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The DNA conformational energy landscape: Sequencedependent conformational equilibria of duplex DNA

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The free energy surfaces of duplex dinucleotide steps were mapped in a principal conformational subspace derived from crystal structure data on DNA duplex oligomers. The three dimensional subspace, spanned by collective degrees of freedom representing linear combinations of the Cartesian coordinates of the backbone and sugar atoms of both strands accounted for 77% o ...

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