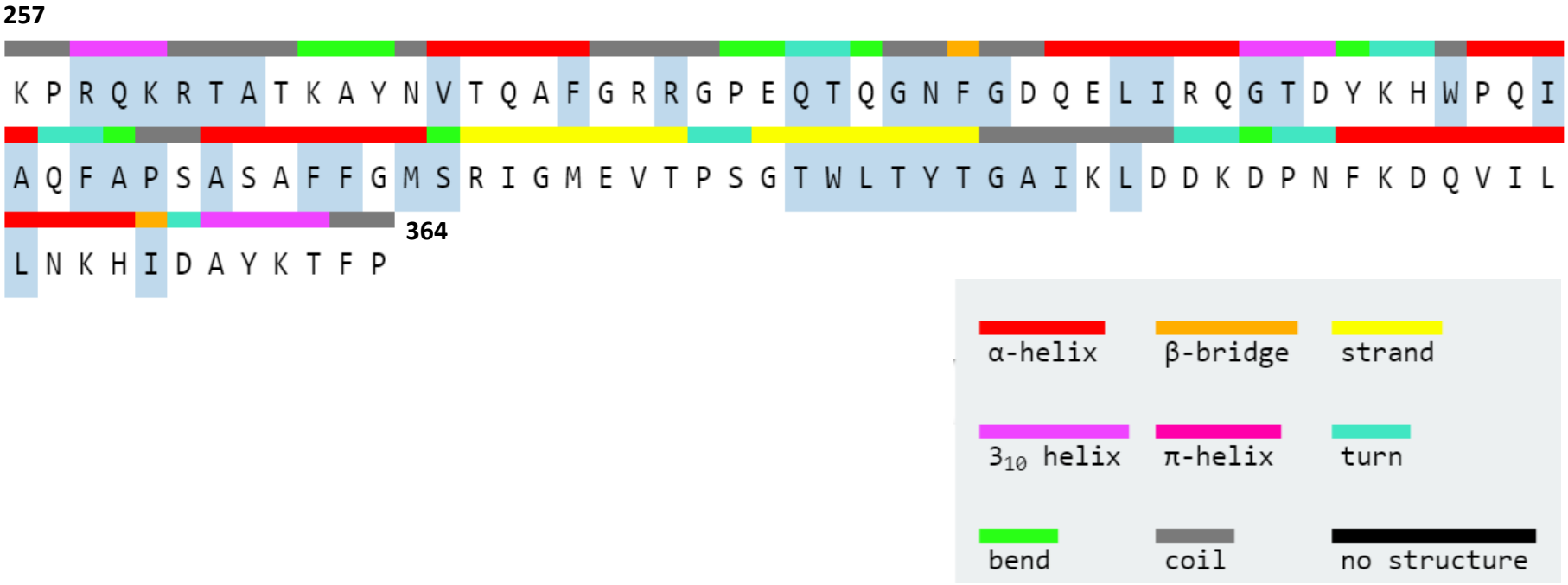

Figure S1. Binding pocket prediction through CASTp. The primary sequence of CTD is represented along with their secondary structure annotation. The residues predicted to be in binding pocket is highlighted in light blue.

