STRUCTURAL
BIOLOGY

Volume 79 (2023)

Supporting information for article:

Structure-based discovery of an antipsychotic drug, paliperidone, as a modulator of human superoxide dismutase 1: a potential therapeutic target in amyotrophic lateral sclerosis

Snehal Aouti, Sivaraman Padavattan and Balasundaram Padmanabhan

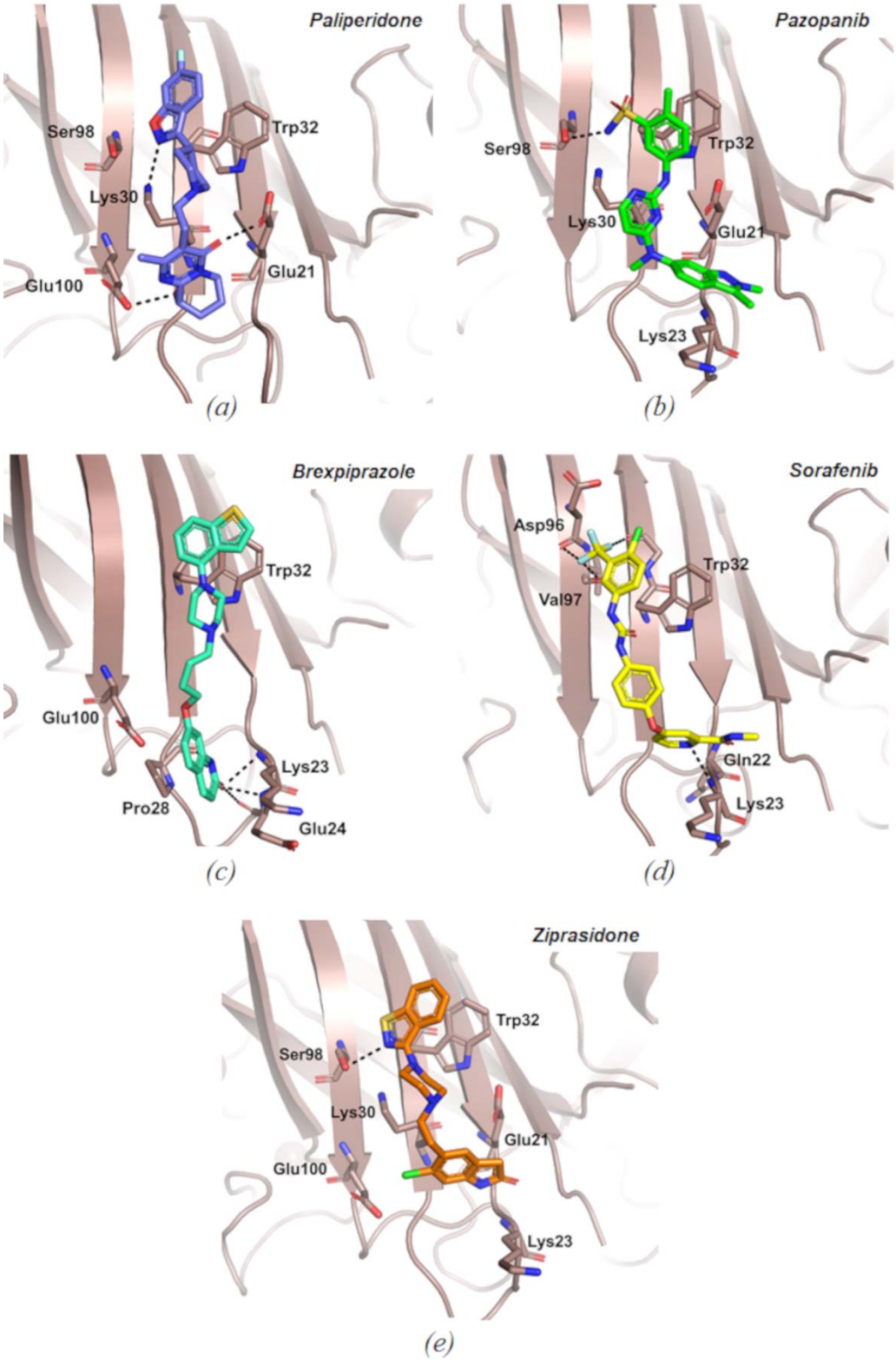


Figure S1 Docking interactions of top compounds screened based on Pharmacophore model 1. The best docking pose of compound at binding site and the interacting residues are represented as sticks. *(a)* Paliperidone; *(b)* Pazopanib; *(c)* Brexpiprazole; *(d)* Sorafenib; and *(e)* Ziprasidone.

