Supporting Information for the manuscript:

# Transferable Mixing Of Atomistic And Coarse-Grain Water Models

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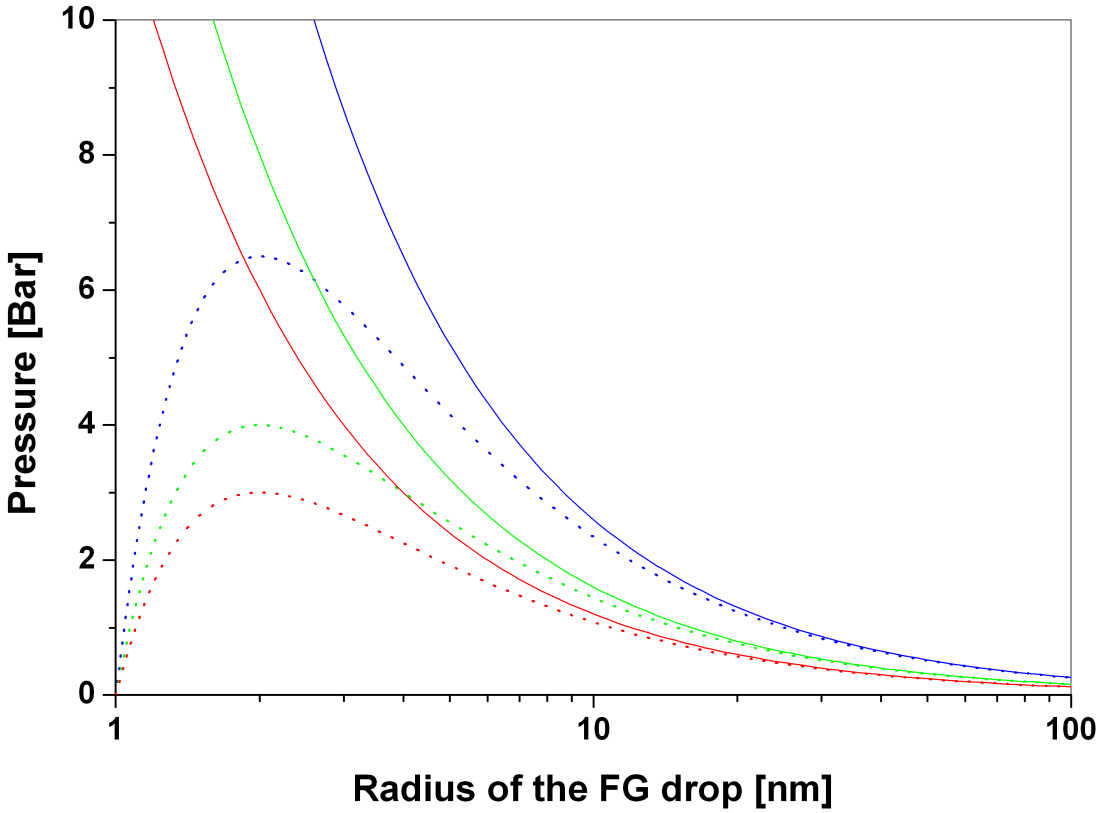


**Figure SI 1**. Variation of the pressure within the FG drop induced by the hybrid interface. Dotted lines correspond to the pressure calculated taking into account a variation of the interface tension as function of the radius of the FG droplet taking a Tolman length of 1 nm. The continuous line corresponds to the standard Young-Laplace equation (see main text). Red, Green and Blue colors indicate the TIP3P, SPC and SPC/E, respectively.

