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2-Acetylphenyl (2E)-3-(4-fluorophenyl)-acrylate

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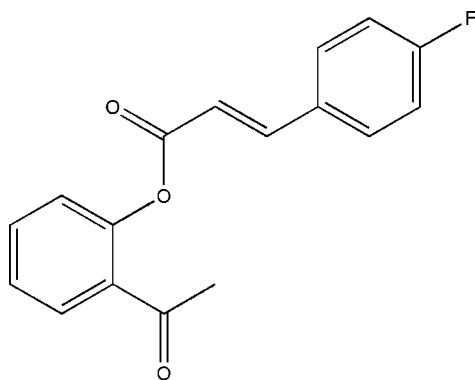
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 Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.041; wR factor = 0.115; data-to-parameter ratio = 16.5.

In the title compound, $\text{C}_{17}\text{H}_{13}\text{FO}_3$, the dihedral angle between the benzene rings is $70.34(5)^\circ$. In the crystal, molecules are linked *via* pairs of bifurcated $\text{C}-\text{H}\cdots(\text{O},\text{O})$ hydrogen bonds, forming inversion dimers. These dimers are linked *via* $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{F}$ interactions, forming a three-dimensional structure.

Related literature

For the preparation, see: Pinto *et al.* (2000). For related structures, see: Santos *et al.* (2009); Ren, Li *et al.* (2006); Ren, Zhang *et al.* (2006). For bond-length data, see: Allen *et al.* (1987). The title compound is a core structure in various natural and pharmaceutically active compounds, displaying a broad spectrum of activity, see: Gomes *et al.* (2010).



Experimental

Crystal data

 $\text{C}_{17}\text{H}_{13}\text{FO}_3$
 $M_r = 284.27$
 Monoclinic, $C2/c$
 $a = 26.574(1)$ Å
 $b = 6.3883(3)$ Å
 $c = 19.3304(6)$ Å

 $\beta = 123.037(2)^\circ$
 $V = 2751.01(19)$ Å³
 $Z = 8$
 Mo $K\alpha$ radiation

 $\mu = 0.10$ mm⁻¹
 $T = 173$ K
 $0.26 \times 0.23 \times 0.09$ mm

Data collection

 Nonius Kappa CCD diffractometer
 6005 measured reflections
 3150 independent reflections
 2201 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.021$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.115$
 $S = 1.05$
 3150 reflections
 191 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.18$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.20$ e Å⁻³
Table 1

Hydrogen-bond geometry (Å, °).

Cg1 is the centroid of the C3–C8 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C7}-\text{H7}\cdots\text{F1}^i$	0.95	2.52	3.2402 (16)	132
$\text{C11}-\text{H11}\cdots\text{O3}^{ii}$	0.95	2.46	3.3369 (16)	154
$\text{C13}-\text{H13}\cdots\text{O3}^{iii}$	0.95	2.45	3.3191 (16)	153
$\text{C16}-\text{H16}\cdots\text{O1}^{iii}$	0.95	2.51	3.3590 (17)	149
$\text{C6}-\text{H6}\cdots\text{Cg1}^{iv}$	0.95	2.99	3.818 (1)	146

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

Data collection: *COLLECT* program (Nonius, 2000); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2596).

References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
- Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
- Gomes, A., Freitas, M., Fernandes, E. & Lima, J. L. F. C. (2010). *Mini Rev. Med. Chem.* **10**, 1–7.
- Nonius (2000). *COLLECT*. Nonius BV, Delft, The Netherlands.
- Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography, Part A*, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
- Pinto, D. C. G. A., Silva, A. M. S. & Cavaleiro, J. A. S. (2000). *New J. Chem.* **24**, 85–92.
- Ren, R., Li, X.-M., Li, Q. & Zhang, S.-S. (2006). *Acta Cryst.* **E62**, o293–o294.
- Ren, R., Zhang, S.-S., Li, Q., Li, X.-M. & Song, X.-Y. (2006). *Acta Cryst.* **E62**, o160–o161.
- Santos, C. M. M., Silva, A. M. S. & Cavaleiro, J. A. S. (2009). *Eur. J. Org. Chem.* pp. 2642–2660.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

supporting information

Acta Cryst. (2012). E68, o3049 [https://doi.org/10.1107/S1600536812040536]

