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(2E)-1-(1,3-Benzodioxol-5-yl)-3-(2-bromophenyl)prop-2-en-1-one

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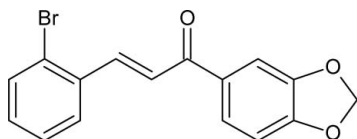
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 Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.034; wR factor = 0.086; data-to-parameter ratio = 14.7.

The molecule of the title compound, $\text{C}_{16}\text{H}_{11}\text{BrO}_3$, is essentially planar with a maximum deviation of 0.178 (4) Å and the configuration of the keto group with respect to the olefinic double bond is typically *s-cis*. In the crystal structure, intermolecular $\text{Br}\cdots\text{O}$ interactions [3.187 (3) Å] give rise to chains parallel to the *b* axis. Adjacent chains are further linked along the *a* axis by $\text{C}-\text{H}\cdots\pi$ interactions. The crystal studied was a racemic twin with a 0.595 (13):0.405 (13) ratio.

Related literature

For chalcones, see: Di Carlo *et al.* (1999); Sarojini *et al.* (2006); Yarishkin *et al.* (2008). For halogen-bonding interactions, see: Thallapally *et al.* (2002); Metrangolo *et al.* (2005); Riley *et al.* (2009). For related structures, see: Harrison *et al.* (2006); Rathore *et al.* (2006); Li *et al.* (2008); Jasinski *et al.* (2010). For racemic twinning, see: Flack (1983); Flack & Bernardinelli (2000); Gómez *et al.* (2010).



Experimental

Crystal data

 $\text{C}_{16}\text{H}_{11}\text{BrO}_3$
 $M_r = 331.16$
 Orthorhombic, $P2_12_12_1$
 $a = 5.0434$ (2) Å

 $b = 12.9354$ (4) Å
 $c = 20.8916$ (7) Å
 $V = 1362.93$ (8) Å³
 $Z = 4$

 Mo $K\alpha$ radiation
 $\mu = 3.02$ mm⁻¹
 $T = 296$ K
 $0.53 \times 0.19 \times 0.16$ mm

Data collection

 Bruker SMART APEXII CCD
 area-detector diffractometer
 Absorption correction: multi-scan
 (SADABS; Bruker, 2004)
 $T_{\min} = 0.576$, $T_{\max} = 0.653$

 17031 measured reflections
 2674 independent reflections
 2437 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.034$
 $wR(F^2) = 0.086$
 $S = 1.06$
 2674 reflections
 182 parameters
 H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.64$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.52$ e Å⁻³
 Absolute structure: Flack (1983),
 1086 Bijvoet pairs
 Flack parameter: 0.595 (13)

Table 1

Hydrogen-bond geometry (Å, °).

Cg3 is the centroid of the C10–C15 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C16—H16B ⁱ ⋯Cg3 ⁱ	0.97	2.76	3.563 (4)	141

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

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT-Plus (Bruker, 2004); data reduction: SAINT-Plus; 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: SHELXL97.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2432).

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(2E)-1-(1,3-Benzodioxol-5-yl)-3-(2-bromophenyl)prop-2-en-1-one**Hongqi Li, R. S. Rathore, K. Prakash Kamath, H. S. Yathirajan and B. Narayana****S1. Comment**

Chalcones possess many interesting biological and pharmacological properties. They are highly reactive substances of varied nature. Recently, it is shown that few of the derivatives are able to block voltage-dependent potassium channels (Yarishkin *et al.*, 2008). Chalcones have been also implicated in organic nonlinear optical materials for their SHG conversion efficiency (Sarojini *et al.*, 2006). The radical quenching property of the phenolic groups present in many chalcones or chalcone-rich plant extracts has led to their use as drugs or food preservatives (Di Carlo *et al.*, 1999). We earlier reported structures of chalcone derivatives (Harrison *et al.*, 2006; Rathore *et al.*, 2006; Jasinski *et al.*, 2010; Li *et al.*, 2008). In continuation of the study, we have synthesized a new chalcone analog, C₁₆H₁₁BrO₃, (I), and discuss its crystal structure herein.

