

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

## 2-(4-Chlorophenyl)-2-oxoethyl 3-(trifluoromethyl)benzoate

 Hoong-Kun Fun,<sup>a\*‡</sup> Wan-Sin Loh,<sup>a§</sup> B. Garudachari,<sup>b</sup>  
Arun M. Isloor<sup>b</sup> and M. N. Satyanarayan<sup>c</sup>

<sup>a</sup>X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, <sup>b</sup>Organic Chemistry Division, Department of Chemistry, National Institute of Technology – Karnataka, Surathkal, Mangalore 575 025, India, and <sup>c</sup>Department of Physics, National Institute of Technology – Karnataka, Surathkal, Mangalore 575 025, India

Correspondence e-mail: hkfun@usm.my

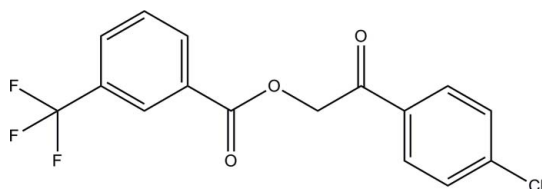
Received 24 May 2011; accepted 30 May 2011

Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.048;  $wR$  factor = 0.121; data-to-parameter ratio = 18.4.

In the title compound,  $\text{C}_{16}\text{H}_{10}\text{ClF}_3\text{O}_3$ , the two benzene rings are slightly twisted from each other, with a dihedral angle of  $15.50$  ( $8$ )° between the planes. In the crystal, intermolecular  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds link the molecules into a layer parallel to the  $bc$  plane.

### Related literature

For the background and applications of phenacyl benzoates, see: Sheehan & Umezaw (1973); Ruzicka *et al.* (2002); Litera *et al.* (2006); Rather & Reid (1919); Huang *et al.* (1996); Gandhi *et al.* (1995). For bond-length data, see: Allen *et al.* (1987). For the stability of the temperature controller used for the data collection, see: Cosier & Glazer (1986).



### Experimental

#### Crystal data

$\text{C}_{16}\text{H}_{10}\text{ClF}_3\text{O}_3$   
 $M_r = 342.69$   
Monoclinic,  $P2_1/c$   
 $a = 14.3036$  (7) Å  
 $b = 12.1335$  (6) Å  
 $c = 8.5464$  (4) Å  
 $\beta = 101.444$  (1)°

$V = 1453.76$  (12) Å<sup>3</sup>  
 $Z = 4$   
Mo  $K\alpha$  radiation  
 $\mu = 0.31$  mm<sup>-1</sup>  
 $T = 100$  K  
 $0.28 \times 0.16 \times 0.11$  mm

#### Data collection

Bruker SMART APEXII CCD  
area-detector diffractometer  
Absorption correction: multi-scan  
(*SADABS*; Bruker, 2009)  
 $T_{\min} = 0.919$ ,  $T_{\max} = 0.966$

15629 measured reflections  
3822 independent reflections  
2963 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.046$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$   
 $wR(F^2) = 0.121$   
 $S = 1.04$   
3822 reflections

208 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.52$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.33$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C1}-\text{H1A}\cdots\text{O1}^i$	0.95	2.53	3.205 (2)	128
$\text{C4}-\text{H4A}\cdots\text{O3}^{ii}$	0.95	2.53	3.289 (2)	137
$\text{C8}-\text{H8A}\cdots\text{O3}^{iii}$	0.99	2.48	3.474 (2)	177

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

H-KF and W-SL thank Universiti Sains Malaysia (USM) for a Research University Grant (No. 1001/PFIZIK/811160). W-SL also thanks the Malaysian government and USM for the award of a Research Fellowship. AMI is thankful to the Department of Atomic Energy, Board for Research in Nuclear Sciences, Government of India, for a 'Young Scientist' award. BG thanks the Department of Information Technology, New Delhi, India, for the financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2720).

