

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

# (E)-1-(Furan-2-yl)-3-(2,4,5-trimethoxyphenyl)prop-2-en-1-one

 Thitipone Suwunwong,<sup>a</sup> Suchada Chantrapromma,<sup>a\*‡</sup> Chatchanok Karalai,<sup>a</sup> Pitikan Wisitsak<sup>b</sup> and Hoong-Kun Fun<sup>c§</sup>

<sup>a</sup>Crystal Materials Research Unit, Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat-Yai, Songkhla 90112, Thailand, <sup>b</sup>Excellence Center, Mae Fah Luang University, Thasud, Muang, Chaing Rai 57100, Thailand, and <sup>c</sup>X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia

Correspondence e-mail: suchada.c@psu.ac.th

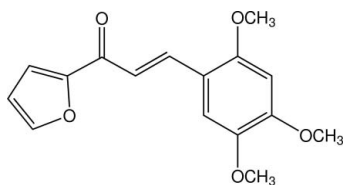
Received 21 December 2011; accepted 1 January 2012

 Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.064;  $wR$  factor = 0.175; data-to-parameter ratio = 13.7.

In the title chalcone derivative,  $\text{C}_{16}\text{H}_{16}\text{O}_5$ , the dihedral angle between the furan and benzene rings is  $2.06$  ( $17^\circ$ ). The two methoxy groups at the *ortho* and *para* positions are essentially coplanar with the benzene ring [ $\text{C}-\text{O}-\text{C}-\text{C}$  angles =  $-1.0$  ( $5^\circ$ ) and  $178.5$  ( $3^\circ$ )], whereas the third one at the *meta* position is slightly twisted [ $\text{C}-\text{O}-\text{C}-\text{C} = 9.6$  ( $5^\circ$ )]. In the crystal, weak  $\text{C}-\text{H}\cdots\text{O}$  interactions link the molecules into a sheet parallel to  $(\bar{1}02)$ . An intermolecular  $\pi-\pi$  interaction between the furan and benzene rings is present [centroid-centroid distance =  $3.772$  ( $2$ ) Å]. A short  $\text{C}\cdots\text{C}$  contact [ $3.173$  ( $5$ ) Å] is also observed between neighbouring furan rings.

## Related literature

For background to and applications of chalcones, see: Cheng *et al.* (2008); Jung *et al.* (2008); Lee *et al.* (2006); Liu *et al.* (2011); Nerya *et al.* (2004); Suwunwong *et al.* (2011); Tewtrakul *et al.* (2003). For related structures, see: Fun *et al.* (2010*a,b*, 2011). For the stability of the temperature controller, see: Cosier & Glazer, (1986). For standard bond-length data, see: Allen *et al.* (1987).



‡ Thomson Reuters ResearcherID: A-5085-2009.

§ Additional correspondence author, e-mail: hkfun@usm.my. Thomson Reuters ResearcherID: A-3561-2009.

## Experimental

## Crystal data

$\text{C}_{16}\text{H}_{16}\text{O}_5$   
 $M_r = 288.29$   
 Monoclinic,  $P2_1/c$   
 $a = 8.338$  ( $2$ ) Å  
 $b = 8.610$  ( $2$ ) Å  
 $c = 18.923$  ( $5$ ) Å  
 $\beta = 94.467$  ( $4$ )°  
 $V = 1354.4$  ( $6$ ) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.11$  mm<sup>-1</sup>  
 $T = 100$  K  
 $0.28 \times 0.21 \times 0.09$  mm

## Data collection

Bruker APEX DUO CCD area-detector diffractometer  
 Absorption correction: multi-scan (SADABS; Bruker, 2009)  
 $T_{\min} = 0.971$ ,  $T_{\max} = 0.991$   
 8001 measured reflections  
 2647 independent reflections  
 1663 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.068$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.064$   
 $wR(F^2) = 0.175$   
 $S = 1.08$   
 2647 reflections  
 193 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.33$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.40$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C14}-\text{H14B}\cdots\text{O2}^i$	0.96	2.47	3.363 (5)	154
$\text{C15}-\text{H15C}\cdots\text{O1}^{ii}$	0.96	2.43	3.365 (4)	165

 Symmetry codes: (i)  $x, y + 1, z$ ; (ii)  $x - 1, -y + \frac{5}{2}, z - \frac{1}{2}$ .

