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# 3-Benzoyl-4-methyl-2-oxo-2*H*-chromen-7-yl acetate

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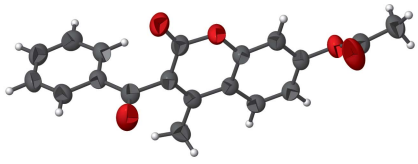
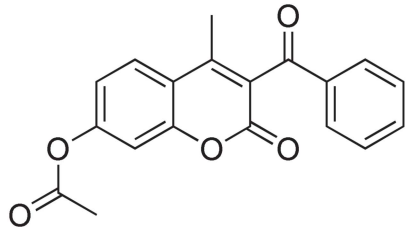
**Structural data**: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{19}H_{14}O_5$, the dihedral angle between the coumarin ring system (r.m.s. deviation = 0.026 Å) and the pendant benzoyl group is 81.91 (7)°. In the crystal, weak C—H···O interactions link the molecules into a three-dimensional network.

**3D view**



**Chemical scheme**



## Structure description

The coumarin nucleus occurs in many natural products (Yu *et al.*, 2003) and it is also widely used in materials chemistry (Swanson *et al.*, 2003). As part of our studies of 3-aroyl coumarins, we report here the synthesis and crystal structure of the title compound (Fig. 1).

The C7—O1, C8—O2 and C18—O5 bond lengths are 1.216 (2), 1.208 (2) and 1.186 (2) Å, respectively. They are shorter than the standard C=O bond length [1.231 (2) Å; Gao *et al.*, 2014]. The C14—O4 [1.393 (2) Å], C18—O4 [1.367 (2) Å], C12—O3 [1.378 (2) Å] and C8—O3 [1.370 (2) Å] bond lengths are obviously longer than the C=O bond length, indicating that they are single bonds. As expected, the coumarin ring is nearly planar (r.m.s. deviation = 0.026 Å) and subtends dihedral angles of 81.91 (7) and 65.35 (9)° with the benzoyl and acetate substituents, respectively.

In the crystal, weak C—H···O interactions (Table 1, Fig. 2) link the molecules into a three-dimensional network. Weak aromatic $\pi$–$\pi$ stacking between inversion-related pairs of C11–C16 rings is also observed [centroid–centroid separation = 3.7482 (10), slippage = 0.98 Å].

## Synthesis and crystallization

A 25 ml Schlenk tube equipped with a magnetic stirring bar was charged with $AgNO_3$ (0.25 mmol, 42.5 mg), potassium persulfate (1.0 mmol, 270 mg), 4-methyl-2-oxo-2*H*-

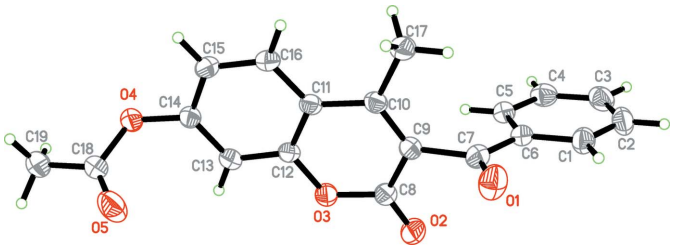



**Figure 1**
The molecular structure showing 50% probability displacement ellipsoids

chromen-7-yl acetate (0.25 mmol, 54.5 mg), 2-oxo-2-phenylacetic acid (0.5 mmol, 75 mg), and 2 ml of $CH_3CN/H_2O$ ($v_1/v_2$ = 1:1) was then added. The reaction mixture was heated in an oil bath at 90°C for 10 h (monitored by TLC). After completion of the reaction, the resulting solution was cooled to room temperature, and the solvent was removed with the aid of a rotary evaporator. The residue was purified by column chromatography on silica gel using ethylacetate/petroleum ether (1:4) as eluant to provide the desired product. Yellow blocks of (I) were recrystallized from trichloromethane solution, m.p. 114–115°C. $^1$H NMR ($CDCl_3$) $\delta$: 7.91 (*dd*, $J_{H-H}$ = 8.0 Hz, $J_{H-H}$ = 0.8 Hz, 2H), 7.71 (*d*, $J_{H-H}$ = 8.7 Hz, 1H), 7.61 (*td*, $J_{H-H}$ = 7.4 Hz, $J_{H-H}$ = 1.2 Hz, 1H), 7.47 (*t*, $J_{H-H}$ = 8.0 Hz, 2H), 7.18 (*d*, $J_{H-H}$ = 2.2 Hz, 1H), 7.14 (*dd*, $J_{H-H}$ = 8.7 Hz, $J_{H-H}$ = 2.2 Hz, 1H), 2.35 (*s*, 3H), 2.33 (*s*, 3H). $^{13}$C NMR ($CDCl_3$) $\delta$: 192.9 (C═O), 168.6, 158.4 (C═O), 153.7, 153.6, 149.7, 136.0, 134.3 (CH), 129.3 (CH), 129.0 (CH), 126.2 (CH), 125.3, 118.7 (CH), 117.4, 110.5 (CH), 21.1 ($CH_3$), 16.0 ($CH_3$). IR (KBr) $\nu$ ($cm^{-1}$): 3066, 2925, 1768, 1720, 1670, 1614, 1450, 1186. HR MS (ESI) *m*/*z* 323.0916 $[M + H]^+$ (calculated for $C_{19}H_{15}O_5^+$ 323.0914).