### References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
- Bruker (2009). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Cosier, J. & Glazer, A. M. (1986). *J. Appl. Cryst.* **19**, 105–107.
- Gandhi, S. S., Bell, K. L. & Gibson, M. S. (1995). *Tetrahedron*, **51**, 13301–13308.
- Huang, W., Pian, J., Chen, B., Pei, W. & Ye, X. (1996). *Tetrahedron*, **52**, 10131–10136.
- Litera, J. K., Loya, A. D. & Klan, P. (2006). *J. Org. Chem.* **71**, 713–723.
- Rather, J. B. & Reid, E. (1919). *J. Am. Chem. Soc.* **41**, 75–83.
- Ruzicka, R., Zabadal, M. & Klan, P. (2002). *Synth. Commun.* **32**, 2581–2590.
- Sheehan, J. C. & Umezaw, K. (1973). *J. Org. Chem.* **58**, 3771–3773.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.

<sup>‡</sup> Thomson Reuters ResearcherID: A-3561-2009.

<sup>§</sup> Thomson Reuters ResearcherID: C-7581-2009.

## supporting information

*Acta Cryst.* (2011). E67, o1597 [doi:10.1107/S1600536811020629]

## 2-(4-Chlorophenyl)-2-oxoethyl 3-(trifluoromethyl)benzoate

Hoong-Kun Fun, Wan-Sin Loh, B. Garudachari, Arun M. Isloor and M. N. Satyanarayan

### S1. Comment

Phenacyl benzoates derivatives are very important in identification of organic acids (Rather & Reid, 1919), they undergo photolysis in neutral and mild conditions (Sheehan & Umezaw, 1973; Ruzicka *et al.*, 2002; Litera *et al.*, 2006). They find applications in the field of synthetic chemistry for the synthesis of oxazoles, imidazoles (Huang *et al.*, 1996), benzoxazepine (Gandhi *et al.*, 1995). We hereby report the crystal structure of 2-(4-chlorophenyl)-2-oxoethyl 3-(trifluoromethyl) benzoate of potential commercial importance.

In the title compound (Fig. 1), the chlorophenyl (C1–C6/Cl1) group is slightly twisted away from the benzene ring (C10–C15) with a dihedral angle of 15.50 (8)°. Bond lengths (Allen *et al.*, 1987) and angles are within the normal ranges.

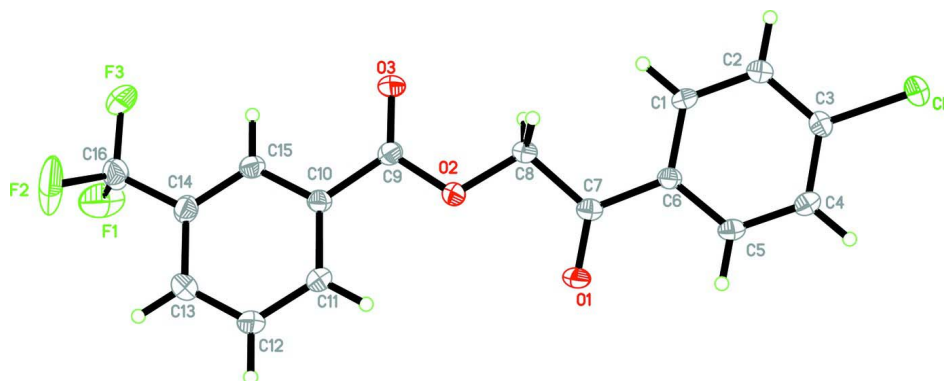
In the crystal packing (Fig. 2), intermolecular C1—H1A···O1<sup>i</sup>, C4—H4A···O3<sup>ii</sup> and C8—H8A···O3<sup>iii</sup> hydrogen bonds (Table 1) link the molecules into a layer parallel to the *bc* plane.

### S2. Experimental

A mixture of 3-(trifluoromethyl)benzoic acid (1.0 g, 0.0052 mol), potassium carbonate (0.80 g, 0.0057 mol) and 2-bromo-1-(4-chlorophenyl)ethanone (1.21 g, 0.0052 mol) in dimethylformamide (10 ml) was stirred at room temperature for 2 h. On cooling, colourless needle-shaped crystals, 2-(4-chlorophenyl)-2-oxoethyl 3-(trifluoromethyl)benzoate begin to separate. It was collected by filtration and recrystallized from ethanol. Yield: 1.60 g, 88.8%, *m.p.*: 387–388 K.

