Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(±)-Ethyl 6,7-dimethoxy-1-(1*H*-pyrrol-2-yl)-1,2,3,4-tetrahydroisoquinoline-2-carboxylate

Rosica Petrova Nikolova,[a] Tsonko Kolev,[b] Stela M. Statkova-Abeghe[c] and Boris Lubomirov Shivachev[d]*

[a]Department of Advanced Materials Science and Engineering, Faculty of Engineering, Yamaguchi University, 2-16-1 Tokiwadai, Ube 755-8611, Japan, [b]Bulgarian Academy of Sciences, Institute of Organic Chemistry, Acad G. Bonchev Str. build. 9, 1113 Sofia, Bulgaria, [c]Plovdiv University, Department of Organic Chemistry, 4000 Plovdiv, Bulgaria, and [d]Department of Structural Biology, University of Pittsburgh School of Medicine, 3501 5th Ave., Pittsburgh 15260, USA
Correspondence e-mail: blc53@pitt.edu

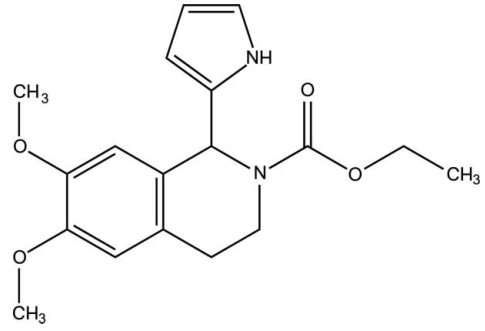
Received 29 July 2008; accepted 12 August 2008

Key indicators: single-crystal X-ray study; T = 290 K; mean σ(C–C) = 0.005 Å; R factor = 0.065; wR factor = 0.157; data-to-parameter ratio = 15.0.

In the title compound, $C_{18}H_{22}N_2O_4$, the dihedral angle between the pyrrolyl and quinolinyl fragments is 68.97 (2)°. Two non-classical intramolecular C—H···O hydrogen bonds stabilize the molecular geometry. In the crystal structure, molecules form infinite chains *via* moderate intermolecular N—H···O(CH$_3$) hydrogen bonds.

Related literature

For related crystal structures, see: Kolev *et al.* (2007); Petrova *et al.* (2007); Petrova *et al.* (2005); Rajnikant *et al.* (2002); Shishkina *et al.* (2005); Venkov *et al.* (2004); Vincente *et al.* (2005).



Experimental

Crystal data

$C_{18}H_{22}N_2O_4$
M_r = 330.38
Monoclinic, $P2_1/c$
a = 8.403 (3) Å
b = 17.046 (3) Å
c = 11.6486 (13) Å
β = 95.260 (13)°
V = 1661.5 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 290 (2) K
0.32 × 0.32 × 0.30 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
6852 measured reflections
3263 independent reflections
1828 reflections with $I > 2\sigma(I)$
R_{int} = 0.110
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.156
S = 1.07
3263 reflections
218 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O1^{i}	0.86	2.49	3.225 (4)	145
N3—H3···O2^{i}	0.86	2.38	3.018 (4)	132
C7—H7···O4	0.98	2.34	2.784 (4)	107
C8—H8*B*···O3	0.97	2.29	2.653 (4)	101

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

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

This work was supported by the National Science Fund of Bulgaria (Project TK357&TK358).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2093).

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supporting information

Acta Cryst. (2008). E**64**, o1796 [doi:10.1107/S1600536808026020]

(±)-Ethyl 6,7-dimethoxy-1-(1*H*-pyrrol-2-yl)-1,2,3,4-tetrahydroisoquinoline-2-carboxylate

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S1. Comment

As part of our research program on tetrahydroisoquinolines (Kolev *et al.*, 2007; Petrova *et al.*, 2007; Petrova *et al.*, 2005) the crystal structure of the title compound,(I), has been solved. The molecule possesses regular geometry with two nearly planar ring systems. The r.m.s. deviation of pyrrolyl and quinolin-2(1*H*)-fragments is 0.161 (7) Å and 0.002 (2) Å, respectively, and the dihedral angle between their mean planes is 68.97 (2)°. The geometrical parameters of both rings are comparable to those observed in other quinoline derivatives (Rajnikant *et al.*, 2002; Vincente *et al.*, 2005; Shishkina *et al.*, 2005). Two non-classsical intramolecular hydrogen bonds (C7—H7···O4 and C8—H8···O3) stabilize the molecular geometry. Only the methoxy O atoms are realised as hydrogen bond acceptors and together with the only possible donor form a bifurcated hydrogen bond of the N—H···(O,*O*) type. Thus neighboring molecules are oriented head-to-tail and connected to form infinite chains along the *b*-axis (Fig. 2).

