

# Ethyl 2-[2-(4-oxo-4*H*-chromen-2-yl)phenoxy]-acetate

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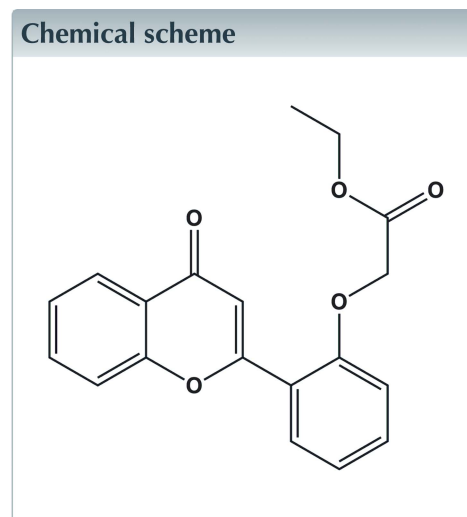
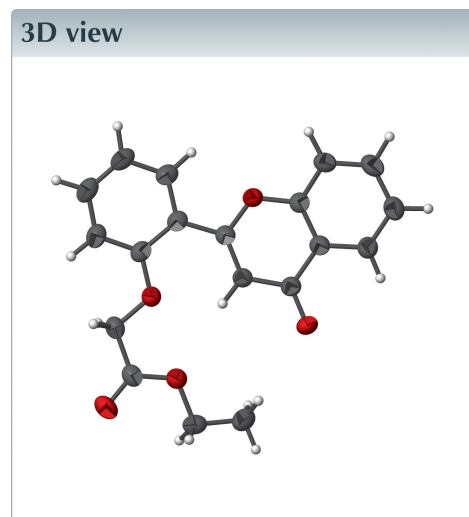
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Keywords: crystal structure; flavonoid derivative; chromene; hydrogen bonding; C—H···O hydrogen bond and to two weak C—H···O contacts. In the crystal, neighboring molecules are linked by a C—H···O hydrogen bond and a C—H··· $\pi$  interaction, forming chains along the *a*-axis direction.

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Structural data: full structural data are available from [iucrdata.iucr.org](http://iucrdata.iucr.org)

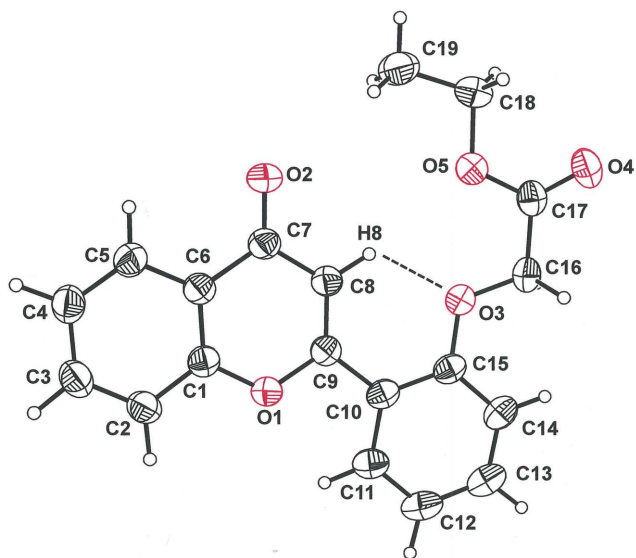
In the title flavonoid derivative, C<sub>19</sub>H<sub>16</sub>O<sub>5</sub>, the chromene portion is planar (r.m.s. deviation = 0.022 Å) with the substituents lying closely to the same plane. The dihedral angle between its mean plane and that of the benzene ring is 4.9 (1)°. This planarity is due, in part, to the presence of a strong intramolecular C—H···O hydrogen bond and to two weak C—H···O contacts. In the crystal, neighboring molecules are linked by a C—H···O hydrogen bond and a C—H··· $\pi$  interaction, forming chains along the *a*-axis direction.



