

Crystal structure of (2*E*)-1-(4-ethoxyphenyl)-3-(4-fluorophenyl)prop-2-en-1-one

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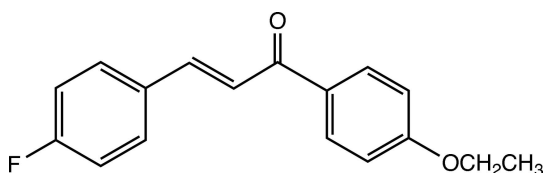
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The title molecule, C₁₇H₁₅FO₂, was synthesized by a Claisen–Schmidt condensation with 4-fluorobenzaldehyde and 4'-ethoxyacetophenone. The torsion angles between the 4-fluorophenyl ring and the alkene and the 4'-ethoxyphenyl ring and the 2-propen-1-one are −1.2 (4)° and 1.2 (3)°, respectively; however, there is a larger torsion between the bonds comprising the 2-propen-1-one unit of 12.0 (4)°. The crystal packing is stabilized by intermolecular C—H···O/F hydrogen bonding, π–π stacking, and H–π interactions.

1. Chemical context

Chalcones are a group of 1,3-diaryl-2-propen-1-one compounds that have been found to exhibit a wide variety of biological activity including anticancer, antimicrobial and anti-inflammatory properties (Sahu *et al.*, 2012). Chalcones are also important starting materials for the synthesis of several pharmacologically interesting classes of heterocyclic compounds such as isoxazoles, pyrazolines and pyrazoles (Kamal *et al.*, 2019). In our research involving the synthesis of chalcone derivatives, we have synthesized and obtained an X-ray structure for the title compound, C₁₇H₁₅FO₂, 2(*E*)-1-(4-ethoxyphenyl)-3-(4-fluorophenyl)-2-propen-1-one.



2. Structural commentary

This chalcone has aromatic rings with substitutions in the 4 position on both ends of the molecule, where the phenyl on the alkene is fluorinated, and the phenyl on the carbonyl contains an ethoxide (Fig. 1). Both phenyl rings are inclined towards the same side of the molecule thanks to the *E* geometry of the chalcone's alkene. The compound is a heavily π-conjugated structure that is nearly planar. To measure the deviation from planarity, three torsion angles were examined. The angles involving the aromatic rings are nearly identical with little bend, where the torsion between the C8—C7 and C5—C4 bonds is −1.2 (4)°, and the torsion between the C8—C9 and C15—C10 bonds is 1.2 (3)°. However, the torsion angle of the chalcone between the O1—C9 and C7—C8 bonds

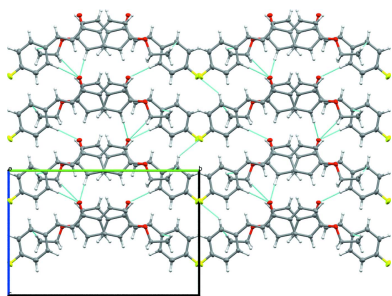


Table 1

Torsions of 4,4' substituted chalcones (°).

All torsions were measured in *Mercury* (v2020.2.0; Macrae *et al.*, 2020), with the exception of the torsion angles from this work, which were calculated using the CONF command of *SHELXL2018/3* (Sheldrick, 2015b).

Entry	-X	-R	Carbonyl-alkene torsion	Aryl-alkene torsion	Aryl-carbonyl torsion	Space group	CCDC Dep. No.
1	F	Me	18.77	12.69	13.71	<i>P2₁/c</i>	660304 ^a
2	F	OH	2.41	0.99	6.18	<i>P1</i>	2184323 ^b
3	F	OMe	18.95	11.50	2.92	<i>Pbca</i>	738291 ^c
4	F	OEt	12.00	1.20	1.20	<i>Pca2₁</i>	This work
5	Cl	OMe	16.38	3.78	25.77	<i>Pbca</i>	2070477 ^d
6	Br	OMe	16.42	6.43	24.69	<i>Pc</i>	2062759 ^e
7	2-Cl	OEt	5.16	4.47	0.44	<i>P1</i>	1550212 ^f
8	3-Cl	OEt	0.86	0.93	2.60	<i>P1</i>	1587066 ^f

