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Methyl 5′-acetyl-2′-amino-6′-methyl-2-oxospiro[indoline-3,4′-4*H*-pyran]-3′-carboxylate

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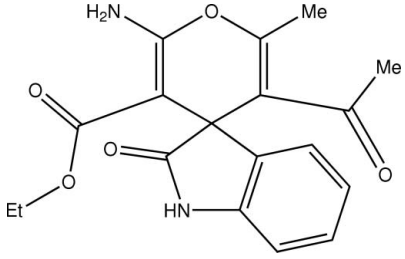
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.149; data-to-parameter ratio = 12.5.

In the title compound, $C_{18}H_{18}N_2O_5$, the two spiro-fused cyclic fragments are planar. The planar system is stabilized by an intramolecular N—H···O hydrogen bond. In the crystal packing, molecules are connected by intermolecular N—H···O hydrogen bonds.

Related literature

For related literature, see: Cingolant *et al.* (1989); Urbahns *et al.* (2000); Zefirov & Zorky (1995); Bürgi & Dunitz (1994).



Experimental

Crystal data

$C_{18}H_{18}N_2O_5$
M_r = 342.34
Monoclinic, $C2/c$
a = 24.5506 (9) Å
b = 10.6729 (4) Å
c = 15.8285 (7) Å
β = 122.818 (3)°
V = 3485.5 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 (2) K
0.30 × 0.10 × 0.05 mm

Data collection

Oxford Diffraction Xcalibur3 diffractometer
Absorption correction: none
10420 measured reflections
3018 independent reflections
2240 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.149
S = 1.09
3018 reflections
241 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O1^{i}	0.90 (3)	1.96 (3)	2.850 (2)	168 (2)
N2—H2NA···O3	0.90 (3)	1.96 (3)	2.667 (3)	134 (2)
N2—H2NB···O1^{ii}	0.91 (3)	2.00 (3)	2.892 (2)	166 (2)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXTL* (Siemens, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *XP* (Siemens, 1998); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2112).

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supplementary materials

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Methyl 5'-acetyl-2'-amino-6'-methyl-2-oxospiro[indoline-3,4'-4*H*-pyran]-3'-carboxylate

S. V. Shishkina, O. V. Shishkin, R. G. Redkin, L. A. Shemchuk and V. P. Chernykh

Comment

Spiro-cyclic derivatives of 2-oxindole are interesting objects for searching of new physiologically active substances (Cingolant *et al.*, 1989, Urbahns *et al.*, 2000). However, such compounds containing the 2-amino-4*H*-pyrane fragment have not been investigated. In this paper we report the molecular and crystal structure of the spiro[indolin-3,4-(5-acetyl-2-amino-3-carbethoxy-6- methyl-4*H*-pyran)]-2-one (Fig. 1) which can be considered as a potential melatonin analogue with a rigid etanamide side chain. Dihydroindolone fragment is planar within 0.01 Å and spiro-joined to the dihydropyrane ring; esterified carboxyl group and the C18, N2, and C16 atoms are co-planar within 0.03 Å and are turned with respect to the bicyclic fragment for 116.2 (2) ° (the C1—C6—C7—C9 torsion angle). The formation of hydrogen bond promotes the elongation of the C11—C12 and C13—O3 bonds (Table 1) in comparison with their mean values (Bürgi & Dunitz, 1994) 1.320 Å and 1.210 Å, respectively and the shortening of the C11—N2 and C12—C13 bonds (the mean value are 1.336 Å and 1.455 Å, respectively). The repulsion between substituents at the C9—C10 double bond (the shortened intramolecular contacts H17*c*···C10 2.81 Å, H17*c*···C18 2.76 Å, H18*b*···C16 2.63 Å, H18*c*···C17 2.64 Å [the sum of van der Waals radii is 2.87 Å (Zefirov & Zorky, 1995)], C18···C17 3.19 Å (3.42 Å) leads to an increase of the C9—C10—C18 bond angle up to 128.6 (2) °. The formation of the N2—H2Na···O3 intramolecular hydrogen bond (Table 2) supports the coplanarity of the carboxyl group and dihydropyrane ring. In the crystal molecules of (I) are connected by the intermolecular hydrogen bonds N1—H1N···O1' and N2—H2Nb···O1' (Table 2, Fig. 2).

