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Crystal structure and Hirshfeld surface analysis of 4-bromo-2-chlorophenyl (*E*)-3-[4-(undecyloxy)-phenyl]acrylate

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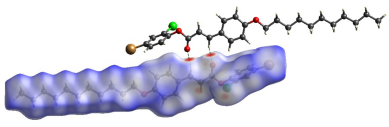
In the title compound, $C_{26}H_{32}BrClO_3$, the dihedral angle between the 4-bromo-2-chlorophenyl ring and the aromatic ring of (alkyloxy)phenyl moiety is found to be 77.21 (2)°. The torsion angle associated with the ester moiety is 173.2 (2)° which is *anti-periplanar*. In the crystal, intermolecular C—H···O hydrogen bonding links the molecules into cyclic hydrogen-bonded inversion dimers with $R_2^2(10)$ motifs. The molecular structure is associated with an inversion centre and connected through two symmetrical C—H···O interactions, forming $R_2^2(10)$ inversion dimer motif. The packing is further consolidated by C—H···π and C—Cl···π interactions. Hirshfeld surface analysis showed that the most significant contributions are from H···H (54.0%), C···H/H···C (15.2%), Br···H/H···Br (10.9%), O···H/H···O (7.8%) and Cl···H/H···Cl (2.6%) contacts.

1. Chemical context

Compounds based on the 4-bromo-2-chlorophenyl scaffold are found to exhibit potent *in vitro* inhibitory activity against *Plasmodium falciparum*, making them promising candidates as transmission-blocking agents for malaria treatment (Vallone *et al.*, 2018; Kos *et al.*, 2022). The incorporation of halogen substituents in the phenyl ring is known to enhance antimicrobial activity in such molecules (Radwan *et al.*, 2014). Acrylate derivatives have demonstrated antitumor potential by inhibiting tubulin polymerization at the cellular level (Pieters *et al.*, 1999; Jung *et al.*, 2019). The presence and prolongation of alkyl groups in the various drug molecules are found to enhance the penetration of the compounds into cells, which make the molecules efficient as drugs. In this context, it is found that caffeic acid phosphanium salt combined with alkyl chains acquire anticancer properties (Lukáč *et al.*, 2024), whereas cinnamic acid-based molecules coupled with alkyl groups exhibit anti-tuberculosis activity (De *et al.*, 2011). Furthermore, increasing the alkyl chain length on amido functional groups has been shown to improve the anti-inflammatory activities of certain drugs (Matta *et al.*, 2020). Studies on 4-bromophenyl piperidine derivatives revealed strong binding affinities towards the COVID-19 main protease, indicating potential antiviral activities (Lorin *et al.*, 2024). Similarly, chlorophenyl derivatives have demonstrated inhibitory effects against the SARS-CoV-2 main protease. Despite the promising pharmacological potential, limited research has been conducted on the medicinal significance of 4-bromo-2-chlorophenyl scaffolds. In view of this gap, we



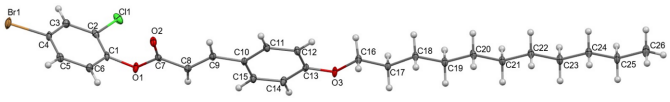
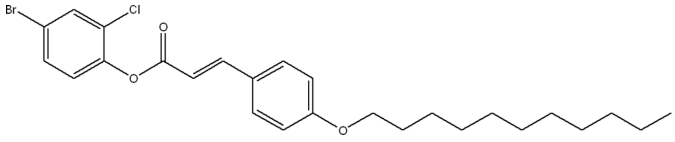


Figure 1
The title molecule with the atom-labelling scheme and 50% probability displacement ellipsoids.

aimed to design and synthesize a novel series of compounds incorporating this moiety. Herein, we present the synthesis and characterization of the title compound, constructed by coupling the 4-bromo-2-chlorophenyl unit with a (undecyloxy) phenyl fragment through an ester linkage.



2. Structural commentary

The title compound (Fig. 1) crystallizes in the space group $P\overline{1}$. The molecule is nearly planar with an r.m.s deviation of 0.076 Å. The dihedral angle between the mean planes of the 4-bromo-2-chlorophenyl ring and the aromatic ring of the (alkyloxy)phenyl moiety is 77.21 (2)°. With respect to the alkyl chain (O3–C26), the dihedral angle formed with the 4-bromo-2-chlorophenyl ring is 66.94 (2)°, while that with the phenyl ring is 10.59 (2)°, indicating a more coplanar orientation between the alkyl chain and the phenyl ring. The torsion angle associated with the ester moiety (C1—O1—C7—C8) is 173.1 (2)°, which is *anti-periplanar*. The molecule does not show any significant deviations in bond distances or angles.

