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(1*E*,4*Z*,6*E*)-5-Hydroxy-1,7-bis(2-methoxyphenyl)-1,4,6-heptatrien-3-one

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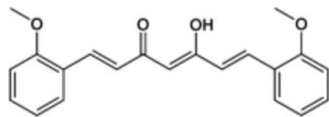
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 Key indicators: single-crystal X-ray study; $T = 150$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.044; wR factor = 0.120; data-to-parameter ratio = 13.1.

In the title compound, $\text{C}_{21}\text{H}_{20}\text{O}_4$, the central heptatrienone unit is approximately planar, with a maximum atomic deviation of 0.1121 (11) Å; the two benzene rings are twisted with respect to the heptatrienone mean plane by 2.73 (5) and 29.31 (4)°. The molecule exists in the enol form and the hydroxy group forms an intramolecular hydrogen bond with the neighboring carbonyl group. Weak intermolecular C—H...O hydrogen bonding is present in the crystal structure.

Related literature

For potential applications of curcumin and its derivatives in medicine, see: Reddy & Lokesh (1992); Sreejayan Rao (1997); Narlawar *et al.* (2008); Qiu *et al.* (2010). For the tautomerism of curcumin and its analogues, see: Gunasekaran *et al.* (2008).



Experimental

Crystal data

$\text{C}_{21}\text{H}_{20}\text{O}_4$
 $M_r = 336.37$
Triclinic, $P\bar{1}$
 $a = 7.3234$ (11) Å
 $b = 7.7960$ (12) Å
 $c = 16.897$ (3) Å

$\alpha = 96.819$ (3)°
 $\beta = 95.641$ (3)°
 $\gamma = 115.520$ (2)°
 $V = 852.3$ (2) Å³
 $Z = 2$
Mo $K\alpha$ radiation

$\mu = 0.09$ mm⁻¹
 $T = 150$ K

0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEXII CCD
diffractometer
5805 measured reflections

2998 independent reflections
2238 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.022$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.120$
 $S = 1.05$
2998 reflections

229 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.19$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.24$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O3}-\text{H3}'\cdots\text{O2}$	0.82	1.77	2.5003 (18)	147
$\text{C5}-\text{H5}\cdots\text{O2}^i$	0.93	2.45	3.351 (2)	162
$\text{C8}-\text{H8}\cdots\text{O2}^i$	0.93	2.49	3.413 (2)	169

Symmetry code: (i) $-x + 2, -y + 2, -z + 1$.

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINTE* (Bruker, 2008); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1999); software used to prepare material for publication: *SHELXL97* and *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5219).

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supporting information

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(1*E*,4*Z*,6*E*)-5-Hydroxy-1,7-bis(2-methoxyphenyl)-1,4,6-heptatrien-3-one

Yiliang Zhao, Paul W. Groundwater, David E. Hibbs, Paul K. Nguyen and Rajeshwar Narlawar

S1. Comment

The title compound is a derivative of curcumin. The curcumin and its derivatives have potent applications in the medicine field (Reddy & Lokesh, 1992; Sreejayan Rao, 1997; Narlawar *et al.*, 2008; Qiu *et al.*, 2010). We synthesized non-natural curcumin analogs in order to increase the NF- κ B inhibitory activity and reduce the cell toxicity.

The molecular structure of the compound is showing in Fig. 1. The bond lengths indicate the electron delocalization in the molecular structure. The central heptatrienone unit is approximately planar with the maximum atomic deviation of $-0.1121(11)$ Å; the two benzene rings are twisted with respect to the heptatrienone mean plane at $2.73(5)$ and $29.31(4)^\circ$, respectively. In the solution, curcumin and its non-natural analogs exist as ketol-enol tautomeric forms (Gunasekaran *et al.*, 2008). In the crystal, the title compound exists as an enol form, the hydroxy group forms an intra-molecular hydrogen bond to the neighboring carbonyl group.

Weak intermolecular C—H \cdots O hydrogen bonding is present in the crystal structure (Table 1).

S2. Experimental

In a dry three-necked flask, 1.03 ml acetylacetone (10 mmol) and 0.488 g boron oxide (3.5 mmol) were dissolved in 10 ml ethyl acetate and heated to 75°C for 1 h. Methoxybenzaldehyde (2.84 ml, 20 mmol) and tributylborate (4.8 ml, 20 mmol) were mixed with 10 ml ethyl acetate, stirred for 45 min and then added to the solution.

The mixture was heated to 100°C for 1 h, then *n*-butylamine (1.54 ml, 15 mmol) dissolved in 15 ml ethyl acetate was added dropwise over a period of 90 min. The reaction was stirred for 18 h at 85°C , cooled to 60°C , then 4*M* HCl solution (5 ml) was added and the mixture stirred at 60°C for 1 h.

