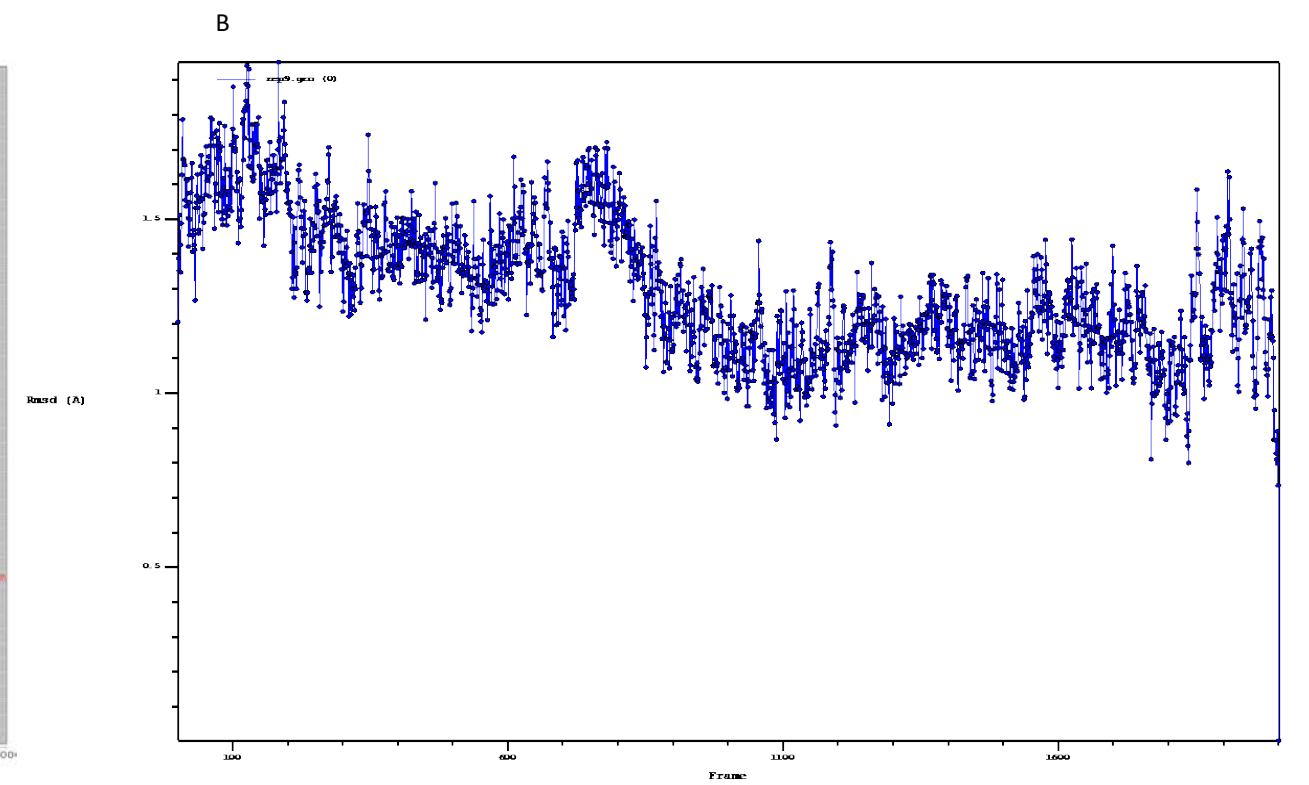
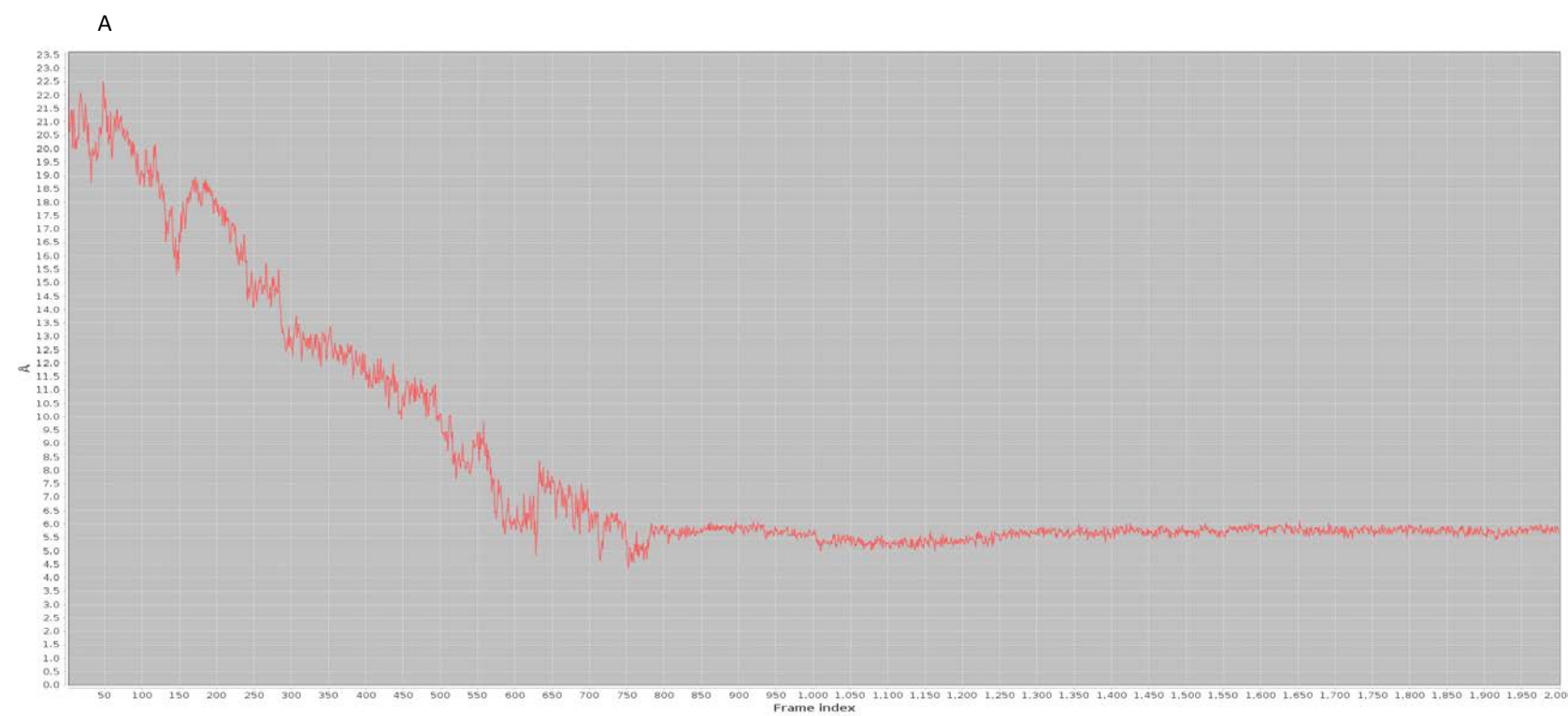


Figure S4. MD-binding: Ligand RMSD calculated from the centroid of binding pocket and protein backbone RMSD (20ns) for Replica 9 (A-B), Replica 10 (C-D), Replica 11 (E-F).