3. Supramolecular features

In the crystal, C—H···O hydrogen bonding links the molecules into cyclic hydrogen-bonded inversion dimers with $R_2^2(10)$ motifs (Table 1, Fig. 2). The crystal packing is further consolidated by weak C—H···π interactions (Table 1, Fig. 3). In addition, a weak non-covalent C—Cl···π halogen···π interaction arising from the electrostatic attraction between the electron-deficient chlorine atom and the electron-rich π-system connects the molecules along the *a*-axis direction

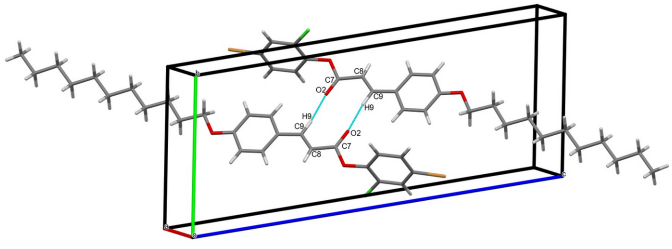


Figure 2
The molecular packing with intermolecular C—H···O interactions depicted by dashed pale- green coloured lines. Symmetry code: (i) $-x-1, -y+1, -z+1$.

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

*Cg*2 is the centroid of the C10–C15 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9···O2^{i}	0.93	2.35	3.248 (3)	164
C16—H16*A*···*Cg*2^{ii}	0.97	2.95	3.824 (3)	150

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

[Cl···*Cg*1 distance = 3.6415 (15) Å; *Cg*1 is the centroid for the 4-bromo-2-chlorophenyl ring (C1–C6); Fig. 4].

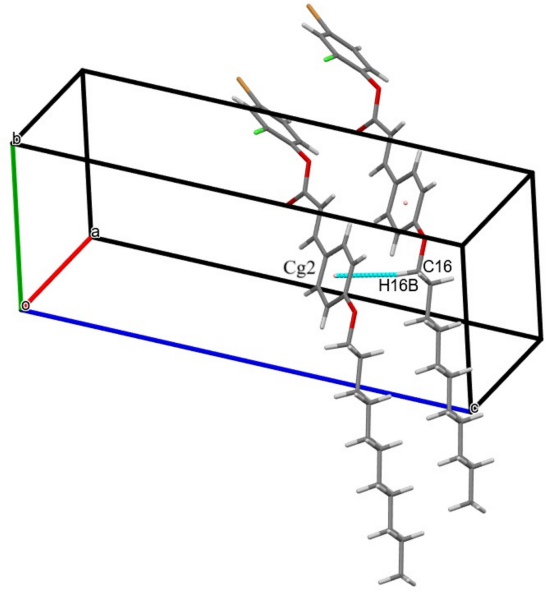


Figure 3
The crystal packing with the C—H···π interactions depicted by dashed pale-green lines. *Cg*2 is the centroid of the (C10–C15)($x+1, y, z$) ring.

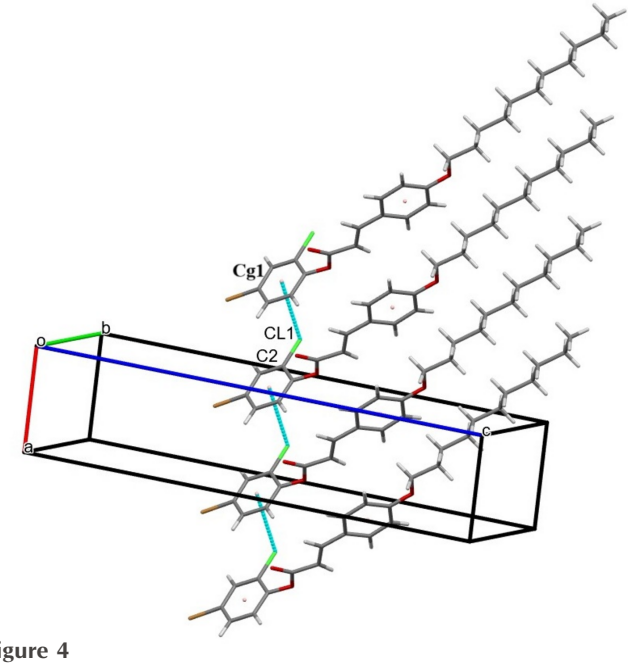


Figure 4
The crystal packing with weak C—Cl···*Cg*1 interactions depicted by dashed pale-green lines. *Cg*1 is the centroid of the C1–C6 ring.

