Crystal structure of (2E)-1-(4-ethoxyphenyl)-3-(4-fluorophenyl)-2-propen-1-one

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The title molecule, C 17H15FO 2, 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 $1.2(3)^\circ$, respectively; however, there is a larger torsion between the bonds comprising the 2-propen-1-one unit of $12.0(4)^\circ$. 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, C 17H15FO 2, 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 $-1.2(4)^\circ$, and the torsion between the C8—C9 and C15—C10 bonds is $1.2(3)^\circ$. However, the torsion angle of the chalcone between the O1—C9 and C7—C8 bonds...
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, 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-

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).
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 remaining two pairs were identified by inspection. In comparison to the other chalcones described in Table 1, our structure packs in a unique space group $P_{c\alpha}$, with alternating molecules related by the $a$ glide plane of the $P_{c\alpha 2}_1$ space group; this orientates these molecules such that adjacent molecules are mirror images of one another with opposing chalcone bond torsions. Lastly, there are $\pi-\pi$ 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 $P_{c\alpha 2}_1$, where many others pack in $P_{b\alpha c}$ or $P\bar{T}$. Common themes that appear among these structures include $\pi-\pi$ stacking and hydrogen bonding to the carbonyl oxygen. However, it is interesting to note that the chloro/methoxy and bromo/methoxy analogs pack with $\pi-\pi$ 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 (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 H$_2$O (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) $v_{\max}$ 3067, 2936, 1653, 1596, 1572, 1504, 1157, 1033 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 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; $^{13}$C($^1$H) NMR (100MHz, CDCl$_3$) $\delta$ 188.4, 163.5, 163.9 ($d$, $J_{C-F} = 252.1$ Hz), 142.6, 131.3 ($d$, $J_{C-F} = 2.9$ Hz), 131.0, 130.8, 130.2 ($d$, $J_{C-F} = 8.6$ Hz), 121.5 ($d$, $J_{C-F} = 1.9$ Hz), 116.0 ($d$, $J_{C-F} = 22.0$ Hz), 113.8, 55.5 ppm. $^1$H NMR data have previously been reported (Liu et al., 2001).

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**Table 1**

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.

| D—H · · · A | D—H | H · · · A | D—A | D—H · · · A |
|-------------|------|-----------|------|-------------|
| C3—H3 · · · F1 | 0.95 | 2.60 | 3.345 (3) | 136 |
| C5—H5 · · · O1ii | 0.95 | 2.70 | 3.544 (3) | 149 |
| C14—H14 · · · O1iii | 0.95 | 2.46 | 3.295 (3) | 146 |
| C16—H16A · · · O1iv | 0.99 | 2.60 | 3.470 (3) | 146 |

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

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**Table 3**

Experimental details.

Crystal data

Chemical formula: C$_7$H$_{15}$FO$_2$

$M_r=270.29$

Crystal system, space group: Orthorhombic, $Pc\alpha_2_1$

Temperature (K): 100

$\alpha$, $\beta$, $\gamma$ (Å$^\circ$): 7.1426 (4), 17.0566 (9), 11.1520 (6)

$V$ (Å$^3$): 1358.63 (13)

$Z$: 4

Radiation type: Mo Kα

$\mu$ (mm$^{-1}$): 0.10

Crystal size (mm$^3$): 0.24 × 0.11 × 0.11

Data collection

Diffractometer: Bruker APEXII CCD

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

$T_{\text{min}}$, $T_{\text{max}}$: 0.691, 0.745

No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections: 23454, 2438, 2365

$R_{\text{int}}$, (sin $\theta$/λ)$_{\text{max}}$ (Å$^{-1}$): 0.061, 0.603

Refinement

$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$: 0.039, 0.104, 1.10

No. of reflections: 2438

No. of parameters: 182

No. of restraints: 1

$\Delta$/$\rho_{\text{max}}$, $\Delta$/$\rho_{\text{min}}$ (e Å$^{-3}$): 0.27, −0.17

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**Table 2**

Hydrogen-bond geometry (Å, °).

Computer programs: APEX4 (Bruker, 2021), SAINT (Bruker, 2002), SHELXTL20182 (Sheldrick, 2015a), SHELXL2018/3 (Sheldrick, 2015b), and SHELXTL (Sheldrick, 2008).

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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. $U_{iso}(H)$ was 1.2 times $U_{eq}(C)$ for aromatic and methylene hydrogen atoms, and 1.5 times $U_{eq}(C)$ 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 e Å$^{-3}$) and there was little improvement in the model.

Funding information

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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\(_2\)
Mr = 270.29
Orthorhombic, Pca\(_2\)\(_1\)
\(a = 7.1426 (4)\) Å
\(b = 17.0566 (9)\) Å
\(c = 11.1520 (6)\) Å
\(V = 1358.63 (13)\) Å\(^3\)
\(Z = 4\)
\(F(000) = 568\)

Data collection
Bruker APEXII CCD diffractometer
\(\phi\) and \(\omega\) scans
Absorption correction: multi-scan (SADABS; Krause et al., 2015)
\(T\)\(_{\text{min}}\) = 0.691, \(T\)\(_{\text{max}}\) = 0.745
23454 measured reflections

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
\(w = 1/[\sigma^2(F^2) + (0.069P)^2 + 0.1828P]\)
where \(P = (F^2 + 2F^2)/3\)
\((\Delta\sigma)_{\text{max}} < 0.001\)
\(\Delta\rho_{\text{max}} = 0.27\) e Å\(^{-3}\)
\(\Delta\rho_{\text{min}} = -0.17\) 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 (Å²)*

|    | x     | y     | z     | Uiso*/Ueq |
|----|-------|-------|-------|-----------|
| 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 | 0.5059(2) | 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 (Å\\(^2\))

|  | \(U_{11}^{\text{I}}\) | \(U_{22}^{\text{I}}\) | \(U_{33}^{\text{I}}\) | \(U_{12}^{\text{I}}\) | \(U_{13}^{\text{I}}\) | \(U_{23}^{\text{I}}\) |
|---|---|---|---|---|---|---|
| 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, °)

| Bond/Angle | Length (Å) | Angle (°) |
|---|---|---|
| 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)  
C1—C2—C3 118.4 (3)  
C1—C2—H2 120.8  
C3—C2—H2 120.8  
C2—C3—C4 121.2 (3)  
C2—C3—H3 119.4  
C3—C4—C5 118.4 (2)  
C3—C4—C7 119.4 (3)  
C5—C4—C7 122.1 (3)  
C6—C5—C4 120.5 (3)  
C6—C5—H5 119.7  
C4—C5—H5 119.7  
C1—C6—C5 118.8 (3)  
C1—C6—H6 120.6  
C5—C6—H6 120.6  
C8—C7—C4 127.7 (3)  
C8—C7—H7 116.2  
C7—C8—C9 121.2 (2)  
C7—C8—H8 119.4  
C9—C8—H8 119.4  
O1—C9—C8 120.3 (2)  
O1—C9—C10 120.4 (2)  
C8—C9—C10 119.3 (2)  
C15—C10—C11 117.8 (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.

| D—H···A | D—H | H···A | D···A | D—H···A |
|---------|------|------|-------|---------|
| 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−1/2; (ii) −x+1/2, y, z+1/2; (iii) −x+1, −y+1, z+1/2.