



# (*E*)-1-(Anthracen-9-yl)-3-(2-chloro-6-fluorophenyl)-prop-2-en-1-one: crystal structure and Hirshfeld surface analysis

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**Keywords:** crystal structure; chalcone; hydrogen bonding; Hirshfeld surface analysis.

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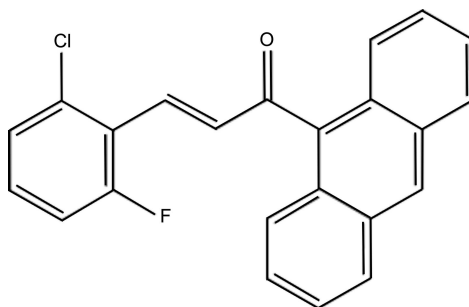
**Supporting information:** this article has supporting information at journals.iucr.org/e

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In the title compound, C<sub>23</sub>H<sub>14</sub>ClFO, the enone moiety adopts an *E* conformation. The dihedral angle between the benzene and anthracene ring is 63.42 (8)° and an intramolecular C—H···F hydrogen bond generates an *S*(6) ring motif. In the crystal, molecules are arranged into centrosymmetric dimers *via* pairs of C—H···F hydrogen bonds. The crystal structure also features C—H···π and π—π interactions. Hirshfeld surface analysis was used to confirm the existence of intermolecular interactions.

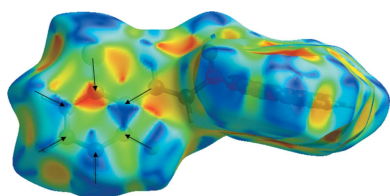
## 1. Chemical context

The biological properties of chalcone derivatives such as anticancer (Bhat *et al.*, 2005), antimalarial (Xue *et al.*, 2004), anti-oxidant and antimicrobial (Yayli *et al.*, 2006), antiplatelet (Zhao *et al.*, 2005) as well as anti-inflammatory (Madan *et al.*, 2000) have been studied extensively and developed. As part of our own studies in this area, we hereby report the synthesis and crystal structure of the title compound.

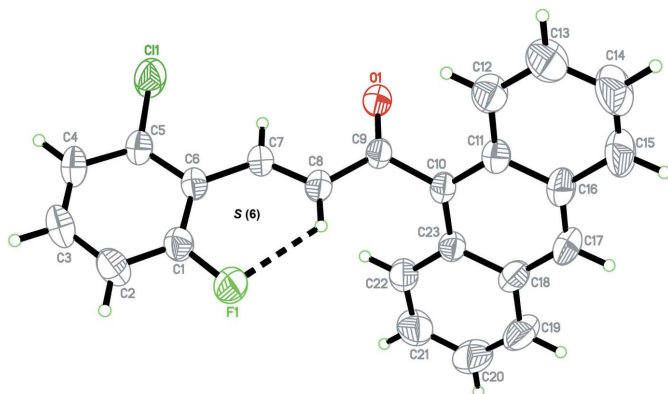


## 2. Structural commentary

The molecular structure of the title chalcone is shown in Fig. 1. The enone moiety (O1/C7–C9) adopts an *E* conformation with respect to the C7=C8 bond. The anthracene ring system (C10–C23) is twisted at the C9–C10 bond from the (*E*)-3-(2-chloro-6-fluorophenyl)acrylaldehyde moiety [maximum deviation = 0.193 (16) Å for atom O1] with a C8–C9–C10–C23 torsion angle of –61.4 (2)°. The terminal benzene and anthracene ring systems (C1–C6 and C10–C23, respectively) form a dihedral angle of 63.42 (8)°. The least-squares plane through the enone moiety [O1/C7–C9] with a maximum deviation of 0.033 (2) Å for atom C9] makes dihedral angles of 5.62 (13) and 59.18 (12)° with the benzene (C1–C6) and anthracene (C10–C23) rings, respectively. An intramolecular



