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Supporting Material

Multiple molecular dynamics simulations of TEM -lactamase: Dynamics and water binding of the -loop

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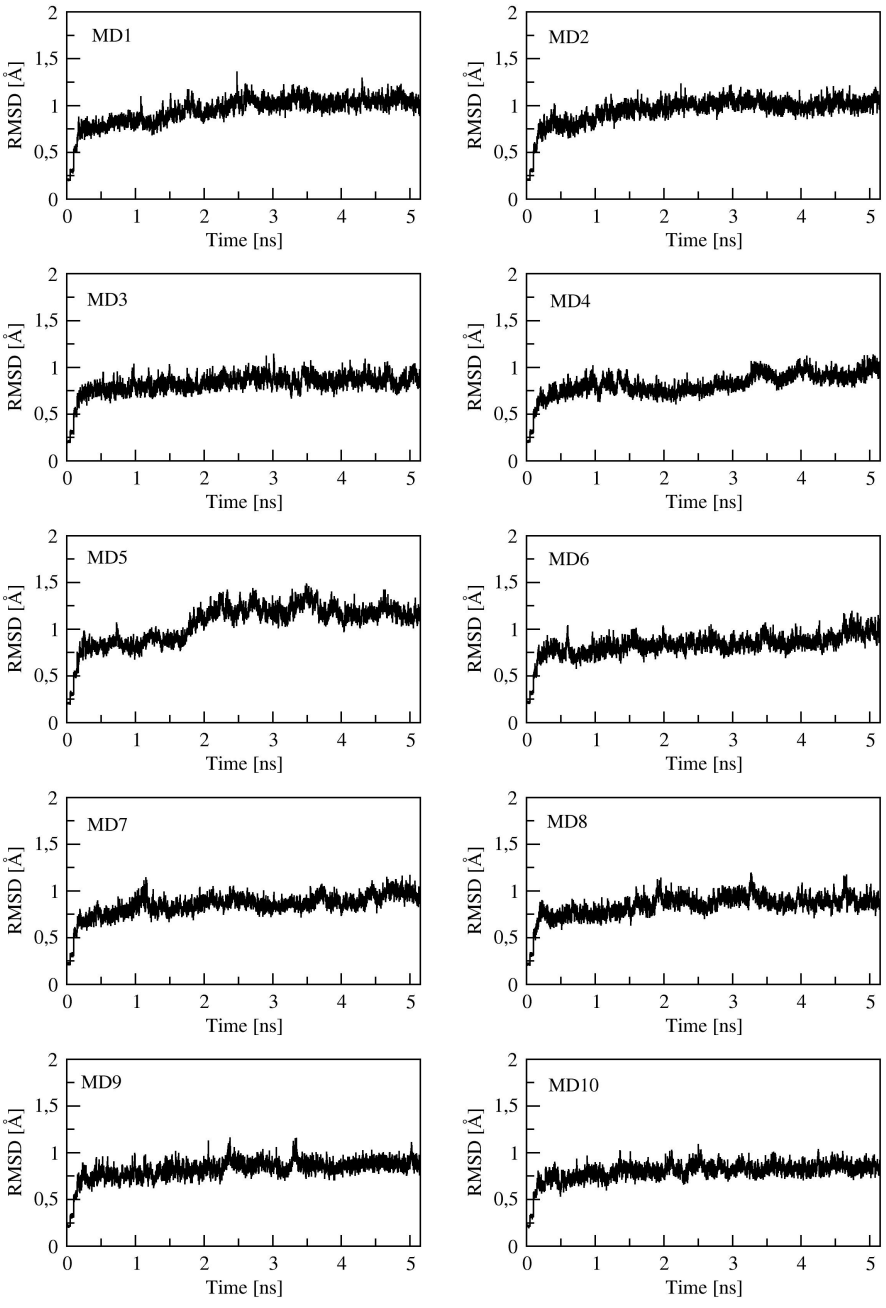

Figure S1: Root mean square deviation of the protein backbone from the minimized starting structure during the 10 MMD_{nowat} simulations.

