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3-(2-Methoxyethyl) 5-methyl 2,6-dimethyl-4-(3-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate

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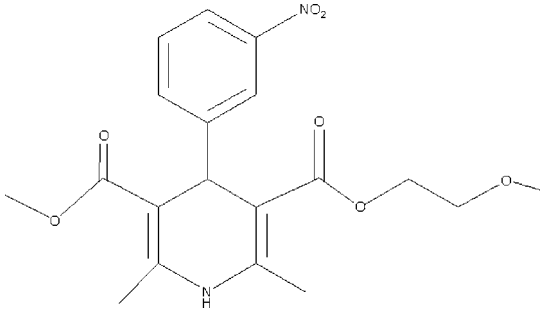
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.055; wR factor = 0.138; data-to-parameter ratio = 17.3.

The title compound, $C_{19}H_{22}N_3O_7$, is a nefidipine analogue. The crystal packing is stabilized by intermolecular N—H···O hydrogen bonds.

Related literature

For related literature, see: Cotta-Ramusino & Varì (1999); Goldmann & Stoltefuss (1991); Hofmann & Cimiraglia (1990); Sun *et al.* (2006); Yiu & Knaus (1999).



Experimental

Crystal data

$C_{19}H_{22}N_2O_7$
M_r = 390.39
Monoclinic, $P2_1/c$
a = 14.575 (3) Å
b = 9.909 (2) Å
c = 14.522 (3) Å
β = 115.11 (3)°
V = 1899.1 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 293 (2) K
0.10 × 0.08 × 0.06 mm

Data collection

Bruker $P4$ diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick 1996)
T_{min} = 0.990, T_{max} = 0.994
14339 measured reflections
4505 independent reflections
3156 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.138
S = 1.06
4505 reflections
261 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.30 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
N1—H1···O2^{i}	0.888 (9)	1.974 (10)	2.8556 (19)	171 (2)

Symmetry code: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SHELXTL* (Bruker, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: EZ2085).

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supplementary materials

Acta Cryst. (2007). E**63**, o3451 [**doi:10.1107/S1600536807032515**]

3-(2-Methoxyethyl) 5-methyl 2,6-dimethyl-4-(3-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate

F.-X. Sun, F.-G. Rong, X.-H. Chu and S.-X. Yan

Comment

4-Aryl-1,4-dihydropyridine-3,5-dicarboxylic diesters of the nefidipine type have become almost indispensable for the treatment of cardiovascular diseases since they first appeared on the market in 1975 (Yiu & Knaus, 1999; Goldmann & Stoltefuss, 1991). The title compound, (I), is a nefidipine analog. The molecular structure of (I) is shown in Fig. 1. The dihydropyridine rings display an envelope conformation, with atom C4 displaced from the mean planes formed by the other atoms in the same ring by 0.170 (1) A°. The dihedral angle between the benzene ring and the N1/C2/C3/C5/C6 plane is 85.50 (0)°. This is similar to the situation found in nefidipine (Hofmann & Cimiraglia, 1990; Cotta-Ramusino & Varì, 1999) and the structure of 3-(2-acetoxyethyl) 5-methyl 2,6-dimethyl-4-(3-nitrophenyl)-1,4-dihydropyridine- 3,5-dicarboxylate (Sun *et al.*, 2006).

Experimental

The title compound was prepared by dissolving 2,6-dimethyl-4-(*m*-nitro-phenyl)-1,4-dihydro-pyridine-3,5-dicarboxylic acid mono-methyl ester (332 mg, 1 mmol) and 2-methoxy-ethanol (76 mg, 1 mmol) in 10 ml CH_2Cl_2. Dicyclohexyl-carbodiimide (206 mg, 1 mmol) was added dropwise to the solution at 278 K. The reaction mixture was stirred at 276–279 K for a further 6 h. The solvent was removed by vacuum evaporation. The desired product was purified by chromatography on a silica gel column (eluted by ethyl acetate and petroleum, 1:6) at room temperature. The product (350 mg) was obtained in a yield of 90%. Suitable crystals were obtained by slow evaporation of a solution in ethyl acetate and petroleum (1:6).

Refinement

The H atom bonded to N1 was located in a difference map and its positional parameters were refined freely [U_{iso}(H) = 1.2Ueq(N)]. All other H atoms were positioned geometrically and refined using a riding model, with C—H = 0.97 A ° and U_{iso}(H) = 1.2Ueq(C) or 1.5Ueq(C).