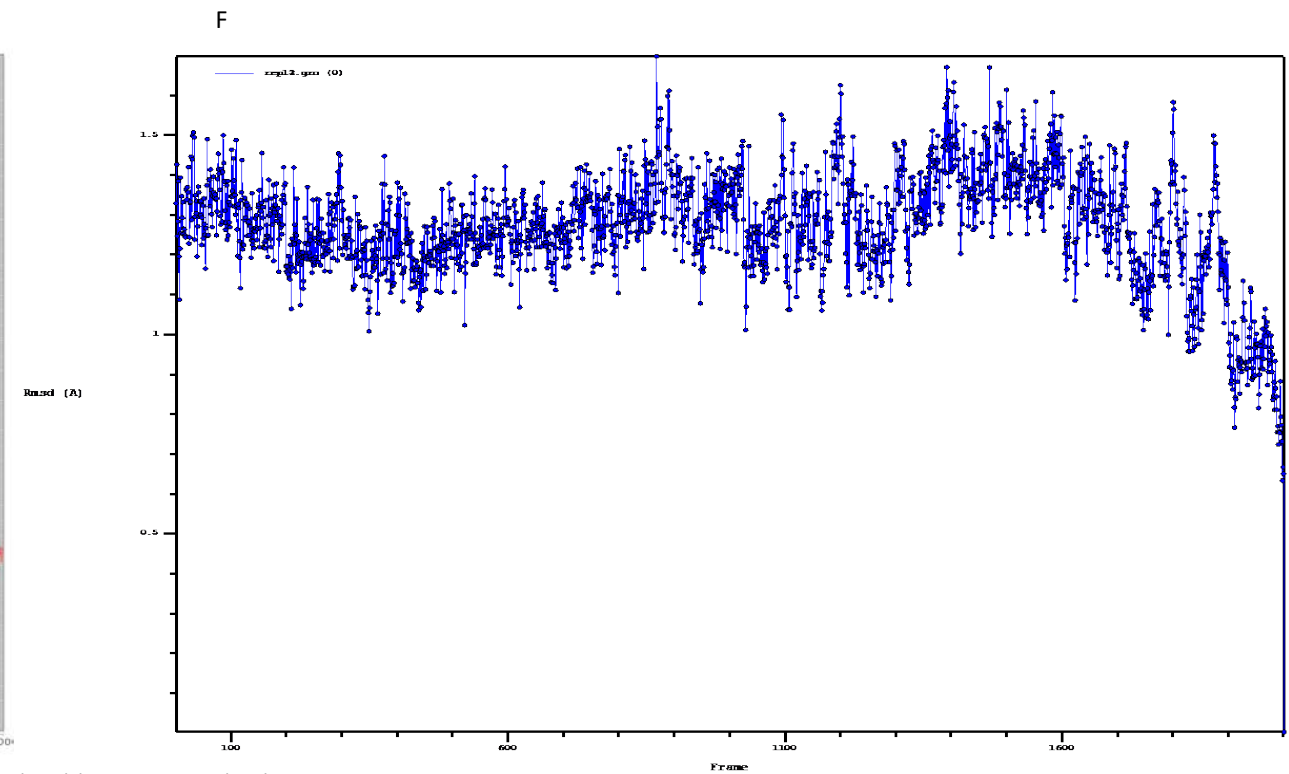
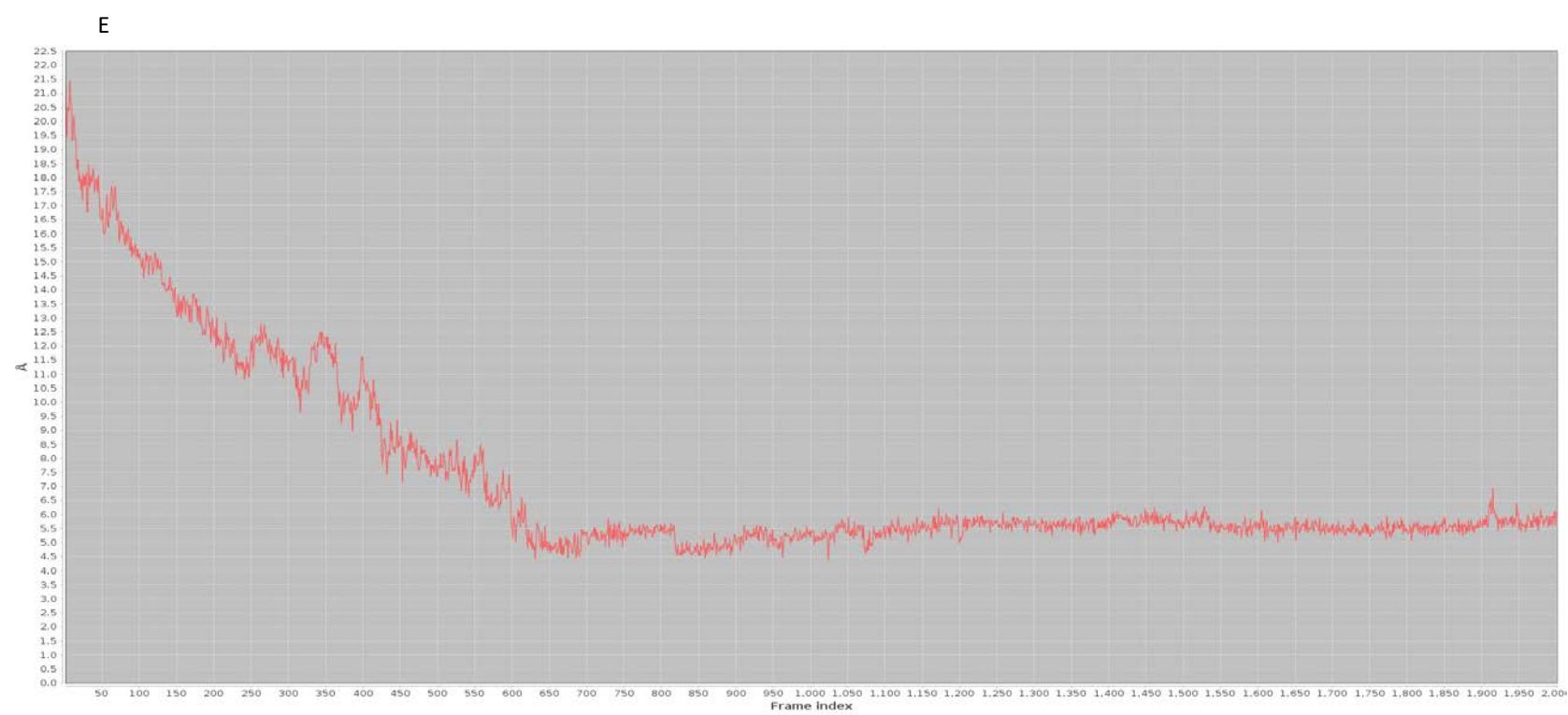
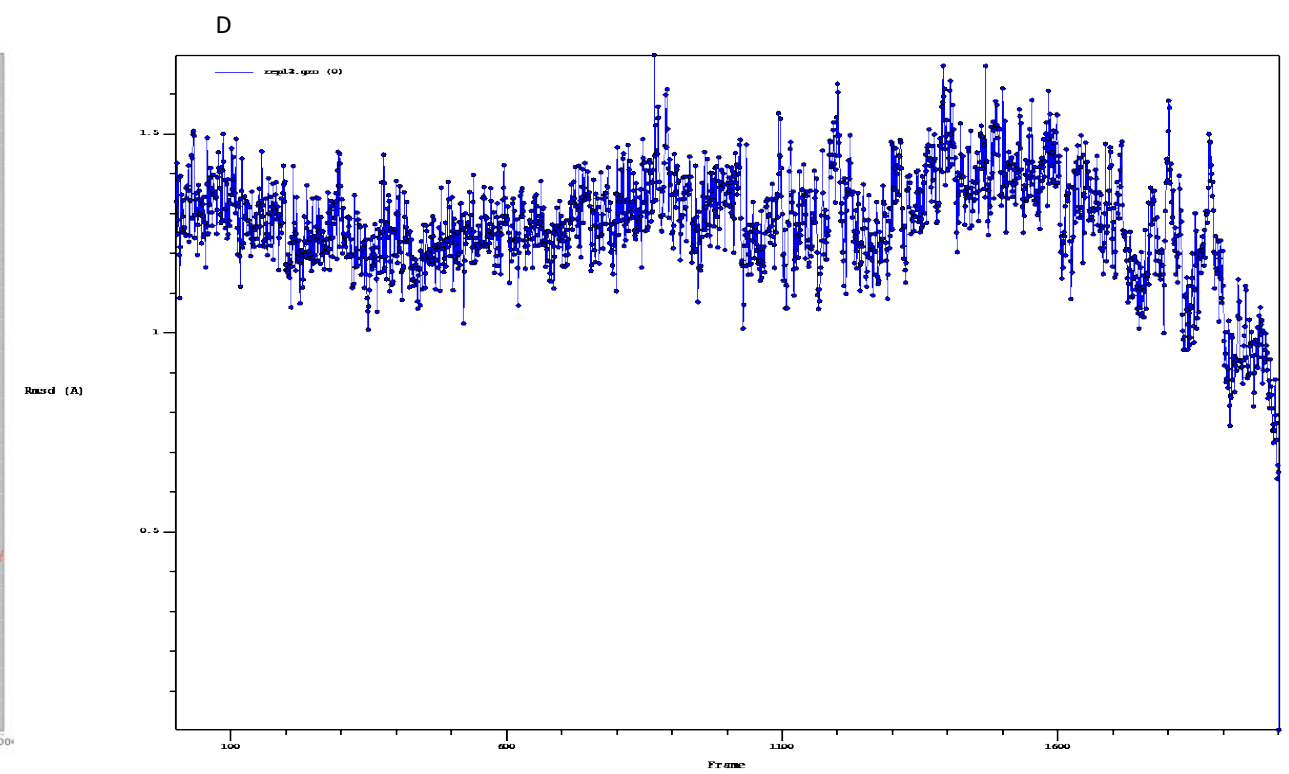
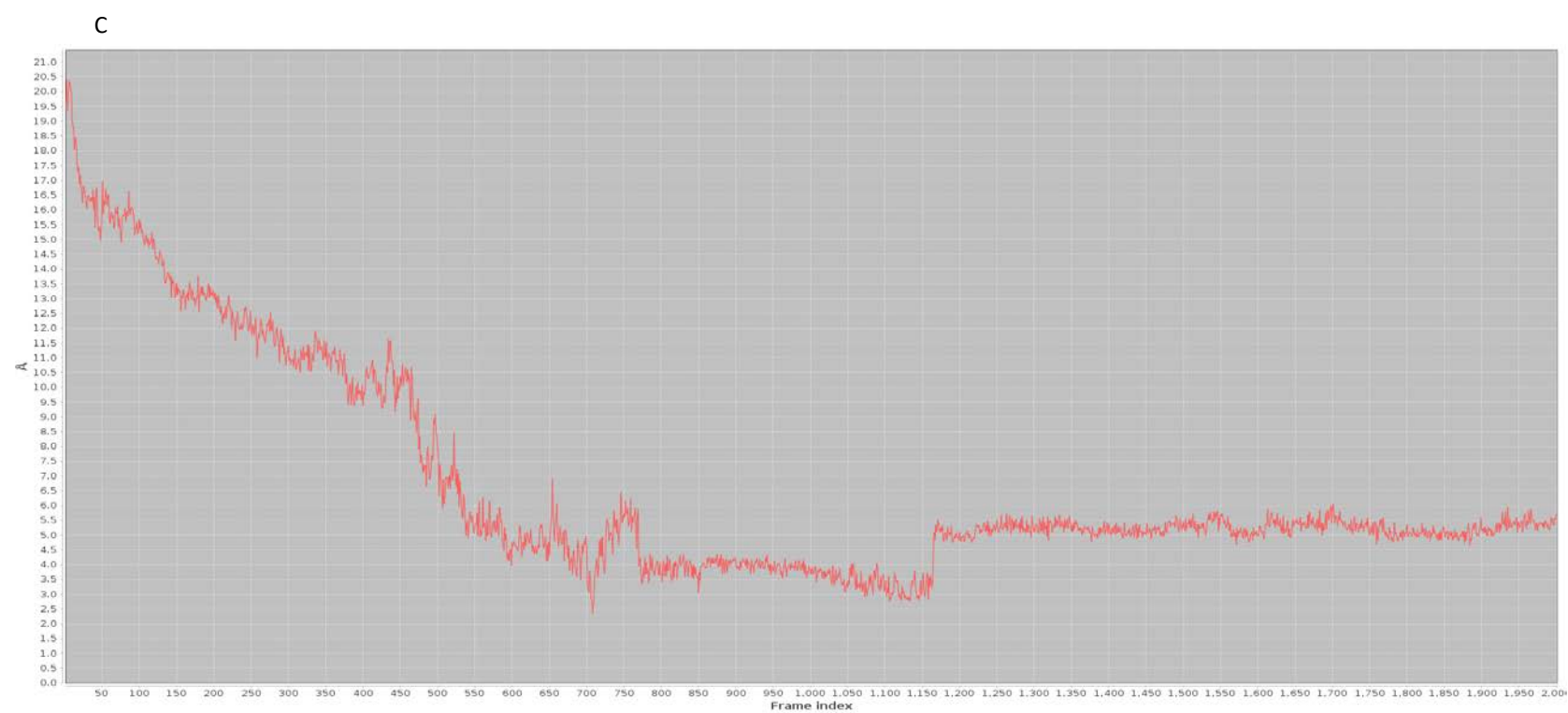
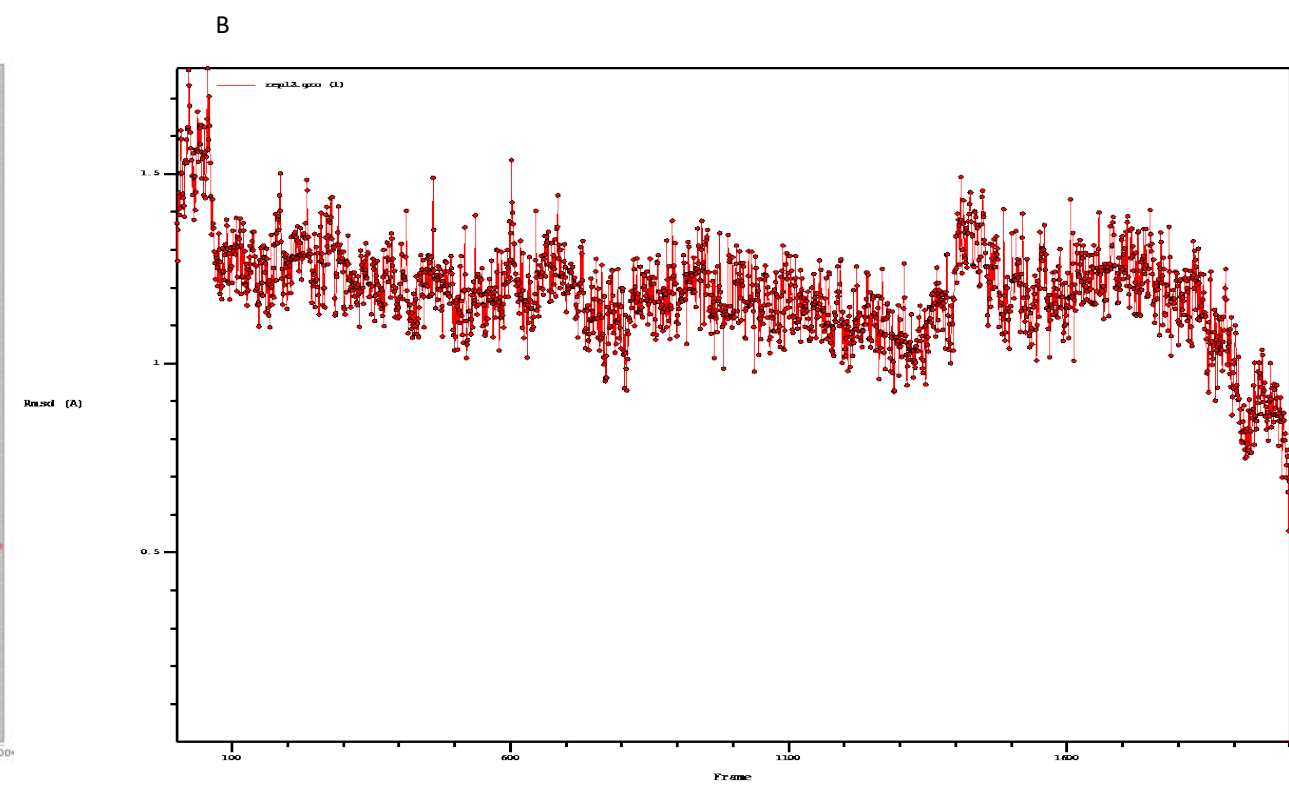
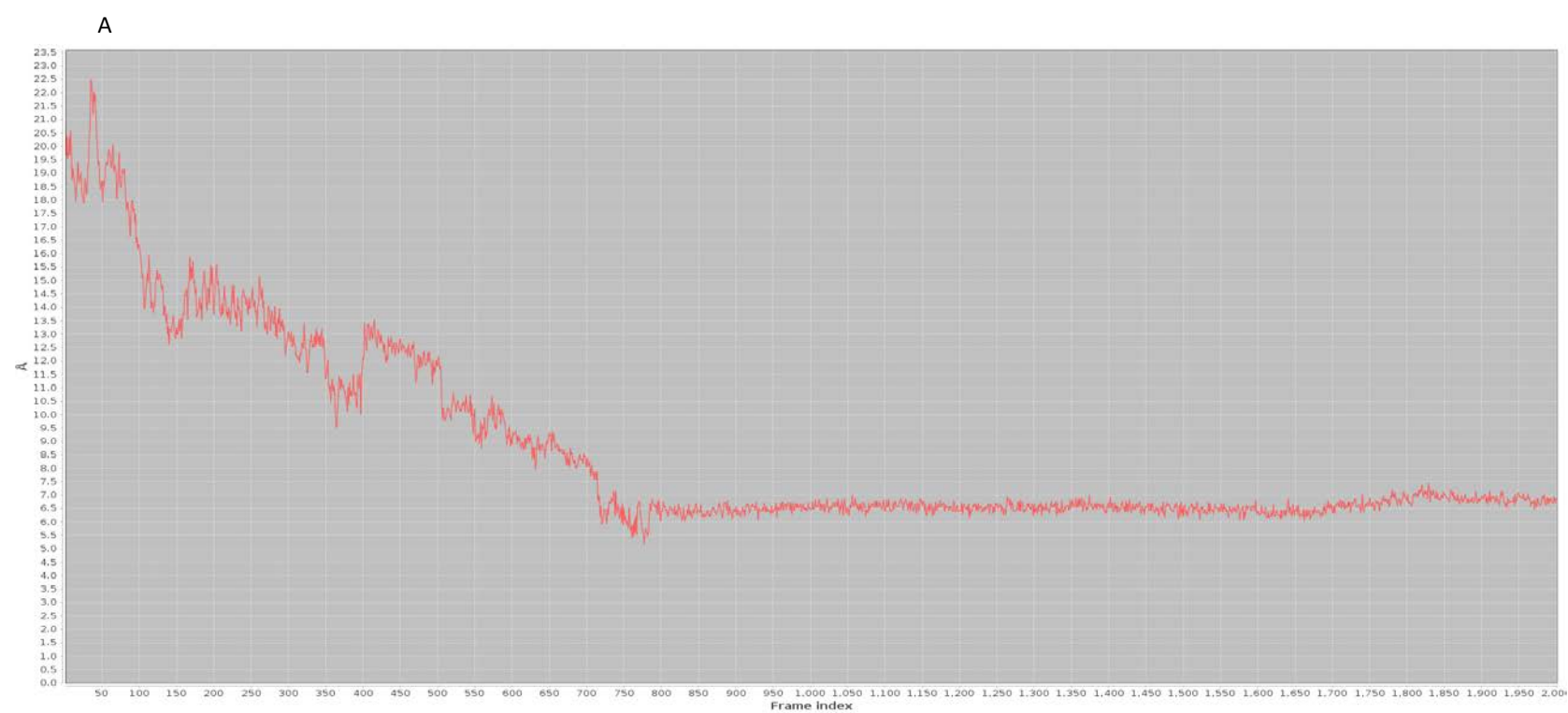


Figure S5. MD-binding: Ligand RMSD calculated from the centroid of binding pocket and protein backbone RMSD (20ns) for Replica 12 (A-B), Replica 13 (C-D), Replica 14 (E-F).