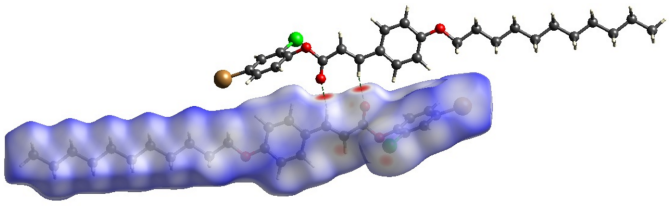


Figure 5
The Hirshfeld surface of the title compound plotted over d_{norm} with dashed lines indicating hydrogen bonds.

4. Hirshfeld surface analysis

The Hirshfeld surface (Spackman & Jayatilaka, 2009) and two-dimensional fingerprint plots (McKinnon *et al.*, 2007) were generated using *CrystalExplorer17* (Spackman *et al.*, 2021) to investigate the intermolecular interactions. The Hirshfeld surface mapped over d_{norm} is shown in Fig. 5. The prominent red spots on the iso-surface indicate the presence of significant intermolecular hydrogen-bond interactions, specifically C9—H9···O2, which play a stabilizing role in the crystal packing. The corresponding 2D fingerprint plots are shown in Fig. 6, quantifying the contribution of various intermolecular interactions to the overall crystal packing. The most significant contributions arise from H···H (54.0%), followed by C···H/H···C (15.3%), Br···H/H···Br (10.9%), O···H/H···O (7.7%) and Cl···H/H···Cl (4.5%) contacts. The sharp spikes in the 2D fingerprint plots correspond to the C9—H9···O2 hydrogen bond (O···H/H···O).

5. Database Survey

A search of the Cambridge Structural Database (CSD version 2.0.4, December 2024; Groom *et al.*, 2016) for molecules containing the 4-bromo-2-chlorophenyl moiety resulted in 15 matches. Among these, the five compounds with CSD codes EBEPUZ (Lehmler *et al.*, 2013), ISOJUX (Koti Reddy *et al.*, 2016), FANFOS (Sangeeta *et al.*, 2017), VIDQUX (Mohan *et al.*, 2018) and EJULUT (Dumitrescu *et al.*, 2020), are found to be substituted with fragments containing alkyloxy chains or substituted aromatic or heterocyclic rings that are in same plane. The dihedral angles between these planes and the 4-bromo-2-chlorophenyl moiety are 59.0, 75.3, 88.78, 37.47, and 2.99°. In the title compound, the dihedral angle between the 4-bromo-2-chlorophenyl ring and the planar (undecyloxy) phenyl)acrylate fragment is found to be 74.23 (3)°. The torsion angle between the *ortho*-substituted chlorine atom and the first atom of the planar side chain in the above compounds is between 1 to 4° whereas in the title compound it is 5.30 (4)°.

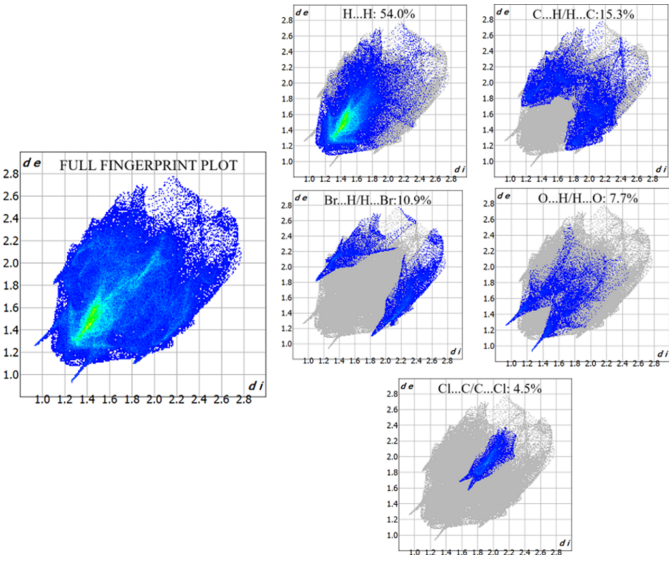
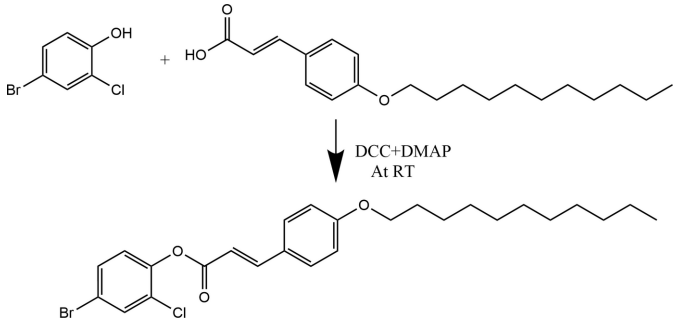