## Structure description

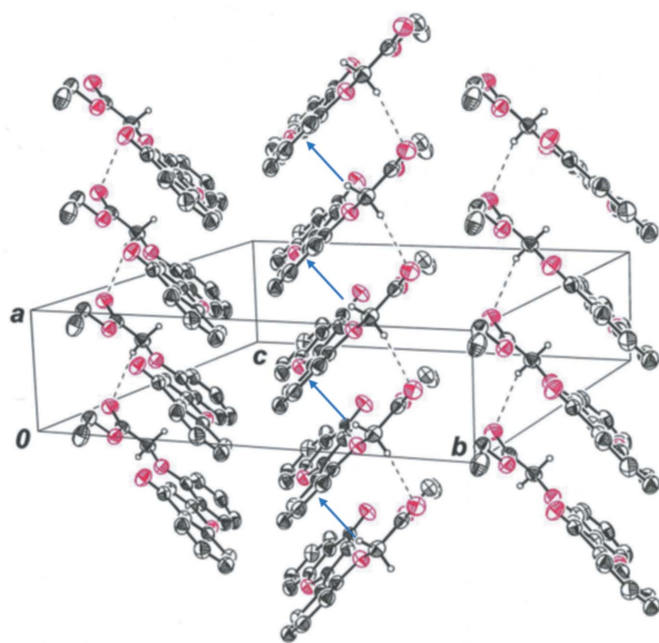
Flavonoids comprise a family of natural compounds with variable phenolic structures that occur in plants. Naturally occurring flavonoids and their chemical derivatives exhibit a variety of pharmacological activities (Kühnau, 1976; Kale *et al.*, 2008; Walle, 2007). It has been shown that biological activity can be affected by the position of the different substituents on the flavone ring. Many studies have been published suggesting that flavonoid-based molecules have therapeutic efficacy in areas such as cardiovascular diseases, cancers, and age-related diseases (Bear & Teel, 2000; Rice-Evans *et al.*, 1995; Pandey, 2007). In general, flavonoids can act as substrates, inducers, and/or inhibitors of P450 enzymes. We have previously reported synthetic flavonoids metabolized by several cytochrome P450 enzymes including P450s 1A1, 1A2, 1B1, 2C9, 3A4 and 3A5 (Sridhar *et al.*, 2012; Foroozesh *et al.*, 1997).

The crystal structure of flavone itself (Waller *et al.*, 2003) is quite similar to that of ethyl 2-(2-(4-oxo-4*H*-chromen-2-yl)phenoxy)acetate in that it occurs in *P*2<sub>1</sub>2<sub>1</sub> with a comparably shaped cell, is essentially planar, and forms  $\pi$  stacks along the *a* axis. The crystallographically characterized flavone derivatives most similar to the title compound



**Figure 1**  
The molecular structure of the title compound, with atom labeling and 50% probability displacement ellipsoids. The intramolecular hydrogen bond is shown by a dashed line (Table 1).

are 2'-hydroxy flavone (Seetharaman & Rajan, 1995) and 2'-methoxy flavone (Wallet *et al.*, 1990), both of which are also planar molecules with hydrogen bonding playing a role in enforcing the molecular conformation. Both 2'-hydroxy flavone and 2'-methoxy flavone also form columnar  $\pi$  stacks, but the latter molecule packs to form two distinct stacks along different directions.



**Figure 2**  
A view of the crystal packing of the title compound. The C—H...O hydrogen bonds are shown as dashed lines, and the C—H... $\pi$  interactions are illustrated by blue arrows for the central column of molecules (see Table 1).

**Table 1**  
Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$Cg3$  is the centroid of the C10–C15 benzene ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C8—H8...O3	0.96 (3)	2.13 (3)	2.771 (3)	122 (2)
C5—H5...O2	0.97 (3)	2.54 (3)	2.876 (3)	100 (2)
C11—H11...O1	0.97 (3)	2.26 (3)	2.631 (3)	101 (2)
C16—H16B...O4 <sup>i</sup>	1.03 (3)	2.56 (3)	3.327 (3)	131 (2)
C16—H16A...Cg3 <sup>ii</sup>	0.99 (3)	2.75 (3)	3.0449 (3)	128 (2)

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

**Table 2**  
Experimental details.

Crystal data	
Chemical formula	$C_{19}H_{16}O_5$
$M_r$	324.32
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	150
$a, b, c$ ( $\text{\AA}$ )	4.6852 (1), 17.5786 (5), 18.8573 (5)
$V$ ( $\text{\AA}^3$ )	1553.07 (7)
$Z$	4
Radiation type	Cu $K\alpha$
$\mu$ ( $\text{mm}^{-1}$ )	0.83
Crystal size (mm)	0.29 $\times$ 0.22 $\times$ 0.07
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (SADABS; Krause <i>et al.</i> , 2015)
$T_{\min}, T_{\max}$	0.77, 0.94
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	11308, 3030, 2800
$R_{\text{int}}$	0.040
$(\sin \theta/\lambda)_{\text{max}}$ ( $\text{\AA}^{-1}$ )	0.618
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.035, 0.089, 1.08
No. of reflections	3030
No. of parameters	281
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ ( $e \text{\AA}^{-3}$ )	0.13, $-0.17$
Absolute structure	Flack $x$ determined using 1052 quotients $[(I^+) - (I^-)] / [(I^+) + (I^-)]$ (Parsons <i>et al.</i> , 2013).
Absolute structure parameter	0.04 (9)