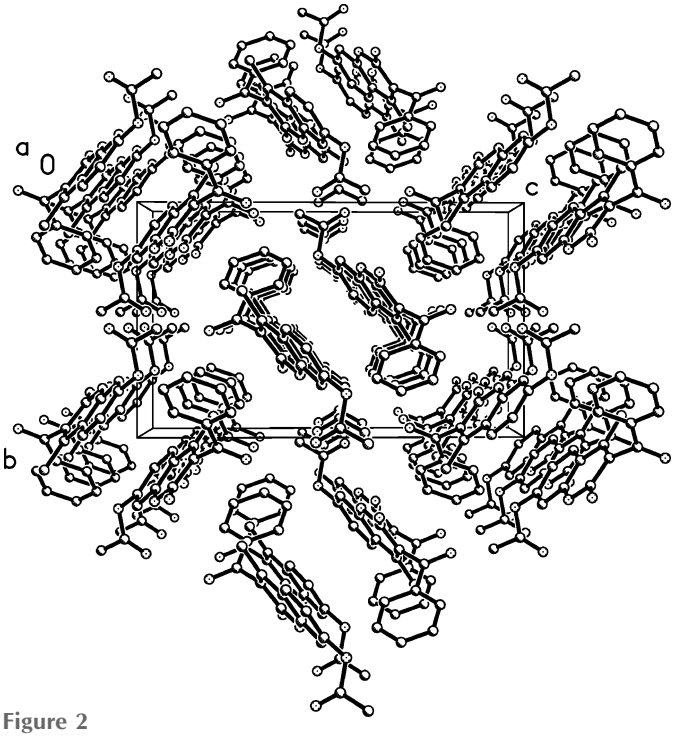



**Figure 2**
The crystal packing viewed down [100].

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C2—H2···O2$^{i}$ | 0.93 | 2.57 | 3.475 (3) | 164 |
| C4—H4···O3$^{ii}$ | 0.93 | 2.56 | 3.361 (3) | 144 |
| C19—H19*C*···O3$^{iii}$ | 0.96 | 2.47 | 3.409 (2) | 165 |

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

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{19}H_{14}O_5$ |
| $M_r$ | 322.30 |
| Crystal system, space group | Monoclinic, $P2_1/n$ |
| Temperature (K) | 291 |
| *a*, *b*, *c* (Å) | 9.1617 (2), 10.2307 (3), 16.8581 (5) |
| $\beta$ (°) | 92.812 (3) |
| $V$ (Å$^3$) | 1578.20 (7) |
| $Z$ | 4 |
| Radiation type | Cu $K\alpha$ |
| $\mu$ ($mm^{-1}$) | 0.82 |
| Crystal size (mm) | 0.25 × 0.2 × 0.18 |
| | |
| Data collection | |
| Diffractometer | Agilent Xcalibur, Eos, Gemini |
| Absorption correction | Multi-scan (*CrysAlis PRO*; Agilent, 2013) |
| $T_{min}$, $T_{max}$ | 0.544, 1.000 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 5738, 2817, 2327 |
| $R_{int}$ | 0.037 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.597 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.048, 0.138, 1.04 |
| No. of reflections | 2817 |
| No. of parameters | 220 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.26, −0.18 |

Computer programs: *CrysAlis PRO* (Agilent, 2013), *SHELXS* (Sheldrick, 2008), SHELXL (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

