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N-(2-Bromophenyl)-2-phenylpropanamide

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Key indicators

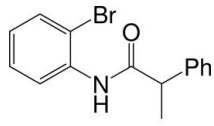
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.037
wR factor = 0.097
Data-to-parameter ratio = 15.8

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

In the title compound, $C_{15}H_{14}BrNO$, N—H···O hydrogen bonds result in the formation of a chain parallel to the *c* axis.

Comment

It is known that 2-phenylacetamide derivatives have significant biological activities and some of them have been tested for anticonvulsant and anti-epileptic activities in mice (Yamagami *et al.*, 1984). In addition, they are important intermediates in the synthesis of benzoxazoles (Evindar & Batey 2006; Pottorf *et al.*, 2002) and oxindoles (Lee & Hartwig, 2001; Shaughnessy *et al.*, 1998). As part of our interest in this field, we have synthesized and characterized the title compound, (I).



(I)

The molecule is built up from two benzene rings linked through a propanamide fragment (Fig. 1). The two aromatic rings make a dihedral angle of 64.9 (1)°. N—H···O hydrogen-bonding interactions link the molecules into chains extending parallel to the *c* axis (Fig. 2 and Table 1).

Experimental

2-Bromobenzenamine (1.72 g, 10 mmol), 2-phenylpropanoic acid (1.5 g, 10 mmol), DCC (*N*,*N*′-methanediylidenedicyclohexanamine; (2.45 g, 12 mmol), DMAP (4-dimethylaminopyridine; 0.12 g, 1 mmol) and CH_2Cl_2 (15 ml) were stirred in a round-bottomed flask at 273 K

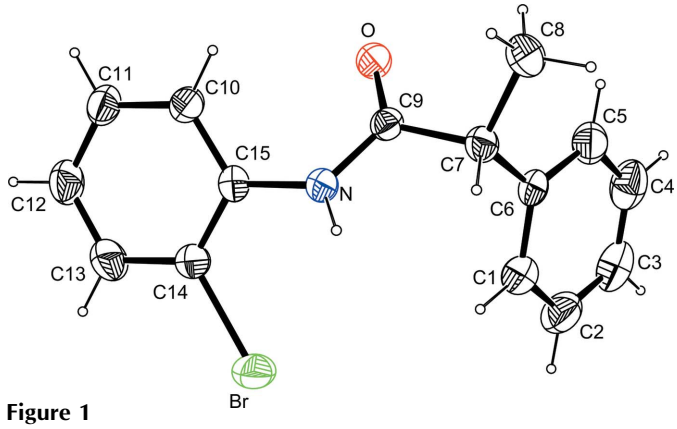


Figure 1
A perspective view of the molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level. H atoms are shown as spheres of arbitrary radii.

for 24 h. The reaction mixture was then cooled to 273 K, filtered and the solvent removed *in vacuo*. The residue was purified by flash column chromatography (SiO_2, 20:1 hexane/EtOAc) to give the desired product (yield 89%). Colourless crystals were obtained from a hexane–EtOAc (2:1) solution after it was left to stand for 6 d.

Crystal data

$C_{15}H_{14}BrNO$
M_r = 304.18
Monoclinic, $P2_1/c$
a = 11.587 (2) Å
b = 13.756 (3) Å
c = 8.433 (2) Å
β = 95.97 (3)°
V = 1336.8 (5) Å^3
Z = 4
D_x = 1.511 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 3.06 mm^{-1}
T = 293 (2) K
Block, colourless
0.41 × 0.36 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.288, T_{max} = 0.546
11223 measured reflections
2590 independent reflections
1687 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.097
S = 1.03
2590 reflections
164 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0474P)^2 + 0.2146P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N—H0···O^{i}	0.86	2.21	3.057 (3)	167

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

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with aromatic C—H = 0.95 Å, methylene C—H = 0.99 Å, methyl C—H = 0.96 Å and N—H = 0.86 Å, with U_{iso}(H) = 1.5U_{eq} for methyl C and 1.2U_{eq} for all other atoms.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *CrystalStructure* and *PLATON*.

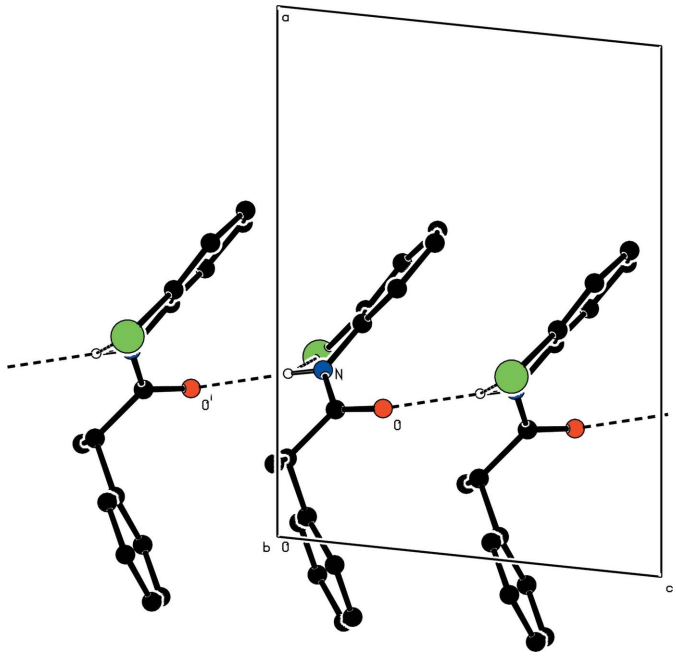


Figure 2
Packing diagram, viewed down the b axis, showing the N—H···O hydrogen bonds as dashed lines. H atoms not involved in hydrogen bonds have been omitted for clarity. [Symmetry code: (i) $x, \frac{1}{2}-y, z-\frac{1}{2}$.]

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