SUPPORTING INFORMATION

Analysis of factors influencing hydration site prediction based on molecular dynamics simulations

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Figure S1. Correlation of energy values of the paired hydration sites between those obtained from the 20ns MD simulations and those obtained from shorter simulation lengths (1.5 ns, 2 ns, 3 ns, 5 ns, 10 ns)

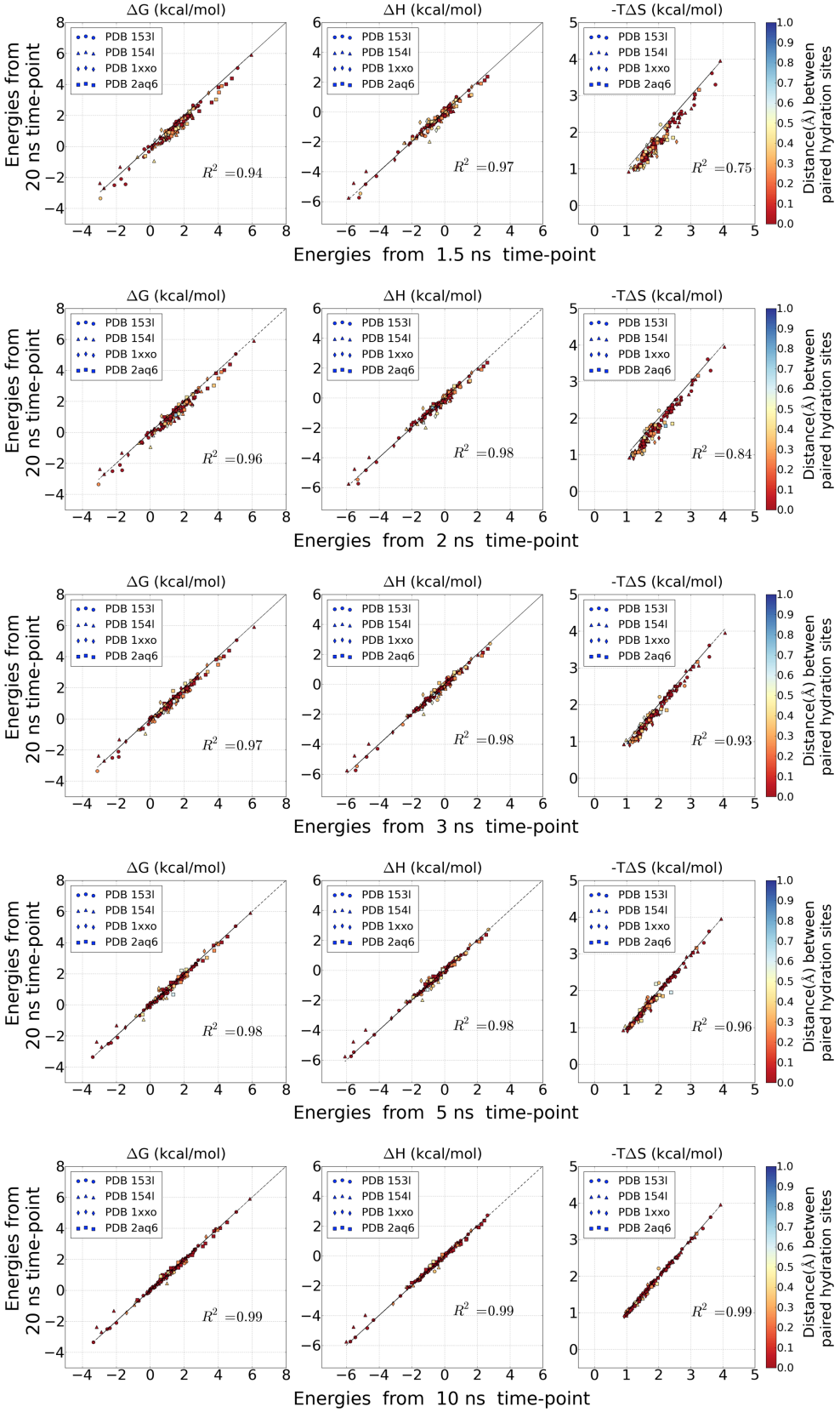

Figure S2. Superimposition of hydration sites in the binding site of pyridoxine 5'-phosphate oxidase. (PDB: 1XXO)