Figures

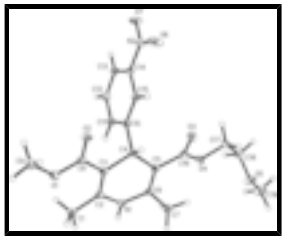


Fig. 1. A view of the title compound (I) showing atom numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

3-(2-Methoxyethyl) 5-methyl 2,6-dimethyl-4-(3-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate

Crystal data

$C_{19}H_{22}N_2O_7$	$D_x = 1.365$ Mg m^{-3}
$M_r = 390.39$	Melting point: 413-414 K
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 14.575$ (3) Å	Cell parameters from 2365 reflections
$b = 9.909$ (2) Å	$\theta = 2.5$–33.6º
$c = 14.522$ (3) Å	$\mu = 0.11$ mm^{-1}
$\beta = 115.11$ (3)º	$T = 293$ (2) K
$V = 1899.1$ (7) Å^3	Block, yellow
$Z = 4$	0.10 × 0.08 × 0.06 mm
$F_{000} = 824$	

Data collection

Bruker P4 diffractometer	4505 independent reflections
Radiation source: fine-focus sealed tube	3156 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.055$
$T = 293$(2) K	$\theta_{max} = 27.9$º
ω scans	$\theta_{min} = 2.6$º
Absorption correction: multi-scan (SADABS; Sheldrick 1996)	$h = -19 \rightarrow 15$
$T_{min} = 0.990$, $T_{max} = 0.994$	$k = -13 \rightarrow 13$
14339 measured reflections	$l = -15 \rightarrow 19$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.055$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.138$	$w = 1/[\sigma^2(F_o^2) + (0.0636P)^2 + 0.0976P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.001$
4505 reflections	$\Delta\rho_{max} = 0.30$ e Å^{-3}
261 parameters	$\Delta\rho_{min} = -0.23$ e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\text{sigma}(F^2)$ 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}
O1	0.60094 (10)	0.61768 (13)	1.13994 (9)	0.0270 (3)
O2	0.49017 (10)	0.70189 (13)	1.19424 (9)	0.0269 (3)
O3	0.24981 (11)	1.05799 (13)	1.00474 (10)	0.0335 (4)
O4	0.20420 (10)	1.08548 (14)	0.83810 (10)	0.0310 (3)
O5	0.12560 (11)	1.32144 (15)	0.70977 (11)	0.0383 (4)
O6	0.14553 (13)	0.79275 (18)	1.19824 (13)	0.0520 (5)
O7	0.04605 (11)	0.62697 (15)	1.12708 (12)	0.0414 (4)
N1	0.45194 (12)	0.83737 (15)	0.86965 (11)	0.0229 (3)
N2	0.11639 (12)	0.70158 (17)	1.13617 (12)	0.0286 (4)
C1	0.58383 (15)	0.67373 (19)	0.94922 (14)	0.0260 (4)
H1A	0.6474	0.6993	1.0033	0.039*
H1B	0.5866	0.6874	0.8850	0.039*
H1C	0.5707	0.5803	0.9564	0.039*
C2	0.50064 (13)	0.75855 (17)	0.95394 (13)	0.0197 (4)
C3	0.47090 (13)	0.76349 (17)	1.03097 (13)	0.0192 (4)
C4	0.37869 (13)	0.84412 (17)	1.02140 (13)	0.0194 (4)
H4	0.3980	0.8990	1.0829	0.023*
C5	0.34163 (14)	0.93896 (17)	0.93035 (13)	0.0203 (4)
C6	0.37773 (13)	0.93152 (17)	0.85898 (13)	0.0204 (4)
C7	0.35141 (16)	1.01866 (19)	0.76676 (13)	0.0276 (4)
H7A	0.3090	1.0918	0.7686	0.041*
H7B	0.3159	0.9658	0.7066	0.041*
H7C	0.4124	1.0541	0.7660	0.041*
C8	0.51996 (13)	0.69282 (17)	1.12730 (13)	0.0199 (4)
C9	0.64973 (16)	0.5507 (2)	1.23687 (14)	0.0329 (5)
H9A	0.6656	0.6156	1.2905	0.049*
H9B	0.7110	0.5085	1.2420	0.049*
H9C	0.6051	0.4834	1.2426	0.049*
C10	0.29293 (13)	0.75040 (17)	1.01454 (12)	0.0189 (4)
C11	0.26034 (14)	0.64731 (18)	0.94289 (14)	0.0241 (4)
H11	0.2917	0.6357	0.8995	0.029*
C12	0.18251 (14)	0.56185 (19)	0.93470 (15)	0.0281 (4)
H12	0.1619	0.4938	0.8860	0.034*

