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

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.043
wR factor = 0.127
Data-to-parameter ratio = 8.1

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

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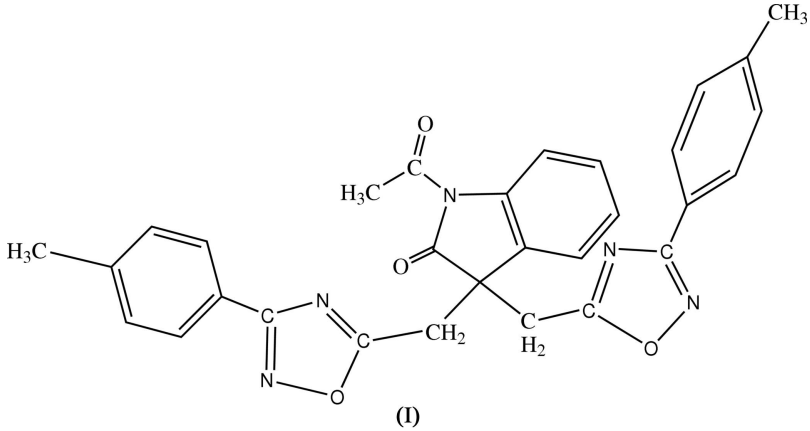
In the crystal structure of the title compound, $C_{30}H_{25}N_5O_4$, there are C—H···O and C—H···N hydrogen bonds.

Comment

Oxindole derivatives, which possess affinity for different receptors, exhibit intrinsic analgesic (Daisley & Walker, 1979), anti-inflammatory (Kadin, 1986), antiviral (Singh & Krishna, 1989), cardiotonic (Andreani & Rambaldi, 1988), anti-convulsant (Valenta *et al.*, 1990), anxiolytic (Sarges *et al.*, 1989) and inotropic (Ogawa *et al.*, 1988) properties. We are focusing our synthetic and structural studies on new oxindole derivatives, and recently we have published the synthesis and structure of 1-acetyl-3,3-bis[(3-(2-methylphenyl)-1,2,4-oxadiazol-5-yl)methyl]-1*H*-indolin-2(3*H*)-one (Yan *et al.*, 2006). We report here the structure of its close analogue, (I), with 2-methylphenyl replaced by the 4-methylphenyl group.



(I)

The molecular structure of (I) is shown in Fig. 1. The indanone ring system is planar and the acetyl group at N5 is twisted by 17.5 (2)°. The dihedral angle between the N4/C22O4/N3/C23 and C24–C29 planes is 11.1 (1)° and that between the N2/C8/N1/O1/C29 and C2–C7 planes is 25.6 (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 1).

Experimental

N-Acetyl-2-indolinone (20 mmol) was dissolved in acetone (40 ml) and potassium carbonate (60 mmol) was added in one portion. 3-(4-Methylphenyl)-5-chloromethyl-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 filtration, the crude compound

was obtained. The pure compound was obtained by crystallization from a mixture of ethyl acetate (4 ml) and petrolum ether (8 ml). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

Crystal data

$C_{30}H_{25}N_5O_4$
M_r = 519.55
Monoclinic, $C2$
a = 15.5510 (16) Å
b = 6.9695 (14) Å
c = 25.220 (2) Å
β = 103.46 (3)°
V = 2658.3 (7) Å^3
Z = 4
D_x = 1.298 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
Block, colourless
0.40 × 0.40 × 0.30 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} = 0.974
5676 measured reflections
2843 independent reflections
2200 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 26.0°
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.127
S = 1.05
2843 reflections
353 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.075P)^2 + 0.19P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0098 (12)

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7A···N1^{i}	0.93	2.62	3.387 (6)	140
C10—H10A···O2^{ii}	0.97	2.46	3.411 (5)	166
C16—H16A···O2	0.93	2.30	2.834 (5)	116
C29—H29A···N4	0.93	2.62	2.935 (4)	100

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

All H atoms were positioned geometrically with C—H distances in the range 0.93–0.97 Å and included in the refinement in the riding-model approximation, with U_{iso}(H) values of 1.2 or 1.5 times U_{eq}(C). In the absence of significant anomalous scattering, Friedel pairs were merged.

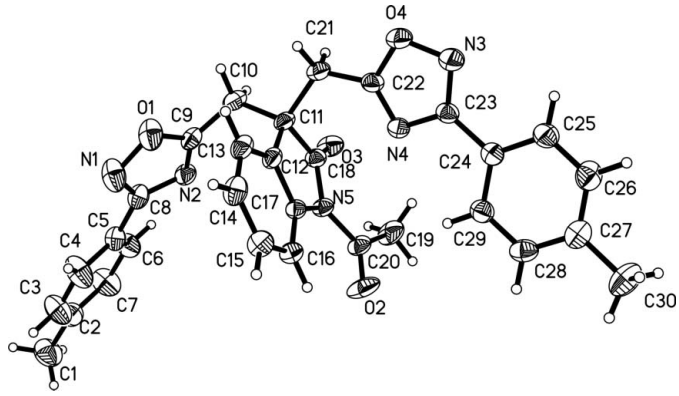


Figure 1
A view of the molecular structure of (I), showing displacement ellipsoids at the 30% probability level.

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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