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2-Oxo-2*H*-chromen-7-yl 4-ethylbenzoate

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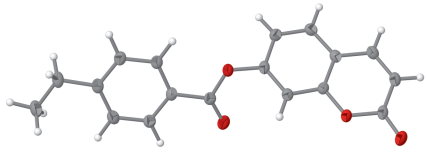
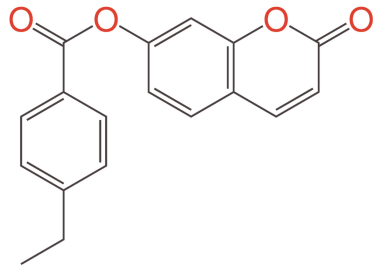
In the title compound, $C_{18}H_{14}O_4$, the benzoate ring is oriented at a dihedral angle of 39.78 (5)° with respect to the coumarin ring system. In the crystal, the molecules are linked by C—H···O hydrogen bonds to generate infinite (101) layers.

3D view



Chemical scheme



Structure description

The title compound, $C_{18}H_{14}O_4$ (**I**), crystallizes in the monoclinic space group $P2_1/c$ with one molecule in the asymmetric unit (Fig. 1). The side chain is titled with respect to the chromen-2-one ring system with torsion angles C18—C10—O2—C9 = −51.22 (16)° and C11—C10—O2—C9 = 133.18 (11)°. The C10–C18/O3 coumarin ring system is almost planar (r.m.s deviation = 0.012 Å) and makes a dihedral angle with the pendant benzoate ring system of 39.78 (5)°. The C14—C15 [1.342 (2) Å] and C15—C16 [1.447 (2) Å] bond lengths are consistent with the double and single bonds in the Lewis structure of (**I**) and with those in similar coumarin derivatives (Gomes *et al.*, 2016; Ouédraogo *et al.*, 2018).

In the extended structure of (**I**), the molecules are connected by C—H···O hydrogen bonds (Table 1): the C11—H11···O1 and C12—H12···O3 bonds lead to [010] chains, which are cross-linked by the C15—H15···O4 bonds to generate (101) layers incorporating $R_2^2(11)$ and $R_3^3(13)$ loops (Fig. 2). The intermolecular interactions in (**I**) were further quantified by Hirshfeld surface (Fig. 3) analysis using *CrystalExplorer* (Spackman *et al.*, 2021): the two-dimensional fingerprint plots for (**I**) (Fig. 4) show that the greatest contributions are from H···H (40.5%), H···O/O···H (26.1%) C···H/H···C (18.4%) and C···C (9.0%) contacts.

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

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11···O1^{i}	0.943 (17)	2.527 (18)	3.4535 (16)	167.8 (14)
C12—H12···O3^{i}	0.972 (18)	2.597 (18)	3.3166 (15)	131.0 (13)
C15—H15···O4^{ii}	0.97 (2)	2.38 (2)	3.2871 (16)	155.1 (15)

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

Synthesis and crystallization

In a 100 ml round-bottom flask equipped with a condenser, 4-ethylbenzoyl chloride (0.95 ml, 6.2 mmol, ∼1 equiv.) was dissolved in 30 ml of tetrahydrofuran and then were added dried triethylamine (2.6 ml, 3 equiv.) and 7-hydroxycoumarin (1 g, 6.17 mmol, 1 equiv.) in small portions over 30 min. While stirring, the mixture was refluxed for 4 h and poured into 40 ml of chloroform. The solution was acidified with dilute hydrochloric acid until its discoloration was complete. The organic phase was extracted, concentrated in a vacuum until a slight cloudiness was obtained and cooled in an ice bath. The resulting precipitate was filtered off with suction, washed with petroleum ether and recrystallized from a chloroform/*n*-hexane (1:3) solvent mixture resulting in a white powder of the title compound (1.15 g, 70% yield, m.p. = 407–409 K). Colorless crystals of (**I**) suitable for single-crystal X-ray diffraction analysis were then obtained by slow evaporation of an acetone solution.