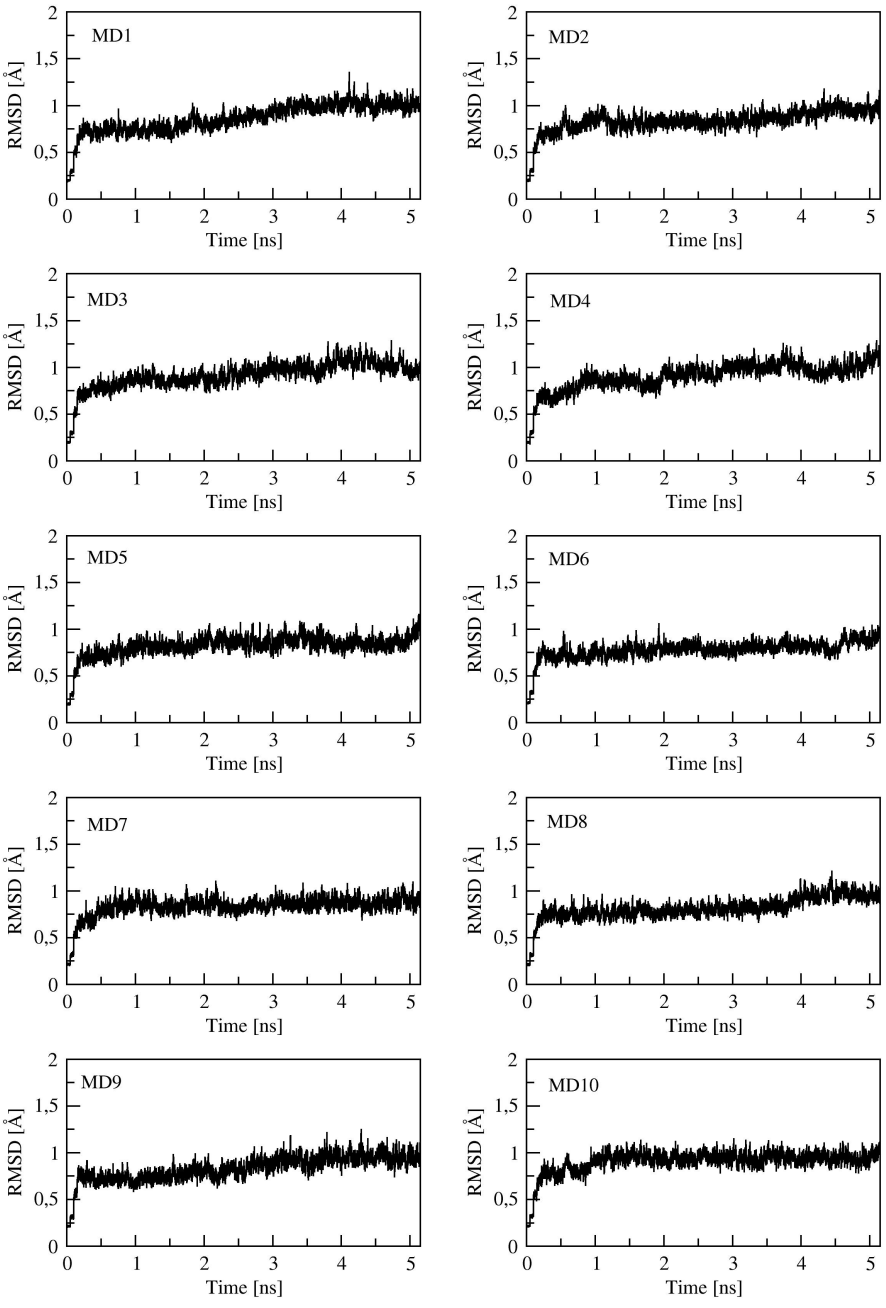

Figure S2: Root mean square deviation of the protein backbone from the minimized starting structure during the 10 MMD_{wat} simulations.

