

# Crystal structure and Hirshfeld surface analysis of (2*E*)-1-(4-bromophenyl)-3-(2-methylphenyl)prop-2-en-1-one

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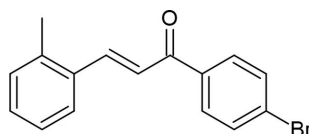
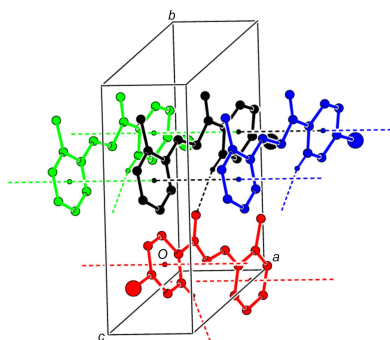
**Supporting information:** this article has supporting information at journals.iucr.org/e

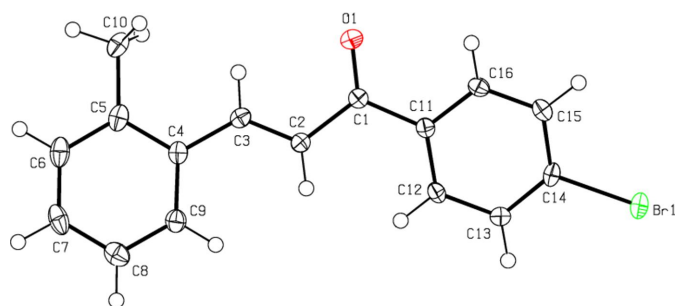
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In the title compound, C<sub>16</sub>H<sub>13</sub>BrO, the planes of the aromatic rings are inclined at an angle of 23.49 (15)°, and the configuration about the C=C bond is *E*. In the crystal, the molecules are linked into chains by weak C—H···O interactions along the *b* axis. Successive chains form a zigzag structure along the *c* axis, and these chains are connected to each other by *face-to-face*  $\pi$ – $\pi$  stacking interactions along the *a* axis. These layers, parallel to the (001) plane, are linked by van der Waals interactions, thus consolidating the crystal structure. Hirshfeld surface analysis showed that the most significant contacts in the structure are H···H (43.1%), C···H/H···C (17.4%), Br···H/H···Br (14.9%), C···C (11.9%) and O···H/H···O (9.8%).

