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(*E*)-1-[4-(Hexyloxy)phenyl]-3-(4-hydroxyphenyl)prop-2-en-1-one

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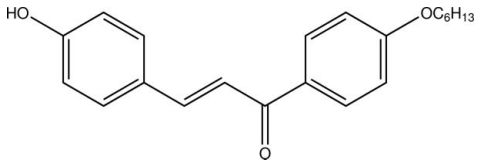
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.048; wR factor = 0.135; data-to-parameter ratio = 26.7.

In the title compound, $C_{21}H_{24}O_3$, intermolecular O—H···O and C—H···O interactions form bifurcated acceptor bonds, generating $R_2^1(6)$ ring motifs. These ring motifs link the molecules into extended chains along [010]. The crystal structure is further stabilized by C—H···π interactions.

Related literature

For the biological properties of chalcone derivatives, see: Bhat *et al.* (2005); Xue *et al.* (2004); Zhao *et al.* (2005); Lee *et al.* (2006). For related structures, see: Razak *et al.* (2009, 2009*a*,*b*); Ngaini, Fadzillah *et al.* (2009); Ngaini, Rahman *et al.* (2009). For details of hydrogen-bond motifs, see: Bernstein *et al.* (1995). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{21}H_{24}O_3$
M_r = 324.40
Monoclinic, $P2_1/c$
a = 10.2807 (2) Å
b = 16.6322 (2) Å
c = 11.4736 (2) Å
β = 113.439 (1)°
V = 1799.99 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 100 K
0.53 × 0.46 × 0.09 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.960, T_{max} = 0.993
35735 measured reflections
5839 independent reflections
4743 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.135
S = 1.03
5839 reflections
219 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

*Cg*2 is the centroid of the C10–C15 ring.

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1^{i}	0.84	1.86	2.694 (1)	175
C4—H4A···O1^{i}	0.95	2.54	3.213 (1)	128
C16—H16A···*Cg*2^{ii}	0.99	2.77	3.666 (1)	151

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2369).

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supporting information

Acta Cryst. (2011). E**67**, o169–o170 [https://doi.org/10.1107/S1600536810052086]

(*E*)-1-[4-(Hexyloxy)phenyl]-3-(4-hydroxyphenyl)prop-2-en-1-one

Zainab Ngaini, Siti Muhaini Haris Fadzillah, Hasnain Hussain, Ibrahim Abdul Razak and Hoong-Kun Fun

S1. Comment

The biological properties of chalcones derivatives have been extensively reported (Bhat *et al.*, 2005; Xue *et al.*, 2004; Lee *et al.*, 2006; Zhao *et al.*, 2005). Synthetic and naturally occurring chalcones have been widely studied and developed as one of the pharmaceutically important molecules. We have synthesized the title chalcone derivative, (I) which showed antimicrobial activity when tested against *E. coli* ATCC 8739 In this paper, we report the crystal structure of the title compound.

The bond lengths observed in the title compound (Fig.1) are comparable with previously reported values (Allen *et al.*, 1987). The conformation of the enone moiety (O1/C7—C9) is *s-cis* as shown by the value of -6.3 (2)° for O1—C9—C8—C7 torsion angle. The enone (O1/C7—C9) moiety adopts *s-cis* conformation with O2—C7—C8—C9 torsion angle being -6.3 (2)°. The dihedral angle between the mean plane through the enone moiety and the benzene rings is 5.1 (1)° for C1—C6 ring and 5.6 (1)° for C10—C15 ring. The two benzene rings make a dihedral angle of 7.8 (1)° between them.

The widening of C1—C6—C7 and C6—C7—C8 angles to 123.0 (1)° and 126.9 (1)° respectively, are the consequences of the close interatomic contact between H1A and H8A which is 2.20 Å. Similarly, the strain induced by short H8A···H11A contact, which is 2.09Å resulted in the opening of C9—C10—C11 angle to 123.8 (1)°. The distortion of angles, which is relative to what is predicted in terms of hybidization principles can also be observed in the related structures previously reported by Razak, Fun, Ngaini, Rahman *et al.* (2009), Razak, Fun, Ngaini, Fadzillah *et al.* (2009*a*,*b*), Ngaini, Fadzillah *et al.* (2009) and Ngaini, Rahman *et al.* (2009).