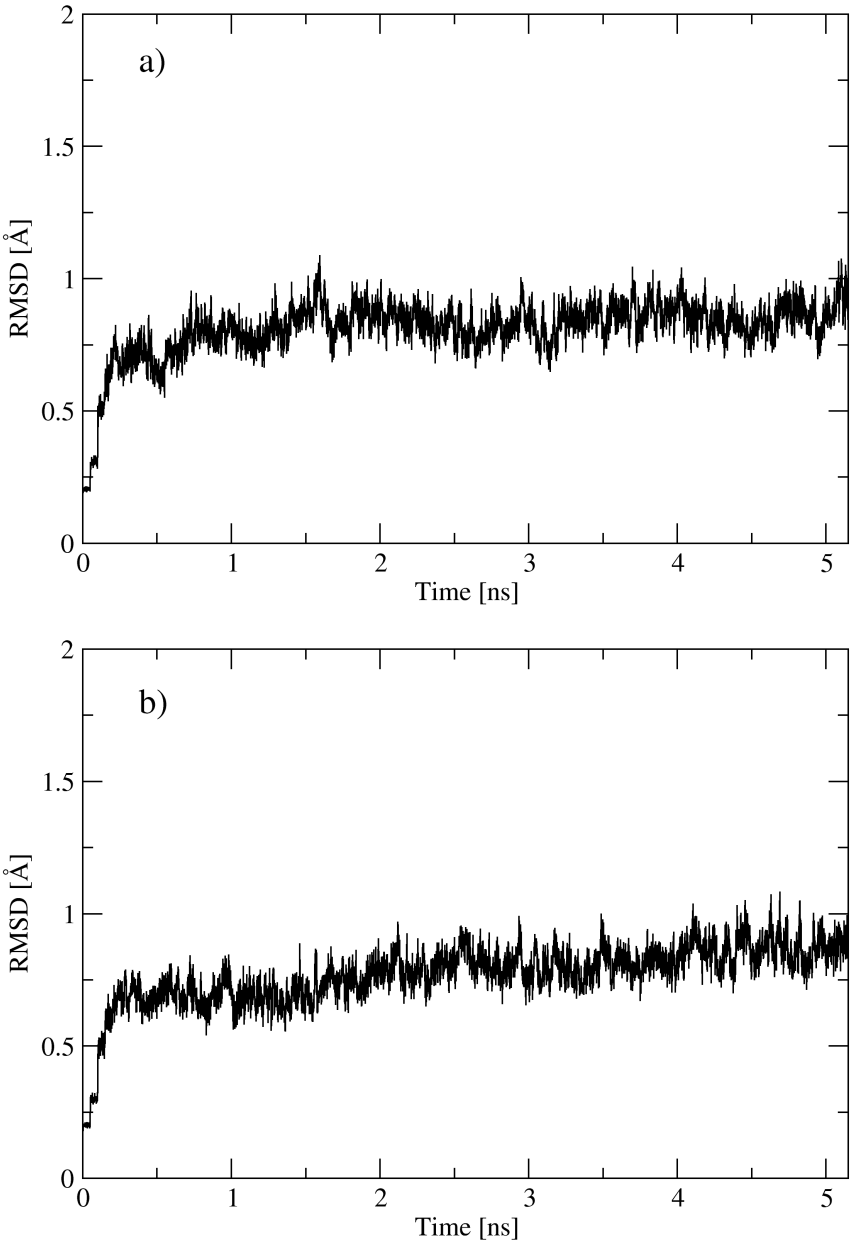

Figure S3: Root mean square deviation of the protein backbone from the minimized starting structure during the simulations using the SPC/E water model. a) simulation without crystal water molecules, b) simulation with crystal water molecules.

