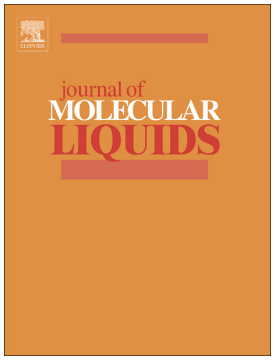

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Characterization of the Supramolecular Assembly in 1,4-Butandiol

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Experimental small- and wide-angle X-ray scattering (SWAXS) data, molecular dynamics simulations, and the complemented-system approach for the calculation of the SWAXS intensities from simulation data were used to study the hydrogen-bonded supramolecular assemblies formed in liquid 1,4-butandiol and to check the structural performance of the well-established force-field models TraPPE-UA, GROMOS96-54a7, CHARMM27, OPLS-AA, and AMBER03 for this diol. We found that all the models were able to reproduce the main scattering peak in the experimental SWAXS curve, though the all-atom models, rather surprisingly, failed to convincingly interpret its scattering shoulder stretching towards smaller values of the scattering vector. The united-atom TraPPE-UA force field showed the best performance in terms of the position of the peak and the absolute values of the scattering intensity. Therefore, its results were further analysed to reveal the various contributions to the total scattering intensity and to visualize the obtained typical molecular conformations and other supramolecular structural details in 1,4-butandiol, reaching up to the colloidal scale. Thus, the importance of the presented results is two-fold. First, they reveal the details of the molecular structure in a model diol that is, due to an additional –OH group per alcohol molecule, rather different in comparison to typical simple alcohols, and second, they nicely illustrate the importance of a careful structural consideration and the necessity for an