



Crystal structure and Hirshfeld surface analysis of a bromochalcone: (*E*)-1-(3-bromophenyl)-3-(2,6-dichlorophenyl)prop-2-en-1-one

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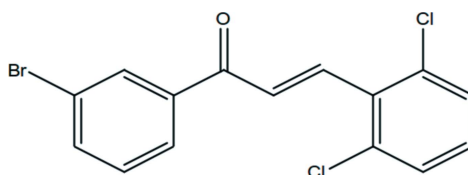
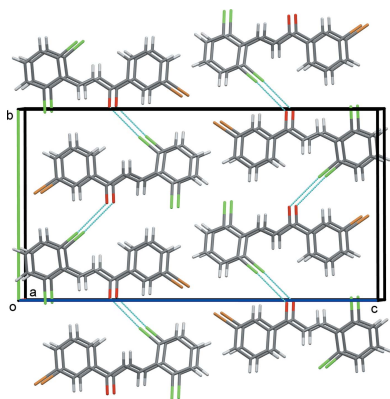
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In the title chalcone derivative, C₁₅H₉BrCl₂O, the aryl rings are inclined to each other by 14.49 (17)°, and the configuration about the C=C bond is *E*. There is a short intramolecular C—H...Cl contact present resulting in the formation of an *S*(6) ring motif. In the crystal, the shortest intermolecular contacts are Cl...O contacts [3.173 (3) Å] that link the molecules to form a 2₁ helix propagating along the *b*-axis direction. The helices stack up the short crystallographic *a* axis, and are linked by offset π - π interactions [intercentroid distance = 3.983 (1) Å], forming layers lying parallel to the *ab* plane. A quantification of the intermolecular contacts in the crystal were estimated using Hirshfeld surface analysis and two-dimensional fingerprint plots.

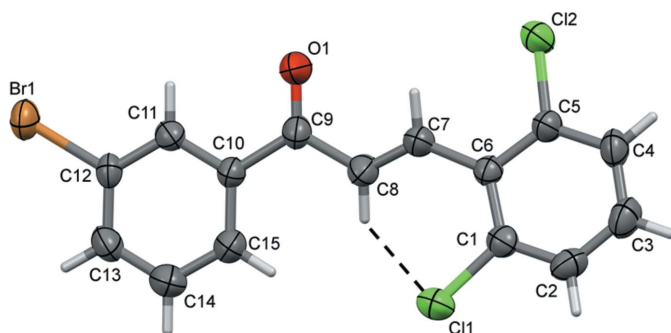
1. Chemical context

Chalcones, considered to be the precursors of flavonoids and isoflavonoids, are abundant in edible plants. Chemically they consist of open-chain flavonoids in which the two aromatic rings are joined by a three-carbon, α -unsaturated carbonyl system and are described by the generic term 'chalcone'. Chalcones are coloured compounds because of the presence of the -CO-CH=CH- chromophore, which depends on the presence of other auxochromes. Chalcones are finding applications as organic non-linear optical materials (NLO) because of their good SHG conversion efficiencies (Chandra Shekhara Shetty *et al.*, 2016; Raghavendra *et al.*, 2017). In view of this interest we have synthesized the title chalcone derivative and report herein on its crystal structure and Hirshfeld surface analysis.



2. Structural commentary

The molecular structure of the title compound is shown in Fig. 1. It comprises two aromatic rings (2,6-dichlorophenyl and

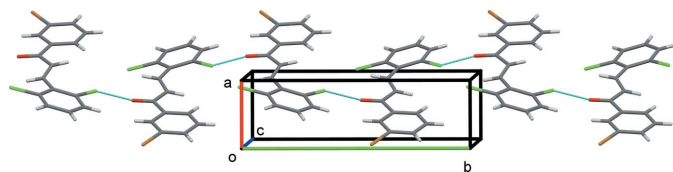

Figure 1

The molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 50% probability level. The intramolecular C—H···Cl hydrogen bond (Table 1) is shown as a dashed line.

