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Crystal structure of 4-methoxyphenyl 2-oxo-2H-chromene-3-carboxylate

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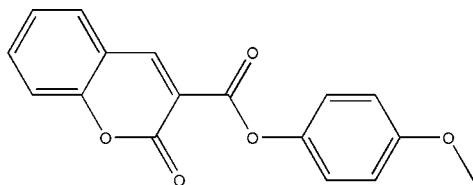
In the title compound, C₁₇H₁₂O₅, the dihedral angle between the planes of the coumarin ring system (r.m.s. deviation = 0.015 Å) and the benzene ring is 48.04 (10)°. The central CO₂ group subtends a dihedral angle of 27.15 (11)° with the coumarin ring system and 74.86 (13)° with the benzene ring. In the crystal, molecules are linked by C—H...O interactions, which generate a three-dimensional network. Very weak C—H...π interactions are also observed.

Keywords: crystal structure; 2-oxo-2H-chromene; C—H...π interactions; C—H...O interactions.

CCDC reference: 1058259

1. Related literature

For details of the biological activities of 2-oxo-2H-chromene derivatives, see: Kawase *et al.* (2001); Traven (2004); Lacy & O'Kennedy (2004); Chimenti *et al.* (2009). For related structures, see: Sreenivasa *et al.* (2013); Devarajegowda *et al.*, (2013).



2. Experimental

2.1. Crystal data

C₁₇H₁₂O₅M_r = 296.27Orthorhombic, P2₁2₁2₁
a = 6.2648 (18) Å
b = 10.435 (3) Å
c = 20.621 (7) Å
V = 1348.0 (7) Å³Z = 4
Mo Kα radiation
μ = 0.11 mm⁻¹
T = 296 K
0.22 × 0.20 × 0.18 mm

2.2. Data collection

Bruker APEXII CCD
diffractometer
Absorption correction: multi-scan
(SADABS; Bruker, 2013)
T_{min} = 0.977, T_{max} = 0.98110472 measured reflections
2385 independent reflections
2150 reflections with I > 2σ(I)
R_{int} = 0.050

2.3. Refinement

R[F² > 2σ(F²)] = 0.035
wR(F²) = 0.085
S = 1.09
1411 reflections201 parameters
H-atom parameters constrained
Δρ_{max} = 0.16 e Å⁻³
Δρ_{min} = -0.16 e Å⁻³**Table 1**

Hydrogen-bond geometry (Å, °).

Cg1 and Cg2 are the centroids of the C1/C6/C7/C8/C9/O1 and C1/C2/C3/C4/C5/C6 rings, respectively.

| D—H...A | D—H | H...A | D...A | D—H...A |
|------------------------------|------|-------|-----------|---------|
| C17—H17B...O5 ⁱ | 0.96 | 2.50 | 3.228 (3) | 132 |
| C12—H12...O2 ⁱⁱ | 0.93 | 2.48 | 3.353 (3) | 156 |
| C15—H15...O2 ⁱⁱⁱ | 0.93 | 2.50 | 3.207 (3) | 133 |
| C3—H3...O3 ^{iv} | 0.93 | 2.47 | 3.272 (4) | 145 |
| C5—H5...Cg1 ^v | 0.93 | 2.82 | 3.303 (3) | 114 |
| C17—H17C...Cg2 ^{vi} | 0.93 | 2.96 | 3.709 (4) | 136 |

Symmetry codes: (i) x - ½, -y + ½, -z + 1; (ii) x - 1, y, z; (iii) -x + 2, y + ½, -z + ½; (iv) -x + ½, -y + 1, z - ½; (v) -x, y + ½, -z + ½; (vi) x + ½, -y + ½, -z - 1.

Data collection: APEX2 (Bruker, 2013); cell refinement: SAINT (Bruker, 2013); data reduction: SAINT (Bruker, 2013); program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL2014 (Sheldrick, 2015); molecular graphics: Mercury (Macrae *et al.*, 2008); software used to prepare material for publication: SHELXL2014 (Sheldrick, 2015).

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7399).