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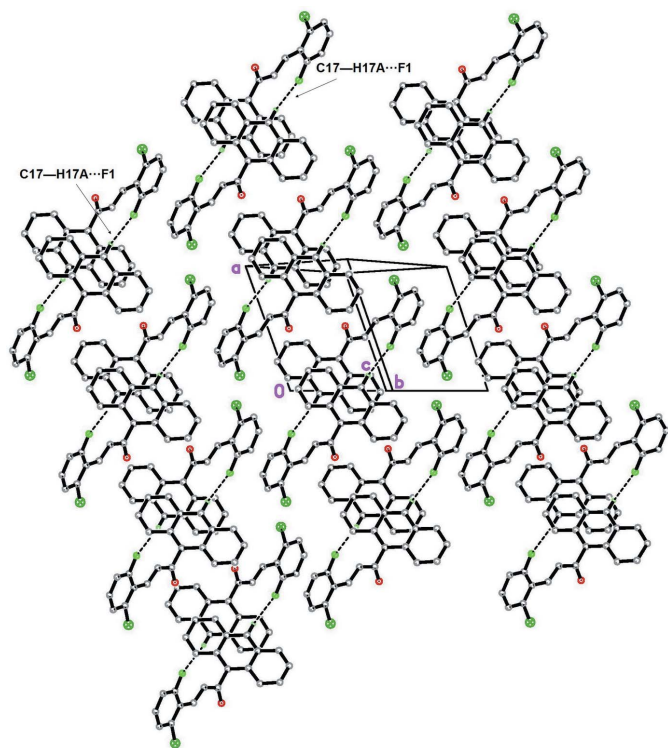


**Figure 1**  
The molecular structure of the title compound, showing 50% probability displacement ellipsoids. The intramolecular C—H···F hydrogen bond is shown as a dashed line.

C8—H8A···F1 hydrogen bond is observed, generating an  $S(6)$  ring motif. The bond lengths and angles are comparable with those in previously reported structures (Razak *et al.*, 2009; Ngaini *et al.*, 2011).

### 3. Supramolecular features

In the crystal (Fig. 2), the molecules are arranged into centrosymmetric dimers *via* pairs of C17—H17A···F1 (Table 1) hydrogen bonds. The crystal structure also features



**Figure 2**  
The crystal packing showing the molecules arranged into centrosymmetric dimers. The H atoms not involved in the intermolecular interactions (dashed lines) have been omitted for clarity.

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

Cg1 is the centroid of the C1—C6 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C8—H8A···F1	0.93	2.19	2.808 (2)	123
C17—H17A···F1 <sup>i</sup>	0.93	2.46	3.353 (2)	161
C14—H14A···Cg1 <sup>ii</sup>	0.93	2.99	3.712 (3)	136

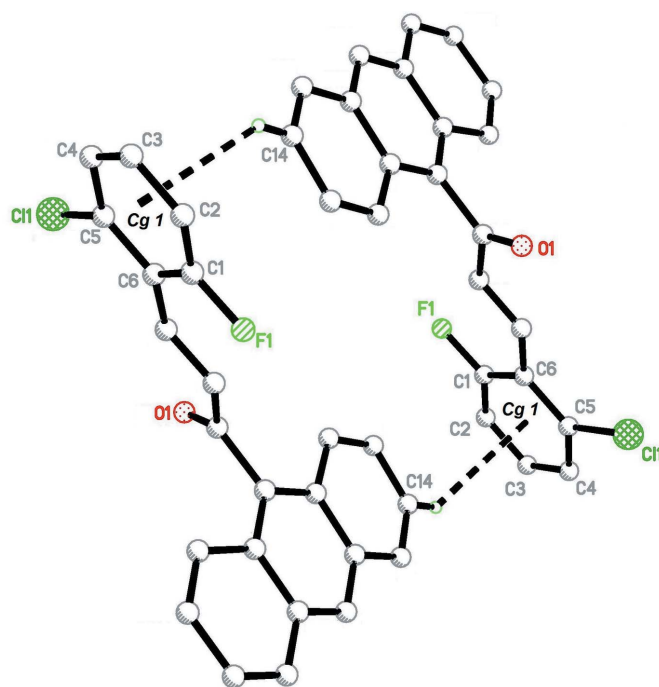
Symmetry codes: (i)  $-x, -y + 1, -z + 1$ ; (ii)  $-x + 1, -y + 1, -z + 1$ .

C14—H14A···Cg1 (Fig. 3) and Cg1···Cg1(1 -  $x$ , - $y$ , 1 -  $z$ ) interactions [centroid-to-centroid distance = 3.7557 (13) Å; Cg1 is the centroid of the C1—C6 ring].

