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Crystal structure and Hirshfeld surface analysis of (2*E*)-1-(3-bromophenyl)-3-(4-fluorophenyl)prop-2-en-1-one

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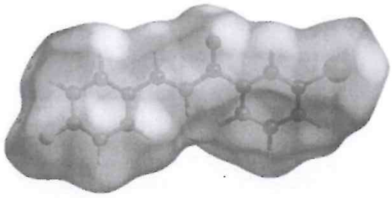
In the title compound, $C_{15}H_{10}BrFO$, the molecular structure consists of a 3-bromophenyl ring and a 4-fluorophenyl ring linked *via* a prop-2-en-1-one spacer. The 3-bromophenyl and 4-fluorophenyl rings make a dihedral angle of 48.90 (15)°. The molecule has an *E* configuration about the C=C bond and the carbonyl group is *syn* with respect to the C=C bond. In the crystal, molecules are linked by C—H$\cdots\pi$ interactions between the bromophenyl and fluorophenyl rings of molecules, resulting in a two-dimensional layered structure parallel to the *ab* plane. The molecular packing is stabilized by weak Br···H and F···H contacts, one of which is on the one side of each layer, and the second is on the other. The intermolecular interactions in the crystal packing were further analysed using Hirshfeld surface analysis, which indicates that the most significant contacts are Cl···H/H···Cl (20.8%), followed by C···H/H···C (31.1%), H···H (21.7%), Br···H/H···Br (14.2%), F···H/H···F (9.8%), O···H/H···O (9.7%).



1. Chemical context

An aromatic ketone and an enone that forms the central core for a variety of important biological compounds, which are known collectively as chalcones or chalconoids. Chalcones are 1,3-diphenyl-2-propene-1-one, in which two aromatic rings are linked by a three carbon α,β-unsaturated carbonyl system. The α,β-unsaturated ketone group in chalcones is responsible for their enzyme inhibitory activity including xanthine oxidase, aldose reductase, soluble epoxide hydrolase, protein tyrosine kinase, quinonone reductase and mono amine oxidase (Amita *et al.*, 2014). Chalcones are abundant in nature starting from ferns to higher plants and a number of them are polyhydroxylated in the aryl rings. They are considered to be precursors of flavonoids and isoflavonoids. Chalcones possess conjugated double bonds and a completely delocalized π-electron system on both benzene rings. Molecules that possess such a system have relatively low redox potentials and have a greater probability of undergoing electron-transfer reactions. Crystal structures have been reported for 3-(3-bromophenyl)-1-(4-bromophenyl)prop-2-en-1-one (Teh *et al.*, 2006), 3-(3-bromophenyl)-1-(2-naphthyl)prop-2-en-1-one (Moorthi *et al.*, 2007), (*E*)-1-(3-bromophenyl)-3-(4-ethoxyphenyl)prop-2-en-1-one (Fun *et al.*, 2008), (*E*)-3-(biphenyl-4-yl)-1-(3-bromophenyl)prop-2-en-1-one (Dutkiewicz *et al.*, 2009), (2*E*)-1-(3-

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

*Cg*1 and *Cg*2 are the centroids of the 3-bromophenyl (C1–C6) and 4-fluorophenyl (C10–C15) rings, respectively.

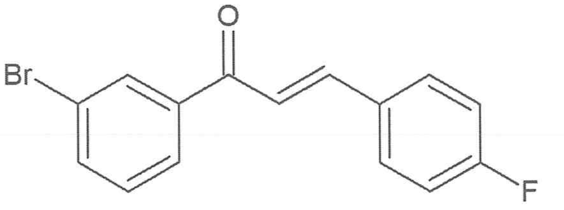
D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C2—H2$A\cdots Cg2^{\rm i}$	0.93	2.93	3.571 (4)	127
C5—H5$A\cdots Cg2^{\rm ii}$	0.93	2.98	3.642 (3)	129
C14—H14$A\cdots Cg1^{\rm iii}$	0.93	2.90	3.590 (3)	132

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

Table 2
Summary of short interatomic contacts (Å) in the title compound.