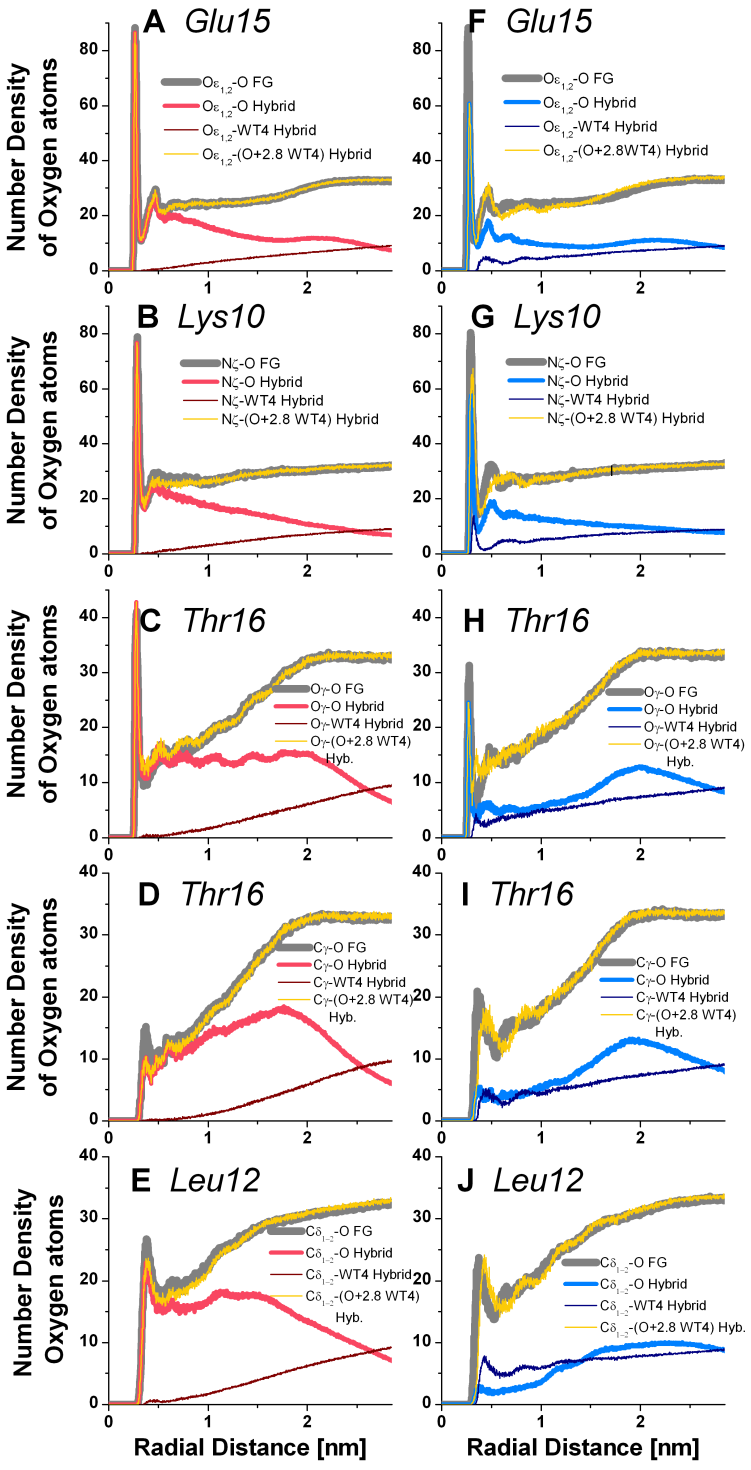


**Figure SI 2**. Solvation structure around FG amino acids calculated along the trajectories of systems 22 to 25 (using the v-rescale thermostat and Parrinello-Rahman barostat, see main text). A to F) Number densities of Oxygen atoms around representative residues using AMBER-TIP3P. G to K) Same as B to F using GROMOS-SPC/E.

