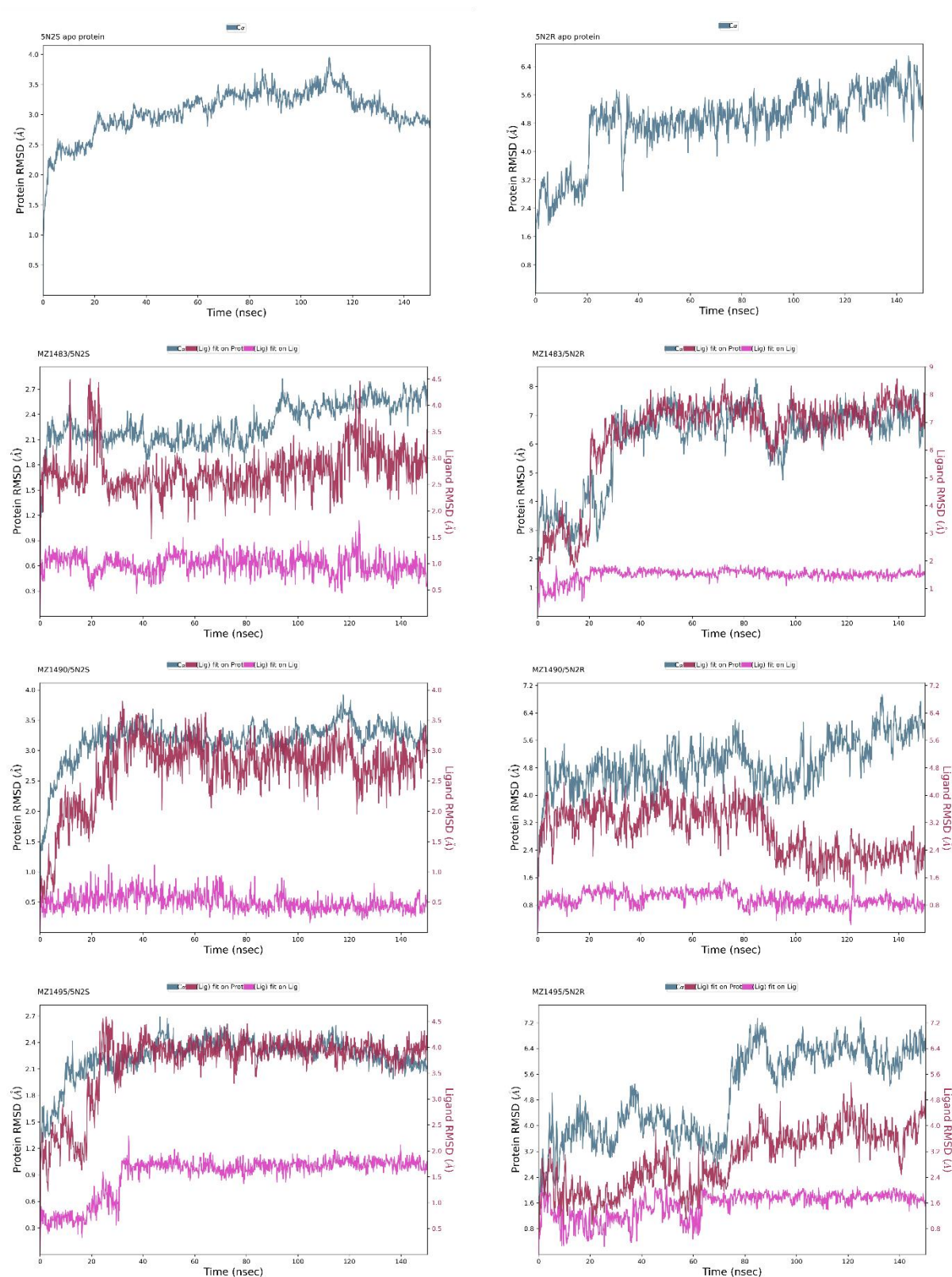
