Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*)-3-(2,4-Dimethoxyphenyl)-1-(3,4,5-trimethoxyphenyl)prop-2-en-1-one

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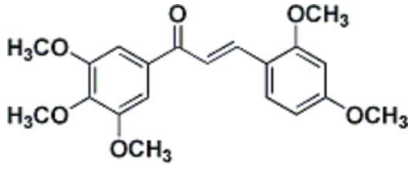
Received 4 December 2011; accepted 9 December 2011

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.046; wR factor = 0.126; data-to-parameter ratio = 14.6.

In the title chalcone derivative, $C_{20}H_{22}O_6$, the dihedral angle between the mean planes of the benzene rings is 15.77 (6)°. The H atoms of the central C=C double bond are in a *trans* configuration. There are a number of C—H···O interactions and a C—H···π interaction present in the crystal structure.

Related literature

For related structures, see: Wu *et al.* (2010, 2011); Huang *et al.* (2010); Peng *et al.* (2010). For applications of chalcones, see: Wu *et al.* (2010, 2011); Nielsen *et al.* (2005). For the hydrogen-bond analysis, see: Spek (2009).



Experimental

Crystal data

$C_{20}H_{22}O_6$
M_r = 358.38
Monoclinic, $P2_1/c$
a = 8.3111 (11) Å
b = 13.8493 (17) Å
c = 15.887 (2) Å
β = 101.588 (2)°
V = 1791.4 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 K
0.40 × 0.37 × 0.31 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.651, T_{max} = 1.000
9663 measured reflections
3512 independent reflections
2452 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.126
S = 0.97
3512 reflections
241 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

*Cg*1 is the centroid of the C4–C9 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···O6^{i}	0.93	2.65	3.562 (2)	166
C18—H18B···O3^{ii}	0.96	2.64	3.404 (2)	136
C16—H16B···O2^{iii}	0.96	2.68	3.389 (2)	132
C16—H16C···O1^{iii}	0.96	2.66	3.608 (3)	169
C19—H19C···$Cg1^{iv}$	0.96	2.79	3.530 (2)	134

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors are grateful to the associate researcher Sun Jie from Shanghai Institute of Organic Chemistry, Chinese academy of Sciences for testing and crystal analysis. This study was partially supported by the Zhejiang Natural Science Funds (Y2101108) and the University Students in Zhejiang Science and Technology Innovation Projects (2011R413025).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZQ2146).

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Wu, J., Wang, C., Cai, Y., Yang, S., Zheng, X., Qiu, P., Peng, J., Wu, X., Liang, G. & Li, X. (2010). *Chin. J. Org. Chem.* **30**, 884–889.

supporting information

Acta Cryst. (2012). E**68**, o154 [doi:10.1107/S1600536811053001]

(*E*)-3-(2,4-Dimethoxyphenyl)-1-(3,4,5-trimethoxyphenyl)prop-2-en-1-one

Jianzhang Wu, Junyan Qiu, Xiaokai Wu, Shulin Yang and Yonggen Liu

S1. Comment

Chalcones are characterized by possessing two aromatic rings linked by a three-carbon α,β-unsaturated carbonyl system (Wu *et al.*, 2010; Wu *et al.*, 2011). Natural chalcones have many kinds of active biological properties such as antiinflammatory, antitumoral, antimalarial, antileishmanial, Antibacterial. Investigations have demonstrated that synthetical chalcones have the same biological properties as natural chalcones. (Wu *et al.* 2010; Wu *et al.* 2011; Nielsen *et al.* 2005). In order to study its anticancer agents, we have synthesized the title chalcone derivative and herein its crystal structure is reported. The crystal structure parameters are similar to those found in some analogous structures reported in the literature (Peng *et al.*, 2010; Huang *et al.*, 2010).The dihedral angle between the mean planes of the phenyl rings is 15.77 (6)°. The H atoms of the central C=C double bond are in a *trans* configuration. In the crystal structure, there are many weak C–H···O intermolecular contacts (Table 1) but no classic hydrogen bonds between the molecules (Spek, 2009).

