Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

7-*p*-Tolyl-10,11-dihydrobenzo[*h*]furo-[3,4-*b*]quinolin-8(7*H*)-one

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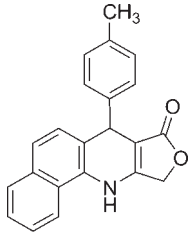
Received 1 February 2010; accepted 13 February 2010

Key indicators: single-crystal X-ray study; T = 223 K; mean σ(C–C) = 0.003 Å; R factor = 0.064; wR factor = 0.138; data-to-parameter ratio = 13.1.

In the title compound, $C_{22}H_{17}NO_2$, the fused ring system is essentially planar (r.m.s. deviation = 0.021 Å) and the dihedral angle between the dihydropyridine and tolyl rings is 80.98 (11)°. In the crystal, the molecules are linked into chains along the b axis by intermolecular N—H···O and C—H···O hydrogen bonds. Adjacent chains are linked by π–π interactions [centroid–centroid separation = 3.5748 (15) Å].

Related literature

For the biological activity of podophyllotoxin and its derivatives, see: Bosmans *et al.* (1989); Eycken *et al.* (1989); Hitosuyanagi *et al.* (1997, 1999); Lienard *et al.* (1991); Magedov *et al.* (2007); Poli & Giambastiani (2002); Tomioka *et al.* (1989, 1993); Tratrat *et al.* (2002). For a related structure, see: Shi & Ji (2009).



Experimental

Crystal data

$C_{22}H_{17}NO_2$
M_r = 327.37
Monoclinic, $P2_1/c$
a = 10.6954 (16) Å
b = 13.0566 (18) Å
c = 12.183 (2) Å
β = 107.322 (3)°
V = 1624.1 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 223 K
0.60 × 0.34 × 0.30 mm

Data collection

Rigaku Mercury diffractometer
Absorption correction: multi-scan (Jacobson, 1998)
T_{min} = 0.770, T_{max} = 0.975
15611 measured reflections
2978 independent reflections
2476 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.138
S = 1.18
2978 reflections
228 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.87	2.00	2.802 (2)	153
C12—H12···O1^{i}	0.94	2.49	3.248 (3)	137

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

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSC, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The author thanks the Scientific Research Item of Xuzhou Institute of Technology (grant No. XKY2009114) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI5030).

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supporting information

Acta Cryst. (2010). E**66**, o668 [doi:10.1107/S160053681000591X]

7-*p*-Tolyl-10,11-dihydrobenzo[*h*]furo[3,4-*b*]quinolin-8(7*H*)-one

Chunling Shi

S1. Comment

Podophyllotoxin is an antitumor lignan that inhibits microtubule assembly (Eycken *et al.*, 1989; Tomioka *et al.*, 1989; Bosmans *et al.*, 1989). Extensive structural modifications have been performed in order to obtain more potent and less toxic anticancer agents (Tomioka *et al.*, 1993; Lienard *et al.*, 1991; Poli *et al.*, 2002). Among them, 4-aza-podophllotoxin (9-aryl-4,9-dihydrofuro[3,4-b]quinolin-1(3*H*)-one) derivatives reported as powerful DNA topoisomerase II inhibitors, have recently attached considerable interest (Hitosuyanagi *et al.*, 1997; Hitosuyanagi *et al.*, 1999; Tratrat *et al.*, 2002; Magedov *et al.*, 2007). We report here the crystal structure of the title compound, which was synthesized by the three-component reaction of naphthalen-1-amine with 4-methylbenzaldehyde and tetronic acid catalyzed by L-proline using ethanol as solvent at 353 K.

In the title compound, the 1,4-dihydropyridine (C1–C5/N1) and furanone rings are planar (Fig. 1) and both are coplanar with the naphthalene ring system i.e the fused ring system is essentially planar (r.m.s. deviation 0.021 Å). The dihedral angle between C1–C5/N1 and C16–C21 planes is 80.98 (11)°. The conformation of the title molecule differs from that of a related molecule, 7-methyl-9-*p*-tolyl-4,9-dihydrofuro[3,4-b]quinolin-1(3*H*)-one (Shi *et al.*, 2009).

