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2-(5-Bromo-1-methyl-1*H*-indol-3-ylcarbonyl)-*N*-methylacetamide

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Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.003 Å
R factor = 0.036
wR factor = 0.104
Data-to-parameter ratio = 16.9

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

The title compound, $C_{12}H_{12}BrN_2O_2$, is a key intermediate in the synthesis of alkaloids such as didemnimides. The crystal packing is stabilized by two intermolecular C—H···O non-classical hydrogen bonds. In addition, there are C—H···π-ring stacking interactions in the crystal structure.

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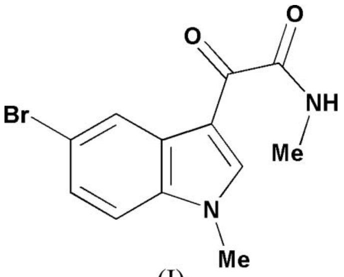
Comment

Pyridoacridine alkaloids have emerged as a class of alkaloids from sponges and ascidians with significant antifungal, cytotoxic, and DNA-binding properties (Vervoort *et al.*, 1997). We report here the structure of the title compound, (I) (Fig. 1).



(I)

The crystal packing is stabilized by two intermolecular C—H···O non-classical hydrogen-bond interactions and C5—H5···*Cg*1 (*Cg*1 is the centroid of the C1–C6 ring) π-ring interactions, forming a dimer. Dimers are further linked by one intermolecular N—H···O hydrogen-bond interaction, forming hydrogen-bonded ribbons (Table 1, Fig. 2).

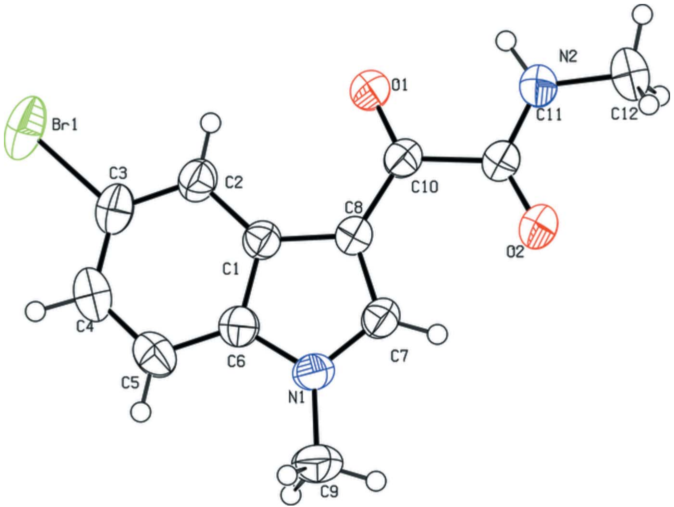


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

Experimental

The title compound was synthesized according to the literature procedure of Reddy *et al.* (1994). Crystals suitable for data collection were obtained by slow evaporation of an acetone–dichloromethane (1:3) solution at 298 K.

Crystal data

$C_{12}H_{11}BrN_2O_2$
$M_r = 295.14$
Monoclinic, $P2_1/n$
$a = 11.8344\ (15)$ Å
$b = 5.6974\ (7)$ Å
$c = 17.651\ (2)$ Å
$\beta = 91.632\ (2)^\circ$
$V = 1189.6\ (3)$ Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 3.45$ mm^{-1}
$T = 299\ (2)$ K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{\min} = 0.425$, $T_{\max} = 0.546$ (expected range = 0.391–0.502)
8629 measured reflections
2693 independent reflections
2023 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.025$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.104$
$S = 1.11$
2693 reflections
159 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max} = 0.55$ e Å^{-3}
$\Delta\rho_{\min} = -0.39$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1$^{\rm i}$	0.90 (3)	2.11 (3)	2.962 (3)	158 (3)
C9—H9A···O2$^{\rm ii}$	0.96	2.46	3.346 (4)	154
N2—H2A···O1	0.90 (3)	2.26 (3)	2.646 (3)	106 (2)
C2—H2···O1	0.93	2.54	3.035 (3)	114
C7—H7···O2	0.93	2.30	2.846 (3)	117
C5—H5···$Cg1^{\rm iii}$	0.93	2.81 (1)	3.54 (1)	137 (1)

Symmetry codes: (i) $-x, -y+2, -z+2$; (ii) $-x-\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (iii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$. *Cg*1 is the centroid of the C1–C6 ring.

C-bound H atoms were positioned geometrically (C—H = 0.93–0.96 Å) and refined using a riding model, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ or $1.5U_{\rm eq}$(methyl C). Atom H2A on N2 was refined isotropically, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm N2})$.

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: *SHELXTL* (Sheldrick, 2001).

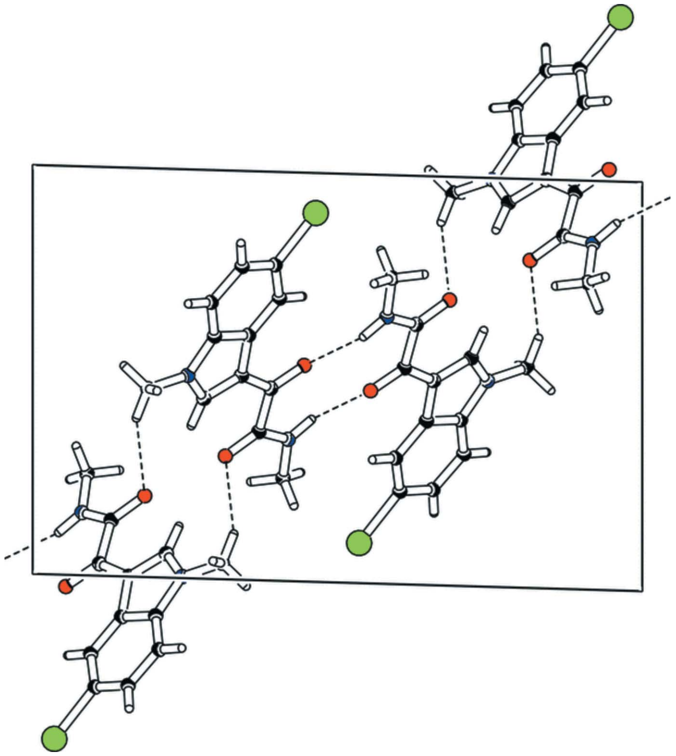


Figure 2
Packing diagram of (I), viewed along the *b* axis. Hydrogen bonds are shown as dashed lines.

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