Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

Crystal structure and Hirshfeld surface studies of 4-bromo-2-chlorophenyl (2*E*)-3-[4-(pentyloxy)-phenyl]prop-2-enoate

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Received 14 February 2025
Accepted 12 April 2025

Edited by F. Di Salvo, University of Buenos Aires, Argentina

Keywords: crystal structure; 4-bromo-2-chlorophenyl; Hirshfeld surface.

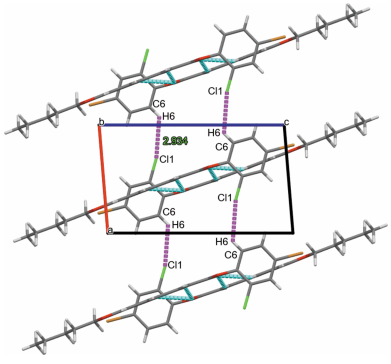
CCDC reference: 2443273

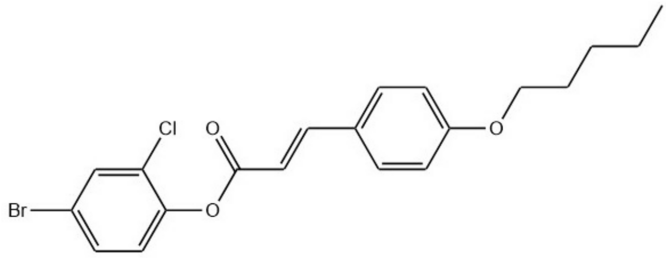
Supporting information: this article has supporting information at journals.iucr.org/e

The asymmetric unit of the compound $C_{20}H_{20}BrClO_3$ contains one independent molecule in which the aromatic rings are oriented at a dihedral angle of 83.30 (2)°. An intramolecular C—H···O contact generates a five-membered $S(5)$ ring motif. In the crystal, C—H···O hydrogen bonds link the molecules through $R_2^1(6)$, $R_2^2(10)$, $R_2^2(14)$ hydrogen-bond motifs. The structure is consolidated by C—H···π interactions. A Hirshfeld surface analysis of the crystal structure indicates that the most important contributions for the crystal packing are from H···H (32.8%), C···H/H···C (28.1%), O···H/H···O (14.0%) Br···H/H···Br (12.5%) and Cl···H/H···Cl (10.6%) interactions.

1. Chemical context

4-Bromo-2-chlorophenyl derivatives possess an interesting *in vitro* inhibitory activity on plasmodium falciparum bacteria and serve as the starting molecule for structure-based design of novel inhibitors for anti-plasmodial and transmission-blocking agents (Vallone *et al.*, 2018). These compounds are known to exhibit anti-malarial activity (Kos *et al.*, 2022). Compounds having halogen atoms at the *ortho* and *meta* positions with respect to the bromine have also been found to exhibit anti-inflammatory activity (Hošek *et al.*, 2019). This class of compounds are very important for the design of drugs for the treatment of diseases such as dengue and chikungunya and furthermore, the introduction of alkyl groups into these compounds will induce better penetration capacity at the cellular level. Compounds obtained by combining 4-bromo-2-chlorophenyl and (alkyloxy)phenyl-derived molecules are well known for their antimicrobial activity (Radwan *et al.*, 2014) and antitumor properties (Jung *et al.*, 2019; Pieters *et al.*, 1999). The role of alkyl groups in the various drug molecules is to speed up the penetration of compounds into the cell *i.e.* into mitochondria. In this context, it is found that decylcaffeic acid inhibits the growth of colorectal cancer cells (Lukáč *et al.*, 2024) and alkyl groups in cinnamic acid-based molecules encourage antituberculosis activity (De *et al.*, 2011). The alkyl group, which makes an amido links with various aromatic or heterocyclic rigid cores, will enhance the degree of inhibition activity of anti-inflammatory drugs (Matta *et al.*, 2020). Keeping these properties in mind, we decided to synthesize and study the title compound, which has both a rigid core (4-bromo-2-chlorophenyl) and an alkyloxy chain linked through the ester group and present the results herein.





