organic compounds

2-(2-Bromophenyl)acetic acid

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In the title molecule, $C_8H_7BrO_2$, the carboxyl group is twisted by 76.2 (3)° from the benzene ring plane. In the crystal, molecules are linked into inversion dimers through pairs of O—H⋯O hydrogen bonds. The dimers are further linked into layers parallel to the *bc* plane by weak C—H⋯O hydrogen bonds.

Related literature

For applications of the title compound, see: Deshpande *et al.* (2008); Rodriguesa *et al.* (2002); Pratt *et al.* (2000). For related structures, see: Hodgson & Asplund (1991); Harris *et al.* (1994); Hartung *et al.* (2004); Yuan *et al.* (2008); Jasinski *et al.*(2010); Li *et al.* (2010).
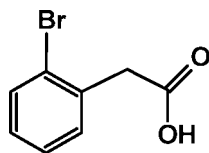
Experimental

Crystal data

$C_8H_7BrO_2$	V = 829.09 (7) Å^3
M_r = 215.05	Z = 4
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
a = 8.9732 (5) Å	μ = 4.90 mm^{-1}
b = 5.9114 (3) Å	T = 293 K
c = 15.8489 (7) Å	0.3 × 0.2 × 0.2 mm
β = 99.529 (5)°	

Data collection

Oxford Diffraction Xcalibur Sapphire3 diffractometer	8471 measured reflections
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)	1628 independent reflections
	1248 reflections with $I > 2\sigma(I)$
	R_{int} = 0.043
T_{min} = 0.370, T_{max} = 1.000	

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.096	
S = 1.07	
1628 reflections	$\Delta\rho_{max}$ = 0.55 e Å^{-3}
105 parameters	$\Delta\rho_{min}$ = −0.69 e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O8—H8⋯O9^i	0.87 (7)	1.76 (7)	2.630 (4)	175 (3)
C6—H6⋯O9^{ii}	0.93	2.57	3.453 (5)	158

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5295).

References

Deshpande, P. P., Nanduri, V. B., Pullockaran, A., Christie, H., Mueller, R. H. & Patel, R. N. (2008). *J. Ind. Microbiol. Biotechnol.* **35**, 901–906.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Harris, K. D. M., Tremayne, M., Lightfoot, P. & Bruce, P. G. (1994). *J. Am. Chem. Soc.* **116**, 3543–3547.
Hartung, J., Špehar, K., Svoboda, I. & Fuess, H. (2004). *Acta Cryst.* E**60**, o95–o96.
Hodgson, D. J. & Asplund, R. O. (1991). *Acta Cryst.* C**47**, 1986–1987.
Jasinski, J. P., Butcher, R. J., Swamy, M. T., Narayana, B., Sarojini, B. K. & Yathirajan, H. S. (2010). *J. Chem. Crystallogr.* **40**, 25–28.
Li, J.-S., He, Q.-X. & Li, P.-Y. (2010). *Acta Cryst.* E**66**, o110.
Oxford Diffraction (2010). *CrysAlis PRO*. Oxford Diffraction Ltd, Yarnton, Oxfordshire, England.
Pratt, J., Jimonet, P., Bohme, G. A., Boireau, A., Damour, D., Debono, M. W., Borella, A. G., Randle, J. C. R., Ribeill, Y., Stutzmann, J.-M., Vuilhorgne, M. & Mignani, S. (2000). *Bioorg. Med. Chem. Lett.* **10**, 2749–2754.
Rodriguesa, D. C., de Meijere, A. & Marsaioli, A. J. (2002). *J. Braz. Chem. Soc.* **13**, 664–668.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Yuan, Y.-Q., Guo, S.-R. & Wang, L.-J. (2008). *Acta Cryst.* E**64**, o2435.

supplementary materials

2-(2-Bromophenyl)acetic acid

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Comment

The title compound, (I), has many applications in various syntheses, for example, in the synthesis of heterocyclic compounds (Deshpande *et al.*, 2008) and in the synthesis of AMPA antagonists - substituted quinoxalinediones, quinolones, isatinoximes and benzodiazepine derivatives (Pratt *et al.*, 2000). It can also be used in a gas chromatography as a phase transfer catalyst (Rodriguesa *et al.*, 2002). Herein we report its crystal structure.