Figure 6
The two-dimensional fingerprint plots for the title compound, showing all interactions, and delineated into H···H, C···H/H···C, Br···H/H···Br, O···H/H···O, Cl···C/C···Cl, Cl···H/H···Cl, Cl···O/O···Cl, O···C/C···O, Cl···Cl, C···C, O···O and Br···C/C···Br interactions.

6. Synthesis and crystallization

A mixture of 4-bromo-2-chlorophenol (0.208 g, 0.001 mol) and (*E*)-3-[4-(undecyloxy)phenyl]acrylic acid (0.319 g, 0.001 mol) was suspended in anhydrous chloroform (10 ml). To this, *N*,*N*-dicyclohexylcarbodiimide (0.206 g, 0.001 mol) and 4-*N*,*N*-dimethylamino pyridine (5 mg) was added 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, which was crystallized from a chloroform–petroleum ether mixture. Yield (0.385 g, 73%), m.p. 338–340 K. Elemental analysis, calculated: C, 61.49; H, 6.35; Br, 15.73; Cl, 6.98; O, 9.45%, found: C, 61.52; H, 6.38; Br, 15.76; Cl, 6.95%.

7. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined using a riding model with $U_{iso}(H) = k*U_{eq}(C)$, where k= 1.5 for methyl hydrogen atoms and 1.2 for all others.

Acknowledgements

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Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{26}H_{32}BrClO_3$
M_r	507.87
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, b, c (Å)	5.5111 (8), 9.5856 (15), 23.532 (4)
α, β, γ (°)	81.251 (4), 86.986 (4), 88.012 (4)
V (Å^3)	1226.5 (3)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.81
Crystal size (mm)	0.27 × 0.24 × 0.20
Data collection	
Diffractometer	Bruker SMART APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.6, 0.7
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	17380, 6085, 5080
R_{int}	0.051
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.669
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.048, 0.114, 1.09
No. of reflections	6085
No. of parameters	281
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.90, −0.96

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2019/2* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2020) and *publCIF* (Westrip,2010).

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Computing details

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

Crystal data

$C_{26}H_{32}BrClO_3$
M_r = 507.87
Triclinic, $P\overline{1}$
a = 5.5111 (8) Å
b = 9.5856 (15) Å
c = 23.532 (4) Å
α = 81.251 (4)°
β = 86.986 (4)°
γ = 88.012 (4)°
V = 1226.5 (3) Å^3
Z = 2
$F(000)$ = 528
D_x = 1.375 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5080 reflections
θ = 2–28.4°
μ = 1.81 mm^{-1}
T = 296 K
Prism, colourless
0.27 × 0.24 × 0.20 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} = 0.6, T_{max} = 0.7
17380 measured reflections
6085 independent reflections
5080 reflections with $I > 2\sigma(I)$
R_{int} = 0.051
θ_{max} = 28.4°, θ_{min} = 2.6°
h = −7→7
k = −12→12
l = −31→31

