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(*E*)-1-(2-Hydroxyphenyl)-3-(3-methoxyphenyl)prop-2-en-1-one

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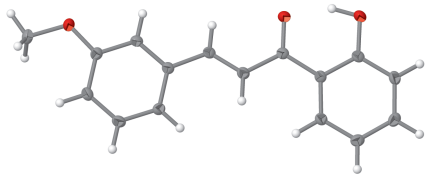
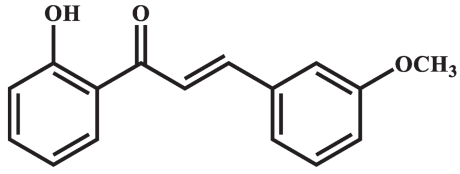
In the title compound, $C_{16}H_{14}O_3$, the phenyl rings are oriented at a dihedral angle of 3.82 (3)° and an intramolecular O—H···O hydrogen bond closes an *S*(6) ring. In the crystal, weak C—H···O and C—H···π hydrogen bonds and aromatic π–π stacking occurs. A Hirshfeld surface analysis of the crystal structure indicates that the most important contributions for the crystal packing are from H···H (48.2%), H···O/O···H (20.0%), H···C/C···H (16.5%) and C···C (12.7%) interactions.

3D view



Chemical scheme



Structure description

Chalcones are open-chain flavonoids, widely recognized as versatile building blocks in organic synthesis, owing to their α,β-unsaturated carbonyl system that facilitates the formation of diverse chemical frameworks (*e.g.*, Khalilov *et al.*, 2022). As part of our ongoing studies in this area, we now report the synthesis and structure of the title compound, $C_{16}H_{14}O_3$, (**I**).

The phenyl rings (C2–C7 and C10–C15) are oriented at a dihedral angle of 3.82 (3)° (Fig. 1) and the C2—C1—C8—C9 and C1—C8—C9—C10 torsion angles are −177.00 (9) and −178.67 (9)°, respectively. A short (and presumably strong) intramolecular O2—H2···O1 hydrogen bond occurs (Table 1).

In the crystal, weak C—H···O hydrogen bonds link the molecules into infinite chains propagating along the *c*-axis direction (Fig. 2). Further, there are π–π interactions between the almost parallel phenyl rings with centroid-to-centroid distances of 3.7124 (6) Å, where the dihedral angle between the phenyl rings is 3.83 (1)° and the slippage is 1.192 Å. A weak C—H···π(ring) interaction (Table 1) is also observed.

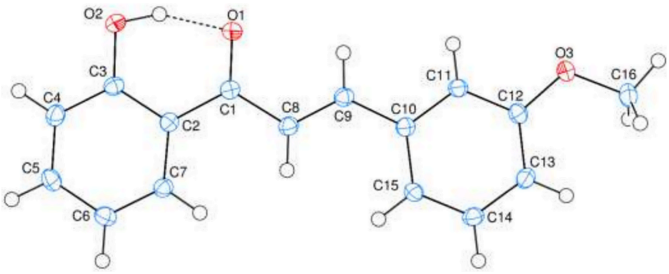


Figure 1
The molecular structure of (**I**) showing 50% probability ellipsoids. The intramolecular O—H···O hydrogen bond is shown as a dashed line.

To confirm and quantifying the intermolecular interactions in the crystal of (**I**), a Hirshfeld surface analysis (Fig. 3) was carried out using *Crystal Explorer 17.5* (Spackman *et al.*, 2021). The overall two-dimensional fingerprint plot, Fig. 4*a*, and those delineated into H···H (48.2% of the surface), H···O/O···H (20.0%), H···C/C···H (16.5%), C···C (12.7%), C···O/O···C (2.6%) and O···O(0.1%) (McKinnon *et al.*, 2007) are illustrated in Fig. 4*b–g*, respectively.

