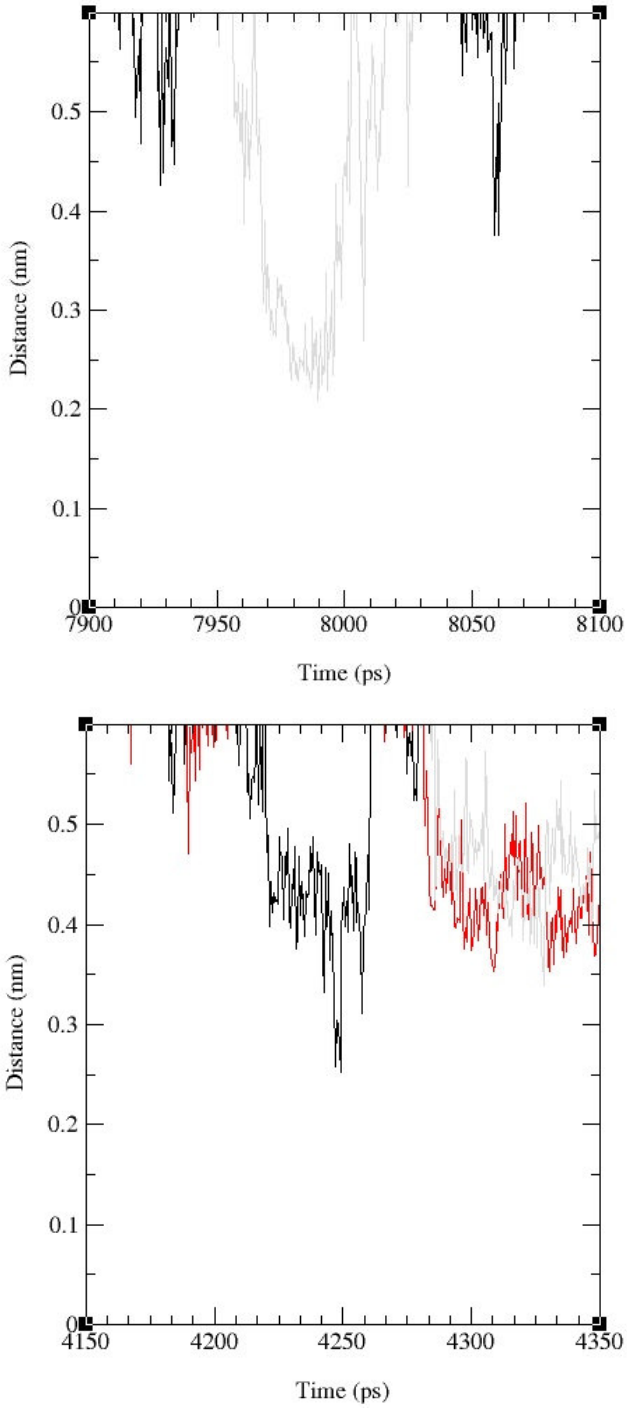
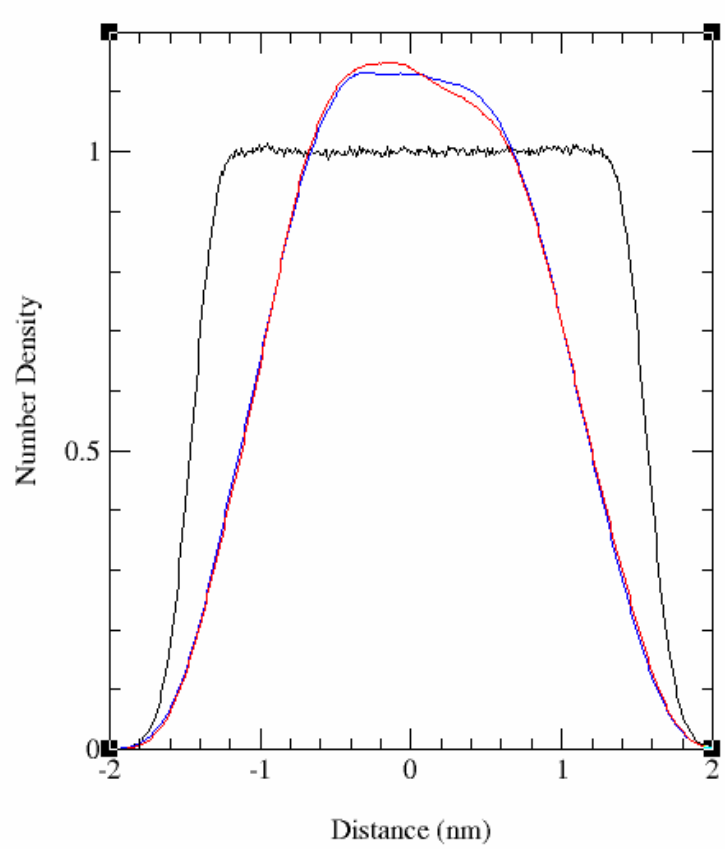


SUPPLEMENTARY FIGURE 1 **A**. The distance between one of the chloride ions and the hydrogen atoms attached to the guanido group of arg28 (black) or the amino group of arg36 (grey), as a function of the simulation time during the simulation MD_E22p. The ion rapidly moves from the vicinity of arg28 to the vicinity of arg36

and back. **B.** The distance between one of the sodium ions and the carboxylate oxygens of glu31 (black), glu38 (red) and glu66 (grey), during the simulation MD_S. The ion is detained by one or two of the negative residues during the presented time frame.



SUPPLEMENTARY FIGURE 2 Number densities of ions (Cl^- in red, Na^+ in blue) and water oxygen atoms (black) plotted versus distance from the center of the solution slab in the direction normal to the water-air interface as calculated over a 10ns simulation of 1.2M salt solution at the water-air interface. The ions are located near the center of the slab, in contrast to the results of Jungwirth and Tobias (Jungwirth and Tobias 2001; Jungwirth and Tobias 2002), in which the Cl^- ions were closer to the interface (see the Discussion in the main text). The number densities are normalized by a division of the values by bulk number densities. Values for Na^+ and Cl^- are averaged over slices of 100ps.

References

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