Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Ethyl 3-acetyl-4-(4-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate

Noor Shahina Begum* and D. E. Vasundhara

Department of Studies in Chemistry, Bangalore University, Bangalore 560 001, India
Correspondence e-mail: noorsb@rediffmail.com

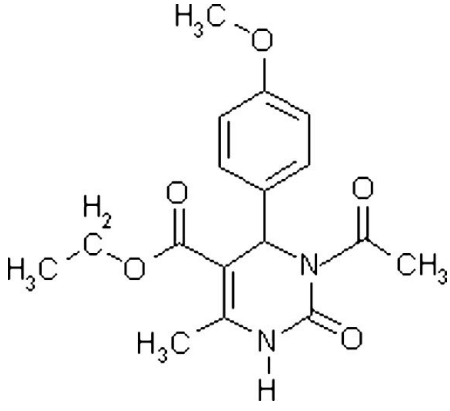
Received 25 July 2007; accepted 1 August 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.058; wR factor = 0.121; data-to-parameter ratio = 11.7.

The crystal structure of the title compound, $C_{17}H_{20}N_2O_5$, is stabilized by C—H···O and N—H···O hydrogen bonds.

Related literature

For related literature, see: Atwal *et al.* (1990, 1991); Cho *et al.* (1989); Grover *et al.* (1995); Hurst & Hull (1961); Janis *et al.* (1987); Jauk *et al.* (2000); Kappe (1998, 2000); Kappe *et al.* (1997); Mayer *et al.* (1999); Rovnyak *et al.* (1992, 1995); Shishkin *et al.* (1997); Triggle & Padmanabhan (1995).



Experimental

Crystal data

$C_{17}H_{20}N_2O_5$
M_r = 332.35
Monoclinic, $P2_1/c$
a = 8.8387 (8) Å
b = 20.2043 (18) Å
c = 10.0232 (9) Å
β = 107.839 (2)°
V = 1703.9 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 (2) K
0.3 × 0.2 × 0.1 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
17507 measured reflections
3343 independent reflections
2369 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.121
S = 1.10
3343 reflections
286 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C17—H17B···O3^{i}	0.929 (4)	2.515 (4)	3.228 (4)	133 (2)
C15—H15B···O4^{ii}	0.911 (5)	2.794 (7)	3.553 (4)	141 (2)
N1—H1N···O4^{ii}	0.892 (6)	2.024 (6)	2.913 (3)	174 (2)
C4—H4···O1^{iii}	0.979 (6)	2.572 (6)	3.310 (3)	132 (1)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

DEV thanks the UGC–FIP for a Teacher Fellowship. NSB thanks the UGC–DRS for financial support. The authors also thank the DST, India, for data collection on the CCD facility set up under the IRPHA DST programme.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2022).

References

Atwal, K., Rovnyak, G. C., Schwartz, J., Moreland, S., Hedberg, A., Gougoutas, J. Z., Malley, M. F. & Floyd, D. M. (1990). *J. Med. Chem.* **33**, 1510–1515.
Atwal, K. S., Swanson, B. N., Unger, S. E., Floyd, D. M., Moreland, S., Hedberg, A. & O'Reilly, B. C. (1991). *J. Med. Chem.* **34**, 806–811.
Bruker (1998). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cho, H., Ueda, M., Shima, K., Mizuno, A., Hayashimatsu, M., Ohnaka, Y., Takeuchi, Y., Hamaguchi, M., Aisaka, K., Hidaka, T., Kawai, M., Takeda, M., Ishihara, T., Funahashi, K., Satah, F., Morita, M. & Noguchi, T. (1989). *J. Med. Chem.* **32**, 2399–2406.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Grover, G. J., Dzwonczyk, S., McMullen, D. M., Normadinam, C. S., Sleph, P. G. & Moreland, S. J. (1995). *J. Cardiovasc. Pharmacol.* **26**, 289–294.
Hurst, E. W. & Hull, R. (1961). *J. Med. Pharm. Chem.* **3**, 215–229.
Janis, R. A., Silver, P. J. & Triggle, D. J. (1987). *Adv. Drug Res.* **16**, 309–312.
Jauk, B., Pernat, T. & Kappe, C. O. (2000). *Molecules*, **5**, 227–239.
Kappe, C. O. (1998). *Molecules*, **3**, 1–20.
Kappe, C. O. (2000). *Eur. J. Med. Chem.* **35**, 1043–1052.
Kappe, C. O., Fabian, W. M. F. & Semones, M. A. (1997). *Tetrahedron*, **53**, 2803–2816.
Mayer, T. U., Kapoor, T. M., Haggarty, S. J., King, R. W., Schreiber, S. I. & Mitchison, T. J. (1999). *Science*, **286**, 971–974.
Rovnyak, G. C., Atwal, K. S., Hedberg, A., Kimball, S. D., Moreland, S., Gougoutas, J. Z., O'Reilly, B. C., Schwartz, J. & Malley, M. F. (1992). *J. Med. Chem.* **35**, 3254–3263.