Contact	Distance	Symmetry operation
Br1$\cdots$Br1	3.7222 (6)	$3-x, 1-y, -z$
H3$A\cdots$Br1	3.19	$2-x, 1-y, -z$
H12$A\cdots$F1	2.66	$1-x, -y, 2-z$
H1$A\cdots$O1	2.82	$-1+x, y, z$
H11$A\cdots$C3	3.01	$2-x, 1-y, 1-z$
H14$A\cdots$C6	2.95	$1-x, -y, 1-z$
H2$A\cdots$C10	2.89	$1-x, 1-y, 1-z$
H5$A\cdots$C15	3.00	$2-x, -y, 1-z$

bromophenyl)-3-(6-methoxy-2-naphthyl)prop-2-en-1-one (Harrison *et al.*, 2010), (2*E*)-1-(3-bromophenyl)-3-(4,5-dimethoxy-2-nitrophenyl)prop-2-en-1-one (Jasinski *et al.*, 2010), (*E*)-1-(3-bromophenyl)-3-(3,4-dimethoxyphenyl)prop-2-en-1-one (Escobar *et al.*, 2012), (*E*)-1-(3-bromophenyl)-3-(4-nitrophenyl)prop-2-en-1-one (Harini *et al.*, 2017) and (*E*)-1-(3-bromophenyl)-3-(3-fluorophenyl)prop-2-en-1-one (Rajendraprasad *et al.*, 2017). We herewith report the crystal and molecular structure of the title compound.



2. Structural commentary

As shown in Fig. 1, the title compound is constructed from two aromatic rings (3-bromophenyl and 4-fluorophenyl rings), which are linked by a C═C—C(═O)—C enone bridge. Probably as a result of the steric repulsion between the fluoride and bromine atoms of adjacent molecules, the C5—C6—C7— O1 and O1—C7—C8—C9 torsion angles about the enone bridge are 25.1 (4) and 14.0 (5) °, respectively. Hence, the dihedral angle between the 3-bromophenyl ring and the 4-fluorophenyl ring increases to 48.90 (15)°. The molecular conformation of the title compound is stabilized by intramolecular C—H$\cdots$Cl contacts (Table 1), producing *S*(6) and *S*(5) ring motifs. The bond lengths and angles are comparable with those found in the related compounds (2*E*)-3-(3-chlorophenyl)-1-(3,4-dimethoxyphenyl)-prop-2-en-1-one (Sheshadri *et al.*, 2018*a*), (2*E*)-3-(3-bromo-4-fluorophenyl)-1-(3,4-dimethoxyphenyl)prop-2-en-1-one (Sheshadri *et al.*, 2018*b*), (*E*)-3-(3,4-dimethoxyphenyl)-1-(1-hydroxynaphthalen-2yl)-prop-2-en-1-one (Ezhilarasi *et al.*, 2015), (*E*)-1-(3-bromophenyl)-3-(3,4-dimethoxyphenyl)prop-2-en-1-one (Escobar *et al.*, 2012) and (*E*)-3-(2-bromophenyl)-1-(3,4-dimethoxyphenyl)prop-2-en-1-one (Li *et al.*, 2012).

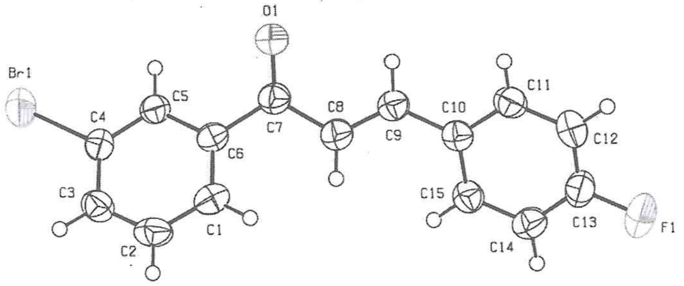


Figure 1
The molecular structure of the title compound, showing the atom labelling and displacement ellipsoids drawn at the 50% probability level.