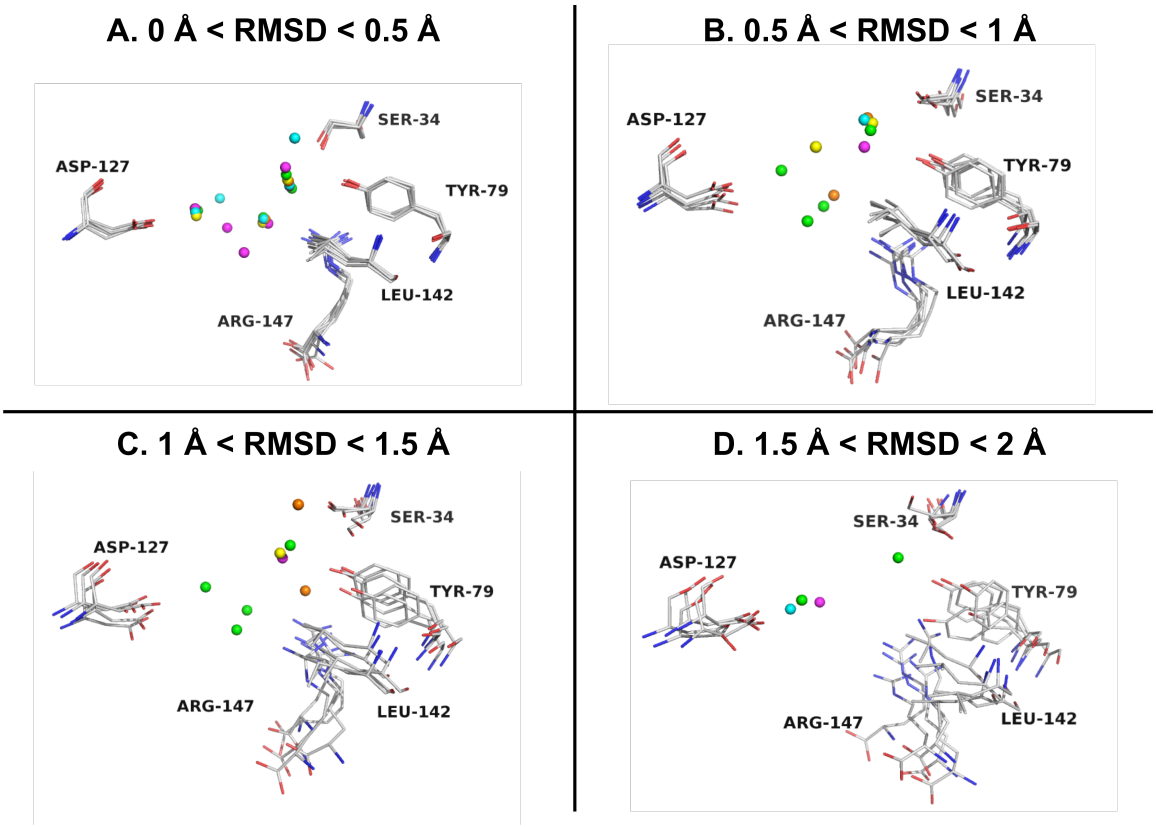

Figure S3. Superimposition of hydration sites in the binding site of goose egg-white lysozyme. (PDB: 153L)

