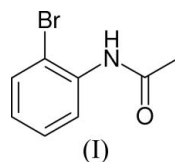


***N*-(2-Bromophenyl)acetamide**Vicki Ronaldson, John. M. D.  
Storey and William T. A.  
Harrison\*Department of Chemistry, University of  
Aberdeen, Meston Walk, Aberdeen AB24 3UE,  
ScotlandCorrespondence e-mail:  
w.harrison@abdn.ac.uk**Key indicators**Single-crystal X-ray study  
 $T = 120$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.032  
 $wR$  factor = 0.074  
Data-to-parameter ratio = 18.0For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.The title compound,  $\text{C}_8\text{H}_8\text{BrNO}$ , possesses normal geometrical parameters. The crystal packing is influenced by an intermolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bond.Received 30 August 2005  
Accepted 1 September 2005  
Online 7 September 2005**Comment**The title compound,  $\text{C}_8\text{H}_8\text{BrNO}$ , (I), (Fig. 1) was prepared as an intermediate in a natural product synthesis.

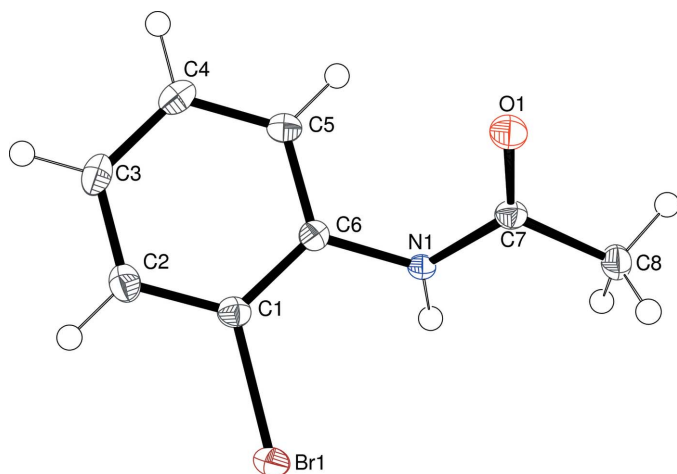
The dihedral angle between the mean planes of the benzene ring (atoms C1–C6) and the N1/O1/C7/C8 side-chain grouping in (I) is  $42.75$  ( $14$ )°. This is intermediate between the situation in acetanilide [*i.e.* (I) without the Br atom],  $\text{C}_8\text{H}_9\text{NO}$  (Brown, 1966; Wasserman *et al.*, 1985), where the aromatic ring and side chain are twisted by  $17.6^\circ$ , and *N*-methylacetanilide,  $\text{C}_9\text{H}_{11}\text{NO}$  (Pederson, 1967), where the two corresponding groups of atoms are constrained by symmetry to be perpendicular. The  $\text{C}_{\text{ar}}-\text{N}$  (ar = aromatic) bond distances are almost identical in (I) and acetanilide (Brown, 1966), being  $1.418$  (4) and  $1.417$  (2) Å respectively, as are the  $\text{C}_{\text{c}}-\text{N}$  (c = carbonyl) distances, at  $1.358$  (4) and  $1.355$  (2) Å, respectively. The equivalent distances in *N*-methylacetanilide (Pederson, 1967), where any electronic conjugation between the benzene ring and amide group is presumably impossible because of their perpendicular orientation, are distinctly different, with  $\text{C}_{\text{ar}}-\text{N}$  much longer at  $1.474$  Å and  $\text{C}_{\text{c}}-\text{N}$  significantly shorter at  $1.325$  Å.

The bond angle sum about N1 in (I) is  $360.0^\circ$ , suggesting that this atom is essentially  $sp^2$ -hybridized. All the other geometrical parameters for (I) lie within their expected ranges (Allen *et al.*, 1995).

