



Crystal structure and Hirshfeld surface analysis of (*E*)-3-(2-chloro-6-fluorophenyl)-1-(3-fluoro-4-methoxyphenyl)prop-2-en-1-one

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Keywords: crystal structure; chalcone; hydrogen bonding; Hirshfeld surface analysis.

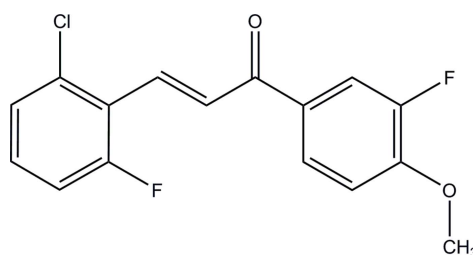
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In the title chalcone derivative, $C_{16}H_{11}ClF_2O_2$, the enone group adopts an *E* conformation. The dihedral angle between the benzene rings is $0.47(9)^\circ$ and an intramolecular $C-H \cdots F$ hydrogen bond closes an *S*(6) ring. In the crystal, molecules are linked into a three-dimensional network by $C-H \cdots O$ hydrogen bonds and aromatic $\pi-\pi$ stacking interactions are also observed [centroid-centroid separation = $3.5629(18)$ Å]. The intermolecular interactions in the crystal structure were quantified and analysed using Hirshfeld surface analysis.

1. Chemical context

Chalcone derivatives possess a wide range of biological properties such as antibacterial (Jarag *et al.*, 2011), anti-inflammatory (Mukherjee *et al.*, 2001) and anti-oxidant (Arty *et al.*, 2000) activities. As part of our ongoing studies on chalcone derivatives, we hereby report the synthesis and crystal structure of the title compound, (I).



2. Structural commentary

The molecular structure of (I) is shown in Fig. 1. The enone moiety (O1/C7–C9) adopts an *E*-conformation with respect to $C7=C8$ bond. The molecule is slightly twisted at the $C9-$

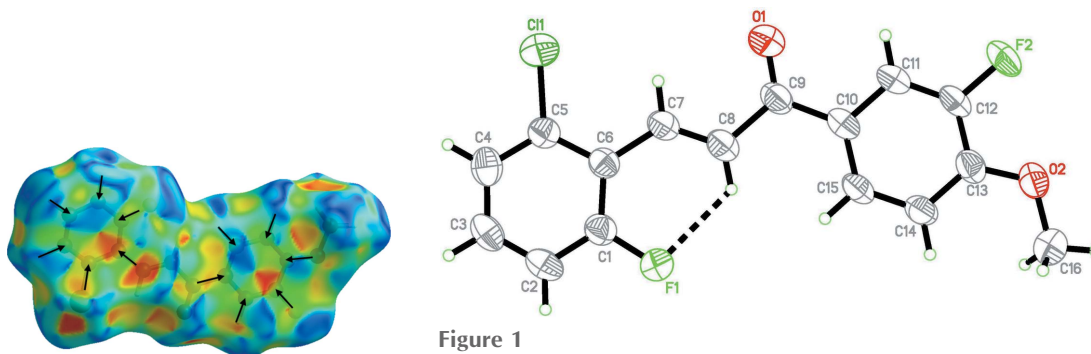


Figure 1
The structure of the title compound, showing 50% probability displacement ellipsoids. The intramolecular $C-H \cdots F$ hydrogen bond is shown as a dashed line.

