

William T. A. Harrison,^{a*}
 S. Bindya,^b H. S. Yathirajan,^b
 B. K. Sarojini^c and B. Narayana^d

^aDepartment of Chemistry, University of Aberdeen, Meston Walk, Aberdeen AB24 3UE, Scotland, ^bDepartment of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India, ^cDepartment of Chemistry, P. A. College of Engineering, Nadupadavu, Mangalore 574 153, India, and ^dDepartment of Chemistry, Mangalore University, Mangalagangotri 574 199, India

Correspondence e-mail:
 w.harrison@abdn.ac.uk

Key indicators

Single-crystal X-ray study
 T = 120 K
 Mean $\sigma(\text{C}-\text{C}) = 0.006 \text{ \AA}$
 R factor = 0.049
 wR factor = 0.104
 Data-to-parameter ratio = 15.9

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

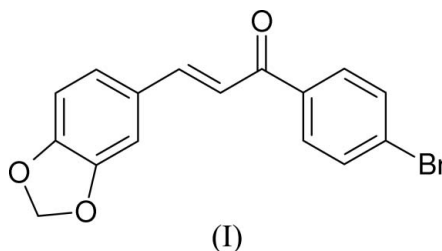
(2E)-3-(1,3-Benzodioxol-5-yl)-1-(4-bromophenyl)prop-2-en-1-one

In the approximately planar molecule of the title compound, $\text{C}_{16}\text{H}_{11}\text{BrO}_3$, the dihedral angle between the two benzene rings is $6.61 (18)^\circ$. This compound crystallizes in a centrosymmetric space group, so it does not display a second-harmonic generation response.

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Comment

Chalcones have important biological (Dimmock *et al.*, 1999) and optical properties (Uchida *et al.*, 1998). As part of our ongoing studies of these compounds (Harrison *et al.*, 2006), the synthesis and structure of the title compound, (I) (Fig. 1), are presented here. Compound (I) is closely related to (*E*)-3-(1,3-benzodioxol-5-yl)-1-(4-phenyl)-2-propen-1-one, (II) (Yathirajan *et al.*, 2006; Yang *et al.*, 2006), with an H atom in (II) replaced by the Br atom in (I).



The crystal structure of compound (I) is centrosymmetric (space group $P2_1/n$), and thus it has no second-harmonic generation (SHG) response (Watson *et al.*, 1993). The geometric parameters for (I) fall within their expected ranges (Allen *et al.*, 1987). For the C1–C6 benzene ring, the r.m.s. deviation from the mean plane is 0.007 \AA [maximum deviation = $0.010 (3) \text{ \AA}$ for atom C1]. For the enone O1/C7/C8/C9 fragment and the C10–C15 benzene ring, the corresponding values are 0.004 \AA [maximum deviation = $0.005 (3) \text{ \AA}$ for atom C7] and 0.004 \AA [maximum deviation = $0.007 (3) \text{ \AA}$ for atom C13]. The dihedral angles between atoms O1/C7/C8/C9 and the C1 and C10 benzene ring mean planes are $4.6 (3)$ and $2.4 (3)^\circ$, respectively. The dihedral angle between the benzene ring best planes (C1–C6 and C10–C15) in (I) is $6.61 (18)^\circ$, which is much less than the corresponding value of $26.89 (5)^\circ$ in (II) (Yathirajan *et al.*, 2006). Atom C16 in (I) is displaced from the C10–C15 benzene ring mean plane by $0.147 (7) \text{ \AA}$.