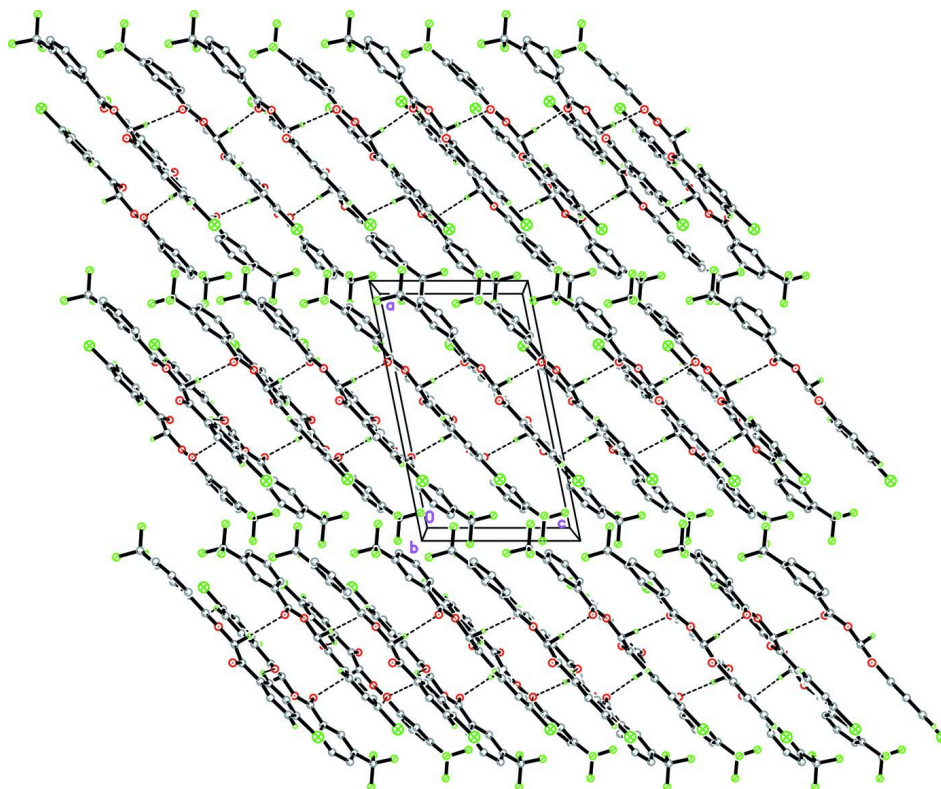
### S3. Refinement

All the H atoms were positioned geometrically (C—H = 0.95 or 0.99 Å) and refined with a riding model, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .



**Figure 1**

The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

**Figure 2**

The crystal packing of the title compound, viewed along the *b* axis. H atoms not involved in the intermolecular interactions (dashed lines) have been omitted for clarity.

### 2-(4-Chlorophenyl)-2-oxoethyl 3-(trifluoromethyl)benzoate

#### Crystal data

$C_{16}H_{10}ClF_3O_3$

$M_r = 342.69$

Monoclinic,  $P2_1/c$

Hall symbol: -P 2ybc

$a = 14.3036 (7) \text{ \AA}$

$b = 12.1335 (6) \text{ \AA}$

$c = 8.5464 (4) \text{ \AA}$

$\beta = 101.444 (1)^\circ$

$V = 1453.76 (12) \text{ \AA}^3$

$Z = 4$

$F(000) = 696$

$D_x = 1.566 \text{ Mg m}^{-3}$

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

Cell parameters from 3750 reflections

$\theta = 2.9\text{--}29.9^\circ$

$\mu = 0.31 \text{ mm}^{-1}$

$T = 100 \text{ K}$

Block, colourless

$0.28 \times 0.16 \times 0.11 \text{ mm}$

#### Data collection

Bruker SMART APEXII CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2009)

