Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

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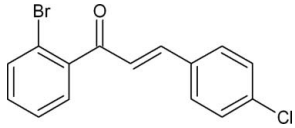
Received 3 June 2010; accepted 7 June 2010

Key indicators: single-crystal X-ray study; T = 110 K; mean σ(C–C) = 0.005 Å; R factor = 0.044; wR factor = 0.126; data-to-parameter ratio = 15.1.

In the title compound, $C_{15}H_{10}BrClO$, the dihedral angle between the mean planes of the benzene rings in the *ortho*-bromo- and *para*-chloro-substituted rings is 70.5 (6)°. The dihedral angles between the mean plane of the prop-2-en-1-one group and the mean planes of the benzene rings in the 4-chlorophenyl and 2-bromophenyl rings are 14.9 (3) and 63.3 (8)°, respectively. In the crystal, inversion dimers linked by pairs of weak C—H···O interactions are observed as well as aromatic π–π stacking interactions.

Related literature

For the radical quenching properties of the phenol groups present in many chalcones, see: Dhar (1981). For the anti-cancer activity of chalcones, see: Dimmock *et al.* (1999) and for their antimalarial activity, see: Troeberg *et al.* (2000). For their non-linear optical properties, see: Sarojini *et al.* (2006). For related structures, see: Fun *et al.* (2008); Li *et al.* (2009); Ng *et al.* (2006); Teh *et al.* (2007); Yang *et al.* (2006), Jasinski *et al.* (2009, 2010). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{15}H_{10}BrClO$
M_r = 321.59
Monoclinic, $P2_1/c$
a = 5.7317 (6) Å
b = 9.3920 (7) Å
c = 23.6517 (18) Å
β = 91.231 (8)°
V = 1272.9 (2) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 6.19 mm^{-1}
T = 110 K
0.84 × 0.49 × 0.13 mm

Data collection

Oxford Diffraction Xcalibur Ruby Gemini R diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.039, T_{max} = 0.512
4362 measured reflections
2466 independent reflections
2275 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.126
S = 1.05
2466 reflections
163 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.80 e Å^{-3}
$\Delta\rho_{min}$ = −1.07 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14A···O^{i}	0.95	2.44	3.319 (4)	154

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2007); 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: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

KV thanks the UGC for the sanction of a Junior Research Fellowship and for a SAP Chemical grant. HSY thanks UOM for sabbatical leave. RJB acknowledges the NSF MRI program (grant No. CHE-0619278) for funds to purchase the X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2282).

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supporting information

Acta Cryst. (2010). E**66**, o1638 [doi:10.1107/S1600536810021562]

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

Jerry P. Jasinski, Ray J. Butcher, K. Veena, B. Narayana and H. S. Yathirajan

S1. Comment

Chalcones, or 1,3-diaryl-2-propen-1-ones, belong to the flavonoid family. Chemically they consist of open-chain flavonoids in which the two aromatic rings are joined by a three-carbon *α*,*β*-unsaturated carbonyl system. A vast number of naturally occurring chalcones are polyhydroxylated in the aryl rings. The radical quenching properties of the phenol groups present in many chalcones have raised interest in using the compounds or chalcone rich plant extracts as drugs or food preservatives (Dhar, 1981). Chalcones have been reported to possess many useful properties, including anti-inflammatory, antimicrobial, antifungal, antioxidant, cytotoxic, anticancer activities (Dimmock *et al.*, 1999). Many chalcones have been described for their high antimalarial activity, probably as a result of Michael addition of nucleophilic species to the double bond of the enone (Troeberg *et al.*, 2000). Chalcones are finding applications as organic non-linear optical materials (NLO) due to their good SHG conversion efficiencies (Sarojini *et al.*, 2006). Hence, in continuation with our synthesis and crystal structure determinations of similar compounds (Jasinski *et al.*, 2009; Jasinski *et al.*, 2010) and also owing to the importance of these flavanoid analogs, this new bromo-chloro substituted chalcone, $C_{15}H_{10}BrClO$, is synthesized and its crystal structure is reported.