In the crystal structure, the molecules are linked by N1—H1···O2 and C12—H12···O1 intermolecular hydrogen bonds (Table 1) to form chains (Fig. 2) along the *b* axis. The adjacent chains are linked through π-π interactions between O1/C14/C4/C5/C15 and C1/C2/C6-C8/C13 rings with a centroid-centroid separation of 3.5748 (15) Å.

S2. Experimental

The title compound was prepared by the reaction of naphthalen-1-amine (1 mmol) and 4-methylbenzalhyde (1 mmol) with tetronic acid (1 mmol) in the presence of L-proline (0.1 mmol) in ethanol (2 ml) at 353 K. Crystals of the title compound suitable for X-ray diffraction were obtained by slow evaporation of a *N*,*N*-dimethylformamide and ethanol solution. ^{1}H NMR (DMSO-d_6, δ): 2.21 (3*H*, s, CH_3), 4.98 (1*H*, d, J = 16.0 Hz, CH_2), 5.07 (1*H*, d, J = 16.0 Hz, CH_2), 5.13 (1*H*, s, CH), 7.05 (2*H*, d, J = 8.0 Hz, ArH), 7.12 (3*H*, dd, J_1 = 6.4 Hz, J_2 = 8.0 Hz, ArH), 7.46 (1*H*, d, J = 8.8 Hz, ArH), 7.51-7.55 (1*H*, m, ArH), 7.60-7.64 (1*H*, m, ArH), 7.84 (1*H*, d, J = 8.0 Hz, ArH), 8.21 (1*H*, d, J = 8.0 Hz, ArH), 10.22 (1*H*, s, NH).

S3. Refinement

H atoms were placed in calculated positions [N–H = 0.87 Å and C–H = 0.94-0.99 Å] and included in the final cycles of refinement using a riding model, with U_{iso}(H) = 1.2-1.5 U_{eq}(C).

