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# Crystal structure of 1-(4-bromophenyl)but-3-yn-1-one

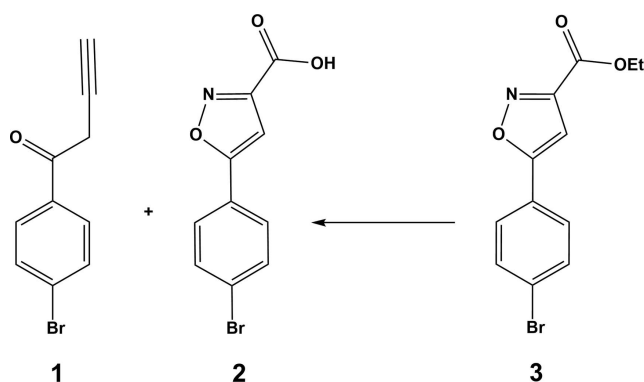
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The title compound, 1-(4-bromophenyl)but-3-yn-1-one, C<sub>10</sub>H<sub>7</sub>BrO, crystallizes in the monoclinic space group *P*2<sub>1</sub>/*n* with one molecule in the asymmetric unit. The structure displays a planar geometry. The crystal structure is consolidated by C—H···O hydrogen bonding and a short C=O···C≡C (acetylene) contacts. Hirshfeld surface analysis indicates that H···H, C···H/H···C and H···Br/Br···H interactions play a more important role in consolidating the crystal structure compared to H···O/O···H and C···C contacts.

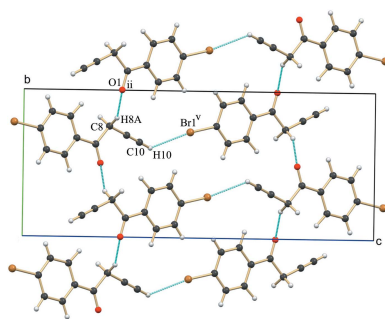
## 1. Chemical context

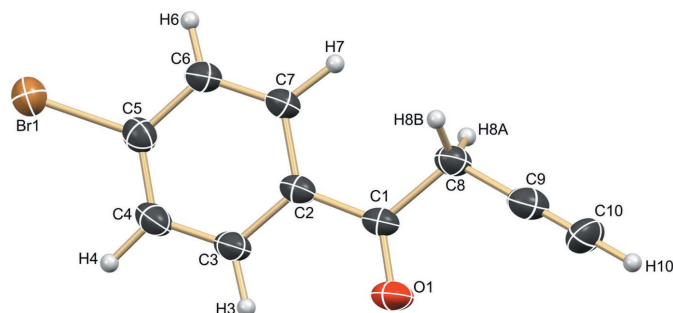
The title compound 1-(4-bromophenyl)but-3-yn-1-one (**1**) was obtained as a side product during the synthesis of 5-(4-bromophenyl)isoxazole-3-carboxylic acid (**2**) from the NaOH-mediated hydrolysis of ethyl 5-(4-bromophenyl)isoxazole-3-carboxylate (**3**). These arylisoxazole carboxylic acids have been identified as potential isosteres of aryl diketo acid in the design of novel HIV-1 integrase inhibitors (Zeng *et al.*, 2008). The presence of three distinct functional groups, viz. alkyne, bromo, and carbonyl, offers an intriguing opportunity to explore how intermolecular interactions contribute to the cohesion of the crystal structure.



## 2. Structural commentary

The title compound crystallizes in the monoclinic *P*2<sub>1</sub>/*n* centrosymmetric space group with one molecule of **1** in the asymmetric unit (Fig. 1). The structure displays a planar geometry [torsion angle C5—C1—C8—C9 = 175.4 (3)°, only the C5 atom of phenyl ring is considered and not the full fragment]. The phenyl ring makes a dihedral angle of 5.4 (2)°



