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Supporting Material

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Table S1. Summary of the protonation states of the extracellular tritratable residues

Standard state:	ASP32, ASP49, ASP115, ASP122, ASP136; GLU104
Protonated state:	ASP13, ASP31, ASP55, ASP86, ASP88, ASP91, ASP97, ASP145, ASP153, ASP154, ASP161, ASP178, ASP185; GLU14, GLU26, GLU35, GLU67, GLU69, GLU75, GLU82, GLU147, GLU163, GLU177, GLU181; HIS127

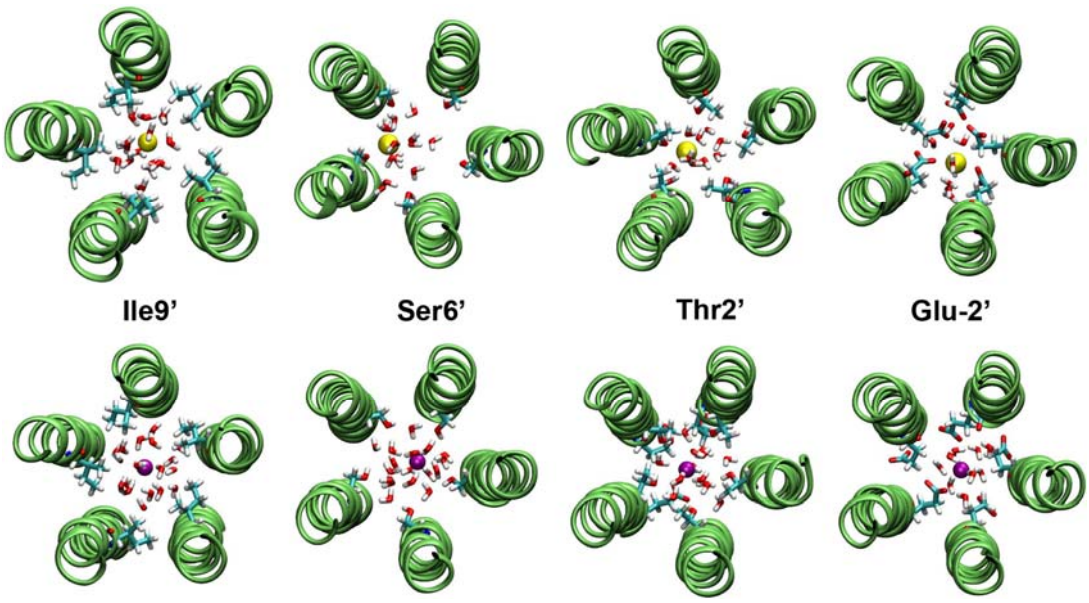

Figure S1 Trajectory snapshots depicting the translocation of a Na^+ ion (yellow, top panel) and a Cl^- ion (purple, bottom panel) at different positions along the pore of GLIC with the closest pore-lining residues labeled.

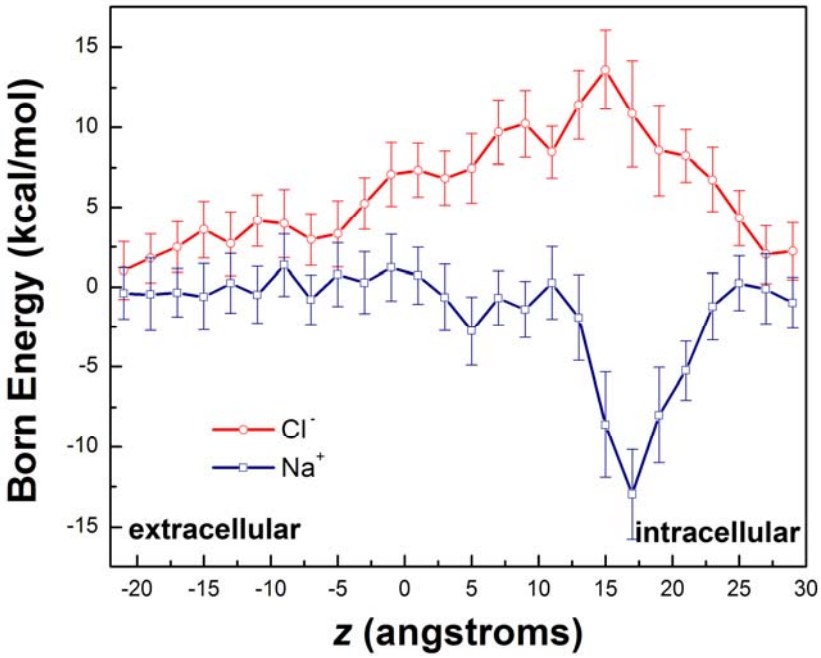

Figure S2 Born energy profiles for sodium (blue line) and chloride (red line) at different z positions along the channel axis. Born energy at each z position is averaged over 500 representative snapshots taken from each umbrella window. The errors are given by the standard deviations; refer to Methods section for details.