In (I) (Fig. 1), all bond lengths and angles are normal and correspond to those observed in related structures (Hodgson & Asplund,1991; Harris *et al.*, 1994; Hartung *et al.*, 2004; Yuan *et al.*, 2008; Jasinski *et al.*, 2010; Li *et al.*, 2010). The carboxyl group is twisted at 76.2 (3)° from the benzene ring plane. Intermolecular O—H···O hydrogen bonds (Table 1) link the molecules into centrosymmetric dimers. Weak intermolecular C—H···O interactions (Table 1) link further these dimers into layers parallel to *bc* plane.

Experimental

The title compound was purchased from the Spectrochem Ltd., Mumbai. Single-crystals were grown from acetone and toluene(1:1) mixture by slow evaporation method.

Refinement

Atom H8 was found in a difference map and isotropically refined. C-bound H atoms were positioned geometrically (C—H 0.93–0.97 Å), and were treated as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Computing details

Data collection: *CrysAlis PRO* CCD (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO* CCD (Oxford Diffraction, 2010); data reduction: *CrysAlis PRO* RED (Oxford Diffraction, 2010); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2009).
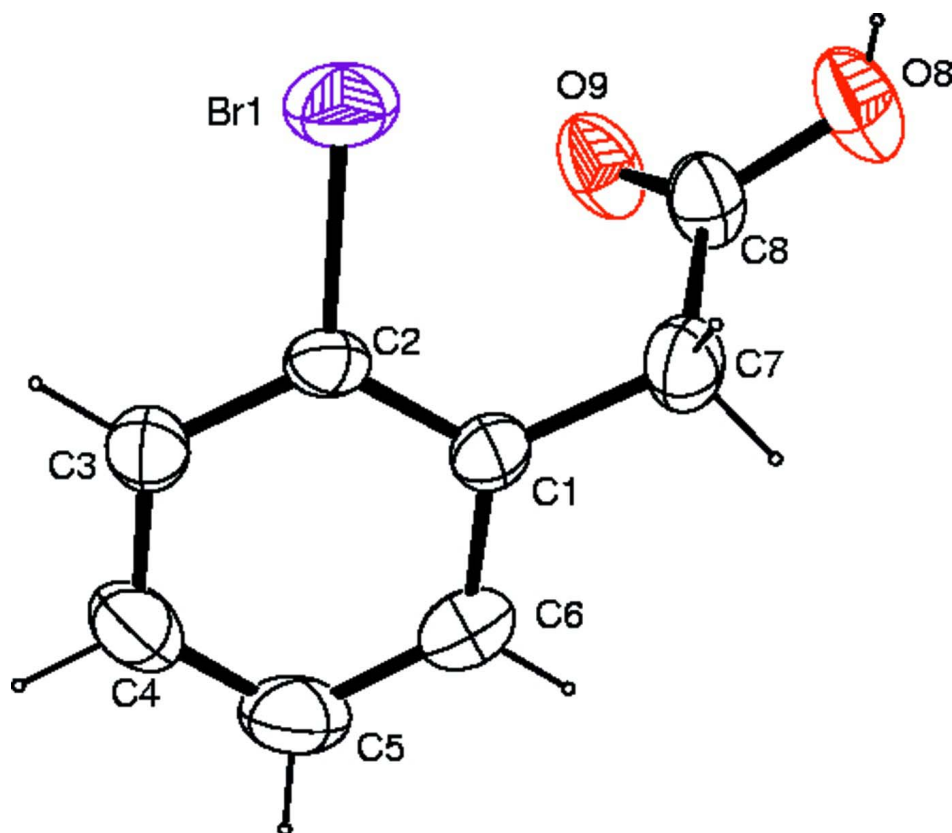
Figure 1

ORTEP view of the molecule with the atom-labeling scheme. The Displacement ellipsoids are drawn at the 40%
probability level. H atoms are shown as small spheres of arbitrary radii.

