

Description of Additional Supplementary Files

File Name: Supplementary Movie 1

Description: The movie shows rapid water movements around the Mn₄Ca-oxo complex and its ligand environment, including the water-wheel region, in the wild-type system. The visualization illustrates the high mobility of water on the picosecond timescale.

Technical details: The movie was prepared using a representative 10 ns segment (460–470 ns) of the MD trajectory from the wild-type system (monomer 1), sampled over 1000 frames. Trajectory smoothing (window size = 10) was applied to improve visual continuity. Frames were rendered in VMD5 and then compiled into a movie for visualization purposes.