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## Structure Reports

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**(2Z,4E)-1-(5-Fluoro-2-hydroxyphenyl)-5-(4-fluorophenyl)-3-hydroxypenta-2,4-dien-1-one**Jing-Wei Chen,<sup>a</sup> Zhuo He,<sup>b</sup> Zhen Wu,<sup>b</sup> Mei-Juan Fang<sup>b\*</sup> and Hua Fang<sup>c</sup><sup>a</sup>The Key Laboratory for Chemical Biology of Fujian Province, Xiamen University, Xiamen 361005, People's Republic of China, <sup>b</sup>School of Pharmaceutical Sciences, Xiamen University, South Xiang-An Road, Xiamen 361100, People's Republic of China, and <sup>c</sup>State Oceanic Administration, Institute of Oceanography 3, Xiamen 361005, People's Republic of China

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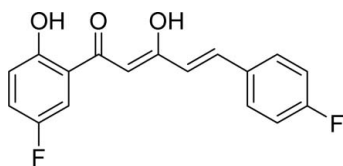
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Key indicators: single-crystal X-ray study;  $T = 173$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.053;  $wR$  factor = 0.147; data-to-parameter ratio = 12.0.

In the title molecule,  $\text{C}_{17}\text{H}_{12}\text{F}_2\text{O}_3$ , the dihedral angle between the benzene rings is  $8.6(2)^\circ$ . In the crystal, two pairs of  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds connect the molecules into inversion dimers. In addition, weak  $\text{C}-\text{H}\cdots\text{F}$  hydrogen bonds link the dimers into a two-dimensional network parallel to  $(10\bar{4})$ . The carbonyl O atom is an acceptor for two weak intramolecular hydrogen bonds.

## Related literature

For the biological activities of chalcones, see: Meng *et al.* (2007); Schobert *et al.* (2009). For the synthesis, see: Baker (1933); Mahal & Venkataraman (1934). For a related structure, see: Fun *et al.* (2012).



## Experimental

## Crystal data

$\text{C}_{17}\text{H}_{12}\text{F}_2\text{O}_3$   
 $M_r = 302.27$   
 Monoclinic,  $P2_1/c$   
 $a = 6.8275(18)$  Å

$b = 14.004(4)$  Å  
 $c = 14.267(4)$  Å  
 $\beta = 91.293(5)^\circ$   
 $V = 1363.8(7)$  Å<sup>3</sup>

$Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.12$  mm<sup>-1</sup>

$T = 173$  K  
 $0.32 \times 0.23 \times 0.18$  mm

## Data collection

Bruker APEX CCD diffractometer  
 Absorption correction: multi-scan  
 (SADABS; Bruker, 2001)  
 $T_{\min} = 0.963$ ,  $T_{\max} = 0.979$

6787 measured reflections  
 2392 independent reflections  
 2040 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.028$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.053$   
 $wR(F^2) = 0.147$   
 $S = 1.08$   
 2392 reflections

199 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.21$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.29$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O1}-\text{H1A}\cdots\text{O2}$	0.82	1.84	2.558 (2)	145
$\text{O1}-\text{H1A}\cdots\text{O3}^i$	0.82	2.55	3.145 (2)	130
$\text{O3}-\text{H3A}\cdots\text{O2}$	0.82	1.81	2.532 (2)	146
$\text{O3}-\text{H3A}\cdots\text{O2}^i$	0.82	2.38	2.856 (2)	118
$\text{C10}-\text{H10A}\cdots\text{F2}^{\text{ii}}$	0.93	2.51	3.326 (3)	147

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

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008) and PLATON (Spek, 2009); software used to prepare material for publication: SHELXL97.

This work was supported financially by the National Science Foundation of China (grants No. 81072549 and 81302652) and the Natural Science Foundation of Fujian Province of China (grant No. 2011 J05101).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5672).