2. Structural commentary

The title compound (Fig. 1) crystallizes in space group $P\overline{1}$. The dihedral angle between the 4-bromo-2-chlorophenyl aromatic ring (C1–C6) and the aromatic ring of the pentyloxy phenyl fragment (C10–C15) is 83.30 (2)°. The torsion angles C1—O1—C7—C8 and C13—O3—C16—C17 are 175.98 (14) and −179.32 (14)°, respectively, which are *anti-periplanar*. The H8—C8═C9—H9 atoms exhibit an *E*-configuration with a torsion angle of 178° and the molecule is non planar with an r.m.s. deviation of 0.065 Å. An intramolecular hydrogen-bond interaction generates an *S*(5) motif (Fig. 2*b*).

3. Supramolecular features

In the crystal, C—H···O hydrogen bonds (Table 1, Fig. 2*a*) link the molecules through $R_2^1(6)$, $R_2^2(10)$ and $R_2^2(14)$ cyclic hydrogen-bond motifs (Bernstein *et al.*, 1995), forming inversion dimers. Together these interactions generate molecular sheets parallel to (010). The inversion dimers are linked through weak C—H···Cl interactions (Table 1) as shown in Fig. 3. The packing is further consolidated by C—H···π interactions (Fig. 4, Table 1).

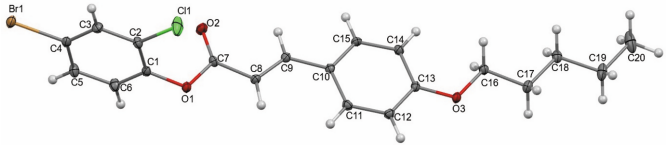


Figure 1
The molecular structure of the title compound, showing displacement ellipsoids drawn at the 50% probability level.

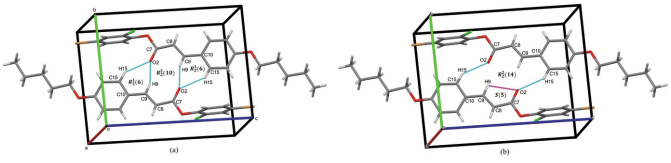


Figure 2
The molecular packing of the title compound. Dashed lines indicate the C—H···O hydrogen-bonding interactions. The $R_2^1(6)$, $R_2^2(10)$ (*a*) and $R_2^2(14)$ (*b*) synthons are indicated by dotted pale-green lines and the *S*(5) ring is shown in pink (*b*).

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

*Cg*1 and *Cg*2 are the centroids of the 4-bromo-2-chlorophenyl (C1–C6) and phenyl (C10–C15) rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···Cl1^{i}	0.93	2.93	3.613 (2)	131
C9—H9···O2	0.93	2.50	2.848 (2)	102
C9—H9···O2^{ii}	0.93	2.46	3.291 (2)	149
C15—H15···O2^{ii}	0.93	2.58	3.371 (2)	143
C11—H11···*Cg*1^{iii}	0.93	2.76	3.5716 (18)	147
C16—H16*B*···*Cg*2^{iv}	0.97	2.79	3.6687 (17)	151
C18—H18*B*···*Cg*2^{v}	0.97	2.85	3.7194 (17)	150

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

4. Hirshfeld surface analysis

Hirshfeld surface analysis (Hirshfeld, 1977; Spackman & Jayatilaka, 2009) was used to visualize and quantify intermolecular interactions using *Crystal Explorer* (Spackman *et*