The crystal of (I) studied was racemically twinned in a 0.595 (13):0.405 (13) ratio. Similar racemic twinning in Br-containing compounds was observed by Gómez *et al.* (2010). The skeleton of (I) is essentially planar possessing two intramolecular short contacts. The bifurcated C1—H7···(Br1, O1) promote planarity of the molecular skeleton (Table 1). The configuration of the keto group with respect to the olefinic double bond is typically *s-cis*, with the C7—C8—C9—O1 torsion angle of -1.6 (7)° (Rathore *et al.*, 2006).

Crystal packing is characterized by halogen···oxygen interactions between molecules related by 2-fold screw axis, with the Br1···O2ⁱ distance of 3.187 (3) Å [symmetry code (i): 0.5+x, 0.5-y, -z] and the C1—Br1···O2 angle of 170.6 (1)°. The Br···O interaction leads to a one-dimensional chain along *b* axis. Crystal packing is shown in Fig 2. Br···O interactions have previously been employed for crystal engineering purposes (Thallapally *et al.*, 2002). Halogen bonding between halogen atoms (Lewis acid) and neutral or anionic Lewis base, has been subject of great interest in recent years, primarily due to their unique noncovalent bonding characteristics (Metrangolo *et al.*, 2005; Riley *et al.*, 2009). The crystal structure additionally contains a C—H···π short contact, giving rise to an alternate linear pattern along the *a* axis (Table 1).

S2. Experimental

The title compound was prepared as follows: to a mixture of 1-(1,3-benzodioxol-5-yl)ethanone (1.64 g, 0.01 mol) and 2-bromobenzaldehyde (1.85 g, 0.01 mol) in 30 ml ethanol, 10 ml of 10 % sodium hydroxide solution was added and stirred at 5-10° C for 3 hours. The precipitate formed was collected by filtration and purified by recrystallization from ethanol. Final yield 79%; m.p. 390-392° K. Crystals suitable for X-ray analysis were grown from (1:1 v/v) mixture of toluene and acetone by slow evaporation method. Anal.: calc. for C₁₆H₁₁BrO₃ : C 58.03 , H 3.35; found: C 57.93, H 3.31.

S3. Refinement

All H atoms were stereochemically fixed and refined using a riding option with C(Sp²)—H = 0.93 Å, C(methylene)—H = 0.97 Å, and U_{iso}(H) = 1.2 U_{eq}(C). The residual electron density observed in the vicinity of Br is due to the result of rotation of the bromophenyl moiety about the C6—C7 bond. The disorder could not be reliably refined presumably due

to very low occupancy of other conformers. The crystal studied was treated as an inversion twin leading to twin fractions of 0.595 (13):0.405 (13).

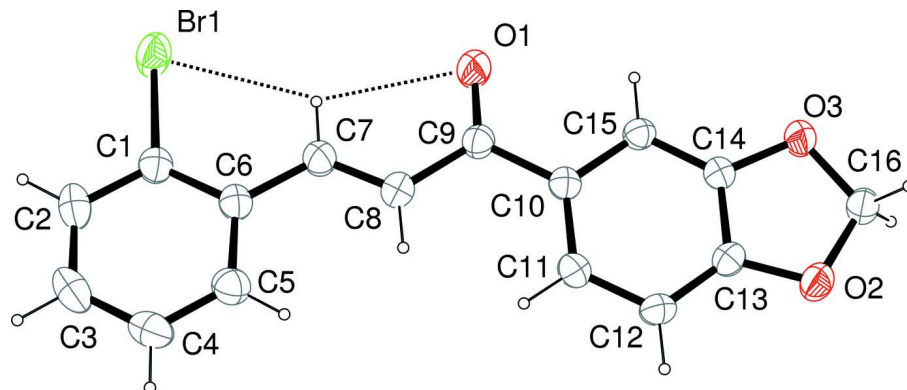


Figure 1

The molecular structure of the title compound. Displacement ellipsoids are drawn at 30% probability level. Dotted lines indicate intramolecular hydrogen bonds.

