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Diethyl 4-(4-bromophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate

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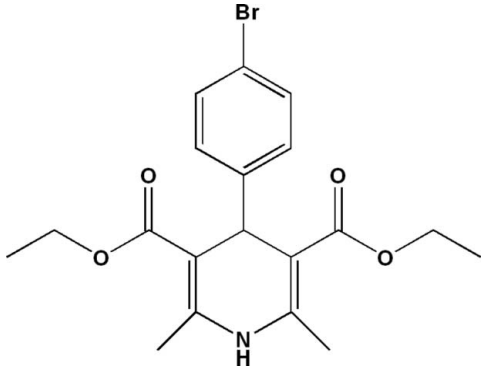
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.027; wR factor = 0.093; data-to-parameter ratio = 18.0.

In the title compound, $C_{19}H_{22}BrNO_4$, the dihydropyridine ring adopts a flattened boat conformation and the plane of the base of the boat forms a dihedral angle of 89.32 (5)° with the benzene ring. The crystal structure can be described as layers in which dihydropyridine rings are parallel to the ($\bar{1}$01) plane. The packing is stabilized by intramolecular C—H···O and intermolecular N—H···O hydrogen bonds, resulting in the formation of a three-dimensional network.

Related literature

For synthesis, see: Dondoni *et al.* (2004); Bennasar *et al.* (2005). For geometry, see: Doreswamy *et al.* (2004); Mahendra *et al.* (2004). For applications, see: Mulder *et al.* (2006); Litvic *et al.* (2005); Moseley (2005). For related literature, see: Bossert *et al.* (1981); Breitenbucher & Figliozzi (2000); Bretzel *et al.* (1993); Debache *et al.* (2006); Geirsson & Johannesdottir (1996); Gómez *et al.* (2005); Hantzsch (1882); Heravi *et al.* (2005); Klusa (1995); Mannhold *et al.* (1992); Nakayama & Kasoka (1996); Sridhar & Perumal (2005); Tewari *et al.* (2004); Tu *et al.* (2001).



Experimental

Crystal data

$C_{19}H_{22}BrNO_4$
M_r = 408.28
Monoclinic, $P2_1/n$
a = 10.0597 (5) Å
b = 7.4244 (4) Å
c = 24.3726 (13) Å
β = 98.126 (2)°
V = 1802.05 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.30 mm^{-1}
T = 295 (2) K
0.15 × 0.11 × 0.1 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: none
19743 measured reflections
4132 independent reflections
3460 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.093
S = 1.13
4132 reflections
230 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O3^{i}	0.86	2.11	2.969 (2)	173
C4—H4···O3	0.98	2.47	2.811 (2)	100

Symmetry code: (i) $x, y-1, z$.

Data collection: *APEX2* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg & Berndt, 2001); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2352).

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supplementary materials

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Diethyl 4-(4-bromophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate

