SUPPLEMENTARY TABLE 1 The probability of finding the Cl^- ions in a detained state, in which an ion is located within 6Å of the terminal group hydrogens of the N-terminus, arginine or lysine, or the hydrogen from the OH group of tyr50, calculated over the simulation MD_N.

Residue	Probability	Detainment Energy (Kcal/mol)
Met1 (NT)	0.01	0.65
Arg 2	0.02	0.23
Arg 3	0.004	1.20
Arg 28	0.001	2.03
Lys 23	0.008	0.78
Arg 36	0.008	0.78
Lys 39	0.03	-0.02
Arg 46	0.01	0.65
Arg 47	0.03	-0.02
Tyr 50	**0.11**	**-0.84**
Lys 54	0.04	-0.20
Arg 71	0.007	0.86
Arg 80	**0.28**	**-1.53**
Arg 82	0.0006	2.34
Arg 86	0.02	0.23
Arg 87	**0.24**	**-1.41**
Lys 92	0.005	1.07

SUPPLEMENTARY TABLE 2 The probability of finding the Na^+ ions in a detained state, in which an ion is within 6Å of the carboxylate oxygens of the C-terminus, aspartate or glutamate and the unprotonated imidazole nitrogen of his16, calculated over the simulation MD_N.

Residue	Probability	Detainment Energy (Kcal/mol)
Glu 5	0.03	-0.02
Asp 15	0.06	-0.45
His 16	0.03	-0.02
Glu 22	0	-
Glu 24	0.004	1.20
Glu 31	0.07	-0.55
Glu 38	0.01	0.65
Glu 41	**0.08**	**-0.64**
Glu 42	0.005	1.07
Asp 55	0	-
Glu 66	0.005	1.07
Glu 69	0	-
Asp 70	0.003	1.37
Asp 74	0	-
Asp 78	0	-
Glu 83	0.01	0.65
Glu 95	**0.12**	**-0.90**
Phe 97 (CT)	**0.08**	**-0.64**

SUPPLEMENTARY TABLE 3 The probability of finding the Cl^- ions in a detained state, in which an ion is within 6Å of the terminal group hydrogens of the N-terminus, arginine or lysine, or the hydrogen from the OH group of tyr50 the calculated over the simulation MD_E22p.

Residue	Probability	Detainment Energy (kcal/mol)
Met1 (NT)	0.03	0.15
Arg 2	**0.09**	**-0.54**
Arg 3	0.02	0.40
Lys 23	0	-
Arg 28	0.05	-0.16
Arg 36	0.007	1.04
Lys 39	0.009	0.89
Arg 46	0.00005	3.99
Arg 47	0.01	0.82
Tyr 50	0.06	-0.28
Lys 54	0.08	-0.46
Arg 71	0.04	-0.02
Arg 80	**0.23**	**-1.20**
Arg 82	0.02	0.40
Arg 86	0.002	1.79
Arg 87	**0.11**	**-0.67**
Lys 92	0.06	-0.28

SUPPLEMENTARY TABLE 4 The probability of finding the Na^+ ions in a detained state, in which an ion is located within 6Å of the carboxylate oxygens of the C-terminus, aspartate or glutamate and the unprotonated imidazole nitrogen of his16, calculated over the simulation MD_E22p.

Residue	Probability	Detainment Energy (kcal/mol)
Glu 5	0	-
Asp 15	0.008	0.78
His 16	0.0006	2.34
Glu 24	0	-
Glu 31	0.006	0.96
Glu 38	0.02	0.23
Glu 41	**0.11**	**-0.85**
Glu 42	0.02	0.23
Asp 55	0.006	0.96
Glu 66	0.02	0.23
Glu 69	0	-
Asp 70	0.02	0.23
Asp 74	0.03	-0.02
Asp 78	0.006	0.96
Glu 83	0.02	0.23
Glu 95	0.02	0.23
Phe 97 (CT)	**0.11**	**-0.85**

SUPPLEMENTARY TABLE 5 The probability of finding the Cl^- ions in a detained state, in which an ion is located within 5Å of the terminal group hydrogens of the N-terminus, arginine or lysine, or the hydrogen from the OH group of tyr50, calculated over the simulation MD_S.

Residue	Probability	Binding Energy (kCal/mol)
Met1	0.003	2.20
Arg 2	0.02	1.06
Arg 3	0.007	1.69
Lys23	0.002	2.44
Arg 28	0.02	1.06
Arg 36	0.02	1.06
Lys39	0.0001	4.23
Arg46	0.03	0.81
Arg47	0.03	0.81
Tyr 50	0.02	1.06
Lys 54	0.03	0.81
Arg 71	0.007	1.69
Arg77	0.03	0.81
Arg 80	0.12	-0.08
Arg82	0.01	1.48
Arg86	0.02	1.06
Arg 87	0.14	-0.18
Lys 92	0.01	1.48

SUPPLEMENTARY TABLE 6 The probability of finding the Na^+ ions in a detained state, in which an ion is located within 5Å of the carboxylate oxygens of the C-terminus, aspartate or glutamate and the unprotonated imidazole nitrogen of his16, calculated over the simulation MD_S.

Residue	Probability	Detainment Energy (Kcal/mol)
Glu 5	0.002	2.44
Asp 15	0.04	0.63
His 16	0.01	1.78
Glu 22	0.01	1.48
Glu 24	0.06	0.38
Glu 31	0.03	0.81
Glu 38	0.007	1.69
Glu 41	0.10	0.05
Glu 42	0.01	1.48
Asp 55	0.01	1.48
Glu 66	0.0004	3.40
Glu 69	0.00	-
Asp 70	0.0007	3.07
Asp 74	0.01	1.48
Asp 78	0.02	1.06
Glu 83	0.02	1.06
Glu 95	0.08	0.19
Phe 97 (CT)	0.02	1.06

SUPPLEMENTARY TABLE 7 Comparison of simulation and experimental results for the increase in surface tension in simulations of 1.2M NaCl solutions relative to water. The results are given in mN/m.

Friedman *et al.* [*]	Jungwirth and Tobias [#]	Experiment [|]
4.1	3.4	2.0

[*] The simulation was carried out with the same software and force field as reported in the main text. A slab of 864 water molecules, 18 Na^+ ions and 18 Cl^- ions was placed into a box of 3nm·3nm·10nm, as in (Jungwirth and Tobias 2001). The system was heated to 250K in 50K step during 100ps, and was then equilibrated for 500ps in 300K before running the data collection (production) stage of 10ns.

[#] (Jungwirth and Tobias 2001)

[|] (Washburn 1928)

References

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