## Refinement

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


## Funding information

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# full crystallographic data

*IUCrData* (2018). **3**, x180015 [https://doi.org/10.1107/S2414314618000159]

## 3-Benzoyl-4-methyl-2-oxo-2*H*-chromen-7-yl acetate

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*Crystal data*

$C_{19}H_{14}O_5$
$M_r$ = 322.30
Monoclinic, $P2_1/n$
$a$ = 9.1617 (2) Å
$b$ = 10.2307 (3) Å
$c$ = 16.8581 (5) Å
$\beta$ = 92.812 (3)°
$V$ = 1578.20 (7) Å$^3$
$Z$ = 4
$F(000)$ = 672
$D_x$ = 1.356 Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda$ = 1.54184 Å
Cell parameters from 2227 reflections
$\theta$ = 5.4–72.2°
$\mu$ = 0.82 mm$^{-1}$
$T$ = 291 K
Block, yellow
0.25 × 0.2 × 0.18 mm

*Data collection*

Agilent Xcalibur, Eos, Gemini diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 16.2312 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (CrysAlisPro; Agilent, 2013)
$T_{min}$ = 0.544, $T_{max}$ = 1.000
5738 measured reflections
2817 independent reflections
2327 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.037
$\theta_{max}$ = 67.0°, $\theta_{min}$ = 5.1°
$h$ = −10→7
$k$ = −12→12
$l$ = −20→20

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.138
$S$ = 1.04
2817 reflections
220 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0713P)^2 + 0.2573P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.26 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 e Å$^{-3}$
Extinction correction: SHELXL-2014/7 (Sheldrick 2014, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0398 (18)

