

2-(4-Chlorophenyl)chromen-4-one

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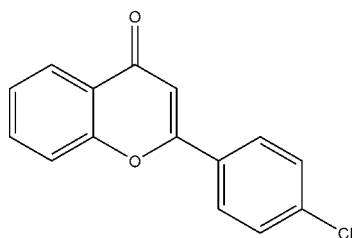
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.049; wR factor = 0.119; data-to-parameter ratio = 13.8.

The title compound, $\text{C}_{15}\text{H}_9\text{ClO}_2$, is a synthetic flavonoid obtained by the cyclization of 3-(4-chlorophenyl)-1-(2-hydroxyphenyl)prop-2-en-1-one. The 4-chlorophenyl ring is twisted at an angle of 11.54° with respect to the chromen-4-one skeleton. In the crystal, pairs of molecules are inter-connected by weak $\text{Cl}\cdots\text{Cl}$ interactions [$3.3089(10)$ Å] forming dimers which are further peripherally connected through intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

For general features and crystal structures of flavanoids, see: Tim Cushnie & Lamb (2005); Wera *et al.* (2011). For crystal structures of small molecules, see: Singh, Agarwal & Awasthi (2011); Singh, Singh *et al.* (2011). For the synthesis, see: Migrdichian (1957); Awasthi *et al.* (2009); Shah *et al.* (1955). For intermolecular interactions and bond lengths and angles, see: Reddy *et al.* (2006); Wang *et al.* (2010); Desiraju & Steiner (1999); Waller *et al.* (2003); Allen *et al.* (1987).



Experimental

Crystal data

$\text{C}_{15}\text{H}_9\text{ClO}_2$
 $M_r = 256.67$
 Monoclinic, $C2/c$
 $a = 22.1564(16)$ Å
 $b = 3.8745(2)$ Å
 $c = 26.7728(18)$ Å
 $\beta = 95.524(6)^\circ$

$V = 2287.6(3)$ Å³
 $Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 0.32$ mm⁻¹
 $T = 293$ K
 $0.40 \times 0.39 \times 0.38$ mm

Data collection

Oxford Xcalibur Eos diffractometer
 Absorption correction: multi-scan
 (*CrysAlis PRO*; Oxford
 Diffraction, 2009)
 $T_{\min} = 0.938$, $T_{\max} = 0.941$
 8152 measured reflections
 2249 independent reflections
 1910 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.037$
 Standard reflections: 0

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.049$
 $wR(F^2) = 0.119$
 $S = 1.10$
 2249 reflections
 163 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.20$ e Å⁻³
 $\Delta\rho_{\min} = -0.24$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C11}-\text{H11}\cdots\text{O2}^i$	0.93	2.64	3.345 (3)	134 (1)

Symmetry code: (i) $-x + 1, y - 1, -z + \frac{1}{2}$

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZJ2023).

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supporting information

Acta Cryst. (2011). E67, o3163 [https://doi.org/10.1107/S1600536811043832]

2-(4-Chlorophenyl)chromen-4-one

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S1. Comment

The term flavonoid generally includes a group of natural products containing a C6—C3—C6 carbon skeleton or more specifically phenylbenzopyran functionality in the molecule. Flavones (*flavus* = yellow), a class of the flavonoids mainly found in cereals and herbs. Flavanoids exhibit a wide range of biological activities such as antibacterial, anti-inflammatory, antioxidants, antifungal, antitumour and antimalarial (Tim Cushnie & Lamb 2005). Recently, few flavanoids have also been characterized in solid state (Wera *et al.*, 2011). Continuing our ongoing work on antimalarials (Awasthi *et al.*, 2009) and crystal structure of small molecules (Singh, Agarwal & Awasthi, 2011; Singh, Singh *et al.*, 2011), here we wish to report the crystal structure of 2-(4-chlorophenyl)chromen-4-one.

