Table 1. *Fractional coordinates and equivalent isotropic thermal parameters* (Å^2) *with their e.s.d.'s in parentheses*

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

	x	y	z	U_{eq}/U_{iso}
C(2)	0·0680 (3)	0·4147 (3)	0·289 (1)	0·050 (2)
C(4)	0·0934 (2)	0·5095 (2)	−0·033 (1)	0·041 (2)
C(5)	0·1589 (2)	0·5138 (2)	−0·095 (1)	0·040 (2)
C(6)	0·1740 (2)	0·4695 (2)	0·032 (1)	0·040 (2)
C(7)	0·2071 (3)	0·5671 (3)	−0·290 (2)	0·060 (2)
C(1′)	0·1513 (3)	0·3732 (3)	0·339 (1)	0·044 (2)
C(2′)	0·1678 (3)	0·3316 (3)	0·138 (1)	0·051 (2)
C(3′)	0·2219 (3)	0·3225 (3)	0·287 (1)	0·053 (2)
C(4′)	0·2616 (3)	0·3882 (3)	0·448 (1)	0·052 (2)
C(5′)	0·3286 (3)	0·4420 (3)	0·325 (1)	0·057 (2)
C(3′1)	0·1817 (3)	0·2044 (2)	0·446 (2)	0·074 (3)
C(3′2)	0·1401 (3)	0·1541 (3)	0·656 (2)	0·095 (3)
N(1)	0·1302 (2)	0·4197 (2)	0·2132 (–)	0·041 (2)
N(3)	0·0534 (2)	0·4611 (2)	0·159 (1)	0·045 (2)
O(2)	0·0286 (2)	0·3735 (2)	0·456 (1)	0·083 (2)
O(4)	0·0718 (2)	0·5454 (2)	−0·141 (1)	0·053 (1)
O(3′)	0·1862 (2)	0·2669 (2)	0·482 (1)	0·093 (2)
O(4′)	0·2142 (2)	0·4153 (2)	0·484 (1)	0·050 (1)
O(5′)	0·3156 (2)	0·4581 (2)	0·059 (1)	0·058 (2)
O(3′1)	0·2047 (5)	0·1940 (3)	0·258 (2)	0·138 (4)*
O(3′2)	0·258 (1)	0·240 (1)	0·436 (5)	0·098 (8)†

* S.o.f. 0·81 (1).
† S.o.f. 0·19 (1) and U_{iso}.

Table 2. *Bond distances* (Å) *and bond angles* (°) *with e.s.d.'s in parentheses*

C(4)—C(5)	1·437 (7)	N(3)—C(2)	1·381 (8)
C(5)—C(6)	1·341 (7)	N(3)—C(4)	1·375 (7)
C(5)—C(7)	1·486 (8)	O(2)—C(2)	1·215 (8)
C(1′)—C(2′)	1·52 (1)	O(4)—C(4)	1·235 (6)
C(2′)—C(3′)	1·50 (1)	O(3′)—C(3′)	1·449 (8)
C(3′)—C(4′)	1·497 (9)	O(3′)—C(3′1)	1·348 (6)
C(4′)—C(5′)	1·490 (9)	O(4′)—C(1′)	1·424 (8)
C(3′1)—C(3′2)	1·46 (1)	O(4′)—C(4′)	1·456 (8)
N(1)—C(2)	1·377 (9)	O(5′)—C(5′)	1·434 (9)
N(1)—C(6)	1·374 (6)	O(3′1)—C(3′1)	1·14 (1)
N(1)—C(1′)	1·465 (8)	O(3′2)—C(3′1)	1·47 (3)