3-bromophenyl) linked by the C7=C8—C9(=O1)—C10 enone bridge. The bond lengths and bond angles are normal and the molecular conformation is characterized by a dihedral angle of 14.49 (17)° between the mean planes of the two aromatic rings. The olefinic double bond [C7=C8 = 1.286 (5) Å] is in an *E* configuration. There is a short intramolecular C—H···Cl contact present resulting in the formation of an *S*(6) ring motif (Fig. 1 and Table 1). The unsaturated keto group is in a *syn*-periplanar conformation with respect to the olefinic double bond, which is evident from the O1—C9—C8—C7 torsion angle of 10.9 (6)°. The *trans* conformation of the C=C double bond in the central enone group is confirmed by the C6—C7—C8=C9 torsion angle of −179.8 (3)°. The bond angles O1—C9—C10 [120.4 (3)°], O1—C9—C8 [119.9 (3)°] and C9—C8—C7 [123.9 (4)°] about C9 indicate that this carbon atom is in a distorted trigonal-planar conformation.

3. Supramolecular features

In the crystal, the molecules stack along the short crystallographic *a* axis. The shortest intermolecular contacts are Cl···O1ⁱ contacts [3.173 (3) Å; symmetry code (i): $-x + 2, y + \frac{1}{2}, -z + \frac{1}{2}$] that link the molecules to form 2₁ helices propagating along the *b*-axis direction (Fig. 2). The helices are linked by offset π - π interactions, forming undulating layers lying parallel to the *ab* plane, see Fig. 3 [Cg1···Cg1ⁱⁱ = 3.983 (2) Å, $\alpha = 0.0$ (2)°, $\beta = 24.7^\circ$, interplanar distance = 3.6193 (14) Å, offset 1.66 Å; Cg2···Cg2ⁱⁱⁱ = 3.984 (2) Å, $\alpha = 0.0$ (2)°, $\beta = 24.8^\circ$, offset = 1.67 Å; Cg1 and Cg2 are the centroids of C1–C6 and


Figure 2

A partial view along the *c* axis of the crystal packing of the title compound. The intermolecular Cl···O interactions are shown as dashed lines.

Table 1

Hydrogen-bond geometry (Å, °).

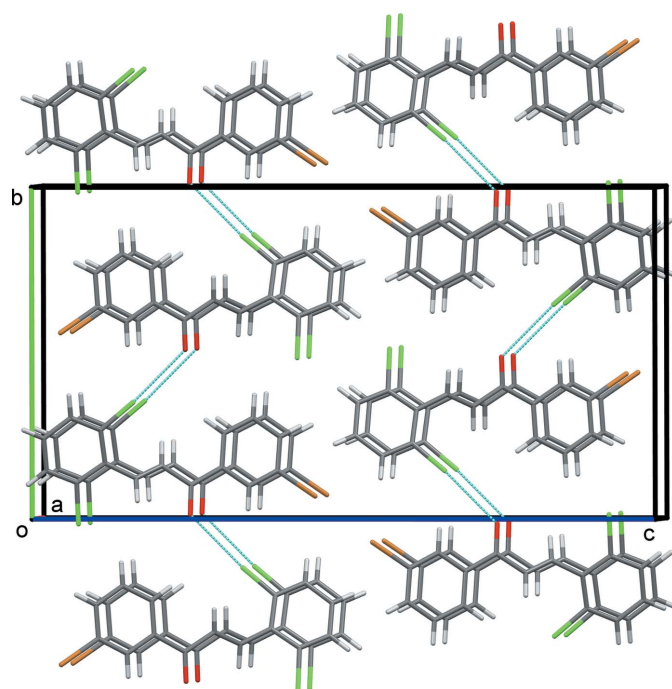
<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C8—H8A···Cl1	0.93	2.54	3.128 (4)	122

C10—C15 rings, respectively; symmetry codes: (ii) $x - 1, y, z$; (iii) $x + 1, y, z$].

4. Hirshfeld surface analysis

Hirshfeld surfaces and fingerprint plots were generated for the title compound using *CrystalExplorer* (Wolff *et al.*, 2012). Hirshfeld surfaces enable the visualization of intermolecular interactions by different colours and colour intensity, representing short or long contacts and indicating the relative strength of the interactions. Fig. 4*a* shows the Hirshfeld surfaces mapped over d_{norm} , while Fig. 4*b* shows the Hirshfeld surfaces mapped over curvedness. In Fig. 4*a*, the red spots near atoms Cl1 and O1 result from the Cl···O interactions, which play a significant role in the molecular packing of the title compound (Figs. 2 and 3), and the Cl···H/H···Cl and O···H/H···O contacts. The curvedness plot (Fig. 4*b*) shows an extensive flat surface characteristic of planar stacking – see the *Supramolecular features* section above.