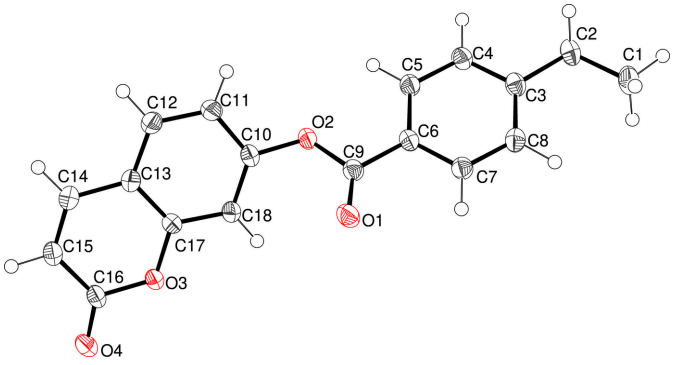


Figure 1
The molecular structure of (**I**) with displacement ellipsoids drawn at the 50% probability level.

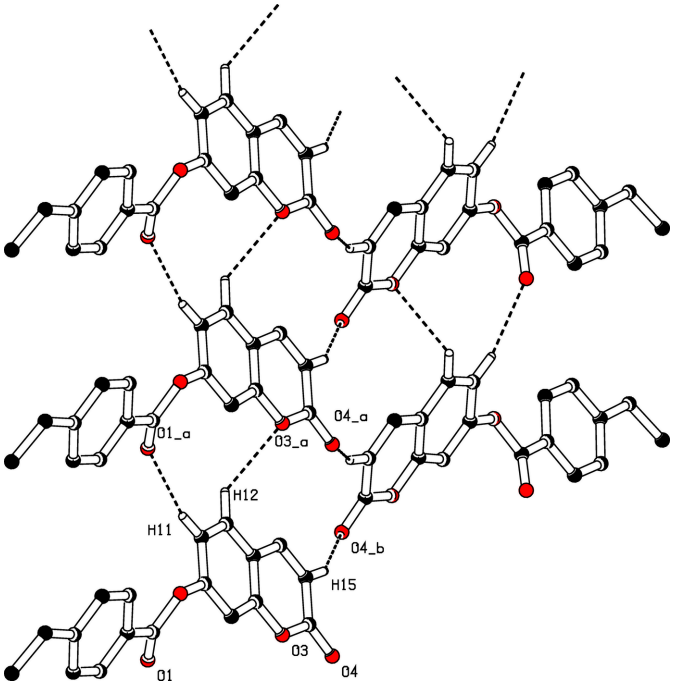


Figure 2
A view of the crystal packing of (**I**) showing C–H···O hydrogen bonds to form $R_2^2(11)$ and $R_3^3(13)$ loops extending parallel to the *ac* plane. H atoms not involved in the hydrogen bonds omitted.

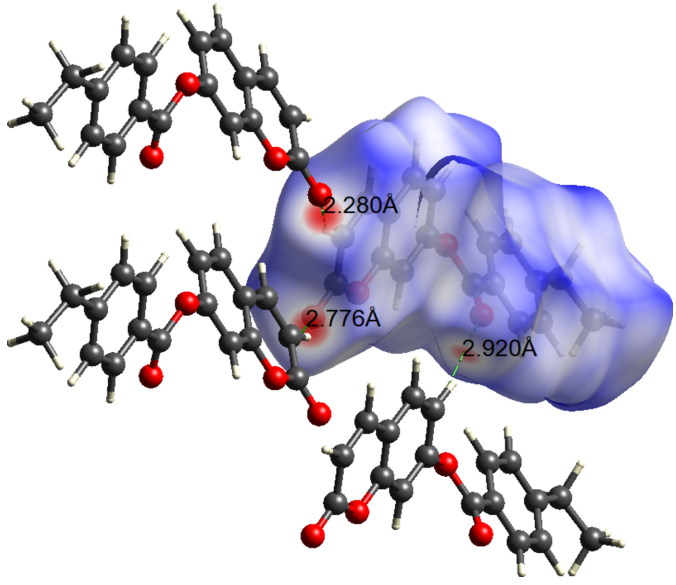


Figure 3
The Hirshfeld surface of (**I**) mapped over d_{norm}. Dotted lines represent hydrogen bonds