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Comment

1,4-Dihydropyridines (1,4-DHPs) have recently received great attention because of their wide range of therapeutic and pharmacological activities, such as antiviral, antitumor, antibacterial, and anti-inflammatory behaviour. Furthermore, these compounds have emerged as the integral backbones of several calcium channel blockers (Litvic *et al.*, 2005), and as drugs for the treatment of cardiovascular diseases and hypertension (Bossert *et al.*, 1981; Nakayama *et al.*, 1996; Mulder *et al.*, 2006). The dihydropyridine skeleton is common in many vasodilator, bronchiodilator, anti-atherosclerotic, anti-tumor, hepatoprotective and anti-diabetic agents (Mannhold *et al.*, 1992). They are also known as neuroprotectants, as anti-platelet treatment of aggregators and are important in Alzheimer's disease as anti-ischaemic agents (Klusa, 1995; Bretzel *et al.*, 1993). Among the 1,4-dihydropyridines there are also drug-resistance modifiers (Sridhar *et al.*, 2005), antioxidants (Heravi *et al.*, 2005) and a drug for the treatment of urinary urge incontinence (Moseley *et al.*, 2005). Interest in 1,4-dihydropyridines is also sustained by their structural closeness to nicotinamide dinucleotide, a cofactor used by many reductases in metabolism (Tewari *et al.*, 2004). Although 1,4-dihydropyridines with various aromatic, heteroaromatic, aliphatic and sugar substituents at C-4 have been reported as anti-tuberculosis agents (Geirsson *et al.*, 1996). The simplest and the most straightforward procedure, originally reported by Hantzsch, involves the three-component, one-pot condensation of an aldehyde, β-keto ester, and ammonia under strongly refluxing conditions (Hantzsch, 1882). Therefore, synthesis of the 1,4-dihydropyridine nucleus continuously received the attention of scientists. This has led to the recent disclosure of several improved reaction procedures for the synthesis of 1,4-dihydropyridines, by either modification of the classical one-pot Hantzsch approach itself, or the development of novel, but more complex multistep strategies (Breitenbucher *et al.*, 2000; Tu *et al.*, 2001; Dondoni *et al.*, 2004; Bennasar *et al.*, 2005; Gómez *et al.*, 2005). As a part of our program aiming at developing selective and environmental friendly methodologies for the reparation of fine chemicals and in continuation of our interest in new catalysts for multi-component reactions (Debache *et al.*, 2006), in this paper, we wish to highlight our finding about the four-component Hantzsch reaction in refluxing ethanol as a solvent. In this study, we have synthesized diethyl 4-(4-bromophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate, (I), and characterized by X-ray diffraction method.

The molecular geometry and the atom-numbering scheme of (I) are shown in Fig. 1. The asymmetric unit of title compound contains a dimethyldihydropyridine group linked to a bromophenyl moiety and two ethylcarboxylate.

The geometric parameters of (I) are in agreement with those of other structures possessing a dihydropyridine substituent previously reported in the literature (Doreswamy *et al.*, 2004; Mahendra *et al.*, 2004).

The dihydropyridine ring adopts a flat boat conformation when C4 and N1 atoms are significantly displaced from dihydropyridine ring by −0.144 and 0.106 Å respectively, and its mean plane forms dihedral angles of 89.32 (5)° with phenyl substituent.

The crystal structure can be described by layers which dihydropyridine ring is parallel to (10$\bar{1}$) plane (Fig. 2).

The packing of (I) is stabilized by classical intramolecular C—H···O and intermolecular N—H···O hydrogen bonds, resulting in the formation of two dimensional network (Fig. 2). Additional hydrogen-bonding parameters are listed in Table 1.

Experimental

A mixture of 4-bromobenzaldehyde (5 mmol), ethyl acetoacetate (10 mmol) and ammonium acetate (10 mmol) was refluxed in ethanol (10 ml) for 5 h. The reaction mixture was poured in cold water and extracted with ethyl acetate. The organic layer was washed with brine, dried over Na_2SO_4 and concentrated to give an analytically pure compound. The crude product was purified by recrystallization from ethanol to afford 1,4-dihydropyridines in 90% yields.

Refinement

All H atoms were localized on Fourier maps, but introduced in calculated positions and treated as riding on their parent C atom, with N—H = 082, C—H = 0.93–0.97 Å, and with U_{iso}(H) = 1.2U_{eq}(C, N) or 1.5U_{eq}(C_{methyl}).

Figures

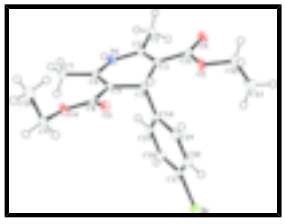

Fig. 1. The structure of the title compound with the atomic labelling scheme. Displacement are drawn at the 50% probability level.

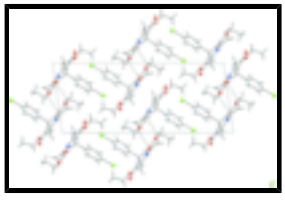

Fig. 2. A diagram of the layered crystal packing of (I) viewed down the *b* axis. Hydrogen bonds are shown as dashed lines.

