

## 2-Oxo-2*H*-chromen-7-yl 4-methylbenzoate

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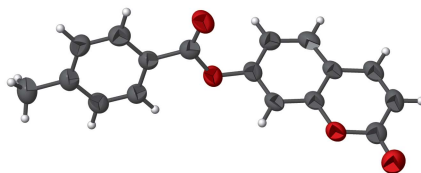
**Keywords:** crystal structure; C—H...O hydrogen bond; coumarin; Hirshfeld surface analysis.

CCDC reference: 1839611

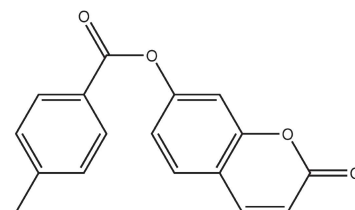
**Structural data:** full structural data are available from [iucrdata.iucr.org](http://iucrdata.iucr.org)

In the title compound, C<sub>17</sub>H<sub>12</sub>O<sub>4</sub>, the benzoate ring is oriented at an acute angle of 60.14 (13)° relative to the coumarin plane (r.m.s. deviation = 0.006 Å). This conformation is stabilized by an intramolecular C—H...O weak hydrogen bond, which forms a five-membered ring. Also present are  $\pi$ – $\pi$  stacking interactions between neighbouring pyrone and benzene rings [centroid-to-centroid distances in the range 3.6286 (1)–3.6459 (1) Å] and C=O... $\pi$  interactions [O...centroid distances in the range 3.2938 (1)–3.6132 (1) Å]. Hirshfeld surface analysis has been used to confirm and quantify the supramolecular interactions.

### 3D view



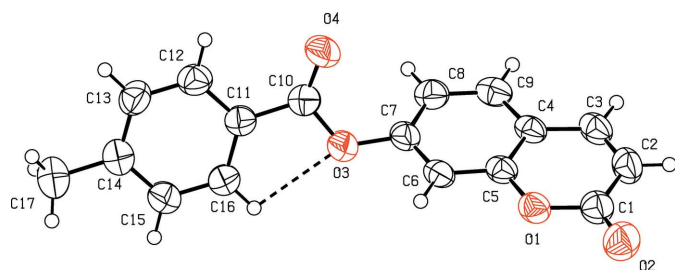
### Chemical scheme



### Structure description

Coumarins and their derivatives constitute one of the major classes of naturally occurring compounds and interest in their chemistry continues unabated because of their usefulness as biologically active agents. They also form the core of several molecules of pharmaceutical importance. Coumarin and its derivatives have been reported to serve as anti-bacterial (Basanagouda *et al.*, 2009), anti-oxidant (Vukovic *et al.*, 2010) and anti-inflammatory agents (Emmanuel-Giota *et al.*, 2001). In view of their importance and as a continuation of our work on the crystal structure analysis of coumarin derivatives (Abou *et al.*, 2012, 2013), we report herein the synthesis, crystal structure and Hirshfeld surface analysis of the title compound.

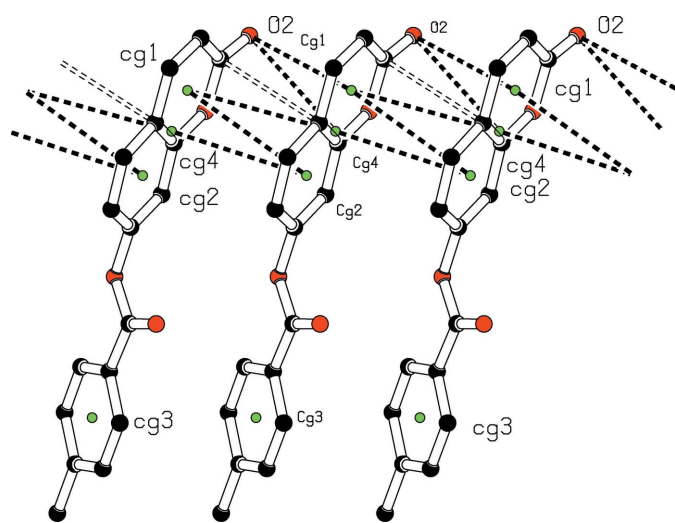
The molecular structure of the title compound is illustrated in Fig. 1. In this structure, an *S*(5) ring motif arises from an intramolecular C16—H16...O3 hydrogen bond



**Figure 1**  
The molecular structure of the title compound with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. The dashed line indicates the intramolecular hydrogen bond.

