Table 2. *Atomic coordinates* ($\times 10^4$) *and equivalent isotropic temperature factors* ($Å^2 \times 10^3$)

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
C(1)	−1823 (3)	3238 (3)	8589 (2)	21 (1)
C(2)	−3553 (4)	3354 (4)	9207 (2)	31 (1)
C(3)	−1732 (4)	3398 (3)	7621 (2)	23 (1)
C(4)	−154 (3)	3282 (3)	7052 (2)	21 (1)
C(5)	1370 (3)	2989 (3)	7452 (2)	17 (1)
C(6)	1291 (3)	2849 (3)	8410 (2)	19 (1)
C(7)	−301 (4)	2972 (3)	8972 (2)	22 (1)
S(1)	3381 (1)	2784 (1)	6716 (1)	19 (1)
O(1)	3281 (3)	1797 (2)	6082 (2)	29 (1)
O(2)	3519 (3)	4236 (2)	6222 (2)	27 (1)
O(3)	4683 (2)	2231 (2)	7332 (2)	27 (1)
O(4)	6834 (3)	5026 (2)	5680 (2)	28 (1)
C(8)	3694 (3)	−2213 (3)	7744 (2)	20 (1)
C(9)	2745 (3)	−953 (3)	8098 (2)	20 (1)
C(10)	1050 (3)	−862 (3)	8504 (2)	21 (1)
C(11)	198 (3)	−2038 (3)	8579 (2)	18 (1)
N(1)	−1507 (3)	−1938 (3)	8949 (2)	23 (1)
C(12)	−2284 (4)	−3217 (3)	9141 (2)	26 (1)
C(13)	−2505 (4)	−597 (3)	9237 (2)	29 (1)
C(14)	1156 (3)	−3325 (3)	8260 (2)	21 (1)
C(15)	2854 (3)	−3389 (3)	7850 (2)	22 (1)
C(16)	5436 (3)	−2311 (3)	7249 (2)	21 (1)
C(17)	6343 (3)	−1236 (3)	7047 (2)	20 (1)
C(18)	8102 (3)	−1371 (3)	6571 (2)	19 (1)
C(19)	9015 (4)	−258 (3)	6539 (2)	21 (1)
C(20)	10701 (4)	−370 (3)	6129 (2)	21 (1)
N(2)	11498 (3)	−1545 (3)	5728 (2)	21 (1)
C(21)	13318 (3)	−1665 (4)	5284 (2)	30 (1)
C(22)	10650 (4)	−2636 (3)	5723 (2)	25 (1)
C(23)	8978 (4)	−2578 (3)	6130 (2)	23 (1)

Table 3. *Selected torsion angles* (°)

C(14)—C(11)—N(1)—C(12)	8.8 (4)	C(16)—C(17)—C(18)—C(23)	10.5 (5)
C(15)—C(8)—C(16)—C(17)	175.5 (3)	C(6)—C(5)—S(1)—O(3)	9.6 (3)
C(8)—C(16)—C(17)—C(18)	178.4 (3)		

(1974, Vol. IV). Atomic coordinates are contained in Table 2. The C—C distances for the phenyl groups range between 1.378 and 1.412 Å. The cation molecule is planar with a mean deviation of 0.081 Å from the 18-atom least-squares plane. Selected torsion angles are in Table 3. Fig. 1 illustrates the molecule with the atomic numbering scheme employed. Fig. 2 illustrates the projected packing of the molecules viewed down the *a* axis.

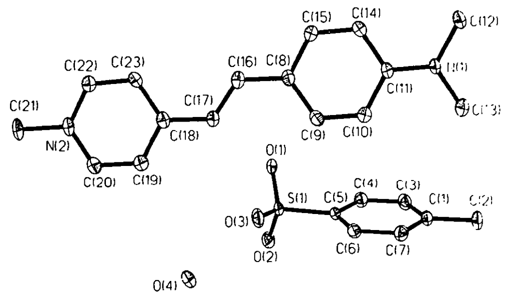

Fig. 1. Thermal-ellipsoid (50% probability) plot showing the atomic numbering scheme.

