Supporting Information

Molecular insights into the binding of carnosine and anserine to human serum carnosinase 1 (CN1)

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Table S1. Gold docking scores for anserine and carnosine to CN1.

Ligand	Fitness Score Chain A	Fitness Score Chain B
Anserine	59.59	86.68
Carnosine	56.61	84.45

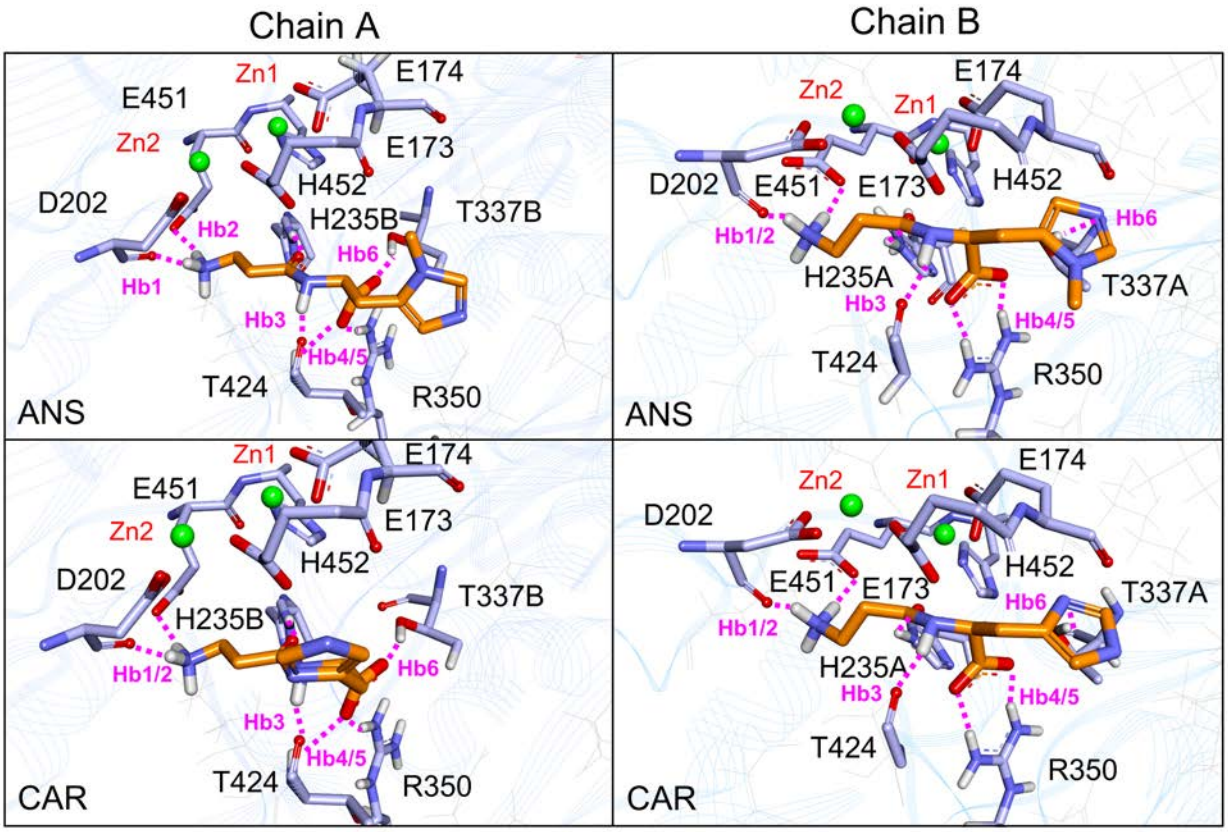

Figure S1. Binding mode of anserine and carnosine to CN1 from docking simulations.