Synthesis and crystallization

To a solution of 2-hydroxyacetophenone (1.36 g, 10 mmol) in ethanol (10 ml) was added 0.1 ml of piperidine as catalyst and the mixture was stirred at room temperature for 0.5 h. Then, 3-methoxybenzaldehyde (1.36 g, 10 mmol) was added to the vigorously stirred reaction mixture and it was left overnight. The precipitated crystals were separated by filtration and recrystallized from an ethanol/water (1:1) solution (yield: 90%, m.p. 359 K). ^{1}H NMR (300 MHz, acetone-d_6, p.p.m.): 3.7 (*s*, 3H, CH_3); 6.94 (*d*, 1H, CH, arom. $^3J_{H-H}$ = 7.8 Hz); 7.2 (*s*, 1H, arom.), 7.3–7.4 (*m*, 5H, arom.), 7.6 (*d*, 1H, CH, $^3J_{H-H}$ = 15.6 HZ); 7.8 (*d*, 1H, CH, $^3J_{H-H}$ = 15.6 Hz); 7.9 (d, 1H, CH, arom. $^3J_{H-H}$ = 7.7 Hz); 11.3 (s, 1H, OH). ^{13}C NMR (75 MHz, acetone-d_6, p.p.m.): 55.1 (CH_3); 112.8 (CH, arom.); 115.7 (CH, arom.); 117.4 (CH, arom); 117.6 (CH, arom.); 119.3 (C_{quat}, arom.); 120.1 (δbCH); 121.1 (CH, arom.); 128.8 (CH, arom.); 129.3 (CH, arom.); 135.7 (C_{quat}, arom.); 136.2 (CH, arom.); 144.7 (=CH); 159.7 (C—O), 160.8 (C—O); 194.9 (CO).

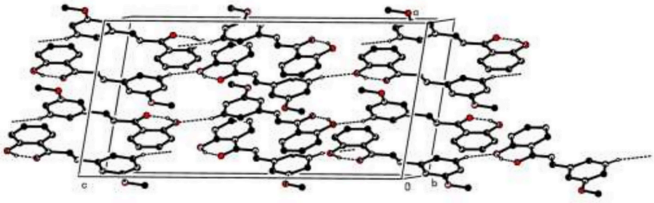


Figure 2
The packing diagram of (**I**) viewed down the *b*-axis direction. Intramolecular O—H···O and intermolecular C—H···O hydrogen bonds are shown as dashed lines. H atoms not involved in these interactions have been omitted for clarity.

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

*Cg*1 is the centroid of the C2–C7 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1	0.96 (2)	1.61 (2)	2.5156 (10)	154.9 (19)
C14—H14···O2^{i}	0.95	2.49	3.4220 (13)	167
C16—H16*C*···*Cg*1^{ii}	0.98	2.71	3.5097 (13)	140

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

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

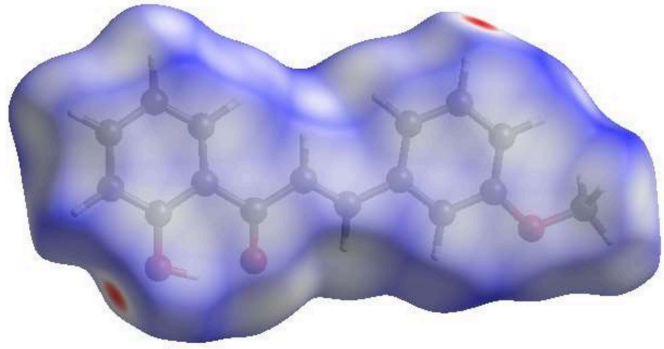


Figure 3
View of the three-dimensional Hirshfeld surface of (**I**) plotted over d_{norm}.

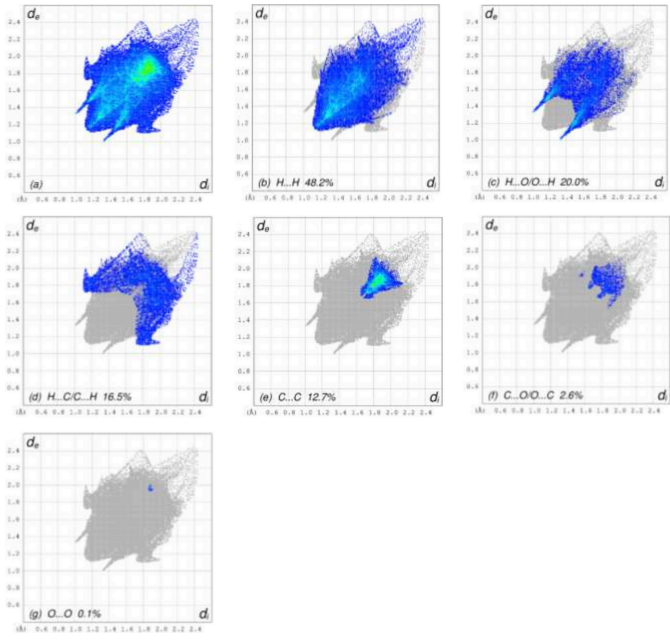


Figure 4
The full two-dimensional fingerprint plots for (**I**), showing (*a*) all interactions, and delineated into (*b*) H···H, (*c*) H···O/O···H, (*d*) H···C/C···H, (*e*) C···C, (*f*) C···O/O···C and (*g*) O···O interactions. The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

Acknowledgements

The authors' contributions are as follows. Conceptualizations, IGM and TH; methodology, FNN and AYZ; investigation, TH, VNK and IGM; writing (original draft), TH, VNK and IGM; writing (review and editing of the manuscript), TH and IGM; visualization, TH and FSK; funding acquisition, VNK, TH and ANB; resources, TH, VNK and FNN; supervision, FNN and TH.