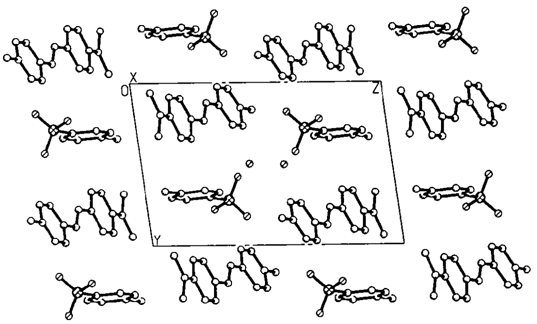

Fig. 2. Projected packing plot viewed down the *a* axis.

Related literature. For additional information on related structures and chemistry, see Williams (1983) and Marder, Perry & Schaefer (1989).

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Structure of 17-(3-Oxazolin-4-yl)androsta-4,16-dien-3-one

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Abstract. 17-(2,5-Dihydro-3-oxazol-4-yl)androsta-4,16-dien-3-one, $C_{22}H_{29}NO_2$, $M_r = 339.48$, orthorhombic, $P2_12_12_1$, $a = 7.715$ (5), $b = 12.033$ (1), $c = 19.199$ (1) Å, $V = 1782.3$ (1) $Å^3$, $Z = 4$, $D_x = 1.265$ g cm^{-3}, λ(Mo $K\bar{\alpha}$) = 0.71073 Å, $\mu = 0.7$ cm^{-1}, $F(000) = 736$, $T = 130$ K, $R(F) = 0.044$ for 1984

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0108-2701/93/020351-04$06.00

Table 1. *Final fractional atomic coordinates and equivalent isotropic thermal displacement parameters* (Å^2) *for non-*H *atoms*

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
O(1)	0.1197 (3)	0.17514 (17)	0.32628 (13)	0.0337 (8)
O(2)	0.5826 (3)	1.21170 (19)	0.46421 (14)	0.0356 (8)
N(1)	0.6000 (3)	1.0290 (2)	0.42372 (14)	0.0238 (8)
C(1)	0.3674 (4)	0.4303 (2)	0.34027 (17)	0.0187 (8)
C(2)	0.3322 (4)	0.3162 (3)	0.30877 (18)	0.0229 (9)
C(3)	0.1538 (4)	0.2743 (2)	0.32608 (15)	0.0236 (9)
C(4)	0.0210 (4)	0.3581 (2)	0.33882 (17)	0.0211 (9)
C(5)	0.0487 (4)	0.4679 (2)	0.33655 (15)	0.0172 (8)
C(6)	−0.1004 (4)	0.5472 (3)	0.34205 (18)	0.0228 (9)
C(7)	−0.0630 (4)	0.6465 (2)	0.38960 (18)	0.0216 (9)
C(8)	0.1038 (3)	0.7047 (2)	0.36676 (15)	0.0147 (8)
C(9)	0.2554 (4)	0.6211 (2)	0.37051 (15)	0.0144 (7)
C(10)	0.2282 (3)	0.5174 (2)	0.32303 (14)	0.0147 (8)
C(11)	0.4343 (4)	0.6757 (2)	0.35897 (17)	0.0192 (9)
C(12)	0.4658 (4)	0.7851 (2)	0.39830 (16)	0.0171 (8)
C(13)	0.3129 (4)	0.8644 (2)	0.38775 (14)	0.0138 (7)
C(14)	0.1487 (3)	0.8030 (2)	0.41292 (15)	0.0148 (8)
C(15)	0.0180 (4)	0.8968 (2)	0.42712 (17)	0.0201 (8)
C(16)	0.1371 (4)	0.9873 (2)	0.45143 (15)	0.0190 (8)
C(17)	0.3018 (4)	0.9689 (2)	0.43218 (14)	0.0165 (8)
C(18)	0.3013 (4)	0.9032 (3)	0.31145 (15)	0.0195 (8)
C(19)	0.2362 (4)	0.5478 (3)	0.24490 (15)	0.0215 (9)
C(20)	0.4424 (4)	1.0472 (2)	0.44164 (15)	0.0183 (8)
C(21)	0.4187 (5)	1.1604 (3)	0.47393 (19)	0.0245 (9)
C(22)	0.6991 (5)	1.1263 (3)	0.44191 (19)	0.0285 (10)