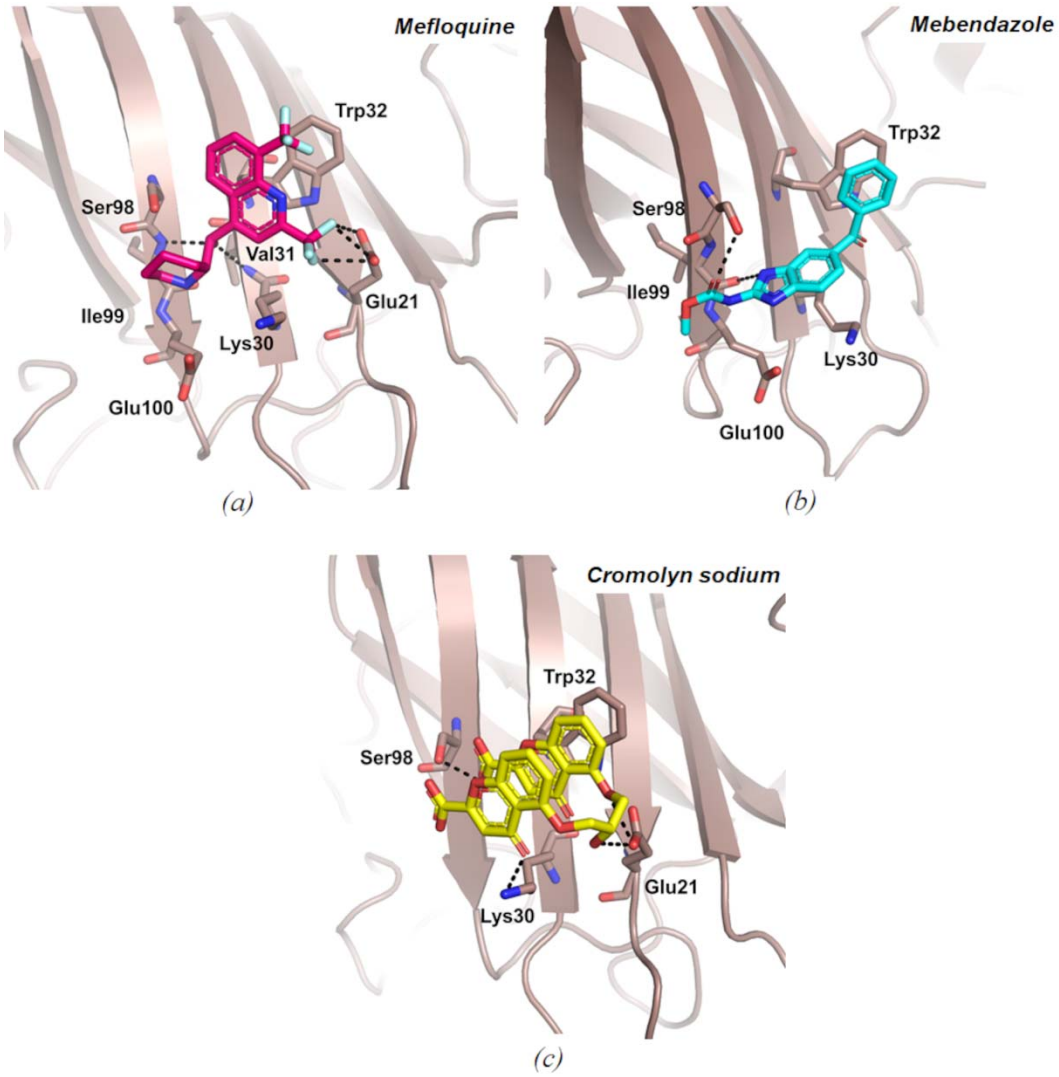


Figure S2 Docking interactions of top compounds screened based on Pharmacophore model 2. The best docking pose of the compound at the binding site and the interacting residues are represented