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Crystal structure and Hirshfeld surface analysis of 3-[(*E*)-2-(2-bromo-4,5-dimethoxyphenyl)ethenyl]-5,5-dimethylcyclohex-2-en-1-one

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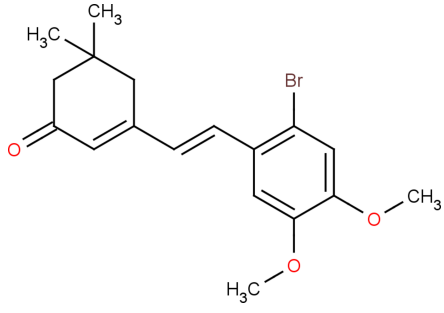
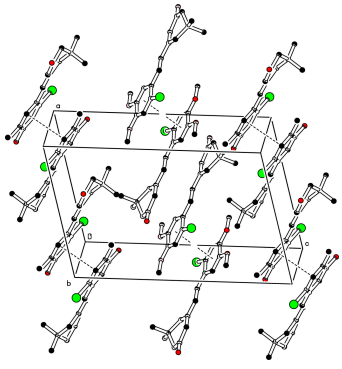
In the title compound, $C_{18}H_{21}BrO_3$, which represents an isophorone (3,5,5-trimethyl-2-cyclohexen-1-one) derivative, the cyclohexene ring adopts a twist-boat conformation. An intramolecular C—H···Br hydrogen bond between a methine H atom and the Br substituent at the phenyl ring leads to the stabilization of the molecular conformation. Intermolecular C—H···O hydrogen bonds as well as π–π interactions are observed in the crystal. The intermolecular interactions were quantified and analysed using Hirshfeld surface analysis, revealing that H···H interactions contribute most (46.9%) to the crystal packing.

1. Chemical context

Isophorone (3,5,5-trimethyl-2-cyclohexen-1-one) is a colourless to pale yellow cyclic α,β-unsaturated ketone, characterized by a distinctive peppermint-like odour (Kataoka *et al.*, 2007). The presence of a conjugated enone system makes isophorone an excellent synthon for carbon–carbon bond-forming reactions, thus establishing its role as a valuable intermediate in synthetic organic chemistry. In recent years, isophorone-derived compounds have garnered considerable attention due to their broad spectrum of biological activities, including anticancer (Logeshwari *et al.*, 2024), antimicrobial and antioxidant (Kozak *et al.*, 2019) effects. These pharmacological properties are primarily attributed to the introduction of styryl or aryl moieties through condensation with bioactive aldehydes, positioning isophorone as an important scaffold in drug discovery.



In the context given above, we synthesized an isophorone derivative and report here the molecular and crystal structure, and Hirshfeld surface analysis of 3-[(*E*)-2-(2-bromo-4,5-di-



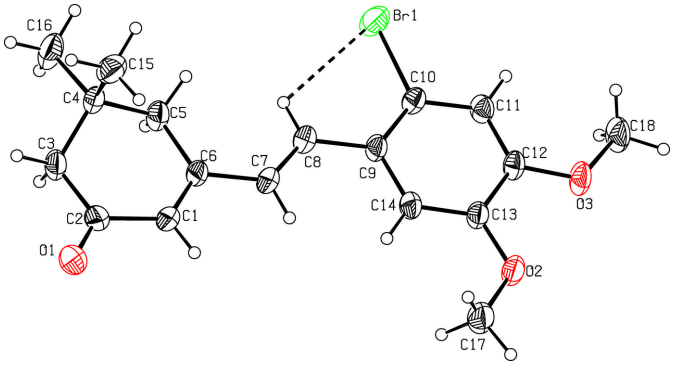


Figure 1
A view of the molecular structure of compound (I), showing the atom labelling. Displacement ellipsoids are drawn at the 30% probability level. The intramolecular hydrogen bond is shown as a dashed line.

methoxyphenyl)ethenyl]-5,5-dimethylcyclohex-2-en-1-one, (I).