S2. Experimental

The title compound has been obtained following the procedure described by Venkov *et al.*, 2004. Colorless crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation from ethanol/water (2:1) solution.

S3. Refinement

All H atoms were placed in idealized positions (*C*—H_{methyl} = 0.96 Å, *C*—$H_{methylen}$ = 0.97 Å, C—$H_{aromatic}$ = 0.93Å and N—H = 0.86 Å) and were constrained to ride on their parent atoms, with U_{iso}(H) = 1.5U_{eq}(C_{methyl}) or U_{iso}(H) = 1.2U_{eq}($C_{aromatic}$, $C_{methylen}$ ~ or N). The high R_{int} value (0.11) and relatively low ratio (0.55) of observed to unique reflections may be a result of the poor diffraction quality of the crystal.

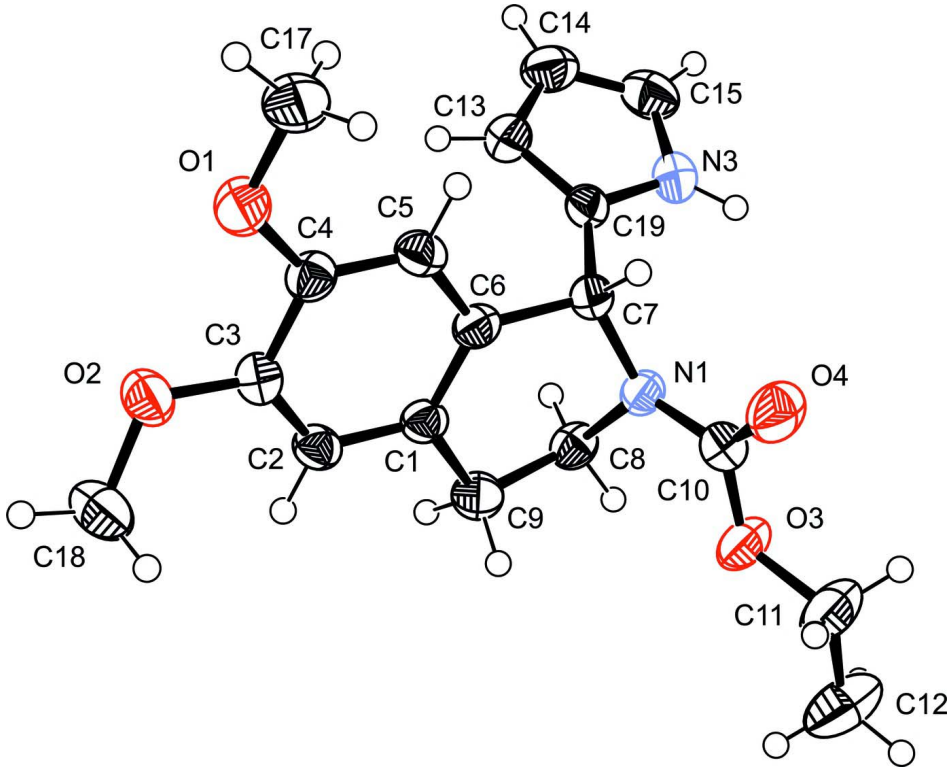

Figure 1

View of the structure and the atom-numbering scheme of (I) showing 50% probability displacement ellipsoids. H atoms are shown as small spheres of arbitrary radii.