as sticks. *(a)* Mefloquine; *(b)* Mebendazole; and *(c)* Cromolyn sodium.

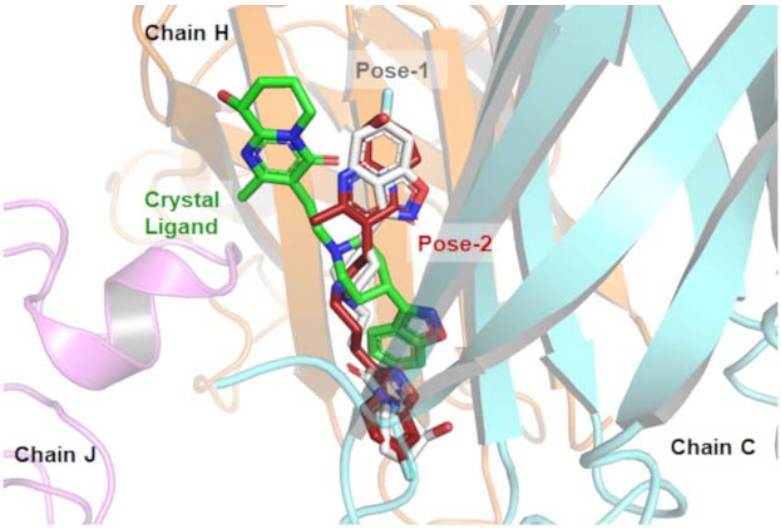


Figure S3 Superimposition of docked poses (pose-1: white and pose-2: marron) on to the crystal ligand (green).

