Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-(4-Fluorophenyl)-3-(4-methoxyphenyl)-prop-2-en-1-one

William T. A. Harrison,[a]* H. S. Yathirajan,[b] H. G. Anilkumar,[b] B. K. Sarojini[c] and B. Narayana[d]

[a]Department of Chemistry, University of Aberdeen, Meston Walk, Aberdeen AB24 3UE, Scotland, [b]Department of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India, [c]Department of Chemistry, P. A. College of Engineering, Nadupadavu, Mangalore 574 153, India, and [d]Department of Chemistry, Mangalore University, Mangalagangotri 574 199, India

Correspondence e-mail: w.harrison@abdn.ac.uk

Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.003 Å
R factor = 0.036
wR factor = 0.083
Data-to-parameter ratio = 9.6

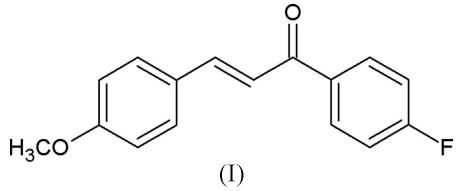
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 27 June 2006
Accepted 30 June 2006

The planar molecules of the title compound, $C_{15}H_{13}FO_2$, are normal. The non-centrosymmetric crystal packing may be influenced by weak C—H···O and C—H···F interactions.

Comment

Among the various organic compounds reported for their non-linear optical (NLO) properties, chalcone derivatives are notable for their excellent blue-light transmittance and good crystallizability (Uchida *et al.*, 1998). They provide a necessary molecular electronic configuration to show NLO effects, with two aromatic rings connected through a conjugated bridge (Goto *et al.*, 1991; Tam *et al.*, 1989; Indira *et al.*, 2002). Substitution on either of the benzene rings appears to increase the likelihood of non-centrosymmetric crystal packing, as well as enhancing the electronic properties of the molecule (Fichou *et al.*, 1988). As part of our ongoing studies in this area (Harrison *et al.*, 2005; Harrison, Yathirajan, Sarojini, Narayana & Vijaya Raj, 2006), we have prepared the title chalcone derivative, (I) (Fig. 1).



(I)

The geometric parameters for (I) are normal. The dihedral angle between the C1–C6 and C10–C15 benzene rings is 7.15 (10)°. The C16 methyl C atom is displaced from the C10–C15 ring plane by 0.059 (4) Å. The enone group is close to planar (r.m.s. deviation from the mean plane of C6–C10 + O1 = 0.028 Å). Overall, the molecule of (I) is approximately planar, which is different from the significantly more twisted conformation of the 4-chloro derivative (Harrison, Yathirajan, Sarojini, Narayana & Indira, 2006), where the dihedral angle between the benzene rings is 21.82 (6)°.

The only possible non-van der Waals intermolecular interactions in (I) are C—H···O and C—H···F bonds arising from the methyl group (Table 2, Fig. 2). There are no π–π stacking interactions in (I).

Compound (I) complements other chalcone derivatives with different substituents *X* at the 4-fluoro position (see scheme), including *X* = Cl (Harrison, Yathirajan, Sarojini, Narayana & Indira, 2006), *X* = OH (Sathiya Moorthi *et al.*, 2005), *X* = CH_3 (Wang *et al.*, 2005), *X* = H (Rabinovich & Schmidt, 1970), *X* = OCH_3 (Zheng *et al.*, 1992) and *X* = NO_2