C13	0.13505 (14)	0.57720 (19)	0.99865 (14)	0.0256 (4)
H13	0.0833	0.5193	0.9947	0.031*
C14	0.16678 (13)	0.68103 (17)	1.06860 (13)	0.0209 (4)
C15	0.24447 (14)	0.76776 (17)	1.07778 (13)	0.0213 (4)
H15	0.2639	0.8368	1.1257	0.026*
C16	0.26331 (14)	1.03323 (17)	0.92952 (13)	0.0231 (4)
C17	0.12072 (16)	1.1692 (2)	0.83370 (16)	0.0344 (5)
H17A	0.1461	1.2441	0.8808	0.041*
H17B	0.0748	1.1168	0.8521	0.041*
C18	0.06682 (15)	1.2205 (2)	0.72745 (16)	0.0322 (5)
H18A	0.0553	1.1469	0.6798	0.039*
H18B	0.0015	1.2573	0.7173	0.039*
C19	0.08013 (19)	1.3655 (3)	0.60699 (18)	0.0504 (6)
H19A	0.0761	1.2913	0.5630	0.076*
H19B	0.1203	1.4363	0.5976	0.076*
H19C	0.0132	1.3988	0.5910	0.076*
H1	0.4693 (16)	0.831 (2)	0.8182 (12)	0.037 (6)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0301 (7)	0.0354 (7)	0.0173 (6)	0.0075 (6)	0.0117 (6)	0.0043 (5)
O2	0.0290 (8)	0.0382 (8)	0.0180 (6)	−0.0013 (6)	0.0145 (6)	0.0023 (6)
O3	0.0477 (9)	0.0309 (7)	0.0308 (8)	0.0091 (6)	0.0253 (7)	0.0010 (6)
O4	0.0328 (8)	0.0357 (8)	0.0289 (7)	0.0114 (6)	0.0173 (6)	0.0050 (6)
O5	0.0365 (9)	0.0461 (9)	0.0307 (8)	−0.0077 (7)	0.0127 (7)	0.0093 (7)
O6	0.0572 (11)	0.0653 (11)	0.0551 (10)	−0.0319 (9)	0.0446 (9)	−0.0335 (9)
O7	0.0369 (9)	0.0500 (9)	0.0501 (10)	−0.0192 (7)	0.0310 (8)	−0.0092 (7)
N1	0.0303 (9)	0.0276 (8)	0.0172 (8)	0.0016 (7)	0.0163 (7)	0.0019 (6)
N2	0.0255 (9)	0.0358 (9)	0.0289 (9)	−0.0054 (7)	0.0158 (8)	−0.0021 (7)
C1	0.0294 (10)	0.0331 (10)	0.0215 (9)	0.0004 (8)	0.0165 (8)	0.0011 (8)
C2	0.0220 (9)	0.0228 (9)	0.0165 (8)	−0.0032 (7)	0.0103 (8)	−0.0015 (7)
C3	0.0234 (10)	0.0216 (9)	0.0161 (8)	−0.0031 (7)	0.0116 (7)	−0.0011 (7)
C4	0.0248 (10)	0.0215 (9)	0.0156 (8)	−0.0037 (7)	0.0122 (8)	−0.0028 (7)
C5	0.0245 (10)	0.0209 (8)	0.0186 (9)	−0.0032 (7)	0.0123 (8)	−0.0016 (7)
C6	0.0244 (10)	0.0206 (9)	0.0185 (9)	−0.0043 (7)	0.0115 (8)	−0.0016 (7)
C7	0.0361 (11)	0.0282 (10)	0.0225 (9)	−0.0014 (8)	0.0165 (9)	0.0017 (8)
C8	0.0224 (9)	0.0229 (9)	0.0162 (8)	−0.0056 (7)	0.0099 (8)	−0.0024 (7)
C9	0.0338 (11)	0.0441 (12)	0.0204 (10)	0.0068 (9)	0.0112 (9)	0.0092 (8)
C10	0.0206 (9)	0.0215 (8)	0.0155 (8)	0.0005 (7)	0.0085 (7)	0.0014 (7)
C11	0.0261 (10)	0.0274 (10)	0.0225 (9)	−0.0015 (8)	0.0138 (8)	−0.0048 (7)
C12	0.0278 (11)	0.0255 (10)	0.0302 (10)	−0.0056 (8)	0.0117 (9)	−0.0087 (8)
C13	0.0214 (10)	0.0259 (10)	0.0287 (10)	−0.0038 (8)	0.0098 (8)	0.0010 (8)
C14	0.0202 (9)	0.0243 (9)	0.0212 (9)	0.0003 (7)	0.0116 (8)	0.0021 (7)
C15	0.0251 (10)	0.0222 (9)	0.0179 (9)	−0.0022 (7)	0.0105 (8)	−0.0016 (7)
C16	0.0303 (10)	0.0194 (9)	0.0239 (10)	−0.0027 (8)	0.0155 (8)	−0.0013 (7)
C17	0.0346 (12)	0.0359 (11)	0.0424 (12)	0.0119 (9)	0.0256 (10)	0.0085 (9)
C18	0.0274 (11)	0.0340 (11)	0.0386 (12)	0.0017 (9)	0.0172 (10)	0.0024 (9)