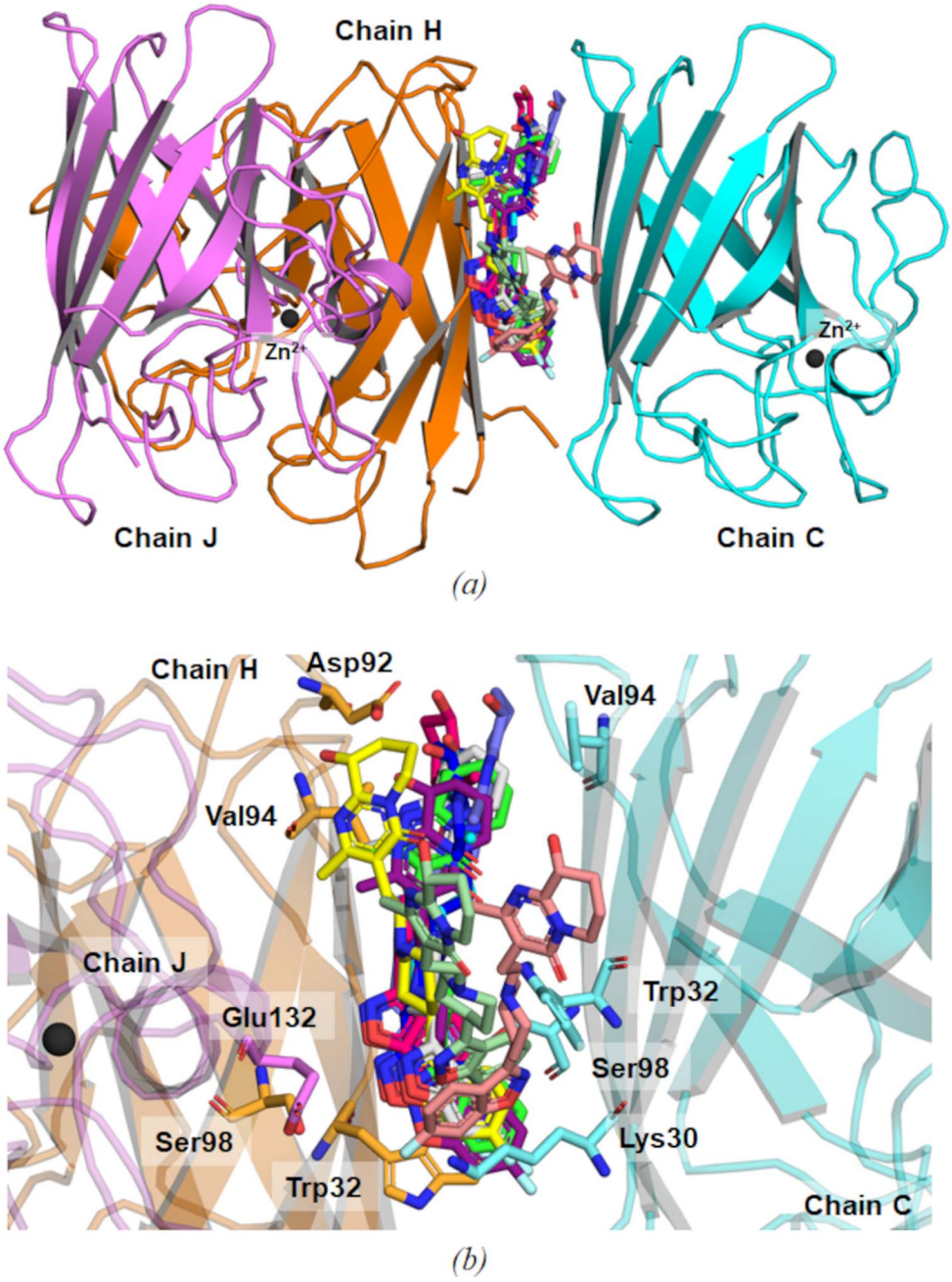


Figure S4 Trajectory cluster analysis of Paliperidone (crystal ligand) over the entire simulation run. (*a*) Ten clustered positions of Paliperidone obtained are superimposed to validate the binding of ligand at Trp32 site. (*b*) Zoom view of (*a*). The residues are shown as sticks.