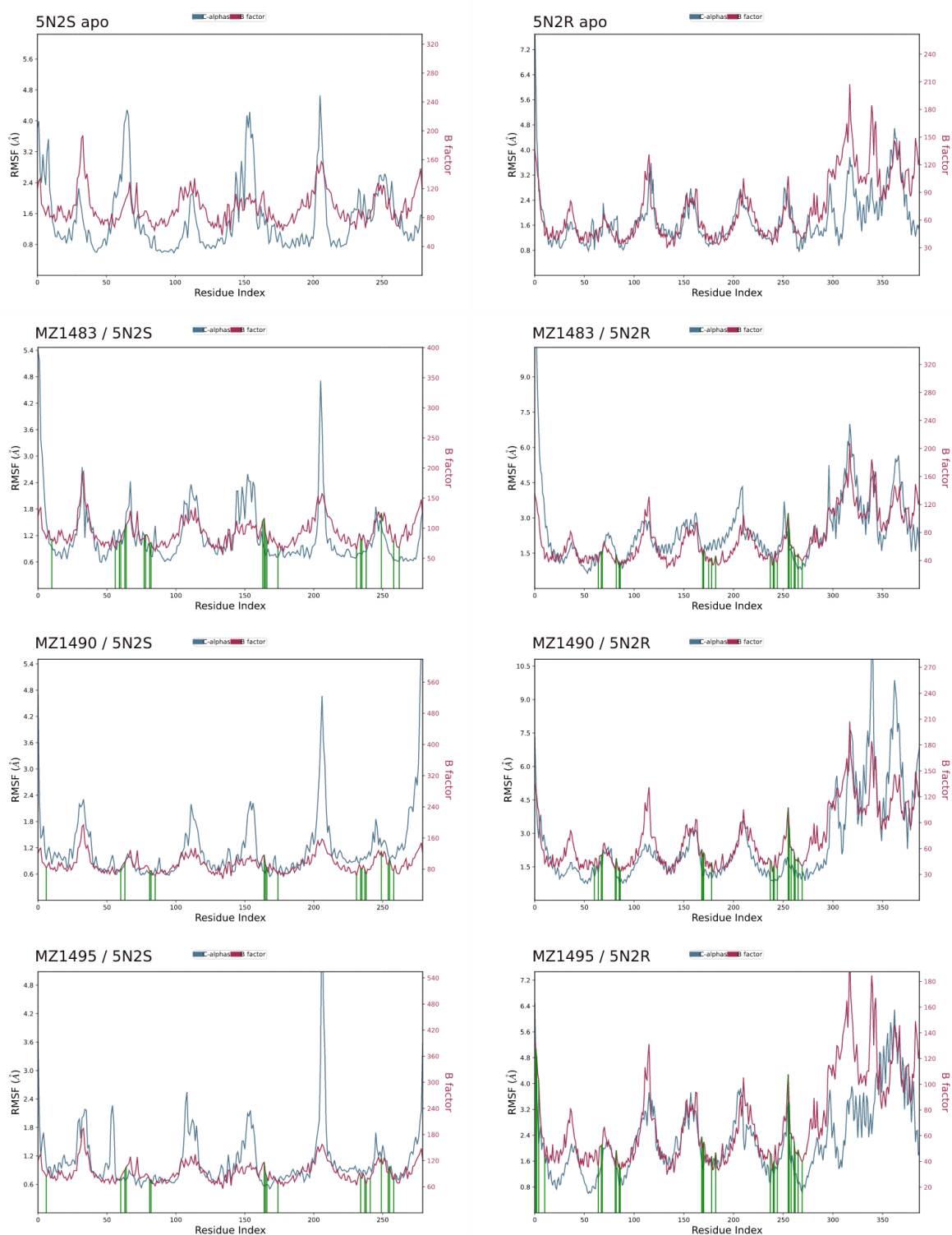


