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(*E*)-2-(3-Chlorobenzylidene)-5,6-dimethoxy-2,3-dihydro-1*H*-inden-1-one

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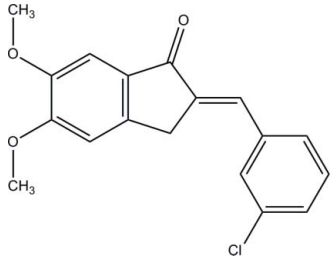
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.031; wR factor = 0.084; data-to-parameter ratio = 17.4.

In the title compound, $C_{18}H_{15}ClO_3$, the dihydroindenone group makes a dihedral angle of 8.56 (6)° with the bezene ring. In the crystal, the molecules are interconnected into a three-dimensional network *via* intermolecular C—H···O hydrogen bonds. Weak C—H···π and π···π [centroid–centroid distances 3.6598 (9)–3.6913 (9) Å] interactions are also observed.

Related literature

For general background to and the biological activity of chalcone derivatives, see: Marzinzik & Felder (1998); Srikanth & Castle (2005); Furusawa *et al.* (2005) Heidenreich *et al.* (2008); Syed *et al.* (2008). For related structures, see: Ali *et al.* (2010*a*,*b*). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).



Experimental

Crystal data

$C_{18}H_{15}ClO_3$
M_r = 314.75
Tetragonal, $P\bar{4}2_1c$
a = 20.5004 (16) Å
c = 7.0241 (7) Å
V = 2952.0 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.27 mm^{-1}
T = 100 K
0.74 × 0.13 × 0.11 mm

Data collection

Bruker APEXII DUO CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.826, T_{max} = 0.971
62722 measured reflections
4499 independent reflections
4251 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.084
S = 1.06
4499 reflections
259 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Absolute structure: Flack (1983), 1966 Friedel pairs
Flack parameter: −0.01 (5)

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

*Cg*2 is the centroid of the C1–C6 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···O1^{i}	0.942 (16)	2.489 (18)	3.2650 (16)	139.6 (15)
C11—H11···O1^{ii}	0.951 (18)	2.561 (17)	3.3229 (16)	137.3 (14)
C18—H18*C*···O3^{iii}	0.96 (2)	2.53 (2)	3.4684 (17)	165.2 (17)
C3—H3···*Cg*2^{iv}	0.87 (2)	2.86 (2)	3.6072 (17)	144.4 (17)

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); 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: SJ5044).

References

Ali, M. A., Ismail, R., Tan, S. C., Yeap, C. S. & Fun, H.-K. (2010*a*). *Acta Cryst.* E**66**, o2531–o2532.
Ali, M. A., Ismail, R., Tan, S. C., Yeap, C. S. & Fun, H.-K. (2010*b*). *Acta Cryst.* E**66**, o2753.
Bruker (2009). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cosier, J. & Glazer, A. M. (1986). *J. Appl. Cryst.* **19**, 105–107.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Furusawa, M., Tanaka, T., Ito, T., Nishiwaka, A., Yamazaki, N., Nakaya, K. I., Matsuura, N., Tsuchiya, H., Nagayama, M. & Iinuma, M. (2005). *J. Health Sci.* **51**, 376–378.
Heidenreich, A., Aus, G., Bolla, M., Joniau, S., Matveev, V. B., Schmid, H. P. & Zattoni, F. (2008). *Eur. Urol.* **53**, 68–80.
Marzinzik, A. L. & Felder, E. R. (1998). *J. Org. Chem.* **63**, 723–727.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Srikanth, G. S. C. & Castle, S. L. (2005). *Tetrahedron*, **61**, 10377–10441.
Syed, D. N., Suh, Y., Afag, F. & Mukhtar, H. (2008). *Cancer Lett.* **265**, 167–176.

