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## Ethyl 3-(2,4-difluorophenoxy)-2-(4-methoxyphenyl)acrylate

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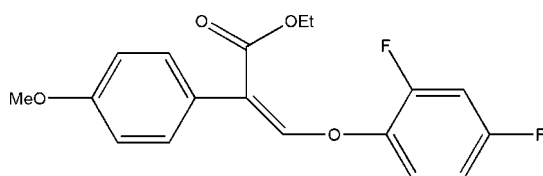
Received 20 October 2008; accepted 10 November 2008

Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.062;  $wR$  factor = 0.173; data-to-parameter ratio = 14.5.

In the title molecule,  $\text{C}_{18}\text{H}_{16}\text{F}_2\text{O}_4$ , the two benzene rings form a dihedral angle of  $55.2(2)^\circ$ . In the crystal structure, weak intermolecular  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds link the molecules into chains propagating along the  $c$  axis.

## Related literature

For a related crystal structure, see Fang *et al.* (2007). For the properties of phenylacetate and styrene derivatives, see: Huang *et al.* (2007); Li *et al.* (2007).



## Experimental

## Crystal data

$\text{C}_{18}\text{H}_{16}\text{F}_2\text{O}_4$   
 $M_r = 334.31$   
 Monoclinic,  $P2_1/c$   
 $a = 17.295(3)$  Å  
 $b = 7.294(2)$  Å  
 $c = 14.233(2)$  Å  
 $\beta = 113.73(3)^\circ$

$V = 1643.7(7)$  Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.11$  mm<sup>-1</sup>  
 $T = 298(2)$  K  
 $0.31 \times 0.30 \times 0.28$  mm

## Data collection

Bruker SMART 1000 CCD area-detector diffractometer  
 Absorption correction: multi-scan (*SADABS*; Bruker, 2001)  
 $T_{\min} = 0.967$ ,  $T_{\max} = 0.970$

3340 measured reflections  
 3198 independent reflections  
 1959 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.017$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.062$   
 $wR(F^2) = 0.173$   
 $S = 1.03$   
 3198 reflections

220 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.43$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.31$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C6}-\text{H6}\cdots\text{O1}^i$	0.93	2.52	3.280 (2)	140

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINTE* (Bruker, 2007); data reduction: *SAINTE*; 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2469).

## References

- Bruker (2001). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Bruker (2007). *SMART* and *SAINTE*. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Fang, R.-Q., Li, H.-Q., Shi, L., Xiao, Z.-P. & Zhu, H.-L. (2007). *Acta Cryst.* **E63**, o3975.  
 Huang, X.-F., Ruan, B.-F., Wang, X.-T., Xu, C., Ge, H.-M. & Zhu, H.-L. (2007). *Eur. J. Med. Chem.* **42**, 263–267.  
 Li, H.-Q., Xu, C., Li, H.-S., Xiao, Z.-P., Shi, L. & Zhu, H.-L. (2007). *ChemMedChem*, **2**, 1361–1369.  
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

## supporting information

*Acta Cryst.* (2008). E64, o2374 [doi:10.1107/S1600536808036945]

## Ethyl 3-(2,4-difluorophenoxy)-2-(4-methoxyphenyl)acrylate

Wu Chen, Yong-Ming Cui, Fei Pan, Dong-Sheng Xia and Qing-Fu Zeng

### S1. Comment

Phenylacetate and styrene derivatives are important in view of their extensive biological activities. Recently, many of such compounds with good activities were synthesized (Huang *et al.*, 2007; Li *et al.*, 2007). We report in this paper the title new compound, (I).