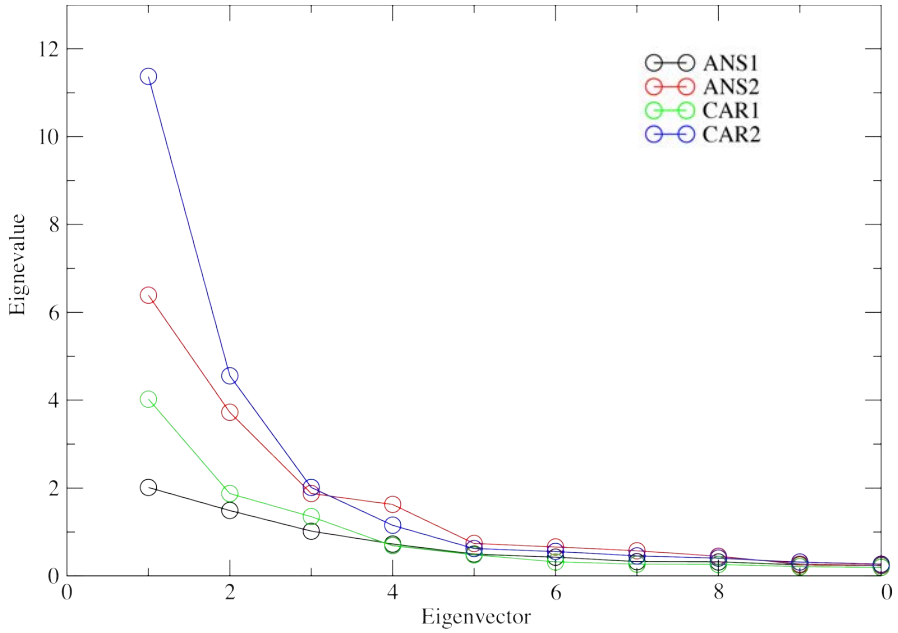

Figure S2. Eigenvalues of all systems

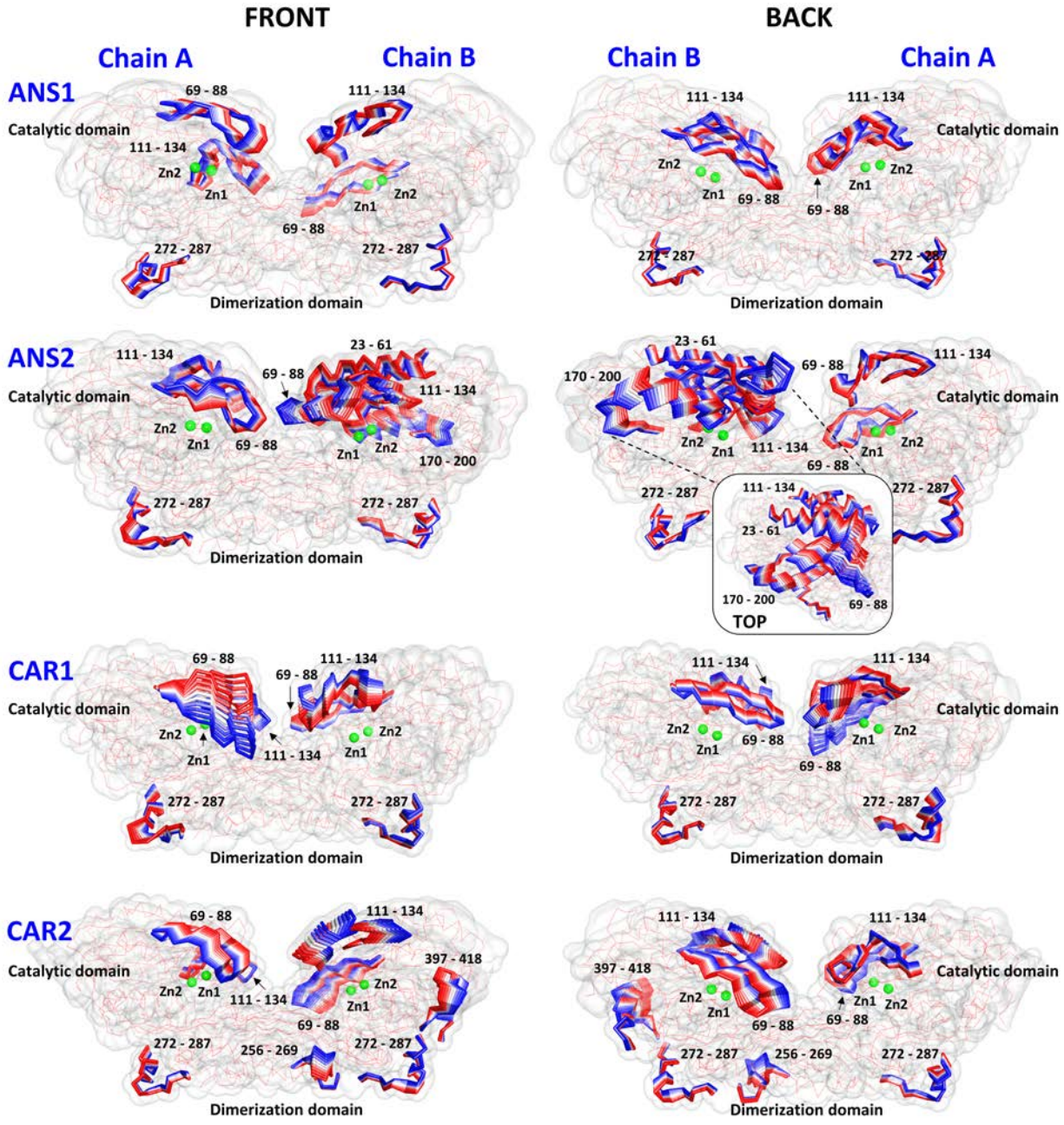

Figure S3. Principal Component analysis (PCA) calculated from the first principal component of all systems. Only highly mobile regions are shown in RWB format.