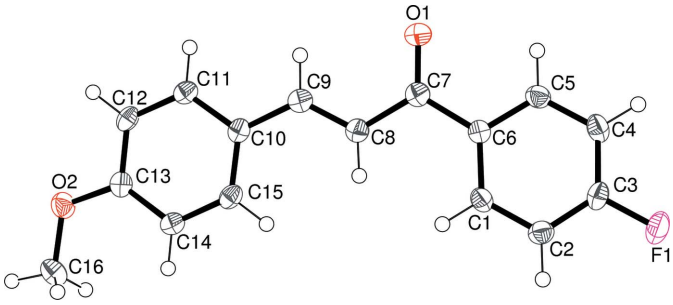


Figure 1
A view of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

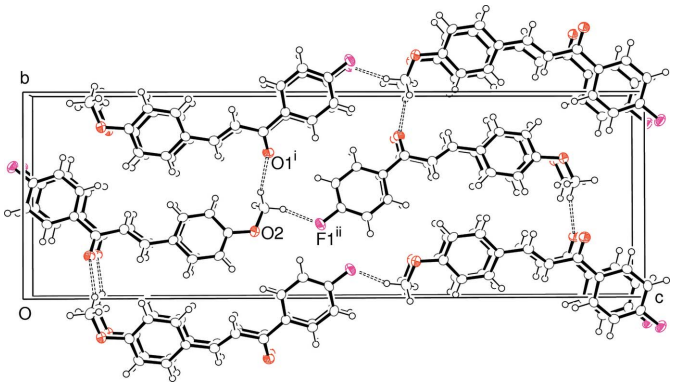


Figure 2
The packing in (I), viewed down [100], with C—H···O and C—H···F interactions indicated by dashed lines.

(Patil *et al.*, 2006). All of these compounds crystallize with different structures.

Experimental

4-Fluoroacetophenone (1.38 g, 0.01 mol) in ethanol (25 ml) was mixed with 4-methoxy-benzaldehyde (1.36 g, 0.01 mol) in ethanol (25 ml) and the mixture was treated with an aqueous solution (20 ml) of potassium hydroxide (20 ml, 5%). The resulting mixture was stirred well and left for 24 h, and the solid product was collected by filtration and dried. Crystals of (I) were recrystallized from ethanol (yield 90%; m.p. 371 K). Analysis, found (calculated) for $C_{16}H_{13}FO_2$: C 74.29 (74.92%), H 5.72 (5.07%).

Crystal data

$C_{16}H_{13}FO_2$
M_r = 256.26
Orthorhombic, $P2_12_12_1$
a = 3.9148 (2) Å
b = 10.1977 (5) Å
c = 30.8052 (14) Å
V = 1229.80 (10) Å^3
Z = 4
D_x = 1.384 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 120 (2) K
Block, colourless
0.65 × 0.20 × 0.15 mm

Data collection

Nonius KappaCCD area-detector diffractometer
ω and φ scans
Absorption correction: multi-scan *SADABS* (Bruker, 2003)
T_{min} = 0.938, T_{max} = 0.985
8063 measured reflections
1669 independent reflections
1402 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.083
S = 1.09
1669 reflections
174 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0274P)^2 + 0.45P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.017 (3)

Table 1
Selected torsion angles (°).

C5—C6—C7—O1	−9.4 (3)	O1—C7—C8—C9	−5.8 (4)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16B···O1^{i}	0.98	2.56	3.502 (3)	161
C16—H16A···F1^{ii}	0.98	2.59	3.458 (3)	148

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

In the absence of significant anomalous scattering effects, Friedel pairs were averaged and the absolute structure of the crystal studied is indeterminate. The H atoms were placed in idealized locations (C—H = 0.95–0.98 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C). The methyl group was rotated to fit the electron density.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK*, *DENZO* (Otwinowski & Minor, 1997), and *SORTAV* (Blessing, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

The authors thank the EPSRC National Crystallography Service (University of Southampton) for data collection. HGS thanks the University of Mysore for provision of research facilities. BKS thanks AICTE, Government of India, New Delhi, for financial assistance under the Career Award for Young Teachers (CAYT) scheme.

References

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Bruker (2003). *SADABS*, Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Fichou, D., Watanabe, T., Takeda, T., Miyata, S., Goto, Y. & Nakayama, M. (1988). *Jpn J. Appl. Phys.* **27**, 429–430.
Goto, Y., Hayashi, A., Kimura, Y. & Nakayama, M. (1991). *J. Cryst. Growth*, **108**, 688–698.
Harrison, W. T. A., Yathirajan, H. S., Sarojini, B. K., Narayana, B. & Anilkumar, H. G. (2005). *Acta Cryst.* C**61**, o728–o730.
Harrison, W. T. A., Yathirajan, H. S., Sarojini, B. K., Narayana, B. & Indira, J. (2006). *Acta Cryst.* E**62**, o1647–o1649.
Harrison, W. T. A., Yathirajan, H. S., Sarojini, B. K., Narayana, B. & Vijaya Raj, K. K. (2006). *Acta Cryst.* E**62**, o1578–o1579.