(Table 1), and generates a pseudo bicyclic ring system (Fig. 1). The coumarin ring system is planar [r.m.s. deviation = 0.006 Å] and is oriented at an acute angle of 60.14 (13)° with respect to the C11–C16 benzene ring, while the angles between the pseudo five-membered ring [r.m.s. deviation = 0.007 Å] and the coumarin ring system and C11–C16 benzene ring are 60.91 (12) and 1.06 (15)°, respectively. These dihedral angles show that the five-membered hydrogen-bonded ring and the C11–C16 benzene ring are almost coplanar. Also, an inspection of the bond lengths shows that there is a slight asymmetry of the electron distribution around the pyrone ring: the C2–C3 [1.336 (5) Å] and C1–C2 [1.446 (5) Å] bond lengths are shorter and longer, respectively, than those expected for a C<sub>ar</sub>–C<sub>ar</sub> bond. This feature suggests that the π electron density is preferentially located on the C2–C3 bond of the pyrone ring, as seen in other coumarin derivatives (e.g. Gomes *et al.*, 2016; Ziki *et al.*, 2016).

In the crystal, no intermolecular hydrogen bonds are observed. The unique close intermolecular contacts present are O2···H17A and C4···C1, with distances shorter than the sum of the van der Waals radii [O2···H17A(*x*, −*y*, ½ + *z*) = 2.65



**Figure 2**  
A view of the crystal packing, showing C···C contacts, C1=O2···π and π–π stacking interactions (dashed lines). The green dots are ring centroids.

**Table 1**  
Hydrogen-bond geometry (Å, °).

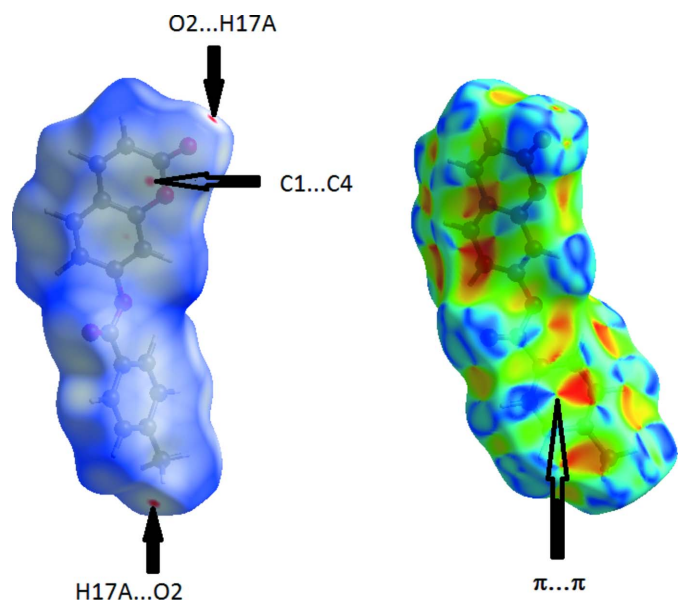
Cg1 and Cg4 are the centroids of the O1/C1–C5 and O1/C1–C4/C7–C9 rings, respectively.