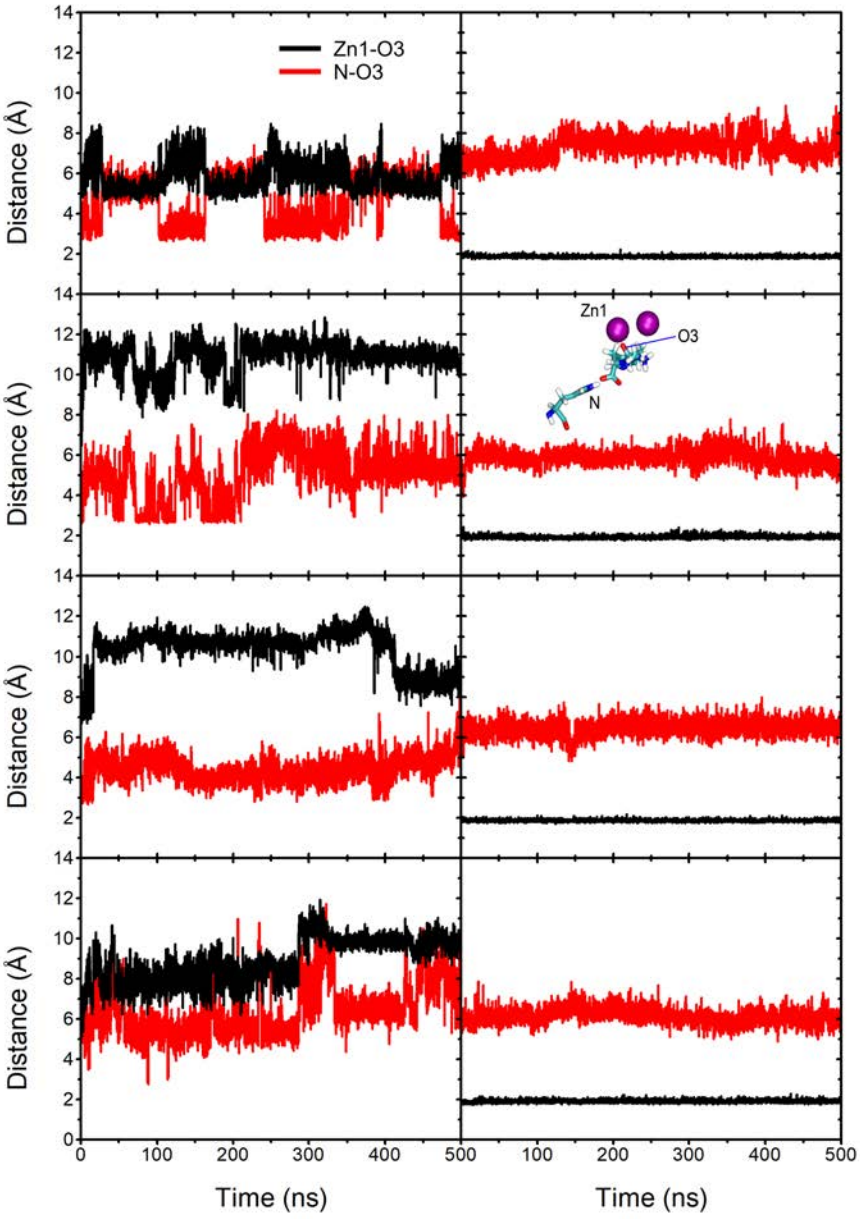

Figure S4. Distances of Zn1-O3 (black) and N-O3 (red). N is a nitrogen atom on histidine ring (H235) and O3 is a carbonyl oxygen (O3) on ligand in all systems.