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.114
S = 1.09
6085 reflections
281 parameters
0 restraints
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0321P)^2 + 1.7821P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.90 e Å^{-3}
$\Delta\rho_{min}$ = −0.96 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	−1.44231 (6)	0.07449 (4)	0.72273 (2)	0.03026 (10)
Cl1	−0.69598 (12)	−0.02663 (8)	0.56674 (3)	0.02653 (16)
O2	−0.7521 (3)	0.3939 (2)	0.51095 (8)	0.0204 (4)
O3	0.2021 (3)	0.4438 (2)	0.21602 (8)	0.0203 (4)
O1	−0.9273 (4)	0.2016 (2)	0.48915 (8)	0.0224 (4)
C4	−1.2718 (5)	0.1195 (3)	0.65019 (11)	0.0181 (5)
C10	−0.2950 (4)	0.4111 (3)	0.35655 (10)	0.0146 (5)
C12	0.0467 (5)	0.5320 (3)	0.30290 (11)	0.0175 (5)
H12	0.158485	0.603779	0.298670	0.021*
C13	0.0446 (4)	0.4401 (3)	0.26272 (10)	0.0157 (5)
C7	−0.7748 (4)	0.3133 (3)	0.47730 (11)	0.0148 (5)
C3	−1.0695 (5)	0.0384 (3)	0.63777 (11)	0.0196 (5)
H3	−1.013572	−0.035248	0.664720	0.024*
C5	−1.3567 (5)	0.2311 (3)	0.61188 (11)	0.0186 (5)
H5	−1.490918	0.285355	0.621850	0.022*
C1	−1.0382 (5)	0.1795 (3)	0.54418 (11)	0.0169 (5)
C8	−0.6485 (4)	0.3140 (3)	0.42096 (11)	0.0159 (5)
H8	−0.697304	0.256542	0.395425	0.019*
C11	−0.1211 (4)	0.5154 (3)	0.34965 (11)	0.0160 (5)
H11	−0.117004	0.575513	0.377070	0.019*
C2	−0.9519 (5)	0.0700 (3)	0.58382 (11)	0.0177 (5)
C17	0.5323 (5)	0.5294 (3)	0.15377 (11)	0.0180 (5)
H17A	0.429058	0.523176	0.122165	0.022*
H17B	0.620095	0.439804	0.162346	0.022*
C6	−1.2378 (5)	0.2615 (3)	0.55788 (11)	0.0189 (5)
H6	−1.292326	0.336328	0.531272	0.023*
C15	−0.2948 (5)	0.3201 (3)	0.31520 (11)	0.0174 (5)
H15	−0.409570	0.250043	0.318702	0.021*
C16	0.3751 (5)	0.5544 (3)	0.20594 (11)	0.0184 (5)
H16A	0.473556	0.551762	0.239077	0.022*
H16B	0.292172	0.645838	0.198952	0.022*
C18	0.7136 (5)	0.6456 (3)	0.13518 (11)	0.0186 (5)
H18A	0.813274	0.654416	0.167141	0.022*
H18B	0.626185	0.734666	0.124933	0.022*
C9	−0.4608 (4)	0.3998 (3)	0.40721 (10)	0.0153 (5)
H9	−0.432562	0.460077	0.433465	0.018*
C19	0.8772 (5)	0.6149 (3)	0.08386 (11)	0.0182 (5)
H19A	0.971302	0.528723	0.095216	0.022*
H19B	0.775702	0.598798	0.053172	0.022*