The reaction mixture was cooled to ambient temperature, the organic layer was separated and the aqueous layer was extracted with ethyl acetate (3×100 ml). The combined organic layers were washed with 100 ml of brine, dried over anhydrous Na_2SO_4 and evaporated *in vacuo*.

The crude compound was purified by flash column chromatography, using 4% ethyl acetate in petroleum ether to give the title compound as a yellow solid (0.35 g, 5%). Single crystals suitable for X-ray data collection were obtained by slow evaporation of an ethyl acetate:petroleum ether (2:8) solution.

S3. Refinement

H atoms were placed in calculated positions with O—H = 0.82, C—H = 0.93 to 0.96 Å, and were refined in a riding mode with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for aromatic H atoms and $1.5U_{\text{eq}}(\text{C}, \text{O})$ for the others.

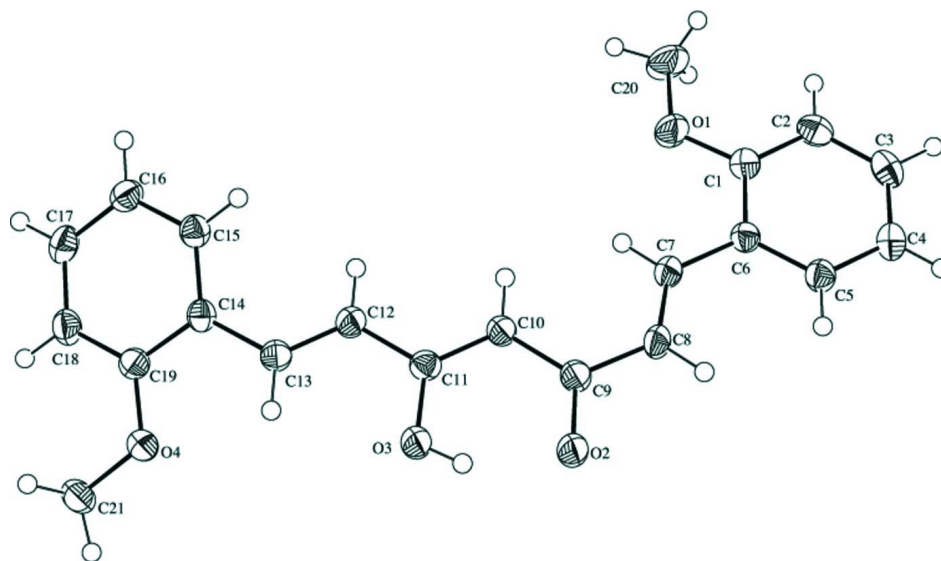


Figure 1

The molecular structure of the title compound with 50% probability displacement ellipsoids for non-H atoms.

(1E,4Z,6E)-5-Hydroxy-1,7-bis(2-methoxyphenyl)-1,4,6-heptatrien-3-one

Crystal data

$C_{21}H_{20}O_4$

$M_r = 336.37$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 7.3234$ (11) Å

$b = 7.7960$ (12) Å

$c = 16.897$ (3) Å

$\alpha = 96.819$ (3)°

$\beta = 95.641$ (3)°

$\gamma = 115.520$ (2)°

$V = 852.3$ (2) Å³

$Z = 2$

$F(000) = 356$

$D_x = 1.311$ Mg m⁻³

Melting point: 397(2) K

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 500 reflections

$\theta = 1.1$ – 28.2 °

$\mu = 0.09$ mm⁻¹

$T = 150$ K

Block, yellow

$0.30 \times 0.20 \times 0.20$ mm

Data collection

Bruker SMART APEXII CCD
diffractometer

Radiation source: fine-focus sealed tube, Bruker
K760

Graphite monochromator

ω scans

5805 measured reflections

2998 independent reflections

2238 reflections with $I > 2\sigma(I)$

$R_{int} = 0.022$

$\theta_{max} = 25.2$ °, $\theta_{min} = 2.5$ °

$h = -8 \rightarrow 8$

$k = -7 \rightarrow 9$

$l = -20 \rightarrow 20$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.044$

$wR(F^2) = 0.120$

$S = 1.05$

2998 reflections

229 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

$$w = 1/[\sigma^2(F_o^2) + (0.0634P)^2 + 0.0684P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.009$

$$\Delta\rho_{\max} = 0.19 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.24 \text{ e } \text{\AA}^{-3}$$

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.