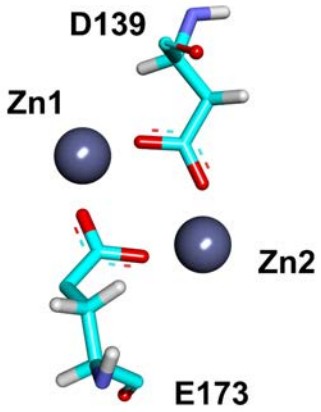

Figure S5. Bridge-like structure of two Zinc ions and D139 and E173

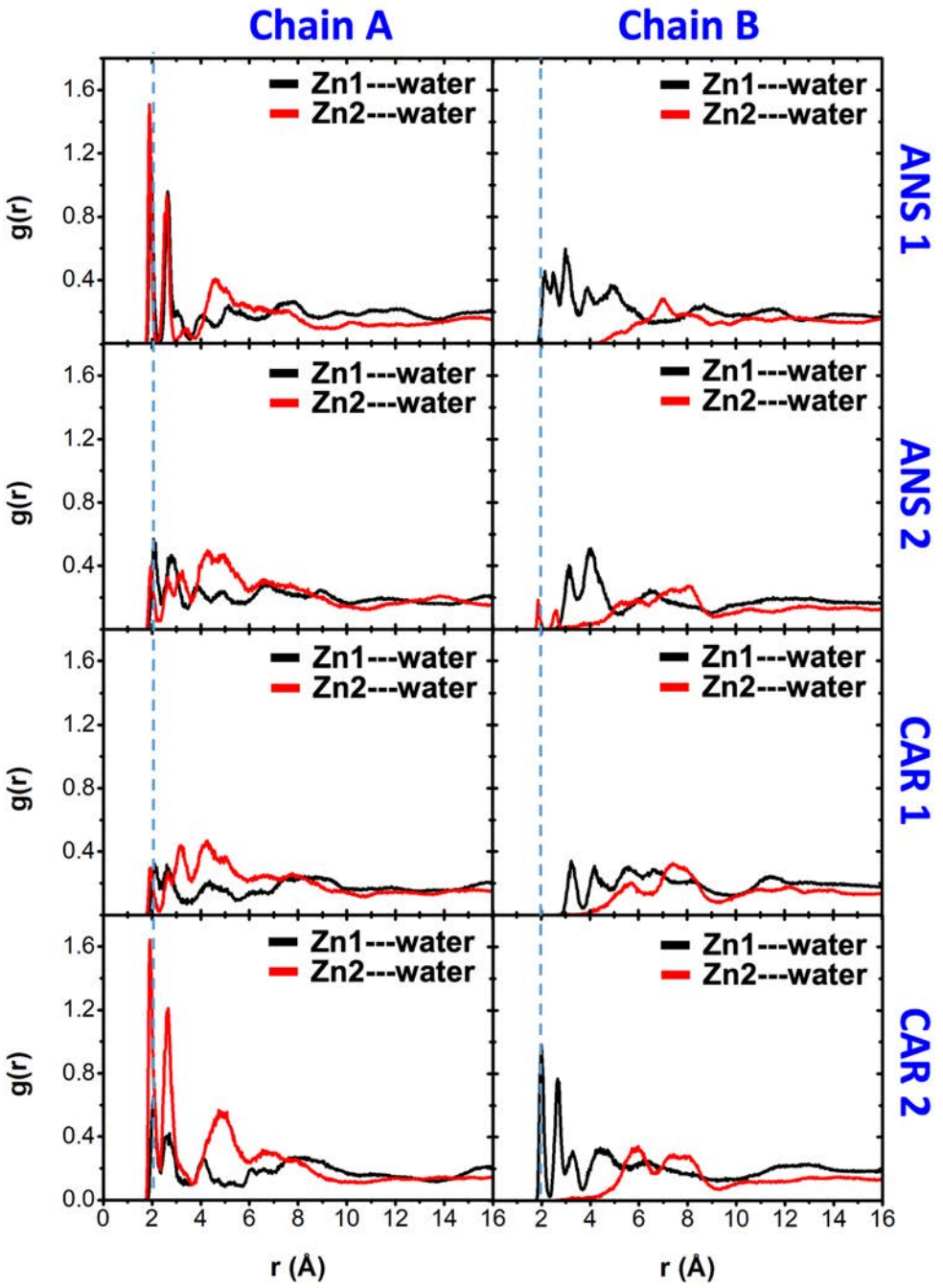

Figure S6. Radial Distribution Function of Zn1 and Zn2 in all systems. The dashed line represents the Zn-O bond length reported in a previous work [1].

