organic compounds

Ethyl 2-methyl-5-oxo-4-(3,4,5-tri-methoxyphenyl)-1,4,5,6,7,8-hexahydro-quinoline-3-carboxylate

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In the molecular structure of the title compound, $C_{22}H_{27}NO_6$, the dihydropyridine ring adopts a flattened boat conformation while the cyclohexenone ring is in an envelope conformation. In the crystal, molecules stack parallel to the crystallographic a axis linked by intermolecular N—H···O and C—H···O hydrogen bonds.

Related literature

For general background to the biological activity of quinoline derivatives, see: Baba (1997); Baba *et al.* (1997,1998); Davies *et al.* (2005); Rose & Draeger *et al.* (1992); Warrior *et al.* (2005).
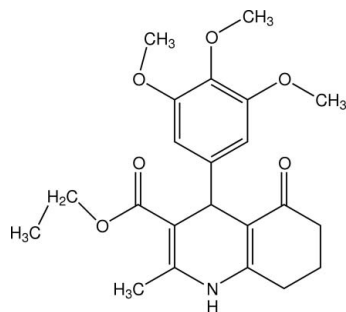
Experimental

Crystal data

$C_{22}H_{27}NO_6$	a = 7.512 (2) Å
M_r = 401.44	b = 10.402 (1) Å
Triclinic, $P\bar{1}$	c = 14.568 (3) Å

α = 109.77 (3)°	Mo $K\alpha$ radiation
β = 95.42 (1)°	μ = 0.10 mm^{-1}
γ = 104.41 (2)°	T = 294 K
V = 1017.4 (4) Å^3	0.26 × 0.24 × 0.21 mm
Z = 2	

Data collection

Nonius MACH3 diffractometer	3574 independent reflections
Absorption correction: ψ scan (North *et al.*, 1968)	2653 reflections with $I > 2\sigma(I)$
T_{min} = 0.976, T_{max} = 0.980	R_{int} = 0.013
4471 measured reflections	3 standard reflections every 60 min intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.129	
S = 1.03	$\Delta\rho_{max}$ = 0.23 e Å^{-3}
3574 reflections	$\Delta\rho_{min}$ = −0.18 e Å^{-3}
268 parameters	

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O1^i	0.83 (3)	2.21 (3)	2.995 (2)	160 (3)
C2—H2B···O4^{ii}	0.97	2.55	3.340 (3)	138
C10—H10B···O1^i	0.96	2.59	3.429 (3)	146

Symmetry codes: (i) $x - 1, y, z$; (ii) $x - 1, y - 1, z$.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JH2183).

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supporting information

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Ethyl 2-methyl-5-oxo-4-(3,4,5-trimethoxyphenyl)-1,4,5,6,7,8-hexahydro-quinoline-3-carboxylate

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S1. Comment

Some derivatives of quinoline are naturally occurring alkaloids and are very attractive for their various bioactivities. For example, they have calcium modulatory properties (Rose &Draeger, 1992), antibacterial activity (Davies *et al.*, 2005),fungicidal activity (Warrior *et al.*, 2005) and selective inhibitor of human immunodeficiency virus type I (HIV-1) transcription (Baba, 1997; Baba *et al.*,1997,1998) *etc*. Due to these significant biological activities, the structure of a quinoline derivative, ethyl 2-methyl-5-oxo -4-(3,4,5-trimethoxyphenyl)-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate is elucidated and reported.

The dihydropyridine ring of the title molecule adopts a flattened boat conformation. The cyclohexenone ring is in an envelope conformation with atom C3 at the flap. The 3,4,5-trimethoxyphenyl ring and the plane of the dihydropyridine ring (N1/C1/C6/C7/C8/C9) are nearly perpendicular to each other, with a dihedral angle of 89.33 (4)°. In the crystal structure, molecules are linked into a sheet (Fig.2) parallel to the *a* axis by N—H···O and C—H···O intra and intermolecular hydrogen bonds (Table 1). Further, it is observed that these sheets are assembled through centrosymmetrically related pairs of molecules by C2—H2B···O4 inter molecular hydrogen bond and weak interactions, which stabilize the structure.

