

SUPPLEMENTARY ANIMATION FILE The movement of one of the sodium ions near the protein surface between $t=800\text{ps}$ and $t=1400\text{ps}$. Residues glu31, glu41 and his16 are presented on the protein scaffold (see also Figure 4A). At the first frame depicted in the movie, the ion is associated with glu95 (simulation MD_N, $t=700$). It then escapes the vicinity of glu95 and starts to diffuse in the bulk. During its diffusion, it is re-attracted by the negative Coloumb cage, and becomes detained by glu41 ($t=890$). The ion's encounter with glu41 is brief. After approximately 20ps , it diffuses away from glu41. Within less than 100ps , it becomes associated with his16, which is located under the negative Coloumb cage umbrella and hence can transiently detain the sodium ion. The ion is associated with his16 for $\sim 100\text{ps}$, before being released into the bulk and detained by glu41. Finally, the ion is driven into the bulk solvent, where it freely diffuses away from the protein surface.