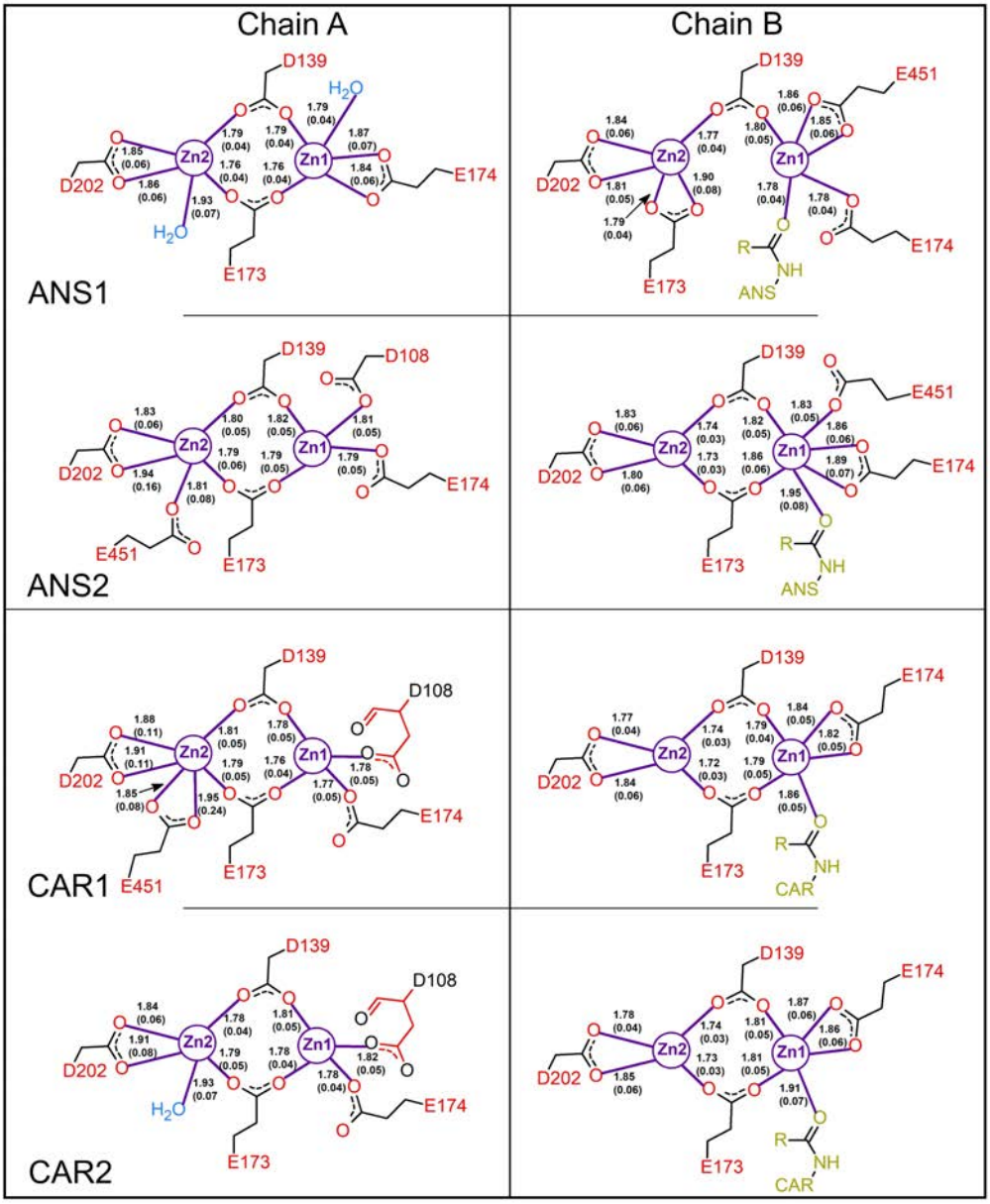

Figure S7. Zn^{2+} environments (first shell (distance $\leq$ 0.2 nm) (Ataie et al. 2008; Tamames et al. 2007)) inside the pocket in all systems. The average distances between Zn^{2+} and