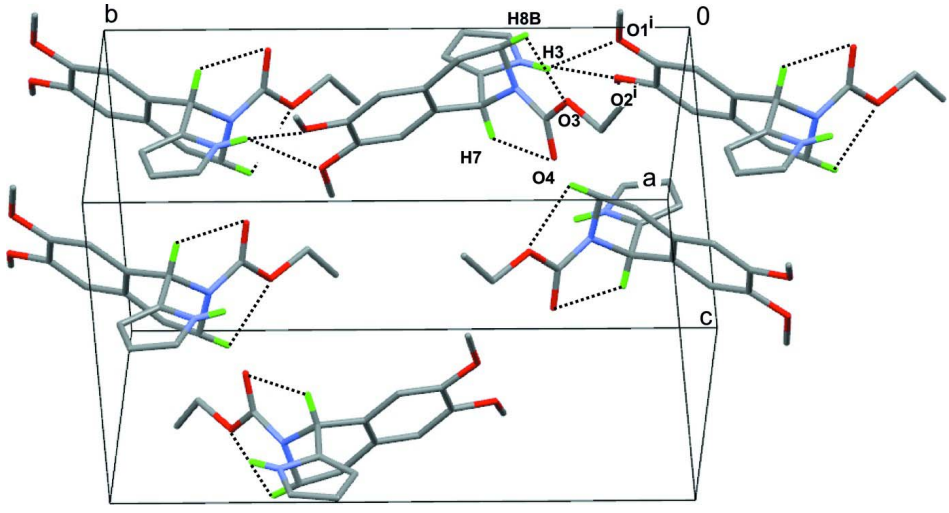

Figure 2

A view of the molecular packing in (I). Hydrogen bonds are represented by dotted lines. H atoms not involved in hydrogen bonding interactions have been omitted. [Symmetry code: (i) -*x*, -1/2 + *y*, 1/2 - *z*].

(±)-Ethyl 6,7-dimethoxy-1-(1*H*-pyrrol-2-yl)-1,2,3,4-tetrahydroisoquinoline- 2-carboxylate

Crystal data

$C_{18}H_{22}N_2O_4$
$M_r = 330.38$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 8.403$ (3) Å
$b = 17.046$ (3) Å
$c = 11.6486$ (13) Å
$\beta = 95.260$ (13)°
$V = 1661.5$ (7) Å^3
$Z = 4$
$F(000) = 704$
$D_x = 1.321$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 22 reflections
$\theta = 18.3$–18.8°
$\mu = 0.09$ mm^{-1}
$T = 290$ K
Prism, colorless
0.32 × 0.32 × 0.30 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Nonprofiled $\omega/2\theta$ scans
6852 measured reflections
3263 independent reflections
1828 reflections with $I > 2\sigma(I)$
$R_{int} = 0.110$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.1°$
$h = 0 \rightarrow 10$
$k = -20 \rightarrow 20$
$l = -14 \rightarrow 14$
3 standard reflections every 120 min
intensity decay: −1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.065$
$wR(F^2) = 0.156$
$S = 1.07$
3263 reflections
218 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
$w = 1/[\sigma^2(F_o^2) + (0.0293P)^2 + 2.0348P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0075 (10)

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}
O1	0.2084 (3)	0.63581 (14)	0.3413 (2)	0.0474 (7)
O2	0.3254 (3)	0.65266 (14)	0.1467 (2)	0.0443 (7)
O3	0.2237 (3)	0.20530 (14)	0.1157 (2)	0.0476 (7)