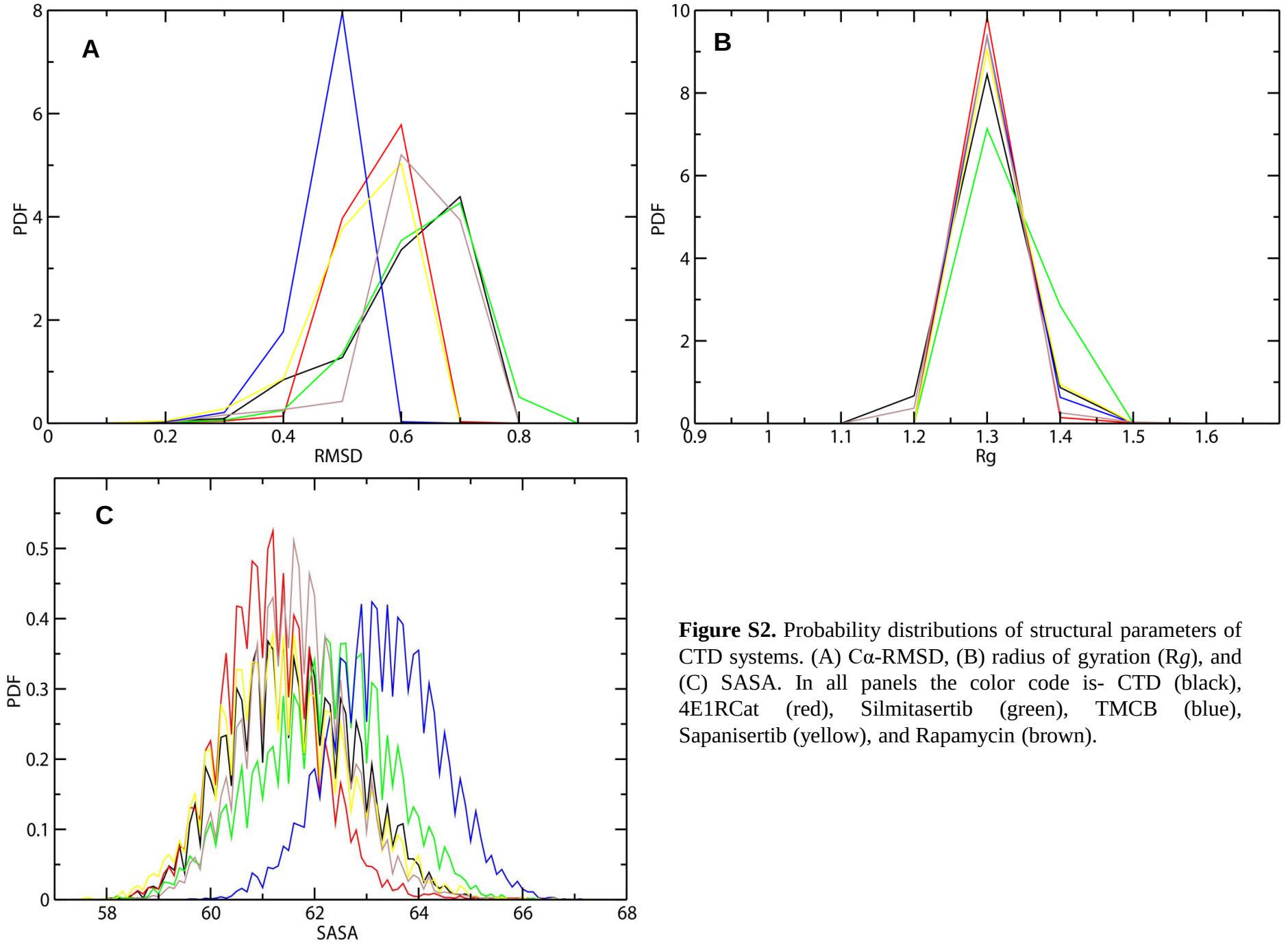

Figure S2. Probability distributions of structural parameters of CTD systems. (A) Cα-RMSD, (B) radius of gyration (R*g*), and (C) SASA. In all panels the color code is- CTD (black), 4E1RCat (red), Silmitasertib (green), TMCB (blue), Sapanisertib (yellow), and Rapamycin (brown).

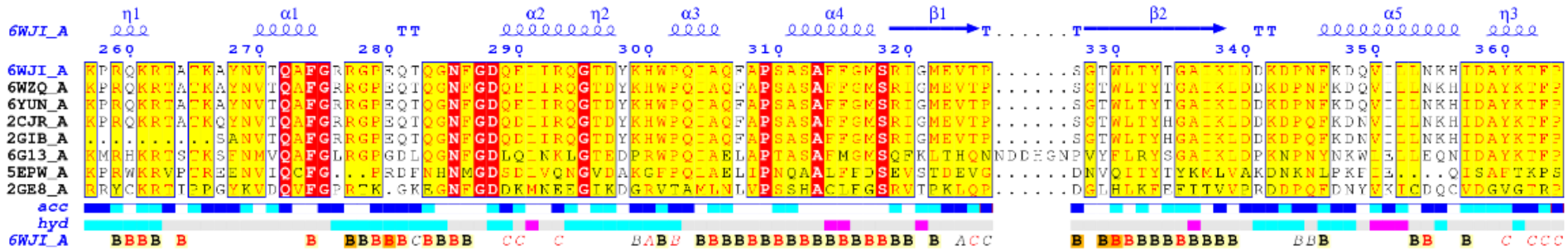

Figure S3. Multiple sequence alignment of N-CTD protein showing the conserved residues. Multiple sequence alignment was performed using ESPript 3.0 using PDB structure 6WJI against the PDB database.