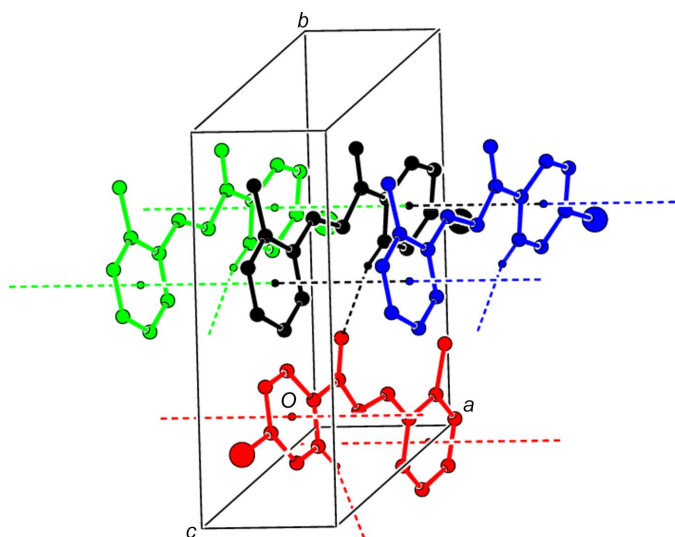
## 1. Chemical context

Diverse C—C, C—N, C—S and C—O bond formations are fundamental and valuable conversions in modern organic chemistry (Gurbanov *et al.*, 2017; Afkhami *et al.*, 2019; Mahmoudi *et al.*, 2021). Chalcones are  $\alpha,\beta$ -unsaturated ketones containing aryl–aryl or aryl–alkyl groups at both ends. They belong to the flavonoid family, and they possess a wide variety of biological activities. Many natural chalcones, such as echinatin, naringenin, isoliquiritigenin, butein, 4-hydroxyderricin, 4-hydroxyonchocarpin, derricin, xanthoangelol, lonchocarpin, licochalcone A, licochalcone E, humulusol, munsericin, flavokawain A, isobavachalcone, mallotophilippen C, D and E, brousochalcone A, crotaorixin, pedicinin and nardoaristolone A have been isolated from plants (Rozmer & Perjési, 2016; Çelik *et al.*, 2023; Chalkha *et al.*, 2023). Moreover, the enone moiety is a widespread structural motif often found in biologically active compounds possessing enzyme inhibitory, anticancer and antimicrobial activity (Poustforoosh *et al.*, 2022; Tapera *et al.*, 2022; Sarkı *et al.*, 2023). Herein, in continuation to our recent investigations (Gurbanov *et al.*, 2022*a,b*), we report the crystal structure and Hirshfeld surface analysis of (2*E*)-1-(4-bromophenyl)-3-(2-methylphenyl)prop-2-en-1-one.





**Figure 1**  
The molecular structure of the title compound, showing the atom labeling and displacement ellipsoids drawn at the 50% probability level.



**Figure 2**  
View of the C–H...O hydrogen bonds and *face-to-face*  $\pi$ – $\pi$  stacking interactions in the title compound along the *c* axis.

## 2. Structural commentary

The title compound (Fig. 1) is composed of two aromatic rings, *i.e.* 2-methylphenyl (C4–C9) and 4-bromophenyl (C11–C16), which are linked by a –CO–CH=CH– *E*-configured enone bridge. The molecule is approximately planar, as indicated by the torsion angles C10–C5–C4–C3 = 1.9 (5)°, C9–C4–

**Table 1**  
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>
C12–H12...O1 <sup>i</sup>	0.95	2.58	3.200 (3)	124

Symmetry code: (i)  $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$ .

**Table 2**  
Summary of short interatomic contacts (Å) in the title compound.

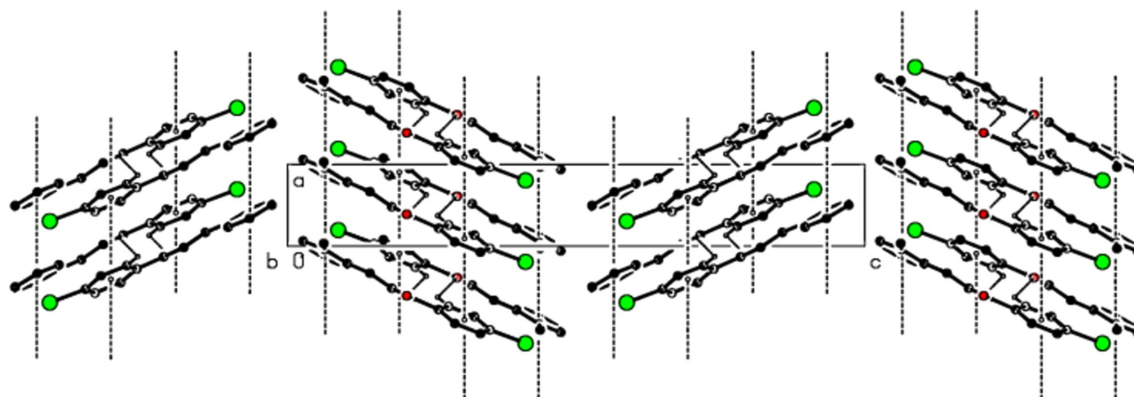
C3...H10 <i>B</i>	2.85	$x + 1, y, z$
Br1...H7	3.17	$-x + \frac{3}{2}, -y + 1, z - \frac{1}{2}$
O1...H12	2.58	$-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$
H15...H9	2.45	$-x + 2, y + \frac{1}{2}, -z + \frac{1}{2}$
C10...H10 <i>A</i>	3.10	$x + \frac{1}{2}, -y + \frac{3}{2}, -z + 1$

C3–C2 = –4.4 (5)°, C4–C3–C2–C1 = –176.3 (3)°, C3–C2–C1–C11 = –168.2 (3)°, C2–C1–C11–C12 = 15.9 (4)° and Br1–C14–C15–C16 = 178.5 (2)°. The dihedral angle between the planes of the 2-methylphenyl and 4-bromophenyl rings is 23.49 (15)°.