Diethyl 4-(4-bromophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate

Crystal data

$C_{19}H_{22}BrNO_4$	F_{000} = 840
M_r = 408.28	D_x = 1.505 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 8206 reflections
a = 10.0597 (5) Å	θ = 2.3–27.5º
b = 7.4244 (4) Å	μ = 2.30 mm^{-1}
c = 24.3726 (13) Å	T = 295 (2) K
β = 98.126 (2)º	Prism, colourless
V = 1802.05 (16) Å^3	0.15 × 0.11 × 0.1 mm
Z = 4	

Data collection

Bruker APEXII diffractometer	θ_{max} = 27.5º
Monochromator: graphite	θ_{min} = 1.7º
T = 295(2) K	h = −12→13
CCD rotation images, thin slices, φ scans, and ω	k = −9→9
Absorption correction: none	l = −31→30
19743 measured reflections	Standard reflections: ?;
4132 independent reflections	every ? reflections
3460 reflections with $I > 2\sigma(I)$	intensity decay: ?
R_{int} = 0.044	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.027	$w = 1/[\sigma^2(F_o^2) + (0.0459P)^2 + 0.9623P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.093	$(\Delta/\sigma)_{max}$ = 0.002
S = 1.13	$\Delta\rho_{max}$ = 0.55 e Å^{-3}
4132 reflections	$\Delta\rho_{min}$ = −0.33 e Å^{-3}
230 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997)
Primary atom site location: structure-invariant direct methods	Extinction coefficient: none
Secondary atom site location: difference Fourier map	

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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 $F^2 > 2\text{sigma}(F^2)$ 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}
Br	0.53359 (2)	0.25548 (3)	0.27107 (1)	0.0231 (1)
O1	1.15604 (14)	−0.0716 (2)	0.14212 (6)	0.0248 (5)
O2	1.07916 (15)	0.2138 (2)	0.13729 (6)	0.0213 (4)
O3	0.72372 (13)	0.42820 (18)	0.00338 (6)	0.0180 (4)
O4	0.57284 (14)	0.24035 (17)	−0.04326 (6)	0.0181 (4)