In the title compound (Fig. 1), the bond lengths and bond angles are usual and are comparable with the analogues structure of 2-phenyl-4*H*-chromen-4-one (flavone) reported earlier (Allen *et al.*, 1987; Waller *et al.*, 2003). The 4-chlorophenyl ring in the molecule is twisted at an angle of 11.54° relative to the chromen-4-one skeleton confirming nearly planar structure. The centroid-centroid distance between two parallel chromone ring in the molecule is 3.87 Å. Further, it is evident from the crystal packing structure (Fig. 2) that 8 molecules are present in a unit cell and adjacent chromone units are parallel in a given column, thus forming a herringbone type pattern. Moreover, crystal packing in the molecule is stabilized by weaker intermolecular hydrogen bonding C11—H11—O2 [$D = 3.34(3)$ Å] which is very well supported by earlier findings (Desiraju & Steiner, 1999). Further, weak interaction among atoms in molecule such as C11—C11 ($x, -1 + y, 1/2 - z$) [3.30 Å] (Reddy *et al.*, 2006) and C8—H8—H8—C8 [2.26 Å] (Wang *et al.*, 2010) are also responsible for stability in the crystal packing. Further, intermolecular C11—C11 short interaction forms a dimeric unit which are further peripherally links to six other molecules through C—H—O and C—H—H—C interactions.

S2. Experimental

The synthesis of the title compound was carried out in two steps according to the published procedure. (Migrdichian 1957; Awasthi *et al.*, 2009). In the first step, an aqueous solution of sodium hydroxide (10% w/v, 10 ml) was added to a solution of 2-hydroxyacetophenone (1.77 g m, 10 mmol) and 4-chlorobenzaldehyde (1.73 g m, 10 mmol) in minimum amount of methanol (3–5 ml) at ice cooled flask. The reaction mixture was allowed to draw closer to room temperature and stirred for 18–20 h yielded a yellow solid. The completion of the reaction was monitored by thin layer chromatography. After completion of the reaction, the mixture was neutralized with 10% hydrochloric acid in water. The compound was characterized by ¹H NMR, ¹³C NMR, FT-IR and EI-MS.

In second step, the cyclization was carried out according to published procedure (Shah *et al.*, 1955). Briefly, 3-(4-chlorophenyl)-1-(2-hydroxyphenyl)propenone (40 mg, 0.12 mmol) & SeO₂ (39 mg, 0.35 mmol) were added to dry amyl alcohol (30 ml) and the mixture was heated in an oil bath at 140–150 °C so that the entire compound was completely dissolved in the solvent. The reaction mixture was refluxed for 12 h and completion of the reaction was monitored by TLC. The reaction mixture was then filtered and dried in vacuum and purified by silica gel column using (Pet. ether:

EtOAc, 2:3) as eluent. The recrystalliation of an isolated compound from PE/ethylacetate to afford 2-(4-chlorophenyl)-chromen-4-one (10 mg, 20.1%) as white solid, m.p 177–178°C. R_f 0.6 (PE; EtOAc, 2:3). FT-IR ν_{\max} (KBr) cm^{-1} : 1651 (C=O), 1606 and 1510 (C=C aromatic), 1263 (C—O); ^1H NMR (300 Mz, CDCl_3) p.p.m.: δ 6.63 (1H, s, H-3, pyrone ring), δ 7.32–7.48 (4H, m, Ar-H, H'-5, H'-6, H'-7, H'-8), 7.20 (2H, dd, $J = 2.4$ Hz, H'-5, H'-3), 7.28 (2H, dd, $J = 2.1$ Hz, H'-2, H'-6), ^{13}C NMR (300 Mz, CDCl_3) ppm: EI-MS: m/z 255 [M^+].

For crystallization 5 mg of compound dissolved in 5 ml mixture of Petroleum ether/ethylacetate (80:20) and left for several days at ambient temperature which yielded fine needle shape crystals.

S3. Refinement

All H atoms were located from Fourier map (range of C—H = 0.93 Å) allowed to refine freely.