2. Structural commentary

The molecular structure of (I) is displayed in Fig. 1. The O1—C2 [1.222 (3) Å], C1—C6 [1.342 (3) Å] and C7—C8 [1.322 (3) Å] bond lengths confirm the double-bond character. The reduction of the bond angle C10—C9—C14 [116.2 (2)°] is due to the short contact H7···H14 (2.05 Å). The cyclohexene ring adopts a twist-boat conformation with puckering parameters (Cremer & Pople, 1975) q_2 = 0.374 (2) Å, q_3 = −0.274 (2) Å, Q_T = 0.464 (2) Å and φ = 349.5 (4)°. Atom C4 deviates by −0.638 (2) Å from the least-squares plane through the remaining five atoms (C1–C3/C5/C6) of the ring. The mean plane calculation of the bromo dimethyl phenyl ring reveals that the methyl atoms C17 and C18 deviate by −0.051 (2) and 0.065 (2) Å, respectively, from the plane while the bromine atom deviates by 0.008 (1) Å. A weak intramolecular contact (Table 1) between a methine H atom and the Br atom attached to the phenyl ring leads to the stabilization of the molecular conformation. This C8—H8···Br1 interaction forms an *S*(5) ring motif (Bernstein *et al.*, 1995), as shown in Fig. 1.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···Br1	0.93	2.76	3.212 (2)	111
C17—H17*C*···O1^{i}	0.96	2.58	3.495 (3)	159

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

3. Supramolecular features

In the crystal, molecules associate pairwise *via* C17—H17*C*···O1^{i} hydrogen bonds (Table 1) into inversion dimers with an $R_2^2(24)$ graph-set motif (Etter *et al.*, 1990), as shown in Fig. 2. Moreover, π–π interactions are observed between the centroids of inversion-related benzene rings (C9–C14) with a centroid-to-centroid distance of 3.825 (1) Å and a slippage of 1.435 Å (Fig. 3).

4. Hirshfeld surface analysis

Intermolecular interactions were quantified by a Hirshfeld surface (HS) analysis (Spackman & Jayatilaka, 2009) using *CrystalExplorer* (Spackman *et al.*, 2021). The HS mapped over

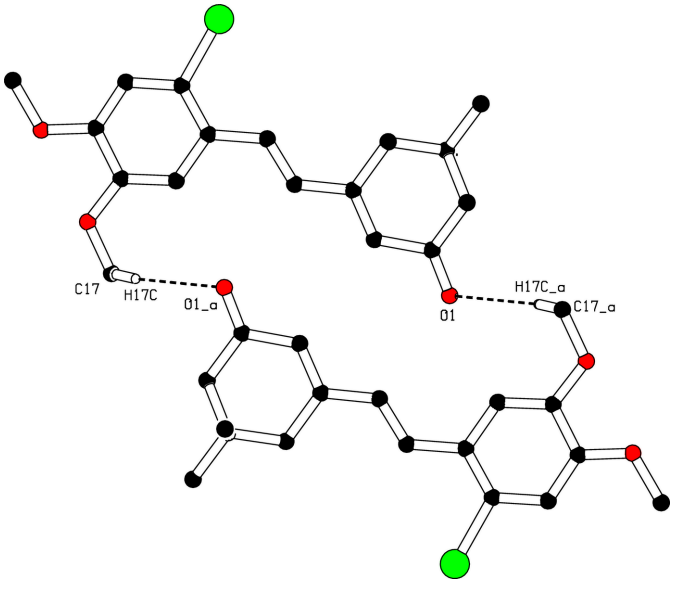


Figure 2
The formation of a centrosymmetric dimer in the crystal structure of (I) through C—H···O hydrogen bonds. [Symmetry code: (*a*) $-x+1, -y+2, -z$.]