*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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.42067 (18) | 0.45664 (18) | 0.79826 (9) | 0.0787 (5) |
| O2 | 0.47734 (14) | 0.30569 (16) | 0.61932 (10) | 0.0695 (5) |
| O3 | 0.24925 (13) | 0.28252 (13) | 0.57529 (8) | 0.0549 (4) |
| O4 | −0.23097 (14) | 0.21970 (13) | 0.46535 (8) | 0.0549 (4) |
| O5 | −0.2083 (2) | 0.03492 (17) | 0.53544 (11) | 0.0900 (6) |
| C1 | 0.6308 (2) | 0.6465 (2) | 0.76609 (12) | 0.0563 (5) |
| H1 | 0.6289 | 0.6163 | 0.8181 | 0.068* |
| C2 | 0.7325 (2) | 0.7391 (2) | 0.74621 (14) | 0.0655 (6) |
| H2 | 0.7983 | 0.7717 | 0.7851 | 0.079* |
| C3 | 0.7372 (2) | 0.7834 (2) | 0.66899 (14) | 0.0650 (6) |
| H3 | 0.8058 | 0.8458 | 0.6560 | 0.078* |
| C4 | 0.6407 (2) | 0.7353 (2) | 0.61166 (13) | 0.0605 (5) |
| H4 | 0.6446 | 0.7646 | 0.5596 | 0.073* |
| C5 | 0.5374 (2) | 0.64341 (18) | 0.63057 (11) | 0.0501 (5) |
| H5 | 0.4720 | 0.6115 | 0.5913 | 0.060* |
| C6 | 0.53109 (19) | 0.59858 (17) | 0.70822 (10) | 0.0452 (4) |
| C7 | 0.4219 (2) | 0.50110 (19) | 0.73141 (11) | 0.0505 (5) |
| C8 | 0.35343 (19) | 0.34511 (19) | 0.62240 (11) | 0.0502 (5) |
| C9 | 0.30657 (19) | 0.45207 (17) | 0.67102 (10) | 0.0459 (4) |
| C10 | 0.16730 (19) | 0.49705 (16) | 0.66636 (10) | 0.0446 (4) |
| C11 | 0.06022 (18) | 0.42967 (16) | 0.61466 (10) | 0.0418 (4) |
| C12 | 0.10533 (18) | 0.32206 (16) | 0.57183 (10) | 0.0435 (4) |
| C13 | 0.0120 (2) | 0.24892 (18) | 0.52289 (11) | 0.0482 (4) |
| H13 | 0.0457 | 0.1777 | 0.4948 | 0.058* |
| C14 | −0.13290 (19) | 0.28508 (17) | 0.51713 (11) | 0.0454 (4) |
| C15 | −0.18368 (19) | 0.39151 (18) | 0.55818 (11) | 0.0492 (5) |
| H15 | −0.2819 | 0.4145 | 0.5534 | 0.059* |
| C16 | −0.08818 (19) | 0.46300 (18) | 0.60608 (11) | 0.0481 (5) |
| H16 | −0.1225 | 0.5349 | 0.6333 | 0.058* |
| C17 | 0.1211 (2) | 0.6136 (2) | 0.71267 (12) | 0.0598 (5) |
| H17A | 0.0810 | 0.6787 | 0.6768 | 0.090* |
| H17B | 0.2042 | 0.6490 | 0.7422 | 0.090* |
| H17C | 0.0485 | 0.5878 | 0.7487 | 0.090* |
| C18 | −0.2599 (2) | 0.09088 (19) | 0.47921 (12) | 0.0528 (5) |
| C19 | −0.3583 (3) | 0.0359 (2) | 0.41586 (14) | 0.0674 (6) |
| H19A | −0.3360 | 0.0740 | 0.3658 | 0.101* |
| H19B | −0.4578 | 0.0551 | 0.4270 | 0.101* |
| H19C | −0.3451 | −0.0571 | 0.4136 | 0.101* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0800 (11) | 0.0931 (13) | 0.0617 (9) | −0.0215 (9) | −0.0092 (7) | 0.0224 (8) |
| O2 | 0.0404 (8) | 0.0679 (10) | 0.0998 (11) | 0.0070 (7) | −0.0007 (7) | −0.0154 (8) |
| O3 | 0.0417 (7) | 0.0473 (8) | 0.0755 (9) | 0.0053 (5) | 0.0001 (6) | −0.0161 (6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O4 | 0.0555 (8) | 0.0433 (7) | 0.0641 (8) | −0.0033 (6) | −0.0143 (6) | 0.0026 (6) |
| O5 | 0.1241 (16) | 0.0584 (10) | 0.0840 (11) | −0.0260 (10) | −0.0321 (10) | 0.0174 (9) |
| C1 | 0.0539 (11) | 0.0613 (13) | 0.0530 (10) | 0.0007 (9) | −0.0040 (8) | −0.0083 (9) |
| C2 | 0.0516 (11) | 0.0637 (14) | 0.0804 (14) | −0.0075 (10) | −0.0044 (10) | −0.0229 (11) |
| C3 | 0.0547 (12) | 0.0505 (12) | 0.0905 (16) | −0.0055 (9) | 0.0108 (10) | −0.0049 (11) |
| C4 | 0.0622 (12) | 0.0525 (12) | 0.0673 (12) | 0.0034 (9) | 0.0084 (9) | 0.0093 (10) |
| C5 | 0.0509 (10) | 0.0444 (10) | 0.0541 (10) | 0.0033 (8) | −0.0057 (8) | −0.0002 (8) |
| C6 | 0.0441 (9) | 0.0403 (9) | 0.0506 (9) | 0.0041 (7) | −0.0030 (7) | −0.0021 (7) |
| C7 | 0.0500 (10) | 0.0494 (11) | 0.0515 (10) | 0.0017 (8) | −0.0034 (8) | 0.0040 (8) |
| C8 | 0.0418 (10) | 0.0437 (10) | 0.0648 (11) | 0.0008 (8) | 0.0002 (8) | −0.0009 (8) |
| C9 | 0.0456 (9) | 0.0401 (9) | 0.0519 (10) | −0.0031 (7) | −0.0001 (7) | 0.0032 (7) |
| C10 | 0.0506 (10) | 0.0356 (9) | 0.0474 (9) | 0.0006 (7) | 0.0005 (7) | 0.0024 (7) |
| C11 | 0.0425 (9) | 0.0348 (9) | 0.0482 (9) | 0.0016 (7) | 0.0028 (7) | 0.0034 (7) |
| C12 | 0.0405 (9) | 0.0347 (9) | 0.0551 (9) | 0.0027 (7) | 0.0019 (7) | 0.0018 (7) |
| C13 | 0.0496 (10) | 0.0366 (9) | 0.0583 (10) | 0.0020 (7) | 0.0013 (8) | −0.0039 (8) |
| C14 | 0.0465 (9) | 0.0382 (9) | 0.0508 (9) | −0.0027 (7) | −0.0053 (7) | 0.0061 (7) |
| C15 | 0.0419 (9) | 0.0467 (10) | 0.0585 (10) | 0.0069 (8) | −0.0016 (7) | 0.0044 (8) |
| C16 | 0.0470 (10) | 0.0415 (10) | 0.0558 (10) | 0.0091 (8) | 0.0013 (8) | −0.0025 (8) |
| C17 | 0.0626 (12) | 0.0530 (12) | 0.0625 (12) | 0.0124 (9) | −0.0096 (9) | −0.0134 (9) |
| C18 | 0.0544 (11) | 0.0425 (10) | 0.0612 (11) | −0.0008 (8) | −0.0013 (8) | −0.0005 (9) |
| C19 | 0.0685 (14) | 0.0523 (12) | 0.0799 (14) | −0.0022 (10) | −0.0106 (11) | −0.0145 (11) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C7 | 1.216 (2) | C8—C9 | 1.445 (3) |
| O2—C8 | 1.208 (2) | C9—C10 | 1.355 (2) |
| O3—C8 | 1.370 (2) | C10—C11 | 1.454 (2) |
| O3—C12 | 1.378 (2) | C10—C17 | 1.497 (2) |
| O4—C14 | 1.393 (2) | C11—C12 | 1.390 (2) |
| O4—C18 | 1.367 (2) | C11—C16 | 1.402 (2) |
| O5—C18 | 1.186 (2) | C12—C13 | 1.379 (2) |
| C1—H1 | 0.9300 | C13—H13 | 0.9300 |
| C1—C2 | 1.381 (3) | C13—C14 | 1.377 (3) |
| C1—C6 | 1.392 (2) | C14—C15 | 1.383 (3) |
| C2—H2 | 0.9300 | C15—H15 | 0.9300 |
| C2—C3 | 1.381 (3) | C15—C16 | 1.372 (2) |
| C3—H3 | 0.9300 | C16—H16 | 0.9300 |
| C3—C4 | 1.369 (3) | C17—H17A | 0.9600 |
| C4—H4 | 0.9300 | C17—H17B | 0.9600 |
| C4—C5 | 1.382 (3) | C17—H17C | 0.9600 |
| C5—H5 | 0.9300 | C18—C19 | 1.475 (3) |
| C5—C6 | 1.391 (3) | C19—H19A | 0.9600 |
| C6—C7 | 1.479 (3) | C19—H19B | 0.9600 |
| C7—C9 | 1.516 (2) | C19—H19C | 0.9600 |
| | | | |
| C8—O3—C12 | 121.69 (14) | C12—C11—C16 | 116.77 (15) |
| C18—O4—C14 | 118.72 (14) | C16—C11—C10 | 124.67 (16) |
| C2—C1—H1 | 120.0 | O3—C12—C11 | 121.25 (15) |