Notes: (a) Butcher *et al.* (2007); (b) Sobolev *et al.* (2022); (c) Zhao *et al.* (2009); (d) Whitwood *et al.* (2021); (e) Wilhelm *et al.* (2022); (f) Harshitha *et al.* (2018).

is 12.0 (4)°, indicating a break in planarity. This single deviation causes a slight concave bend in the molecule. The title compound crystallized as a racemic mixture in the space group *Pca2₁*; thus, a clockwise and anticlockwise torsion of the chalcone are present with a 1:1 ratio in the unit cell.

There are several other chalcones with a comparable 4 and 4' set of substitutions that are summarized in Table 1 from a CSD database search. If the halogen (-X) is maintained as a fluorine, the other substituent (-R) varies as either a methyl,

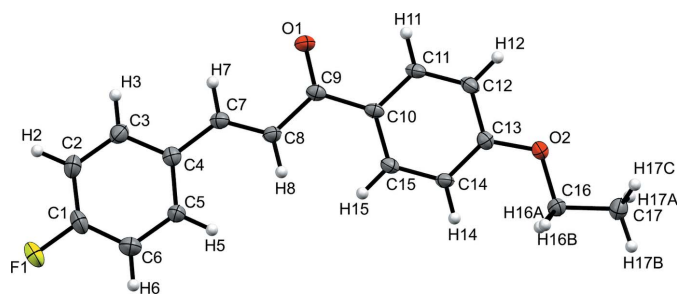


Figure 1
The molecular structure of 2(*E*)-1-(4-ethoxyphenyl)-3-(4-fluorophenyl)-2-propen-1-one. Displacement ellipsoids are drawn at the 50% probability level.

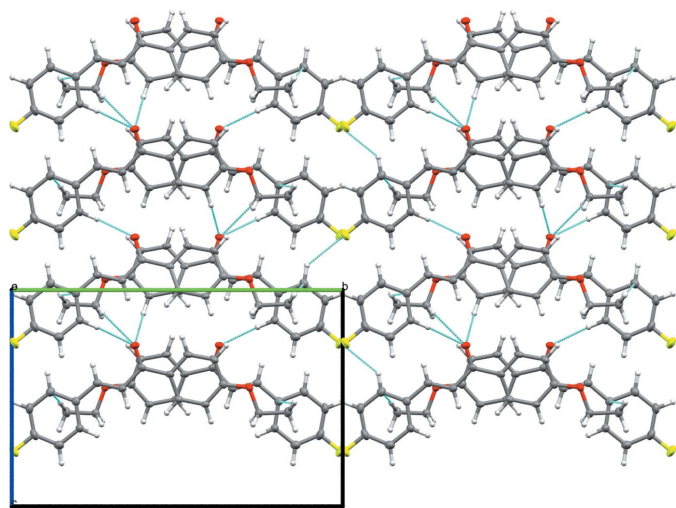


Figure 2
Packing of the title compound viewed along the *a* axis. Hydrogen bonds and H- π bonds are shown as blue lines.

hydroxyl, methoxy, or ethoxy group. Examination of the three torsion angles described above suggests that there is a trend in the degree of distortion from planarity, with an order of methyl, methoxy, ethoxy, to hydroxy by increasing planarity. While there are no direct examples that contain a halogen and an ethoxy, we felt comparison of our compound to the nearest chloro- and bromo-substituted compounds was warranted. The closest examples are a bromo/methoxy and a chloro/methoxy 4,4' -substituted chalcone. Both cases are more distorted from planar than our fluoro/ethoxy chalcone. Lastly, we found a set of chalcones with an ethoxy substituent, where there are chlorine atoms in the 2 and 3 position of the respective phenyl ring. Both of these cases are more planar than our chalcone.