## 3. Supramolecular features and Hirshfeld surface analysis

In the crystal, the molecules are linked into *C*(5) chains (Bernstein *et al.*, 1995) by weak C–H...O interactions (Table 1 and Fig. 2) along the *a* axis. Successive chains form a zigzag structure along the *b* axis (Fig. 3) and these chains are connected to each other along the *c* axis by *face-to-face*  $\pi$ – $\pi$  stacking interactions [*Cg*1...*Cg*1<sup>*a*</sup> = 3.942 (2) Å, slippage = 1.890 Å; *Cg*2...*Cg*2<sup>*a*</sup> = 3.9420 (18) Å, slippage = 1.942 Å; symmetry code: (*a*)  $x - 1, y, z$ ; *Cg*1 and *Cg*2 are the centroids of the 2-methylphenyl (C4–C9) and 4-bromophenyl (C11–C16) rings, respectively]. They form layers parallel to the (001) plane through van der Waals interactions, thus consolidating the crystal structure.

*CrystalExplorer17.5* (Spackman *et al.*, 2021) was used to compute the Hirshfeld surfaces and the two-dimensional fingerprints of the title molecule. The  $d_{\text{norm}}$  mappings for the title compound were performed in the range from –0.0627 to +1.1373 a.u., on the  $d_{\text{norm}}$  surfaces, allowing the location of the C–H...O interactions (Tables 1 and 2).



**Figure 3**  
Zigzag packing of the title compound along the *b* axis.

**Table 3**  
 Experimental details.

Crystal data	
Chemical formula	C <sub>16</sub> H <sub>13</sub> BrO
<i>M<sub>r</sub></i>	301.17
Crystal system, space group	Orthorhombic, <i>P</i> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	3.942, 11.5915 (2), 28.0387 (4)
<i>V</i> (Å <sup>3</sup> )	1281.19 (3)
<i>Z</i>	4
Radiation type	Cu <i>K</i> α
<i>μ</i> (mm <sup>-1</sup> )	4.23
Crystal size (mm)	0.35 × 0.09 × 0.07
Data collection	
Diffractometer	Rigaku XtaLAB Synergy Dualflex diffractometer with a HyPix detector
Absorption correction	Gaussian ( <i>CrysAlis PRO</i> ; Rigaku OD, 2022)
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.251, 1.000
No. of measured, independent and observed [ <i>I</i> > 2σ( <i>I</i> )] reflections	14537, 2657, 2627
<i>R<sub>int</sub></i>	0.025
(sin θ/λ) <sub>max</sub> (Å <sup>-1</sup> )	0.632
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.022, 0.052, 1.14
No. of reflections	2657
No. of parameters	165
H-atom treatment	H-atom parameters constrained
Δρ <sub>max</sub> , Δρ <sub>min</sub> (e Å <sup>-3</sup> )	0.51, -0.42
Absolute structure	Refined as an inversion twin
Absolute structure parameter	0.53 (2)

Computer programs: *CrysAlis PRO* (Rigaku OD, 2022), *SHELXT2018* (Sheldrick, 2015a), *SHELXL2018* (Sheldrick, 2015b), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2020).

The fingerprint plots (Fig. 4) show that H...H [Fig. 4(b); 43.1%], C...H/H...C [Fig. 4(c); 17.4%], Br...H/H...Br [Fig. 4(d); 14.9%], C...C [Fig. 4(e); 11.9%] and O...H/H...O [Fig. 4(f); 9.8%] interactions contribute the most to the surface contacts. The crystal packing is additionally influenced by Br...C/C...Br (2.0%), Br...Br (0.8%), N...N (2.6%) and O...C/C...O (0.2%) contacts. The Hirshfeld surface study confirms the significance of H-atom interactions in the packing formation. The large number of H...H, C...H/H...C, Br...H/H...Br, C...C and O...H/H...O interactions indicates that van der Waals interactions and hydrogen bonding are important in the crystal packing (Hathwar *et al.*, 2015).