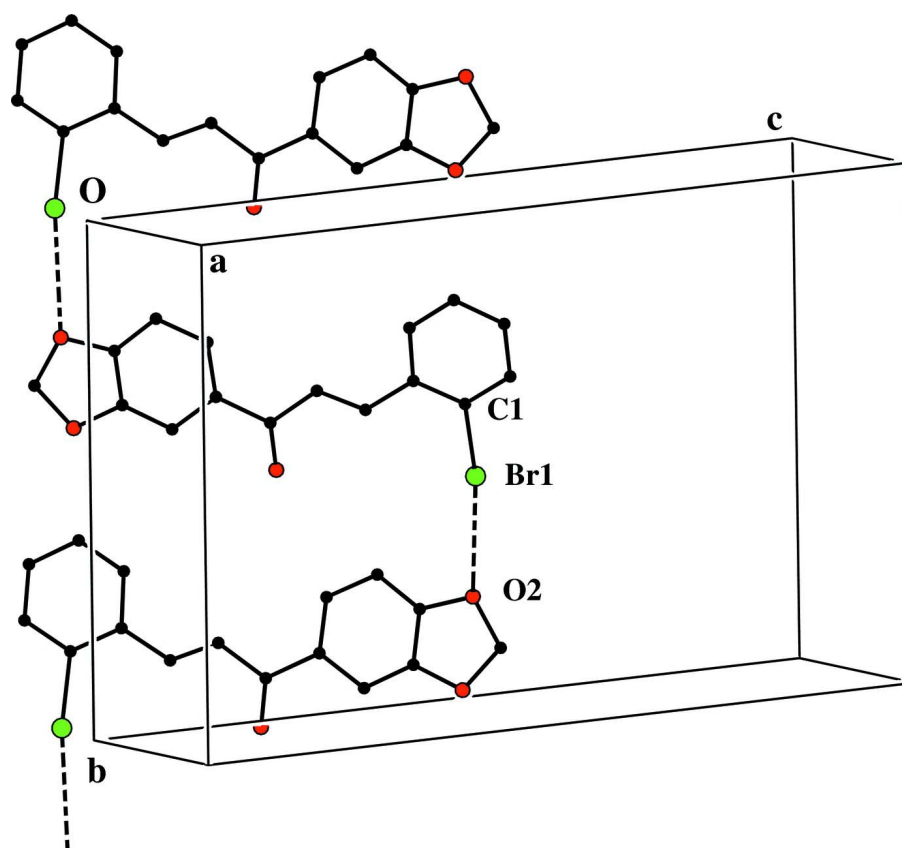


Figure 2

Molecular packing of the title compound showing the halogen...oxygen interactions (dashed lines) forming one-dimensional chains along the *b* axis.

(2E)-1-(1,3-Benzodioxol-5-yl)-3-(2-bromophenyl)prop-2-en-1-one

Crystal data

 $C_{16}H_{11}BrO_3$ $M_r = 331.16$ Orthorhombic, $P2_12_12_1$

Hall symbol: P 2ac 2ab

 $a = 5.0434 (2) \text{ \AA}$ $b = 12.9354 (4) \text{ \AA}$ $c = 20.8916 (7) \text{ \AA}$ $V = 1362.93 (8) \text{ \AA}^3$ $Z = 4$ $F(000) = 664$ $D_x = 1.614 \text{ Mg m}^{-3}$

Melting point = 390–392 K

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 7488 reflections

 $\theta = 2.5\text{--}25.7^\circ$ $\mu = 3.02 \text{ mm}^{-1}$ $T = 296 \text{ K}$

Block, colorless

 $0.53 \times 0.19 \times 0.16 \text{ mm}$

Data collection

Bruker SMART APEXII CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 φ and ω scansAbsorption correction: multi-scan
(SADABS; Bruker, 2004) $T_{\min} = 0.576$, $T_{\max} = 0.653$