3. Supramolecular features

2(*E*)-1-(4-Ethoxyphenyl)-3-(4-fluorophenyl)-2-propen-1-one crystallizes in the orthorhombic space group *Pca2₁*, with four molecules occupying one unit cell. The molecules pack using hydrogen bonding, π - π stacking, and H- π interactions (Figs. 2, 3, 4). There are four hydrogen bonds (Table 2) that inter-

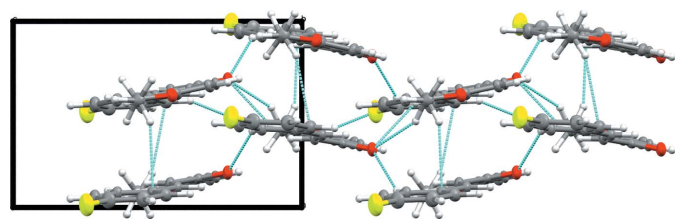


Figure 3
Packing of the title compound viewed along the *b* axis. Hydrogen bonds and H- π bonds are shown as blue lines.

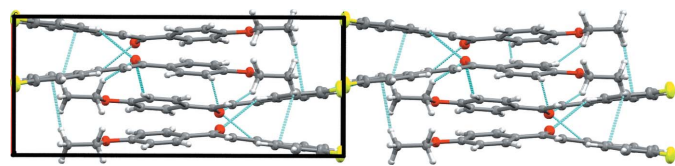


Figure 4
Packing of the title compound viewed along the *c* axis. Hydrogen bonds and H- π bonds are shown as blue lines.

Table 2

Hydrogen-bond geometry (Å, °).

Two hydrogen bonds were found automatically by *SHELXL*; including the C14–H14 and O1, and C16–H16A and O1 donor–acceptor pairs. The remaining two pairs were identified by inspection.

<i>D</i> –H... <i>A</i>	<i>D</i> –H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> –H... <i>A</i>
C3–H3...F1 ⁱ	0.95	2.60	3.345 (3)	136
C5–H5...O1 ⁱⁱ	0.95	2.70	3.544 (3)	149
C14–H14...O1 ⁱⁱⁱ	0.95	2.46	3.295 (3)	146
C16–H16A...O1 ⁱⁱⁱ	0.99	2.60	3.470 (3)	146

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

connect each molecule to three of its neighbors. The first is between the C3–H3 bond and an adjacent F1 atom, the second pairs the C5–H5 bond and a nearby O1 atom, and the final two involve the C14–H14 and C16–H16A bonds with a neighboring O1 atom. Given the extent of conjugated π bonds throughout this molecule, π – π stacking is present between adjacent molecules along the *a* axis [centroid–centroid distance = 4.240 Å], with alternating molecules related by the *a* glide plane of the *Pca*₂₁ space group; this orients these molecules such that adjacent molecules are mirror images of one another with opposing chalcone bond torsions. Lastly, there are H– π interactions present between H17A and the aromatic ring comprised of C1–C6, as well as between H17C and this same ring on another molecule, forming a chain of interactions that parallel the *a* axis.

In comparison to the other chalcones described in Table 1, our structure packs in a unique space group *Pca*₂₁, where many others pack in *Pbca* or *P* $\bar{1}$. Common themes that appear among these structures include π – π stacking and hydrogen bonding to the carbonyl oxygen. However, it is interesting to note that the chloro/methoxy and bromo/methoxy analogs pack with π – π stacking where the molecules are mirror images from a plane that is colinear with the molecular mean plane, rather than images related to a plane that is orthogonal to the molecular mean plane as observed in our structure. Also, in the case where the $-R$ substituent is a hydroxide, hydrogen bonding between the hydroxyl group and the carbonyl oxygen dominates the packing.

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.43, update March 2022; Groom *et al.*, 2016) for 4,4'-phenyl-substituted chalcones resulted in multiple hits. Most closely related to the title compound are three 4-fluorophenyl-substituted chalcones: (*E*)-3-(4-fluorophenyl)-1-(4-methylphenyl)prop-2-en-1-one (Butcher *et al.*, 2007), (*E*)-3-(4-fluorophenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one (Sobolev *et al.*, 2022), (*E*)-3-(4-fluorophenyl)-1-(4-methoxyphenyl)prop-2-en-1-one (Zhao *et al.*, 2009). Additionally, two 4'-methoxy-substituted compounds with 4-chloro or bromophenyl substitution were found, (*E*)-3-(4-chlorophenyl)-1-(4-methoxyphenyl)prop-2-en-1-one (Whitwood *et al.*, 2021) and (*E*)-3-(4-bromophenyl)-1-(4-methoxyphenyl)prop-2-en-1-one

Table 3

Experimental details.