The title compound, $C_{15}H_{10}BrClO$, is a chalcone with 4-chlorophenyl and 2-bromophenyl rings bonded to opposite sides of a propenone group (Fig. 2). The dihedral angle between mean planes of the benzene rings in the *ortho*-bromo and *para*-chloro substituted rings is 70.5 (6)°. The angle between the mean plane of the prop-2-ene-1-one group (C1/C7/O/C8) and the mean planes of the benzene rings in the 4-chlorophenyl (C10–CC15) and 2-bromophenyl rings (C1–C6) are 14.9 (3)° and 63.3 (8)°, respectively. Bond distances and angles are in normal ranges (Allen *et al.*, 1987). While no classical hydrogen bonds are present, a weak intermolecular C14—H14A···O interaction (Table 1) and weak *π*-*π* stacking interactions [Cg2_perp···Cg2_perp = 3.3466 (14) Å; slippage = 2.931 Å; 1-x, 2-y, 1-z] are observed which contribute to the stability of crystal packing (Fig. 3).

S2. Experimental

A 50% KOH solution was added to a mixture of 2-bromo acetophenone (0.01 mol, 1.99 g) and 4-chloro benzaldehyde (0.01 mol, 1.40 g) in 25 ml of ethanol (Fig. 1). The mixture was stirred for an hour at room temperature and the precipitate was collected by filtration and purified by recrystallization from ethanol. The single-crystal was grown from ethyl acetate by slow evaporation and the yield of the compound was 58% (m.p.368–370 K). Analytical data: Composition (%) found (Calculated): C: 55.97 (56.02); H: 3.09(3.13).

S3. Refinement

The H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C–H distances = 0.95Å and with U_{iso}(H) = 1.18–1.22 U_{eq}(C).

