Biomolecular Solvation Structure Revealed by Molecular Dynamics Simulations

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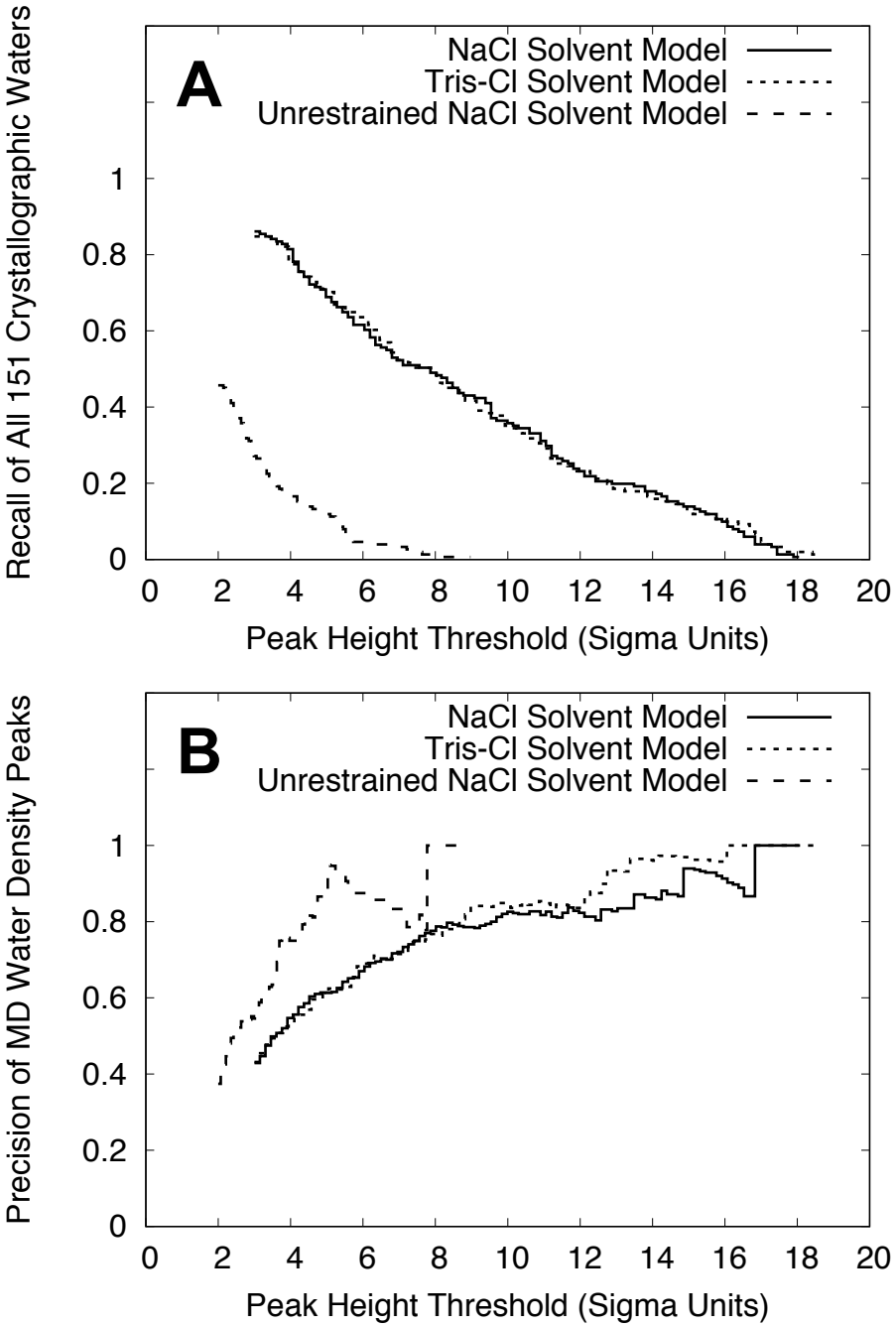

Supporting Figure S1. Dependence of recall and precision on MD water density peak height threshold. (A) Recall. (B) Precision. Statistics were computed using all 151 crystallographic waters, using a cutoff distance of 1.0 Å. Results for the restrained NaCl and Tris-Cl models were obtained using the last 10 ns of the trajectories. Results for the unrestrained NCl model were obtained using the first 100 ns of the trajectory.