The overall two-dimensional fingerprint plot (McKinnon *et al.*, 2007), for the title compound and those delineated into Cl···H/H···Cl, H···H, C···C, Br···H/H···Br, C···H/H···C, O···H/H···O contacts are illustrated in Fig. 5; the most significant contributions from the different interatomic


Figure 3

A view along the *a* axis of the crystal packing of the title compound. The intermolecular Cl···O interactions are shown as dashed lines.

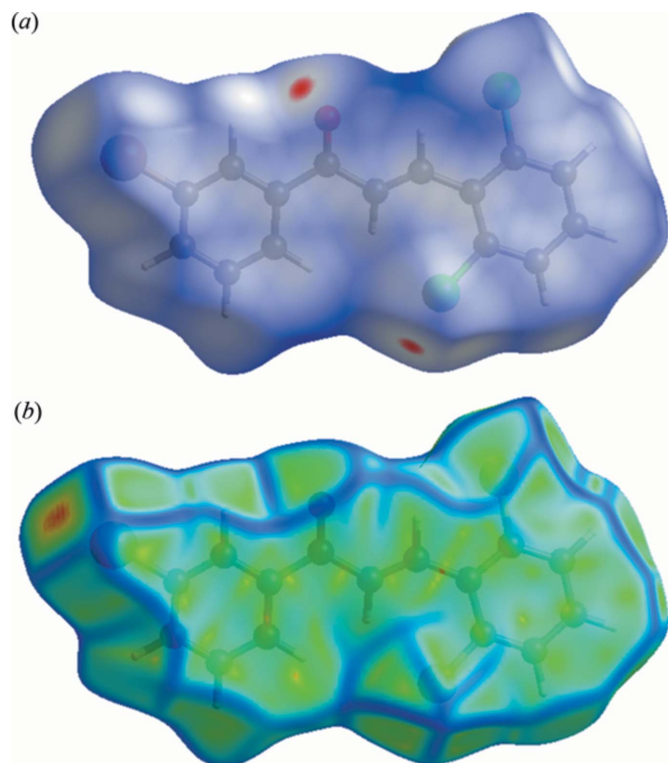


Figure 4
A view of the three-dimensional Hirshfeld surface of the title compound mapped over (a) d_{norm} and (b) curvedness.

contacts to the Hirshfeld surfaces are as follows: Cl...H (23.6%), H...H (19.2%), C...C (14.8%), Br...H (14.2%), C...H (12%) and O...H (8%). Other intermolecular contacts contribute less than 5% to the Hirshfeld surface mapping. Interestingly, the Cl...O interactions (Fig. 2) make a contribution of only 2.2% to the Hirshfeld surface.