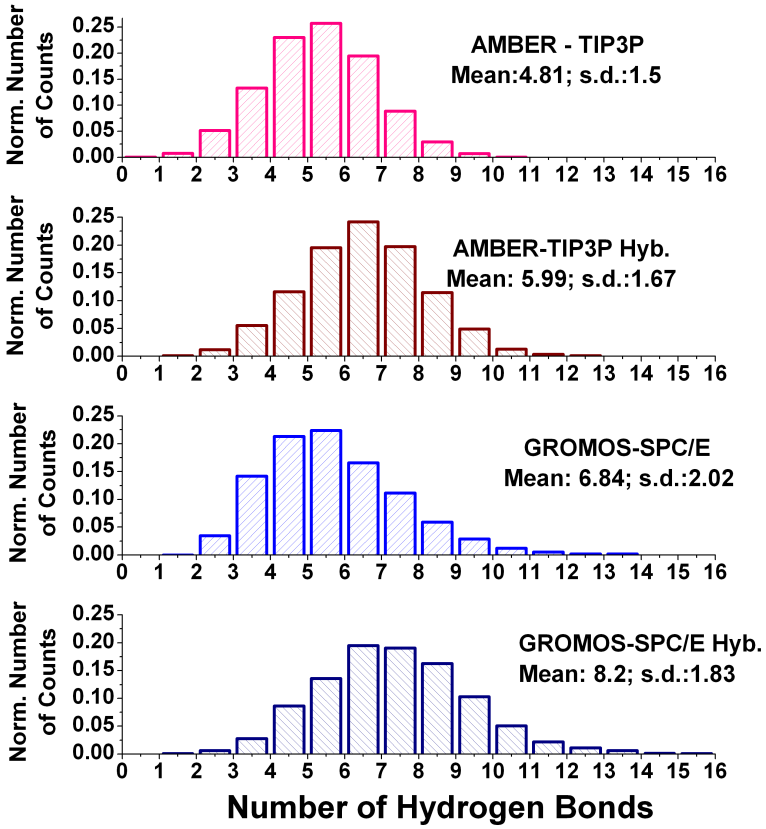


**Figure SI 3.** Inter side chain Hydrogen bonds calculated along the trajectories of systems 22 to 25 (using the v-rescale thermostat and Parrinello-Rahman barostat, see main text). Distribution of the normalized number of Hydrogen bonds for FG (light red or blue) and hybrid (dark red or blue) simulations for AMBER-TIP3P (top) and GROMOS-SPC/E (bottom). Mean values and standard deviation of each distribution are reported on the corresponding panels.

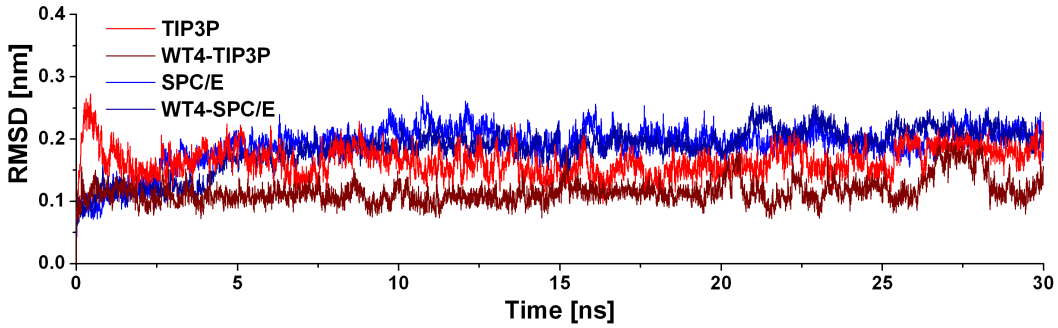


**Figure SI4**. Structural comparison of simulations with different force fields and solvation approaches, using the V-rescale thermostat and Parrinello-Rahman barostat (systems 22 to 25 in Table 1, main text). The instantaneous RMSD are calculated on the Cα carbons. Light and dark colors indicate FG and hybrid solvation schemes, respectively.

