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Crystal structure and Hirshfeld surface analysis of (2*E*)-3-(4-chloro-3-fluorophenyl)-1-(3,4-dimethoxyphenyl)prop-2-en-1-one

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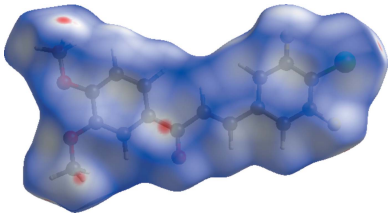
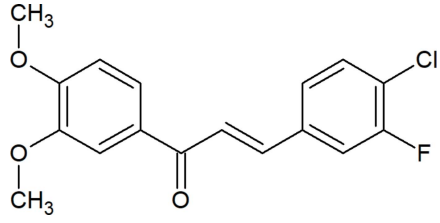
The molecular structure of the title compound, $C_{17}H_{14}ClFO_3$, consists of a 4-chloro-3-fluorophenyl ring and a 3,4-dimethoxyphenyl ring linked *via* a prop-2-en-1-one spacer. The molecule has an *E* configuration about the C═C bond and the carbonyl group is *syn* with respect to the C═C bond. The F and H atoms at the *meta* positions of the 4-chloro-3-fluorophenyl ring are disordered over two orientations, with an occupancy ratio of 0.785 (3):0.215 (3). In the crystal, molecules are linked *via* pairs of C—H···O interactions with an $R_2^2(14)$ ring motif, forming inversion dimers. The dimers are linked into a tape structure running along $[10\bar{1}]$ by a C—H···π interaction. The intermolecular contacts in the crystal were further analysed using Hirshfield surface analysis, which indicates that the most significant contacts are H···H (25.0%), followed by C···H/H···C (20.6%), O···H/H···O (15.6%), Cl···H/H···Cl (10.7%), F···H/H···F (10.4%), F···C/C···F (7.2%) and C···C (3.0%).

1. Chemical context

Chalcones, compounds with a 1,3-diphenylprop-2-en-1-one framework, are considered to be the precursors of flavonoids and isoflavonoids, which are abundant in edible plants. These compounds are coloured *via* the –CO—CH═CH– chromophore and other auxochromes. Chalcones attract significant attention because of their availability of high optical nonlinearities arising from the delocalization of π-conjugated electron clouds throughout the chalcone system, which provides a large charge-transfer axis with appropriate substituents on the terminal aromatic rings. π-conjugated systems have been studied extensively for their optoelectronic properties (Shetty *et al.*, 2016, 2017) because of the possibility of developing low-cost, large-area and flexible electronic devices. In view of all the above and in a continuation of our previous work on 3,4-dimethoxy chalcones (Sheshadri *et al.*, 2018*a*,*b*), we report herein the crystal and molecular structure of the title compound.





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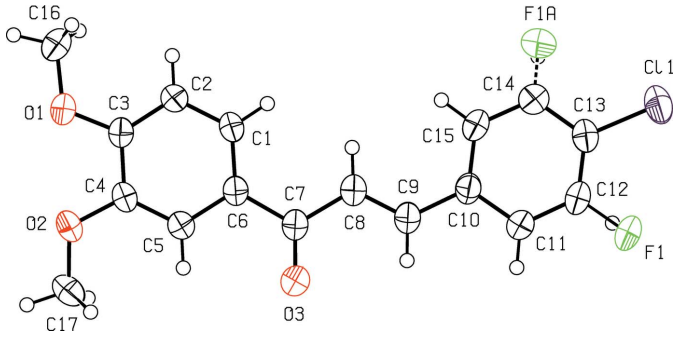

Figure 1
The molecular structure of the title compound, showing the atom labelling and displacement ellipsoids drawn at the 50% probability level.

2. Structural commentary

The title compound (Fig. 1) is composed of two aromatic rings, 4-chloro-3-fluorophenyl and 3,4-dimethoxyphenyl, which are linked by a –CO—CH═CH– enone bridge. The molecule is approximately planar as indicated by the torsion angles C1—C6—C7—O3 = 174.71 (16)°, C1—C6—C7—C8 = −3.8 (2)°, C6—C7—C8—C9 = 178.49 (15)°, O3—C7—C8—C9 = 0.0 (3)°, C8—C9—C10—C11 = 178.22 (17)° and C7—C8—C9—C10 = −179.00 (15)°. The dihedral angle between the 4-chloro-3-fluorophenyl and 3,4-dimethoxyphenyl rings is 5.40 (7)°. The H atoms of the central propenone group are *trans* configured. The two methoxy groups attached to atoms C3 and C4 are almost coplanar with the benzene ring, with deviations of 0.214 (2) Å for C16 and 0.209 (2) Å for C17. The 4-chloro-3-fluorophenyl fragment is disordered over two orientations around the C9—C10 bond axis, with an occupancy ratio of 0.785 (3):0.215 (3).

