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Methyl 5-phenyl-1,2,3,4,4a,5,5a,13c-octahydro-6*H*-benzo[*f*]chromeno[3,4-*b*]-indolizine-5a-carboxylate

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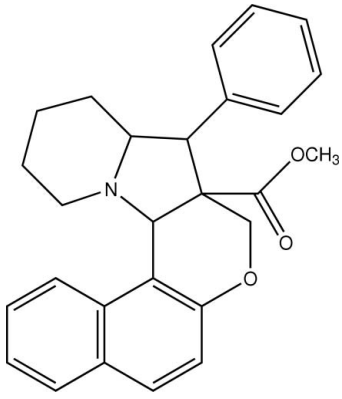
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.044; wR factor = 0.122; data-to-parameter ratio = 16.5.

In the title compound, $C_{27}H_{27}NO_3$, the pyrrolidine ring exhibits a twist conformation and the piperidine ring exhibits a chair conformation. The pyrrolidine ring makes dihedral angles of 54.47 (5), 51.50 (5) and 73.37 (6)° with the naphthalene ring system and the tetrahydropyran and phenyl rings, respectively. The structure is stabilized by intramolecular C—H···O and C—H···N interactions.

Related literature

For general background to the applications and biological activity of indolizine derivatives, see: Gubin *et al.* (1992); Gupta *et al.* (2003); Poty *et al.* (1994); Hema *et al.* (2003); Malonne *et al.* (1998); Medda *et al.* (2003). For puckering parameters, see: Cremer and Pople (1975). For asymmetry parameters, see: Nardelli (1983).



Experimental

Crystal data

$C_{27}H_{27}NO_3$
M_r = 413.50
Triclinic, $P\overline{1}$
a = 9.4201 (3) Å
b = 10.6752 (3) Å
c = 11.0761 (3) Å
α = 78.262 (2)°
β = 77.911 (2)°
γ = 87.346 (2)°
V = 1066.34 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 K
0.30 × 0.20 × 0.15 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.975, T_{max} = 0.988
22685 measured reflections
4641 independent reflections
3461 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.122
S = 1.00
4641 reflections
281 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···O3	0.98	2.47	2.8240 (19)	101
C19—H19B···N1	0.97	2.55	2.885 (2)	100

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *APEX2* and *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2988).

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supporting information

Acta Cryst. (2009). E**65**, o1923–o1924 [doi:10.1107/S1600536809026774]

Methyl 5-phenyl-1,2,3,4,4a,5,5a,13c-octahydro-6*H*-benzo[*f*]chromeno[3,4-*b*]indolizine-5a-carboxylate

E. Theboral Sugi Kamala, S. Nirmala, L. Sudha, S. Kathiravan and R. Raghunathan

S1. Comment

Indolizines, the nitrogen containing heterocyclic systems, are widely distributed in nature; in particular, indolizine derivatives are an important class of heterocyclic bioactive compounds with a wide range of applications, such as pharmaceutical drugs, potential central nervous system depressants, calcium entry blockers, cardiovascular agents, spectral sensitizers and novel dyes(Gubin *et al.*, 1992; Gupta *et al.*, 2003; Poty *et al.*, 1994; Hema *et al.*, 2003).Moreover indolizine derivatives have been found to possess a variety of biological activities such as antiinflammatory (Malonne *et al.*, 1998), antiviral (Medda *et al.*, 2003).

Fig 1 shows the *ORTEP* plot of compound (I). Bond lengths and angles are comparable with other reported values.