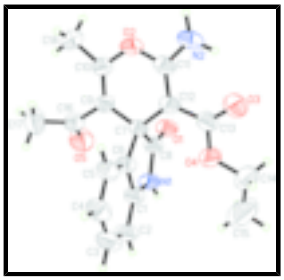
Experimental

A solution of isatin (0.01 mol), triethanolamine (1.3 ml, 0.01 mol) and pentane-2,4-dione (1.01 ml, 0.01 mol) in absolute ethanol (10.0 ml) were gradually added to the cyano-acetic acid ethyl ester (1.1 ml, 0.01 mol). The resulting reaction mixture was refluxed for 2 h. The mixture was allowed to form the precipitate. The resulting precipitate was filtered, washed with hexane, and recrystallized from the ethanol and DMF mixture (1:1) and dried. Yield 0.22 g (65%), m.p. 508 K. ^{1}H NMR (DMSO-d$_6$) δ p.p.m.: 065 t (3*H*, OCH_2CH_3), 1.80 s (3*H*, CH_3), 2.05 s (3*H*, $COCH_3$), 3.65 q (2*H*, OCH_2CH_3), 6.65 d (1*H*), 6.80 t (1*H*), 6.98 d (1*H*), 7.05 t (1*H*), 7.72 s (1*H*, NH_2, D_2O) exchangeable), 10.25 s (1*H*, NH, D_2O exchangeable.). Analysis, required for $C_{18}H_{18}N_2O_5$: C 63.15; H 5.30; N 8.18%; found: C63.15; H 5.30; N 8.18%.

Refinement

All hydrogen atoms were located from electron density difference maps and included in the refinement in the riding motion approximation with U_{iso} constrained to be 1.5 times U_{eq} of the carrier atom for the methyl groups and 1.2 times U_{eq} of the carrier atom for the other atoms·The hydrogen atoms which are take part in the formation of hydrogen bonds are refined in isotropic approximation.

Figures



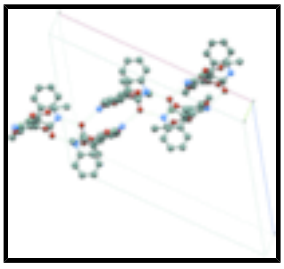


Fig. 1. View of the title compound with atomic membering. All atoms are shown with displacement ellipsoids drawn at the 50% probability level. Fig. 2. The crystal packing is stabilized by N—H···O hydrogen bonds.

Methyl 5'-acetyl-2'-amino-6'-methyl-2-oxospiro[indoline-3,4'-4*H*-pyran]-3'-carboxylate

Crystal data

$C_{18}H_{18}N_2O_5$	F_{000} = 1440
M_r = 342.34	D_x = 1.305 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
a = 24.5506 (9) Å	Cell parameters from 6306 reflections
b = 10.6729 (4) Å	θ = 3–35º
c = 15.8285 (7) Å	μ = 0.10 mm^{-1}
β = 122.818 (3)º	*T* = 293 (2) K
V = 3485.5 (2) Å^3	Plate, colourless
Z = 8	0.30 × 0.10 × 0.05 mm

Data collection

Oxford Diffraction Xcalibur3 diffractometer	R_{int} = 0.031
Radiation source: Enhance (Mo) X-ray Source	θ_{max} = 25.0º
Monochromator: graphite	θ_{min} = 2.9º
T = 293(2) K	*h* = −29→29
ω scans	*k* = −12→12
Absorption correction: none	*l* = −18→17
10420 measured reflections	2 standard reflections
3018 independent reflections	every 50 reflections
2240 reflections with $I > 2\sigma(I)$	intensity decay: 5%