C19	0.0452 (14)	0.0649 (16)	0.0367 (13)	−0.0055 (12)	0.0132 (11)	0.0147 (12)

Geometric parameters (Å, °)

O1—C8	1.341 (2)	C6—C7	1.500 (2)
O1—C9	1.441 (2)	C7—H7A	0.9600
O2—C8	1.225 (2)	C7—H7B	0.9600
O3—C16	1.214 (2)	C7—H7C	0.9600
O4—C16	1.342 (2)	C9—H9A	0.9600
O4—C17	1.452 (2)	C9—H9B	0.9600
O5—C18	1.410 (2)	C9—H9C	0.9600
O5—C19	1.421 (3)	C10—C15	1.386 (2)
O6—N2	1.218 (2)	C10—C11	1.390 (2)
O7—N2	1.225 (2)	C11—C12	1.380 (3)
N1—C2	1.369 (2)	C11—H11	0.9300
N1—C6	1.386 (2)	C12—C13	1.382 (3)
N1—H1	0.888 (9)	C12—H12	0.9300
N2—C14	1.468 (2)	C13—C14	1.380 (3)
C1—C2	1.501 (2)	C13—H13	0.9300
C1—H1A	0.9600	C14—C15	1.382 (2)
C1—H1B	0.9600	C15—H15	0.9300
C1—H1C	0.9600	C17—C18	1.492 (3)
C2—C3	1.361 (2)	C17—H17A	0.9700
C3—C8	1.452 (2)	C17—H17B	0.9700
C3—C4	1.518 (2)	C18—H18A	0.9700
C4—C5	1.522 (2)	C18—H18B	0.9700
C4—C10	1.526 (2)	C19—H19A	0.9600
C4—H4	0.9800	C19—H19B	0.9600
C5—C6	1.349 (2)	C19—H19C	0.9600
C5—C16	1.471 (3)		
C8—O1—C9	115.48 (14)	H9A—C9—H9B	109.5
C16—O4—C17	115.99 (14)	O1—C9—H9C	109.5
C18—O5—C19	111.16 (16)	H9A—C9—H9C	109.5
C2—N1—C6	124.58 (14)	H9B—C9—H9C	109.5
C2—N1—H1	119.0 (14)	C15—C10—C11	118.60 (16)
C6—N1—H1	116.4 (14)	C15—C10—C4	120.98 (15)
O6—N2—O7	122.71 (16)	C11—C10—C4	120.41 (15)
O6—N2—C14	118.76 (15)	C12—C11—C10	121.52 (17)
O7—N2—C14	118.52 (16)	C12—C11—H11	119.2
C2—C1—H1A	109.5	C10—C11—H11	119.2
C2—C1—H1B	109.5	C11—C12—C13	120.16 (17)
H1A—C1—H1B	109.5	C11—C12—H12	119.9
C2—C1—H1C	109.5	C13—C12—H12	119.9
H1A—C1—H1C	109.5	C14—C13—C12	118.01 (17)
H1B—C1—H1C	109.5	C14—C13—H13	121.0
C3—C2—N1	119.28 (16)	C12—C13—H13	121.0
C3—C2—C1	127.08 (16)	C13—C14—C15	122.64 (16)
N1—C2—C1	113.64 (14)	C13—C14—N2	119.26 (16)
C2—C3—C8	125.15 (16)	C15—C14—N2	118.10 (16)