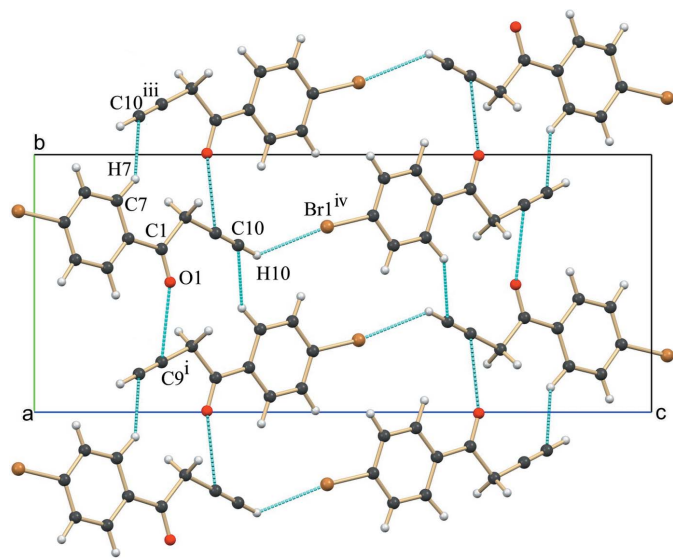


**Figure 1**  
The asymmetric unit of **1** with the atom labelling. Displacement ellipsoids represent 30% probability levels.

with the least-squares plane through the O1/C1/C8–C10 fragment.

### 3. Supramolecular features

In the crystal, the closely associated molecules of **1** generate two different helical assemblies across the crystallographic  $2_1$ -screw axis ( $b$ -axis). The helical assembly generated using C1=O1...C9<sup>i</sup>≡C10<sup>i</sup> (acetylene, C=O... $\pi$ ) contacts [symmetry code: (i)  $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{3}{2}$ ] (Li *et al.*, 2019; Mooibroek, *et al.*, 2008) has a sheet structure (Fig. 2, Table 1), while the helical assembly created using C–H...O (C8–H8A...O1<sup>ii</sup>) contacts [symmetry code: (ii)  $-x + \frac{3}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$ ] (Desiraju & Steiner, 2001) has a proper helical structure (Fig. 3, Table 1). The helical assembly created using the short C1=O1...C9≡C10 contacts is further supported by marginal C–H... $\pi$  [symmetry code: (iii)  $-x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$ ] contacts



**Figure 2**  
A view of the molecular packing of **1** along the helical  $b$ -axis showing the association of closely linked molecules by C=O...C≡C (acetylene, C=O... $\pi$ ) and marginal C–H... $\pi$  ( $\pi$ -cloud of acetylene molecules) contacts. Neighbouring helices along the longer  $c$  axis are linked by C–H...Br contacts. Symmetry codes as in Table 1.

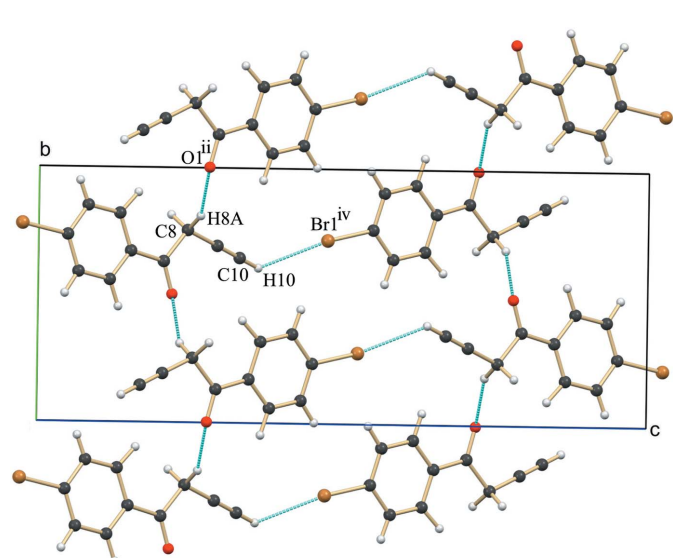
**Table 1**  
Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C1–O1...C9 <sup>i</sup>		3.13 (1)		154 (1)
C8–H8A...O1 <sup>ii</sup>	1.02 (4)	2.31 (4)	3.259 (5)	156 (3)
C7–H7...C10 <sup>iii</sup>	1.06 (3)	2.71 (4)	3.626 (5)	144 (3)
C10–H10...Br1 <sup>iv</sup>	0.93	2.68	3.305 (5)	126