## References

- Baker, W. J. (1933). *J. Chem. Soc.* pp. 1381–1389.  
 Bruker (2001). SAINT, SMART and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Fun, H.-K., Farhadikoutenaqi, A., Narayana, B., Nayak, P. S. & Sarojini, B. K. (2012). *Acta Cryst.* **E68**, o2658.  
 Mahal, H. S. & Venkataraman, K. (1934). *J. Chem. Soc.* pp. 1767–1769.  
 Meng, C. Q., Ni, L. M., Worsencroft, K. J., Ye, Z., Weingarten, D. M., Simpson, J. E., Skudlarek, J. W., Marino, E. M., Suen, K. L., Kunsch, C., Souder, A., Howard, R. B., Sundell, C. L., Wasserman, M. A. & Sikorski, J. A. (2007). *J. Med. Chem.* **50**, 1304–1315.  
 Schobert, R., Biersack, B., Dietrich, A., Knauer, S., Zoldakova, M., Fruehauf, A. & Mueller, T. (2009). *J. Med. Chem.* **52**, 241–246.  
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
 Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.

## supporting information

*Acta Cryst.* (2014). E70, o88 [https://doi.org/10.1107/S1600536813033564]

**(2Z,4E)-1-(5-Fluoro-2-hydroxyphenyl)-5-(4-fluorophenyl)-3-hydroxypenta-2,4-dien-1-one**

**Jing-Wei Chen, Zhuo He, Zhen Wu, Mei-Juan Fang and Hua Fang**

**S1. Comment**

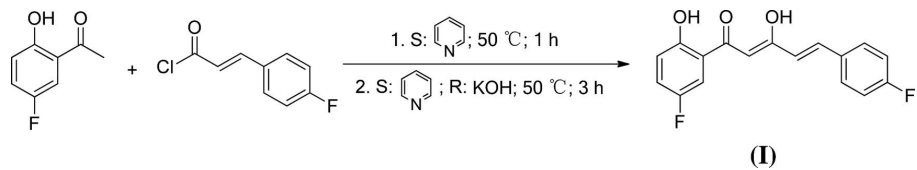
Dibenzoylmethane (1,3-Diphenyl-propane-1,3-dione, DBM) and chalcones have been found to exhibit a variety of biological activities, such as anti-tumor, anti-inflammatory, antibacterial, anti-parasitic, anti-oxidation and anti-viral effect (Schobert *et al.*, 2009; Meng *et al.*, 2007). Recently, we carried out to synthesis a series of (*E*)-1,5-diphenylpent-4-ene-1,3-dione derivatives. These compounds have keto-enol tautomerism, however, the enol form predominates. The dihedral angle between the planes of the phenyl rings (C2–C7) and (C12–C17) is 8.6 (3) °. Bond lengths and angles in (I, Fig. 2) are agreement with values reported for a similar compound (Fun *et al.*, 2012). In the crystal, two pairs of O—H···O hydrogen bonds connect the molecules into inversion dimers (Fig. 3). In addition, weak C—H···F hydrogen bonds link dimers into a two-dimensional network parallel to (10 $\bar{4}$ ) (Fig. 4). The oxygen atom of the —C=O group is an acceptor for two intramolecular hydrogen bonds (Fig. 2).

**S2. Experimental**

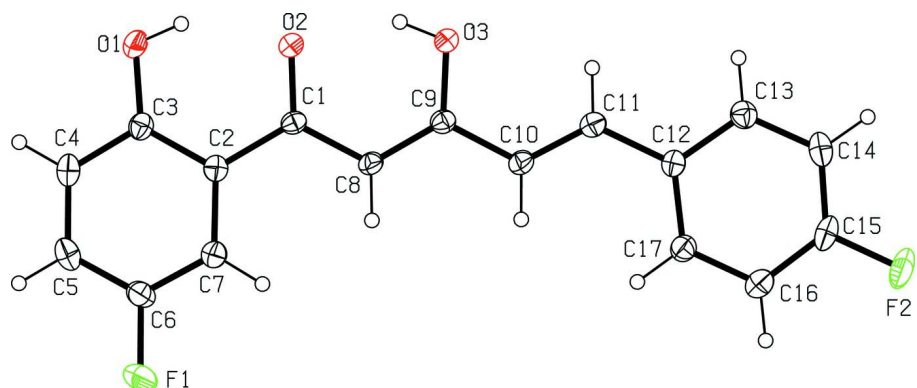
The reaction scheme is shown in Fig. 1. A reaction mixture of (*E*)-3-(4-fluorophenyl) acryloyl chloride (0.37 g, 2.0 mmol) and 1-(5-fluoro-2-hydroxyphenyl)ethanone (0.31 g, 2.0 mmol) in pyridine (10 ml) was stirred for 1 h at 323K (Baker *et al.*, 1933). The mixture was then neutralized with dilute hydrochloric acid, and extracted with ethyl acetate (3×15 ml). The organic phase was concentrated under vacuum to obtain a slurry residue to which was added pyridine (10 ml) and potassium hydroxide (0.21 g, 1.5 mmol). The solution was stirred for 3 h at 323K. The mixture was then neutralized with dilute hydrochloric acid, and extracted with ethyl acetate (3×15 ml). The organic phase was dried over anhydrous MgSO<sub>4</sub> and concentrated under vacuum to obtain a slurry residue. The residue was purified by chromatography using petroleum ether and ethyl acetate (v:v=5:1) as eluent to give a light yellow solid (Mahal & Venkataraman, 1934). Single crystals were obtained by crystallization of a petroleum ether and ethyl acetate (v:v=1:4) solution of the title compound.