S2. Experimental

The title compound was synthesized by Claisen-Schmidt condensation between 2,4-dimethoxybenzaldehyde and 1-(3,4,5-trimethoxyphenyl)ethanone. 2,4-Dimethoxybenzaldehyde (1 mmol) and 1-(3,4,5-trimethoxyphenyl)ethanone (1 mmol) were dissolved in ehanol (20 ml). The reaction temperature was controlled at 283 K, and then NaOH (20%, 3 drops) was added. The reaction was monitored by thin-layer chromatography. 20 ml H_2O was added 5 h later and the yellow solid precipitated. It was washed with a mixture of water and cold ethanol, and dried (yield: 70%; mp 125.7–127.7°C). Single crystals of the title compound were obtained by recrystallization from a solution of CH_3CH_2OH / CH_2Cl_2 at 293 K.

S3. Refinement

All H atoms were placed in geometrical positions and constrained to ride on their parent atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic H atoms, and with C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms.

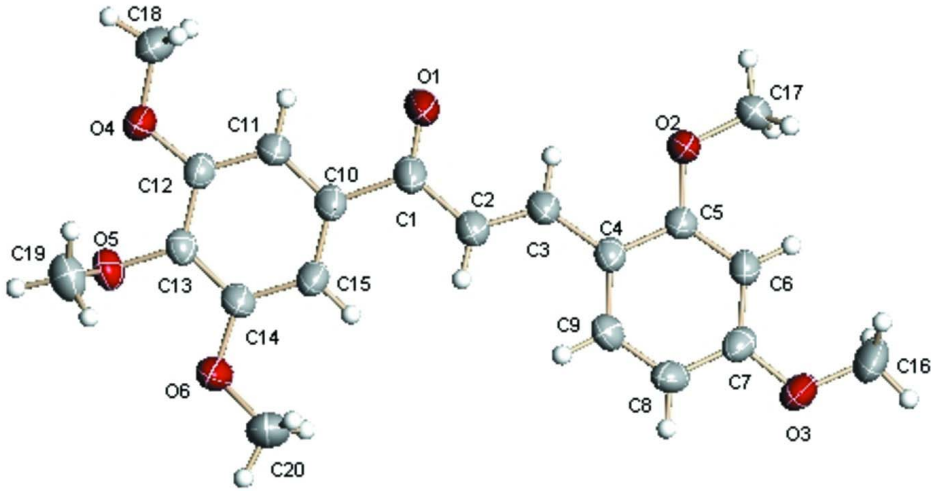

Figure 1

Molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

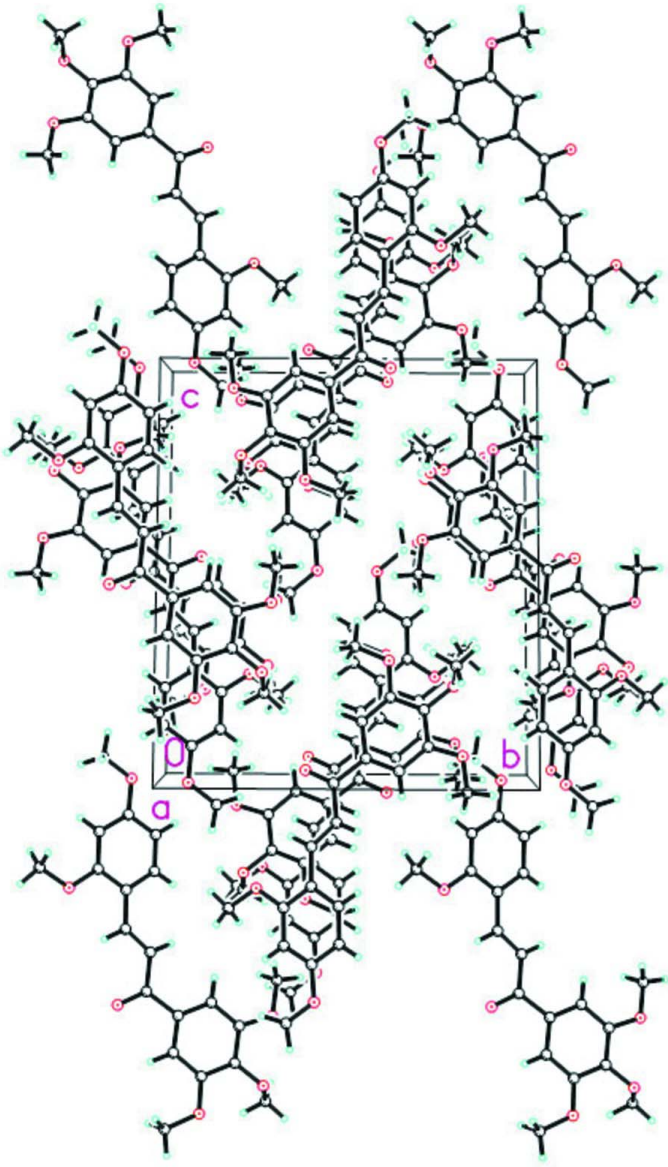

Figure 2

Crystal packing of the title compound viewed down the *a* axis.

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Crystal data

$C_{20}H_{22}O_6$
$M_r = 358.38$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 8.3111$ (11) Å
$b = 13.8493$ (17) Å
$c = 15.887$ (2) Å
$\beta = 101.588$ (2)°
$V = 1791.4$ (4) Å^3
$Z = 4$

$F(000) = 760$
$D_x = 1.329$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2728 reflections