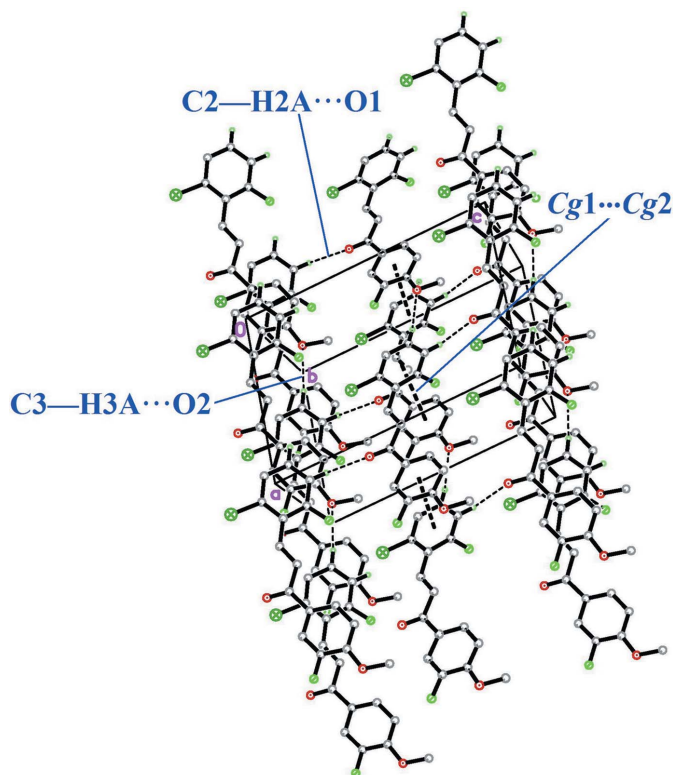


Figure 2
The packing in (I) showing C—H...O and π — π interactions as dashed lines.

Table 1
Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C2-H2A\cdots O1^i$	0.93	2.50	3.391 (4)	162
$C3-H3A\cdots O2^{ii}$	0.93	2.52	3.441 (4)	171
$C8-H8A\cdots F1$	0.93	2.21	2.842 (4)	124

Symmetry codes: (i) $x - \frac{1}{2}, -y + \frac{3}{2}, z + \frac{1}{2}$; (ii) $x - \frac{3}{2}, y + \frac{1}{2}, z$.

C10 bond with a C8—C9—C10—C15 torsion angle of -2.2 (4°) and a maximum deviation of 0.193 (16) \AA for atom O1. The dihedral angle between the terminal benzene rings (C1—C6 and C10—C15) is 0.47 (9°). The least-squares plane through the enone moiety (O1/C7—C9) makes dihedral angles of 2.87 (14) and 3.33 (14) $^\circ$ with the C1—C6 and C10—C15 benzene rings, respectively. An intramolecular C8—H8A...F1 hydrogen bond (Table 1) is observed, generating an $S(6)$ ring motif. The bond lengths and angles are comparable with the equivalent data for previously reported structures; (Razak *et al.*, 2009; Harrison *et al.*, 2006a).

3. Supramolecular features

In the crystal, molecules are linked into a three-dimensional network *via* C2—H2A...O1 ($x - \frac{1}{2}, -y + \frac{3}{2}, z + \frac{1}{2}$) and C3—H3A...O2 ($x - \frac{3}{2}, y + \frac{1}{2}, z$) hydrogen bonds (Table 1), as shown