17031 measured reflections

2674 independent reflections

2437 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.023$ $\theta_{\max} = 26.0^\circ$, $\theta_{\min} = 1.9^\circ$ $h = -6 \rightarrow 6$ $k = -13 \rightarrow 15$ $l = -25 \rightarrow 25$

Refinement

Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.034$ $wR(F^2) = 0.086$ $S = 1.06$

2674 reflections

182 parameters

0 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0412P)^2 + 0.7667P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.001$ $\Delta\rho_{\max} = 0.64 \text{ e \AA}^{-3}$ $\Delta\rho_{\min} = -0.52 \text{ e \AA}^{-3}$ Absolute structure: Flack (1983), 1086 Bijvoet
pairs

Absolute structure parameter: 0.595 (13)

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 $F^2 > \sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.74414 (9)	0.52368 (3)	0.425085 (18)	0.07369 (16)
O1	0.0651 (6)	0.5167 (2)	0.25271 (15)	0.0779 (9)
O2	-0.6166 (5)	0.26394 (18)	0.06042 (12)	0.0586 (6)

O3	-0.6165 (5)	0.44083 (18)	0.07678 (11)	0.0554 (5)
C1	0.7744 (7)	0.3802 (2)	0.40661 (13)	0.0493 (7)
C2	0.9616 (7)	0.3239 (3)	0.44092 (16)	0.0610 (9)
H2	1.0660	0.3561	0.4717	0.073*
C3	0.9903 (8)	0.2201 (3)	0.42877 (19)	0.0679 (11)
H3	1.1121	0.1813	0.4520	0.081*
C4	0.8394 (8)	0.1738 (3)	0.3824 (2)	0.0661 (10)
H4	0.8595	0.1036	0.3741	0.079*
C5	0.6594 (7)	0.2304 (3)	0.34812 (17)	0.0576 (9)
H5	0.5603	0.1975	0.3166	0.069*
C6	0.6196 (6)	0.3355 (3)	0.35892 (14)	0.0461 (7)
C7	0.4282 (7)	0.3947 (3)	0.32148 (16)	0.0533 (8)
H7	0.4276	0.4658	0.3280	0.064*
C8	0.2596 (7)	0.3595 (2)	0.28037 (14)	0.0524 (7)
H8	0.2561	0.2885	0.2732	0.063*
C9	0.0717 (6)	0.4246 (3)	0.24404 (15)	0.0461 (7)
C10	-0.1054 (6)	0.3754 (2)	0.19621 (13)	0.0413 (6)
C11	-0.1108 (7)	0.2691 (3)	0.18603 (16)	0.0486 (7)
H11	0.0015	0.2268	0.2097	0.058*
C12	-0.2804 (7)	0.2245 (2)	0.14116 (15)	0.0522 (8)
H12	-0.2842	0.1534	0.1347	0.063*
C13	-0.4395 (6)	0.2889 (2)	0.10737 (14)	0.0436 (7)
C14	-0.4375 (6)	0.3942 (2)	0.11713 (13)	0.0398 (6)
C15	-0.2737 (7)	0.4401 (2)	0.16089 (12)	0.0430 (6)
H15	-0.2739	0.5113	0.1670	0.052*
C16	-0.7382 (8)	0.3593 (2)	0.04180 (13)	0.0498 (7)
H16A	-0.7151	0.3704	-0.0038	0.060*
H16B	-0.9267	0.3572	0.0510	0.060*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0729 (2)	0.0700 (2)	0.0781 (3)	0.0085 (2)	-0.0259 (2)	-0.02381 (18)
O1	0.096 (2)	0.0487 (15)	0.0889 (19)	0.0021 (15)	-0.0448 (17)	-0.0083 (14)
O2	0.0621 (14)	0.0532 (13)	0.0605 (13)	0.0012 (11)	-0.0161 (12)	-0.0129 (11)
O3	0.0580 (13)	0.0492 (12)	0.0589 (13)	0.0062 (11)	-0.0187 (11)	-0.0013 (11)
C1	0.0454 (16)	0.0575 (17)	0.0449 (14)	-0.0019 (17)	0.0005 (14)	0.0032 (12)
C2	0.0490 (18)	0.088 (3)	0.0466 (17)	0.0060 (18)	-0.0039 (15)	0.0082 (18)
C3	0.057 (2)	0.083 (3)	0.064 (2)	0.0180 (19)	0.0026 (19)	0.027 (2)
C4	0.064 (2)	0.054 (2)	0.081 (2)	0.0069 (16)	0.0111 (19)	0.017 (2)
C5	0.056 (2)	0.056 (2)	0.0608 (19)	-0.0020 (15)	0.0003 (16)	0.0071 (17)
C6	0.0418 (15)	0.0552 (19)	0.0415 (15)	-0.0003 (15)	0.0029 (12)	0.0046 (13)
C7	0.0564 (19)	0.0461 (18)	0.0575 (18)	0.0046 (15)	-0.0111 (16)	-0.0041 (15)
C8	0.0509 (16)	0.0510 (16)	0.0553 (16)	-0.003 (2)	-0.0075 (18)	-0.0004 (13)
C9	0.0473 (17)	0.0479 (19)	0.0432 (15)	-0.0038 (15)	-0.0021 (13)	-0.0006 (13)
C10	0.0411 (15)	0.0450 (16)	0.0378 (13)	-0.0004 (13)	0.0037 (12)	0.0025 (13)
C11	0.0464 (17)	0.0473 (18)	0.0522 (17)	0.0055 (15)	-0.0052 (15)	0.0026 (15)
C12	0.058 (2)	0.0368 (14)	0.0621 (17)	-0.0016 (17)	-0.0073 (18)	-0.0041 (13)