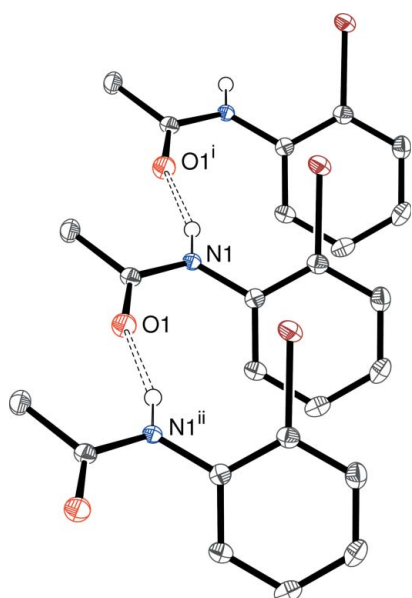
The crystal packing in (I) is influenced by an  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bond (Table 1 and Fig. 2) that links the molecules into chains propagating along [100]. There are no  $\pi-\pi$  stacking interactions in (I). The packing is shown in Fig. 3.

**Experimental**

2-Bromoaniline (3.44 g, 20.0 mmol) was added to a solution of acetyl chloride (1.88 g, 24.0 mmol) and DIPEA (*N,N*-diisopropylethylamine) (3.12 g, 24.0 mmol) in dry tetrahydrofuran (20 ml) at 273 K. On completion (as monitored by thin-layer chromatography), the reaction mixture was diluted with water (20 ml) and the product was

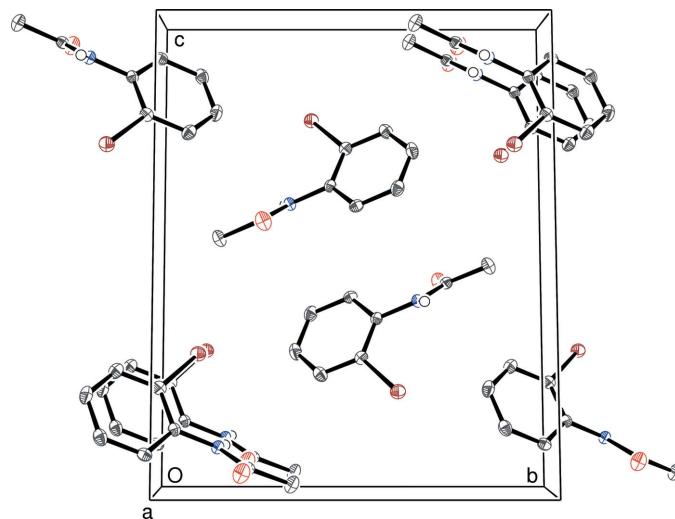


**Figure 1**  
View of (I) (50% probability displacement ellipsoids; H atoms are drawn as small spheres of arbitrary radii).



**Figure 2**  
Detail of (I) showing how the N–H...O hydrogen bond (dashed lines) links molecules into a chain. The view direction is perpendicular to the mean plane of the benzene ring of the central molecule, showing that no  $\pi$ – $\pi$  stacking occurs. All H atoms except atom H1 and its symmetry equivalents have been omitted for clarity. [Symmetry codes: (i)  $x - 1, y, z$ ; (ii)  $x + 1, y, z$ .]

extracted with EtOAc (3  $\times$  20 ml). The organic phase was then washed with water (2  $\times$  20 ml) and brine (20 ml), then dried (MgSO<sub>4</sub>) and evaporated under reduced pressure to yield the crude product, which was recrystallized from CH<sub>2</sub>Cl<sub>2</sub> to give (I) (yield 97%, 4.13 g) as clear needles; one of these was cut to a block for data collection; m.p. 363–364 K;  $R_F$  = 0.12 [hexane/EtOAc (5:1)]. IR (KBr disc, cm<sup>-1</sup>):  $\nu_{\max}$  3272 (NH), 3159 (Ar–H), 1647 (C=O), 1518 (Ar C=C); <sup>1</sup>H NMR (250 MHz; CDCl<sub>3</sub>):  $\delta_H$  2.21 (3H, s, CH<sub>3</sub>), 6.97 (1H, t,  $J$  = 7.5 Hz, Ar–H), 7.29 (1H, t,  $J$  = 7.5 Hz, Ar–H), 7.51 (1H, d,  $J$  = 8.0 Hz, Ar–H), 7.61 (1H, bs, NH), 8.31 (1H, d,  $J$  = 7.5 Hz, Ar–H); <sup>13</sup>C NMR (CDCl<sub>3</sub>):  $\delta_C$  24.9 (–COCH<sub>3</sub>), 113.2 (Ar C–Br), 122.0, 125.2, 128.4, 132.2 (4  $\times$  Ar C), 135.7 (–CO–NH–C–), 168.3 (–C=O). Mass spectrum:  $[M+H]^+$  212.979, C<sub>8</sub>H<sub>8</sub>BrNO requires 212.979.