C23	1.5469 (5)	0.7803 (3)	−0.06600 (11)	0.0187 (5)
H23A	1.640127	0.694139	−0.054020	0.022*
H23B	1.443821	0.762871	−0.096192	0.022*
C20	1.0514 (5)	0.7326 (3)	0.06060 (11)	0.0185 (5)
H20A	1.154647	0.748415	0.091027	0.022*
H20B	0.958141	0.819163	0.049260	0.022*
C14	−0.1262 (5)	0.3332 (3)	0.26937 (11)	0.0183 (5)
H14	−0.125992	0.270754	0.242746	0.022*
C21	1.2113 (5)	0.6993 (3)	0.00905 (11)	0.0184 (5)
H21A	1.304137	0.612633	0.020503	0.022*
H21B	1.107613	0.683149	−0.021230	0.022*
C25	1.8825 (5)	0.8593 (3)	−0.14085 (12)	0.0217 (6)
H25A	1.780445	0.842081	−0.171282	0.026*
H25B	1.974251	0.772814	−0.128449	0.026*
C24	1.7217 (5)	0.8967 (3)	−0.09043 (11)	0.0189 (5)
H24A	1.628795	0.982639	−0.102987	0.023*
H24B	1.823950	0.915000	−0.060221	0.023*
C22	1.3861 (5)	0.8153 (3)	−0.01485 (11)	0.0189 (5)
H22A	1.488999	0.832089	0.015483	0.023*
H22B	1.293413	0.901732	−0.026726	0.023*
C26	2.0588 (6)	0.9755 (3)	−0.16466 (13)	0.0295 (7)
H26A	2.157249	0.946694	−0.195930	0.044*
H26B	2.161360	0.992456	−0.134811	0.044*
H26C	1.968879	1.060577	−0.178209	0.044*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.03308 (17)	0.03720 (19)	0.01798 (14)	−0.00773 (13)	0.01127 (11)	0.00119 (11)
Cl1	0.0175 (3)	0.0268 (4)	0.0378 (4)	0.0014 (3)	0.0032 (3)	−0.0148 (3)
O2	0.0206 (9)	0.0218 (10)	0.0197 (9)	−0.0075 (8)	0.0081 (7)	−0.0078 (8)
O3	0.0223 (9)	0.0216 (10)	0.0170 (9)	−0.0089 (8)	0.0112 (7)	−0.0049 (7)
O1	0.0266 (10)	0.0254 (10)	0.0166 (9)	−0.0153 (8)	0.0099 (8)	−0.0076 (8)
C4	0.0214 (12)	0.0197 (13)	0.0129 (11)	−0.0079 (10)	0.0054 (9)	−0.0020 (9)
C10	0.0142 (11)	0.0148 (12)	0.0133 (11)	−0.0002 (9)	0.0035 (9)	0.0004 (9)
C12	0.0159 (11)	0.0174 (12)	0.0194 (12)	−0.0053 (10)	0.0035 (10)	−0.0034 (10)
C13	0.0156 (11)	0.0175 (12)	0.0131 (11)	−0.0010 (10)	0.0042 (9)	−0.0008 (9)
C7	0.0107 (10)	0.0150 (12)	0.0183 (12)	−0.0017 (9)	0.0005 (9)	−0.0014 (9)
C3	0.0218 (12)	0.0174 (13)	0.0187 (12)	−0.0033 (10)	−0.0010 (10)	0.0011 (10)
C5	0.0163 (11)	0.0194 (13)	0.0199 (12)	−0.0019 (10)	0.0038 (10)	−0.0031 (10)
C1	0.0172 (11)	0.0185 (12)	0.0155 (12)	−0.0089 (10)	0.0054 (9)	−0.0043 (10)
C8	0.0157 (11)	0.0181 (12)	0.0140 (11)	−0.0012 (10)	0.0015 (9)	−0.0033 (9)
C11	0.0156 (11)	0.0163 (12)	0.0163 (11)	−0.0001 (10)	0.0023 (9)	−0.0042 (9)
C2	0.0146 (11)	0.0162 (12)	0.0232 (13)	−0.0027 (10)	0.0024 (10)	−0.0065 (10)
C17	0.0177 (11)	0.0213 (13)	0.0146 (11)	−0.0040 (10)	0.0050 (9)	−0.0028 (10)
C6	0.0204 (12)	0.0171 (12)	0.0176 (12)	−0.0038 (10)	0.0012 (10)	0.0029 (10)
C15	0.0201 (12)	0.0158 (12)	0.0162 (12)	−0.0058 (10)	0.0034 (10)	−0.0017 (9)
C16	0.0193 (12)	0.0185 (13)	0.0173 (12)	−0.0060 (10)	0.0054 (10)	−0.0031 (10)

C18	0.0167 (11)	0.0202 (13)	0.0185 (12)	−0.0050 (10)	0.0067 (10)	−0.0030 (10)
C9	0.0150 (11)	0.0157 (12)	0.0143 (11)	−0.0001 (9)	0.0021 (9)	−0.0007 (9)
C19	0.0176 (11)	0.0201 (13)	0.0167 (12)	−0.0038 (10)	0.0064 (10)	−0.0036 (10)
C23	0.0184 (12)	0.0169 (12)	0.0203 (13)	−0.0034 (10)	0.0068 (10)	−0.0032 (10)
C20	0.0148 (11)	0.0191 (13)	0.0213 (13)	−0.0045 (10)	0.0059 (10)	−0.0038 (10)
C14	0.0224 (12)	0.0167 (12)	0.0161 (12)	−0.0056 (10)	0.0055 (10)	−0.0047 (10)
C21	0.0173 (11)	0.0181 (13)	0.0194 (12)	−0.0046 (10)	0.0071 (10)	−0.0037 (10)
C25	0.0227 (13)	0.0212 (13)	0.0208 (13)	−0.0072 (11)	0.0102 (10)	−0.0039 (10)
C24	0.0183 (12)	0.0188 (13)	0.0197 (12)	−0.0054 (10)	0.0058 (10)	−0.0041 (10)
C22	0.0182 (12)	0.0194 (13)	0.0189 (12)	−0.0050 (10)	0.0064 (10)	−0.0040 (10)
C26	0.0307 (15)	0.0310 (16)	0.0262 (14)	−0.0122 (13)	0.0154 (12)	−0.0054 (12)