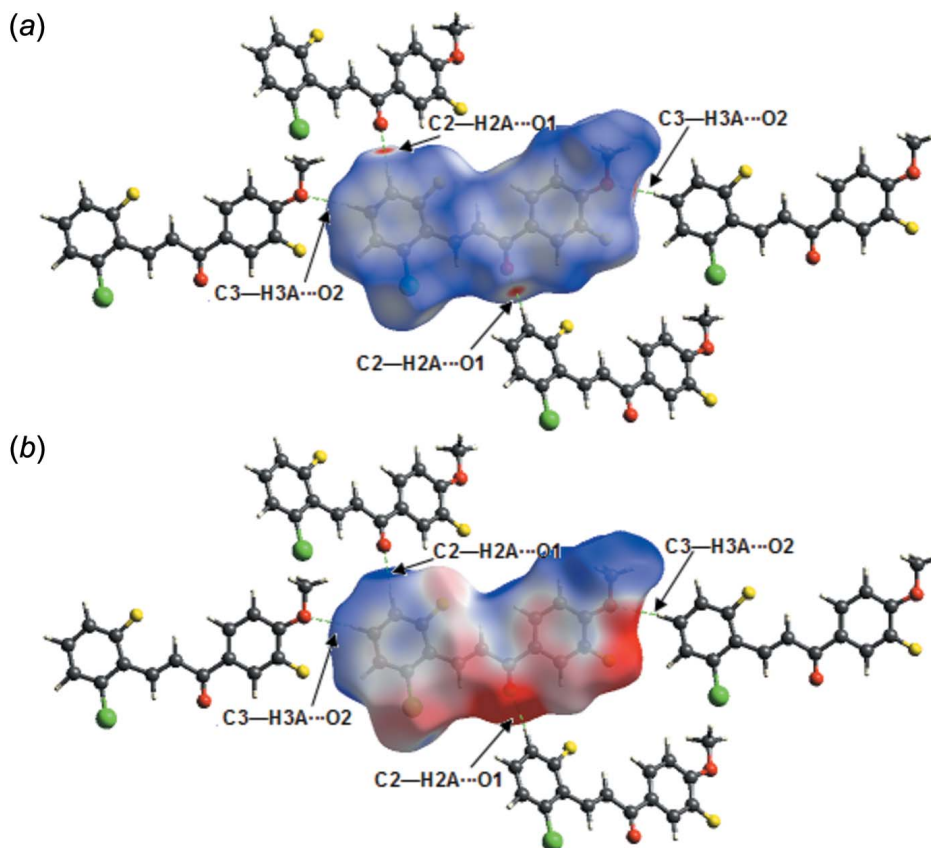


Figure 3
(a) d_{norm} mapped on Hirshfeld surfaces for visualizing the intermolecular interactions of the title chalcone compound. (b) Hirshfeld surfaces mapped over the electrostatic potential. Dotted lines (green) represent hydrogen bonds.

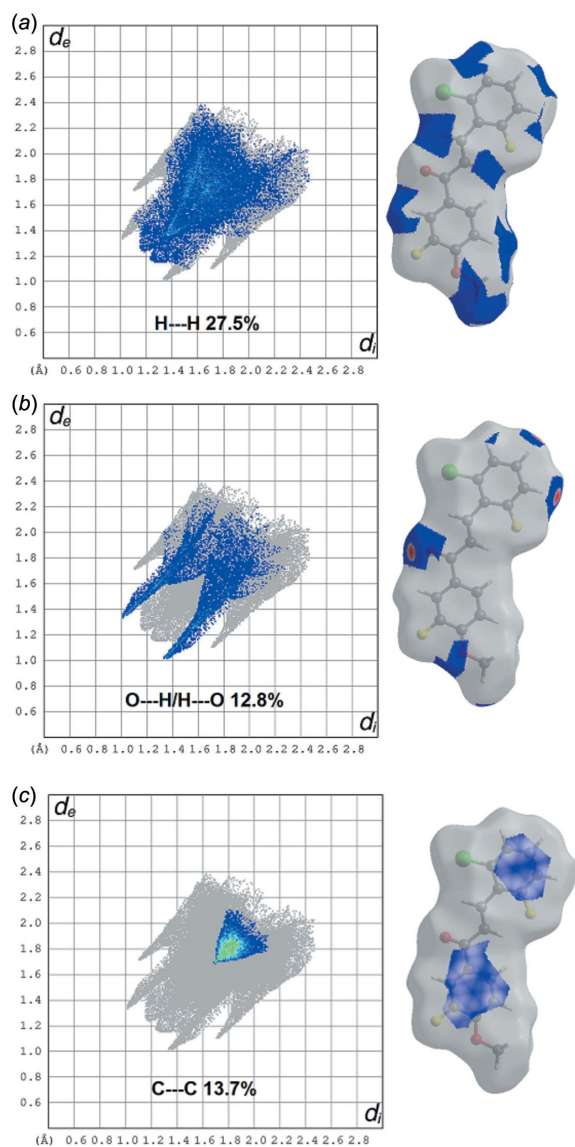


Figure 4
Fingerprint plots for the title chalcone compound, broken down into contributions from specific pairs of atom types. For each plot, the grey shadow is an outline of the complete fingerprint plot. Surfaces to the right highlight the relevant surface patches associated with the specific contacts, with d_{norm} mapped in the same manner as Fig. 3a.

in Fig. 2. The crystal structure also features π - π interactions [$Cg1 \cdots Cg2$ ($-1 + x, y, z$), centroid-to-centroid distance = 3.5629 (18) Å, where $Cg1$ and $Cg2$ are the centroids of the C1–C6 and C10–C15 rings, respectively].