Table 2. *Selected data on the geometry* (Å, °)

O(1)—C(3)	1.222 (3)	C(8)—C(14)	1.518 (4)
O(2)—C(21)	1.419 (5)	C(9)—C(10)	1.560 (4)
O(2)—C(22)	1.431 (4)	C(9)—C(11)	1.545 (4)
N(1)—C(20)	1.282 (4)	C(10)—C(19)	1.545 (4)
N(1)—C(22)	1.441 (4)	C(11)—C(12)	1.537 (4)
C(1)—C(2)	1.525 (5)	C(12)—C(13)	1.531 (4)
C(1)—C(10)	1.537 (4)	C(13)—C(14)	1.544 (4)
C(2)—C(3)	1.503 (4)	C(13)—C(17)	1.522 (4)
C(3)—C(4)	1.458 (4)	C(13)—C(18)	1.540 (4)
C(4)—C(5)	1.339 (4)	C(14)—C(15)	1.538 (4)
C(5)—C(6)	1.498 (4)	C(15)—C(16)	1.499 (4)
C(5)—C(10)	1.530 (4)	C(16)—C(17)	1.342 (4)
C(6)—C(7)	1.531 (5)	C(17)—C(20)	1.448 (4)
C(7)—C(8)	1.529 (4)	C(20)—C(21)	1.508 (5)
C(8)—C(9)	1.544 (4)		

C(21)—O(2)—C(22)	106.7 (3)	C(13)—C(17)—C(20)	124.4 (3)
C(20)—N(1)—C(22)	107.4 (3)	C(16)—C(17)—C(20)	124.6 (2)
C(14)—C(13)—C(17)	100.0 (2)	N(1)—C(20)—C(17)	124.4 (2)
C(17)—C(13)—C(18)	106.2 (2)	N(1)—C(20)—C(21)	112.3 (3)
C(13)—C(14)—C(15)	104.0 (2)	C(17)—C(20)—C(21)	123.3 (3)
C(14)—C(15)—C(16)	100.7 (2)	O(2)—C(21)—C(20)	103.3 (3)
C(15)—C(16)—C(17)	112.0 (2)	O(2)—C(22)—N(1)	108.8 (3)
C(13)—C(17)—C(16)	110.1 (2)		

C(12)—C(13)—C(14)—C(15)	159.4 (2)	C(15)—C(16)—C(17)—C(13)	3.3 (3)
C(17)—C(13)—C(14)—C(8)	168.2 (2)	C(15)—C(16)—C(17)—C(20)	173.1 (3)
C(17)—C(13)—C(14)—C(15)	34.8 (3)	C(13)—C(17)—C(20)—N(1)	−12.3 (4)
C(18)—C(13)—C(14)—C(15)	−77.8 (3)	C(13)—C(17)—C(20)—C(21)	167.6 (3)
C(12)—C(13)—C(17)—C(16)	−140.0 (3)	C(16)—C(17)—C(20)—N(1)	179.4 (3)
C(12)—C(13)—C(17)—C(20)	50.2 (4)	C(16)—C(17)—C(20)—C(21)	−0.7 (5)
C(14)—C(13)—C(17)—C(16)	−24.1 (3)	C(17)—C(20)—N(1)—C(22)	−179.9 (3)
C(14)—C(13)—C(17)—C(20)	166.1 (3)	C(21)—C(20)—N(1)—C(22)	0.2 (4)
C(18)—C(13)—C(17)—C(16)	93.9 (3)	N(1)—C(20)—C(21)—O(2)	7.1 (4)
C(18)—C(13)—C(17)—C(20)	−75.9 (3)	C(17)—C(20)—C(21)—O(2)	−172.8 (3)
C(8)—C(14)—C(15)—C(16)	−160.9 (2)	C(20)—C(21)—O(2)—C(22)	−11.3 (3)
C(13)—C(14)—C(15)—C(16)	−33.2 (3)	N(1)—C(22)—O(2)—C(21)	12.2 (4)
C(14)—C(15)—C(16)—C(17)	19.1 (3)	O(2)—C(22)—N(1)—C(20)	−7.7 (4)