D–H···A	D–H	H···A	D···A	D–H···A
C16–H16···O3	0.93	2.38	2.708 (4)	100
C1–O2···Cg1 <sup>1</sup>	1.21 (1)	3.29 (1)	3.431 (4)	86 (1)
C1–O2···Cg4 <sup>4</sup>	1.21 (1)	3.61 (1)	3.412 (4)	71 (1)

Symmetry code: (i) *x*, *y* + 1, *z*.

and C4···C1 (*x*, *y* − 1, *z*) = 3.364 (5) Å], and unusual C1=O2···π interactions [O2···Cg1 (*x*, 1 + *y*, *z*) = 3.294 (3), O2···Cg4(*x*, 1 + *y*, *z*) = 3.613 (3) Å, where Cg1 and Cg4 are respectively the centroids of the pyrone ring and the coumarin ring system]. The resulting supramolecular aggregation is completed by the presence of π–π stacking between the coumarin and the pyrone and the benzene C11–C16 rings. The centroid–centroid distances of those rings, Cg1···Cg2(*x*, 1 + *y*, *z*) = 3.6286 (18), Cg1···Cg4 (*x*, 1 + *y*, *z*) = 3.6459 (16) and Cg2···Cg4 (*x*, −1 + *y*, *z*) = 3.6407 (16), where Cg2 is the centroid of the C4–C9 benzene ring, are less than 3.8 Å, the threshold (Janiak, 2000) considered to be suitable for an effective π–π interaction (Fig. 2). The perpendicular distances of Cg(*I*) on ring *J* and distances between Cg(*I*) and perpendicular projection of Cg(*J*) on ring *I* (slippage) are summarized in Table 2.

To confirm and quantify the supramolecular interactions, molecular Hirshfeld surfaces of the title compound were calculated using a standard (high) surface resolution with the three-dimensional *d*<sub>norm</sub> surfaces mapped over a fixed colour scale of −0.043 (red) to 1.281 a.u. (blue), with the program



**Figure 3**  
Hirshfeld surfaces mapped over *d*<sub>norm</sub> (−0.043 to 1.281 a.u.) (left) and shape-index (right).

Table 2

Analysis of short ring interactions (Å).

$Cg(I)$  and  $Cg(J)$  are centroids of rings;  $CgI\_Perp$  is the perpendicular distance of  $Cg(I)$  on ring  $J$  and slippage is the distance between  $Cg(I)$  and the perpendicular projection of  $Cg(J)$  on ring  $I$ .

$Cg(I)$	$Cg(J)$	Symmetry $Cg(J)$	$Cg(I) \cdots Cg(J)$	$CgI\_Perp$	$CgJ\_Perp$	Slippage
$Cg1$	$Cg2$	$x, y + 1, z$	3.6285 (18)	−3.3321 (13)	3.3284 (12)	1.445
$Cg1$	$Cg4$	$x, y + 1, z$	3.6457 (16)	−3.3306 (13)	3.3242 (10)	1.497
$Cg2$	$Cg4$	$x, y - 1, z$	3.6408 (16)	3.3298 (12)	−3.3354 (10)	1.460

CrystalExplorer3.1 (Wolff *et al.*, 2012). The analysis of intermolecular interactions through the mapping of three-dimensional  $d_{norm}$  involves the contact distances  $d_i$  and  $d_e$  from the Hirshfeld surface to the nearest atom inside and outside, respectively. In the studied coumarin, the surface mapped over  $d_{norm}$  highlights three red spots, reflecting distances shorter than the sum of the van der Waals radii. These dominant interactions correspond to intermolecular  $O2 \cdots H17A$ ,  $C4 \cdots C1$  contacts,  $O \cdots \pi$  and  $\pi-\pi$  stacking interactions between the surface and the neighbouring environment. The mapping also shows white spots, with distances equal to the sum of the van der Waals radii, and blue regions, with distances longer than the sum of the van der Waals radii. Transparent surfaces are displayed in order to visualize the molecule (Fig. 3a). In the shape-index map (−1.00 to 1.00 a.u., Fig. 3b), the adjacent red and blue triangle-like patches show concave regions that indicate  $\pi-\pi$  stacking interactions (Bitzer *et al.*, 2017). Furthermore, the two-dimensional fingerprint plots (FP) are decomposed to highlight particular close contacts of atom pairs, and the contributions from different contacts are provided in Fig. 4. The red spots in the middle of the surface appearing near  $d_e = d_i \simeq 1.8-2.0$  Å correspond to close  $C \cdots C$  interplanar contacts. These contacts, which comprise 9.0% of the total Hirshfeld surface area, are related to  $\pi-\pi$  interactions (Fig. 4a) as predicted by the X-ray study. The most significant contribution to the Hirshfeld surface (40.4%) is from  $H \cdots H$  contacts, which appear in the central region of the FP with a central blue spike at  $d_e = d_i = 1.10$  Å (Fig. 4b).  $H \cdots O/O \cdots H$  interactions with a 26.1% contribution

