Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

A fast-slow method to treat solute dynamics in explicit solvent

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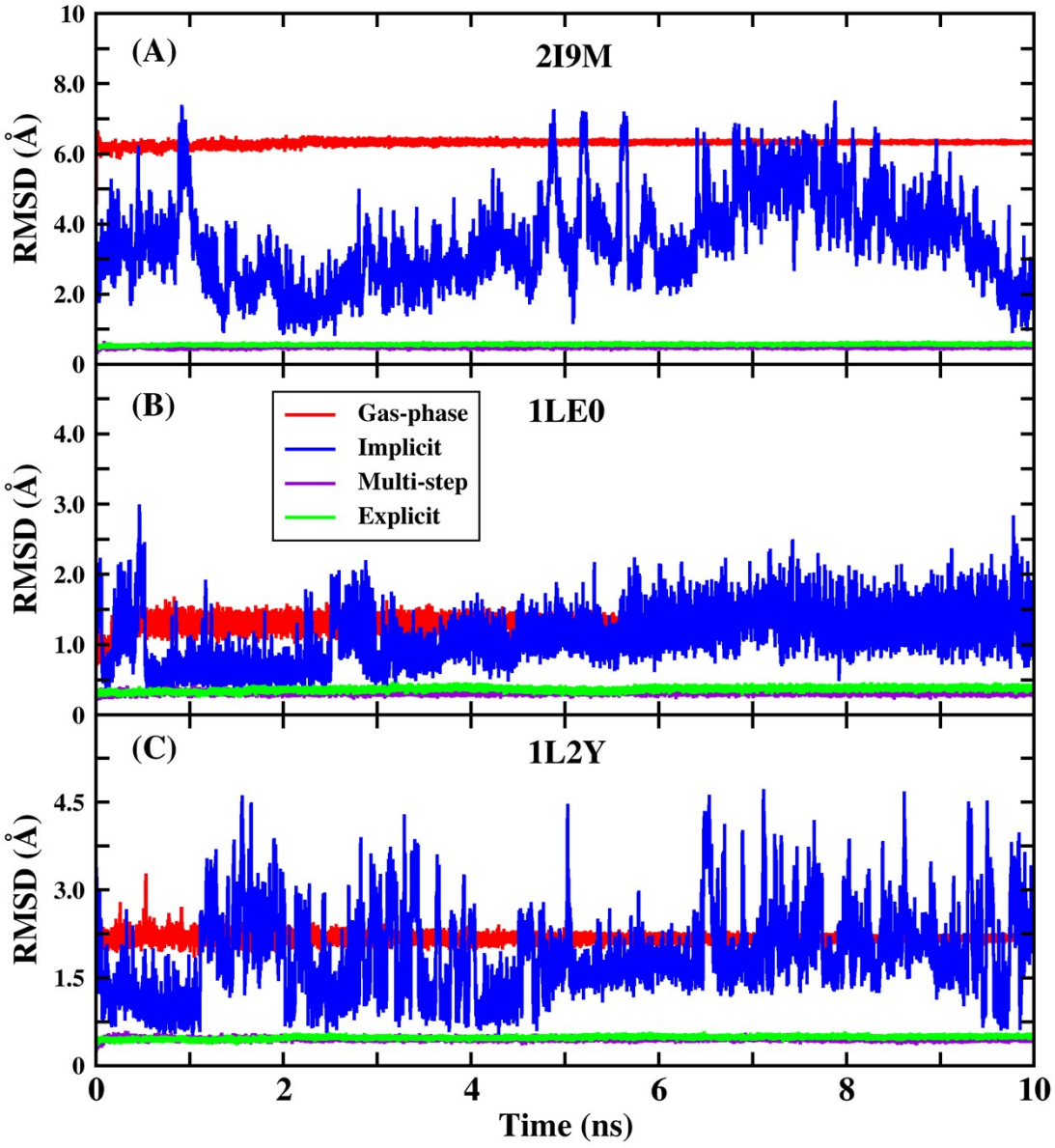

Figure S1. RMSD of protein backbone atoms based on the second simulated trajectory relative to the initial NMR structure as a function of time.