A PLATON (Spek, 2003) analysis of (I) indicated two possible intermolecular C–H...O interactions (Table 1) that might help to establish the crystal packing, which results in [110] chains of molecules (Fig. 2). A slightly short $\text{Br1}\cdots\text{O3}^i$ [symmetry code: (i) $\frac{3}{2} + x, \frac{3}{2} - y, z - \frac{1}{2}$] contact of $3.237 (3) \text{ \AA}$

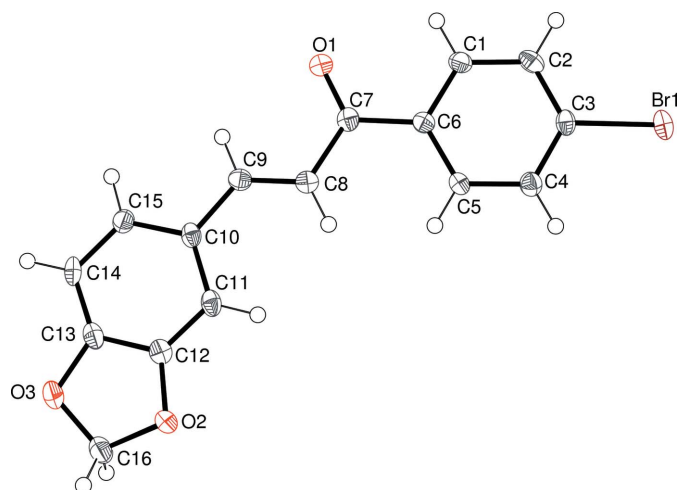


Figure 1
A view of the molecular structure of (I), showing 50% probability displacement ellipsoids (arbitrary spheres for H atoms).

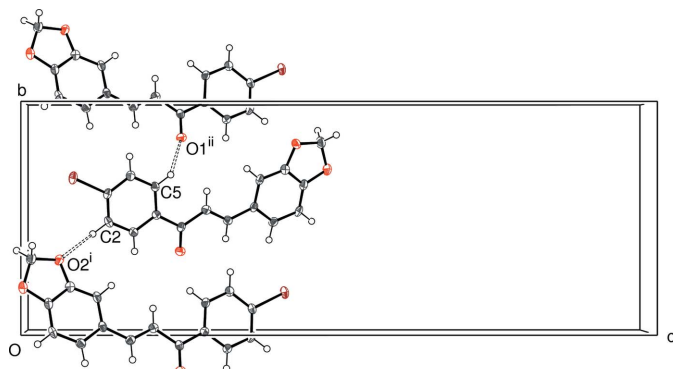


Figure 2
A fragment of the packing of (I), with the C—H...O interactions shown as dashed lines (symmetry codes as in Table 1).

arises, compared with the expected separation of 3.37 Å for these atoms (Bondi, 1964).

Any π - π stacking effects in (I) are probably weak. Although equivalent atoms in adjacent molecules in the [100] direction are separated by the *a* unit-cell dimension of 3.9221 (2) Å, the aromatic ring systems of the molecules are substantially offset (Fig. 3). The packing in (II) is different and results in herring-bone sheets of molecules in space group *Pbca*, consolidated by possible C—H... π interactions (Yang *et al.*, 2006), which might also correlate with the different dihedral angles between the benzene rings in the two structures.

Experimental

An aqueous solution of potassium hydroxide (5%, 5 ml) was added slowly with stirring to a mixture of piperonal (1.50 g, 0.01 mol) and 4-bromoacetophenone (1.99 g, 0.01 mol) in ethanol (25 ml). The mixture was stirred at room temperature for 12 h. The precipitated solid was filtered off, washed with water and dried, and crystals of (I) were recrystallized from acetone by slow evaporation (yield 78%;