**S3. Refinement**

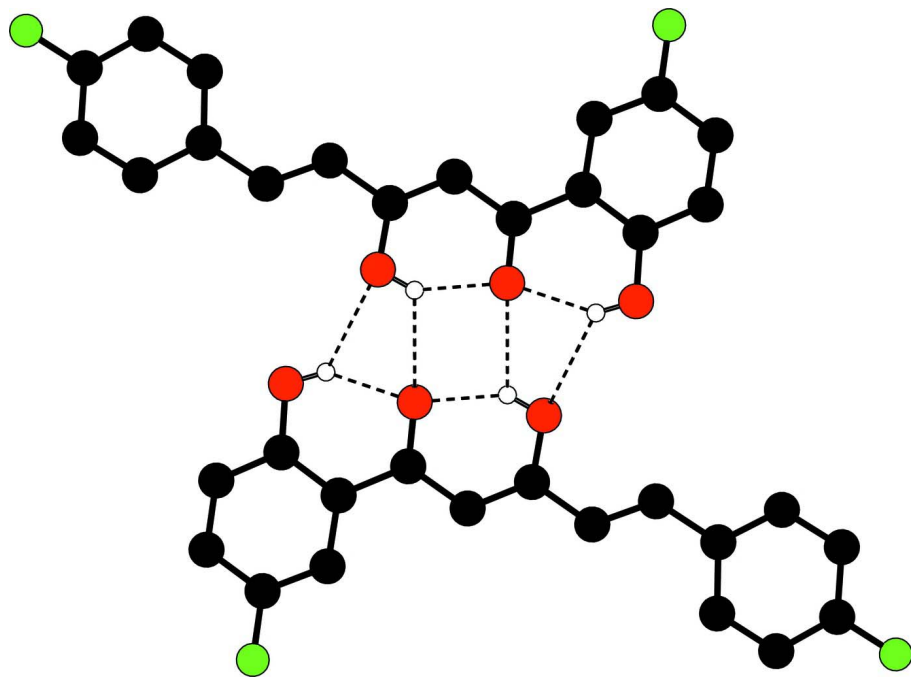
All H atoms were placed in geometrically idealized positions and treated as riding on their parent atoms, with C—H = 0.93 (aromatic) or 0.98 (CH), O—H = 0.82 Å and isotropic displacement parameters for were set at  $U_{iso}(H) = x U_{eq}$  (carried atom), with  $x = 1.5$  for hydroxy, and  $x = 1.2$  for methyne.

**Figure 1**

The reaction scheme.

**Figure 2**

The molecular structure of (I) with displacement ellipsoids drawn at the 30% probability level and H atoms drawn as small spheres of arbitrary radii.

**Figure 3**

An inversion dimers of (I). Hydrogen bonds are shown as dashed lines.