C(3′)—O(3′)—C(3′1)	120·7 (6)	O(4′)—C(1′)—N(1)	107·9 (4)
C(1′)—O(4′)—C(4′)	109·7 (4)	O(4′)—C(1′)—C(2′)	106·1 (6)
C(2)—N(1)—C(6)	121·4 (4)	N(1)—C(1′)—C(2′)	113·8 (5)
C(2)—N(1)—C(1′)	118·9 (4)	C(1′)—C(2′)—C(3′)	101·8 (5)
C(6)—N(1)—C(1′)	119·7 (5)	O(3′)—C(3′)—C(2′)	108·1 (5)
C(2)—N(3)—C(4)	127·2 (5)	O(3′)—C(3′)—C(4′)	105·9 (5)
O(2)—C(2)—N(1)	124·1 (6)	C(2′)—C(3′)—C(4′)	104·6 (5)
O(2)—C(2)—N(3)	121·9 (6)	O(4′)—C(4′)—C(3′)	105·7 (5)
N(1)—C(2)—N(3)	114·0 (5)	O(4′)—C(4′)—C(5′)	110·8 (5)
O(4)—C(4)—N(3)	119·8 (5)	C(3′)—C(4′)—C(5′)	115·1 (6)
O(4)—C(4)—C(5)	124·5 (5)	O(5′)—C(5′)—C(4′)	109·4 (6)
N(3)—C(4)—C(5)	115·8 (4)	O(3′)—C(3′1)—O(3′1)	120·3 (6)
C(4)—C(5)—C(6)	117·5 (5)	O(3′)—C(3′1)—O(3′2)	89 (1)
C(4)—C(5)—C(7)	119·4 (5)	O(3′)—C(3′1)—C(3′2)	112·4 (6)
C(6)—C(5)—C(7)	123·0 (5)	O(3′1)—C(3′1)—C(3′2)	127·1 (5)
N(1)—C(6)—C(5)	124·0 (5)	O(3′2)—C(3′1)—C(3′2)	123 (1)

Related literature. The molecular geometry of the title compound is very similar to that of the recently reported structure of the orthorhombic modification (Eccleston, Wilson & Howie, 1988). In the two modifications the base residues are head-to-head linked by N(3)—H···O(4) hydrogen bonds. However, the modifications differ in the second hydrogen bond: in the hexagonal form the bond is between sugar O(5′)—H and base O(4), whereas in the orthorhombic form the bond connects O(5′)—H and O(4′) of neighbouring sugar residues.

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Structure of 6-Allyl-3-hydroxymethyl-6,10b-dimethyl-2-phenyl-2,3,5,6-tetrahydroisoquinolino[1,2-*b*][1,3]oxazol-5-one

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Abstract. $C_{23}H_{25}NO_3$, $M_r = 363{\cdot}46$, orthorhombic, $P2_12_12_1$, $a = 10{\cdot}047$ (4), $b = 10{\cdot}599$ (4), $c = 19{\cdot}003$ (6) Å, $V = 2024$ (1) Å^3, $Z = 4$, $D_x = 1{\cdot}19$ g cm^{-3}, λ(Mo $K\alpha$) = 0·7107 Å, $\mu = 0{\cdot}9$ cm^{-1}, $F(000) = 776$, $T = 151$ K, $R = 0{\cdot}050$ ($wR = 0{\cdot}068$) for 1888 unique observed reflections. Three fused (six-, six- and five-membered) heteroatom rings contain an amide N bridgehead atom.

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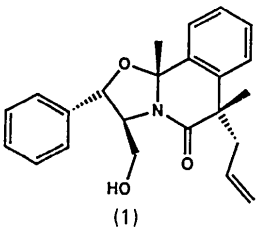
Experimental. Crystals (colorless prisms) of $C_{23}H_{25}NO_3$ [hereafter (1)] were obtained from a dichloromethane/hexane solution by Dr Thomas Wünsch and Professor A. I. Meyers. Crystal size 0·51 × 0·52 × 0·62 mm. Nicolet *R3m* diffractometer, unit-cell constants from least-squares fit of setting angles for 25 reflections ($2\theta_{av} = 23{\cdot}16°$). Data collected (Wyckoff ω scans) to $(\sin\theta)/\lambda = 0{\cdot}5947$ Å^{-1}, $0 \le h \le 12$, $0 \le k \le 13$, $-23 \le l \le 0$. Three standard reflections (400, 040, 006) measured every 97 reflections, approximately linear 11% decrease in intensity for each over course of data collection, correction applied; Lorentz and polarization corrections; no absorption correction applied because of the low absorption coefficient; 2060 reflections measured, 2039 unique, 1888 reflections with $F_o > 2{\cdot}5\sigma(F_o)$ observed.