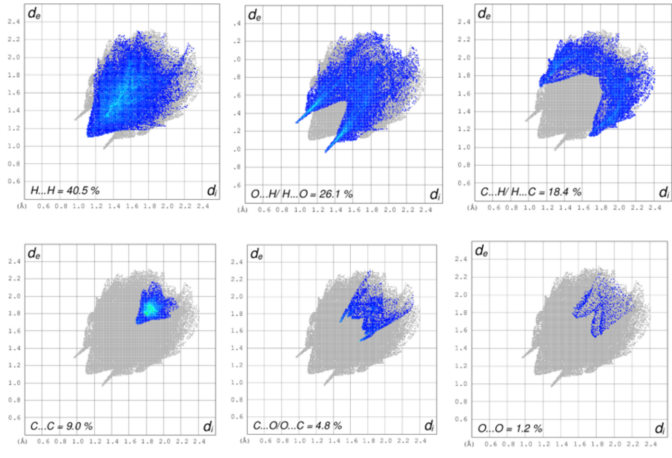


Figure 4
Fingerprint plots for (**I**) showing (*a*) H···H, (*b*) O···H, (*c*) C···H, (*d*) C···C, (*e*) C···O, (*f*) O···O interactions. The outline of the full fingerprint is shown in grey: d_i is the closest internal distance from a given point on the Hirshfeld surface and d_e is the closest external contact.

Refinement

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

Acknowledgements

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Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{14}O_4$
M_r	294.29
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, b, c (Å)	11.4837 (5), 6.1481 (3), 19.9255 (9)
β (°)	97.386 (2)
V (Å^3)	1395.13 (11)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.10
Crystal size (mm)	0.24 × 0.06 × 0.06
Data collection	
Diffractometer	Bruker D8 Venture
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.712, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	70676, 4305, 3095
R_{int}	0.058
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.717
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.050, 0.156, 1.06
No. of reflections	4305
No. of parameters	255
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.22, −0.31

Computer programs: *CrysAlis PRO* (Rigaku OD, 2022), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*), *PLATON* (Spek,2020) and *WinGX* (Farrugia, 2012) and *publCIF* (Westrip, 2010).

full crystallographic data

IUCrData (2025). **10**, x251030 [https://doi.org/10.1107/S2414314625010302]

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2-Oxo-2*H*-chromen-7-yl 4-ethylbenzoate

Crystal data

$C_{18}H_{14}O_4$
M_r = 294.29
Monoclinic, $P2_1/c$
a = 11.4837 (5) Å
b = 6.1481 (3) Å
c = 19.9255 (9) Å
β = 97.386 (2)°
V = 1395.13 (11) Å^3
Z = 4
$F(000)$ = 616
D_x = 1.401 Mg m^{-3}
Melting point = 407–409 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4940 reflections
θ = 5.1–61.3°
μ = 0.10 mm^{-1}
T = 293 K
Prism, colourless
0.24 × 0.06 × 0.06 mm

Data collection

Bruker D8 Venture diffractometer
Radiation source: micro-focus sealed X-ray tube
ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.712, T_{max} = 0.746
70676 measured reflections
4305 independent reflections
3095 reflections with $I > 2\sigma(I)$
R_{int} = 0.058
θ_{max} = 30.7°, θ_{min} = 2.6°
h = −16→16
k = −8→8
l = −28→28

