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2-(4-Bromophenyl)-*N*-(2,6-dimethylphenyl)acetamide

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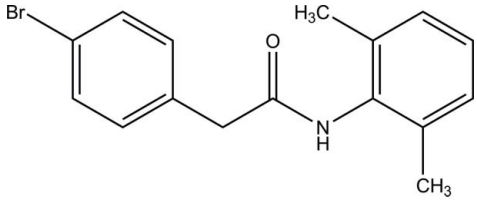
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.006 Å; R factor = 0.052; wR factor = 0.143; data-to-parameter ratio = 18.8.

In the title compound, $C_{16}H_{16}BrNO$, the dihedral angle between the benzene rings is 69.8 (2)°. In the crystal, N—H···O hydrogen bonds link the molecules into $C(4)$ chains propagating in [100]. Adjacent molecules in the chains are also linked by C—H···O interactions which, along with the N—H···O hydrogen bonds, generate $R_2^1(6)$ loops.

Related literature

For general background to the title compound and for related structures, see: Fun *et al.* (2011*a*,*b*, 2012*a*,*b*). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{16}H_{16}BrNO$
M_r = 318.21
Monoclinic, $P2_1/c$
a = 4.7146 (6) Å
b = 22.999 (3) Å
c = 13.5350 (15) Å
β = 91.138 (3)°
V = 1467.3 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.79 mm^{-1}
T = 296 K
0.18 × 0.09 × 0.07 mm

Data collection

Bruker SMART APEXII DUO CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.635, T_{max} = 0.822
14048 measured reflections
3352 independent reflections
1593 reflections with $I > 2\sigma(I)$
R_{int} = 0.074

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.143
S = 1.01
3352 reflections
178 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.57 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*1···O1^{i}	0.91 (4)	1.95 (4)	2.847 (4)	166 (3)
C7—H7*B*···O1^{i}	0.97	2.38	3.240 (5)	148

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6926).

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§ Thomson Reuters ResearcherID: A-5525-2009.

supplementary materials

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2-(4-Bromophenyl)-*N*-(2,6-dimethylphenyl)acetamide

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Comment

In continuation of our work on synthesis of amides (Fun *et al.*, 2011*a*, 2011*b*, 2012*a*, 2012*b*), we report herein the crystal structure of the title compound.

In the title molecule (Fig. 1), the two benzene rings (C1-C6 and C9-C14) make a dihedral angle of 69.8 (2)°. Bond lengths and angles are within normal ranges and are comparable to related structures (Fun *et al.*, 2011*a*, 2011*b*, 2012*a*, 2012*b*).

In the crystal structure, Fig. 2, molecules are linked *via* N1–H1N1···O1 and C7–H7B···O1 hydrogen bonds (Table 1) into one-dimensional [100] chains which contain $R_2^1(6)$ ring motifs (Bernstein *et al.*, 1995).

Experimental

4-Bromophenylacetic acid (0.213 g, 1 mmol), 2,6-Dimethylaniline (0.1 ml, 1 mmol) and 1-ethyl-3-(3-dimethylamino-propyl)-carbodiimide hydrochloride (1.0 g, 0.01 mol) were dissolved in dichloromethane (20 ml). The mixture was stirred in presence of triethylamine at 273 K for about 3 h. The contents were poured into 100 ml of ice-cold aqueous hydrochloric acid with stirring. The resulting solution was extracted thrice with dichloromethane. The organic layer was washed with saturated $NaHCO_3$ solution and brine solution, dried and concentrated under reduced pressure to give the title compound (I). Colourless plates were grown from a methanol and *N,N*-dimethylformamide (1:1) solvent mixture by the slow evaporation method (*m.p.*:479-481 K).

Refinement

Atom H1N1 was located in a difference Fourier map and refined freely [N–H = 0.91 (4) Å]. The remaining H atoms were positioned geometrically and refined using a riding model with C–H = 0.93-0.97 Å and U_{iso}(H) = 1.2 or 1.5 U_{eq}(C). A rotating-group model was applied for the methyl groups.

Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

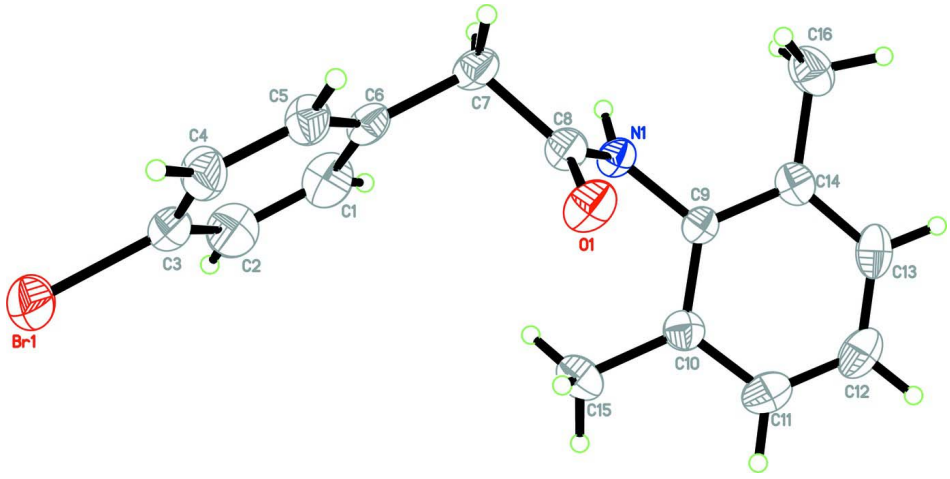

Figure 1

The molecular structure of the title compound showing 30% probability displacement ellipsoids for non-H atoms.

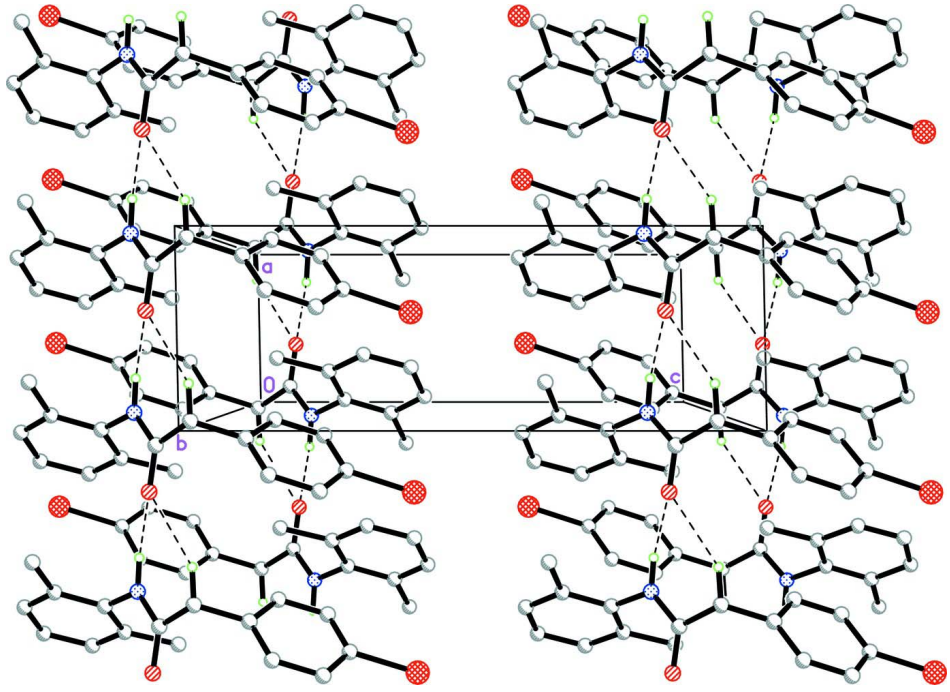

Figure 2

The crystal structure of the title compound, viewed along the *b* axis. H atoms not involved in hydrogen bonds (dashed lines) have been omitted for clarity.

