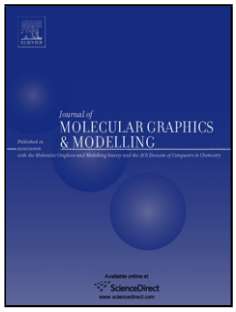

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Effect of solvent model when probing protein dynamics with molecular dynamics

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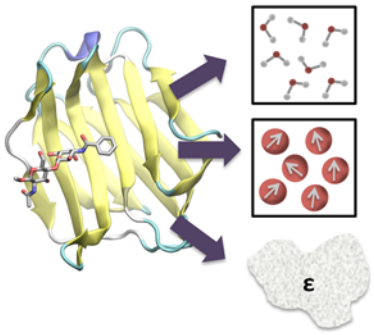
Graphical abstract



Highlights

- Three solvent model at different resolution were compared on protein dynamics
- The three solvent model have different inherent time scales
- All solvent models reproduce, on average, the NMR observables equally well
- Deviations for side-chains are significantly larger than the deviation for the backbone

Abstract

We probe the dynamics of the Bpti and Galectin-3 proteins using molecular dynamics simulations employing three water models at different levels of resolution, viz. the atomistic TIP4P-Ewald, the coarse-grained Elba and an implicit generalised Born model. The dynamics are quantified indirectly by model-free order parameters, S^2 of the backbone N–H and selected side-chain bond vectors, which also have been determined experimentally through NMR relaxation measurements. For the backbone, the order parameters produced with the three solvent models agree to a large extent with experiments, giving average unsigned deviations between 0.03 and 0.06. For the side-chains, for which the experimental data is incomplete, the deviations are considerably larger with mean deviations between 0.13 and 0.17. However, for both backbone and side-chains, it is difficult to pick a winner, as all models perform equally well overall. For a more complete set of side-chain vectors, we resort to analysing the variation among the estimates from different solvent models. Unfortunately, the variations are found to be sizeable with mean deviations between 0.11 and 0.15. Implications for computational assessment of protein dynamics are discussed.