**Figure 3**  
The packing in (I), viewed down [100], with all H atoms except H1 omitted for clarity.

#### Crystal data

C<sub>8</sub>H<sub>8</sub>BrNO  
 $M_r$  = 214.06  
Monoclinic,  $P2_1/n$   
 $a$  = 4.7790 (1) Å  
 $b$  = 11.9257 (4) Å  
 $c$  = 14.6703 (3) Å  
 $\beta$  = 96.8173 (16)°  
 $V$  = 830.19 (4) Å<sup>3</sup>  
 $Z$  = 4

$D_x$  = 1.713 Mg m<sup>-3</sup>  
Mo  $K\alpha$  radiation  
Cell parameters from 1977 reflections  
 $\theta$  = 2.9–27.5°  
 $\mu$  = 4.89 mm<sup>-1</sup>  
 $T$  = 120 (2) K  
Block, colourless  
0.24  $\times$  0.10  $\times$  0.07 mm

#### Data collection

Nonius KappaCCD diffractometer  
 $\omega$  and  $\varphi$  scans  
Absorption correction: multi-scan (SADABS; Bruker, 2003)  
 $T_{\min}$  = 0.387,  $T_{\max}$  = 0.726  
9212 measured reflections  
1905 independent reflections

1750 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}}$  = 0.037  
 $\theta_{\max}$  = 27.5°  
 $h$  = –6  $\rightarrow$  5  
 $k$  = –15  $\rightarrow$  15  
 $l$  = –18  $\rightarrow$  19

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)]$  = 0.032  
 $wR(F^2)$  = 0.074  
 $S$  = 1.26  
1905 reflections  
106 parameters  
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + 1.9011P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max}$  = 0.001  
 $\Delta\rho_{\max}$  = 0.76 e Å<sup>-3</sup>  
 $\Delta\rho_{\min}$  = –0.38 e Å<sup>-3</sup>  
Extinction correction: SHELXL97  
Extinction coefficient: 0.0163 (11)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1–H1 <sup>i</sup> ...O1 <sup>i</sup>	0.83 (4)	2.10 (4)	2.896 (3)	161 (3)

Symmetry code: (i)  $x - 1, y, z$ .

All the C-bound H atoms were placed in idealized positions (C–H = 0.95–0.98 Å) and refined as riding on their carriers with the constraint  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$  or  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{methyl carrier})$  applied. The methyl group was allowed to rotate about the C7–C8 bond as a rigid group. The N-bound H atom was located in a

difference map and its position was freely refined with the constraint  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$ .

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK*, *DENZO* (Otwinowski & Minor, 1997) and *SORTAV* (Blessing, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

We thank the EPSRC National Mass Spectrometry Service (University of Swansea) and the EPSRC National Crystallography Service (University of Southampton) for data collections.

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## supporting information

*Acta Cryst.* (2005). E61, o3156–o3158 [doi:10.1107/S1600536805027492]

## ***N*-(2-Bromophenyl)acetamide**

**Vicki Ronaldson, John. M. D. Storey and William T. A. Harrison**

### **S1. Comment**

The title compound, C<sub>8</sub>H<sub>8</sub>BrNO, (I), (Fig. 1) was prepared as an intermediate in a natural product synthesis.

