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Methyl 2-[4-(4-chlorobenzoyl)phenoxy]-2-methylpropanoate

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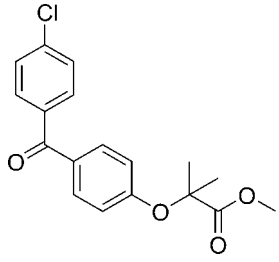
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.067; wR factor = 0.194; data-to-parameter ratio = 14.7.

In the title compound, $C_{18}H_{17}ClO_4$, the dihedral angle between the mean planes of the benzene rings is 53.4 (1)°. Weak intermolecular C—H···O interactions are observed.

Related literature

For background, see: Guichard *et al.* (2000). For the synthesis of the title compound, see: Bandgar *et al.* (2011). For bond lengths, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{18}H_{17}ClO_4$
M_r = 332.77
Orthorhombic, *Pbca*
a = 19.657 (4) Å
b = 7.5860 (15) Å
c = 22.436 (5) Å
V = 3345.6 (12) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.25 mm^{-1}
T = 293 K
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.930, T_{max} = 0.976
6018 measured reflections
3065 independent reflections
1432 reflections with $I > 2\sigma(I)$
R_{int} = 0.092

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.194
S = 1.00
3065 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1A···O3^{i}	0.93	2.37	3.254 (6)	159

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

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1989); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL-Plus* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JJ2129).

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supplementary materials

Acta Cryst. (2012). E**68**, o1676 [doi:10.1107/S1600536812019812]

Methyl 2-[4-(4-chlorobenzoyl)phenoxy]-2-methylpropanoate

Baohua Zou, Zheng Fang, Hui Zhong, Kai Guo and Ping Wei

Comment

The title compound, $C_{18}H_{17}ClO_4$, (I), is a derivative of Fenofibrate, a antihypertensive drug (Guichard *et al.* 2000). We report herein its crystal structure.

In the title compound, (I), the dihedral angle between the mean planes of the benzene and phenyl rings is 53.4 (1)°. Crystal packing is influenced by weak C—H···O intermolecular interactions. Bond lengths are in normal ranges (Allen *et al.* 1987).

Experimental

2-(4-(4-chlorobenzoyl)phenoxy)-2-methylpropanoic acid (6.28 mmol, 2.00 g) was dissolved in 35% hydrochloric acid methanol solution (15 mL), the solution was heated to 338.15 K under N2 atmosphere for 3 h. The reaction mexture was cooled to room temperature and the solvent was distilled to get the crude compound. The crude compond was dissolved in dichloromethane (15 mL), washed with water (10 mL) three times, dried, and concentrated to get the title compound (1.95 g). pure: white solid (Bandgar *et al.* 2011). Crystals of the title compound suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

Refinement

H atoms were positioned geometrically with C—H = 0.93, 0.98 and 0.97 Å for aromatic, methine and methylene H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2 (or 1.5 for methyl groups) times U_{eq}(C).

Computing details

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1989); cell refinement: *CAD-4 EXPRESS* (Enraf–Nonius, 1989); data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL-Plus* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

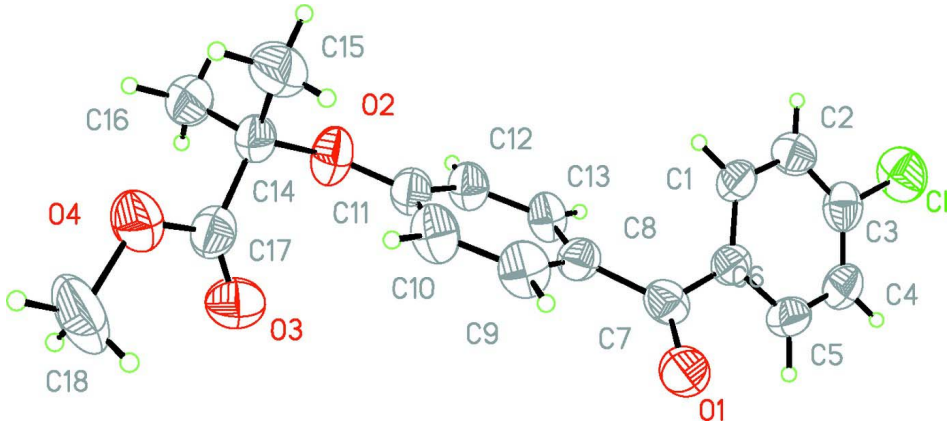

Figure 1

The molecular structure of the title compound, (I), showing the atom labeling scheme and 50% probability displacement ellipsoids.