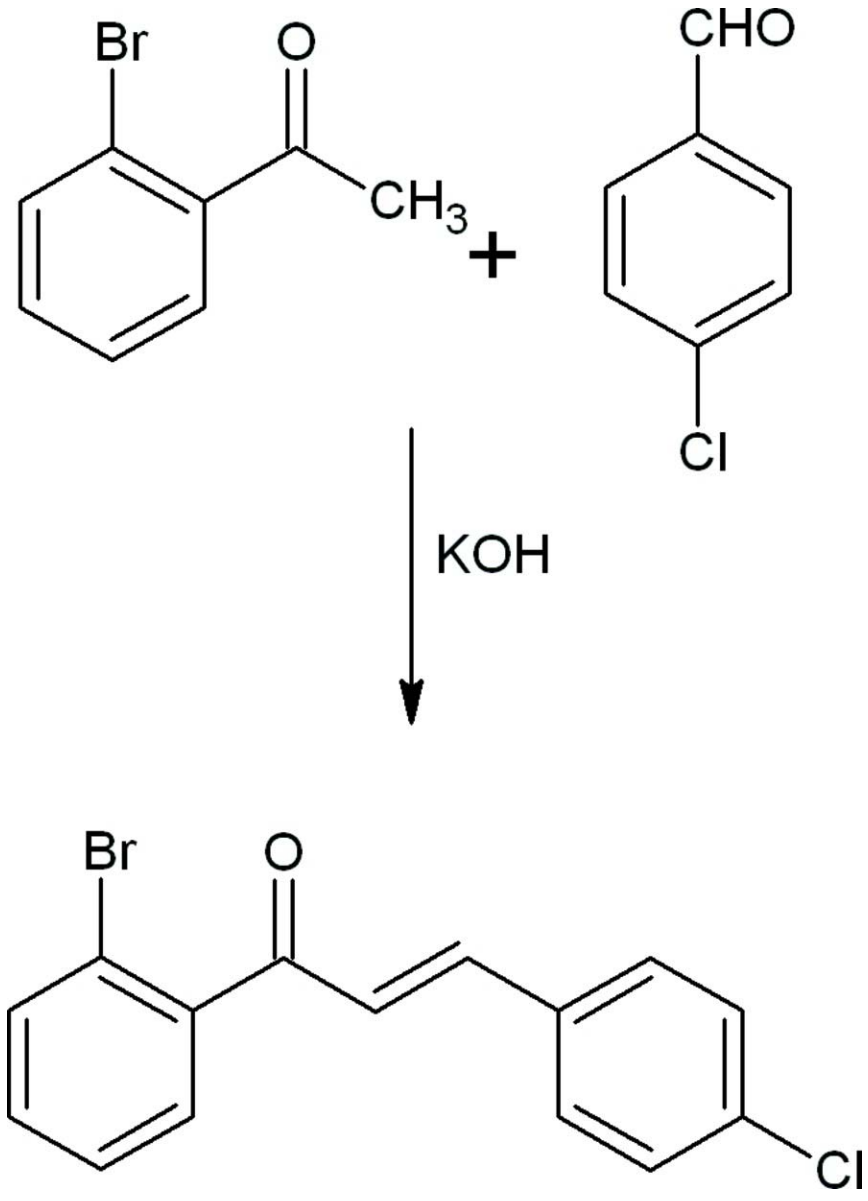

Figure 1

Reaction Scheme for the title compound.

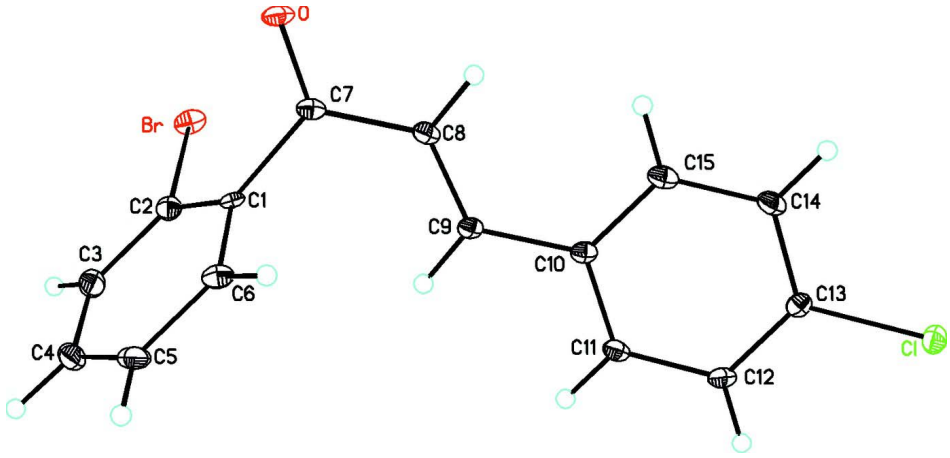

Figure 2

Molecular structure of the title compound, $C_{15}H_{10}BrClO$, showing the atom labeling scheme and 50% probability displacement ellipsoids.