3. Supramolecular features and Hirshfeld surface analysis

In the crystal, molecules are linked by C—H$\cdots\pi$ interactions between the bromophenyl and fluorophenyl rings of molecules, resulting in a two-dimensional layered structure parallel to the *ab* plane (Table 1; Fig. 2). The molecular packing is stabilized by weak Br$\cdots$H and $\cdots$H contacts, one of which is on the one side of a layer, and the second is on the other. A summary of the short contacts is given in Table 2.

Hirshfeld surfaces and fingerprint plots were generated for the title compound using *CrystalExplorer* (McKinnon *et al.*, 2007). Hirshfeld surfaces enable the visualization of intermolecular interactions by different colours and colour inten-

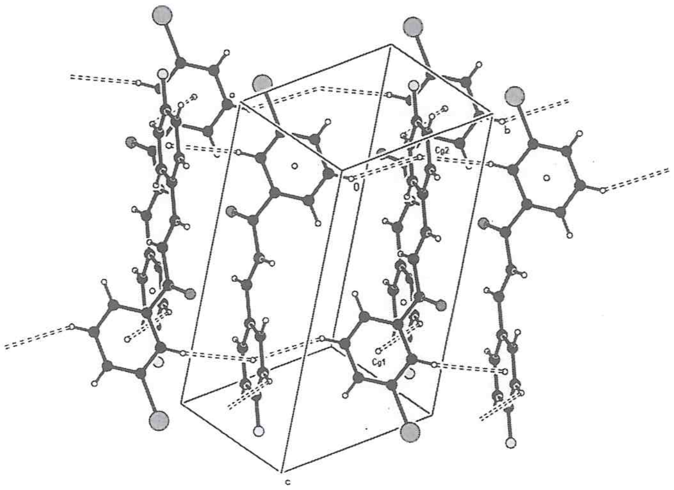


Figure 2
A view of the C—H$\cdots\pi$ interactions in the title compound.

Table 3
Percentage contributions of interatomic contacts to the Hirshfeld surface for the compound.

Contact	Percentage contribution
C···H/H···C	31.1
H···H	21.7
Br···H/H···Br	14.2
F···H/H···F	9.8
O···H/H···O	9.7
C···C	3.4
Br···F/F···Br	3.1
F···C/C···F	1.8
Br.·C/C···Br	1.5
C···O/O···C	1.5
F···F	1.3
Br···Br	0.9

sity, representing short or long contacts and indicating the relative strength of the interactions.

The function $d_{\rm norm}$ is a ratio enclosing the distances of any surface point to the nearest interior ($d_{\rm i}$) and exterior ($d_{\rm e}$) atom and the van der Waals radii of the atoms (Hirshfeld, 1977; Soman *et al.*, 2014). The function $d_{\rm norm}$ will be equal to zero when intermolecular distances are close to van der Waals contacts. They are indicated by a white colour on the Hirshfeld surface, while contacts longer than the sum of van der Waals radii with positive $d_{\rm norm}$ values are coloured in blue. The surface plot for $d_{\rm norm}$ (Fig. 3) was generated using a high standard surface resolution over a colour scale of −0.0186 to 1.3784 a.u.

The overall two-dimensional fingerprint plot for the title compound and those delineated into C···H/H···C, H···H, Br···H/H···Br, F···H/H···F and O···H/H···O contacts are illustrated in Fig. 4. The percentage contributions of the various interatomic contacts to the Hirshfeld surfaces are given in Table 3. The presence of C—H···π interactions in the crystal is indicated by the pair of characteristic wings in the fingerprint plot delineated into C···H/H···C contacts (31.1% contribution to the Hirshfeld surface). The C···H/H···C interactions are represented by the spikes at the bottom right and left ($d_{\rm e} + d_{\rm i} \simeq 2.75$ Å). H···H contacts are disfavoured when the number of H atoms on the molecular surface is large.