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Acta Cryst. (2015). E71, o374–o375 [doi:10.1107/S2056989015006970]

Crystal structure of 4-methoxyphenyl 2-oxo-2H-chromene-3-carboxylate

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S1. Chemical context

The 2-oxo-2H-chromene is a useful starting material for the construction of heterocyclic compounds with a broad spectrum of biological activities. Especially the 3-substituted derivatives exhibits pharmacological effects such as analgesic, anti-arthritis, anti-inflammatory, anti-pyretic, anti-viral, anti-cancer and anticoagulant properties (Chimenti *et al.*, 2009; Traven *et al.*, 2004; Lacy *et al.*, 2004). Moreover, these derivatives are well known for their anti-microbial activity toward different microorganisms, they show anti-microbial activity with reference to anti-*H. pylori* activity. (Kawase *et al.*, 2001).

2-oxo-2H-chromenes (coumarins) have been also used in the field of medicine, cosmetics and fluorescent dyes. They are efficient fluorophores characterized by good emission quantum yields and are used as materials for lasers in organic light emitting devices, non-linear optical chromophores and fluorescent labels. Keeping these facts in mind and in continuation of our work on 2-oxo-2H-chromene derivatives (Sreenivasa *et al.*, 2013; Palakshamurthy, Sreenivasa *et al.*, 2013; Palakshamurthy, Devarajegowda *et al.*, 2013; Devarajegowda, *et al.*, 2013), herein we report the synthesis and crystal structure of 4-Methoxyphenyl 2-oxo-2H-chromene-3-carboxylate (I).

S2. Structural commentary

In the title molecule (I), C₁₇H₁₂O₅, the coumarin ring is almost planar, the rms deviation (considering non Hydrogen atom) being 0.012 (1) Å. The dihedral angle between the coumarin ring and the phenyl ring in (I) is 48.04 (10)°. Compared to this, the dihedral angle is 21.11 (1)° in 4-(octyloxy)phenyl 2-oxo-2H-chromene-3-carboxylate (II) (Palakshamurthy, Devarajegowda *et al.*, 2013), 62.97 (2)° in 4-(decyloxy)phenyl 7-(trifluoromethyl)-2-oxo-2H-chromene-3-carboxylate (III) (Palakshamurthy, Sreenivasa *et al.*, 2013b), 22.95 (11)° in 4'-Cyanobiphenyl-4-yl 7-diethylamino-2-oxo-2H-chromene-3-carboxylate (IV) (Sreenivasa *et al.*, 2013) and 54.46 (17)° in 4-[4-(Heptyloxy)benzoyloxy] phenyl 2-oxo-7-trifluoromethyl-2H-chromene-3-carboxylate (V) (Devarajegowda, *et al.*, 2013). Further, in (I), the dihedral angle between the central ester chain [C8—C10(O3)—O4] and the phenyl ring and the coumarin ring are 74.86 (10)° and 27.16 (8)° respectively. The methoxy group is slightly out of plane from the attached benzene ring, the C17—O5—C14—C13 torsion being 10.3 (3)°.

S3. Supramolecular features

In the crystal structure, the molecules are linked into zig-zag C9 chains along *c* axis via C3—H3···O3 intermolecular interactions. Further, C12—H12···O2 interactions between the molecules in the neighbouring chains leads to C8 chains along *a* axis, and thus forming sheets in the *ac* plane. These sheets are interconnected via an intermolecular C15—H15···O2 interactions which form helical C7 chains running along *b* axis, and hence a three dimensional architecture is displayed. An additional C17—H17B···O5 interactions between the molecules in the neighbouring C7 helical chains leading to the formation of C3 chains along *a* axis results in sheets along *ab* plane. Thus, a grid like three dimensional

structure is observed. Packing of the molecules displaying the columns formed along a axis is shown in Figure 2.

The packing also features $C5-H5\cdots Cg1$ and $C17-H17C\cdots Cg2$ interactions (where $Cg1$ and the $Cg2$ are the centroids of the rings $C1/C6/C7/C8/C9/O1$ and $C1/C2/C3/C4/C5/C6$ respectively), as shown in Figure 3.

S4. Synthesis and crystallization

A solution of dicyclohexylcarbodiimide (DCC) dissolved in dried CH_2Cl_2 was added to a solution containing coumarin 3-carboxylic acid (1.0 mmol) and 4-methoxyphenol (1.0 mmol) and a catalytic amount of $N-N$ -Dimethylaminopyrimidine (DMAP) in anhydrous dichloromethane (CH_2Cl_2), under stirring, After 24 hrs of stirring, dicyclohexylurea was filtered off and the solution was concentrated. The solid residue was purified by column chromatography on silica gel (60–120) using chloroform ($CHCl_3$) as an eluent. Colourless prisms of the title compound were grown by slow evaporation of an ethanol solution at room temperature.