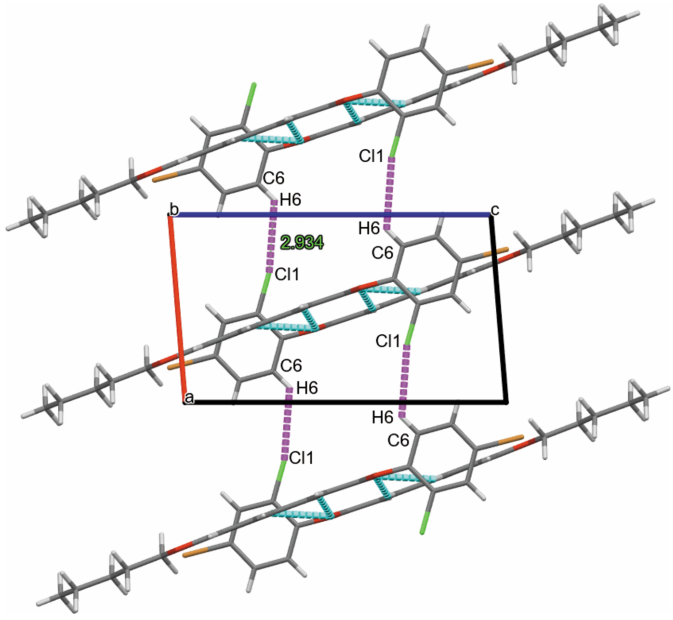


Figure 3
The molecular packing of the title compound with weak C—H···Cl interactions indicated by magenta coloured dashed lines.

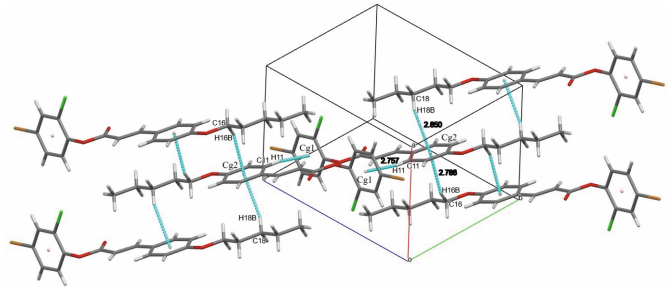


Figure 4
The molecular packing of the title compound. Dashed lines indicate the C—H···π interactions.

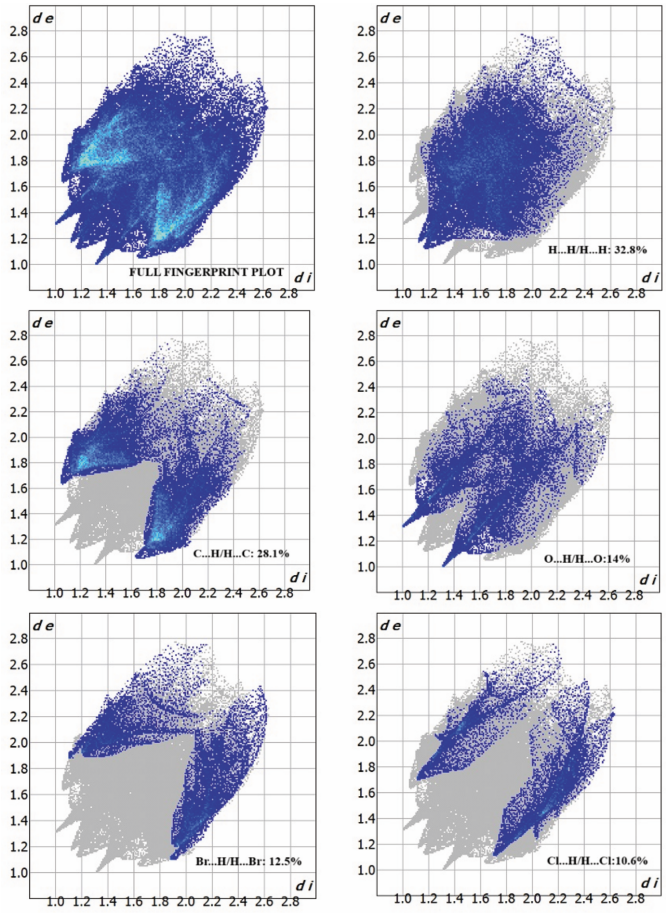


Figure 5
The two-dimensional fingerprint plots for the title compound, showing all interactions, and those delineated into H···H, C···H/H···C, O···H/H···O, Br···H/H···Br and Cl···H/H···Cl contacts.

al., 2021). The two-dimensional fingerprint plots (Fig. 5) quantifying the various intermolecular interactions indicate that the major contributions to the crystal packing of the title molecule are from H···H (32.8%), C··· H/H ···C (28.1%), O···H/H···O (14.0%), Br···H/H···Br (12.5%) and Cl···H/H···Cl (10.6%) contacts.

