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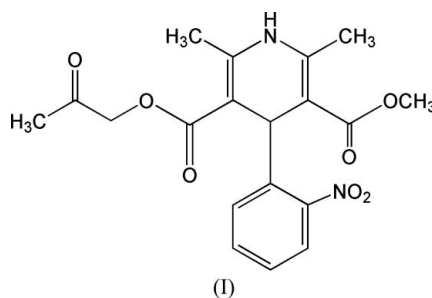
## Key indicators

Single-crystal X-ray study  
 $T = 293\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$   
 $R$  factor = 0.041  
 $wR$  factor = 0.118  
Data-to-parameter ratio = 12.7For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Acetyl methyl 1,4-dihydro-2,6-dimethyl-  
4-(2-nitrophenyl)pyridine-3,5-dicarboxylate

In the title compound,  $\text{C}_{19}\text{H}_{20}\text{N}_2\text{O}_7$ , the C atom in the 4-position of the dihydropyridine ring is displaced out of the plane by 0.0461 (2) Å. The dihydropyridine ring plane is almost perpendicular to the benzene ring, with a dihedral angle of 88.9 (3)°.

## Comment

4-Phenyl-1,4-dihydropyridines are useful in treating diseases of the circulation, especially those concerning coronaries (Bossert *et al.*, 1972; Ohno *et al.*, 1986). We present here the structure of the title compound, (I).



In (I), the dihydropyridine ring is almost perpendicular to the benzene ring, with a dihedral angle of 88.9 (3)° (Fig. 1). C7 is displaced from the dihydropyridine ring plane by 0.0461 (2) Å. Intermolecular N—H...O and C—H...O hydrogen bonds stabilize the crystal structure (Fig. 2 and Table 2).

## Experimental

The title compound was prepared according to the method described by Phillips (1949) and Berson & Brown (1955). To a mixture of 2-nitrobenzaldehyde (15.1 g, 0.1 mol), acetoacetate-2-epoxyethylpropionate (14.4 g, 0.1 mol) and methyl acetoacetate (11.6 g, 0.1 mol), methanol (100 ml) and ammonia solution (32 ml) were added under reflux for 10 h hours, then the solution was filtered. The product was placed in a 100 ml three-neck flask, 30 ml of acetic acid and 50 ml of distilled water were added, and the mixture was heated under reflux for 24 h hours. The crude product was cooled, and filtered off. Yellow crystals (20.1 g, yield 50%) were obtained, and single crystals (m.p. 423–424 K) suitable for crystallographic analysis were obtained by slow evaporation of an ethanol solution. Spectroscopic analysis: IR (KBr,  $\nu\text{ cm}^{-1}$ ): 3332, 3100, 2952, 1708, 1679, 1649, 1645, 1620, 1526, 1495, 1350, 1430, 1382, 1206, 716;  $^1\text{H NMR}$  ( $\text{CDCl}_3$ ,  $\delta$ , p.p.m.): 7.25–7.67(*m*, 4H), 6.61(*sw*, 1H), 5.74(*d*, 1H), 4.59(*q*, 2H), 3.56(*s*, 3H), 2.29–2.34(*s*, 6H), 2.03(*s*, 3H). Analysis, calculated for  $\text{C}_{19}\text{H}_{20}\text{N}_2\text{O}_7$ : C 58.76, H 5.19, N 7.21%; found: C 58.80, H 5.20, N 7.25%.

Crystal data

C<sub>19</sub>H<sub>20</sub>N<sub>2</sub>O<sub>7</sub>  
*M<sub>r</sub>* = 388.37  
 Monoclinic, *C2/c*  
*a* = 26.462 (15) Å  
*b* = 9.566 (6) Å  
*c* = 16.159 (9) Å  
 β = 115.155 (6)°  
*V* = 3703 (4) Å<sup>3</sup>  
*Z* = 8

*D<sub>x</sub>* = 1.393 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 Cell parameters from 2469 reflections  
 θ = 2.3–25.5°  
 μ = 0.11 mm<sup>-1</sup>  
*T* = 293 (2) K  
 Block, yellow  
 0.36 × 0.22 × 0.16 mm

Data collection

Bruker APEX-II CCD area-detector diffractometer  
 φ and ω scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
*T<sub>min</sub>* = 0.972, *T<sub>max</sub>* = 0.983  
 9700 measured reflections