appear on the left side as blue spikes with the tip at  $d_e + d_i \simeq 2.5$  Å, top and bottom (Fig. 4c), showing the presence of  $O \cdots H$  contacts, whereas the  $C \cdots H/H \cdots C$  plot (16.7%) reveals the information on intermolecular contacts (Fig. 4d). Other visible spots in the Hirshfeld surfaces showing  $C \cdots O/O \cdots C$  and  $O \cdots O$  contacts make contributions for only 6.5 and 1.3%, respectively (Fig. 4e and 4f).

### Synthesis and crystallization

To a solution of *p*-toluoyl chloride (6.17 mmol, 0.85 ml) in dried tetrahydrofuran (40 ml) was added dried trimethylamine (3 molar equivalents, 2.6 ml) and 7-hydroxycoumarin (6.17 mmol, 1 g) by small portions over 30 min. The mixture was then refluxed for 4 h and poured into 40 ml of chloroform.

Table 3

Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{12}O_4$
$M_r$	280.27
Crystal system, space group	Monoclinic, $Pc$
Temperature (K)	298
$a, b, c$ (Å)	5.7029 (2), 4.0346 (1), 28.9081 (10)
$\beta$ (°)	90.751 (3)
$V$ (Å <sup>3</sup> )	665.09 (4)
$Z$	2
Radiation type	Cu $K\alpha$
$\mu$ (mm <sup>−1</sup> )	0.83
Crystal size (mm)	0.25 × 0.16 × 0.09
Data collection	
Diffractometer	Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, Atlas S2
Absorption correction	Multi-scan (CrysAlis PRO; Rigaku OD, 2015)
$T_{min}, T_{max}$	0.858, 1.000
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	4661, 1780, 1713
$R_{int}$	0.018
$(\sin \theta/\lambda)_{max}$ (Å <sup>−1</sup> )	0.604
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.030, 0.079, 1.12
No. of reflections	1780
No. of parameters	191
No. of restraints	2
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å <sup>−3</sup> )	0.10, −0.10
Absolute structure	Flack $x$ determined using 559 quotients $[(I^-) - (I^+)] / [(I^-) + (I^+)]$ (Parsons <i>et al.</i> , 2013)
Absolute structure parameter	−0.02 (10)

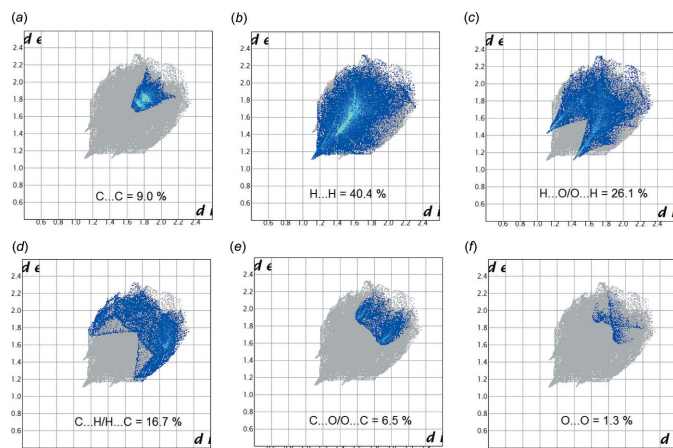


Figure 4

Decomposed two-dimensional fingerprint plots for the title compound. Various close contacts and their relative contributions are indicated.