#### 4. Database survey

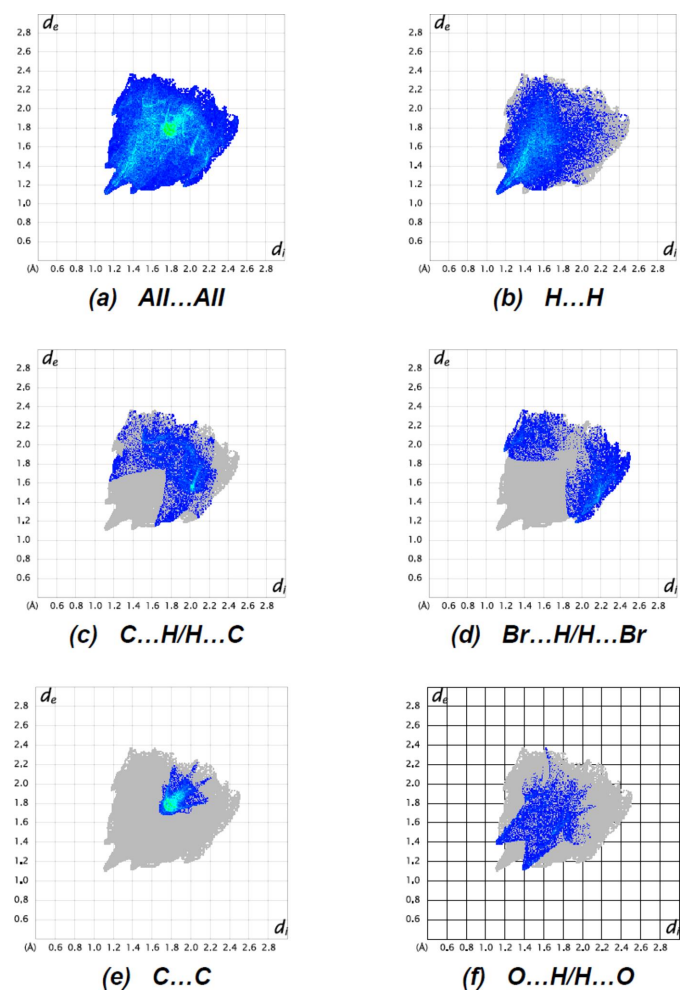
Four related compounds were found as a result of a search for the '(2*E*)-1,3-diphenylprop-2-en-1-one' unit in the Cambridge Structural Database (CSD, Version 5.42, update of September 2021; Groom *et al.*, 2016), *viz.* CSD refcodes KOCZUA (Bindya *et al.*, 2019), RUCKIM (Spruce *et al.*, 2020), XOLLOC (Çelikesir *et al.*, 2019) and OBIYUW01 (Atioğlu *et al.*, 2019).

In the crystal of KOCZUA, the shortest intermolecular contacts are Cl...O [3.173 (3) Å]; these link the molecules to form a 2<sub>1</sub> helix propagating along the *b*-axis direction. The helices are linked by offset π-π interactions [intercentroid distance = 3.983 (1) Å], forming layers lying parallel to the *ab*

plane. In the crystal of RUCKIM, the molecules are linked through type II halogen bonds, forming a sheet structure parallel to the *bc* plane. Weak intermolecular C—H...π interactions are observed between the sheets. In the crystal of XOLLOC, molecules are linked *via* pairs of C—H...O interactions with an *R*<sub>2</sub><sup>2</sup>(14) ring motif, forming inversion dimers. The dimers are linked into a tape structure running along [101] *via* C—H...π interactions. In the crystal of OBIYUW01, molecules are linked by C—H...π interactions between the bromophenyl and fluorophenyl rings, resulting in a two-dimensional layered structure parallel to the *ab* plane. The molecular packing is consolidated by weak Br...H and F...H contacts.

#### 5. Synthesis and crystallization

The title compound was synthesized using a reported procedure (Chithiraikumar *et al.*, 2021) and colourless crystals were



**Figure 4**  
 The two-dimensional fingerprint plots of the title compound, showing (a) all interactions, and delineated into (b) H...H, (c) C...H/H...C, (d) Br...H/H...Br, (e) C...C and (f) O...H/H...O interactions. *d<sub>e</sub>* and *d<sub>i</sub>* represent the distances from a point on the Hirshfeld surface to the nearest atoms outside (external) and inside (internal) the surface.

obtained upon recrystallization from an ethanol/water (3:1 v/v) solution at room temperature.

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All H atoms were placed in their geometrically calculated positions and refined using a riding model, with C–H = 0.95 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for aromatic H atoms, and C–H = 0.98 Å and  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$  for methyl H atoms.