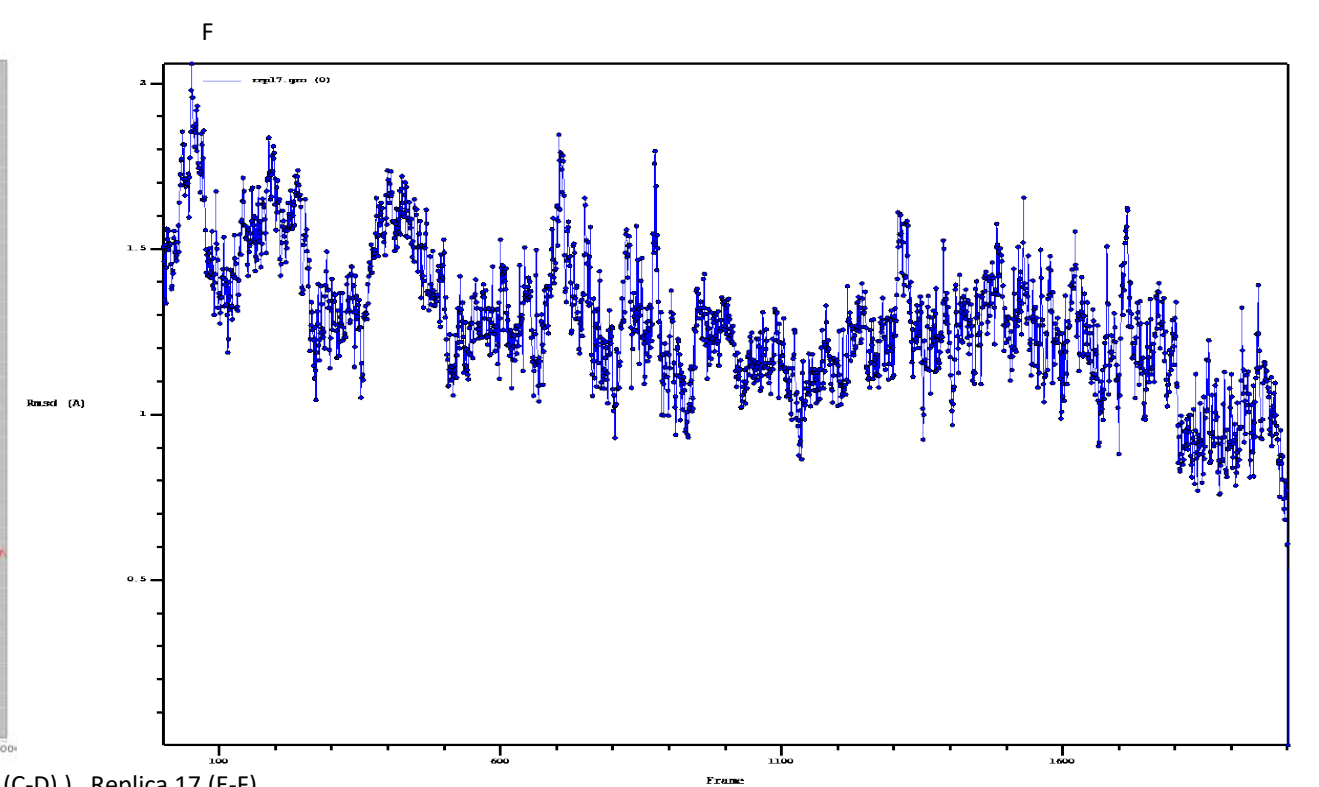
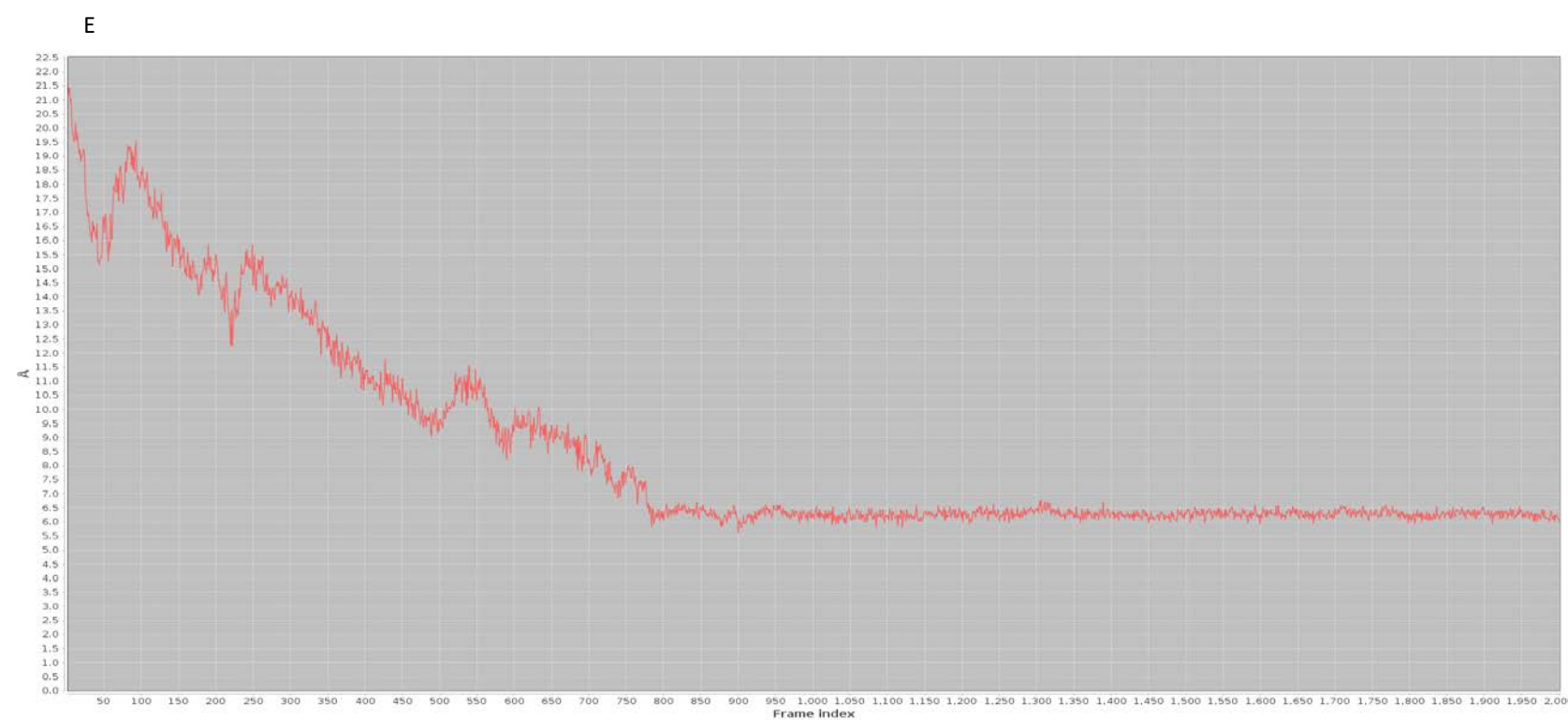
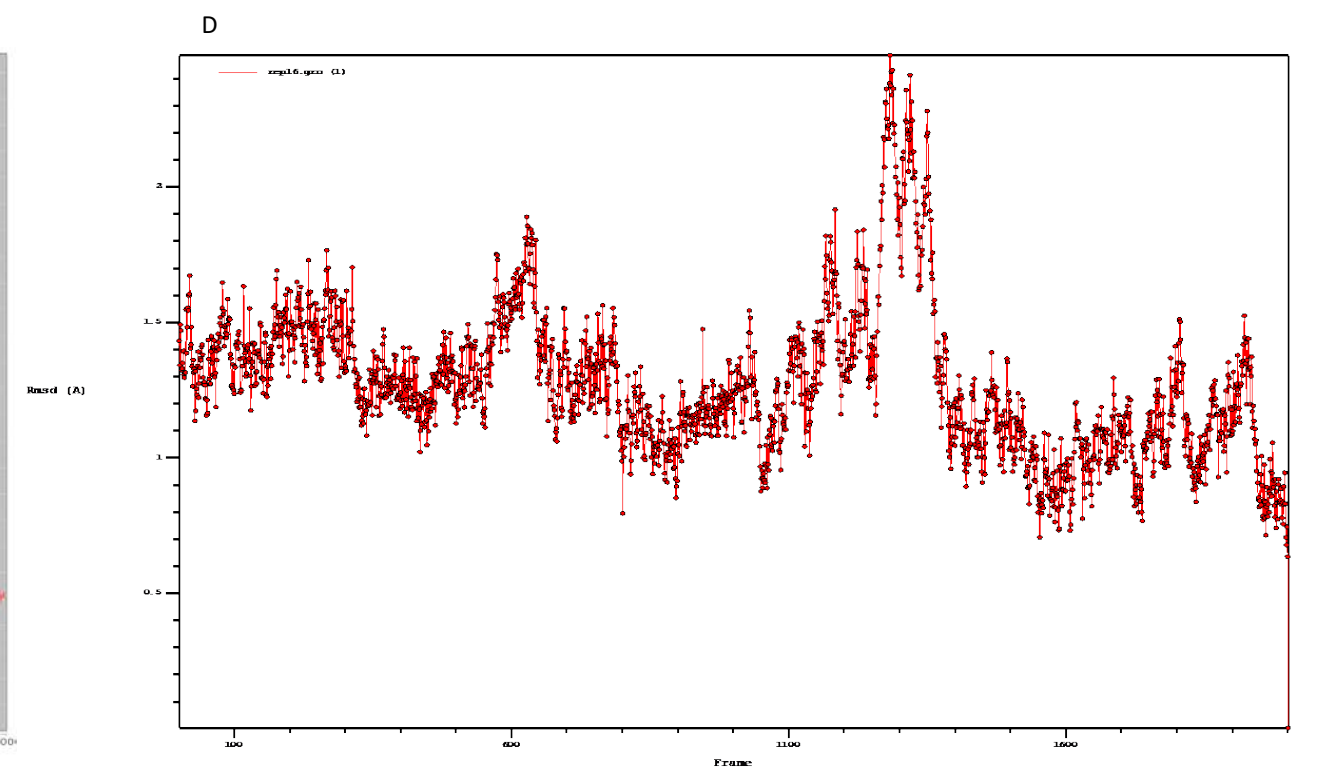