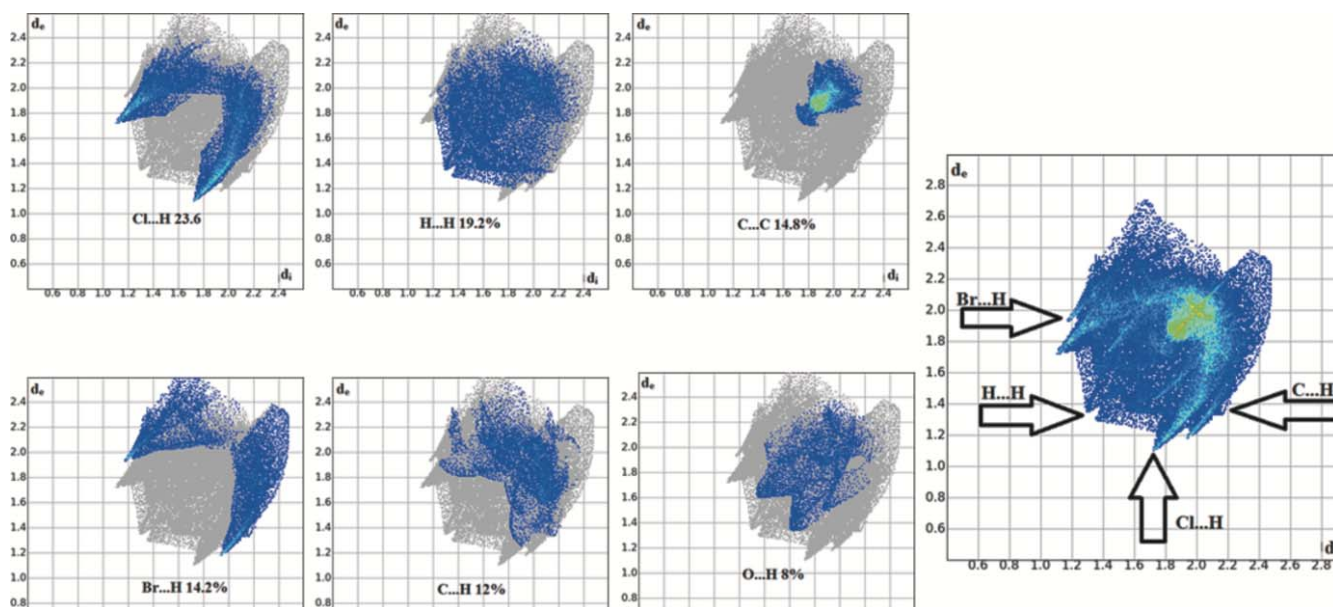


Figure 5
Two-dimensional fingerprint plots of the title compound showing the percentage contributions of all interactions, and the most significant individual types of interactions.

5. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.40, last update November 2018; Groom *et al.*, 2016) using 1-(3-bromophenyl)-3-phenylprop-2-en-1-one as the main skeleton revealed the presence of 12 structures (see supporting information), including 1-(3-bromophenyl)-3-phenylprop-2-en-1-one itself (CSD refcode CICLUW; Rosli *et al.*, 2007). The other structures closest to the title compound with a second halogen-substituted phenyl ring are: 1-(3-bromophenyl)-3-(4-chlorophenyl)prop-2-en-1-one (VIDFEU; Teh *et al.*, 2007), 1-(3-bromophenyl)-3-(3-fluorophenyl)prop-2-en-1-one (GASBEK; Rajendraprasad *et al.*, 2017), and 1-(3-bromophenyl)-3-(4-fluorophenyl)prop-2-en-1-one (OBIYUW; Ekbote *et al.*, 2017). In these four compounds, the two benzene rings are inclined to each other by *ca* 49.93, 46.71, 48.92 and 47.74°, respectively. The same dihedral angle in the title compound is only 14.49 (17)° because of the presence of the intramolecular C—H...Cl hydrogen bond, as shown in Fig. 1 (Table 1).

6. Synthesis and crystallization

The title compound was synthesized according to a reported procedure (Chidan Kumar *et al.*, 2014). 1-(3-Bromophenyl)ethanone (0.01 mol) and 2,6-dichlorobenzaldehyde (0.01 mol) were dissolved in 20 ml of methanol. A catalytic amount of NaOH was added dropwise with vigorous stirring. The reaction mixture was stirred for about 3 h at room temperature. The crude product was filtered, washed several times with distilled water and recrystallized from methanol. On slow evaporation of the solvent, colourless plate-like crystals of the title compound were obtained (m.p. 327–330 K).

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The C-bound H atoms were positioned geometrically ($C-H = 0.95 \text{ \AA}$) and refined using a riding model with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Acknowledgements

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Table 2

Experimental details.

Crystal data	
Chemical formula	$C_{15}H_9BrCl_2O$
M_r	356.02
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	294
a, b, c (Å)	3.9834 (7), 13.471 (2), 25.661 (4)
β (°)	92.736 (4)
V (Å ³)	1375.4 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	3.36
Crystal size (mm)	0.47 × 0.14 × 0.05
Data collection	
Diffractometer	Bruker APEXII DUO CCD area-detector
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2012)
$T_{\text{min}}, T_{\text{max}}$	0.303, 0.842
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10857, 3242, 2260
R_{int}	0.037
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.657
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.041, 0.124, 1.04
No. of reflections	3242
No. of parameters	172
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.47, -0.33

Computer programs: *APEX2* and *SAINT* (Bruker, 2012), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008), *PLATON* (Spek, 2009) and *pubCIF* (Westrip, 2010).