In the molecule the pyrrolidine ring N1/C5/C6/C7/C8 exhibits *twist* conformation with assymetry parameters (Nardelli, 1983) ΔC_s(N1) =23.66 (1)/ (C8) = 14.95 (1) and with the puckering parameters (Cremer and Pople, 1975) q2 = 0.4749 (1)Å and φ2 = 155.74 (2)°. The six membered ring N1/C1—C5 exhibits *chair* conformation with assymetry parameters ΔC_s(N1) = 2.78 (1)/(C3) = 2.78 (1) and with the puckering parameters Q = 0.5788 (2) Å, Θ = 175.62 (2)° and φ = 145 (2)°. The sum of bond angles around N1 [331.99 (3)°] indicates sp^3 hybridization. The pyrrolidine ring makes dihedral angles of 54.47 (5)°, 51.50 (5)° and 73.37 (6)° with the napthalene,tetrahydro pyran and phenyl rings respectively. The napthalene and tetrahydro pyran rings are almost planar with each other with a dihedral angle of 8.88 (4)°,

In the crystal packing, atom O3 is involved in intramolecular C - H···O interactions and atom N1 contributes to C - H···N intramolecular interactions.

S2. Experimental

A mixture of (*Z*)-methyl 2-(1-formylnaphthalen-2-yloxy)-3-*p*-tolylacrylate and pipecolinic acid were refluxed in benzene for 20 h and the solvent was removed under reduced pressure. The crude product was subjected to column chromatography to get the pure product. The product was recrystallized from dry benzene by slow evaporation.

S3. Refinement

H atoms were placed in idealized positions and allowed to ride on their parent atoms, with C–H = 0.93 or 0.96 Å and Uĩso~(H)= 1.2–1.5U~eq~(C).

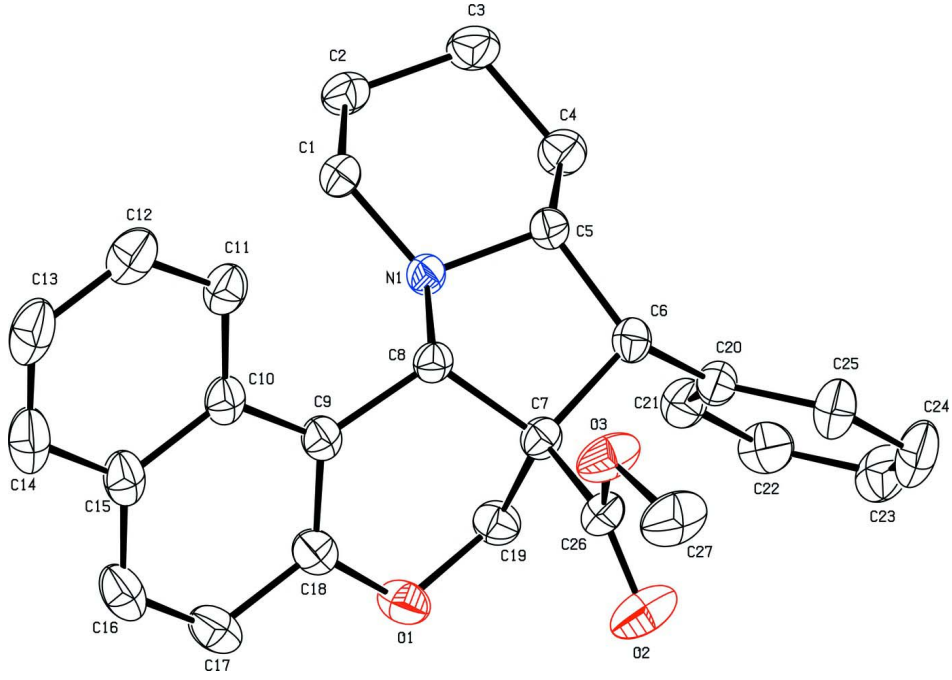

Figure 1

The molecular structure of (I) with 30% probability displacement ellipsoids.