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.6037 (2)	0.3920 (3)	0.64590 (10)	0.0297 (4)
C2	0.5514 (3)	0.3937 (3)	0.72270 (10)	0.0344 (4)
H2	0.4929	0.2793	0.7428	0.041*
C3	0.5873 (3)	0.5672 (3)	0.76908 (10)	0.0354 (5)
H3	0.5524	0.5687	0.8205	0.042*
C4	0.6743 (3)	0.7384 (3)	0.74013 (10)	0.0338 (4)
H4	0.6964	0.8541	0.7716	0.041*
C5	0.7279 (2)	0.7363 (3)	0.66415 (9)	0.0297 (4)
H5	0.7877	0.8518	0.6450	0.036*
C6	0.6946 (2)	0.5643 (2)	0.61529 (9)	0.0268 (4)
C7	0.7506 (2)	0.5582 (2)	0.53473 (9)	0.0281 (4)
H7	0.7175	0.4365	0.5058	0.034*
C8	0.8438 (2)	0.7075 (3)	0.49809 (10)	0.0304 (4)
H8	0.8820	0.8307	0.5266	0.036*
C9	0.8905 (2)	0.6913 (3)	0.41590 (9)	0.0280 (4)
C10	0.8584 (2)	0.5123 (2)	0.37012 (9)	0.0272 (4)
H10	0.8122	0.4023	0.3937	0.033*
C11	0.8942 (2)	0.4988 (2)	0.29240 (9)	0.0268 (4)
C12	0.8535 (2)	0.3168 (2)	0.24370 (9)	0.0283 (4)
H12	0.8155	0.2092	0.2687	0.034*
C13	0.8668 (2)	0.2926 (3)	0.16534 (9)	0.0281 (4)
H13	0.9086	0.4020	0.1415	0.034*
C14	0.8221 (2)	0.1110 (2)	0.11348 (9)	0.0264 (4)
C15	0.8139 (2)	-0.0505 (2)	0.14426 (10)	0.0293 (4)
H15	0.8443	-0.0406	0.1999	0.035*
C16	0.7621 (2)	-0.2245 (3)	0.09447 (10)	0.0315 (4)
H16	0.7570	-0.3302	0.1163	0.038*
C17	0.7178 (3)	-0.2390 (3)	0.01173 (10)	0.0348 (4)
H17	0.6811	-0.3559	-0.0221	0.042*
C18	0.7274 (3)	-0.0814 (3)	-0.02129 (10)	0.0335 (4)
H18	0.6975	-0.0930	-0.0770	0.040*
C19	0.7815 (2)	0.0937 (2)	0.02861 (9)	0.0275 (4)