| | | | |
|---|---|---|---|
| C2—C1—C6 | 119.91 (19) | O3—C12—C13 | 115.48 (15) |
| C6—C1—H1 | 120.0 | C13—C12—C11 | 123.27 (16) |
| C1—C2—H2 | 119.8 | C12—C13—H13 | 121.2 |
| C3—C2—C1 | 120.39 (19) | C14—C13—C12 | 117.64 (17) |
| C3—C2—H2 | 119.8 | C14—C13—H13 | 121.2 |
| C2—C3—H3 | 120.0 | C13—C14—O4 | 120.35 (17) |
| C4—C3—C2 | 119.9 (2) | C13—C14—C15 | 121.53 (16) |
| C4—C3—H3 | 120.0 | C15—C14—O4 | 117.99 (16) |
| C3—C4—H4 | 119.8 | C14—C15—H15 | 120.2 |
| C3—C4—C5 | 120.5 (2) | C16—C15—C14 | 119.59 (16) |
| C5—C4—H4 | 119.8 | C16—C15—H15 | 120.2 |
| C4—C5—H5 | 119.9 | C11—C16—H16 | 119.4 |
| C4—C5—C6 | 120.12 (18) | C15—C16—C11 | 121.20 (17) |
| C6—C5—H5 | 119.9 | C15—C16—H16 | 119.4 |
| C1—C6—C7 | 118.77 (17) | C10—C17—H17A | 109.5 |
| C5—C6—C1 | 119.16 (18) | C10—C17—H17B | 109.5 |
| C5—C6—C7 | 122.08 (16) | C10—C17—H17C | 109.5 |
| O1—C7—C6 | 122.32 (17) | H17A—C17—H17B | 109.5 |
| O1—C7—C9 | 117.43 (18) | H17A—C17—H17C | 109.5 |
| C6—C7—C9 | 120.25 (15) | H17B—C17—H17C | 109.5 |
| O2—C8—O3 | 116.64 (17) | O4—C18—C19 | 111.14 (17) |
| O2—C8—C9 | 125.67 (18) | O5—C18—O4 | 121.96 (18) |
| O3—C8—C9 | 117.69 (15) | O5—C18—C19 | 126.90 (19) |
| C8—C9—C7 | 114.50 (16) | C18—C19—H19A | 109.5 |
| C10—C9—C7 | 123.35 (17) | C18—C19—H19B | 109.5 |
| C10—C9—C8 | 121.97 (16) | C18—C19—H19C | 109.5 |
| C9—C10—C11 | 118.65 (16) | H19A—C19—H19B | 109.5 |
| C9—C10—C17 | 121.98 (16) | H19A—C19—H19C | 109.5 |
| C11—C10—C17 | 119.37 (15) | H19B—C19—H19C | 109.5 |
| C12—C11—C10 | 118.54 (15) | | |