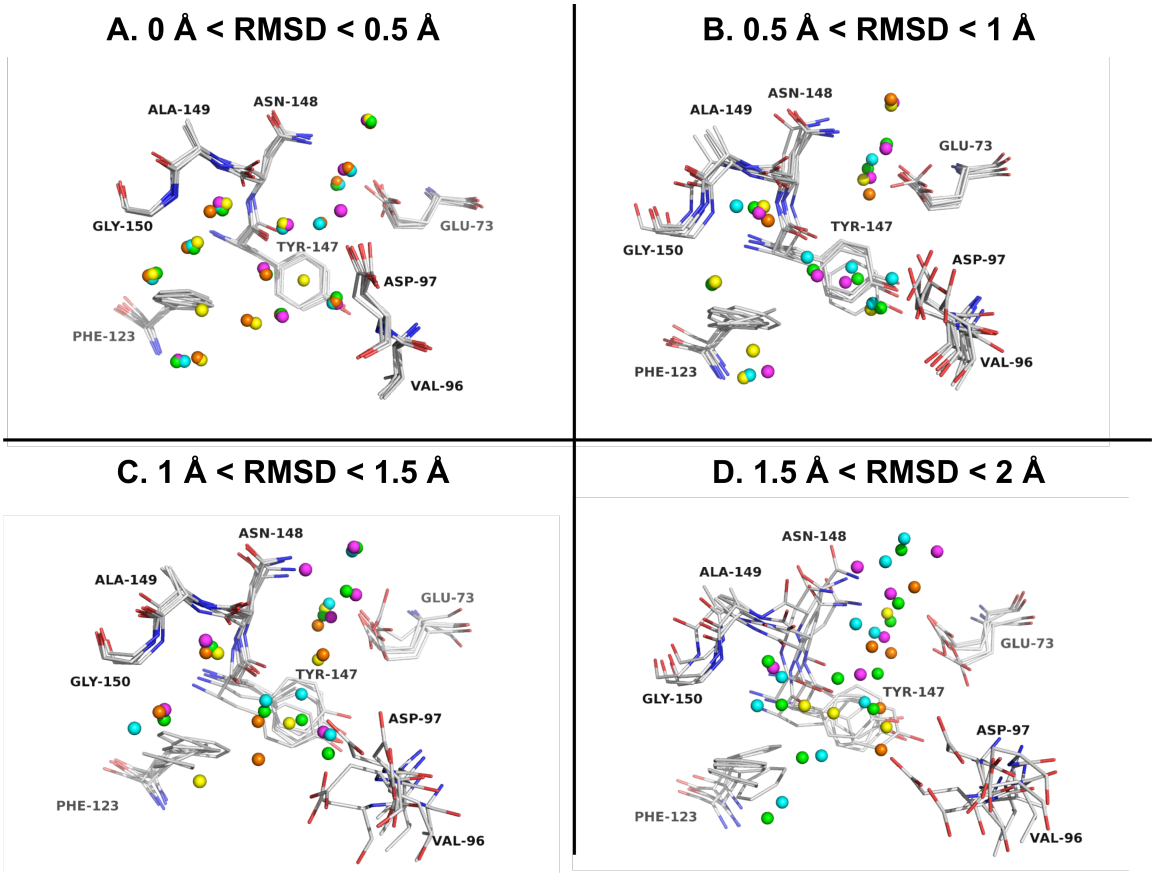

Figure S4. Superimposition of hydration sites in the binding site of goose lysozyme. (PDB: 154L)