2-(2-Bromophenyl)acetic acid

Crystal data

$C_8H_7BrO_2$	$F(000) = 424$
$M_r = 215.05$	$D_x = 1.723$ Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point = 381–377 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 8.9732\ (5)$ Å	Cell parameters from 3025 reflections
$b = 5.9114\ (3)$ Å	$\theta = 3.4–29.1°$
$c = 15.8489\ (7)$ Å	$\mu = 4.90$ mm^{-1}
$\beta = 99.529\ (5)°$	$T = 293$ K
$V = 829.09\ (7)$ Å^3	Prism, white
$Z = 4$	$0.3 \times 0.2 \times 0.2$ mm

Data collection

Oxford Diffraction Xcalibur Sapphire3 diffractometer	Absorption correction: multi-scan (*CrysAlis PRO* RED; Oxford Diffraction, 2010)
Radiation source: fine-focus sealed tube	$T_{min} = 0.370$, $T_{max} = 1.000$
Graphite monochromator	8471 measured reflections
Detector resolution: 16.1049 pixels mm^{-1}	1628 independent reflections
ω scan	1248 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.043$

$\theta_{max} = 26.0°$, $\theta_{min} = 3.7°$

$h = -11 \rightarrow 11$

$k = -7 \rightarrow 7$

$l = -19 \rightarrow 19$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.042$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.096$	
$S = 1.07$	$w = 1/[\sigma^2(F_o^2) + (0.0324P)^2 + 1.055P]$
1628 reflections	where $P = (F_o^2 + 2F_c^2)/3$
105 parameters	$(\Delta/\sigma)_{max} = 0.001$
0 restraints	$\Delta\rho_{max} = 0.55$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{min} = -0.69$ e Å^{-3}
	Extinction correction: *SHELXL97* (Sheldrick, 2008), Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.071 (3)

Special details

Experimental. *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.34.40 (release 27–08-2010 CrysAlis171. NET) (compiled Aug 27 2010,11:50:40) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Br1	0.42140 (6)	0.23223 (8)	0.92648 (3)	0.0681 (3)
C1	0.2498 (4)	0.4863 (6)	0.7908 (2)	0.0427 (9)
C2	0.3352 (4)	0.2936 (6)	0.8109 (2)	0.0395 (8)
C3	0.3640 (4)	0.1404 (7)	0.7497 (3)	0.0498 (10)
H3	0.4208	0.0110	0.7654	0.060*
C4	0.3078 (6)	0.1819 (8)	0.6660 (3)	0.0627 (12)
H4	0.3275	0.0813	0.6241	0.075*
C5	0.2223 (6)	0.3715 (9)	0.6430 (3)	0.0689 (13)
H5	0.1839	0.3990	0.5857	0.083*
C6	0.1935 (5)	0.5208 (7)	0.7051 (3)	0.0599 (12)
H6	0.1347	0.6480	0.6890	0.072*
C7	0.2239 (5)	0.6574 (7)	0.8568 (3)	0.0570 (11)
H7A	0.3211	0.7023	0.8887	0.068*
H7B	0.1779	0.7906	0.8276	0.068*
O8	0.1337 (4)	0.7126 (6)	0.9850 (2)	0.0710 (10)
C8	0.1266 (4)	0.5795 (7)	0.9188 (3)	0.0520 (10)
O9	0.0457 (3)	0.4130 (5)	0.9081 (2)	0.0650 (9)
H8	0.072 (7)	0.678 (10)	1.020 (5)	0.11 (2)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0835 (4)	0.0712 (4)	0.0440 (3)	−0.0020 (2)	−0.0059 (2)	0.0091 (2)
C1	0.049 (2)	0.0354 (19)	0.047 (2)	−0.0069 (16)	0.0158 (18)	0.0034 (16)
C2	0.045 (2)	0.041 (2)	0.0330 (19)	−0.0082 (16)	0.0085 (16)	0.0050 (15)
C3	0.058 (2)	0.043 (2)	0.052 (3)	−0.0005 (18)	0.021 (2)	0.0007 (19)
C4	0.085 (3)	0.059 (3)	0.049 (3)	−0.015 (2)	0.026 (2)	−0.014 (2)
C5	0.088 (3)	0.079 (3)	0.038 (3)	−0.007 (3)	0.004 (2)	0.007 (2)
C6	0.070 (3)	0.053 (2)	0.055 (3)	0.007 (2)	0.006 (2)	0.016 (2)
C7	0.070 (3)	0.040 (2)	0.067 (3)	−0.005 (2)	0.029 (2)	−0.004 (2)
O8	0.080 (2)	0.069 (2)	0.071 (2)	−0.0264 (17)	0.0341 (19)	−0.0325 (17)
C8	0.053 (2)	0.048 (2)	0.058 (3)	−0.0015 (19)	0.019 (2)	−0.010 (2)
O9	0.0697 (19)	0.0631 (19)	0.069 (2)	−0.0253 (16)	0.0323 (16)	−0.0258 (16)