$\theta = 5.2$–$49.2°$
$\mu = 0.10$ mm^{-1}
$T = 293$ K
Prismatic, green
0.40 × 0.37 × 0.31 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.651, T_{max} = 1.000
9663 measured reflections
3512 independent reflections
2452 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 26.0°, θ_{min} = 2.0°
h = −10→9
k = −17→15
l = −16→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.126
S = 0.97
3512 reflections
241 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
$w = 1/[\sigma^2(F_o^2) + (0.0689P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0069 (15)

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.

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 $F^2 > \sigma(F^2)$ 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	0.3078 (3)	0.60842 (10)	−0.03257 (9)	0.0969 (7)
O2	0.45908 (16)	0.73756 (8)	0.24726 (7)	0.0510 (4)
O3	0.34229 (18)	0.58134 (9)	0.49898 (7)	0.0629 (4)
O4	0.20538 (17)	0.38935 (8)	−0.28996 (7)	0.0549 (4)
O5	0.11723 (15)	0.21987 (8)	−0.23292 (7)	0.0487 (3)
O6	0.07241 (18)	0.19802 (8)	−0.07336 (8)	0.0614 (4)
C1	0.2622 (3)	0.53394 (12)	−0.00427 (11)	0.0532 (5)
C2	0.2513 (2)	0.52558 (12)	0.08616 (11)	0.0494 (5)
H2	0.1994	0.4719	0.1037	0.059*
C3	0.3124 (2)	0.59147 (12)	0.14391 (11)	0.0478 (5)
H3	0.3597	0.6450	0.1231	0.057*
C4	0.3155 (2)	0.59116 (11)	0.23532 (10)	0.0397 (4)
C5	0.3969 (2)	0.66447 (11)	0.28813 (10)	0.0395 (4)
C6	0.4097 (2)	0.66259 (11)	0.37629 (10)	0.0438 (4)
H6	0.4670	0.7109	0.4104	0.053*