5. Database survey

A search of the Cambridge Structural Database (CSD version 2.0.4, December 2019; Groom *et al.*, 2016) for molecules containing the 4-bromo-2-chlorophenyl moiety resulted in 15 matches. Of these, the six compounds with CSD codes EBEPUZ (Lehmler *et al.*, 2013), EJULUT (Dumitrescu *et al.*, 2020), ISOJUX (Reddy *et al.*, 2016), FANFOS (Sangeeta *et al.*, 2017) and VIDQUX (Mohan *et al.*, 2018) have either alkyloxy or substituted aromatic or heterocyclic rings connected fragments that are found to be in the same plane. The dihedral angle made by these planes with the 4-bromo-2-chlorophenyl moiety are 59.0, 75.3, 88.78, 37.47, and 2.99°, respectively, whereas in the title compound, the dihedral angle between the 4-bromo-2-chlorophenyl and (pentyloxy)phenylprop-2-enoate moieties is 82.15 (2)°. The torsion angle between the *ortho*-substituted chlorine atom and the first atom of the planar functional group in the above compounds is between 1 and 3° while in the title compound this torsion angle is 1.2 (2)°.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{20}BrClO_3$
M_r	423.72
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, b, c (Å)	7.5850 (7), 9.825 (1), 12.8466 (13)
α, β, γ (°)	87.176 (3), 85.069 (3), 82.934 (3)
V (Å^3)	945.85 (16)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	2.33
Crystal size (mm)	0.32 × 0.27 × 0.24
Data collection	
Diffractometer	Bruker *SMART* APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.476, 0.570
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14284, 4721, 4105
R_{int}	0.035
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.668
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.027, 0.066, 1.03
No. of reflections	4721
No. of parameters	227
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.39, −0.45

Computer programs: *APEX2* and *SAINT* (Bruker, 2017), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*) and *Mercury* (Macrae *et al.*, 2020).

6. Synthesis and crystallization

A mixture of 4-bromo-2-chlorophenol (0.208 g, 0.001 mol) and (*E*)-3-[4-(pentyloxy)phenyl]acrylic acid (0.234 g, 0.001 mol) was suspended in anhydrous chloroform (10 ml). To this was added *N*,*N*-dicyclohexylcarbodiimide (0.206 g, 0.001 mol) and 4-*N*,*N*-dimethylamino pyridine (5 mg) and the mixture stirred overnight at room temperature. The *N*,*N*-dicyclohexyl urea formed was filtered off and the filtrate diluted with chloroform (25 ml). This solution was washed successively with 5% aqueous acetic acid solution (2 × 25 ml) and water (2 × 25 ml) and dried on sodium sulfate. The residue obtained on removal of solvent was chromatographed on silica gel using chloroform as eluent. Removal of solvent from the eluate afforded a white material that was crystallized from a chloroform–petroleum ether mixture. Yield 75%. Elemental analysis calculated: C, 56.69; H, 4.76; Br, 18.86; Cl, 8.37; O, 11.33%; found: C, 56.71; H, 4.79; Cl, 8.42%, m.p. 371–373 K.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C).

Acknowledgements

The authors acknowledge the Raman Research Institute, Bangalore, and Centre of Innovative Science, Engineering and Education (CISEE), UCS, Tumkur University, for constant support in extending the laboratory facilities. MHK thankful to BSPM's lab for use of their computing facilities at the Department of PG Studies and Research in Physics, Tumkur University.

Funding information

Funding for this research was provided by: Vission Group of Science and Technology (award No. GRD319 to B. S. Palakshamurthy).