2-(4-Bromophenyl)-*N*-(2,6-dimethylphenyl)acetamide

Crystal data

$C_{16}H_{16}BrNO$
$M_r = 318.21$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 4.7146\ (6)$ Å
$b = 22.999\ (3)$ Å
$c = 13.5350\ (15)$ Å
$\beta = 91.138\ (3)°$
$V = 1467.3\ (3)$ Å^3
$Z = 4$

$F(000) = 648$
$D_x = 1.440$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1376 reflections
$\theta = 3.0–20.1°$
$\mu = 2.79$ mm^{-1}
$T = 296$ K
Plate, colourless
0.18 × 0.09 × 0.07 mm

Data collection

Bruker SMART APEXII DUO CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.635$, $T_{max} = 0.822$
14048 measured reflections
3352 independent reflections
1593 reflections with $I > 2\sigma(I)$
$R_{int} = 0.074$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.8°$
$h = -6\rightarrow6$
$k = -26\rightarrow29$
$l = -17\rightarrow17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.143$
$S = 1.01$
3352 reflections
178 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0518P)^2 + 0.539P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.57$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2$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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.41005 (16)	0.35233 (3)	0.61576 (4)	0.1038 (3)
O1	0.4016 (5)	0.33510 (13)	1.1247 (2)	0.0615 (8)
N1	−0.0290 (7)	0.37234 (13)	1.1589 (2)	0.0416 (7)
C1	0.0074 (10)	0.35773 (19)	0.8830 (4)	0.0688 (13)
H1A	−0.1203	0.3825	0.9134	0.083*
C2	0.0970 (11)	0.3706 (2)	0.7894 (4)	0.0744 (14)
H2A	0.0300	0.4037	0.7570	0.089*
C3	0.2837 (10)	0.33480 (19)	0.7448 (3)	0.0614 (11)
C4	0.3828 (10)	0.28624 (19)	0.7918 (3)	0.0652 (12)
H4A	0.5100	0.2616	0.7609	0.078*
C5	0.2916 (9)	0.27413 (17)	0.8861 (3)	0.0550 (10)