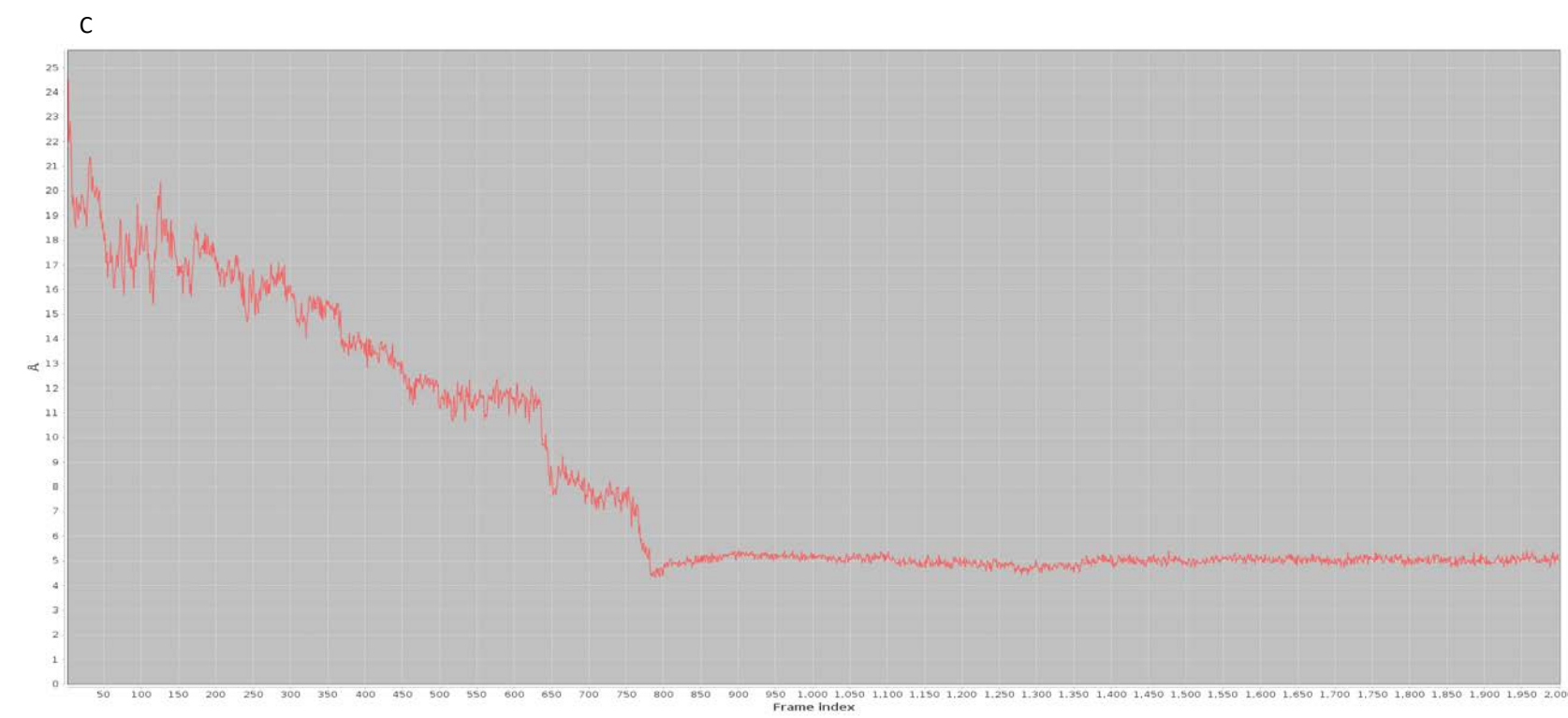
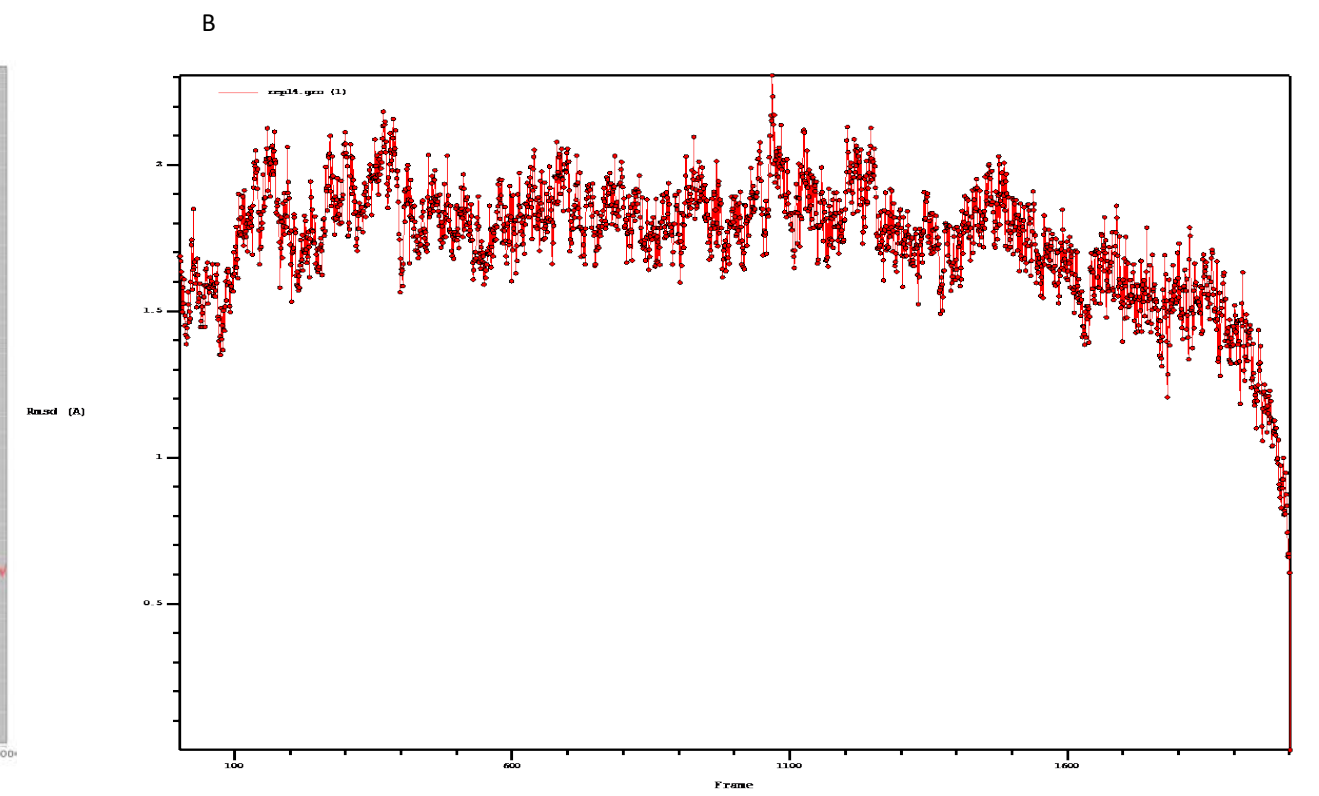
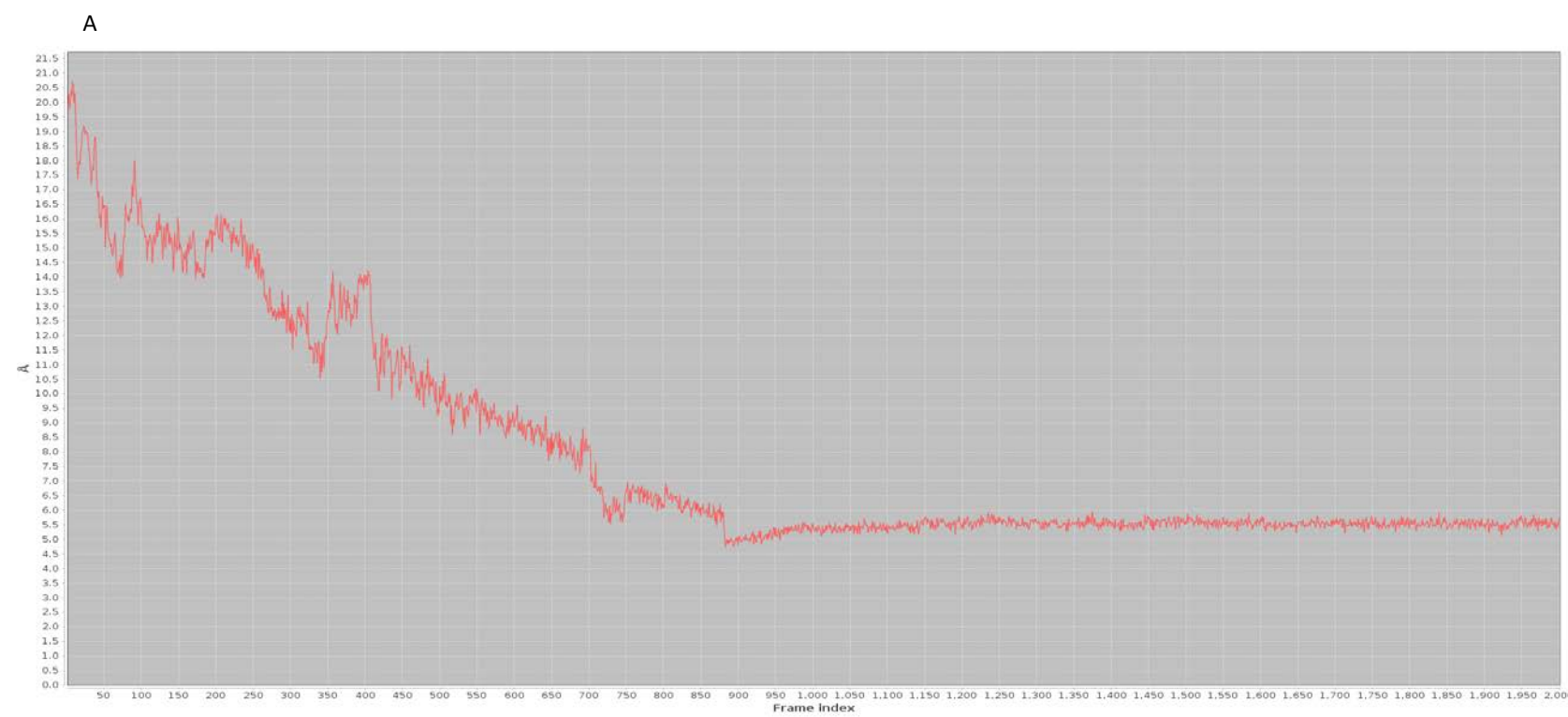