The conformation assumed by the zigzag alkoxyl tail is *trans*. Even though the torsion angle of C12—C13—O3—C16 is -1.3 (2)°, which shows that it is roughly coplanar with the attached benzene ring, the alkoxyl tail is actually twisted about the C18—C19 bond. Within the aliphatic chain, the C17—C18—C19—C20 torsion angle shows the value of -167.0 (1)°

In the crystal structure, intermolecular O2—H2···O1(-*x*,*y* - 1/2,-*z* + 3/2) and C4—H4A···O1(-*x*,*y* - 1/2,-*z* + 3/2) interactions form bifurcated acceptor bonds generating $R^1_2(6)$ ring motifs (Bernstein *et al.*, 1995). These intermolecular interactions link the molecules into extended chains along the [0 1 0] direction. The crystal structure is further stabilized by C—H···π interactions (Table 1).

S2. Experimental

A mixture of 4-hydroxybenzaldehyde (1.22 g, 10 mmol), 4-hexyloxyacetophenone (2.20 g, 10 mmol) and KOH (2.02 g, 36 mmol) in 30 ml of methanol was heated at reflux for 24 h. The reaction was cooled to room temperature and acidified with cold diluted HCl (2 N). The resulting precipitate was filtered, washed and dried. After redissolving in hexane-ethanol mixture, followed by few days of slow evaporation, suitable crystals were collected for X-ray analysis.

S3. Refinement

All the C– and O-bound H atoms were positioned geometrically and refined using a riding model with C—H = 0.93–0.97Å and O—H = 0.84 Å. The U_{iso} values were constrained to be -1.5U_{equ} (methyl H and O atoms) and -1.2U_{equ} (other H atoms). The rotating model group was applied for the methyl group.

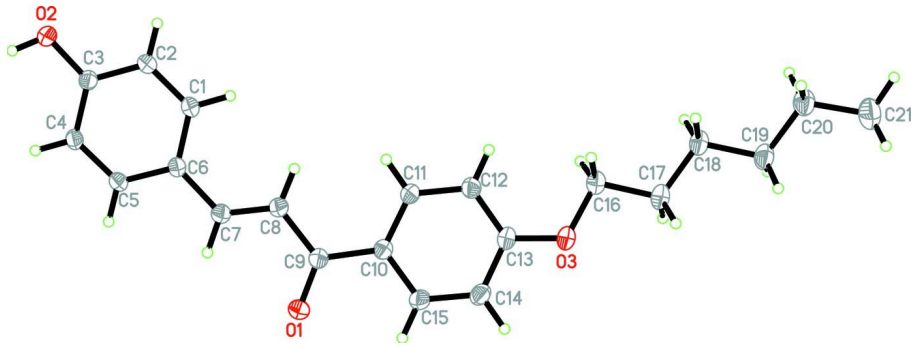

Figure 1

The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom numbering scheme.