C7	0.3368 (2)	0.58853 (12)	0.41331 (11)	0.0454 (4)
C8	0.2505 (2)	0.51675 (12)	0.36245 (12)	0.0495 (5)
H8	0.1993	0.4677	0.3872	0.059*
C9	0.2416 (2)	0.51894 (11)	0.27580 (11)	0.0456 (5)
H9	0.1839	0.4703	0.2423	0.055*
C10	0.2178 (2)	0.44929 (11)	−0.06312 (10)	0.0441 (5)
C11	0.2324 (2)	0.46042 (11)	−0.14787 (11)	0.0451 (4)
H11	0.2675	0.5192	−0.1662	0.054*
C12	0.1956 (2)	0.38529 (11)	−0.20524 (10)	0.0428 (4)
C13	0.1453 (2)	0.29723 (11)	−0.17775 (10)	0.0407 (4)
C14	0.1279 (2)	0.28626 (11)	−0.09326 (11)	0.0436 (4)
C15	0.1647 (2)	0.36210 (11)	−0.03595 (11)	0.0468 (5)
H15	0.1538	0.3545	0.0208	0.056*
C16	0.4271 (3)	0.65505 (15)	0.55295 (12)	0.0817 (8)
H16A	0.5415	0.6534	0.5505	0.123*
H16B	0.4147	0.6445	0.6110	0.123*
H16C	0.3821	0.7169	0.5336	0.123*
C17	0.5458 (2)	0.81254 (12)	0.29860 (11)	0.0517 (5)
H17A	0.4751	0.8421	0.3321	0.078*
H17B	0.5805	0.8601	0.2621	0.078*
H17C	0.6402	0.7859	0.3363	0.078*
C18	0.2455 (3)	0.47971 (13)	−0.32250 (12)	0.0632 (6)
H18A	0.1629	0.5263	−0.3168	0.095*
H18B	0.2508	0.4730	−0.3820	0.095*
H18C	0.3501	0.5010	−0.2907	0.095*
C19	−0.0442 (2)	0.21605 (14)	−0.28238 (13)	0.0635 (6)
H19A	−0.1204	0.2052	−0.2452	0.095*
H19B	−0.0523	0.1643	−0.3232	0.095*
H19C	−0.0697	0.2761	−0.3123	0.095*
C20	0.0313 (3)	0.18677 (15)	0.00746 (13)	0.0796 (7)
H20A	0.1280	0.1943	0.0515	0.119*
H20B	−0.0141	0.1236	0.0115	0.119*
H20C	−0.0483	0.2347	0.0147	0.119*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.196 (2)	0.0472 (8)	0.0459 (9)	−0.0398 (10)	0.0199 (10)	−0.0057 (6)
O2	0.0720 (9)	0.0430 (7)	0.0373 (7)	−0.0161 (6)	0.0091 (6)	−0.0008 (5)
O3	0.1002 (12)	0.0532 (8)	0.0383 (7)	−0.0019 (7)	0.0214 (7)	0.0041 (6)
O4	0.0851 (10)	0.0457 (7)	0.0366 (7)	−0.0065 (6)	0.0188 (6)	−0.0026 (5)
O5	0.0564 (8)	0.0391 (6)	0.0498 (7)	0.0031 (6)	0.0088 (6)	−0.0121 (5)
O6	0.0974 (11)	0.0389 (7)	0.0520 (8)	−0.0099 (7)	0.0252 (7)	−0.0010 (6)
C1	0.0786 (14)	0.0389 (10)	0.0384 (10)	−0.0011 (9)	0.0028 (9)	−0.0016 (8)
C2	0.0649 (13)	0.0396 (9)	0.0429 (10)	−0.0037 (9)	0.0092 (9)	−0.0034 (8)
C3	0.0658 (13)	0.0363 (9)	0.0400 (10)	−0.0048 (8)	0.0076 (8)	−0.0006 (7)
C4	0.0486 (11)	0.0334 (8)	0.0364 (9)	0.0030 (7)	0.0067 (8)	−0.0017 (7)
C5	0.0473 (10)	0.0338 (8)	0.0375 (9)	−0.0002 (7)	0.0087 (8)	0.0010 (7)

C6	0.0574 (12)	0.0376 (9)	0.0353 (9)	−0.0013 (8)	0.0065 (8)	−0.0034 (7)
C7	0.0625 (12)	0.0395 (9)	0.0361 (10)	0.0095 (8)	0.0141 (8)	0.0039 (7)
C8	0.0659 (13)	0.0354 (9)	0.0514 (11)	−0.0025 (8)	0.0217 (9)	0.0041 (8)
C9	0.0551 (12)	0.0338 (9)	0.0484 (11)	−0.0019 (8)	0.0119 (9)	−0.0064 (7)
C10	0.0560 (12)	0.0377 (9)	0.0353 (9)	0.0018 (8)	0.0018 (8)	−0.0013 (7)
C11	0.0581 (12)	0.0353 (9)	0.0410 (10)	−0.0034 (8)	0.0078 (8)	0.0011 (7)
C12	0.0520 (11)	0.0412 (9)	0.0354 (9)	0.0038 (8)	0.0094 (8)	−0.0016 (7)
C13	0.0466 (11)	0.0343 (9)	0.0402 (10)	0.0047 (7)	0.0066 (8)	−0.0052 (7)
C14	0.0537 (11)	0.0328 (9)	0.0440 (10)	0.0007 (8)	0.0086 (8)	0.0008 (7)
C15	0.0641 (13)	0.0422 (10)	0.0334 (9)	0.0020 (9)	0.0082 (8)	0.0010 (7)
C16	0.138 (2)	0.0694 (14)	0.0348 (11)	−0.0064 (14)	0.0103 (12)	−0.0023 (10)
C17	0.0619 (13)	0.0421 (10)	0.0515 (11)	−0.0131 (9)	0.0125 (9)	−0.0037 (8)
C18	0.0934 (17)	0.0537 (12)	0.0456 (11)	−0.0055 (11)	0.0211 (11)	0.0058 (9)
C19	0.0649 (14)	0.0589 (12)	0.0627 (13)	−0.0058 (10)	0.0032 (10)	−0.0159 (10)
C20	0.117 (2)	0.0644 (14)	0.0642 (14)	−0.0289 (14)	0.0338 (13)	0.0030 (11)