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).

The authors thank the Thailand Research Fund (grant No. RSA5280033) and the Prince of Songkla University for financial support. TS thanks the Graduate School, Prince of Songkla University, for partial financial support. The authors also thank Universiti Sains Malaysia for the Research University Grant No. 1001/PFIZIK/811160.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS5037).

## 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.  
 Cheng, J.-H., Hung, C.-F., Yang, S.-C., Wang, J.-P., Won, S.-J. & Lin, C.-N. (2008). *Bioorg. Med. Chem.* **16**, 7270–7276.  
 Cosier, J. & Glazer, A. M. (1986). *J. Appl. Cryst.* **19**, 105–107.  
 Fun, H.-K., Chantrapromma, S. & Suwunwong, T. (2011). *Acta Cryst. E* **67**, o2789–o2790.  
 Fun, H.-K., Suwunwong, T., Chantrapromma, S. & Karalai, C. (2010*a*). *Acta Cryst. E* **66**, o2559–o2560.  
 Fun, H.-K., Suwunwong, T., Chantrapromma, S. & Karalai, C. (2010*b*). *Acta Cryst. E* **66**, o3070–o3071.  
 Jung, Y. J., Son, K. I., Oh, Y. E. & Noh, D. Y. (2008). *Polyhedron*, **27**, 861–867.

- Lee, S. H., Seo, G. S., Kim, J. Y., Jin, X. Y., Kim, H.-D. & Sohn, D. H. (2006). *Eur. J. Pharmacol.* **532**, 178–186.
- Liu, X.-F., Zheng, C.-J., Sun, L.-P., Liu, X.-K. & Piao, H.-R. (2011). *Eur. J. Med. Chem.* **46**, 3469–3473.
- Nerya, O., Musa, R., Khatib, S., Tamir, S. & Vaya, J. (2004). *Phytochemistry*, **65**, 1389–1395.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.
- Suwunwong, T., Chantrapromma, S. & Fun, H. K. (2011). *Chem. Pap.* **65**, 890–897.
- Tewtrakul, S., Subhadhirasakul, S., Puripattanavong, J. & Panphadung, T. (2003). *Songklanakarin J. Sci. Technol.* **25**, 503–508.

## supporting information

*Acta Cryst.* (2012). E68, o317–o318 [doi:10.1107/S1600536812000037]

**(E)-1-(Furan-2-yl)-3-(2,4,5-trimethoxyphenyl)prop-2-en-1-one**

**Thitipone Suwunwong, Suchada Chantrapromma, Chatchanok Karalai, Pitikan Wisitsak and Hoong-Kun Fun**

**S1. Comment**

Chalcones and heteroaryl chalcones have been reported to possess a wide range of biological activities such as antibacterial (Liu *et al.*, 2011), anti-inflammatory (Lee *et al.*, 2006), anti-oxidant (Cheng *et al.*, 2008), HIV-1 protease inhibitory (Tewtrakul *et al.*, 2003) as well as anti-tyrosinase activities (Nerya *et al.*, 2004), including fluorescent property (Jung *et al.*, 2008; Suwunwong *et al.*, 2011). The title heteroaryl chalcones (I) was synthesized to study for its fluorescence property and tyrosinase inhibitory activity and also to compare its property with the previously published related compounds (Suwunwong *et al.*, 2011). Our experiment shows that (I) exhibits fluorescence property (Suwunwong *et al.*, 2011) and tyrosinase inhibitory activity with the  $IC_{50}$  value of  $0.143 \pm 0.002$  mg.ml<sup>-1</sup>. Herein the crystal structure of (I) is reported.