S2. Experimental

3,4,5-trimethoxy benzaldehyde (10 mmol), 1,3-cyclohexanedione (10 mmol) and ethyl acetoacetate (10 mmol) were mixed along with 20 ml of ethanol. Ammonium acetate (10 mmol) was added to the mixture and refluxed on water bath for about 1 h. The progress of the reaction was monitored by TLC. After confirming that the reaction got completed, the reaction mixture was allowed to cool to room temperature and left aside for a day. Solid crystals started to grow from the mother liquor. It was filtered and washed with diethyl ether to ensure pure crystals [yield: 60%, m.p. 576–578 K].

S3. Refinement

H atoms were placed at calculated positions and allowed to ride on their carrier atoms with N—H = 0.83 Å, C—H = 0.93–0.97 Å, and $U_{iso} = 1.2U_{eq}(C)$ for CH$_2$ and CH groups and $U_{iso} = 1.5U_{eq}(C)$ for CH$_3$ group.
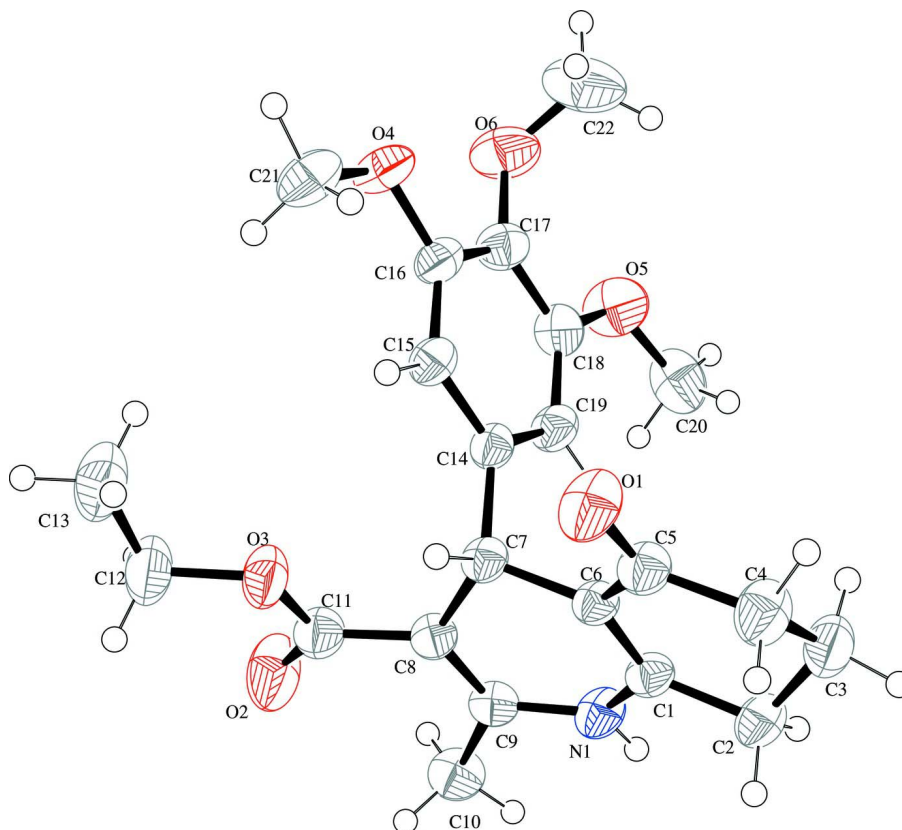
Figure 1