nitrogen or oxygen atoms are shown with standard deviation in a bracket. Such average distances are computed using the data after 250 ns.

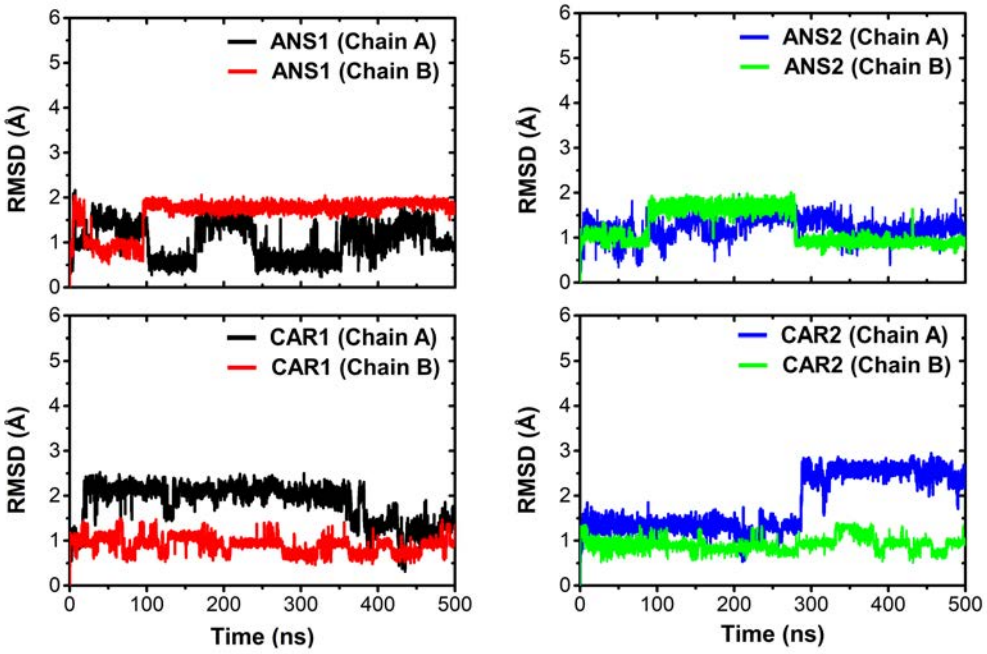

Figure S8. Ligand RMSDs of all systems.