The dihedral angle between the mean planes of the benzene ring (atoms C1–C6) and the N1/O1/C7/C8 side-chain grouping in (I) is 42.75 (14)°. This is intermediate between the situation in acetanilide [*i.e.* (I) without the Br atom], C<sub>8</sub>H<sub>9</sub>NO (Brown, 1966; Wasserman *et al.*, 1985), where the aromatic ring and side chain are twisted by 17.6°, and *N*-methylacetanilide, C<sub>9</sub>H<sub>11</sub>NO (Pederson, 1967), where the two equivalent groups of atoms are constrained by symmetry to be perpendicular. The C<sub>ar</sub>—N (ar = aromatic) bond distances are almost identical in (I) and acetanilide (Brown, 1966), being 1.418 (4) and 1.417 (2) Å respectively, as are the C<sub>c</sub>—N (c = carbonyl) distances, at 1.358 (4) and 1.355 (2) Å, respectively. The equivalent distances in *N*-methylacetanilide (Pederson, 1967), where any electronic conjugation between the benzene ring and amine group is presumably impossible because of their perpendicular orientation, are distinctly different, with C<sub>ar</sub>—N much longer at 1.474 Å and C<sub>c</sub>—N significantly shorter at 1.325 Å.

The bond angle sum about N1 in (I) is 360.0°, suggesting that this atom is more or less *sp*<sup>2</sup>-hybridized. All the other geometrical parameters for (I) lie within their expected ranges (Allen *et al.*, 1995).

The crystal packing in (I) is influenced by an N—H···O hydrogen bond (Table 1 and Fig. 2) that links the molecules into chains propagating in [100]. There are no *π*–*π* stacking interactions in (I). The unit-cell packing is shown in Fig. 3.

### **S2. Experimental**

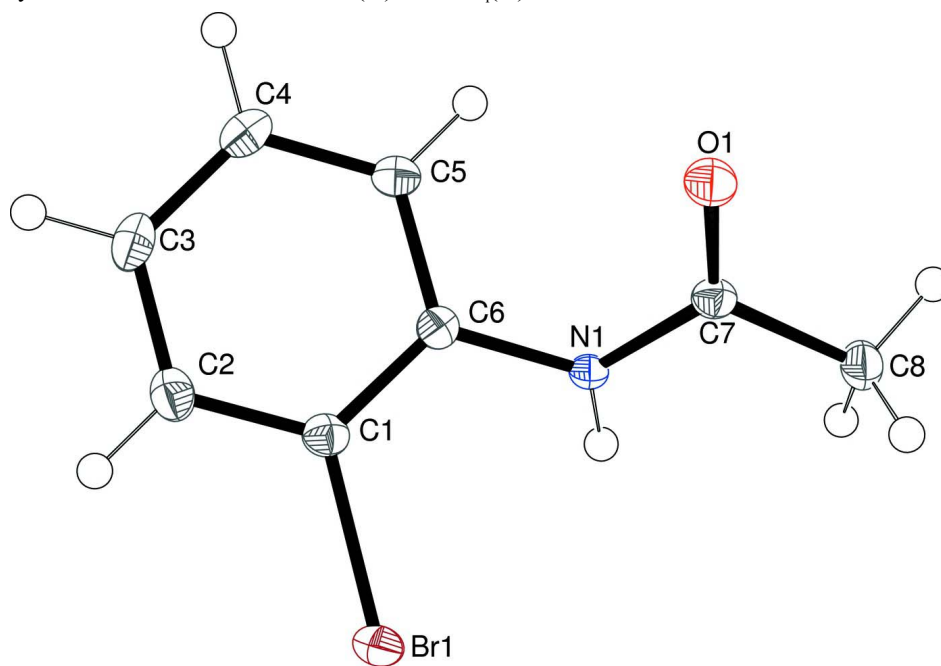
2-Bromoaniline (3.44 g, 20.0 mmol) was added to a solution of acetyl chloride (1.88 g, 24.0 mmol) and DIPEA (*N,N*-diisopropylethylamine) (3.12 g, 24.0 mmol) in dry tetrahydrofuran (20 ml) at 273 K. On completion (as monitored by thin-layer chromatography), the reaction mixture was diluted with water (20 ml) and the product was extracted with EtOAc (3 × 20 ml). The organic phase was then washed with water (2 × 20 ml) and brine (20 ml), then dried (MgSO<sub>4</sub>) and evaporated under reduced pressure to yield the crude product, which was recrystallized from CH<sub>2</sub>Cl<sub>2</sub> to give (I) (yield 97%, 4.13 g) as clear needles; one of these was cut to a block for data collection; m.p. 363–364 K; *R*<sub>F</sub> = 0.12

