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N′-(2-Hydroxybenzoyl)-2-oxo-2*H*-chromene-3-carbohydrazide

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The coumarin system and the 2-hydroxybenzoyl group in the title compound, $C_{17}H_{12}N_2O_5$, are approximately coplanar. There are some intermolecular O—H···O hydrogen bonds and intramolecular N—H···O hydrogen bonds; the intermolecular O—H···O hydrogen bonds result in a chain along the *a* axis.

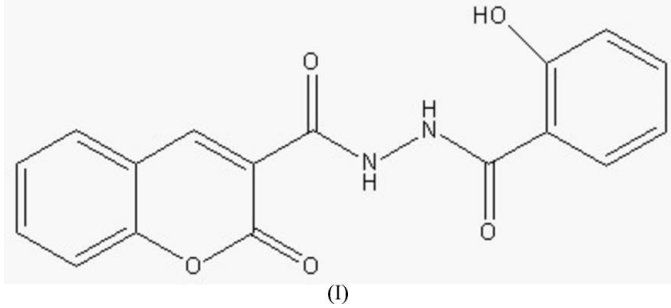
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.040
wR factor = 0.120
Data-to-parameter ratio = 14.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Recently, coumarin derivatives have attracted increasing attention due to their remarkable biological properties (Feurer, 1974; Budzisz *et al.*, 2004). Such derivatives represent a class of organic compounds which have extensive and diverse applications (Krasovitskii, 1988; Guilardi *et al.*, 2002). These compounds can exhibit anti-inflammatory activity (Adam *et al.*, 2005), and have been described as agents with potential for anticancer (Georgieva *et al.*, 2004) and anti-coagulant activity (Creaven *et al.*, 2005). We present here the crystal structure of the title compound, (I).



(I)

The molecular structure of (I) is shown in Fig. 1. The coumarin system (C2–C10/O1/O2) of the molecule is planar. The dihedral angle between the benzene ring C5–C10 and the fused pyrone ring in the coumarin system is 1.05 (8)°. The

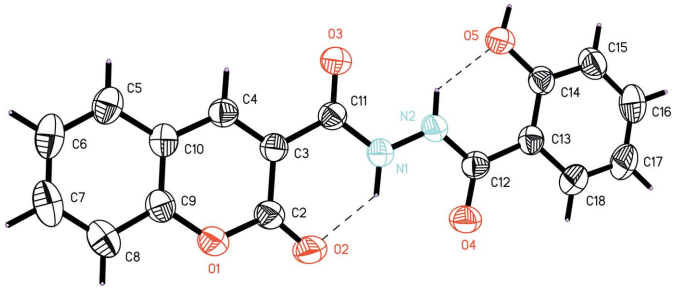


Figure 1
The molecular structure of (I), showing the atom-numbering scheme and 50% probability displacement ellipsoids. The intramolecular hydrogen bonds are shown as dashed lines.

average deviation of these atoms from the mean plane of the coumarin system is 0.015 (1) Å; this value is in agreement with those found in analogous coumarin derivatives (Dobson & Gerkin, 1996; Kokila *et al.*, 1996). The whole molecule is nearly planar. The dihedral angle between the coumarin system and the 2-hydroxybenzohydrazide unit is 0.67 (5) Å.

The hydrogen bonds are listed in Table 1. There are two intramolecular N—H···O hydrogen bonds and one intermolecular O—H···O hydrogen bond in the crystal structure; the intermolecular hydrogen bond O5—H5*O*···O4 links neighbouring molecules, forming a chain (Fig. 2).

Experimental

All chemicals used in this work were of analytical grade available commercially. The title compound was prepared by reacting ethyl coumarin-3-carboxylate with an equivalent amount of 2-hydroxybenzohydrazide ethanol solution by refluxing for 3 h, resulting in a yellow powder. This was dissolved in ethanol and kept at room temperature for several days to obtain yellow single crystals of (I).

Crystal data

$C_{17}H_{12}N_2O_5$
$M_r = 324.29$
Monoclinic, $P2_1/c$
$a = 9.467$ (4) Å
$b = 11.766$ (4) Å
$c = 13.268$ (7) Å
$\beta = 100.96$ (2)°
$V = 1450.9$ (11) Å^3
$Z = 4$
$D_x = 1.485$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.11$ mm^{-1}
$T = 293$ (2) K
Block, yellow
0.60 × 0.25 × 0.15 mm

Data collection

Rigaku Weissenberg IP diffractometer
ω scans
Absorption correction: none
14024 measured reflections
3321 independent reflections
2401 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.120$
$S = 1.07$
3321 reflections
229 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0742P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5*O*···O4^{i}	0.91	1.75	2.6527 (15)	174
N1—H1*N*···O2	0.93	1.90	2.6392 (15)	134
N2—H2*N*···O5	0.85	1.98	2.6135 (15)	131

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

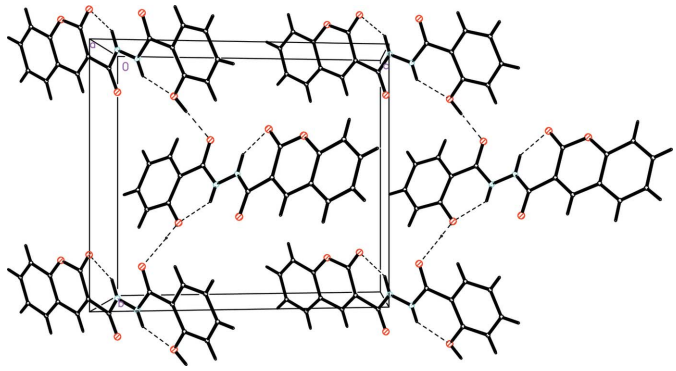


Figure 2
A packing diagram for the title compound. Dashed lines represent hydrogen bonds.

All H atoms were located in difference Fourier maps. Those bonded to N and O atoms were refined as riding in their as-found relative positions, giving bond lengths shown in Table 1. Those bonded to C atoms were idealized, with C—H = 0.93 Å. U_{iso} values of all H atoms were refined freely.

Data collection: *TEXRAY* (Molecular Structure Corporation, 1999) ; cell refinement: *TEXRAY*; data reduction: *TEXSAN*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEX* (McArdle, 1995); software used to prepare material for publication: *SHELXL97*.

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