C20	0.4696 (3)	0.0470 (3)	0.62014 (13)	0.0528 (6)
H20A	0.5460	0.0455	0.6694	0.079*
H20B	0.4574	-0.0550	0.5788	0.079*
H20C	0.3353	0.0284	0.6290	0.079*
C21	0.7528 (3)	0.2469 (3)	-0.08326 (9)	0.0361 (4)
H21A	0.8425	0.2087	-0.1101	0.054*
H21B	0.7722	0.3714	-0.0938	0.054*
H21C	0.6129	0.1539	-0.1030	0.054*
O1	0.57382 (19)	0.22818 (18)	0.59524 (7)	0.0404 (3)
O2	0.95885 (19)	0.84396 (17)	0.38537 (7)	0.0373 (3)
O3	0.96478 (19)	0.65274 (18)	0.25677 (7)	0.0355 (3)
H3'	0.9801	0.7482	0.2883	0.053*
O4	0.79859 (17)	0.25673 (17)	0.00178 (6)	0.0335 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0299 (9)	0.0292 (10)	0.0291 (9)	0.0131 (8)	0.0038 (7)	0.0041 (8)
C2	0.0337 (10)	0.0361 (11)	0.0333 (10)	0.0132 (8)	0.0080 (7)	0.0138 (8)
C3	0.0332 (9)	0.0475 (13)	0.0250 (9)	0.0171 (9)	0.0072 (7)	0.0067 (8)
C4	0.0335 (9)	0.0356 (11)	0.0288 (9)	0.0142 (8)	0.0035 (7)	-0.0010 (8)
C5	0.0314 (9)	0.0268 (10)	0.0273 (9)	0.0102 (8)	0.0047 (7)	0.0027 (7)
C6	0.0269 (8)	0.0258 (10)	0.0261 (9)	0.0108 (7)	0.0030 (7)	0.0040 (7)
C7	0.0315 (9)	0.0241 (10)	0.0258 (9)	0.0110 (8)	0.0033 (7)	0.0003 (7)
C8	0.0383 (10)	0.0222 (10)	0.0258 (9)	0.0102 (8)	0.0059 (7)	-0.0008 (7)
C9	0.0288 (9)	0.0245 (10)	0.0270 (9)	0.0085 (7)	0.0045 (7)	0.0046 (7)
C10	0.0312 (9)	0.0234 (9)	0.0245 (8)	0.0100 (7)	0.0046 (7)	0.0042 (7)
C11	0.0262 (8)	0.0236 (9)	0.0282 (9)	0.0091 (7)	0.0032 (7)	0.0052 (7)
C12	0.0313 (9)	0.0241 (10)	0.0287 (9)	0.0113 (8)	0.0066 (7)	0.0049 (7)
C13	0.0287 (9)	0.0260 (10)	0.0283 (9)	0.0107 (7)	0.0063 (7)	0.0052 (7)
C14	0.0243 (8)	0.0281 (10)	0.0264 (9)	0.0113 (7)	0.0065 (6)	0.0035 (7)
C15	0.0287 (9)	0.0302 (10)	0.0283 (9)	0.0122 (8)	0.0067 (7)	0.0048 (7)
C16	0.0328 (9)	0.0268 (10)	0.0371 (10)	0.0143 (8)	0.0099 (7)	0.0066 (8)
C17	0.0365 (10)	0.0283 (11)	0.0361 (10)	0.0133 (8)	0.0079 (8)	-0.0028 (8)
C18	0.0383 (10)	0.0351 (11)	0.0254 (9)	0.0157 (8)	0.0063 (7)	0.0005 (8)
C19	0.0262 (8)	0.0263 (10)	0.0299 (9)	0.0109 (7)	0.0076 (7)	0.0061 (7)
C20	0.0698 (14)	0.0275 (12)	0.0646 (14)	0.0198 (11)	0.0241 (11)	0.0186 (10)
C21	0.0405 (10)	0.0443 (12)	0.0284 (9)	0.0212 (9)	0.0099 (8)	0.0125 (8)
O1	0.0556 (8)	0.0249 (7)	0.0414 (7)	0.0157 (6)	0.0178 (6)	0.0098 (6)
O2	0.0537 (8)	0.0227 (7)	0.0312 (7)	0.0114 (6)	0.0141 (6)	0.0051 (5)
O3	0.0508 (8)	0.0248 (7)	0.0288 (6)	0.0138 (6)	0.0124 (6)	0.0052 (5)
O4	0.0454 (7)	0.0302 (7)	0.0265 (6)	0.0177 (6)	0.0079 (5)	0.0065 (5)

Geometric parameters (Å, °)

C1—O1	1.369 (2)	C12—H12	0.9300
C1—C2	1.389 (2)	C13—C14	1.460 (2)
C1—C6	1.406 (2)	C13—H13	0.9300

C2—C3	1.384 (3)	C14—C15	1.398 (2)
C2—H2	0.9300	C14—C19	1.414 (2)
C3—C4	1.382 (3)	C15—C16	1.384 (2)
C3—H3	0.9300	C15—H15	0.9300
C4—C5	1.380 (2)	C16—C17	1.384 (2)
C4—H4	0.9300	C16—H16	0.9300
C5—C6	1.398 (2)	C17—C18	1.386 (2)
C5—H5	0.9300	C17—H17	0.9300
C6—C7	1.461 (2)	C18—C19	1.388 (3)
C7—C8	1.332 (2)	C18—H18	0.9300
C7—H7	0.9300	C19—O4	1.359 (2)
C8—C9	1.466 (2)	C20—O1	1.425 (2)
C8—H8	0.9300	C20—H20A	0.9600
C9—O2	1.271 (2)	C20—H20B	0.9600
C9—C10	1.424 (2)	C20—H20C	0.9600
C10—C11	1.365 (2)	C21—O4	1.4283 (18)
C10—H10	0.9300	C21—H21A	0.9600
C11—O3	1.3297 (19)	C21—H21B	0.9600
C11—C12	1.445 (2)	C21—H21C	0.9600
C12—C13	1.334 (2)	O3—H3'	0.8200
O1—C1—C2	123.87 (16)	C12—C13—C14	126.25 (16)
O1—C1—C6	115.31 (14)	C12—C13—H13	116.9
C2—C1—C6	120.82 (16)	C14—C13—H13	116.9
C3—C2—C1	119.36 (17)	C15—C14—C19	117.82 (15)
C3—C2—H2	120.3	C15—C14—C13	122.64 (14)
C1—C2—H2	120.3	C19—C14—C13	119.53 (15)
C4—C3—C2	121.01 (16)	C16—C15—C14	121.97 (15)
C4—C3—H3	119.5	C16—C15—H15	119.0
C2—C3—H3	119.5	C14—C15—H15	119.0
C5—C4—C3	119.41 (17)	C17—C16—C15	119.04 (16)
C5—C4—H4	120.3	C17—C16—H16	120.5
C3—C4—H4	120.3	C15—C16—H16	120.5
C4—C5—C6	121.47 (16)	C16—C17—C18	120.78 (17)
C4—C5—H5	119.3	C16—C17—H17	119.6
C6—C5—H5	119.3	C18—C17—H17	119.6
C5—C6—C1	117.92 (15)	C17—C18—C19	120.17 (16)
C5—C6—C7	122.55 (15)	C17—C18—H18	119.9
C1—C6—C7	119.53 (15)	C19—C18—H18	119.9
C8—C7—C6	127.18 (16)	O4—C19—C18	124.39 (15)
C8—C7—H7	116.4	O4—C19—C14	115.44 (14)
C6—C7—H7	116.4	C18—C19—C14	120.18 (16)
C7—C8—C9	124.57 (16)	O1—C20—H20A	109.5
C7—C8—H8	117.7	O1—C20—H20B	109.5
C9—C8—H8	117.7	H20A—C20—H20B	109.5
O2—C9—C10	120.10 (14)	O1—C20—H20C	109.5
O2—C9—C8	117.60 (15)	H20A—C20—H20C	109.5
C10—C9—C8	122.29 (15)	H20B—C20—H20C	109.5

