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Methyl *N*-(2-bromo-4-chlorophenyl)carbamate

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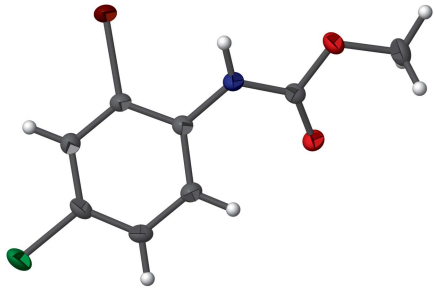
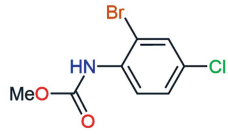
Structural data: full structural data are available from iucrdata.iucr.org

In the title molecule, $C_8H_7BrClNO_2$, the bromochlorophenyl ring is inclined to the methylcarbamate unit by 32.73 (7)°. In the crystal, N—H···O hydrogen bonds form chains of molecules parallel to [100].

3D view



Chemical scheme



Structure description

Carbamate derivatives show a variety of biological activities (Krátký *et al.*, 2014; Smith *et al.*, 2014; Yang *et al.*, 2012). They can be synthesized using a variety of convenient processes (Blaser *et al.*, 2012; Smith *et al.*, 2012; Ibrahim *et al.*, 2011; Porzelle *et al.*, 2009; Lee *et al.*, 2009; Lebel & Leogane, 2006; Caddick *et al.*, 2003). The X-ray crystal structure of the related *tert*-butyl 2-phenylethylcarbamate was published recently (El-Hiti *et al.*, 2016).

In the title molecule (Fig. 1), the dihedral angle between the bromochlorophenyl and methylcarbamate groups is 32.73 (7)°. In the crystal, N—H···O hydrogen bonds, Table 1, form chains parallel to [100], (Fig. 2).

Synthesis and crystallization

The title compound was synthesized from the reaction of 2-bromo-4-chloroaniline and dimethyl dicarbonate in dichloromethane in the presence of triethylamine. Recrystallization of the crude product from diethyl ether solution gave the title compound as colourless crystals, m.p. 88–89°C (lit. 86–89 °C; Moghaddam *et al.*, 2016).

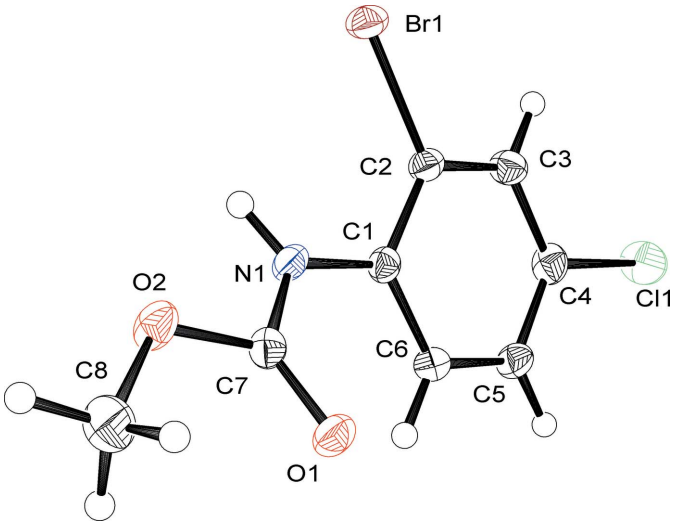


Figure 1
An *ORTEP* representation (50% probability level) of the title molecule.

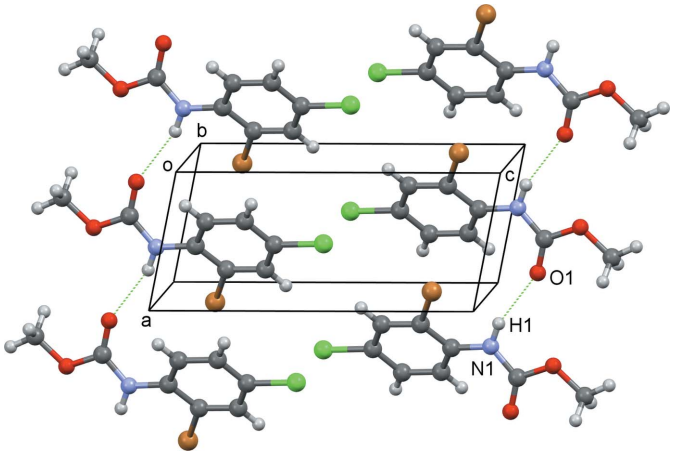


Figure 2
A segment of the crystal structure, viewed along *b*, showing the N—H···O hydrogen bonds as dotted lines.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Funding information