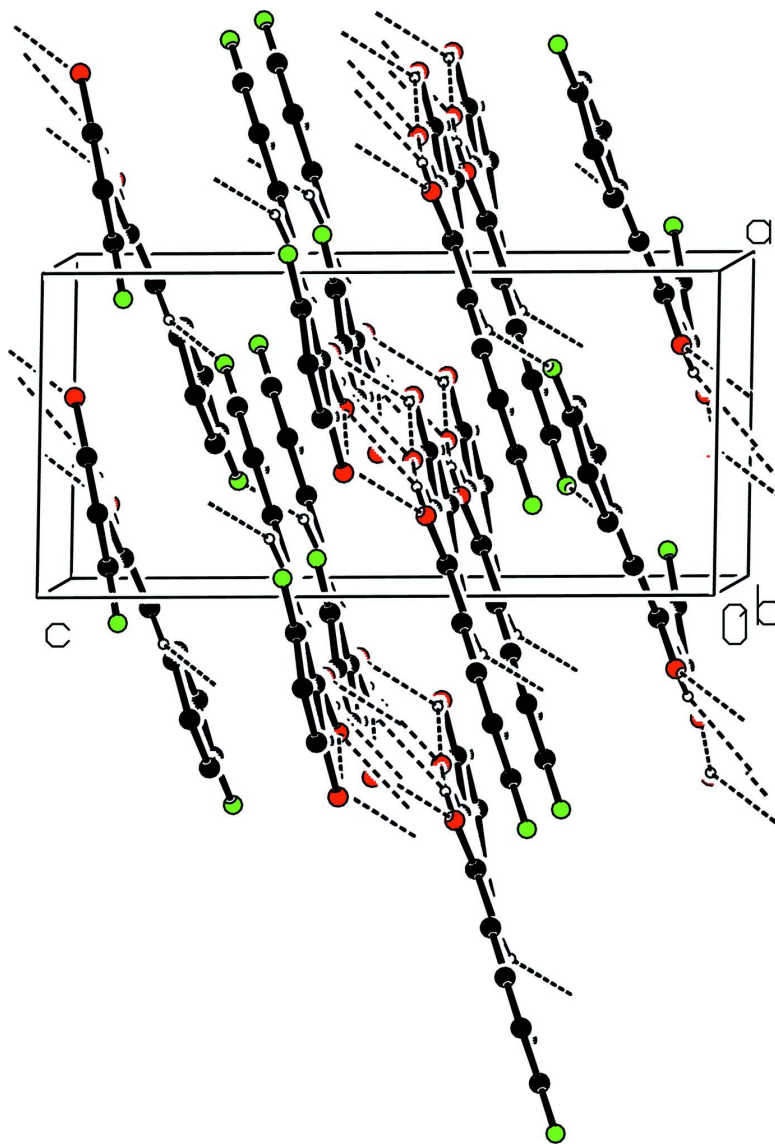


Figure 4

Part of the crystal structure with hydrogen bonds shown as dashed lines.

**(2Z,4E)-1-(5-Fluoro-2-hydroxyphenyl)-5-(4-fluorophenyl)-3-hydroxypenta-2,4-dien-1-one**

*Crystal data*

$C_{17}H_{12}F_2O_3$

$M_r = 302.27$

Monoclinic,  $P2_1/c$

Hall symbol:  $-P\ 2_1/c$

$a = 6.8275$  (18) Å

$b = 14.004$  (4) Å

$c = 14.267$  (4) Å

$\beta = 91.293$  (5)°

$V = 1363.8$  (7) Å<sup>3</sup>

$Z = 4$

$F(000) = 624$

$D_x = 1.472$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 2113 reflections

$\theta = 1.6$ – $27.3$ °

$\mu = 0.12$  mm<sup>-1</sup>

$T = 173$  K

Block, yellow

$0.32 \times 0.23 \times 0.18$  mm

*Data collection*

Bruker APEX CCD  
diffractometer  
Radiation source: fine-focus sealed tube  
Graphite monochromator  
 $\varphi$  and  $\omega$  scan  
Absorption correction: multi-scan  
(*SADABS*; Bruker, 2001)  
 $T_{\min} = 0.963$ ,  $T_{\max} = 0.979$