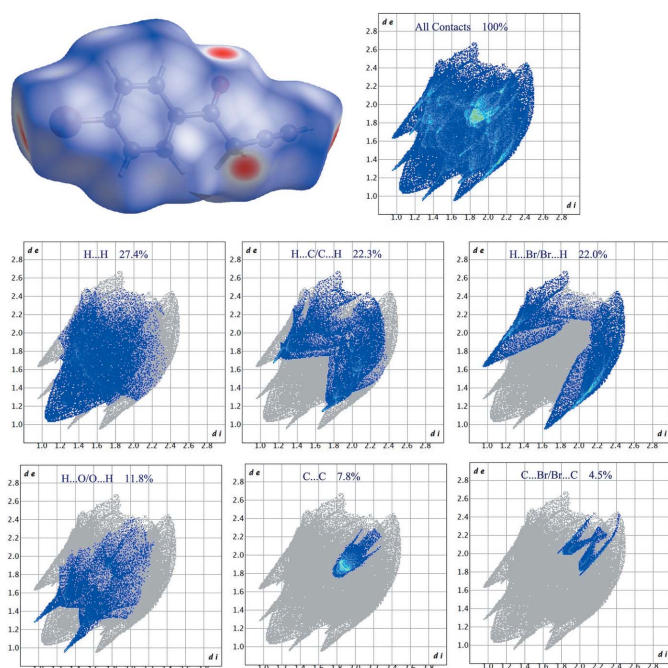
Symmetry codes: (i)  $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{3}{2}$ ; (ii)  $-x + \frac{3}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$ ; (iii)  $-x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$ ; (iv)  $x - \frac{3}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$ .

involving the phenyl ring (C7–H7) and the  $\pi$  cloud of the acetylene moiety. Both helices are intertwined and form a two-dimensional sheet structure roughly along the  $a$ -axis direction. Along the longer  $c$ -axis, molecules are loosely connected using weak C–H...Br (C10–H10...Br1<sup>iv</sup>) contacts [symmetry code: (iv)  $x - \frac{3}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$ ] (van den Berg & Seddon, 2003), generating the extended assembly (Figs. 2 and 3, Table 1).

In order to visualize and quantify intermolecular interactions in **1**, a Hirshfeld surface analysis (Spackman & Jayatilaka, 2009) was performed using *Crystal Explorer 21.5* (Spackman *et al.*, 2021), and the associated two-dimensional fingerprint plots (McKinnon *et al.*, 2007) were generated. The Hirshfeld surfaces for the molecule in **1** are shown in Fig. 4 in which the two-dimensional fingerprint plots of the most dominant contacts are also presented. H...H (27.4%), H...C/C...H (22.3%) and H...Br/Br...H (22.0%) contacts are responsible for the largest contributions to the Hirshfeld surface. Besides these contacts, H...O/O...H (11.8%) and C...C (7.8%) interactions contribute significantly to the total Hirshfeld surface. The contributions of further contacts are only minor and amount to C...Br/Br...C (4.5%) and C...O/O...C (3.6%).



**Figure 3**  
A view of the molecular packing of **1** along the helical  $b$ -axis showing the association of closely linked molecules by C–H...O contacts. Neighbouring helices along the longer  $c$  axis are linked by C–H...Br contacts. Symmetry codes as in Table 1.


**Figure 4**

Three-dimensional Hirshfeld surfaces of compound **1** plotted over  $d_{\text{norm}}$  in the range  $-0.2760$  to  $0.9829$  a.u., and Hirshfeld fingerprint plots for all contacts and those decomposed into H $\cdots$ H, H $\cdots$ C/C $\cdots$ H, H $\cdots$ Br/Br $\cdots$ H, H $\cdots$ O/O $\cdots$ H, C $\cdots$ C and C $\cdots$ Br/Br $\cdots$ C contacts.  $d_i$  and  $d_e$  denote the closest internal and external distances (in Å) from a point on the surface.