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supplementary materials

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(*E*)-2-(3-Chlorobenzylidene)-5,6-dimethoxy-2,3-dihydro-1*H*-inden-1-one

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Comment

α,β-unsaturated ketones are useful key intermediates (Marzinzik & Felder, 1998, Srikanth & Castle, 2005) bearing the well known chalcone pharmacophore. Chalcones can be isolated from several plants and are precursors of flavones and anthocyan compounds. Some of them also exhibit antioxidant and anticancer properties. In fact, the pharmacological properties of chalcones are due to the presence of both α,β-unsaturation (Furusawa *et al.*, 2005) and an aromatic ring. Many antitumor drugs have been developed for prostate cancer patients, but their intolerable systemic toxicity often limits their clinical use. Chemoprevention is one of the most promising approaches in prostate cancer research, in which natural or synthetic agents are used to prevent this malignant disease (Heidenreich *et al.*, 2008, Syed *et al.*, 2008).

The molecular structure of the title compound is essentially planar (Fig. 1). The torsion angles of the two methoxy groups are [C18–O3–C13–C14] 4.38 (18) and [C17–O2–C12–C11] -2.01 (17)°. The maximum deviation of the dihydroindenone group is 0.024 (1) Å and it makes dihedral angle of 8.56 (6)° with the benzene ring [C1–C6]. The geometric parameters are comparable to those observed in closely related structures (Ali *et al.*, 2010*a*,*b*).

In the crystal structure, the molecules are linked together into a three dimensional network by the intermolecular C7—H7···O1, C11—H11···O1 and C18—H18C···O3 hydrogen bonds (Fig. 2, Table 1). Weak C—H···π and π···π interactions are also observed [*Cg*1···*Cg*2^{v} of 3.6913 (9) Å and *Cg*2···*Cg*3^{vi} of 3.6598 (9) Å; (v) *x*, *y*, 1 + *z*; (vi) *x*, *y*, -1 + *z*. *Cg*1, *Cg*2 and *Cg*3 are centroids of C8–C10/C15–C16, C1–C6 and C10–C15 rings, respectively].

Experimental

A mixture of 5,6-dimethoxy-2,3-dihydro-1*H*-indene-1-one (0.001 mmol) and 3-chlorobenzaldehyde (0.001 mmol) were dissolved in methanol (10 ml) and 30% sodium hydroxide solution (5 ml) was added and the mixture stirred for 5 h. After the completion of the reaction as evident from TLC, the mixture was poured into crushed ice then neutralized with concentrated HCl. The precipitated solid was filtered, washed with water and recrystallized from ethanol to reveal the title compound as light yellow crystals.

Refinement

All hydrogen atoms were located from difference Fourier map and refined freely. A total of 1966 Friedel pairs were use to determine the absolute structure.

Figures

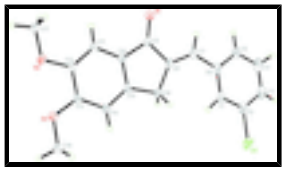

Fig. 1. The molecular structure of the title compound with atom labels and 50% probability ellipsoids for non-H atoms.

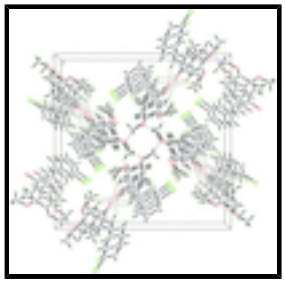

Fig. 2. The crystal packing of title compound, showing a three-dimensional network. Intermolecular hydrogen bonds are shown as dashed lines.

(*E*)-2-(3-Chlorobenzylidene)-5,6-dimethoxy-2,3-dihydro-1*H*-inden-1-one

Crystal data

$C_{18}H_{15}ClO_3$	$D_x = 1.416$ Mg m^{-3}
$M_r = 314.75$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Tetragonal, $P\bar{4}2_1c$	Cell parameters from 9872 reflections
Hall symbol: P -4 2n	$\theta = 2.8$–$30.4°$
$a = 20.5004$ (16) Å	$\mu = 0.27$ mm^{-1}
$c = 7.0241$ (7) Å	$T = 100$ K
$V = 2952.0$ (4) Å^3	Needle, yellow
$Z = 8$	0.74 × 0.13 × 0.11 mm
$F(000) = 1312$	