The molecule of (I) in Fig. 1 exists in an *E* configuration with respect to the C6=C7 double bond [1.335 (5) Å]. The molecule is planar with the dihedral angle between the furan and the benzene rings being 2.06 (17)°. The middle prop-2-en-1-one unit (O2/C5–C7) is also planar with the *r.m.s.* 0.0013 (2) and the torsion angle O1–C5–C6–C7 = -0.4 (5)°. The mean plane through this unit makes dihedral angles of 4.1 (2)° and 3.6 (2)° with the furan and the benzene rings, respectively. The two methoxy groups at *ortho* (at atom 9) and *para* (at atom C11) positions of 2,4,5-trimethoxyphenyl unit are essentially co-planar with the attached benzene ring with torsion angles C14–O3–C9–C10 = -1.0 (5)° and C15–O4–C11–C12 = 178.5 (3)°, whereas the third one at *meta* (at atom C12) position is slightly twisted with the torsion angle of C16–O5–C12–C13 = 9.6 (5)°. These angle values also indicated that the methyl group at *para* position points toward the one at *ortho* but point away from the one at *meta* positions due to the steric effect. The bond distances have normal values (Allen *et al.*, 1987) and are comparable with closely related structures (Fun *et al.*, 2010a,b, 2011).

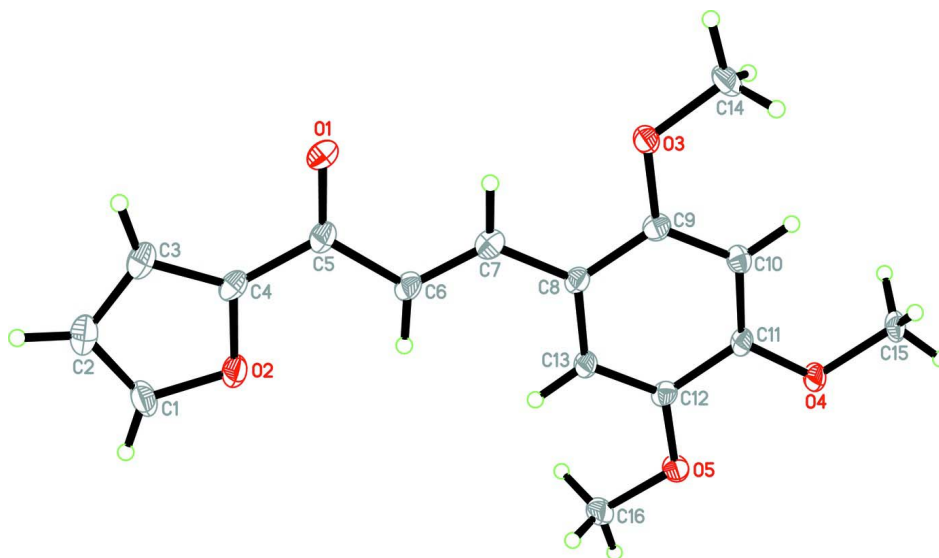
In the crystal packing (Fig. 2), weak C14—H14B⋯O2<sup>i</sup> and C15—H15C⋯O1<sup>ii</sup> interactions (Table 1) link the molecules into sheets parallel to the ( $\bar{1}$  0 2) plane and these sheets are stacked along the *a* axis by  $\pi$ - $\pi$  interactions with  $Cg1 \cdots Cg2^{iii} = 3.772$  (2) Å [symmetry code: (iii) 1-x, 2-y, 1-z]; *Cg1* and *Cg2* are the centroids of C1–C4/O2 furan and C8–C13 benzene rings, respectively. A C1⋯C1<sup>iv</sup>[3.173 (5) Å; symmetry code: (iv) 2-x, 1-y, 1-z] short contact is also observed.

**S2. Experimental**

The title compound was prepared by the condensation of the solution of 2-furyl methylketone (2 mmol, 0.22 g) in ethanol (15 ml) with the solution of 2,4,5-trimethoxybenzaldehyde (2 mmol, 0.40 g) in ethanol (15 ml) in the presence of 20% NaOH (aq) 5 ml at 278 K for 4 hr. The resulting solid which was obtained was collected by filtration, washed with distilled water and dried in air. Yellow slab-shaped single crystals of the title compound suitable for X-ray structure determination were recrystallized from acetone:ethanol (1:1 *v/v*) by the slow evaporation of the solvent at room temperature after several days (m.p. 356–357 K).