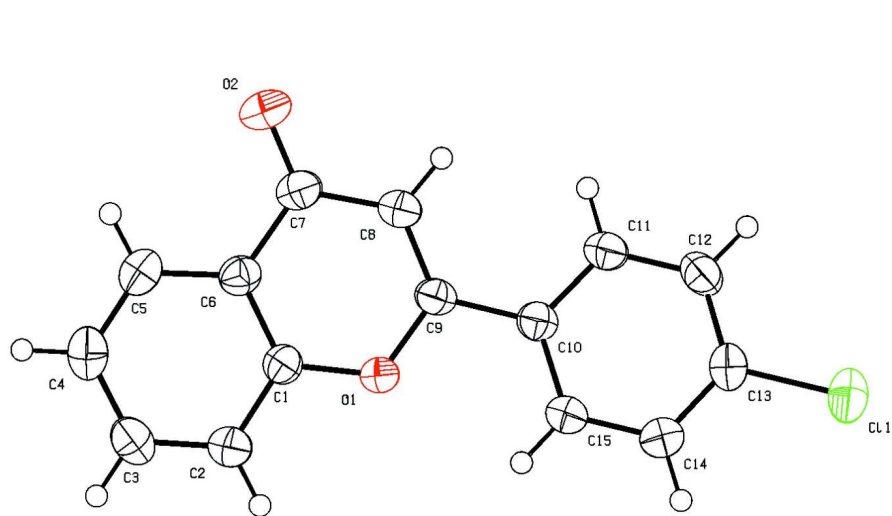


Figure 1

ORTEP diagram of the molecule with thermal ellipsoids drawn at 50% probability level Color code: White: C; red: O; green: Cl; white: H.