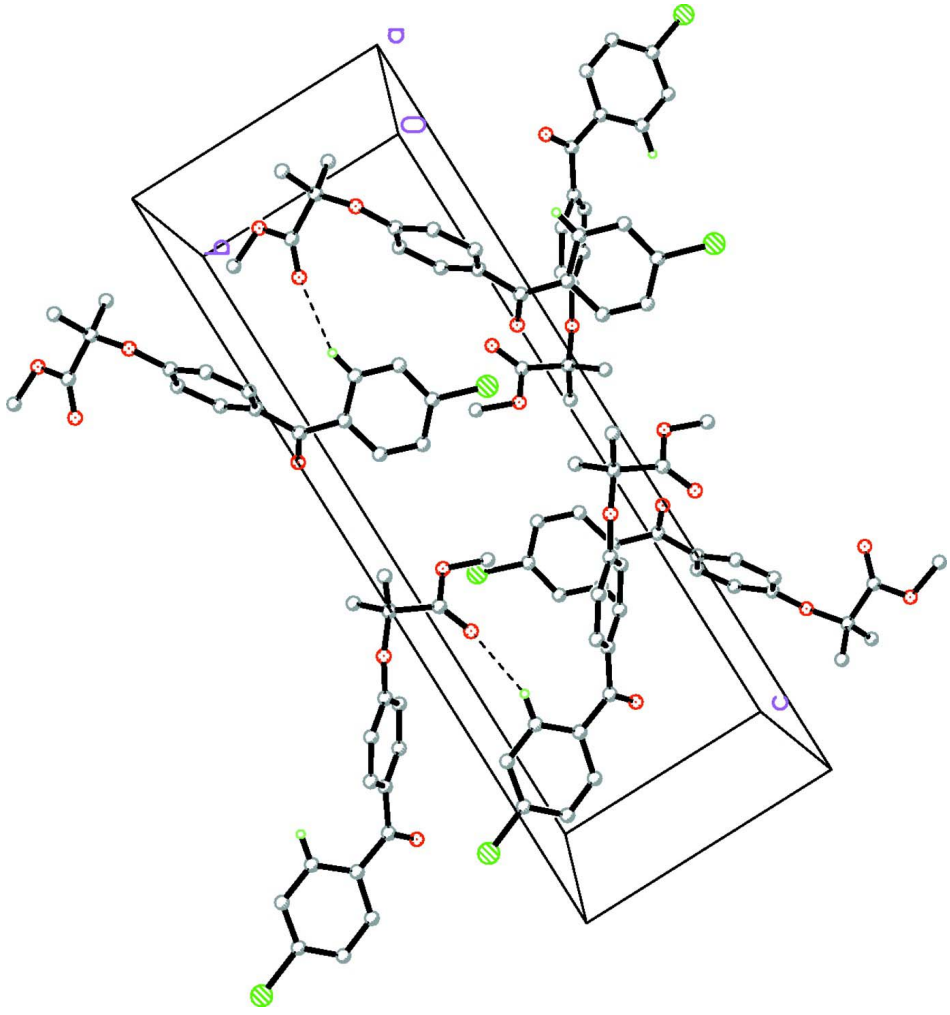

Figure 2

Packing diagram of the title compound viewed along the *a* axis. Dashed lines indicate weak C—H···O intermolecular interactions. Remaining H atoms have been omitted for clarity.