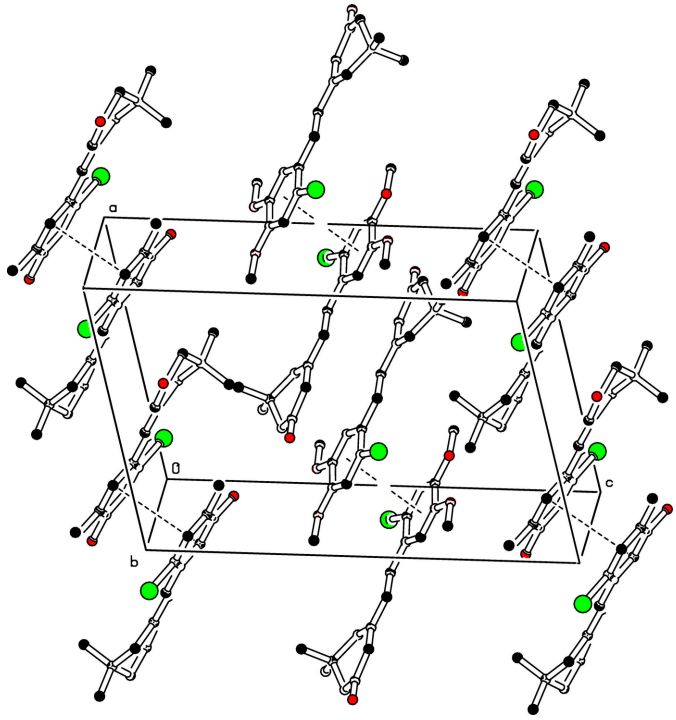


Figure 3
The crystal packing of (I) with π–π intermolecular interactions shown as dashed lines. For clarity, H atoms have been omitted.

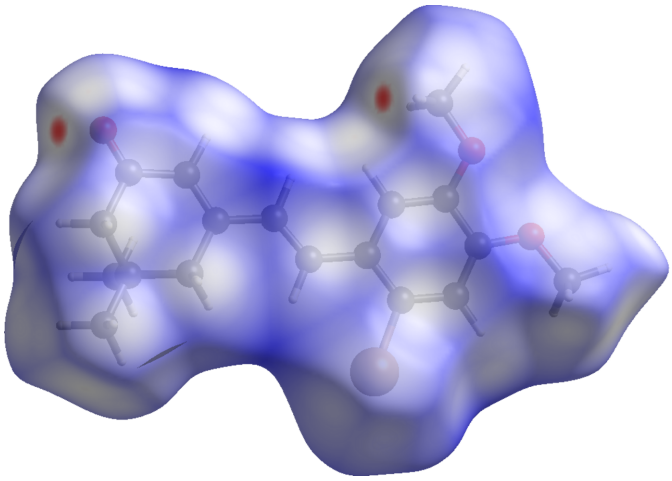


Figure 4
A view of the Hirshfeld surface mapped over d_{norm} for compound (I).