Crystal data	
Chemical formula	C ₁₇ H ₁₅ FO ₂
<i>M_r</i>	270.29
Crystal system, space group	Orthorhombic, <i>Pca</i> ₂₁
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	7.1426 (4), 17.0566 (9), 11.1520 (6)
<i>V</i> (Å ³)	1358.63 (13)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.10
Crystal size (mm)	0.24 × 0.11 × 0.11
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015) [†]
<i>T</i> _{min} , <i>T</i> _{max}	0.691, 0.745
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	23454, 2438, 2365
<i>R</i> _{int}	0.061
(sin θ/λ) _{max} (Å ⁻¹)	0.603
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.039, 0.104, 1.10
No. of reflections	2438
No. of parameters	182
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	0.27, -0.17

Computer programs: *APEX4* (Bruker, 2021), *SAINT* (Bruker, 2002), *SHELXT2018/2* (Sheldrick, 2015a), *SHELXL2018/3* (Sheldrick, 2015b), and *SHELXTL* (Sheldrick, 2008).

(Wilhelm *et al.*, 2022). Two 4'-ethoxy-substituted compounds were also found, (*E*)-3-(2-chlorophenyl)-1-(4-ethoxyphenyl)prop-2-en-1-one (Harshitha *et al.*, 2018) and (*E*)-3-(3-chlorophenyl)-1-(4-ethoxyphenyl)prop-2-en-1-one (Harshitha *et al.*, 2018). See Table 1 for relevant data from these structures.

5. Synthesis and crystallization

4-Fluorobenzaldehyde (3 mmol) and 4-ethoxyacetophenone (3 mmol) were mixed in 95% EtOH (2.5 mL). An aqueous solution of sodium hydroxide (0.3 mL, 15 mM) was added to the mixture dropwise. The mixture was allowed to stir at room temperature for 45 min. Cold distilled H₂O (4 mL) was added and the mixture was cooled in an ice bath before isolating the solid product by vacuum filtration. The chalcone was purified by recrystallization with dichloromethane/hexane (4:1) to yield colorless crystals (77% yield). High-quality crystals for diffraction were grown from slow evaporation of 190 proof ethanol at room temperature, m.p. 392–394 K; IR (ATR) ν_{\max} 3067, 2936, 1653, 1596, 1572, 1504, 1157, 1033 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.03 (*d*, *J* = 9.2 Hz, 2H), 7.76 (*d*, *J* = 15.6 Hz, 1H), 7.62 (*dd*, *J* = 5.5, 3.2 Hz, 2H), 7.46 (*d*, *J* = 15.6 Hz, 1H), 7.10 (*t*, *J* = 8.7 Hz, 2H), 6.79 (*d*, *J* = 8.7 Hz, 2H), 3.88 (*s*, 3H) ppm; ¹³C{¹H} NMR (100MHz, CDCl₃) δ 188.4, 163.5, 163.9 (*d*, ¹*J*_{C-F} = 252.1 Hz), 142.6, 131.3 (*d*, ⁴*J*_{C-F} = 2.9 Hz), 131.0, 130.8, 130.2 (*d*, ³*J*_{C-F} = 8.6 Hz), 121.5 (*d*, ⁶*J*_{C-F} = 1.9 Hz), 116.0 (*d*, ²*J*_{C-F} = 22.0 Hz), 113.8, 55.5 ppm. ¹H NMR data have previously been reported (Liu *et al.*, 2001).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. Hydrogen atoms were generated using a riding model with geometric constraints and refined isotropically. Aromatic C—H distances are 0.95 Å, methylene C—H distances are 0.99 Å, and methyl C—H distances are 0.98 Å. $U_{\text{iso}}(\text{H})$ was 1.2 times $U_{\text{eq}}(\text{C})$ for aromatic and methylene hydrogen atoms, and 1.5 times $U_{\text{eq}}(\text{C})$ for methyl hydrogen atoms. There is minor whole molecule disorder visible in the residual peaks that was not refined since these peaks are rather small ($< 0.26 \text{ e \AA}^{-3}$) and there was little improvement in the model.