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Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{14}O_3$
M_r	254.27
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	100
a, *b*, *c* (Å)	10.72243 (10), 10.51268 (9), 22.22491 (18)
β (°)	99.4688 (8)
V (Å^3)	2471.09 (4)
Z	8
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.76
Crystal size (mm)	0.15 × 0.10 × 0.10
Data collection	
Diffractometer	Rigaku XtaLAB Synergy-S, HyPix-6000HE area-detector
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2021)
T_{min}, T_{max}	0.770, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14193, 2689, 2527
R_{int}	0.031
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.639
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.036, 0.099, 1.06
No. of reflections	2689
No. of parameters	178
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.26, −0.19

Computer programs: *CrysAlis PRO* (Rigaku OD, 2021), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*) and *SHELXTL* (Sheldrick, 2015), *SHELXTL* (Sheldrick, 2008).

full crystallographic data

IUCrData (2025). **10**, x250182 [https://doi.org/10.1107/S2414314625001828]

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Crystal data

$C_{16}H_{14}O_3$
M_r = 254.27
Monoclinic, *C*2/*c*
a = 10.72243 (10) Å
b = 10.51268 (9) Å
c = 22.22491 (18) Å
β = 99.4688 (8)°
V = 2471.09 (4) Å^3
Z = 8
F(000) = 1072
D_x = 1.367 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54184 Å
Cell parameters from 10243 reflections
θ = 4.0–79.8°
μ = 0.76 mm^{-1}
T = 100 K
Prism, colourless
0.15 × 0.10 × 0.10 mm

Data collection

Rigaku XtaLAB Synergy-S, HyPix-6000HE area-detector diffractometer
Radiation source: micro-focus sealed X-ray tube
φ and *ω* scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2021)
T_{min} = 0.770, T_{max} = 1.000
14193 measured reflections
2689 independent reflections
2527 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 80.0°, θ_{min} = 4.0°
h = −13→13
k = −8→13
l = −28→28

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.099
S = 1.06
2689 reflections
178 parameters
0 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0493P)^2 + 1.7373P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00040 (4)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. The OH hydrogen atom was located in a difference Fourier map, and refined freely. The C-bound hydrogen atom positions were geometrically placed (C—H = 0.95–0.98 Å and refined using a riding model by applying the constraint of U_{iso} = k U_{eq} (C), where k = 1.5 for methyl H atoms and k = 1.2 for the other C-bound H atoms.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.38451 (7)	0.58069 (7)	0.35542 (3)	0.02097 (19)
O2	0.33559 (8)	0.41446 (8)	0.27352 (3)	0.0227 (2)
H2	0.3655 (18)	0.489 (2)	0.2965 (9)	0.056 (5)*
O3	0.54949 (8)	1.01783 (8)	0.60473 (3)	0.0223 (2)
C1	0.34130 (9)	0.51250 (10)	0.39322 (5)	0.0169 (2)
C2	0.28385 (9)	0.38836 (10)	0.37447 (5)	0.0163 (2)
C3	0.28323 (10)	0.34535 (10)	0.31402 (5)	0.0178 (2)
C4	0.22718 (10)	0.22920 (11)	0.29458 (5)	0.0209 (2)
H4	0.2271	0.2010	0.2540	0.025*
C5	0.17196 (10)	0.15544 (10)	0.33442 (5)	0.0212 (2)
H5	0.1338	0.0767	0.3210	0.025*
C6	0.17186 (10)	0.19577 (11)	0.39429 (5)	0.0203 (2)
H6	0.1339	0.1445	0.4215	0.024*
C7	0.22712 (10)	0.31026 (10)	0.41383 (5)	0.0184 (2)
H7	0.2269	0.3370	0.4547	0.022*
C8	0.34912 (10)	0.55674 (10)	0.45654 (5)	0.0186 (2)
H8	0.3206	0.5031	0.4859	0.022*
C9	0.39600 (10)	0.67174 (10)	0.47329 (5)	0.0176 (2)
H9	0.4217	0.7228	0.4422	0.021*
C10	0.41176 (9)	0.72683 (10)	0.53452 (5)	0.0168 (2)
C11	0.47212 (10)	0.84450 (10)	0.54386 (5)	0.0178 (2)
H11	0.5011	0.8858	0.5107	0.021*
C12	0.49052 (10)	0.90231 (10)	0.60123 (5)	0.0180 (2)
C13	0.44902 (10)	0.84144 (11)	0.64993 (5)	0.0196 (2)
H13	0.4617	0.8797	0.6892	0.024*
C14	0.38859 (10)	0.72374 (11)	0.64062 (5)	0.0205 (2)
H14	0.3605	0.6822	0.6739	0.025*
C15	0.36886 (10)	0.66657 (10)	0.58381 (5)	0.0187 (2)
H15	0.3266	0.5870	0.5781	0.022*
C16	0.56917 (11)	1.08037 (11)	0.66276 (5)	0.0225 (2)
H16A	0.6094	1.1631	0.6591	0.034*
H16B	0.6239	1.0279	0.6926	0.034*
H16C	0.4876	1.0930	0.6764	0.034*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0264 (4)	0.0192 (4)	0.0185 (4)	−0.0042 (3)	0.0074 (3)	0.0001 (3)
O2	0.0306 (4)	0.0225 (4)	0.0164 (4)	−0.0047 (3)	0.0081 (3)	−0.0007 (3)
O3	0.0296 (4)	0.0177 (4)	0.0203 (4)	−0.0056 (3)	0.0059 (3)	−0.0032 (3)
C1	0.0165 (5)	0.0172 (5)	0.0172 (5)	0.0016 (4)	0.0034 (4)	0.0010 (4)