3272 independent reflections  
 2456 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.021  
 θ<sub>max</sub> = 25.0°  
*h* = -31 → 31  
*k* = -11 → 7  
*l* = -19 → 19

Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.042  
*wR* (*F*<sup>2</sup>) = 0.118  
*S* = 1.06  
 3272 reflections  
 257 parameters  
 H-atom parameters constrained

*w* = 1/[σ<sup>2</sup>(*F<sub>o</sub>*<sup>2</sup>) + (0.0544*P*)<sup>2</sup> + 2.0965*P*]  
 where *P* = (*F<sub>o</sub>*<sup>2</sup> + 2*F<sub>c</sub>*<sup>2</sup>)/3  
 (Δ/σ)<sub>max</sub> = 0.001  
 Δρ<sub>max</sub> = 0.29 e Å<sup>-3</sup>  
 Δρ<sub>min</sub> = -0.26 e Å<sup>-3</sup>

Table 1

Selected geometric parameters (Å, °).

O1–N1	1.226 (2)	O6–C16	1.353 (2)
O2–N1	1.217 (2)	O6–C17	1.436 (2)
O3–C9	1.331 (2)	O7–C18	1.204 (3)
O3–C10	1.435 (2)	N1–C1	1.475 (3)
O4–C9	1.216 (2)	N2–C11	1.373 (3)
O5–C16	1.204 (2)	N2–C13	1.374 (2)
C15–C7–C8	111.45 (14)	C8–C7–C6	110.53 (14)
C15–C7–C6	109.09 (14)		
O2–N1–C1–C6	-41.6 (3)	C1–C6–C7–C8	132.86 (18)

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> –H... <i>A</i>	<i>D</i> –H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> –H... <i>A</i>
N2–H2A...O4 <sup>i</sup>	0.86	2.16	2.958 (2)	154
C2–H2...O7 <sup>ii</sup>	0.93	2.44	3.237 (4)	144

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

All H atoms were initially located in a difference Fourier map. The methyl H atoms were then constrained to an ideal geometry, with C–H distances of 0.96 Å and *U*<sub>iso</sub>(H) = 1.5*U*<sub>eq</sub>(C), but each group was allowed to rotate freely about its C–C bond. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C–H = 0.93–0.98 Å and N–H = 0.86 Å, and with *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C or N).

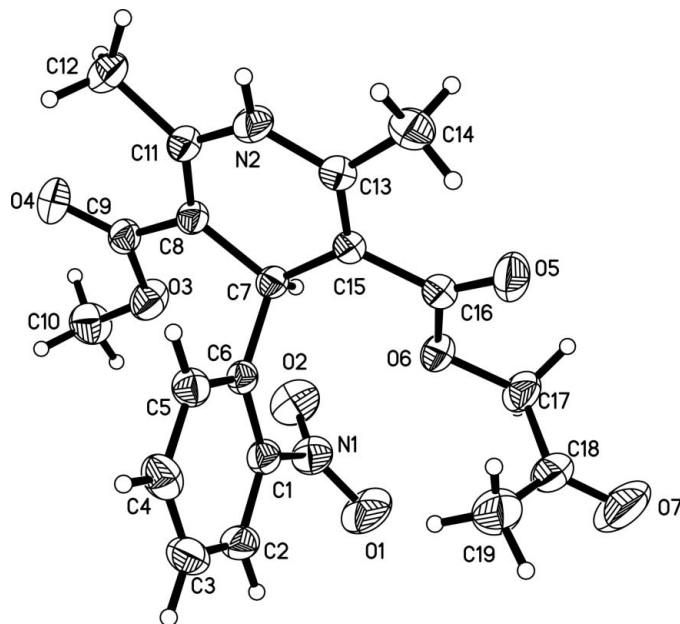


Figure 1  
 View of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 35% probability level.

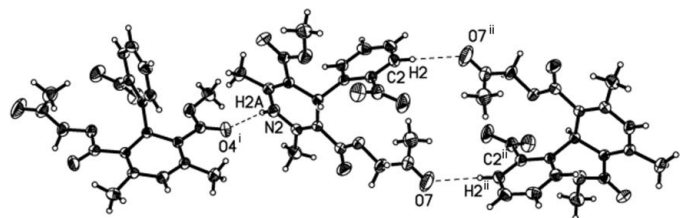


Figure 2  
 The hydrogen-bonding scheme in (I). N–H...O and C–H...O hydrogen bonds are shown as dashed lines (symmetry codes are as in Table 2).

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

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