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supporting information

Acta Cryst. (2025). E**81**, 912-915 [https://doi.org/10.1107/S2056989025003317]

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Computing details

4-Bromo-2-chlorophenyl (2*E*)-3-[4-(pentyloxy)phenyl]prop-2-enoate

Crystal data

$C_{20}H_{20}BrClO_3$
M_r = 423.72
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 7.5850 (7) Å
b = 9.825 (1) Å
c = 12.8466 (13) Å
α = 87.176 (3)°
β = 85.069 (3)°
γ = 82.934 (3)°
V = 945.85 (16) Å^3
Z = 2
$F(000)$ = 432
Prism
D_x = 1.488 Mg m^{-3}
Melting point: 458 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4105 reflections
θ = 2.5–29.0°
μ = 2.33 mm^{-1}
T = 296 K
Prism, colourless
0.32 × 0.27 × 0.24 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 1.02 pixels mm^{-1}
φ and Ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.476, T_{max} = 0.570
14284 measured reflections
4721 independent reflections
4105 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 28.4°, θ_{min} = 2.7°
h = −10→10
k = −13→13
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.066
S = 1.03
4721 reflections
227 parameters
0 restraints
0.123 constraints
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
$w = 1/[\sigma^2(F_o^2) + (0.023P)^2 + 0.4253P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.18439 (3)	0.12617 (2)	1.03966 (2)	0.02099 (6)
Cl1	0.69315 (6)	0.12132 (7)	0.70527 (4)	0.03690 (13)
O3	0.78618 (16)	0.38029 (12)	−0.06342 (9)	0.0169 (2)
O1	0.38962 (16)	0.12409 (12)	0.57472 (9)	0.0169 (2)
O2	0.3931 (2)	0.35324 (13)	0.57369 (10)	0.0260 (3)
C4	0.2485 (2)	0.12778 (16)	0.89331 (13)	0.0159 (3)
C10	0.5853 (2)	0.35279 (16)	0.24860 (12)	0.0134 (3)
C12	0.6902 (2)	0.24985 (17)	0.08324 (13)	0.0154 (3)
H12	0.716007	0.172269	0.043468	0.018*
C8	0.4799 (2)	0.23374 (17)	0.41618 (13)	0.0151 (3)
H8	0.492031	0.148155	0.386742	0.018*
C7	0.4187 (2)	0.24945 (17)	0.52630 (13)	0.0155 (3)
C11	0.6237 (2)	0.23732 (17)	0.18630 (13)	0.0155 (3)
H11	0.604072	0.151208	0.214998	0.019*
C13	0.7190 (2)	0.37875 (17)	0.03838 (12)	0.0140 (3)
C9	0.5182 (2)	0.34530 (17)	0.35835 (13)	0.0147 (3)
H9	0.499875	0.427875	0.392337	0.018*
C1	0.3422 (2)	0.12854 (16)	0.68166 (13)	0.0147 (3)
C5	0.1161 (2)	0.12990 (18)	0.82517 (14)	0.0202 (4)
H5	−0.002839	0.131054	0.850218	0.024*
C3	0.4258 (2)	0.12611 (17)	0.85862 (13)	0.0184 (3)
H3	0.512420	0.124852	0.905778	0.022*
C15	0.6154 (2)	0.48017 (17)	0.20237 (13)	0.0154 (3)
H15	0.590935	0.557698	0.242285	0.018*
C14	0.6808 (2)	0.49489 (17)	0.09858 (13)	0.0156 (3)
H14	0.699023	0.581115	0.069501	0.019*
C17	0.8891 (2)	0.49610 (18)	−0.22259 (13)	0.0180 (3)
H17A	0.802673	0.458591	−0.260963	0.022*
H17B	0.997676	0.432518	−0.225787	0.022*
C18	0.9276 (2)	0.63480 (18)	−0.27262 (13)	0.0186 (3)
H18A	0.819067	0.698353	−0.266778	0.022*
H18B	1.014894	0.670824	−0.234011	0.022*
C2	0.4721 (2)	0.12635 (18)	0.75163 (14)	0.0176 (3)
C16	0.8173 (2)	0.51254 (17)	−0.11028 (13)	0.0159 (3)
H16A	0.902213	0.552149	−0.072138	0.019*
H16B	0.706771	0.573970	−0.107005	0.019*
C6	0.1655 (2)	0.13025 (18)	0.71820 (14)	0.0200 (4)
H6	0.078790	0.131658	0.671066	0.024*
C19	0.9971 (3)	0.6278 (2)	−0.38731 (14)	0.0263 (4)