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.88	2.19	2.885 (2)	135

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_8H_7BrClNO_2$
M_r	264.51
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	150
a, b, c (Å)	4.6637 (3), 9.4598 (6), 11.9898 (7)
α, β, γ (°)	111.639 (5), 101.035 (5), 93.712 (5)
V (Å^3)	477.25 (5)
Z	2
Radiation type	Cu $K\alpha$
μ (mm^{-1})	8.19
Crystal size (mm)	0.31 × 0.20 × 0.15
Data collection	
Diffractometer	Agilent SuperNova, Dual, Cu at zero, Atlas
Absorption correction	Gaussian (*CrysAlis PRO*; Agilent, 2014)
T_{min}, T_{max}	0.776, 0.891
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	2938, 1847, 1777
R_{int}	0.019
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.623
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.024, 0.063, 1.08
No. of reflections	1847
No. of parameters	119
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.30, −0.61

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SHELXS2013* (Sheldrick, 2008), *SHELXL2013* (Sheldrick, 2015), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *CHEMDRAW Ultra* (Cambridge Soft, 2001).

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full crystallographic data

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Methyl *N*-(2-bromo-4-chlorophenyl)carbamate

Crystal data

$C_8H_7BrClNO_2$
M_r = 264.51
Triclinic, $P\overline{1}$
a = 4.6637 (3) Å
b = 9.4598 (6) Å
c = 11.9898 (7) Å
α = 111.639 (5)°
β = 101.035 (5)°
γ = 93.712 (5)°
V = 477.25 (5) Å^3
Z = 2
$F(000)$ = 260
D_x = 1.841 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 2127 reflections
θ = 5.1–74.1°
μ = 8.19 mm^{-1}
T = 150 K
Block, colourless
0.31 × 0.20 × 0.15 mm