Computer programs: APEX3 and SAINT (Bruker, 2016), SHELXT (Sheldrick, 2015a), SHELXL2018/1 (Sheldrick, 2015b), SHELXTL (Sheldrick, 2008), DIAMOND (Brandenburg & Putz, 2012), Mercury (Macrae *et al.*, 2008) and publCIF (Westrip, 2010).

In the title compound, the 10-membered bicyclic moiety is planar to within 0.028 (3)  $\text{\AA}$  (r.m.s. deviation of the fitted atoms = 0.022  $\text{\AA}$ ), while the dihedral angle between its mean plane and that of the C10–C15 benzene ring is only 4.9 (1) $^\circ$ . This planarity is likely due to the intramolecular C8—H8...O3 hydrogen bond (Fig. 1 and Table 1). The conformation of the ester grouping may be due in part to C19—H19B...O2 and C8—H8...O5 hydrogen bonds, but since the H...O distances are only 0.04 and 0.08  $\text{\AA}$  less than the sum of the van der Waals radii, respectively, these interactions would be quite weak at best.

In the crystal, molecules are linked by C—H...O hydrogen bonds, forming chains extending along the  $a$ -axis direction

(Table 1 and Fig. 2). Within the chains there are also C—H... $\pi$  interactions present (Table 1, Fig. 2).

### Synthesis and crystallization

Potassium carbonate (0.86 g, 6.291 mmol) was added to a stirred solution of flavon-2'-ol (0.500 g, 2.097 mmol) in 30 ml of acetone. The mixture was stirred for 30 min at 298 K. Bromo ethyl acetate (0.761 g, 5.24 mmol) was added slowly to the mixture. The reaction mixture was heated at 303 K overnight and then filtered and concentrated on a rotary evaporator. The crude material was then purified by flash chromatography on silica gel with ethyl acetate:hexanes (20:80, *v:v*) as the eluent to yield the title compound as a white solid (yield 0.652 g, 96%; m.p. 361–363 K). Colorless plate-like crystals were obtained by slow cooling of a warm solution of ethyl acetate:hexanes (2:1, *v:v*).

<sup>1</sup>H NMR (300 MHz,  $\delta$ , p.p.m. in CDCl<sub>3</sub>): 8.23 (*d*, *J* = 9.1 Hz, 1H), 7.93 (*d*, *J* = 8.1 Hz, 1H), 7.68 (*d*, *J* = 7.3 Hz, 1H), 7.56–7.38 (*m*, 3H), 7.24 (*s*, 1H), 7.16 (*t*, *J* = 7.6 Hz, 1H), 6.91 (*d*, *J* = 7.7 Hz, 1H), 4.76 (*s*, 2H), 4.28 (*q*, *J* = 7.2 Hz, 2H), 1.31 (*t*, *J* = 7.2 Hz, 3H). <sup>13</sup>C NMR (75 MHz,  $\delta$ , p.p.m. in CDCl<sub>3</sub>): 178.7, 168.1, 160.4, 156.4, 156.0, 133.5, 132.2, 129.6, 125.6, 124.9, 123.8, 121.7, 121.5, 118.0, 112.9, 112.5, 65.6, 61.6, 14.0. Anal. calcd. for C<sub>19</sub>H<sub>16</sub>O<sub>5</sub>: C, 70.36; H, 4.97. Found: C, 70.55; H, 4.91.

### Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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## full crystallographic data

*IUCrData* (2018). 3, x180993 [https://doi.org/10.1107/S2414314618009938]

Ethyl 2-[2-(4-oxo-4*H*-chromen-2-yl)phenoxy]acetate

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Ethyl 2-[2-(4-oxo-4*H*-chromen-2-yl)phenoxy]acetate*Crystal data*

$C_{19}H_{16}O_5$	$D_x = 1.387 \text{ Mg m}^{-3}$
$M_r = 324.32$	Cu $K\alpha$ radiation, $\lambda = 1.54178 \text{ \AA}$
Orthorhombic, $P2_12_12_1$	Cell parameters from 9900 reflections
$a = 4.6852 (1) \text{ \AA}$	$\theta = 3.4\text{--}72.4^\circ$
$b = 17.5786 (5) \text{ \AA}$	$\mu = 0.83 \text{ mm}^{-1}$
$c = 18.8573 (5) \text{ \AA}$	$T = 150 \text{ K}$
$V = 1553.07 (7) \text{ \AA}^3$	Plate, colourless
$Z = 4$	$0.29 \times 0.22 \times 0.07 \text{ mm}$
$F(000) = 680$	

*Data collection*

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer	$T_{\min} = 0.77, T_{\max} = 0.94$
Radiation source: INCOATEC $I\mu$ S micro-focus source	11308 measured reflections
Mirror monochromator	3030 independent reflections
Detector resolution: $10.4167 \text{ pixels mm}^{-1}$	2800 reflections with $I > 2\sigma(I)$
$\omega$ scans	$R_{\text{int}} = 0.040$
Absorption correction: multi-scan (SADABS; Krause <i>et al.</i> , 2015)	$\theta_{\max} = 72.4^\circ, \theta_{\min} = 3.4^\circ$
	$h = -5 \rightarrow 4$
	$k = -21 \rightarrow 21$
	$l = -23 \rightarrow 22$

*Refinement*

Refinement on $F^2$	Hydrogen site location: difference Fourier map
Least-squares matrix: full	All H-atom parameters refined
$R[F^2 > 2\sigma(F^2)] = 0.035$	$w = 1/[\sigma^2(F_o^2) + (0.0432P)^2 + 0.2094P]$
$wR(F^2) = 0.089$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{\max} < 0.001$
3030 reflections	$\Delta\rho_{\max} = 0.13 \text{ e \AA}^{-3}$
281 parameters	$\Delta\rho_{\min} = -0.17 \text{ e \AA}^{-3}$
0 restraints	Absolute structure: Flack $x$ determined using
Primary atom site location: structure-invariant direct methods	1052 quotients $[(I^-)-(I^+)]/[(I^-)+(I^+)]$ (Parsons <i>et al.</i> , 2013).
Secondary atom site location: difference Fourier map	Absolute structure parameter: 0.04 (9)