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.047$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.149$	$w = 1/[\sigma^2(F_o^2) + (0.0851P)^2 + 1.3474P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{max} < 0.001$
3018 reflections	$\Delta\rho_{max} = 0.32$ e Å^{-3}
241 parameters	$\Delta\rho_{min} = -0.21$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2$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	0.08678 (6)	0.67104 (13)	0.34768 (10)	0.0526 (4)
O2	0.28466 (6)	0.64340 (14)	0.44108 (11)	0.0602 (4)
O3	0.19920 (8)	0.99077 (15)	0.32023 (13)	0.0770 (5)
O4	0.10457 (7)	0.89331 (14)	0.22049 (12)	0.0695 (5)
O5	0.09930 (8)	0.40131 (17)	0.26489 (14)	0.0787 (5)
N1	0.03680 (7)	0.65486 (15)	0.17652 (12)	0.0483 (4)
H1N	−0.0044 (13)	0.663 (2)	0.1598 (19)	0.070 (7)*
N2	0.29878 (9)	0.8478 (2)	0.45134 (15)	0.0626 (5)
H2NB	0.3365 (13)	0.830 (2)	0.511 (2)	0.067 (7)*
H2NA	0.2827 (13)	0.926 (3)	0.430 (2)	0.084 (9)*
C1	0.05499 (9)	0.64990 (16)	0.10680 (14)	0.0457 (4)
C2	0.01655 (10)	0.64695 (19)	0.00309 (15)	0.0584 (6)
H2	−0.0284	0.6499	−0.0306	0.070*
C3	0.04697 (12)	0.6395 (2)	−0.04904 (16)	0.0641 (6)
H3	0.0221	0.6381	−0.1189	0.077*
C4	0.11360 (12)	0.6342 (2)	0.00091 (16)	0.0610 (6)
H4	0.1330	0.6278	−0.0356	0.073*
C5	0.15193 (10)	0.63820 (18)	0.10521 (15)	0.0510 (5)