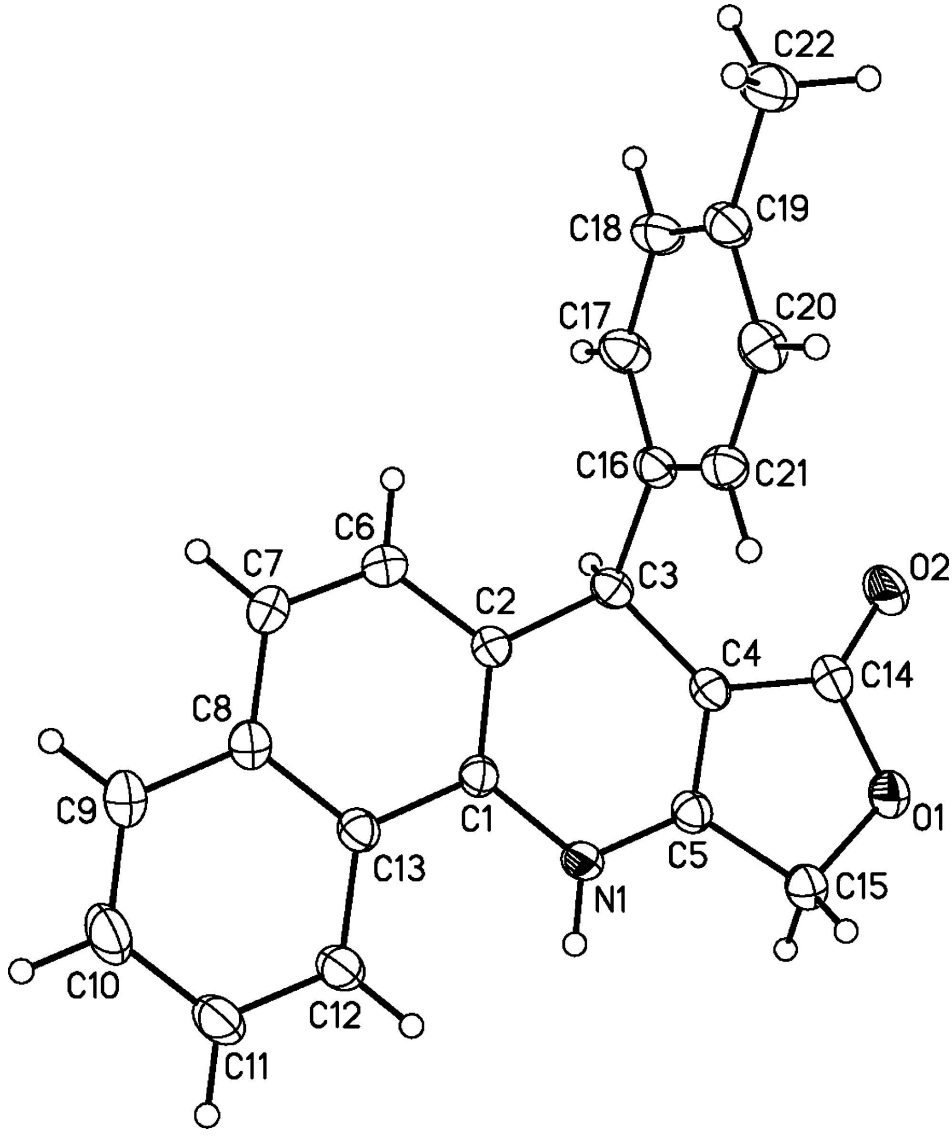

Figure 1

The molecular structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

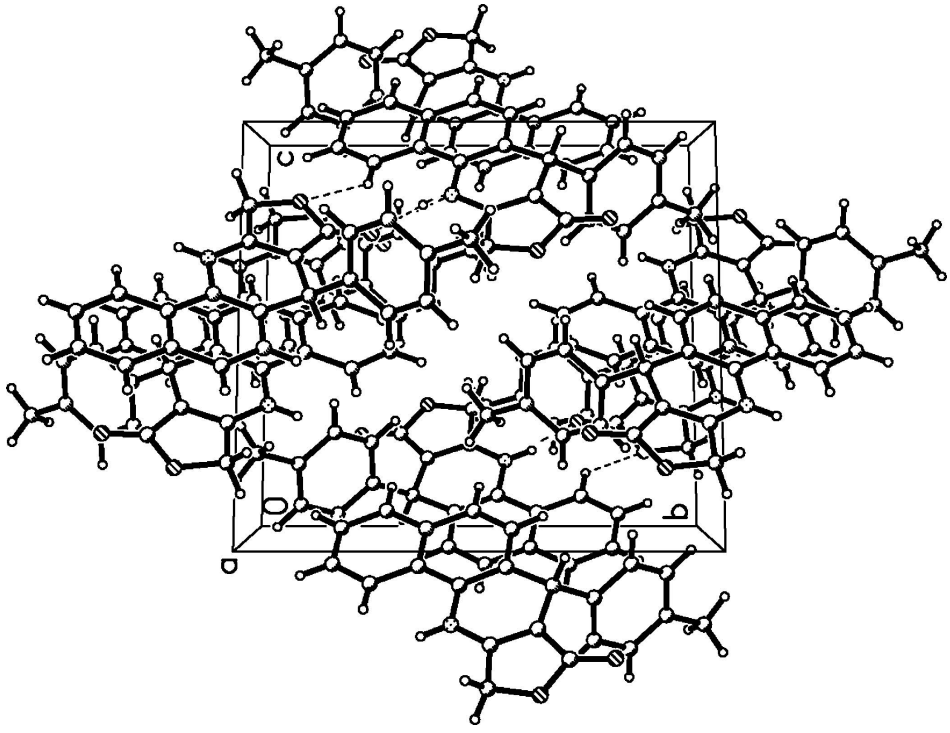

Figure 2

The crystal packing of the title compound.

