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Ethyl 2-(1-benzyl-5-bromo-1*H*-indol-3-yl)-2-hydroxyacetate

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
Disorder in main residue
R factor = 0.043
wR factor = 0.110
Data-to-parameter ratio = 15.9

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

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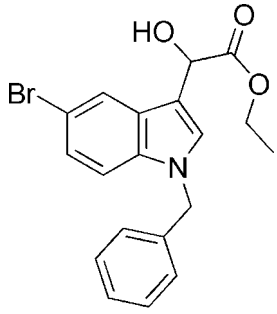
The crystal structure of the title compound, $C_{19}H_{18}BrNO_3$, there are both intra- and intermolecular hydrogen bonds.

Comment

Indolylarylmaleimides have valuable pharmacological properties. For example, indolylarylmaleimide derivatives are reported to be useful in the control and prevention of cancer, central nervous system disorders, Alzheimer's disease, cardiovascular diseases, dermatological diseases, inflammation, autoimmune diseases, diabetic complications and viral diseases (Sudipta *et al.*, 2006). We report here the structure of the title compound, (I) (Fig. 1), a key intermediate in the synthesis of indolylarylmaleimides. The hydrogen bonding (Table 1) is depicted in Fig. 2.



(I)

Experimental

The title compound was synthesized according to the procedure of Yuan *et al.* (2004). Crystals appropriate for data collection were obtained by slow evaporation of a CH_2Cl_2–acetone (3:1 *v*/*v*) solution at 283 K.

Crystal data

$C_{19}H_{18}BrNO_3$
M_r = 388.25
Monoclinic, $P2_1/n$
a = 8.9104 (7) Å
b = 9.4736 (7) Å
c = 20.5732 (16) Å
β = 92.0560 (10)°
V = 1735.5 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.38 mm^{-1}
T = 298 (2) K
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART 4K CCD diffractometer
Absorption correction: none
18902 measured reflections
3790 independent reflections
2742 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

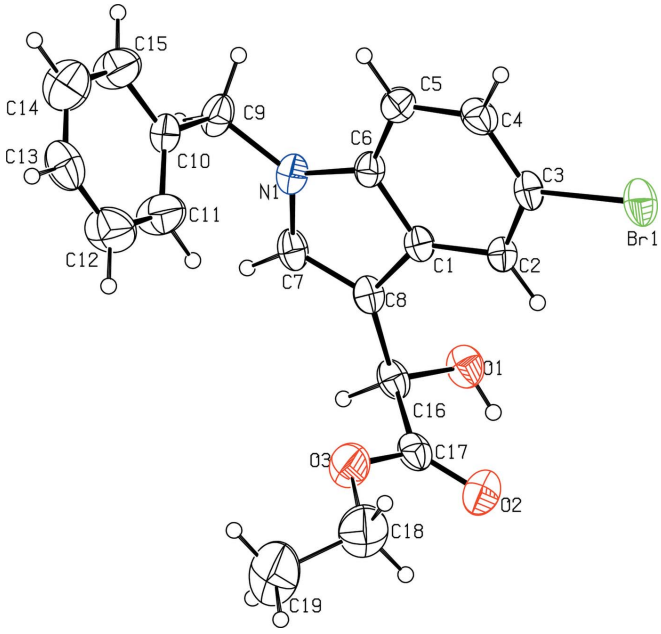


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. The minor disorder component is not shown. Atoms of the minor disorder components are joined with dashed lines.

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$	6 restraints
$wR(F^2) = 0.110$	H-atom parameters constrained
$S = 1.02$	$\Delta\rho_{max} = 0.67$ e Å^{-3}
3790 reflections	$\Delta\rho_{min} = -0.18$ e Å^{-3}
239 parameters	

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.82	2.24	3.006 (3)	155
C7—H7···O1^{ii}	0.93	2.54	3.420 (3)	157
C9—H9A···O2^{iii}	0.97	2.48	3.428 (3)	166
O1—H1···O2	0.82	2.30	2.693 (3)	110

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $-x+2, -y+1, -z$; (iii) $x+1, y, z$.

All H atoms were initially located in a difference Fourier map. The methyl H atoms were then constrained to an ideal geometry, with C—H distances of 0.98 Å and U_{iso}(H) = 1.5U_{eq}(C), but each group was allowed to rotate freely about its C—C bond. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.95–1.00 Å and U_{iso}(H) = 1.2U_{eq}(C). The occupancies of the disordered atoms C18/C18′ and C19/C19′ refined to 0.63 (3):0.37 (3).

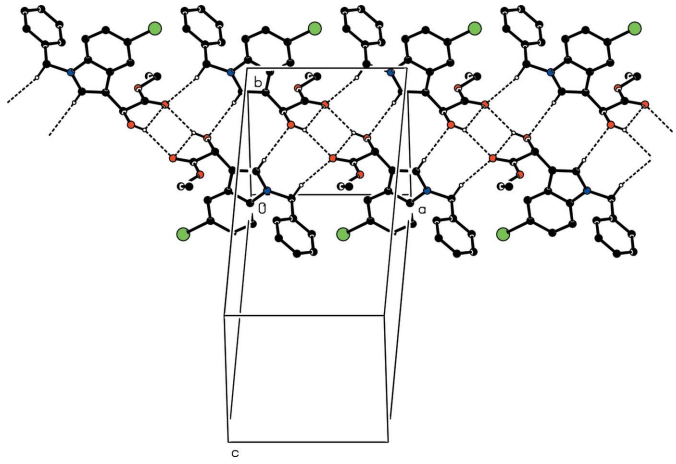


Figure 2
The molecular packing of (I), showing chain formation along the *a* axis. Hydrogen bonds are drawn as dashed lines. H atoms not involved in hydrogen bonds have been omitted.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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References

Bruker (2001). *SMART* (Version 5.628) and *SAINT* (Version 6.45). Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Sudipta, R., Sujata, R. & Gribble, G. W. (2006). *Org. Lett.* **8**, 4975–4977.
Yuan, Y., Wang, X. L. X. & Ding, K. (2004). *J. Org. Chem.* **69**, 146–149.