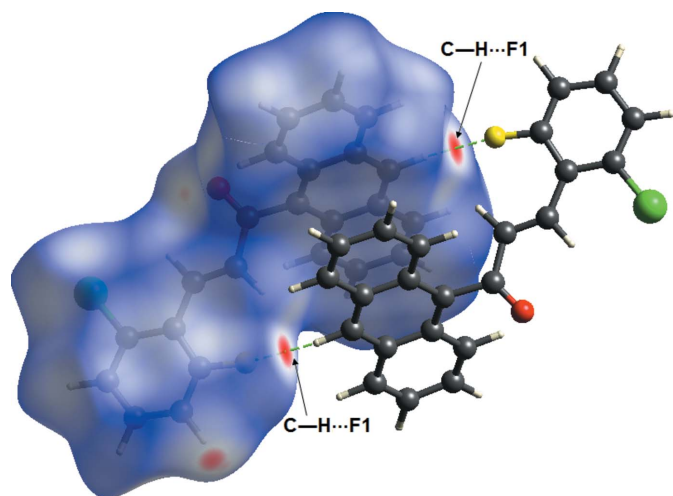
### 4. Hirshfeld surfaces analysis

The intermolecular interactions of the title compound can be visualized using Hirshfeld surface analysis (Wolff *et al.*, 2012). The Hirshfeld surfaces mapped over  $d_{\text{norm}}$  are shown in Fig. 4. The 2-D fingerprint plots showing the occurrence of different kinds of intermolecular contacts are shown in Fig. 5.

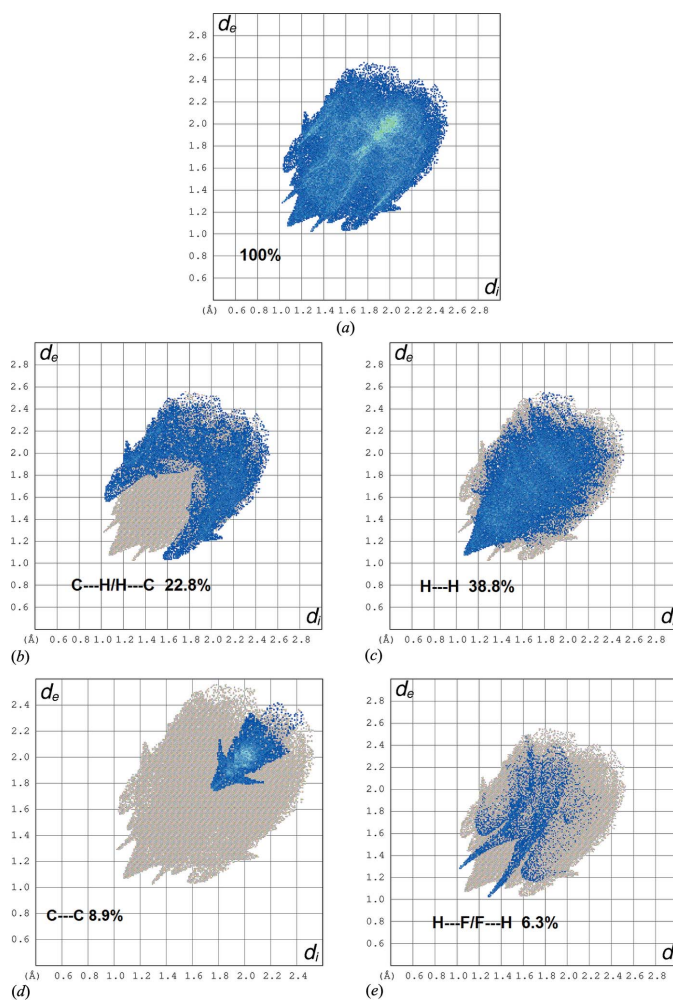
The C17—H17A···F1 interactions are shown on the Hirshfeld surfaces marked with a bright-red spot for short contacts. The H···F/F···H contacts comprise 6.3% of the total Hirshfeld surface, represented by two symmetrical narrow pointed spikes with  $d_e + d_i \sim 2.3$  Å, suggesting the presence of a non-classical C—H···F hydrogen bond. The H···H contacts are shown on the fingerprint plot as one distinct spike with the minimum value of  $d_e + d_i$ . These contacts represent the largest contribution within the Hirshfeld surfaces (38.8%).



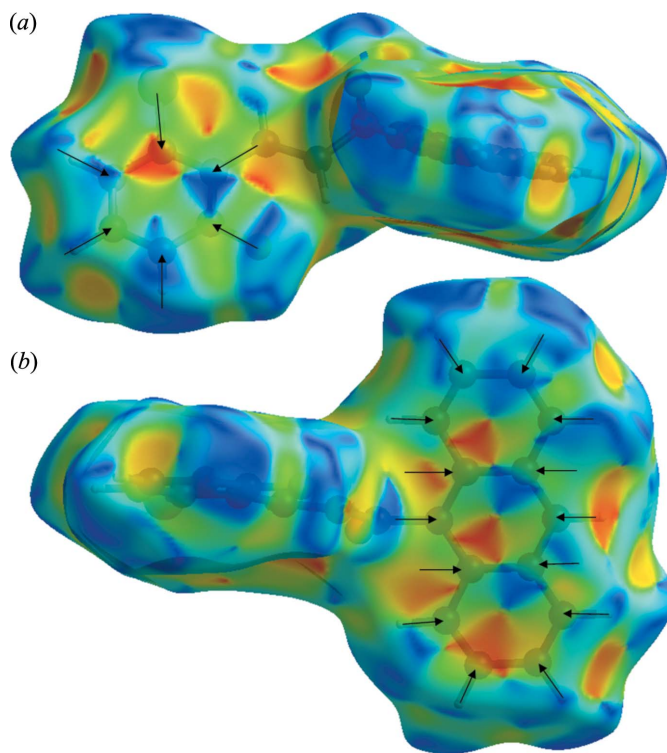
**Figure 3**  
Detail of the crystal structure showing the C14—H14A···Cg1 interaction where Cg1 is the centroid of C1—C6 ring.