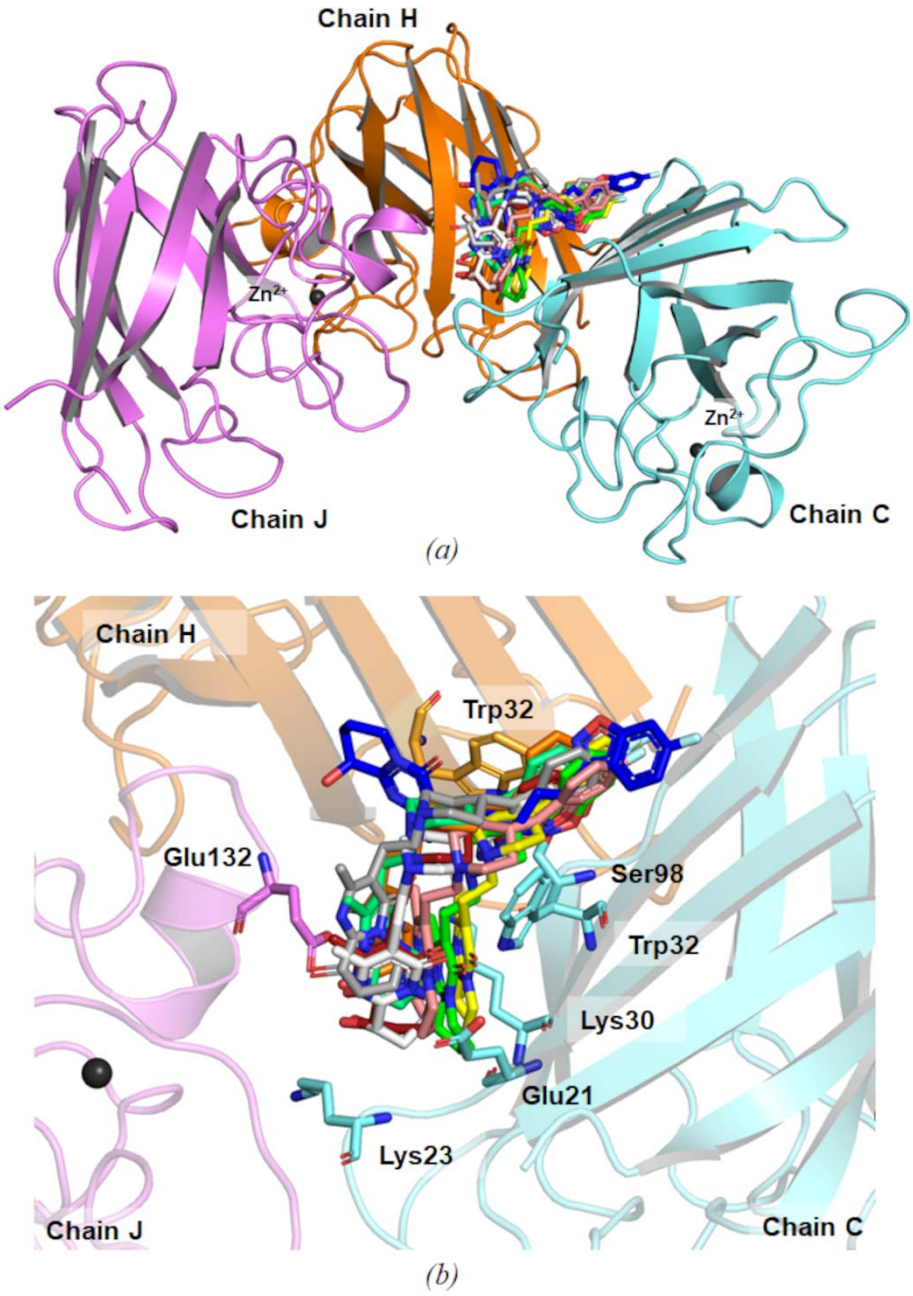
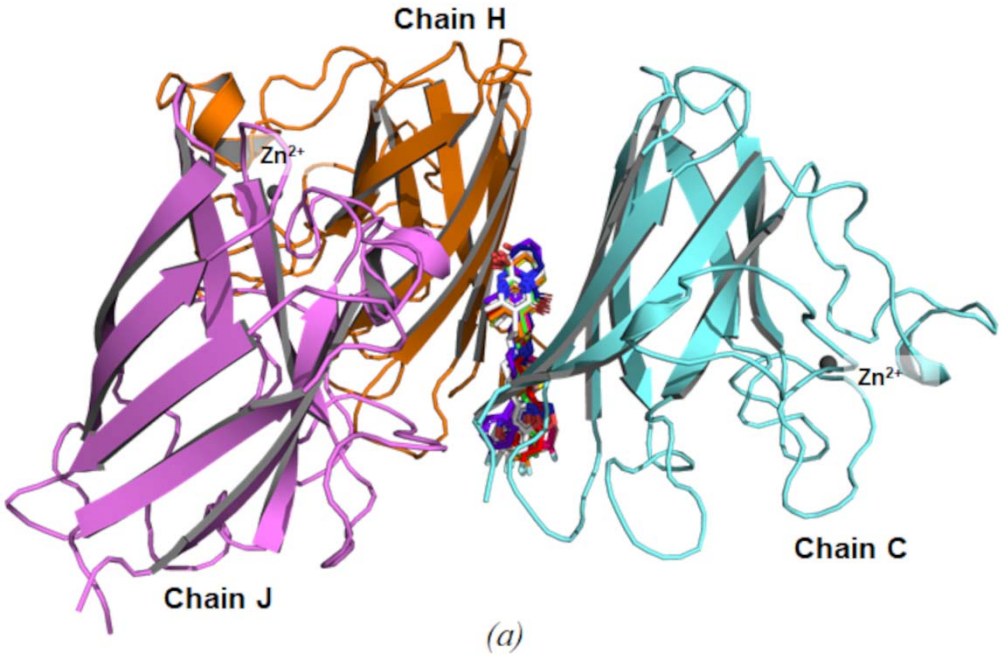