Computer programs: CrysAlis PRO (Rigaku OD, 2015), SIR2014 (Burla *et al.*, 2015), SHELXL2014 (Sheldrick, 2015), PLATON (Spek, 2009), Mercury (Macrae *et al.*, 2008), WinGX (Farrugia, 2012) and publCIF (Westrip, 2010).

The solution was acidified with diluted hydrochloric acid until the pH was 2–3. The organic layer was extracted, washed with water to neutrality, dried over MgSO<sub>4</sub> and the solvent removed. The resulting precipitate (crude product) was filtered off with suction, washed with petroleum ether and recrystallized from chloroform. Pale-yellow crystals of the title compound were obtained in a good yield: 88%, m.p. 435–436 K.

### Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3.

### Acknowledgements

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## full crystallographic data

*IUCrData* (2018). 3, x180927 [https://doi.org/10.1107/S2414314618009276]

2-Oxo-2*H*-chromen-7-yl 4-methylbenzoate

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2-Oxo-2*H*-chromen-7-yl 4-methylbenzoate*Crystal data*

$C_{17}H_{12}O_4$

$M_r = 280.27$

Monoclinic, *Pc*

$a = 5.7029$  (2) Å

$b = 4.0346$  (1) Å

$c = 28.9081$  (10) Å

$\beta = 90.751$  (3)°

$V = 665.09$  (4) Å<sup>3</sup>

$Z = 2$

$F(000) = 292$

$D_x = 1.399$  Mg m<sup>-3</sup>

Melting point: 435 K

Cu  $K\alpha$  radiation,  $\lambda = 1.54184$  Å

Cell parameters from 2863 reflections

$\theta = 4.6$ – $68.2$ °

$\mu = 0.83$  mm<sup>-1</sup>

$T = 298$  K

Prism, pale-yellow

$0.25 \times 0.16 \times 0.09$  mm

*Data collection*

Rigaku Oxford Diffraction SuperNova, Dual,

Cu at zero, Atlas S2

diffractometer

Radiation source: micro-focus sealed X-ray

tube, SuperNova (Cu) X-ray Source

Mirror monochromator

Detector resolution: 5.3048 pixels mm<sup>-1</sup>

$\omega$  scans

Absorption correction: multi-scan

(CrysAlis PRO; Rigaku OD, 2015)

$T_{\min} = 0.858$ ,  $T_{\max} = 1.000$

4661 measured reflections

1780 independent reflections

1713 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.018$

$\theta_{\max} = 68.5$ °,  $\theta_{\min} = 6.1$ °

$h = -6 \rightarrow 6$

$k = -4 \rightarrow 4$

$l = -34 \rightarrow 34$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.030$

$wR(F^2) = 0.079$

$S = 1.12$

1780 reflections

191 parameters

2 restraints

48 constraints

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

$w = 1/[\sigma^2(F_o^2) + (0.0313P)^2 + 0.1164P]$

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

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

$\Delta\rho_{\max} = 0.10$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.10$  e Å<sup>-3</sup>

Absolute structure: Flack  $x$  determined using

559 quotients  $[(I^-)-(I)]/[(I^+)+(I)]$  (Parsons *et al.*, 2013)

Absolute structure parameter:  $-0.02$  (10)

*Special details*

**Refinement.** H atoms were placed in calculated positions [C—H = 0.93 (aromatic) or 0.96 Å (methyl group)] and refined using a riding model approximation with  $U_{\text{iso}}(\text{H})$  constrained to 1.2 (aromatic) or 1.5 (methyl) times  $U_{\text{eq}}$  of the respective parent atom.