#### 4. Database survey

A survey of the Cambridge Structural Database (version 5.43, update 4, November 2022; Groom *et al.*, 2016) revealed that no crystal structure of compound **1** has been reported. Moreover, no crystal structure similar to that of compound **1** has been reported. However, focusing only on the 1-phenylbut-3-yn-1-one unit yielded 24 hits with not much similarity with the title compound. The most similar structure with respect to compound **1** is 3-phenyl-2-(phenylethynyl)-1*H*-inden-1-one (FEGDOO; Kumar *et al.*, 2022).

#### 5. Synthesis and crystallization

A solution of methyl ester **3** (100 mg, 0.35 mmol) and 1*N* NaOH (3 mL) and methanol (3 mL) was heated to reflux for 3 h. After completion of the reaction as indicated by TLC, the reaction mixture was cooled to room temperature and neutralized with a solution of 3*N* HCl and then extracted with dichloromethane ( $3 \times 10$  mL). The combined organic layer was washed with brine and concentrated. The resulting crude was purified by column chromatography (30% ethyl acetate in petroleum ether) to afford the acid **2** (70 mg, 74% yield) and an alkyne, the title compound **1** (8 mg, 11% yield) as colourless solids. Colourless crystals of the title compound **1** suitable for single crystal X-ray diffraction analysis were obtained by slow evaporation of an ethanol solution.

**Table 2**

Experimental details.

Crystal data	
Chemical formula	C <sub>10</sub> H <sub>7</sub> BrO
$M_r$	223.07
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	297
$a, b, c$ (Å)	4.471 (2), 9.032 (4), 21.652 (11)
$\beta$ (°)	92.252 (8)
$V$ (Å <sup>3</sup> )	873.7 (7)
$Z$	4
Radiation type	Mo $K\alpha$
$\mu$ (mm <sup>-1</sup> )	4.65
Crystal size (mm)	0.35 $\times$ 0.28 $\times$ 0.13
Data collection	
Diffractometer	Bruker SMART APEX
Absorption correction	Multi-scan (SADABS; Bruker 2016)
$T_{\text{min}}, T_{\text{max}}$	0.293, 0.583
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	4994, 1965, 1397
$R_{\text{int}}$	0.043
$(\sin \theta/\lambda)_{\text{max}}$ (Å <sup>-1</sup> )	0.664
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.048, 0.140, 1.02
No. of reflections	1965
No. of parameters	133
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å <sup>-3</sup> )	0.40, $-0.62$

Computer programs: APEX3 and SAINT-Plus (Bruker, 2016), SHELXS97 (Sheldrick, 2008), SHELXL20147 (Sheldrick, 2015), ORTEP-3 for Windows (Farrugia, 2012), Mercury (Macrae *et al.*, 2020), SHELXTL (Sheldrick, 2008), PLATON (Spek, 2020) and publCIF (Westrip, 2010).

#### 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms (except the acetylene H atom) were located in difference-Fourier map and refined isotropically. The acetylene ( $-\text{C}\equiv\text{C}-\text{H}$ ) H atom was placed in a geometrically idealized position using HFIX 163. It was constrained to ride on its parent atom, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for acetylene. The long C8–H8A distance [1.02 (4) Å] could be the result of its involvement in the directional C–H $\cdots$ O hydrogen-bond formation with O1.

#### Acknowledgements

SKS thanks the DST-INSPIRE program for a research fellowship.

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## supporting information

*Acta Cryst.* (2023). E79, 633-636 [https://doi.org/10.1107/S205698902300508X]

## Crystal structure of 1-(4-bromophenyl)but-3-yn-1-one

Shaziyarveen K. Siddiqui, C. V. Ramana and Rajesh G. Gonnade

## Computing details

Data collection: *APEX3* (Bruker, 2016); cell refinement: *SAINT-Plus* (Bruker, 2016); data reduction: *SAINT-Plus* (Bruker, 2016); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014/7* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2020); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008), *PLATON* (Spek, 2020) and *publCIF* (Westrip, 2010).