Indira, J., Karat, P. P. & Sarojini, B. K. (2002). *J. Cryst. Growth*, **242**, 209–214.
Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Patil, P. S., Teh, J. B.-J., Fun, H.-K., Razak, I. A. & Dharmaprakash, S. M. (2006). *Acta Cryst.* E**62**, o896–o898.
Rabinovich, D. & Schmidt, G. M. J. (1970). *J. Chem. Soc. B*, pp. 6–9.
Sathiya Moorthi, S., Chinnakali, K., Nanjundan, S., Radhika, R., Fun, H.-K. & Yu, X.-L. (2005). *Acta Cryst.* E**61**, o480–o482.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Tam, W., Guerin, B., Calabrese, J. C. & Stevenson, S. H. (1989). *Chem. Phys. Lett.* **154**, 93–96.
Uchida, T., Kozawa, K., Sakai, T., Aoki, M., Yoguchi, H., Abduryim, A. & Watanabe, Y. (1998). *Mol. Cryst. Liq. Cryst.* **315**, 135–140.
Wang, L., Lu, C.-R., Zhang, Y. & Zhang, D.-C. (2005). *Jiegou Huaxue (Chin. J. Struct. Chem.)*, **24**, 191–195. (In Chinese).
Zheng, J., Zhang, D., Sheng, P., Wang, H. & Yao, X. (1992). *Yingyong Huaxue (Chin. J. Appl. Chem.)*, **9**, 66–69. (In Chinese).

supporting information

Acta Cryst. (2006). E**62**, o3251–o3253 [https://doi.org/10.1107/S160053680602530X]

1-(4-Fluorophenyl)-3-(4-methoxyphenyl)prop-2-en-1-one

William T. A. Harrison, H. S. Yathirajan, H. G. Anilkumar, B. K. Sarojini and B. Narayana

1-(4-Fluorophenyl)-3-(4-methoxyphenyl)prop-2-en-1-one

Crystal data

$C_{16}H_{13}FO_2$
$M_r = 256.26$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 3.9148$ (2) Å
$b = 10.1977$ (5) Å
$c = 30.8052$ (14) Å
$V = 1229.80$ (10) Å^3
$Z = 4$
$F(000) = 536$
$D_x = 1.384$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1541 reflections
$\theta = 1.0$–$27.5°$
$\mu = 0.10$ mm^{-1}
$T = 120$ K
Block, colourless
0.65 × 0.20 × 0.15 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan SADABS (Bruker, 2003)
$T_{min} = 0.938$, $T_{max} = 0.985$
8063 measured reflections
1669 independent reflections
1402 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.3°$
$h = -5 \rightarrow 4$
$k = -13 \rightarrow 13$
$l = -40 \rightarrow 40$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.083$
$S = 1.09$
1669 reflections
174 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: none
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0274P)^2 + 0.45P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}
Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.017 (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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.3302 (6)	0.5221 (2)	0.08621 (6)	0.0249 (5)
H1	0.3789	0.5496	0.1150	0.030*
C2	0.4042 (7)	0.6047 (2)	0.05194 (6)	0.0271 (5)
H2	0.5029	0.6886	0.0568	0.033*
C3	0.3309 (6)	0.5622 (2)	0.01070 (6)	0.0259 (5)
C4	0.1873 (7)	0.4417 (2)	0.00202 (6)	0.0285 (6)
H4	0.1399	0.4153	−0.0269	0.034*
C5	0.1141 (7)	0.3604 (2)	0.03656 (6)	0.0265 (5)
H5	0.0140	0.2770	0.0313	0.032*
C6	0.1850 (6)	0.39877 (19)	0.07920 (6)	0.0216 (5)
C7	0.0968 (6)	0.3057 (2)	0.11487 (6)	0.0257 (5)
C8	0.2157 (6)	0.3353 (2)	0.15937 (6)	0.0265 (5)
H8	0.3639	0.4078	0.1639	0.032*
C9	0.1196 (6)	0.2625 (2)	0.19346 (6)	0.0249 (5)
H9	−0.0287	0.1909	0.1876	0.030*
C10	0.2193 (6)	0.2817 (2)	0.23866 (6)	0.0227 (5)
C11	0.1246 (6)	0.1895 (2)	0.26996 (6)	0.0242 (5)
H11	−0.0011	0.1142	0.2613	0.029*
C12	0.2094 (6)	0.2053 (2)	0.31321 (6)	0.0241 (5)
H12	0.1451	0.1406	0.3338	0.029*
C13	0.3895 (6)	0.3162 (2)	0.32649 (6)	0.0232 (5)
C14	0.4832 (6)	0.4105 (2)	0.29607 (6)	0.0236 (5)
H14	0.6024	0.4871	0.3049	0.028*
C15	0.4010 (6)	0.39162 (19)	0.25281 (6)	0.0245 (5)
H15	0.4704	0.4553	0.2321	0.029*
C16	0.6316 (7)	0.4400 (2)	0.38472 (7)	0.0323 (6)
H16A	0.6783	0.4321	0.4159	0.048*
H16B	0.4846	0.5162	0.3796	0.048*
H16C	0.8472	0.4512	0.3690	0.048*
O1	−0.0729 (5)	0.20711 (14)	0.10708 (5)	0.0344 (4)
O2	0.4625 (4)	0.32341 (14)	0.36970 (4)	0.0303 (4)
F1	0.4078 (4)	0.64183 (12)	−0.02341 (4)	0.0381 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0287 (14)	0.0251 (10)	0.0210 (9)	0.0020 (10)	−0.0018 (10)	−0.0029 (8)
C2	0.0290 (13)	0.0227 (10)	0.0296 (10)	−0.0013 (11)	0.0023 (10)	−0.0004 (8)
C3	0.0282 (14)	0.0268 (11)	0.0228 (9)	0.0060 (11)	0.0036 (10)	0.0061 (8)
C4	0.0358 (15)	0.0296 (12)	0.0200 (9)	0.0064 (12)	−0.0017 (10)	−0.0030 (8)