*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	0.5429 (3)	0.0843 (6)	0.49733 (7)	0.0518 (5)
O2	0.4691 (5)	0.3534 (7)	0.56175 (10)	0.0743 (7)
O3	0.6523 (4)	−0.4691 (6)	0.35649 (8)	0.0610 (6)
O4	0.9336 (4)	−0.2152 (7)	0.31623 (9)	0.0716 (7)
C1	0.6049 (6)	0.1755 (9)	0.54165 (12)	0.0565 (8)
C2	0.8274 (6)	0.0560 (9)	0.55949 (12)	0.0590 (8)
H2	0.8734	0.1118	0.5895	0.071*
C3	0.9685 (5)	−0.1326 (8)	0.53400 (11)	0.0543 (8)
H3	1.1104	−0.2068	0.5464	0.065*
C4	0.9024 (5)	−0.2212 (7)	0.48762 (11)	0.0454 (6)
C5	0.6875 (5)	−0.1073 (7)	0.47053 (10)	0.0451 (7)
C6	0.6086 (5)	−0.1821 (7)	0.42646 (11)	0.0467 (7)
H6	0.4639	−0.1057	0.4158	0.056*
C7	0.7490 (5)	−0.3724 (8)	0.39873 (10)	0.0503 (7)
C8	0.9663 (5)	−0.4892 (8)	0.41398 (11)	0.0541 (8)
H8	1.0600	−0.6153	0.3946	0.065*
C9	1.0394 (5)	−0.4145 (8)	0.45818 (12)	0.0526 (8)
H9	1.1833	−0.4940	0.4688	0.063*
C10	0.7591 (5)	−0.3791 (8)	0.31640 (11)	0.0493 (7)
C11	0.6263 (5)	−0.5016 (7)	0.27583 (11)	0.0464 (6)
C12	0.7106 (6)	−0.4371 (8)	0.23191 (11)	0.0565 (8)
H12	0.8512	−0.3235	0.2286	0.068*
C13	0.5873 (6)	−0.5405 (9)	0.19322 (11)	0.0595 (9)
H13	0.6466	−0.4965	0.1640	0.071*
C14	0.3763 (6)	−0.7088 (8)	0.19696 (11)	0.0545 (8)
C15	0.2946 (6)	−0.7738 (8)	0.24099 (12)	0.0570 (8)
H15	0.1542	−0.8880	0.2443	0.068*
C16	0.4162 (5)	−0.6737 (8)	0.27977 (11)	0.0522 (7)
H16	0.3578	−0.7212	0.3089	0.063*
C17	0.2387 (8)	−0.8184 (10)	0.15511 (14)	0.0719 (10)
H17A	0.2586	−0.6605	0.1306	0.108*
H17B	0.0756	−0.8333	0.1627	0.108*
H17C	0.2939	−1.0315	0.1453	0.108*

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0435 (11)	0.0589 (13)	0.0530 (13)	0.0018 (9)	−0.0057 (10)	0.0054 (10)
O2	0.0723 (16)	0.0801 (18)	0.0708 (16)	0.0088 (14)	0.0031 (13)	−0.0090 (14)
O3	0.0560 (13)	0.0790 (16)	0.0480 (12)	−0.0217 (11)	−0.0004 (10)	0.0008 (11)