6787 measured reflections  
2392 independent reflections  
2040 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.028$   
 $\theta_{\max} = 25.0^\circ$ ,  $\theta_{\min} = 2.0^\circ$   
 $h = -8 \rightarrow 8$   
 $k = -16 \rightarrow 16$   
 $l = -12 \rightarrow 16$

*Refinement*

Refinement on  $F^2$   
Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.053$   
 $wR(F^2) = 0.147$   
 $S = 1.08$   
2392 reflections  
199 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  
 $w = 1/[\sigma^2(F_o^2) + (0.073P)^2 + 0.3861P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.21 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.29 \text{ e } \text{\AA}^{-3}$

*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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
F1	-1.0830 (2)	1.43310 (10)	0.38367 (11)	0.0579 (5)
F2	-1.6953 (2)	0.59884 (10)	0.25050 (10)	0.0577 (5)
O3	-0.7476 (2)	0.93089 (10)	0.42390 (11)	0.0383 (4)
H3A	-0.6598	0.9675	0.4404	0.057*
O2	-0.5856 (2)	1.09111 (10)	0.45331 (11)	0.0348 (4)
O1	-0.3972 (2)	1.24886 (10)	0.46202 (11)	0.0391 (4)
H1A	-0.4108	1.1908	0.4649	0.059*
C16	-1.5714 (3)	0.75182 (16)	0.27847 (15)	0.0371 (5)
H16A	-1.6915	0.7780	0.2602	0.045*
C6	-0.9127 (3)	1.38522 (15)	0.40188 (16)	0.0371 (5)
C9	-0.9017 (3)	0.98066 (14)	0.39432 (13)	0.0276 (5)
C1	-0.7404 (3)	1.13263 (14)	0.42564 (13)	0.0258 (5)
C7	-0.9178 (3)	1.28835 (15)	0.40533 (15)	0.0328 (5)
H7A	-1.0352	1.2559	0.3952	0.039*
C5	-0.7442 (4)	1.43672 (16)	0.41622 (16)	0.0401 (6)
H5A	-0.7455	1.5030	0.4127	0.048*