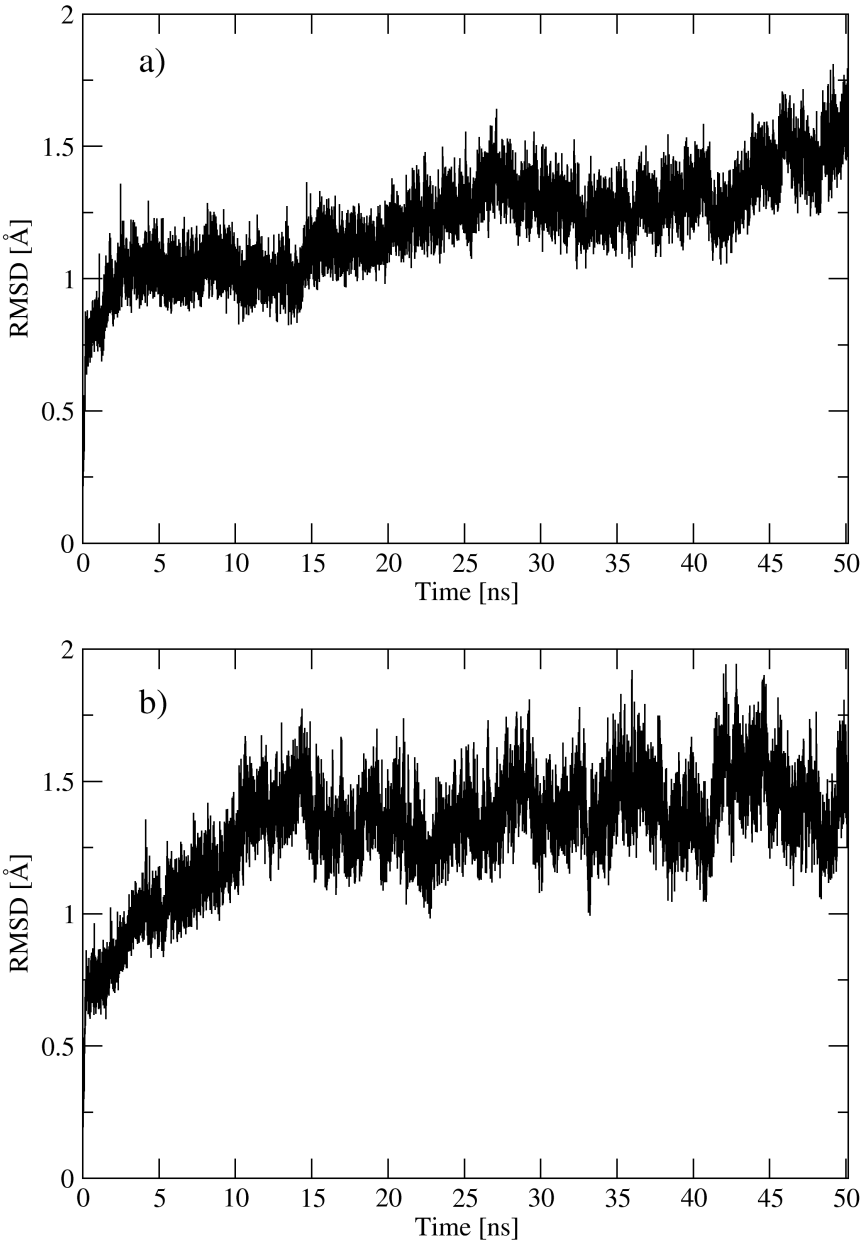

Figure S4: Root mean square deviation of the protein backbone from the minimized starting structure during the extended 50 ns simulations. a) simulation without crystal water molecules, b) simulation with crystal water molecules.