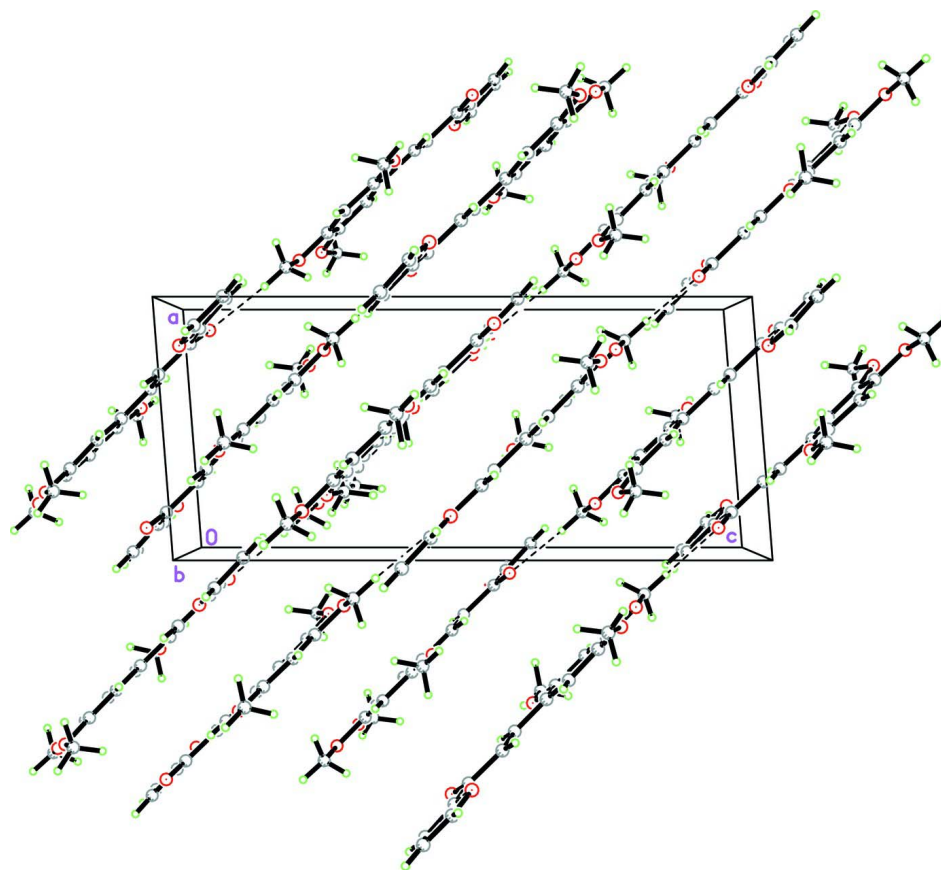
### S3. Refinement

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with  $d(\text{C—H}) = 0.93 \text{ \AA}$  for aromatic and CH, and  $0.96 \text{ \AA}$  for  $\text{CH}_3$  atoms. The  $U_{\text{iso}}(\text{H})$  values were constrained to be  $1.5U_{\text{eq}}$  of the carrier atom for methyl H atoms and  $1.2U_{\text{eq}}$  for the remaining H atoms. A rotating group model was used for the methyl groups. The highest residual electron density peak is located at  $0.83 \text{ \AA}$  from C10 and the deepest hole is located at  $0.89 \text{ \AA}$  from C4.



**Figure 1**

The molecular structure of the title compound, showing 50% probability displacement ellipsoids.

**Figure 2**

The crystal packing of the title compound viewed along the  $b$  axis, showing molecular sheets parallel to the  $(\bar{1} 0 2)$  plane. Hydrogen bonds are shown as dashed lines.

**(*E*)-1-(Furan-2-yl)-3-(2,4,5-trimethoxyphenyl)prop-2-en-1-one**

*Crystal data*

$C_{16}H_{16}O_5$

$M_r = 288.29$

Monoclinic,  $P2_1/c$

Hall symbol:  $-P 2_1/c$

$a = 8.338$  (2) Å

$b = 8.610$  (2) Å

$c = 18.923$  (5) Å

$\beta = 94.467$  (4)°

$V = 1354.4$  (6) Å<sup>3</sup>

$Z = 4$

$F(000) = 608$

$D_x = 1.414$  Mg m<sup>-3</sup>

Melting point = 356–357 K

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 2647 reflections

$\theta = 2.2$ – $26.0$ °

$\mu = 0.11$  mm<sup>-1</sup>

$T = 100$  K

Plate, yellow

$0.28 \times 0.21 \times 0.09$  mm

*Data collection*

Bruker APEX DUO CCD area-detector  
diffractometer

Radiation source: sealed tube

Graphite monochromator

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan  
(*SADABS*; Bruker, 2009)