S5. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 1. The H atoms were positioned with idealized geometry using a riding model with $C-H = 0.93-0.99$ Å. All H-atoms were refined with isotropic displacement parameters (set to 1.2-1.5 times of the U eq of the parent atom).

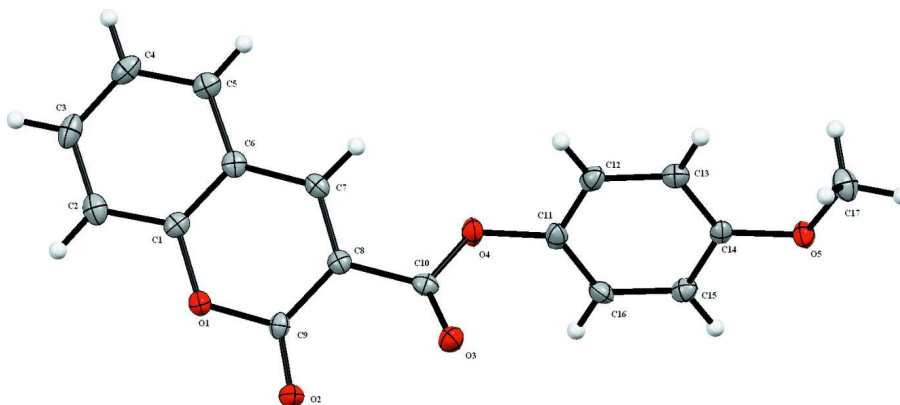


Figure 1

The molecular structure of the title compound, showing displacement ellipsoids drawn at the 50% probability level.

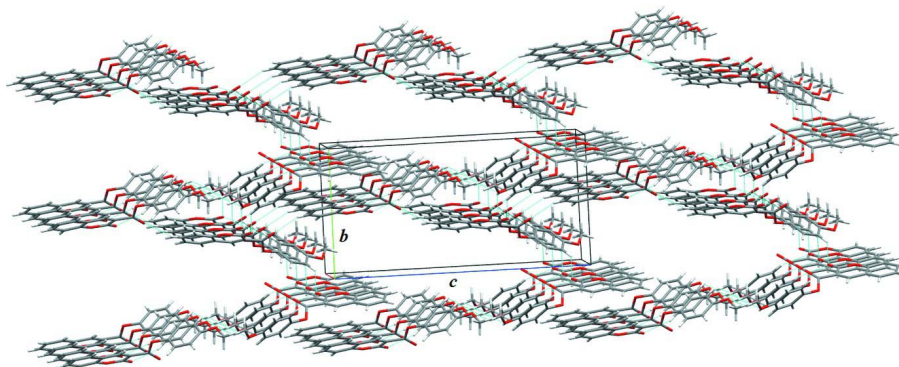
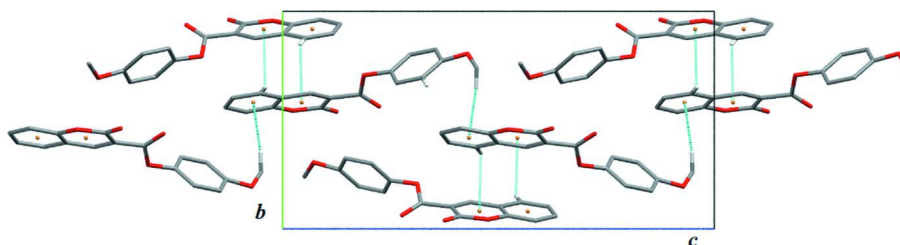
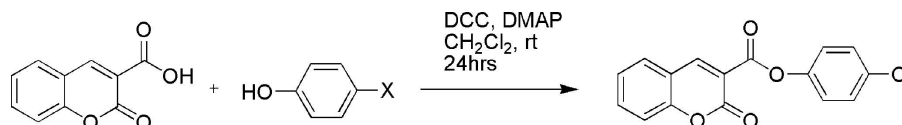


Figure 2

The packing of (I) showing grid like structure when viewed along a axis.