Figure S6. MD-binding: Ligand RMSD calculated from the centroid of binding pocket and protein backbone RMSD (20ns) for Replica 15 (A-B), Replica 16 (C-D), Replica 17 (E-F).



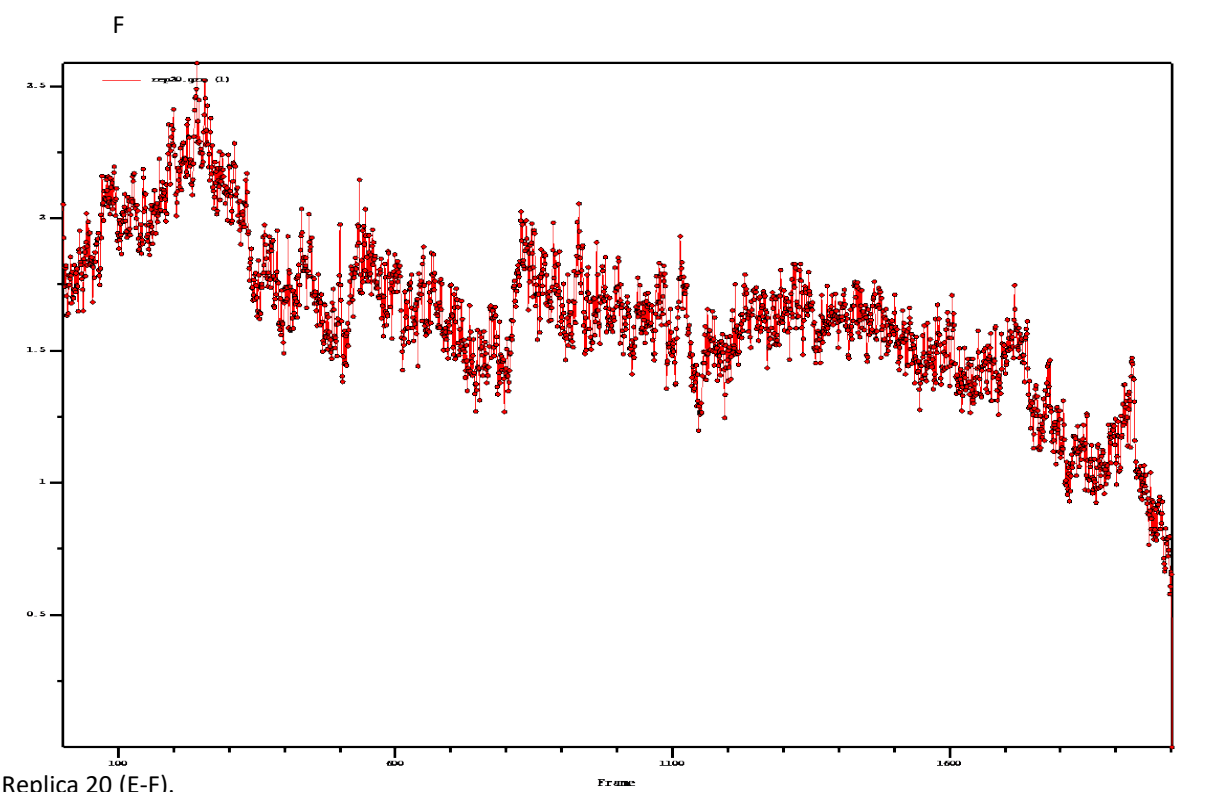
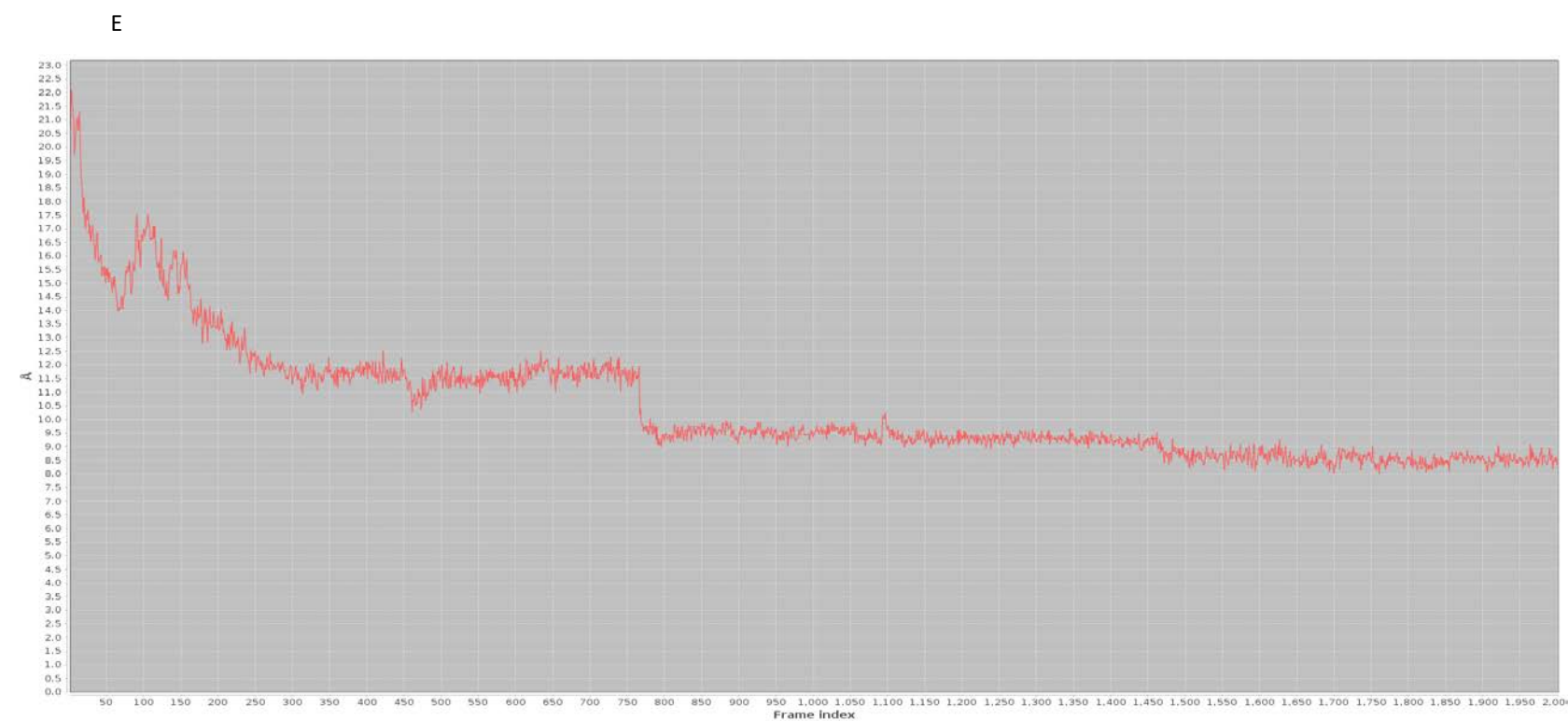
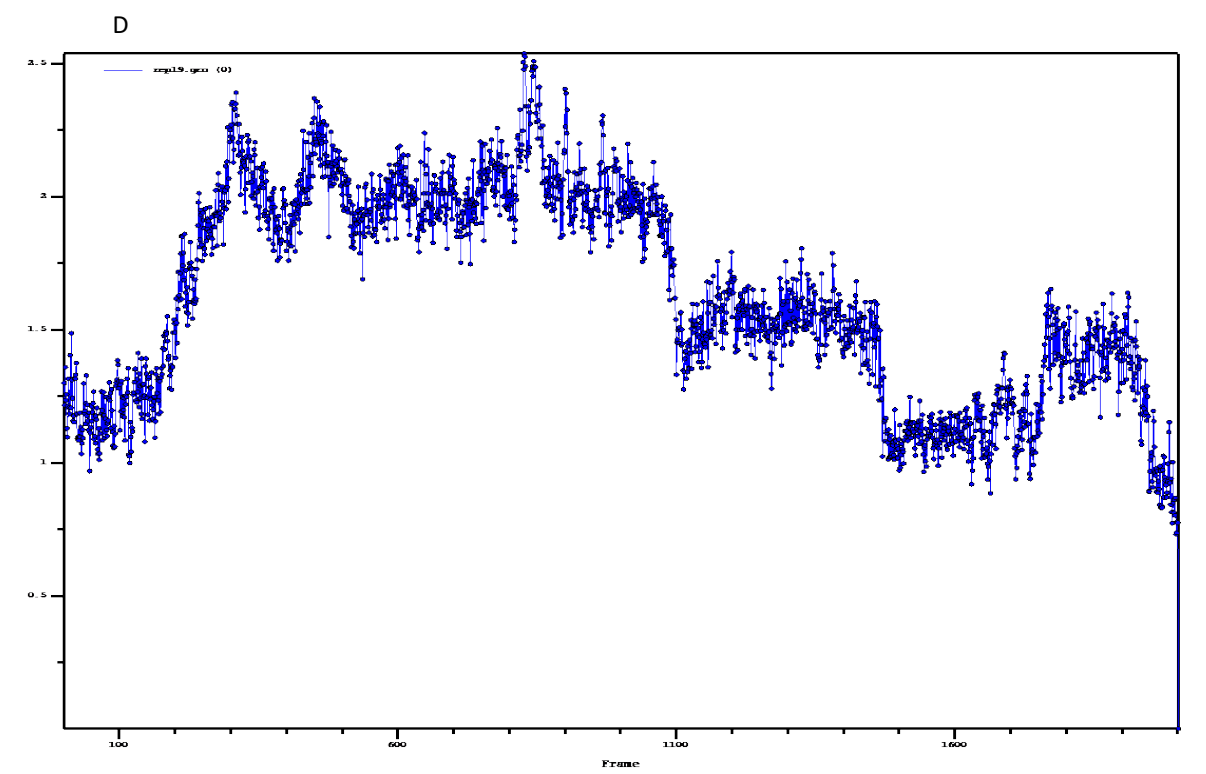
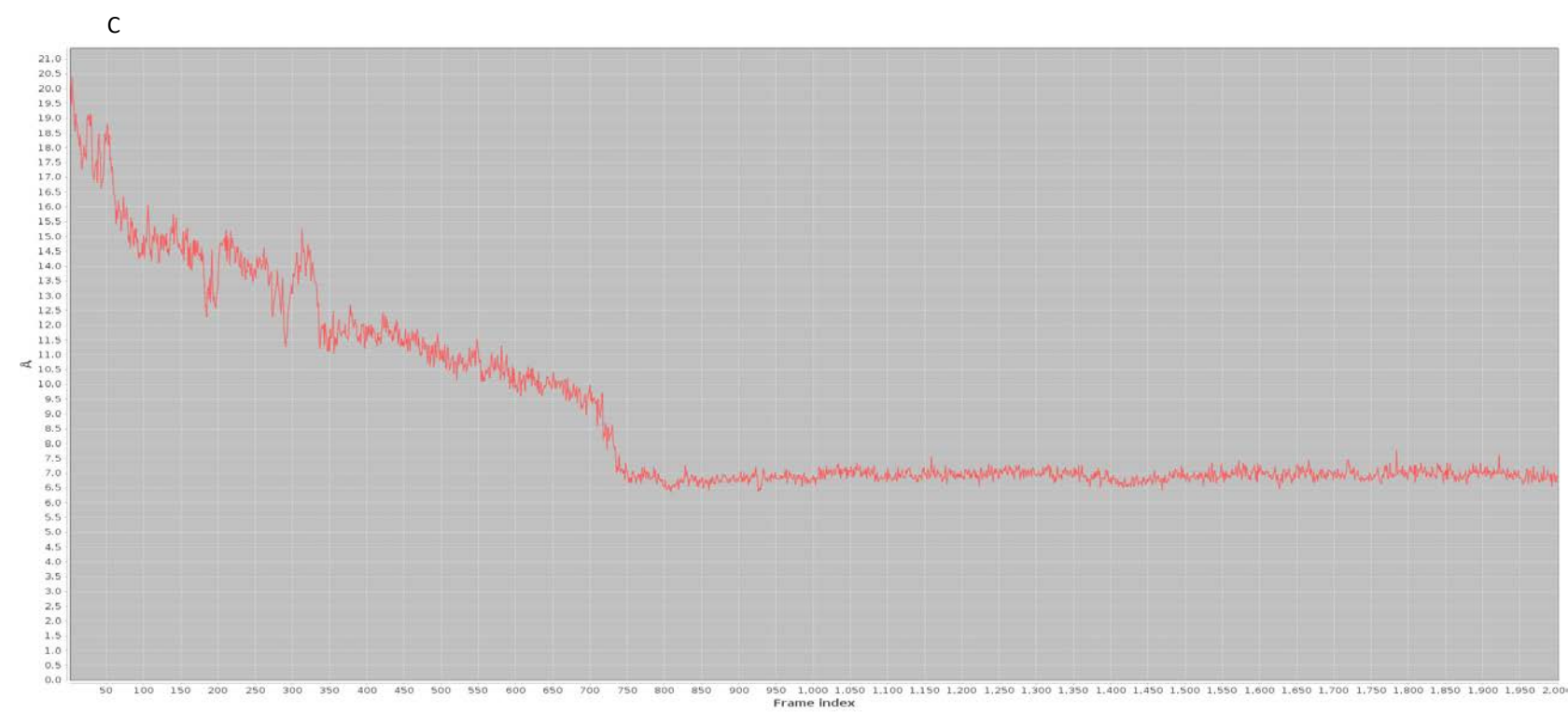
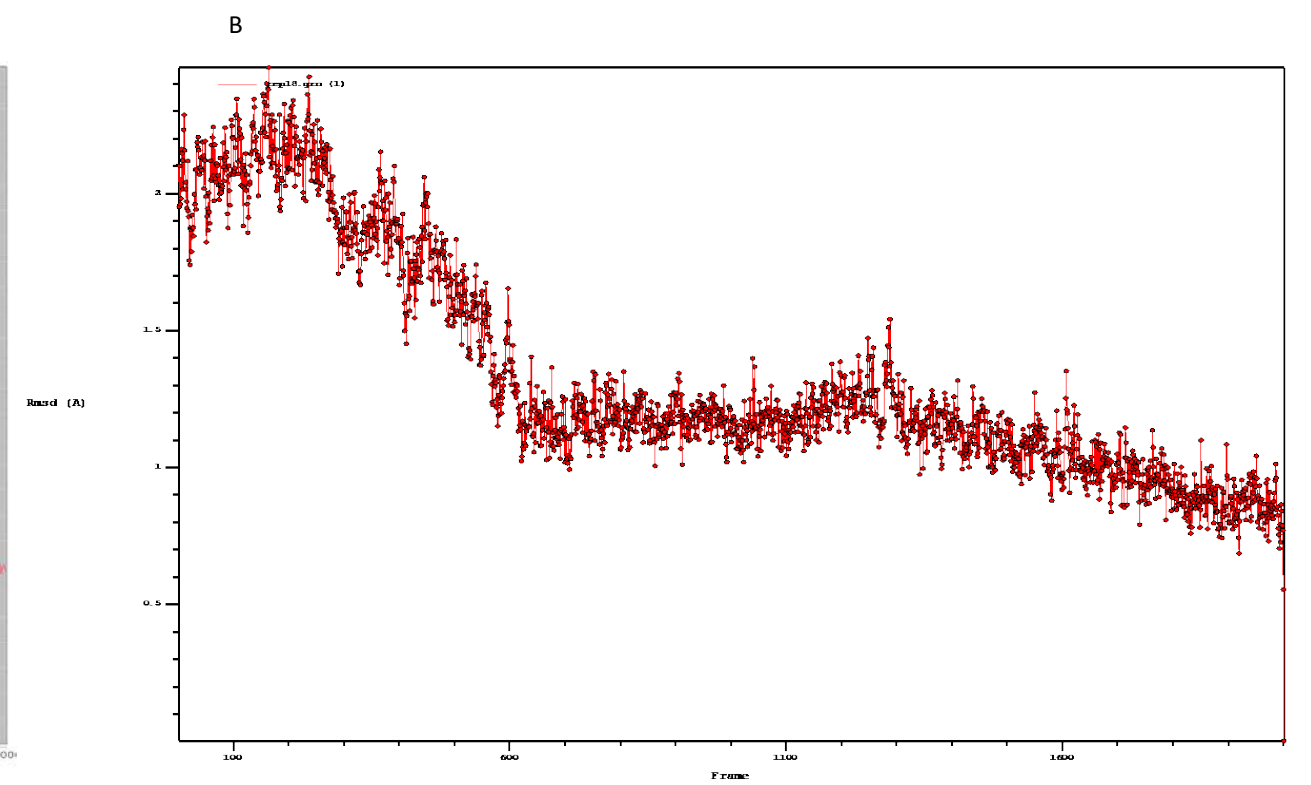
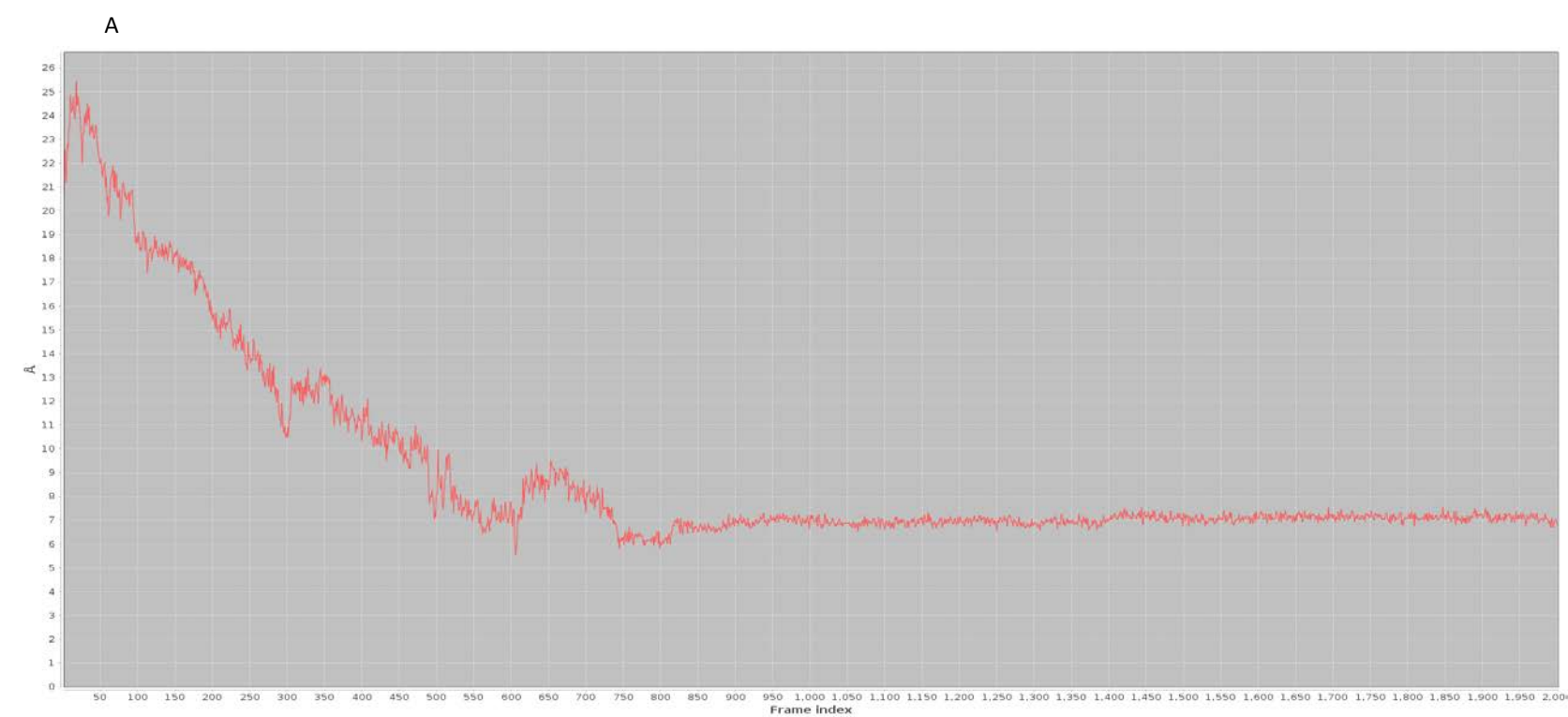