O4	0.2206 (3)	0.23765 (16)	0.3033 (2)	0.0573 (8)
N1	0.0630 (3)	0.30217 (16)	0.1633 (2)	0.0336 (7)
C2	0.2399 (4)	0.5223 (2)	0.0832 (3)	0.0339 (8)
H2	0.2815	0.5290	0.0126	0.041*
C19	−0.1547 (4)	0.37433 (19)	0.2412 (3)	0.0339 (8)
C6	0.1037 (4)	0.44139 (19)	0.2113 (3)	0.0329 (8)
C3	0.2542 (4)	0.58174 (19)	0.1623 (3)	0.0337 (8)
C13	−0.2492 (4)	0.4391 (2)	0.2366 (3)	0.0415 (9)
H13	−0.2154	0.4906	0.2277	0.050*
C7	0.0237 (4)	0.36515 (18)	0.2422 (3)	0.0347 (8)
H7	0.0659	0.3503	0.3204	0.042*
C9	0.1515 (4)	0.3882 (2)	0.0146 (3)	0.0408 (9)
H9A	0.2564	0.3657	0.0085	0.049*
H9B	0.1157	0.4115	−0.0593	0.049*
C5	0.1184 (4)	0.5026 (2)	0.2922 (3)	0.0352 (8)
H5	0.0780	0.4956	0.3632	0.042*
N3	−0.2512 (3)	0.31109 (17)	0.2555 (2)	0.0418 (8)
H3	−0.2197	0.2631	0.2616	0.050*
C10	0.1731 (4)	0.2482 (2)	0.2028 (3)	0.0395 (9)
C4	0.1907 (4)	0.5724 (2)	0.2694 (3)	0.0349 (8)
C18	0.4219 (5)	0.6587 (2)	0.0526 (3)	0.0555 (11)
H18A	0.4648	0.7109	0.0499	0.083*
H18B	0.3580	0.6479	−0.0182	0.083*
H18C	0.5080	0.6216	0.0626	0.083*
C1	0.1642 (4)	0.45151 (19)	0.1057 (3)	0.0323 (8)
C15	−0.4056 (5)	0.3361 (2)	0.2588 (3)	0.0498 (10)
H15	−0.4936	0.3042	0.2672	0.060*
C8	0.0366 (4)	0.3237 (2)	0.0414 (3)	0.0356 (8)
H8A	−0.0725	0.3415	0.0240	0.043*
H8B	0.0529	0.2782	−0.0061	0.043*
C17	0.1649 (5)	0.6268 (2)	0.4555 (3)	0.0527 (11)
H17A	0.1816	0.6754	0.4965	0.079*
H17B	0.2294	0.5865	0.4941	0.079*
H17C	0.0543	0.6123	0.4532	0.079*
C14	−0.4078 (5)	0.4148 (2)	0.2476 (3)	0.0491 (10)
H14	−0.4971	0.4471	0.2471	0.059*
C11	0.3387 (6)	0.1452 (3)	0.1464 (4)	0.0675 (14)
H11A	0.2972	0.1094	0.2010	0.081*
H11B	0.4361	0.1685	0.1824	0.081*
C12	0.3725 (6)	0.1029 (3)	0.0433 (4)	0.0812 (16)
H12A	0.4508	0.0630	0.0633	0.122*
H12B	0.4129	0.1387	−0.0106	0.122*
H12C	0.2761	0.0790	0.0090	0.122*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0666 (18)	0.0391 (15)	0.0374 (14)	−0.0089 (13)	0.0099 (13)	−0.0089 (12)

O2	0.0514 (15)	0.0414 (15)	0.0412 (14)	−0.0117 (12)	0.0110 (12)	−0.0012 (12)
O3	0.0551 (17)	0.0418 (15)	0.0455 (15)	0.0201 (13)	0.0028 (13)	−0.0023 (13)
O4	0.073 (2)	0.0578 (18)	0.0403 (16)	0.0254 (15)	0.0029 (14)	0.0079 (14)
N1	0.0403 (17)	0.0308 (16)	0.0298 (14)	0.0073 (14)	0.0035 (13)	0.0008 (13)
C2	0.0360 (19)	0.039 (2)	0.0275 (17)	0.0023 (16)	0.0060 (15)	0.0038 (15)
C19	0.043 (2)	0.0306 (19)	0.0297 (18)	−0.0011 (16)	0.0094 (16)	0.0005 (15)
C6	0.0326 (19)	0.0323 (19)	0.0339 (18)	0.0051 (15)	0.0040 (16)	−0.0011 (15)
C3	0.0330 (19)	0.0326 (19)	0.0351 (19)	−0.0019 (15)	0.0009 (16)	0.0030 (16)
C13	0.046 (2)	0.037 (2)	0.043 (2)	0.0064 (18)	0.0088 (18)	0.0034 (17)
C7	0.044 (2)	0.0297 (18)	0.0317 (18)	0.0025 (16)	0.0092 (16)	0.0011 (15)
C9	0.047 (2)	0.042 (2)	0.0335 (19)	0.0006 (18)	0.0074 (18)	−0.0034 (17)
C5	0.037 (2)	0.041 (2)	0.0289 (17)	0.0009 (17)	0.0065 (15)	0.0007 (17)
N3	0.0453 (19)	0.0350 (17)	0.0460 (18)	−0.0009 (15)	0.0084 (15)	0.0054 (15)
C10	0.043 (2)	0.037 (2)	0.039 (2)	0.0001 (18)	0.0094 (18)	0.0029 (17)
C4	0.041 (2)	0.0339 (19)	0.0297 (18)	0.0008 (16)	0.0014 (16)	−0.0043 (16)
C18	0.053 (3)	0.064 (3)	0.052 (2)	−0.016 (2)	0.016 (2)	0.000 (2)
C1	0.0322 (19)	0.0352 (19)	0.0299 (17)	0.0062 (15)	0.0043 (15)	0.0019 (15)
C15	0.041 (2)	0.060 (3)	0.050 (2)	−0.009 (2)	0.0124 (19)	−0.001 (2)
C8	0.041 (2)	0.0345 (19)	0.0306 (18)	0.0032 (16)	−0.0010 (15)	−0.0055 (16)
C17	0.067 (3)	0.054 (3)	0.038 (2)	−0.003 (2)	0.009 (2)	−0.011 (2)
C14	0.044 (2)	0.057 (3)	0.047 (2)	0.013 (2)	0.009 (2)	0.000 (2)
C11	0.077 (3)	0.052 (3)	0.073 (3)	0.030 (2)	0.006 (3)	−0.004 (2)
C12	0.083 (4)	0.076 (3)	0.084 (4)	0.035 (3)	0.004 (3)	−0.023 (3)