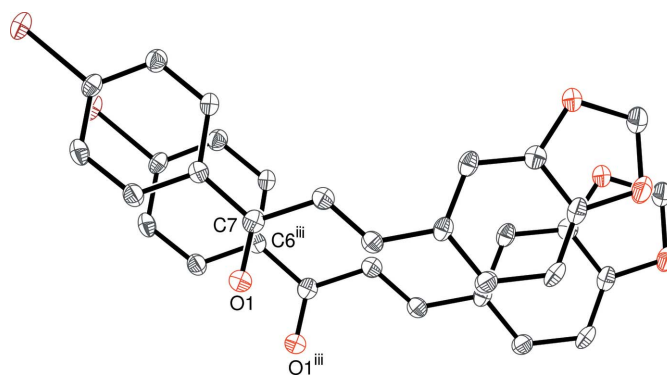


Figure 3
A fragment of the packing of (I), with the drawing projected on to the best plane of the O1 molecule, showing the offset of the aromatic rings of adjacent molecules stacked in the [100] direction. H atoms have been omitted for clarity. The closest intermolecular contact is 3.460 (5) Å for C7...C6ⁱⁱⁱ. [Symmetry code: (iii) $x - 1, y, z$.]

m.p. 413–415 K). Analysis, found (calculated for C₁₆H₁₁BrO₃): C 59.91 (58.03%), H 3.26 (3.35%).

Crystal data

C₁₆H₁₁BrO₃
M_r = 331.16
 Monoclinic, *P*₂₁/*n*
a = 3.9221 (2) Å
b = 10.9795 (8) Å
c = 29.840 (2) Å
 β = 90.299 (4)°
V = 1284.97 (14) Å³

Z = 4
D_x = 1.712 Mg m⁻³
 Mo *K* α radiation
 μ = 3.20 mm⁻¹
T = 120 (2) K
 Lath, colourless
 0.53 × 0.10 × 0.03 mm

Data collection

Nonius KappaCCD area-detector diffractometer
 ω and φ scans
 Absorption correction: multi-scan (SADABS; Bruker, 2003)
T_{min} = 0.282, *T_{max}* = 0.910

10550 measured reflections
 2886 independent reflections
 2176 reflections with *I* > 2 σ (*I*)
R_{int} = 0.057
 θ_{\max} = 27.5°

Refinement

Refinement on *F*²
R[*F*² > 2 σ (*F*²)] = 0.049
wR(*F*²) = 0.104
S = 1.05
 2886 reflections
 181 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0205P)^2 + 3.9272P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.58 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.51 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C2—H2...O2 ⁱ	0.95	2.54	3.384 (5)	148
C5—H5...O1 ⁱⁱ	0.95	2.61	3.336 (5)	134

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

H atoms were positioned geometrically, with C—H = 0.95–0.98 Å, and refined as riding, with *U_{iso}*(H) = 1.2*U_{eq}*(C).

Data collection: COLLECT (Nonius, 1998); cell refinement: SCALEPACK (Otwinowski & Minor, 1997); data reduction: SCALEPACK and DENZO (Otwinowski & Minor, 1997) and

SORTAV (Blessing, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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supporting information

Acta Cryst. (2006). E62, o5293–o5295 [https://doi.org/10.1107/S1600536806041547]

(2E)-3-(1,3-Benzodioxol-5-yl)-1-(4-bromophenyl)prop-2-en-1-one

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(2E)-3-(1,3-Benzodioxol-5-yl)-1-(4-bromophenyl)prop-2-en-1-one*Crystal data*

$C_{16}H_{11}BrO_3$	$F(000) = 664$
$M_r = 331.16$	$D_x = 1.712 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: $-P 2_1n$	Cell parameters from 2533 reflections
$a = 3.9221 (2) \text{ \AA}$	$\theta = 2.9\text{--}27.5^\circ$
$b = 10.9795 (8) \text{ \AA}$	$\mu = 3.20 \text{ mm}^{-1}$
$c = 29.840 (2) \text{ \AA}$	$T = 120 \text{ K}$
$\beta = 90.299 (4)^\circ$	Lath, colourless
$V = 1284.97 (14) \text{ \AA}^3$	$0.53 \times 0.10 \times 0.03 \text{ mm}$
$Z = 4$	