2-Acetylphenyl (2*E*)-3-(4-fluorophenyl)acrylate

Mehubub I. K. Momin, Sunayna Pawar, Neil Anthony Koorbanally, Hong Su and Deresh Ramjugernath

S1. Comment

The title compound (*E*)-2-acetylphenyl-3-(4-fluorophenyl) acrylate was obtained as an intermediate en route to the synthesis of 4'-fluoro-2-styrylchromone and easily converts to the 2-hydroxyphenyl pentadienone with DMSO in the presence of a strong base (Santos *et al.*, 2009). It was synthesized according to the procedure by Pinto *et al.* (2000) with modification. The title compound is a core structure in various natural and pharmaceutically active compounds, displaying a broad spectrum of activity (Gomes *et al.*, 2010).

In the molecule of the title compound (Fig. 1), the two aromatic rings (ring 1: C3—C4—C5—C6—C7—C8; ring 2: C12—C13—C14—C15—C16—C17—C18) are almost perpendicular to each other with a dihedral angle of 70.34 (5)°. The torsion angle C9—C10—C11—C12 is -178.8 (1)°, indicating a *trans* configuration of the double bond. All bond lengths and angles are within normal ranges (Allen *et al.*, 1987). In the crystal packing, ring 1 adopts a parallel offset arrangement with itself of the neighbouring molecule with centroidal distance of 4.125 (1) Å. The crystal is further stabilized by a number of weak hydrogen bonds with the type C—H...X (*X* = O or F) and C—H... π (Table 1).

S2. Experimental

Phosphorous oxychloride (15.6 mmol) was added to a solution of 2-hydroxyacetophenone (12.0 mmol) and 4'-fluoro cinnamic acid (15.6 mmol) in dry pyridine. The solution was stirred at 60–70 °C for 3 h, then poured into ice and water and the reaction mixture acidified with hydrochloric acid (pH 3–4). The obtained solid was removed by filtration and dissolved in ethyl acetate (100 ml) and purified by silica gel column chromatography using a 7:3 mixture of ethyl acetate:n-hexane as the eluent. The solvent was evaporated to dryness and the residue recrystallized from ethanol, resulting in the title compound with a 72% yield and a m.p of 80–82°C.

IR (KBr) ν_{\max} (cm⁻¹): 1729 (C=O), 1670 (C=O), 1624 (C=C), 1590, 1446, 1221 (C—F), 1202, 1159, 1050. ¹H NMR (CDCl₃, 400 MHz): δ 7.84 (d, *J* = 15.96 Hz, 1H, H β), 7.81 (dd, *J* = 7.56, 1.60 Hz, 1H), 7.58 (dd, *J* = 8.60, 5.44, 2H), 7.54 (ddd, *J* = 8.04, 7.88, 1.60 Hz, 1H), 7.33 (ddd, *J* = 8.04, 7.56, 0.72 Hz, 1H), 7.17 (d, *J* = 8.04 Hz, 1H), 7.09 (t, *J* = 8.60 Hz, 2H), 6.58 (d, *J* = 15.96 Hz, 1H, H α), 2.54 (s, 3H, CH₃). ¹³C NMR (CDCl₃, 100 MHz): δ 197.78 (C=O), 165.14 (C=O), 164.25 (d, *J*_{CF} = 250.70 Hz), 149.07, 145.99, 133.36, 131.30, 130.43, 130.24 ((d, *J*_{CF} = 19.46 Hz), 130.15, 126.10, 123.78, 116.58, 116.20 (d, *J*_{CF} = 21.85 Hz), 29.71 (CH₃). ¹⁹F NMR (CDCl₃, 376.5 MHz): δ -108.54. EIMS (probe) 70 eV (*m/z*, *rel. int.*) 284 (*M*⁺) (21.42), 149 (100), 121 (25), 101 (20).