[hexane/EtOAc (5:1)]. IR (KBr disc, cm<sup>-1</sup>): *v*<sub>max</sub> 3272 (NH), 3159 (Ar—H), 1647 (C=O), 1518 (Ar C=C); <sup>1</sup>H NMR (250 MHz; CDCl<sub>3</sub>): *δ*<sub>H</sub> 2.21 (3H, *s*, CH<sub>3</sub>), 6.97 (1H, *t*, *J* = 7.5 Hz, Ar—H), 7.29 (1H, *t*, *J* = 7.5 Hz, Ar—H), 7.51 (1H, *d*, *J* = 8.0 Hz, Ar—H), 7.61 (1H, *bs*, NH), 8.31 (1H, *d*, *J* = 7.5 Hz, Ar—H); <sup>13</sup>C NMR (CDCl<sub>3</sub>): *δ*<sub>C</sub> 24.9 (—COCH<sub>3</sub>), 113.2 (Ar C—Br), 122.0, 125.2, 128.4, 132.2 (4 × Ar C), 135.7 (—CO—NH—C—), 168.3 (—C=O). Mass spectrum: [*M*+H]<sup>+</sup> 212.979, C<sub>8</sub>H<sub>8</sub>BrNO requires 212.979.

### **S3. Refinement**

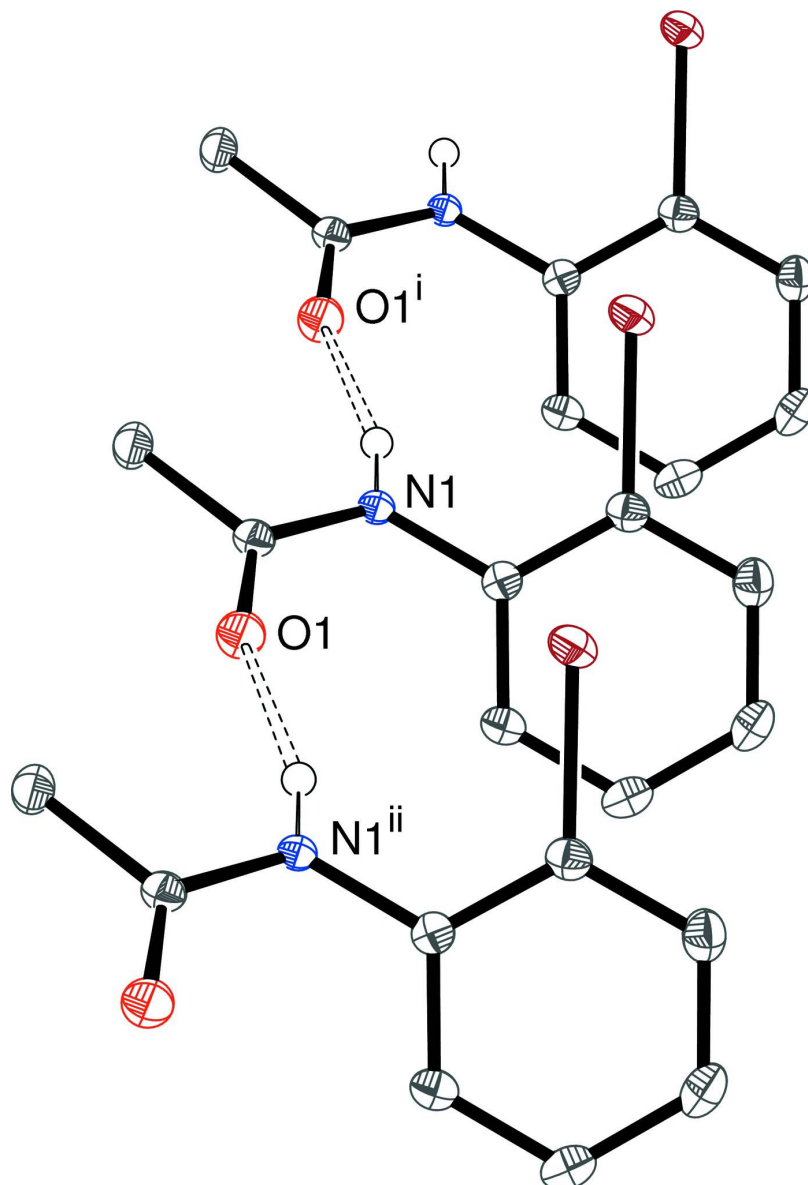
All the C-bound hydrogen atoms were placed in idealized positions (C—H = 0.95–0.98 Å) and refined as riding on their carriers with the constraint *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(carrier) or *U*<sub>iso</sub>(H) = 1.5*U*<sub>eq</sub>(methyl carrier) applied. The methyl moiety was allowed to rotate about the C7—C8 bond as a rigid group. The N-bound H atom was located in a difference map and its