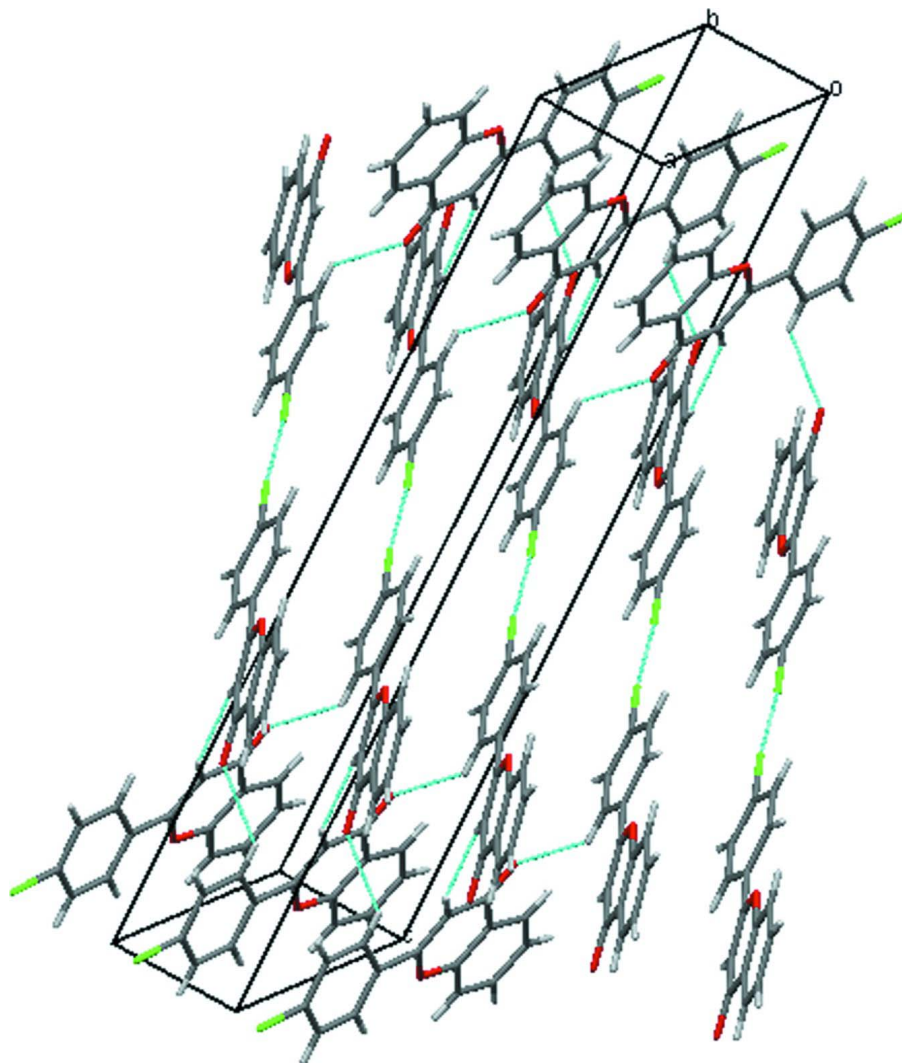


Figure 2

Packing diagram of molecule showing centroid-centroid distance between two parallel lying chromone ring and intermolecular hydrogen bonding.

2-(4-Chlorophenyl)chromen-4-one

Crystal data

$C_{15}H_9ClO_2$

$M_r = 256.67$

Monoclinic, $C2/c$

Hall symbol: $-C 2yc$

$a = 22.1564 (16) \text{ \AA}$

$b = 3.8745 (2) \text{ \AA}$

$c = 26.7728 (18) \text{ \AA}$

$\beta = 95.524 (6)^\circ$

$V = 2287.6 (3) \text{ \AA}^3$

$Z = 8$

$F(000) = 528$

$D_x = 1.490 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 3949 reflections

$\theta = 3.1\text{--}32.6^\circ$

$\mu = 0.32 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Needle, colourless

$0.40 \times 0.39 \times 0.38 \text{ mm}$

Data collection

Oxford Xcalibur Eos
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
 ω scans
Absorption correction: multi-scan
(*CrysAlis PRO*; Oxford Diffraction, 2009)
 $T_{\min} = 0.938$, $T_{\max} = 0.941$

8152 measured reflections
2249 independent reflections
1910 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.037$
 $\theta_{\max} = 26.0^\circ$, $\theta_{\min} = 3.4^\circ$
 $h = -26 \rightarrow 26$
 $k = -4 \rightarrow 4$
 $l = -33 \rightarrow 33$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.049$
 $wR(F^2) = 0.119$
 $S = 1.10$
2249 reflections
163 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
 $w = 1/[\sigma^2(F_o^2) + (0.0483P)^2 + 1.836P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.009$
 $\Delta\rho_{\max} = 0.20 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.24 \text{ e } \text{\AA}^{-3}$

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>	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	0.31934 (3)	0.85487 (18)	0.02358 (2)	0.0570 (2)
C9	0.53822 (9)	1.4266 (6)	0.14239 (7)	0.0337 (5)
C6	0.64493 (9)	1.7175 (6)	0.18541 (7)	0.0354 (5)
C10	0.48486 (9)	1.2780 (6)	0.11311 (7)	0.0337 (5)
C1	0.63679 (9)	1.6341 (5)	0.13486 (7)	0.0339 (5)
C13	0.38335 (9)	1.0144 (6)	0.05827 (8)	0.0397 (5)
C15	0.48053 (10)	1.2743 (6)	0.06106 (8)	0.0400 (5)
H15	0.5123	1.3606	0.0445	0.048*
C8	0.54262 (10)	1.5012 (7)	0.19128 (8)	0.0461 (6)
H8	0.5095	1.4573	0.2092	0.055*
C5	0.70028 (10)	1.8653 (6)	0.20370 (8)	0.0428 (5)
H5	0.7069	1.9248	0.2374	0.051*
C2	0.68118 (10)	1.6940 (6)	0.10315 (8)	0.0431 (5)
H2	0.6748	1.6370	0.0693	0.052*
C14	0.42994 (10)	1.1448 (6)	0.03366 (8)	0.0436 (6)
H14	0.4273	1.1455	-0.0012	0.052*