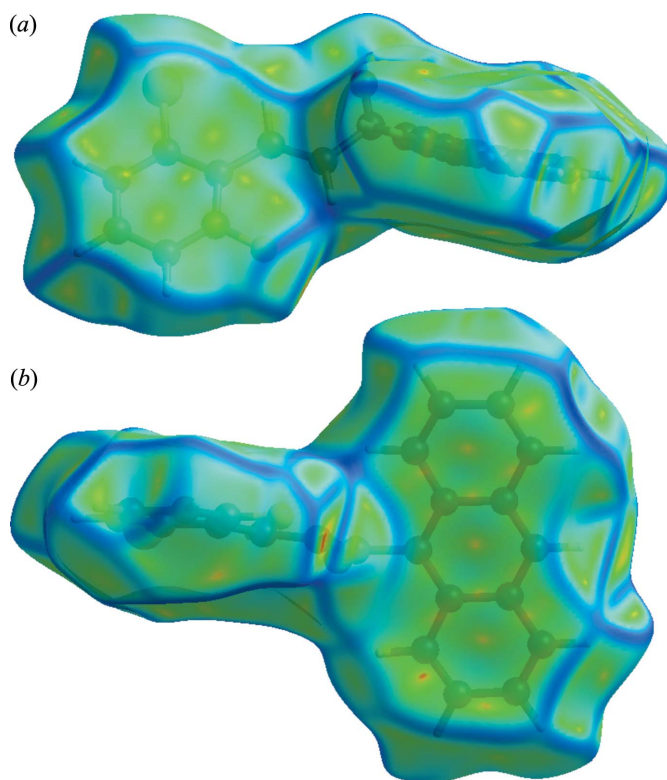
**Figure 4**  
 $d_{\text{norm}}$  mapped on the Hirshfeld surface for visualizing the intermolecular interactions of the title chalcone compound. Dotted lines (green) represent hydrogen bonds.



**Figure 5**  
 The 2-Dimensional fingerprint plot for the title chalcone compound showing contributions from different contacts.



**Figure 6**  
 Hirshfeld surface mapped over the shape index of the chalcone compound in (a) front view and (b) back view.



**Figure 7**  
 Hirshfeld surface mapped over curvedness of the chalcone compound in (a) front view and (b) back view.

**Table 2**  
Experimental details.

Crystal data	
Chemical formula	C <sub>23</sub> H <sub>14</sub> ClFO
<i>M</i> <sub>r</sub>	360.79
Crystal system, space group	Triclinic, <i>P</i> $\bar{1}$
Temperature (K)	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	9.2846 (9), 9.8777 (10), 10.3624 (11)
$\alpha$ , $\beta$ , $\gamma$ (°)	94.364 (2), 113.3517 (19), 92.866 (2)
<i>V</i> (Å <sup>3</sup> )	866.63 (15)
<i>Z</i>	2
Radiation type	Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	0.24
Crystal size (mm)	0.43 × 0.39 × 0.11
Data collection	
Diffractometer	Bruker SMART APEXII DUO CCD
Absorption correction	Multi-scan ( <i>SADABS</i> ; Bruker, 2009)
<i>T</i> <sub>min</sub> , <i>T</i> <sub>max</sub>	0.905, 0.974
No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections	15408, 3917, 2973
<i>R</i> <sub>int</sub>	0.027
( <i>sin</i> $\theta$ / $\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.650
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2 $\sigma$ ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.046, 0.159, 1.04
No. of reflections	3917
No. of parameters	235
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}$ , $\Delta\rho_{\text{min}}$ (e Å <sup>-3</sup> )	0.27, -0.38

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXTL* (Sheldrick, 2008) and *SHELXL2014* (Sheldrick, 2015).

