

Supporting Information

Mechanistic Insights into Glycosylation-Driven Structural Rearrangements in Human Aquaporin 1

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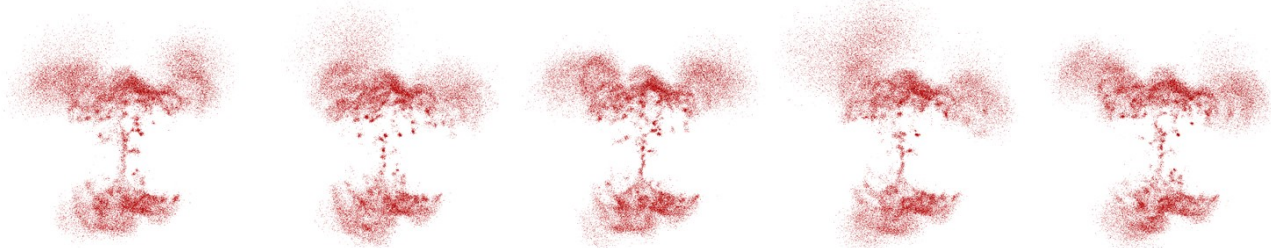
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+glycan



-glycan

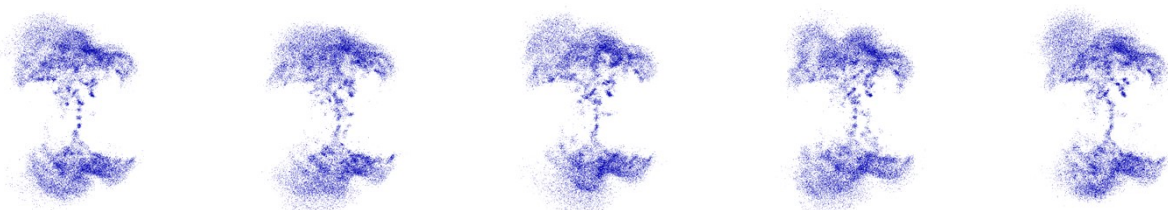
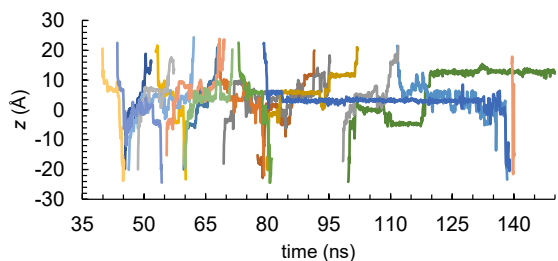
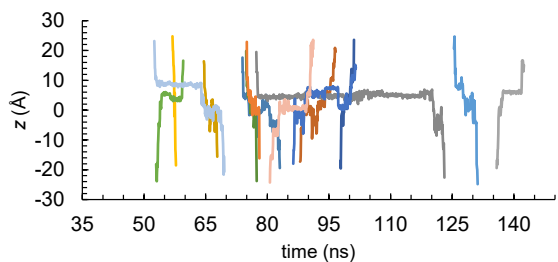
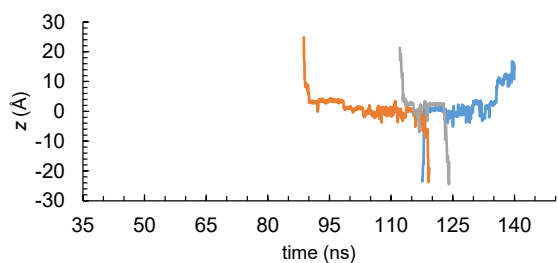
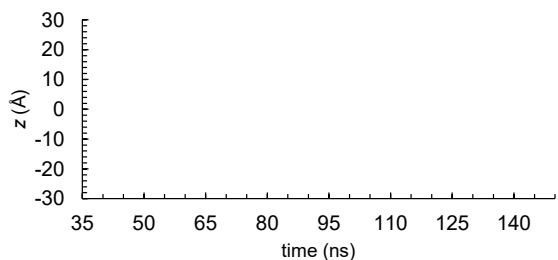
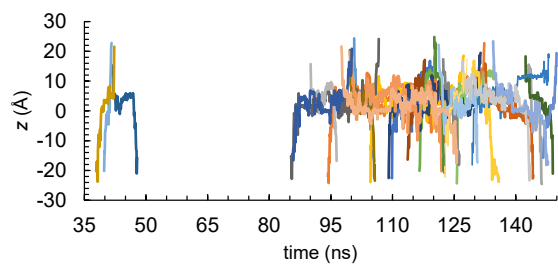


Figure S1. Water molecule distributions within 3.2 Å of the protein and glycan surfaces for each of the five individual MD trajectories. Each panel represents a separate MD trajectory. Top panels: glycosylated AQP1. Bottom panels: non-glycosylated AQP1. Red and blue dots represent accumulated positions of water molecules, respectively.