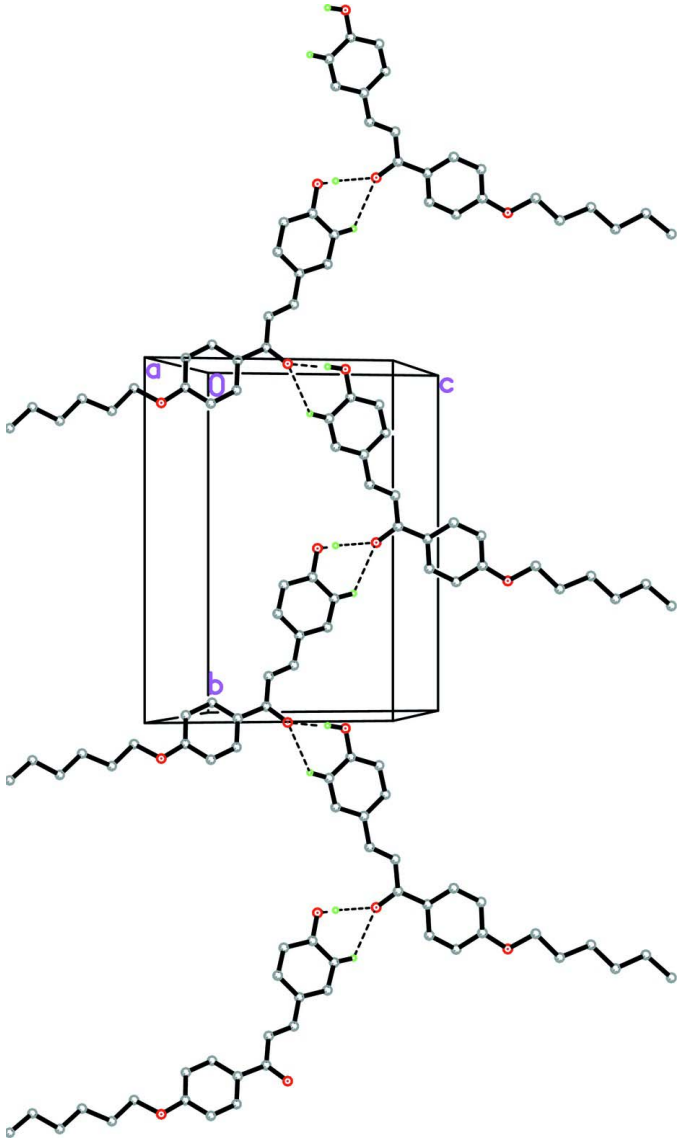

Figure 2

A molecular chain of the title compound along the b axis.

(*E*)-1-[4-(hexyloxy)phenyl]-3-(4-hydroxyphenyl)prop-2-en-1-one

Crystal data

$C_{21}H_{24}O_3$
$M_r = 324.40$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 10.2807\ (2)$ Å
$b = 16.6322\ (2)$ Å
$c = 11.4736\ (2)$ Å
$\beta = 113.439\ (1)°$
$V = 1799.99\ (5)$ Å^3
$Z = 4$

$F(000) = 696$
$D_x = 1.197$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9960 reflections
$\theta = 2.3–31.1°$
$\mu = 0.08$ mm^{-1}
$T = 100$ K
Plate, yellow
0.53 × 0.46 × 0.09 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: sealed tube
Graphite monochromator
π and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.960, T_{max} = 0.993
35735 measured reflections
5839 independent reflections
4743 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 31.3°, θ_{min} = 2.2°
h = −15→14
k = −24→24
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.135
S = 1.03
5839 reflections
219 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
$w = 1/[\sigma^2(F_o^2) + (0.0702P)^2 + 0.4086P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
O1	0.15448 (9)	0.50631 (5)	0.96314 (7)	0.02611 (17)
O2	−0.08883 (8)	0.02224 (4)	0.78756 (7)	0.02446 (16)
H2	−0.1115	0.0146	0.7095	0.037*
O3	0.37607 (9)	0.61122 (5)	1.53438 (7)	0.02772 (18)
C1	0.03955 (11)	0.20205 (6)	0.97710 (9)	0.0226 (2)
H1A	0.0805	0.2163	1.0645	0.027*
C2	0.00156 (11)	0.12297 (6)	0.94356 (9)	0.0231 (2)
H2A	0.0155	0.0836	1.0074	0.028*
C3	−0.05759 (10)	0.10104 (6)	0.81509 (9)	0.02014 (19)
C4	−0.08238 (10)	0.15987 (6)	0.72177 (9)	0.02078 (19)
H4A	−0.1251	0.1457	0.6344	0.025*
C5	−0.04439 (11)	0.23904 (6)	0.75716 (9)	0.02089 (19)
H5A	−0.0618	0.2787	0.6931	0.025*
C6	0.01911 (10)	0.26189 (6)	0.88518 (9)	0.01983 (18)