*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.** 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  $F^2 > 2\sigma(F^2)$  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>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.2034 (3)	0.36678 (8)	0.51445 (8)	0.0368 (4)
O2	0.7780 (4)	0.46099 (10)	0.65057 (8)	0.0460 (4)
O3	0.6284 (4)	0.55035 (9)	0.41929 (8)	0.0401 (4)
O4	1.1532 (4)	0.69398 (10)	0.40606 (10)	0.0513 (5)
O5	0.9663 (4)	0.62778 (9)	0.49699 (8)	0.0423 (4)
C1	0.2302 (5)	0.33774 (12)	0.58204 (11)	0.0346 (5)
C2	0.0567 (6)	0.27625 (14)	0.59824 (13)	0.0423 (6)
H2	-0.075 (7)	0.2546 (16)	0.5610 (14)	0.049 (8)*
C3	0.0689 (6)	0.24647 (14)	0.66622 (14)	0.0474 (6)
H3	-0.056 (7)	0.2035 (18)	0.6761 (16)	0.059 (8)*
C4	0.2536 (6)	0.27732 (14)	0.71673 (13)	0.0465 (6)
H4	0.247 (7)	0.2551 (16)	0.7655 (15)	0.052 (8)*
C5	0.4281 (6)	0.33689 (14)	0.69871 (12)	0.0421 (6)
H5	0.560 (6)	0.3608 (16)	0.7313 (15)	0.047 (7)*
C6	0.4182 (5)	0.36879 (12)	0.63074 (11)	0.0350 (5)
C7	0.6005 (5)	0.43284 (12)	0.61004 (11)	0.0361 (5)
C8	0.5556 (5)	0.46043 (13)	0.53864 (12)	0.0362 (5)
H8	0.669 (6)	0.5030 (16)	0.5230 (14)	0.046 (7)*
C9	0.3641 (5)	0.42812 (12)	0.49416 (11)	0.0330 (4)
C10	0.3013 (5)	0.44765 (12)	0.41940 (11)	0.0346 (5)
C11	0.0962 (5)	0.40542 (13)	0.38233 (13)	0.0405 (5)
H11	-0.012 (6)	0.3664 (15)	0.4072 (14)	0.042 (7)*
C12	0.0415 (6)	0.41769 (14)	0.31085 (13)	0.0469 (6)
H12	-0.103 (6)	0.3856 (15)	0.2880 (15)	0.047 (7)*
C13	0.1946 (6)	0.47231 (14)	0.27468 (13)	0.0458 (6)
H13	0.159 (6)	0.4829 (16)	0.2251 (15)	0.050 (7)*
C14	0.3935 (6)	0.51654 (14)	0.30949 (12)	0.0422 (6)
H14	0.488 (7)	0.5559 (17)	0.2835 (16)	0.057 (8)*
C15	0.4429 (5)	0.50577 (12)	0.38172 (12)	0.0358 (5)
C16	0.7779 (5)	0.60771 (14)	0.38187 (12)	0.0404 (5)
H16A	0.886 (6)	0.5842 (14)	0.3420 (13)	0.041 (7)*
H16B	0.642 (6)	0.6484 (14)	0.3621 (13)	0.035 (6)*
C17	0.9869 (5)	0.64768 (13)	0.42946 (12)	0.0382 (5)
C18	1.1644 (7)	0.66578 (16)	0.54554 (14)	0.0479 (6)
H18A	1.363 (7)	0.6452 (17)	0.5326 (17)	0.058 (8)*
H18B	1.143 (6)	0.7245 (17)	0.5402 (15)	0.053 (8)*
C19	1.0807 (9)	0.64282 (19)	0.61898 (16)	0.0607 (8)
H19A	1.224 (9)	0.663 (2)	0.650 (2)	0.083 (11)*
H19B	1.074 (7)	0.588 (2)	0.6227 (17)	0.070 (10)*
H19C	0.887 (10)	0.662 (2)	0.632 (2)	0.104 (15)*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0381 (8)	0.0372 (7)	0.0350 (7)	-0.0042 (7)	-0.0006 (6)	-0.0031 (6)
O2	0.0501 (10)	0.0495 (9)	0.0384 (8)	-0.0137 (8)	-0.0087 (7)	-0.0020 (7)
O3	0.0434 (9)	0.0433 (8)	0.0337 (7)	-0.0057 (7)	0.0017 (7)	-0.0005 (6)
O4	0.0484 (11)	0.0482 (9)	0.0573 (10)	-0.0074 (9)	0.0135 (9)	0.0052 (8)
O5	0.0443 (9)	0.0421 (8)	0.0405 (8)	-0.0049 (7)	0.0005 (7)	-0.0001 (7)
C1	0.0359 (12)	0.0331 (10)	0.0348 (10)	0.0033 (9)	0.0033 (9)	-0.0036 (8)
C2	0.0421 (14)	0.0389 (12)	0.0460 (12)	-0.0057 (11)	0.0030 (10)	-0.0047 (10)
C3	0.0526 (15)	0.0374 (12)	0.0523 (14)	-0.0073 (12)	0.0104 (12)	-0.0006 (10)
C4	0.0570 (16)	0.0414 (12)	0.0411 (12)	-0.0014 (12)	0.0083 (12)	0.0009 (10)
C5	0.0503 (15)	0.0403 (12)	0.0358 (11)	-0.0025 (11)	0.0031 (10)	-0.0027 (9)
C6	0.0360 (11)	0.0329 (10)	0.0362 (10)	0.0011 (10)	0.0044 (9)	-0.0050 (8)
C7	0.0377 (12)	0.0352 (11)	0.0354 (10)	-0.0004 (10)	0.0018 (9)	-0.0046 (9)
C8	0.0380 (12)	0.0350 (11)	0.0356 (11)	-0.0020 (10)	0.0010 (9)	-0.0024 (9)
C9	0.0323 (11)	0.0311 (9)	0.0355 (10)	0.0039 (9)	0.0032 (9)	-0.0037 (8)
C10	0.0352 (12)	0.0340 (10)	0.0346 (10)	0.0077 (9)	0.0001 (9)	-0.0064 (8)
C11	0.0418 (13)	0.0360 (11)	0.0437 (11)	0.0056 (10)	-0.0067 (10)	-0.0051 (10)
C12	0.0539 (16)	0.0410 (13)	0.0458 (12)	0.0095 (12)	-0.0162 (11)	-0.0092 (11)
C13	0.0551 (16)	0.0446 (13)	0.0376 (12)	0.0174 (12)	-0.0095 (11)	-0.0067 (10)
C14	0.0486 (15)	0.0434 (12)	0.0347 (11)	0.0108 (12)	-0.0010 (10)	-0.0016 (10)
C15	0.0358 (12)	0.0376 (11)	0.0340 (10)	0.0082 (10)	0.0000 (9)	-0.0070 (8)
C16	0.0405 (13)	0.0431 (12)	0.0377 (11)	0.0014 (11)	0.0083 (10)	0.0033 (10)
C17	0.0374 (12)	0.0346 (11)	0.0427 (12)	0.0060 (10)	0.0088 (10)	0.0011 (9)
C18	0.0464 (16)	0.0450 (14)	0.0523 (14)	-0.0064 (12)	-0.0055 (11)	-0.0063 (11)
C19	0.079 (2)	0.0539 (17)	0.0492 (14)	-0.0116 (16)	-0.0156 (16)	-0.0003 (13)