Methyl 2-[4-(4-chlorobenzoyl)phenoxy]-2-methylpropanoate

Crystal data

$C_{18}H_{17}ClO_4$
$M_r = 332.77$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 19.657$ (4) Å
$b = 7.5860$ (15) Å
$c = 22.436$ (5) Å
$V = 3345.6$ (12) Å^3
$Z = 8$
$F(000) = 1392$
$D_x = 1.321$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 9$–12°
$\mu = 0.25$ mm^{-1}
$T = 293$ K
Block, colorless
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 16.0355 pixels mm^{-1}
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.930$, $T_{max} = 0.976$
6018 measured reflections
3065 independent reflections
1432 reflections with $I > 2\sigma(I)$
$R_{int} = 0.092$
$\theta_{max} = 25.4°$, $\theta_{min} = 1.8°$
$h = 0 \rightarrow 23$
$k = 0 \rightarrow 9$
$l = -27 \rightarrow 27$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.067$
$wR(F^2) = 0.194$
$S = 1.00$
3065 reflections
208 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
$w = 1/[\sigma^2(F_o^2) + (0.070P)^2 + 1.P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ e Å^{-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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl	0.19155 (8)	0.28985 (19)	0.10094 (7)	0.0861 (5)
O1	0.03598 (16)	1.0570 (4)	0.15179 (15)	0.0650 (10)
O2	0.18493 (16)	1.3480 (4)	0.38182 (14)	0.0641 (9)
O3	0.1333 (2)	1.6697 (5)	0.34807 (16)	0.0758 (11)
O4	0.07842 (17)	1.7018 (4)	0.43384 (15)	0.0688 (10)

C1	0.1314 (2)	0.6897 (6)	0.2032 (2)	0.0513 (12)
H1A	0.1311	0.7155	0.2437	0.062*
C2	0.1552 (2)	0.5266 (6)	0.1842 (2)	0.0569 (12)
H2A	0.1694	0.4429	0.2119	0.068*
C3	0.1576 (2)	0.4899 (7)	0.1245 (2)	0.0576 (13)
C4	0.1335 (3)	0.6088 (7)	0.0831 (2)	0.0627 (13)
H4A	0.1341	0.5815	0.0427	0.075*
C5	0.1087 (2)	0.7686 (7)	0.1024 (2)	0.0579 (13)
H5A	0.0917	0.8481	0.0745	0.069*
C6	0.1083 (2)	0.8146 (6)	0.16303 (18)	0.0451 (11)
C7	0.0807 (2)	0.9881 (6)	0.1814 (2)	0.0496 (11)
C8	0.1063 (2)	1.0766 (6)	0.23639 (19)	0.0461 (11)
C9	0.0652 (2)	1.1914 (6)	0.2664 (2)	0.0583 (13)
H9A	0.0207	1.2071	0.2534	0.070*
C10	0.0875 (2)	1.2857 (6)	0.3158 (2)	0.0576 (12)
H10A	0.0584	1.3619	0.3359	0.069*
C11	0.1539 (2)	1.2636 (6)	0.33445 (19)	0.0502 (11)
C12	0.1967 (2)	1.1497 (6)	0.3040 (2)	0.0523 (12)
H12A	0.2417	1.1368	0.3162	0.063*
C13	0.1730 (2)	1.0555 (6)	0.2559 (2)	0.0519 (11)
H13A	0.2017	0.9773	0.2363	0.062*
C14	0.1484 (2)	1.4503 (6)	0.42572 (19)	0.0488 (11)
C15	0.0947 (3)	1.3430 (6)	0.4578 (2)	0.0746 (16)
H15A	0.1154	1.2408	0.4753	0.112*
H15B	0.0604	1.3066	0.4299	0.112*
H15C	0.0742	1.4134	0.4885	0.112*
C16	0.2051 (2)	1.5112 (7)	0.4665 (2)	0.0657 (14)
H16A	0.2249	1.4110	0.4861	0.099*
H16B	0.1870	1.5904	0.4959	0.099*
H16D	0.2392	1.5707	0.4435	0.099*
C17	0.1192 (2)	1.6172 (6)	0.3962 (2)	0.0544 (12)
C18	0.0490 (3)	1.8640 (6)	0.4124 (3)	0.096 (2)
H18D	0.0206	1.9141	0.4428	0.143*
H18A	0.0223	1.8405	0.3775	0.143*
H18B	0.0847	1.9454	0.4026	0.143*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl	0.1045 (12)	0.0681 (9)	0.0857 (11)	0.0090 (8)	0.0163 (9)	−0.0196 (8)
O1	0.055 (2)	0.055 (2)	0.085 (2)	−0.0014 (17)	−0.0228 (18)	0.0061 (18)
O2	0.058 (2)	0.069 (2)	0.065 (2)	0.0090 (17)	−0.0062 (16)	−0.0251 (18)
O3	0.095 (3)	0.070 (2)	0.063 (2)	−0.005 (2)	0.008 (2)	0.0145 (19)
O4	0.081 (2)	0.054 (2)	0.072 (2)	0.0153 (18)	0.008 (2)	−0.0068 (18)
C1	0.058 (3)	0.057 (3)	0.039 (2)	−0.009 (2)	−0.005 (2)	−0.001 (2)
C2	0.059 (3)	0.051 (3)	0.060 (3)	0.004 (2)	0.000 (2)	0.003 (2)
C3	0.055 (3)	0.060 (3)	0.058 (3)	−0.006 (2)	0.008 (2)	−0.014 (3)
C4	0.080 (4)	0.065 (3)	0.043 (3)	−0.009 (3)	−0.005 (3)	−0.009 (3)
C5	0.067 (3)	0.064 (3)	0.043 (3)	−0.010 (3)	−0.007 (2)	0.010 (2)
C6	0.043 (2)	0.051 (3)	0.041 (2)	−0.008 (2)	−0.001 (2)	0.003 (2)