Significant C–H... $\pi$  interactions (22.8%) can be also be seen, indicated by the wings of *d*<sub>e</sub> + *d*<sub>i</sub> ~ 2.6 Å on the fingerprint plot. The presence of  $\pi$ – $\pi$  interactions is shown as C...C contacts, which contribute 8.9% of the Hirshfeld surfaces. The presence of these interactions can also be shown by the Hirshfeld surfaces mapped by shape index (Fig. 6) and the Hirshfeld surfaces mapped with curvedness (Fig. 7).

## 5. Synthesis and crystallization

A mixture of 9-acetylanthracene (0.1 mol, 0.11 g) and 2-chloro-6-fluorobenzaldehyde (0.1 mol, 0.08 g) was dissolved in methanol (20 ml). A catalytic amount of NaOH (5 ml, 20%)

was added to the solution dropwise with vigorous stirring. The reaction mixture was stirred for about 5–6 h at room temperature. After stirring, the contents of the flask were poured into ice-cold water (50 ml) and the resulting crude solid was collected by filtration. The compound was dried and purified by repeated recrystallization from acetone solution, forming yellow plates.

## 6. Refinement details

Crystal data collection and structure refinement details are summarized in Table 2. All H atoms were positioned geometrically (C–H = 0.93 Å) and refined using a riding model with *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C). The most disagreeable reflections (–1 –2 4 and –1 1 0) were omitted from the final refinement.

## Acknowledgements

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## supporting information

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## (E)-1-(Anthracen-9-yl)-3-(2-chloro-6-fluorophenyl)prop-2-en-1-one: crystal structure and Hirshfeld surface analysis

**Amzar Ahlami Abdullah, Nur Hafiq Hanif Hassan, Suhana Arshad, Nuridayanti Che Khalib and Ibrahim Abdul Razak**

### Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

### (E)-1-(Anthracen-9-yl)-3-(2-chloro-6-fluorophenyl)prop-2-en-1-one

#### Crystal data

$C_{23}H_{14}ClFO$

$M_r = 360.79$

Triclinic,  $P\bar{1}$

$a = 9.2846$  (9) Å

$b = 9.8777$  (10) Å

$c = 10.3624$  (11) Å

$\alpha = 94.364$  (2)°

$\beta = 113.3517$  (19)°

$\gamma = 92.866$  (2)°

$V = 866.63$  (15) Å<sup>3</sup>

$Z = 2$

$F(000) = 372$

$D_x = 1.383$  Mg m<sup>-3</sup>

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

Cell parameters from 4550 reflections

$\theta = 2.5$ – $29.4$ °

$\mu = 0.24$  mm<sup>-1</sup>

$T = 296$  K

Plate, yellow

$0.43 \times 0.39 \times 0.11$  mm

#### Data collection

Bruker SMART APEXII DUO CCD  
diffractometer

Radiation source: fine-focus sealed tube

$\varphi$  and  $\omega$  scans

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

$T_{\min} = 0.905$ ,  $T_{\max} = 0.974$

15408 measured reflections

3917 independent reflections

2973 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.027$

$\theta_{\max} = 27.5$ °,  $\theta_{\min} = 2.1$ °

$h = -12 \rightarrow 12$

$k = -12 \rightarrow 12$

$l = -13 \rightarrow 13$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.046$

$wR(F^2) = 0.159$

$S = 1.04$

3917 reflections

235 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 atoms treated by a mixture of independent  
and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0894P)^2 + 0.1829P]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$

$$\Delta\rho_{\max} = 0.27 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.38 \text{ e } \text{\AA}^{-3}$$