Data collection

Bruker APEXII DUO CCD area-detector diffractometer	4499 independent reflections
Radiation source: fine-focus sealed tube	4251 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.045$
φ and ω scans	$\theta_{max} = 30.5°$, $\theta_{min} = 2.0°$
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)	$h = -29 \rightarrow 29$
$T_{min} = 0.826$, $T_{max} = 0.971$	$k = -28 \rightarrow 29$
62722 measured reflections	$l = -10 \rightarrow 10$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.031$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.084$	$w = 1/[\sigma^2(F_o^2) + (0.0483P)^2 + 0.5709P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.001$
4499 reflections	$\Delta\rho_{max} = 0.37$ e Å^{-3}
259 parameters	$\Delta\rho_{min} = -0.19$ e Å^{-3}
0 restraints	Absolute structure: Flack (1983), 1966 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: −0.01 (5)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.658402 (17)	0.24083 (2)	0.07331 (5)	0.03382 (9)
O1	0.35460 (5)	0.18458 (5)	0.76502 (14)	0.0273 (2)
O2	0.38949 (4)	0.34023 (5)	1.38581 (13)	0.02125 (18)
O3	0.49925 (5)	0.39341 (5)	1.30773 (13)	0.02196 (19)
C1	0.55261 (6)	0.20587 (6)	0.27855 (18)	0.0204 (2)
C2	0.59058 (6)	0.19228 (7)	0.11923 (18)	0.0235 (3)
C3	0.57575 (8)	0.14194 (8)	−0.0056 (2)	0.0300 (3)
C4	0.52078 (9)	0.10399 (8)	0.0310 (2)	0.0326 (3)
C5	0.48177 (8)	0.11719 (7)	0.1883 (2)	0.0275 (3)
C6	0.49729 (7)	0.16787 (6)	0.31451 (17)	0.0206 (2)
C7	0.45338 (6)	0.17840 (6)	0.47637 (17)	0.0207 (2)
C8	0.45819 (6)	0.21831 (6)	0.62791 (17)	0.0183 (2)
C9	0.40455 (6)	0.21715 (6)	0.77302 (17)	0.0190 (2)
C10	0.42366 (6)	0.26270 (6)	0.92367 (16)	0.0166 (2)
C11	0.38957 (6)	0.27681 (6)	1.09221 (17)	0.0173 (2)
C12	0.41636 (6)	0.32139 (6)	1.21623 (17)	0.0169 (2)
C13	0.47750 (6)	0.35135 (6)	1.17248 (16)	0.0168 (2)
C14	0.51055 (6)	0.33681 (6)	1.00419 (17)	0.0168 (2)
C15	0.48283 (6)	0.29164 (6)	0.87923 (16)	0.0156 (2)
C16	0.50915 (6)	0.26751 (6)	0.68977 (16)	0.0178 (2)