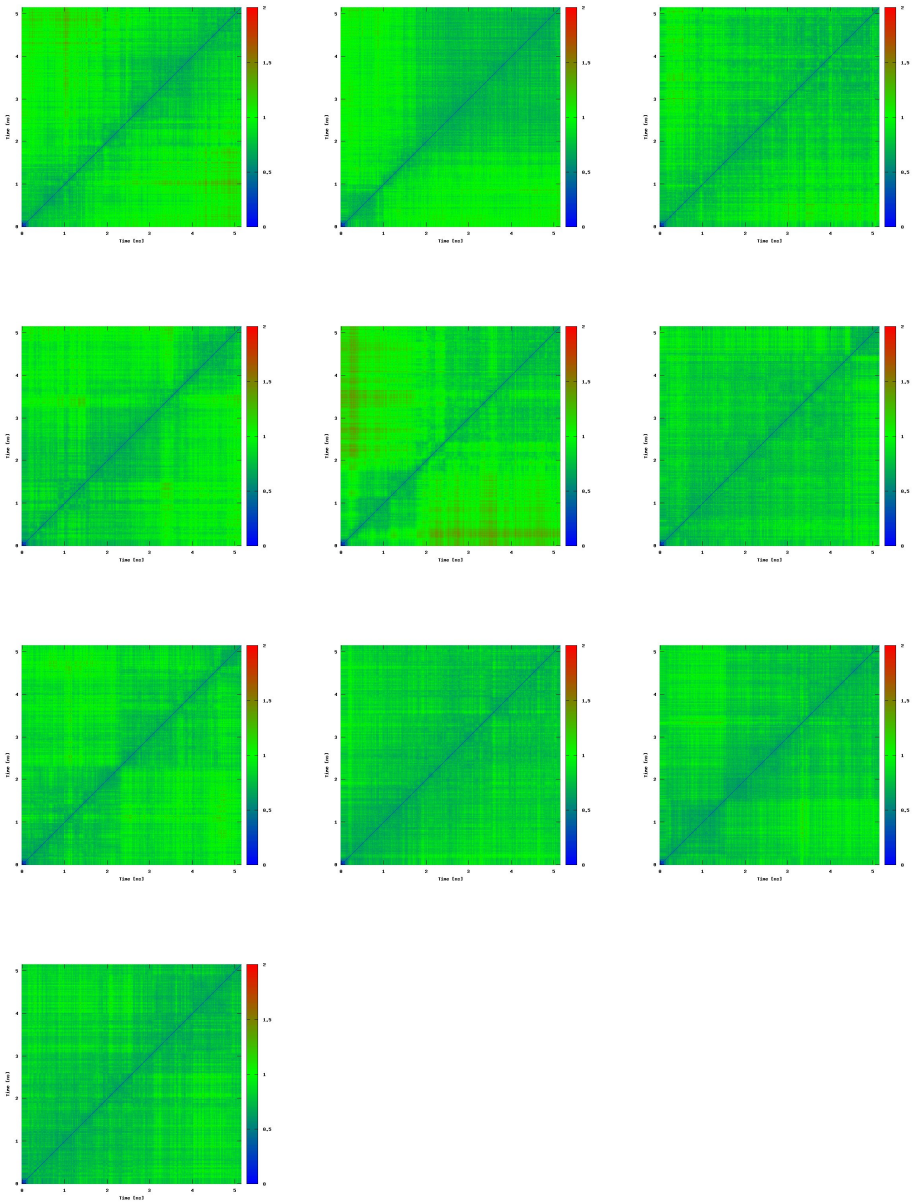

Figure S5: 2D-RMSD plots of the protein backbone during the 10 MMD_{nowat} simulations.