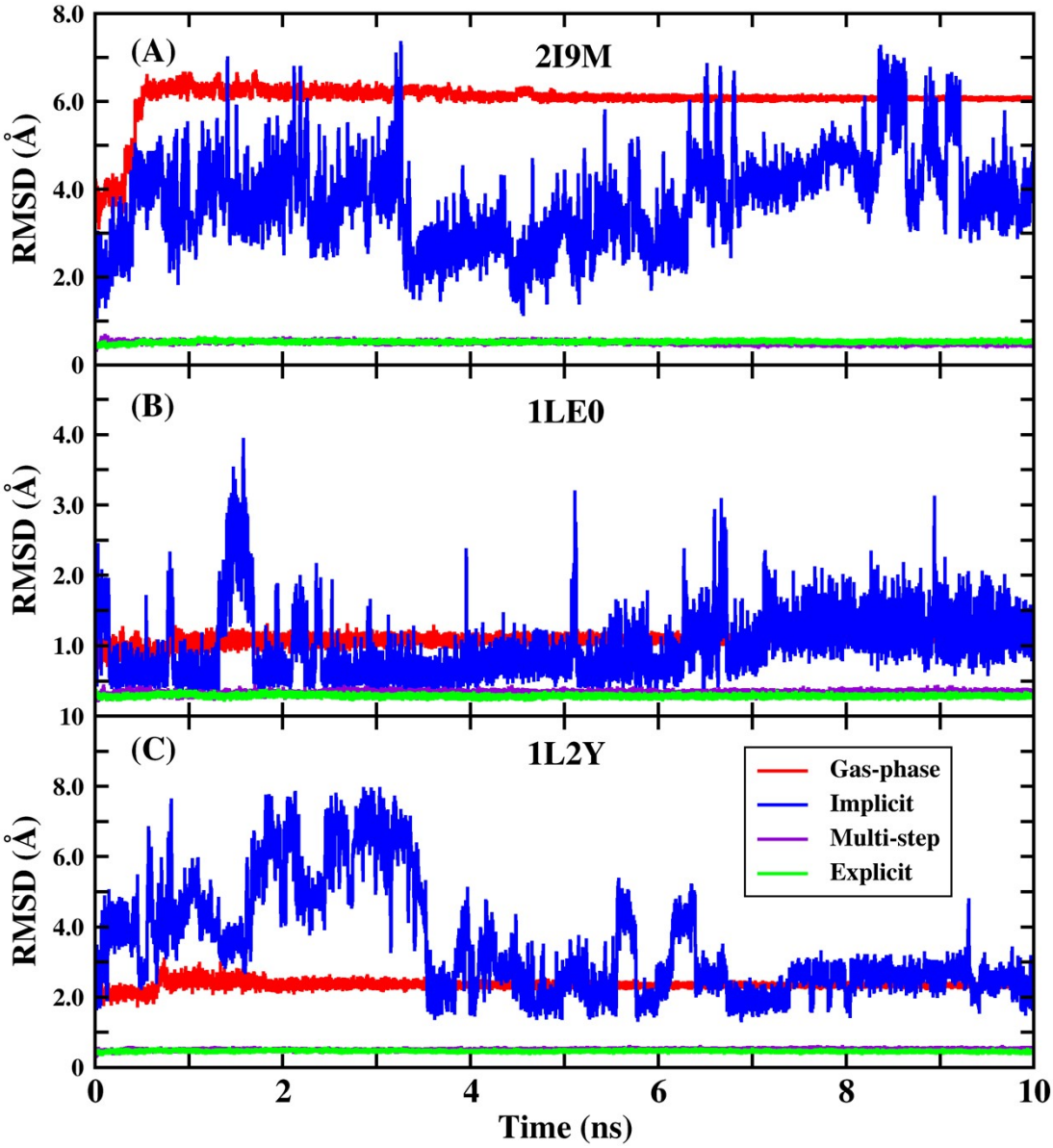

Figure S2. RMSD of protein backbone atoms based on the third simulated trajectory relative to the initial NMR structure as a function of time.