**Figure 3**

The packing of (I) showing C—H... π interactions when viewed along a axis.

**Figure 4**

The formation of the title compound.

4-Methoxyphenyl 2-oxo-2H-chromene-3-carboxylate

Crystal data

$C_{17}H_{12}O_5$
 $M_r = 296.27$
 Orthorhombic, $P2_12_12_1$
 $a = 6.2648$ (18) Å
 $b = 10.435$ (3) Å
 $c = 20.621$ (7) Å
 $V = 1348.0$ (7) Å³
 $Z = 4$
 $F(000) = 616$
 prism

$D_x = 1.460$ Mg m⁻³
 Melting point: 435 K
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 2385 reflections
 $\theta = 2.0$ – 25.0°
 $\mu = 0.11$ mm⁻¹
 $T = 296$ K
 Prism, colourless
 $0.22 \times 0.20 \times 0.18$ mm

Data collection

Bruker APEXII CCD
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 Detector resolution: 2.01 pixels mm⁻¹
 ϕ and ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2013)
 $T_{\min} = 0.977$, $T_{\max} = 0.981$

10472 measured reflections
 2385 independent reflections
 2150 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.050$
 $\theta_{\max} = 25.0^\circ$, $\theta_{\min} = 2.0^\circ$
 $h = -7 \rightarrow 5$
 $k = -12 \rightarrow 12$
 $l = -24 \rightarrow 23$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.035$
 $wR(F^2) = 0.085$
 $S = 1.09$
 1411 reflections
 201 parameters
 0 restraints
 0 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
 $w = 1/[\sigma^2(F_o^2) + (0.0342P)^2 + 0.2933P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.16$ e Å⁻³
 $\Delta\rho_{\min} = -0.16$ e Å⁻³