C2—C3—C4	121.45 (15)	C14—C15—C10	119.06 (16)
C8—C3—C4	113.38 (14)	C14—C15—H15	120.5
C3—C4—C5	112.24 (14)	C10—C15—H15	120.5
C3—C4—C10	110.75 (14)	O3—C16—O4	122.05 (17)
C5—C4—C10	109.88 (14)	O3—C16—C5	122.84 (16)
C3—C4—H4	107.9	O4—C16—C5	115.03 (15)
C5—C4—H4	107.9	O4—C17—C18	107.68 (15)
C10—C4—H4	107.9	O4—C17—H17A	110.2
C6—C5—C16	125.65 (16)	C18—C17—H17A	110.2
C6—C5—C4	121.55 (16)	O4—C17—H17B	110.2
C16—C5—C4	112.79 (14)	C18—C17—H17B	110.2
C5—C6—N1	119.42 (15)	H17A—C17—H17B	108.5
C5—C6—C7	128.25 (17)	O5—C18—C17	109.62 (17)
N1—C6—C7	112.27 (15)	O5—C18—H18A	109.7
C6—C7—H7A	109.5	C17—C18—H18A	109.7
C6—C7—H7B	109.5	O5—C18—H18B	109.7
H7A—C7—H7B	109.5	C17—C18—H18B	109.7
C6—C7—H7C	109.5	H18A—C18—H18B	108.2
H7A—C7—H7C	109.5	O5—C19—H19A	109.5
H7B—C7—H7C	109.5	O5—C19—H19B	109.5
O2—C8—O1	121.34 (16)	H19A—C19—H19B	109.5
O2—C8—C3	122.25 (16)	O5—C19—H19C	109.5
O1—C8—C3	116.40 (14)	H19A—C19—H19C	109.5
O1—C9—H9A	109.5	H19B—C19—H19C	109.5
O1—C9—H9B	109.5		

C6—N1—C2—C3	5.0 (3)	C5—C4—C10—C15	−106.64 (18)
C6—N1—C2—C1	−175.04 (16)	C3—C4—C10—C11	−52.6 (2)
N1—C2—C3—C8	−175.56 (16)	C5—C4—C10—C11	72.0 (2)
C1—C2—C3—C8	4.5 (3)	C15—C10—C11—C12	−0.9 (3)
N1—C2—C3—C4	5.9 (2)	C4—C10—C11—C12	−179.55 (16)
C1—C2—C3—C4	−174.06 (17)	C10—C11—C12—C13	−0.2 (3)
C2—C3—C4—C5	−12.9 (2)	C11—C12—C13—C14	1.1 (3)
C8—C3—C4—C5	168.40 (14)	C12—C13—C14—C15	−1.0 (3)
C2—C3—C4—C10	110.34 (18)	C12—C13—C14—N2	178.76 (17)
C8—C3—C4—C10	−68.37 (18)	O6—N2—C14—C13	179.37 (19)
C3—C4—C5—C6	10.6 (2)	O7—N2—C14—C13	−1.3 (3)
C10—C4—C5—C6	−113.10 (18)	O6—N2—C14—C15	−0.8 (3)
C3—C4—C5—C16	−170.61 (14)	O7—N2—C14—C15	178.47 (17)
C10—C4—C5—C16	65.68 (18)	C13—C14—C15—C10	−0.1 (3)
C16—C5—C6—N1	179.96 (16)	N2—C14—C15—C10	−179.84 (15)
C4—C5—C6—N1	−1.4 (3)	C11—C10—C15—C14	1.0 (3)
C16—C5—C6—C7	3.0 (3)	C4—C10—C15—C14	179.64 (16)
C4—C5—C6—C7	−178.38 (17)	C17—O4—C16—O3	−2.3 (3)
C2—N1—C6—C5	−7.3 (3)	C17—O4—C16—C5	174.69 (16)
C2—N1—C6—C7	170.09 (16)	C6—C5—C16—O3	−162.51 (18)
C9—O1—C8—O2	−0.5 (2)	C4—C5—C16—O3	18.8 (2)
C9—O1—C8—C3	178.75 (15)	C6—C5—C16—O4	20.5 (3)
C2—C3—C8—O2	179.45 (17)	C4—C5—C16—O4	−158.19 (15)
C4—C3—C8—O2	−1.9 (2)	C16—O4—C17—C18	178.25 (16)