Geometric parameters (Å, º)

Br1—C4	1.902 (2)	C15—H15	0.9300
Cl1—C2	1.724 (3)	C16—H16A	0.9700
O2—C7	1.201 (3)	C16—H16B	0.9700
O3—C13	1.361 (3)	C18—C19	1.527 (3)
O3—C16	1.435 (3)	C18—H18A	0.9700
O1—C7	1.370 (3)	C18—H18B	0.9700
O1—C1	1.392 (3)	C9—H9	0.9300
C4—C5	1.376 (4)	C19—C20	1.525 (3)
C4—C3	1.381 (4)	C19—H19A	0.9700
C10—C11	1.395 (3)	C19—H19B	0.9700
C10—C15	1.402 (3)	C23—C24	1.524 (3)
C10—C9	1.456 (3)	C23—C22	1.529 (3)
C12—C13	1.388 (4)	C23—H23A	0.9700
C12—C11	1.393 (3)	C23—H23B	0.9700
C12—H12	0.9300	C20—C21	1.529 (3)
C13—C14	1.401 (3)	C20—H20A	0.9700
C7—C8	1.464 (3)	C20—H20B	0.9700
C3—C2	1.391 (4)	C14—H14	0.9300
C3—H3	0.9300	C21—C22	1.519 (3)
C5—C6	1.393 (3)	C21—H21A	0.9700
C5—H5	0.9300	C21—H21B	0.9700
C1—C6	1.383 (4)	C25—C24	1.523 (3)
C1—C2	1.383 (4)	C25—C26	1.526 (4)
C8—C9	1.339 (3)	C25—H25A	0.9700
C8—H8	0.9300	C25—H25B	0.9700
C11—H11	0.9300	C24—H24A	0.9700
C17—C16	1.510 (3)	C24—H24B	0.9700
C17—C18	1.521 (3)	C22—H22A	0.9700
C17—H17A	0.9700	C22—H22B	0.9700
C17—H17B	0.9700	C26—H26A	0.9600
C6—H6	0.9300	C26—H26B	0.9600
C15—C14	1.380 (3)	C26—H26C	0.9600
C13—O3—C16	117.9 (2)	C19—C18—H18B	109.3

C7—O1—C1	116.30 (19)	H18A—C18—H18B	107.9
C5—C4—C3	122.6 (2)	C8—C9—C10	128.5 (2)
C5—C4—Br1	118.51 (19)	C8—C9—H9	115.7
C3—C4—Br1	118.9 (2)	C10—C9—H9	115.7
C11—C10—C15	118.0 (2)	C20—C19—C18	114.1 (2)
C11—C10—C9	118.2 (2)	C20—C19—H19A	108.7
C15—C10—C9	123.8 (2)	C18—C19—H19A	108.7
C13—C12—C11	119.1 (2)	C20—C19—H19B	108.7
C13—C12—H12	120.5	C18—C19—H19B	108.7
C11—C12—H12	120.5	H19A—C19—H19B	107.6
O3—C13—C12	124.5 (2)	C24—C23—C22	113.6 (2)
O3—C13—C14	115.6 (2)	C24—C23—H23A	108.8
C12—C13—C14	119.8 (2)	C22—C23—H23A	108.8
O2—C7—O1	121.8 (2)	C24—C23—H23B	108.8
O2—C7—C8	127.6 (2)	C22—C23—H23B	108.8
O1—C7—C8	110.5 (2)	H23A—C23—H23B	107.7
C4—C3—C2	118.1 (2)	C19—C20—C21	112.8 (2)
C4—C3—H3	120.9	C19—C20—H20A	109.0
C2—C3—H3	120.9	C21—C20—H20A	109.0
C4—C5—C6	118.8 (2)	C19—C20—H20B	109.0
C4—C5—H5	120.6	C21—C20—H20B	109.0
C6—C5—H5	120.6	H20A—C20—H20B	107.8
C6—C1—C2	120.9 (2)	C15—C14—C13	120.4 (2)
C6—C1—O1	120.4 (2)	C15—C14—H14	119.8
C2—C1—O1	118.7 (2)	C13—C14—H14	119.8
C9—C8—C7	118.1 (2)	C22—C21—C20	113.7 (2)
C9—C8—H8	120.9	C22—C21—H21A	108.8
C7—C8—H8	120.9	C20—C21—H21A	108.8
C12—C11—C10	121.9 (2)	C22—C21—H21B	108.8
C12—C11—H11	119.0	C20—C21—H21B	108.8
C10—C11—H11	119.0	H21A—C21—H21B	107.7
C1—C2—C3	120.2 (2)	C24—C25—C26	112.6 (2)
C1—C2—Cl1	120.1 (2)	C24—C25—H25A	109.1
C3—C2—Cl1	119.8 (2)	C26—C25—H25A	109.1
C16—C17—C18	112.7 (2)	C24—C25—H25B	109.1
C16—C17—H17A	109.1	C26—C25—H25B	109.1
C18—C17—H17A	109.1	H25A—C25—H25B	107.8
C16—C17—H17B	109.1	C25—C24—C23	112.9 (2)
C18—C17—H17B	109.1	C25—C24—H24A	109.0
H17A—C17—H17B	107.8	C23—C24—H24A	109.0
C1—C6—C5	119.5 (2)	C25—C24—H24B	109.0
C1—C6—H6	120.3	C23—C24—H24B	109.0
C5—C6—H6	120.3	H24A—C24—H24B	107.8
C14—C15—C10	120.8 (2)	C21—C22—C23	113.3 (2)
C14—C15—H15	119.6	C21—C22—H22A	108.9
C10—C15—H15	119.6	C23—C22—H22A	108.9
O3—C16—C17	106.8 (2)	C21—C22—H22B	108.9
O3—C16—H16A	110.4	C23—C22—H22B	108.9

