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4-(4-Methoxyphenyl)-5,7-dimethylchroman-2-one

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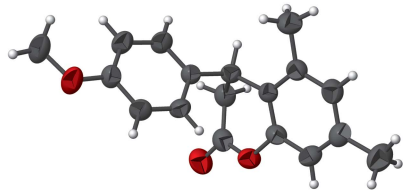
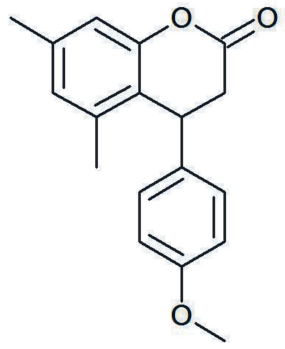
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{18}H_{18}O_3$, a dihydrocoumarin synthesized *via* a microwave-assisted hydroarylation reaction, the 4-methoxyphenyl ring is inclined to the mean plane of the coumarin moiety by 78.21 (9)°. The pyran ring has a screw-boat conformation and its mean plane is inclined to the fused benzene ring by 13.88 (11)°. In the crystal, molecules are linked *via* C—H···O hydrogen bonds, forming ribbons along the *b*-axis direction. The ribbons are linked *via* C—H···π interactions, forming slabs parallel to the *ab* plane.

3D view



Chemical scheme



Structure description

Coumarin derivatives exist widely in nature, especially in plants (Asai *et al.*, 1991), and show a wide range of biological effects such as anti-inflammatory, anti-oxidative, anti-ageing and anti-cancer activities. 4-Aryl-3,4-dihydrocoumarins are of synthetic interest because they are present in a number of natural molecules, such as neoflavonoids and other complex flavonoids. Dihydrocoumarins may be obtained by methods based on acid-mediated hydroarylation of alkenes (Jagdale & Sudalai, 2007). However, these methods use toxic solvents and long reaction times. In the present work the hydroarylation was carried out using microwave irradiation and using trifluoroacetic acid as solvent. The simplicity of this approach makes it particularly attractive for use in combinatorial synthesis. Herein we report on the synthesis and crystal structure of the title dihydrocoumarin compound.

The title compound, Fig. 1, is L-shaped with the 4-methoxyphenyl ring being inclined to the mean plane of the coumarin moiety by 78.21 (9)°. In the crystal, molecules are linked *via* C—H···O hydrogen bonds (Table 1 and Fig. 2), forming ribbons along [010]. The ribbons are linked by C—H···π interactions, forming slabs parallel to (001); see Fig. 2 and Table 1.

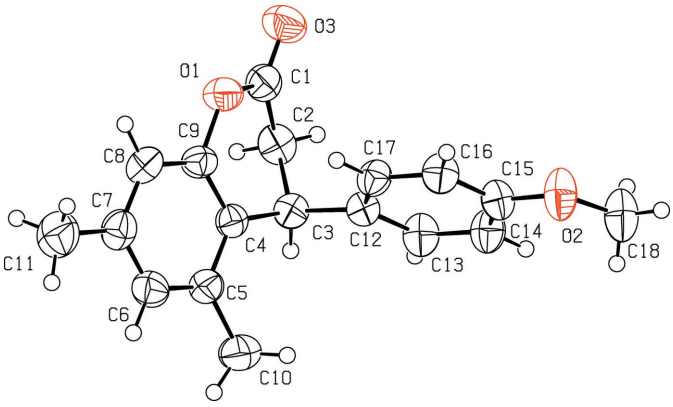


Figure 1
A view of the molecular structure of the title compound, showing the atom labelling and 50% probability displacement ellipsoids.