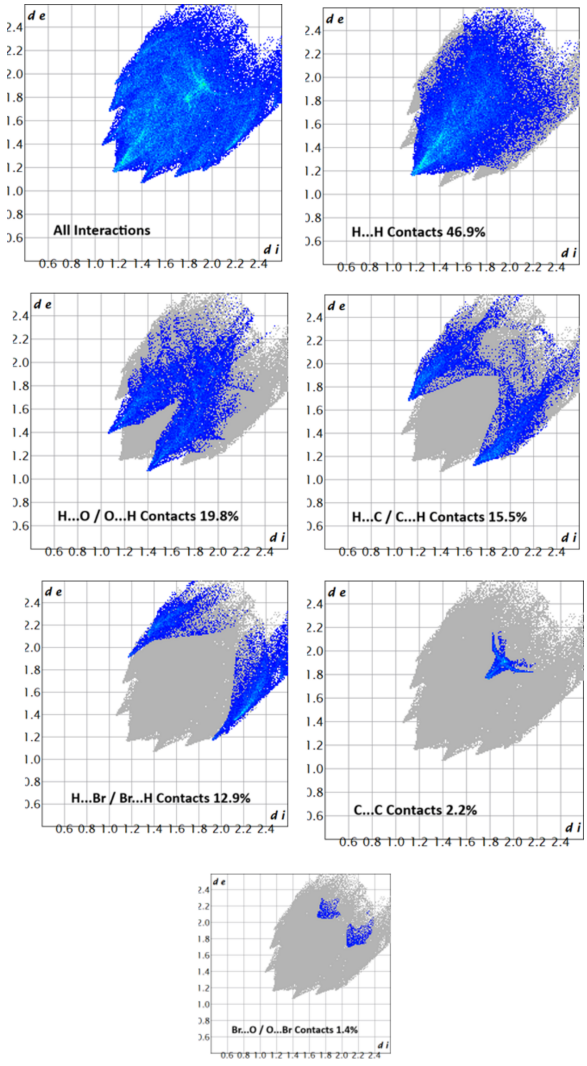


Figure 5
Two-dimensional fingerprint plots for compound (I), showing all interactions, and delineated into H···H, H···O/O···H, H···C/C···H, H···Br/Br···H, C···C and Br···O/O···Br interactions. The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{21}BrO_3$
M_r	365.26
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	300
a, b, c (Å)	11.9084 (8), 8.1667 (5), 18.1737 (13)
β (°)	102.231 (2)
V (Å^3)	1727.3 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	2.39
Crystal size (mm)	0.19 × 0.17 × 0.09
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.636, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	33400, 4282, 2767
R_{int}	0.045
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.036, 0.084, 1.03
No. of reflections	4282
No. of parameters	199
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.25, −0.38

Computer programs: *APEX3* and *SAINT* (Bruker, 2017), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012), *PLATON* (Spek, 2020) and *publCIF* (Westrip, 2010).

d_{norm} is illustrated in Fig. 4. where the deep-red spots at O1 and H17*C* represent distances shorter than van der Waals radii and are indicative of the intermolecular C—H···O hydrogen bond discussed above.

The associated two-dimensional fingerprint plots (McKinnon *et al.*, 2007) provide quantitative information about the non-covalent interactions in the crystal packing in terms of the percentage contribution of the interatomic contacts (Spackman & McKinnon, 2002). The overall two-dimensional fingerprint plot is shown in Fig. 5 (top left). The HS analysis reveals that H···H and H···O/O···H contacts are the main contributors to the crystal packing, followed by H···C/C···H, H···Br/Br···H, C···C and Br···O/O···Br contacts (Fig. 5).

5. Synthesis and crystallization

Compound (I) was synthesized by dissolving isophorone (1 mmol, 0.140 g) and 2-bromo-4,5-dimethoxybenzaldehyde (1 mmol, 0.247 g) in absolute ethanol (15 ml) in a round-bottom flask of 50 ml and stirring. Following that, a 20%$_{wt}$ sodium hydroxide solution (1 mmol, 0.04 g) was added dropwise under continuous stirring. The reaction mixture was then stirred at ambient temperature (298 K) for 6 h. The progress of the condensation reaction was monitored from time to time by thin-layer chromatography (TLC) on a hexane–ethyl acetate (7:3) solvent system. After completion, the mixture was transferred to crushed ice, which caused the development

of a yellow precipitate. The solid was filtered off under reduced pressure, washed with cold distilled water, and dried at room temperature. The crude product was recrystallized from ethanol to obtain crystals of (I).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms were placed in idealized positions and allowed to ride on their parent atoms: C—H = 0.93–0.97 Å with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and U_{iso}(H) = 1.2U_{eq}(C) for other H atoms.