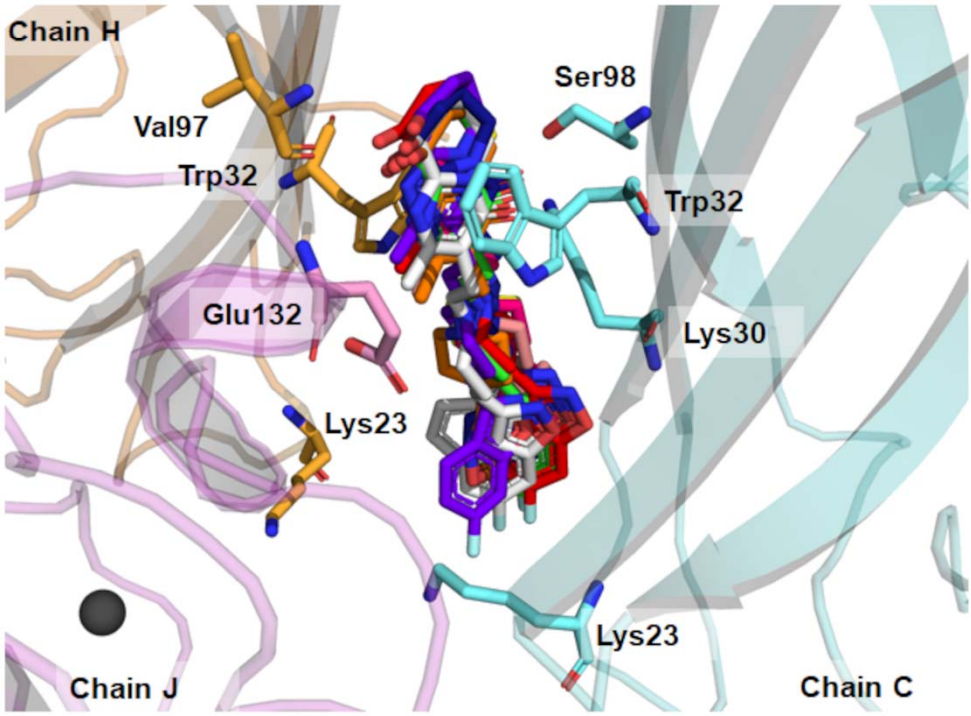