 doi:10.1107/S1600536807037890

Rovnyak, G. C., Kimball, S. D., Beyer, B., Cucinotta, G., DiMarco, J. D., Gougoutas, J., Hedberg, A., Malley, M., McCarthy, J. P., Zhang, R. & Moreland, S. (1995). *J. Med. Chem.* **38**, 119–129.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Shishkin, O. V., Solomovich, E. V., Vakula, V. M. & Yaremenko, F. G. (1997). *Russ. Chem. Bull.* **46**, 1941–1946.
Triggle, D. J. & Padmanabhan, S. (1995). *Chemtracts Org. Chem.* **8**, 191–196.

supplementary materials

Acta Cryst. (2007). E**63**, o3741-o3742 [**doi:10.1107/S1600536807037890**]

Ethyl 3-acetyl-4-(4-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate

N. S. Begum and D. E. Vasundhara

Comment

4-Aryldihydropyrimidines (DHPMs) represent a heterocyclic system of remarkable pharmacological efficiency. They have recently emerged as important target molecules due to their therapeutic and medicinal properties (Kappe, 2000) such as antiviral (Hurst *et al.*, 1961), antimitotic (Mayer *et al.*, 1999), and antihypertensive (Atwal *et al.*, 1991). They are also the most studied class of organic calcium channel modulators (Kappe, 1998; Jauk *et al.*, 2000) and since their introduction into clinical medicine in 1975, they have become almost indispensable for the treatment of cardiovascular diseases such as hypertension, cardiac arrhythmias, or angina (Janis *et al.*, 1987). These inherently asymmetric compounds have been studied extensively to expand the existing structure-activity relationships and to get further insight into molecular interactions at the receptor-site level (Cho *et al.*, 1989; Atwal *et al.*, 1990; Rovnyak *et al.*, 1992 and Grover *et al.*, 1995).

The title compound (I) is a calcium antagonist and belongs to dihydropyrimidine heterocycles. In this molecule (Fig. 1) the substituted aryl ring is positioned axially, perpendicular to, and nearly bisects the boat-like dihydropyrimidine ring. This is evident as the dihedral angle between the planes of both ring systems is 84.92 (7)°. The 4-aryl substitutent (methoxy group) adopts a synperiplanar position. These features have been found mandatory for optimum calcium channel modulatory activity according to the recently proposed new binding-site model for this class of cardiovascular drugs (Rovnyak *et al.*, 1995; Triggle *et al.*, 1995). The exocyclic ester at C8 adopts a *trans* orientation with respect to C8—C9 double bond. DHPM's of this type are known to show conformational flexibility, where, the aryl ring and the ester group can rotate and the conformation of dihydropyrimidine ring can change (Kappe *et al.*, 1997; Shishkin *et al.*, 1997). The crystal structure is stabilized by intermolecular C—H···O and N—H···O hydrogen bonds (Fig. 2).

Experimental

5-Ethoxycarbonyl-6-methyl-4-(4-methoxyphynyl)- 3,4-dihydropyrimidine-2(1*H*)-one was prepared by refluxing a mixture of ethyl acetoacetate solution (3.12 g, 24 m*M*), acetaldehyde (2.72 g, 20 m*M*) and lithium bromide (0.175 g, 2 m*M*) in acetonitrile (25 ml) for 5 h, in a 100 ml round bottom flask. After cooling, the reaction mixture was poured in to crushed ice and stirred for several minutes. The solid product was filtered, washed with cold water, dried and recrystallized from ethanol (yield = 5.17 g, 89.1% and the melting point = 474 K). To prepare the acetyl derivative (title compound), 2 g of this product was mixed with 10 ml of acetic anhydride and refluxed for 4 h in a 25 ml round bottom flask. The reaction mixture was cooled and diluted by adding 20 ml of water·The acetyl derivative seperated out as an oil. The mixture was vigorously stirred and was allowed to solidify. It was filtered, washed thoroughly with water and crystallized from an acetone-water mixture. The yield was 1.94 g (85.0%) and the melting point was 413 K. X-ray diffraction quality single crystals were grown from a solution of chloroform by slow evaporation.