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.156
S = 1.06
4305 reflections
255 parameters
0 restraints
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0889P)^2 + 0.2456P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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 H atoms were located in difference maps and their positions and U_{iso} values were freely refined.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O2	0.71504 (8)	0.42159 (14)	0.38731 (4)	0.0248 (2)
O3	0.55289 (8)	0.14242 (14)	0.57921 (4)	0.0252 (2)
O1	0.80649 (9)	0.09594 (16)	0.40536 (5)	0.0323 (2)
O4	0.46888 (9)	0.00631 (16)	0.66357 (5)	0.0344 (2)
C17	0.60586 (10)	0.31085 (19)	0.54905 (6)	0.0219 (2)
C10	0.68769 (10)	0.4389 (2)	0.45336 (6)	0.0231 (2)
C9	0.77633 (10)	0.2465 (2)	0.36850 (6)	0.0244 (2)
C6	0.80475 (10)	0.2753 (2)	0.29849 (6)	0.0235 (2)
C18	0.63433 (11)	0.2719 (2)	0.48430 (6)	0.0235 (2)
C5	0.78305 (11)	0.4703 (2)	0.26297 (6)	0.0258 (2)
C13	0.62824 (10)	0.50917 (19)	0.58229 (6)	0.0234 (2)
C3	0.87510 (11)	0.3251 (2)	0.16904 (6)	0.0262 (3)
C11	0.71028 (11)	0.6413 (2)	0.48389 (6)	0.0256 (2)
C8	0.89493 (11)	0.1307 (2)	0.20483 (7)	0.0275 (3)
C7	0.86050 (11)	0.1057 (2)	0.26900 (6)	0.0263 (2)
C16	0.51819 (11)	0.1624 (2)	0.64297 (6)	0.0259 (3)
C4	0.81888 (11)	0.4938 (2)	0.19946 (6)	0.0273 (3)
C14	0.59507 (11)	0.5311 (2)	0.64935 (6)	0.0266 (3)
C15	0.54372 (11)	0.3659 (2)	0.67835 (6)	0.0267 (3)
C12	0.68011 (11)	0.6754 (2)	0.54797 (7)	0.0269 (3)
C2	0.91348 (12)	0.3636 (2)	0.10002 (6)	0.0302 (3)
C1	0.98427 (15)	0.1831 (3)	0.07278 (8)	0.0391 (3)
H2A	0.9611 (14)	0.505 (3)	0.1025 (8)	0.034 (4)*
H7	0.8742 (14)	−0.032 (3)	0.2945 (8)	0.035 (4)*
H8	0.9368 (15)	0.002 (3)	0.1848 (8)	0.038 (4)*
H4	0.8076 (14)	0.636 (3)	0.1754 (8)	0.035 (4)*
H2B	0.8427 (15)	0.393 (3)	0.0674 (8)	0.036 (4)*
H5	0.7432 (15)	0.596 (3)	0.2835 (8)	0.036 (4)*
H1B	1.0623 (18)	0.151 (3)	0.1047 (10)	0.052 (5)*
H11	0.7455 (14)	0.751 (3)	0.4603 (8)	0.033 (4)*
H1C	0.9376 (17)	0.043 (3)	0.0665 (11)	0.059 (6)*
H18	0.6161 (15)	0.136 (3)	0.4624 (8)	0.034 (4)*
H1A	1.0048 (16)	0.222 (3)	0.0264 (9)	0.044 (5)*
H12	0.6935 (15)	0.816 (3)	0.5699 (9)	0.043 (5)*
H15	0.5194 (16)	0.377 (3)	0.7232 (10)	0.045 (5)*
H14	0.6115 (15)	0.671 (3)	0.6738 (8)	0.037 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0296 (4)	0.0253 (4)	0.0205 (4)	0.0027 (3)	0.0076 (3)	0.0016 (3)
O3	0.0322 (5)	0.0251 (4)	0.0193 (4)	−0.0033 (3)	0.0070 (3)	−0.0004 (3)
O1	0.0364 (5)	0.0323 (5)	0.0300 (5)	0.0082 (4)	0.0115 (4)	0.0091 (4)
O4	0.0460 (6)	0.0333 (5)	0.0259 (4)	−0.0070 (4)	0.0115 (4)	0.0030 (4)
C17	0.0226 (5)	0.0231 (5)	0.0201 (5)	−0.0005 (4)	0.0033 (4)	0.0018 (4)