*Geometric parameters (Å, °)*

O1—C9	1.370 (3)	C8—H8	0.96 (3)
O1—C1	1.379 (3)	C9—C10	1.481 (3)
O2—C7	1.233 (3)	C10—C11	1.401 (3)
O3—C15	1.368 (3)	C10—C15	1.410 (3)
O3—C16	1.416 (3)	C11—C12	1.389 (3)
O4—C17	1.210 (3)	C11—H11	0.97 (3)
O5—C17	1.324 (3)	C12—C13	1.379 (4)
O5—C18	1.465 (3)	C12—H12	0.98 (3)
C1—C6	1.385 (3)	C13—C14	1.380 (4)
C1—C2	1.386 (3)	C13—H13	0.97 (3)
C2—C3	1.386 (4)	C14—C15	1.394 (3)
C2—H2	1.01 (3)	C14—H14	0.96 (3)
C3—C4	1.396 (4)	C16—C17	1.503 (4)
C3—H3	0.97 (3)	C16—H16A	0.99 (3)
C4—C5	1.371 (4)	C16—H16B	1.03 (3)
C4—H4	1.00 (3)	C18—C19	1.495 (4)
C5—C6	1.400 (3)	C18—H18A	1.03 (3)
C5—H5	0.97 (3)	C18—H18B	1.04 (3)