C7	0.06282 (10)	0.34531 (6)	0.91739 (9)	0.02114 (19)
H7A	0.0432	0.3814	0.8483	0.025*
C8	0.12779 (10)	0.37647 (6)	1.03444 (9)	0.02112 (19)
H8A	0.1482	0.3426	1.1062	0.025*
C9	0.16801 (10)	0.46172 (6)	1.05398 (9)	0.01995 (18)
C10	0.22628 (10)	0.49587 (6)	1.18407 (9)	0.01980 (19)
C11	0.24298 (10)	0.45194 (6)	1.29304 (9)	0.02125 (19)
H11A	0.2192	0.3964	1.2853	0.025*
C12	0.29373 (11)	0.48771 (6)	1.41261 (10)	0.0228 (2)
H12A	0.3043	0.4570	1.4856	0.027*
C13	0.32897 (11)	0.56930 (6)	1.42408 (10)	0.0227 (2)
C14	0.31631 (11)	0.61369 (6)	1.31623 (10)	0.0256 (2)
H14A	0.3432	0.6687	1.3244	0.031*
C15	0.26496 (11)	0.57768 (6)	1.19849 (10)	0.0239 (2)
H15A	0.2555	0.6085	1.1258	0.029*
C16	0.38894 (11)	0.57030 (7)	1.64912 (10)	0.0251 (2)
H16A	0.4594	0.5263	1.6688	0.030*
H16B	0.2966	0.5472	1.6399	0.030*
C17	0.43689 (12)	0.63306 (7)	1.75310 (10)	0.0281 (2)
H17A	0.3622	0.6745	1.7340	0.034*
H17B	0.5234	0.6597	1.7539	0.034*
C18	0.46809 (12)	0.59804 (7)	1.88375 (10)	0.0269 (2)
H18A	0.5392	0.5546	1.9007	0.032*
H18B	0.3803	0.5737	1.8838	0.032*
C19	0.52330 (13)	0.65975 (7)	1.99042 (11)	0.0298 (2)
H19A	0.4449	0.6959	1.9856	0.036*
H19B	0.5975	0.6928	1.9792	0.036*
C20	0.58473 (13)	0.61976 (7)	2.12078 (11)	0.0321 (2)
H20A	0.5103	0.5862	2.1308	0.038*
H20B	0.6628	0.5836	2.1247	0.038*
C21	0.64050 (18)	0.67832 (10)	2.23034 (13)	0.0502 (4)
H21A	0.6852	0.6485	2.3102	0.075*
H21B	0.5619	0.7105	2.2330	0.075*
H21C	0.7105	0.7139	2.2189	0.075*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0332 (4)	0.0223 (3)	0.0210 (4)	0.0006 (3)	0.0089 (3)	0.0028 (3)
O2	0.0315 (4)	0.0194 (3)	0.0214 (4)	−0.0027 (3)	0.0093 (3)	−0.0019 (3)
O3	0.0343 (4)	0.0242 (4)	0.0233 (4)	−0.0042 (3)	0.0100 (3)	−0.0070 (3)
C1	0.0279 (5)	0.0224 (4)	0.0164 (4)	−0.0004 (4)	0.0076 (4)	−0.0011 (3)
C2	0.0293 (5)	0.0217 (4)	0.0179 (4)	0.0000 (4)	0.0091 (4)	0.0016 (3)
C3	0.0213 (4)	0.0196 (4)	0.0199 (4)	−0.0004 (3)	0.0086 (4)	−0.0015 (3)
C4	0.0230 (4)	0.0220 (4)	0.0167 (4)	0.0003 (4)	0.0073 (4)	−0.0018 (3)
C5	0.0243 (4)	0.0214 (4)	0.0164 (4)	0.0012 (4)	0.0075 (4)	0.0011 (3)
C6	0.0220 (4)	0.0200 (4)	0.0177 (4)	0.0002 (3)	0.0081 (3)	−0.0011 (3)
C7	0.0225 (4)	0.0205 (4)	0.0202 (4)	0.0008 (3)	0.0083 (4)	0.0004 (3)