### Special details

**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  $F^2 > 2\text{sigma}(F^2)$  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	0.34800 (14)	0.90969 (12)	0.72673 (15)	0.0699 (4)
Cl1	0.88071 (6)	0.82117 (5)	1.09430 (6)	0.0677 (2)
O1	0.52128 (16)	0.43191 (13)	0.84772 (16)	0.0550 (4)
C1	0.4948 (2)	0.95649 (18)	0.8188 (2)	0.0458 (4)
C2	0.5336 (3)	1.09407 (19)	0.8323 (2)	0.0550 (5)
H2A	0.4608	1.1517	0.7807	0.066*
C3	0.6821 (3)	1.14449 (19)	0.9237 (2)	0.0570 (5)
H3A	0.7116	1.2372	0.9327	0.068*
C4	0.7881 (2)	1.05996 (19)	1.0024 (2)	0.0526 (5)
H4A	0.8886	1.0950	1.0648	0.063*
C5	0.7438 (2)	0.92195 (17)	0.98776 (19)	0.0429 (4)
C6	0.5955 (2)	0.86314 (16)	0.89285 (17)	0.0380 (4)
C7	0.5552 (2)	0.71650 (16)	0.87498 (19)	0.0404 (4)
H7A	0.6308	0.6670	0.9364	0.048*
C8	0.4263 (2)	0.64341 (17)	0.7838 (2)	0.0434 (4)
H8A	0.3445	0.6871	0.7217	0.052*
C9	0.4112 (2)	0.49374 (17)	0.77988 (19)	0.0398 (4)
C10	0.2559 (2)	0.41801 (16)	0.68598 (18)	0.0382 (4)
C11	0.2509 (2)	0.31627 (17)	0.58084 (18)	0.0417 (4)
C12	0.3822 (3)	0.2912 (2)	0.5479 (2)	0.0565 (5)
H12A	0.4763	0.3456	0.5947	0.068*
C13	0.3721 (3)	0.1887 (3)	0.4489 (3)	0.0718 (7)
H13A	0.4600	0.1736	0.4295	0.086*
C14	0.2325 (4)	0.1053 (3)	0.3755 (3)	0.0800 (8)
H14A	0.2291	0.0344	0.3096	0.096*
C15	0.1029 (3)	0.1272 (3)	0.3997 (2)	0.0700 (6)
H15A	0.0103	0.0718	0.3496	0.084*
C16	0.1060 (2)	0.23471 (19)	0.50155 (19)	0.0496 (4)
C17	-0.0258 (2)	0.2597 (2)	0.5264 (2)	0.0551 (5)
H17A	-0.1191	0.2055	0.4748	0.066*
C18	-0.0244 (2)	0.3629 (2)	0.6260 (2)	0.0479 (4)
C19	-0.1599 (2)	0.3878 (3)	0.6524 (3)	0.0683 (6)

H19A	-0.2546	0.3364	0.5986	0.082*
C20	-0.1546 (3)	0.4844 (3)	0.7537 (3)	0.0756 (7)
H20A	-0.2455	0.5004	0.7677	0.091*
C21	-0.0121 (3)	0.5609 (2)	0.8381 (3)	0.0679 (6)
H21A	-0.0092	0.6263	0.9087	0.081*
C22	0.1212 (2)	0.5408 (2)	0.8184 (2)	0.0528 (5)
H22A	0.2147	0.5916	0.8769	0.063*
C23	0.1206 (2)	0.44299 (16)	0.70929 (18)	0.0397 (4)

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
F1	0.0491 (7)	0.0501 (7)	0.0787 (9)	0.0030 (5)	-0.0066 (6)	0.0012 (6)
C11	0.0519 (3)	0.0535 (3)	0.0713 (4)	-0.0034 (2)	-0.0026 (3)	0.0099 (2)
O1	0.0412 (7)	0.0393 (7)	0.0702 (9)	0.0012 (5)	0.0087 (6)	-0.0007 (6)
C1	0.0465 (10)	0.0396 (9)	0.0443 (9)	0.0005 (7)	0.0124 (8)	-0.0026 (7)
C2	0.0695 (13)	0.0368 (9)	0.0554 (11)	0.0083 (9)	0.0216 (10)	0.0036 (8)
C3	0.0770 (14)	0.0323 (9)	0.0588 (12)	-0.0059 (9)	0.0269 (11)	-0.0033 (8)
C4	0.0562 (11)	0.0411 (9)	0.0514 (11)	-0.0150 (8)	0.0166 (9)	-0.0070 (8)
C5	0.0447 (9)	0.0392 (8)	0.0405 (9)	-0.0053 (7)	0.0145 (7)	-0.0009 (7)
C6	0.0423 (9)	0.0335 (8)	0.0377 (8)	-0.0024 (6)	0.0170 (7)	-0.0011 (6)
C7	0.0403 (9)	0.0334 (8)	0.0452 (9)	-0.0010 (7)	0.0161 (7)	0.0006 (7)
C8	0.0388 (9)	0.0353 (8)	0.0504 (10)	-0.0022 (7)	0.0128 (8)	0.0026 (7)
C9	0.0368 (8)	0.0360 (8)	0.0455 (9)	-0.0032 (7)	0.0173 (7)	-0.0026 (7)
C10	0.0376 (8)	0.0336 (8)	0.0403 (8)	-0.0034 (6)	0.0137 (7)	0.0011 (6)
C11	0.0439 (9)	0.0408 (9)	0.0368 (8)	-0.0021 (7)	0.0136 (7)	0.0007 (7)
C12	0.0575 (12)	0.0626 (12)	0.0523 (11)	-0.0026 (10)	0.0281 (10)	-0.0063 (9)
C13	0.0805 (17)	0.0812 (16)	0.0618 (14)	0.0067 (13)	0.0405 (13)	-0.0115 (12)
C14	0.101 (2)	0.0781 (16)	0.0578 (14)	-0.0017 (15)	0.0358 (14)	-0.0256 (12)
C15	0.0773 (15)	0.0670 (14)	0.0508 (12)	-0.0131 (12)	0.0171 (11)	-0.0213 (10)
C16	0.0523 (11)	0.0490 (10)	0.0376 (9)	-0.0053 (8)	0.0102 (8)	-0.0034 (7)
C17	0.0403 (10)	0.0614 (12)	0.0475 (10)	-0.0108 (8)	0.0043 (8)	-0.0053 (9)
C18	0.0357 (9)	0.0537 (10)	0.0470 (10)	-0.0008 (7)	0.0096 (8)	0.0051 (8)
C19	0.0352 (10)	0.0876 (16)	0.0737 (15)	-0.0047 (10)	0.0160 (10)	-0.0008 (13)
C20	0.0488 (12)	0.0917 (18)	0.0939 (19)	0.0084 (12)	0.0379 (13)	0.0001 (15)
C21	0.0670 (14)	0.0652 (13)	0.0828 (16)	0.0050 (11)	0.0444 (13)	-0.0055 (12)
C22	0.0486 (10)	0.0475 (10)	0.0636 (12)	-0.0039 (8)	0.0273 (9)	-0.0080 (9)
C23	0.0383 (8)	0.0362 (8)	0.0422 (9)	-0.0005 (7)	0.0140 (7)	0.0040 (7)