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

*Cg*1 is the centroid of the C1–C6 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···O3^{i}	0.93	2.57	3.426 (2)	152
C2—H2···*Cg*1^{ii}	0.93	2.81	3.5832 (16)	142

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

3. Supramolecular features and Hirshfeld surface analysis

In the crystal, the molecules are connected into inversion dimers with an $R_2^2(14)$ ring motif (Fig. 2) *via* pairs of C—H···O interactions (Table 1). The dimers are further linked by a C—H···π interaction (Table 1), forming a tape structure along [10$\bar{1}$] (Fig. 3).

The Hirshfeld surface and two-dimensional fingerprint plots of the title compound were calculated using *CrystalExplorer17.5* (Turner *et al.*, 2017). In the Hirshfeld surface

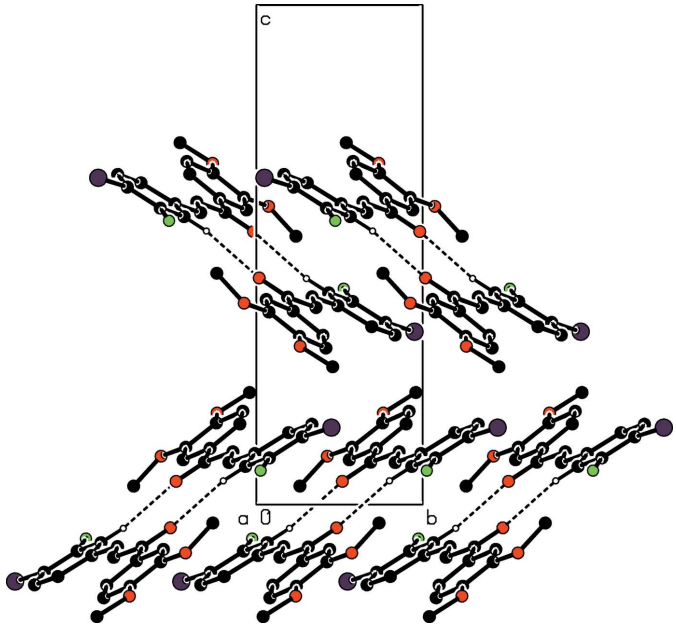

Figure 2
A packing diagram of the title compound viewed along the *a* axis, showing molecular dimers formed by the intermolecular C—H···O hydrogen bonds (dashed lines). The minor disorder component and H atoms not involved in the hydrogen bonds are omitted for clarity.

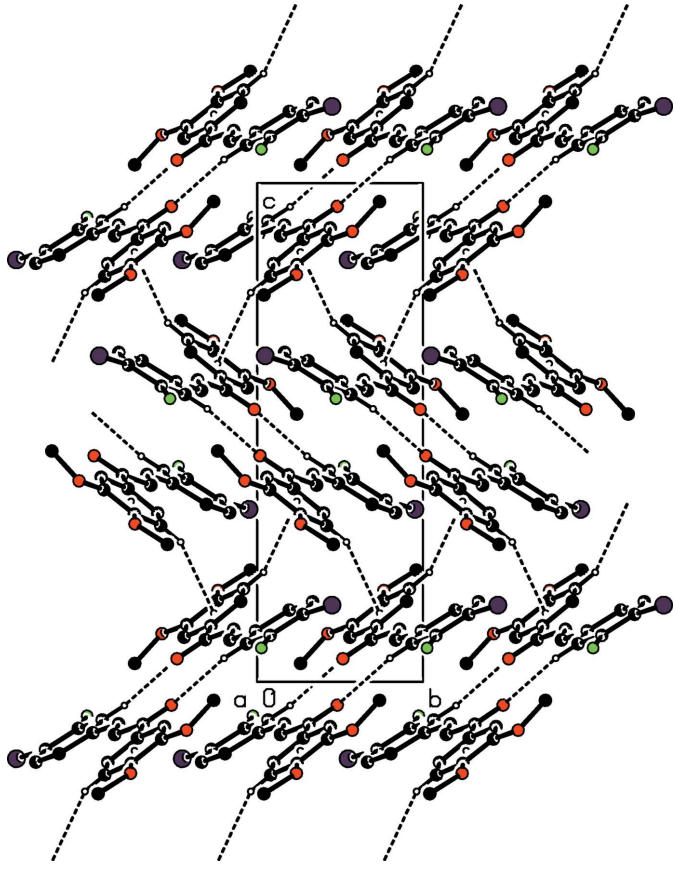

Figure 3
A packing diagram of the title compound viewed along the *a* axis, showing intermolecular C—H···O and C—H···π interactions (dashed lines). The minor disorder component and H atoms not involved in the hydrogen bonds are omitted for clarity.