C11	0.43729 (10)	1.1410 (6)	0.13715 (8)	0.0416 (5)
H11	0.4397	1.1385	0.1720	0.050*
C12	0.38674 (10)	1.0092 (6)	0.10974 (8)	0.0431 (5)
H12	0.3551	0.9172	0.1260	0.052*
C7	0.59653 (11)	1.6468 (6)	0.21751 (8)	0.0445 (6)
O2	0.60167 (9)	1.7078 (6)	0.26277 (6)	0.0690 (6)
C3	0.73488 (10)	1.8388 (6)	0.12232 (9)	0.0472 (6)
H3	0.7651	1.8809	0.1013	0.057*
C4	0.74463 (11)	1.9233 (6)	0.17286 (9)	0.0475 (6)
H4	0.7814	2.0193	0.1856	0.057*
O1	0.58414 (6)	1.4868 (4)	0.11337 (5)	0.0382 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0454 (4)	0.0656 (5)	0.0582 (4)	-0.0157 (3)	-0.0049 (3)	-0.0043 (3)
C9	0.0323 (10)	0.0380 (12)	0.0317 (10)	0.0045 (9)	0.0076 (8)	0.0045 (9)
C6	0.0365 (11)	0.0363 (12)	0.0332 (11)	0.0054 (9)	0.0013 (9)	0.0023 (9)
C10	0.0323 (11)	0.0353 (11)	0.0337 (10)	0.0045 (9)	0.0033 (8)	0.0035 (9)
C1	0.0319 (10)	0.0358 (12)	0.0336 (10)	0.0005 (9)	0.0011 (8)	0.0027 (9)
C13	0.0326 (11)	0.0390 (12)	0.0466 (12)	-0.0030 (10)	-0.0011 (9)	-0.0010 (10)
C15	0.0375 (11)	0.0492 (13)	0.0342 (11)	-0.0041 (10)	0.0082 (9)	0.0025 (10)
C8	0.0389 (12)	0.0672 (16)	0.0331 (11)	-0.0059 (11)	0.0085 (9)	0.0006 (11)
C5	0.0437 (12)	0.0432 (13)	0.0398 (12)	0.0003 (11)	-0.0045 (10)	-0.0018 (10)
C2	0.0408 (12)	0.0529 (14)	0.0361 (11)	-0.0015 (11)	0.0060 (9)	-0.0002 (10)
C14	0.0444 (13)	0.0533 (15)	0.0331 (11)	-0.0050 (11)	0.0038 (10)	-0.0002 (10)
C11	0.0393 (12)	0.0529 (14)	0.0334 (11)	-0.0009 (11)	0.0076 (9)	0.0040 (10)
C12	0.0347 (11)	0.0496 (14)	0.0461 (12)	-0.0054 (10)	0.0103 (10)	0.0052 (11)
C7	0.0451 (13)	0.0563 (15)	0.0321 (11)	0.0007 (12)	0.0038 (9)	-0.0031 (10)
O2	0.0648 (12)	0.1114 (17)	0.0314 (9)	-0.0159 (11)	0.0068 (8)	-0.0149 (10)
C3	0.0379 (12)	0.0508 (15)	0.0539 (14)	-0.0036 (11)	0.0105 (10)	0.0053 (12)
C4	0.0382 (12)	0.0450 (14)	0.0574 (14)	-0.0045 (11)	-0.0045 (11)	0.0018 (12)
O1	0.0326 (7)	0.0541 (10)	0.0282 (7)	-0.0041 (7)	0.0045 (6)	-0.0028 (7)

Geometric parameters (Å, °)

C11—C13	1.733 (2)	C8—C7	1.441 (3)
C9—C8	1.335 (3)	C8—H8	0.9300
C9—O1	1.358 (2)	C5—C4	1.362 (3)
C9—C10	1.471 (3)	C5—H5	0.9300
C6—C1	1.386 (3)	C2—C3	1.370 (3)
C6—C5	1.399 (3)	C2—H2	0.9300
C6—C7	1.463 (3)	C14—H14	0.9300
C10—C15	1.388 (3)	C11—C12	1.377 (3)
C10—C11	1.392 (3)	C11—H11	0.9300
C1—O1	1.374 (2)	C12—H12	0.9300
C1—C2	1.379 (3)	C7—O2	1.229 (3)
C13—C14	1.373 (3)	C3—C4	1.389 (3)