S3. Refinement

All non-hydrogen atoms were refined anisotropically. All hydrogen atoms could be found in the difference electron density maps but were finally placed in idealized positions refining in riding models with *U*_{iso} set at 1.2 or 1.5 times *U*_{eq} of their parent atoms.

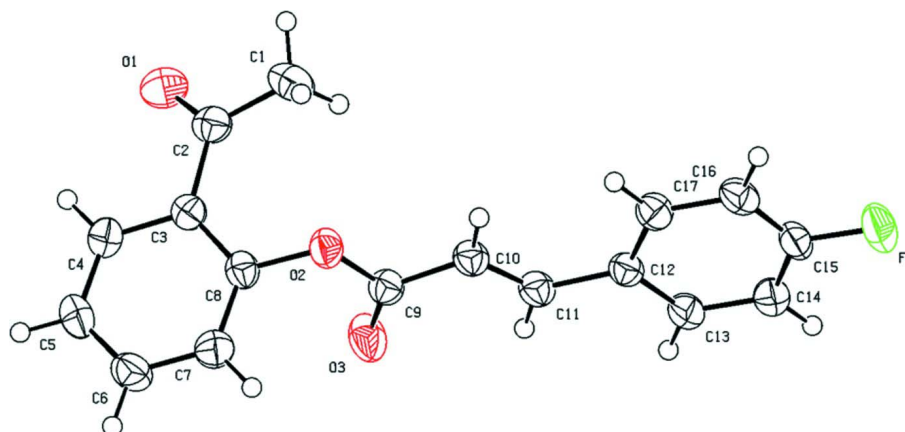


Figure 1

ORTEP diagram showing the molecular structure of the titled compound with atomic labelling scheme. Non-H atoms are drawn with 50% probability displacement ellipsoids and H atoms are shown as open circles.

2-Acetylphenyl (2E)-3-(4-fluorophenyl)acrylate

Crystal data

$C_{17}H_{13}FO_3$

$M_r = 284.27$

Monoclinic, $C2/c$

Hall symbol: $-C\ 2yc$

$a = 26.574\ (1)\ \text{\AA}$

$b = 6.3883\ (3)\ \text{\AA}$

$c = 19.3304\ (6)\ \text{\AA}$

$\beta = 123.037\ (2)^\circ$

$V = 2751.01\ (19)\ \text{\AA}^3$

$Z = 8$

$F(000) = 1184$

$D_x = 1.373\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 6005 reflections

$\theta = 3.1\text{--}27.5^\circ$

$\mu = 0.10\ \text{mm}^{-1}$

$T = 173\ \text{K}$

Plate, colourless

$0.26 \times 0.23 \times 0.09\ \text{mm}$

Data collection

Nonius Kappa CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$1.2^\circ\ \varphi$ scans and ω scans

6005 measured reflections

3150 independent reflections

2201 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.021$

$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 3.1^\circ$

$h = -33 \rightarrow 34$

$k = -8 \rightarrow 8$

$l = -25 \rightarrow 24$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.041$