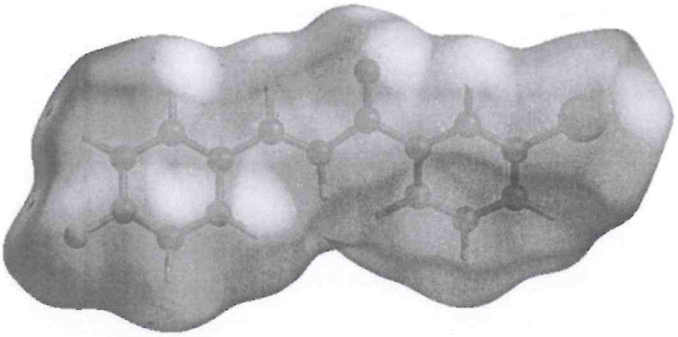
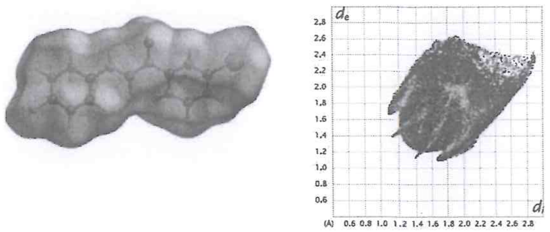
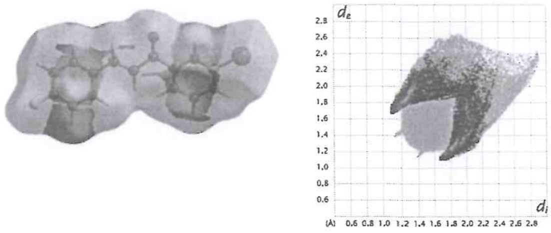


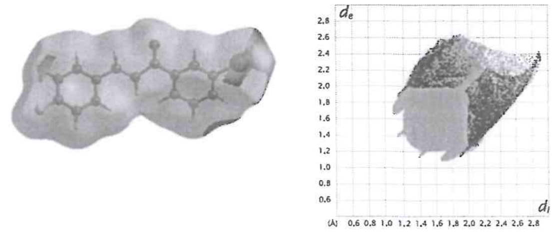
Figure 3
A view of the Hirshfeld surface of the title compound mapped over $d_{\rm norm}$, using a fixed colour scale of −0.0186 (red) to 1.3784 (blue) a.u.



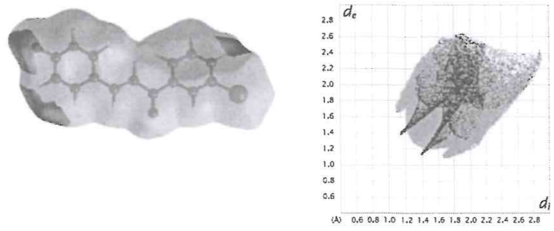
All...All 100 %



C...H / H...C 31.1 %



Br...H / H...Br 14.2 %



F...H / H...F 9.8 %

Figure 4
The two-dimensional fingerprint plots of the title compound.

The Br···H/H···Br and F···H/H···F contacts (Fig. 4) in the structure with 14.2 and 9.8% contributions, respectively, to the Hirshfeld surface are viewed as pairs of spikes with the tips at $d_{\rm e} + d_{\rm i} \simeq 3.05$ and 2.45 Å, respectively.

4. Synthesis and crystallization

The title compound was synthesized as per the procedure reported earlier (Kumar *et al.*, 2013*a*,*b*). 1-(3-Bromophenyl)ethanone (0.01 mol) and 4-fluorobenzaldehyde (0.01 mol) were dissolved in 30 ml methanol. A catalytic amount of NaOH was added to the solution dropwise under vigorous stirring. The reaction mixture was stirred for about 4 h at room temperature. The formed crude products were filtered, washed successively with distilled water and recrystallized from methanol to obtain the title chalcone. The melting point (338–

342 K) was determined using a Stuart Scientific (UK) apparatus.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 4. H atoms were positioned geometrically and refined using riding model, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. Owing to poor agreement between observed and calculated intensities, thirteen outliers ($\bar{1}15$, 131, $\bar{3}26$, 043, 254, $\bar{1}23$, $\bar{2}28$, 150, 253, $\bar{1}11$, $\bar{3}25$, 543, 623) were omitted in the final cycles of refinement.

