Structure and Hydration of Bam HI DNA recognition site: a molecular dynamics investigation

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The results of a 3 ns molecular dynamics simulation of the dodecamer duplex d(TATGGATCCATA)2 recognised by the Bam HI endonuclease are here presented. The DNA has been simulated as a flexible molecule using AMBER force field and the Ewald summation method which eliminates the undesired effects of truncation and permits to evaluate the full effects of electrostatic forces. The starting B conformation evolves toward a configuration quite close to that observed through X-ray diffraction in its complex with Bam HI. This configuration is fairly stable and the Watson-Crick hydrogen bonds are well maintained over the simulation trajectory. Hydration analysis indicates a preferential hydration for the phosphate than for the ester oxygens. Hydration shells in both the major and minor groove were observed. In both grooves the C-G pairs were found to be more hydrated than A-T pairs. The "spine of hydration" in the minor groove was clear. Water residence time are longer in the minor groove than in the major groove, although relatively short in both cases. No special long values are observed for sites where water molecules were observed by X-ray diffraction indicating that water molecules having an high probability to be located in a specific site are also fast exchanging.