$T_{\min} = 0.919$ ,  $T_{\max} = 0.966$

15629 measured reflections

3822 independent reflections

2963 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.046$

$\theta_{\max} = 29.0^\circ$ ,  $\theta_{\min} = 1.5^\circ$

$h = -19 \rightarrow 19$

$k = -10 \rightarrow 16$

$l = -11 \rightarrow 11$

Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.048$   
 $wR(F^2) = 0.121$   
 $S = 1.04$   
 3822 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0486P)^2 + 1.0347P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.52 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.33 \text{ e } \text{\AA}^{-3}$

Special details

**Experimental.** The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

**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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	0.22643 (4)	0.86068 (4)	1.07291 (6)	0.02896 (14)
F1	0.92991 (14)	0.87892 (13)	0.01853 (17)	0.0580 (5)
F2	1.04777 (11)	0.85923 (17)	0.2147 (2)	0.0727 (6)
F3	0.93614 (10)	0.73951 (11)	0.17107 (16)	0.0371 (3)
O1	0.53911 (10)	1.07226 (11)	0.66621 (15)	0.0222 (3)
O2	0.66428 (9)	0.93394 (11)	0.59360 (15)	0.0214 (3)
O3	0.69311 (10)	0.76708 (11)	0.49795 (17)	0.0260 (3)
C1	0.43295 (14)	0.83441 (15)	0.8232 (2)	0.0202 (4)
H1A	0.4678	0.7774	0.7845	0.024*
C2	0.36390 (14)	0.80774 (16)	0.9092 (2)	0.0225 (4)
H2A	0.3509	0.7329	0.9297	0.027*
C3	0.31378 (14)	0.89225 (16)	0.9650 (2)	0.0207 (4)
C4	0.33093 (13)	1.00257 (16)	0.9356 (2)	0.0202 (4)
H4A	0.2957	1.0593	0.9742	0.024*
C5	0.39992 (13)	1.02787 (15)	0.8495 (2)	0.0191 (4)
H5A	0.4122	1.1028	0.8285	0.023*
C6	0.45214 (13)	0.94487 (15)	0.7924 (2)	0.0171 (4)
C7	0.52797 (13)	0.97681 (15)	0.7041 (2)	0.0182 (4)
C8	0.59082 (14)	0.88503 (15)	0.6632 (2)	0.0199 (4)
H8A	0.6195	0.8437	0.7609	0.024*
H8B	0.5526	0.8332	0.5868	0.024*
C9	0.71079 (13)	0.86489 (15)	0.5125 (2)	0.0190 (4)
C10	0.78492 (13)	0.92229 (15)	0.4433 (2)	0.0185 (4)