(1)

Structure solved by direct methods [*RANT* (Sheldrick, 1983)]; block-diagonal (maximum 103 parameters/block, 255 parameters total, data/parameters = 7·40) weighted $\{w = [\sigma^2(F) + gF^2]^{-1}, g = 1{\cdot}81 \times 10^{-3}\}$ least-squares refinement on F. H atoms in idealized positions [C—H = 0·96 Å, U(H) = 1·2 × U_{iso}(C)] with exception of H(O3) (located in difference map and refined with isotropic thermal parameter). Non-H atoms refined with anisotropic thermal parameters. Extinction correction applied, $x = 0{\cdot}012$ (1) (Larson, 1967; Sheldrick, 1983). At convergence [$(\Delta/\sigma)_{max} = 0{\cdot}126$, $(\Delta/\sigma)_{mean} = 0{\cdot}019$ for last three cycles] $R = 0{\cdot}050$, $wR = 0{\cdot}068$, $S = 1{\cdot}31$, slope of normal probability plot = 1·13, $(\Delta\rho)_{max} = 0{\cdot}24$, $(\Delta\rho)_{min} = -0{\cdot}17$ e Å^{-3}. Known stereochemistry at C(10) (*S*) and C(11) (*S*) (Wünsch, 1990) from synthetic precursor gave relative stereochemistry at C(8) (*S*) and fixed the enantiomorph. Neutral-atom scattering factors and anomalous-dispersion corrections used (*International Tables for X-ray Crystallography*, 1974, Vol. IV); all calculations performed using *SHELXTL* (Sheldrick, 1983). Table 1 gives atomic coordinates and Table 2 gives bond lengths and angles.* Fig. 1 shows the structure of (1) and the numbering scheme used.

* Lists of anisotropic thermal parameters, H-atom coordinates and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53754 (16 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Atomic coordinates and equivalent isotropic thermal parameters* (Å^2 × 10^3) *for* (1)

Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U
C(1)	0·0987 (3)	0·9175 (3)	0·7189 (1)	36 (1)
C(2)	0·2041 (3)	0·9145 (3)	0·7755 (1)	35 (1)
C(3)	0·1947 (4)	0·9994 (3)	0·8324 (1)	42 (1)
C(4)	0·2817 (4)	0·9916 (3)	0·8888 (2)	47 (1)
C(5)	0·3776 (4)	0·8952 (4)	0·8903 (2)	50 (1)
C(6)	0·3892 (4)	0·8128 (3)	0·8336 (2)	49 (1)
C(7)	0·3053 (3)	0·8226 (3)	0·7743 (1)	39 (1)
C(8)	0·3221 (3)	0·7336 (3)	0·7102 (2)	41 (1)
C(9)	0·2532 (3)	0·7844 (3)	0·6437 (1)	37 (1)
C(10)	0·0854 (3)	0·9288 (2)	0·5917 (1)	36 (1)
C(11)	0·0227 (3)	1·0472 (3)	0·6270 (1)	35 (1)
C(12)	0·0632 (3)	1·1739 (3)	0·5947 (1)	37 (1)
C(13)	−0·0317 (4)	1·2501 (3)	0·5605 (1)	42 (1)
C(14)	0·0058 (4)	1·3659 (3)	0·5314 (2)	52 (1)
C(15)	0·1372 (4)	1·4076 (3)	0·5371 (2)	52 (1)
C(16)	0·2308 (4)	1·3336 (3)	0·5715 (2)	49 (1)
C(17)	0·1948 (4)	1·2161 (3)	0·5999 (2)	42 (1)
C(18)	−0·0152 (4)	0·8448 (3)	0·5529 (1)	40 (1)
C(19)	−0·0299 (3)	0·8520 (3)	0·7439 (2)	40 (1)
C(20)	0·2583 (4)	0·6039 (3)	0·7265 (2)	50 (1)
C(21)	0·4732 (3)	0·7138 (3)	0·6919 (2)	47 (1)
C(22)	0·5492 (4)	0·8334 (4)	0·6790 (2)	58 (1)
C(23)	0·6092 (5)	0·8655 (4)	0·6205 (2)	72 (1)
N(1)	0·1473 (3)	0·8633 (2)	0·6520 (1)	36 (1)
O(1)	0·2879 (3)	0·7515 (2)	0·5829 (1)	49 (1)
O(2)	0·0711 (2)	1·0463 (2)	0·6991 (1)	37 (1)
O(3)	−0·0697 (3)	0·9187 (2)	0·4965 (1)	50 (1)
H(O3)	−0·1189 (43)	0·8554 (34)	0·4660 (19)	77 (12)*

* Refined isotropically.