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supporting information

Acta Cryst. (2019). E75, 264-267 [https://doi.org/10.1107/S205698901900104X]

Crystal structure and Hirshfeld surface analysis of a bromochalcone: (*E*)-1-(3-bromophenyl)-3-(2,6-dichlorophenyl)prop-2-en-1-one

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Computing details

Data collection: *APEX2* (Bruker, 2012); cell refinement: *SAINTE* (Bruker, 2012); data reduction: *SAINTE* (Bruker, 2012); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

(*E*)-1-(3-bromophenyl)-3-(2,6-dichlorophenyl)prop-2-en-1-one

Crystal data

$C_{15}H_9BrCl_2O$

$M_r = 356.02$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 3.9834$ (7) Å

$b = 13.471$ (2) Å

$c = 25.661$ (4) Å

$\beta = 92.736$ (4)°

$V = 1375.4$ (4) Å³

$Z = 4$

$F(000) = 704$

$D_x = 1.719$ Mg m⁻³

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

Cell parameters from 2260 reflections

$\theta = 1.6$ – 27.8°

$\mu = 3.36$ mm⁻¹

$T = 294$ K

Plate, colourless

$0.47 \times 0.14 \times 0.05$ mm

Data collection

Bruker APEXII DUO CCD area-detector diffractometer

Radiation source: Rotating Anode

Graphite monochromator

Detector resolution: 18.4 pixels mm⁻¹

φ and ω scans

Absorption correction: multi-scan (SADABS; Bruker, 2012)

$T_{\min} = 0.303$, $T_{\max} = 0.842$

10857 measured reflections

3242 independent reflections

2260 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.037$

$\theta_{\max} = 27.8^\circ$, $\theta_{\min} = 1.6^\circ$

$h = -5 \rightarrow 5$

$k = -17 \rightarrow 15$

$l = -31 \rightarrow 33$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.041$

$wR(F^2) = 0.124$

$S = 1.04$

3242 reflections

172 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent
and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0691P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$$\begin{aligned}(\Delta/\sigma)_{\max} &= 0.001 \\ \Delta\rho_{\max} &= 0.47 \text{ e } \text{\AA}^{-3} \\ \Delta\rho_{\min} &= -0.33 \text{ e } \text{\AA}^{-3}\end{aligned}$$