C8	0.0233 (4)	0.0191 (4)	0.0201 (4)	0.0002 (3)	0.0076 (4)	0.0002 (3)
C9	0.0185 (4)	0.0201 (4)	0.0201 (4)	0.0016 (3)	0.0064 (3)	−0.0002 (3)
C10	0.0179 (4)	0.0193 (4)	0.0205 (4)	0.0007 (3)	0.0058 (3)	−0.0008 (3)
C11	0.0214 (4)	0.0202 (4)	0.0213 (5)	−0.0028 (3)	0.0077 (4)	−0.0016 (3)
C12	0.0229 (4)	0.0239 (5)	0.0207 (5)	−0.0029 (4)	0.0078 (4)	−0.0017 (4)
C13	0.0209 (4)	0.0231 (5)	0.0226 (5)	−0.0015 (4)	0.0071 (4)	−0.0049 (4)
C14	0.0283 (5)	0.0183 (4)	0.0274 (5)	−0.0006 (4)	0.0082 (4)	−0.0025 (4)
C15	0.0265 (5)	0.0197 (4)	0.0234 (5)	0.0011 (4)	0.0076 (4)	0.0015 (4)
C16	0.0247 (5)	0.0269 (5)	0.0234 (5)	−0.0025 (4)	0.0093 (4)	−0.0054 (4)
C17	0.0294 (5)	0.0276 (5)	0.0256 (5)	−0.0027 (4)	0.0091 (4)	−0.0088 (4)
C18	0.0260 (5)	0.0267 (5)	0.0257 (5)	−0.0008 (4)	0.0077 (4)	−0.0071 (4)
C19	0.0310 (5)	0.0274 (5)	0.0271 (5)	0.0000 (4)	0.0074 (4)	−0.0078 (4)
C20	0.0324 (6)	0.0314 (6)	0.0295 (6)	0.0017 (5)	0.0093 (5)	−0.0061 (4)
C21	0.0633 (10)	0.0464 (8)	0.0306 (7)	−0.0042 (7)	0.0078 (6)	−0.0100 (6)

Geometric parameters (Å, º)

O1—C9	1.2410 (12)	C12—C13	1.3971 (14)
O2—C3	1.3563 (12)	C12—H12A	0.9500
O2—H2	0.8400	C13—C14	1.4018 (15)
O3—C13	1.3545 (12)	C14—C15	1.3766 (15)
O3—C16	1.4406 (13)	C14—H14A	0.9500
C1—C2	1.3824 (14)	C15—H15A	0.9500
C1—C6	1.4039 (14)	C16—C17	1.5127 (14)
C1—H1A	0.9500	C16—H16A	0.9900
C2—C3	1.4009 (14)	C16—H16B	0.9900
C2—H2A	0.9500	C17—C18	1.5187 (16)
C3—C4	1.3971 (13)	C17—H17A	0.9900
C4—C5	1.3874 (14)	C17—H17B	0.9900
C4—H4A	0.9500	C18—C19	1.5235 (15)
C5—C6	1.4019 (13)	C18—H18A	0.9900
C5—H5A	0.9500	C18—H18B	0.9900
C6—C7	1.4598 (14)	C19—C20	1.5253 (17)
C7—C8	1.3435 (14)	C19—H19A	0.9900
C7—H7A	0.9500	C19—H19B	0.9900
C8—C9	1.4690 (13)	C20—C21	1.5113 (18)
C8—H8A	0.9500	C20—H20A	0.9900
C9—C10	1.4826 (14)	C20—H20B	0.9900
C10—C11	1.3985 (14)	C21—H21A	0.9800
C10—C15	1.4088 (14)	C21—H21B	0.9800
C11—C12	1.3925 (14)	C21—H21C	0.9800
C11—H11A	0.9500		
C3—O2—H2	109.5	C15—C14—H14A	119.9
C13—O3—C16	118.65 (8)	C13—C14—H14A	119.9
C2—C1—C6	121.61 (9)	C14—C15—C10	121.04 (10)
C2—C1—H1A	119.2	C14—C15—H15A	119.5
C6—C1—H1A	119.2	C10—C15—H15A	119.5