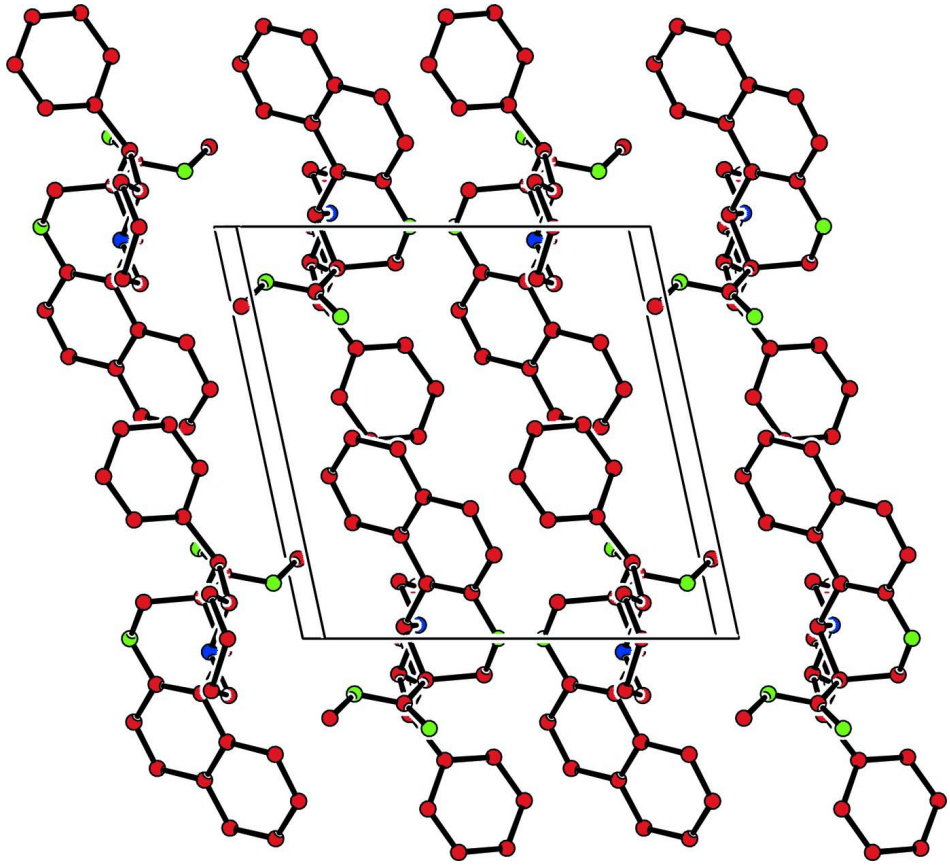

Figure 2

The packing of the molecules viewed along *b* axis.

Methyl 5-phenyl-1,2,3,4,4a,5,5a,13c-octahydro-6*H*- benzo[*f*]chromeno[3,4-*b*]indolizine-5a-carboxylate

Crystal data

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Triclinic, $P\overline{1}$
Hall symbol: -P 1
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$b = 10.6752$ (3) Å
$c = 11.0761$ (3) Å
$\alpha = 78.262$ (2)°
$\beta = 77.911$ (2)°
$\gamma = 87.346$ (2)°
$V = 1066.34$ (5) Å^3
$Z = 2$
$F(000) = 440$
$D_x = 1.288$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 22685 reflections
$\theta = 2.0$–$27.0°$
$\mu = 0.08$ mm^{-1}
$T = 293$ K
Needle, colourless
0.30 × 0.20 × 0.15 mm

