

Supplementary information: assessing the performance of implicit solvation models at a nucleic acid surface

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To assess the sensitivity of our results to the discretization used in our solution of the Poisson equation, we recalculated solvation forces and solvent polarization at several different grid dimensions. In particular, polar solvation forces were obtained from solutions of the Poisson equation calculated on grids of fixed length using 97^3 , 129^3 , 161^3 , 193^3 , 225^3 , 257^3 , 289^3 , and 321^3 resulting in isotropic grid spacings of approximately 0.69, 0.52, 0.42, 0.35, 0.30, 0.26, 0.23, and 0.21 Å, respectively. Solvent polarization values were obtained from solutions of the Poisson equation calculated on grids of fixed length using 97^3 , 129^3 , 161^3 , 193^3 , and 225^3 resulting in isotropic grid spacings of approximately 0.69, 0.52, 0.42, 0.35, and 0.30 Å, respectively. The regression coefficient of the explicit-implicit force and polarization correlation changed very little ($\sim 1\%$) over these sets of grid dimensions. However, the Pearson correlation coefficient showed a somewhat larger change, as illustrated in Fig. S1. Note that both quantities are well converged at the 0.3 Å grid resolution used in this study.

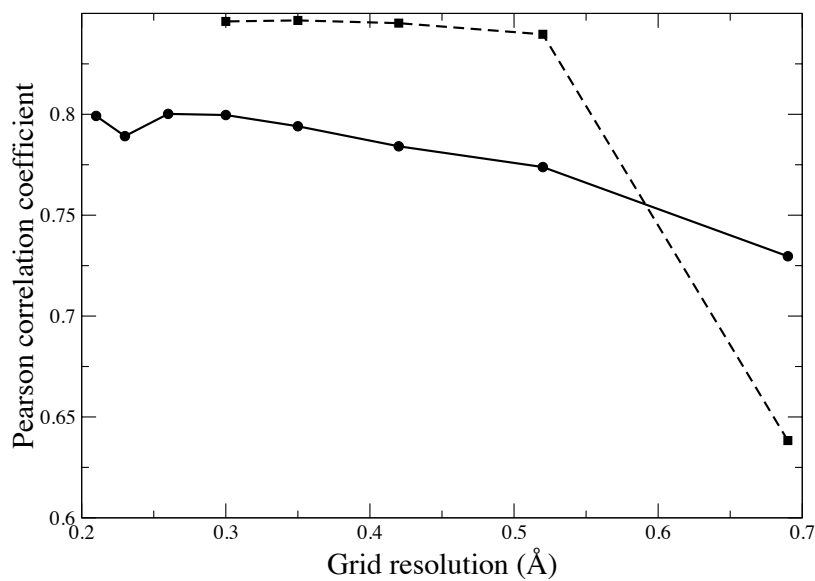


Figure S1: Sensitivity of the Pearson correlation coefficient for explicit-implicit polar solvation comparisons to Poisson equation domain discretization. The solid line depicts the correlation of polar solvation forces while the dotted line depicts correlation of solvent polarization.