H5	0.1969	0.6347	0.1389	0.061*
C6	0.12235 (8)	0.64741 (16)	0.15742 (13)	0.0431 (4)
C7	0.15141 (8)	0.65374 (16)	0.27042 (13)	0.0388 (4)
C8	0.08823 (8)	0.66018 (17)	0.27184 (14)	0.0431 (4)
C9	0.18856 (8)	0.53477 (17)	0.32161 (13)	0.0433 (4)
C10	0.24992 (9)	0.53452 (19)	0.39961 (15)	0.0525 (5)
C11	0.25668 (9)	0.75611 (19)	0.40164 (14)	0.0487 (5)
C12	0.19375 (8)	0.76803 (18)	0.32151 (13)	0.0450 (4)
C13	0.16859 (10)	0.89299 (19)	0.28959 (15)	0.0545 (5)
C14	0.07229 (14)	1.0115 (3)	0.1836 (2)	0.0975 (10)
H14B	0.0863	1.0522	0.1437	0.117*
H14A	0.0824	1.0660	0.2393	0.117*
C15	−0.00001 (19)	0.9856 (4)	0.1196 (4)	0.1426 (16)
H15C	−0.0092	0.9300	0.0657	0.214*
H15B	−0.0230	1.0630	0.0923	0.214*
H15A	−0.0135	0.9476	0.1603	0.214*
C16	0.15250 (9)	0.41441 (18)	0.27901 (14)	0.0492 (5)
C17	0.17974 (14)	0.3148 (2)	0.2462 (2)	0.0835 (8)
H17C	0.2221	0.3394	0.2628	0.125*
H17B	0.1518	0.3032	0.1748	0.125*
H17A	0.1828	0.2377	0.2798	0.125*
C18	0.29125 (12)	0.4255 (3)	0.45825 (19)	0.0831 (8)
H18C	0.3242	0.4135	0.4438	0.125*
H18B	0.2649	0.3516	0.4399	0.125*
H18A	0.3113	0.4414	0.5288	0.125*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0338 (7)	0.0759 (9)	0.0445 (8)	−0.0015 (6)	0.0188 (6)	−0.0062 (6)
O2	0.0326 (7)	0.0714 (10)	0.0538 (9)	0.0016 (6)	0.0085 (6)	−0.0094 (7)
O3	0.0651 (10)	0.0576 (10)	0.0789 (11)	−0.0174 (8)	0.0198 (9)	−0.0042 (8)
O4	0.0492 (9)	0.0526 (9)	0.0694 (10)	0.0000 (6)	0.0078 (8)	0.0017 (7)
O5	0.0548 (10)	0.0833 (12)	0.0920 (13)	−0.0154 (8)	0.0359 (9)	−0.0148 (9)
N1	0.0248 (8)	0.0650 (10)	0.0432 (9)	−0.0036 (6)	0.0108 (7)	−0.0015 (7)
N2	0.0408 (10)	0.0775 (14)	0.0499 (11)	−0.0170 (9)	0.0117 (9)	−0.0105 (9)
C1	0.0374 (9)	0.0490 (10)	0.0394 (10)	−0.0074 (7)	0.0134 (8)	−0.0021 (8)
C2	0.0434 (11)	0.0633 (13)	0.0440 (11)	−0.0091 (9)	0.0076 (9)	−0.0012 (9)
C3	0.0713 (15)	0.0683 (14)	0.0374 (11)	−0.0151 (10)	0.0195 (11)	−0.0039 (9)
C4	0.0712 (15)	0.0679 (14)	0.0466 (12)	−0.0111 (10)	0.0336 (11)	−0.0055 (9)
C5	0.0486 (11)	0.0551 (12)	0.0480 (11)	−0.0079 (8)	0.0252 (10)	−0.0044 (8)
C6	0.0375 (9)	0.0460 (10)	0.0387 (10)	−0.0069 (7)	0.0161 (8)	−0.0045 (7)
C7	0.0289 (8)	0.0465 (10)	0.0363 (9)	−0.0033 (7)	0.0145 (7)	−0.0028 (7)
C8	0.0319 (9)	0.0502 (10)	0.0416 (10)	−0.0021 (7)	0.0163 (8)	−0.0034 (7)
C9	0.0382 (9)	0.0521 (11)	0.0393 (9)	0.0024 (7)	0.0209 (8)	−0.0015 (8)
C10	0.0417 (10)	0.0595 (12)	0.0466 (11)	0.0061 (8)	0.0176 (9)	−0.0054 (9)
C11	0.0361 (9)	0.0635 (13)	0.0435 (10)	−0.0077 (8)	0.0197 (8)	−0.0082 (9)
C12	0.0336 (9)	0.0581 (11)	0.0391 (9)	−0.0063 (8)	0.0170 (8)	−0.0054 (8)

C13	0.0484 (11)	0.0555 (12)	0.0477 (11)	−0.0098 (9)	0.0183 (9)	−0.0058 (9)
C14	0.0754 (17)	0.0617 (15)	0.098 (2)	0.0061 (13)	0.0102 (15)	0.0115 (14)
C15	0.090 (2)	0.113 (3)	0.158 (4)	0.031 (2)	0.024 (2)	0.027 (2)
C16	0.0481 (11)	0.0542 (11)	0.0415 (10)	−0.0006 (8)	0.0218 (9)	0.0040 (8)
C17	0.0882 (18)	0.0638 (15)	0.104 (2)	−0.0079 (13)	0.0556 (17)	−0.0230 (14)
C18	0.0654 (15)	0.0803 (17)	0.0650 (15)	0.0258 (13)	0.0102 (12)	−0.0028 (12)

Geometric parameters (Å, °)