Refinement

All H atoms were located from Fourier difference maps and refined with isotropic thermal displacement parameters; the H-atoms bonded to C13 were included in the refinement at geometrically idealized positions with C—H = 0.96 A° and U_{iso} = 1.5xU_{eq} C13.

Figures

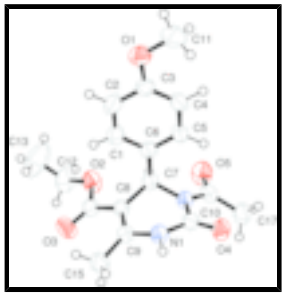


Fig. 1. The molecular structure of (I), showing 50% probability displacement ellipsoids.

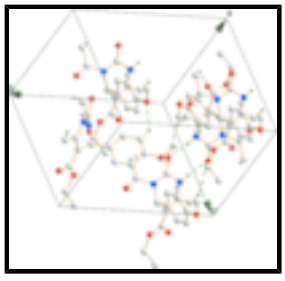


Fig. 2. A view of the unit cell showing intermolecular C—H···O and N—H···O hydrogen bonding interactions.

Ethyl 3-acetyl-6-methyl-4-(4-methoxyphenyl)-2-oxo-\ 1,2,3,4-tetrahydropyrimidine-5-carboxylate

Crystal data

$C_{17}H_{20}N_2O_5$	F_{000} = 704
M_r = 332.35	D_x = 1.296 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 8.8387 (8) Å	Cell parameters from 500 reflections
b = 20.2043 (18) Å	θ = 1.0–25.0º
c = 10.0232 (9) Å	μ = 0.10 mm^{-1}
β = 107.839 (2)º	T = 293 (2) K
V = 1703.9 (3) Å^3	Rectangular, colourless
Z = 4	0.3 × 0.2 × 0.1 mm

Data collection

Bruker SMART CCD area-detector diffractometer	2369 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.045
Monochromator: graphite	θ_{max} = 26.0º

ω/2θ scans	θ_{min} = 2.0º
Absorption correction: none	h = −10→10
17507 measured reflections	k = −24→24
3343 independent reflections	l = −12→12

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0393P)^2 + 0.4822P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.058$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.121$	$\Delta\rho_{max} = 0.20$ e Å^{-3}
$S = 1.10$	$\Delta\rho_{min} = -0.17$ e Å^{-3}
3343 reflections	Extinction correction: none
286 parameters	

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
C1	0.1807 (3)	0.62671 (14)	−0.4147 (3)	0.0578 (7)
H1	0.258 (3)	0.5977 (12)	−0.434 (2)	0.064 (7)*
C2	0.0648 (3)	0.65191 (14)	−0.5284 (3)	0.0610 (7)
H2	0.062 (3)	0.6393 (12)	−0.620 (3)	0.067 (8)*
C3	−0.0503 (3)	0.69434 (11)	−0.5095 (2)	0.0467 (6)
C4	−0.0447 (3)	0.71195 (11)	−0.3757 (3)	0.0468 (6)
H4	−0.122 (3)	0.7428 (12)	−0.358 (2)	0.063 (7)*
C5	0.0738 (3)	0.68632 (11)	−0.2623 (3)	0.0440 (6)
H5	0.070 (2)	0.6976 (10)	−0.169 (2)	0.046 (6)*
C6	0.1872 (2)	0.64294 (10)	−0.2785 (2)	0.0392 (5)
C7	0.3185 (3)	0.61621 (11)	−0.1535 (2)	0.0397 (5)
H7	0.409 (2)	0.6440 (10)	−0.140 (2)	0.041 (6)*
C8	0.3650 (2)	0.54550 (10)	−0.1719 (2)	0.0381 (5)
C9	0.2724 (2)	0.49805 (11)	−0.1439 (2)	0.0399 (5)
C10	0.1584 (3)	0.57494 (10)	−0.0123 (2)	0.0407 (5)
C11	−0.2841 (4)	0.75841 (19)	−0.6132 (4)	0.0755 (9)
H11A	−0.228 (4)	0.8003 (16)	−0.564 (3)	0.097 (11)*
H11B	−0.348 (4)	0.7666 (15)	−0.709 (3)	0.089 (10)*
H11C	−0.340 (4)	0.7379 (17)	−0.553 (4)	0.113 (13)*
C12	0.7234 (4)	0.5743 (2)	−0.2778 (4)	0.0732 (9)
H12A	0.787 (4)	0.6143 (18)	−0.245 (3)	0.110 (12)*