## Molecular docking studies – Figures S1-S4



**Figure S1** – Plots showing the RMSD evolution of 6 complexes and corresponding apo proteins (each protein structure used for each ligand) of a protein (left Y-axis) and ligand (right Y-axis). All protein frames are first aligned on the reference frame backbone, and then the RMSD is calculated based on the atom selection. Pink – Ligand fit on ligand (1st frame), Grayblue – Ca, maroon – Ligand fit on protein.



**Figure S2** – Plots showing the RMSF 6 complexes and corresponding apo proteins (each protein structure used for each ligand), colored grey. Peaks indicate areas of the protein that fluctuate the most during the simulation. Protein residues that interact with the ligand are marked with green-colored vertical bars. The experimental x-ray B-factor (right Y-axis) is showed in magenta.

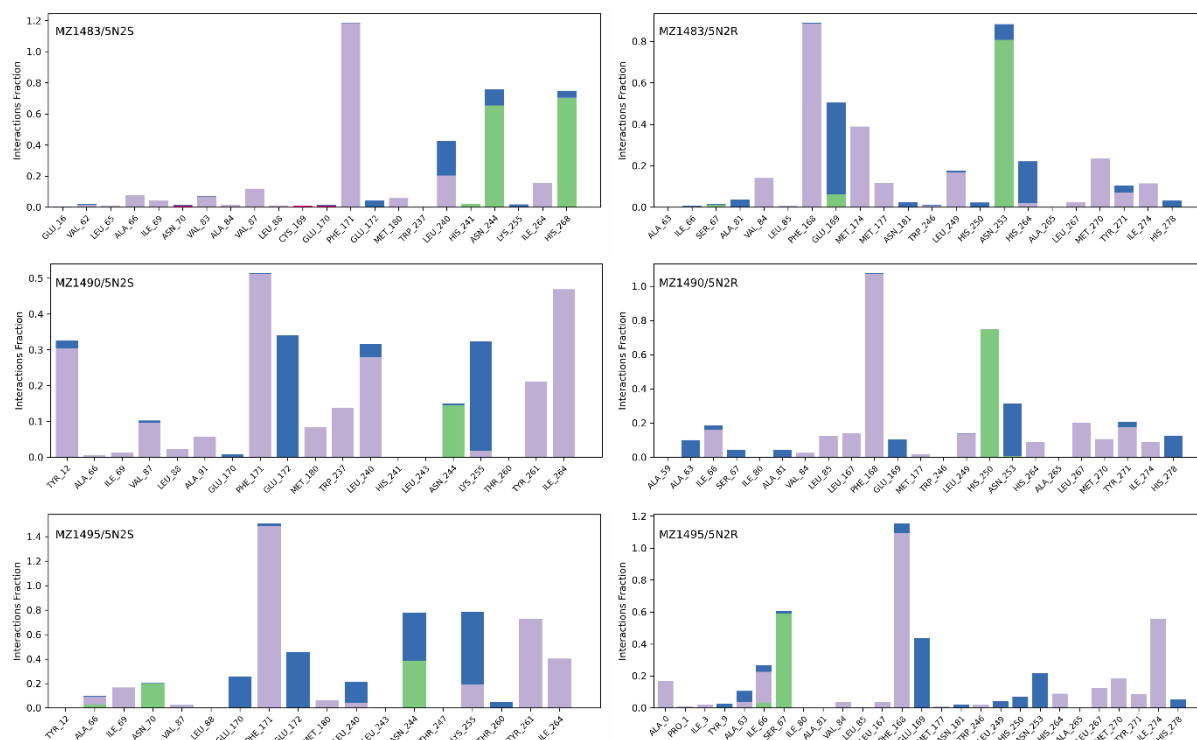


Figure S3 –Histograms of Protein -ligand interactions monitored throughout the simulation for 6 simulated complexes (each protein structure used for each ligand). Green – H-bonds, Violet – hydrophobic interactions, Pink – Ionic interactions, Blue – water bridges.

