Supplementary Material

Molecular simulation of conformational transitions in biomolecules using a combination of structure-based potential and empirical valence bond theory

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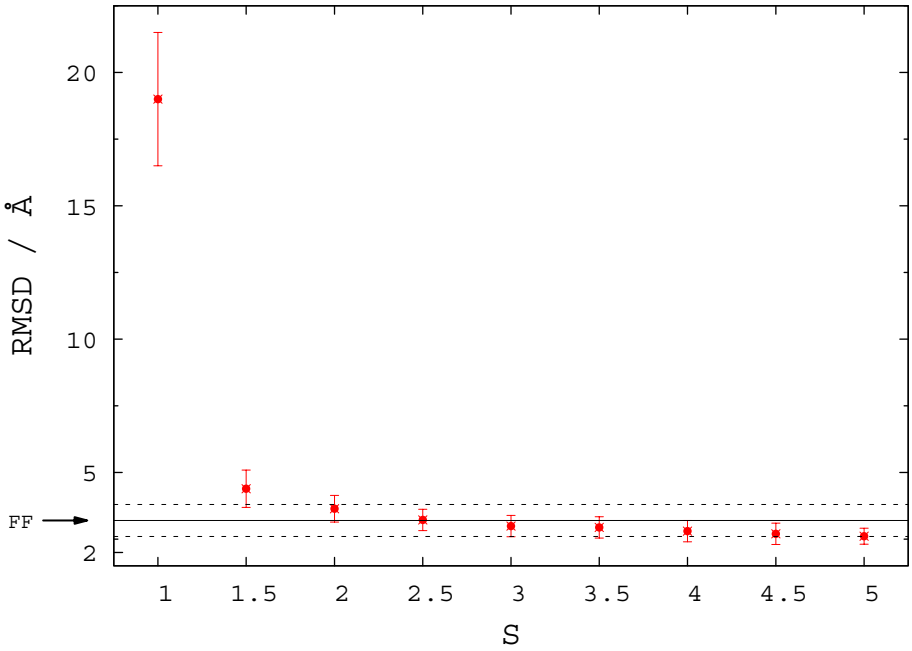

Figure S1. Calculated average root mean square deviation (RMSD) of the Cartesian coordinates of all atoms in the DNA duplex from the canonical B-DNA simulated using the structure-based potential with different scaling factors, *S*; error bars indicate one standard deviation from the average. For reference, data using the parmbsc0 force field (FF) is shown as a horizontal solid line with dashed lines indicating one standard deviation from the average.