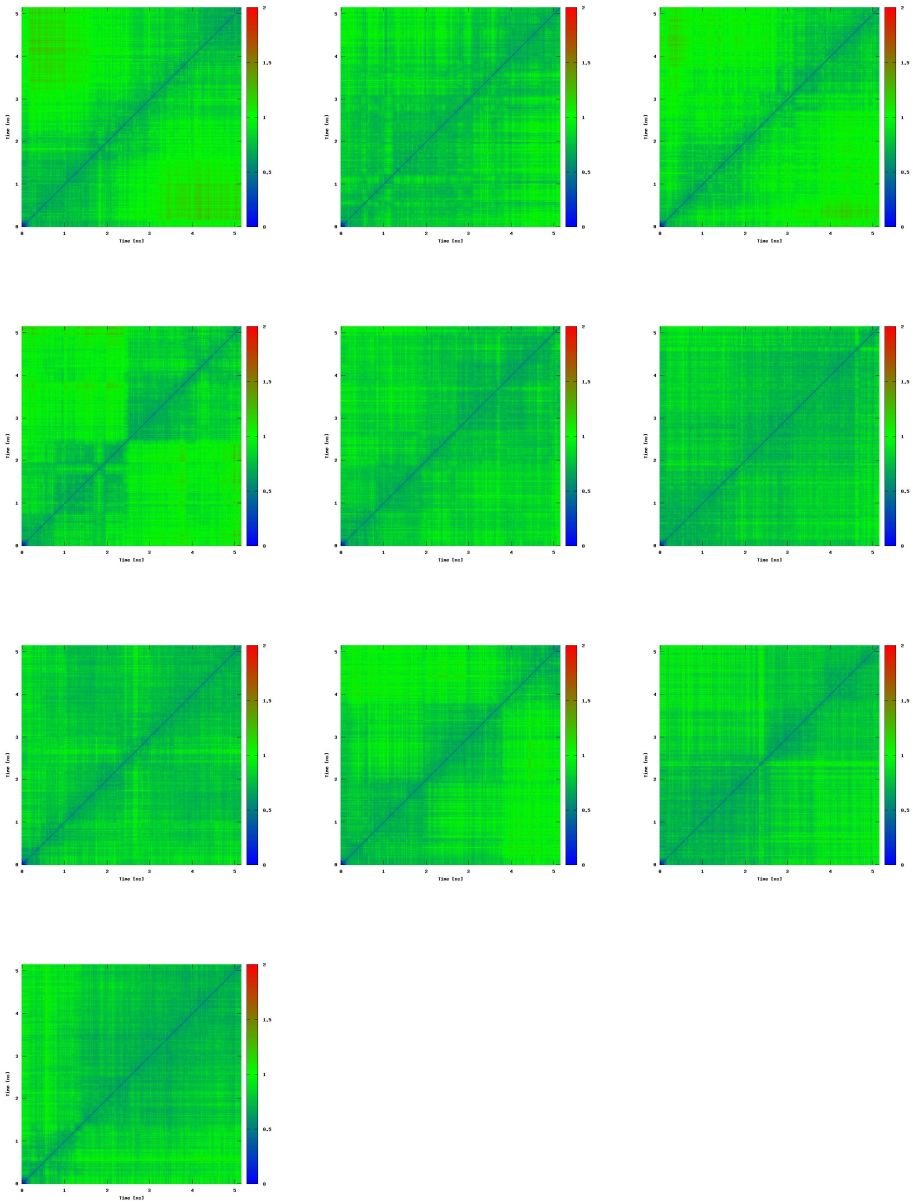

Figure S6: 2D-RMSD plots of the protein backbone during the 10 MMD_{wat} simulations.

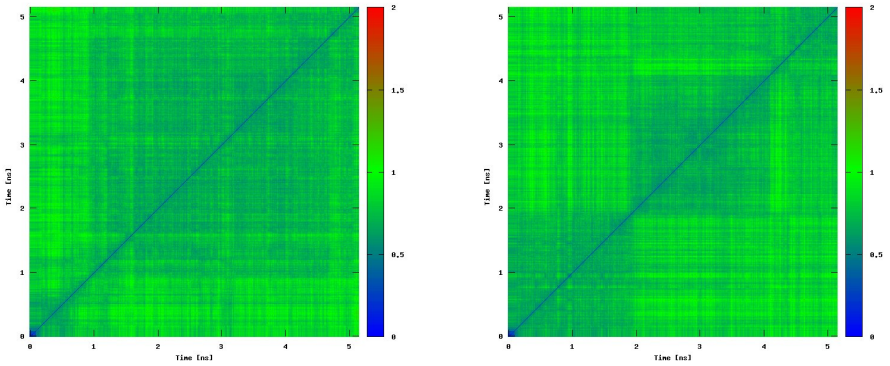

Figure S7: 2D-RMSD plots of the protein backbone during the simulations using the SPC/E water model. Left: simulation without crystal water molecules, right: simulation with crystal water molecules.

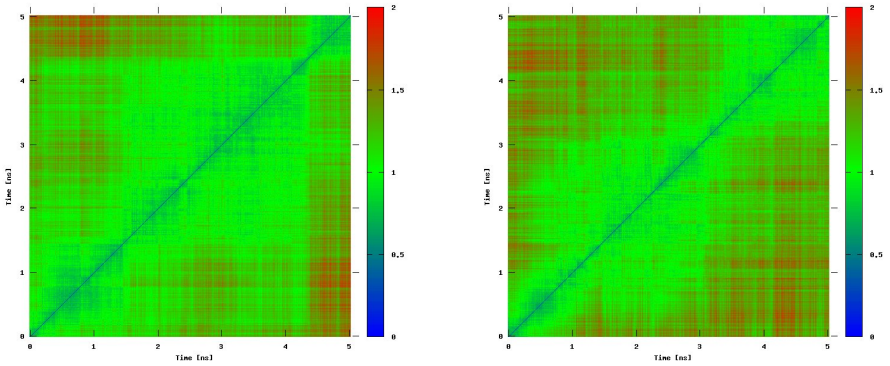

Figure S8: 2D-RMSD plots of the protein backbone during the extended 50 ns simulations. Left: simulation without crystal water molecules, right: simulation with crystal water molecules.