H12B	0.785 (5)	0.533 (2)	−0.233 (4)	0.135 (15)*
C13	0.6866 (5)	0.5672 (2)	−0.4278 (4)	0.1348 (18)
H13A	0.6245	0.5278	−0.4578	0.202*
H13B	0.7835	0.564	−0.4518	0.202*
H13C	0.6272	0.605	−0.4735	0.202*
C14	0.5045 (3)	0.52967 (12)	−0.2155 (2)	0.0438 (5)
C15	0.2798 (4)	0.42479 (13)	−0.1633 (4)	0.0560 (7)
H15A	0.297 (4)	0.4137 (17)	−0.246 (4)	0.113 (13)*
H15B	0.189 (4)	0.4038 (15)	−0.162 (3)	0.094 (11)*
H15C	0.353 (5)	0.4051 (18)	−0.088 (4)	0.130 (15)*
C16	0.3369 (3)	0.67056 (11)	0.0735 (2)	0.0471 (6)
C17	0.3006 (4)	0.67190 (17)	0.2084 (3)	0.0591 (7)
H17A	0.191 (4)	0.6850 (15)	0.193 (3)	0.098 (11)*
H17B	0.308 (4)	0.6307 (17)	0.251 (3)	0.094 (11)*
H17C	0.361 (3)	0.7043 (15)	0.268 (3)	0.084 (10)*
O1	−0.1630 (2)	0.71530 (9)	−0.62888 (17)	0.0611 (5)
O2	0.57984 (19)	0.58430 (8)	−0.2372 (2)	0.0627 (5)
O3	0.5508 (2)	0.47512 (9)	−0.2308 (2)	0.0711 (6)
O4	0.06853 (18)	0.58291 (8)	0.05764 (17)	0.0536 (4)
O5	0.4247 (2)	0.71030 (9)	0.04514 (19)	0.0704 (6)
N1	0.1531 (2)	0.51820 (9)	−0.0891 (2)	0.0438 (5)
H1N	0.089 (3)	0.4869 (12)	−0.074 (2)	0.059 (7)*
N2	0.2716 (2)	0.62013 (8)	−0.02432 (18)	0.0388 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0586 (16)	0.0689 (18)	0.0530 (16)	0.0169 (14)	0.0274 (14)	0.0014 (13)
C2	0.0663 (17)	0.080 (2)	0.0411 (15)	0.0147 (15)	0.0236 (14)	0.0033 (14)
C3	0.0484 (14)	0.0458 (13)	0.0492 (14)	0.0001 (11)	0.0200 (12)	0.0091 (11)
C4	0.0495 (14)	0.0383 (13)	0.0563 (16)	0.0046 (11)	0.0218 (13)	0.0014 (11)
C5	0.0484 (14)	0.0408 (13)	0.0459 (14)	0.0027 (11)	0.0190 (12)	−0.0020 (11)
C6	0.0405 (12)	0.0353 (12)	0.0453 (13)	−0.0049 (10)	0.0182 (10)	0.0023 (10)
C7	0.0378 (12)	0.0381 (12)	0.0475 (14)	−0.0060 (10)	0.0195 (11)	−0.0030 (10)
C8	0.0357 (12)	0.0391 (12)	0.0406 (12)	0.0013 (9)	0.0134 (10)	−0.0006 (10)
C9	0.0364 (12)	0.0409 (12)	0.0417 (13)	−0.0002 (10)	0.0108 (10)	−0.0016 (10)
C10	0.0385 (12)	0.0392 (13)	0.0461 (13)	0.0007 (10)	0.0155 (11)	0.0017 (10)
C11	0.066 (2)	0.081 (2)	0.074 (2)	0.0226 (18)	0.0129 (19)	0.016 (2)
C12	0.0596 (18)	0.082 (2)	0.095 (2)	−0.0158 (18)	0.0481 (18)	−0.017 (2)
C13	0.137 (4)	0.194 (5)	0.097 (3)	−0.079 (3)	0.070 (3)	−0.032 (3)
C14	0.0412 (13)	0.0463 (14)	0.0452 (14)	0.0026 (11)	0.0150 (11)	0.0006 (11)
C15	0.0632 (18)	0.0417 (15)	0.069 (2)	−0.0047 (14)	0.0292 (17)	−0.0047 (14)
C16	0.0428 (13)	0.0403 (13)	0.0579 (15)	0.0024 (11)	0.0152 (12)	−0.0052 (11)
C17	0.068 (2)	0.0549 (18)	0.0590 (18)	−0.0015 (15)	0.0254 (16)	−0.0141 (15)
O1	0.0598 (11)	0.0713 (12)	0.0508 (10)	0.0136 (9)	0.0147 (9)	0.0134 (9)
O2	0.0525 (10)	0.0545 (10)	0.0973 (14)	−0.0090 (8)	0.0468 (10)	−0.0080 (10)
O3	0.0733 (13)	0.0509 (11)	0.1076 (16)	0.0149 (9)	0.0551 (12)	0.0059 (10)
O4	0.0513 (10)	0.0548 (10)	0.0666 (11)	−0.0061 (8)	0.0357 (9)	−0.0072 (8)