The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.
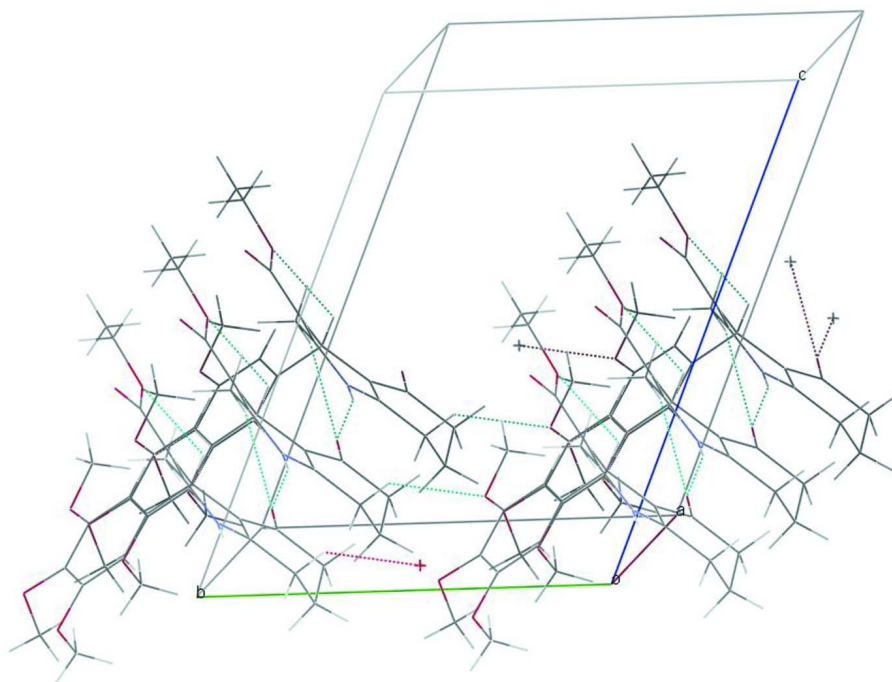
Figure 2

The packing diagram showing the sheets of hydrogen bonds along the *a* axis

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Crystal data

$C_{22}H_{27}NO_6$	$Z = 2$
$M_r = 401.44$	$F(000) = 428$
Triclinic, $P\bar{1}$	$D_x = 1.310$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 7.512$ (2) Å	Cell parameters from 25 reflections
$b = 10.402$ (1) Å	$\theta = 2–25°$
$c = 14.568$ (3) Å	$\mu = 0.10$ mm^{-1}
$\alpha = 109.77$ (3)°	$T = 294$ K
$\beta = 95.42$ (1)°	Block, colourless
$\gamma = 104.41$ (2)°	$0.26 \times 0.24 \times 0.21$ mm
$V = 1017.4$ (4) Å^3	

Data collection

Nonius MACH3 diffractometer	3574 independent reflections
Radiation source: fine-focus sealed tube	2653 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.013$
$\omega–2\theta$ scans	$\theta_{max} = 25.0°$, $\theta_{min} = 2.1°$
Absorption correction: ψ scan (North *et al.*, 1968)	$h = -1 \rightarrow 8$
	$k = -12 \rightarrow 12$
	$l = -17 \rightarrow 17$
$T_{min} = 0.976$, $T_{max} = 0.980$	3 standard reflections every 60 min
4471 measured reflections	intensity decay: none