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Acta Cryst. (2022). E78, 821-824 [https://doi.org/10.1107/S2056989022007423]

Crystal structure of (2*E*)-1-(4-ethoxyphenyl)-3-(4-fluorophenyl)prop-2-en-1-one

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Computing details

Data collection: *APEX4* (Bruker, 2021); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT* (Bruker, 2002); program(s) used to solve structure: *SHELXT2018/2* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015b); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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

Crystal data

$C_{17}H_{15}FO_2$

$M_r = 270.29$

Orthorhombic, *Pca*2₁

$a = 7.1426$ (4) Å

$b = 17.0566$ (9) Å

$c = 11.1520$ (6) Å

$V = 1358.63$ (13) Å³

$Z = 4$

$F(000) = 568$

$D_x = 1.321$ Mg m⁻³

Melting point = 119–121 K

Mo *K*α radiation, $\lambda = 0.71073$ Å

Cell parameters from 7611 reflections

$\theta = 3.1$ – 25.3°

$\mu = 0.10$ mm⁻¹

$T = 100$ K

Block, colorless

$0.24 \times 0.11 \times 0.11$ mm

Data collection

Bruker APEXII CCD
diffractometer

φ and ω scans

Absorption correction: multi-scan
(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.691$, $T_{\max} = 0.745$

23454 measured reflections

2438 independent reflections

2365 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.061$

$\theta_{\max} = 25.4^\circ$, $\theta_{\min} = 2.4^\circ$

$h = -8 \rightarrow 8$

$k = -20 \rightarrow 20$

$l = -13 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.039$

$wR(F^2) = 0.104$

$S = 1.10$

2438 reflections

182 parameters

1 restraint

Primary atom site location: dual

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.069P)^2 + 0.1828P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.27$ e Å⁻³

$\Delta\rho_{\min} = -0.17$ 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.