$T_{\min} = 0.971$ ,  $T_{\max} = 0.991$

8001 measured reflections

2647 independent reflections

1663 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.068$   
 $\theta_{\text{max}} = 26.0^\circ$ ,  $\theta_{\text{min}} = 2.2^\circ$   
 $h = -8 \rightarrow 10$

$k = -10 \rightarrow 7$   
 $l = -23 \rightarrow 23$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.064$   
 $wR(F^2) = 0.175$   
 $S = 1.08$   
 2647 reflections  
 193 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0653P)^2 + 1.5283P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.33 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.40 \text{ e } \text{\AA}^{-3}$

*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 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.** 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  $F^2 > 2\sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.8947 (3)	1.0580 (3)	0.56583 (11)	0.0221 (6)
O2	0.8198 (3)	0.6581 (3)	0.53014 (11)	0.0219 (6)
O3	0.5846 (3)	1.3849 (3)	0.41496 (11)	0.0234 (6)
O4	0.1930 (3)	1.2112 (3)	0.22782 (11)	0.0203 (6)
O5	0.2463 (3)	0.9265 (3)	0.26329 (11)	0.0211 (6)
C1	0.8927 (5)	0.5329 (4)	0.56403 (17)	0.0249 (9)
H1A	0.8673	0.4297	0.5539	0.030*
C2	1.0063 (4)	0.5797 (4)	0.61407 (17)	0.0244 (9)
H2A	1.0717	0.5167	0.6440	0.029*
C3	1.0061 (4)	0.7441 (4)	0.61196 (17)	0.0218 (8)
H3A	1.0719	0.8098	0.6404	0.026*
C4	0.8920 (4)	0.7884 (4)	0.56070 (15)	0.0177 (7)
C5	0.8371 (4)	0.9414 (4)	0.53558 (15)	0.0181 (8)
C6	0.7141 (4)	0.9497 (4)	0.47546 (15)	0.0177 (8)
H6A	0.6743	0.8590	0.4539	0.021*
C7	0.6597 (4)	1.0876 (4)	0.45188 (16)	0.0174 (8)
H7A	0.7039	1.1740	0.4756	0.021*
C8	0.5399 (4)	1.1191 (4)	0.39374 (15)	0.0157 (7)
C9	0.5031 (4)	1.2735 (4)	0.37474 (16)	0.0172 (8)
C10	0.3898 (4)	1.3086 (4)	0.31901 (15)	0.0162 (7)