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.043$	
$wR(F^2) = 0.129$	$w = 1/[\sigma^2(F_o^2) + (0.0609P)^2 + 0.3979P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	
3574 reflections	$(\Delta/\sigma)_{max} < 0.001$
268 parameters	$\Delta\rho_{max} = 0.23$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.18$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: *SHELXL97* (Sheldrick, 2008), Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.013 (3)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C22	0.4600 (4)	0.2952 (4)	0.0056 (2)	0.0841 (9)
H22A	0.4922	0.3586	−0.0293	0.101*
H22B	0.3534	0.2153	−0.0339	0.101*
H22C	0.5642	0.2613	0.0178	0.101*
H1N	−0.286 (4)	−0.135 (3)	0.2897 (18)	0.061 (7)*
O4	0.68460 (19)	0.35699 (15)	0.22606 (11)	0.0519 (4)
O3	0.36747 (19)	0.26111 (15)	0.50993 (10)	0.0523 (4)
N1	−0.1712 (2)	−0.09684 (18)	0.30488 (13)	0.0405 (4)
O1	0.41288 (19)	−0.16053 (16)	0.25103 (12)	0.0588 (4)
C6	0.1238 (2)	−0.11864 (19)	0.27165 (13)	0.0323 (4)
C1	−0.0644 (2)	−0.17812 (19)	0.25700 (13)	0.0347 (4)
C8	0.0925 (2)	0.09809 (19)	0.40306 (13)	0.0346 (4)
C9	−0.0944 (2)	0.0320 (2)	0.38398 (14)	0.0356 (4)
C15	0.4536 (2)	0.20151 (19)	0.27900 (14)	0.0371 (4)
H15	0.5452	0.1991	0.3256	0.044*
O2	0.0990 (2)	0.30115 (19)	0.54511 (14)	0.0765 (6)
C5	0.2404 (3)	−0.2085 (2)	0.23209 (15)	0.0407 (5)
C16	0.5036 (3)	0.28065 (19)	0.22121 (15)	0.0388 (4)
O6	0.4166 (2)	0.36880 (18)	0.09651 (13)	0.0659 (5)
C19	0.1316 (3)	0.1295 (2)	0.19881 (14)	0.0393 (4)
H19	0.0068	0.0788	0.1914	0.047*
C7	0.2165 (2)	0.03861 (18)	0.33288 (13)	0.0330 (4)
H7	0.3332	0.0471	0.3740	0.040*
C14	0.2679 (2)	0.12545 (18)	0.26814 (13)	0.0332 (4)
O5	0.0588 (2)	0.21801 (19)	0.06860 (13)	0.0656 (5)
C3	−0.0564 (3)	−0.3963 (2)	0.12134 (17)	0.0557 (6)
H3A	−0.0602	−0.3578	0.0694	0.067*
H3B	−0.1143	−0.4991	0.0910	0.067*
C18	0.1810 (3)	0.2088 (2)	0.14062 (15)	0.0430 (5)
C17	0.3684 (3)	0.2858 (2)	0.15175 (15)	0.0438 (5)
C11	0.1788 (3)	0.2281 (2)	0.49145 (15)	0.0446 (5)
C2	−0.1646 (3)	−0.3315 (2)	0.19699 (16)	0.0448 (5)
H2A	−0.2869	−0.3398	0.1631	0.054*
H2B	−0.1832	−0.3840	0.2408	0.054*
C10	−0.2342 (3)	0.0813 (2)	0.44419 (16)	0.0479 (5)
H10A	−0.1986	0.0885	0.5112	0.058*
H10B	−0.3565	0.0135	0.4152	0.058*
H10C	−0.2366	0.1733	0.4445	0.058*
C4	0.1457 (3)	−0.3643 (2)	0.16960 (18)	0.0539 (6)
H4A	0.1496	−0.4198	0.2111	0.065*
H4B	0.2156	−0.3952	0.1179	0.065*
C20	−0.1304 (3)	0.1336 (3)	0.04654 (18)	0.0630 (7)
H20A	−0.1993	0.1503	−0.0050	0.076*
H20B	−0.1835	0.1588	0.1051	0.076*
H20C	−0.1369	0.0342	0.0244	0.076*