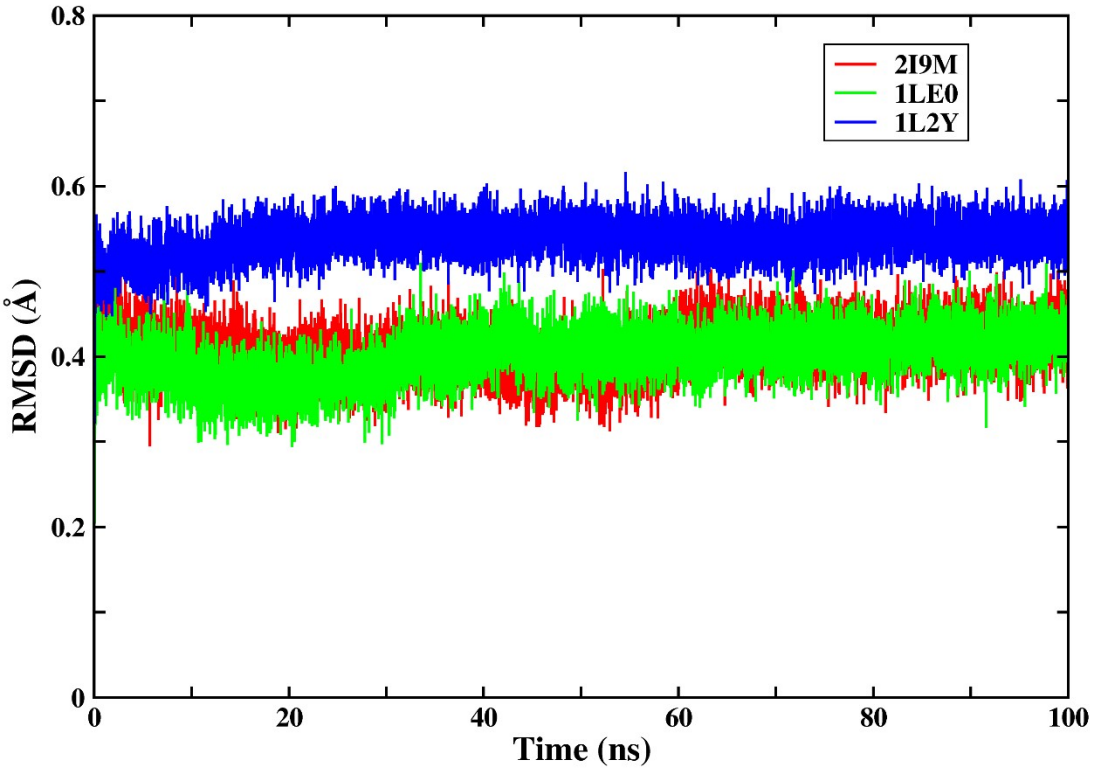

Figure S3. RMSD of protein backbone atoms based on the 100-ns long-term simulation relative to the initial NMR structure as a function of time.