Acknowledgements

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References

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bruker (2017). *APEX3* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, U. S. A.
Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
Etter, M. C., MacDonald, J. C. & Bernstein, J. (1990). *Acta Cryst.* B**46**, 256–262.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Kataoka, H., Terada, Y., Inoue, R. & Mitani, K. (2007). *J. Chromatogr. A* **1155**, 100–104.
Kozak, Z., Pıravadılı Mucur, S., Canımkurbey, B., İdil, Ö., Eryılmaz, S. & Gul, M. (2019). *Res. Chem. Intermed.* **45**, 5625–5639.
Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.
Logeshwari, G., Jeyashri, K. R., Rajkumar, M., Manikandan, H., Sivakumar, K., Selvanayagam, S. & Rajathi, V. (2024). *Spectrochim. Acta A Mol. Biomol. Spectrosc.* **319**, 124577.
McKinnon, J. J., Jayatilaka, D. & Spackman, M. A. (2007). *Chem. Commun.* pp. 3814–3816.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Spackman, M. A. & Jayatilaka, D. (2009). *CrystEngComm* **11**, 19–32.
Spackman, M. A. & McKinnon, J. J. (2002). *CrystEngComm* **4**, 378–392.
Spackman, P. R., Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Jayatilaka, D. & Spackman, M. A. (2021). *J. Appl. Cryst.* **54**, 1006–1011.
Spek, A. L. (2020). *Acta Cryst.* E**76**, 1–11.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

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Muruganandham Rajkumar, Uthirapathi Rajapandiyan, Haridoss Manikandan, Velusamy Rajathi and Sivashanmugam Selvanayagam

Computing details

3-[(*E*)-2-(2-Bromo-4,5-dimethoxyphenyl)ethenyl]-5,5-dimethylcyclohex-2-en-1-one

Crystal data

$C_{18}H_{21}BrO_3$
$M_r = 365.26$
Monoclinic, $P2_1/c$
$a = 11.9084$ (8) Å
$b = 8.1667$ (5) Å
$c = 18.1737$ (13) Å
$\beta = 102.231$ (2)°
$V = 1727.3$ (2) Å^3
$Z = 4$
$F(000) = 752$
$D_x = 1.405$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9892 reflections
$\theta = 2.6$–24.9°
$\mu = 2.39$ mm^{-1}
$T = 300$ K
Block, yellow
0.19 × 0.17 × 0.09 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: i-mu-s microfocus source
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
$T_{min} = 0.636$, $T_{max} = 0.746$
33400 measured reflections
4282 independent reflections
2767 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 28.3°$, $\theta_{min} = 2.6°$
$h = -15 \rightarrow 15$
$k = -10 \rightarrow 10$
$l = -24 \rightarrow 24$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.084$
$S = 1.03$
4282 reflections
199 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.032P)^2 + 0.5285P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.38$ 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	0.21244 (2)	0.20268 (3)	0.03311 (2)	0.06997 (12)
O1	0.66634 (15)	1.0834 (2)	0.14033 (11)	0.0836 (6)
O2	−0.01107 (12)	0.74963 (19)	−0.16748 (9)	0.0603 (4)
O3	−0.11576 (12)	0.47454 (18)	−0.16639 (9)	0.0600 (4)
C1	0.52228 (18)	0.8950 (3)	0.09158 (12)	0.0569 (6)
H1	0.477268	0.976060	0.063868	0.068*
C2	0.63384 (19)	0.9412 (3)	0.13716 (12)	0.0586 (6)
C3	0.70601 (18)	0.8051 (3)	0.17758 (13)	0.0554 (6)
H3A	0.757898	0.849533	0.221475	0.067*
H3B	0.752286	0.759373	0.144658	0.067*
C4	0.63502 (16)	0.6684 (2)	0.20260 (11)	0.0441 (5)
C5	0.54760 (17)	0.6074 (3)	0.13380 (12)	0.0511 (5)
H5A	0.587780	0.544519	0.102108	0.061*
H5B	0.493931	0.534370	0.150666	0.061*
C6	0.48127 (17)	0.7415 (3)	0.08760 (11)	0.0471 (5)
C7	0.37120 (18)	0.7062 (3)	0.03714 (11)	0.0536 (6)
H7	0.335261	0.793272	0.008546	0.064*
C8	0.31710 (17)	0.5639 (3)	0.02768 (11)	0.0496 (5)
H8	0.352859	0.475488	0.055327	0.060*
C9	0.20528 (16)	0.5337 (3)	−0.02282 (10)	0.0444 (5)
C10	0.14791 (17)	0.3853 (3)	−0.02615 (11)	0.0452 (5)
C11	0.04082 (17)	0.3600 (3)	−0.07330 (11)	0.0478 (5)
H11	0.004492	0.259107	−0.073778	0.057*
C12	−0.01094 (16)	0.4839 (3)	−0.11895 (11)	0.0452 (5)
C13	0.04507 (16)	0.6359 (3)	−0.11840 (11)	0.0449 (5)
C14	0.15029 (17)	0.6574 (3)	−0.07094 (11)	0.0478 (5)
H14	0.186674	0.758185	−0.070673	0.057*
C15	0.5738 (2)	0.7347 (3)	0.26188 (12)	0.0638 (6)
H15A	0.523896	0.822936	0.240823	0.096*
H15B	0.529205	0.648981	0.277875	0.096*
H15C	0.629523	0.774031	0.304298	0.096*
C16	0.7137 (2)	0.5289 (3)	0.23628 (15)	0.0737 (7)
H16A	0.752552	0.486776	0.199091	0.111*
H16B	0.769349	0.568486	0.278733	0.111*
H16C	0.669031	0.443436	0.252311	0.111*
C17	0.0350 (2)	0.9103 (3)	−0.16221 (16)	0.0733 (7)
H17A	−0.011771	0.978807	−0.199475	0.110*
H17B	0.036049	0.953757	−0.112985	0.110*
H17C	0.111881	0.907246	−0.170618	0.110*