H10A	0.3691	1.4115	0.3065	0.019*
C11	0.3084 (4)	1.1903 (4)	0.28248 (15)	0.0145 (7)
C12	0.3391 (4)	1.0334 (4)	0.30161 (15)	0.0152 (7)
C13	0.4544 (4)	1.0014 (4)	0.35535 (15)	0.0155 (7)
H13A	0.4769	0.8982	0.3668	0.019*
C14	0.5532 (5)	1.5429 (4)	0.39800 (19)	0.0317 (10)
H14B	0.6202	1.6080	0.4291	0.048*
H14C	0.4421	1.5656	0.4036	0.048*
H14D	0.5759	1.5621	0.3498	0.048*
C15	0.1539 (4)	1.3692 (4)	0.20725 (16)	0.0190 (8)
H15C	0.0763	1.3687	0.1670	0.029*
H15D	0.2495	1.4216	0.1951	0.029*
H15A	0.1098	1.4221	0.2460	0.029*
C16	0.2548 (5)	0.7704 (4)	0.28869 (17)	0.0234 (8)
H16D	0.1717	0.7097	0.2640	0.035*
H16A	0.2406	0.7694	0.3385	0.035*
H16B	0.3580	0.7272	0.2806	0.035*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0219 (15)	0.0236 (14)	0.0194 (11)	-0.0015 (11)	-0.0062 (10)	-0.0033 (10)
O2	0.0214 (15)	0.0215 (14)	0.0214 (11)	0.0010 (11)	-0.0076 (10)	0.0023 (10)
O3	0.0271 (16)	0.0136 (13)	0.0269 (12)	-0.0014 (11)	-0.0148 (11)	0.0006 (10)
O4	0.0225 (15)	0.0167 (13)	0.0198 (11)	0.0022 (11)	-0.0106 (10)	0.0018 (9)
O5	0.0236 (15)	0.0138 (13)	0.0239 (11)	-0.0038 (11)	-0.0105 (10)	-0.0012 (9)
C1	0.029 (2)	0.0191 (19)	0.0261 (17)	0.0075 (18)	0.0009 (16)	0.0063 (15)
C2	0.020 (2)	0.033 (2)	0.0205 (16)	0.0054 (17)	0.0015 (15)	0.0070 (15)
C3	0.016 (2)	0.030 (2)	0.0187 (15)	-0.0001 (16)	-0.0019 (14)	0.0027 (14)
C4	0.0135 (19)	0.0238 (19)	0.0153 (14)	-0.0026 (16)	-0.0016 (13)	-0.0002 (14)
C5	0.015 (2)	0.024 (2)	0.0155 (15)	0.0011 (16)	-0.0012 (13)	0.0006 (14)
C6	0.014 (2)	0.0200 (19)	0.0183 (15)	-0.0021 (15)	-0.0049 (13)	-0.0002 (13)
C7	0.0129 (19)	0.0218 (19)	0.0174 (15)	-0.0026 (14)	0.0011 (13)	-0.0004 (13)
C8	0.0157 (19)	0.0169 (18)	0.0140 (14)	-0.0004 (15)	-0.0018 (13)	0.0002 (13)
C9	0.0143 (19)	0.0176 (18)	0.0189 (15)	-0.0029 (15)	-0.0032 (14)	-0.0008 (13)
C10	0.0144 (19)	0.0155 (18)	0.0184 (15)	0.0016 (15)	0.0000 (13)	0.0022 (13)
C11	0.0096 (18)	0.0189 (18)	0.0146 (14)	0.0037 (14)	-0.0017 (13)	0.0016 (13)
C12	0.0115 (18)	0.0181 (18)	0.0155 (14)	-0.0002 (15)	-0.0023 (13)	-0.0017 (13)
C13	0.0132 (19)	0.0161 (18)	0.0166 (15)	0.0008 (14)	-0.0035 (13)	0.0006 (12)
C14	0.044 (3)	0.0117 (19)	0.036 (2)	-0.0027 (19)	-0.0158 (18)	0.0021 (16)
C15	0.019 (2)	0.0172 (18)	0.0196 (15)	0.0027 (15)	-0.0046 (14)	0.0063 (13)
C16	0.029 (2)	0.0140 (19)	0.0259 (17)	-0.0021 (16)	-0.0058 (15)	-0.0004 (14)

*Geometric parameters (Å, °)*

O1—C5	1.234 (4)	C7—C8	1.453 (5)
O2—C1	1.372 (4)	C7—H7A	0.9300
O2—C4	1.379 (4)	C8—C9	1.405 (5)