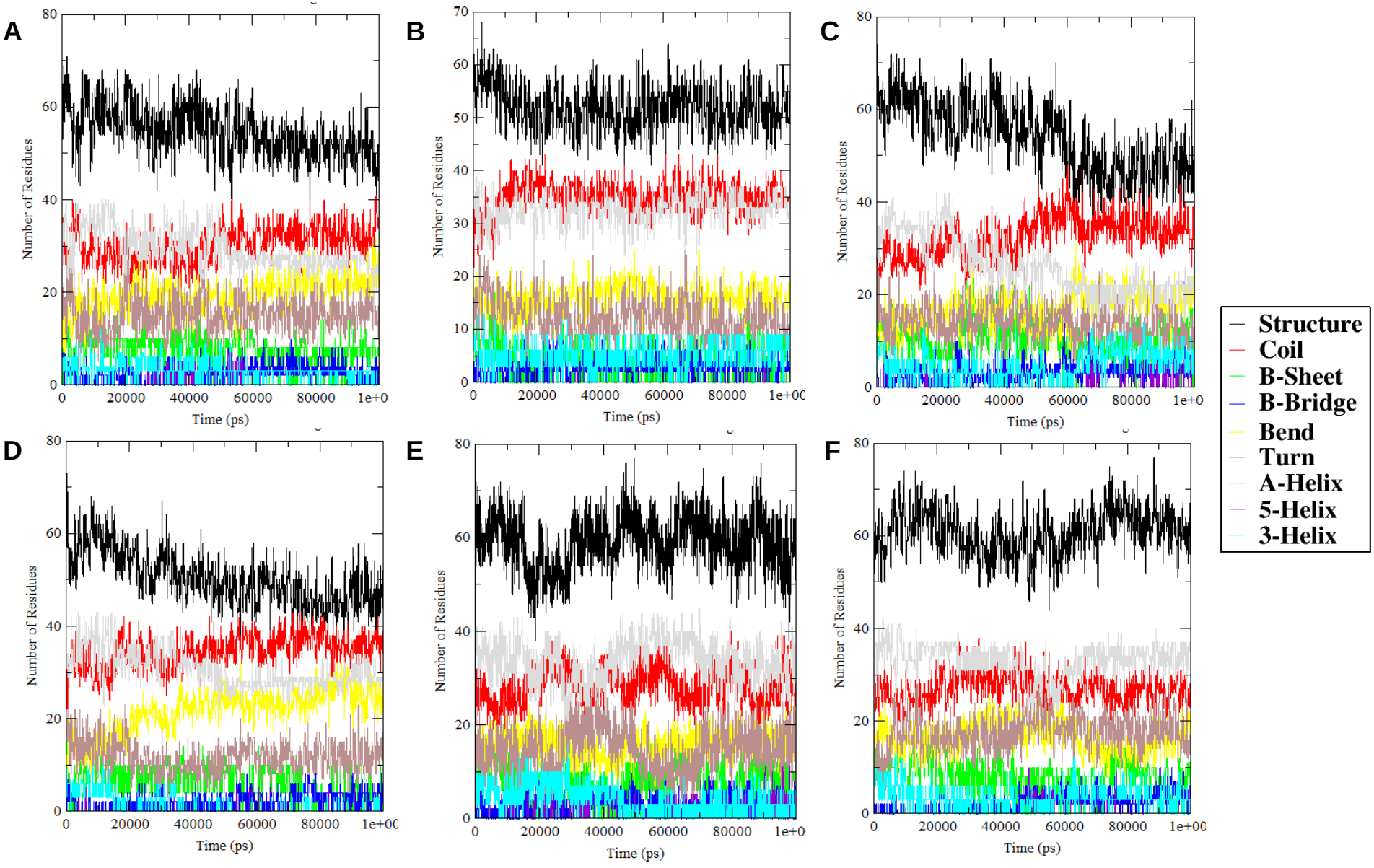

Figure S4. Secondary structure content in N-CTD systems calculated after MD simulation of 100 ns at 300K. (A) CTD, (B) CTD-4E1RCat, (C) CTD-Silmitasertib, (D) CTD-TMCB, (E) CTD-Sapanisertib, and (F) CTD-Rapamycin.
Structure = α helix + β-sheet + β-bridge +Turn + Coil