Geometric parameters (Å, º)

O1—C4	1.367 (4)	C9—C8	1.515 (5)
O1—C17	1.420 (4)	C9—H9A	0.9700
O2—C3	1.369 (4)	C9—H9B	0.9700
O2—C18	1.426 (4)	C5—C4	1.374 (5)
O3—C10	1.350 (4)	C5—H5	0.9300
O3—C11	1.431 (5)	N3—C15	1.369 (5)
O4—C10	1.216 (4)	N3—H3	0.8600
N1—C10	1.355 (4)	C18—H18A	0.9600
N1—C8	1.464 (4)	C18—H18B	0.9600
N1—C7	1.470 (4)	C18—H18C	0.9600
C2—C3	1.367 (5)	C15—C14	1.349 (5)
C2—C1	1.399 (4)	C15—H15	0.9300
C2—H2	0.9300	C8—H8A	0.9700
C19—C13	1.359 (5)	C8—H8B	0.9700
C19—N3	1.368 (4)	C17—H17A	0.9600
C19—C7	1.506 (5)	C17—H17B	0.9600
C6—C1	1.385 (4)	C17—H17C	0.9600
C6—C5	1.403 (4)	C14—H14	0.9300
C6—C7	1.521 (4)	C11—C12	1.451 (6)
C3—C4	1.410 (4)	C11—H11A	0.9700
C13—C14	1.413 (5)	C11—H11B	0.9700
C13—H13	0.9300	C12—H12A	0.9600

C7—H7	0.9800	C12—H12B	0.9600
C9—C1	1.510 (4)	C12—H12C	0.9600
C4—O1—C17	117.8 (3)	O1—C4—C5	126.3 (3)
C3—O2—C18	116.9 (3)	O1—C4—C3	115.1 (3)
C10—O3—C11	116.9 (3)	C5—C4—C3	118.6 (3)
C10—N1—C8	122.5 (3)	O2—C18—H18A	109.5
C10—N1—C7	118.0 (3)	O2—C18—H18B	109.5
C8—N1—C7	113.6 (3)	H18A—C18—H18B	109.5
C3—C2—C1	121.8 (3)	O2—C18—H18C	109.5
C3—C2—H2	119.1	H18A—C18—H18C	109.5
C1—C2—H2	119.1	H18B—C18—H18C	109.5
C13—C19—N3	107.1 (3)	C6—C1—C2	118.9 (3)
C13—C19—C7	131.5 (3)	C6—C1—C9	121.8 (3)
N3—C19—C7	121.2 (3)	C2—C1—C9	119.3 (3)
C1—C6—C5	119.2 (3)	C14—C15—N3	108.2 (3)
C1—C6—C7	121.5 (3)	C14—C15—H15	125.9
C5—C6—C7	119.3 (3)	N3—C15—H15	125.9
O2—C3—C2	125.3 (3)	N1—C8—C9	109.8 (3)
O2—C3—C4	115.0 (3)	N1—C8—H8A	109.7
C2—C3—C4	119.7 (3)	C9—C8—H8A	109.7
C19—C13—C14	108.1 (3)	N1—C8—H8B	109.7
C19—C13—H13	125.9	C9—C8—H8B	109.7
C14—C13—H13	125.9	H8A—C8—H8B	108.2
N1—C7—C19	110.6 (3)	O1—C17—H17A	109.5
N1—C7—C6	110.3 (2)	O1—C17—H17B	109.5
C19—C7—C6	111.7 (3)	H17A—C17—H17B	109.5
N1—C7—H7	108.0	O1—C17—H17C	109.5
C19—C7—H7	108.0	H17A—C17—H17C	109.5
C6—C7—H7	108.0	H17B—C17—H17C	109.5
C1—C9—C8	112.3 (3)	C15—C14—C13	107.2 (3)
C1—C9—H9A	109.1	C15—C14—H14	126.4
C8—C9—H9A	109.1	C13—C14—H14	126.4
C1—C9—H9B	109.1	O3—C11—C12	109.2 (4)
C8—C9—H9B	109.1	O3—C11—H11A	109.8
H9A—C9—H9B	107.9	C12—C11—H11A	109.8
C4—C5—C6	121.8 (3)	O3—C11—H11B	109.8
C4—C5—H5	119.1	C12—C11—H11B	109.8
C6—C5—H5	119.1	H11A—C11—H11B	108.3
C19—N3—C15	109.4 (3)	C11—C12—H12A	109.5
C19—N3—H3	125.3	C11—C12—H12B	109.5
C15—N3—H3	125.3	H12A—C12—H12B	109.5
O4—C10—O3	123.1 (3)	C11—C12—H12C	109.5
O4—C10—N1	125.5 (3)	H12A—C12—H12C	109.5
O3—C10—N1	111.4 (3)	H12B—C12—H12C	109.5
C18—O2—C3—C2	−14.4 (5)	C8—N1—C10—O3	−14.8 (5)
C18—O2—C3—C4	166.3 (3)	C7—N1—C10—O3	−166.0 (3)