H19A	1.108096	0.567089	−0.393177	0.032*
H19B	0.911805	0.589191	−0.425798	0.032*
C20	1.0284 (3)	0.7680 (3)	−0.43626 (17)	0.0380 (6)
H20A	1.074526	0.758169	−0.507796	0.057*
H20B	1.112534	0.806870	−0.398383	0.057*
H20C	0.917802	0.827400	−0.433463	0.057*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.02982 (11)	0.01924 (9)	0.01305 (9)	−0.00280 (7)	0.00343 (6)	−0.00147 (6)
Cl1	0.0158 (2)	0.0705 (4)	0.0242 (3)	−0.0090 (2)	0.00258 (18)	0.0020 (2)
O3	0.0247 (7)	0.0142 (6)	0.0112 (6)	−0.0028 (5)	0.0034 (5)	−0.0005 (4)
O1	0.0242 (6)	0.0139 (6)	0.0123 (6)	−0.0038 (5)	0.0028 (5)	0.0001 (4)
O2	0.0471 (9)	0.0141 (6)	0.0165 (6)	−0.0068 (6)	0.0047 (6)	−0.0028 (5)
C4	0.0220 (9)	0.0108 (8)	0.0141 (8)	−0.0016 (6)	0.0028 (6)	−0.0003 (6)
C10	0.0129 (8)	0.0148 (8)	0.0125 (8)	−0.0018 (6)	−0.0020 (6)	0.0005 (6)
C12	0.0177 (8)	0.0135 (8)	0.0149 (8)	−0.0010 (6)	−0.0008 (6)	−0.0026 (6)
C8	0.0171 (8)	0.0142 (8)	0.0139 (8)	−0.0019 (6)	0.0011 (6)	−0.0027 (6)
C7	0.0173 (8)	0.0147 (8)	0.0142 (8)	−0.0033 (6)	−0.0002 (6)	0.0022 (6)
C11	0.0170 (8)	0.0128 (8)	0.0166 (8)	−0.0031 (6)	−0.0006 (6)	0.0012 (6)
C13	0.0145 (8)	0.0161 (8)	0.0111 (8)	−0.0018 (6)	−0.0006 (6)	0.0000 (6)
C9	0.0150 (8)	0.0158 (8)	0.0135 (8)	−0.0015 (6)	−0.0010 (6)	−0.0019 (6)
C1	0.0206 (8)	0.0103 (7)	0.0125 (8)	−0.0015 (6)	0.0012 (6)	0.0009 (6)
C5	0.0162 (8)	0.0247 (9)	0.0186 (9)	−0.0022 (7)	0.0024 (7)	0.0028 (7)
C3	0.0190 (9)	0.0205 (9)	0.0162 (8)	−0.0041 (7)	−0.0024 (7)	−0.0006 (6)
C15	0.0189 (8)	0.0128 (8)	0.0147 (8)	−0.0025 (6)	−0.0003 (6)	−0.0034 (6)
C14	0.0192 (8)	0.0126 (8)	0.0147 (8)	−0.0024 (6)	−0.0001 (6)	0.0010 (6)
C17	0.0189 (8)	0.0211 (9)	0.0131 (8)	−0.0006 (7)	0.0011 (6)	−0.0013 (6)
C18	0.0171 (8)	0.0236 (9)	0.0144 (8)	−0.0022 (7)	0.0002 (6)	0.0022 (6)
C2	0.0146 (8)	0.0197 (9)	0.0184 (9)	−0.0043 (6)	0.0019 (6)	−0.0003 (6)
C16	0.0184 (8)	0.0151 (8)	0.0138 (8)	−0.0025 (6)	0.0012 (6)	0.0006 (6)
C6	0.0180 (8)	0.0253 (9)	0.0167 (9)	−0.0033 (7)	−0.0021 (7)	0.0021 (7)
C19	0.0214 (9)	0.0406 (12)	0.0145 (9)	0.0012 (8)	0.0016 (7)	0.0044 (8)
C20	0.0250 (11)	0.0560 (15)	0.0298 (12)	−0.0034 (10)	0.0016 (9)	0.0219 (10)