Synthesis and crystallization

A mixture of 3,5-dimethyl-phenol (0.245 g, 2.00 mmol) and 4-methoxycinnamic acid (0.356 g, 2 mmol) was placed in a cylindrical quartz reactor (4 cm diameter). The reactor was then introduced into a CEM Discover microwave reactor [2.45 GHz, adjusted power of 250 W, and an IR temperature detector]. The stirred liquid mixture was irradiated for 5 min at 333 K. The mixture was then allowed to cool and a white solid formed rapidly (< 5 min) at 298 K. This crude solid was filtered off (under nitrogen), washed with anhydrous ethanol (3 × 5 ml), and vacuum dried for 1 h. The solid was further dried under high vacuum (10^{-2} Torr) at 298 K for 8 h. Recrystallization from dry ethanol solution gave the title compound as colourless needle-like crystals (yield 65%; m.p. = 413–418 K). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.14 (*s*, 3H); 2.34 (*s*, 3H); 2.97 (*dd*, 1H, *J* = 15.6 and 2.58 Hz); 3.00 (*dd*, 1H, *J* = 15.6 and 6.0 Hz); 4.32 (*dd*, 1H, *J* = 6.0 and 2.58 Hz); 6.79–6.76 (*m*, 2H); 6.81–6.80 (*m*, 2H); 6.96–6.94 (*m*, 2H). ^{13}C NMR (101 MHz,$CDCl_3$) δ p.p.m. 18.62; 21.08; 37.21; 37.98; 55.25; 114.45; 115.42; 120.47; 127.28; 128.02; 132.32; 136.54; 138.68; 152.03; 158.80; 167.66.

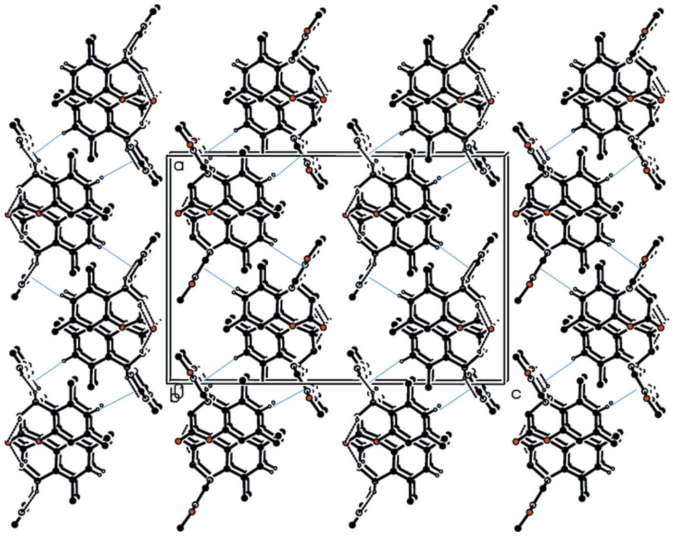


Figure 2
A view along the *b* axis of thec crystal packing of the title compound, showing the C—H···O hydrogen bonds as dashed lines, and with the C—H···π interactions represented by thin blue lines. Details are given in Table 1 and H atoms not involved in these interactions have been omitted for clarity.

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

*Cg*3 is the centroid of the C12–C17 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2*B*···O3^{i}	0.97	2.52	3.327 (3)	140
C3—H3···O2^{ii}	0.98	2.53	3.446 (3)	156
C6—H6···*Cg*3^{iii}	0.93	2.95	3.853 (3)	165

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{18}O_3$
M_r	282.32
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	293
a, *b*, *c* (Å)	16.1115 (19), 7.7040 (9), 23.873 (3)
V (Å^3)	2963.2 (6)
Z	8
Radiation type	Mo *K*α
μ (mm^{-1})	0.09
Crystal size (mm)	0.35 × 0.20 × 0.12
Data collection	
Diffractometer	Bruker APEX CCD area-detector
Absorption correction	Multi-scan (*SADABS*; Sheldrick, 2000)
T_{min}, T_{max}	0.303, 0.999
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13132, 2786, 1563
R_{int}	0.070
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.610
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.050, 0.155, 0.97
No. of reflections	2786
No. of parameters	194
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.19, −0.18

Computer programs: *SMART* (Bruker, 2003), *SAINT* (Bruker, 2003), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *PLATON* (Spek, 2009), *publCIF* (Westrip, 2010).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Reflections 1 0 2, 2 0 2, 2 0 0 and 1 1 1 affected by the backstop were removed during the final cycles of refinement.