Figure S5 Trajectory cluster analysis of Paliperidone docked pose-1 over the entire simulation run. (*a*) Ten clustered positions of pose-1 obtained are superimposed to validate the binding of ligand at Trp32 site. (*b*) Zoom view of (*a*). The residues are shown as sticks.



(a)



(b)

Figure S6 Trajectory cluster analysis of Paliperidone docked pose-2 over the entire simulation run. (*a*) Ten clustered positions of pose-2 obtained are superimposed to validate the binding of ligand at Trp32 site. (*b*) Zoom view of (*a*). The residues are shown as sticks.

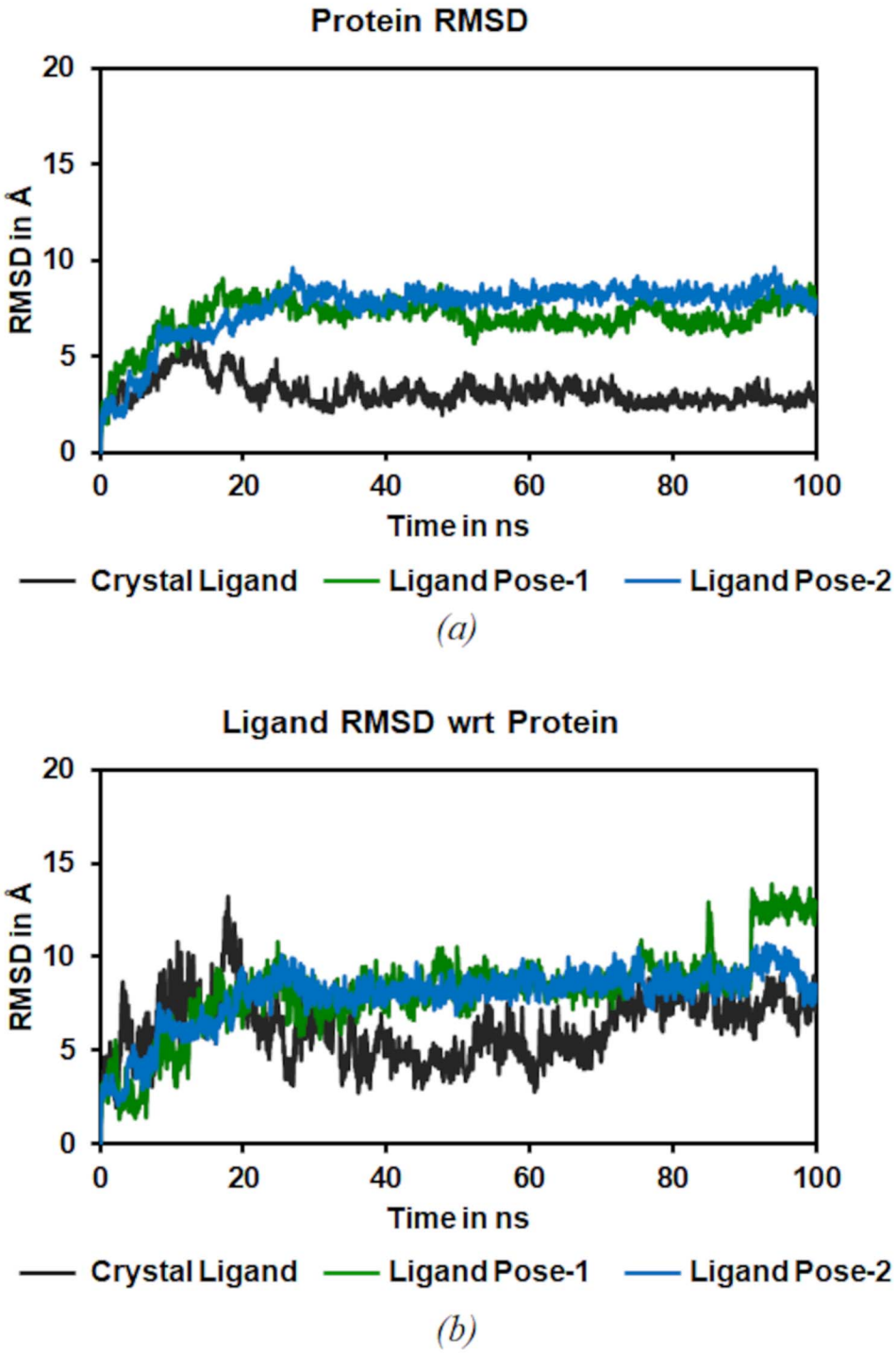


Figure S7 Analysis of MD simulation trajectories for different SOD1-Paliperidone complexes. *(a)* RMSD of protein in complex with Paliperidone poses; *(b)* RMSD plots of ligands with respect to protein.