C6—C7	1.466 (3)	C19—H19A	0.97 (4)
C7—C8	1.446 (3)	C19—H19B	0.97 (4)
C8—C9	1.353 (3)	C19—H19C	1.00 (5)
C9—O1—C1	119.97 (17)	C10—C11—H11	119.4 (16)
C15—O3—C16	117.64 (17)	C13—C12—C11	119.5 (3)
C17—O5—C18	115.8 (2)	C13—C12—H12	122.9 (16)
O1—C1—C6	121.68 (19)	C11—C12—H12	117.6 (16)
O1—C1—C2	116.0 (2)	C12—C13—C14	120.6 (2)
C6—C1—C2	122.3 (2)	C12—C13—H13	121.6 (17)
C3—C2—C1	118.3 (2)	C14—C13—H13	117.8 (17)
C3—C2—H2	121.7 (16)	C13—C14—C15	120.0 (2)
C1—C2—H2	120.0 (16)	C13—C14—H14	118.5 (19)
C2—C3—C4	120.6 (2)	C15—C14—H14	121.4 (19)
C2—C3—H3	116.4 (18)	O3—C15—C14	122.2 (2)
C4—C3—H3	122.9 (18)	O3—C15—C10	116.94 (19)
C5—C4—C3	119.8 (2)	C14—C15—C10	120.8 (2)
C5—C4—H4	123.0 (18)	O3—C16—C17	110.95 (19)
C3—C4—H4	117.1 (18)	O3—C16—H16A	109.3 (15)
C4—C5—C6	120.9 (2)	C17—C16—H16A	108.3 (15)
C4—C5—H5	123.8 (16)	O3—C16—H16B	111.7 (14)
C6—C5—H5	115.3 (16)	C17—C16—H16B	107.2 (13)
C1—C6—C5	118.1 (2)	H16A—C16—H16B	109 (2)
C1—C6—C7	119.8 (2)	O4—C17—O5	125.1 (2)
C5—C6—C7	122.1 (2)	O4—C17—C16	121.1 (2)
O2—C7—C8	122.7 (2)	O5—C17—C16	113.8 (2)
O2—C7—C6	122.4 (2)	O5—C18—C19	106.8 (2)
C8—C7—C6	114.9 (2)	O5—C18—H18A	105.4 (17)
C9—C8—C7	122.2 (2)	C19—C18—H18A	111.3 (18)
C9—C8—H8	120.0 (16)	O5—C18—H18B	109.3 (17)
C7—C8—H8	117.8 (16)	C19—C18—H18B	109.4 (16)
C8—C9—O1	121.46 (19)	H18A—C18—H18B	114 (3)
C8—C9—C10	128.7 (2)	C18—C19—H19A	107 (2)
O1—C9—C10	109.83 (18)	C18—C19—H19B	110.1 (19)
C11—C10—C15	117.1 (2)	H19A—C19—H19B	110 (3)
C11—C10—C9	119.2 (2)	C18—C19—H19C	113 (3)
C15—C10—C9	123.7 (2)	H19A—C19—H19C	111 (3)
C12—C11—C10	121.9 (3)	H19B—C19—H19C	107 (4)
C12—C11—H11	118.7 (16)		
C9—O1—C1—C6	-0.3 (3)	C8—C9—C10—C11	178.7 (2)
C9—O1—C1—C2	179.21 (19)	O1—C9—C10—C11	1.5 (3)
O1—C1—C2—C3	-178.0 (2)	C8—C9—C10—C15	0.6 (4)
C6—C1—C2—C3	1.6 (4)	O1—C9—C10—C15	-176.63 (19)
C1—C2—C3—C4	-0.6 (4)	C15—C10—C11—C12	2.6 (3)
C2—C3—C4—C5	-1.0 (4)	C9—C10—C11—C12	-175.7 (2)
C3—C4—C5—C6	1.8 (4)	C10—C11—C12—C13	0.8 (4)
O1—C1—C6—C5	178.7 (2)	C11—C12—C13—C14	-2.4 (4)

C2—C1—C6—C5	-0.8 (3)	C12—C13—C14—C15	0.6 (4)
O1—C1—C6—C7	-1.7 (3)	C16—O3—C15—C14	-1.6 (3)
C2—C1—C6—C7	178.7 (2)	C16—O3—C15—C10	178.42 (19)
C4—C5—C6—C1	-0.9 (4)	C13—C14—C15—O3	-177.0 (2)
C4—C5—C6—C7	179.6 (2)	C13—C14—C15—C10	2.9 (3)
C1—C6—C7—O2	-177.6 (2)	C11—C10—C15—O3	175.58 (19)
C5—C6—C7—O2	1.9 (3)	C9—C10—C15—O3	-6.3 (3)
C1—C6—C7—C8	2.5 (3)	C11—C10—C15—C14	-4.4 (3)
C5—C6—C7—C8	-177.9 (2)	C9—C10—C15—C14	173.8 (2)
O2—C7—C8—C9	178.7 (2)	C15—O3—C16—C17	-176.01 (18)
C6—C7—C8—C9	-1.5 (3)	C18—O5—C17—O4	-0.2 (3)
C7—C8—C9—O1	-0.5 (3)	C18—O5—C17—C16	-179.5 (2)
C7—C8—C9—C10	-177.5 (2)	O3—C16—C17—O4	173.4 (2)
C1—O1—C9—C8	1.5 (3)	O3—C16—C17—O5	-7.3 (3)
C1—O1—C9—C10	179.00 (18)	C17—O5—C18—C19	173.0 (2)

### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

Cg3 is the centroid of the C10—C15 benzene 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>
C8—H8 $\cdots$ O3	0.96 (3)	2.13 (3)	2.771 (3)	122 (2)
C5—H5 $\cdots$ O2	0.97 (3)	2.54 (3)	2.876 (3)	100 (2)
C11—H11 $\cdots$ O1	0.97 (3)	2.26 (3)	2.631 (3)	101 (2)
C16—H16 <i>B</i> $\cdots$ O4 <sup>i</sup>	1.03 (3)	2.56 (3)	3.327 (3)	131 (2)
C16—H16 <i>A</i> $\cdots$ Cg3 <sup>ii</sup>	0.99 (3)	2.75 (3)	3.0449 (3)	128 (2)

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