7-*p*-Tolyl-10,11-dihydrobenzo[*h*]furo[3,4-*b*]quinolin-8(7*H*)-one

Crystal data

$C_{22}H_{17}NO_2$
$M_r = 327.37$
Monoclinic, $P2_1/c$
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$a = 10.6954\ (16)$ Å
$b = 13.0566\ (18)$ Å
$c = 12.183\ (2)$ Å
$\beta = 107.322\ (3)°$
$V = 1624.1\ (4)$ Å^3
$Z = 4$
$F(000) = 688$
$D_x = 1.339$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71070$ Å
Cell parameters from 5302 reflections
$\theta = 3.0–25.3°$
$\mu = 0.09$ mm^{-1}
$T = 223$ K
Block, colourless
0.60 × 0.34 × 0.30 mm

Data collection

Rigaku Mercury diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 7.31 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (Jacobson, 1998)
$T_{min} = 0.770$, $T_{max} = 0.975$
15611 measured reflections
2978 independent reflections
2476 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 25.4°$, $\theta_{min} = 3.1°$
$h = -12\rightarrow11$
$k = -15\rightarrow12$
$l = -14\rightarrow14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.064$
$wR(F^2) = 0.138$
$S = 1.18$
2978 reflections
228 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0503P)^2 + 0.6601P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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}
O1	1.04628 (16)	0.87892 (12)	0.19046 (14)	0.0446 (4)
O2	1.02197 (17)	0.72658 (13)	0.26734 (16)	0.0520 (5)
N1	0.88595 (17)	1.05854 (13)	0.32900 (16)	0.0357 (5)
H1	0.8921	1.1200	0.3035	0.043*
C1	0.8218 (2)	1.04144 (15)	0.41266 (18)	0.0303 (5)
C2	0.8127 (2)	0.94420 (16)	0.45353 (18)	0.0321 (5)
C3	0.8734 (2)	0.84879 (15)	0.41573 (19)	0.0323 (5)
H3	0.9455	0.8252	0.4827	0.039*
C4	0.9332 (2)	0.88088 (16)	0.32405 (18)	0.0327 (5)
C5	0.9376 (2)	0.97791 (16)	0.28925 (19)	0.0330 (5)
C6	0.7450 (2)	0.93198 (18)	0.5358 (2)	0.0442 (6)
H6	0.7384	0.8661	0.5648	0.053*
C7	0.6888 (3)	1.01196 (18)	0.5748 (2)	0.0481 (7)
H7	0.6436	1.0004	0.6291	0.058*
C8	0.6977 (2)	1.11247 (17)	0.5345 (2)	0.0398 (6)
C9	0.6407 (3)	1.19767 (19)	0.5729 (2)	0.0518 (7)
H9	0.5941	1.1878	0.6264	0.062*
C10	0.6521 (3)	1.2934 (2)	0.5338 (3)	0.0570 (7)
H10	0.6140	1.3493	0.5605	0.068*
C11	0.7207 (3)	1.30888 (18)	0.4538 (2)	0.0515 (7)
H11	0.7296	1.3755	0.4279	0.062*
C12	0.7747 (2)	1.22844 (16)	0.4130 (2)	0.0413 (6)
H12	0.8189	1.2400	0.3580	0.050*
C13	0.7652 (2)	1.12779 (16)	0.45230 (19)	0.0330 (5)
C14	1.0009 (2)	0.81812 (18)	0.2636 (2)	0.0392 (6)