*Geometric parameters (Å, °)*

F1—C1	1.350 (2)	C12—C13	1.358 (3)
C11—C5	1.734 (2)	C12—H12A	0.9300
O1—C9	1.212 (2)	C13—C14	1.398 (4)
C1—C2	1.371 (3)	C13—H13A	0.9300
C1—C6	1.392 (3)	C14—C15	1.347 (4)
C2—C3	1.367 (3)	C14—H14A	0.9300
C2—H2A	0.9300	C15—C16	1.430 (3)

C3—C4	1.371 (3)	C15—H15A	0.9300
C3—H3A	0.9300	C16—C17	1.377 (3)
C4—C5	1.383 (2)	C17—C18	1.391 (3)
C4—H4A	0.9300	C17—H17A	0.9300
C5—C6	1.400 (2)	C18—C19	1.419 (3)
C6—C7	1.457 (2)	C18—C23	1.432 (2)
C7—C8	1.326 (2)	C19—C20	1.348 (4)
C7—H7A	0.9300	C19—H19A	0.9300
C8—C9	1.474 (2)	C20—C21	1.403 (4)
C8—H8A	0.9300	C20—H20A	0.9300
C9—C10	1.501 (2)	C21—C22	1.353 (3)
C10—C23	1.401 (2)	C21—H21A	0.9300
C10—C11	1.410 (2)	C22—C23	1.429 (3)
C11—C12	1.418 (3)	C22—H22A	0.9300
C11—C16	1.431 (2)		
F1—C1—C2	116.89 (17)	C11—C12—H12A	119.6
F1—C1—C6	118.40 (15)	C12—C13—C14	121.4 (2)
C2—C1—C6	124.72 (18)	C12—C13—H13A	119.3
C3—C2—C1	118.30 (19)	C14—C13—H13A	119.3
C3—C2—H2A	120.9	C15—C14—C13	120.3 (2)
C1—C2—H2A	120.9	C15—C14—H14A	119.9
C2—C3—C4	120.80 (17)	C13—C14—H14A	119.9
C2—C3—H3A	119.6	C14—C15—C16	120.8 (2)
C4—C3—H3A	119.6	C14—C15—H15A	119.6
C3—C4—C5	119.26 (18)	C16—C15—H15A	119.6
C3—C4—H4A	120.4	C17—C16—C15	121.58 (19)
C5—C4—H4A	120.4	C17—C16—C11	119.60 (17)
C4—C5—C6	122.82 (17)	C15—C16—C11	118.81 (19)
C4—C5—C11	117.09 (14)	C16—C17—C18	122.30 (17)
C6—C5—C11	120.08 (13)	C16—C17—H17A	118.8
C1—C6—C5	114.05 (15)	C18—C17—H17A	118.8
C1—C6—C7	124.47 (16)	C17—C18—C19	122.26 (18)
C5—C6—C7	121.48 (16)	C17—C18—C23	118.89 (17)
C8—C7—C6	129.39 (17)	C19—C18—C23	118.79 (18)
C8—C7—H7A	115.3	C20—C19—C18	121.4 (2)
C6—C7—H7A	115.3	C20—C19—H19A	119.3
C7—C8—C9	120.76 (17)	C18—C19—H19A	119.3
C7—C8—H8A	119.6	C19—C20—C21	120.1 (2)
C9—C8—H8A	119.6	C19—C20—H20A	120.0
O1—C9—C8	121.54 (15)	C21—C20—H20A	120.0
O1—C9—C10	120.20 (15)	C22—C21—C20	121.0 (2)
C8—C9—C10	118.24 (15)	C22—C21—H21A	119.5
C23—C10—C11	120.91 (15)	C20—C21—H21A	119.5
C23—C10—C9	119.90 (14)	C21—C22—C23	121.0 (2)
C11—C10—C9	119.07 (15)	C21—C22—H22A	119.5
C10—C11—C12	123.31 (16)	C23—C22—H22A	119.5
C10—C11—C16	118.82 (16)	C10—C23—C22	122.97 (16)



