Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# Ethyl *N*-(5-bromo-3-phenylindol-2-yl)carbamate

**B. H. M. Mruthyunjayaswamy,[a] Omkar B. Ijare,[a] Y Jadegoud,[a] A. Ray Chaudhuri[b] and T. N. Guru Row[b]***

[a]Department of Chemistry, University of Gulbarga, Gulbarga, Karnataka 585 106, India, and [b]Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore, Karnataka 560 012, India

Correspondence e-mail: ssctng@sscu.iisc.ernet.in

Received 15 May 2002
Accepted 6 June 2002
Online 14 June 2002

The crystal structure of the title compound, $C_{17}H_{15}BrN_2O_2$, has been determined at room temperature. The indole moiety is essentially planar and the structure is stabilized by intra- and intermolecular N—H···O hydrogen bonds.

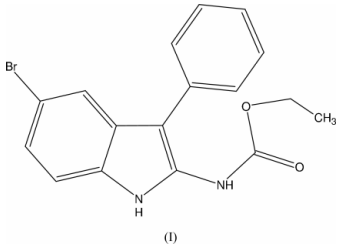
**Key indicators**

Single-crystal X-ray study
$T$ = 293 K
Mean $\sigma$(C–C) = 0.004 Å
$R$ factor = 0.037
$wR$ factor = 0.084
Data-to-parameter ratio = 16.8

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

## Comment

The title compound, (I), shows 80% antifilerial activity *in vitro* against *O. Gutturosa* (Mruthyunjayaswamy *et al.*, 2002). The indole moiety is planar. The activity is due to the presence of the ethyl carbamate moiety. Hydrogen bonds are given in Table 1.




(I)

## Experimental

The title compound was prepared by nitrosation of 5-bromo-3-phenylindole-2-carboxyhydrazide followed by the resulting product in ethanol for 5 h (Hiremath *et al.*, 1978). Crystals were grown from ?tpbgc=^st_head3_bgcolour]>2-propanol.

### *Crystal data*

$C_{17}H_{15}BrN_2O_2$
$M_r$ = 359.21
Monoclinic, $P2_1/n$
$a$ = 13.602 (2) Å
$b$ = 10.1781 (17) Å
$c$ = 23.565 (4) Å
$\beta$ = 106.267 (3)°
$V$ = 3131.8 (9) Å$^3$
$Z$ = 8
$D_x$ = 1.524 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 9585 reflections
$\theta$ = 2.2–23.3°
$\mu$ = 2.63 mm$^{-1}$
$T$ = 293 (2) K
Prism, pale brown
0.32 × 0.21 × 0.10 mm

### *Data collection*

Bruker SMART CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*XPREP*; Bruker, 1998)
$T_{min}$ = 0.514, $T_{max}$ = 0.769
39464 measured reflections
6698 independent reflections
4047 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.061
$\theta_{max}$ = 27.4°
$h = -17 \rightarrow 17$
$k = -13 \rightarrow 13$
$l = -30 \rightarrow 28$

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.084
$S$ = 0.87
6698 reflections
399 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0456P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.47 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.38 e Å$^{-3}$

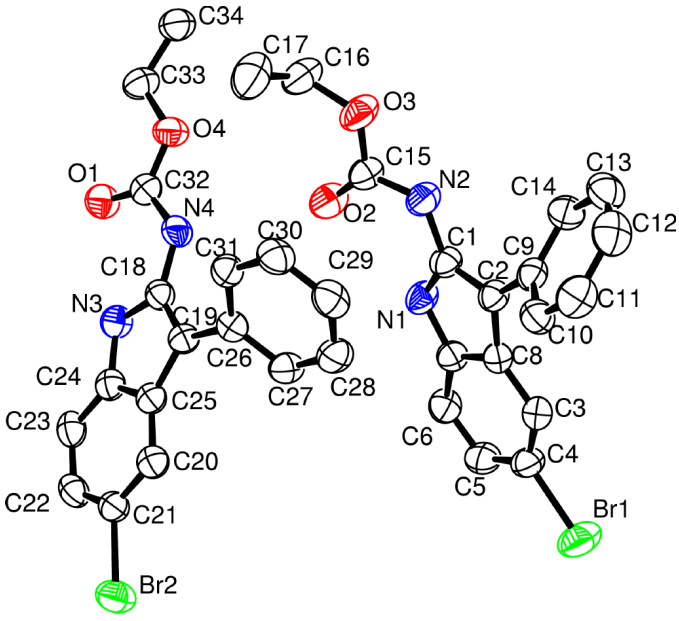



**Figure 1**
The asymmetric unit of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity.

**Table 1**
Hydrogen-bonding geometry (Å, °).

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O1 | 0.86 | 2.19 | 2.722 (3) | 120 |
| N1—H1···O3$^{i}$ | 0.86 | 2.28 | 2.926 (3) | 132 |
| N2—H2···O3$^{ii}$ | 0.86 | 2.48 | 3.282 (3) | 155 |
| N3—H3···O3 | 0.86 | 2.33 | 2.797 (2) | 114 |
| N3—H3···O1$^{iii}$ | 0.86 | 2.33 | 3.049 (3) | 142 |
| C33—H33*B*···O3 | 0.98 | 2.37 | 2.739 (3) | 102 |

Symmetry codes: (i) $\frac{1}{2}+x, \frac{3}{2}-y, z-\frac{1}{2}$; (ii) $\frac{1}{2}-x, y-\frac{1}{2}, \frac{1}{2}-z$; (iii) $x-\frac{1}{2}, \frac{3}{2}-y, \frac{1}{2}+z$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 for Windows (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *PLATON* (Spek, 1990).

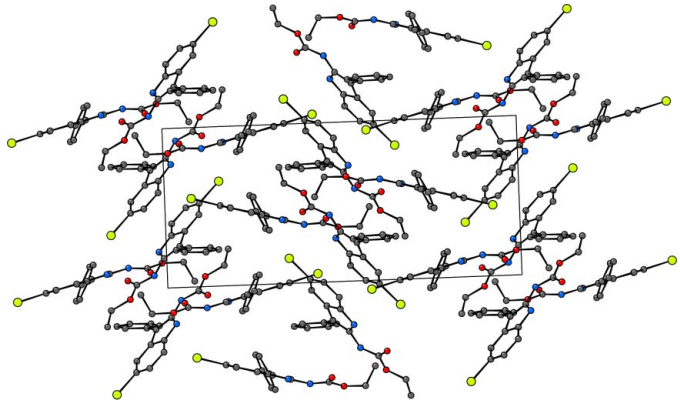


**Figure 2**
Packing diagram of the title compound, viewed down the *a* axis, with *b* vertical and *c* horizontal. H atoms have been omitted for clarity.

The authors thank the Department of Science and Technology, India, for data collection on the CCD facility of the IRFA-DST program, and the Chairman, Department of Chemistry, Gulbarga University, for providing facilities to carry out the synthesis of the compound.

## References

Bruker (1998). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Hiremath, S. P., Mruthyunjayaswamy, B. H. M. & Purohit, M. G. (1978). *Indian J. Chem. Sect. B*, **16**, 789.
Mruthyunjayaswamy, B. H. M., Hiremath, S. P. & Hooper, M. (2002). Unpublished results.
Sheldrick, G. M. (1997). *SHELXL*97 and *SHELXS*97. University of Göttingen, Germany.
Spek, A. L. (1990). *Acta Cryst.* A**46**, C-34.
Watkin, D. J., Pearce, L. & Prout, C. K. (1993). *CAMERON*. Chemical Crystallography Laboratory, University of Oxford, England.