C15	1.0079 (2)	0.98353 (17)	0.2007 (2)	0.0410 (6)
H15A	0.9500	1.0088	0.1274	0.049*
H15B	1.0846	1.0284	0.2258	0.049*
C16	0.7751 (2)	0.76137 (15)	0.38090 (19)	0.0332 (5)
C17	0.7769 (2)	0.68286 (17)	0.4572 (2)	0.0436 (6)
H17	0.8420	0.6822	0.5288	0.052*
C18	0.6844 (3)	0.60477 (17)	0.4302 (2)	0.0463 (6)
H18	0.6875	0.5527	0.4842	0.056*
C19	0.5881 (2)	0.60229 (17)	0.3254 (2)	0.0395 (6)
C20	0.5876 (2)	0.68095 (17)	0.2488 (2)	0.0407 (6)
H20	0.5239	0.6809	0.1765	0.049*
C21	0.6785 (2)	0.75938 (17)	0.2760 (2)	0.0376 (5)
H21	0.6747	0.8121	0.2225	0.045*
C22	0.4884 (3)	0.51737 (19)	0.2961 (3)	0.0541 (7)
H22A	0.5015	0.4722	0.3618	0.081*
H22B	0.4985	0.4788	0.2312	0.081*
H22C	0.4010	0.5464	0.2763	0.081*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0519 (10)	0.0402 (9)	0.0490 (10)	0.0012 (7)	0.0264 (9)	−0.0075 (8)
O2	0.0626 (12)	0.0345 (10)	0.0664 (12)	0.0061 (8)	0.0305 (10)	−0.0097 (8)
N1	0.0415 (11)	0.0252 (9)	0.0463 (12)	0.0009 (8)	0.0222 (9)	0.0003 (8)
C1	0.0299 (11)	0.0312 (12)	0.0313 (12)	−0.0018 (9)	0.0113 (9)	−0.0033 (9)
C2	0.0358 (12)	0.0297 (12)	0.0310 (12)	−0.0014 (9)	0.0101 (10)	−0.0026 (9)
C3	0.0336 (12)	0.0266 (11)	0.0348 (12)	0.0022 (8)	0.0076 (10)	0.0009 (9)
C4	0.0306 (12)	0.0307 (12)	0.0357 (13)	−0.0018 (9)	0.0084 (10)	−0.0052 (9)
C5	0.0316 (12)	0.0320 (12)	0.0367 (13)	−0.0003 (9)	0.0119 (10)	−0.0032 (9)
C6	0.0605 (16)	0.0341 (13)	0.0444 (15)	−0.0012 (11)	0.0254 (12)	0.0034 (11)
C7	0.0632 (17)	0.0431 (14)	0.0503 (16)	0.0005 (12)	0.0355 (14)	−0.0009 (11)
C8	0.0432 (14)	0.0387 (13)	0.0404 (13)	0.0012 (10)	0.0171 (11)	−0.0048 (10)
C9	0.0601 (17)	0.0476 (16)	0.0573 (17)	0.0051 (12)	0.0321 (14)	−0.0091 (12)
C10	0.0614 (18)	0.0427 (16)	0.075 (2)	0.0090 (12)	0.0321 (16)	−0.0141 (13)
C11	0.0565 (16)	0.0305 (13)	0.0739 (19)	0.0039 (11)	0.0291 (14)	−0.0036 (12)
C12	0.0426 (13)	0.0309 (12)	0.0540 (16)	0.0001 (10)	0.0198 (12)	−0.0020 (11)
C13	0.0313 (12)	0.0312 (12)	0.0368 (13)	−0.0018 (9)	0.0108 (10)	−0.0039 (9)
C14	0.0393 (13)	0.0370 (14)	0.0409 (14)	−0.0001 (10)	0.0114 (11)	−0.0074 (10)
C15	0.0456 (14)	0.0368 (13)	0.0450 (15)	−0.0006 (10)	0.0201 (11)	−0.0048 (10)
C16	0.0366 (12)	0.0256 (11)	0.0379 (13)	0.0019 (9)	0.0118 (10)	−0.0013 (9)
C17	0.0518 (15)	0.0333 (13)	0.0394 (14)	−0.0025 (11)	0.0038 (11)	0.0035 (10)
C18	0.0605 (16)	0.0293 (12)	0.0495 (16)	−0.0050 (11)	0.0168 (13)	0.0046 (10)
C19	0.0372 (13)	0.0318 (12)	0.0523 (15)	−0.0022 (9)	0.0178 (11)	−0.0070 (10)
C20	0.0358 (13)	0.0414 (13)	0.0410 (14)	−0.0001 (10)	0.0056 (10)	−0.0050 (11)
C21	0.0418 (13)	0.0320 (12)	0.0383 (14)	0.0018 (10)	0.0109 (11)	0.0027 (10)
C22	0.0510 (15)	0.0437 (15)	0.071 (2)	−0.0125 (12)	0.0231 (14)	−0.0085 (13)

