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1-Acetyl-3,3-bis[3-(2-methylphenyl)-1,2,4-oxadiazol-5-yl]-1*H*-indolin-2(3*H*)-one

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.067
wR factor = 0.172
Data-to-parameter ratio = 14.4

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

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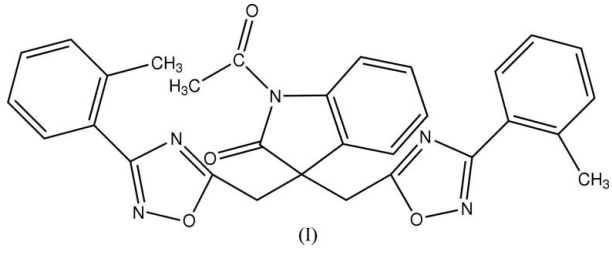
In the title compound, $C_{30}H_{25}N_5O_4$, the indanone ring system is planar. The dihedral angle between the benzene and attached oxadiazole rings are different [9.3 (2) and 43.9 (1)°] in the two phenyloxadiazole fragments. In the crystal packing, intermolecular C—H···O and C—H···N hydrogen-bond interactions are observed.

Comment

Some oxindole derivatives have intrinsic analgesic (Daisley & Walker, 1979), anti-inflammatory (Kadin *et al.*, 1986), antiviral (Singh & Krishna, 1989), cardiotonic (Andreani *et al.*, 1988), anticonvulsant (Valenta *et al.*, 1990), anxiolytic (Sarges *et al.*, 1989) and inotropic (Ogawa *et al.*, 1988) properties. We report here the crystal structure of the title compound, (I).



(I)

The molecular structure of (I) is shown in Fig. 1 and selected bond lengths and angles are given in Table 1. The indanone ring system is planar and the acetyl group at N5 is twisted by 11.8 (2)°. The dihedral angle between the O1/N1/N2/C8/C9 and C1–C6 planes is 9.3 (2)° and that between the O4/N3/N4/C22/C23 and C25–C30 planes is 43.9 (1)°. Intramolecular C—H···N and C—H···O hydrogen bonds are observed in the molecular structure. The crystal structure is stabilized by intermolecular C—H···O and C—H···N hydrogen bonds (Table 2).

Experimental

N-Acetyl-2-indolinone (20 mmol) was dissolved in acetone (40 ml) and potassium carbonate (60 mmol) was added in one portion. 5-Chloromethyl-3-(2-methylphenyl)-1,2,4-oxadiazole (40 mmol) in acetone (40 ml) was added to this mixture. The resulting mixture was refluxed for 72 h. After cooling and filtering, crude compound (I) was obtained. Pure compound (I) was obtained by crystallizing from a mixture of ethyl acetate (4 ml) and petroleum ether (8 ml). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution. ^{1}H NMR ($CDCl_3$): δ 8.20–8.23 (*m*, 1H), 7.74–7.77 (*m*, 2H), 7.33–7.38 (*m*, 2H), 7.23–7.30 (*s*, 5H), 7.09–7.14 (*m*, 2H), 3.69–3.84 (*s*, 4H), 2.75 (*s*, 3H), 2.44 (*s*, 6H).

Crystal data

$C_{30}H_{25}N_5O_4$
M_r = 519.55
Monoclinic, $P2_1/c$
a = 11.680 (2) Å
b = 12.234 (2) Å
c = 18.396 (4) Å
β = 93.85 (3)°
V = 2622.7 (8) Å^3
Z = 4
D_x = 1.316 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 10–13°
μ = 0.09 mm^{-1}
T = 293 (2) K
Block, colourless
0.40 × 0.20 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.965, T_{max} = 0.982
5405 measured reflections
5144 independent reflections
2860 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 26.0°
$h = 0 \rightarrow 14$
$k = 0 \rightarrow 15$
$l = -22 \rightarrow 22$
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.172
S = 1.06
5144 reflections
356 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.07P)^2 + 0.4P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.010
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0073 (10)

Table 1
Selected geometric parameters (Å, °).

O1—C9	1.339 (3)	N2—C8	1.391 (3)
O1—N1	1.421 (3)	N3—C22	1.281 (3)
O2—C12	1.201 (3)	N3—C23	1.384 (3)
O3—C20	1.202 (4)	N4—C23	1.285 (3)
O4—C22	1.328 (3)	N5—C12	1.402 (3)
O4—N4	1.422 (3)	N5—C20	1.402 (4)
N1—C8	1.284 (4)	N5—C13	1.423 (4)
N2—C9	1.272 (3)		
C9—C10—C11	113.6 (2)	N5—C20—C19	118.7 (3)
O3—C20—N5	119.0 (4)	C22—C21—C11	112.2 (2)
O3—C20—C19	122.3 (3)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3B···N2	0.93	2.45	2.822 (4)	104
C14—H14A···O3	0.93	2.32	2.843 (5)	115
C16—H16A···N1^{i}	0.93	2.62	3.395 (6)	142
C24—H24B···O3^{ii}	0.96	2.59	3.509 (5)	160

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

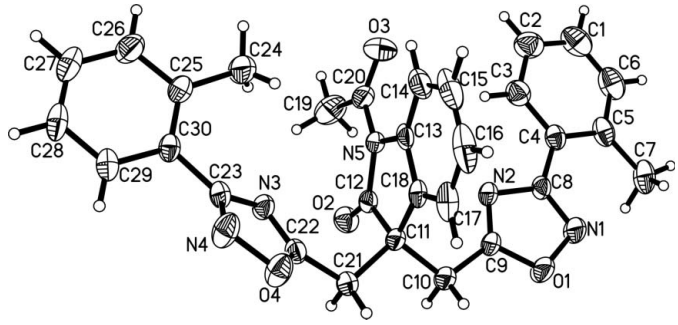


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids.

All H atoms were positioned geometrically at distances of 0.93–0.97 Å, and included in the refinement in the riding-model approximation with U_{iso}(H) = 1.2 or 1.5U_{eq} of the carrier atom.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXL97*.

References

Andreani, A. & Rambaldi, M. (1988). *J. Heterocycl. Chem.* **25**, 1519–1523.
Daisley, R. W. & Walker, J. (1979). *Eur. J. Med. Chem. Chim. Ther.* **14**, 47–52.
Enraf–Nonius (1989). *CAD-4 Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
Kadin, S. B. (1986). Eur. Patent No. EP 175551.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Ogawa, H., Tamada, S., Fujioka, T., Teramoto, S., Kondo, K., Yamashita, S., Yabuuchi, Y., Tominaga, M. & Nakagawa, K. (1988). *Chem. Pharm. Bull.* **36**, 2253–2258.
Sarges, R., Howard, H. R., Koe, B. K. & Weissman, A. (1989). *J. Med. Chem.* **32**, 437–444.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Siemens (1996). *SHELXTL*. Version 5.06. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Singh, S. P. & Krishna, J. (1989). *Zentralbl. Mikrobiol.* **144**, 105–109.
Valenta, V., Holubek, J., Svatek, E., Valchar, M., Krejci, I. & Protiva, M. (1990). *Collect. Czech. Chem. Commun.* **55**, 2756–2764.