Refinement. There is a minor disordered component visible in the residual peaks that is not refined, since there is little improvement in the model.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
F1	0.4847 (3)	0.00701 (11)	0.7445 (2)	0.0476 (6)
O1	0.3123 (3)	0.37163 (10)	0.25635 (16)	0.0242 (4)
O2	0.3964 (2)	0.71755 (10)	0.44972 (18)	0.0227 (4)
C1	0.4610 (4)	0.06802 (16)	0.6686 (3)	0.0326 (7)
C2	0.4545 (4)	0.05380 (16)	0.5477 (3)	0.0301 (6)
H2	0.465389	0.001957	0.517328	0.036*
C3	0.4316 (4)	0.11687 (16)	0.4708 (3)	0.0257 (6)
H3	0.426726	0.107993	0.386721	0.031*
C4	0.4154 (3)	0.19357 (15)	0.5148 (2)	0.0205 (6)
C5	0.4225 (4)	0.20530 (15)	0.6394 (2)	0.0220 (6)
H5	0.410714	0.256768	0.671075	0.026*
C6	0.4464 (4)	0.14242 (17)	0.7165 (3)	0.0301 (6)
H6	0.452542	0.150326	0.800692	0.036*
C7	0.3907 (3)	0.25841 (15)	0.4307 (2)	0.0208 (6)
H7	0.390057	0.244965	0.348020	0.025*
C8	0.3692 (4)	0.33370 (14)	0.4560 (2)	0.0199 (5)
H8	0.369696	0.350200	0.537401	0.024*
C9	0.3442 (3)	0.39260 (15)	0.3600 (2)	0.0185 (5)
C10	0.3596 (3)	0.47712 (15)	0.3897 (2)	0.0179 (5)
C11	0.3348 (4)	0.53263 (15)	0.2981 (2)	0.0211 (5)
H11	0.309041	0.515191	0.218899	0.025*
C12	0.3470 (3)	0.61131 (15)	0.3206 (2)	0.0225 (6)
H12	0.328745	0.647740	0.257190	0.027*
C13	0.3862 (3)	0.63855 (14)	0.4366 (2)	0.0195 (6)
C14	0.4132 (3)	0.58453 (15)	0.5286 (2)	0.0192 (5)
H14	0.440382	0.602146	0.607528	0.023*
C15	0.4002 (4)	0.50479 (15)	0.5046 (2)	0.0198 (5)
H15	0.419362	0.468300	0.567816	0.024*
C16	0.4192 (4)	0.74662 (15)	0.5705 (3)	0.0236 (6)
H16A	0.536921	0.726316	0.605590	0.028*
H16B	0.313446	0.729185	0.621292	0.028*
C17	0.4247 (4)	0.83493 (15)	0.5646 (3)	0.0264 (6)
H17A	0.540214	0.851724	0.524786	0.040*
H17B	0.420936	0.856464	0.646047	0.040*
H17C	0.316396	0.853991	0.519179	0.040*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0811 (15)	0.0254 (9)	0.0364 (10)	0.0047 (9)	-0.0034 (10)	0.0135 (8)
O1	0.0317 (10)	0.0254 (9)	0.0156 (9)	-0.0012 (7)	0.0005 (8)	-0.0020 (8)
O2	0.0303 (10)	0.0174 (9)	0.0204 (10)	-0.0012 (7)	-0.0030 (8)	0.0031 (7)
C1	0.0432 (18)	0.0207 (14)	0.0338 (18)	0.0018 (12)	-0.0004 (13)	0.0099 (13)
C2	0.0397 (15)	0.0172 (12)	0.0334 (16)	0.0016 (11)	0.0008 (13)	-0.0019 (12)
C3	0.0283 (14)	0.0233 (13)	0.0256 (15)	0.0002 (11)	-0.0012 (11)	-0.0040 (11)
C4	0.0185 (12)	0.0206 (12)	0.0225 (14)	-0.0004 (9)	-0.0001 (10)	0.0007 (11)
C5	0.0281 (14)	0.0191 (13)	0.0190 (13)	0.0004 (10)	0.0017 (11)	0.0002 (10)
C6	0.0391 (16)	0.0305 (15)	0.0208 (14)	0.0000 (12)	0.0007 (12)	0.0009 (12)
C7	0.0221 (12)	0.0237 (13)	0.0166 (13)	-0.0011 (10)	0.0004 (10)	-0.0002 (11)
C8	0.0234 (11)	0.0211 (12)	0.0153 (12)	-0.0009 (10)	0.0014 (10)	-0.0016 (11)
C9	0.0157 (11)	0.0237 (13)	0.0161 (13)	-0.0003 (9)	0.0031 (9)	0.0015 (10)
C10	0.0160 (11)	0.0244 (13)	0.0134 (12)	-0.0005 (9)	0.0025 (9)	0.0022 (10)
C11	0.0234 (13)	0.0275 (13)	0.0125 (12)	-0.0021 (10)	-0.0020 (10)	0.0023 (10)
C12	0.0257 (14)	0.0239 (13)	0.0181 (14)	-0.0019 (10)	-0.0040 (11)	0.0060 (11)
C13	0.0191 (11)	0.0193 (12)	0.0200 (14)	0.0001 (9)	0.0010 (10)	0.0021 (11)
C14	0.0227 (13)	0.0227 (13)	0.0121 (12)	0.0010 (10)	0.0000 (10)	0.0002 (10)
C15	0.0215 (12)	0.0222 (13)	0.0158 (13)	0.0020 (10)	-0.0013 (10)	0.0037 (10)
C16	0.0306 (13)	0.0200 (13)	0.0202 (13)	-0.0007 (10)	0.0029 (11)	-0.0006 (11)
C17	0.0287 (13)	0.0204 (13)	0.0301 (15)	0.0000 (10)	0.0022 (12)	-0.0021 (12)