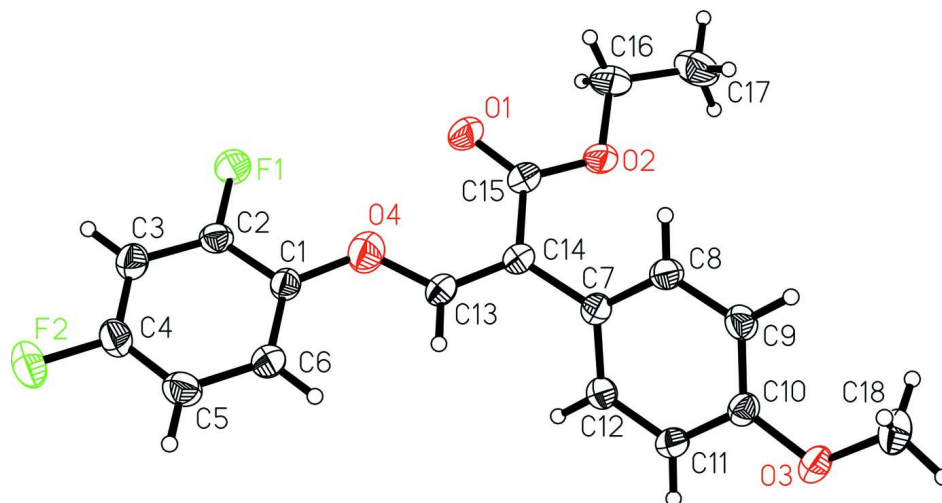
In (I) (Fig. 1), all bond lengths and angles are normal and correspond to those observed in the related compound (Fang *et al.*, 2007). The dihedral angles between C1—C6 and C7—C12 benzene rings is 55.2 (2)°. The O4/C13—C15/O1/O2 plane forms dihedral angles of 5.9 (2)° and 50.2 (2)°, respectively, with C1—C6 and C7—C12 benzene rings. In the crystal, weak intermolecular C—H···O hydrogen bonds (Table 1) link the molecules into chains propagated along *c* axis.

### S2. Experimental

Ethyl 3-bromo-2-(2,4-difluorophenyl)acrylate (0.1 mmol) and 4-methoxyphenol (0.1 mmol) were reacted in chloroform (20 ml) for 12 h, giving a clear colorless solution. Crystals of the compound were formed by gradual evaporation of the solution.

### S3. Refinement

All H atoms were placed in calculated positions with C—H = 0.93–0.97 Å, and refined as riding, with  $U_{\text{iso}}(\text{H}) = 1.2\text{--}1.5U_{\text{eq}}(\text{C})$ .



**Figure 1**

The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

## Ethyl 3-(2,4-difluorophenoxy)-2-(4-methoxyphenyl)acrylate

## Crystal data

C<sub>18</sub>H<sub>16</sub>F<sub>2</sub>O<sub>4</sub> $M_r = 334.31$ Monoclinic,  $P2_1/c$ 

Hall symbol: -P 2ybc

 $a = 17.295 (3) \text{ \AA}$  $b = 7.294 (2) \text{ \AA}$  $c = 14.233 (2) \text{ \AA}$  $\beta = 113.73 (3)^\circ$  $V = 1643.7 (7) \text{ \AA}^3$  $Z = 4$  $F(000) = 696$  $D_x = 1.351 \text{ Mg m}^{-3}$ Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$ 

Cell parameters from 1232 reflections

 $\theta = 2.3\text{--}24.5^\circ$  $\mu = 0.11 \text{ mm}^{-1}$  $T = 298 \text{ K}$ 

Block, colorless

 $0.31 \times 0.30 \times 0.28 \text{ mm}$ 

## Data collection

Bruker SMART 1000 CCD area-detector  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 $\omega$  scansAbsorption correction: multi-scan  
(SADABS; Bruker, 2001) $T_{\min} = 0.967$ ,  $T_{\max} = 0.970$ 

3340 measured reflections

3198 independent reflections

1959 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.017$  $\theta_{\max} = 26.0^\circ$ ,  $\theta_{\min} = 1.3^\circ$  $h = -21 \rightarrow 19$  $k = -8 \rightarrow 0$  $l = 0 \rightarrow 17$ 

## Refinement

Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.062$  $wR(F^2) = 0.173$  $S = 1.03$ 

3198 reflections

220 parameters

0 restraints

Primary atom site location: structure-invariant  
direct methodsSecondary atom site location: difference Fourier  
mapHydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0671P)^2 + 1.0598P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\max} = 0.001$  $\Delta\rho_{\max} = 0.43 \text{ e \AA}^{-3}$  $\Delta\rho_{\min} = -0.31 \text{ e \AA}^{-3}$ Extinction correction: SHELXTL (Sheldrick,  
2008),  $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$ 

Extinction coefficient: 0.021 (2)

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

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
F1	-0.10160 (10)	0.2759 (3)	0.53359 (13)	0.0659 (6)
F2	-0.21582 (12)	0.0299 (3)	0.20055 (15)	0.0819 (7)
O1	0.11843 (13)	0.3874 (4)	0.73642 (16)	0.0643 (7)