Extinction correction: *SHELXL2014* (Sheldrick, 2015), $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.010 (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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | U_{iso}^*/U_{eq} |
|------|------------|--------------|---------------|--------------------|
| O5 | 0.2218 (3) | 0.80557 (17) | 0.42819 (9) | 0.0181 (5) |
| O4 | 0.5756 (3) | 0.70623 (17) | 0.18810 (9) | 0.0213 (5) |
| O1 | 1.0215 (3) | 0.54316 (17) | 0.02385 (9) | 0.0172 (5) |
| O2 | 1.1382 (3) | 0.53880 (19) | 0.12431 (9) | 0.0221 (5) |
| O3 | 0.8203 (3) | 0.56290 (18) | 0.22324 (9) | 0.0216 (5) |
| C17 | 0.0344 (5) | 0.7406 (3) | 0.44957 (15) | 0.0235 (7) |
| H17A | -0.0827 | 0.7619 | 0.4215 | 0.035* |
| H17B | 0.0014 | 0.7664 | 0.4931 | 0.035* |
| H17C | 0.0584 | 0.6497 | 0.4484 | 0.035* |
| C14 | 0.3033 (5) | 0.7725 (2) | 0.36853 (13) | 0.0146 (6) |
| C13 | 0.1987 (5) | 0.6954 (2) | 0.32378 (13) | 0.0185 (6) |
| H13 | 0.0656 | 0.6606 | 0.3333 | 0.022* |
| C12 | 0.2960 (5) | 0.6709 (2) | 0.26457 (14) | 0.0195 (7) |
| H12 | 0.2284 | 0.6191 | 0.2341 | 0.023* |
| C11 | 0.4914 (5) | 0.7230 (2) | 0.25097 (13) | 0.0189 (6) |
| C10 | 0.7332 (4) | 0.6180 (2) | 0.17961 (14) | 0.0164 (6) |
| C8 | 0.7751 (4) | 0.6021 (2) | 0.10923 (13) | 0.0143 (6) |
| C9 | 0.9873 (5) | 0.5583 (2) | 0.08977 (13) | 0.0153 (6) |
| C1 | 0.8638 (5) | 0.5612 (2) | -0.02156 (13) | 0.0155 (6) |
| C2 | 0.9148 (5) | 0.5377 (2) | -0.08562 (14) | 0.0204 (7) |
| H2 | 1.0497 | 0.5080 | -0.0969 | 0.024* |
| C3 | 0.7610 (5) | 0.5592 (3) | -0.13272 (14) | 0.0223 (7) |
| H3 | 0.7935 | 0.5448 | -0.1761 | 0.027* |
| C7 | 0.6224 (5) | 0.6229 (2) | 0.06469 (13) | 0.0148 (6) |
| H7 | 0.4887 | 0.6511 | 0.0781 | 0.018* |
| C6 | 0.6609 (4) | 0.6025 (2) | -0.00282 (13) | 0.0153 (6) |
| C5 | 0.5082 (5) | 0.6226 (2) | -0.05175 (13) | 0.0181 (6) |
| H5 | 0.3717 | 0.6500 | -0.0407 | 0.022* |
| C4 | 0.5591 (5) | 0.6021 (3) | -0.11558 (14) | 0.0204 (7) |
| H4 | 0.4575 | 0.6169 | -0.1476 | 0.024* |
| C15 | 0.5015 (5) | 0.8245 (2) | 0.35439 (13) | 0.0173 (6) |
| H15 | 0.5705 | 0.8756 | 0.3849 | 0.021* |
| C16 | 0.5972 (5) | 0.8008 (3) | 0.29511 (14) | 0.0187 (7) |
| H16 | 0.7294 | 0.8361 | 0.2851 | 0.022* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| O5 | 0.0178 (11) | 0.0206 (9) | 0.0160 (11) | -0.0012 (9) | 0.0043 (8) | -0.0010 (8) |
| O4 | 0.0249 (12) | 0.0249 (10) | 0.0140 (11) | 0.0105 (9) | 0.0029 (8) | 0.0000 (8) |
| O1 | 0.0158 (11) | 0.0205 (9) | 0.0154 (11) | 0.0007 (9) | 0.0018 (8) | -0.0017 (8) |
| O2 | 0.0175 (12) | 0.0299 (11) | 0.0189 (11) | 0.0057 (9) | -0.0032 (9) | -0.0045 (8) |
| O3 | 0.0218 (12) | 0.0276 (10) | 0.0153 (11) | 0.0042 (10) | -0.0001 (9) | 0.0035 (8) |
| C17 | 0.0247 (19) | 0.0205 (14) | 0.0252 (17) | -0.0036 (13) | 0.0078 (14) | 0.0008 (12) |
| C14 | 0.0177 (16) | 0.0133 (12) | 0.0128 (15) | 0.0039 (12) | 0.0004 (12) | 0.0022 (10) |
| C13 | 0.0173 (16) | 0.0183 (13) | 0.0198 (16) | 0.0002 (13) | -0.0019 (13) | 0.0006 (12) |
| C12 | 0.0230 (18) | 0.0187 (14) | 0.0169 (16) | 0.0033 (13) | -0.0034 (13) | -0.0039 (11) |
| C11 | 0.0223 (17) | 0.0198 (14) | 0.0146 (15) | 0.0070 (13) | 0.0012 (12) | 0.0007 (12) |
| C10 | 0.0139 (16) | 0.0148 (13) | 0.0204 (17) | -0.0021 (12) | 0.0000 (13) | 0.0012 (12) |
| C8 | 0.0154 (16) | 0.0114 (12) | 0.0163 (15) | -0.0017 (11) | 0.0004 (12) | -0.0005 (11) |
| C9 | 0.0195 (17) | 0.0125 (12) | 0.0138 (15) | -0.0008 (12) | 0.0019 (13) | -0.0013 (10) |
| C1 | 0.0186 (17) | 0.0118 (12) | 0.0162 (15) | -0.0028 (12) | -0.0013 (12) | 0.0016 (11) |
| C2 | 0.0233 (17) | 0.0151 (13) | 0.0228 (17) | -0.0018 (12) | 0.0056 (13) | -0.0018 (12) |
| C3 | 0.034 (2) | 0.0186 (13) | 0.0145 (16) | -0.0064 (13) | 0.0031 (14) | -0.0009 (12) |
| C7 | 0.0135 (16) | 0.0108 (12) | 0.0202 (17) | -0.0005 (11) | 0.0021 (12) | -0.0003 (11) |
| C6 | 0.0183 (17) | 0.0097 (11) | 0.0178 (16) | -0.0030 (12) | 0.0017 (13) | 0.0010 (11) |
| C5 | 0.0211 (17) | 0.0127 (13) | 0.0206 (16) | 0.0006 (12) | -0.0020 (14) | 0.0011 (11) |
| C4 | 0.0298 (19) | 0.0143 (13) | 0.0171 (16) | -0.0027 (13) | -0.0056 (13) | 0.0017 (11) |
| C15 | 0.0188 (16) | 0.0143 (12) | 0.0189 (15) | -0.0001 (12) | -0.0030 (13) | -0.0019 (11) |
| C16 | 0.0125 (15) | 0.0220 (14) | 0.0216 (16) | 0.0013 (12) | 0.0020 (12) | 0.0013 (12) |