+glycan



-glycan

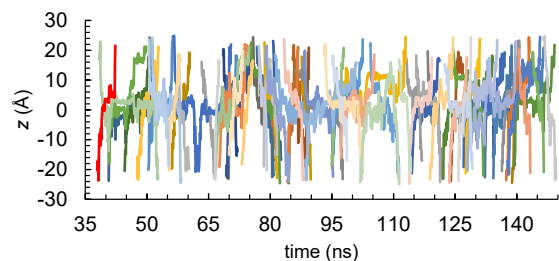
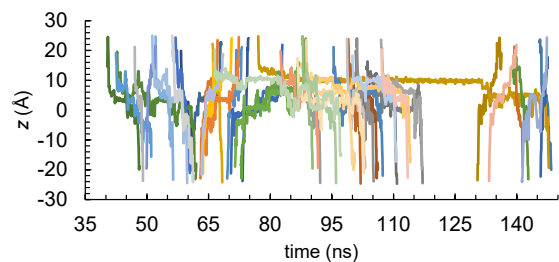
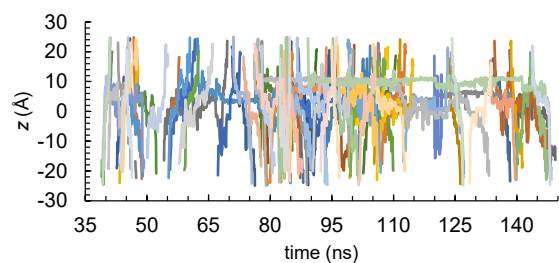
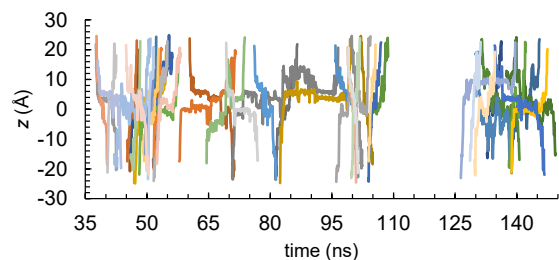
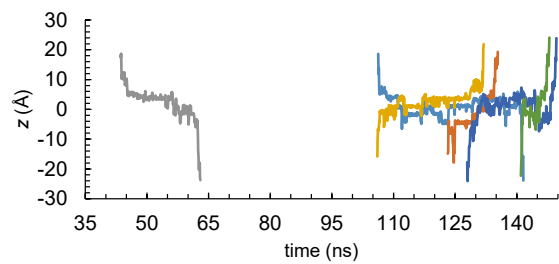
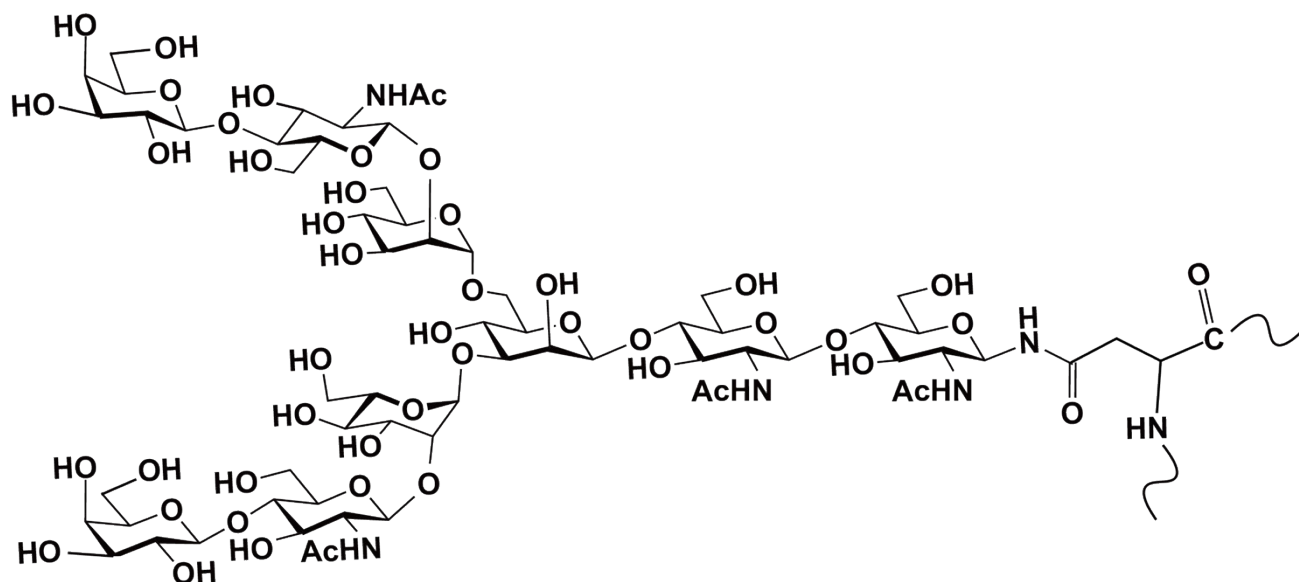


Figure S2. MD trajectories along the z -axis of oxygen atoms of water molecules that permeate the channel. Each panel represents a separate MD trajectory. Left panels: glycosylated AQP1. Right panels: non-glycosylated AQP1. Each line corresponds to the trajectory of an individual permeating water molecule.



Gal- β -1,4-GlcNAc- α -1,2-Man- α -1,6-
 Gal- β -1,4-GlcNAc- α -1,2-Man- α -1,3-
 Man- β -1,4-GlcNAc- β -1,4-GlcNAc- β -Asparagine

Gal: D-Galactoside; GlcNAc: N-acetyl-D-glucosamine; Man: D-Mannoside

Figure S3. Structure of the N-linked glycan modeled at Asn42 and Asn205 in AQP1.