O1—C8	1.226 (2)	C6—C7	1.526 (2)
O2—C11	1.358 (2)	C7—C9	1.516 (2)
O2—C10	1.379 (2)	C7—C12	1.520 (2)
O3—C13	1.222 (2)	C7—C8	1.565 (2)
O4—C13	1.343 (2)	C9—C10	1.333 (3)
O4—C14	1.435 (3)	C9—C16	1.497 (3)
O5—C16	1.208 (2)	C10—C18	1.491 (3)
N1—C8	1.345 (2)	C11—C12	1.374 (3)
N1—C1	1.398 (3)	C12—C13	1.441 (3)
N1—H1N	0.90 (3)	C14—C15	1.518 (5)
N2—C11	1.328 (2)	C14—H14B	0.9700
N2—H2NB	0.91 (3)	C14—H14A	0.9700
N2—H2NA	0.90 (3)	C15—H15C	0.9600
C1—C2	1.381 (3)	C15—H15B	0.9600
C1—C6	1.393 (3)	C15—H15A	0.9600
C2—C3	1.383 (3)	C16—C17	1.491 (3)
C2—H2	0.9300	C17—H17C	0.9600
C3—C4	1.379 (3)	C17—H17B	0.9600
C3—H3	0.9300	C17—H17A	0.9600
C4—C5	1.389 (3)	C18—H18C	0.9600
C4—H4	0.9300	C18—H18B	0.9600
C5—C6	1.368 (3)	C18—H18A	0.9600
C5—H5	0.9300		
C11—O2—C10	119.97 (14)	C9—C10—C18	128.6 (2)
C13—O4—C14	118.56 (17)	O2—C10—C18	108.93 (17)
C8—N1—C1	112.32 (15)	N2—C11—O2	110.06 (17)
C8—N1—H1N	123.3 (16)	N2—C11—C12	127.1 (2)
C1—N1—H1N	124.1 (16)	O2—C11—C12	122.82 (16)
C11—N2—H2NB	119.2 (15)	C11—C12—C13	117.59 (17)
C11—N2—H2NA	114.4 (18)	C11—C12—C7	121.29 (17)
H2NB—N2—H2NA	125 (2)	C13—C12—C7	121.10 (15)
C2—C1—C6	121.10 (19)	O3—C13—O4	121.16 (19)
C2—C1—N1	129.37 (18)	O3—C13—C12	126.63 (18)
C6—C1—N1	109.52 (16)	O4—C13—C12	112.20 (16)
C1—C2—C3	117.93 (19)	O4—C14—C15	107.5 (2)
C1—C2—H2	121.0	O4—C14—H14B	110.2
C3—C2—H2	121.0	C15—C14—H14B	110.2
C4—C3—C2	121.10 (19)	O4—C14—H14A	110.2
C4—C3—H3	119.5	C15—C14—H14A	110.2
C2—C3—H3	119.5	H14B—C14—H14A	108.5