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Table 4
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{10}BrFO$
M_r	305.14
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	294
a, b, c (Å)	5.9255 (6), 7.5867 (8), 14.1427 (15)
α, β, γ (°)	89.774 (2), 82.671 (2), 87.712 (2)
V (Å^3)	630.09 (11)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	3.26
Crystal size (mm)	0.30 × 0.28 × 0.26
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2007)
T_{min}, T_{max}	0.398, 0.431
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9618, 2442, 2101
R_{int}	0.023
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.105, 1.10
No. of reflections	2442
No. of parameters	163
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.76, −0.40

Computer programs: *APEX2* and *SAINT* (Bruker, 2007), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009).

supporting information

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Crystal structure and Hirshfeld surface analysis of (2*E*)-1-(3-bromophenyl)-3-(4-fluorophenyl)prop-2-en-1-one

Zeliha Atioğlu, S. Bindya, Mehmet Akkurt and C. S. Chidan Kumar

Computing details

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2009).

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

Crystal data

$C_{15}H_{10}BrFO$
$M_r = 305.14$
Triclinic, $P\overline{1}$
$a = 5.9255$ (6) Å
$b = 7.5867$ (8) Å
$c = 14.1427$ (15) Å
$\alpha = 89.774$ (2)°
$\beta = 82.671$ (2)°
$\gamma = 87.712$ (2)°
$V = 630.09$ (11) Å^3
$Z = 2$
$F(000) = 304$
$D_x = 1.608$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4763 reflections
$\theta = 3.6$–27.3°
$\mu = 3.26$ mm^{-1}
$T = 294$ K
Block, colourless
0.30 × 0.28 × 0.26 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2007)
$T_{min} = 0.398$, $T_{max} = 0.431$
9618 measured reflections
2442 independent reflections
2101 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.5°$
$h = -7 \rightarrow 7$
$k = -7 \rightarrow 9$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.105$
$S = 1.10$
2442 reflections
163 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0481P)^2 + 0.4984P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.76$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ 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	1.29286 (6)	0.37541 (6)	0.08193 (2)	0.06864 (18)
F1	0.2394 (4)	−0.0245 (4)	0.91227 (16)	0.0855 (7)
O1	1.2246 (4)	0.2758 (4)	0.46700 (17)	0.0609 (6)
C1	0.7494 (5)	0.4234 (4)	0.3499 (2)	0.0485 (7)
H1A	0.639101	0.432526	0.402871	0.058*
C2	0.7020 (5)	0.4863 (5)	0.2621 (3)	0.0553 (8)
H2A	0.560236	0.540073	0.257032	0.066*
C3	0.8602 (5)	0.4709 (4)	0.1826 (2)	0.0530 (8)
H3A	0.825976	0.511138	0.123703	0.064*
C4	1.0720 (5)	0.3940 (4)	0.1920 (2)	0.0440 (6)
C5	1.1280 (5)	0.3320 (4)	0.2783 (2)	0.0408 (6)
H5A	1.271938	0.281871	0.283008	0.049*
C6	0.9640 (5)	0.3463 (4)	0.3583 (2)	0.0401 (6)
C7	1.0259 (5)	0.2821 (4)	0.4522 (2)	0.0453 (7)
C8	0.8399 (5)	0.2254 (4)	0.5237 (2)	0.0491 (7)
H8A	0.697720	0.207874	0.504874	0.059*
C9	0.8697 (5)	0.1987 (4)	0.6141 (2)	0.0437 (6)
H9A	1.012966	0.220989	0.630447	0.052*
C10	0.7013 (5)	0.1380 (4)	0.6910 (2)	0.0402 (6)
C11	0.7434 (5)	0.1542 (4)	0.7850 (2)	0.0479 (7)
H11A	0.878507	0.202032	0.797670	0.058*
C12	0.5888 (6)	0.1008 (5)	0.8598 (2)	0.0585 (8)
H12A	0.617731	0.112494	0.922560	0.070*
C13	0.3923 (6)	0.0304 (5)	0.8394 (2)	0.0550 (8)
C14	0.3445 (5)	0.0080 (4)	0.7482 (2)	0.0500 (7)
H14A	0.211180	−0.044035	0.736707	0.060*
C15	0.4981 (5)	0.0640 (4)	0.6738 (2)	0.0456 (7)
H15A	0.466180	0.052442	0.611505	0.055*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0651 (3)	0.0932 (3)	0.0443 (2)	0.00443 (19)	0.00298 (15)	0.01381 (18)
F1	0.0780 (15)	0.117 (2)	0.0573 (13)	−0.0210 (14)	0.0140 (11)	0.0172 (13)
O1	0.0431 (12)	0.0916 (19)	0.0486 (13)	−0.0062 (12)	−0.0076 (9)	0.0087 (12)
C1	0.0376 (14)	0.0507 (18)	0.0559 (18)	−0.0022 (13)	−0.0009 (13)	−0.0040 (14)
C2	0.0405 (15)	0.0551 (19)	0.072 (2)	0.0047 (14)	−0.0157 (15)	0.0050 (16)
C3	0.0502 (17)	0.0548 (19)	0.0564 (19)	−0.0041 (14)	−0.0162 (14)	0.0139 (15)
C4	0.0426 (14)	0.0470 (16)	0.0416 (15)	−0.0025 (13)	−0.0023 (12)	0.0043 (12)