4. Analysis of the Hirshfeld Surfaces

Crystal Explorer 3.1 (Wolff *et al.*, 2012) was used to analyse the close contacts in the crystal of (I), which can be summarized with fingerprint plots mapped over d_{norm} , electrostatic potential, shape index and curvedness. The electrostatic potentials were calculated using *TONTO* (Spackman *et al.*, 2008; Jayatilaka *et al.*, 2005) integrated within *Crystal Explorer*. The electrostatic potentials were mapped on

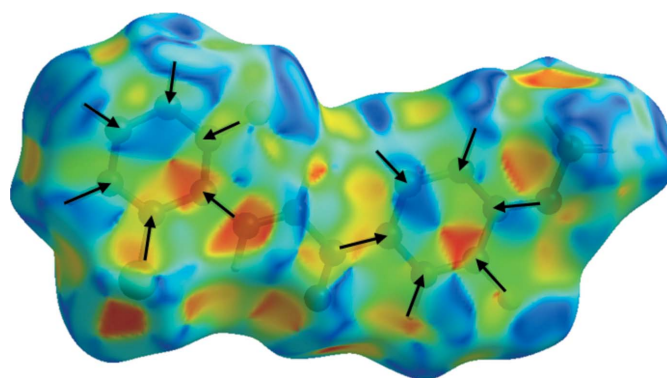


Figure 5
Hirshfeld surfaces mapped over the shape index of the title chalcone compound.

Hirshfeld surfaces using the STO-3G basis set at Hartree-Fock level theory over a range ± 0.03 au.

The strong C–H \cdots O interactions are visualized as bright-red spots between the respective donor and acceptor atoms on the Hirshfeld surfaces mapped over d_{norm} (Fig. 3a) with neighbouring molecules connected by C2–H2A \cdots O1 and C3–H3A \cdots O2 hydrogen bonds. This finding is corroborated by Hirshfeld surfaces mapped over the electrostatic potential (Fig. 3b) showing the negative potential around the oxygen atoms as light-red clouds and the positive potential around hydrogen atoms as light-blue clouds.

Significant intermolecular interactions are plotted in Fig. 4: the H \cdots H interactions appear as the largest region of the fingerprint plot with a high concentration in the middle region, shown in light blue, at $d_e = d_i \sim 1.4$ Å (Fig. 4a) with overall Hirshfeld surfaces of 27.5%. The contribution from the O \cdots H/H \cdots O contacts, corresponding to C–H \cdots O interactions, is represented by a pair of sharp spikes characteristic of a strong hydrogen-bond interaction having almost the same $d_e + d_i \sim 2.3$ Å (Fig. 4b).

The C \cdots C contacts, which refer to π - π stacking interactions, contribute 13.7% of the Hirshfeld surfaces. This appears as a distinct triangle at around $d_e = d_i \sim 1.8$ Å (Fig. 4c). The presence of the π - π stacking interactions is also indicated

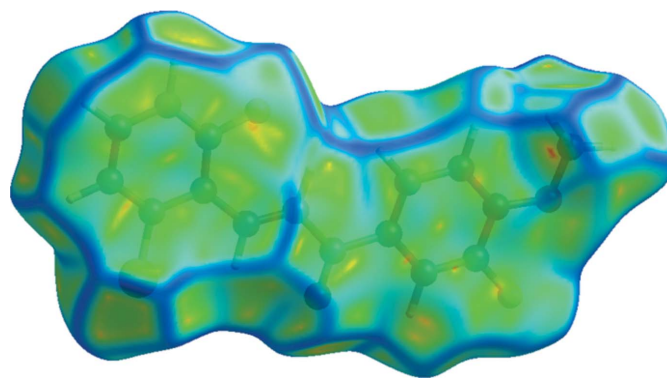


Figure 6
Hirshfeld surfaces mapped over curvedness of the title chalcone compound.