D—H···*A*	*D*···*A*	*D*—H	H···*A*	*D*—H···*A*
C(6)—H(61)···O(1$^{\rm i}$)	3.583 (5)	1.01 (3)	2.59 (3)	169 (2)
C(12)—H(121)···N(1$^{\rm ii}$)	3.150 (4)	0.96 (3)	2.62 (2)	116 (2)
C(19)—H(192)···O(1$^{\rm i}$)	3.429 (4)	0.99 (3)	2.51 (3)	154 (3)

Symmetry code: (i) $-x, \frac{1}{2}+y, \frac{1}{2}-z$; (ii) x, y, z.

unique reflections with $I \geq 2.5\sigma(I)$ and 343 parameters. In the crystalline state, the conjugated double-bond system of the *D* ring of the steroid skeleton and the oxazoline ring apparently adopt a *transoid* configuration.

Experimental. The title compound was prepared as one of the isomers of a series of 16- and 17-dehydrosteroids with 17-oxazolinyl substituents (van Leusen, Brouwer, Lei & van Leusen, 1992). A suitable colourless crystal of prismatic habit with dimensions 0.15 × 0.20 × 0.45 mm was glued on top of a glass fibre and transferred into the cold nitrogen stream of the low-temperature unit on an Enraf–Nonius CAD-4F diffractometer interfaced to a VAX 730 computer. Graphite-monochromated Mo $K\bar{\alpha}$ radiation was used to obtain 2947 reflections [h 0→10, k 0→16, l 0→26; $1.07 < \theta < 30.0°$; $(\sin\theta)_{\rm max}/\lambda$ = 0.7035 Å^{-1}; $\omega/2\theta$ scan, $\Delta\omega = (0.90 + 0.35\tan\theta)°$]. Cell dimensions were derived from setting angles of 17 reflections in the range $9.16 < \theta < 12.63°$. The unit cell was identified as orthorhombic with space group $P2_12_12_1$. The cell was checked for the presence of higher lattice symmetry (Spek, 1988) and examination of the final atomic coordinates of the structure did not yield extra metric symmetry elements (Le Page, 1987, 1988). Three reference reflections measured every 3 h (440, r.m.s. deviation 2.9%; $3\bar{5}\bar{3}$, r.m.s. deviation 2.4%; $\bar{3}3\bar{4}$, r.m.s. deviation 2.2%) showed no indication of crystal decomposition during the 67.6 h of X-ray exposure time. The data were corrected for long-term instability, Lorentz and polarization effects, but not for absorption. Variance $\sigma^2(I)$, calculated on the basis of counting statistics plus the term $(PI)^2$, where P (=0.044) is the instability constant as derived from the excess variance in the reference reflections (McCandlish, Stout & Andrews, 1975), resulted in the unique set of 2921 reflections with 1984 satisfying the $I \geq 2.5\sigma(I)$ criterion of observability. The structure was solved by direct methods using *GENTAN* (Hall, 1990) and refined on F_o by block-diagonal least-squares techniques with anisotropic thermal parameters for non-H atoms using *CRYLSQ* (Olthof-Hazekamp, 1990) minimizing the function $Q = \Sigma_{\mathbf{h}}[\Sigma w(|F_o| - |F_c|)^2]$. H atoms were located on a subsequent difference Fourier map and included in the final refinement with isotropic thermal displacement factors. Final refinement with full-matrix least-squares techniques converged at $R(F) = 0.044$; $wR = 0.048$ [$w = 1/\sigma^2(F)$]; $S = 1.389$. Minimum and maximum residual densities in the final difference Fourier map were −0.25 and 0.29 e Å^{-3}, respectively. The maximum shift/σ in the final cycle was 0.3211, with an average value of 0.0166. 343 parameters were refined. Correction for isotropic secondary extinction was applied (Zachariasen, 1967), $g = 1.0\,(1) \times 10^{-4}$. Final fractional atomic coordinates and equivalent isotropic thermal parameters for the non-H atoms are given in Table 1. Selected molecular geometry data are collected in Table 2.*