C12—C11—C16	117.86 (16)	C10—C23—C18	119.40 (16)
C13—C12—C11	120.8 (2)	C22—C23—C18	117.55 (16)
C13—C12—H12A	119.6		
F1—C1—C2—C3	-179.33 (18)	C11—C12—C13—C14	0.5 (4)
C6—C1—C2—C3	0.7 (3)	C12—C13—C14—C15	1.5 (4)
C1—C2—C3—C4	-1.6 (3)	C13—C14—C15—C16	-0.7 (4)
C2—C3—C4—C5	0.5 (3)	C14—C15—C16—C17	179.2 (2)
C3—C4—C5—C6	1.7 (3)	C14—C15—C16—C11	-1.9 (4)
C3—C4—C5—C11	-177.92 (16)	C10—C11—C16—C17	1.9 (3)
F1—C1—C6—C5	-178.72 (16)	C12—C11—C16—C17	-177.37 (19)
C2—C1—C6—C5	1.2 (3)	C10—C11—C16—C15	-177.00 (19)
F1—C1—C6—C7	1.9 (3)	C12—C11—C16—C15	3.7 (3)
C2—C1—C6—C7	-178.11 (18)	C15—C16—C17—C18	179.4 (2)
C4—C5—C6—C1	-2.4 (2)	C11—C16—C17—C18	0.5 (3)
C11—C5—C6—C1	177.15 (13)	C16—C17—C18—C19	-179.5 (2)
C4—C5—C6—C7	176.95 (17)	C16—C17—C18—C23	-2.3 (3)
C11—C5—C6—C7	-3.5 (2)	C17—C18—C19—C20	177.0 (2)
C1—C6—C7—C8	4.7 (3)	C23—C18—C19—C20	-0.1 (4)
C5—C6—C7—C8	-174.62 (18)	C18—C19—C20—C21	-1.5 (4)
C6—C7—C8—C9	177.73 (16)	C19—C20—C21—C22	1.0 (4)
C7—C8—C9—O1	-8.3 (3)	C20—C21—C22—C23	1.2 (4)
C7—C8—C9—C10	173.29 (16)	C11—C10—C23—C22	177.24 (17)
O1—C9—C10—C23	120.22 (19)	C9—C10—C23—C22	1.3 (3)
C8—C9—C10—C23	-61.4 (2)	C11—C10—C23—C18	0.7 (3)
O1—C9—C10—C11	-55.8 (2)	C9—C10—C23—C18	-175.30 (15)
C8—C9—C10—C11	122.59 (18)	C21—C22—C23—C10	-179.4 (2)
C23—C10—C11—C12	176.76 (17)	C21—C22—C23—C18	-2.8 (3)
C9—C10—C11—C12	-7.2 (3)	C17—C18—C23—C10	1.7 (3)
C23—C10—C11—C16	-2.5 (3)	C19—C18—C23—C10	178.96 (19)
C9—C10—C11—C16	173.54 (16)	C17—C18—C23—C22	-175.05 (19)
C10—C11—C12—C13	177.7 (2)	C19—C18—C23—C22	2.2 (3)
C16—C11—C12—C13	-3.0 (3)		

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

Cg1 is the centroid of the C1—C6 ring.

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C8—H8 <i>A</i> ...F1	0.93	2.19	2.808 (2)	123
C17—H17 <i>A</i> ...F1 <sup>i</sup>	0.93	2.46	3.353 (2)	161
C14—H14 <i>A</i> ...Cg1 <sup>ii</sup>	0.93	2.99	3.712 (3)	136

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