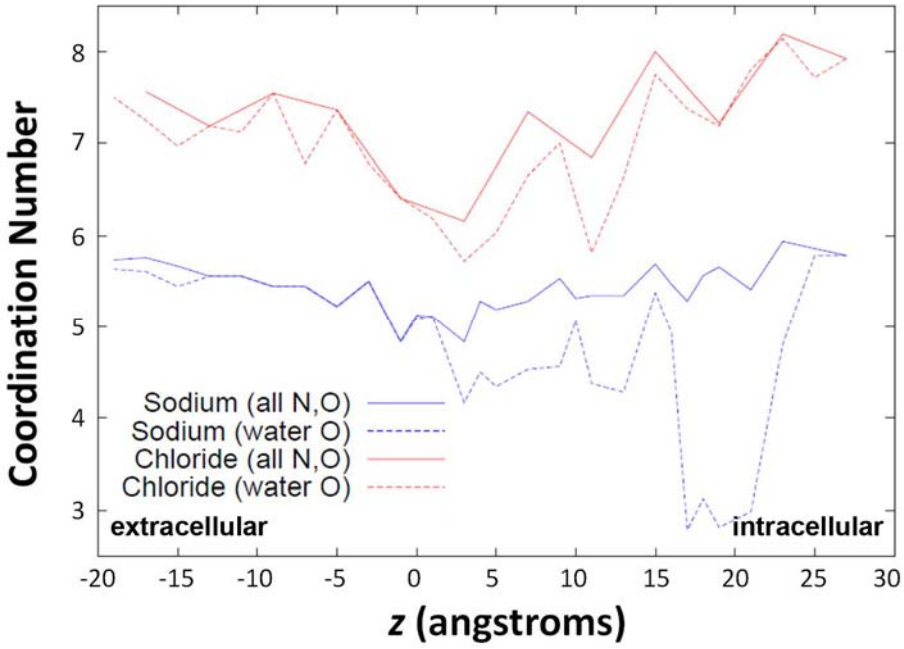

Figure S3 Coordination number of sodium (blue lines) and chloride (red lines) ions inside the GLIC channel, obtained by integrating the time-averaged RDFs (for individual umbrella windows) of water oxygen, protein nitrogen and oxygen atoms around the ion at their first minima r_m, where r_m = 3.3Å for sodium and r_m = 4.1Å for chloride. Average number of water molecules in the first solvation shell of sodium and chloride are also shown separately in dotted lines.

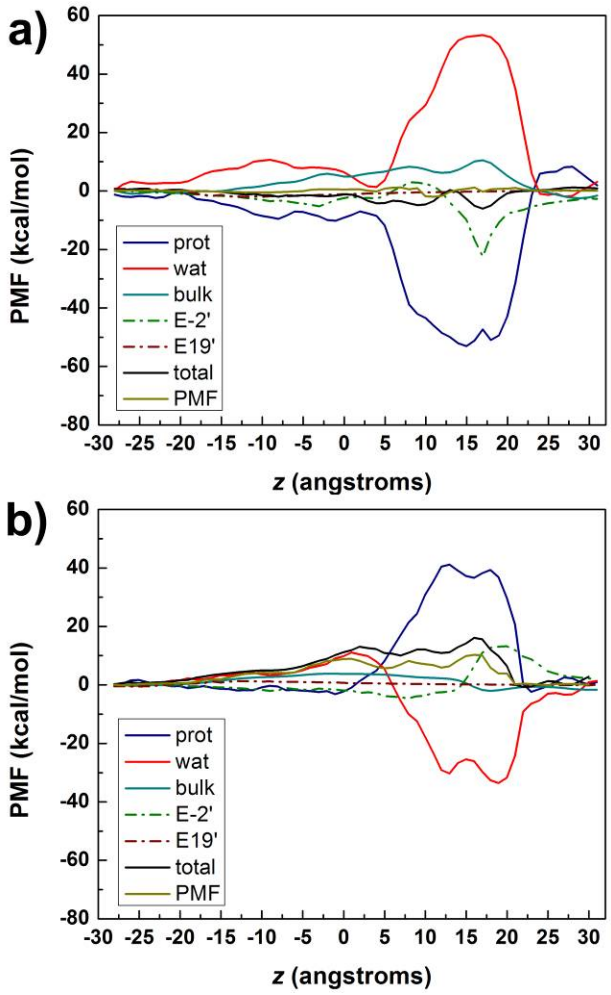

Figure S4 Mean force decomposition of the PMFs due to interactions of the ion with its first solvation shell (wat), the residues E-2' and E19', and the protein excluding E-2' and E19' (prot), and the remaining bulk solution and membrane (bulk) for (a) Na^+; (b) Cl^-. *Total* denotes the sum of all the contributions (black lines). *PMF* denotes the reference PMF calculated with the umbrella sampling method (dark yellow lines). For the sodium PMFs, the mean difference between the black and yellow lines is 1.7 kcal/mol, while the maximum difference is 6.2 kcal/mol. For the chloride PMFs, the mean difference is 2.3 kcal/mol, while the maximum difference is 5.9 kcal/mol. These differences give a low bound of the errors of the decomposition method.