C18	−0.1695 (2)	0.3181 (3)	−0.17712 (15)	0.0699 (7)
H18A	−0.242412	0.327809	−0.211566	0.105*
H18B	−0.121412	0.243649	−0.197319	0.105*
H18C	−0.180950	0.277343	−0.129703	0.105*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.07534 (19)	0.05863 (17)	0.06375 (17)	−0.00047 (12)	−0.01275 (12)	0.01078 (12)
O1	0.0711 (11)	0.0741 (12)	0.0917 (13)	−0.0346 (10)	−0.0141 (10)	0.0226 (10)
O2	0.0468 (9)	0.0514 (9)	0.0701 (10)	−0.0037 (7)	−0.0158 (8)	0.0076 (8)
O3	0.0446 (8)	0.0494 (9)	0.0727 (10)	−0.0071 (7)	−0.0174 (7)	−0.0094 (7)
C1	0.0484 (12)	0.0665 (15)	0.0475 (12)	−0.0123 (11)	−0.0084 (10)	0.0180 (11)
C2	0.0511 (13)	0.0709 (16)	0.0493 (13)	−0.0201 (12)	0.0006 (10)	0.0117 (11)
C3	0.0369 (11)	0.0714 (15)	0.0527 (13)	−0.0080 (11)	−0.0025 (9)	−0.0028 (11)
C4	0.0350 (10)	0.0482 (12)	0.0439 (11)	0.0024 (9)	−0.0034 (9)	−0.0009 (9)
C5	0.0413 (11)	0.0528 (13)	0.0534 (12)	−0.0024 (10)	−0.0030 (9)	−0.0061 (10)
C6	0.0389 (11)	0.0640 (13)	0.0338 (10)	−0.0089 (10)	−0.0022 (8)	0.0018 (9)
C7	0.0449 (12)	0.0648 (15)	0.0432 (11)	−0.0074 (11)	−0.0087 (9)	0.0096 (10)
C8	0.0426 (11)	0.0579 (13)	0.0431 (11)	−0.0016 (10)	−0.0025 (9)	−0.0001 (10)
C9	0.0379 (11)	0.0529 (12)	0.0381 (10)	−0.0046 (9)	−0.0020 (8)	−0.0038 (9)
C10	0.0443 (11)	0.0480 (12)	0.0388 (10)	0.0015 (10)	−0.0012 (9)	−0.0024 (9)
C11	0.0452 (12)	0.0455 (11)	0.0488 (12)	−0.0087 (10)	0.0011 (10)	−0.0084 (10)
C12	0.0375 (11)	0.0474 (12)	0.0454 (11)	−0.0022 (9)	−0.0033 (9)	−0.0099 (9)
C13	0.0373 (11)	0.0473 (11)	0.0458 (11)	−0.0017 (9)	−0.0011 (9)	−0.0018 (9)
C14	0.0396 (11)	0.0489 (12)	0.0496 (12)	−0.0090 (9)	−0.0024 (9)	−0.0016 (9)
C15	0.0647 (15)	0.0781 (16)	0.0462 (13)	0.0081 (13)	0.0062 (11)	0.0081 (12)
C16	0.0533 (14)	0.0646 (16)	0.0885 (18)	0.0120 (12)	−0.0180 (13)	0.0019 (14)
C17	0.0567 (15)	0.0519 (14)	0.099 (2)	−0.0056 (12)	−0.0103 (13)	0.0167 (14)
C18	0.0552 (14)	0.0580 (15)	0.0837 (18)	−0.0178 (12)	−0.0141 (13)	−0.0112 (13)