Data collection

Nonius KappaCCD area-detector diffractometer	10550 measured reflections
Radiation source: fine-focus sealed tube	2886 independent reflections
Graphite monochromator	2176 reflections with $I > 2\sigma(I)$
ω and φ scans	$R_{\text{int}} = 0.057$
Absorption correction: multi-scan (SADABS; Bruker, 2003)	$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 3.3^\circ$
$T_{\text{min}} = 0.282$, $T_{\text{max}} = 0.910$	$h = -5 \rightarrow 5$
	$k = -13 \rightarrow 14$
	$l = -38 \rightarrow 38$

Refinement

Refinement on F^2	Secondary atom site location: none
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.049$	H-atom parameters constrained
$wR(F^2) = 0.104$	$w = 1/[\sigma^2(F_o^2) + (0.0205P)^2 + 3.9272P]$
$S = 1.05$	where $P = (F_o^2 + 2F_c^2)/3$
2886 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
181 parameters	$\Delta\rho_{\text{max}} = 0.58 \text{ e \AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -0.51 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.3310 (10)	0.4388 (4)	0.17536 (13)	0.0216 (9)
H1	0.3885	0.3549	0.1768	0.026*
C2	0.1758 (10)	0.4840 (4)	0.13692 (14)	0.0231 (9)
H2	0.1314	0.4324	0.1120	0.028*
C3	0.0878 (9)	0.6051 (4)	0.13562 (13)	0.0189 (8)
C4	0.1491 (10)	0.6820 (4)	0.17167 (13)	0.0218 (8)
H4	0.0829	0.7652	0.1704	0.026*
C5	0.3091 (10)	0.6355 (4)	0.20971 (14)	0.0214 (9)
H5	0.3539	0.6874	0.2345	0.026*
C6	0.4041 (9)	0.5132 (4)	0.21166 (13)	0.0180 (8)
C7	0.5891 (9)	0.4595 (4)	0.25081 (13)	0.0187 (8)
C8	0.6549 (10)	0.5346 (4)	0.29119 (14)	0.0229 (9)
H8	0.5765	0.6164	0.2922	0.027*
C9	0.8237 (10)	0.4878 (4)	0.32608 (13)	0.0203 (8)
H9	0.9017	0.4064	0.3227	0.024*
C10	0.9034 (9)	0.5462 (4)	0.36885 (13)	0.0191 (8)
C11	0.8019 (10)	0.6677 (4)	0.37820 (13)	0.0217 (8)
H11	0.6803	0.7153	0.3569	0.026*
C12	0.8879 (9)	0.7128 (4)	0.41944 (14)	0.0203 (9)
C13	1.0677 (10)	0.6453 (4)	0.45084 (13)	0.0225 (9)
C14	1.1662 (10)	0.5281 (4)	0.44332 (14)	0.0235 (9)
H14	1.2852	0.4818	0.4653	0.028*
C15	1.0814 (10)	0.4799 (4)	0.40119 (14)	0.0223 (9)
H15	1.1480	0.3988	0.3944	0.027*
C16	0.9960 (11)	0.8330 (4)	0.47829 (14)	0.0286 (10)
H16A	1.1925	0.8887	0.4746	0.034*
H16B	0.8494	0.8652	0.5025	0.034*
O1	0.6843 (7)	0.3529 (2)	0.24915 (10)	0.0263 (7)
O2	0.8060 (7)	0.8252 (3)	0.43716 (9)	0.0277 (7)
O3	1.1131 (8)	0.7136 (3)	0.48956 (10)	0.0299 (7)
Br1	-0.11012 (10)	0.67243 (4)	0.082945 (13)	0.02512 (14)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.027 (2)	0.019 (2)	0.019 (2)	-0.0030 (17)	0.0002 (17)	-0.0016 (17)
C2	0.025 (2)	0.027 (2)	0.017 (2)	-0.0008 (18)	0.0016 (16)	-0.0072 (18)
C3	0.0149 (19)	0.025 (2)	0.016 (2)	-0.0008 (16)	-0.0003 (15)	0.0037 (16)
C4	0.023 (2)	0.024 (2)	0.019 (2)	0.0008 (18)	0.0000 (15)	0.0007 (18)
C5	0.025 (2)	0.022 (2)	0.017 (2)	0.0006 (17)	-0.0046 (16)	-0.0021 (16)