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > 2\sigma(F^2)$ is used only for calculating -R-factor-obs 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	0.05103 (10)	0.56559 (3)	0.06384 (1)	0.0533 (2)
Cl1	1.1724 (3)	0.85319 (6)	0.33444 (4)	0.0585 (3)
Cl2	1.1077 (3)	0.48639 (7)	0.42380 (4)	0.0629 (4)
O1	0.6757 (10)	0.5127 (2)	0.25232 (11)	0.0795 (13)
C1	1.2349 (8)	0.7699 (2)	0.38553 (13)	0.0400 (10)
C2	1.3925 (9)	0.8068 (3)	0.43034 (14)	0.0482 (11)
C3	1.4602 (10)	0.7456 (3)	0.47251 (15)	0.0551 (12)
C4	1.3682 (9)	0.6477 (3)	0.46994 (13)	0.0489 (11)
C5	1.2137 (9)	0.6115 (2)	0.42448 (13)	0.0411 (10)
C6	1.1375 (8)	0.6695 (2)	0.38034 (12)	0.0344 (9)
C7	0.9826 (9)	0.6237 (2)	0.33364 (13)	0.0423 (11)
C8	0.8005 (9)	0.6605 (3)	0.29567 (13)	0.0464 (11)
C9	0.6625 (9)	0.6020 (3)	0.25107 (13)	0.0433 (11)
C10	0.5026 (8)	0.6542 (2)	0.20468 (12)	0.0386 (10)
C11	0.3737 (8)	0.5979 (2)	0.16350 (12)	0.0386 (10)
C12	0.2288 (8)	0.6434 (2)	0.12041 (12)	0.0377 (10)
C13	0.2083 (10)	0.7454 (3)	0.11687 (14)	0.0512 (12)
C14	0.3403 (11)	0.8019 (3)	0.15749 (15)	0.0572 (14)
C15	0.4858 (10)	0.7575 (3)	0.20135 (15)	0.0494 (11)
H2A	1.45350	0.87340	0.43210	0.0580*
H3A	1.56810	0.77070	0.50260	0.0660*
H4A	1.40930	0.60610	0.49850	0.0590*
H7A	1.02250	0.55590	0.33080	0.0510*
H8A	0.75310	0.72810	0.29640	0.0560*
H11A	0.38530	0.52900	0.16500	0.0460*
H13A	0.10710	0.77540	0.08750	0.0620*
H14A	0.33120	0.87080	0.15540	0.0680*
H15A	0.57290	0.79640	0.22870	0.0590*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0585 (3)	0.0625 (3)	0.0375 (2)	-0.0001 (2)	-0.0130 (2)	-0.0037 (2)
C11	0.0795 (7)	0.0395 (5)	0.0556 (6)	-0.0046 (4)	-0.0054 (5)	0.0095 (4)
C12	0.0904 (8)	0.0433 (5)	0.0526 (6)	-0.0130 (5)	-0.0208 (5)	0.0112 (4)
O1	0.140 (3)	0.0403 (16)	0.0538 (17)	0.0047 (16)	-0.0406 (19)	-0.0011 (13)
C1	0.0414 (18)	0.0401 (18)	0.0388 (18)	0.0025 (14)	0.0054 (15)	-0.0002 (14)
C2	0.048 (2)	0.0391 (19)	0.057 (2)	-0.0045 (15)	-0.0027 (18)	-0.0106 (17)
C3	0.055 (2)	0.063 (2)	0.046 (2)	-0.0017 (19)	-0.0109 (18)	-0.0121 (19)
C4	0.054 (2)	0.059 (2)	0.0326 (18)	0.0010 (17)	-0.0085 (16)	0.0005 (16)
C5	0.0442 (18)	0.0386 (18)	0.0397 (18)	-0.0044 (14)	-0.0064 (15)	0.0003 (15)
C6	0.0350 (16)	0.0346 (16)	0.0334 (16)	0.0022 (12)	-0.0016 (13)	-0.0028 (13)
C7	0.052 (2)	0.0357 (17)	0.0386 (18)	-0.0035 (14)	-0.0037 (16)	0.0023 (14)
C8	0.056 (2)	0.0400 (19)	0.0422 (19)	0.0092 (16)	-0.0095 (17)	-0.0037 (15)
C9	0.051 (2)	0.045 (2)	0.0334 (18)	0.0050 (15)	-0.0044 (15)	-0.0037 (15)
C10	0.0458 (19)	0.0355 (17)	0.0337 (17)	0.0019 (14)	-0.0057 (14)	-0.0033 (13)
C11	0.0445 (18)	0.0369 (17)	0.0346 (17)	0.0044 (14)	0.0028 (14)	0.0011 (14)
C12	0.0393 (17)	0.047 (2)	0.0262 (15)	0.0021 (14)	-0.0030 (13)	-0.0013 (14)
C13	0.062 (2)	0.052 (2)	0.039 (2)	0.0088 (17)	-0.0042 (17)	0.0087 (17)
C14	0.078 (3)	0.041 (2)	0.052 (2)	0.0057 (18)	-0.002 (2)	0.0036 (17)
C15	0.065 (2)	0.0416 (19)	0.0409 (19)	0.0018 (17)	-0.0048 (17)	-0.0043 (16)

Geometric parameters (Å, °)