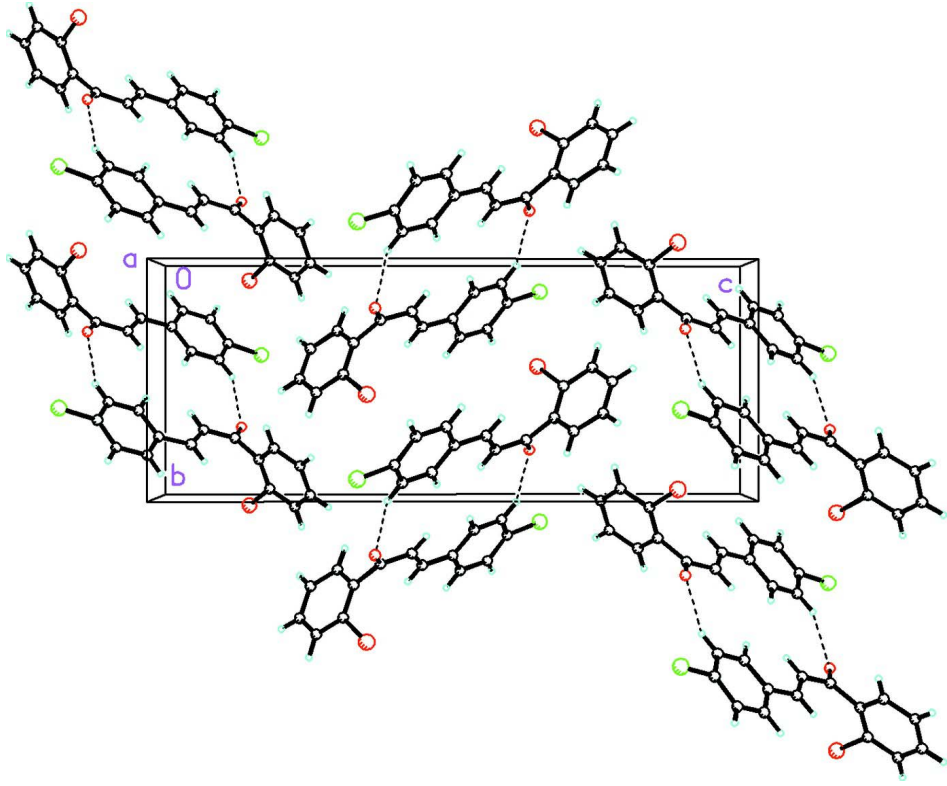

Figure 3

Packing diagram of the title compound, $C_{15}H_{10}BrClO$ viewed down the *a* axis. Dashed lines indicate a weak C—H···O intermolecular hydrogen bond interaction which links the molecules into chains along the (011) direction.

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Crystal data

$C_{15}H_{10}BrClO$
$M_r = 321.59$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 5.7317$ (6) Å
$b = 9.3920$ (7) Å
$c = 23.6517$ (18) Å
$\beta = 91.231$ (8)°
$V = 1272.9$ (2) Å^3
$Z = 4$
$F(000) = 640$
$D_x = 1.678$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 2738 reflections
$\theta = 4.7$–$74.2°$
$\mu = 6.19$ mm^{-1}
$T = 110$ K
Plate, yellow
0.84 × 0.49 × 0.13 mm

Data collection

Oxford Diffraction Xcalibur Ruby Gemini R diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 10.5081 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
$T_{min} = 0.039$, $T_{max} = 0.512$
4362 measured reflections
2466 independent reflections
2275 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 74.2°$, $\theta_{min} = 5.1°$
$h = -6 \rightarrow 6$
$k = -11 \rightarrow 10$
$l = -25 \rightarrow 29$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.126$
$S = 1.05$
2466 reflections
163 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0875P)^2 + 2.2371P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.80$ e Å^{-3}
$\Delta\rho_{min} = -1.07$ e Å^{-3}

Special details

Experimental. IR data (KBr) *v* cm^{-1}: 2837 cm^{-1}, 2966 cm^{-1}, (C—H al. str) 3061 cm^{-1}, (C—H ar. str), 1655 cm^{-1} (C=O), 1584 cm^{-1} (C=C); 1254 cm^{-1} (C—O—C).

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}
Br	−0.27391 (6)	0.44265 (4)	0.639317 (15)	0.02097 (17)
Cl	0.85133 (14)	0.88426 (9)	0.35152 (3)	0.0207 (2)