O3—C9	1.371 (4)	C8—C13	1.408 (4)
O3—C14	1.418 (4)	C9—C10	1.393 (5)
O4—C11	1.369 (4)	C10—C11	1.379 (5)
O4—C15	1.445 (4)	C10—H10A	0.9300
O5—C12	1.373 (4)	C11—C12	1.416 (5)
O5—C16	1.427 (4)	C12—C13	1.372 (4)
C1—C2	1.347 (5)	C13—H13A	0.9300
C1—H1A	0.9300	C14—H14B	0.9600
C2—C3	1.416 (5)	C14—H14C	0.9600
C2—H2A	0.9300	C14—H14D	0.9600
C3—C4	1.359 (5)	C15—H15C	0.9600
C3—H3A	0.9300	C15—H15D	0.9600
C4—C5	1.462 (5)	C15—H15A	0.9600
C5—C6	1.473 (4)	C16—H16D	0.9600
C6—C7	1.335 (5)	C16—H16A	0.9600
C6—H6A	0.9300	C16—H16B	0.9600
C1—O2—C4	106.3 (3)	C11—C10—C9	119.9 (3)
C9—O3—C14	118.1 (3)	C11—C10—H10A	120.1
C11—O4—C15	117.3 (3)	C9—C10—H10A	120.1
C12—O5—C16	116.2 (3)	O4—C11—C10	124.8 (3)
C2—C1—O2	110.8 (3)	O4—C11—C12	114.9 (3)
C2—C1—H1A	124.6	C10—C11—C12	120.2 (3)
O2—C1—H1A	124.6	C13—C12—O5	126.2 (3)
C1—C2—C3	106.3 (3)	C13—C12—C11	118.9 (3)
C1—C2—H2A	126.9	O5—C12—C11	114.9 (3)
C3—C2—H2A	126.9	C12—C13—C8	122.3 (3)
C4—C3—C2	107.4 (3)	C12—C13—H13A	118.8
C4—C3—H3A	126.3	C8—C13—H13A	118.8
C2—C3—H3A	126.3	O3—C14—H14B	109.5
C3—C4—O2	109.2 (3)	O3—C14—H14C	109.5
C3—C4—C5	132.0 (3)	H14B—C14—H14C	109.5
O2—C4—C5	118.8 (3)	O3—C14—H14D	109.5
O1—C5—C4	118.8 (3)	H14B—C14—H14D	109.5
O1—C5—C6	122.7 (3)	H14C—C14—H14D	109.5
C4—C5—C6	118.5 (3)	O4—C15—H15C	109.5
C7—C6—C5	120.0 (3)	O4—C15—H15D	109.5
C7—C6—H6A	120.0	H15C—C15—H15D	109.5
C5—C6—H6A	120.0	O4—C15—H15A	109.5
C6—C7—C8	128.0 (3)	H15C—C15—H15A	109.5
C6—C7—H7A	116.0	H15D—C15—H15A	109.5
C8—C7—H7A	116.0	O5—C16—H16D	109.5
C9—C8—C13	117.2 (3)	O5—C16—H16A	109.5
C9—C8—C7	119.6 (3)	H16D—C16—H16A	109.5
C13—C8—C7	123.1 (3)	O5—C16—H16B	109.5
O3—C9—C10	123.1 (3)	H16D—C16—H16B	109.5
O3—C9—C8	115.5 (3)	H16A—C16—H16B	109.5
C10—C9—C8	121.4 (3)		



C4—O2—C1—C2	0.1 (4)	C7—C8—C9—O3	-1.1 (4)
O2—C1—C2—C3	-0.1 (4)	C13—C8—C9—C10	-1.6 (5)
C1—C2—C3—C4	0.1 (4)	C7—C8—C9—C10	179.5 (3)
C2—C3—C4—O2	0.0 (4)	O3—C9—C10—C11	-177.7 (3)
C2—C3—C4—C5	179.1 (3)	C8—C9—C10—C11	1.6 (5)
C1—O2—C4—C3	0.0 (3)	C15—O4—C11—C10	-0.1 (4)
C1—O2—C4—C5	-179.3 (3)	C15—O4—C11—C12	178.5 (3)
C3—C4—C5—O1	-3.5 (5)	C9—C10—C11—O4	178.8 (3)
O2—C4—C5—O1	175.6 (3)	C9—C10—C11—C12	0.3 (4)
C3—C4—C5—C6	177.0 (3)	C16—O5—C12—C13	9.6 (5)
O2—C4—C5—C6	-3.9 (4)	C16—O5—C12—C11	-170.0 (3)
O1—C5—C6—C7	-0.4 (5)	O4—C11—C12—C13	179.2 (3)
C4—C5—C6—C7	179.1 (3)	C10—C11—C12—C13	-2.1 (4)
C5—C6—C7—C8	179.9 (3)	O4—C11—C12—O5	-1.1 (4)
C6—C7—C8—C9	-177.3 (3)	C10—C11—C12—O5	177.6 (3)
C6—C7—C8—C13	4.0 (5)	O5—C12—C13—C8	-177.5 (3)
C14—O3—C9—C10	-1.0 (5)	C11—C12—C13—C8	2.1 (5)
C14—O3—C9—C8	179.6 (3)	C9—C8—C13—C12	-0.2 (5)
C13—C8—C9—O3	177.7 (3)	C7—C8—C13—C12	178.5 (3)

*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>
C14—H14B $\cdots$ O2 <sup>i</sup>	0.96	2.47	3.363 (5)	154
C15—H15C $\cdots$ O1 <sup>ii</sup>	0.96	2.43	3.365 (4)	165

Symmetry codes: (i)  $x, y+1, z$ ; (ii)  $x-1, -y+5/2, z-1/2$ .