Geometric parameters (Å, º)

O1—C1	1.216 (2)	C9—H9	0.9300
O2—C5	1.3595 (19)	C10—C15	1.384 (2)
O2—C17	1.4235 (18)	C10—C11	1.385 (2)
O3—C7	1.3564 (19)	C11—C12	1.377 (2)
O3—C16	1.425 (2)	C11—H11	0.9300
O4—C12	1.366 (2)	C12—C13	1.388 (2)
O4—C18	1.419 (2)	C13—C14	1.387 (2)
O5—C13	1.3742 (18)	C14—C15	1.383 (2)
O5—C19	1.413 (2)	C15—H15	0.9300
O6—C14	1.3656 (19)	C16—H16A	0.9600
O6—C20	1.402 (2)	C16—H16B	0.9600
C1—C2	1.462 (2)	C16—H16C	0.9600
C1—C10	1.499 (2)	C17—H17A	0.9600
C2—C3	1.321 (2)	C17—H17B	0.9600
C2—H2	0.9300	C17—H17C	0.9600
C3—C4	1.447 (2)	C18—H18A	0.9600
C3—H3	0.9300	C18—H18B	0.9600
C4—C9	1.396 (2)	C18—H18C	0.9600
C4—C5	1.402 (2)	C19—H19A	0.9600
C5—C6	1.383 (2)	C19—H19B	0.9600
C6—C7	1.381 (2)	C19—H19C	0.9600
C6—H6	0.9300	C20—H20A	0.9600
C7—C8	1.387 (2)	C20—H20B	0.9600
C8—C9	1.364 (2)	C20—H20C	0.9600
C8—H8	0.9300		
C5—O2—C17	117.82 (13)	C11—C12—C13	119.79 (16)
C7—O3—C16	117.64 (15)	O5—C13—C14	119.64 (14)
C12—O4—C18	117.40 (13)	O5—C13—C12	120.52 (15)
C13—O5—C19	113.86 (13)	C14—C13—C12	119.82 (14)

C14—O6—C20	117.86 (14)	O6—C14—C15	124.57 (16)
O1—C1—C2	121.06 (15)	O6—C14—C13	115.33 (14)
O1—C1—C10	119.26 (16)	C15—C14—C13	120.10 (15)
C2—C1—C10	119.67 (15)	C14—C15—C10	119.96 (16)
C3—C2—C1	122.45 (17)	C14—C15—H15	120.0
C3—C2—H2	118.8	C10—C15—H15	120.0
C1—C2—H2	118.8	O3—C16—H16A	109.5
C2—C3—C4	128.42 (17)	O3—C16—H16B	109.5
C2—C3—H3	115.8	H16A—C16—H16B	109.5
C4—C3—H3	115.8	O3—C16—H16C	109.5
C9—C4—C5	116.56 (15)	H16A—C16—H16C	109.5
C9—C4—C3	122.93 (14)	H16B—C16—H16C	109.5
C5—C4—C3	120.50 (15)	O2—C17—H17A	109.5
O2—C5—C6	122.56 (14)	O2—C17—H17B	109.5
O2—C5—C4	115.95 (14)	H17A—C17—H17B	109.5
C6—C5—C4	121.48 (15)	O2—C17—H17C	109.5
C7—C6—C5	119.61 (15)	H17A—C17—H17C	109.5
C7—C6—H6	120.2	H17B—C17—H17C	109.5
C5—C6—H6	120.2	O4—C18—H18A	109.5
O3—C7—C6	123.55 (15)	O4—C18—H18B	109.5
O3—C7—C8	116.18 (16)	H18A—C18—H18B	109.5
C6—C7—C8	120.26 (16)	O4—C18—H18C	109.5
C9—C8—C7	119.28 (16)	H18A—C18—H18C	109.5
C9—C8—H8	120.4	H18B—C18—H18C	109.5
C7—C8—H8	120.4	O5—C19—H19A	109.5
C8—C9—C4	122.75 (16)	O5—C19—H19B	109.5
C8—C9—H9	118.6	H19A—C19—H19B	109.5
C4—C9—H9	118.6	O5—C19—H19C	109.5
C15—C10—C11	119.75 (15)	H19A—C19—H19C	109.5
C15—C10—C1	122.81 (15)	H19B—C19—H19C	109.5
C11—C10—C1	117.44 (15)	O6—C20—H20A	109.5
C12—C11—C10	120.55 (16)	O6—C20—H20B	109.5
C12—C11—H11	119.7	H20A—C20—H20B	109.5
C10—C11—H11	119.7	O6—C20—H20C	109.5
O4—C12—C11	124.89 (16)	H20A—C20—H20C	109.5
O4—C12—C13	115.31 (14)	H20B—C20—H20C	109.5