C6	0.0169 (19)	0.019 (2)	0.018 (2)	-0.0016 (16)	0.0010 (15)	-0.0010 (16)
C7	0.0177 (19)	0.022 (2)	0.017 (2)	-0.0025 (16)	0.0052 (15)	0.0028 (16)
C8	0.026 (2)	0.020 (2)	0.022 (2)	-0.0005 (17)	-0.0017 (17)	-0.0004 (17)
C9	0.020 (2)	0.020 (2)	0.021 (2)	0.0000 (16)	0.0015 (16)	-0.0017 (17)
C10	0.018 (2)	0.024 (2)	0.0153 (19)	-0.0047 (16)	0.0010 (15)	0.0040 (16)
C11	0.022 (2)	0.027 (2)	0.0158 (19)	-0.0046 (18)	0.0000 (15)	0.0047 (18)
C12	0.0149 (19)	0.025 (2)	0.021 (2)	-0.0007 (16)	0.0008 (15)	0.0002 (17)
C13	0.023 (2)	0.028 (2)	0.016 (2)	-0.0079 (17)	-0.0021 (16)	0.0028 (17)
C14	0.024 (2)	0.030 (2)	0.016 (2)	-0.0001 (18)	-0.0034 (16)	0.0088 (17)
C15	0.023 (2)	0.021 (2)	0.022 (2)	-0.0001 (17)	-0.0027 (16)	0.0025 (17)
C16	0.032 (2)	0.033 (2)	0.021 (2)	0.003 (2)	-0.0048 (18)	-0.003 (2)
O1	0.0347 (17)	0.0194 (16)	0.0246 (16)	0.0023 (13)	-0.0051 (13)	-0.0013 (13)
O2	0.0392 (17)	0.0239 (15)	0.0198 (15)	0.0040 (14)	-0.0073 (12)	-0.0038 (13)
O3	0.0391 (18)	0.0324 (17)	0.0182 (16)	-0.0005 (14)	-0.0072 (13)	0.0015 (13)
Br1	0.0227 (2)	0.0354 (3)	0.0172 (2)	-0.0005 (2)	-0.00468 (14)	0.0035 (2)

Geometric parameters (Å, °)

C1—C6	1.385 (5)	C9—H9	0.9500
C1—C2	1.387 (5)	C10—C15	1.393 (5)
C1—H1	0.9500	C10—C11	1.420 (6)
C2—C3	1.374 (6)	C11—C12	1.367 (5)
C2—H2	0.9500	C11—H11	0.9500
C3—C4	1.388 (5)	C12—O2	1.381 (5)
C3—Br1	1.899 (4)	C12—C13	1.385 (6)
C4—C5	1.391 (5)	C13—C14	1.362 (6)
C4—H4	0.9500	C13—O3	1.388 (5)
C5—C6	1.395 (5)	C14—C15	1.402 (6)
C5—H5	0.9500	C14—H14	0.9500
C6—C7	1.493 (5)	C15—H15	0.9500
C7—O1	1.229 (5)	C16—O3	1.429 (5)
C7—C8	1.482 (6)	C16—O2	1.435 (5)
C8—C9	1.334 (5)	C16—H16A	0.9900
C8—H8	0.9500	C16—H16B	0.9900
C9—C10	1.461 (5)		
C6—C1—C2	121.6 (4)	C15—C10—C11	119.6 (4)
C6—C1—H1	119.2	C15—C10—C9	118.7 (4)
C2—C1—H1	119.2	C11—C10—C9	121.7 (4)
C3—C2—C1	118.6 (4)	C12—C11—C10	116.7 (4)
C3—C2—H2	120.7	C12—C11—H11	121.6
C1—C2—H2	120.7	C10—C11—H11	121.6
C2—C3—C4	121.6 (4)	C11—C12—O2	127.7 (4)
C2—C3—Br1	120.1 (3)	C11—C12—C13	122.5 (4)
C4—C3—Br1	118.3 (3)	O2—C12—C13	109.8 (3)
C3—C4—C5	119.0 (4)	C14—C13—C12	122.6 (4)
C3—C4—H4	120.5	C14—C13—O3	127.7 (4)
C5—C4—H4	120.5	C12—C13—O3	109.7 (4)

