Table 23.3.2.1. *Average torsion-angle properties of A-, B- and Z-DNA (°)*

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	293 (17)	174 (14)	56 (14)	81 (7)	203 (12)	289 (12)	199 (8)
Conformation	g^-	*t*	g^+	C3′-*endo*	*t*	g^-	*t*
B-DNA	298 (15)	176 (9)	48 (11)	128 (13)	184 (11)	265 (10)	249 (16)
Conformation	g^-	*t*	g^+	C1′-*exo*	*t*	g^-	g^-
B_{II}-DNA		146 (8)		144 (7)	246 (15)	174 (14)	271 (8)
Conformation		—		C2′-*endo*	g^-	*t*	g^-
Z_I-DNA – purines	71 (13)	183 (9)	179 (9)	95 (8)	95 (8)	301 (16)	63 (5)
Conformation	g^+	*t*	*t*	O4′-*endo*	g^+	g^-	g^+
Z_{II}-DNA – purines					189 (12)	52 (14)	58 (5)
Conformation					*t*	g^+	g^+
Z_I-DNA – pyrimidines	201 (20)	225 (16)	54 (13)	141 (8)	267 (9)	75 (9)	204 (98)
Conformation	*t*	—	g^+	C2′-*endo*	g^-	g^+	*t*
Z_{II}-DNA – pyrimidines	168 (16)	166 (14)					
Conformation	*t*	*t*					

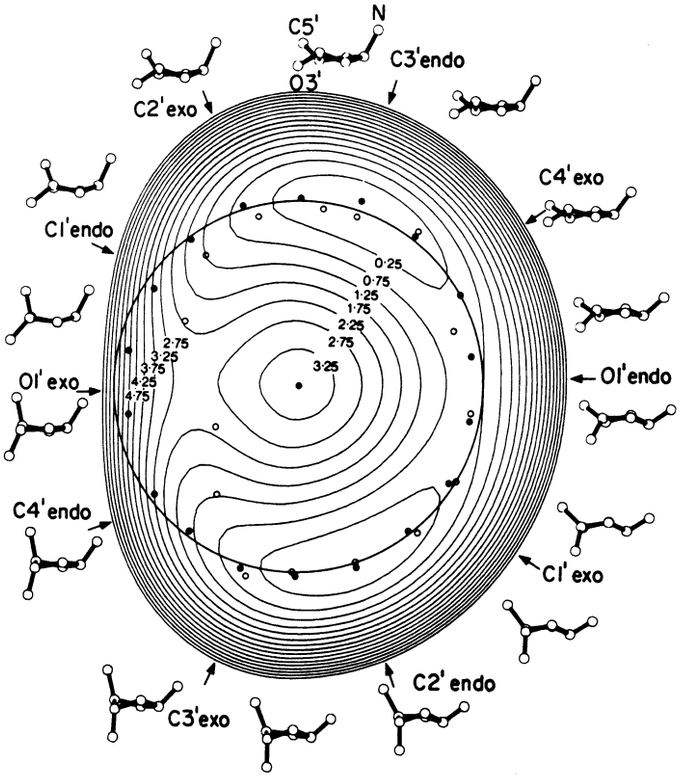

Fig. 23.3.2.5. Potential plot of all furanose ring conformations. Energies are in kcal mol^{-1}. The distance from the central point gives the maximum displacement of the out-of-plane atom from the plane of the other four. The circle is a constant-displacement trajectory chosen to pass through the potential 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 (°)	Torsion angle δ (°)
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

NEWHELIX 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, 1998*c*). *NEWHELIX* 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 *NEWHELIX*, 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).

references