C13	-1.2171 (3)	0.67182 (15)	0.33270 (14)	0.0336 (5)
H13A	-1.0979	0.6447	0.3511	0.040*
C8	-0.9043 (3)	1.07757 (14)	0.39450 (14)	0.0287 (5)
H8A	-1.0170	1.1090	0.3736	0.034*
C3	-0.5709 (3)	1.28979 (15)	0.44117 (14)	0.0297 (5)
C14	-1.3700 (4)	0.61349 (16)	0.30486 (16)	0.0400 (6)
H14A	-1.3558	0.5474	0.3041	0.048*
C11	-1.0733 (3)	0.83020 (14)	0.36333 (14)	0.0287 (5)
H11A	-0.9613	0.7987	0.3852	0.034*
C2	-0.7438 (3)	1.23770 (14)	0.42429 (13)	0.0271 (5)
C17	-1.4183 (3)	0.80885 (16)	0.30625 (15)	0.0331 (5)
H17A	-1.4352	0.8747	0.3068	0.040*
C10	-1.0668 (3)	0.92464 (14)	0.36235 (14)	0.0294 (5)
H10A	-1.1766	0.9571	0.3394	0.035*
C15	-1.5432 (3)	0.65543 (17)	0.27832 (15)	0.0385 (6)
C12	-1.2379 (3)	0.77070 (14)	0.33372 (13)	0.0265 (5)
C4	-0.5740 (3)	1.38854 (15)	0.43586 (16)	0.0374 (6)
H4A	-0.4585	1.4226	0.4458	0.045*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
F1	0.0450 (9)	0.0381 (8)	0.0906 (12)	0.0127 (6)	0.0004 (8)	0.0083 (8)
F2	0.0554 (10)	0.0552 (9)	0.0619 (10)	-0.0309 (7)	-0.0138 (7)	-0.0001 (7)
O3	0.0275 (8)	0.0281 (8)	0.0588 (11)	0.0005 (6)	-0.0106 (7)	-0.0042 (7)
O2	0.0258 (8)	0.0298 (8)	0.0483 (9)	-0.0013 (6)	-0.0062 (7)	0.0013 (7)
O1	0.0295 (9)	0.0346 (8)	0.0530 (10)	-0.0088 (7)	-0.0058 (7)	0.0058 (7)
C16	0.0306 (12)	0.0444 (13)	0.0363 (13)	-0.0028 (10)	0.0002 (9)	-0.0039 (10)
C6	0.0374 (13)	0.0306 (11)	0.0434 (13)	0.0058 (10)	0.0033 (10)	0.0042 (10)
C9	0.0268 (11)	0.0301 (11)	0.0258 (11)	0.0005 (9)	-0.0012 (8)	0.0017 (8)
C1	0.0235 (10)	0.0308 (11)	0.0231 (10)	0.0005 (8)	0.0001 (8)	0.0016 (8)
C7	0.0307 (12)	0.0318 (11)	0.0358 (12)	-0.0020 (9)	0.0008 (9)	0.0010 (9)
C5	0.0508 (15)	0.0260 (11)	0.0438 (14)	-0.0027 (10)	0.0066 (11)	0.0006 (10)
C13	0.0369 (13)	0.0324 (11)	0.0313 (12)	-0.0010 (9)	0.0002 (9)	0.0019 (9)
C8	0.0251 (11)	0.0297 (11)	0.0310 (11)	-0.0015 (8)	-0.0066 (8)	0.0042 (9)
C3	0.0307 (12)	0.0315 (11)	0.0269 (11)	-0.0046 (9)	0.0012 (9)	0.0016 (9)
C14	0.0535 (15)	0.0282 (11)	0.0383 (13)	-0.0097 (11)	0.0018 (11)	-0.0012 (10)
C11	0.0271 (12)	0.0333 (11)	0.0257 (11)	0.0009 (9)	0.0005 (8)	-0.0027 (9)
C2	0.0305 (11)	0.0284 (11)	0.0224 (10)	-0.0028 (9)	0.0023 (8)	0.0013 (8)
C17	0.0296 (12)	0.0331 (11)	0.0367 (12)	-0.0009 (9)	0.0014 (9)	-0.0043 (9)
C10	0.0274 (11)	0.0316 (11)	0.0290 (11)	-0.0011 (9)	-0.0051 (9)	0.0000 (9)
C15	0.0398 (14)	0.0441 (13)	0.0317 (12)	-0.0205 (11)	-0.0008 (10)	-0.0013 (10)
C12	0.0299 (11)	0.0291 (10)	0.0206 (10)	-0.0032 (9)	0.0018 (8)	-0.0019 (8)
C4	0.0413 (14)	0.0312 (11)	0.0397 (13)	-0.0108 (10)	0.0026 (10)	-0.0030 (10)