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₁₆ H ₁₁ ClF ₂ O ₂
<i>M_r</i>	308.70
Crystal system, space group	Monoclinic, <i>Cc</i>
Temperature (K)	294
<i>a</i> , <i>b</i> , <i>c</i> (Å)	9.0832 (13), 11.1072 (13), 13.9564 (17)
β (°)	102.027 (3)
<i>V</i> (Å ³)	1377.1 (3)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.30
Crystal size (mm)	0.45 × 0.17 × 0.13
Data collection	
Diffraction	Bruker <i>SMART</i> APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2009)
<i>T_{min}</i> , <i>T_{max}</i>	0.791, 0.889
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	14473, 4003, 3111
<i>R_{int}</i>	0.031
($\sin \theta/\lambda$) _{max} (Å ⁻¹)	0.705
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.039, 0.116, 1.05
No. of reflections	4003
No. of parameters	191
No. of restraints	2
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	0.20, -0.27
Absolute structure	Flack <i>x</i> determined using 1298 quotients [(<i>I</i> ⁺) - (<i>I</i> ⁻)] / [(<i>I</i> ⁺) + (<i>I</i> ⁻)] Parsons <i>et al.</i> (2013)
Absolute structure parameter	0.08 (2)

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS97* and *SHELXTL* (Sheldrick 2008), *SHELXL2014* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

by the appearance of red and blue triangles on the shape-indexed surfaces, identified with black arrows in Fig. 5, and in the flat regions on the Hirshfeld surfaces mapped over curvedness in Fig. 6.

5. Synthesis and crystallization

A mixture of 3-fluoro-4-methoxyacetophenone (0.1 mol, 0.08 g) and 2-chloro-6-fluorobenzaldehyde (0.1 mol, 0.08 g) was dissolved in methanol (20 ml). A catalytic amount of NaOH (5 ml, 20%) was added to the solution dropwise with vigorous stirring. The reaction mixture was stirred for about 5–

6 h at room temperature. After stirring, the contents of the flask were poured into ice-cold water (50 ml) and the resulting crude solid was collected by filtration. Brownish blocks of (I) were grown from an acetone solution by slow evaporation.

6. Refinement details

Crystal data collection and structure refinement details are summarized in Table 2. All H atoms were positioned geometrically (C–H = 0.93 Å) and refined using a riding model with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. In the final refinement, the most disagreeable reflection (020) was omitted.

Acknowledgements

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Computing details

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

(*E*)-3-(2-Chloro-6-fluorophenyl)-1-(3-fluoro-4-methoxyphenyl)prop-2-en-1-one

Crystal data

$C_{16}H_{11}ClF_2O_2$

$M_r = 308.70$

Monoclinic, *Cc*

$a = 9.0832$ (13) Å

$b = 11.1072$ (13) Å

$c = 13.9564$ (17) Å

$\beta = 102.027$ (3)°

$V = 1377.1$ (3) Å³

$Z = 4$

$F(000) = 632$

$D_x = 1.489$ Mg m⁻³

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

Cell parameters from 4692 reflections

$\theta = 2.9$ – 28.9 °

$\mu = 0.30$ mm⁻¹

$T = 294$ K

Block, brown

$0.45 \times 0.17 \times 0.13$ mm

Data collection

Bruker SMART APEXII CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2009)