C10	0.0230 (5)	0.0280 (6)	0.0187 (5)	0.0018 (4)	0.0041 (4)	0.0009 (4)
C9	0.0233 (5)	0.0255 (6)	0.0252 (5)	0.0004 (4)	0.0055 (4)	0.0008 (4)
C6	0.0231 (5)	0.0272 (6)	0.0206 (5)	−0.0016 (4)	0.0042 (4)	0.0000 (4)
C18	0.0262 (6)	0.0247 (5)	0.0197 (5)	−0.0006 (4)	0.0035 (4)	−0.0013 (4)
C5	0.0279 (6)	0.0273 (6)	0.0226 (5)	0.0013 (5)	0.0051 (4)	0.0006 (4)
C13	0.0225 (5)	0.0256 (5)	0.0220 (5)	0.0017 (4)	0.0031 (4)	−0.0021 (4)
C3	0.0233 (5)	0.0335 (6)	0.0217 (5)	−0.0021 (5)	0.0031 (4)	−0.0019 (5)
C11	0.0263 (6)	0.0245 (5)	0.0270 (6)	−0.0005 (4)	0.0069 (5)	0.0017 (4)
C8	0.0258 (6)	0.0303 (6)	0.0272 (6)	0.0011 (5)	0.0061 (5)	−0.0039 (5)
C7	0.0260 (6)	0.0272 (6)	0.0260 (6)	0.0008 (5)	0.0049 (5)	0.0005 (5)
C16	0.0287 (6)	0.0310 (6)	0.0187 (5)	0.0011 (5)	0.0057 (4)	0.0018 (4)
C4	0.0296 (6)	0.0300 (6)	0.0226 (5)	0.0002 (5)	0.0044 (5)	0.0017 (5)
C14	0.0277 (6)	0.0279 (6)	0.0244 (5)	0.0010 (5)	0.0043 (4)	−0.0044 (4)
C15	0.0290 (6)	0.0311 (6)	0.0207 (5)	0.0021 (5)	0.0052 (4)	−0.0016 (4)
C12	0.0285 (6)	0.0240 (6)	0.0290 (6)	−0.0002 (4)	0.0070 (5)	−0.0027 (4)
C2	0.0282 (6)	0.0411 (7)	0.0218 (6)	−0.0004 (5)	0.0056 (5)	−0.0016 (5)
C1	0.0434 (8)	0.0451 (8)	0.0315 (7)	0.0000 (7)	0.0157 (6)	−0.0066 (6)

Geometric parameters (Å, º)

O2—C9	1.3644 (14)	C3—C4	1.4003 (18)
O2—C10	1.3958 (13)	C3—C2	1.5157 (17)
O3—C17	1.3774 (14)	C11—C12	1.3813 (17)
O3—C16	1.3850 (14)	C11—H11	0.941 (17)
O1—C9	1.2048 (15)	C8—C7	1.3946 (17)
O4—C16	1.2126 (15)	C8—H8	1.035 (17)
C17—C18	1.3918 (15)	C7—H7	0.990 (17)
C17—C13	1.3956 (16)	C16—C15	1.4474 (18)
C10—C18	1.3807 (16)	C4—H4	0.995 (17)
C10—C11	1.3948 (17)	C14—C15	1.3417 (18)
C9—C6	1.4836 (16)	C14—H14	0.994 (17)
C6—C7	1.3925 (17)	C15—H15	0.973 (18)
C6—C5	1.3980 (17)	C12—H12	0.972 (18)
C18—H18	0.952 (17)	C2—C1	1.517 (2)
C5—C4	1.3876 (16)	C2—H2A	1.022 (17)
C5—H5	1.009 (17)	C2—H2B	0.990 (17)
C13—C12	1.4040 (17)	C1—H1B	1.05 (2)
C13—C14	1.4421 (16)	C1—H1C	1.01 (2)
C3—C8	1.3956 (18)	C1—H1A	1.011 (18)
C9—O2—C10	120.37 (9)	C3—C8—H8	120.9 (9)
C17—O3—C16	121.92 (9)	C6—C7—C8	120.29 (12)
O3—C17—C18	116.40 (10)	C6—C7—H7	118.4 (9)
O3—C17—C13	120.96 (10)	C8—C7—H7	121.4 (9)
C18—C17—C13	122.63 (11)	O4—C16—O3	116.24 (11)
C18—C10—C11	122.47 (11)	O4—C16—C15	126.41 (11)
C18—C10—O2	122.07 (10)	O3—C16—C15	117.35 (10)
C11—C10—O2	115.30 (10)	C5—C4—C3	121.65 (12)