C17	0.32745 (6)	0.31173 (7)	1.4304 (2)	0.0237 (2)
C18	0.55815 (7)	0.42822 (7)	1.2670 (2)	0.0266 (3)
H1	0.5664 (9)	0.2390 (9)	0.359 (3)	0.029 (5)*
H3	0.6019 (10)	0.1348 (10)	−0.102 (3)	0.044 (6)*
H4	0.5118 (11)	0.0700 (10)	−0.069 (4)	0.051 (6)*
H5	0.4430 (11)	0.0892 (10)	0.215 (3)	0.051 (6)*
H7	0.4154 (8)	0.1528 (8)	0.465 (3)	0.025 (4)*
H11	0.3500 (9)	0.2539 (8)	1.115 (3)	0.026 (4)*
H14	0.5503 (8)	0.3565 (9)	0.974 (3)	0.024 (4)*
H18A	0.5551 (10)	0.4571 (9)	1.158 (3)	0.031 (5)*
H18B	0.5953 (9)	0.3989 (9)	1.237 (3)	0.031 (5)*
H18C	0.5683 (11)	0.4553 (10)	1.375 (3)	0.047 (6)*
H16A	0.5126 (8)	0.3044 (8)	0.600 (3)	0.020 (4)*
H16B	0.5517 (8)	0.2491 (8)	0.703 (2)	0.020 (4)*
H17A	0.3144 (9)	0.3303 (9)	1.556 (3)	0.031 (5)*
H17B	0.2950 (8)	0.3251 (8)	1.341 (2)	0.020 (4)*
H17C	0.3292 (8)	0.2645 (8)	1.439 (3)	0.022 (4)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.02695 (16)	0.0484 (2)	0.02614 (16)	0.00242 (14)	0.00952 (13)	0.00399 (15)
O1	0.0264 (5)	0.0360 (5)	0.0195 (4)	−0.0121 (4)	0.0032 (4)	−0.0053 (4)
O2	0.0214 (4)	0.0246 (4)	0.0178 (4)	−0.0037 (3)	0.0070 (3)	−0.0051 (3)
O3	0.0234 (4)	0.0250 (4)	0.0175 (4)	−0.0077 (4)	0.0032 (3)	−0.0038 (3)
C1	0.0232 (6)	0.0233 (6)	0.0147 (5)	0.0064 (4)	0.0015 (4)	0.0019 (4)
C2	0.0227 (6)	0.0293 (6)	0.0184 (5)	0.0103 (5)	0.0031 (4)	0.0062 (5)
C3	0.0372 (8)	0.0338 (7)	0.0189 (5)	0.0146 (6)	0.0066 (6)	−0.0015 (5)
C4	0.0449 (8)	0.0292 (7)	0.0238 (6)	0.0079 (6)	0.0037 (6)	−0.0084 (5)
C5	0.0341 (7)	0.0271 (6)	0.0213 (6)	0.0015 (5)	0.0031 (5)	−0.0048 (5)
C6	0.0241 (6)	0.0228 (6)	0.0150 (5)	0.0053 (4)	0.0005 (4)	0.0008 (4)
C7	0.0234 (6)	0.0235 (6)	0.0154 (5)	0.0006 (5)	0.0024 (4)	−0.0003 (4)
C8	0.0197 (5)	0.0213 (5)	0.0139 (5)	−0.0001 (4)	0.0024 (4)	0.0001 (4)
C9	0.0205 (5)	0.0222 (5)	0.0144 (5)	−0.0021 (4)	0.0022 (4)	−0.0004 (4)
C10	0.0176 (5)	0.0191 (5)	0.0130 (4)	0.0002 (4)	0.0010 (4)	0.0005 (4)
C11	0.0173 (5)	0.0195 (5)	0.0152 (5)	−0.0011 (4)	0.0027 (4)	−0.0001 (4)
C12	0.0179 (5)	0.0182 (5)	0.0148 (5)	0.0008 (4)	0.0027 (4)	0.0006 (4)
C13	0.0184 (5)	0.0172 (5)	0.0150 (5)	0.0000 (4)	−0.0003 (4)	0.0011 (4)
C14	0.0155 (5)	0.0186 (5)	0.0163 (4)	0.0004 (4)	0.0003 (4)	0.0013 (4)
C15	0.0166 (5)	0.0180 (5)	0.0122 (4)	0.0018 (4)	0.0012 (4)	0.0015 (4)
C16	0.0183 (5)	0.0216 (5)	0.0136 (5)	0.0005 (4)	0.0037 (4)	0.0004 (4)
C17	0.0206 (6)	0.0310 (6)	0.0195 (5)	−0.0026 (5)	0.0064 (5)	−0.0010 (5)
C18	0.0240 (6)	0.0327 (7)	0.0232 (6)	−0.0098 (5)	0.0013 (5)	−0.0047 (5)

Geometric parameters (Å, °)

Cl1—C2	1.7401 (15)	C8—C16	1.5160 (17)
O1—C9	1.2237 (15)	C9—C10	1.4647 (16)
O2—C12	1.3680 (14)	C10—C15	1.3860 (16)