Geometric parameters (Å, º)

Br1—C4	1.9009 (16)	C5—C6	1.393 (2)
Cl1—C2	1.7263 (17)	C5—H5	0.9300
O3—C13	1.3623 (18)	C3—C2	1.389 (2)
O3—C16	1.4424 (19)	C3—H3	0.9300
O1—C7	1.3858 (19)	C15—C14	1.389 (2)
O1—C1	1.3914 (19)	C15—H15	0.9300
O2—C7	1.200 (2)	C14—H14	0.9300
C4—C3	1.378 (2)	C17—C16	1.507 (2)
C4—C5	1.385 (3)	C17—C18	1.528 (2)
C10—C15	1.395 (2)	C17—H17A	0.9700

C10—C11	1.407 (2)	C17—H17B	0.9700
C10—C9	1.459 (2)	C18—C19	1.523 (2)
C12—C11	1.381 (2)	C18—H18A	0.9700
C12—C13	1.399 (2)	C18—H18B	0.9700
C12—H12	0.9300	C16—H16A	0.9700
C8—C9	1.341 (2)	C16—H16B	0.9700
C8—C7	1.460 (2)	C6—H6	0.9300
C8—H8	0.9300	C19—C20	1.523 (3)
C11—H11	0.9300	C19—H19A	0.9700
C13—C14	1.397 (2)	C19—H19B	0.9700
C9—H9	0.9300	C20—H20A	0.9600
C1—C6	1.380 (2)	C20—H20B	0.9600
C1—C2	1.387 (2)	C20—H20C	0.9600

C13—O3—C16	116.35 (12)	C15—C14—C13	119.26 (15)
C7—O1—C1	114.71 (13)	C15—C14—H14	120.4
C3—C4—C5	122.21 (16)	C13—C14—H14	120.4
C3—C4—Br1	118.70 (13)	C16—C17—C18	110.16 (14)
C5—C4—Br1	119.09 (13)	C16—C17—H17A	109.6
C15—C10—C11	117.68 (15)	C18—C17—H17A	109.6
C15—C10—C9	118.90 (15)	C16—C17—H17B	109.6
C11—C10—C9	123.42 (14)	C18—C17—H17B	109.6
C11—C12—C13	120.30 (15)	H17A—C17—H17B	108.1
C11—C12—H12	119.8	C19—C18—C17	113.57 (15)
C13—C12—H12	119.8	C19—C18—H18A	108.9
C9—C8—C7	118.63 (15)	C17—C18—H18A	108.9
C9—C8—H8	120.7	C19—C18—H18B	108.9
C7—C8—H8	120.7	C17—C18—H18B	108.9
O2—C7—O1	121.15 (15)	H18A—C18—H18B	107.7
O2—C7—O1	121.15 (15)	C1—C2—C3	120.49 (15)
O2—C7—C8	127.83 (15)	C1—C2—Cl1	119.66 (13)
O2—C7—C8	127.83 (15)	C3—C2—Cl1	119.84 (14)
O1—C7—C8	111.02 (14)	O3—C16—C17	109.47 (13)
C12—C11—C10	121.05 (15)	O3—C16—H16A	109.8
C12—C11—H11	119.5	C17—C16—H16A	109.8
C10—C11—H11	119.5	O3—C16—H16B	109.8
O3—C13—C14	124.48 (14)	C17—C16—H16B	109.8
O3—C13—C12	115.88 (14)	H16A—C16—H16B	108.2
C14—C13—C12	119.64 (15)	C1—C6—C5	120.49 (17)
C8—C9—C10	127.86 (16)	C1—C6—H6	119.8
C8—C9—H9	116.1	C5—C6—H6	119.8
C10—C9—H9	116.1	C20—C19—C18	112.52 (18)
C6—C1—C2	119.99 (15)	C20—C19—H19A	109.1
C6—C1—O1	119.64 (15)	C18—C19—H19A	109.1
C2—C1—O1	120.32 (15)	C20—C19—H19B	109.1
C4—C5—C6	118.32 (16)	C18—C19—H19B	109.1
C4—C5—H5	120.8	H19A—C19—H19B	107.8
C6—C5—H5	120.8	C19—C20—H20A	109.5