Data collection

Bruker Kappa APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.975$, $T_{max} = 0.988$
22685 measured reflections
4641 independent reflections
3461 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 27.0°$, $\theta_{min} = 2.0°$
$h = -11 \rightarrow 12$
$k = -13 \rightarrow 13$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.122$
$S = 1.00$
4641 reflections
281 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
$w = 1/[\sigma^2(F_o^2) + (0.0534P)^2 + 0.3168P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.012 (2)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.54853 (15)	0.76212 (14)	0.13837 (13)	0.0396 (3)
H1A	0.4898	0.7171	0.2165	0.047*
H1B	0.5454	0.8527	0.1403	0.047*
C2	0.70388 (16)	0.71426 (15)	0.12642 (15)	0.0453 (4)
H2A	0.7052	0.6221	0.1343	0.054*
H2B	0.7439	0.7339	0.1943	0.054*
C3	0.79742 (17)	0.77508 (18)	0.00095 (16)	0.0540 (4)
H3A	0.8930	0.7357	−0.0077	0.065*
H3B	0.8089	0.8655	−0.0016	0.065*
C4	0.72958 (17)	0.75893 (18)	−0.10770 (16)	0.0504 (4)
H4A	0.7854	0.8056	−0.1864	0.060*
H4B	0.7295	0.6692	−0.1125	0.060*
C5	0.57534 (15)	0.80960 (13)	−0.08654 (13)	0.0366 (3)
H5	0.5812	0.8987	−0.0780	0.044*
C6	0.47933 (16)	0.80945 (13)	−0.18463 (13)	0.0378 (3)
H6	0.4643	0.8996	−0.2206	0.045*
C7	0.32917 (15)	0.76056 (13)	−0.10062 (13)	0.0365 (3)
C8	0.33931 (14)	0.78431 (12)	0.02922 (13)	0.0340 (3)
H8	0.3313	0.8762	0.0288	0.041*
C9	0.22386 (15)	0.71384 (13)	0.13304 (13)	0.0376 (3)
C10	0.17673 (15)	0.75355 (14)	0.25133 (14)	0.0412 (3)
C11	0.23444 (18)	0.86035 (16)	0.28129 (15)	0.0476 (4)
H11	0.3068	0.9082	0.2220	0.057*

C12	0.1870 (2)	0.8954 (2)	0.39497 (17)	0.0612 (5)
H12	0.2275	0.9661	0.4118	0.073*
C13	0.0784 (2)	0.8262 (2)	0.48593 (17)	0.0714 (6)
H13	0.0478	0.8495	0.5638	0.086*
C14	0.0178 (2)	0.7247 (2)	0.46007 (17)	0.0658 (5)
H14	−0.0558	0.6797	0.5205	0.079*
C15	0.06357 (17)	0.68546 (16)	0.34362 (15)	0.0501 (4)
C16	−0.00152 (18)	0.58123 (17)	0.31539 (17)	0.0572 (5)
H16	−0.0748	0.5357	0.3758	0.069*
C17	0.04018 (17)	0.54627 (16)	0.20290 (18)	0.0540 (4)
H17	−0.0050	0.4782	0.1857	0.065*
C18	0.15284 (16)	0.61359 (14)	0.11133 (15)	0.0431 (4)
C19	0.30894 (17)	0.61779 (14)	−0.08800 (15)	0.0441 (4)
H19A	0.3044	0.6000	−0.1696	0.053*
H19B	0.3921	0.5724	−0.0612	0.053*
C20	0.53277 (16)	0.74536 (14)	−0.29578 (14)	0.0413 (3)
C21	0.59051 (17)	0.62247 (15)	−0.28796 (15)	0.0478 (4)
H21	0.6021	0.5754	−0.2102	0.057*
C22	0.63086 (19)	0.56903 (18)	−0.39354 (18)	0.0571 (4)
H22	0.6691	0.4866	−0.3863	0.069*
C23	0.6149 (2)	0.6367 (2)	−0.50911 (18)	0.0688 (5)
H23	0.6415	0.6004	−0.5801	0.083*
C24	0.5594 (2)	0.7582 (2)	−0.51919 (17)	0.0750 (6)
H24	0.5486	0.8048	−0.5974	0.090*
C25	0.5192 (2)	0.81199 (18)	−0.41372 (15)	0.0589 (5)
H25	0.4823	0.8949	−0.4222	0.071*
C26	0.20768 (16)	0.83093 (14)	−0.15768 (14)	0.0420 (4)
C27	0.0803 (2)	1.02515 (18)	−0.1933 (2)	0.0728 (6)
H27A	0.0737	1.1075	−0.1703	0.109*
H27B	−0.0126	0.9839	−0.1656	0.109*
H27C	0.1093	1.0355	−0.2832	0.109*
N1	0.49017 (12)	0.74134 (10)	0.03267 (10)	0.0349 (3)
O1	0.17989 (12)	0.57199 (10)	0.00045 (11)	0.0524 (3)
O2	0.13962 (15)	0.78741 (13)	−0.21840 (14)	0.0738 (4)
O3	0.18643 (13)	0.94760 (11)	−0.13447 (13)	0.0610 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0406 (8)	0.0426 (8)	0.0360 (8)	0.0003 (6)	−0.0123 (6)	−0.0045 (6)
C2	0.0417 (8)	0.0485 (8)	0.0495 (9)	0.0022 (7)	−0.0186 (7)	−0.0092 (7)
C3	0.0359 (8)	0.0718 (11)	0.0571 (11)	−0.0019 (8)	−0.0116 (7)	−0.0172 (9)
C4	0.0384 (8)	0.0672 (10)	0.0466 (9)	−0.0003 (7)	−0.0068 (7)	−0.0153 (8)
C5	0.0401 (8)	0.0355 (7)	0.0331 (7)	−0.0035 (6)	−0.0068 (6)	−0.0042 (6)
C6	0.0427 (8)	0.0346 (7)	0.0344 (8)	0.0016 (6)	−0.0092 (6)	−0.0020 (6)
C7	0.0380 (7)	0.0355 (7)	0.0368 (8)	0.0032 (6)	−0.0112 (6)	−0.0062 (6)
C8	0.0354 (7)	0.0320 (6)	0.0348 (7)	0.0028 (5)	−0.0116 (6)	−0.0035 (5)
C9	0.0332 (7)	0.0377 (7)	0.0384 (8)	0.0052 (6)	−0.0093 (6)	0.0010 (6)