O1—C1—C2—C3	−10.4 (3)	O1—C1—C10—C11	0.4 (3)
C10—C1—C2—C3	169.13 (18)	C2—C1—C10—C11	−179.08 (17)
C1—C2—C3—C4	−177.75 (18)	C15—C10—C11—C12	−0.4 (3)
C2—C3—C4—C9	−3.8 (3)	C1—C10—C11—C12	179.24 (17)
C2—C3—C4—C5	175.28 (19)	C18—O4—C12—C11	−4.6 (3)
C17—O2—C5—C6	2.4 (2)	C18—O4—C12—C13	175.86 (16)
C17—O2—C5—C4	−178.70 (15)	C10—C11—C12—O4	179.65 (16)
C9—C4—C5—O2	−175.91 (14)	C10—C11—C12—C13	−0.8 (3)
C3—C4—C5—O2	5.0 (2)	C19—O5—C13—C14	94.45 (19)
C9—C4—C5—C6	3.0 (2)	C19—O5—C13—C12	−87.4 (2)
C3—C4—C5—C6	−176.14 (16)	O4—C12—C13—O5	3.3 (2)

O2—C5—C6—C7	176.89 (15)	C11—C12—C13—O5	−176.24 (15)
C4—C5—C6—C7	−1.9 (3)	O4—C12—C13—C14	−178.56 (15)
C16—O3—C7—C6	0.5 (3)	C11—C12—C13—C14	1.9 (3)
C16—O3—C7—C8	−178.72 (18)	C20—O6—C14—C15	7.9 (3)
C5—C6—C7—O3	−179.56 (16)	C20—O6—C14—C13	−171.57 (17)
C5—C6—C7—C8	−0.4 (3)	O5—C13—C14—O6	−4.1 (2)
O3—C7—C8—C9	−179.29 (16)	C12—C13—C14—O6	177.80 (15)
C6—C7—C8—C9	1.5 (3)	O5—C13—C14—C15	176.41 (15)
C7—C8—C9—C4	−0.3 (3)	C12—C13—C14—C15	−1.7 (3)
C5—C4—C9—C8	−1.9 (3)	O6—C14—C15—C10	−178.97 (16)
C3—C4—C9—C8	177.22 (17)	C13—C14—C15—C10	0.5 (3)
O1—C1—C10—C15	−180.0 (2)	C11—C10—C15—C14	0.6 (3)
C2—C1—C10—C15	0.6 (3)	C1—C10—C15—C14	−179.05 (17)

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C4–C9 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···O6^{i}	0.93	2.65	3.562 (2)	166
C18—H18*B*···O3^{ii}	0.96	2.64	3.404 (2)	136
C16—H16*B*···O2^{iii}	0.96	2.68	3.389 (2)	132
C16—H16*C*···O1^{iii}	0.96	2.66	3.608 (3)	169
C19—H19*C*···*Cg*1^{iv}	0.96	2.79	3.530 (2)	134

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