O2—C17	1.4343 (15)	C10—C11	1.4048 (16)
O3—C13	1.3582 (14)	C11—C12	1.3768 (17)
O3—C18	1.4314 (16)	C11—H11	0.951 (18)
C1—C2	1.3914 (17)	C12—C13	1.4293 (16)
C1—C6	1.3988 (19)	C13—C14	1.3948 (16)
C1—H1	0.926 (19)	C14—C15	1.3968 (16)
C2—C3	1.388 (2)	C14—H14	0.935 (17)
C3—C4	1.393 (2)	C15—C16	1.5188 (16)
C3—H3	0.87 (2)	C16—H16A	0.989 (17)
C4—C5	1.390 (2)	C16—H16B	0.955 (17)
C4—H4	1.01 (2)	C17—H17A	0.994 (19)
C5—C6	1.4025 (18)	C17—H17B	0.953 (17)
C5—H5	1.00 (2)	C17—H17C	0.971 (17)
C6—C7	1.4661 (17)	C18—H18A	0.97 (2)
C7—C8	1.3461 (17)	C18—H18B	0.994 (19)
C7—H7	0.943 (17)	C18—H18C	0.96 (2)
C8—C9	1.4995 (16)		
C12—O2—C17	115.60 (10)	C12—C11—H11	124.0 (11)
C13—O3—C18	116.98 (10)	C10—C11—H11	117.8 (11)
C2—C1—C6	119.16 (12)	O2—C12—C11	125.30 (11)
C2—C1—H1	117.7 (12)	O2—C12—C13	114.76 (10)
C6—C1—H1	123.1 (12)	C11—C12—C13	119.94 (11)
C3—C2—C1	122.31 (14)	O3—C13—C14	124.68 (11)
C3—C2—Cl1	118.89 (11)	O3—C13—C12	114.23 (10)
C1—C2—Cl1	118.79 (11)	C14—C13—C12	121.09 (11)
C2—C3—C4	118.40 (13)	C13—C14—C15	118.47 (11)
C2—C3—H3	118.6 (14)	C13—C14—H14	121.7 (12)
C4—C3—H3	123.0 (14)	C15—C14—H14	119.9 (12)
C5—C4—C3	120.22 (14)	C10—C15—C14	119.89 (11)
C5—C4—H4	125.7 (14)	C10—C15—C16	111.65 (10)
C3—C4—H4	113.9 (14)	C14—C15—C16	128.46 (11)
C4—C5—C6	121.06 (14)	C8—C16—C15	102.88 (9)
C4—C5—H5	119.9 (13)	C8—C16—H16A	112.0 (10)
C6—C5—H5	119.0 (13)	C15—C16—H16A	109.8 (10)
C1—C6—C5	118.84 (12)	C8—C16—H16B	113.2 (10)
C1—C6—C7	123.76 (12)	C15—C16—H16B	111.7 (10)
C5—C6—C7	117.39 (12)	H16A—C16—H16B	107.4 (14)
C8—C7—C6	131.13 (12)	O2—C17—H17A	106.0 (11)
C8—C7—H7	117.8 (11)	O2—C17—H17B	111.0 (10)
C6—C7—H7	111.1 (11)	H17A—C17—H17B	106.4 (14)
C7—C8—C9	118.31 (11)	O2—C17—H17C	112.8 (10)
C7—C8—C16	132.96 (11)	H17A—C17—H17C	109.7 (15)
C9—C8—C16	108.73 (10)	H17B—C17—H17C	110.5 (14)
O1—C9—C10	127.22 (11)	O3—C18—H18A	114.1 (12)
O1—C9—C8	126.23 (11)	O3—C18—H18B	112.8 (11)
C10—C9—C8	106.55 (10)	H18A—C18—H18B	104.5 (15)
C15—C10—C11	122.49 (11)	O3—C18—H18C	108.2 (14)
C15—C10—C9	110.14 (10)	H18A—C18—H18C	106.5 (16)
C11—C10—C9	127.37 (11)	H18B—C18—H18C	110.5 (17)

