

Description of Additional Supplementary Files

Supplementary Movie 1 | Representative O₂-trapping events. The video was created using MD simulation snapshots obtained from VMD program (one frame per 100 ps). A smoothing window size of 2 frames was applied to all atoms, and the video speed was set to 80 frames per second. The simulation time span for the video corresponds to 620–700 ns of simulation #1. In the video, MBP is shown as a yellow cartoon representation. The Trp residues are shown as van der Waals surface representation and colored blue. O₂ is also shown as van der Waals surface representation and colored red. For clear visualization of the O₂-trapping events, water molecules, chloride and potassium ions, and other O₂ molecules except for the trapped O₂, are not shown.

Supplementary Movie 2 | Representative maltose-binding events. The video was created using MD simulation snapshots obtained from VMD program (one frame per 1 ns). A smoothing window size of 2 frames was applied to all atoms, and the video speed was set to 25 frames per second. The simulation time span for the video corresponds to 2950–3150 ns of the simulation. In the video, MBP is shown as a yellow cartoon representation. The maltose-binding site is shown as transparent surface representation and colored blue. Maltose is shown as van der Waals surface representation and colored red. Chloride and potassium ions are shown as ball-and-stick representation. Water molecules are not shown for clear visualization of the maltose-binding events.