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1-Acetyl-3,3-bis[3-(3-methoxyphenyl)-1,2,4-oxadiazol-5-ylmethyl]indolin-2-one

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
R factor = 0.090
wR factor = 0.223
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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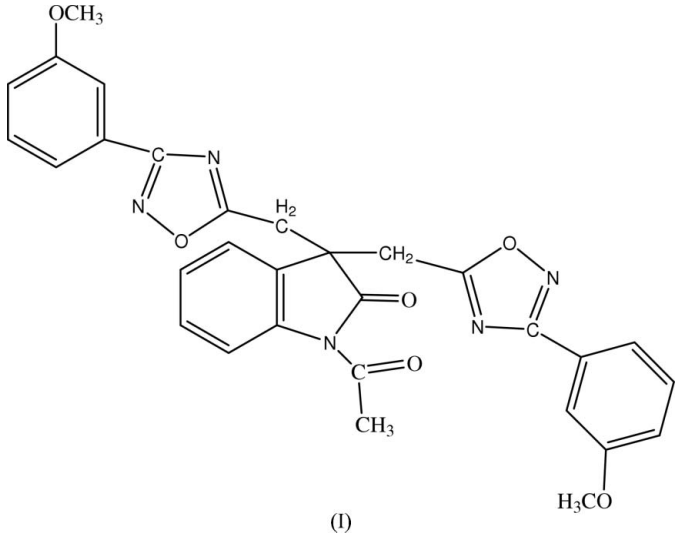
In the title compound, $C_{30}H_{25}N_5O_6$, a derivative of oxindole, intramolecular C—H···O and C—H···N interactions help to establish the molecular conformation.

Comment

Oxindole derivatives show many important biologial effects, such as anti-inflammatory (Kadin *et al.*, 1986) and anti-convulsant (Valenta *et al.*, 1990) properties. As part of our studies of these compounds, we have recently reported the synthesis and structure of 1-acetyl-3,3-bis[(3-(2-methylphenyl)-1,2,4-oxadiazol-5-ylmethyl]indolin-2-one, (II) (Yan *et al.*, 2006). We report here the structure of the title compound, (I) (Fig. 1), a close analogue of (II), in which the 2-methylphenyl group is replaced by a 3-methoxyphenyl group.



(I)

The indanone ring system in (I) is planar and the acetyl group at N3 is twisted from it by 1.4 (2)°. The dihedral angle between the N4/C22/O6/N5/C23 and C24–C29 planes is 6.7 (1)° and that between the N2/C8/N1/O2/C9 and C2–C7 planes is 2.8 (2)°. Three acute intramolecular C—H···N and C—H···O hydrogen bonds (Table 1) may help to establish the molecular conformation of (I).

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-(3-methoxyphenyl)-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, the crude title compound was obtained. The pure compound was obstained by recrystallization from a mixture of ethyl acetate (4 ml) and

petrolum ether (8 ml). Crystals of (I) suitable for X-ray diffraction analysis were obstained by slow evaporation of an ethanol solution.

Crystal data

$C_{30}H_{25}N_5O_6$
M_r = 551.55
Triclinic, $P\overline{1}$
a = 8.6300 (17) Å
b = 11.866 (2) Å
c = 14.616 (3) Å
α = 108.95 (3)°
β = 99.02 (3)°
γ = 101.17 (3)°
V = 1349.3 (6) Å^3
Z = 2
D_x = 1.358 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 (2) K
Block, colourless
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.977, T_{max} = 0.990
5644 measured reflections
5289 independent reflections
2900 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 26.0°
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.090
$wR(F^2)$ = 0.223
S = 1.03
5289 reflections
365 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.06P)^2 + 2P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.016 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7A···N2	0.93	2.59	2.910 (7)	101
C16—H16A···O4	0.93	2.27	2.805 (7)	116
C25—H25A···N4	0.93	2.52	2.858 (6)	102

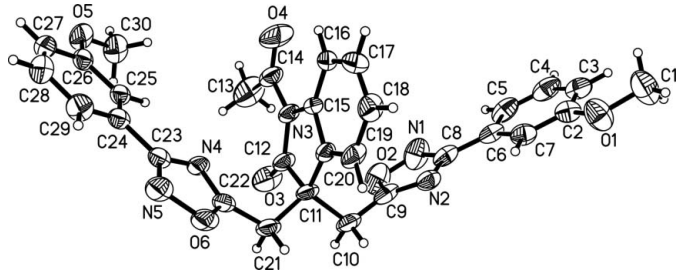


Figure 1
A view of the molecular structure of (I), showing displacement ellipsoids at the 30% probability level (arbitrary spheres for the H atoms).

All H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding, with U_{iso}(H) = 1.2 or 1.5U_{eq}(C).

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*.

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