C4—C5—C6	120.5 (4)	C13—C14—C15	116.0 (4)
C4—C5—H5	119.8	C13—C14—H14	122.0
C6—C5—H5	119.8	C15—C14—H14	122.0
C1—C6—C5	118.7 (4)	C10—C15—C14	122.6 (4)
C1—C6—C7	118.5 (4)	C10—C15—H15	118.7
C5—C6—C7	122.8 (4)	C14—C15—H15	118.7
O1—C7—C8	120.7 (4)	O3—C16—O2	108.1 (3)
O1—C7—C6	119.4 (4)	O3—C16—H16A	110.1
C8—C7—C6	119.9 (3)	O2—C16—H16A	110.1
C9—C8—C7	120.3 (4)	O3—C16—H16B	110.1
C9—C8—H8	119.9	O2—C16—H16B	110.1
C7—C8—H8	119.9	H16A—C16—H16B	108.4
C8—C9—C10	128.0 (4)	C12—O2—C16	105.1 (3)
C8—C9—H9	116.0	C13—O3—C16	105.1 (3)
C10—C9—H9	116.0		
C6—C1—C2—C3	-1.3 (6)	C15—C10—C11—C12	0.0 (5)
C1—C2—C3—C4	-0.3 (6)	C9—C10—C11—C12	179.5 (4)
C1—C2—C3—Br1	177.7 (3)	C10—C11—C12—O2	-176.8 (4)
C2—C3—C4—C5	1.1 (6)	C10—C11—C12—C13	0.6 (6)
Br1—C3—C4—C5	-176.9 (3)	C11—C12—C13—C14	-1.3 (6)
C3—C4—C5—C6	-0.4 (6)	O2—C12—C13—C14	176.5 (4)
C2—C1—C6—C5	2.0 (6)	C11—C12—C13—O3	-179.1 (4)
C2—C1—C6—C7	-176.6 (4)	O2—C12—C13—O3	-1.2 (5)
C4—C5—C6—C1	-1.1 (6)	C12—C13—C14—C15	1.4 (6)
C4—C5—C6—C7	177.4 (4)	O3—C13—C14—C15	178.7 (4)
C1—C6—C7—O1	3.1 (5)	C11—C10—C15—C14	0.1 (6)
C5—C6—C7—O1	-175.4 (4)	C9—C10—C15—C14	-179.4 (4)
C1—C6—C7—C8	-176.7 (3)	C13—C14—C15—C10	-0.8 (6)
C5—C6—C7—C8	4.8 (6)	C11—C12—O2—C16	-172.2 (4)
O1—C7—C8—C9	1.1 (6)	C13—C12—O2—C16	10.1 (4)
C6—C7—C8—C9	-179.2 (4)	O3—C16—O2—C12	-15.1 (4)
C7—C8—C9—C10	-178.1 (4)	C14—C13—O3—C16	174.2 (4)
C8—C9—C10—C15	179.4 (4)	C12—C13—O3—C16	-8.2 (4)
C8—C9—C10—C11	-0.1 (6)	O2—C16—O3—C13	14.4 (4)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2 \cdots O2 ⁱ	0.95	2.54	3.384 (5)	148
C5—H5 \cdots O1 ⁱⁱ	0.95	2.61	3.336 (5)	134

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