N1	0.81110 (17)	−0.1926 (2)	0.02334 (7)	0.0158 (4)
C1	1.0102 (2)	−0.3304 (3)	0.07312 (9)	0.0204 (6)
C2	0.92482 (18)	−0.1649 (3)	0.06168 (8)	0.0151 (5)
C3	0.95008 (18)	0.0016 (3)	0.08344 (8)	0.0138 (5)
C4	0.84771 (18)	0.1524 (3)	0.07128 (7)	0.0133 (5)
C5	0.75149 (18)	0.1147 (3)	0.01826 (7)	0.0127 (5)
C6	0.73320 (18)	−0.0549 (3)	−0.00198 (7)	0.0136 (5)
C7	0.63769 (19)	−0.1155 (3)	−0.05182 (8)	0.0181 (6)
C8	0.68440 (19)	0.2753 (2)	−0.00735 (8)	0.0130 (5)
C9	0.51398 (19)	0.3921 (3)	−0.07597 (8)	0.0193 (6)
C10	0.5891 (2)	0.4244 (3)	−0.12397 (9)	0.0303 (7)
C11	1.07165 (18)	0.0371 (3)	0.12318 (8)	0.0169 (6)
C12	1.1835 (2)	0.2660 (3)	0.18190 (10)	0.0264 (7)
C13	1.1395 (3)	0.2357 (3)	0.23741 (10)	0.0292 (7)
C14	0.76975 (18)	0.1802 (3)	0.12001 (7)	0.0137 (5)
C15	0.6847 (2)	0.0454 (3)	0.13475 (8)	0.0184 (6)
C16	0.6134 (2)	0.0666 (3)	0.17933 (8)	0.0201 (6)
C17	0.6288 (2)	0.2243 (3)	0.20965 (8)	0.0170 (6)
C18	0.7117 (2)	0.3610 (3)	0.19590 (8)	0.0208 (6)
C19	0.7813 (2)	0.3375 (3)	0.15105 (8)	0.0193 (6)
H1	0.78782	−0.30168	0.01486	0.0190*
H1A	1.09448	−0.31251	0.05973	0.0305*
H1B	0.96477	−0.43187	0.05462	0.0305*
H1C	1.02581	−0.35245	0.11231	0.0305*
H4	0.89637	0.26388	0.06592	0.0159*
H7A	0.54706	−0.10591	−0.04401	0.0271*
H7B	0.65646	−0.23841	−0.06021	0.0271*
H7C	0.64872	−0.04066	−0.08299	0.0271*
H9A	0.51786	0.49911	−0.05295	0.0232*
H9B	0.42047	0.36700	−0.08950	0.0232*
H10A	0.68067	0.45441	−0.11041	0.0455*
H10B	0.54807	0.52207	−0.14601	0.0455*
H10C	0.58662	0.31751	−0.14624	0.0455*
H12A	1.20504	0.39234	0.17800	0.0317*
H12B	1.26403	0.19640	0.17941	0.0317*
H13A	1.05396	0.29215	0.23823	0.0437*
H13B	1.20446	0.28677	0.26579	0.0437*
H13C	1.13192	0.10873	0.24375	0.0437*
H15	0.67545	−0.06086	0.11435	0.0220*
H16	0.55656	−0.02388	0.18853	0.0241*
H18	0.72077	0.46701	0.21640	0.0249*
H19	0.83673	0.42932	0.14163	0.0232*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br	0.0243 (1)	0.0300 (2)	0.0161 (1)	0.0065 (1)	0.0068 (1)	−0.0015 (1)
O1	0.0172 (7)	0.0324 (9)	0.0236 (8)	0.0037 (6)	−0.0011 (6)	0.0056 (6)

O2	0.0174 (7)	0.0263 (8)	0.0184 (8)	−0.0045 (6)	−0.0032 (6)	−0.0026 (6)
O3	0.0208 (7)	0.0123 (7)	0.0201 (7)	0.0007 (5)	0.0004 (5)	−0.0008 (5)
O4	0.0179 (7)	0.0148 (7)	0.0195 (8)	−0.0010 (5)	−0.0044 (6)	0.0042 (5)
N1	0.0183 (8)	0.0097 (7)	0.0187 (8)	−0.0010 (6)	0.0002 (6)	−0.0012 (6)
C1	0.0202 (10)	0.0182 (10)	0.0234 (11)	0.0044 (8)	0.0055 (8)	0.0035 (8)
C2	0.0147 (9)	0.0167 (10)	0.0144 (9)	0.0010 (7)	0.0041 (7)	0.0033 (7)
C3	0.0138 (8)	0.0164 (9)	0.0117 (9)	0.0003 (7)	0.0032 (7)	0.0016 (7)
C4	0.0149 (8)	0.0124 (9)	0.0122 (9)	−0.0023 (7)	0.0011 (7)	−0.0003 (7)
C5	0.0132 (8)	0.0133 (9)	0.0118 (9)	−0.0005 (7)	0.0027 (7)	0.0008 (7)
C6	0.0151 (9)	0.0149 (10)	0.0110 (9)	−0.0006 (7)	0.0027 (7)	0.0013 (7)
C7	0.0215 (10)	0.0153 (10)	0.0163 (10)	−0.0016 (8)	−0.0011 (8)	−0.0030 (7)
C8	0.0137 (9)	0.0157 (10)	0.0103 (9)	−0.0004 (7)	0.0044 (7)	−0.0002 (7)
C9	0.0176 (9)	0.0165 (10)	0.0218 (10)	0.0019 (8)	−0.0043 (8)	0.0053 (8)
C10	0.0378 (13)	0.0325 (13)	0.0202 (11)	0.0103 (10)	0.0023 (9)	0.0078 (9)
C11	0.0144 (9)	0.0242 (11)	0.0127 (9)	−0.0024 (7)	0.0038 (7)	0.0024 (7)
C12	0.0195 (10)	0.0386 (14)	0.0198 (11)	−0.0103 (9)	−0.0013 (9)	−0.0050 (9)
C13	0.0273 (12)	0.0371 (14)	0.0226 (12)	−0.0052 (9)	0.0020 (9)	−0.0058 (9)
C14	0.0135 (9)	0.0157 (9)	0.0111 (8)	0.0013 (7)	−0.0007 (7)	0.0003 (7)
C15	0.0242 (10)	0.0152 (10)	0.0162 (9)	−0.0022 (8)	0.0048 (8)	−0.0034 (7)
C16	0.0222 (10)	0.0206 (10)	0.0180 (10)	−0.0028 (8)	0.0047 (8)	0.0007 (8)
C17	0.0163 (9)	0.0242 (11)	0.0106 (9)	0.0064 (7)	0.0027 (7)	0.0003 (7)
C18	0.0226 (10)	0.0185 (10)	0.0210 (10)	−0.0001 (8)	0.0022 (8)	−0.0070 (8)
C19	0.0202 (10)	0.0173 (10)	0.0205 (10)	−0.0025 (8)	0.0028 (8)	−0.0032 (8)