C2	0.0163 (5)	0.0158 (5)	0.0168 (5)	0.0023 (4)	0.0029 (4)	−0.0002 (4)
C3	0.0184 (5)	0.0187 (5)	0.0171 (5)	0.0020 (4)	0.0048 (4)	0.0010 (4)
C4	0.0244 (5)	0.0205 (5)	0.0183 (5)	0.0005 (4)	0.0046 (4)	−0.0038 (4)
C5	0.0213 (5)	0.0157 (5)	0.0268 (5)	−0.0009 (4)	0.0045 (4)	−0.0032 (4)
C6	0.0210 (5)	0.0173 (5)	0.0236 (5)	0.0000 (4)	0.0066 (4)	0.0019 (4)
C7	0.0207 (5)	0.0176 (5)	0.0173 (5)	0.0012 (4)	0.0046 (4)	0.0001 (4)
C8	0.0216 (5)	0.0178 (5)	0.0168 (5)	0.0007 (4)	0.0041 (4)	0.0012 (4)
C9	0.0179 (5)	0.0179 (5)	0.0178 (5)	0.0016 (4)	0.0053 (4)	0.0006 (4)
C10	0.0169 (5)	0.0161 (5)	0.0178 (5)	0.0022 (4)	0.0040 (4)	0.0004 (4)
C11	0.0197 (5)	0.0166 (5)	0.0179 (5)	0.0005 (4)	0.0060 (4)	0.0011 (4)
C12	0.0178 (5)	0.0154 (5)	0.0208 (5)	0.0009 (4)	0.0029 (4)	−0.0005 (4)
C13	0.0227 (5)	0.0202 (5)	0.0159 (5)	0.0013 (4)	0.0033 (4)	−0.0015 (4)
C14	0.0248 (5)	0.0198 (5)	0.0179 (5)	0.0006 (4)	0.0067 (4)	0.0028 (4)
C15	0.0219 (5)	0.0148 (5)	0.0199 (5)	−0.0006 (4)	0.0052 (4)	0.0005 (4)
C16	0.0255 (5)	0.0189 (5)	0.0219 (5)	−0.0019 (4)	0.0006 (4)	−0.0048 (4)

Geometric parameters (Å, º)