Geometric parameters (Å, º)

O1—C14	1.385 (3)	C9—H9	0.94
O1—C15	1.442 (3)	C10—C11	1.398 (4)
O2—C14	1.215 (3)	C10—H10	0.94
N1—C5	1.344 (3)	C11—C12	1.362 (3)
N1—C1	1.406 (3)	C11—H11	0.94
N1—H1	0.87	C12—C13	1.413 (3)
C1—C2	1.378 (3)	C12—H12	0.94
C1—C13	1.430 (3)	C15—H15A	0.98
C2—C6	1.409 (3)	C15—H15B	0.98
C2—C3	1.538 (3)	C16—C17	1.380 (3)
C3—C4	1.503 (3)	C16—C21	1.384 (3)
C3—C16	1.524 (3)	C17—C18	1.390 (3)
C3—H3	0.99	C17—H17	0.94
C4—C5	1.341 (3)	C18—C19	1.382 (3)
C4—C14	1.433 (3)	C18—H18	0.94
C5—C15	1.489 (3)	C19—C20	1.387 (3)
C6—C7	1.359 (3)	C19—C22	1.506 (3)
C6—H6	0.94	C20—C21	1.383 (3)
C7—C8	1.414 (3)	C20—H20	0.94
C7—H7	0.94	C21—H21	0.94
C8—C13	1.413 (3)	C22—H22A	0.97
C8—C9	1.413 (3)	C22—H22B	0.97
C9—C10	1.356 (4)	C22—H22C	0.97
C14—O1—C15	108.88 (16)	C11—C12—C13	120.8 (2)
C5—N1—C1	118.59 (18)	C11—C12—H12	119.6
C5—N1—H1	120.7	C13—C12—H12	119.6
C1—N1—H1	120.7	C8—C13—C12	118.4 (2)
C2—C1—N1	120.70 (18)	C8—C13—C1	119.01 (19)
C2—C1—C13	121.46 (19)	C12—C13—C1	122.6 (2)
N1—C1—C13	117.83 (18)	O2—C14—O1	119.4 (2)
C1—C2—C6	117.90 (19)	O2—C14—C4	131.3 (2)
C1—C2—C3	123.82 (18)	O1—C14—C4	109.28 (19)
C6—C2—C3	118.28 (19)	O1—C15—C5	103.55 (18)
C4—C3—C16	114.39 (18)	O1—C15—H15A	111.1
C4—C3—C2	107.95 (17)	C5—C15—H15A	111.1
C16—C3—C2	111.84 (17)	O1—C15—H15B	111.1
C4—C3—H3	107.5	C5—C15—H15B	111.1
C16—C3—H3	107.5	H15A—C15—H15B	109.0
C2—C3—H3	107.5	C17—C16—C21	117.7 (2)
C5—C4—C14	107.9 (2)	C17—C16—C3	119.9 (2)
C5—C4—C3	124.11 (19)	C21—C16—C3	122.32 (19)
C14—C4—C3	127.9 (2)	C16—C17—C18	121.3 (2)
C4—C5—N1	124.7 (2)	C16—C17—H17	119.4
C4—C5—C15	110.36 (19)	C18—C17—H17	119.4
N1—C5—C15	124.93 (19)	C19—C18—C17	121.2 (2)

C7—C6—C2	122.4 (2)	C19—C18—H18	119.4
C7—C6—H6	118.8	C17—C18—H18	119.4
C2—C6—H6	118.8	C18—C19—C20	117.2 (2)
C6—C7—C8	120.6 (2)	C18—C19—C22	121.2 (2)
C6—C7—H7	119.7	C20—C19—C22	121.7 (2)
C8—C7—H7	119.7	C21—C20—C19	121.7 (2)
C13—C8—C9	119.0 (2)	C21—C20—H20	119.1
C13—C8—C7	118.6 (2)	C19—C20—H20	119.1
C9—C8—C7	122.4 (2)	C20—C21—C16	120.9 (2)
C10—C9—C8	121.1 (2)	C20—C21—H21	119.6
C10—C9—H9	119.4	C16—C21—H21	119.6
C8—C9—H9	119.4	C19—C22—H22A	109.5
C9—C10—C11	119.9 (2)	C19—C22—H22B	109.5
C9—C10—H10	120.0	H22A—C22—H22B	109.5
C11—C10—H10	120.0	C19—C22—H22C	109.5
C12—C11—C10	120.7 (2)	H22A—C22—H22C	109.5
C12—C11—H11	119.6	H22B—C22—H22C	109.5
C10—C11—H11	119.6		