Geometric parameters (Å, °)

| | | | |
|------------|-----------|----------|-----------|
| O5—C14 | 1.376 (3) | C10—C8 | 1.484 (4) |
| O5—C17 | 1.426 (3) | C8—C7 | 1.344 (4) |
| O4—C10 | 1.361 (3) | C8—C9 | 1.462 (4) |
| O4—C11 | 1.411 (3) | C1—C2 | 1.381 (4) |
| O1—C1 | 1.374 (3) | C1—C6 | 1.397 (4) |
| O1—C9 | 1.385 (3) | C2—C3 | 1.386 (4) |
| O2—C9 | 1.201 (3) | C2—H2 | 0.9300 |
| O3—C10 | 1.199 (3) | C3—C4 | 1.388 (4) |
| C17—H17A | 0.9600 | C3—H3 | 0.9300 |
| C17—H17B | 0.9600 | C7—C6 | 1.429 (4) |
| C17—H17C | 0.9600 | C7—H7 | 0.9300 |
| C14—C15 | 1.386 (4) | C6—C5 | 1.406 (4) |
| C14—C13 | 1.389 (4) | C5—C4 | 1.371 (4) |
| C13—C12 | 1.388 (4) | C5—H5 | 0.9300 |
| C13—H13 | 0.9300 | C4—H4 | 0.9300 |
| C12—C11 | 1.368 (4) | C15—C16 | 1.384 (4) |
| C12—H12 | 0.9300 | C15—H15 | 0.9300 |
| C11—C16 | 1.388 (4) | C16—H16 | 0.9300 |
| C14—O5—C17 | 117.6 (2) | O1—C9—C8 | 116.5 (2) |