C11—C10—C9	121.33 (15)	O4—C21—H21A	109.5
C11—C10—H10	119.3	O4—C21—H21B	109.5
C9—C10—H10	119.3	H21A—C21—H21B	109.5
O3—C11—C10	121.55 (15)	O4—C21—H21C	109.5
O3—C11—C12	116.30 (14)	H21A—C21—H21C	109.5
C10—C11—C12	122.14 (15)	H21B—C21—H21C	109.5
C13—C12—C11	124.44 (16)	C1—O1—C20	118.23 (14)
C13—C12—H12	117.8	C11—O3—H3'	109.5
C11—C12—H12	117.8	C19—O4—C21	118.11 (13)
O1—C1—C2—C3	-179.73 (15)	O3—C11—C12—C13	-5.5 (2)
C6—C1—C2—C3	0.8 (2)	C10—C11—C12—C13	173.19 (15)
C1—C2—C3—C4	0.0 (3)	C11—C12—C13—C14	-178.32 (15)
C2—C3—C4—C5	-0.7 (2)	C12—C13—C14—C15	-18.2 (3)
C3—C4—C5—C6	0.6 (2)	C12—C13—C14—C19	160.64 (15)
C4—C5—C6—C1	0.1 (2)	C19—C14—C15—C16	-1.9 (2)
C4—C5—C6—C7	-179.81 (14)	C13—C14—C15—C16	176.95 (14)
O1—C1—C6—C5	179.67 (14)	C14—C15—C16—C17	0.3 (2)
C2—C1—C6—C5	-0.8 (2)	C15—C16—C17—C18	0.8 (2)
O1—C1—C6—C7	-0.4 (2)	C16—C17—C18—C19	-0.1 (3)
C2—C1—C6—C7	179.11 (15)	C17—C18—C19—O4	178.77 (14)
C5—C6—C7—C8	2.5 (3)	C17—C18—C19—C14	-1.6 (2)
C1—C6—C7—C8	-177.40 (16)	C15—C14—C19—O4	-177.76 (13)
C6—C7—C8—C9	-178.05 (15)	C13—C14—C19—O4	3.3 (2)
C7—C8—C9—O2	172.23 (16)	C15—C14—C19—C18	2.6 (2)
C7—C8—C9—C10	-6.7 (3)	C13—C14—C19—C18	-176.36 (15)
O2—C9—C10—C11	-1.9 (2)	C2—C1—O1—C20	4.7 (2)
C8—C9—C10—C11	177.04 (14)	C6—C1—O1—C20	-175.74 (15)
C9—C10—C11—O3	1.5 (2)	C18—C19—O4—C21	1.7 (2)
C9—C10—C11—C12	-177.04 (14)	C14—C19—O4—C21	-177.93 (13)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3' \cdots O2	0.82	1.77	2.5003 (18)	147
C5—H5' \cdots O2 ⁱ	0.93	2.45	3.351 (2)	162
C8—H8' \cdots O2 ⁱ	0.93	2.49	3.413 (2)	169

Symmetry code: (i) $-x+2, -y+2, -z+1$.