

WHY DO DNA HELICAL MODELS EXHIBIT WEDGE ROLLS? A MATHEMATICAL RATIONALE*

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ABSTRACT

The base-pair parameters wedge-tilt and wedge-roll are extremely useful for describing curved DNA structures. The wedge effect has generally been assumed to be due to the differences between the base-pair tilts and rolls of two successive base-pairs in a DNA molecule. A mathematical formalism has been established here, which shows that, wedge-roll is a function of base-pair tilt and helical twist, similarly the wedge-tilt is a function of base-pair roll and helical twist. This provides a straightforward explanation for the reported wedge-roll in *A*-DNA helical model of 12° and gives a value of -3.8° for *B*-DNA fiber model. The wedge-rolls and wedge-tilts calculated for the oligonucleotide crystal structures, using these relations, are in excellent agreement with the values reported earlier, which were calculated directly from the coordinates, using a global helix axis.

INTRODUCTION

THE uniform helical models proposed on the basis of X-ray fiber data assume that all the nucleotide units have an identical structure. Since there is no variation between the units, the base-pairs in them are simply characterized in terms of their orientation with respect to the helix axis (*Z*-axis). The base-pair orientation is described in terms of two angles: tilt (Θ_x) and roll (Θ_y) and the displacement ($D \text{ \AA}$) of the base-pair centre from the helix axis¹⁻³. However the recently studied oligonucleotide crystal structures^{2,4} and the models for curved DNA⁵⁻⁹ indicate that the relative orientations of neighbouring base-pairs may also be described in terms of two wedge parameters, wedge-roll (Θ_R) and wedge-tilt (Θ_T). The wedge-roll in a straight *B*-DNA model has been assumed to be zero while the large wedge-roll value for fiber *A*-DNA has been explained descriptively and pictorially^{4,6} as being due to the large displacement of the tilted base-pairs from the helix axis. However no rigorous mathematical or geometrical explanation is available. We show here, from simple mathematical relations between the orientation vectors of two neighbouring base-pairs in a regular helix that the wedge-roll can be simply expressed in terms of the base-pair tilts and helical twist, a relationship shown graphically in our earlier paper³. Similarly the wedge-tilt is related to the intrinsic rolls of the base-pairs.

METHOD

The orientation vectors for each base-pair have been termed as the local base-pair axes. The average of the two base normals defines the base-pair normal (local *Z*-axis) while the line joining C8 (purine)-C6 (pyrimidine) defines the *Y*-axis. The *X*-axis is now defined by the direction normal to both this axis and the base-pair normal, such that a right-handed frame of reference is obtained (figure 1). These axes can be defined in an external cartesian frame of reference by their direction cosines (l_x, m_x, n_x) and (l_y, m_y, n_y), and the unit vectors along the *X* and *Y*-axes of the first base-pair are given by

$$X_1 = l_x i + m_x j + n_x k \quad (1)$$

$$Y_1 = l_y i + m_y j + n_y k. \quad (2)$$

Since the *Z*-axis of the external frame can be chosen to coincide with the helix axis, the second base-pair is related to the first by a rotation (corresponding to helical twist Θ) and a translation (helical rise) about this axis. The unit vectors X_2 and Y_2 are therefore given by the following relations

$$X_2 = (l_x \cos \Theta - m_x \sin \Theta) i + (l_x \sin \Theta + m_x \cos \Theta) j + n_x k \quad (3)$$

$$Y_2 = (l_y \cos \Theta - m_y \sin \Theta) i + (l_y \sin \Theta + m_y \cos \Theta) j + n_y k, \quad (4)$$

where Θ = helical twist angle; $n_x = \sin(\Theta_y)$ and $n_y = \sin(\Theta_x)$.

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