C3—C4—C5	120.6 (2)	C14—C15—H15C	109.5
C3—C4—H4	119.7	C14—C15—H15B	109.5
C5—C4—H4	119.7	H15C—C15—H15B	109.5
C6—C5—C4	118.74 (19)	C14—C15—H15A	109.5
C6—C5—H5	120.6	H15C—C15—H15A	109.5
C4—C5—H5	120.6	H15B—C15—H15A	109.5
C5—C6—C1	120.49 (17)	O5—C16—C17	119.8 (2)
C5—C6—C7	130.34 (16)	O5—C16—C9	119.91 (18)
C1—C6—C7	109.16 (15)	C17—C16—C9	120.08 (18)
C9—C7—C12	110.36 (14)	C16—C17—H17C	109.5
C9—C7—C6	110.66 (14)	C16—C17—H17B	109.5
C12—C7—C6	114.17 (14)	H17C—C17—H17B	109.5
C9—C7—C8	110.05 (14)	C16—C17—H17A	109.5
C12—C7—C8	110.76 (14)	H17C—C17—H17A	109.5
C6—C7—C8	100.45 (13)	H17B—C17—H17A	109.5
O1—C8—N1	126.49 (17)	C10—C18—H18C	109.5
O1—C8—C7	124.99 (16)	C10—C18—H18B	109.5
N1—C8—C7	108.50 (16)	H18C—C18—H18B	109.5
C10—C9—C16	120.72 (17)	C10—C18—H18A	109.5
C10—C9—C7	123.15 (16)	H18C—C18—H18A	109.5
C16—C9—C7	116.12 (14)	H18B—C18—H18A	109.5
C9—C10—O2	122.41 (17)		
C8—N1—C1—C2	−178.18 (19)	C6—C7—C9—C16	−52.80 (19)
C8—N1—C1—C6	2.1 (2)	C8—C7—C9—C16	57.31 (19)
C6—C1—C2—C3	1.0 (3)	C16—C9—C10—O2	−179.83 (16)
N1—C1—C2—C3	−178.70 (19)	C7—C9—C10—O2	0.7 (3)
C1—C2—C3—C4	0.5 (3)	C16—C9—C10—C18	−2.4 (3)
C2—C3—C4—C5	−1.0 (3)	C7—C9—C10—C18	178.2 (2)
C3—C4—C5—C6	0.1 (3)	C11—O2—C10—C9	−0.8 (3)
C4—C5—C6—C1	1.4 (3)	C11—O2—C10—C18	−178.72 (19)
C4—C5—C6—C7	−179.93 (18)	C10—O2—C11—N2	−178.78 (17)
C2—C1—C6—C5	−2.0 (3)	C10—O2—C11—C12	1.0 (3)
N1—C1—C6—C5	177.77 (16)	N2—C11—C12—C13	−3.3 (3)
C2—C1—C6—C7	179.12 (16)	O2—C11—C12—C13	177.05 (17)
N1—C1—C6—C7	−1.15 (19)	N2—C11—C12—C7	178.69 (18)
C5—C6—C7—C9	−62.6 (2)	O2—C11—C12—C7	−1.0 (3)
C1—C6—C7—C9	116.19 (16)	C9—C7—C12—C11	0.8 (2)
C5—C6—C7—C12	62.6 (2)	C6—C7—C12—C11	−124.59 (19)
C1—C6—C7—C12	−118.60 (16)	C8—C7—C12—C11	122.91 (18)
C5—C6—C7—C8	−178.84 (18)	C9—C7—C12—C13	−177.20 (16)
C1—C6—C7—C8	−0.05 (18)	C6—C7—C12—C13	57.4 (2)
C1—N1—C8—O1	176.39 (18)	C8—C7—C12—C13	−55.1 (2)
C1—N1—C8—C7	−2.1 (2)	C14—O4—C13—O3	−0.6 (3)
C9—C7—C8—O1	66.1 (2)	C14—O4—C13—C12	178.2 (2)
C12—C7—C8—O1	−56.2 (2)	C11—C12—C13—O3	7.4 (3)
C6—C7—C8—O1	−177.25 (17)	C7—C12—C13—O3	−174.5 (2)
C9—C7—C8—N1	−115.41 (16)	C11—C12—C13—O4	−171.36 (18)
C12—C7—C8—N1	122.29 (16)	C7—C12—C13—O4	6.7 (3)
C6—C7—C8—N1	1.28 (18)	C13—O4—C14—C15	−171.6 (3)

C12—C7—C9—C10	−0.7 (2)	C10—C9—C16—O5	130.3 (2)
C6—C7—C9—C10	126.69 (19)	C7—C9—C16—O5	−50.2 (2)
C8—C7—C9—C10	−123.20 (19)	C10—C9—C16—C17	−54.7 (3)
C12—C7—C9—C16	179.85 (15)	C7—C9—C16—C17	124.8 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1N···O1^{i}	0.90 (3)	1.96 (3)	2.850 (2)	168 (2)
N2—H2NA···O3	0.90 (3)	1.96 (3)	2.667 (3)	134 (2)
N2—H2NB···O1^{ii}	0.91 (3)	2.00 (3)	2.892 (2)	166 (2)