Geometric parameters (Å, °)

Br—C17	1.902 (2)	C16—C17	1.382 (3)
O1—C11	1.214 (2)	C17—C18	1.385 (3)
O2—C11	1.356 (3)	C18—C19	1.390 (3)
O2—C12	1.453 (3)	C1—H1A	0.9600
O3—C8	1.218 (2)	C1—H1B	0.9600
O4—C8	1.347 (2)	C1—H1C	0.9600
O4—C9	1.457 (3)	C4—H4	0.9800
N1—C2	1.386 (3)	C7—H7A	0.9600
N1—C6	1.380 (3)	C7—H7B	0.9600
N1—H1	0.8600	C7—H7C	0.9600
C1—C2	1.503 (3)	C9—H9A	0.9700
C2—C3	1.355 (3)	C9—H9B	0.9700
C3—C11	1.473 (3)	C10—H10A	0.9600
C3—C4	1.522 (3)	C10—H10B	0.9600
C4—C14	1.527 (2)	C10—H10C	0.9600
C4—C5	1.527 (2)	C12—H12A	0.9700
C5—C6	1.355 (3)	C12—H12B	0.9700
C5—C8	1.466 (3)	C13—H13A	0.9600
C6—C7	1.507 (3)	C13—H13B	0.9600
C9—C10	1.499 (3)	C13—H13C	0.9600
C12—C13	1.499 (3)	C15—H15	0.9300
C14—C19	1.387 (3)	C16—H16	0.9300
C14—C15	1.396 (3)	C18—H18	0.9300