Geometric parameters (Å, °)

F1—C1	1.352 (3)	C8—H8	0.9500
O1—C9	1.231 (3)	C9—C10	1.483 (3)
O2—C13	1.357 (3)	C10—C15	1.396 (4)
O2—C16	1.444 (3)	C10—C11	1.404 (3)
C1—C2	1.371 (5)	C11—C12	1.368 (4)
C1—C6	1.381 (4)	C11—H11	0.9500
C2—C3	1.385 (4)	C12—C13	1.404 (4)
C2—H2	0.9500	C12—H12	0.9500
C3—C4	1.402 (4)	C13—C14	1.392 (3)
C3—H3	0.9500	C14—C15	1.389 (4)
C4—C5	1.405 (4)	C14—H14	0.9500
C4—C7	1.461 (4)	C15—H15	0.9500
C5—C6	1.385 (4)	C16—C17	1.508 (4)
C5—H5	0.9500	C16—H16A	0.9900
C6—H6	0.9500	C16—H16B	0.9900
C7—C8	1.324 (3)	C17—H17A	0.9800
C7—H7	0.9500	C17—H17B	0.9800
C8—C9	1.480 (3)	C17—H17C	0.9800
C13—O2—C16	116.6 (2)	C15—C10—C9	123.3 (2)
F1—C1—C2	118.9 (3)	C11—C10—C9	118.9 (2)
F1—C1—C6	118.3 (3)	C12—C11—C10	121.3 (2)

C2—C1—C6	122.7 (3)	C12—C11—H11	119.3
C1—C2—C3	118.4 (3)	C10—C11—H11	119.3
C1—C2—H2	120.8	C11—C12—C13	120.4 (2)
C3—C2—H2	120.8	C11—C12—H12	119.8
C2—C3—C4	121.2 (3)	C13—C12—H12	119.8
C2—C3—H3	119.4	O2—C13—C14	124.8 (2)
C4—C3—H3	119.4	O2—C13—C12	116.0 (2)
C3—C4—C5	118.4 (2)	C14—C13—C12	119.2 (2)
C3—C4—C7	119.4 (3)	C15—C14—C13	119.8 (2)
C5—C4—C7	122.1 (3)	C15—C14—H14	120.1
C6—C5—C4	120.5 (3)	C13—C14—H14	120.1
C6—C5—H5	119.7	C14—C15—C10	121.4 (2)
C4—C5—H5	119.7	C14—C15—H15	119.3
C1—C6—C5	118.8 (3)	C10—C15—H15	119.3
C1—C6—H6	120.6	O2—C16—C17	107.8 (2)
C5—C6—H6	120.6	O2—C16—H16A	110.2
C8—C7—C4	127.7 (3)	C17—C16—H16A	110.2
C8—C7—H7	116.2	O2—C16—H16B	110.2
C4—C7—H7	116.2	C17—C16—H16B	110.2
C7—C8—C9	121.2 (2)	H16A—C16—H16B	108.5
C7—C8—H8	119.4	C16—C17—H17A	109.5
C9—C8—H8	119.4	C16—C17—H17B	109.5
O1—C9—C8	120.3 (2)	H17A—C17—H17B	109.5
O1—C9—C10	120.4 (2)	C16—C17—H17C	109.5
C8—C9—C10	119.3 (2)	H17A—C17—H17C	109.5
C15—C10—C11	117.8 (2)	H17B—C17—H17C	109.5

Hydrogen-bond geometry (\AA , $^\circ$)

Two hydrogen bonds were found automatically by *SHELXL*; including the C14—H14 and O1, and C16—H16A and O1 donor–acceptor pairs. The remaining two pairs were identified by inspection.

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C3—H3 \cdots F1 ⁱ	0.95	2.60	3.345 (3)	136
C5—H5 \cdots O1 ⁱⁱ	0.95	2.70	3.544 (3)	149
C14—H14 \cdots O1 ⁱⁱⁱ	0.95	2.46	3.295 (3)	146
C16—H16A \cdots O1 ⁱⁱⁱ	0.99	2.60	3.470 (3)	146

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