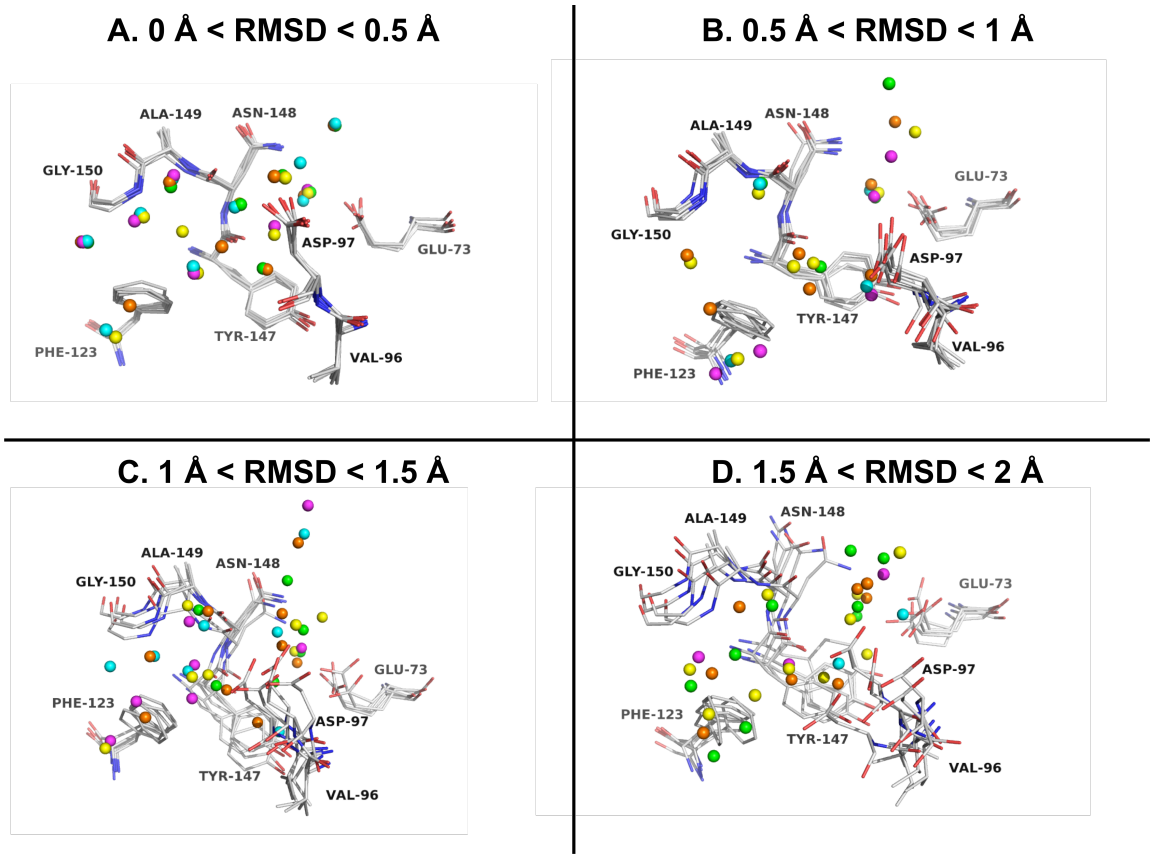

Figure S5. Pairwise comparison between two different simulations of Goose lysozyme apo structure (PDB: 153L)