Table 2. *Bond lengths* (Å) *and bond angles* (°) *for* (1) *with e.s.d.'s in parentheses*

C(1)—C(2)	1·510 (4)	C(1)—C(19)	1·542 (4)
C(1)—N(1)	1·478 (3)	C(1)—O(2)	1·442 (3)
C(2)—C(3)	1·410 (4)	C(2)—C(7)	1·408 (4)
C(3)—C(4)	1·385 (4)	C(4)—C(5)	1·405 (5)
C(5)—C(6)	1·392 (5)	C(6)—C(7)	1·412 (4)
C(7)—C(8)	1·550 (4)	C(8)—C(9)	1·538 (4)
C(8)—C(20)	1·548 (4)	C(8)—C(21)	1·572 (5)
C(9)—N(1)	1·362 (4)	C(9)—O(1)	1·255 (3)
C(10)—C(11)	1·556 (4)	C(10)—C(18)	1·536 (4)
C(10)—N(1)	1·477 (4)	C(11)—C(12)	1·531 (4)
C(11)—O(2)	1·455 (3)	C(12)—C(13)	1·408 (4)
C(12)—C(17)	1·400 (5)	C(13)—C(14)	1·398 (4)
C(14)—C(15)	1·396 (6)	C(15)—C(16)	1·388 (5)
C(16)—C(17)	1·405 (4)	C(18)—O(3)	1·436 (4)
C(21)—C(22)	1·500 (5)	C(22)—C(23)	1·310 (5)
O(3)—H(O3)	1·015 (39)		

C(2)—C(1)—C(19)	111·0 (2)	C(2)—C(1)—N(1)	111·9 (2)
C(19)—C(1)—N(1)	111·5 (2)	C(2)—C(1)—O(2)	109·9 (2)
C(19)—C(1)—O(2)	110·2 (2)	N(1)—C(1)—O(2)	102·0 (2)
C(1)—C(2)—C(3)	119·1 (3)	C(1)—C(2)—C(7)	120·6 (2)
C(3)—C(2)—C(7)	120·2 (3)	C(2)—C(3)—C(4)	120·9 (3)
C(3)—C(4)—C(5)	119·4 (3)	C(4)—C(5)—C(6)	119·9 (3)
C(5)—C(6)—C(7)	121·4 (3)	C(2)—C(7)—C(6)	118·0 (3)
C(2)—C(7)—C(8)	120·9 (3)	C(6)—C(7)—C(8)	121·1 (3)
C(7)—C(8)—C(9)	112·5 (2)	C(7)—C(8)—C(20)	109·7 (2)
C(9)—C(8)—C(20)	106·9 (3)	C(7)—C(8)—C(21)	111·1 (3)
C(9)—C(8)—C(21)	107·5 (2)	C(20)—C(8)—C(21)	109·0 (3)
C(8)—C(9)—N(1)	118·1 (2)	C(8)—C(9)—O(1)	122·2 (3)
N(1)—C(9)—O(1)	119·6 (3)	C(11)—C(10)—C(18)	114·1 (3)
C(11)—C(10)—N(1)	102·5 (2)	C(18)—C(10)—N(1)	112·2 (2)
C(10)—C(11)—C(12)	115·3 (2)	C(10)—C(11)—O(2)	105·4 (2)
C(12)—C(11)—O(2)	107·1 (2)	C(11)—C(12)—C(13)	120·5 (3)
C(11)—C(12)—C(17)	120·2 (3)	C(13)—C(12)—C(17)	119·2 (3)
C(12)—C(13)—C(14)	120·3 (3)	C(13)—C(14)—C(15)	120·1 (3)
C(14)—C(15)—C(16)	119·9 (3)	C(15)—C(16)—C(17)	120·5 (3)
C(12)—C(17)—C(16)	120·0 (3)	C(10)—C(18)—O(3)	107·0 (2)
C(8)—C(21)—C(22)	114·6 (3)	C(21)—C(22)—C(23)	126·4 (4)
C(1)—N(1)—C(9)	126·6 (2)	C(1)—N(1)—C(10)	110·1 (2)
C(9)—N(1)—C(10)	121·9 (2)	C(1)—O(2)—C(11)	108·4 (2)
C(18)—O(3)—H(O3)	104·5 (20)		