Geometric parameters (Å, º)

Br1—C10	1.904 (2)	C8—C9	1.469 (3)
O1—C2	1.222 (3)	C8—H8	0.9300
O2—C13	1.361 (2)	C9—C10	1.386 (3)
O2—C17	1.418 (3)	C9—C14	1.404 (3)
O3—C12	1.361 (2)	C10—C11	1.393 (3)
O3—C18	1.424 (3)	C11—C12	1.369 (3)
C1—C6	1.342 (3)	C11—H11	0.9300
C1—C2	1.458 (3)	C12—C13	1.408 (3)
C1—H1	0.9300	C13—C14	1.374 (3)
C2—C3	1.499 (3)	C14—H14	0.9300
C3—C4	1.526 (3)	C15—H15A	0.9600
C3—H3A	0.9700	C15—H15B	0.9600
C3—H3B	0.9700	C15—H15C	0.9600
C4—C16	1.519 (3)	C16—H16A	0.9600
C4—C15	1.523 (3)	C16—H16B	0.9600

C4—C5	1.531 (3)	C16—H16C	0.9600
C5—C6	1.499 (3)	C17—H17A	0.9600
C5—H5A	0.9700	C17—H17B	0.9600
C5—H5B	0.9700	C17—H17C	0.9600
C6—C7	1.460 (3)	C18—H18A	0.9600
C7—C8	1.322 (3)	C18—H18B	0.9600
C7—H7	0.9300	C18—H18C	0.9600