C10	0.0353 (7)	0.0467 (8)	0.0377 (8)	0.0105 (6)	−0.0105 (6)	0.0016 (6)
C11	0.0452 (9)	0.0583 (9)	0.0393 (8)	0.0089 (7)	−0.0116 (7)	−0.0083 (7)
C12	0.0594 (11)	0.0808 (13)	0.0485 (10)	0.0128 (9)	−0.0170 (9)	−0.0209 (9)
C13	0.0698 (13)	0.1044 (17)	0.0372 (10)	0.0179 (12)	−0.0085 (9)	−0.0145 (10)
C14	0.0548 (11)	0.0877 (14)	0.0406 (10)	0.0156 (10)	0.0001 (8)	0.0062 (9)
C15	0.0393 (8)	0.0583 (10)	0.0431 (9)	0.0113 (7)	−0.0065 (7)	0.0075 (7)
C16	0.0392 (9)	0.0582 (10)	0.0591 (11)	0.0025 (8)	0.0005 (8)	0.0119 (8)
C17	0.0380 (8)	0.0464 (9)	0.0707 (12)	−0.0031 (7)	−0.0078 (8)	0.0018 (8)
C18	0.0356 (7)	0.0408 (8)	0.0492 (9)	0.0031 (6)	−0.0088 (7)	−0.0013 (7)
C19	0.0437 (8)	0.0409 (8)	0.0480 (9)	−0.0014 (6)	−0.0076 (7)	−0.0113 (7)
C20	0.0406 (8)	0.0486 (8)	0.0342 (8)	−0.0004 (6)	−0.0088 (6)	−0.0058 (6)
C21	0.0476 (9)	0.0520 (9)	0.0443 (9)	0.0055 (7)	−0.0102 (7)	−0.0111 (7)
C22	0.0482 (9)	0.0654 (11)	0.0605 (11)	0.0050 (8)	−0.0059 (8)	−0.0255 (9)
C23	0.0632 (12)	0.0998 (16)	0.0486 (11)	0.0020 (11)	−0.0046 (9)	−0.0338 (11)
C24	0.0890 (15)	0.1004 (16)	0.0344 (10)	0.0088 (13)	−0.0153 (10)	−0.0098 (10)
C25	0.0689 (12)	0.0660 (11)	0.0385 (9)	0.0091 (9)	−0.0128 (8)	−0.0031 (8)
C26	0.0432 (8)	0.0482 (8)	0.0380 (8)	0.0029 (7)	−0.0154 (7)	−0.0098 (6)
C27	0.0742 (13)	0.0566 (11)	0.0990 (16)	0.0198 (9)	−0.0548 (12)	−0.0080 (10)
N1	0.0328 (6)	0.0373 (6)	0.0334 (6)	0.0007 (5)	−0.0090 (5)	−0.0022 (5)
O1	0.0482 (6)	0.0477 (6)	0.0609 (7)	−0.0112 (5)	−0.0050 (5)	−0.0140 (5)
O2	0.0823 (10)	0.0762 (9)	0.0850 (10)	0.0176 (7)	−0.0542 (8)	−0.0328 (8)
O3	0.0680 (8)	0.0456 (6)	0.0851 (9)	0.0183 (5)	−0.0509 (7)	−0.0167 (6)