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| O1—C7—C9—C8 | −94.8 (2) | C8—O3—C12—C13 | −179.03 (16) |
| O1—C7—C9—C10 | 80.4 (3) | C8—C9—C10—C11 | 4.1 (3) |
| O2—C8—C9—C7 | −10.1 (3) | C8—C9—C10—C17 | −175.79 (17) |
| O2—C8—C9—C10 | 174.6 (2) | C9—C10—C11—C12 | −0.3 (2) |
| O3—C8—C9—C7 | 170.11 (16) | C9—C10—C11—C16 | 177.90 (17) |
| O3—C8—C9—C10 | −5.1 (3) | C10—C11—C12—O3 | −2.7 (3) |
| O3—C12—C13—C14 | −179.65 (16) | C10—C11—C12—C13 | 178.08 (16) |
| O4—C14—C15—C16 | −176.12 (16) | C10—C11—C16—C15 | −177.57 (16) |
| C1—C2—C3—C4 | −0.1 (3) | C11—C12—C13—C14 | −0.3 (3) |
| C1—C6—C7—O1 | −3.7 (3) | C12—O3—C8—O2 | −177.65 (17) |
| C1—C6—C7—C9 | 176.75 (17) | C12—O3—C8—C9 | 2.2 (3) |
| C2—C1—C6—C5 | 1.1 (3) | C12—C11—C16—C15 | 0.6 (3) |
| C2—C1—C6—C7 | −179.06 (19) | C12—C13—C14—O4 | 176.41 (15) |
| C2—C3—C4—C5 | 0.6 (3) | C12—C13—C14—C15 | 0.6 (3) |
| C3—C4—C5—C6 | −0.3 (3) | C13—C14—C15—C16 | −0.2 (3) |
| C4—C5—C6—C1 | −0.6 (3) | C14—O4—C18—O5 | 2.9 (3) |
| C4—C5—C6—C7 | 179.57 (18) | C14—O4—C18—C19 | −176.37 (17) |

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| C5—C6—C7—O1 | 176.2 (2) | C14—C15—C16—C11 | −0.4 (3) |
| C5—C6—C7—C9 | −3.4 (3) | C16—C11—C12—O3 | 179.04 (16) |
| C6—C1—C2—C3 | −0.8 (3) | C16—C11—C12—C13 | −0.2 (3) |
| C6—C7—C9—C8 | 84.8 (2) | C17—C10—C11—C12 | 179.68 (17) |
| C6—C7—C9—C10 | −100.1 (2) | C17—C10—C11—C16 | −2.2 (3) |
| C7—C9—C10—C11 | −170.69 (15) | C18—O4—C14—C13 | 65.0 (2) |
| C7—C9—C10—C17 | 9.4 (3) | C18—O4—C14—C15 | −118.98 (19) |
| C8—O3—C12—C11 | 1.6 (3) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C2—H2···O2$^{i}$ | 0.93 | 2.57 | 3.475 (3) | 164 |
| C4—H4···O3$^{ii}$ | 0.93 | 2.56 | 3.361 (3) | 144 |
| C19—H19*C*···O3$^{iii}$ | 0.96 | 2.47 | 3.409 (2) | 165 |

Symmetry codes: (i) −*x*+3/2, *y*+1/2, −*z*+3/2; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) −*x*, −*y*, −*z*+1.