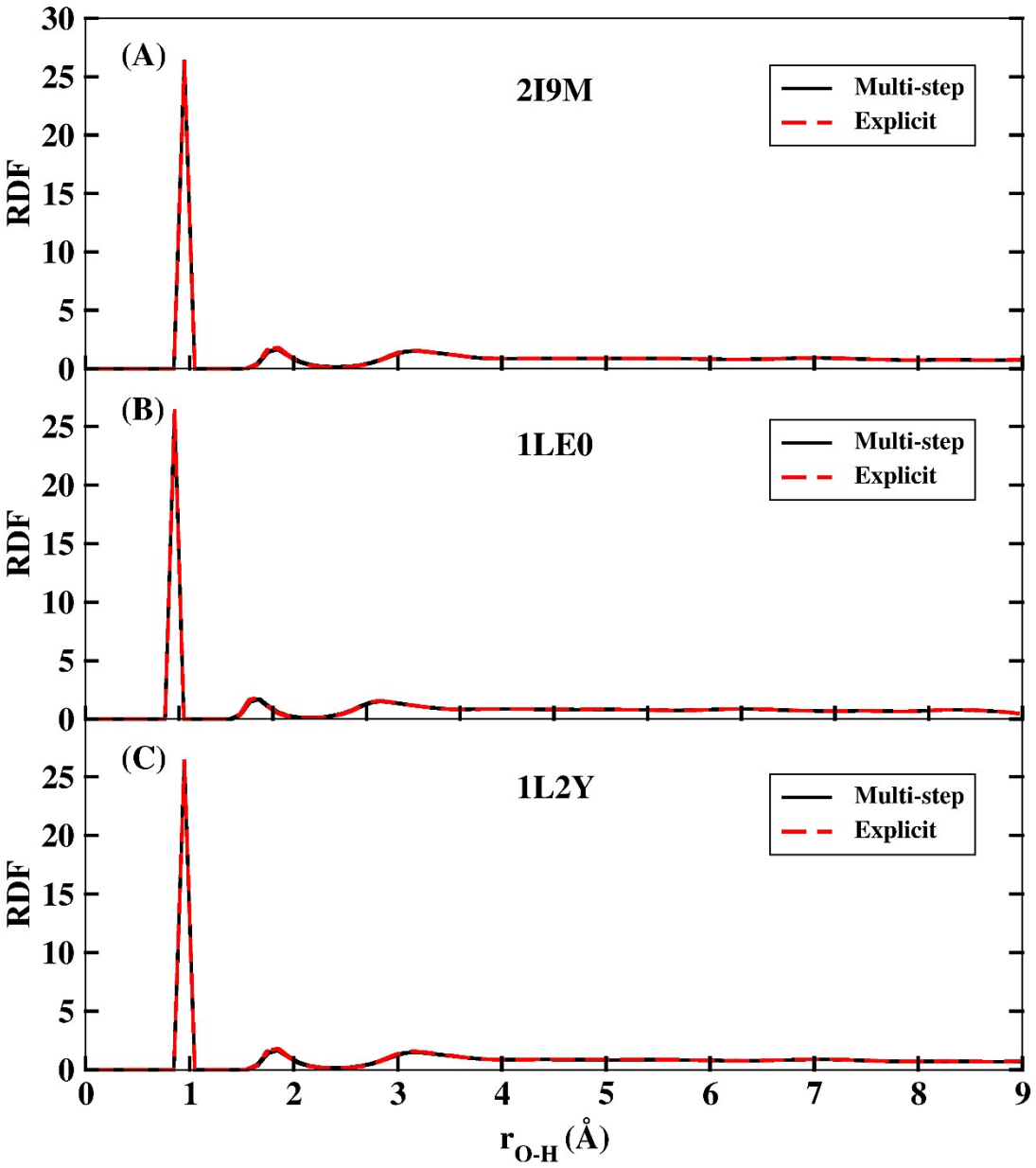

Figure S4. The radial distribution function (RDF) between oxygen and hydrogen atoms (O-H) of water in the multi-step explicit solvent and standard explicit solvent.