$T_{\min} = 0.791$, $T_{\max} = 0.889$

14473 measured reflections

4003 independent reflections

3111 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.031$

$\theta_{\max} = 30.1$ °, $\theta_{\min} = 2.9$ °

$h = -12 \rightarrow 12$

$k = -15 \rightarrow 15$

$l = -19 \rightarrow 19$

Refinement

Refinement on F^2

Least-squares matrix: full

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

$wR(F^2) = 0.116$

$S = 1.05$

4003 reflections

191 parameters

2 restraints

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0664P)^2 + 0.0639P]$

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

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

$\Delta\rho_{\max} = 0.20$ e Å⁻³

$\Delta\rho_{\min} = -0.27$ e Å⁻³

Absolute structure: Flack x determined using
 1298 quotients $[(F^+)-(F^-)]/[(F^+)+(F^-)]$ Parsons *et al.*
 (2013)
 Absolute structure parameter: 0.08 (2)

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	0.01382 (11)	0.90043 (10)	0.28908 (7)	0.0766 (3)
F1	0.2567 (2)	0.7732 (2)	0.63725 (14)	0.0679 (6)
F2	1.0123 (2)	0.5464 (2)	0.42338 (15)	0.0676 (5)
O1	0.5069 (4)	0.7363 (3)	0.3366 (2)	0.0864 (9)
O2	1.0692 (2)	0.5000 (2)	0.61111 (18)	0.0654 (6)
C1	0.1380 (3)	0.8232 (3)	0.5705 (2)	0.0473 (6)
C2	0.0177 (4)	0.8618 (3)	0.6081 (2)	0.0558 (7)
H2A	0.0181	0.8538	0.6745	0.067*
C3	-0.1020 (3)	0.9121 (3)	0.5458 (3)	0.0555 (7)
H3A	-0.1844	0.9391	0.5698	0.067*
C4	-0.1017 (3)	0.9231 (3)	0.4480 (3)	0.0533 (7)
H4A	-0.1837	0.9573	0.4057	0.064*
C5	0.0209 (3)	0.8832 (2)	0.4124 (2)	0.0447 (6)
C6	0.1479 (3)	0.8313 (2)	0.47289 (19)	0.0409 (5)
C7	0.2772 (3)	0.7932 (3)	0.4327 (2)	0.0480 (6)
H7A	0.2670	0.8034	0.3655	0.058*
C8	0.4052 (4)	0.7467 (3)	0.4783 (2)	0.0527 (6)
H8A	0.4215	0.7321	0.5453	0.063*
C9	0.5248 (3)	0.7170 (3)	0.4236 (2)	0.0501 (6)
C10	0.6672 (3)	0.6632 (2)	0.4787 (2)	0.0428 (6)
C11	0.7762 (3)	0.6300 (3)	0.4255 (2)	0.0458 (6)
H11A	0.7598	0.6433	0.3583	0.055*
C12	0.9060 (3)	0.5780 (2)	0.4739 (2)	0.0463 (6)
C13	0.9367 (3)	0.5544 (3)	0.5741 (2)	0.0478 (6)
C14	0.8298 (3)	0.5889 (3)	0.6265 (2)	0.0505 (6)
H14A	0.8471	0.5762	0.6938	0.061*
C15	0.6969 (3)	0.6426 (3)	0.5783 (2)	0.0480 (6)
H15A	0.6259	0.6653	0.6142	0.058*
C16	1.1014 (5)	0.4726 (5)	0.7133 (3)	0.0857 (13)
H16A	1.1972	0.4329	0.7304	0.129*
H16B	1.0245	0.4206	0.7278	0.129*
H16C	1.1041	0.5457	0.7502	0.129*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0769 (5)	0.1065 (7)	0.0450 (4)	0.0182 (5)	0.0090 (3)	0.0033 (4)
F1	0.0590 (11)	0.0974 (14)	0.0482 (10)	0.0220 (9)	0.0137 (8)	0.0121 (10)
F2	0.0564 (9)	0.0931 (14)	0.0632 (11)	0.0103 (9)	0.0350 (9)	-0.0092 (10)
O1	0.0880 (18)	0.125 (2)	0.0543 (14)	0.0458 (17)	0.0320 (13)	0.0164 (15)
O2	0.0398 (10)	0.1009 (18)	0.0566 (13)	0.0060 (11)	0.0124 (9)	-0.0102 (12)
C1	0.0477 (13)	0.0491 (14)	0.0478 (14)	0.0008 (11)	0.0161 (11)	0.0033 (12)
C2	0.0601 (17)	0.0623 (17)	0.0529 (16)	-0.0056 (14)	0.0297 (14)	-0.0028 (14)
C3	0.0464 (14)	0.0587 (16)	0.0685 (19)	-0.0037 (12)	0.0281 (13)	-0.0069 (14)
C4	0.0398 (13)	0.0518 (15)	0.068 (2)	-0.0015 (11)	0.0099 (12)	-0.0036 (14)
C5	0.0441 (13)	0.0465 (14)	0.0436 (13)	-0.0029 (11)	0.0098 (11)	-0.0027 (10)
C6	0.0421 (12)	0.0388 (12)	0.0435 (13)	-0.0024 (9)	0.0130 (10)	-0.0011 (10)
C7	0.0517 (14)	0.0520 (15)	0.0441 (14)	0.0054 (12)	0.0189 (11)	0.0010 (11)
C8	0.0542 (15)	0.0589 (16)	0.0501 (15)	0.0084 (13)	0.0225 (12)	-0.0005 (13)
C9	0.0540 (14)	0.0515 (14)	0.0510 (15)	0.0076 (12)	0.0247 (12)	-0.0003 (12)
C10	0.0471 (13)	0.0385 (12)	0.0490 (14)	-0.0052 (10)	0.0242 (11)	-0.0053 (10)
C11	0.0503 (14)	0.0491 (14)	0.0437 (13)	-0.0043 (11)	0.0229 (11)	-0.0057 (11)
C12	0.0426 (12)	0.0540 (15)	0.0491 (14)	-0.0051 (11)	0.0246 (11)	-0.0112 (12)
C13	0.0365 (12)	0.0564 (15)	0.0527 (15)	-0.0066 (11)	0.0147 (11)	-0.0110 (12)
C14	0.0449 (13)	0.0684 (18)	0.0418 (14)	-0.0043 (12)	0.0174 (11)	-0.0068 (13)
C15	0.0446 (12)	0.0583 (15)	0.0473 (14)	-0.0024 (11)	0.0236 (11)	-0.0070 (12)
C16	0.0552 (19)	0.142 (4)	0.057 (2)	0.014 (2)	0.0050 (16)	-0.002 (2)