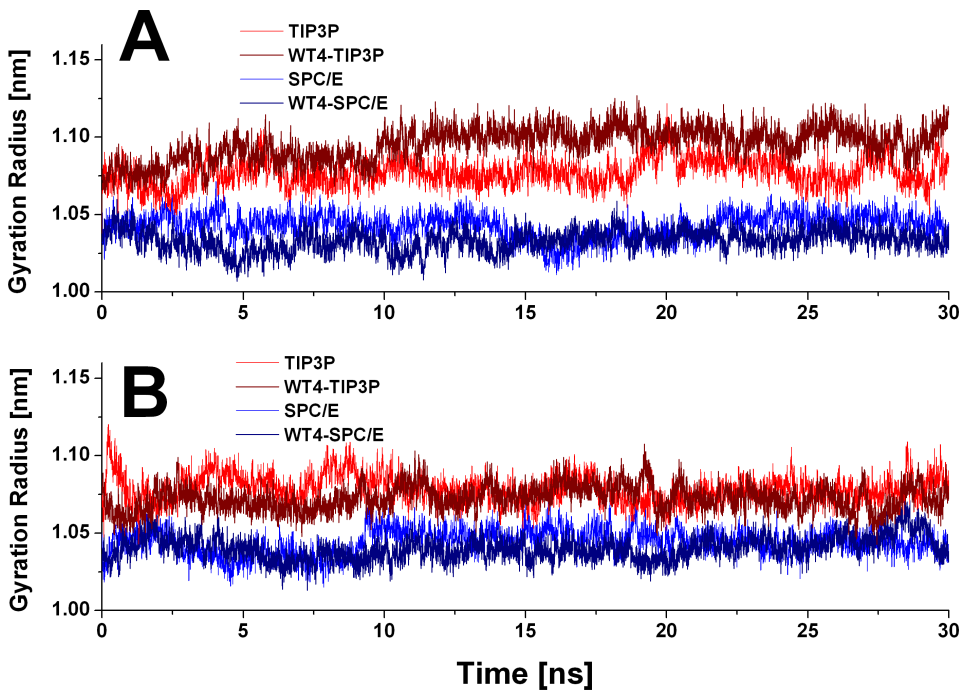


**Figure SI 5.** Gyration radii along MD trajectories of β1 domain of the streptococcal protein G (PDB id: 1FCL). A) Simulations performed using the Berendsen's thermostat and barostats (systems 16 to 19 in Table 1, main text). B) Idem to A for simulations performed using the V-rescale and Parrinello-Rahman thermostat and barostats, respectively (systems 22 to 25 in Table 1, main text).

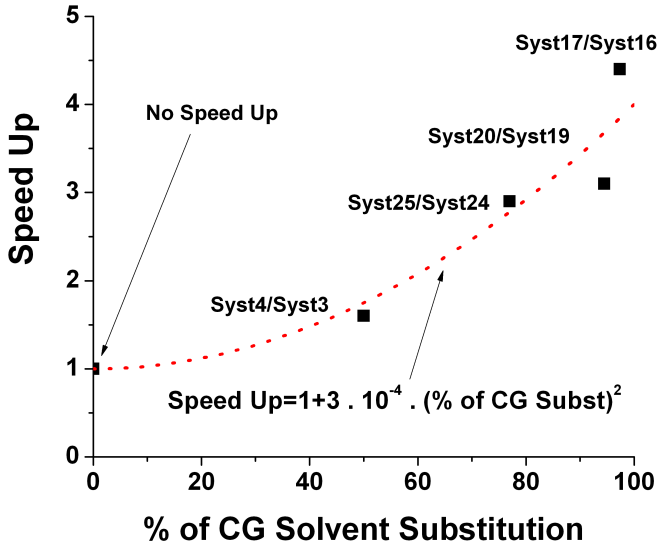


**Figure SI 6.** Speed up as a function of the percent of substitution of FG water by CG molecules. The speed up is calculated as the ratio between the wall-time needed to perform the simulations of the systems indicated. The quadratic function shown in the figure fits the data with a R value of 0.95.