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Key indicators

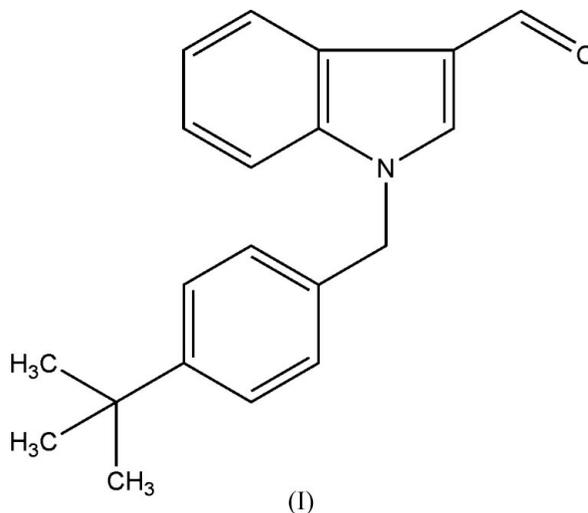
Single-crystal X-ray study
 $T = 90\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$
 R factor = 0.040
 wR factor = 0.107
Data-to-parameter ratio = 13.9For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.1-(4-*tert*-Butylbenzyl)-1*H*-indole-3-carbaldehyde

The title compound, $\text{C}_{20}\text{H}_{21}\text{NO}$, was obtained by the reaction of indole-3-carbaldehyde with 4-*tert*-butylbenzyl chloride and recrystallization of the product from ethanol. The indole ring system is nearly planar and makes a dihedral angle of $74.45(3)^\circ$ with the plane of the 4-*tert*-butylphenyl ring.

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Comment

1-Benzylindole-3-carbaldehyde readily undergoes base-catalysed condensation with azabicyclo[2.2.2]octan-3-one (Sonar *et al.*, 2003). However, 1-(4-*tert*-butylbenzyl)indole-3-carbaldehyde failed to undergo a similar condensation reaction. In view of the unusual behavior of this aldehyde, its X-ray crystallographic structure was determined to obtain details of the molecular conformation.



1-(4-*tert*-Butylbenzyl)-1*H*-indole-3-carbaldehyde, (I), was prepared by the reaction of indole-3-carbaldehyde with 4-*tert*-butylbenzyl chloride in the presence of potassium carbonate and dimethylformamide under reflux, and the resultant product was crystallized from ethanol.

Fig. 1 shows a view of (I) and selected geometric parameters are presented in Table 1. The indole ring system is planar, with bond distances and bond angles comparable with those reported for other indole derivatives (Mason *et al.*, 2003). The plane of the indole ring system makes a dihedral angle of $74.45(3)^\circ$ with the plane of the benzene ring of the 4-*tert*-butylbenzyl group.

Experimental

A mixture of 1.45 g (10 mmol) of indole-3-carbaldehyde, 1.982 g (10.85 mmol) of 4-*tert*-butylbenzyl chloride, 1.4 g of anhydrous

K_2CO_3 and 10 ml DMF was vigorously stirred and refluxed for 2 h. The cooled reaction mixture was poured into 40 ml of water and the precipitated solid was collected by filtration and air dried. Recrystallization from ethanol afforded pale-yellow crystals.

Crystal data

$C_{20}H_{21}NO$	$Z = 4$
$M_r = 291.38$	$D_x = 1.233 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Cu $K\alpha$ radiation
$a = 11.5242 (11) \text{ \AA}$	$\mu = 0.58 \text{ mm}^{-1}$
$b = 10.2024 (10) \text{ \AA}$	$T = 90.0 (2) \text{ K}$
$c = 13.4072 (13) \text{ \AA}$	Block, pale yellow
$\beta = 95.446 (4)^\circ$	$0.20 \times 0.18 \times 0.15 \text{ mm}$
$V = 1569.2 (3) \text{ \AA}^3$	

Data collection

Bruker–Nonius X8 Proteum diffractometer	18596 measured reflections
ω and φ scans	2817 independent reflections
Absorption correction: multi-scan (SADABS; Bruker–Nonius, 2004)	2691 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.892$, $T_{\max} = 0.918$	$R_{\text{int}} = 0.032$
	$\theta_{\text{max}} = 68.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0507P)^2 + 0.8252P]$
$R[F^2 > 2\sigma(F^2)] = 0.040$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.107$	$(\Delta/\sigma)_{\text{max}} = 0.002$
$S = 1.08$	$\Delta\rho_{\text{max}} = 0.32 \text{ e \AA}^{-3}$
2817 reflections	$\Delta\rho_{\text{min}} = -0.23 \text{ e \AA}^{-3}$
203 parameters	Extinction correction: <i>SHELXL97</i>
H-atom parameters constrained	Extinction coefficient: 0.0053 (5)

Table 1

Selected geometric parameters (\AA , $^\circ$).

N1–C2	1.3573 (17)	C2–C3	1.3762 (19)
N1–C11	1.4671 (16)	C3–C10	1.4289 (18)
O1–C10	1.2268 (17)		
N1–C2–C3	110.56 (11)	N1–C11–C12	112.43 (10)
C2–C3–C10	123.96 (12)	C13–C12–C11	121.59 (11)
C10–C3–C4	129.64 (12)	C14–C15–C18	123.35 (12)
O1–C10–C3	125.26 (13)	C16–C15–C18	119.57 (11)
C2–C3–C10–O1	−179.58 (13)	C4–C3–C10–O1	2.9 (2)

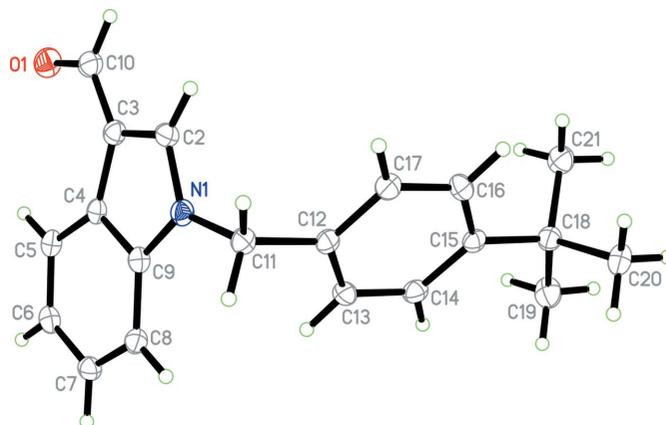


Figure 1

The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

H atoms were found in difference Fourier maps and subsequently placed in idealized positions with constrained C–H distances of 0.99 (CH_2), 0.98 (CH_3) and 0.95 \AA (Csp^2). $U_{\text{iso}}(\text{H})$ values were set at either 1.5 U_{eq} (methyl C) or 1.2 U_{eq} (other C).

Data collection: *APEX2* (Bruker–Nonius, 2004); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP in SHELXTL/PC* (Sheldrick, 1995); software used to prepare material for publication: *SHELXL97* (Sheldrick, 1997) and local procedures.

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