C21	0.8277 (3)	0.3578 (3)	0.29756 (19)	0.0573 (6)
H21A	0.9466	0.4146	0.2935	0.069*
H21B	0.8305	0.2616	0.2845	0.069*
H21C	0.8025	0.3978	0.3630	0.069*
C13	0.6642 (3)	0.4322 (3)	0.5930 (2)	0.0768 (8)
H13A	0.7287	0.5156	0.6512	0.092*
H13B	0.6768	0.4544	0.5347	0.092*
H13C	0.7174	0.3564	0.5904	0.092*
C12	0.4662 (3)	0.3867 (3)	0.59723 (18)	0.0667 (7)
H12A	0.4530	0.3652	0.6565	0.080*
H12B	0.4124	0.4635	0.6007	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C22	0.0715 (18)	0.133 (3)	0.080 (2)	0.0367 (18)	0.0272 (15)	0.072 (2)
O4	0.0339 (8)	0.0517 (9)	0.0690 (10)	0.0004 (6)	0.0116 (7)	0.0298 (8)
O3	0.0343 (8)	0.0524 (9)	0.0480 (8)	0.0054 (6)	0.0031 (6)	−0.0016 (7)
N1	0.0211 (8)	0.0445 (9)	0.0519 (10)	0.0076 (7)	0.0058 (7)	0.0150 (8)
O1	0.0272 (8)	0.0560 (9)	0.0804 (11)	0.0141 (7)	0.0118 (7)	0.0085 (8)
C6	0.0257 (9)	0.0357 (10)	0.0354 (9)	0.0083 (7)	0.0064 (7)	0.0137 (8)
C1	0.0276 (9)	0.0381 (10)	0.0394 (10)	0.0079 (8)	0.0057 (8)	0.0172 (8)
C8	0.0294 (9)	0.0378 (10)	0.0375 (10)	0.0117 (8)	0.0073 (8)	0.0139 (8)
C9	0.0310 (10)	0.0411 (10)	0.0407 (10)	0.0154 (8)	0.0094 (8)	0.0189 (8)
C15	0.0280 (9)	0.0374 (10)	0.0428 (11)	0.0072 (8)	0.0046 (8)	0.0139 (8)
O2	0.0504 (10)	0.0693 (11)	0.0758 (12)	0.0162 (8)	0.0164 (9)	−0.0140 (9)
C5	0.0321 (10)	0.0433 (11)	0.0455 (11)	0.0111 (8)	0.0085 (8)	0.0152 (9)
C16	0.0322 (10)	0.0323 (10)	0.0487 (11)	0.0065 (8)	0.0120 (8)	0.0128 (8)
O6	0.0674 (11)	0.0684 (11)	0.0800 (12)	0.0172 (9)	0.0201 (9)	0.0508 (10)
C19	0.0279 (9)	0.0405 (10)	0.0452 (11)	0.0065 (8)	0.0061 (8)	0.0138 (9)
C7	0.0230 (8)	0.0367 (10)	0.0379 (10)	0.0082 (7)	0.0054 (7)	0.0129 (8)
C14	0.0278 (9)	0.0311 (9)	0.0370 (10)	0.0084 (7)	0.0077 (7)	0.0082 (8)
O5	0.0493 (10)	0.0834 (12)	0.0730 (11)	0.0173 (8)	−0.0018 (8)	0.0458 (10)
C3	0.0474 (13)	0.0447 (12)	0.0554 (13)	0.0020 (10)	0.0087 (10)	0.0035 (10)
C18	0.0408 (11)	0.0454 (11)	0.0438 (11)	0.0160 (9)	0.0042 (9)	0.0167 (9)
C17	0.0456 (12)	0.0406 (11)	0.0496 (12)	0.0129 (9)	0.0128 (9)	0.0215 (9)
C11	0.0380 (11)	0.0462 (11)	0.0463 (11)	0.0114 (9)	0.0111 (9)	0.0133 (9)
C2	0.0322 (10)	0.0419 (11)	0.0521 (12)	0.0030 (8)	0.0034 (9)	0.0145 (9)
C10	0.0340 (11)	0.0593 (13)	0.0570 (13)	0.0217 (9)	0.0163 (9)	0.0223 (10)
C4	0.0470 (12)	0.0435 (12)	0.0636 (14)	0.0163 (10)	0.0146 (11)	0.0080 (10)
C20	0.0466 (13)	0.0887 (18)	0.0515 (13)	0.0309 (13)	0.0002 (10)	0.0186 (13)
C21	0.0307 (11)	0.0586 (14)	0.0789 (16)	0.0055 (10)	0.0112 (11)	0.0268 (12)
C13	0.0482 (14)	0.0747 (17)	0.0697 (17)	0.0042 (12)	−0.0008 (12)	−0.0059 (14)
C12	0.0475 (13)	0.0650 (15)	0.0528 (14)	0.0008 (11)	0.0051 (11)	−0.0078 (12)

Geometric parameters (Å, º)

