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

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## Supporting Information

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

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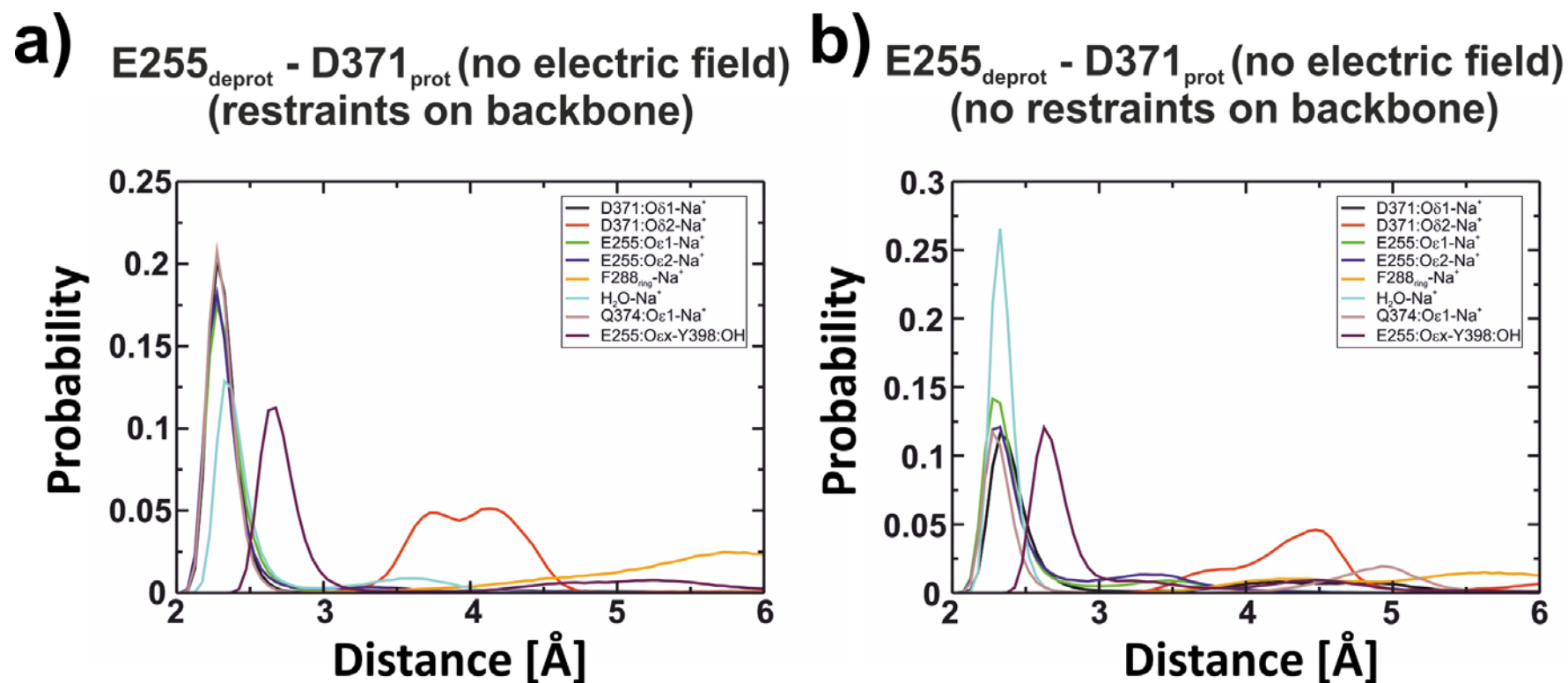


Figure S1: a) Distribution of ion binding distances in the state E255<sub>deprot</sub>/D371<sub>prot</sub> using 10 kJ/(mol\*nm<sup>2</sup>) backbone restraints. b) Distance distributions within the binding site in an unrestrained simulation. In both simulations no electric field was applied.

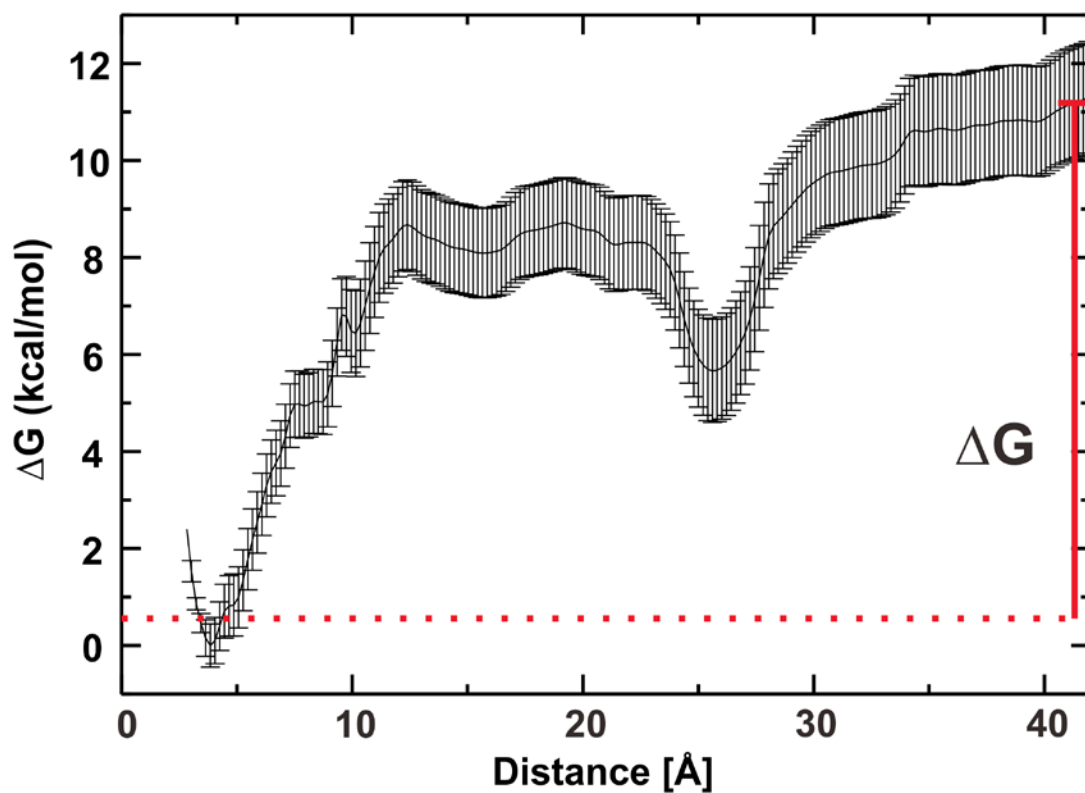


Figure S2: Potential of Mean Force (PMF) of Na<sup>+</sup> ion translocation from the binding site to the bulk solution in the E255<sub>prot</sub>/D371<sub>deprot</sub> state. The free energy difference is 11.2 $\pm$  1.0 kcal/mol. This free energy difference is not in good agreement with experimental data (5.6 kcal/mol).