C11	0.80562 (14)	1.03401 (16)	0.4691 (2)	0.0219 (4)
H11A	0.7732	1.0758	0.5358	0.026*
C12	0.87340 (15)	1.08395 (17)	0.3975 (3)	0.0276 (4)
H12A	0.8872	1.1601	0.4149	0.033*
C13	0.92112 (15)	1.02351 (17)	0.3007 (2)	0.0264 (4)
H13A	0.9673	1.0580	0.2511	0.032*
C14	0.90109 (14)	0.91177 (17)	0.2764 (2)	0.0228 (4)
C15	0.83340 (13)	0.86101 (16)	0.3467 (2)	0.0198 (4)
H15A	0.8200	0.7848	0.3292	0.024*
C16	0.95338 (16)	0.84786 (19)	0.1713 (3)	0.0314 (5)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C11	0.0281 (3)	0.0281 (3)	0.0351 (3)	−0.0017 (2)	0.0170 (2)	0.0031 (2)
F1	0.1082 (15)	0.0398 (9)	0.0358 (8)	0.0034 (9)	0.0380 (9)	−0.0024 (6)
F2	0.0272 (8)	0.0992 (15)	0.0989 (14)	−0.0158 (8)	0.0301 (8)	−0.0676 (12)
F3	0.0439 (8)	0.0256 (7)	0.0466 (8)	0.0074 (6)	0.0204 (6)	−0.0064 (6)
O1	0.0289 (7)	0.0134 (6)	0.0255 (6)	−0.0011 (5)	0.0082 (6)	0.0029 (5)
O2	0.0242 (7)	0.0165 (6)	0.0263 (6)	−0.0022 (5)	0.0121 (5)	−0.0020 (5)
O3	0.0311 (8)	0.0137 (6)	0.0362 (8)	−0.0031 (6)	0.0140 (6)	−0.0030 (6)
C1	0.0241 (9)	0.0131 (9)	0.0243 (9)	0.0023 (7)	0.0070 (7)	0.0001 (7)
C2	0.0257 (10)	0.0162 (9)	0.0272 (9)	0.0001 (7)	0.0088 (8)	0.0023 (7)
C3	0.0212 (9)	0.0214 (9)	0.0210 (8)	−0.0017 (7)	0.0078 (7)	0.0011 (7)
C4	0.0214 (9)	0.0167 (9)	0.0219 (8)	0.0035 (7)	0.0030 (7)	−0.0010 (7)
C5	0.0224 (9)	0.0140 (8)	0.0199 (8)	0.0012 (7)	0.0020 (7)	0.0013 (7)
C6	0.0200 (9)	0.0140 (8)	0.0175 (7)	−0.0005 (7)	0.0039 (6)	0.0007 (7)
C7	0.0212 (9)	0.0153 (8)	0.0173 (8)	−0.0007 (7)	0.0021 (7)	0.0010 (7)
C8	0.0232 (9)	0.0152 (9)	0.0225 (8)	−0.0007 (7)	0.0074 (7)	0.0011 (7)
C9	0.0203 (9)	0.0170 (9)	0.0200 (8)	0.0011 (7)	0.0046 (7)	−0.0008 (7)
C10	0.0186 (9)	0.0156 (9)	0.0214 (8)	0.0003 (7)	0.0038 (7)	0.0018 (7)
C11	0.0227 (9)	0.0175 (9)	0.0268 (9)	0.0015 (7)	0.0078 (7)	−0.0019 (7)
C12	0.0265 (10)	0.0168 (10)	0.0413 (11)	−0.0027 (8)	0.0112 (9)	−0.0028 (8)
C13	0.0249 (10)	0.0237 (10)	0.0323 (10)	−0.0034 (8)	0.0100 (8)	0.0020 (8)
C14	0.0210 (9)	0.0238 (10)	0.0246 (9)	0.0010 (8)	0.0068 (7)	−0.0039 (8)
C15	0.0216 (9)	0.0161 (9)	0.0219 (8)	0.0000 (7)	0.0043 (7)	−0.0014 (7)
C16	0.0298 (11)	0.0325 (12)	0.0356 (11)	−0.0061 (9)	0.0155 (9)	−0.0119 (9)

*Geometric parameters (Å, °)*

C11—C3	1.7364 (19)	C5—H5A	0.9500
F1—C16	1.336 (3)	C6—C7	1.490 (3)
F2—C16	1.335 (3)	C7—C8	1.515 (3)
F3—C16	1.338 (3)	C8—H8A	0.9900
O1—C7	1.222 (2)	C8—H8B	0.9900
O2—C9	1.344 (2)	C9—C10	1.486 (3)
O2—C8	1.435 (2)	C10—C15	1.394 (3)
O3—C9	1.215 (2)	C10—C11	1.396 (3)