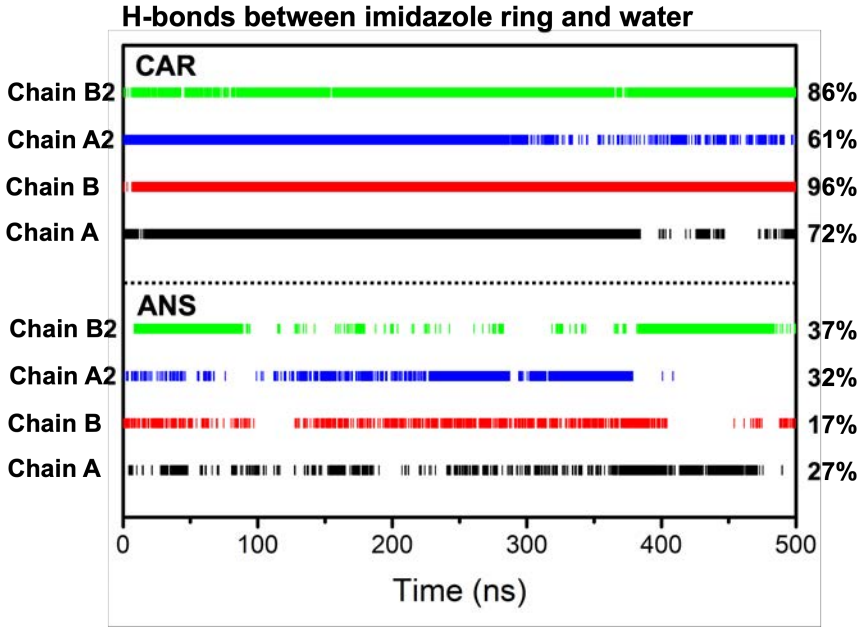

Figure S9. Average hydrogen bonds between imidazole moiety and water

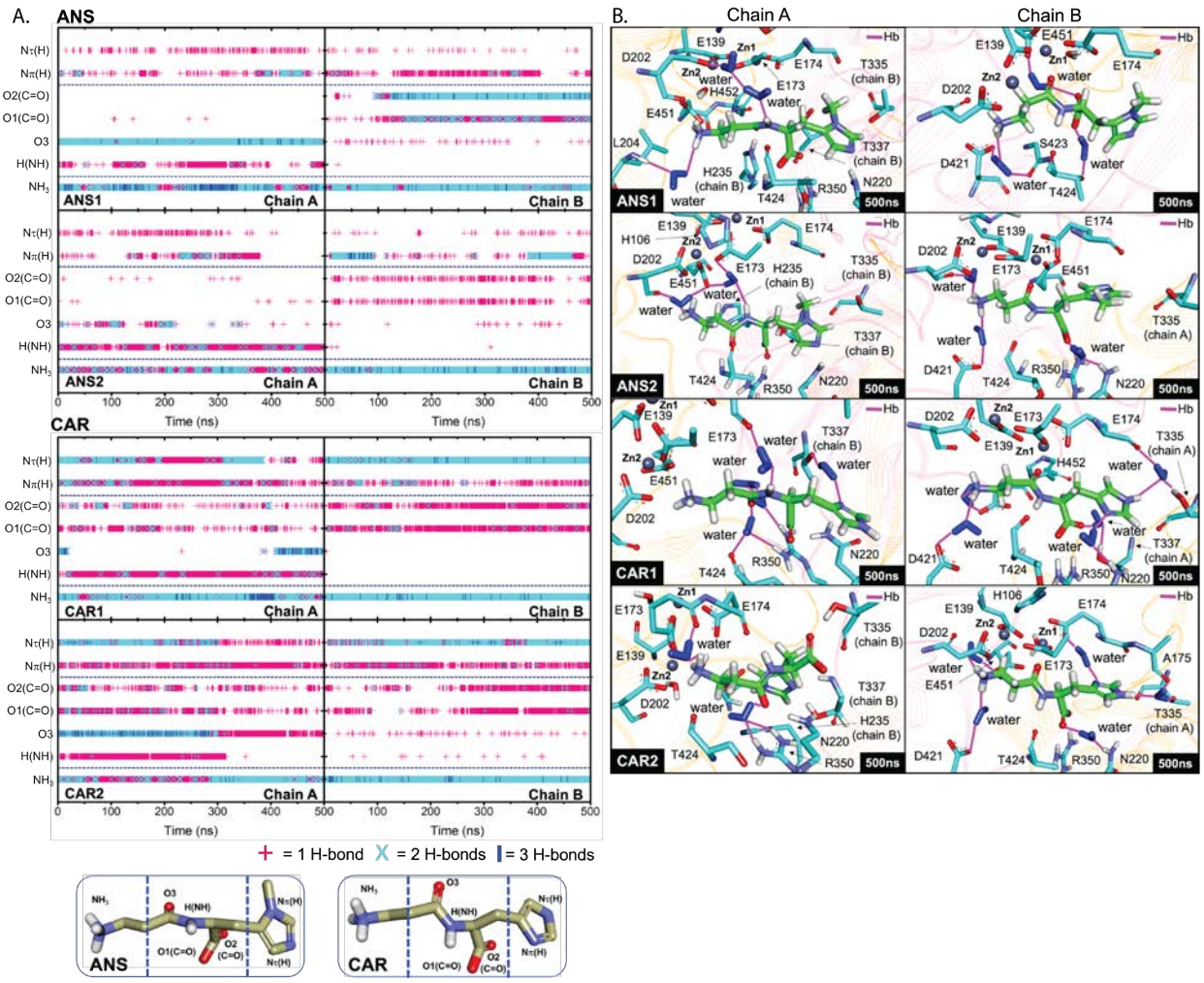

Figure S10 (A) Hydrogen bonds between polar atoms on a ligand and water. The locations of each atom are shown at the bottom. (B) Orientations of ligand inside a pocket and cavity-lining residues in all