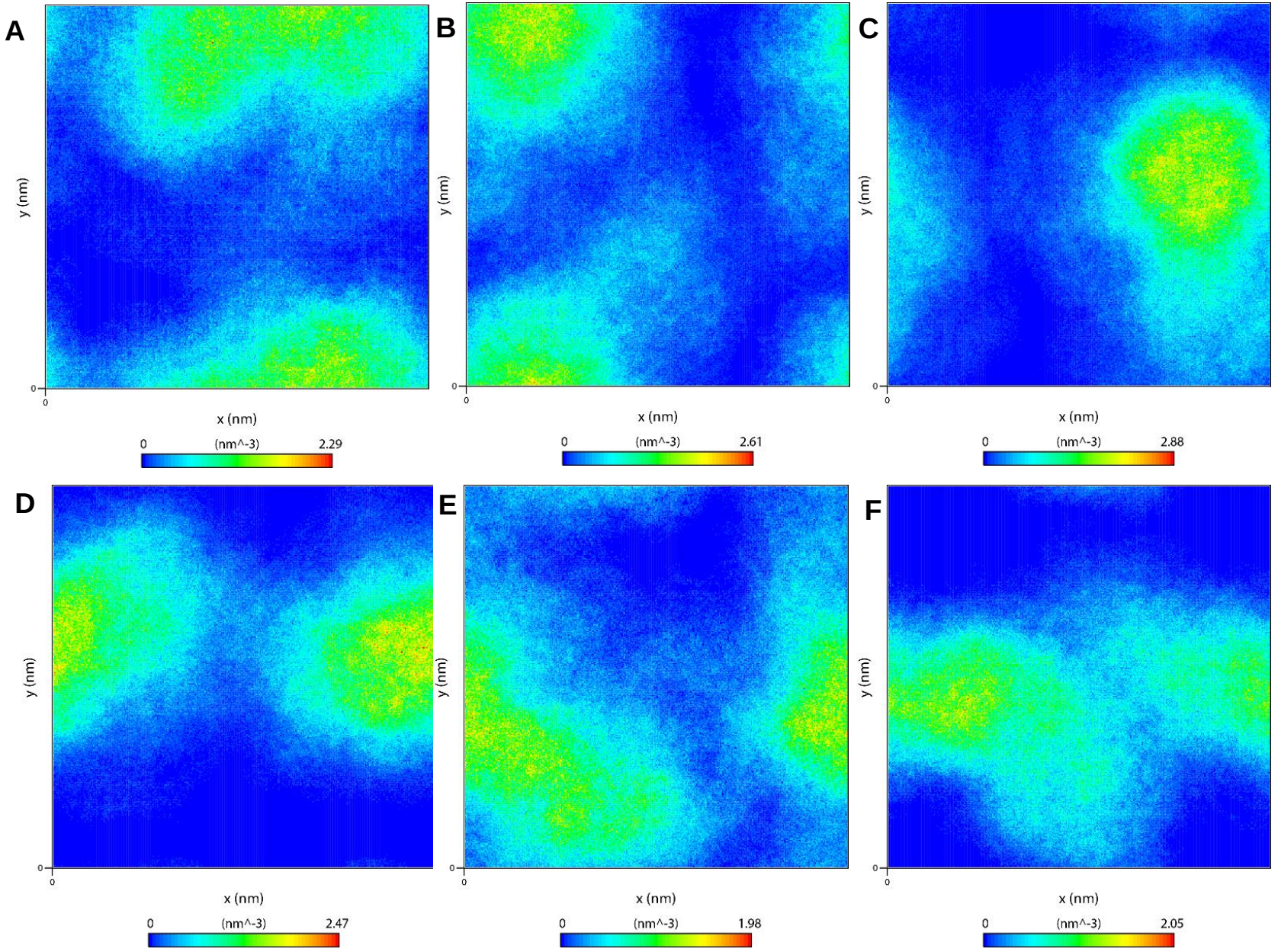

Figure S5. Density distribution plot for protein and protein-drug complexes. (A) CTD, (B) CTD-4E1RCat, (C) CTD-Silmitasertib, (D) CTD-TMCB, (E) CTD-Sapanisertib, and (F) CTD-Rapamycin.