H5A	0.3608	0.2413	0.9186	0.066*
C6	0.1019 (8)	0.30930 (17)	0.9327 (3)	0.0469 (9)
C7	0.0048 (8)	0.29567 (17)	1.0356 (3)	0.0531 (10)
H7A	0.0515	0.2557	1.0517	0.064*
H7B	−0.1996	0.3000	1.0383	0.064*
C8	0.1443 (8)	0.33567 (16)	1.1105 (3)	0.0464 (9)
C9	0.0737 (7)	0.41182 (15)	1.2329 (2)	0.0380 (8)
C10	0.2465 (8)	0.45805 (16)	1.2062 (3)	0.0477 (9)
C11	0.3468 (10)	0.49491 (18)	1.2805 (3)	0.0664 (12)
H11A	0.4670	0.5254	1.2645	0.080*
C12	0.2719 (10)	0.4871 (2)	1.3765 (3)	0.0704 (13)
H12A	0.3412	0.5122	1.4251	0.084*
C13	0.0963 (10)	0.4428 (2)	1.4010 (3)	0.0618 (12)
H13A	0.0450	0.4383	1.4666	0.074*
C14	−0.0091 (8)	0.40372 (16)	1.3301 (3)	0.0470 (9)
C15	0.3245 (11)	0.4697 (2)	1.1008 (3)	0.0736 (13)
H15A	0.1636	0.4621	1.0581	0.110*
H15B	0.4787	0.4448	1.0829	0.110*
H15C	0.3808	0.5096	1.0941	0.110*
C16	−0.2007 (10)	0.35451 (19)	1.3576 (3)	0.0680 (12)
H16A	−0.1351	0.3192	1.3278	0.102*
H16B	−0.3903	0.3627	1.3344	0.102*
H16C	−0.1992	0.3502	1.4281	0.102*
H1N1	−0.220 (8)	0.3663 (14)	1.153 (3)	0.042 (10)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.1668 (7)	0.0908 (4)	0.0537 (3)	−0.0423 (4)	0.0020 (3)	0.0035 (3)
O1	0.0288 (15)	0.081 (2)	0.0748 (19)	0.0040 (14)	0.0040 (14)	−0.0234 (15)
N1	0.0260 (17)	0.0529 (19)	0.0457 (17)	0.0002 (15)	−0.0001 (15)	−0.0070 (14)
C1	0.063 (3)	0.064 (3)	0.079 (3)	0.022 (2)	−0.002 (3)	−0.012 (3)
C2	0.085 (4)	0.061 (3)	0.076 (3)	0.013 (3)	−0.014 (3)	0.008 (2)
C3	0.077 (3)	0.055 (3)	0.052 (2)	−0.015 (2)	−0.003 (2)	−0.005 (2)
C4	0.083 (3)	0.056 (3)	0.057 (3)	0.007 (2)	0.015 (3)	−0.011 (2)
C5	0.064 (3)	0.047 (2)	0.053 (2)	0.010 (2)	0.005 (2)	−0.0060 (18)
C6	0.038 (2)	0.050 (2)	0.053 (2)	−0.0018 (19)	−0.0050 (19)	−0.0126 (19)
C7	0.036 (2)	0.062 (3)	0.061 (2)	−0.0096 (19)	0.010 (2)	−0.021 (2)
C8	0.033 (2)	0.057 (2)	0.050 (2)	0.0006 (19)	0.0076 (19)	−0.0070 (18)
C9	0.0304 (19)	0.041 (2)	0.0421 (19)	0.0044 (16)	−0.0021 (17)	−0.0023 (16)
C10	0.047 (2)	0.044 (2)	0.052 (2)	0.0030 (19)	−0.0013 (19)	0.0040 (18)
C11	0.067 (3)	0.052 (3)	0.079 (3)	−0.009 (2)	−0.005 (3)	−0.010 (2)
C12	0.079 (3)	0.066 (3)	0.066 (3)	0.000 (3)	−0.011 (3)	−0.024 (2)
C13	0.071 (3)	0.074 (3)	0.040 (2)	0.016 (3)	0.000 (2)	−0.010 (2)
C14	0.042 (2)	0.052 (2)	0.048 (2)	0.0086 (19)	0.0069 (19)	0.0016 (18)
C15	0.090 (4)	0.069 (3)	0.062 (3)	−0.014 (3)	0.006 (3)	0.019 (2)
C16	0.061 (3)	0.084 (3)	0.059 (3)	0.002 (3)	0.017 (2)	0.010 (2)

Geometric parameters (Å, º)