C22—O6	1.402 (3)	C19—H19	0.9300
C22—H22A	0.9600	C7—C14	1.525 (2)
C22—H22B	0.9600	C7—H7	0.9800
C22—H22C	0.9600	O5—C18	1.372 (2)
O4—C16	1.375 (2)	O5—C20	1.413 (3)
O4—C21	1.421 (3)	C3—C2	1.506 (3)
O3—C11	1.350 (2)	C3—C4	1.516 (3)
O3—C12	1.446 (3)	C3—H3A	0.9700
N1—C1	1.374 (2)	C3—H3B	0.9700
N1—C9	1.379 (3)	C18—C17	1.399 (3)
N1—H1N	0.83 (3)	C2—H2A	0.9700
O1—C5	1.234 (2)	C2—H2B	0.9700
C6—C1	1.358 (2)	C10—H10A	0.9600
C6—C5	1.453 (3)	C10—H10B	0.9600
C6—C7	1.512 (3)	C10—H10C	0.9600
C1—C2	1.486 (3)	C4—H4A	0.9700
C8—C9	1.355 (2)	C4—H4B	0.9700
C8—C11	1.461 (3)	C20—H20A	0.9600
C8—C7	1.528 (2)	C20—H20B	0.9600
C9—C10	1.508 (3)	C20—H20C	0.9600
C15—C16	1.379 (3)	C21—H21A	0.9600
C15—C14	1.386 (2)	C21—H21B	0.9600
C15—H15	0.9300	C21—H21C	0.9600
O2—C11	1.209 (2)	C13—C12	1.458 (3)
C5—C4	1.505 (3)	C13—H13A	0.9600
C16—C17	1.389 (3)	C13—H13B	0.9600
O6—C17	1.376 (2)	C13—H13C	0.9600
C19—C18	1.384 (3)	C12—H12A	0.9700
C19—C14	1.387 (3)	C12—H12B	0.9700
O6—C22—H22A	109.5	O5—C18—C19	125.06 (18)
O6—C22—H22B	109.5	O5—C18—C17	114.73 (18)
H22A—C22—H22B	109.5	C19—C18—C17	120.20 (18)
O6—C22—H22C	109.5	O6—C17—C16	120.62 (18)
H22A—C22—H22C	109.5	O6—C17—C18	120.21 (18)
H22B—C22—H22C	109.5	C16—C17—C18	119.13 (18)
C16—O4—C21	117.61 (16)	O2—C11—O3	121.13 (19)
C11—O3—C12	116.21 (17)	O2—C11—C8	126.93 (19)
C1—N1—C9	122.70 (16)	O3—C11—C8	111.93 (16)
C1—N1—H1N	116.1 (17)	C1—C2—C3	111.44 (16)
C9—N1—H1N	120.6 (17)	C1—C2—H2A	109.3
C1—C6—C5	119.71 (16)	C3—C2—H2A	109.3
C1—C6—C7	121.31 (16)	C1—C2—H2B	109.3
C5—C6—C7	118.90 (15)	C3—C2—H2B	109.3
C6—C1—N1	119.52 (17)	H2A—C2—H2B	108.0
C6—C1—C2	124.04 (17)	C9—C10—H10A	109.5

N1—C1—C2	116.30 (16)	C9—C10—H10B	109.5
C9—C8—C11	120.34 (17)	H10A—C10—H10B	109.5
C9—C8—C7	120.86 (17)	C9—C10—H10C	109.5
C11—C8—C7	118.80 (16)	H10A—C10—H10C	109.5
C8—C9—N1	119.58 (17)	H10B—C10—H10C	109.5
C8—C9—C10	126.59 (18)	C5—C4—C3	113.84 (18)
N1—C9—C10	113.77 (16)	C5—C4—H4A	108.8
C16—C15—C14	120.44 (18)	C3—C4—H4A	108.8
C16—C15—H15	119.8	C5—C4—H4B	108.8
C14—C15—H15	119.8	C3—C4—H4B	108.8
O1—C5—C6	121.43 (18)	H4A—C4—H4B	107.7
O1—C5—C4	120.26 (18)	O5—C20—H20A	109.5
C6—C5—C4	118.29 (16)	O5—C20—H20B	109.5
O4—C16—C15	124.14 (18)	H20A—C20—H20B	109.5
O4—C16—C17	115.44 (17)	O5—C20—H20C	109.5
C15—C16—C17	120.42 (17)	H20A—C20—H20C	109.5
C17—O6—C22	113.52 (19)	H20B—C20—H20C	109.5
C18—C19—C14	120.14 (17)	O4—C21—H21A	109.5
C18—C19—H19	119.9	O4—C21—H21B	109.5
C14—C19—H19	119.9	H21A—C21—H21B	109.5
C6—C7—C14	112.18 (15)	O4—C21—H21C	109.5
C6—C7—C8	110.40 (14)	H21A—C21—H21C	109.5
C14—C7—C8	111.39 (14)	H21B—C21—H21C	109.5
C6—C7—H7	107.6	C12—C13—H13A	109.5
C14—C7—H7	107.6	C12—C13—H13B	109.5
C8—C7—H7	107.6	H13A—C13—H13B	109.5
C15—C14—C19	119.66 (17)	C12—C13—H13C	109.5
C15—C14—C7	119.36 (16)	H13A—C13—H13C	109.5
C19—C14—C7	120.98 (16)	H13B—C13—H13C	109.5
C18—O5—C20	118.35 (18)	O3—C12—C13	110.0 (2)
C2—C3—C4	110.79 (18)	O3—C12—H12A	109.7
C2—C3—H3A	109.5	C13—C12—H12A	109.7
C4—C3—H3A	109.5	O3—C12—H12B	109.7
C2—C3—H3B	109.5	C13—C12—H12B	109.7
C4—C3—H3B	109.5	H12A—C12—H12B	108.2
H3A—C3—H3B	108.1		
C5—C6—C1—N1	171.81 (16)	C6—C7—C14—C15	−120.58 (18)
C7—C6—C1—N1	−5.1 (3)	C8—C7—C14—C15	115.10 (18)
C5—C6—C1—C2	−3.6 (3)	C6—C7—C14—C19	59.5 (2)
C7—C6—C1—C2	179.45 (17)	C8—C7—C14—C19	−64.8 (2)
C9—N1—C1—C6	−14.9 (3)	C20—O5—C18—C19	−4.4 (3)
C9—N1—C1—C2	160.86 (18)	C20—O5—C18—C17	174.56 (19)
C11—C8—C9—N1	−174.65 (17)	C14—C19—C18—O5	178.62 (19)
C7—C8—C9—N1	5.4 (3)	C14—C19—C18—C17	−0.3 (3)
C11—C8—C9—C10	2.4 (3)	C22—O6—C17—C16	91.5 (3)
C7—C8—C9—C10	−177.55 (17)	C22—O6—C17—C18	−90.4 (3)
C1—N1—C9—C8	14.7 (3)	O4—C16—C17—O6	−3.2 (3)