$wR(F^2) = 0.115$

$S = 1.05$

3150 reflections

191 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0612P)^2 + 0.6743P]$

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

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

$\Delta\rho_{\text{max}} = 0.18\ \text{e \AA}^{-3}$

$\Delta\rho_{\text{min}} = -0.20\ \text{e \AA}^{-3}$

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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	0.04188 (4)	1.49324 (13)	0.22111 (6)	0.0580 (3)
O1	0.26072 (5)	-0.02536 (18)	0.16114 (6)	0.0556 (3)
O2	0.16132 (4)	0.49823 (13)	0.02908 (6)	0.0379 (2)
O3	0.06857 (4)	0.41188 (17)	-0.00442 (7)	0.0522 (3)
C1	0.25590 (7)	0.3344 (3)	0.18081 (9)	0.0512 (4)
H1A	0.2225	0.3695	0.1867	0.077*
H1B	0.2633	0.4515	0.1548	0.077*
H1C	0.2921	0.3074	0.2354	0.077*
C2	0.24038 (6)	0.1439 (2)	0.12848 (8)	0.0377 (3)
C3	0.19990 (5)	0.1519 (2)	0.03588 (7)	0.0315 (3)
C4	0.19941 (6)	-0.0253 (2)	-0.00725 (8)	0.0369 (3)
H4	0.2241	-0.1415	0.0228	0.044*
C5	0.16398 (6)	-0.0351 (2)	-0.09234 (9)	0.0430 (4)
H5	0.1643	-0.1569	-0.1203	0.052*
C6	0.12814 (7)	0.1330 (2)	-0.13652 (8)	0.0447 (4)
H6	0.1039	0.1274	-0.1951	0.054*
C7	0.12732 (6)	0.3091 (2)	-0.09597 (8)	0.0418 (3)
H7	0.1026	0.4247	-0.1265	0.050*
C8	0.16273 (6)	0.3169 (2)	-0.01042 (8)	0.0327 (3)
C9	0.11003 (6)	0.5312 (2)	0.02865 (8)	0.0337 (3)
C10	0.11450 (6)	0.72268 (19)	0.07306 (8)	0.0339 (3)
H10	0.1496	0.8069	0.0972	0.041*
C11	0.06885 (6)	0.7778 (2)	0.07935 (8)	0.0346 (3)
H11	0.0355	0.6853	0.0548	0.042*
C12	0.06392 (6)	0.96377 (19)	0.11951 (7)	0.0321 (3)
C13	0.01102 (6)	0.9974 (2)	0.11673 (8)	0.0379 (3)
H13	-0.0204	0.8971	0.0906	0.045*
C14	0.00350 (6)	1.1745 (2)	0.15135 (8)	0.0418 (3)
H14	-0.0326	1.1971	0.1493	0.050*
C15	0.04946 (6)	1.3164 (2)	0.18860 (8)	0.0388 (3)
C16	0.10298 (6)	1.2888 (2)	0.19487 (8)	0.0385 (3)
H16	0.1344	1.3885	0.2226	0.046*
C17	0.10980 (6)	1.1118 (2)	0.15972 (8)	0.0360 (3)
H17	0.1464	1.0903	0.1629	0.043*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0663 (6)	0.0476 (5)	0.0611 (6)	-0.0033 (4)	0.0354 (5)	-0.0236 (4)
O1	0.0560 (7)	0.0582 (7)	0.0411 (6)	0.0116 (5)	0.0191 (5)	0.0104 (5)
O2	0.0366 (5)	0.0330 (5)	0.0456 (5)	-0.0029 (4)	0.0234 (4)	-0.0093 (4)
O3	0.0453 (6)	0.0485 (6)	0.0693 (7)	-0.0152 (5)	0.0354 (6)	-0.0258 (5)
C1	0.0492 (9)	0.0627 (10)	0.0346 (8)	-0.0076 (7)	0.0183 (7)	-0.0089 (7)
C2	0.0314 (7)	0.0486 (8)	0.0358 (7)	-0.0011 (6)	0.0201 (6)	-0.0001 (6)
C3	0.0303 (6)	0.0351 (7)	0.0331 (7)	-0.0026 (5)	0.0200 (5)	-0.0011 (5)
C4	0.0397 (7)	0.0348 (7)	0.0413 (8)	0.0037 (6)	0.0254 (6)	0.0013 (6)
C5	0.0512 (9)	0.0416 (8)	0.0440 (8)	-0.0030 (7)	0.0311 (7)	-0.0103 (7)
C6	0.0468 (8)	0.0541 (9)	0.0317 (7)	-0.0014 (7)	0.0205 (6)	-0.0045 (7)
C7	0.0437 (8)	0.0426 (8)	0.0361 (7)	0.0060 (6)	0.0199 (6)	0.0037 (6)
C8	0.0346 (7)	0.0305 (7)	0.0366 (7)	-0.0031 (5)	0.0217 (6)	-0.0039 (5)
C9	0.0348 (7)	0.0327 (7)	0.0334 (7)	0.0005 (6)	0.0183 (6)	0.0001 (5)
C10	0.0355 (7)	0.0296 (7)	0.0341 (7)	-0.0025 (5)	0.0174 (6)	-0.0019 (5)
C11	0.0352 (7)	0.0305 (7)	0.0344 (7)	-0.0032 (5)	0.0165 (6)	-0.0030 (5)
C12	0.0352 (7)	0.0295 (7)	0.0283 (6)	0.0002 (5)	0.0151 (5)	-0.0001 (5)
C13	0.0340 (7)	0.0377 (7)	0.0372 (7)	-0.0044 (6)	0.0164 (6)	-0.0086 (6)
C14	0.0366 (7)	0.0463 (8)	0.0408 (8)	0.0010 (6)	0.0199 (6)	-0.0080 (6)
C15	0.0492 (8)	0.0322 (7)	0.0313 (7)	0.0017 (6)	0.0196 (6)	-0.0063 (6)
C16	0.0424 (8)	0.0332 (7)	0.0343 (7)	-0.0080 (6)	0.0172 (6)	-0.0048 (6)
C17	0.0377 (7)	0.0338 (7)	0.0364 (7)	-0.0026 (6)	0.0201 (6)	-0.0015 (6)