O5	0.0779 (13)	0.0593 (11)	0.0818 (13)	−0.0300 (10)	0.0360 (11)	−0.0210 (10)
N1	0.0406 (11)	0.0401 (11)	0.0563 (12)	−0.0084 (9)	0.0231 (10)	−0.0038 (9)
N2	0.0385 (10)	0.0369 (10)	0.0445 (11)	−0.0051 (8)	0.0178 (8)	−0.0042 (8)

Geometric parameters (Å, °)

C1—C2	1.375 (4)	C11—H11A	1.02 (3)
C1—C6	1.387 (3)	C11—H11B	0.97 (3)
C1—H1	0.96 (2)	C11—H11C	0.98 (4)
C2—C3	1.387 (3)	C12—C13	1.444 (5)
C2—H2	0.95 (3)	C12—O2	1.460 (3)
C3—O1	1.369 (3)	C12—H12A	0.98 (4)
C3—C4	1.374 (3)	C12—H12B	1.02 (4)
C4—C5	1.389 (3)	C13—H13A	0.96
C4—H4	0.98 (2)	C13—H13B	0.96
C5—C6	1.378 (3)	C13—H13C	0.96
C5—H5	0.97 (2)	C14—O3	1.201 (3)
C6—C7	1.523 (3)	C14—O2	1.341 (3)
C7—N2	1.478 (3)	C15—H15A	0.91 (4)
C7—C8	1.513 (3)	C15—H15B	0.91 (3)
C7—H7	0.95 (2)	C15—H15C	0.92 (4)
C8—C9	1.345 (3)	C16—O5	1.210 (3)
C8—C14	1.464 (3)	C16—N2	1.409 (3)
C9—N1	1.391 (3)	C16—C17	1.483 (4)
C9—C15	1.497 (3)	C17—H17A	0.97 (3)
C10—O4	1.221 (2)	C17—H17B	0.93 (3)
C10—N1	1.373 (3)	C17—H17C	0.94 (3)
C10—N2	1.387 (3)	N1—H1N	0.89 (3)
C11—O1	1.426 (3)		
C2—C1—C6	121.6 (2)	C13—C12—O2	111.5 (3)
C2—C1—H1	117.0 (14)	C13—C12—H12A	110.8 (19)
C6—C1—H1	121.4 (15)	O2—C12—H12A	104.3 (19)
C1—C2—C3	120.5 (2)	C13—C12—H12B	107 (2)
C1—C2—H2	119.7 (15)	O2—C12—H12B	113 (2)
C3—C2—H2	119.8 (15)	H12A—C12—H12B	111 (3)
O1—C3—C4	124.9 (2)	C12—C13—H13A	109.5
O1—C3—C2	116.1 (2)	C12—C13—H13B	109.5
C4—C3—C2	119.0 (2)	H13A—C13—H13B	109.5
C3—C4—C5	119.7 (2)	C12—C13—H13C	109.5
C3—C4—H4	121.8 (14)	H13A—C13—H13C	109.5
C5—C4—H4	118.5 (14)	H13B—C13—H13C	109.5
C6—C5—C4	122.3 (2)	O3—C14—O2	121.9 (2)
C6—C5—H5	120.1 (13)	O3—C14—C8	126.1 (2)
C4—C5—H5	117.5 (13)	O2—C14—C8	111.97 (19)
C5—C6—C1	117.0 (2)	C9—C15—H15A	113 (2)
C5—C6—C7	121.8 (2)	C9—C15—H15B	112.7 (19)
C1—C6—C7	121.2 (2)	H15A—C15—H15B	107 (3)
N2—C7—C8	108.50 (17)	C9—C15—H15C	112 (2)
N2—C7—C6	110.76 (17)	H15A—C15—H15C	111 (3)