Data collection

Agilent SuperNova, Dual, Cu at zero, Atlas diffractometer
ω scans
Absorption correction: gaussian (CrysAlis PRO; Agilent, 2014)
T_{min} = 0.776, T_{max} = 0.891
2938 measured reflections
1847 independent reflections
1777 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 74.0°, θ_{min} = 4.1°
h = −5→5
k = −10→11
l = −14→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.063
S = 1.08
1847 reflections
119 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.040P)^2 + 0.157P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.61 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.5832 (4)	0.2508 (2)	0.08977 (18)	0.0178 (4)
C2	0.7774 (4)	0.3658 (2)	0.19208 (19)	0.0189 (4)
C3	0.7777 (5)	0.3806 (2)	0.31131 (19)	0.0226 (4)
H3	0.9115	0.4585	0.3796	0.027*
C4	0.5803 (5)	0.2806 (3)	0.3295 (2)	0.0242 (4)
C5	0.3866 (5)	0.1654 (2)	0.2315 (2)	0.0230 (4)
H5	0.2525	0.0973	0.2455	0.028*
C6	0.3903 (5)	0.1504 (2)	0.1125 (2)	0.0210 (4)
H6	0.2592	0.0704	0.0449	0.025*
C7	0.3560 (5)	0.1832 (2)	−0.12754 (19)	0.0194 (4)
C8	0.2102 (6)	0.1130 (3)	−0.3419 (2)	0.0324 (5)
H8A	0.1401	0.0058	−0.3581	0.049*
H8B	0.2882	0.1174	−0.4110	0.049*
H8C	0.0459	0.1726	−0.3323	0.049*
N1	0.5916 (4)	0.2373 (2)	−0.02987 (16)	0.0204 (3)
H1	0.7618	0.2661	−0.0424	0.024*
O1	0.1036 (3)	0.14673 (18)	−0.12501 (14)	0.0242 (3)
O2	0.4400 (3)	0.17650 (19)	−0.23043 (14)	0.0264 (3)
Cl1	0.57621 (15)	0.30115 (7)	0.47984 (5)	0.03750 (16)
Br1	1.04171 (4)	0.50705 (2)	0.16904 (2)	0.02356 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0170 (9)	0.0181 (9)	0.0196 (10)	0.0047 (7)	0.0063 (7)	0.0075 (7)
C2	0.0177 (9)	0.0181 (9)	0.0223 (10)	0.0019 (7)	0.0058 (8)	0.0091 (8)
C3	0.0241 (10)	0.0215 (9)	0.0200 (10)	−0.0003 (8)	0.0033 (8)	0.0070 (8)
C4	0.0310 (11)	0.0269 (11)	0.0194 (10)	0.0054 (9)	0.0097 (8)	0.0121 (8)
C5	0.0239 (10)	0.0219 (10)	0.0264 (11)	0.0013 (8)	0.0099 (8)	0.0115 (8)
C6	0.0202 (10)	0.0197 (9)	0.0222 (10)	0.0002 (7)	0.0058 (8)	0.0072 (8)
C7	0.0208 (10)	0.0194 (9)	0.0194 (10)	0.0048 (7)	0.0066 (8)	0.0079 (8)
C8	0.0341 (12)	0.0413 (13)	0.0194 (10)	0.0026 (10)	0.0017 (9)	0.0117 (10)
N1	0.0157 (8)	0.0256 (9)	0.0198 (8)	−0.0002 (6)	0.0058 (6)	0.0084 (7)
O1	0.0159 (7)	0.0315 (8)	0.0243 (8)	0.0010 (6)	0.0052 (6)	0.0101 (6)
O2	0.0219 (8)	0.0402 (9)	0.0198 (7)	0.0013 (6)	0.0049 (6)	0.0152 (7)
Cl1	0.0549 (4)	0.0381 (3)	0.0208 (3)	−0.0052 (3)	0.0122 (2)	0.0132 (2)
Br1	0.02532 (14)	0.02146 (14)	0.02454 (14)	−0.00329 (9)	0.00644 (9)	0.01045 (10)

Geometric parameters (Å, º)

C1—C6	1.400 (3)	C5—H5	0.9500
C1—N1	1.401 (3)	C6—H6	0.9500
C1—C2	1.404 (3)	C7—O1	1.214 (3)
C2—C3	1.384 (3)	C7—O2	1.345 (2)
C2—Br1	1.890 (2)	C7—N1	1.354 (3)

C3—C4	1.381 (3)	C8—O2	1.439 (3)
C3—H3	0.9500	C8—H8A	0.9800
C4—C5	1.381 (3)	C8—H8B	0.9800
C4—Cl1	1.744 (2)	C8—H8C	0.9800
C5—C6	1.384 (3)	N1—H1	0.8800
C6—C1—N1	122.34 (18)	C5—C6—H6	119.3
C6—C1—C2	117.59 (19)	C1—C6—H6	119.3
N1—C1—C2	120.06 (18)	O1—C7—O2	123.82 (19)
C3—C2—C1	121.46 (19)	O1—C7—N1	126.17 (19)
C3—C2—Br1	118.43 (15)	O2—C7—N1	110.00 (17)
C1—C2—Br1	120.11 (15)	O2—C8—H8A	109.5
C4—C3—C2	119.0 (2)	O2—C8—H8B	109.5
C4—C3—H3	120.5	H8A—C8—H8B	109.5
C2—C3—H3	120.5	O2—C8—H8C	109.5
C5—C4—C3	121.44 (19)	H8A—C8—H8C	109.5
C5—C4—Cl1	119.54 (17)	H8B—C8—H8C	109.5
C3—C4—Cl1	119.02 (17)	C7—N1—C1	124.53 (17)
C4—C5—C6	119.14 (19)	C7—N1—H1	117.7
C4—C5—H5	120.4	C1—N1—H1	117.7
C6—C5—H5	120.4	C7—O2—C8	115.05 (17)
C5—C6—C1	121.39 (19)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.88	2.19	2.885 (2)	135

Symmetry code: (i) *x*+1, *y*, *z*.