Br1—C3	1.899 (4)	C7—H7B	0.9700
O1—C8	1.224 (4)	C9—C10	1.392 (5)
N1—C8	1.353 (5)	C9—C14	1.392 (5)
N1—C9	1.429 (4)	C10—C11	1.391 (5)
N1—H1N1	0.91 (4)	C10—C15	1.504 (5)
C1—C6	1.371 (6)	C11—C12	1.365 (6)
C1—C2	1.376 (6)	C11—H11A	0.9300
C1—H1A	0.9300	C12—C13	1.358 (6)
C2—C3	1.356 (6)	C12—H12A	0.9300
C2—H2A	0.9300	C13—C14	1.400 (5)
C3—C4	1.363 (6)	C13—H13A	0.9300
C4—C5	1.383 (5)	C14—C16	1.500 (5)
C4—H4A	0.9300	C15—H15A	0.9600
C5—C6	1.369 (5)	C15—H15B	0.9600
C5—H5A	0.9300	C15—H15C	0.9600
C6—C7	1.508 (5)	C16—H16A	0.9600
C7—C8	1.510 (5)	C16—H16B	0.9600
C7—H7A	0.9700	C16—H16C	0.9600
C8—N1—C9	122.4 (3)	C10—C9—C14	121.6 (3)
C8—N1—H1N1	118 (2)	C10—C9—N1	119.7 (3)
C9—N1—H1N1	118 (2)	C14—C9—N1	118.7 (3)
C6—C1—C2	121.6 (4)	C11—C10—C9	118.0 (4)
C6—C1—H1A	119.2	C11—C10—C15	119.4 (4)
C2—C1—H1A	119.2	C9—C10—C15	122.6 (4)
C3—C2—C1	119.5 (4)	C12—C11—C10	121.2 (4)
C3—C2—H2A	120.2	C12—C11—H11A	119.4
C1—C2—H2A	120.2	C10—C11—H11A	119.4
C2—C3—C4	120.6 (4)	C13—C12—C11	120.2 (4)
C2—C3—Br1	119.9 (4)	C13—C12—H12A	119.9
C4—C3—Br1	119.5 (3)	C11—C12—H12A	119.9
C3—C4—C5	119.1 (4)	C12—C13—C14	121.6 (4)
C3—C4—H4A	120.5	C12—C13—H13A	119.2
C5—C4—H4A	120.5	C14—C13—H13A	119.2
C6—C5—C4	121.6 (4)	C9—C14—C13	117.4 (4)
C6—C5—H5A	119.2	C9—C14—C16	121.2 (3)
C4—C5—H5A	119.2	C13—C14—C16	121.4 (4)
C5—C6—C1	117.6 (4)	C10—C15—H15A	109.5
C5—C6—C7	121.0 (4)	C10—C15—H15B	109.5
C1—C6—C7	121.3 (4)	H15A—C15—H15B	109.5
C6—C7—C8	110.9 (3)	C10—C15—H15C	109.5
C6—C7—H7A	109.5	H15A—C15—H15C	109.5
C8—C7—H7A	109.5	H15B—C15—H15C	109.5
C6—C7—H7B	109.5	C14—C16—H16A	109.5
C8—C7—H7B	109.5	C14—C16—H16B	109.5
H7A—C7—H7B	108.0	H16A—C16—H16B	109.5
O1—C8—N1	122.4 (3)	C14—C16—H16C	109.5
O1—C8—C7	121.1 (3)	H16A—C16—H16C	109.5

N1—C8—C7	116.5 (3)	H16B—C16—H16C	109.5
C6—C1—C2—C3	−0.1 (7)	C8—N1—C9—C10	67.8 (5)
C1—C2—C3—C4	0.1 (7)	C8—N1—C9—C14	−113.9 (4)
C1—C2—C3—Br1	−179.7 (3)	C14—C9—C10—C11	3.0 (5)
C2—C3—C4—C5	−0.4 (7)	N1—C9—C10—C11	−178.8 (3)
Br1—C3—C4—C5	179.4 (3)	C14—C9—C10—C15	−176.3 (4)
C3—C4—C5—C6	0.8 (7)	N1—C9—C10—C15	2.0 (5)
C4—C5—C6—C1	−0.9 (6)	C9—C10—C11—C12	−1.8 (6)
C4—C5—C6—C7	−179.8 (4)	C15—C10—C11—C12	177.4 (4)
C2—C1—C6—C5	0.5 (6)	C10—C11—C12—C13	0.0 (7)
C2—C1—C6—C7	179.5 (4)	C11—C12—C13—C14	0.9 (7)
C5—C6—C7—C8	104.8 (4)	C10—C9—C14—C13	−2.2 (5)
C1—C6—C7—C8	−74.1 (5)	N1—C9—C14—C13	179.6 (3)
C9—N1—C8—O1	−2.2 (6)	C10—C9—C14—C16	178.6 (4)
C9—N1—C8—C7	178.9 (3)	N1—C9—C14—C16	0.3 (5)
C6—C7—C8—O1	−63.7 (5)	C12—C13—C14—C9	0.2 (6)
C6—C7—C8—N1	115.2 (4)	C12—C13—C14—C16	179.4 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*1···O1^{i}	0.91 (4)	1.95 (4)	2.847 (4)	166 (3)
C7—H7*B*···O1^{i}	0.97	2.38	3.240 (5)	148

Symmetry code: (i) *x*−1, *y*, *z*.