Figure S7. MD-binding: Ligand RMSD calculated from the centroid of binding pocket and protein backbone RMSD (20ns) for Replica 18 (A-B), Replica 19 (C-D), Replica 20 (E-F).

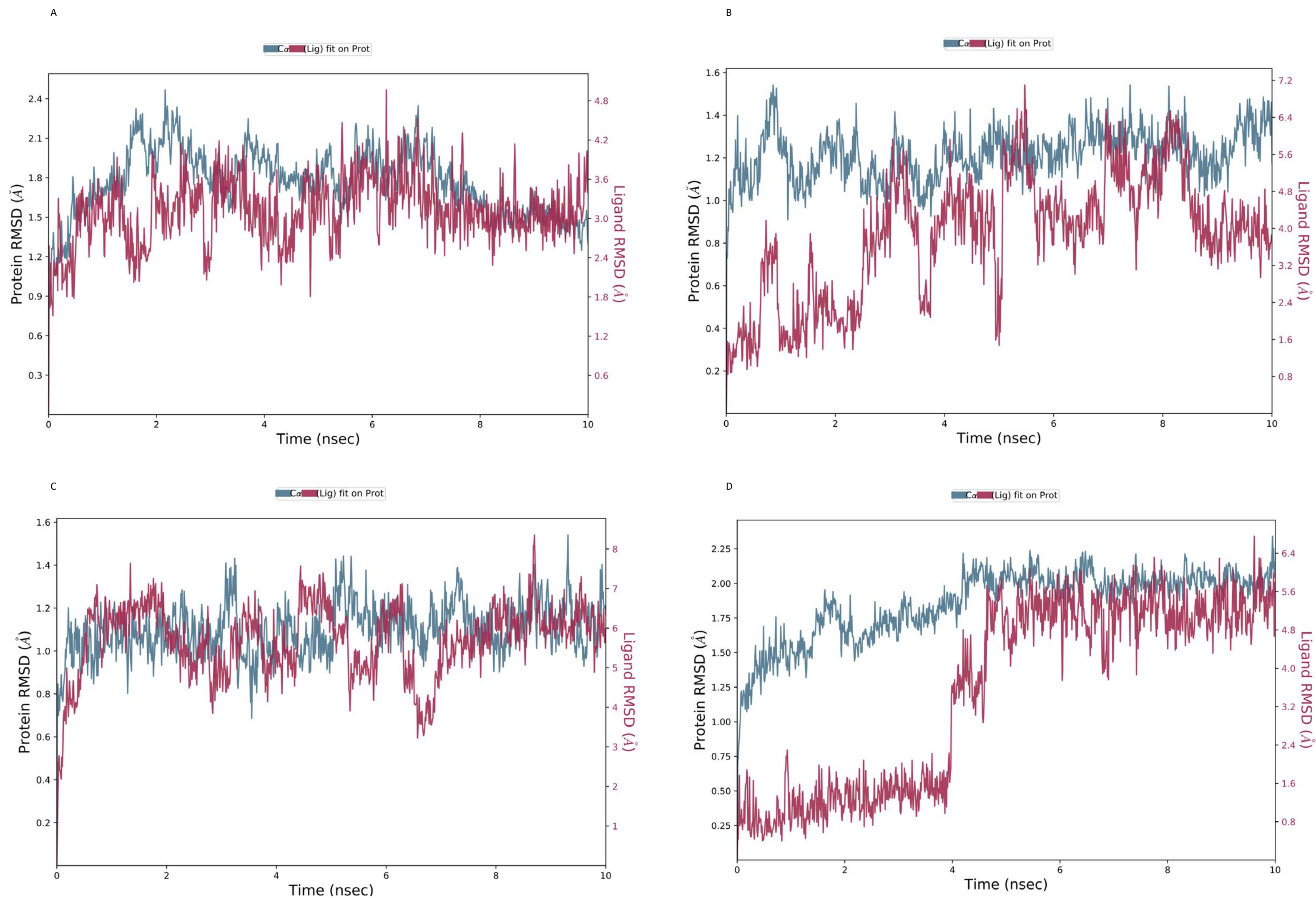


Figure S8. Ligand and protein RMSD during MD-plain(10ns). Replica 1(A); Replica 2(B); Replica 8 (C); Replica10 (D).