C15—C16	1.393 (3)	C19—H19	0.9300
C11—O2—C12	117.15 (16)	H1A—C1—H1C	110.00
C8—O4—C9	116.32 (14)	H1B—C1—H1C	109.00
C2—N1—C6	123.64 (17)	C3—C4—H4	108.00
C6—N1—H1	118.00	C5—C4—H4	108.00
C2—N1—H1	118.00	C14—C4—H4	108.00
N1—C2—C3	119.37 (18)	C6—C7—H7A	109.00
N1—C2—C1	113.54 (18)	C6—C7—H7B	109.00
C1—C2—C3	127.07 (18)	C6—C7—H7C	109.00
C4—C3—C11	118.21 (18)	H7A—C7—H7B	109.00
C2—C3—C4	120.71 (17)	H7A—C7—H7C	109.00
C2—C3—C11	120.87 (19)	H7B—C7—H7C	109.00
C3—C4—C14	110.84 (16)	O4—C9—H9A	110.00
C3—C4—C5	111.13 (17)	O4—C9—H9B	110.00
C5—C4—C14	110.44 (15)	C10—C9—H9A	110.00
C4—C5—C8	114.20 (18)	C10—C9—H9B	110.00
C4—C5—C6	121.03 (18)	H9A—C9—H9B	108.00
C6—C5—C8	124.76 (16)	C9—C10—H10A	109.00
N1—C6—C7	113.35 (18)	C9—C10—H10B	109.00
C5—C6—C7	127.52 (18)	C9—C10—H10C	109.00
N1—C6—C5	119.10 (16)	H10A—C10—H10B	109.00
O4—C8—C5	114.28 (14)	H10A—C10—H10C	109.00
O3—C8—O4	122.29 (16)	H10B—C10—H10C	109.00
O3—C8—C5	123.41 (18)	O2—C12—H12A	109.00
O4—C9—C10	109.88 (16)	O2—C12—H12B	109.00
O2—C11—C3	110.57 (17)	C13—C12—H12A	109.00
O1—C11—C3	127.0 (2)	C13—C12—H12B	109.00
O1—C11—O2	122.40 (18)	H12A—C12—H12B	108.00
O2—C12—C13	111.17 (18)	C12—C13—H13A	109.00
C15—C14—C19	118.05 (17)	C12—C13—H13B	109.00
C4—C14—C15	120.27 (18)	C12—C13—H13C	109.00
C4—C14—C19	121.69 (18)	H13A—C13—H13B	109.00
C14—C15—C16	121.44 (19)	H13A—C13—H13C	109.00
C15—C16—C17	118.8 (2)	H13B—C13—H13C	109.00
Br—C17—C18	119.27 (16)	C14—C15—H15	119.00
Br—C17—C16	119.56 (16)	C16—C15—H15	119.00
C16—C17—C18	121.17 (19)	C15—C16—H16	121.00
C17—C18—C19	119.1 (2)	C17—C16—H16	121.00
C14—C19—C18	121.46 (19)	C17—C18—H18	120.00
C2—C1—H1A	109.00	C19—C18—H18	120.00
C2—C1—H1B	109.00	C14—C19—H19	119.00
C2—C1—H1C	109.00	C18—C19—H19	119.00
H1A—C1—H1B	109.00		
C11—O2—C12—C13	−83.5 (2)	C14—C4—C5—C6	−102.3 (2)
C12—O2—C11—O1	−7.9 (3)	C14—C4—C5—C8	78.0 (2)
C12—O2—C11—C3	171.77 (16)	C3—C4—C14—C15	−65.5 (2)
C8—O4—C9—C10	80.4 (2)	C3—C4—C14—C19	114.0 (2)
C9—O4—C8—O3	10.3 (3)	C5—C4—C14—C15	58.1 (2)

C9—O4—C8—C5	−171.06 (15)	C5—C4—C14—C19	−122.3 (2)
C6—N1—C2—C1	−166.26 (17)	C4—C5—C6—C7	176.77 (17)
C6—N1—C2—C3	12.1 (3)	C8—C5—C6—N1	174.40 (17)
C2—N1—C6—C5	−12.9 (3)	C8—C5—C6—C7	−3.5 (3)
C2—N1—C6—C7	165.30 (17)	C4—C5—C8—O3	17.5 (3)
C1—C2—C3—C11	−0.3 (3)	C4—C5—C8—O4	−161.12 (16)
N1—C2—C3—C4	6.9 (3)	C6—C5—C8—O3	−162.23 (19)
N1—C2—C3—C11	−178.42 (17)	C6—C5—C8—O4	19.1 (3)
C1—C2—C3—C4	−174.97 (18)	C4—C5—C6—N1	−5.4 (3)
C2—C3—C4—C14	101.3 (2)	C4—C14—C15—C16	179.40 (18)
C11—C3—C4—C5	163.28 (17)	C19—C14—C15—C16	−0.2 (3)
C11—C3—C4—C14	−73.5 (2)	C4—C14—C19—C18	−178.99 (18)
C2—C3—C11—O1	−3.2 (3)	C15—C14—C19—C18	0.6 (3)
C2—C3—C11—O2	177.10 (17)	C14—C15—C16—C17	−0.6 (3)
C4—C3—C11—O1	171.59 (19)	C15—C16—C17—Br	−179.49 (15)
C4—C3—C11—O2	−8.1 (2)	C15—C16—C17—C18	1.0 (3)
C2—C3—C4—C5	−21.9 (2)	Br—C17—C18—C19	179.87 (15)
C3—C4—C5—C6	21.2 (2)	C16—C17—C18—C19	−0.6 (3)
C3—C4—C5—C8	−158.58 (16)	C17—C18—C19—C14	−0.2 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O3^{i}	0.86	2.11	2.969 (2)	173
C4—H4···O3	0.98	2.47	2.811 (2)	100