C1—C2—C3—O2	−179.6 (3)	C17—O1—C4—C5	7.6 (5)
C1—C2—C3—C4	−0.4 (5)	C17—O1—C4—C3	−172.4 (3)
N3—C19—C13—C14	−0.4 (4)	C6—C5—C4—O1	178.8 (3)
C7—C19—C13—C14	−175.2 (4)	C6—C5—C4—C3	−1.2 (5)
C10—N1—C7—C19	−132.3 (3)	O2—C3—C4—O1	0.6 (5)
C8—N1—C7—C19	74.0 (3)	C2—C3—C4—O1	−178.7 (3)
C10—N1—C7—C6	103.6 (3)	O2—C3—C4—C5	−179.4 (3)
C8—N1—C7—C6	−50.1 (4)	C2—C3—C4—C5	1.3 (5)
C13—C19—C7—N1	−135.5 (4)	C5—C6—C1—C2	0.7 (5)
N3—C19—C7—N1	50.3 (4)	C7—C6—C1—C2	−178.5 (3)
C13—C19—C7—C6	−12.3 (5)	C5—C6—C1—C9	−179.6 (3)
N3—C19—C7—C6	173.6 (3)	C7—C6—C1—C9	1.2 (5)
C1—C6—C7—N1	16.3 (5)	C3—C2—C1—C6	−0.6 (5)
C5—C6—C7—N1	−162.9 (3)	C3—C2—C1—C9	179.7 (3)
C1—C6—C7—C19	−107.1 (4)	C8—C9—C1—C6	12.8 (5)
C5—C6—C7—C19	73.7 (4)	C8—C9—C1—C2	−167.5 (3)
C1—C6—C5—C4	0.2 (5)	C19—N3—C15—C14	−0.5 (4)
C7—C6—C5—C4	179.4 (3)	C10—N1—C8—C9	−86.6 (4)
C13—C19—N3—C15	0.6 (4)	C7—N1—C8—C9	65.8 (4)
C7—C19—N3—C15	176.0 (3)	C1—C9—C8—N1	−44.0 (4)
C11—O3—C10—O4	0.0 (5)	N3—C15—C14—C13	0.2 (5)
C11—O3—C10—N1	−179.1 (3)	C19—C13—C14—C15	0.1 (4)
C8—N1—C10—O4	166.2 (4)	C10—O3—C11—C12	177.0 (4)
C7—N1—C10—O4	15.0 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···O1^{i}	0.86	2.49	3.225 (4)	145
N3—H3···O2^{i}	0.86	2.38	3.018 (4)	132
C7—H7···O4	0.98	2.34	2.784 (4)	107
C8—H8*B*···O3	0.97	2.29	2.653 (4)	101

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