Acknowledgements

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full crystallographic data

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Crystal data

$C_{18}H_{18}O_3$
M_r = 282.32
Orthorhombic, *Pbca*
a = 16.1115 (19) Å
b = 7.7040 (9) Å
c = 23.873 (3) Å
V = 2963.2 (6) Å^3
Z = 8
$F(000)$ = 1200
D_x = 1.266 Mg m^{-3}
Melting point: 418 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1347 reflections
θ = 3.1–20.8°
μ = 0.09 mm^{-1}
T = 293 K
Block, colorless
0.35 × 0.20 × 0.12 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)
T_{min} = 0.303, T_{max} = 0.999
13132 measured reflections
2786 independent reflections
1563 reflections with $I > 2\sigma(I)$
R_{int} = 0.070
θ_{max} = 25.7°, θ_{min} = 3.4°
h = −17→19
k = −9→9
l = −15→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.155
S = 0.97
2786 reflections
194 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
$w = 1/[\sigma^2(F_o^2) + (0.0794P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Extinction correction: *SHELXL2014* (Sheldrick, 2015), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0059 (10)

Special details

Experimental. A mixture of 3,5-dimethyl-phenol (0,245 g, 2,00 mmol) and 4-methoxycinnamic acid (0.356 g, 2 mmol) was placed in a cylindrical quartz reactor (4 cm diameter). The reactor was then introduced into a CEM Discover microwave reactor [2.45 GHz, adjusted power of 250 W, and an IR temperature detector]. The stirred liquid mixture was irradiated for 5 min at 333 K. The mixture was then allowed to cool and a white solid formed rapidly (< 5 min) at 298 K. This crude solid was filtered off (under nitrogen), washed with anhydrous ethanol (3 × 5 ml), and vacuum dried for 1 h. The solid was further dried under high vacuum (10–2 Torr) at 298 K for 8 h. Recrystallization from dry ethanol gave the title compound as colourless needle-like crystals (yield 65%; m.p. = 413–418 K). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.14 (*s*, 3H); 2.34 (*s*, 3H); 2.97 (*dd*, 1H, J = 15.6 and 2.58 Hz); 3.00 (*dd*, 1H, J = 15.6 and 6.0 Hz); 4.32 (*dd*, 1H, J = 6.0 and 2.58 Hz); 6.79–6.76 (*m*, 2H); 6.81–6.80 (*m*, 2H); 6.96–6.94 (*m*, 2H). ^{13}C NMR (101 MHz,$CDCl_3$) δ p.p.m. 18.62; 21.08; 37.21; 37.98; 55.25; 114.45; 115.42; 120.47; 127.28; 128.02; 132.32; 136.54; 138.68; 152.03; 158.80; 167.66.