C13—O2—C17	117.28 (16)	C9—C10—Br1	121.60 (14)
C12—O3—C18	117.56 (17)	C11—C10—Br1	116.06 (16)
C6—C1—C2	123.3 (2)	C12—C11—C10	119.95 (19)
C6—C1—H1	118.3	C12—C11—H11	120.0
C2—C1—H1	118.3	C10—C11—H11	120.0
O1—C2—C1	120.9 (2)	O3—C12—C11	125.25 (18)
O1—C2—C3	122.6 (2)	O3—C12—C13	115.06 (18)
C1—C2—C3	116.4 (2)	C11—C12—C13	119.69 (17)
C2—C3—C4	113.08 (17)	O2—C13—C14	125.48 (19)
C2—C3—H3A	109.0	O2—C13—C12	115.52 (17)
C4—C3—H3A	109.0	C14—C13—C12	118.99 (19)
C2—C3—H3B	109.0	C13—C14—C9	122.85 (19)
C4—C3—H3B	109.0	C13—C14—H14	118.6
H3A—C3—H3B	107.8	C9—C14—H14	118.6
C16—C4—C15	109.19 (19)	C4—C15—H15A	109.5
C16—C4—C3	109.57 (18)	C4—C15—H15B	109.5
C15—C4—C3	109.23 (18)	H15A—C15—H15B	109.5
C16—C4—C5	109.85 (18)	C4—C15—H15C	109.5
C15—C4—C5	110.41 (17)	H15A—C15—H15C	109.5
C3—C4—C5	108.58 (17)	H15B—C15—H15C	109.5
C6—C5—C4	113.95 (18)	C4—C16—H16A	109.5
C6—C5—H5A	108.8	C4—C16—H16B	109.5
C4—C5—H5A	108.8	H16A—C16—H16B	109.5
C6—C5—H5B	108.8	C4—C16—H16C	109.5
C4—C5—H5B	108.8	H16A—C16—H16C	109.5
H5A—C5—H5B	107.7	H16B—C16—H16C	109.5
C1—C6—C7	119.1 (2)	O2—C17—H17A	109.5
C1—C6—C5	120.65 (18)	O2—C17—H17B	109.5
C7—C6—C5	120.26 (19)	H17A—C17—H17B	109.5
C8—C7—C6	127.1 (2)	O2—C17—H17C	109.5
C8—C7—H7	116.5	H17A—C17—H17C	109.5
C6—C7—H7	116.5	H17B—C17—H17C	109.5
C7—C8—C9	125.5 (2)	O3—C18—H18A	109.5
C7—C8—H8	117.2	O3—C18—H18B	109.5
C9—C8—H8	117.2	H18A—C18—H18B	109.5
C10—C9—C14	116.18 (17)	O3—C18—H18C	109.5
C10—C9—C8	123.18 (19)	H18A—C18—H18C	109.5
C14—C9—C8	120.64 (19)	H18B—C18—H18C	109.5
C9—C10—C11	122.34 (19)		

C6—C1—C2—O1	−178.3 (2)	C8—C9—C10—C11	178.66 (19)
C6—C1—C2—C3	3.2 (3)	C14—C9—C10—Br1	178.11 (15)
O1—C2—C3—C4	148.4 (2)	C8—C9—C10—Br1	−2.1 (3)
C1—C2—C3—C4	−33.1 (3)	C9—C10—C11—C12	0.5 (3)
C2—C3—C4—C16	174.69 (19)	Br1—C10—C11—C12	−178.78 (16)
C2—C3—C4—C15	−65.7 (2)	C18—O3—C12—C11	−8.8 (3)
C2—C3—C4—C5	54.7 (2)	C18—O3—C12—C13	171.6 (2)
C16—C4—C5—C6	−168.58 (19)	C10—C11—C12—O3	−178.98 (19)
C15—C4—C5—C6	71.0 (2)	C10—C11—C12—C13	0.6 (3)
C3—C4—C5—C6	−48.8 (2)	C17—O2—C13—C14	−9.0 (3)
C2—C1—C6—C7	−176.7 (2)	C17—O2—C13—C12	172.3 (2)
C2—C1—C6—C5	2.9 (3)	O3—C12—C13—O2	−2.6 (3)
C4—C5—C6—C1	21.4 (3)	C11—C12—C13—O2	177.80 (19)
C4—C5—C6—C7	−159.02 (19)	O3—C12—C13—C14	178.63 (19)
C1—C6—C7—C8	−178.2 (2)	C11—C12—C13—C14	−1.0 (3)
C5—C6—C7—C8	2.2 (4)	O2—C13—C14—C9	−178.3 (2)
C6—C7—C8—C9	178.9 (2)	C12—C13—C14—C9	0.3 (3)
C7—C8—C9—C10	−174.6 (2)	C10—C9—C14—C13	0.8 (3)
C7—C8—C9—C14	5.2 (3)	C8—C9—C14—C13	−179.09 (19)
C14—C9—C10—C11	−1.2 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···Br1	0.93	2.76	3.212 (2)	111
C17—H17*C*···O1^{i}	0.96	2.58	3.495 (3)	159

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