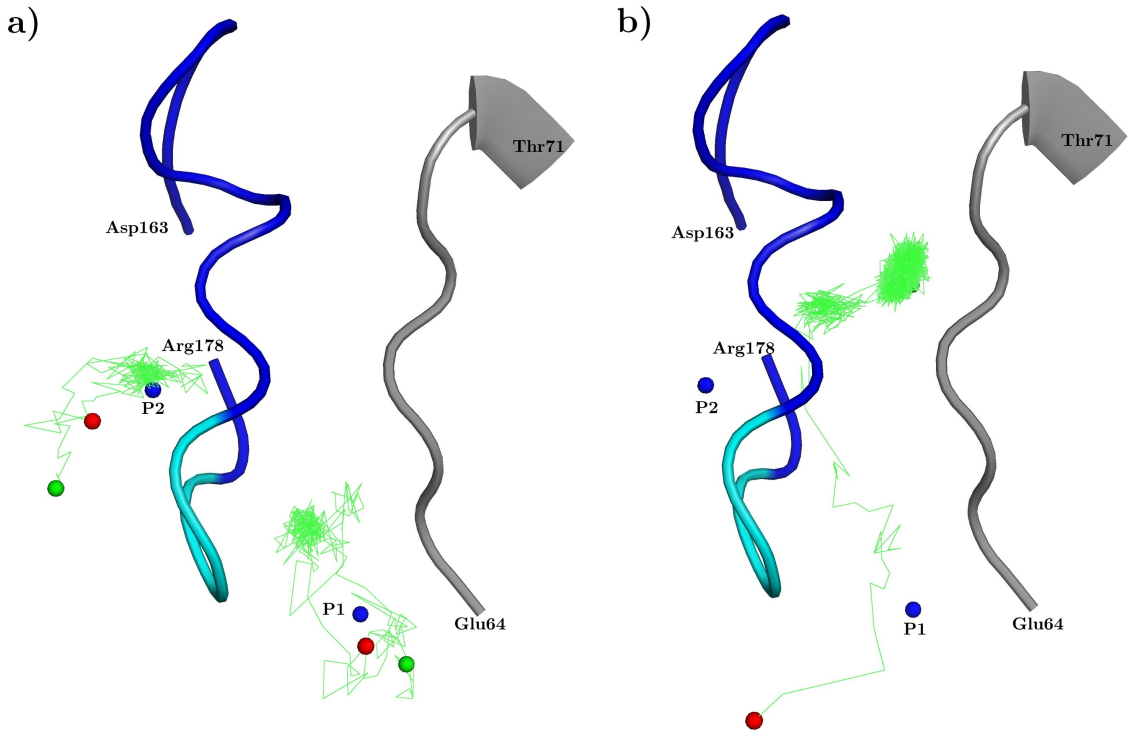

Figure S9: Examples of water molecules passing through and interacting with the Ω-loop cavity. The beginning and end of the water paths are marked as red and green sphere, respectively. Small blue spheres (P1 and P2) represent the coordinates used in assigning individual water paths to the entry and exit points 1 and 2. a) Two water molecules with a path length of less than 500 ps. The water molecules are located only for a short amount of time near the entry and exit points of the Ω-loop cavity. b) A water molecule with a path length of 5 ns. It moves deeply into the Ω-loop cavity and stays at well defined positions.

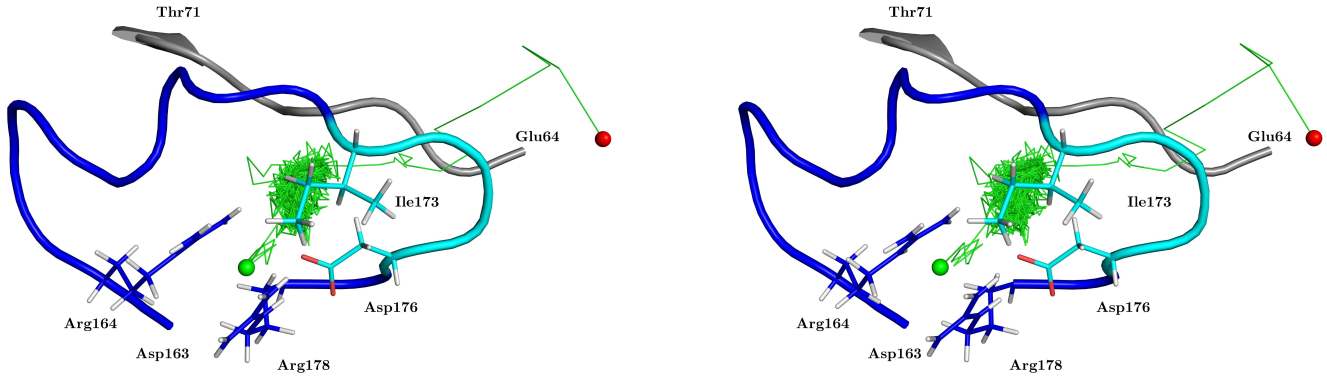

Figure S 10: Stereo view of the path of a water molecule entering the Ω-loop cavity (formed by the Ω-loop, dark blue, and the protein core, grey) at the flexible tip of the Ω-loop (cyan) and leaving the cavity through a dynamical formed opening. The beginning and end of the water path is marked as red and green sphere, respectively.

