Insights into the ion-coupling mechanism in the MATE transporter NorM-VC

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Published in:
Physical Biology

DOI:
10.1088/1478-3975/aa5ee7

Publication date:
2017

Document Version
Peer reviewed version

Supporting Information

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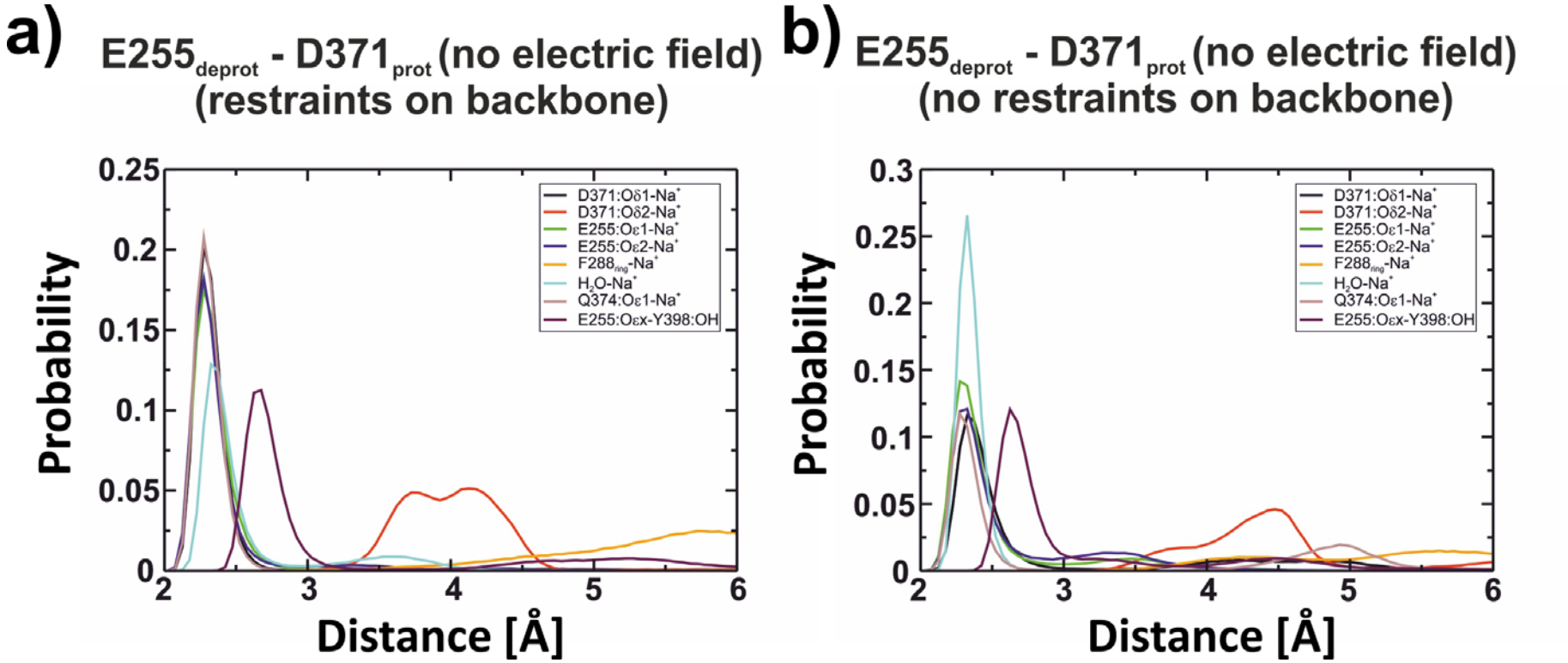

Figure S1: a) Distribution of ion binding distances in the state $E255_{deprot}/D371_{prot}$ using 10 kJ/(mol*nm^2) backbone restraints. b) Distance distributions within the binding site in an unrestrained simulation. In both simulations no electric field was applied.

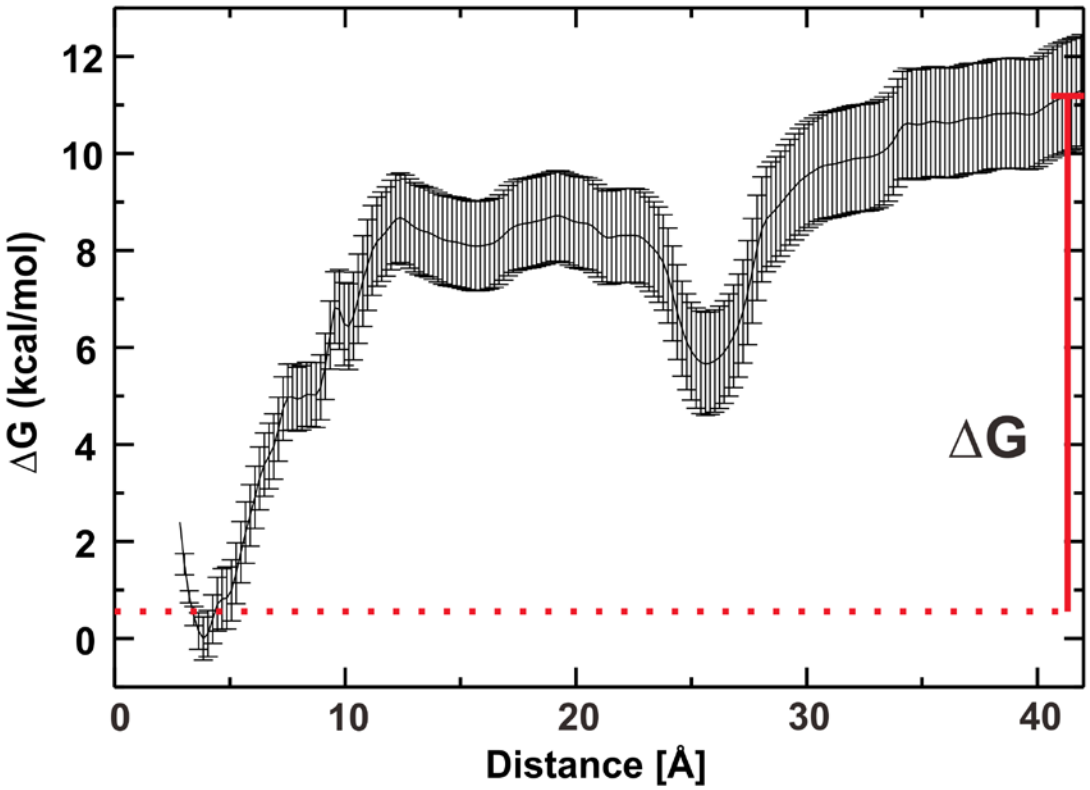

Figure S2: Potential of Mean Force (PMF) of Na^+ ion translocation from the binding site to the bulk solution in the $E255_{prot}/D371_{deprot}$ state. The free energy difference is 11.2+/- 1.0 kcal/mol. This free energy difference is not in good agreement with experimental data (5.6 kcal/mol).