C13—C12	1.373 (3)	C3—H3	0.9300
C15—C14	1.374 (3)	C4—H4	0.9300
C15—H15	0.9300		
C8—C9—O1	122.4 (2)	C6—C5—H5	119.5
C8—C9—C10	125.9 (2)	C3—C2—C1	118.9 (2)
O1—C9—C10	111.72 (17)	C3—C2—H2	120.5
C1—C6—C5	117.7 (2)	C1—C2—H2	120.5
C1—C6—C7	119.74 (19)	C13—C14—C15	119.4 (2)
C5—C6—C7	122.57 (19)	C13—C14—H14	120.3
C15—C10—C11	118.6 (2)	C15—C14—H14	120.3
C15—C10—C9	120.89 (19)	C12—C11—C10	120.5 (2)
C11—C10—C9	120.54 (18)	C12—C11—H11	119.7
O1—C1—C2	116.05 (18)	C10—C11—H11	119.7
O1—C1—C6	122.07 (18)	C13—C12—C11	119.5 (2)
C2—C1—C6	121.9 (2)	C13—C12—H12	120.2
C14—C13—C12	121.1 (2)	C11—C12—H12	120.2
C14—C13—C11	119.24 (17)	O2—C7—C8	123.3 (2)
C12—C13—C11	119.70 (17)	O2—C7—C6	122.7 (2)
C14—C15—C10	120.9 (2)	C8—C7—C6	114.01 (18)
C14—C15—H15	119.5	C2—C3—C4	120.6 (2)
C10—C15—H15	119.5	C2—C3—H3	119.7
C9—C8—C7	122.8 (2)	C4—C3—H3	119.7
C9—C8—H8	118.6	C5—C4—C3	119.9 (2)
C7—C8—H8	118.6	C5—C4—H4	120.1
C4—C5—C6	121.0 (2)	C3—C4—H4	120.1
C4—C5—H5	119.5	C9—O1—C1	118.96 (15)
C8—C9—C10—C15	167.0 (2)	C15—C10—C11—C12	-0.9 (3)
O1—C9—C10—C15	-12.2 (3)	C9—C10—C11—C12	178.5 (2)
C8—C9—C10—C11	-12.3 (4)	C14—C13—C12—C11	0.9 (4)
O1—C9—C10—C11	168.48 (19)	C11—C13—C12—C11	-179.02 (18)
C5—C6—C1—O1	179.74 (19)	C10—C11—C12—C13	-0.2 (4)
C7—C6—C1—O1	0.3 (3)	C9—C8—C7—O2	-178.0 (3)
C5—C6—C1—C2	-0.2 (3)	C9—C8—C7—C6	2.2 (4)
C7—C6—C1—C2	-179.6 (2)	C1—C6—C7—O2	178.3 (2)
C11—C10—C15—C14	1.3 (4)	C5—C6—C7—O2	-1.1 (4)
C9—C10—C15—C14	-178.1 (2)	C1—C6—C7—C8	-1.9 (3)
O1—C9—C8—C7	-0.9 (4)	C5—C6—C7—C8	178.7 (2)
C10—C9—C8—C7	180.0 (2)	C1—C2—C3—C4	0.2 (4)
C1—C6—C5—C4	-0.3 (3)	C6—C5—C4—C3	0.7 (4)
C7—C6—C5—C4	179.1 (2)	C2—C3—C4—C5	-0.7 (4)
O1—C1—C2—C3	-179.7 (2)	C8—C9—O1—C1	-0.9 (3)
C6—C1—C2—C3	0.3 (3)	C10—C9—O1—C1	178.32 (17)
C12—C13—C14—C15	-0.5 (4)	C2—C1—O1—C9	-178.86 (19)
C11—C13—C14—C15	179.43 (18)	C6—C1—O1—C9	1.2 (3)
C10—C15—C14—C13	-0.6 (4)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C11—H11 \cdots O2 ⁱ	0.93	2.64	3.345 (3)	134 (1)

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