

23.3. NUCLEIC ACIDS

Table 23.3.2.1. Average torsion-angle properties of A-, B- and Z-DNA ($^{\circ}$)

Values listed are mean torsion angles, with standard deviations in parentheses. Conformations are only approximate; — indicates a non-*gauche/trans* conformation. B_{II} and Z_{II} are less common variants. For δ , the sugar ring geometry is quoted in place of *gauche/trans*. χ for B-DNA combines pyrimidines and purines. Values were obtained from a sample of 30 A-DNAs, 34 B-DNAs, 22 Z-DNAs and ten nonstandard DNAs in the Nucleic Acid Database. From Schneider *et al.* (1997).

	α	β	γ	δ	ϵ	ζ	χ
A-DNA Conformation	293 (17) g^-	174 (14) t	56 (14) g^+	81 (7) C3'-endo	203 (12) t	289 (12) g^-	199 (8) t
B-DNA Conformation	298 (15) g^-	176 (9) t	48 (11) g^+	128 (13) C1'-exo	184 (11) t	265 (10) g^-	249 (16) g^-
B _{II} -DNA Conformation		146 (8) —		144 (7) C2'-endo	246 (15) g^-	174 (14) t	271 (8) g^-
Z _I -DNA – purines Conformation	71 (13) g^+	183 (9) t	179 (9) t	95 (8) O4'-endo	95 (8) g^+	301 (16) g^-	63 (5) g^+
Z _{II} -DNA – purines Conformation					189 (12) t	52 (14) g^+	58 (5) g^+
Z _I -DNA – pyrimidines Conformation	201 (20) t	225 (16) —	54 (13) g^+	141 (8) C2'-endo	267 (9) g^-	75 (9) g^+	204 (98) t
Z _{II} -DNA – pyrimidines Conformation	168 (16) t	166 (14) t					

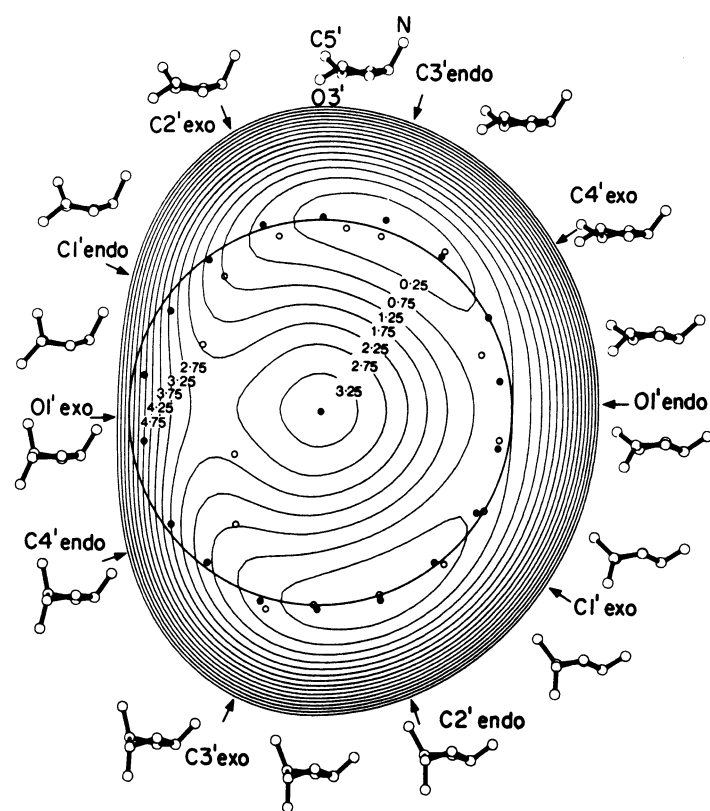


Fig. 23.3.2.5. Potential plot of all furanose ring conformations. Energies are in kcal mol⁻¹. The distance from the central point gives the maximum displacement of the out-of-plane atom from the plane of the other four. The circle is a constant-displacement trajectory chosen to pass through the potential minima on the right three-quarters of the plot. C2'-endo and C3'-endo are especially favoured, whereas O1'-exo on the left is highly disfavoured. The path from C2'-endo through C1'-exo, O1'-endo and C4'-exo to C3'-endo is a low-energy path, and many examples all along this path are known in B-DNA helices. Reprinted with permission from Levitt & Warshel (1978). Copyright (1978) American Chemical Society.

Table 23.3.2.2. Sugar ring conformations, pseudorotation angles and torsion angle δ

Ring conformation	Pseudorotation angle ($^{\circ}$)	Torsion angle δ ($^{\circ}$)
C3'-endo	18	82
C4'-exo	54	82
O4'-endo	90	96
C1'-exo	126	120
C2'-endo	162	144
C3'-exo	198	158
C4'-endo	234	158
O4'-exo	270	144
C1'-endo	306	120
C2'-exo	342	96

NEWHHELIX by Dickerson (B7, B46), *CURVES* by Lavery & Sklenar (1988, 1989), *BABCOCK* by Babcock & Olson (Babcock *et al.*, 1993, 1994; Babcock & Olson, 1994) and *FREEHELIX* (Dickerson, 1998c). *NEWHHELIX* was the earliest of these, but it performs all calculations relative to a best overall helix axis. This is satisfactory for single-crystal DNA structures, but makes the program unusable for the 180° bending observed in some protein–DNA complexes. *CURVES* is especially convenient for mapping the axis of a bent or curved helix. *FREEHELIX*, which evolved from *NEWHHELIX*, calculates all parameters relative to local base-pair geometry, without assuming an overall axis, and permits display of normal vector plots that are especially useful in analysing bending in DNA–protein complexes (Dickerson & Chiu, 1997).