Geometric parameters (Å, º)

C1—N1	1.4521 (18)	C12—H12	0.9300
C1—C2	1.5157 (19)	C13—C14	1.355 (3)
C1—H1A	0.9700	C13—H13	0.9300
C1—H1B	0.9700	C14—C15	1.412 (3)
C2—C3	1.517 (2)	C14—H14	0.9300
C2—H2A	0.9700	C15—C16	1.413 (3)
C2—H2B	0.9700	C16—C17	1.348 (3)
C3—C4	1.518 (2)	C16—H16	0.9300
C3—H3A	0.9700	C17—C18	1.412 (2)
C3—H3B	0.9700	C17—H17	0.9300
C4—C5	1.515 (2)	C18—O1	1.3604 (19)
C4—H4A	0.9700	C19—O1	1.4276 (18)
C4—H4B	0.9700	C19—H19A	0.9700
C5—N1	1.4618 (17)	C19—H19B	0.9700
C5—C6	1.553 (2)	C20—C25	1.383 (2)
C5—H5	0.9800	C20—C21	1.390 (2)
C6—C20	1.5128 (19)	C21—C22	1.379 (2)
C6—C7	1.568 (2)	C21—H21	0.9300
C6—H6	0.9800	C22—C23	1.370 (3)
C7—C26	1.5178 (19)	C22—H22	0.9300
C7—C19	1.5191 (19)	C23—C24	1.368 (3)
C7—C8	1.5328 (19)	C23—H23	0.9300
C8—N1	1.4788 (16)	C24—C25	1.380 (3)

C8—C9	1.5070 (19)	C24—H24	0.9300
C8—H8	0.9800	C25—H25	0.9300
C9—C18	1.375 (2)	C26—O2	1.1892 (18)
C9—C10	1.435 (2)	C26—O3	1.3203 (18)
C10—C11	1.412 (2)	C27—O3	1.4445 (18)
C10—C15	1.422 (2)	C27—H27A	0.9600
C11—C12	1.366 (2)	C27—H27B	0.9600
C11—H11	0.9300	C27—H27C	0.9600
C12—C13	1.393 (3)		