C5	0.0359 (13)	0.0421 (15)	0.0444 (15)	−0.0014 (12)	−0.0049 (11)	0.0028 (12)
C6	0.0368 (13)	0.0397 (15)	0.0442 (15)	−0.0062 (11)	−0.0052 (11)	−0.0003 (12)
C7	0.0435 (15)	0.0490 (17)	0.0440 (15)	−0.0073 (13)	−0.0059 (12)	−0.0013 (13)
C8	0.0437 (15)	0.0570 (19)	0.0474 (17)	−0.0093 (14)	−0.0067 (13)	0.0011 (14)
C9	0.0398 (14)	0.0441 (16)	0.0468 (16)	−0.0008 (12)	−0.0048 (12)	0.0003 (13)
C10	0.0418 (14)	0.0342 (14)	0.0445 (15)	0.0027 (11)	−0.0062 (12)	0.0009 (12)
C11	0.0460 (16)	0.0496 (17)	0.0495 (17)	−0.0009 (13)	−0.0117 (13)	0.0032 (13)
C12	0.065 (2)	0.071 (2)	0.0397 (16)	−0.0030 (17)	−0.0085 (14)	0.0045 (15)
C13	0.0530 (18)	0.060 (2)	0.0490 (18)	0.0006 (15)	0.0050 (14)	0.0107 (15)
C14	0.0425 (15)	0.0476 (17)	0.0597 (19)	−0.0055 (13)	−0.0049 (13)	0.0022 (14)
C15	0.0478 (16)	0.0470 (17)	0.0424 (15)	−0.0023 (13)	−0.0071 (12)	−0.0008 (13)

Geometric parameters (Å, º)

Br1—C4	1.903 (3)	C8—C9	1.327 (4)
F1—C13	1.358 (4)	C8—H8A	0.9300
O1—C7	1.221 (4)	C9—C10	1.465 (4)
C1—C2	1.387 (5)	C9—H9A	0.9300
C1—C6	1.397 (4)	C10—C11	1.390 (4)
C1—H1A	0.9300	C10—C15	1.398 (4)
C2—C3	1.371 (5)	C11—C12	1.379 (5)
C2—H2A	0.9300	C11—H11A	0.9300
C3—C4	1.384 (4)	C12—C13	1.364 (5)
C3—H3A	0.9300	C12—H12A	0.9300
C4—C5	1.382 (4)	C13—C14	1.368 (5)
C5—C6	1.396 (4)	C14—C15	1.378 (4)
C5—H5A	0.9300	C14—H14A	0.9300
C6—C7	1.496 (4)	C15—H15A	0.9300
C7—C8	1.474 (4)		