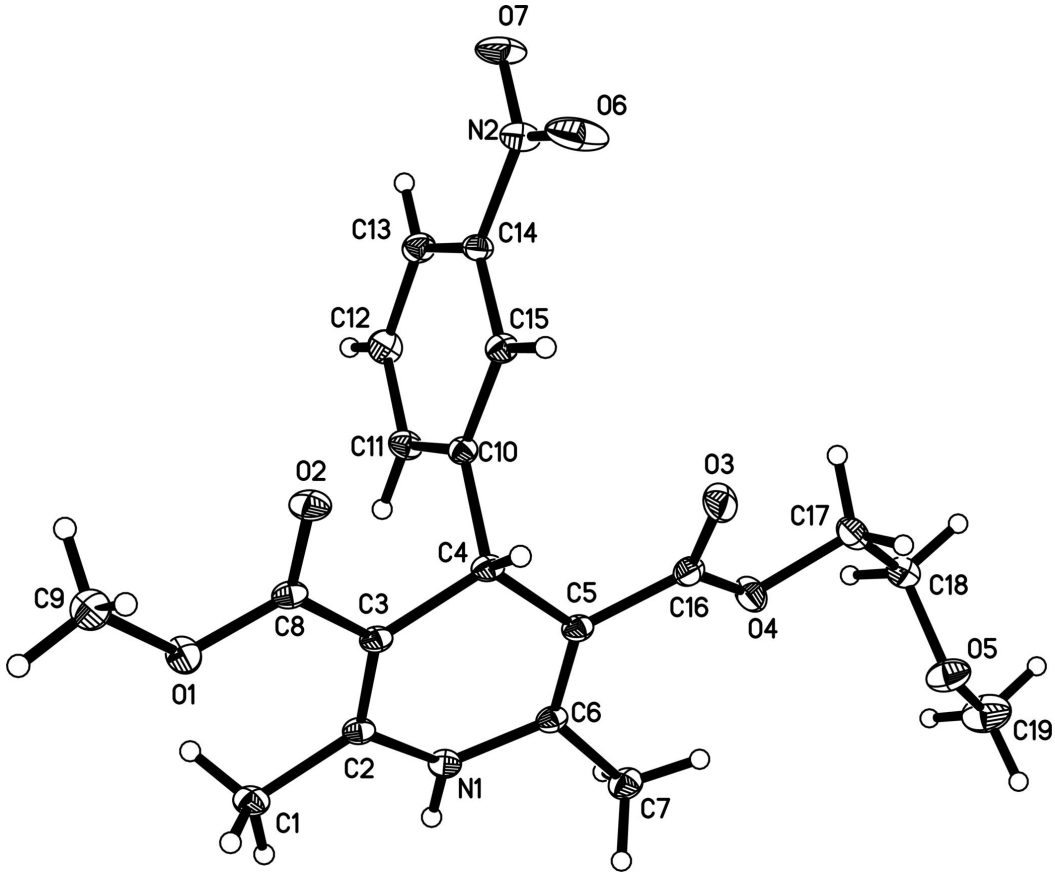
C2—C3—C8—O1	0.2 (3)	C19—O5—C18—C17	175.64 (18)
C4—C3—C8—O1	178.86 (14)	O4—C17—C18—O5	−73.8 (2)
C3—C4—C10—C15	128.79 (17)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.888 (9)	1.974 (10)	2.8556 (19)	171 (2)

Symmetry codes: (i) *x*, −*y*+3/2, *z*−1/2.

Fig. 1


O7
O6
N2
C13
C14
C12
C15
C11
C10
O2
O3
C17
C4
C9
C8
C3
C5
C16
O4
C18
O5
O1
C6
C19
C2
N1
C7
C1