Neutral-atom scattering factors were taken from Cromer & Mann (1968). Anomalous-dispersion factors for the non-H atoms were taken from Cromer & Liberman (1970). All calculations were carried out on the CDC-Cyber 962-31 computer at Groningen University with the program packages *Xtal* (Hall & Stewart, 1990) and *EUCLID* (Spek, 1990), for calculation of geometric data, and a locally modified version of the program *PLUTO* (Meetsma, 1991; Motherwell & Clegg, 1978) for the preparation of illustrations. The orthorhombic unit cell contains four discrete molecules (Fig. 1) of the title compound; each asymmetric unit contains one complete molecule with no atom sitting at a special position, separated by normal van der Waals distances (Bondi, 1964) and some weak hydrogen bonds (Berkovitch-Yellin & Leiserowitz, 1984) (Table 2). A view of the puckering of the title compound, including the adopted numbering scheme, is presented in Fig. 2.

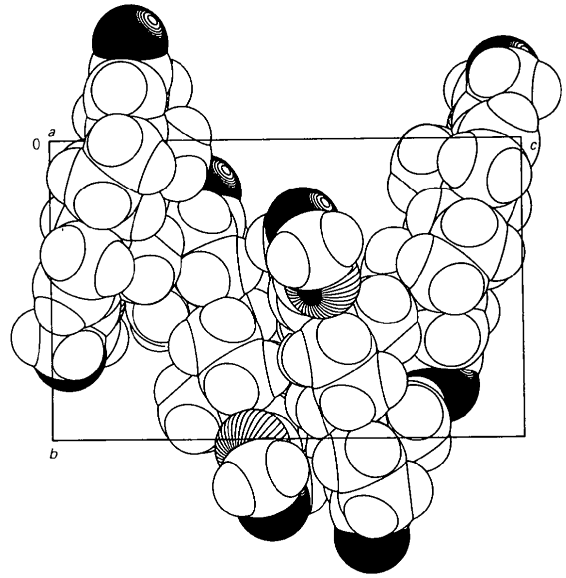

Fig. 1. Space-filling molecular packing viewed down [100]. O atoms are circular and N atoms are meridionally hatched for the sake of clarity.

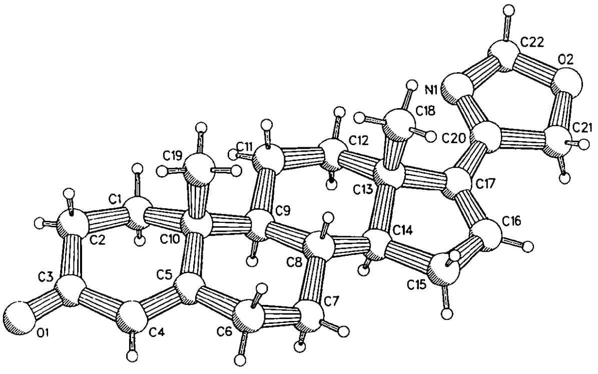

Fig. 2. *PLUTO* drawing of the molecule illustrating the conformation and the adopted numbering scheme.