C2—C1—C6	119.6 (3)	C7—C8—H8A	119.1
C2—C1—H1A	120.2	C8—C9—C10	127.1 (3)
C6—C1—H1A	120.2	C8—C9—H9A	116.5
C3—C2—C1	121.2 (3)	C10—C9—H9A	116.5
C3—C2—H2A	119.4	C11—C10—C15	118.2 (3)
C1—C2—H2A	119.4	C11—C10—C9	119.2 (3)
C2—C3—C4	118.6 (3)	C15—C10—C9	122.5 (3)
C2—C3—H3A	120.7	C12—C11—C10	121.3 (3)
C4—C3—H3A	120.7	C12—C11—H11A	119.3
C5—C4—C3	122.2 (3)	C10—C11—H11A	119.3
C5—C4—Br1	119.3 (2)	C13—C12—C11	118.3 (3)
C3—C4—Br1	118.5 (2)	C13—C12—H12A	120.9
C4—C5—C6	118.6 (3)	C11—C12—H12A	120.9
C4—C5—H5A	120.7	F1—C13—C12	119.0 (3)
C6—C5—H5A	120.7	F1—C13—C14	118.2 (3)
C5—C6—C1	119.8 (3)	C12—C13—C14	122.8 (3)
C5—C6—C7	118.6 (3)	C13—C14—C15	118.6 (3)
C1—C6—C7	121.5 (3)	C13—C14—H14A	120.7

O1—C7—C8	122.3 (3)	C15—C14—H14A	120.7
O1—C7—C6	120.2 (3)	C14—C15—C10	120.7 (3)
C8—C7—C6	117.5 (2)	C14—C15—H15A	119.6
C9—C8—C7	121.9 (3)	C10—C15—H15A	119.6
C9—C8—H8A	119.1		

C6—C1—C2—C3	1.5 (5)	C6—C7—C8—C9	−166.9 (3)
C1—C2—C3—C4	−1.4 (5)	C7—C8—C9—C10	−178.2 (3)
C2—C3—C4—C5	0.3 (5)	C8—C9—C10—C11	−165.8 (3)
C2—C3—C4—Br1	−179.2 (3)	C8—C9—C10—C15	14.1 (5)
C3—C4—C5—C6	0.7 (5)	C15—C10—C11—C12	−0.7 (5)
Br1—C4—C5—C6	−179.9 (2)	C9—C10—C11—C12	179.2 (3)
C4—C5—C6—C1	−0.6 (4)	C10—C11—C12—C13	0.3 (5)
C4—C5—C6—C7	−179.0 (3)	C11—C12—C13—F1	179.3 (3)
C2—C1—C6—C5	−0.5 (4)	C11—C12—C13—C14	1.2 (6)
C2—C1—C6—C7	177.9 (3)	F1—C13—C14—C15	179.7 (3)
C5—C6—C7—O1	25.1 (4)	C12—C13—C14—C15	−2.1 (5)
C1—C6—C7—O1	−153.3 (3)	C13—C14—C15—C10	1.7 (5)
C5—C6—C7—C8	−154.0 (3)	C11—C10—C15—C14	−0.3 (5)
C1—C6—C7—C8	27.6 (4)	C9—C10—C15—C14	179.8 (3)
O1—C7—C8—C9	14.0 (5)		

Hydrogen-bond geometry (Å, º)

*Cg*1 and *Cg*2 are the centroids of the 3-bromophenyl (C1–C6) and 4-fluorophenyl (C10–C15) rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9*A*···O1	0.93	2.53	2.840 (4)	100
C2—H2*A*···$Cg2^{\mathrm{i}}$	0.93	2.93	3.571 (4)	127
C5—H5*A*···$Cg2^{\mathrm{ii}}$	0.93	2.98	3.642 (3)	129
C14—H14*A*···$Cg1^{\mathrm{iii}}$	0.93	2.90	3.590 (3)	132

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

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