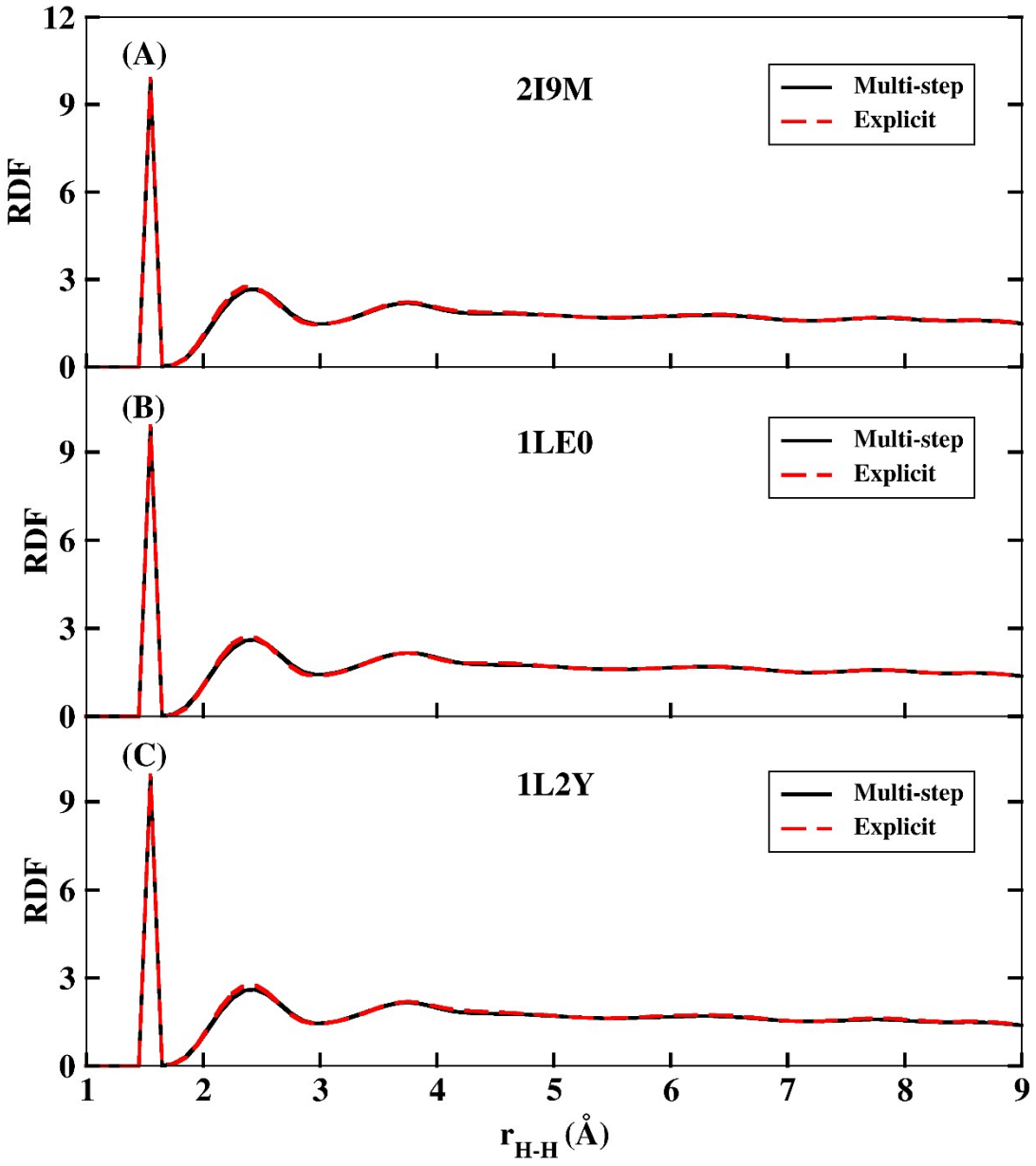

Figure S5. The radial distribution function (RDF) between hydrogen atoms (H-H) of water in the multi-step explicit solvent and standard explicit solvent.

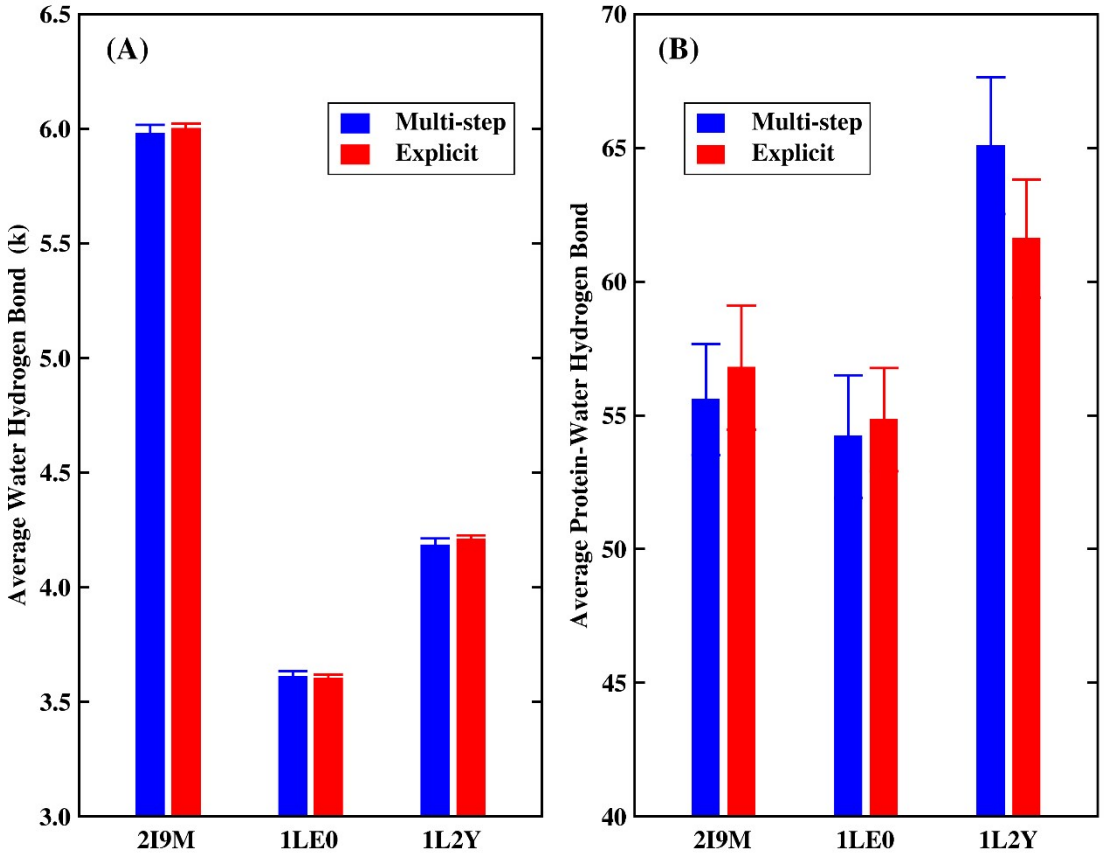

Figure S6. The average and standard deviation (STD) of hydrogen bond number. (A) water hydrogen bond; (B) protein-water hydrogen bond.