C7	0.045 (2)	0.042 (3)	0.061 (3)	0.002 (2)	−0.001 (2)	0.004 (2)
C8	0.041 (2)	0.049 (3)	0.048 (3)	−0.003 (2)	−0.006 (2)	0.003 (2)
C9	0.041 (2)	0.059 (3)	0.075 (3)	0.004 (2)	−0.001 (2)	−0.005 (3)
C10	0.043 (2)	0.053 (3)	0.076 (3)	0.007 (2)	0.006 (3)	−0.012 (3)
C11	0.052 (3)	0.048 (3)	0.051 (3)	−0.001 (2)	−0.005 (2)	−0.006 (2)
C12	0.046 (2)	0.049 (3)	0.062 (3)	0.004 (2)	−0.006 (2)	−0.009 (2)
C13	0.044 (3)	0.044 (3)	0.067 (3)	0.001 (2)	−0.002 (2)	−0.011 (2)
C14	0.055 (3)	0.045 (3)	0.046 (3)	−0.006 (2)	−0.003 (2)	−0.006 (2)
C15	0.095 (4)	0.057 (3)	0.072 (4)	−0.009 (3)	0.013 (3)	0.007 (3)
C16	0.078 (3)	0.060 (3)	0.059 (3)	0.001 (3)	−0.013 (3)	−0.004 (3)
C17	0.059 (3)	0.055 (3)	0.049 (3)	−0.005 (2)	−0.002 (2)	−0.008 (3)
C18	0.105 (5)	0.048 (3)	0.134 (6)	0.028 (3)	−0.013 (4)	−0.021 (4)

Geometric parameters (Å, º)

Cl—C3	1.740 (5)	C9—C10	1.390 (6)
O1—C7	1.219 (5)	C9—H9A	0.9300
O2—C11	1.382 (5)	C10—C11	1.381 (6)
O2—C14	1.445 (5)	C10—H10A	0.9300
O3—C17	1.183 (5)	C11—C12	1.386 (6)
O4—C17	1.330 (5)	C12—C13	1.377 (6)
O4—C18	1.442 (6)	C12—H12A	0.9300
C1—C6	1.385 (6)	C13—H13A	0.9300
C1—C2	1.390 (6)	C14—C15	1.514 (6)
C1—H1A	0.9300	C14—C16	1.515 (6)
C2—C3	1.370 (6)	C14—C17	1.539 (6)
C2—H2A	0.9300	C15—H15A	0.9600
C3—C4	1.378 (7)	C15—H15B	0.9600
C4—C5	1.376 (6)	C15—H15C	0.9600
C4—H4A	0.9300	C16—H16A	0.9600
C5—C6	1.405 (6)	C16—H16B	0.9600
C5—H5A	0.9300	C16—H16D	0.9600
C6—C7	1.482 (6)	C18—H18D	0.9600
C7—C8	1.493 (6)	C18—H18A	0.9600
C8—C9	1.367 (6)	C18—H18B	0.9600
C8—C13	1.391 (5)		

C11—O2—C14	123.6 (3)	O2—C11—C12	113.5 (4)
C17—O4—C18	116.2 (4)	C13—C12—C11	120.3 (4)
C6—C1—C2	121.3 (4)	C13—C12—H12A	119.9
C6—C1—H1A	119.3	C11—C12—H12A	119.9
C2—C1—H1A	119.3	C12—C13—C8	120.4 (4)
C3—C2—C1	119.5 (5)	C12—C13—H13A	119.8
C3—C2—H2A	120.3	C8—C13—H13A	119.8
C1—C2—H2A	120.3	O2—C14—C15	112.4 (4)
C2—C3—C4	121.0 (5)	O2—C14—C16	102.1 (3)
C2—C3—Cl	119.2 (4)	C15—C14—C16	112.9 (4)
C4—C3—Cl	119.9 (4)	O2—C14—C17	109.5 (4)
C5—C4—C3	119.2 (4)	C15—C14—C17	112.8 (4)
C5—C4—H4A	120.4	C16—C14—C17	106.4 (3)