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

F1—C15	1.3600 (15)	C7—C8	1.3878 (18)
O1—C2	1.2195 (17)	C7—H7	0.9500
O2—C9	1.3748 (16)	C9—C10	1.4614 (17)
O2—C8	1.3993 (15)	C10—C11	1.3310 (19)
O3—C9	1.1982 (16)	C10—H10	0.9500
C1—C2	1.490 (2)	C11—C12	1.4636 (17)
C1—H1A	0.9800	C11—H11	0.9500
C1—H1B	0.9800	C12—C13	1.3937 (18)
C1—H1C	0.9800	C12—C17	1.3972 (18)
C2—C3	1.5048 (19)	C13—C14	1.3835 (18)
C3—C8	1.3869 (18)	C13—H13	0.9500
C3—C4	1.4014 (18)	C14—C15	1.369 (2)
C4—C5	1.381 (2)	C14—H14	0.9500
C4—H4	0.9500	C15—C16	1.371 (2)
C5—C6	1.379 (2)	C16—C17	1.3814 (19)
C5—H5	0.9500	C16—H16	0.9500
C6—C7	1.378 (2)	C17—H17	0.9500
C6—H6	0.9500		
C9—O2—C8	116.42 (9)	O3—C9—O2	121.72 (12)
C2—C1—H1A	109.5	O3—C9—C10	127.06 (12)