C13	0.0435 (16)	0.0458 (17)	0.0415 (14)	-0.0033 (13)	0.0011 (13)	-0.0046 (13)
C14	0.0371 (14)	0.0441 (16)	0.0383 (13)	0.0011 (12)	0.0031 (12)	0.0026 (12)
C15	0.0463 (16)	0.0397 (13)	0.0429 (13)	-0.0003 (16)	-0.0004 (13)	-0.0022 (11)
C16	0.0492 (16)	0.0540 (17)	0.0463 (14)	-0.005 (2)	-0.0056 (16)	0.0007 (12)

Geometric parameters (Å, °)

Br1—C1	1.902 (3)	C7—C8	1.292 (5)
O1—C9	1.206 (4)	C7—H7	0.9300
O2—C13	1.365 (4)	C8—C9	1.478 (5)
O2—C16	1.431 (4)	C8—H8	0.9300
O3—C14	1.374 (4)	C9—C10	1.484 (4)
O3—C16	1.423 (4)	C10—C11	1.391 (4)
C1—C2	1.391 (5)	C10—C15	1.402 (4)
C1—C6	1.392 (4)	C11—C12	1.394 (4)
C2—C3	1.374 (6)	C11—H11	0.9300
C2—H2	0.9300	C12—C13	1.355 (4)
C3—C4	1.371 (6)	C12—H12	0.9300
C3—H3	0.9300	C13—C14	1.378 (4)
C4—C5	1.368 (5)	C14—C15	1.368 (4)
C4—H4	0.9300	C15—H15	0.9300
C5—C6	1.393 (5)	C16—H16A	0.9700
C5—H5	0.9300	C16—H16B	0.9700
C6—C7	1.459 (4)		
C13—O2—C16	105.8 (2)	O1—C9—C10	120.6 (3)
C14—O3—C16	105.9 (2)	C8—C9—C10	119.1 (3)
C2—C1—C6	122.1 (3)	C11—C10—C15	119.9 (3)
C2—C1—Br1	117.4 (3)	C11—C10—C9	122.6 (3)
C6—C1—Br1	120.4 (2)	C15—C10—C9	117.5 (3)
C3—C2—C1	119.2 (4)	C10—C11—C12	121.6 (3)
C3—C2—H2	120.4	C10—C11—H11	119.2
C1—C2—H2	120.4	C12—C11—H11	119.2
C4—C3—C2	120.0 (3)	C13—C12—C11	117.3 (3)
C4—C3—H3	120.0	C13—C12—H12	121.3
C2—C3—H3	120.0	C11—C12—H12	121.3
C5—C4—C3	120.3 (4)	C12—C13—O2	128.1 (3)
C5—C4—H4	119.9	C12—C13—C14	121.8 (3)
C3—C4—H4	119.9	O2—C13—C14	110.2 (3)
C4—C5—C6	122.2 (4)	C15—C14—O3	128.0 (3)
C4—C5—H5	118.9	C15—C14—C13	122.2 (3)
C6—C5—H5	118.9	O3—C14—C13	109.8 (3)
C1—C6—C5	116.2 (3)	C14—C15—C10	117.3 (3)
C1—C6—C7	122.4 (3)	C14—C15—H15	121.4
C5—C6—C7	121.4 (3)	C10—C15—H15	121.4
C8—C7—C6	127.4 (3)	O3—C16—O2	108.3 (2)
C8—C7—H7	116.3	O3—C16—H16A	110.0
C6—C7—H7	116.3	O2—C16—H16A	110.0