## 1-(4-Bromophenyl)but-3-yn-1-one

## Crystal data

$C_{10}H_7BrO$

$M_r = 223.07$

Monoclinic,  $P2_1/n$

$a = 4.471$  (2) Å

$b = 9.032$  (4) Å

$c = 21.652$  (11) Å

$\beta = 92.252$  (8)°

$V = 873.7$  (7) Å<sup>3</sup>

$Z = 4$

$F(000) = 440$

$D_x = 1.696$  Mg m<sup>-3</sup>

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

Cell parameters from 1876 reflections

$\theta = 2.4$ – $24.9$ °

$\mu = 4.65$  mm<sup>-1</sup>

$T = 297$  K

Block, colourless

$0.35 \times 0.28 \times 0.13$  mm

## Data collection

Bruker SMART APEX  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Phi and  $\omega$  Scan scans

Absorption correction: multi-scan  
(SADABS; Bruker 2016)

$T_{\min} = 0.293$ ,  $T_{\max} = 0.583$

4994 measured reflections

1965 independent reflections

1397 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.043$

$\theta_{\max} = 28.2$ °,  $\theta_{\min} = 2.4$ °

$h = -4 \rightarrow 5$

$k = -11 \rightarrow 11$

$l = -27 \rightarrow 27$

## Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.048$

$wR(F^2) = 0.140$

$S = 1.02$

1965 reflections

133 parameters

0 restraints

Primary atom site location: structure-invariant  
direct methods

Hydrogen site location: mixed

H atoms treated by a mixture of independent  
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0812P)^2 + 0.1069P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.002$

$\Delta\rho_{\max} = 0.40$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.62$  e Å<sup>-3</sup>

*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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.5990 (7)	0.3666 (3)	0.79382 (16)	0.0508 (8)
Br1	1.37959 (10)	0.22006 (5)	1.02549 (2)	0.0743 (2)
C2	0.7972 (7)	0.3261 (3)	0.84766 (16)	0.0488 (7)
C3	0.9384 (9)	0.4391 (4)	0.88181 (17)	0.0581 (9)
H3	0.887 (9)	0.545 (5)	0.8679 (19)	0.080 (12)*
C4	1.1186 (9)	0.4079 (4)	0.93323 (18)	0.0615 (9)
H4	1.217 (9)	0.494 (5)	0.9555 (19)	0.077 (11)*
C5	1.1578 (9)	0.2628 (4)	0.95122 (18)	0.0556 (8)
C6	1.0233 (9)	0.1475 (4)	0.91808 (18)	0.0609 (9)
H6	1.065 (9)	0.051 (5)	0.9319 (19)	0.070 (11)*
C7	0.8439 (9)	0.1783 (4)	0.86619 (17)	0.0560 (8)
H7	0.752 (8)	0.096 (4)	0.8364 (15)	0.054 (9)*
C8	0.4544 (9)	0.2439 (4)	0.7551 (2)	0.0555 (9)
H8B	0.342 (9)	0.184 (4)	0.7824 (18)	0.056 (10)*
C9	0.2564 (10)	0.3048 (4)	0.7064 (2)	0.0666 (11)
H8A	0.617 (10)	0.187 (5)	0.734 (2)	0.068 (12)*
C10	0.1011 (10)	0.3516 (5)	0.6698 (2)	0.0783 (12)
H10	−0.0283	0.3905	0.6393	0.094*
O1	0.5514 (7)	0.4954 (2)	0.77985 (13)	0.0718 (8)

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0553 (18)	0.0353 (15)	0.0622 (19)	−0.0025 (13)	0.0097 (15)	−0.0018 (14)
Br1	0.0827 (4)	0.0702 (3)	0.0688 (3)	−0.00322 (18)	−0.0116 (2)	−0.00504 (18)
C2	0.0542 (18)	0.0368 (14)	0.0563 (18)	−0.0031 (13)	0.0125 (15)	−0.0051 (14)
C3	0.076 (2)	0.0382 (16)	0.061 (2)	−0.0070 (15)	0.0057 (18)	−0.0033 (15)
C4	0.074 (2)	0.0484 (19)	0.062 (2)	−0.0152 (17)	0.0072 (18)	−0.0110 (17)
C5	0.060 (2)	0.0547 (19)	0.0524 (19)	−0.0042 (15)	0.0068 (15)	−0.0065 (16)
C6	0.077 (2)	0.0415 (18)	0.064 (2)	−0.0030 (17)	0.0016 (18)	−0.0003 (16)
C7	0.069 (2)	0.0386 (15)	0.060 (2)	−0.0030 (15)	0.0009 (17)	−0.0053 (15)
C8	0.057 (2)	0.0396 (15)	0.069 (2)	0.0016 (15)	−0.0034 (19)	−0.0029 (16)
C9	0.067 (2)	0.0464 (18)	0.087 (3)	−0.0048 (17)	0.002 (2)	−0.0019 (19)
C10	0.084 (3)	0.060 (2)	0.088 (3)	0.005 (2)	−0.032 (2)	0.017 (2)
O1	0.0875 (18)	0.0377 (12)	0.0895 (19)	0.0002 (12)	−0.0066 (16)	0.0024 (13)