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## supporting information

*Acta Cryst.* (2023). E79, 847-851 [https://doi.org/10.1107/S2056989023007387]

## Crystal structure and Hirshfeld surface analysis of (2*E*)-1-(4-bromophenyl)-3-(2-methylphenyl)prop-2-en-1-one

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### Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2022); cell refinement: *CrysAlis PRO* (Rigaku OD, 2022); data reduction: *CrysAlis PRO* (Rigaku OD, 2022); program(s) used to solve structure: SHELXT2018 (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015b); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2020).

### (2*E*)-1-(4-Bromophenyl)-3-(2-methylphenyl)prop-2-en-1-one

#### Crystal data

C<sub>16</sub>H<sub>13</sub>BrO

*M<sub>r</sub>* = 301.17

Orthorhombic, *P*2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>

*a* = 3.942 Å

*b* = 11.5915 (2) Å

*c* = 28.0387 (4) Å

*V* = 1281.19 (3) Å<sup>3</sup>

*Z* = 4

*F*(000) = 608

*D<sub>x</sub>* = 1.561 Mg m<sup>-3</sup>

Cu *Kα* radiation, λ = 1.54184 Å

Cell parameters from 12560 reflections

θ = 3.8–76.9°

μ = 4.23 mm<sup>-1</sup>

*T* = 100 K

Needle, colourless

0.35 × 0.09 × 0.07 mm

#### Data collection

Rigaku XtaLAB Synergy Dualflex  
diffractometer with a HyPix detector

Radiation source: micro-focus sealed X-ray tube

φ and ω scans

Absorption correction: gaussian

(*CrysAlis PRO*; Rigaku OD, 2022)

*T<sub>min</sub>* = 0.251, *T<sub>max</sub>* = 1.000

14537 measured reflections

2657 independent reflections

2627 reflections with *I* > 2σ(*I*)

*R<sub>int</sub>* = 0.025

θ<sub>max</sub> = 77.1°, θ<sub>min</sub> = 3.2°

*h* = -4→4

*k* = -14→14

*l* = -35→34

#### Refinement

Refinement on *F*<sup>2</sup>

Least-squares matrix: full

*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.022

*wR*(*F*<sup>2</sup>) = 0.052

*S* = 1.14

2657 reflections

165 parameters

0 restraints

Hydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

*w* = 1/[σ<sup>2</sup>(*F<sub>o</sub>*<sup>2</sup>) + (0.0121*P*)<sup>2</sup> + 1.3924*P*]

where *P* = (*F<sub>o</sub>*<sup>2</sup> + 2*F<sub>c</sub>*<sup>2</sup>)/3

(Δ/σ)<sub>max</sub> = 0.001

Δρ<sub>max</sub> = 0.51 e Å<sup>-3</sup>

Δρ<sub>min</sub> = -0.42 e Å<sup>-3</sup>



Absolute structure: Refined as an inversion twin

Absolute structure parameter: 0.53 (2)

*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.** Refined as a 2-component inversion twin.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.6338 (7)	0.6732 (2)	0.28488 (10)	0.0156 (6)
C2	0.5186 (8)	0.5849 (3)	0.31975 (11)	0.0179 (6)
H2	0.576288	0.506108	0.315259	0.021*
C3	0.3333 (8)	0.6169 (3)	0.35751 (10)	0.0167 (6)
H3	0.272264	0.696111	0.359037	0.020*
C4	0.2138 (8)	0.5441 (3)	0.39673 (9)	0.0162 (5)
C5	0.0419 (8)	0.5941 (3)	0.43586 (11)	0.0199 (6)
C6	-0.0614 (9)	0.5231 (3)	0.47322 (11)	0.0243 (7)
H6	-0.174643	0.556148	0.499821	0.029*
C7	-0.0025 (9)	0.4050 (3)	0.47241 (12)	0.0260 (8)
H7	-0.075592	0.358302	0.498276	0.031*
C8	0.1629 (10)	0.3552 (3)	0.43386 (11)	0.0244 (7)
H8	0.202810	0.274348	0.433117	0.029*
C9	0.2691 (8)	0.4245 (3)	0.39655 (10)	0.0200 (6)
H9	0.382068	0.390249	0.370170	0.024*
C10	-0.0317 (9)	0.7216 (3)	0.43748 (12)	0.0225 (7)
H10A	-0.155611	0.739898	0.466828	0.034*
H10B	-0.169550	0.743225	0.409802	0.034*
H10C	0.182210	0.764687	0.436880	0.034*
C11	0.7811 (8)	0.6341 (2)	0.23829 (10)	0.0151 (5)
C12	0.7419 (7)	0.5219 (2)	0.22102 (9)	0.0170 (6)
H12	0.629276	0.465770	0.239962	0.020*
C13	0.8664 (8)	0.4916 (2)	0.17629 (11)	0.0180 (6)
H13	0.839832	0.415359	0.164401	0.022*
C14	1.0295 (8)	0.5750 (3)	0.14959 (10)	0.0170 (6)
C15	1.0768 (8)	0.6869 (3)	0.16597 (11)	0.0178 (6)
H15	1.193503	0.742210	0.147111	0.021*
C16	0.9500 (8)	0.7159 (3)	0.21041 (11)	0.0172 (6)
H16	0.978056	0.792262	0.222085	0.021*
Br1	1.19480 (8)	0.53645 (3)	0.08770 (2)	0.02188 (9)
O1	0.6109 (6)	0.77583 (19)	0.29371 (8)	0.0242 (5)