C7—C8—C9	124.3 (3)	O3—C16—H16B	110.0
C7—C8—H8	117.9	O2—C16—H16B	110.0
C9—C8—H8	117.9	H16A—C16—H16B	108.4
O1—C9—C8	120.3 (3)		
C6—C1—C2—C3	-1.8 (5)	C15—C10—C11—C12	0.1 (5)
Br1—C1—C2—C3	-179.7 (3)	C9—C10—C11—C12	179.5 (3)
C1—C2—C3—C4	1.4 (5)	C10—C11—C12—C13	0.4 (5)
C2—C3—C4—C5	-0.2 (6)	C11—C12—C13—O2	178.6 (3)
C3—C4—C5—C6	-0.6 (6)	C11—C12—C13—C14	-0.7 (5)
C2—C1—C6—C5	1.0 (5)	C16—O2—C13—C12	178.4 (3)
Br1—C1—C6—C5	178.8 (2)	C16—O2—C13—C14	-2.3 (3)
C2—C1—C6—C7	-178.2 (3)	C16—O3—C14—C15	-179.3 (3)
Br1—C1—C6—C7	-0.4 (4)	C16—O3—C14—C13	1.5 (3)
C4—C5—C6—C1	0.2 (5)	C12—C13—C14—C15	0.6 (5)
C4—C5—C6—C7	179.4 (3)	O2—C13—C14—C15	-178.8 (3)
C1—C6—C7—C8	-173.5 (4)	C12—C13—C14—O3	180.0 (3)
C5—C6—C7—C8	7.4 (6)	O2—C13—C14—O3	0.5 (4)
C6—C7—C8—C9	-179.8 (3)	O3—C14—C15—C10	-179.3 (3)
C7—C8—C9—O1	-1.5 (6)	C13—C14—C15—C10	-0.1 (4)
C7—C8—C9—C10	177.6 (3)	C11—C10—C15—C14	-0.2 (4)
O1—C9—C10—C11	-177.9 (4)	C9—C10—C15—C14	-179.7 (3)
C8—C9—C10—C11	3.0 (4)	C14—O3—C16—O2	-2.8 (3)
O1—C9—C10—C15	1.5 (5)	C13—O2—C16—O3	3.1 (3)
C8—C9—C10—C15	-177.6 (3)		

Hydrogen-bond geometry (Å, °)

Cg3 is the centroid of the C10–C15 ring.

<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>
C7—H7...Br1	0.93	2.69	3.164 (4)	113
C7—H7...O1	0.93	2.50	2.812 (6)	100
C16—H16B...Cg3 ⁱ	0.97	2.76	3.563 (4)	141

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