| | | | |
|-----------------|------------|-----------------|------------|
| C10—O4—C11 | 118.2 (2) | O1—C1—C2 | 117.5 (3) |
| C1—O1—C9 | 122.8 (2) | O1—C1—C6 | 120.5 (2) |
| O5—C17—H17A | 109.5 | C2—C1—C6 | 122.0 (3) |
| O5—C17—H17B | 109.5 | C1—C2—C3 | 118.7 (3) |
| H17A—C17—H17B | 109.5 | C1—C2—H2 | 120.6 |
| O5—C17—H17C | 109.5 | C3—C2—H2 | 120.6 |
| H17A—C17—H17C | 109.5 | C2—C3—C4 | 120.5 (3) |
| H17B—C17—H17C | 109.5 | C2—C3—H3 | 119.8 |
| O5—C14—C15 | 115.0 (2) | C4—C3—H3 | 119.8 |
| O5—C14—C13 | 124.4 (3) | C8—C7—C6 | 121.4 (3) |
| C15—C14—C13 | 120.7 (3) | C8—C7—H7 | 119.3 |
| C12—C13—C14 | 118.9 (3) | C6—C7—H7 | 119.3 |
| C12—C13—H13 | 120.5 | C1—C6—C5 | 117.8 (3) |
| C14—C13—H13 | 120.5 | C1—C6—C7 | 118.0 (3) |
| C11—C12—C13 | 120.0 (3) | C5—C6—C7 | 124.2 (3) |
| C11—C12—H12 | 120.0 | C4—C5—C6 | 120.5 (3) |
| C13—C12—H12 | 120.0 | C4—C5—H5 | 119.8 |
| C12—C11—C16 | 121.7 (3) | C6—C5—H5 | 119.8 |
| C12—C11—O4 | 118.3 (3) | C5—C4—C3 | 120.5 (3) |
| C16—C11—O4 | 119.8 (3) | C5—C4—H4 | 119.8 |
| O3—C10—O4 | 123.9 (3) | C3—C4—H4 | 119.8 |
| O3—C10—C8 | 126.8 (3) | C16—C15—C14 | 120.2 (3) |
| O4—C10—C8 | 109.2 (2) | C16—C15—H15 | 119.9 |
| C7—C8—C9 | 120.7 (3) | C14—C15—H15 | 119.9 |
| C7—C8—C10 | 121.6 (3) | C15—C16—C11 | 118.5 (3) |
| C9—C8—C10 | 117.7 (2) | C15—C16—H16 | 120.7 |
| O2—C9—O1 | 116.2 (3) | C11—C16—H16 | 120.7 |
| O2—C9—C8 | 127.3 (3) | | |
| | | | |
| C17—O5—C14—C15 | -170.9 (2) | C9—O1—C1—C6 | 3.2 (3) |
| C17—O5—C14—C13 | 10.3 (4) | O1—C1—C2—C3 | -177.9 (2) |
| O5—C14—C13—C12 | 178.8 (2) | C6—C1—C2—C3 | 1.8 (4) |
| C15—C14—C13—C12 | 0.1 (4) | C1—C2—C3—C4 | -0.8 (4) |
| C14—C13—C12—C11 | -0.3 (4) | C9—C8—C7—C6 | 0.3 (4) |
| C13—C12—C11—C16 | 0.0 (4) | C10—C8—C7—C6 | -177.4 (2) |
| C13—C12—C11—O4 | -174.0 (2) | O1—C1—C6—C5 | 178.3 (2) |
| C10—O4—C11—C12 | -103.6 (3) | C2—C1—C6—C5 | -1.4 (4) |
| C10—O4—C11—C16 | 82.4 (3) | O1—C1—C6—C7 | -1.1 (3) |
| C11—O4—C10—O3 | -8.0 (4) | C2—C1—C6—C7 | 179.3 (2) |
| C11—O4—C10—C8 | 171.6 (2) | C8—C7—C6—C1 | -0.6 (4) |
| O3—C10—C8—C7 | 151.7 (3) | C8—C7—C6—C5 | -179.9 (2) |
| O4—C10—C8—C7 | -27.9 (3) | C1—C6—C5—C4 | 0.0 (4) |
| O3—C10—C8—C9 | -26.2 (4) | C7—C6—C5—C4 | 179.3 (2) |
| O4—C10—C8—C9 | 154.2 (2) | C6—C5—C4—C3 | 1.0 (4) |
| C1—O1—C9—O2 | 179.5 (2) | C2—C3—C4—C5 | -0.6 (4) |
| C1—O1—C9—C8 | -3.3 (3) | O5—C14—C15—C16 | -178.4 (2) |
| C7—C8—C9—O2 | 178.4 (3) | C13—C14—C15—C16 | 0.5 (4) |
| C10—C8—C9—O2 | -3.8 (4) | C14—C15—C16—C11 | -0.8 (4) |

| | | | |
|--------------|------------|-----------------|-----------|
| C7—C8—C9—O1 | 1.6 (3) | C12—C11—C16—C15 | 0.6 (4) |
| C10—C8—C9—O1 | 179.4 (2) | O4—C11—C16—C15 | 174.4 (2) |
| C9—O1—C1—C2 | -177.2 (2) | | |

Hydrogen-bond geometry (Å, °)

Cg1 and Cg2 are the centroids of the C1/C6/C7/C8/C9/O1 and C1/C2/C3/C4/C5/C6 rings, respectively.

| <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> |
|-------------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| C17—H17B \cdots O5 ⁱ | 0.96 | 2.50 | 3.228 (3) | 132 |
| C12—H12 \cdots O2 ⁱⁱ | 0.93 | 2.48 | 3.353 (3) | 156 |
| C15—H15 \cdots O2 ⁱⁱⁱ | 0.93 | 2.50 | 3.207 (3) | 133 |
| C3—H3 \cdots O3 ^{iv} | 0.93 | 2.47 | 3.272 (4) | 145 |
| C5—H5 \cdots Cg1 ^v | 0.93 | 2.82 | 3.303 (3) | 114 |
| C17—H17C \cdots Cg2 ^{vi} | 0.93 | 2.96 | 3.709 (4) | 136 |

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