O2	0.25578 (13)	0.4637 (3)	0.80903 (15)	0.0544 (6)
O3	0.52673 (12)	0.3660 (3)	0.63131 (16)	0.0587 (6)
O4	0.05420 (13)	0.2906 (4)	0.53932 (19)	0.0709 (7)
C1	-0.01146 (16)	0.2255 (4)	0.4503 (2)	0.0429 (7)
C2	-0.09183 (17)	0.2176 (4)	0.4484 (2)	0.0469 (7)
C3	-0.16113 (18)	0.1544 (5)	0.3667 (2)	0.0565 (9)
H3	-0.2144	0.1520	0.3682	0.068*
C4	-0.14818 (19)	0.0949 (5)	0.2827 (2)	0.0562 (8)
C5	-0.0706 (2)	0.0975 (5)	0.2794 (2)	0.0585 (9)
H5	-0.0637	0.0558	0.2215	0.070*
C6	-0.00211 (18)	0.1628 (5)	0.3632 (2)	0.0524 (8)
H6	0.0510	0.1649	0.3612	0.063*
C7	0.28913 (16)	0.3613 (4)	0.6413 (2)	0.0411 (7)
C8	0.35658 (17)	0.2736 (4)	0.7170 (2)	0.0457 (7)
H8	0.3479	0.2147	0.7699	0.055*
C9	0.43628 (17)	0.2708 (4)	0.7167 (2)	0.0485 (8)
H9	0.4803	0.2108	0.7686	0.058*
C10	0.45029 (17)	0.3582 (4)	0.6383 (2)	0.0440 (7)
C11	0.38402 (17)	0.4463 (4)	0.5619 (2)	0.0490 (8)
H11	0.3928	0.5041	0.5087	0.059*
C12	0.30513 (17)	0.4491 (4)	0.5639 (2)	0.0460 (7)
H12	0.2615	0.5109	0.5124	0.055*
C13	0.13631 (16)	0.3039 (4)	0.5529 (2)	0.0450 (7)
H13	0.1485	0.2747	0.4967	0.054*
C14	0.20244 (17)	0.3551 (4)	0.6398 (2)	0.0427 (7)
C15	0.18686 (18)	0.4008 (4)	0.7308 (2)	0.0476 (7)
C16	0.2474 (2)	0.5001 (6)	0.9039 (2)	0.0755 (11)
H16A	0.2254	0.3927	0.9251	0.091*
H16B	0.2085	0.6009	0.8950	0.091*
C17	0.3315 (3)	0.5472 (6)	0.9827 (3)	0.0840 (12)
H17A	0.3700	0.4482	0.9896	0.126*
H17B	0.3273	0.5675	1.0472	0.126*
H17C	0.3517	0.6565	0.9626	0.126*
C18	0.59573 (18)	0.2753 (5)	0.7078 (3)	0.0696 (10)
H18A	0.6035	0.3215	0.7741	0.104*
H18B	0.6460	0.2967	0.6962	0.104*
H18C	0.5846	0.1460	0.7049	0.104*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
F1	0.0494 (10)	0.1005 (16)	0.0561 (11)	0.0024 (10)	0.0299 (9)	-0.0084 (11)
F2	0.0591 (12)	0.1104 (18)	0.0587 (12)	-0.0114 (12)	0.0053 (10)	-0.0136 (12)
O1	0.0527 (13)	0.0918 (19)	0.0608 (14)	-0.0086 (12)	0.0358 (11)	-0.0089 (13)
O2	0.0562 (13)	0.0704 (16)	0.0429 (11)	-0.0079 (11)	0.0267 (10)	-0.0086 (11)
O3	0.0403 (11)	0.0748 (16)	0.0661 (14)	0.0039 (11)	0.0267 (10)	0.0059 (12)
O4	0.0547 (13)	0.0828 (18)	0.0761 (17)	-0.0016 (13)	0.0272 (12)	-0.0027 (14)
C1	0.0374 (14)	0.0455 (17)	0.0454 (16)	0.0002 (13)	0.0162 (13)	0.0024 (14)