Related literature. The structural parameters of the steroid skeleton can be compared with those found for 6α-methylpregna-4,16-diene-3,20-dione (Duax, Weeks & Strong, 1979), 3,20-dioxopregna-4,16-dien-21-yl acetate (Khazheeva, Simonov, Kamernitskii, Pavlova-Grishina & Skorova, 1982), and (*E*)-17-(diethylphosphonoisocyanomethylene)-3-methoxy-19-norandrosta-1,3,5(10)-triene (Meetsma, Stoelwinder & van Leusen, 1992). The structural parameters of the oxazoline moiety can be compared with those of (−)-[*p*-(2,2-dimethyl-4-phenyl-Δ^3-1,3-oxazolin-5-yl)phenyl]trimethylammonium [2-oxo-10-bornanesulfonate] (Foricher, Montavon, Pfoertner & Schönholzer, 1985) and 2,2,4,5-tetraphenyl-5-[4-(*p*-chlorobenzoyl)-2-cyclooctenyl]-3-oxazoline (Mohedano, Florencio & García-Blanco, 1985).

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* Lists of structure factors, anisotropic thermal displacement parameters, H-atom parameters, bond lengths, bond angles, and torsion angles, including those involving H atoms, have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55529 (28 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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1,3-Dicyanomethylhexahydropyrimidine

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Abstract. Hexahydropyrimidine-1,3-diacetonitrile, $C_8H_{12}N_4$, $M_r = 164.21$, monoclinic, $P2_1/c$, $a = 8.303$ (1), $b = 8.733$ (1), $c = 12.998$ (2) Å, $\beta = 107.73$ (2)°, $V = 897.7$ (4) Å^3, $Z = 4$, $D_x = 1.21$ g cm^{-3}, Cu $K\alpha$ radiation, $\lambda = 1.5418$ Å, $\mu = 6.4$ cm^{-1}, $F(000) = 352$, $T = 293$ K, final $R = 0.035$ ($wR = 0.050$) for 1005 observed reflections. The pyrimidine ring adopts the chair conformation with C(7) and C(9) in equatorial positions.

Experimental. The title compound (Fig. 1) was prepared by dropwise addition of a saturated aqueous solution of potassium cyanide (2 equivalents) to an ice-bath-cooled aqueous solution of formaldehyde (3 equivalents) containing 1,3-propanediamine dihydrochloride (1 equivalent). The aqueous solution was extracted several times with ether and the combined ether layers were dried. The solvent was then removed by distillation at reduced pressure and the residue crystallized from absolute ethanol. Data were collected on an Enraf–Nonius CAD-4 diffractometer with graphite monochromator, for a crystal of dimensions 0.25 × 0.25 × 0.30 mm. Cell parameters were measured on the diffractometer using 25 reflections in the 2θ range 20–40°. Data were collected over range of indices $-9 \leq h \leq 9$, $0 \leq k \leq 9$, $0 \leq l \leq 14$ ($\theta \leq 60°$). Three standards (110, 022 and 102), measured after every 200 reflections, showed a variation of 0.1%. No absorption corrections but Lorentz and polarization corrections were applied. 1333 unique ($R_{\rm int} = 0.013$) reflections were measured, of which 1005 were observed with $|F_o| > 3\sigma(|F_o|)$. Direct methods (*MULTAN*82; Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982) were used for structure determination. H atoms were located by difference Fourier synthesis. Anisotropic full-matrix least-squares refinement (on F) was performed for non-H atoms, isotropic for H atoms. In the last cycle the H atoms were fixed at idealized positions (0.94–1.06 Å). $\sum w(|F_o| - |F_c|)^2$ was minimized, where the non-Poisson $w = 4F^2/[\sigma(I)^2 + (pF^2)^2]$; $p = 0.04$, $R = 0.035$, $wR = 0.050$, $S = 1.650$, for 158 variables. Maximum $\Delta/\sigma = 0.01$. Maximum peak height in the final difference Fourier map was 0.24 e Å^{-3}. Atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV). Computing used the Enraf–Nonius *SDP* (Frenz, 1984). Atomic parameters are given in