O4	0.0611 (14)	0.0904 (19)	0.0631 (14)	-0.0315 (13)	-0.0038 (12)	0.0086 (13)
C1	0.0577 (19)	0.0562 (18)	0.0555 (18)	-0.0068 (16)	-0.0008 (16)	0.0037 (15)
C2	0.061 (2)	0.066 (2)	0.0491 (17)	-0.0048 (16)	-0.0131 (16)	0.0047 (15)
C3	0.0461 (17)	0.0604 (18)	0.0561 (18)	-0.0053 (14)	-0.0127 (14)	0.0142 (16)
C4	0.0378 (14)	0.0474 (15)	0.0507 (16)	-0.0084 (11)	-0.0060 (12)	0.0135 (12)
C5	0.0406 (15)	0.0448 (15)	0.0496 (16)	-0.0067 (11)	-0.0019 (13)	0.0100 (13)
C6	0.0375 (14)	0.0535 (16)	0.0490 (15)	-0.0086 (12)	-0.0064 (12)	0.0114 (13)
C7	0.0486 (17)	0.0569 (17)	0.0454 (16)	-0.0170 (13)	-0.0025 (14)	0.0068 (13)
C8	0.0478 (17)	0.0570 (18)	0.0577 (19)	-0.0041 (13)	0.0045 (15)	0.0049 (14)
C9	0.0404 (16)	0.0528 (18)	0.0646 (19)	-0.0014 (12)	-0.0020 (15)	0.0131 (14)
C10	0.0484 (17)	0.0478 (15)	0.0517 (17)	0.0017 (13)	0.0008 (13)	0.0055 (13)
C11	0.0446 (15)	0.0454 (15)	0.0493 (16)	0.0034 (12)	0.0006 (13)	0.0014 (12)
C12	0.0550 (18)	0.0554 (18)	0.0591 (19)	-0.0072 (13)	0.0055 (16)	0.0060 (15)
C13	0.064 (2)	0.069 (2)	0.0448 (17)	0.0011 (16)	0.0041 (16)	0.0050 (15)
C14	0.0597 (18)	0.0492 (17)	0.0544 (18)	0.0052 (14)	-0.0066 (15)	-0.0024 (14)
C15	0.0531 (17)	0.0596 (19)	0.0584 (19)	-0.0084 (14)	-0.0007 (15)	-0.0006 (15)
C16	0.0517 (17)	0.0563 (18)	0.0488 (16)	-0.0045 (14)	0.0034 (14)	0.0016 (14)
C17	0.084 (3)	0.072 (2)	0.059 (2)	-0.0031 (19)	-0.0116 (19)	-0.0060 (18)

*Geometric parameters (Å, °)*

O1—C1	1.375 (4)	C9—C8	1.372 (5)
O1—C5	1.377 (3)	C9—H9	0.9300
O2—C1	1.210 (4)	C11—C10	1.473 (5)
O3—C7	1.389 (4)	C11—C12	1.388 (4)
O3—C10	1.366 (4)	C11—C16	1.391 (4)
O4—C10	1.195 (4)	C12—H12	0.9300
C2—C1	1.446 (5)	C13—C12	1.378 (5)
C2—C3	1.336 (5)	C13—H13	0.9300
C2—H2	0.9300	C14—C13	1.387 (5)
C3—H3	0.9300	C14—C17	1.500 (5)
C4—C3	1.434 (4)	C15—C14	1.386 (4)
C4—C9	1.400 (4)	C15—H15	0.9300
C5—C4	1.393 (4)	C16—C15	1.371 (5)
C6—C5	1.379 (4)	C16—H16	0.9300
C6—C7	1.375 (4)	C17—H17A	0.9600
C6—H6	0.9300	C17—H17B	0.9600
C7—C8	1.392 (5)	C17—H17C	0.9600
C8—H8	0.9300		
C1—O1—C5	121.7 (2)	C4—C9—H9	119.2
C10—O3—C7	119.7 (2)	O4—C10—O3	122.1 (3)
O2—C1—O1	116.6 (3)	O4—C10—C11	127.0 (3)
O2—C1—C2	126.2 (4)	O3—C10—C11	110.9 (2)
O1—C1—C2	117.2 (3)	C12—C11—C16	118.5 (3)
C3—C2—C1	121.7 (3)	C12—C11—C10	119.0 (3)
C3—C2—H2	119.2	C16—C11—C10	122.5 (3)
C1—C2—H2	119.2	C13—C12—C11	120.4 (3)