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

Fig. 1

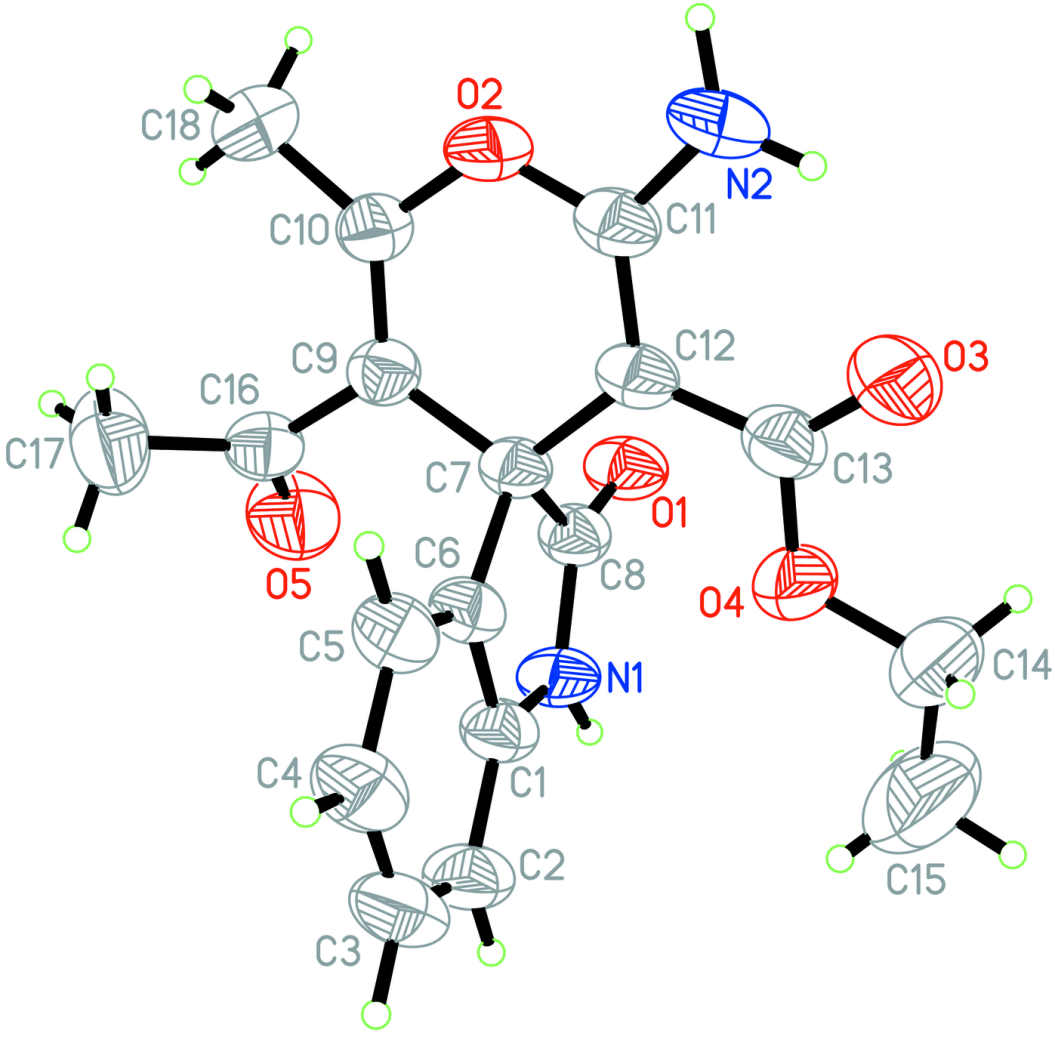

O2
C18
N2
C10
C11
C9
C12
O3
C16
C17
C7
C13
O1
O5
C6
C8
O4
C5
N1
C14
C4
C1
C2
C15
C3

Fig. 2