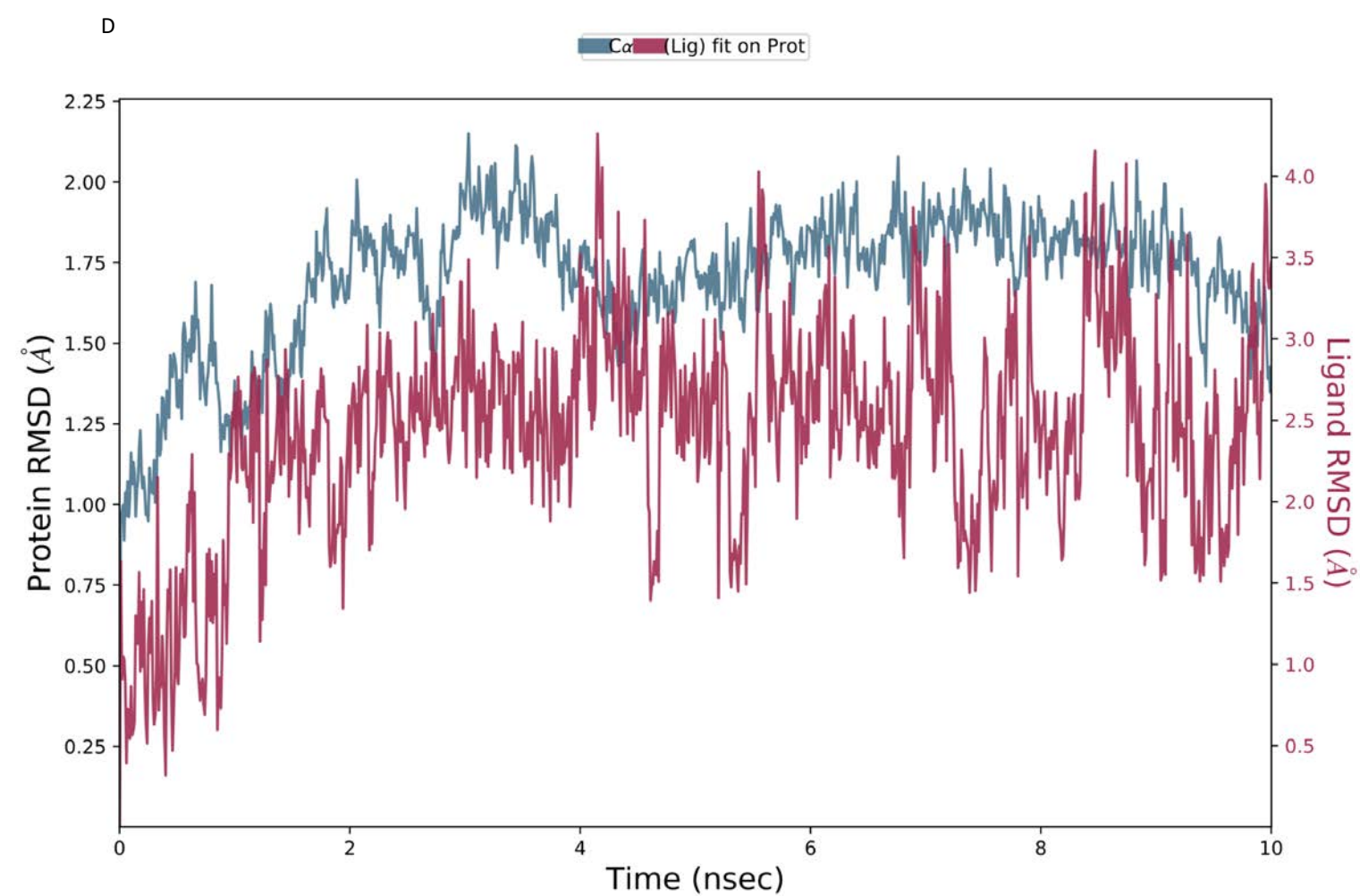
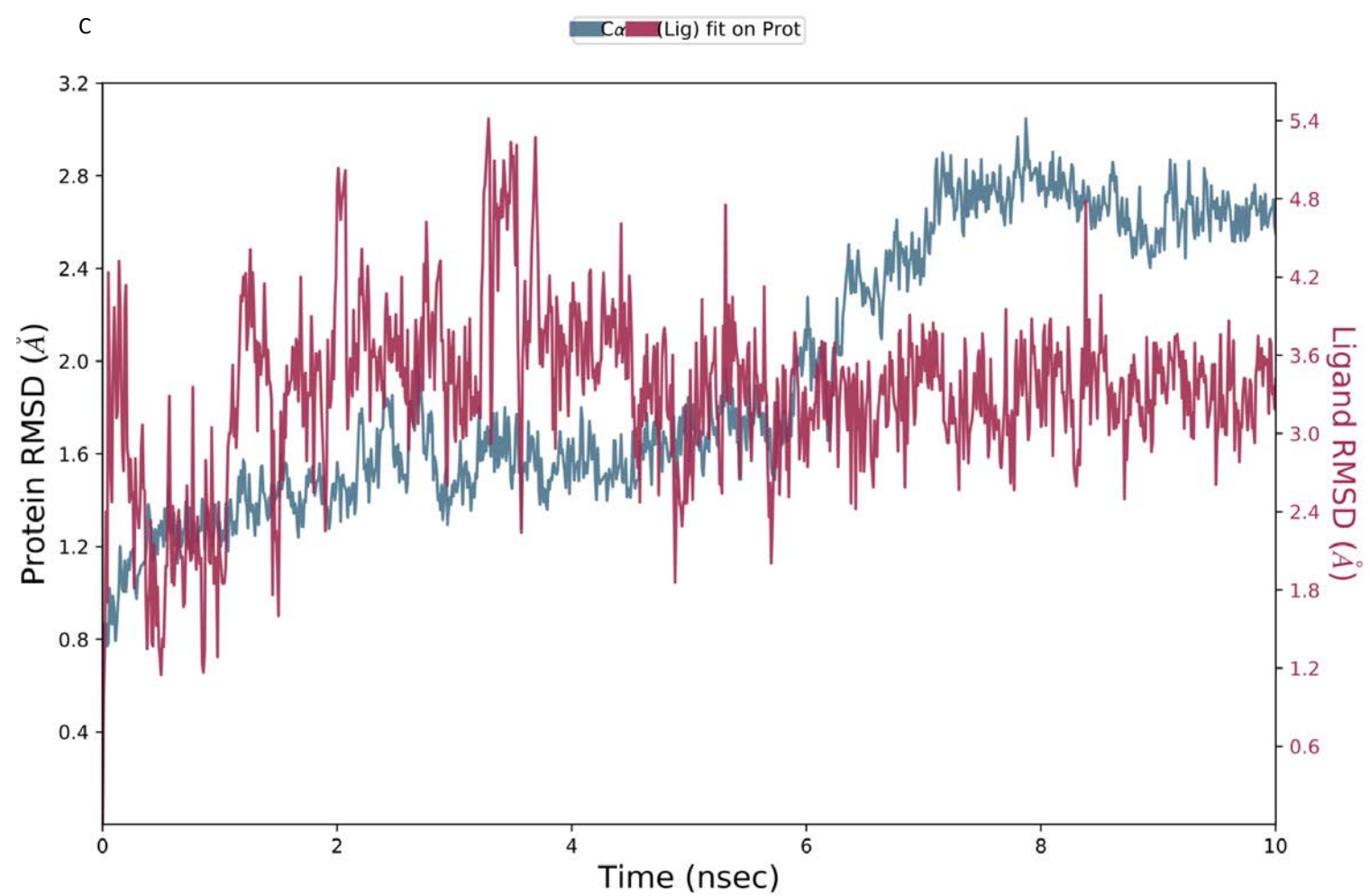
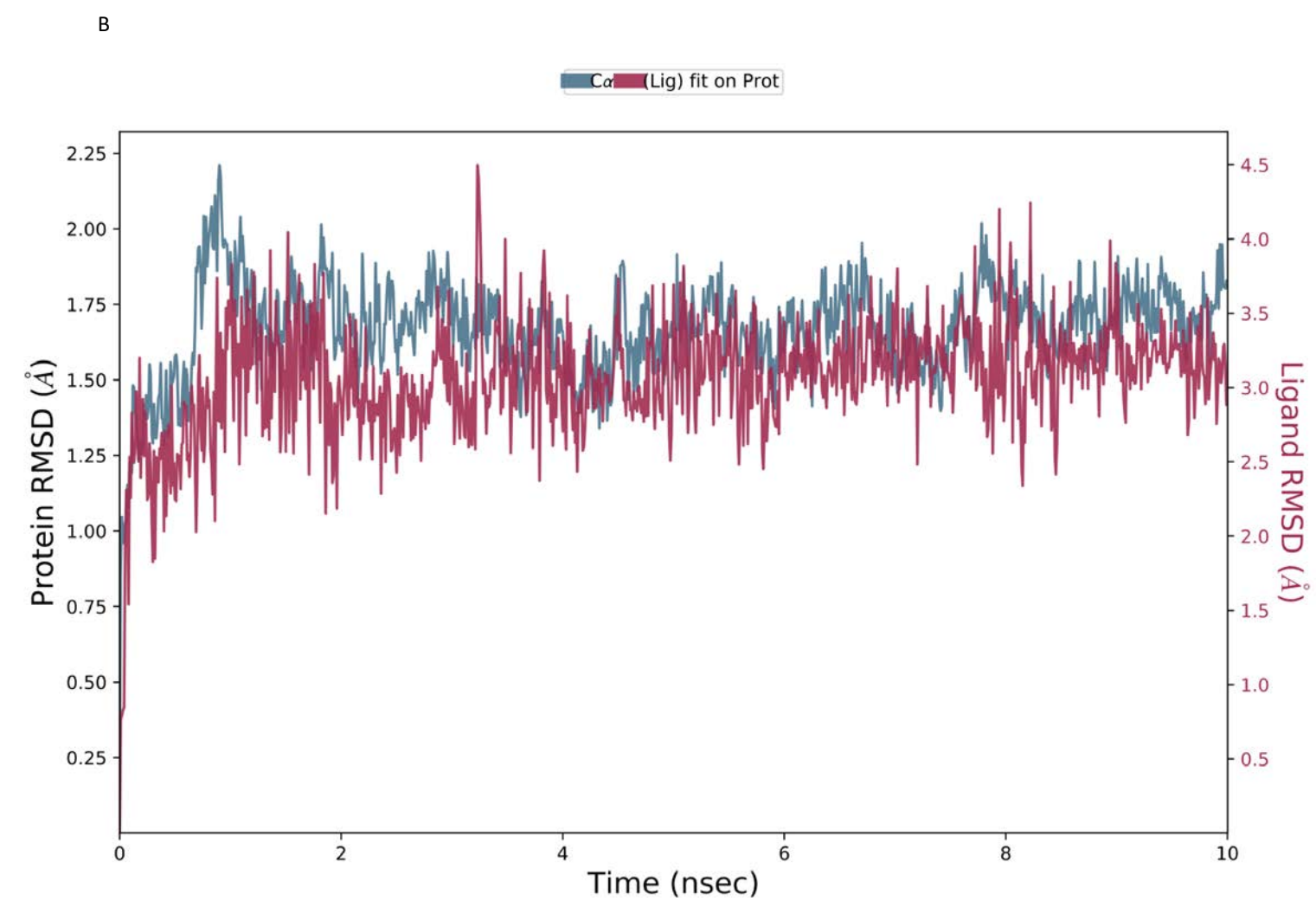
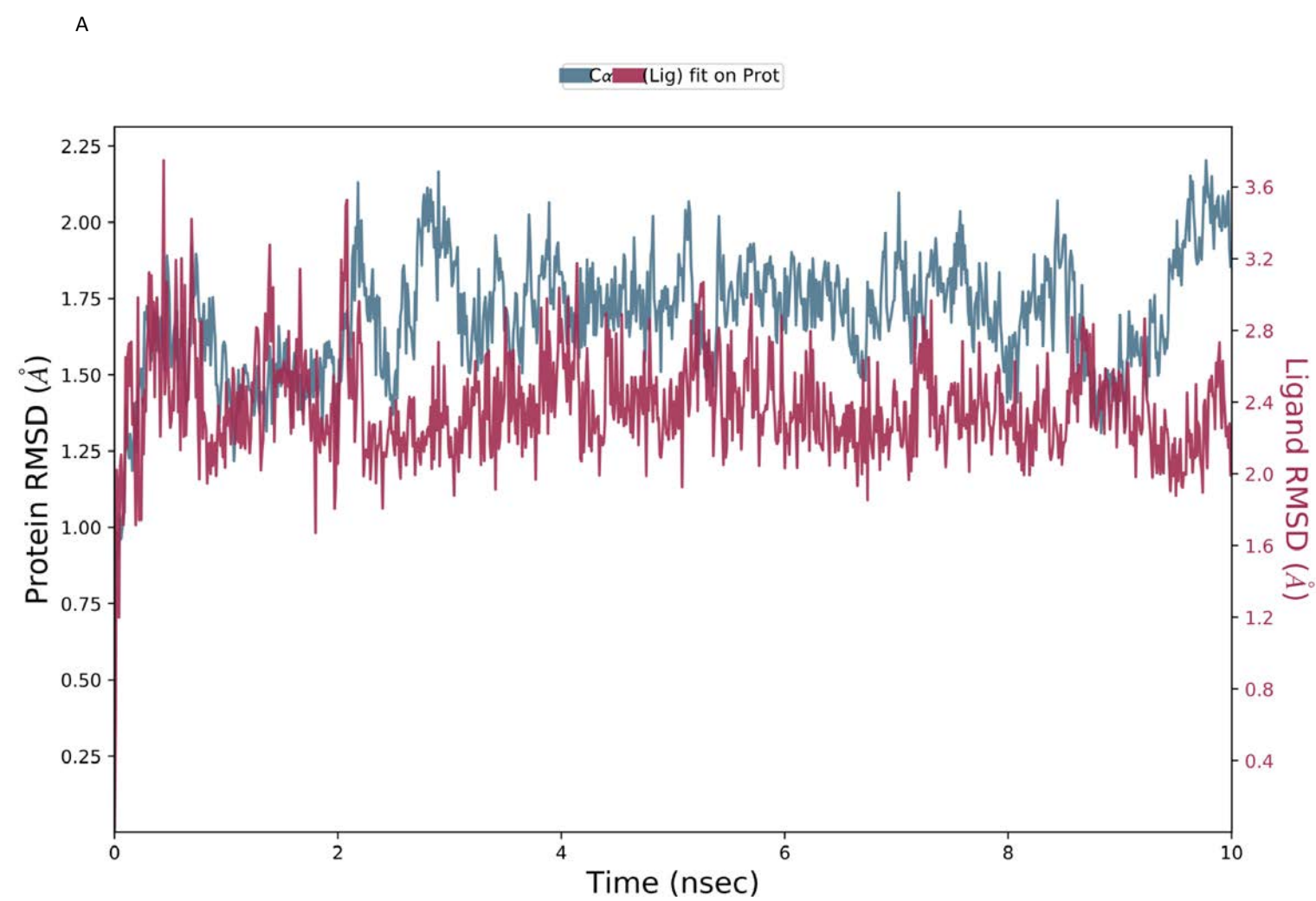


Figure S9. Ligand and protein RMSD during MD-plain(10ns). Replica 11 (A); Replica 12 (B); Replica 13 (C); Replica 14 (D).