Geometric parameters (\AA , $^\circ$)

C11—C5	1.720 (3)	C7—H7A	0.9300
F1—C1	1.386 (3)	C8—C9	1.489 (4)
F2—C12	1.354 (3)	C8—H8A	0.9300
O1—C9	1.209 (4)	C9—C10	1.485 (4)
O2—C13	1.349 (4)	C10—C15	1.379 (4)
O2—C16	1.427 (5)	C10—C11	1.405 (3)
C1—C2	1.376 (4)	C11—C12	1.359 (4)
C1—C6	1.387 (4)	C11—H11A	0.9300
C2—C3	1.363 (5)	C12—C13	1.393 (4)
C2—H2A	0.9300	C13—C14	1.386 (4)
C3—C4	1.371 (5)	C14—C15	1.389 (4)
C3—H3A	0.9300	C14—H14A	0.9300
C4—C5	1.383 (4)	C15—H15A	0.9300
C4—H4A	0.9300	C16—H16A	0.9600
C5—C6	1.403 (4)	C16—H16B	0.9600
C6—C7	1.466 (3)	C16—H16C	0.9600
C7—C8	1.309 (4)		
C13—O2—C16	117.3 (3)	O1—C9—C8	121.0 (3)
C2—C1—F1	115.9 (3)	C10—C9—C8	118.2 (3)
C2—C1—C6	125.0 (3)	C15—C10—C11	118.5 (3)