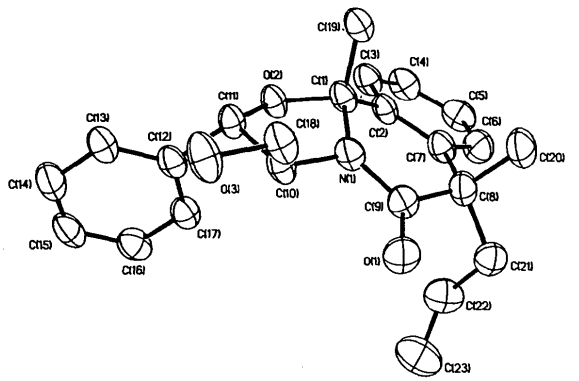


Fig. 1. The structure of $C_{23}H_{25}NO_3$ (50% probability thermal ellipsoids). H atoms have been omitted for clarity.

Related literature. Two compounds have been previously studied that contain five- and six-membered fused rings with an amide N atom at the bridgehead and an ether functionality in the five-membered ring bound to the other bridgehead atom: 3-benzyl-9-hydroxymethyl-3,6-dimethyl-8-phenyl-7,1-oxazabicyclo[4.3.0]nonan-2-one [(2), Meyers, Lefker, Wanner & Aitken (1986)]; 6,7,8,8aα-tetrahydro-2α-phenyl-5*H*-oxazolo[3,2-*a*]pyridin-3(2*H*)-one (Malmros & Wagner, 1977). In the structure of (1), hydrogen bonds from the hydroxymethyl O atom to the amide O atom link molecules of (1) into chains [O(1)—O(3^i) 2·753 (3), O(1)—H(O3^i) 1·74 (4) Å, O(1)—H(O3^i)—O(3^i) 176 (4)°; (i) $x-\frac{1}{2}, \frac{3}{2}-y, \frac{3}{2}-z$].

The out-of-plane deformation of the amide group in (1) and (2) can be described by three parameters: χ_N, χ_C and τ (Winkler & Dunitz, 1971). The deviation from planarity of the amide in (1) is significant, given that $\chi_N = 14{\cdot}7$ and $\chi_C = 2{\cdot}9°$. The torsional angles ω_1 [C(8)—C(9)—N(1)—C(10) = 172·5 (3)°] and ω_2 [O(1)—C(9)—N(1)—C(1) = −175·8 (3)°] added together give the twist angle $\tau = -3{\cdot}3°$. N(1) is 0·07 Å out of the least-squares plane through the amide linkage and associated C atoms bound to the N atom [N(1), C(9), O(1), C(1) and C(10)]. Corresponding parameters in (2) are $\chi_N = 155{\cdot}3$, $\chi_C = 1{\cdot}0°$, $\omega_1 = 167{\cdot}9$, $\omega_2 = -168{\cdot}3°$ and $\tau = -0{\cdot}4°$, and the amide N is 0·13 Å out of the corresponding plane. While the geometry at the amide N atom is non-planar in both (1) and (2), the degree of deformation is smaller in (1) possibly as a result of the fused benzene ring constraining the geometry of the unsaturated six-membered ring.

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(Benzimidazolyl-1)-3 Méthyl-1 *N*-(α-Méthylbenzyl)propylamine

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Abstract. $C_{19}H_{23}N_3$, $M_r = 293{\cdot}4$, monoclinic, $P2_1$, $a = 11{\cdot}510$ (3), $b = 6{\cdot}148$ (2), $c = 12{\cdot}183$ (3) Å, $\beta = 94{\cdot}12$ (1)°, $V = 859{\cdot}9$ (7) Å^3, $Z = 2$, $D_x = 1{\cdot}133$ Mg m^{-3}, λ(Mo $K\bar{\alpha}$) = 0·7107 Å, $\mu = 0{\cdot}063$ mm^{-1}, $F(000) = 316$, $T = 294$ (1) K, $R = 0{\cdot}035$ for 1363 independent observed reflections. All bond

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