C1—C2—C3	119.80 (9)	O3—C16—C17	106.11 (9)
C1—C2—H2A	120.1	O3—C16—H16A	110.5
C3—C2—H2A	120.1	C17—C16—H16A	110.5
O2—C3—C4	122.97 (9)	O3—C16—H16B	110.5
O2—C3—C2	117.40 (9)	C17—C16—H16B	110.5
C4—C3—C2	119.64 (9)	H16A—C16—H16B	108.7
C5—C4—C3	119.74 (9)	C16—C17—C18	112.85 (9)
C5—C4—H4A	120.1	C16—C17—H17A	109.0
C3—C4—H4A	120.1	C18—C17—H17A	109.0
C4—C5—C6	121.57 (9)	C16—C17—H17B	109.0
C4—C5—H5A	119.2	C18—C17—H17B	109.0
C6—C5—H5A	119.2	H17A—C17—H17B	107.8
C5—C6—C1	117.59 (9)	C17—C18—C19	113.55 (9)
C5—C6—C7	119.41 (9)	C17—C18—H18A	108.9
C1—C6—C7	122.99 (9)	C19—C18—H18A	108.9
C8—C7—C6	126.90 (9)	C17—C18—H18B	108.9
C8—C7—H7A	116.6	C19—C18—H18B	108.9
C6—C7—H7A	116.6	H18A—C18—H18B	107.7
C7—C8—C9	121.52 (9)	C18—C19—C20	111.76 (10)
C7—C8—H8A	119.2	C18—C19—H19A	109.3
C9—C8—H8A	119.2	C20—C19—H19A	109.3
O1—C9—C8	121.19 (9)	C18—C19—H19B	109.3
O1—C9—C10	118.82 (9)	C20—C19—H19B	109.3
C8—C9—C10	119.99 (9)	H19A—C19—H19B	107.9
C11—C10—C15	118.10 (9)	C21—C20—C19	114.00 (11)
C11—C10—C9	123.83 (9)	C21—C20—H20A	108.8
C15—C10—C9	118.06 (9)	C19—C20—H20A	108.8
C12—C11—C10	121.48 (9)	C21—C20—H20B	108.8
C12—C11—H11A	119.3	C19—C20—H20B	108.8
C10—C11—H11A	119.3	H20A—C20—H20B	107.6
C11—C12—C13	119.29 (10)	C20—C21—H21A	109.5
C11—C12—H12A	120.4	C20—C21—H21B	109.5
C13—C12—H12A	120.4	H21A—C21—H21B	109.5
O3—C13—C12	124.81 (10)	C20—C21—H21C	109.5
O3—C13—C14	115.26 (9)	H21A—C21—H21C	109.5
C12—C13—C14	119.93 (9)	H21B—C21—H21C	109.5
C15—C14—C13	120.12 (10)		

C6—C1—C2—C3	0.63 (16)	C8—C9—C10—C15	179.28 (9)
C1—C2—C3—O2	177.98 (9)	C15—C10—C11—C12	1.21 (15)
C1—C2—C3—C4	−2.28 (15)	C9—C10—C11—C12	−177.74 (9)
O2—C3—C4—C5	−178.39 (9)	C10—C11—C12—C13	−0.09 (15)
C2—C3—C4—C5	1.89 (15)	C16—O3—C13—C12	−1.30 (15)
C3—C4—C5—C6	0.16 (15)	C16—O3—C13—C14	178.63 (9)
C4—C5—C6—C1	−1.76 (15)	C11—C12—C13—O3	178.38 (9)
C4—C5—C6—C7	177.29 (9)	C11—C12—C13—C14	−1.55 (15)
C2—C1—C6—C5	1.36 (15)	O3—C13—C14—C15	−177.87 (9)
C2—C1—C6—C7	−177.65 (10)	C12—C13—C14—C15	2.07 (16)

C5—C6—C7—C8	−178.26 (10)	C13—C14—C15—C10	−0.93 (16)
C1—C6—C7—C8	0.73 (16)	C11—C10—C15—C14	−0.70 (15)
C6—C7—C8—C9	179.19 (9)	C9—C10—C15—C14	178.32 (9)
C7—C8—C9—O1	−6.32 (15)	C13—O3—C16—C17	−177.53 (9)
C7—C8—C9—C10	173.83 (9)	O3—C16—C17—C18	−175.01 (9)
O1—C9—C10—C11	178.37 (9)	C16—C17—C18—C19	177.23 (9)
C8—C9—C10—C11	−1.77 (14)	C17—C18—C19—C20	−166.95 (10)
O1—C9—C10—C15	−0.58 (14)	C18—C19—C20—C21	−179.71 (11)

Hydrogen-bond geometry (Å, º)

Cg2 is the centroid of C10–C15 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1^{i}	0.84	1.86	2.694 (1)	175
C4—H4*A*···O1^{i}	0.95	2.54	3.213 (1)	128
C16—H16*A*···*Cg*2^{ii}	0.99	2.77	3.666 (1)	151

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