position was freely refined with the constraint  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$ .

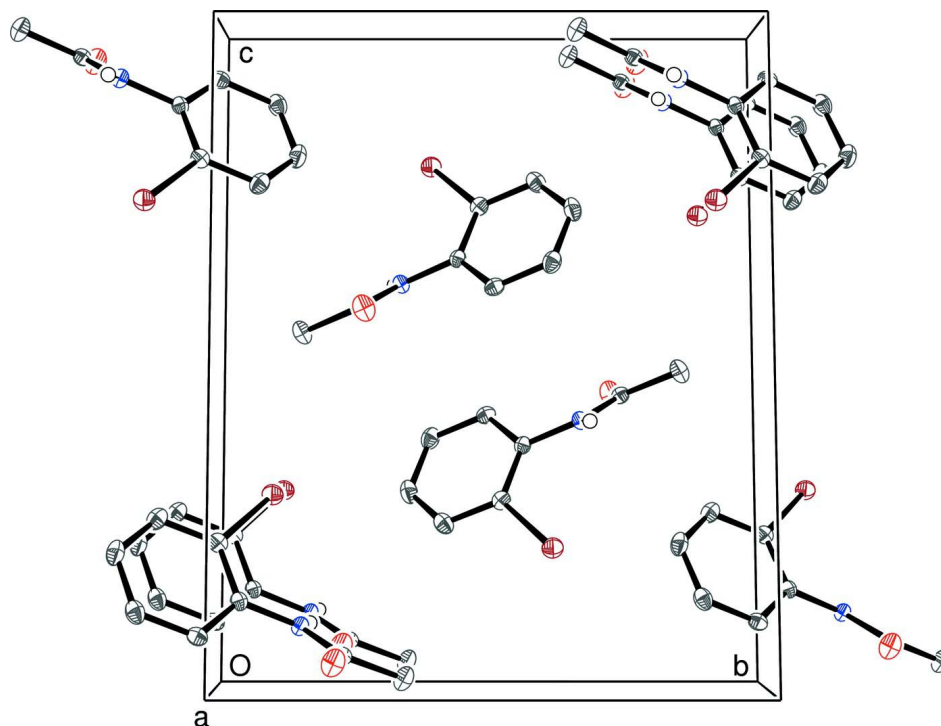


**Figure 1**

View of (I) (50% probability displacement ellipsoids; H atoms are drawn as small spheres of arbitrary radii).

**Figure 2**

Detail of (I) showing how the N—H···O hydrogen bond (dashed lines) links molecules into a chain. The view direction is perpendicular to the mean plane of the benzene ring of the central molecule, showing that no  $\pi$ - $\pi$  stacking occurs. All H atoms except atom H1 have been omitted for clarity. [Symmetry codes: (i)  $x - 1, y, z$ ; (ii)  $x + 1, y, z$ .]