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0136 (15)	0.0168 (14)	0.0164 (13)	0.0005 (11)	-0.0014 (11)	0.0006 (11)
C2	0.0207 (16)	0.0164 (14)	0.0165 (14)	0.0013 (12)	0.0014 (12)	-0.0001 (11)

C3	0.0164 (13)	0.0177 (13)	0.0160 (13)	0.0015 (13)	-0.0028 (12)	-0.0018 (11)
C4	0.0129 (13)	0.0224 (13)	0.0134 (11)	-0.0004 (13)	-0.0030 (9)	0.0003 (11)
C5	0.0137 (14)	0.0316 (18)	0.0145 (14)	-0.0011 (13)	-0.0031 (12)	-0.0034 (13)
C6	0.0193 (14)	0.040 (2)	0.0142 (13)	-0.0042 (16)	-0.0013 (11)	-0.0015 (14)
C7	0.0249 (18)	0.038 (2)	0.0153 (15)	-0.0111 (15)	-0.0042 (13)	0.0066 (14)
C8	0.0264 (17)	0.0242 (16)	0.0226 (15)	-0.0024 (15)	-0.0079 (15)	0.0043 (12)
C9	0.0205 (17)	0.0229 (14)	0.0166 (13)	0.0004 (12)	-0.0016 (11)	0.0005 (10)
C10	0.0194 (16)	0.0280 (17)	0.0203 (16)	0.0003 (14)	0.0009 (13)	-0.0072 (13)
C11	0.0128 (13)	0.0171 (13)	0.0155 (13)	0.0022 (11)	-0.0008 (11)	0.0023 (10)
C12	0.0162 (15)	0.0178 (14)	0.0170 (12)	-0.0007 (12)	0.0021 (10)	0.0043 (11)
C13	0.0200 (16)	0.0151 (14)	0.0190 (14)	0.0005 (11)	0.0005 (12)	-0.0003 (10)
C14	0.0133 (14)	0.0253 (16)	0.0123 (13)	0.0024 (11)	0.0009 (11)	-0.0012 (11)
C15	0.0160 (14)	0.0194 (15)	0.0181 (14)	-0.0021 (12)	-0.0007 (11)	0.0042 (11)
C16	0.0172 (14)	0.0151 (14)	0.0194 (14)	-0.0023 (12)	-0.0019 (12)	0.0009 (11)
Br1	0.02033 (14)	0.03011 (16)	0.01522 (13)	-0.00038 (13)	0.00375 (12)	-0.00153 (13)
O1	0.0303 (14)	0.0171 (11)	0.0252 (11)	0.0010 (9)	0.0064 (10)	-0.0025 (9)