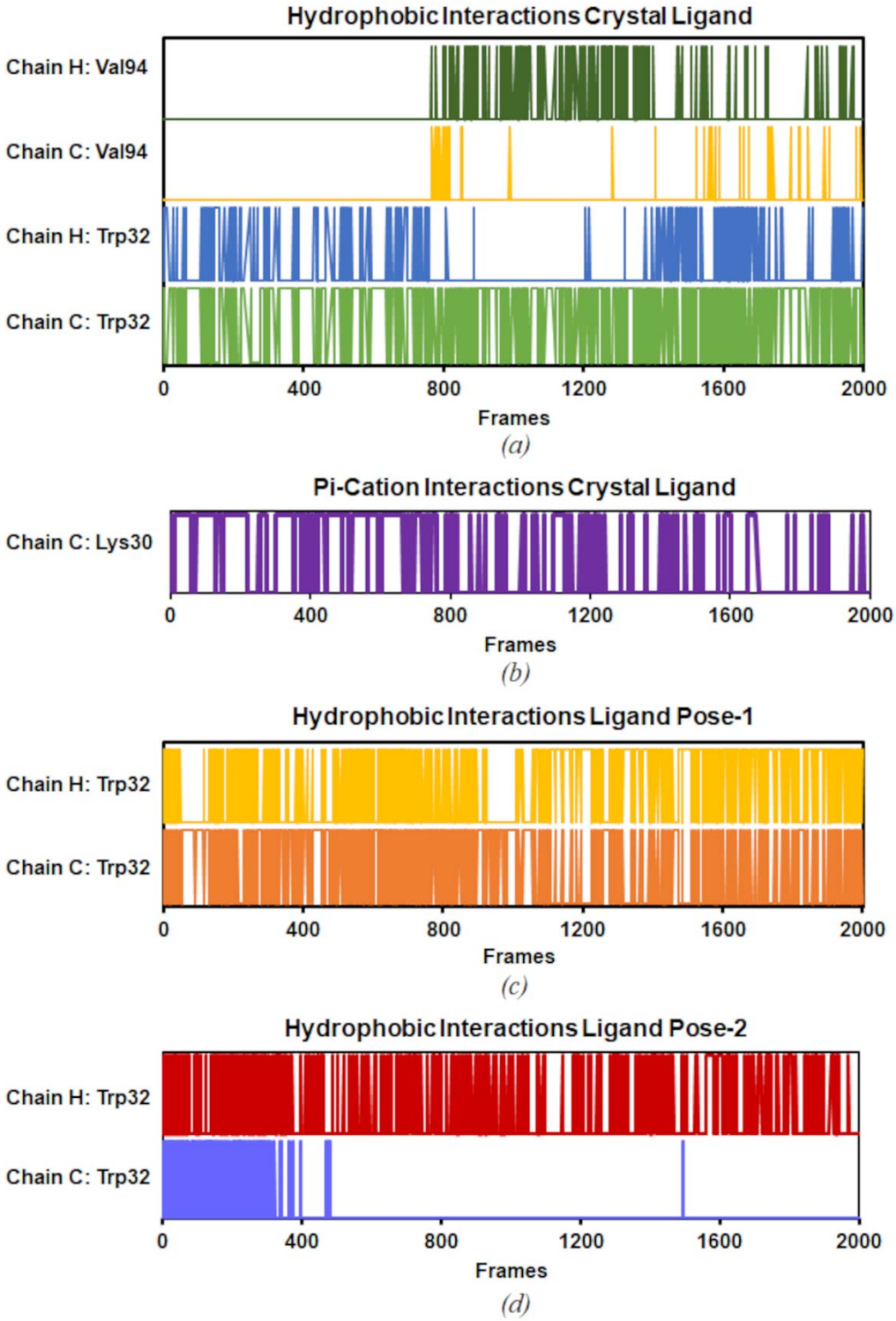


Figure S8 Detailed interaction analysis of SOD1-Paliperidone complexes.