Br1—C12	1.900 (3)	C10—C15	1.396 (5)
C11—C1	1.735 (3)	C11—C12	1.368 (4)
C12—C5	1.737 (3)	C12—C13	1.379 (5)
O1—C9	1.205 (5)	C13—C14	1.375 (5)
C1—C2	1.376 (5)	C14—C15	1.378 (6)
C1—C6	1.412 (4)	C2—H2A	0.9300
C2—C3	1.377 (5)	C3—H3A	0.9300
C3—C4	1.370 (6)	C4—H4A	0.9300
C4—C5	1.382 (5)	C7—H7A	0.9300
C5—C6	1.397 (4)	C8—H8A	0.9300
C6—C7	1.458 (4)	C11—H11A	0.9300
C7—C8	1.286 (5)	C13—H13A	0.9300
C8—C9	1.474 (5)	C14—H14A	0.9300
C9—C10	1.498 (5)	C15—H15A	0.9300
C10—C11	1.380 (4)		
C11—C1—C2	116.2 (2)	C11—C12—C13	121.4 (3)
C11—C1—C6	121.3 (2)	C12—C13—C14	118.8 (3)
C2—C1—C6	122.5 (3)	C13—C14—C15	120.7 (4)
C1—C2—C3	120.3 (4)	C10—C15—C14	120.0 (4)
C2—C3—C4	119.8 (4)	C1—C2—H2A	120.00
C3—C4—C5	119.2 (3)	C3—C2—H2A	120.00
C12—C5—C4	116.7 (3)	C2—C3—H3A	120.00

C12—C5—C6	119.4 (2)	C4—C3—H3A	120.00
C4—C5—C6	123.9 (3)	C3—C4—H4A	120.00
C1—C6—C5	114.3 (3)	C5—C4—H4A	120.00
C1—C6—C7	125.9 (3)	C6—C7—H7A	114.00
C5—C6—C7	119.8 (3)	C8—C7—H7A	114.00
C6—C7—C8	131.4 (3)	C7—C8—H8A	118.00
C7—C8—C9	123.9 (4)	C9—C8—H8A	118.00
O1—C9—C8	119.9 (3)	C10—C11—H11A	120.00
O1—C9—C10	120.4 (3)	C12—C11—H11A	120.00
C8—C9—C10	119.6 (3)	C12—C13—H13A	121.00
C9—C10—C11	118.6 (3)	C14—C13—H13A	121.00
C9—C10—C15	122.3 (3)	C13—C14—H14A	120.00
C11—C10—C15	119.1 (3)	C15—C14—H14A	120.00
C10—C11—C12	120.0 (3)	C10—C15—H15A	120.00
Br1—C12—C11	119.9 (2)	C14—C15—H15A	120.00
Br1—C12—C13	118.7 (2)		
C11—C1—C2—C3	-178.4 (3)	C7—C8—C9—O1	10.9 (6)
C6—C1—C2—C3	-0.3 (5)	C7—C8—C9—C10	-169.8 (3)
C11—C1—C6—C5	178.3 (2)	O1—C9—C10—C11	-0.5 (5)
C11—C1—C6—C7	0.8 (5)	O1—C9—C10—C15	-179.2 (4)
C2—C1—C6—C5	0.2 (5)	C8—C9—C10—C11	-179.7 (3)
C2—C1—C6—C7	-177.3 (3)	C8—C9—C10—C15	1.6 (5)
C1—C2—C3—C4	-0.4 (6)	C9—C10—C11—C12	-179.4 (3)
C2—C3—C4—C5	1.2 (6)	C15—C10—C11—C12	-0.7 (5)
C3—C4—C5—C12	179.4 (3)	C9—C10—C15—C14	179.1 (4)
C3—C4—C5—C6	-1.3 (6)	C11—C10—C15—C14	0.4 (5)
C12—C5—C6—C1	179.9 (3)	C10—C11—C12—Br1	-179.9 (2)
C12—C5—C6—C7	-2.4 (4)	C10—C11—C12—C13	0.2 (5)
C4—C5—C6—C1	0.6 (5)	Br1—C12—C13—C14	-179.2 (3)
C4—C5—C6—C7	178.3 (3)	C11—C12—C13—C14	0.7 (5)
C1—C6—C7—C8	-26.8 (6)	C12—C13—C14—C15	-1.0 (6)
C5—C6—C7—C8	155.8 (4)	C13—C14—C15—C10	0.5 (6)
C6—C7—C8—C9	-179.8 (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>
C8—H8A...C11	0.93	2.54	3.128 (4)	122