**Figure 3**

Unit cell packing in (I), viewed down [010], with all H atoms except H1 omitted for clarity.

### *N*-(2-Bromophenyl)acetamide

#### Crystal data

$C_8H_8BrNO$

$M_r = 214.06$

Monoclinic,  $P2_1/n$

Hall symbol: -P 2yn

$a = 4.7790$  (1) Å

$b = 11.9257$  (4) Å

$c = 14.6703$  (3) Å

$\beta = 96.8173$  (16)°

$V = 830.19$  (4) Å<sup>3</sup>

$Z = 4$

$F(000) = 424$

$D_x = 1.713$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 1977 reflections

$\theta = 2.9$ – $27.5$ °

$\mu = 4.89$  mm<sup>-1</sup>

$T = 120$  K

Block, colourless

$0.24 \times 0.10 \times 0.07$  mm

#### Data collection

Nonius KappaCCD  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\omega$  and  $\varphi$  scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2003)

$T_{\min} = 0.387$ ,  $T_{\max} = 0.726$

9212 measured reflections

1905 independent reflections

1750 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.037$

$\theta_{\max} = 27.5$ °,  $\theta_{\min} = 3.3$ °

$h = -6 \rightarrow 5$

$k = -15 \rightarrow 15$

$l = -18 \rightarrow 19$

Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.032$   
 $wR(F^2) = 0.074$   
 $S = 1.26$   
 1905 reflections  
 106 parameters  
 0 restraints  
 Primary atom site location: structure-invariant  
 direct methods  
 Secondary atom site location: difference Fourier  
 map

Hydrogen site location: difmap (N-H) and geom  
 (others)  
 H atoms treated by a mixture of independent  
 and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + 1.9011P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.76 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\min} = -0.38 \text{ e } \text{Å}^{-3}$   
 Extinction correction: *SHELXL97*,  
 $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$   
 Extinction coefficient: 0.0163 (11)

Special details

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{Å}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.4653 (6)	0.4807 (2)	0.7214 (2)	0.0159 (6)
C2	0.5507 (7)	0.5852 (3)	0.7562 (2)	0.0203 (6)
H2	0.4860	0.6123	0.8109	0.024*
C3	0.7304 (7)	0.6492 (3)	0.7106 (2)	0.0219 (7)
H3	0.7915	0.7203	0.7343	0.026*
C4	0.8223 (7)	0.6099 (3)	0.6300 (2)	0.0205 (6)
H4	0.9479	0.6538	0.5992	0.025*
C5	0.7307 (6)	0.5067 (3)	0.5946 (2)	0.0167 (6)
H5	0.7918	0.4807	0.5390	0.020*
C6	0.5493 (6)	0.4406 (2)	0.63992 (19)	0.0140 (6)
C7	0.6102 (6)	0.2594 (2)	0.56501 (19)	0.0153 (6)
C8	0.4592 (7)	0.1544 (3)	0.5295 (2)	0.0209 (7)
H8A	0.2575	0.1702	0.5151	0.031*
H8B	0.4863	0.0957	0.5765	0.031*
H8C	0.5355	0.1291	0.4739	0.031*
N1	0.4490 (5)	0.3362 (2)	0.60299 (16)	0.0135 (5)
H1	0.280 (8)	0.322 (3)	0.604 (2)	0.017 (9)*
O1	0.8634 (4)	0.27188 (19)	0.56131 (16)	0.0229 (5)
Br1	0.23224 (6)	0.39129 (3)	0.78845 (2)	0.02046 (13)

Atomic displacement parameters ( $\text{Å}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0132 (13)	0.0170 (14)	0.0177 (14)	0.0019 (11)	0.0025 (11)	0.0014 (11)