C5	0.0310 (13)	0.0214 (10)	0.0271 (10)	−0.0002 (11)	−0.0030 (11)	−0.0023 (8)
C6	0.0201 (12)	0.0226 (10)	0.0222 (9)	0.0022 (9)	0.0000 (9)	−0.0001 (8)
C7	0.0250 (12)	0.0248 (10)	0.0273 (10)	0.0021 (11)	0.0012 (10)	−0.0008 (8)
C8	0.0278 (13)	0.0266 (11)	0.0252 (10)	−0.0022 (11)	−0.0012 (10)	0.0012 (9)
C9	0.0230 (12)	0.0233 (10)	0.0285 (10)	0.0017 (11)	0.0004 (10)	0.0002 (8)
C10	0.0227 (12)	0.0214 (10)	0.0241 (9)	0.0049 (10)	0.0032 (9)	0.0026 (8)
C11	0.0232 (12)	0.0206 (10)	0.0289 (10)	0.0020 (11)	0.0031 (10)	0.0014 (8)
C12	0.0224 (12)	0.0232 (10)	0.0267 (10)	0.0033 (10)	0.0033 (9)	0.0077 (9)
C13	0.0189 (12)	0.0267 (10)	0.0240 (9)	0.0063 (11)	0.0005 (9)	0.0016 (8)
C14	0.0211 (12)	0.0210 (10)	0.0285 (10)	0.0013 (10)	0.0010 (10)	0.0012 (8)
C15	0.0243 (13)	0.0211 (10)	0.0282 (10)	0.0034 (10)	0.0054 (11)	0.0044 (8)
C16	0.0328 (14)	0.0349 (12)	0.0291 (10)	0.0033 (13)	−0.0056 (11)	−0.0064 (9)
O1	0.0414 (10)	0.0291 (8)	0.0327 (8)	−0.0111 (9)	−0.0038 (8)	0.0015 (6)
O2	0.0356 (10)	0.0309 (8)	0.0245 (7)	0.0013 (8)	−0.0037 (7)	0.0016 (6)
F1	0.0527 (10)	0.0345 (7)	0.0270 (6)	0.0042 (8)	0.0086 (7)	0.0092 (5)

Geometric parameters (Å, º)