C8—C7—C6	113.64 (18)	H15B—C15—H15C	101 (3)
N2—C7—H7	107.0 (12)	O5—C16—N2	118.2 (2)
C8—C7—H7	109.2 (12)	O5—C16—C17	122.4 (2)
C6—C7—H7	107.5 (12)	N2—C16—C17	119.4 (2)
C9—C8—C14	121.9 (2)	C16—C17—H17A	110.3 (18)
C9—C8—C7	116.22 (19)	C16—C17—H17B	113.6 (19)
C14—C8—C7	121.85 (19)	H17A—C17—H17B	104 (3)
C8—C9—N1	117.23 (19)	C16—C17—H17C	110.7 (17)
C8—C9—C15	128.6 (2)	H17A—C17—H17C	105 (2)
N1—C9—C15	114.2 (2)	H17B—C17—H17C	113 (3)
O4—C10—N1	121.0 (2)	C3—O1—C11	117.6 (2)
O4—C10—N2	125.2 (2)	C14—O2—C12	116.6 (2)
N1—C10—N2	113.75 (19)	C10—N1—C9	124.47 (19)
O1—C11—H11A	106.9 (18)	C10—N1—H1N	114.2 (15)
O1—C11—H11B	103.1 (18)	C9—N1—H1N	117.2 (15)
H11A—C11—H11B	112 (3)	C10—N2—C16	124.65 (18)
O1—C11—H11C	110 (2)	C10—N2—C7	116.39 (17)
H11A—C11—H11C	108 (3)	C16—N2—C7	118.87 (17)
H11B—C11—H11C	115 (3)		
C6—C1—C2—C3	−0.4 (4)	C9—C8—C14—O2	−179.7 (2)
C1—C2—C3—O1	−178.3 (2)	C7—C8—C14—O2	−0.8 (3)
C1—C2—C3—C4	1.4 (4)	C4—C3—O1—C11	−0.3 (4)
O1—C3—C4—C5	178.6 (2)	C2—C3—O1—C11	179.4 (3)
C2—C3—C4—C5	−1.0 (3)	O3—C14—O2—C12	−1.2 (4)
C3—C4—C5—C6	−0.4 (3)	C8—C14—O2—C12	178.5 (2)
C4—C5—C6—C1	1.4 (3)	C13—C12—O2—C14	87.1 (4)
C4—C5—C6—C7	178.8 (2)	O4—C10—N1—C9	−164.1 (2)
C2—C1—C6—C5	−1.0 (4)	N2—C10—N1—C9	16.4 (3)
C2—C1—C6—C7	−178.4 (2)	C8—C9—N1—C10	−26.6 (3)
C5—C6—C7—N2	22.6 (3)	C15—C9—N1—C10	153.2 (2)
C1—C6—C7—N2	−160.2 (2)	O4—C10—N2—C16	22.0 (3)
C5—C6—C7—C8	145.0 (2)	N1—C10—N2—C16	−158.49 (19)
C1—C6—C7—C8	−37.7 (3)	O4—C10—N2—C7	−154.6 (2)
N2—C7—C8—C9	41.5 (3)	N1—C10—N2—C7	24.9 (3)
C6—C7—C8—C9	−82.2 (2)	O5—C16—N2—C10	−173.8 (2)
N2—C7—C8—C14	−137.50 (19)	C17—C16—N2—C10	8.2 (3)
C6—C7—C8—C14	98.8 (2)	O5—C16—N2—C7	2.7 (3)
C14—C8—C9—N1	173.31 (19)	C17—C16—N2—C7	−175.3 (2)
C7—C8—C9—N1	−5.7 (3)	C8—C7—N2—C10	−52.1 (2)
C14—C8—C9—C15	−6.4 (4)	C6—C7—N2—C10	73.3 (2)
C7—C8—C9—C15	174.6 (2)	C8—C7—N2—C16	131.08 (19)
C9—C8—C14—O3	0.0 (4)	C6—C7—N2—C16	−103.5 (2)
C7—C8—C14—O3	178.9 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C17—H17B···O3^{i}	0.929 (4)	2.515 (4)	3.228 (4)	133 (2)