F1—C1—C6	119.1 (2)	C15—C10—C9	123.7 (2)
C3—C2—C1	118.4 (3)	C11—C10—C9	117.7 (2)
C3—C2—H2A	120.8	C12—C11—C10	118.9 (3)
C1—C2—H2A	120.8	C12—C11—H11A	120.6
C2—C3—C4	120.3 (3)	C10—C11—H11A	120.6
C2—C3—H3A	119.8	F2—C12—C11	119.4 (3)
C4—C3—H3A	119.8	F2—C12—C13	117.3 (3)
C3—C4—C5	119.9 (3)	C11—C12—C13	123.3 (2)
C3—C4—H4A	120.1	O2—C13—C14	126.0 (3)
C5—C4—H4A	120.1	O2—C13—C12	116.4 (2)
C4—C5—C6	122.5 (3)	C14—C13—C12	117.6 (3)
C4—C5—C11	117.3 (2)	C13—C14—C15	119.8 (3)
C6—C5—C11	120.1 (2)	C13—C14—H14A	120.1
C1—C6—C5	113.8 (2)	C15—C14—H14A	120.1
C1—C6—C7	125.3 (3)	C10—C15—C14	121.9 (2)
C5—C6—C7	120.9 (2)	C10—C15—H15A	119.1
C8—C7—C6	129.1 (3)	C14—C15—H15A	119.1
C8—C7—H7A	115.5	O2—C16—H16A	109.5
C6—C7—H7A	115.5	O2—C16—H16B	109.5
C7—C8—C9	120.5 (3)	H16A—C16—H16B	109.5
C7—C8—H8A	119.7	O2—C16—H16C	109.5
C9—C8—H8A	119.7	H16A—C16—H16C	109.5
O1—C9—C10	120.8 (3)	H16B—C16—H16C	109.5
F1—C1—C2—C3	179.8 (3)	O1—C9—C10—C15	177.8 (3)
C6—C1—C2—C3	0.1 (5)	C8—C9—C10—C15	-2.2 (4)
C1—C2—C3—C4	0.2 (5)	O1—C9—C10—C11	-3.2 (4)
C2—C3—C4—C5	-0.1 (5)	C8—C9—C10—C11	176.9 (3)
C3—C4—C5—C6	-0.3 (4)	C15—C10—C11—C12	0.5 (4)
C3—C4—C5—C11	-179.8 (2)	C9—C10—C11—C12	-178.5 (2)
C2—C1—C6—C5	-0.4 (4)	C10—C11—C12—F2	-179.6 (2)
F1—C1—C6—C5	179.9 (2)	C10—C11—C12—C13	0.7 (4)
C2—C1—C6—C7	178.4 (3)	C16—O2—C13—C14	1.7 (5)
F1—C1—C6—C7	-1.3 (4)	C16—O2—C13—C12	-178.6 (3)
C4—C5—C6—C1	0.5 (4)	F2—C12—C13—O2	-1.1 (4)
C11—C5—C6—C1	180.0 (2)	C11—C12—C13—O2	178.6 (3)
C4—C5—C6—C7	-178.3 (3)	F2—C12—C13—C14	178.7 (2)
C11—C5—C6—C7	1.2 (3)	C11—C12—C13—C14	-1.7 (4)
C1—C6—C7—C8	-0.7 (5)	O2—C13—C14—C15	-179.0 (3)
C5—C6—C7—C8	178.0 (3)	C12—C13—C14—C15	1.3 (4)
C6—C7—C8—C9	-178.2 (3)	C11—C10—C15—C14	-0.9 (4)
C7—C8—C9—O1	0.8 (5)	C9—C10—C15—C14	178.2 (3)
C7—C8—C9—C10	-179.3 (3)	C13—C14—C15—C10	-0.1 (4)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2A \cdots O1 ⁱ	0.93	2.50	3.391 (4)	162

C3—H3A···O2 ⁱⁱ	0.93	2.52	3.441 (4)	171
C8—H8A···F1	0.93	2.21	2.842 (4)	124

Symmetry codes: (i) $x-1/2, -y+3/2, z+1/2$; (ii) $x-3/2, y+1/2, z$.