C5—N1—C1—C2	0.4 (3)	C9—C8—C13—C1	−179.4 (2)
C5—N1—C1—C13	−178.79 (19)	C7—C8—C13—C1	0.1 (3)
N1—C1—C2—C6	−178.9 (2)	C11—C12—C13—C8	0.3 (4)
C13—C1—C2—C6	0.3 (3)	C11—C12—C13—C1	−179.3 (2)
N1—C1—C2—C3	1.9 (3)	C2—C1—C13—C8	−0.5 (3)
C13—C1—C2—C3	−178.92 (19)	N1—C1—C13—C8	178.7 (2)
C1—C2—C3—C4	−3.7 (3)	C2—C1—C13—C12	179.1 (2)
C6—C2—C3—C4	177.1 (2)	N1—C1—C13—C12	−1.7 (3)
C1—C2—C3—C16	−130.4 (2)	C15—O1—C14—O2	179.3 (2)
C6—C2—C3—C16	50.4 (3)	C15—O1—C14—C4	−0.6 (2)
C16—C3—C4—C5	128.9 (2)	C5—C4—C14—O2	179.8 (3)
C2—C3—C4—C5	3.7 (3)	C3—C4—C14—O2	3.2 (4)
C16—C3—C4—C14	−54.9 (3)	C5—C4—C14—O1	−0.3 (3)
C2—C3—C4—C14	179.9 (2)	C3—C4—C14—O1	−176.95 (19)
C14—C4—C5—N1	−178.8 (2)	C14—O1—C15—C5	1.1 (2)
C3—C4—C5—N1	−2.0 (4)	C4—C5—C15—O1	−1.3 (3)
C14—C4—C5—C15	1.0 (3)	N1—C5—C15—O1	178.54 (19)
C3—C4—C5—C15	177.8 (2)	C4—C3—C16—C17	137.1 (2)
C1—N1—C5—C4	−0.4 (3)	C2—C3—C16—C17	−99.8 (2)
C1—N1—C5—C15	179.8 (2)	C4—C3—C16—C21	−45.9 (3)
C1—C2—C6—C7	0.4 (4)	C2—C3—C16—C21	77.3 (3)
C3—C2—C6—C7	179.6 (2)	C21—C16—C17—C18	−0.5 (3)
C2—C6—C7—C8	−0.8 (4)	C3—C16—C17—C18	176.7 (2)
C6—C7—C8—C13	0.5 (4)	C16—C17—C18—C19	0.7 (4)
C6—C7—C8—C9	−180.0 (2)	C17—C18—C19—C20	−0.1 (4)
C13—C8—C9—C10	−1.3 (4)	C17—C18—C19—C22	179.7 (2)
C7—C8—C9—C10	179.2 (3)	C18—C19—C20—C21	−0.7 (3)
C8—C9—C10—C11	0.3 (4)	C22—C19—C20—C21	179.5 (2)
C9—C10—C11—C12	1.0 (4)	C19—C20—C21—C16	0.9 (3)

C10—C11—C12—C13	−1.3 (4)	C17—C16—C21—C20	−0.3 (3)
C9—C8—C13—C12	1.0 (3)	C3—C16—C21—C20	−177.4 (2)
C7—C8—C13—C12	−179.5 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.87	2.00	2.802 (2)	153
C12—H12···O1^{i}	0.94	2.49	3.248 (3)	137

Symmetry code: (i) −*x*+2, *y*+1/2, −*z*+1/2.