C1—C2	1.382 (3)	C9—H9	0.9500
C1—C6	1.397 (3)	C10—C11	1.397 (3)
C1—H1	0.9500	C10—C15	1.397 (3)
C2—C3	1.373 (3)	C11—C12	1.382 (3)
C2—H2	0.9500	C11—H11	0.9500
C3—F1	1.362 (2)	C12—C13	1.394 (3)
C3—C4	1.377 (3)	C12—H12	0.9500
C4—C5	1.379 (3)	C13—O2	1.363 (2)
C4—H4	0.9500	C13—C14	1.392 (3)
C5—C6	1.398 (3)	C14—C15	1.384 (3)
C5—H5	0.9500	C14—H14	0.9500
C6—C7	1.493 (3)	C15—H15	0.9500
C7—O1	1.229 (3)	C16—O2	1.437 (3)
C7—C8	1.479 (3)	C16—H16A	0.9800
C8—C9	1.340 (3)	C16—H16B	0.9800
C8—H8	0.9500	C16—H16C	0.9800
C9—C10	1.460 (3)		
C2—C1—C6	121.08 (19)	C10—C9—H9	116.6
C2—C1—H1	119.5	C11—C10—C15	117.37 (18)
C6—C1—H1	119.5	C11—C10—C9	119.79 (19)
C3—C2—C1	118.06 (19)	C15—C10—C9	122.81 (18)
C3—C2—H2	121.0	C12—C11—C10	121.5 (2)
C1—C2—H2	121.0	C12—C11—H11	119.2
F1—C3—C2	118.63 (19)	C10—C11—H11	119.2
F1—C3—C4	118.20 (18)	C11—C12—C13	119.91 (19)
C2—C3—C4	123.16 (19)	C11—C12—H12	120.0
C3—C4—C5	118.11 (18)	C13—C12—H12	120.0
C3—C4—H4	120.9	O2—C13—C14	124.38 (19)
C5—C4—H4	120.9	O2—C13—C12	115.88 (18)

C4—C5—C6	121.03 (19)	C14—C13—C12	119.74 (18)
C4—C5—H5	119.5	C15—C14—C13	119.4 (2)
C6—C5—H5	119.5	C15—C14—H14	120.3
C1—C6—C5	118.56 (18)	C13—C14—H14	120.3
C1—C6—C7	123.56 (18)	C14—C15—C10	122.01 (19)
C5—C6—C7	117.88 (18)	C14—C15—H15	119.0
O1—C7—C8	121.24 (19)	C10—C15—H15	119.0
O1—C7—C6	120.10 (18)	O2—C16—H16A	109.5
C8—C7—C6	118.66 (19)	O2—C16—H16B	109.5
C9—C8—C7	121.6 (2)	H16A—C16—H16B	109.5
C9—C8—H8	119.2	O2—C16—H16C	109.5
C7—C8—H8	119.2	H16A—C16—H16C	109.5
C8—C9—C10	126.7 (2)	H16B—C16—H16C	109.5
C8—C9—H9	116.6	C13—O2—C16	117.11 (16)

C6—C1—C2—C3	0.0 (4)	C7—C8—C9—C10	180.0 (2)
C1—C2—C3—F1	−178.9 (2)	C8—C9—C10—C11	−173.7 (2)
C1—C2—C3—C4	0.2 (4)	C8—C9—C10—C15	8.0 (4)
F1—C3—C4—C5	179.1 (2)	C15—C10—C11—C12	−0.6 (3)
C2—C3—C4—C5	0.0 (4)	C9—C10—C11—C12	−179.0 (2)
C3—C4—C5—C6	−0.3 (4)	C10—C11—C12—C13	0.9 (3)
C2—C1—C6—C5	−0.2 (3)	C11—C12—C13—O2	−179.9 (2)
C2—C1—C6—C7	−179.5 (2)	C11—C12—C13—C14	−0.1 (3)
C4—C5—C6—C1	0.4 (3)	O2—C13—C14—C15	178.7 (2)
C4—C5—C6—C7	179.7 (2)	C12—C13—C14—C15	−1.1 (3)
C1—C6—C7—O1	169.8 (2)	C13—C14—C15—C10	1.5 (3)
C5—C6—C7—O1	−9.4 (3)	C11—C10—C15—C14	−0.6 (3)
C1—C6—C7—C8	−9.8 (3)	C9—C10—C15—C14	177.7 (2)
C5—C6—C7—C8	171.0 (2)	C14—C13—O2—C16	3.5 (3)
O1—C7—C8—C9	−5.8 (4)	C12—C13—O2—C16	−176.71 (19)
C6—C7—C8—C9	173.8 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16*B*···O1^{i}	0.98	2.56	3.502 (3)	161
C16—H16*A*···F1^{ii}	0.98	2.59	3.458 (3)	148

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