Geometric parameters (Å, º)

Br1—C2	1.901 (4)	C5—C6	1.378 (6)
C1—C2	1.380 (5)	C5—H5	0.9300
C1—C6	1.383 (5)	C6—H6	0.9300
C1—C7	1.502 (5)	C7—C8	1.491 (6)
C2—C3	1.383 (5)	C7—H7A	0.9700
C3—C4	1.361 (6)	C7—H7B	0.9700
C3—H3	0.9300	O8—C8	1.304 (5)
C4—C5	1.373 (7)	O8—H8	0.87 (7)
C4—H4	0.9300	C8—O9	1.218 (5)
C2—C1—C6	116.6 (4)	C6—C5—H5	120.2
C2—C1—C7	122.6 (4)	C5—C6—C1	121.7 (4)
C6—C1—C7	120.8 (4)	C5—C6—H6	119.1
C1—C2—C3	122.6 (4)	C1—C6—H6	119.1
C1—C2—Br1	120.1 (3)	C8—C7—C1	115.2 (3)
C3—C2—Br1	117.2 (3)	C8—C7—H7A	108.5
C4—C3—C2	118.9 (4)	C1—C7—H7A	108.5
C4—C3—H3	120.5	C8—C7—H7B	108.5
C2—C3—H3	120.5	C1—C7—H7B	108.5
C3—C4—C5	120.4 (4)	H7A—C7—H7B	107.5
C3—C4—H4	119.8	C8—O8—H8	115 (4)
C5—C4—H4	119.8	O9—C8—O8	123.3 (4)
C4—C5—C6	119.7 (4)	O9—C8—C7	123.9 (4)
C4—C5—H5	120.2	O8—C8—C7	112.8 (4)
C6—C1—C2—C3	−0.2 (5)	C4—C5—C6—C1	0.6 (7)
C7—C1—C2—C3	−177.4 (3)	C2—C1—C6—C5	−0.6 (6)
C6—C1—C2—Br1	178.8 (3)	C7—C1—C6—C5	176.8 (4)
C7—C1—C2—Br1	1.5 (5)	C2—C1—C7—C8	−68.9 (5)
C1—C2—C3—C4	0.9 (6)	C6—C1—C7—C8	114.0 (4)
Br1—C2—C3—C4	−178.1 (3)	C1—C7—C8—O9	−15.8 (6)
C2—C3—C4—C5	−0.9 (6)	C1—C7—C8—O8	166.1 (4)
C3—C4—C5—C6	0.2 (7)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O8—H8···O9[i]	0.87 (7)	1.76 (7)	2.630 (4)	175 (3)
C6—H6···O9[ii]	0.93	2.57	3.453 (5)	158

Symmetry codes: (i) −*x*, −*y*+1, −*z*+2; (ii) −*x*, *y*+1/2, −*z*+3/2.