O1—C1	1.2498 (13)	C8—C9	1.3384 (16)
O2—C3	1.3489 (13)	C8—H8	0.9500
O2—H2	0.96 (2)	C9—C10	1.4631 (14)
O3—C12	1.3654 (13)	C9—H9	0.9500
O3—C16	1.4321 (13)	C10—C11	1.3957 (15)
C1—C8	1.4714 (14)	C10—C15	1.4066 (14)
C1—C2	1.4737 (15)	C11—C12	1.3968 (14)
C2—C7	1.4087 (14)	C11—H11	0.9500
C2—C3	1.4165 (14)	C12—C13	1.3921 (15)
C3—C4	1.3977 (15)	C13—C14	1.3963 (16)
C4—C5	1.3815 (16)	C13—H13	0.9500
C4—H4	0.9500	C14—C15	1.3828 (15)
C5—C6	1.3967 (15)	C14—H14	0.9500
C5—H5	0.9500	C15—H15	0.9500
C6—C7	1.3797 (15)	C16—H16A	0.9800
C6—H6	0.9500	C16—H16B	0.9800
C7—H7	0.9500	C16—H16C	0.9800
C3—O2—H2	102.8 (12)	C8—C9—H9	116.7
C12—O3—C16	117.25 (8)	C10—C9—H9	116.7
O1—C1—C8	119.50 (10)	C11—C10—C15	119.11 (9)
O1—C1—C2	120.12 (9)	C11—C10—C9	117.96 (9)
C8—C1—C2	120.38 (9)	C15—C10—C9	122.93 (9)
C7—C2—C3	117.90 (9)	C10—C11—C12	120.91 (9)
C7—C2—C1	122.93 (9)	C10—C11—H11	119.5
C3—C2—C1	119.16 (9)	C12—C11—H11	119.5
O2—C3—C4	117.98 (9)	O3—C12—C13	124.67 (10)
O2—C3—C2	121.57 (10)	O3—C12—C11	115.69 (9)
C4—C3—C2	120.45 (10)	C13—C12—C11	119.64 (10)
C5—C4—C3	120.00 (10)	C12—C13—C14	119.47 (10)

C5—C4—H4	120.0	C12—C13—H13	120.3
C3—C4—H4	120.0	C14—C13—H13	120.3
C4—C5—C6	120.52 (10)	C15—C14—C13	121.20 (10)
C4—C5—H5	119.7	C15—C14—H14	119.4
C6—C5—H5	119.7	C13—C14—H14	119.4
C7—C6—C5	119.81 (10)	C14—C15—C10	119.66 (10)
C7—C6—H6	120.1	C14—C15—H15	120.2
C5—C6—H6	120.1	C10—C15—H15	120.2
C6—C7—C2	121.33 (10)	O3—C16—H16A	109.5
C6—C7—H7	119.3	O3—C16—H16B	109.5
C2—C7—H7	119.3	H16A—C16—H16B	109.5
C9—C8—C1	120.74 (10)	O3—C16—H16C	109.5
C9—C8—H8	119.6	H16A—C16—H16C	109.5
C1—C8—H8	119.6	H16B—C16—H16C	109.5
C8—C9—C10	126.64 (10)		

O1—C1—C2—C7	−176.32 (10)	C2—C1—C8—C9	−177.00 (9)
C8—C1—C2—C7	4.13 (15)	C1—C8—C9—C10	−178.67 (9)
O1—C1—C2—C3	2.66 (15)	C8—C9—C10—C11	174.88 (10)
C8—C1—C2—C3	−176.89 (9)	C8—C9—C10—C15	−5.16 (17)
C7—C2—C3—O2	−179.98 (9)	C15—C10—C11—C12	0.19 (15)
C1—C2—C3—O2	0.99 (15)	C9—C10—C11—C12	−179.85 (9)
C7—C2—C3—C4	0.32 (15)	C16—O3—C12—C13	−0.29 (15)
C1—C2—C3—C4	−178.71 (9)	C16—O3—C12—C11	179.57 (9)
O2—C3—C4—C5	−179.76 (10)	C10—C11—C12—O3	−179.36 (9)
C2—C3—C4—C5	−0.04 (16)	C10—C11—C12—C13	0.50 (16)
C3—C4—C5—C6	−0.18 (17)	O3—C12—C13—C14	179.34 (10)
C4—C5—C6—C7	0.11 (17)	C11—C12—C13—C14	−0.51 (16)
C5—C6—C7—C2	0.18 (16)	C12—C13—C14—C15	−0.16 (16)
C3—C2—C7—C6	−0.39 (15)	C13—C14—C15—C10	0.86 (16)
C1—C2—C7—C6	178.60 (9)	C11—C10—C15—C14	−0.86 (15)
O1—C1—C8—C9	3.45 (16)	C9—C10—C15—C14	179.18 (10)

Hydrogen-bond geometry (Å, º)

*Cg*1 is the centroid of the C2–C7 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1	0.96 (2)	1.61 (2)	2.5156 (10)	154.9 (19)
C14—H14···O2^{i}	0.95	2.49	3.4220 (13)	167
C16—H16*C*···*Cg*1^{ii}	0.98	2.71	3.5097 (13)	140

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