C3—C4—H4A	120.4	C14—C15—H15A	109.5
C4—C5—C6	121.6 (4)	C14—C15—H15B	109.5
C4—C5—H5A	119.2	H15A—C15—H15B	109.5
C6—C5—H5A	119.2	C14—C15—H15C	109.5
C1—C6—C5	117.4 (4)	H15A—C15—H15C	109.5
C1—C6—C7	123.2 (4)	H15B—C15—H15C	109.5
C5—C6—C7	119.4 (4)	C14—C16—H16A	109.5
O1—C7—C6	119.6 (4)	C14—C16—H16B	109.5
O1—C7—C8	120.0 (4)	H16A—C16—H16B	109.5
C6—C7—C8	120.4 (4)	C14—C16—H16D	109.5
C9—C8—C13	118.4 (4)	H16A—C16—H16D	109.5
C9—C8—C7	119.6 (4)	H16B—C16—H16D	109.5
C13—C8—C7	121.8 (4)	O3—C17—O4	123.9 (5)
C8—C9—C10	122.3 (4)	O3—C17—C14	125.6 (5)
C8—C9—H9A	118.9	O4—C17—C14	110.4 (4)
C10—C9—H9A	118.9	O4—C18—H18D	109.5
C11—C10—C9	118.6 (4)	O4—C18—H18A	109.5
C11—C10—H10A	120.7	H18D—C18—H18A	109.5
C9—C10—H10A	120.7	O4—C18—H18B	109.5
C10—C11—O2	126.4 (4)	H18D—C18—H18B	109.5
C10—C11—C12	120.0 (4)	H18A—C18—H18B	109.5

C6—C1—C2—C3	1.8 (7)	C9—C10—C11—O2	179.0 (4)
C1—C2—C3—C4	−3.3 (7)	C9—C10—C11—C12	0.1 (7)
C1—C2—C3—Cl	176.7 (4)	C14—O2—C11—C10	11.3 (7)
C2—C3—C4—C5	1.9 (7)	C14—O2—C11—C12	−169.7 (4)
Cl—C3—C4—C5	−178.1 (4)	C10—C11—C12—C13	−1.2 (7)
C3—C4—C5—C6	1.1 (7)	O2—C11—C12—C13	179.7 (4)
C2—C1—C6—C5	1.1 (6)	C11—C12—C13—C8	1.5 (7)
C2—C1—C6—C7	178.2 (4)	C9—C8—C13—C12	−0.5 (7)
C4—C5—C6—C1	−2.5 (6)	C7—C8—C13—C12	174.8 (4)
C4—C5—C6—C7	−179.8 (4)	C11—O2—C14—C15	58.5 (5)
C1—C6—C7—O1	−147.6 (4)	C11—O2—C14—C16	179.8 (4)
C5—C6—C7—O1	29.5 (6)	C11—O2—C14—C17	−67.7 (5)
C1—C6—C7—C8	31.1 (6)	C18—O4—C17—O3	1.8 (7)
C5—C6—C7—C8	−151.8 (4)	C18—O4—C17—C14	178.3 (4)
O1—C7—C8—C9	25.5 (6)	O2—C14—C17—O3	−11.3 (6)
C6—C7—C8—C9	−153.2 (4)	C15—C14—C17—O3	−137.3 (5)
O1—C7—C8—C13	−149.8 (4)	C16—C14—C17—O3	98.3 (5)
C6—C7—C8—C13	31.5 (6)	O2—C14—C17—O4	172.2 (3)
C13—C8—C9—C10	−0.6 (7)	C15—C14—C17—O4	46.3 (5)
C7—C8—C9—C10	−176.1 (4)	C16—C14—C17—O4	−78.1 (5)
C8—C9—C10—C11	0.9 (7)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*A*···O3^{i}	0.93	2.37	3.254 (6)	159

Symmetry code: (i) *x*, *y*−1, *z*.