systems. Key water molecules that can bridge residue and ligand are displayed in blue.

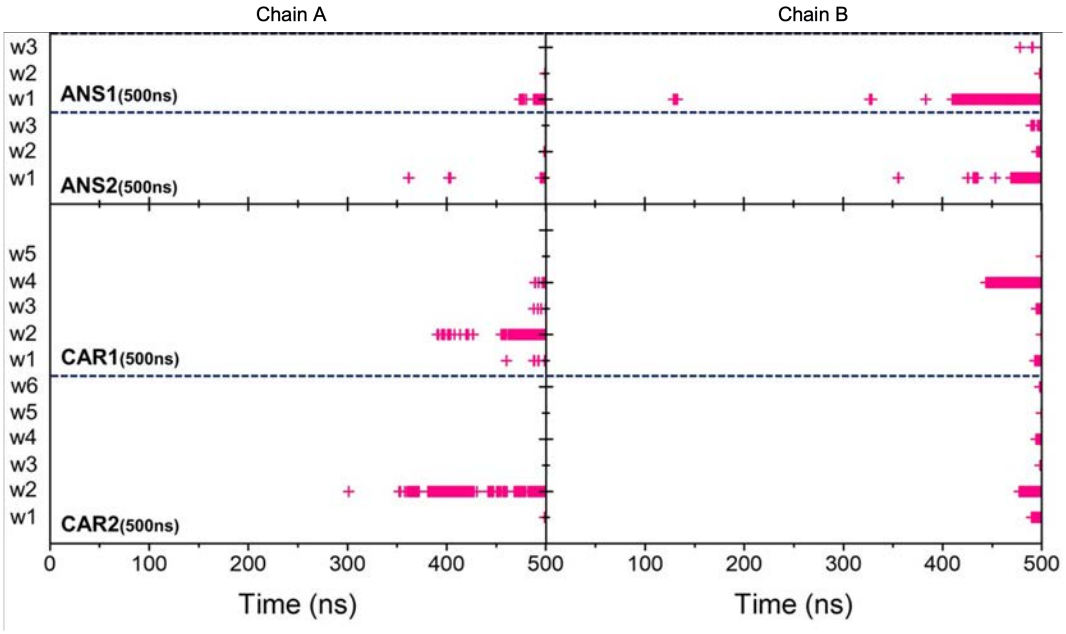

Figure S11 Hydrogen bonds between residues and water molecules that form hydrogen bonds with ligand from chains A and B. Water molecules (w1-w6) forming hydrogen bonds with each ligand at 500ns are used for residue-bridging hydrogen bonds.