O	−0.2348 (4)	0.7916 (3)	0.62618 (11)	0.0207 (5)
C1	0.0767 (5)	0.6542 (3)	0.66371 (13)	0.0132 (6)
C2	−0.0160 (6)	0.5245 (4)	0.68014 (13)	0.0168 (7)
C3	0.0796 (7)	0.4490 (4)	0.72552 (15)	0.0228 (8)
H3A	0.0157	0.3598	0.7360	0.027*
C4	0.2681 (7)	0.5048 (4)	0.75513 (15)	0.0257 (8)
H4A	0.3305	0.4549	0.7869	0.031*
C5	0.3679 (6)	0.6328 (4)	0.73916 (14)	0.0230 (8)
H5A	0.4999	0.6697	0.7593	0.028*
C6	0.2715 (6)	0.7065 (4)	0.69309 (14)	0.0192 (7)
H6A	0.3399	0.7937	0.6816	0.023*
C7	−0.0380 (6)	0.7467 (3)	0.61912 (14)	0.0150 (6)
C8	0.0907 (6)	0.7835 (4)	0.56835 (13)	0.0163 (6)
H8A	0.0264	0.8560	0.5447	0.020*
C9	0.2903 (5)	0.7243 (3)	0.55238 (13)	0.0139 (6)
H9A	0.3548	0.6525	0.5763	0.017*
C10	0.4194 (5)	0.7595 (3)	0.50142 (13)	0.0143 (6)
C11	0.6205 (6)	0.6846 (4)	0.48865 (13)	0.0167 (7)
H11A	0.6685	0.6077	0.5122	0.020*
C12	0.7537 (6)	0.7200 (4)	0.44200 (14)	0.0173 (7)
H12A	0.8904	0.6676	0.4335	0.021*
C13	0.6820 (6)	0.8334 (4)	0.40819 (13)	0.0151 (6)
C14	0.4794 (6)	0.9079 (4)	0.41904 (14)	0.0189 (7)
H14A	0.4303	0.9836	0.3950	0.023*
C15	0.3494 (6)	0.8706 (4)	0.46533 (15)	0.0201 (7)
H15A	0.2100	0.9213	0.4728	0.024*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br	0.0157 (2)	0.0143 (2)	0.0329 (3)	−0.00300 (13)	0.00039 (15)	−0.00360 (12)
Cl	0.0199 (4)	0.0216 (4)	0.0206 (4)	−0.0025 (3)	0.0026 (3)	0.0022 (3)
O	0.0112 (12)	0.0199 (13)	0.0311 (12)	0.0037 (10)	0.0003 (9)	0.0024 (10)
C1	0.0071 (14)	0.0153 (15)	0.0173 (14)	0.0035 (12)	0.0011 (10)	−0.0007 (12)
C2	0.0191 (17)	0.0126 (15)	0.0187 (15)	0.0031 (13)	0.0017 (12)	−0.0013 (12)
C3	0.027 (2)	0.0180 (18)	0.0232 (16)	0.0062 (14)	0.0053 (14)	0.0054 (13)
C4	0.0289 (19)	0.030 (2)	0.0177 (15)	0.0130 (17)	−0.0004 (13)	0.0023 (14)
C5	0.0163 (17)	0.0297 (19)	0.0227 (16)	0.0080 (15)	−0.0047 (13)	−0.0056 (14)
C6	0.0130 (16)	0.0191 (17)	0.0255 (16)	0.0005 (13)	−0.0020 (12)	−0.0024 (13)
C7	0.0125 (15)	0.0094 (14)	0.0230 (15)	−0.0002 (12)	−0.0031 (11)	−0.0009 (12)
C8	0.0149 (16)	0.0143 (15)	0.0196 (15)	0.0009 (13)	−0.0029 (12)	0.0023 (12)
C9	0.0097 (15)	0.0122 (14)	0.0197 (14)	−0.0037 (12)	−0.0027 (11)	0.0012 (12)
C10	0.0113 (15)	0.0124 (15)	0.0190 (14)	−0.0022 (12)	−0.0030 (11)	−0.0017 (12)
C11	0.0143 (16)	0.0150 (15)	0.0207 (15)	−0.0005 (13)	−0.0045 (12)	0.0033 (12)
C12	0.0118 (15)	0.0161 (16)	0.0240 (15)	0.0016 (13)	−0.0021 (12)	−0.0005 (13)
C13	0.0121 (15)	0.0156 (16)	0.0176 (14)	−0.0046 (13)	−0.0019 (11)	−0.0022 (12)
C14	0.0186 (18)	0.0148 (15)	0.0232 (15)	0.0017 (14)	−0.0038 (12)	0.0030 (13)
C15	0.0187 (17)	0.0166 (17)	0.0249 (16)	0.0045 (14)	−0.0032 (13)	0.0011 (13)

Geometric parameters (Å, º)