C1—C2	1.381 (3)	C11—C12	1.385 (3)
C1—C6	1.403 (3)	C11—H11A	0.9500
C1—H1A	0.9500	C12—C13	1.383 (3)
C2—C3	1.389 (3)	C12—H12A	0.9500
C2—H2A	0.9500	C13—C14	1.393 (3)
C3—C4	1.393 (3)	C13—H13A	0.9500
C4—C5	1.378 (3)	C14—C15	1.381 (3)
C4—H4A	0.9500	C14—C16	1.495 (3)
C5—C6	1.398 (3)	C15—H15A	0.9500
C9—O2—C8	115.72 (14)	O3—C9—O2	123.20 (17)
C2—C1—C6	120.70 (17)	O3—C9—C10	124.57 (17)
C2—C1—H1A	119.6	O2—C9—C10	112.22 (16)
C6—C1—H1A	119.6	C15—C10—C11	119.79 (17)
C1—C2—C3	118.83 (18)	C15—C10—C9	117.65 (17)
C1—C2—H2A	120.6	C11—C10—C9	122.55 (17)
C3—C2—H2A	120.6	C12—C11—C10	120.03 (18)
C2—C3—C4	121.75 (18)	C12—C11—H11A	120.0
C2—C3—C11	119.64 (15)	C10—C11—H11A	120.0
C4—C3—C11	118.61 (15)	C13—C12—C11	120.28 (19)
C5—C4—C3	118.75 (17)	C13—C12—H12A	119.9
C5—C4—H4A	120.6	C11—C12—H12A	119.9
C3—C4—H4A	120.6	C12—C13—C14	119.61 (19)
C4—C5—C6	120.98 (17)	C12—C13—H13A	120.2
C4—C5—H5A	119.5	C14—C13—H13A	120.2
C6—C5—H5A	119.5	C15—C14—C13	120.71 (18)
C5—C6—C1	118.99 (17)	C15—C14—C16	120.48 (19)
C5—C6—C7	118.83 (16)	C13—C14—C16	118.80 (18)
C1—C6—C7	122.16 (16)	C14—C15—C10	119.58 (18)
O1—C7—C6	121.81 (17)	C14—C15—H15A	120.2
O1—C7—C8	121.41 (17)	C10—C15—H15A	120.2
C6—C7—C8	116.78 (15)	F2—C16—F1	106.7 (2)
O2—C8—C7	107.97 (14)	F2—C16—F3	106.1 (2)
O2—C8—H8A	110.1	F1—C16—F3	105.40 (17)
C7—C8—H8A	110.1	F2—C16—C14	112.24 (17)
O2—C8—H8B	110.1	F1—C16—C14	112.5 (2)
C7—C8—H8B	110.1	F3—C16—C14	113.35 (18)
H8A—C8—H8B	108.4		
C6—C1—C2—C3	-0.1 (3)	O2—C9—C10—C15	-175.47 (15)
C1—C2—C3—C4	0.5 (3)	O3—C9—C10—C11	-177.10 (18)
C1—C2—C3—C11	179.84 (15)	O2—C9—C10—C11	3.2 (2)
C2—C3—C4—C5	-0.4 (3)	C15—C10—C11—C12	0.7 (3)
C11—C3—C4—C5	-179.73 (14)	C9—C10—C11—C12	-178.00 (18)
C3—C4—C5—C6	-0.1 (3)	C10—C11—C12—C13	-0.2 (3)
C4—C5—C6—C1	0.4 (3)	C11—C12—C13—C14	-0.4 (3)
C4—C5—C6—C7	-178.17 (16)	C12—C13—C14—C15	0.7 (3)
C2—C1—C6—C5	-0.3 (3)	C12—C13—C14—C16	179.9 (2)

C2—C1—C6—C7	178.24 (17)	C13—C14—C15—C10	-0.2 (3)
C5—C6—C7—O1	-7.6 (2)	C16—C14—C15—C10	-179.49 (17)
C1—C6—C7—O1	173.85 (17)	C11—C10—C15—C14	-0.4 (3)
C5—C6—C7—C8	172.43 (16)	C9—C10—C15—C14	178.31 (16)
C1—C6—C7—C8	-6.1 (2)	C15—C14—C16—F2	-128.0 (2)
C9—O2—C8—C7	-163.11 (14)	C13—C14—C16—F2	52.7 (3)
O1—C7—C8—O2	5.7 (2)	C15—C14—C16—F1	111.7 (2)
C6—C7—C8—O2	-174.34 (14)	C13—C14—C16—F1	-67.6 (2)
C8—O2—C9—O3	-0.2 (3)	C15—C14—C16—F3	-7.8 (3)
C8—O2—C9—C10	179.50 (14)	C13—C14—C16—F3	172.98 (18)
O3—C9—C10—C15	4.2 (3)		

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )

<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>
C1—H1 <i>A</i> $\cdots$ O1 <sup>i</sup>	0.95	2.53	3.205 (2)	128
C4—H4 <i>A</i> $\cdots$ O3 <sup>ii</sup>	0.95	2.53	3.289 (2)	137
C8—H8 <i>A</i> $\cdots$ O3 <sup>iii</sup>	0.99	2.48	3.474 (2)	177

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