C17—C16—H16A	110.4	H22A—C22—H22B	107.7
O3—C16—H16B	110.4	C25—C26—H26A	109.5
C17—C16—H16B	110.4	C25—C26—H26B	109.5
H16A—C16—H16B	108.6	H26A—C26—H26B	109.5
C17—C18—C19	111.7 (2)	C25—C26—H26C	109.5
C17—C18—H18A	109.3	H26A—C26—H26C	109.5
C19—C18—H18A	109.3	H26B—C26—H26C	109.5
C17—C18—H18B	109.3		

C16—O3—C13—C12	−3.1 (4)	C4—C3—C2—Cl1	179.0 (2)
C16—O3—C13—C14	177.7 (2)	C2—C1—C6—C5	−1.5 (4)
C11—C12—C13—O3	−178.6 (2)	O1—C1—C6—C5	175.5 (2)
C11—C12—C13—C14	0.5 (4)	C4—C5—C6—C1	−0.2 (4)
C1—O1—C7—O2	−5.4 (4)	C11—C10—C15—C14	0.4 (4)
C1—O1—C7—C8	173.1 (2)	C9—C10—C15—C14	−177.4 (2)
C5—C4—C3—C2	−1.4 (4)	C13—O3—C16—C17	177.4 (2)
Br1—C4—C3—C2	178.0 (2)	C18—C17—C16—O3	175.7 (2)
C3—C4—C5—C6	1.7 (4)	C16—C17—C18—C19	177.7 (2)
Br1—C4—C5—C6	−177.7 (2)	C7—C8—C9—C10	174.4 (2)
C7—O1—C1—C6	78.9 (3)	C11—C10—C9—C8	175.9 (3)
C7—O1—C1—C2	−104.1 (3)	C15—C10—C9—C8	−6.3 (4)
O2—C7—C8—C9	10.5 (4)	C17—C18—C19—C20	176.0 (2)
O1—C7—C8—C9	−167.9 (2)	C18—C19—C20—C21	−179.6 (2)
C13—C12—C11—C10	−1.6 (4)	C10—C15—C14—C13	−1.4 (4)
C15—C10—C11—C12	1.1 (4)	O3—C13—C14—C15	−179.9 (2)
C9—C10—C11—C12	179.0 (2)	C12—C13—C14—C15	0.9 (4)
C6—C1—C2—C3	1.8 (4)	C19—C20—C21—C22	179.9 (2)
O1—C1—C2—C3	−175.3 (2)	C26—C25—C24—C23	−179.4 (2)
C6—C1—C2—Cl1	−177.6 (2)	C22—C23—C24—C25	179.3 (2)
O1—C1—C2—Cl1	5.4 (3)	C20—C21—C22—C23	179.4 (2)
C4—C3—C2—C1	−0.3 (4)	C24—C23—C22—C21	179.6 (2)

Hydrogen-bond geometry (Å, º)

*Cg*2 is the centroid of the C10–C15 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9···O2^{i}	0.93	2.35	3.248 (3)	164
C16—H16*A*···*Cg*2^{ii}	0.97	2.95	3.824 (3)	150

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