C2—C3—C4	120.3 (3)	C13—C12—H12	119.8
C2—C3—H3	119.8	C11—C12—H12	119.8
C4—C3—H3	119.8	C12—C13—C14	121.3 (3)
C5—C4—C9	117.6 (3)	C12—C13—H13	119.4
C5—C4—C3	118.0 (3)	C14—C13—H13	119.4
C9—C4—C3	124.4 (3)	C15—C14—C13	117.8 (3)
O1—C5—C6	116.9 (3)	C15—C14—C17	120.4 (3)
O1—C5—C4	121.1 (3)	C13—C14—C17	121.8 (3)
C6—C5—C4	122.0 (3)	C16—C15—C14	121.5 (3)
C7—C6—C5	118.4 (3)	C16—C15—H15	119.2
C7—C6—H6	120.8	C14—C15—H15	119.2
C5—C6—H6	120.8	C15—C16—C11	120.5 (3)
C6—C7—O3	116.2 (3)	C15—C16—H16	119.8
C6—C7—C8	121.8 (3)	C11—C16—H16	119.8
O3—C7—C8	121.7 (3)	C14—C17—H17A	109.5
C9—C8—C7	118.6 (3)	C14—C17—H17B	109.5
C9—C8—H8	120.7	H17A—C17—H17B	109.5
C7—C8—H8	120.7	C14—C17—H17C	109.5
C8—C9—C4	121.6 (3)	H17A—C17—H17C	109.5
C8—C9—H9	119.2	H17B—C17—H17C	109.5
C5—C6—C7—O3	173.7 (2)	C7—O3—C10—C11	-179.0 (3)
C5—C6—C7—C8	-0.1 (4)	C12—C11—C10—O4	2.7 (5)
C10—O3—C7—C6	120.7 (3)	C16—C11—C10—O4	-175.8 (3)
C10—O3—C7—C8	-65.6 (4)	C12—C11—C10—O3	-179.2 (3)
C1—O1—C5—C6	-179.5 (3)	C16—C11—C10—O3	2.3 (4)
C1—O1—C5—C4	0.9 (4)	C11—C16—C15—C14	0.2 (5)
C7—C6—C5—O1	179.8 (2)	C4—C9—C8—C7	-0.9 (4)
C7—C6—C5—C4	-0.6 (4)	C6—C7—C8—C9	0.8 (4)
O1—C5—C4—C9	-179.9 (2)	O3—C7—C8—C9	-172.6 (3)
C6—C5—C4—C9	0.6 (4)	C16—C15—C14—C13	0.5 (5)
O1—C5—C4—C3	0.0 (4)	C16—C15—C14—C17	-179.4 (3)
C6—C5—C4—C3	-179.5 (3)	C15—C14—C13—C12	-0.8 (5)
C5—C4—C9—C8	0.2 (4)	C17—C14—C13—C12	179.1 (3)
C3—C4—C9—C8	-179.7 (3)	C5—O1—C1—O2	177.6 (3)
C12—C11—C16—C15	-0.7 (5)	C5—O1—C1—C2	-1.2 (4)
C10—C11—C16—C15	177.9 (3)	C3—C2—C1—O2	-178.0 (3)
C1—C2—C3—C4	0.3 (5)	C3—C2—C1—O1	0.6 (5)
C5—C4—C3—C2	-0.6 (4)	C14—C13—C12—C11	0.4 (5)
C9—C4—C3—C2	179.3 (3)	C16—C11—C12—C13	0.4 (5)
C7—O3—C10—O4	-0.8 (5)	C10—C11—C12—C13	-178.2 (3)

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

Cg1 and Cg4 are the centroids of the O1/C1—C5 and O1/C1—C4/C7—C9 rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C16—H16 $\cdots$ O3	0.93	2.38	2.708 (4)	100



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C1—O2...Cg1 <sup>i</sup>	1.21 (1)	3.29 (1)	3.431 (4)	86 (1)
C1—O2...Cg4 <sup>i</sup>	1.21 (1)	3.61 (1)	3.412 (4)	71 (1)

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Symmetry code: (i)  $x, y+1, z$ .