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.24519 (9)	0.54914 (19)	0.37344 (6)	0.0544 (5)
O2	−0.05956 (11)	1.14738 (19)	0.42345 (7)	0.0669 (6)
O3	0.25110 (11)	0.5854 (2)	0.46470 (7)	0.0708 (6)
C1	0.21280 (17)	0.5261 (3)	0.42587 (11)	0.0522 (6)
C2	0.13392 (15)	0.4270 (3)	0.42946 (9)	0.0536 (7)
H2A	0.1080	0.4497	0.4654	0.064*
H2B	0.1461	0.3039	0.4275	0.064*
C3	0.07319 (14)	0.4745 (3)	0.38271 (8)	0.0440 (6)
H3	0.0278	0.3899	0.3834	0.053*
C4	0.11783 (14)	0.4546 (2)	0.32795 (8)	0.0412 (5)
C5	0.07948 (14)	0.4014 (3)	0.27818 (10)	0.0476 (6)
C6	0.12741 (15)	0.3855 (3)	0.23005 (10)	0.0550 (7)
H6	0.1018	0.3488	0.1972	0.066*
C7	0.21175 (16)	0.4217 (3)	0.22875 (10)	0.0542 (6)
C8	0.24902 (14)	0.4748 (3)	0.27819 (10)	0.0516 (6)
H8	0.3054	0.5007	0.2789	0.062*
C9	0.20234 (15)	0.4889 (3)	0.32602 (9)	0.0449 (6)
C10	−0.01234 (15)	0.3653 (4)	0.27682 (11)	0.0681 (7)
H10A	−0.0275	0.3224	0.2405	0.102*
H10B	−0.0423	0.4705	0.2844	0.102*
H10C	−0.0258	0.2800	0.3047	0.102*
C11	0.26174 (16)	0.4012 (4)	0.17614 (11)	0.0772 (9)
H11A	0.2989	0.3045	0.1801	0.116*
H11B	0.2932	0.5050	0.1695	0.116*
H11C	0.2251	0.3808	0.1451	0.116*
C12	0.03573 (14)	0.6540 (3)	0.39205 (8)	0.0408 (6)
C13	−0.03718 (15)	0.6726 (3)	0.42207 (9)	0.0530 (7)
H13	−0.0644	0.5735	0.4347	0.064*
C14	−0.07116 (16)	0.8339 (3)	0.43401 (9)	0.0548 (7)
H14	−0.1203	0.8421	0.4543	0.066*

C15	−0.03148 (15)	0.9819 (3)	0.41561 (9)	0.0484 (6)
C16	0.04172 (15)	0.9657 (3)	0.38571 (9)	0.0514 (6)
H16	0.0691	1.0648	0.3733	0.062*
C17	0.07453 (14)	0.8045 (3)	0.37405 (9)	0.0468 (6)
H17	0.1236	0.7966	0.3537	0.056*
C18	−0.13033 (18)	1.1710 (3)	0.45774 (12)	0.0735 (8)
H18A	−0.1760	1.1063	0.4426	0.110*
H18B	−0.1445	1.2920	0.4589	0.110*
H18C	−0.1185	1.1308	0.4950	0.110*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0486 (10)	0.0639 (11)	0.0507 (10)	−0.0048 (8)	−0.0065 (8)	−0.0001 (8)
O2	0.0769 (13)	0.0432 (9)	0.0805 (12)	0.0072 (9)	0.0317 (10)	0.0016 (8)
O3	0.0775 (13)	0.0771 (13)	0.0577 (11)	0.0022 (10)	−0.0186 (10)	−0.0092 (9)
C1	0.0570 (16)	0.0476 (14)	0.0519 (16)	0.0095 (12)	−0.0073 (13)	0.0013 (11)
C2	0.0670 (17)	0.0464 (13)	0.0476 (14)	0.0017 (13)	0.0008 (13)	0.0073 (10)
C3	0.0450 (14)	0.0394 (12)	0.0476 (14)	−0.0039 (10)	0.0030 (11)	0.0050 (10)
C4	0.0429 (14)	0.0358 (11)	0.0448 (13)	0.0014 (10)	−0.0008 (11)	0.0016 (9)
C5	0.0455 (15)	0.0470 (13)	0.0505 (14)	0.0020 (11)	−0.0035 (12)	−0.0012 (10)
C6	0.0592 (18)	0.0603 (15)	0.0454 (14)	0.0060 (13)	−0.0070 (13)	−0.0041 (11)
C7	0.0554 (17)	0.0577 (15)	0.0495 (15)	0.0090 (12)	0.0044 (13)	0.0044 (11)
C8	0.0407 (14)	0.0593 (15)	0.0547 (15)	0.0043 (12)	0.0011 (12)	0.0069 (12)
C9	0.0444 (15)	0.0450 (13)	0.0453 (14)	−0.0003 (11)	−0.0071 (12)	0.0029 (10)
C10	0.0512 (17)	0.0841 (18)	0.0691 (17)	−0.0054 (15)	−0.0056 (14)	−0.0105 (15)
C11	0.072 (2)	0.101 (2)	0.0585 (18)	0.0071 (17)	0.0115 (15)	−0.0025 (15)
C12	0.0443 (14)	0.0381 (12)	0.0398 (12)	−0.0016 (10)	0.0020 (11)	0.0037 (9)
C13	0.0587 (16)	0.0439 (14)	0.0563 (15)	−0.0034 (12)	0.0165 (13)	0.0079 (10)
C14	0.0580 (16)	0.0522 (14)	0.0543 (15)	0.0013 (12)	0.0193 (12)	0.0060 (11)
C15	0.0581 (16)	0.0409 (13)	0.0463 (14)	0.0010 (11)	0.0087 (12)	0.0013 (10)
C16	0.0543 (16)	0.0401 (13)	0.0597 (15)	−0.0057 (11)	0.0104 (13)	0.0060 (11)
C17	0.0400 (13)	0.0461 (13)	0.0543 (14)	−0.0024 (11)	0.0078 (11)	0.0030 (10)
C18	0.083 (2)	0.0583 (16)	0.0797 (19)	0.0108 (15)	0.0294 (17)	−0.0049 (13)