C2	0.0463 (16)	0.0555 (19)	0.0440 (17)	0.0047 (14)	0.0235 (14)	0.0027 (15)
C3	0.0394 (16)	0.070 (2)	0.056 (2)	-0.0007 (16)	0.0150 (14)	0.0078 (18)
C4	0.0479 (18)	0.064 (2)	0.0462 (18)	-0.0024 (16)	0.0084 (15)	0.0012 (16)
C5	0.061 (2)	0.072 (2)	0.0460 (18)	0.0042 (18)	0.0242 (16)	-0.0044 (17)
C6	0.0447 (16)	0.067 (2)	0.0501 (18)	-0.0004 (15)	0.0239 (14)	-0.0033 (16)
C7	0.0401 (15)	0.0405 (17)	0.0440 (16)	-0.0023 (13)	0.0184 (13)	-0.0062 (13)
C8	0.0460 (16)	0.0496 (18)	0.0452 (16)	0.0030 (14)	0.0220 (13)	0.0043 (14)
C9	0.0431 (15)	0.053 (2)	0.0453 (17)	0.0089 (14)	0.0136 (13)	0.0044 (15)
C10	0.0392 (15)	0.0469 (18)	0.0484 (17)	0.0003 (13)	0.0201 (13)	-0.0052 (14)
C11	0.0462 (16)	0.058 (2)	0.0468 (17)	0.0006 (15)	0.0232 (14)	0.0080 (15)
C12	0.0409 (15)	0.0530 (19)	0.0424 (16)	0.0041 (14)	0.0151 (13)	0.0049 (15)
C13	0.0394 (15)	0.0490 (18)	0.0511 (17)	0.0018 (13)	0.0230 (13)	0.0003 (14)
C14	0.0417 (15)	0.0436 (17)	0.0470 (17)	-0.0008 (13)	0.0220 (13)	0.0003 (14)
C15	0.0500 (17)	0.0467 (18)	0.0510 (18)	-0.0026 (14)	0.0256 (15)	0.0012 (15)
C16	0.085 (3)	0.104 (3)	0.0470 (19)	-0.005 (2)	0.0371 (19)	-0.005 (2)
C17	0.109 (3)	0.090 (3)	0.047 (2)	-0.014 (3)	0.025 (2)	-0.006 (2)
C18	0.0424 (17)	0.086 (3)	0.077 (2)	0.0103 (18)	0.0202 (17)	0.003 (2)

*Geometric parameters (Å, °)*

F1—C2	1.358 (3)	C8—C9	1.380 (4)
F2—C4	1.364 (3)	C8—H8	0.9300
O1—C15	1.222 (3)	C9—C10	1.388 (4)
O2—C15	1.343 (3)	C9—H9	0.9300
O2—C16	1.440 (4)	C10—C11	1.381 (4)
O3—C10	1.366 (3)	C11—C12	1.376 (4)
O3—C18	1.415 (4)	C11—H11	0.9300
O4—C13	1.357 (3)	C12—H12	0.9300
O4—C1	1.401 (3)	C13—C14	1.356 (4)
C1—C2	1.380 (4)	C13—H13	0.9300
C1—C6	1.391 (4)	C14—C15	1.464 (4)
C2—C3	1.370 (4)	C16—C17	1.475 (5)
C3—C4	1.373 (4)	C16—H16A	0.9700
C3—H3	0.9300	C16—H16B	0.9700
C4—C5	1.362 (4)	C17—H17A	0.9600
C5—C6	1.384 (4)	C17—H17B	0.9600
C5—H5	0.9300	C17—H17C	0.9600
C6—H6	0.9300	C18—H18A	0.9600
C7—C8	1.385 (4)	C18—H18B	0.9600
C7—C12	1.395 (4)	C18—H18C	0.9600
C7—C14	1.491 (4)		
C15—O2—C16	116.8 (2)	C12—C11—C10	120.4 (3)
C10—O3—C18	117.7 (2)	C12—C11—H11	119.8
C13—O4—C1	125.0 (2)	C10—C11—H11	119.8
C2—C1—C6	116.5 (3)	C11—C12—C7	121.5 (3)
C2—C1—O4	118.4 (3)	C11—C12—H12	119.2
C6—C1—O4	125.1 (2)	C7—C12—H12	119.2