C15—H15B···O4^{ii}	0.911 (5)	2.794 (7)	3.553 (4)	141 (2)
N1—H1N···O4^{ii}	0.892 (6)	2.024 (6)	2.913 (3)	174 (2)
C4—H4···O1^{iii}	0.979 (6)	2.572 (6)	3.310 (3)	132 (1)

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

Fig. 1

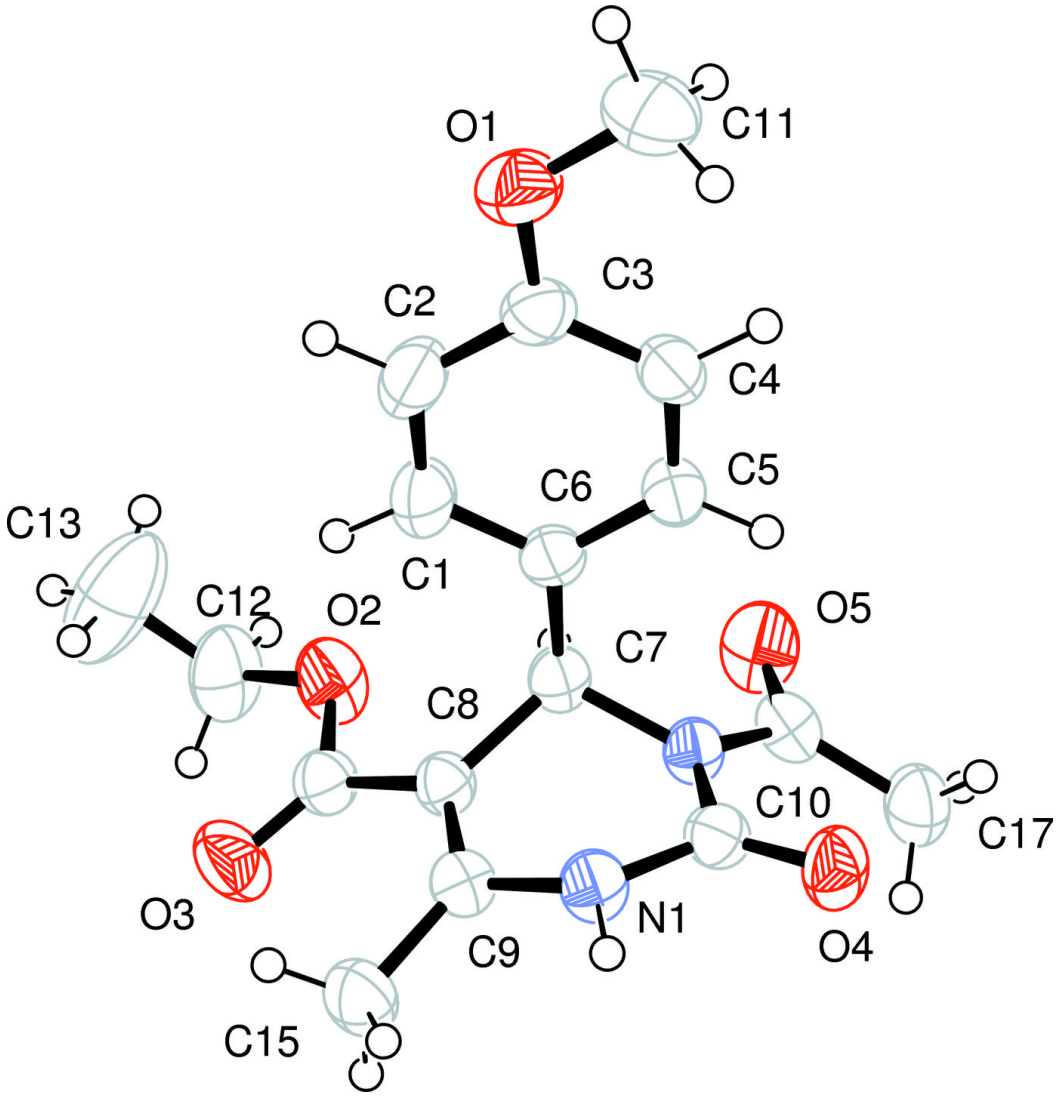


Fig. 2