## Geometric parameters (Å, °)

C1—O1	1.218 (4)	C5—C6	1.388 (5)
C1—C2	1.482 (5)	C6—C7	1.383 (5)
C1—C8	1.518 (5)	C6—H6	0.93 (4)
Br1—C5	1.895 (4)	C7—H7	1.06 (3)
C2—C3	1.397 (5)	C8—C9	1.458 (7)
C2—C7	1.407 (5)	C8—H8B	0.96 (4)
C3—C4	1.378 (6)	C8—H8A	1.02 (4)
C3—H3	1.03 (5)	C9—C10	1.117 (6)
C4—C5	1.377 (5)	C10—H10	0.9300
C4—H4	1.01 (5)		
O1—C1—C2	121.6 (3)	C7—C6—C5	119.7 (3)
O1—C1—C8	119.6 (3)	C7—C6—H6	123 (3)
C2—C1—C8	118.8 (3)	C5—C6—H6	117 (3)
C3—C2—C7	118.9 (3)	C6—C7—C2	119.8 (3)
C3—C2—C1	118.7 (3)	C6—C7—H7	123.5 (18)
C7—C2—C1	122.4 (3)	C2—C7—H7	116.4 (18)
C4—C3—C2	121.1 (3)	C9—C8—C1	110.9 (3)
C4—C3—H3	123 (2)	C9—C8—H8B	110 (2)
C2—C3—H3	116 (2)	C1—C8—H8B	107 (2)
C5—C4—C3	119.2 (3)	C9—C8—H8A	107 (2)
C5—C4—H4	123 (2)	C1—C8—H8A	109 (2)
C3—C4—H4	117 (3)	H8B—C8—H8A	113 (3)
C4—C5—C6	121.3 (4)	C10—C9—C8	178.8 (6)
C4—C5—Br1	119.4 (3)	C9—C10—H10	180.0
C6—C5—Br1	119.2 (3)		
O1—C1—C2—C3	-1.9 (5)	C3—C4—C5—Br1	-175.1 (3)
C8—C1—C2—C3	177.7 (3)	C4—C5—C6—C7	-0.6 (6)
O1—C1—C2—C7	177.0 (3)	Br1—C5—C6—C7	175.5 (3)
C8—C1—C2—C7	-3.4 (5)	C5—C6—C7—C2	-0.5 (6)
C7—C2—C3—C4	-0.7 (5)	C3—C2—C7—C6	1.1 (6)
C1—C2—C3—C4	178.3 (3)	C1—C2—C7—C6	-177.8 (3)
C2—C3—C4—C5	-0.4 (6)	O1—C1—C8—C9	-3.3 (6)
C3—C4—C5—C6	1.0 (6)	C2—C1—C8—C9	177.1 (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>
C1—O1...C9 <sup>i</sup>		3.13 (1)		154 (1)
C8—H8A...O1 <sup>ii</sup>	1.02 (4)	2.31 (4)	3.259 (5)	156 (3)
C7—H7...C10 <sup>iii</sup>	1.06 (3)	2.71 (4)	3.626 (5)	144 (3)
C10—H10...Br1 <sup>iv</sup>	0.93	2.68	3.305 (5)	126

Symmetry codes: (i)  $-x+1/2, y+1/2, -z+3/2$ ; (ii)  $-x+3/2, y-1/2, -z+3/2$ ; (iii)  $-x+1/2, y-1/2, -z+3/2$ ; (iv)  $x-3/2, -y+1/2, z-1/2$ .