*Geometric parameters (Å, °)*

C1—O1	1.218 (4)	C8—H8	0.9500
C1—C2	1.487 (4)	C9—H9	0.9500
C1—C11	1.500 (4)	C10—H10A	0.9800
C2—C3	1.339 (4)	C10—H10B	0.9800
C2—H2	0.9500	C10—H10C	0.9800
C3—C4	1.464 (4)	C11—C12	1.396 (4)
C3—H3	0.9500	C11—C16	1.398 (4)
C4—C9	1.404 (4)	C12—C13	1.392 (4)
C4—C5	1.414 (4)	C12—H12	0.9500
C5—C6	1.393 (5)	C13—C14	1.381 (4)
C5—C10	1.507 (5)	C13—H13	0.9500
C6—C7	1.388 (5)	C14—C15	1.389 (4)
C6—H6	0.9500	C14—Br1	1.907 (3)
C7—C8	1.389 (5)	C15—C16	1.384 (4)
C7—H7	0.9500	C15—H15	0.9500
C8—C9	1.384 (4)	C16—H16	0.9500
O1—C1—C2	121.1 (3)	C4—C9—H9	119.2
O1—C1—C11	120.1 (3)	C5—C10—H10A	109.5
C2—C1—C11	118.9 (3)	C5—C10—H10B	109.5
C3—C2—C1	119.7 (3)	H10A—C10—H10B	109.5
C3—C2—H2	120.1	C5—C10—H10C	109.5
C1—C2—H2	120.1	H10A—C10—H10C	109.5
C2—C3—C4	127.6 (3)	H10B—C10—H10C	109.5
C2—C3—H3	116.2	C12—C11—C16	119.4 (3)
C4—C3—H3	116.2	C12—C11—C1	122.8 (3)
C9—C4—C5	118.8 (3)	C16—C11—C1	117.8 (3)
C9—C4—C3	121.1 (3)	C13—C12—C11	120.6 (3)
C5—C4—C3	120.1 (3)	C13—C12—H12	119.7



C6—C5—C4	118.8 (3)	C11—C12—H12	119.7
C6—C5—C10	120.0 (3)	C14—C13—C12	118.4 (3)
C4—C5—C10	121.2 (3)	C14—C13—H13	120.8
C7—C6—C5	121.4 (3)	C12—C13—H13	120.8
C7—C6—H6	119.3	C13—C14—C15	122.5 (3)
C5—C6—H6	119.3	C13—C14—Br1	119.2 (2)
C6—C7—C8	120.1 (3)	C15—C14—Br1	118.3 (2)
C6—C7—H7	119.9	C16—C15—C14	118.4 (3)
C8—C7—H7	119.9	C16—C15—H15	120.8
C9—C8—C7	119.3 (3)	C14—C15—H15	120.8
C9—C8—H8	120.4	C15—C16—C11	120.7 (3)
C7—C8—H8	120.4	C15—C16—H16	119.7
C8—C9—C4	121.6 (3)	C11—C16—H16	119.7
C8—C9—H9	119.2		
O1—C1—C2—C3	12.0 (5)	C3—C4—C9—C8	178.7 (3)
C11—C1—C2—C3	-168.2 (3)	O1—C1—C11—C12	-164.3 (3)
C1—C2—C3—C4	-176.3 (3)	C2—C1—C11—C12	15.9 (4)
C2—C3—C4—C9	-4.4 (5)	O1—C1—C11—C16	12.6 (4)
C2—C3—C4—C5	175.1 (3)	C2—C1—C11—C16	-167.2 (3)
C9—C4—C5—C6	1.1 (5)	C16—C11—C12—C13	-0.6 (4)
C3—C4—C5—C6	-178.4 (3)	C1—C11—C12—C13	176.2 (3)
C9—C4—C5—C10	-178.6 (3)	C11—C12—C13—C14	0.1 (4)
C3—C4—C5—C10	1.9 (5)	C12—C13—C14—C15	0.8 (5)
C4—C5—C6—C7	-0.8 (5)	C12—C13—C14—Br1	-178.8 (2)
C10—C5—C6—C7	178.9 (3)	C13—C14—C15—C16	-1.1 (5)
C5—C6—C7—C8	0.1 (6)	Br1—C14—C15—C16	178.5 (2)
C6—C7—C8—C9	0.3 (5)	C14—C15—C16—C11	0.6 (5)
C7—C8—C9—C4	0.1 (5)	C12—C11—C16—C15	0.3 (5)
C5—C4—C9—C8	-0.7 (5)	C1—C11—C16—C15	-176.7 (3)

*Hydrogen-bond geometry* ( $\text{\AA}$ ,  $^\circ$ )

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
C3—H3 $\cdots$ O1	0.95	2.45	2.791 (4)	101
C12—H12 $\cdots$ O1 <sup>i</sup>	0.95	2.58	3.200 (3)	124

Symmetry code: (i)  $-x+1, y-1/2, -z+1/2$ .