N1—C1—C2	110.04 (12)	C11—C12—H12	119.7
N1—C1—H1A	109.7	C13—C12—H12	119.7
C2—C1—H1A	109.7	C14—C13—C12	119.46 (18)
N1—C1—H1B	109.7	C14—C13—H13	120.3
C2—C1—H1B	109.7	C12—C13—H13	120.3
H1A—C1—H1B	108.2	C13—C14—C15	121.63 (18)
C1—C2—C3	111.46 (13)	C13—C14—H14	119.2
C1—C2—H2A	109.3	C15—C14—H14	119.2
C3—C2—H2A	109.3	C14—C15—C16	121.75 (17)
C1—C2—H2B	109.3	C14—C15—C10	119.33 (18)
C3—C2—H2B	109.3	C16—C15—C10	118.91 (15)
H2A—C2—H2B	108.0	C17—C16—C15	121.48 (16)
C2—C3—C4	110.99 (14)	C17—C16—H16	119.3
C2—C3—H3A	109.4	C15—C16—H16	119.3
C4—C3—H3A	109.4	C16—C17—C18	119.65 (17)
C2—C3—H3B	109.4	C16—C17—H17	120.2
C4—C3—H3B	109.4	C18—C17—H17	120.2
H3A—C3—H3B	108.0	O1—C18—C9	124.15 (14)
C5—C4—C3	108.85 (13)	O1—C18—C17	113.58 (14)
C5—C4—H4A	109.9	C9—C18—C17	122.24 (15)
C3—C4—H4A	109.9	O1—C19—C7	111.98 (12)
C5—C4—H4B	109.9	O1—C19—H19A	109.2
C3—C4—H4B	109.9	C7—C19—H19A	109.2
H4A—C4—H4B	108.3	O1—C19—H19B	109.2
N1—C5—C4	110.61 (12)	C7—C19—H19B	109.2
N1—C5—C6	104.91 (11)	H19A—C19—H19B	107.9
C4—C5—C6	120.75 (12)	C25—C20—C21	117.25 (15)
N1—C5—H5	106.6	C25—C20—C6	117.84 (14)
C4—C5—H5	106.6	C21—C20—C6	124.88 (13)
C6—C5—H5	106.6	C22—C21—C20	121.16 (16)
C20—C6—C5	120.22 (12)	C22—C21—H21	119.4
C20—C6—C7	115.04 (12)	C20—C21—H21	119.4
C5—C6—C7	103.10 (11)	C23—C22—C21	120.37 (17)
C20—C6—H6	105.8	C23—C22—H22	119.8
C5—C6—H6	105.8	C21—C22—H22	119.8
C7—C6—H6	105.8	C24—C23—C22	119.46 (17)
C26—C7—C19	108.51 (12)	C24—C23—H23	120.3
C26—C7—C8	115.68 (11)	C22—C23—H23	120.3

C19—C7—C8	107.65 (11)	C23—C24—C25	120.25 (18)
C26—C7—C6	109.40 (11)	C23—C24—H24	119.9
C19—C7—C6	112.66 (11)	C25—C24—H24	119.9
C8—C7—C6	102.97 (11)	C24—C25—C20	121.49 (18)
N1—C8—C9	115.59 (10)	C24—C25—H25	119.3
N1—C8—C7	99.80 (10)	C20—C25—H25	119.3
C9—C8—C7	112.33 (12)	O2—C26—O3	123.07 (14)
N1—C8—H8	109.6	O2—C26—C7	124.22 (14)
C9—C8—H8	109.6	O3—C26—C7	112.70 (12)
C7—C8—H8	109.6	O3—C27—H27A	109.5
C18—C9—C10	118.14 (13)	O3—C27—H27B	109.5
C18—C9—C8	119.29 (13)	H27A—C27—H27B	109.5
C10—C9—C8	122.39 (13)	O3—C27—H27C	109.5
C11—C10—C15	117.06 (15)	H27A—C27—H27C	109.5
C11—C10—C9	123.40 (14)	H27B—C27—H27C	109.5
C15—C10—C9	119.52 (15)	C1—N1—C5	110.91 (11)
C12—C11—C10	121.81 (17)	C1—N1—C8	116.93 (11)
C12—C11—H11	119.1	C5—N1—C8	104.15 (10)
C10—C11—H11	119.1	C18—O1—C19	116.88 (12)
C11—C12—C13	120.7 (2)	C26—O3—C27	116.46 (13)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···O3	0.98	2.47	2.8240 (19)	101
C19—H19*B*···N1	0.97	2.55	2.885 (2)	100