O1—C9—O2	123.83 (11)	C5—C4—H4	119.7 (9)
O1—C9—C6	125.74 (11)	C3—C4—H4	118.6 (9)
O2—C9—C6	110.36 (10)	C15—C14—C13	120.76 (11)
C7—C6—C5	119.36 (11)	C15—C14—H14	120.6 (10)
C7—C6—C9	118.44 (11)	C13—C14—H14	118.6 (10)
C5—C6—C9	122.12 (11)	C14—C15—C16	121.14 (11)
C10—C18—C17	117.17 (11)	C14—C15—H15	122.6 (11)
C10—C18—H18	122.0 (10)	C16—C15—H15	116.2 (11)
C17—C18—H18	120.8 (10)	C11—C12—C13	120.82 (11)
C4—C5—C6	119.78 (11)	C11—C12—H12	120.4 (11)
C4—C5—H5	119.5 (9)	C13—C12—H12	118.8 (10)
C6—C5—H5	120.7 (9)	C3—C2—C1	116.26 (12)
C17—C13—C12	117.94 (11)	C3—C2—H2A	107.8 (9)
C17—C13—C14	117.83 (11)	C1—C2—H2A	109.2 (9)
C12—C13—C14	124.23 (11)	C3—C2—H2B	108.3 (9)
C8—C3—C4	117.86 (11)	C1—C2—H2B	109.3 (10)
C8—C3—C2	123.35 (11)	H2A—C2—H2B	105.4 (13)
C4—C3—C2	118.77 (11)	C2—C1—H1B	112.1 (10)
C12—C11—C10	118.94 (11)	C2—C1—H1C	111.5 (11)
C12—C11—H11	121.9 (10)	H1B—C1—H1C	108.3 (16)
C10—C11—H11	119.2 (10)	C2—C1—H1A	110.5 (11)
C7—C8—C3	121.06 (11)	H1B—C1—H1A	108.5 (14)
C7—C8—H8	118.1 (9)	H1C—C1—H1A	105.7 (15)

C16—O3—C17—C18	−178.68 (10)	O2—C10—C11—C12	176.73 (11)
C16—O3—C17—C13	0.87 (17)	C4—C3—C8—C7	−0.39 (19)
C9—O2—C10—C18	−51.22 (17)	C2—C3—C8—C7	178.31 (12)
C9—O2—C10—C11	133.19 (11)	C5—C6—C7—C8	0.37 (19)
C10—O2—C9—O1	2.72 (18)	C9—C6—C7—C8	−176.26 (11)
C10—O2—C9—C6	−174.39 (10)	C3—C8—C7—C6	0.4 (2)
O1—C9—C6—C7	7.17 (19)	C17—O3—C16—O4	177.58 (11)
O2—C9—C6—C7	−175.79 (10)	C17—O3—C16—C15	−2.29 (16)
O1—C9—C6—C5	−169.36 (13)	C6—C5—C4—C3	1.05 (19)
O2—C9—C6—C5	7.68 (16)	C8—C3—C4—C5	−0.32 (19)
C11—C10—C18—C17	−1.63 (18)	C2—C3—C4—C5	−179.08 (11)
O2—C10—C18—C17	−176.91 (10)	C17—C13—C14—C15	−0.42 (18)
O3—C17—C18—C10	−179.88 (10)	C12—C13—C14—C15	178.69 (12)
C13—C17—C18—C10	0.58 (18)	C13—C14—C15—C16	−1.07 (19)
C7—C6—C5—C4	−1.06 (19)	O4—C16—C15—C14	−177.46 (13)
C9—C6—C5—C4	175.44 (11)	O3—C16—C15—C14	2.40 (18)
O3—C17—C13—C12	−178.62 (10)	C10—C11—C12—C13	0.43 (19)
C18—C17—C13—C12	0.90 (18)	C17—C13—C12—C11	−1.41 (18)
O3—C17—C13—C14	0.54 (17)	C14—C13—C12—C11	179.49 (12)
C18—C17—C13—C14	−179.94 (11)	C8—C3—C2—C1	−4.46 (19)
C18—C10—C11—C12	1.16 (19)	C4—C3—C2—C1	174.23 (12)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···O1^{i}	0.943 (17)	2.527 (18)	3.4535 (16)	167.8 (14)
C12—H12···O3^{i}	0.972 (18)	2.597 (18)	3.3166 (15)	131.0 (13)
C15—H15···O4^{ii}	0.97 (2)	2.38 (2)	3.2871 (16)	155.1 (15)

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