C2	0.0200 (15)	0.0194 (15)	0.0214 (15)	0.0018 (12)	0.0023 (12)	-0.0045 (12)
C3	0.0218 (16)	0.0149 (15)	0.0281 (17)	-0.0019 (12)	-0.0007 (13)	-0.0035 (13)
C4	0.0187 (15)	0.0175 (14)	0.0249 (16)	-0.0034 (12)	0.0012 (12)	0.0037 (13)
C5	0.0158 (14)	0.0193 (15)	0.0154 (14)	-0.0002 (11)	0.0029 (11)	0.0023 (12)
C6	0.0122 (13)	0.0136 (13)	0.0159 (13)	0.0021 (11)	0.0006 (10)	0.0013 (11)
C7	0.0157 (14)	0.0161 (14)	0.0143 (13)	0.0000 (11)	0.0029 (11)	0.0017 (11)
C8	0.0191 (15)	0.0181 (15)	0.0264 (16)	-0.0023 (12)	0.0059 (12)	-0.0065 (13)
N1	0.0107 (12)	0.0141 (12)	0.0164 (12)	-0.0016 (9)	0.0048 (9)	-0.0018 (10)
O1	0.0129 (10)	0.0239 (12)	0.0330 (13)	-0.0014 (9)	0.0069 (9)	-0.0054 (10)
Br1	0.02191 (19)	0.02130 (19)	0.01987 (19)	-0.00046 (12)	0.00956 (12)	0.00033 (12)

*Geometric parameters (Å, °)*

C1—C2	1.390 (4)	C5—H5	0.9500
C1—C6	1.390 (4)	C6—N1	1.418 (4)
C1—Br1	1.899 (3)	C7—O1	1.227 (4)
C2—C3	1.380 (5)	C7—N1	1.358 (4)
C2—H2	0.9500	C7—C8	1.507 (4)
C3—C4	1.390 (4)	C8—H8A	0.9800
C3—H3	0.9500	C8—H8B	0.9800
C4—C5	1.387 (4)	C8—H8C	0.9800
C4—H4	0.9500	N1—H1	0.83 (4)
C5—C6	1.397 (4)		
C2—C1—C6	121.6 (3)	C1—C6—C5	118.3 (3)
C2—C1—Br1	118.5 (2)	C1—C6—N1	120.8 (3)
C6—C1—Br1	119.9 (2)	C5—C6—N1	121.0 (3)
C3—C2—C1	119.3 (3)	O1—C7—N1	123.2 (3)
C3—C2—H2	120.3	O1—C7—C8	121.3 (3)
C1—C2—H2	120.3	N1—C7—C8	115.5 (3)
C2—C3—C4	120.3 (3)	C7—C8—H8A	109.5
C2—C3—H3	119.9	C7—C8—H8B	109.5
C4—C3—H3	119.9	H8A—C8—H8B	109.5
C5—C4—C3	120.0 (3)	C7—C8—H8C	109.5
C5—C4—H4	120.0	H8A—C8—H8C	109.5
C3—C4—H4	120.0	H8B—C8—H8C	109.5
C4—C5—C6	120.6 (3)	C7—N1—C6	124.5 (2)
C4—C5—H5	119.7	C7—N1—H1	118 (2)
C6—C5—H5	119.7	C6—N1—H1	118 (2)
C6—C1—C2—C3	-2.1 (5)	Br1—C1—C6—N1	3.9 (4)
Br1—C1—C2—C3	177.1 (2)	C4—C5—C6—C1	-0.4 (4)
C1—C2—C3—C4	0.7 (5)	C4—C5—C6—N1	178.4 (3)
C2—C3—C4—C5	0.8 (5)	O1—C7—N1—C6	2.2 (5)
C3—C4—C5—C6	-0.9 (5)	C8—C7—N1—C6	-179.6 (3)
C2—C1—C6—C5	2.0 (4)	C1—C6—N1—C7	-138.6 (3)
Br1—C1—C6—C5	-177.3 (2)	C5—C6—N1—C7	42.6 (4)
C2—C1—C6—N1	-176.9 (3)		

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
N1—H1···O1 <sup>i</sup>	0.83 (4)	2.10 (4)	2.896 (3)	161 (3)

Symmetry code: (i)  $x-1, y, z$ .