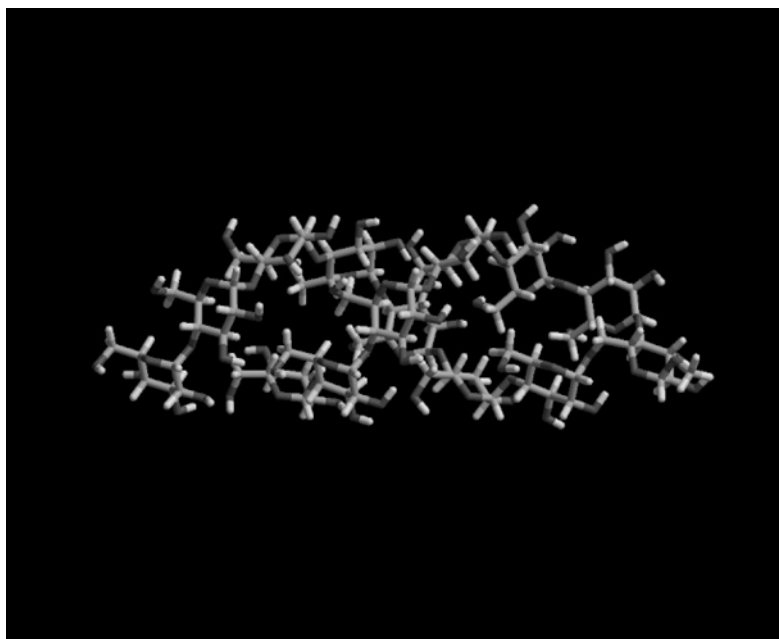


## HYDRATION OF THE DOUBLE HELICAL SEGMENT OF AMYLOPECTIN

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As a continuation of previous investigations of starch structural motifs, including the starch branch point[1], a model of the double helical segment of amylopectin consisting of 14 glucose units has been synthesized (see figure). The hydration of this miniature double helical segment has been thoroughly investigated by molecular dynamics simulations in explicit water, starting from a structure in agreement with crystallographic data [2]. Analysis of solute-water interactions shows the importance of water as a stabilizer of the double helical structure. Moreover, the analyses indicate that the double helical motif has significant flexibility in terms of overall bending.



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