C1—N1—C9—C10	−162.71 (17)	C15—C16—C17—O6	177.59 (18)
C1—C6—C5—O1	−173.80 (19)	O4—C16—C17—C18	178.77 (17)
C7—C6—C5—O1	3.2 (3)	C15—C16—C17—C18	−0.5 (3)
C1—C6—C5—C4	4.2 (3)	O5—C18—C17—O6	3.4 (3)
C7—C6—C5—C4	−178.84 (18)	C19—C18—C17—O6	−177.62 (18)
C21—O4—C16—C15	−2.2 (3)	O5—C18—C17—C16	−178.56 (18)
C21—O4—C16—C17	178.60 (18)	C19—C18—C17—C16	0.5 (3)
C14—C15—C16—O4	−178.84 (17)	C12—O3—C11—O2	0.6 (3)
C14—C15—C16—C17	0.3 (3)	C12—O3—C11—C8	−178.82 (19)
C1—C6—C7—C14	−103.04 (19)	C9—C8—C11—O2	−12.8 (3)
C5—C6—C7—C14	80.0 (2)	C7—C8—C11—O2	167.2 (2)
C1—C6—C7—C8	21.8 (2)	C9—C8—C11—O3	166.62 (17)
C5—C6—C7—C8	−155.10 (16)	C7—C8—C11—O3	−13.4 (2)
C9—C8—C7—C6	−22.0 (2)	C6—C1—C2—C3	−24.4 (3)
C11—C8—C7—C6	158.08 (16)	N1—C1—C2—C3	160.04 (18)
C9—C8—C7—C14	103.36 (19)	C4—C3—C2—C1	49.9 (3)
C11—C8—C7—C14	−76.6 (2)	O1—C5—C4—C3	−158.6 (2)
C16—C15—C14—C19	−0.2 (3)	C6—C5—C4—C3	23.5 (3)
C16—C15—C14—C7	179.89 (16)	C2—C3—C4—C5	−50.4 (3)
C18—C19—C14—C15	0.1 (3)	C11—O3—C12—C13	−164.3 (2)
C18—C19—C14—C7	−179.92 (17)		

Hydrogen-bond geometry (Å, °)

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C7—H7⋯O3	0.98	2.36	2.720 (2)	101
N1—H1*N*⋯O1[i]	0.83 (3)	2.21 (3)	2.995 (2)	160 (3)
C2—H2*B*⋯O4[ii]	0.97	2.55	3.340 (3)	138
C10—H10*B*⋯O1[i]	0.96	2.59	3.429 (3)	146

Symmetry codes: (i) $x-1, y, z$; (ii) $x-1, y-1, z$.