F1—C2—C3	118.8 (3)	C14—C13—O4	126.9 (3)
F1—C2—C1	117.1 (3)	C14—C13—H13	116.6
C3—C2—C1	124.1 (3)	O4—C13—H13	116.6
C2—C3—C4	116.8 (3)	C13—C14—C15	118.8 (2)
C2—C3—H3	121.6	C13—C14—C7	119.7 (2)
C4—C3—H3	121.6	C15—C14—C7	121.5 (3)
C5—C4—F2	119.5 (3)	O1—C15—O2	122.2 (3)
C5—C4—C3	122.3 (3)	O1—C15—C14	124.6 (3)
F2—C4—C3	118.2 (3)	O2—C15—C14	113.2 (2)
C4—C5—C6	119.3 (3)	O2—C16—C17	108.4 (3)
C4—C5—H5	120.4	O2—C16—H16A	110.0
C6—C5—H5	120.4	C17—C16—H16A	110.0
C5—C6—C1	121.0 (3)	O2—C16—H16B	110.0
C5—C6—H6	119.5	C17—C16—H16B	110.0
C1—C6—H6	119.5	H16A—C16—H16B	108.4
C8—C7—C12	117.0 (2)	C16—C17—H17A	109.5
C8—C7—C14	121.6 (3)	C16—C17—H17B	109.5
C12—C7—C14	121.3 (3)	H17A—C17—H17B	109.5
C9—C8—C7	122.3 (3)	C16—C17—H17C	109.5
C9—C8—H8	118.9	H17A—C17—H17C	109.5
C7—C8—H8	118.9	H17B—C17—H17C	109.5
C8—C9—C10	119.6 (3)	O3—C18—H18A	109.5
C8—C9—H9	120.2	O3—C18—H18B	109.5
C10—C9—H9	120.2	H18A—C18—H18B	109.5
O3—C10—C11	116.3 (3)	O3—C18—H18C	109.5
O3—C10—C9	124.4 (3)	H18A—C18—H18C	109.5
C11—C10—C9	119.3 (3)	H18B—C18—H18C	109.5
C13—O4—C1—C2	179.1 (3)	C8—C9—C10—C11	-0.1 (5)
C13—O4—C1—C6	0.8 (5)	O3—C10—C11—C12	-178.6 (3)
C6—C1—C2—F1	179.1 (3)	C9—C10—C11—C12	0.6 (5)
O4—C1—C2—F1	0.6 (4)	C10—C11—C12—C7	-1.1 (5)
C6—C1—C2—C3	-0.6 (5)	C8—C7—C12—C11	1.0 (4)
O4—C1—C2—C3	-179.1 (3)	C14—C7—C12—C11	-176.3 (3)
F1—C2—C3—C4	-179.2 (3)	C1—O4—C13—C14	-175.5 (3)
C1—C2—C3—C4	0.4 (5)	O4—C13—C14—C15	0.6 (5)
C2—C3—C4—C5	0.0 (5)	O4—C13—C14—C7	179.7 (3)
C2—C3—C4—F2	179.5 (3)	C8—C7—C14—C13	-128.4 (3)
F2—C4—C5—C6	-179.7 (3)	C12—C7—C14—C13	48.7 (4)
C3—C4—C5—C6	-0.2 (6)	C8—C7—C14—C15	50.7 (4)
C4—C5—C6—C1	0.0 (5)	C12—C7—C14—C15	-132.1 (3)
C2—C1—C6—C5	0.4 (5)	C16—O2—C15—O1	5.3 (5)
O4—C1—C6—C5	178.7 (3)	C16—O2—C15—C14	-175.9 (3)
C12—C7—C8—C9	-0.4 (4)	C13—C14—C15—O1	3.9 (5)
C14—C7—C8—C9	176.8 (3)	C7—C14—C15—O1	-175.2 (3)
C7—C8—C9—C10	0.0 (5)	C13—C14—C15—O2	-174.9 (3)
C18—O3—C10—C11	-179.3 (3)	C7—C14—C15—O2	6.0 (4)
C18—O3—C10—C9	1.5 (4)	C15—O2—C16—C17	173.7 (3)

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C8—C9—C10—O3                    179.1 (3)

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*Hydrogen-bond geometry (Å, °)*

<i>D—H···A</i>	<i>D—H</i>	<i>H···A</i>	<i>D···A</i>	<i>D—H···A</i>
C6—H6···O1 <sup>i</sup>	0.93	2.52	3.280 (2)	140

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