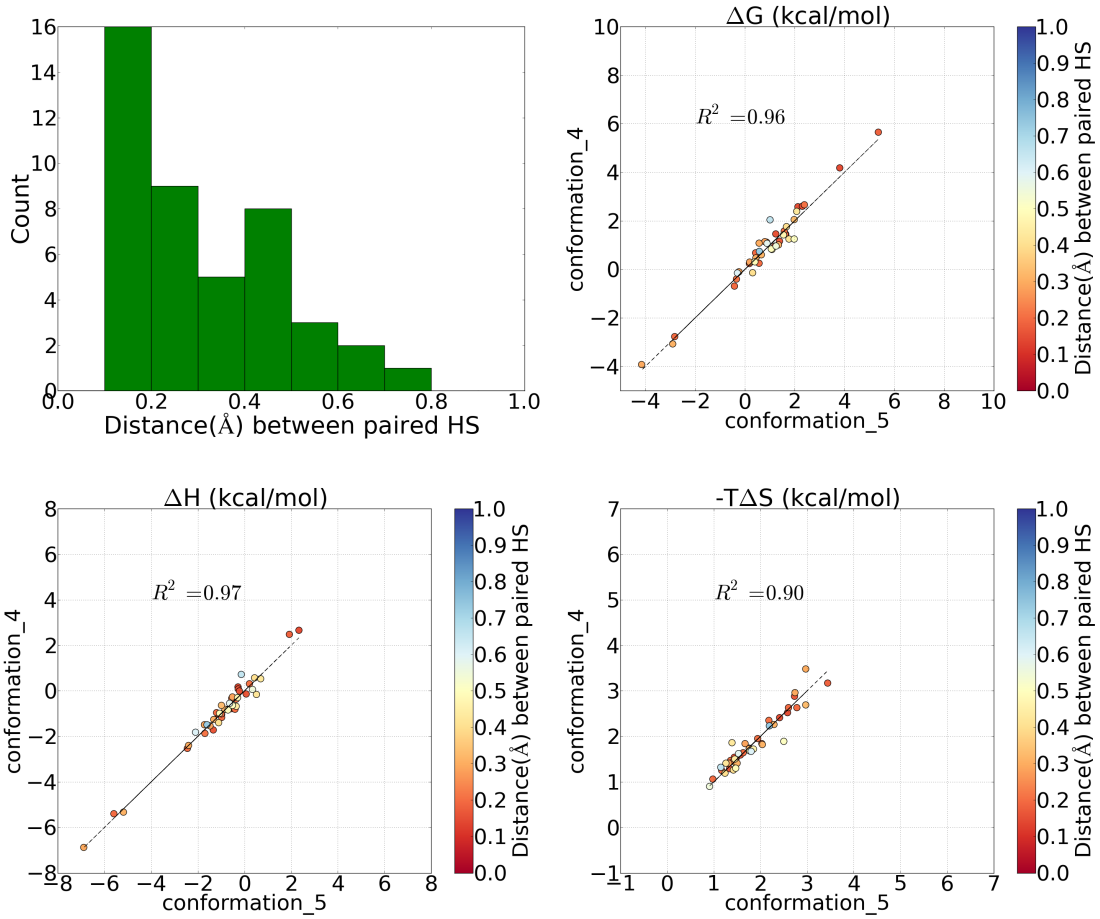

Figure S6. Pairwise comparison between two different simulations of pyridoxine 5'-phosphate oxidase (PDB: 1XXO)

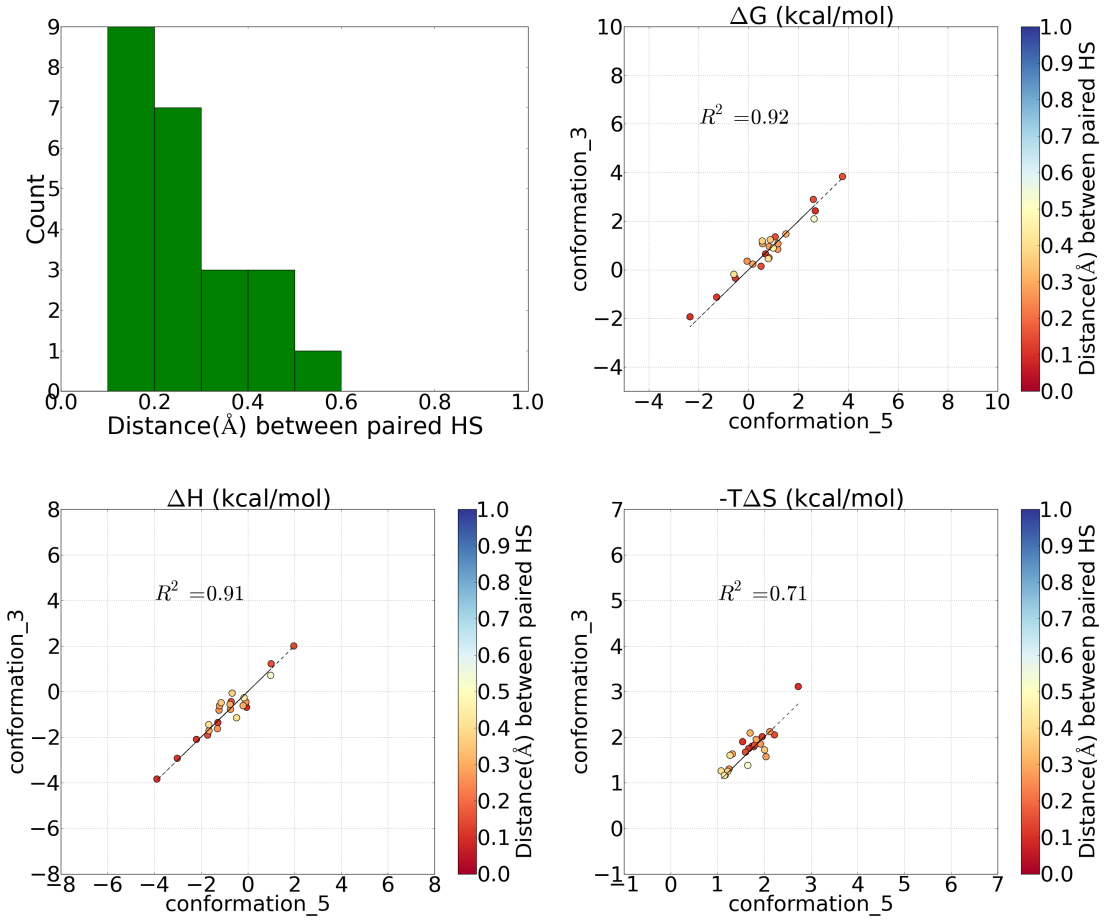

Figure S7. Pairwise comparison between two different simulations of pyridoxine 5'-phosphate oxidase (PDB: 2AQ6)