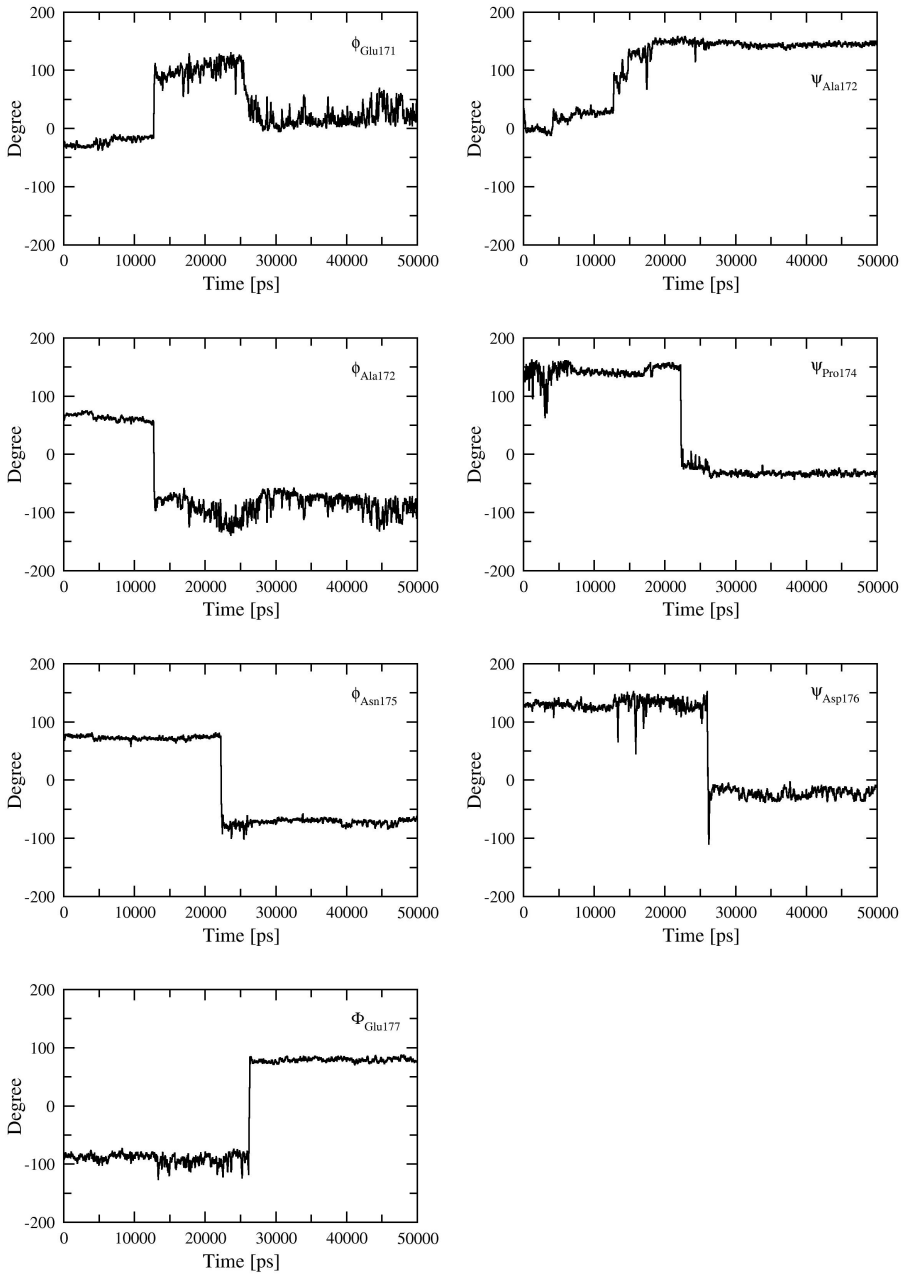

Figure S11: Backbone dihedral angles of those Ω-loop residues that showed changes correlated to the opening and closing movement.