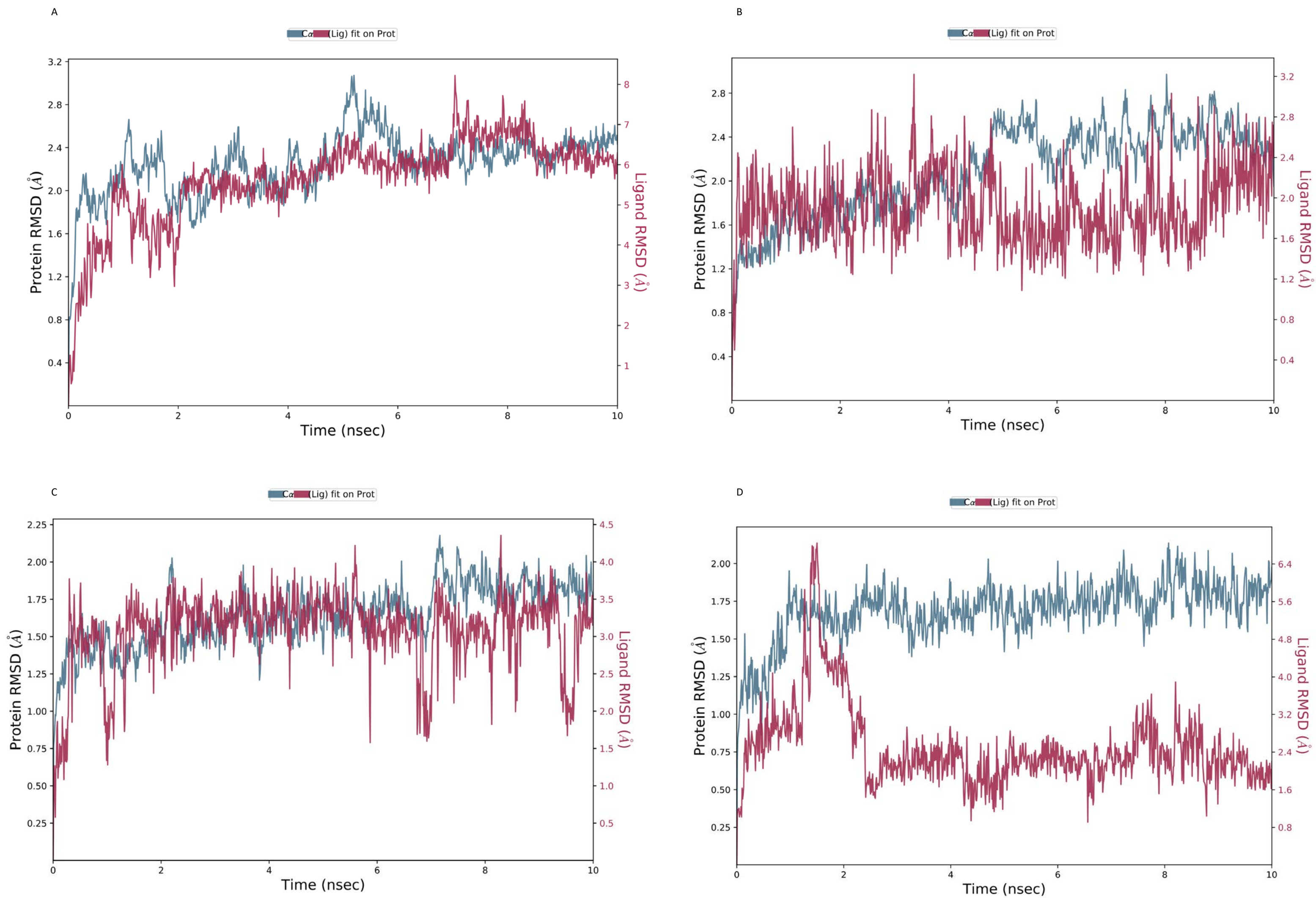
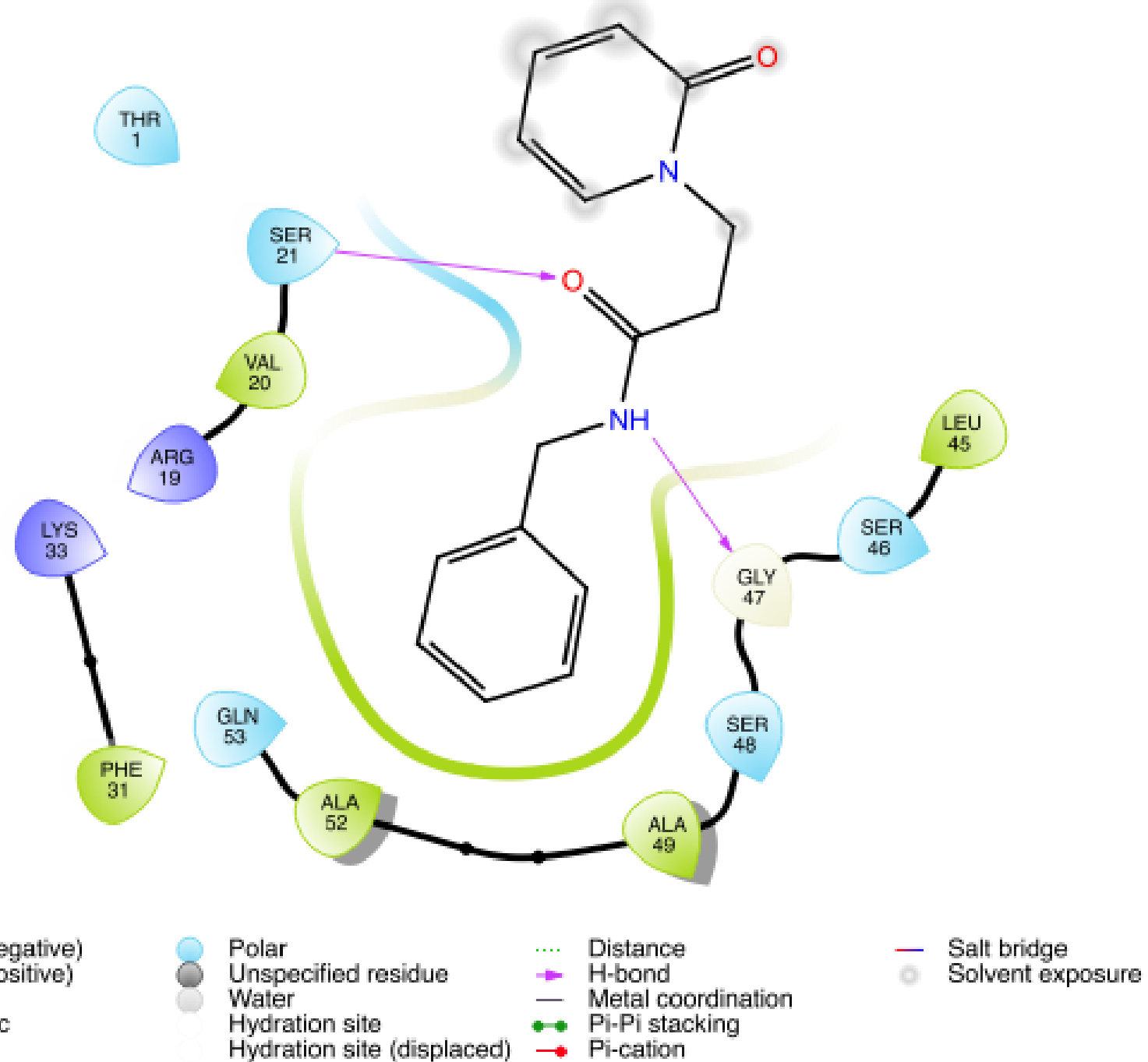


Figure S10. Ligand and protein RMSD during MD-plain(10ns). Replica 15 (A); Replica 16 (B); Replica 17 (C); Replica 20 (D).



A



B

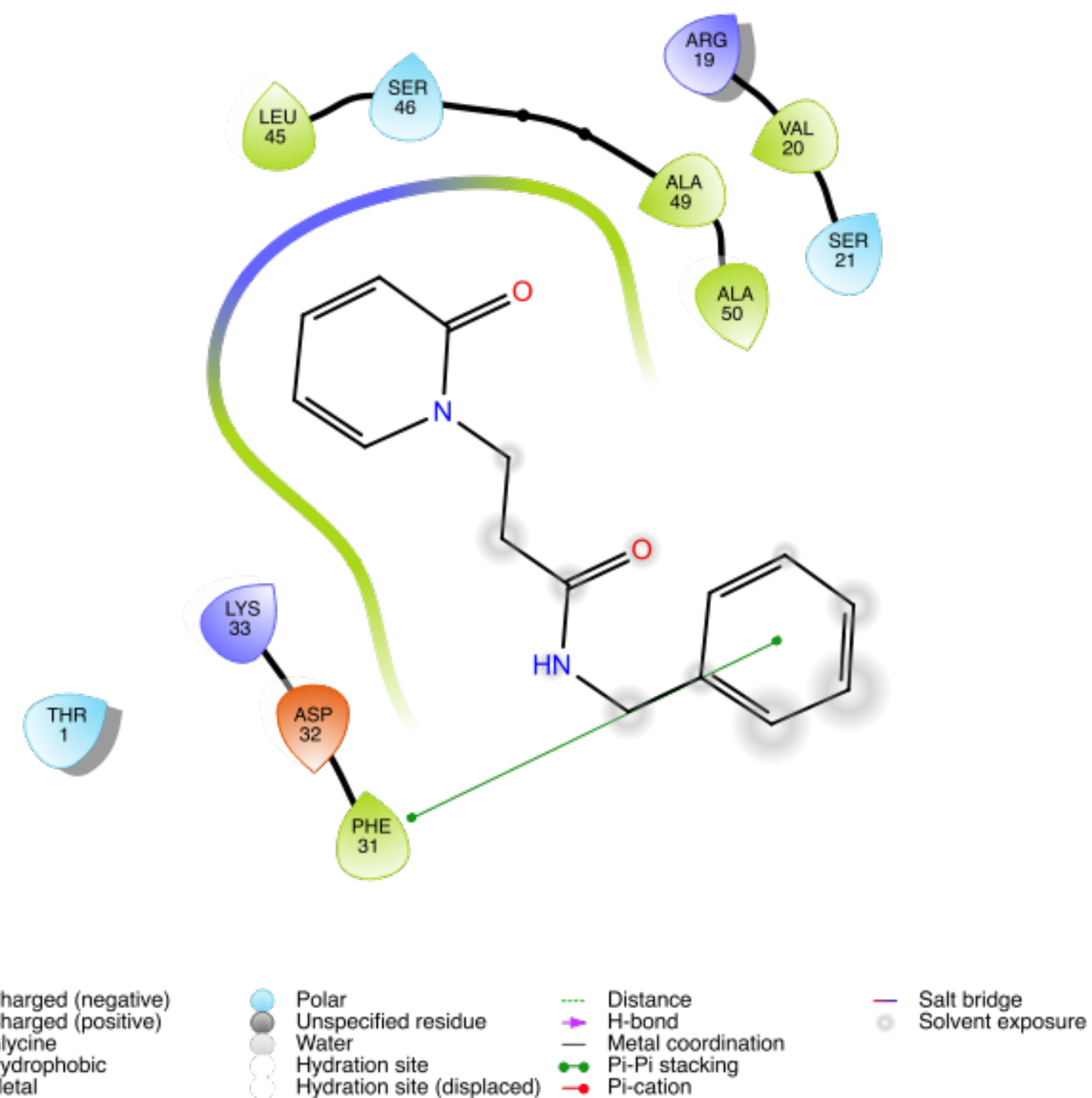


Figure S11. Ligand Interaction Diagram of pose1 (A) and pose2 (B). Purple arrows show H-bond interactions and green line Pi-Pi stacking

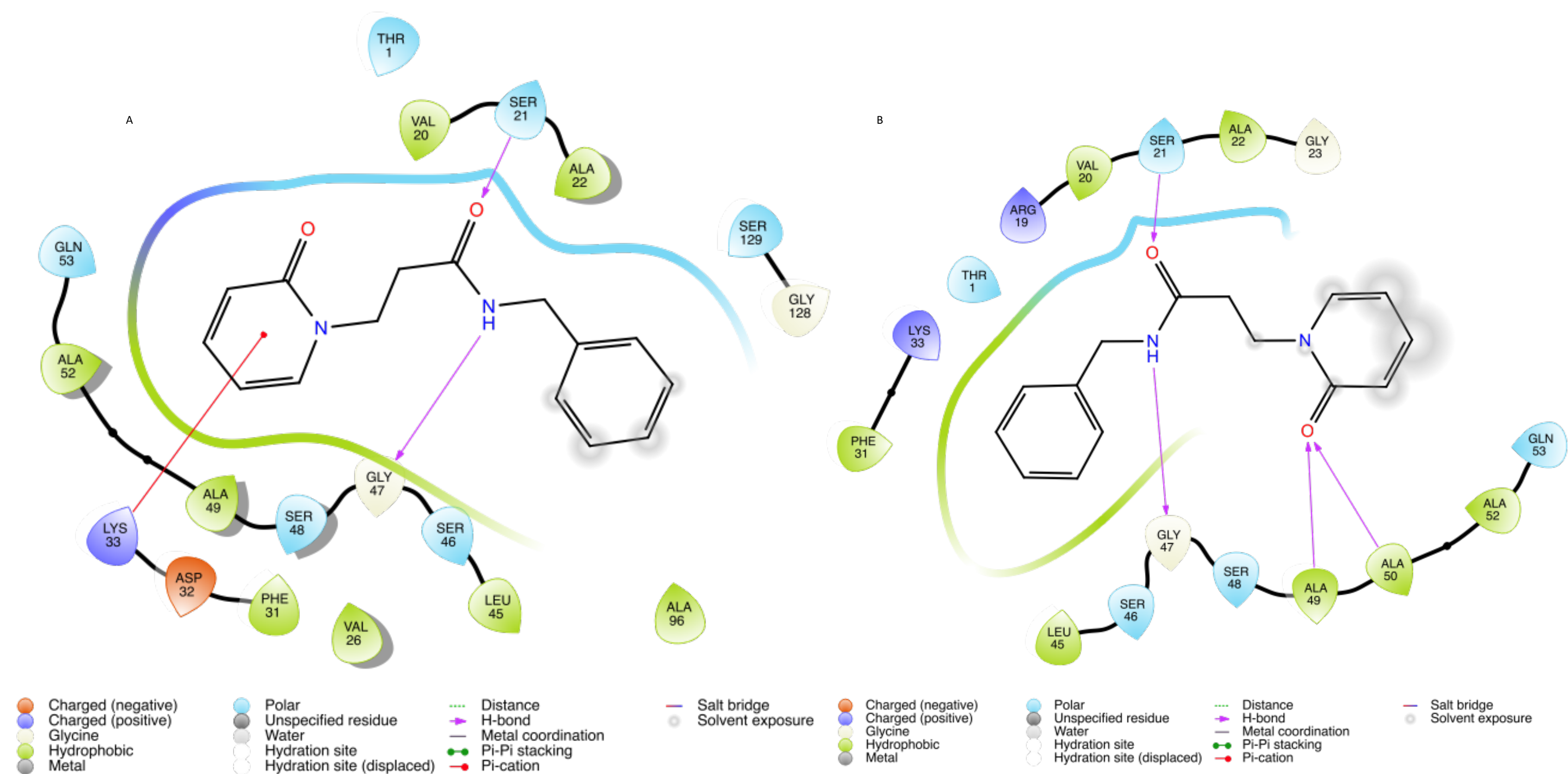


Figure S12. Ligand Interaction Diagram of pose3 (A) and IFD pose (B). Purple arrows show H-bond interactions and red line Pi-cation.