Geometric parameters (Å, º)

O1—C1	1.368 (3)	C8—H8	0.9300
O1—C9	1.405 (2)	C10—H10A	0.9600
O2—C15	1.366 (2)	C10—H10B	0.9600
O2—C18	1.415 (3)	C10—H10C	0.9600
O3—C1	1.203 (3)	C11—H11A	0.9600
C1—C2	1.485 (3)	C11—H11B	0.9600
C2—C3	1.529 (3)	C11—H11C	0.9600
C2—H2A	0.9700	C12—C13	1.383 (3)
C2—H2B	0.9700	C12—C17	1.386 (3)
C3—C4	1.500 (3)	C13—C14	1.387 (3)
C3—C12	1.525 (3)	C13—H13	0.9300

C3—H3	0.9800	C14—C15	1.379 (3)
C4—C9	1.388 (3)	C14—H14	0.9300
C4—C5	1.400 (3)	C15—C16	1.384 (3)
C5—C6	1.390 (3)	C16—C17	1.378 (3)
C5—C10	1.506 (3)	C16—H16	0.9300
C6—C7	1.388 (3)	C17—H17	0.9300
C6—H6	0.9300	C18—H18A	0.9600
C7—C8	1.386 (3)	C18—H18B	0.9600
C7—C11	1.500 (3)	C18—H18C	0.9600
C8—C9	1.372 (3)		

C1—O1—C9	120.47 (19)	C5—C10—H10B	109.5
C15—O2—C18	117.79 (18)	H10A—C10—H10B	109.5
O3—C1—O1	117.4 (2)	C5—C10—H10C	109.5
O3—C1—C2	126.1 (2)	H10A—C10—H10C	109.5
O1—C1—C2	116.5 (2)	H10B—C10—H10C	109.5
C1—C2—C3	112.50 (18)	C7—C11—H11A	109.5
C1—C2—H2A	109.1	C7—C11—H11B	109.5
C3—C2—H2A	109.1	H11A—C11—H11B	109.5
C1—C2—H2B	109.1	C7—C11—H11C	109.5
C3—C2—H2B	109.1	H11A—C11—H11C	109.5
H2A—C2—H2B	107.8	H11B—C11—H11C	109.5
C4—C3—C12	114.20 (16)	C13—C12—C17	117.19 (19)
C4—C3—C2	107.76 (19)	C13—C12—C3	120.38 (18)
C12—C3—C2	111.32 (17)	C17—C12—C3	122.3 (2)
C4—C3—H3	107.8	C12—C13—C14	122.3 (2)
C12—C3—H3	107.8	C12—C13—H13	118.9
C2—C3—H3	107.8	C14—C13—H13	118.9
C9—C4—C5	117.4 (2)	C15—C14—C13	119.5 (2)
C9—C4—C3	118.67 (19)	C15—C14—H14	120.3
C5—C4—C3	123.9 (2)	C13—C14—H14	120.3
C6—C5—C4	118.8 (2)	O2—C15—C14	125.1 (2)
C6—C5—C10	120.8 (2)	O2—C15—C16	115.91 (19)
C4—C5—C10	120.4 (2)	C14—C15—C16	119.0 (2)
C7—C6—C5	123.0 (2)	C17—C16—C15	120.8 (2)
C7—C6—H6	118.5	C17—C16—H16	119.6
C5—C6—H6	118.5	C15—C16—H16	119.6
C8—C7—C6	117.7 (2)	C16—C17—C12	121.2 (2)
C8—C7—C11	120.8 (2)	C16—C17—H17	119.4
C6—C7—C11	121.5 (2)	C12—C17—H17	119.4
C9—C8—C7	119.7 (2)	O2—C18—H18A	109.5
C9—C8—H8	120.2	O2—C18—H18B	109.5
C7—C8—H8	120.2	H18A—C18—H18B	109.5
C8—C9—C4	123.4 (2)	O2—C18—H18C	109.5
C8—C9—O1	115.3 (2)	H18A—C18—H18C	109.5
C4—C9—O1	121.2 (2)	H18B—C18—H18C	109.5
C5—C10—H10A	109.5		