C2—C1—H1B	109.5	O2—C9—C10	111.22 (11)
H1A—C1—H1B	109.5	C11—C10—C9	119.26 (12)
C2—C1—H1C	109.5	C11—C10—H10	120.4
H1A—C1—H1C	109.5	C9—C10—H10	120.4
H1B—C1—H1C	109.5	C10—C11—C12	127.80 (12)
O1—C2—C1	119.47 (12)	C10—C11—H11	116.1
O1—C2—C3	118.28 (12)	C12—C11—H11	116.1
C1—C2—C3	122.25 (12)	C13—C12—C17	118.24 (12)
C8—C3—C4	117.21 (11)	C13—C12—C11	119.00 (11)
C8—C3—C2	126.11 (11)	C17—C12—C11	122.76 (12)
C4—C3—C2	116.67 (11)	C14—C13—C12	121.07 (12)
C5—C4—C3	121.63 (13)	C14—C13—H13	119.5
C5—C4—H4	119.2	C12—C13—H13	119.5
C3—C4—H4	119.2	C15—C14—C13	118.25 (13)
C6—C5—C4	119.62 (13)	C15—C14—H14	120.9
C6—C5—H5	120.2	C13—C14—H14	120.9
C4—C5—H5	120.2	F1—C15—C14	118.60 (13)
C7—C6—C5	120.20 (12)	F1—C15—C16	118.28 (12)
C7—C6—H6	119.9	C14—C15—C16	123.12 (12)
C5—C6—H6	119.9	C15—C16—C17	118.02 (12)
C6—C7—C8	119.76 (13)	C15—C16—H16	121.0
C6—C7—H7	120.1	C17—C16—H16	121.0
C8—C7—H7	120.1	C16—C17—C12	121.26 (12)
C3—C8—C7	121.56 (12)	C16—C17—H17	119.4
C3—C8—O2	119.91 (11)	C12—C17—H17	119.4
C7—C8—O2	118.51 (11)		
O1—C2—C3—C8	164.97 (13)	C8—O2—C9—O3	-0.64 (18)
C1—C2—C3—C8	-14.7 (2)	C8—O2—C9—C10	178.87 (10)
O1—C2—C3—C4	-14.28 (18)	O3—C9—C10—C11	0.0 (2)
C1—C2—C3—C4	166.04 (12)	O2—C9—C10—C11	-179.43 (12)
C8—C3—C4—C5	0.71 (19)	C9—C10—C11—C12	-178.78 (11)
C2—C3—C4—C5	-179.97 (12)	C10—C11—C12—C13	177.62 (13)
C3—C4—C5—C6	0.1 (2)	C10—C11—C12—C17	-1.4 (2)
C4—C5—C6—C7	-0.5 (2)	C17—C12—C13—C14	1.26 (19)
C5—C6—C7—C8	0.0 (2)	C11—C12—C13—C14	-177.78 (12)
C4—C3—C8—C7	-1.21 (18)	C12—C13—C14—C15	0.0 (2)
C2—C3—C8—C7	179.54 (12)	C13—C14—C15—F1	178.52 (11)
C4—C3—C8—O2	-179.87 (11)	C13—C14—C15—C16	-1.6 (2)
C2—C3—C8—O2	0.88 (19)	F1—C15—C16—C17	-178.23 (11)
C6—C7—C8—C3	0.9 (2)	C14—C15—C16—C17	1.9 (2)
C6—C7—C8—O2	179.56 (12)	C15—C16—C17—C12	-0.56 (19)
C9—O2—C8—C3	-109.06 (13)	C13—C12—C17—C16	-0.95 (19)
C9—O2—C8—C7	72.24 (15)	C11—C12—C17—C16	178.05 (12)

Hydrogen-bond geometry (Å, °)

Cg1 is the centroid of the C3–C8 ring.

<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>
C1—H1 <i>B</i> \cdots O2	0.98	2.48	2.8245 (18)	100
C7—H7 \cdots F1 ⁱ	0.95	2.52	3.2402 (16)	132
C11—H11 \cdots O3	0.95	2.50	2.8415 (16)	101
C11—H11 \cdots O3 ⁱⁱ	0.95	2.46	3.3369 (16)	154
C13—H13 \cdots O3 ⁱⁱ	0.95	2.45	3.3191 (16)	153
C16—H16 \cdots O1 ⁱⁱⁱ	0.95	2.51	3.3590 (17)	149
C6—H6 \cdots Cg1 ^{iv}	0.95	2.99	3.818 (1)	146

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