Br—C2	1.910 (3)	C8—C9	1.334 (5)
Cl—C13	1.739 (3)	C8—H8A	0.9500
O—C7	1.219 (4)	C9—C10	1.466 (4)
C1—C2	1.388 (5)	C9—H9A	0.9500
C1—C6	1.392 (4)	C10—C11	1.389 (5)
C1—C7	1.506 (4)	C10—C15	1.402 (5)
C2—C3	1.389 (5)	C11—C12	1.395 (5)
C3—C4	1.378 (6)	C11—H11A	0.9500
C3—H3A	0.9500	C12—C13	1.389 (5)
C4—C5	1.387 (6)	C12—H12A	0.9500
C4—H4A	0.9500	C13—C14	1.384 (5)
C5—C6	1.395 (5)	C14—C15	1.383 (5)
C5—H5A	0.9500	C14—H14A	0.9500
C6—H6A	0.9500	C15—H15A	0.9500
C7—C8	1.464 (4)		
C2—C1—C6	118.5 (3)	C7—C8—H8A	117.1
C2—C1—C7	122.6 (3)	C8—C9—C10	126.2 (3)
C6—C1—C7	118.6 (3)	C8—C9—H9A	116.9
C1—C2—C3	121.2 (3)	C10—C9—H9A	116.9
C1—C2—Br	120.6 (2)	C11—C10—C15	118.2 (3)
C3—C2—Br	118.3 (3)	C11—C10—C9	120.0 (3)
C4—C3—C2	119.4 (3)	C15—C10—C9	121.7 (3)
C4—C3—H3A	120.3	C10—C11—C12	121.5 (3)
C2—C3—H3A	120.3	C10—C11—H11A	119.3
C3—C4—C5	121.0 (3)	C12—C11—H11A	119.3
C3—C4—H4A	119.5	C13—C12—C11	118.5 (3)
C5—C4—H4A	119.5	C13—C12—H12A	120.7
C4—C5—C6	118.9 (3)	C11—C12—H12A	120.7
C4—C5—H5A	120.5	C14—C13—C12	121.3 (3)
C6—C5—H5A	120.5	C14—C13—Cl	119.3 (3)
C1—C6—C5	121.0 (3)	C12—C13—Cl	119.4 (3)
C1—C6—H6A	119.5	C15—C14—C13	119.2 (3)
C5—C6—H6A	119.5	C15—C14—H14A	120.4
O—C7—C8	120.9 (3)	C13—C14—H14A	120.4
O—C7—C1	119.7 (3)	C14—C15—C10	121.2 (3)
C8—C7—C1	119.4 (3)	C14—C15—H15A	119.4
C9—C8—C7	125.7 (3)	C10—C15—H15A	119.4
C9—C8—H8A	117.1		
C6—C1—C2—C3	1.2 (5)	O—C7—C8—C9	−169.4 (3)
C7—C1—C2—C3	−172.9 (3)	C1—C7—C8—C9	11.8 (5)
C6—C1—C2—Br	−177.0 (2)	C7—C8—C9—C10	179.4 (3)
C7—C1—C2—Br	8.8 (4)	C8—C9—C10—C11	−177.2 (3)
C1—C2—C3—C4	0.8 (5)	C8—C9—C10—C15	4.7 (5)
Br—C2—C3—C4	179.0 (3)	C15—C10—C11—C12	1.4 (5)

C2—C3—C4—C5	−2.1 (6)	C9—C10—C11—C12	−176.8 (3)
C3—C4—C5—C6	1.3 (5)	C10—C11—C12—C13	0.4 (5)
C2—C1—C6—C5	−2.0 (5)	C11—C12—C13—C14	−2.0 (5)
C7—C1—C6—C5	172.4 (3)	C11—C12—C13—Cl	177.4 (2)
C4—C5—C6—C1	0.7 (5)	C12—C13—C14—C15	1.7 (5)
C2—C1—C7—O	60.4 (4)	Cl—C13—C14—C15	−177.7 (3)
C6—C1—C7—O	−113.7 (4)	C13—C14—C15—C10	0.2 (5)
C2—C1—C7—C8	−120.8 (3)	C11—C10—C15—C14	−1.7 (5)
C6—C1—C7—C8	65.1 (4)	C9—C10—C15—C14	176.5 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14*A*···O^{i}	0.95	2.44	3.319 (4)	154

Symmetry code: (i) −*x*, −*y*+2, −*z*+1.