C9—O1—C1—O3	−177.71 (19)	C5—C4—C9—C8	0.6 (3)
C9—O1—C1—C2	3.3 (3)	C3—C4—C9—C8	−179.98 (19)
O3—C1—C2—C3	140.3 (2)	C5—C4—C9—O1	177.58 (18)
O1—C1—C2—C3	−40.8 (3)	C3—C4—C9—O1	−3.0 (3)
C1—C2—C3—C4	53.4 (2)	C1—O1—C9—C8	−162.75 (19)
C1—C2—C3—C12	−72.6 (2)	C1—O1—C9—C4	20.1 (3)
C12—C3—C4—C9	91.7 (2)	C4—C3—C12—C13	147.3 (2)
C2—C3—C4—C9	−32.5 (2)	C2—C3—C12—C13	−90.4 (3)
C12—C3—C4—C5	−88.9 (3)	C4—C3—C12—C17	−36.4 (3)
C2—C3—C4—C5	146.8 (2)	C2—C3—C12—C17	85.9 (2)
C9—C4—C5—C6	0.2 (3)	C17—C12—C13—C14	0.1 (4)
C3—C4—C5—C6	−179.20 (19)	C3—C12—C13—C14	176.6 (2)
C9—C4—C5—C10	−178.8 (2)	C12—C13—C14—C15	−0.1 (4)
C3—C4—C5—C10	1.8 (3)	C18—O2—C15—C14	6.6 (3)
C4—C5—C6—C7	−0.7 (3)	C18—O2—C15—C16	−174.8 (2)
C10—C5—C6—C7	178.2 (2)	C13—C14—C15—O2	178.3 (2)
C5—C6—C7—C8	0.5 (3)	C13—C14—C15—C16	−0.2 (4)
C5—C6—C7—C11	179.3 (2)	O2—C15—C16—C17	−178.3 (2)
C6—C7—C8—C9	0.3 (3)	C14—C15—C16—C17	0.4 (4)
C11—C7—C8—C9	−178.6 (2)	C15—C16—C17—C12	−0.3 (4)
C7—C8—C9—C4	−0.9 (3)	C13—C12—C17—C16	0.1 (3)
C7—C8—C9—O1	−177.98 (19)	C3—C12—C17—C16	−176.36 (19)

Hydrogen-bond geometry (Å, º)

Cg3 is the centroid of the C12–C17 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2*B*···O3^{i}	0.97	2.52	3.327 (3)	140
C3—H3···O2^{ii}	0.98	2.53	3.446 (3)	156
C6—H6···*Cg*3^{iii}	0.93	2.95	3.853 (3)	165

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