## Geometric parameters (Å, °)

F1—C6	1.362 (2)	C5—C4	1.368 (3)
F2—C15	1.358 (2)	C5—H5A	0.9300
O3—C9	1.323 (2)	C13—C14	1.377 (3)
O3—H3A	0.8200	C13—C12	1.392 (3)
O2—C1	1.262 (2)	C13—H13A	0.9300
O1—C3	1.345 (2)	C8—H8A	0.9300
O1—H1A	0.8200	C3—C4	1.385 (3)
C16—C15	1.363 (3)	C3—C2	1.404 (3)
C16—C17	1.367 (3)	C14—C15	1.366 (3)
C16—H16A	0.9300	C14—H14A	0.9300
C6—C7	1.358 (3)	C11—C10	1.323 (3)
C6—C5	1.369 (3)	C11—C12	1.454 (3)
C9—C8	1.357 (3)	C11—H11A	0.9300
C9—C10	1.439 (3)	C17—C12	1.391 (3)
C1—C8	1.422 (3)	C17—H17A	0.9300
C1—C2	1.472 (3)	C10—H10A	0.9300
C7—C2	1.404 (3)	C4—H4A	0.9300
C7—H7A	0.9300		
C9—O3—H3A	109.5	O1—C3—C2	123.41 (18)
C3—O1—H1A	109.5	C4—C3—C2	119.84 (19)
C15—C16—C17	118.1 (2)	C15—C14—C13	118.1 (2)
C15—C16—H16A	120.9	C15—C14—H14A	121.0
C17—C16—H16A	120.9	C13—C14—H14A	121.0
C7—C6—F1	118.4 (2)	C10—C11—C12	126.55 (19)
C7—C6—C5	122.9 (2)	C10—C11—H11A	116.7
F1—C6—C5	118.66 (19)	C12—C11—H11A	116.7
O3—C9—C8	122.42 (18)	C3—C2—C7	118.35 (18)
O3—C9—C10	115.18 (17)	C3—C2—C1	120.26 (18)
C8—C9—C10	122.40 (18)	C7—C2—C1	121.38 (18)
O2—C1—C8	119.71 (18)	C16—C17—C12	121.6 (2)
O2—C1—C2	118.55 (17)	C16—C17—H17A	119.2
C8—C1—C2	121.72 (18)	C12—C17—H17A	119.2
C6—C7—C2	119.3 (2)	C11—C10—C9	124.61 (19)
C6—C7—H7A	120.4	C11—C10—H10A	117.7
C2—C7—H7A	120.4	C9—C10—H10A	117.7
C4—C5—C6	118.6 (2)	F2—C15—C16	118.1 (2)
C4—C5—H5A	120.7	F2—C15—C14	118.8 (2)
C6—C5—H5A	120.7	C16—C15—C14	123.1 (2)
C14—C13—C12	121.1 (2)	C17—C12—C13	117.98 (19)
C14—C13—H13A	119.5	C17—C12—C11	122.39 (18)
C12—C13—H13A	119.5	C13—C12—C11	119.63 (19)
C9—C8—C1	122.19 (19)	C5—C4—C3	121.0 (2)
C9—C8—H8A	118.9	C5—C4—H4A	119.5
C1—C8—H8A	118.9	C3—C4—H4A	119.5
O1—C3—C4	116.75 (18)		

F1—C6—C7—C2	-179.82 (18)	C8—C1—C2—C7	9.5 (3)
C5—C6—C7—C2	0.0 (4)	C15—C16—C17—C12	0.0 (3)
C7—C6—C5—C4	-0.7 (4)	C12—C11—C10—C9	178.58 (19)
F1—C6—C5—C4	179.0 (2)	O3—C9—C10—C11	1.7 (3)
O3—C9—C8—C1	0.7 (3)	C8—C9—C10—C11	-178.0 (2)
C10—C9—C8—C1	-179.63 (18)	C17—C16—C15—F2	-179.84 (19)
O2—C1—C8—C9	0.8 (3)	C17—C16—C15—C14	0.2 (4)
C2—C1—C8—C9	179.13 (19)	C13—C14—C15—F2	179.86 (19)
C12—C13—C14—C15	-0.1 (3)	C13—C14—C15—C16	-0.2 (4)
O1—C3—C2—C7	178.50 (19)	C16—C17—C12—C13	-0.3 (3)
C4—C3—C2—C7	-2.1 (3)	C16—C17—C12—C11	179.90 (19)
O1—C3—C2—C1	-2.1 (3)	C14—C13—C12—C17	0.3 (3)
C4—C3—C2—C1	177.29 (19)	C14—C13—C12—C11	-179.87 (19)
C6—C7—C2—C3	1.4 (3)	C10—C11—C12—C17	-4.8 (3)
C6—C7—C2—C1	-177.92 (19)	C10—C11—C12—C13	175.4 (2)
O2—C1—C2—C3	8.5 (3)	C6—C5—C4—C3	0.1 (3)
C8—C1—C2—C3	-169.85 (18)	O1—C3—C4—C5	-179.18 (19)
O2—C1—C2—C7	-172.14 (18)	C2—C3—C4—C5	1.3 (3)

*Hydrogen-bond geometry (Å, °)*

<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>
O1—H1A...O2	0.82	1.84	2.558 (2)	145
O1—H1A...O3 <sup>i</sup>	0.82	2.55	3.145 (2)	130
O3—H3A...O2	0.82	1.81	2.532 (2)	146
O3—H3A...O2 <sup>i</sup>	0.82	2.38	2.856 (2)	118
C10—H10A...F2 <sup>ii</sup>	0.93	2.51	3.326 (3)	147

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