C4—C3—C2	118.49 (16)	C19—C20—H20B	109.5
C4—C3—H3	120.8	H20A—C20—H20B	109.5
C2—C3—H3	120.8	C19—C20—H20C	109.5
C14—C15—C10	122.07 (15)	H20A—C20—H20C	109.5
C14—C15—H15	119.0	H20B—C20—H20C	109.5
C10—C15—H15	119.0		

C1—O1—C7—O2	−4.4 (2)	C5—C4—C3—C2	−0.1 (3)
C1—O1—C7—O2	−4.4 (2)	Br1—C4—C3—C2	179.57 (12)
C1—O1—C7—C8	175.98 (14)	C11—C10—C15—C14	0.1 (2)
C9—C8—C7—O2	1.9 (3)	C9—C10—C15—C14	179.33 (16)
C9—C8—C7—O2	1.9 (3)	C10—C15—C14—C13	−0.4 (3)
C9—C8—C7—O1	−178.50 (15)	O3—C13—C14—C15	−178.89 (15)
C13—C12—C11—C10	−0.7 (3)	C12—C13—C14—C15	0.2 (3)
C15—C10—C11—C12	0.5 (2)	C16—C17—C18—C19	−178.75 (15)
C9—C10—C11—C12	−178.75 (15)	C6—C1—C2—C3	−0.1 (3)
C16—O3—C13—C14	−0.5 (2)	O1—C1—C2—C3	−177.82 (15)
C16—O3—C13—C12	−179.66 (14)	C6—C1—C2—Cl1	178.92 (13)
C11—C12—C13—O3	179.49 (15)	O1—C1—C2—Cl1	1.2 (2)
C11—C12—C13—C14	0.3 (3)	C4—C3—C2—C1	0.1 (3)
C7—C8—C9—C10	178.25 (16)	C4—C3—C2—Cl1	−178.89 (13)
C15—C10—C9—C8	179.46 (17)	C13—O3—C16—C17	−179.32 (14)
C11—C10—C9—C8	−1.3 (3)	C18—C17—C16—O3	−178.46 (14)
C7—O1—C1—C6	100.14 (18)	O1—C1—C6—C5	177.77 (15)
C7—O1—C1—C2	−82.15 (19)	C17—C18—C19—C20	178.03 (16)
Br1—C4—C5—C6	−179.64 (13)		

Hydrogen-bond geometry (Å, º)

*Cg*1 and *Cg*2 are the centroids of the 4-bromo-2-chlorophenyl (C1–C6) and phenyl (C10–C15) rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···Cl1^{i}	0.93	2.93	3.613 (2)	131
C9—H9···O2	0.93	2.50	2.848 (2)	102
C9—H9···O2^{ii}	0.93	2.46	3.291 (2)	149
C15—H15···O2^{ii}	0.93	2.58	3.371 (2)	143
C11—H11···*Cg*1^{iii}	0.93	2.76	3.5716 (18)	147
C16—H16*B*···*Cg*2^{iv}	0.97	2.79	3.6687 (17)	151
C18—H18*B*···*Cg*2^{v}	0.97	2.85	3.7194 (17)	150

Symmetry codes: (i) *x*−1, *y*, *z*; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) −*x*+1, −*y*, −*z*+1; (iv) −*x*+1, −*y*+1, −*z*; (v) −*x*+2, −*y*+1, −*z*.