C12—C11—C10	118.13 (11)		
C6—C1—C2—C3	−0.32 (19)	C9—C10—C11—C12	179.81 (12)
C6—C1—C2—Cl1	178.78 (10)	C17—O2—C12—C11	−2.01 (17)
C1—C2—C3—C4	0.0 (2)	C17—O2—C12—C13	178.74 (11)
Cl1—C2—C3—C4	−179.06 (12)	C10—C11—C12—O2	−179.80 (11)
C2—C3—C4—C5	0.7 (2)	C10—C11—C12—C13	−0.59 (17)
C3—C4—C5—C6	−1.1 (2)	C18—O3—C13—C14	4.38 (18)
C2—C1—C6—C5	−0.09 (19)	C18—O3—C13—C12	−176.10 (11)
C2—C1—C6—C7	−179.15 (12)	O2—C12—C13—O3	0.50 (15)
C4—C5—C6—C1	0.8 (2)	C11—C12—C13—O3	−178.79 (11)
C4—C5—C6—C7	179.91 (14)	O2—C12—C13—C14	−179.96 (11)
C1—C6—C7—C8	−7.7 (2)	C11—C12—C13—C14	0.74 (18)
C5—C6—C7—C8	173.26 (14)	O3—C13—C14—C15	178.91 (11)
C6—C7—C8—C9	−179.20 (12)	C12—C13—C14—C15	−0.58 (17)
C6—C7—C8—C16	0.6 (2)	C11—C10—C15—C14	−0.16 (18)
C7—C8—C9—O1	−2.7 (2)	C9—C10—C15—C14	−179.73 (11)
C16—C8—C9—O1	177.46 (13)	C11—C10—C15—C16	179.72 (10)
C7—C8—C9—C10	177.72 (11)	C9—C10—C15—C16	0.15 (14)
C16—C8—C9—C10	−2.16 (13)	C13—C14—C15—C10	0.29 (17)
O1—C9—C10—C15	−178.36 (13)	C13—C14—C15—C16	−179.57 (11)
C8—C9—C10—C15	1.25 (13)	C7—C8—C16—C15	−177.69 (13)
O1—C9—C10—C11	2.1 (2)	C9—C8—C16—C15	2.15 (12)
C8—C9—C10—C11	−178.30 (11)	C10—C15—C16—C8	−1.44 (13)
C15—C10—C11—C12	0.32 (18)	C14—C15—C16—C8	178.43 (12)

Hydrogen-bond geometry (Å, °)

*Cg*2 is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O1^{i}	0.942 (16)	2.489 (18)	3.2650 (16)	139.6 (15)
C11—H11···O1^{ii}	0.951 (18)	2.561 (17)	3.3229 (16)	137.3 (14)
C18—H18C···O3^{iii}	0.96 (2)	2.53 (2)	3.4684 (17)	165.2 (17)
C3—H3···Cg2^{iv}	0.87 (2)	2.86 (2)	3.6072 (17)	144.4 (17)

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

Fig. 1

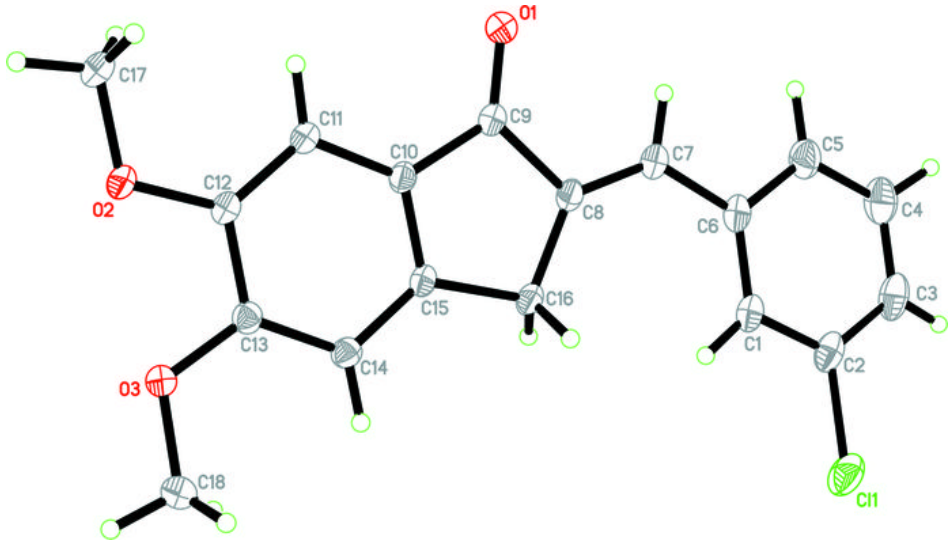
O1
C17
C11
C9
C10
C7
C5
C12
O2
C8
C6
C4
C15
C16
C3
C13
C1
C14
C2
O3
C18
Cl1

Fig. 2