Symmetry codes: (i) *x*, *y*−1, *z*.

Fig. 1

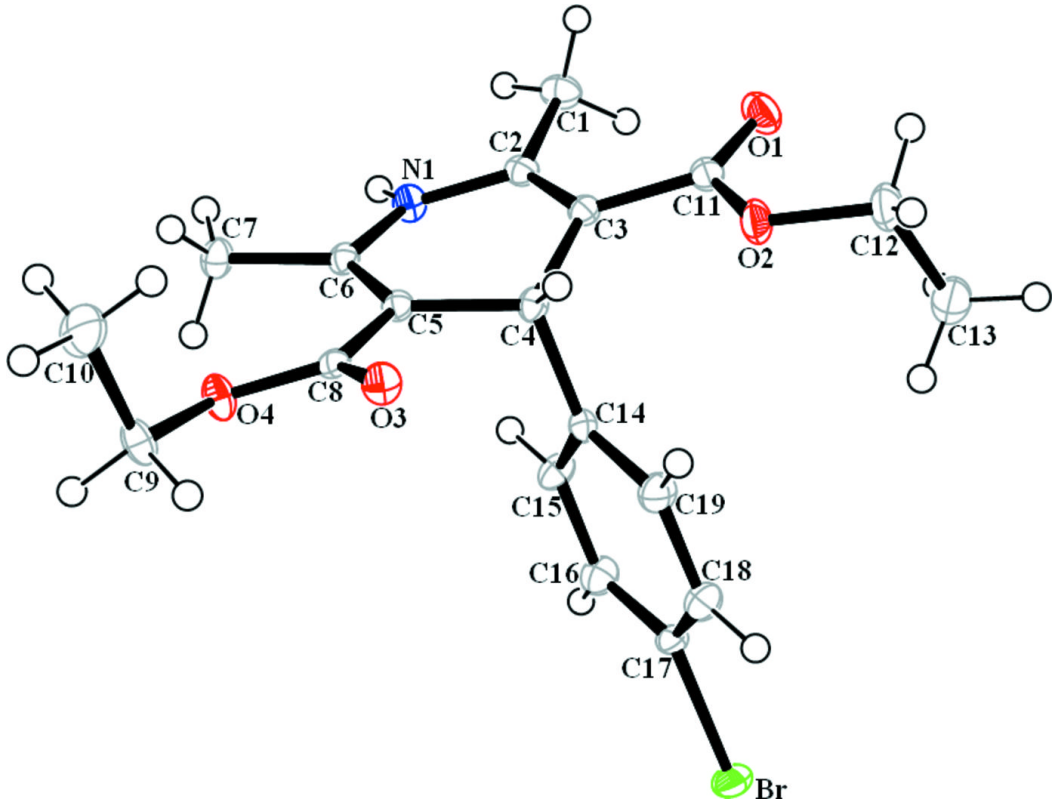
C1
C2
O1
N1
C11
C7
C3
O2
C12
C6
C5
C4
C13
C10
C8
O4
O3
C14
C9
C15
C19
C16
C18
C17
Br

Fig. 2