Table 1. *Final fractional coordinates and equivalent isotropic temperature factors* (Å^2) *for non*-H *atoms with e.s.d.'s in parentheses*

$$B_{\rm eq} = \tfrac{4}{3}\textstyle\sum_i \sum_j \beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$B_{\rm eq}$
N(1)	0.5997 (2)	0.1089 (2)	0.4213 (1)	3.30 (3)
N(2)	1.0267 (3)	0.3770 (2)	0.2759 (1)	7.43 (6)
N(3)	0.8891 (2)	0.1775 (2)	0.4632 (1)	3.40 (3)
N(4)	0.3418 (2)	0.1822 (2)	0.1619 (1)	5.96 (5)
C(2)	0.7417 (2)	0.1249 (2)	0.3781 (1)	3.26 (3)
C(4)	0.8595 (2)	0.3275 (2)	0.5048 (1)	3.88 (4)
C(5)	0.7066 (2)	0.3201 (2)	0.5449 (1)	4.29 (4)
C(6)	0.5558 (2)	0.2569 (2)	0.4583 (1)	3.92 (4)
C(7)	1.0385 (2)	0.1755 (2)	0.4280 (2)	4.26 (4)
C(8)	1.0339 (2)	O.2874 (2)	0.3406 (2)	4.69 (4)
C(9)	0.4559 (2)	0.0342 (2)	0.3453 (1)	3.82 (4)
C(10)	0.3882 (2)	0.1173 (2)	0.2408 (1)	4.05 (4)

Table 2. *Bond lengths* (Å), *bond angles* (°) *and selected torsion angles* (°) *with e.s.d.'s in parentheses*

N(1)—C(2)	1.459 (2)	N(3)—C(7)	1.447 (3)
N(1)—C(6)	1.464 (2)	N(4)—C(10)	1.132 (2)
N(1)—C(9)	1.452 (2)	C(4)—C(5)	1.513 (3)
N(2)—C(8)	1.137 (3)	C(5)—C(6)	1.510 (2)
N(3)—C(2)	1.452 (2)	C(7)—C(8)	1.490 (3)
N(3)—C(4)	1.467 (2)	C(9)—C(10)	1.490 (2)
C(2)—N(1)—C(6)	110.7 (1)	N(3)—C(4)—C(5)	109.9 (1)
C(2)—N(1)—C(9)	112.0 (1)	C(4)—C(5)—C(6)	110.6 (2)
C(6)—N(1)—C(9)	112.6 (1)	N(1)—C(6)—C(5)	109.5 (1)
C(2)—N(3)—C(4)	111.5 (1)	N(3)—C(7)—C(8)	114.1 (2)
C(2)—N(3)—C(7)	111.1 (1)	N(2)—C(8)—C(7)	177.0 (2)
C(4)—N(3)—C(7)	112.5 (1)	N(1)—C(9)—C(10)	113.9 (2)
N(1)—C(2)—N(3)	109.2 (1)	N(4)—C(10)—C(9)	177.8 (2)
C(6)—N(1)—C(2)—N(3)	62.4 (2)	C(2)—N(3)—C(4)—C(5)	57.0 (2)
C(2)—N(1)—C(6)—C(5)	−59.3 (2)	N(1)—C(6)—C(5)—C(4)	54.5 (2)
C(4)—N(3)—C(2)—N(1)	−61.2 (2)	N(3)—C(4)—C(5)—C(6)	−53.2 (2)

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