



Figure S10: Persistence of the activated and bridging water at their respective positions calculated through the analysis of the unbiased MD trajectories of the apo-TadA* models ((A) to (D)) and for TadA*-RNA models ((E) to (G)). The different colors signify a unique water molecule that visited these critical water positions. Note that the data was obtained using a distance-based mask of 3.5 Å from the Zn⁺² ion, for activated water and from the peptide backbone of the 84 residue, for the bridging water.