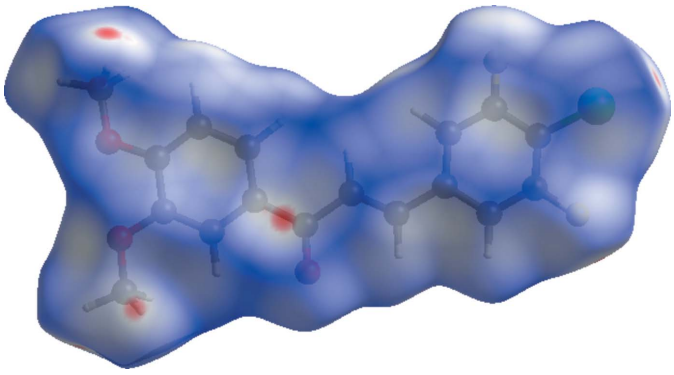

Figure 4
Plot of d_{norm} mapped on the Hirshfeld surfaces of the title compound showing the short H···O contacts.

plotted over d_{norm} (Fig. 4), the white surfaces indicate contacts with distances equal to the sum of van der Waals radii, and the red and blue colours indicate distances shorter or longer than the van der Waals radii, respectively (Venkatesan *et al.*, 2016). The overall two-dimensional fingerprint plot and those delineated into H···H (25.0%), C···H/H···C (20.6%), O···H/H···O (15.6%), Cl···H/H···Cl (10.7%), F···H/H···F (10.4%), F···C/C···F (7.2%) and C···C (3.0%) contacts (McKinnon *et al.*, 2007) are illustrated in Fig. 5*a–h*, respectively. The small percentage contributions from the other different interatomic contacts to the Hirshfeld surfaces are as follows: Cl···O/O···Cl (2.7%), O···C/C···O (1.7%), Cl···C/C···Cl (1.1%), F···F (0.9%), Cl···F/F···Cl (0.7%) and F···O/O···F (0.2%).

4. Database survey

A search of the Cambridge Structural Database (CSD, version 5.40, update of February 2019; Groom *et al.*, 2016) using (*E*)-1,3-diphenylprop-2-en-1-one as the main skeleton revealed 3314 hits. Six structures containing the (*E*)-1,3-diphenylprop-2-en-1-one framework with different substituents that are similar to the title compound were found, *viz.* 3-(3-chlorophenyl)-1-(3,4-dimethoxyphenyl)prop-2-en-1-one (VIDVEM; Sheshadri *et al.*, 2018*a*), 3-(3-bromo-4-fluorophenyl)-1-(3,4-dimethoxyphenyl)prop-2-en-1-one (BIBWOB; Sheshadri *et al.*, 2018*b*), (*E*)-3-(2-bromophenyl)-1-(3,4-dimethoxyphenyl)-prop-2-en-1-one (LAPREB; Li *et al.*, 2012), (*E*)-1-(3,5-difluorophenyl)-3-(2,4-dimethoxyphenyl)prop-2-en-1-one (KUZFOB; Huang *et al.*, 2010), (*E*)-1-(3-bromophenyl)-3-(3,4-dimethoxyphenyl)prop-2-en-1-one (LAQWUX; Escobar *et al.*, 2012) and 3-(3,4-dimethoxyphenyl)-1-(4-fluorophenyl)-prop-2-en-1-one(MEGQOF; Butcher *et al.*, 2006).

For these similar compounds, the dihedral angles between the two terminal benzene rings, which are linked by a –CO—CH═CH– enone bridge are 18.46 (7)° for VIDVEM, 17.91 (17)° for BIBWOB, 9.3 (2) and 19.4 (2)° (two crystallographically independent molecules) for LAPREB, 5.46 (2)° for KUZFOB, 26.59 (9)° for LAQWUX and 47.81 (6) and 50.18 (5)° (two crystallographically independent molecules) for MEGQOF. In the crystals of VIDVEM and BIBWOB, molecules are linked by C—H···O hydrogen bonds, forming dimers with $R_2^2(14)$ ring motifs, and the dimers are further linked by other C—H···O hydrogen contacts, forming two-dimensional supramolecular structures. In the crystal of LAPREB, molecules are also linked through weak intermolecular C—H···O hydrogen bonds. The crystal structure of KUZFOB is stabilized by intermolecular C—H···F hydrogen bonds.

5. Synthesis and crystallization

The title compound was synthesized as per the procedure reported earlier (Kumar *et al.*, 2013*a*,*b*). 1-(3,4-Dimethoxyphenyl)ethanone (0.01 mol) and 4-chloro-3-fluorobenzaldehyde (0.01 mol) were dissolved in 20 ml of methanol. A catalytic amount of NaOH was added to the solution dropwise with vigorous stirring. The reaction mixture was stirred for about 3 h at room temperature. The formed crude products were filtered, washed successively with distilled water and recrystallized from methanol to get the title compound (m.p. 384–388 K).

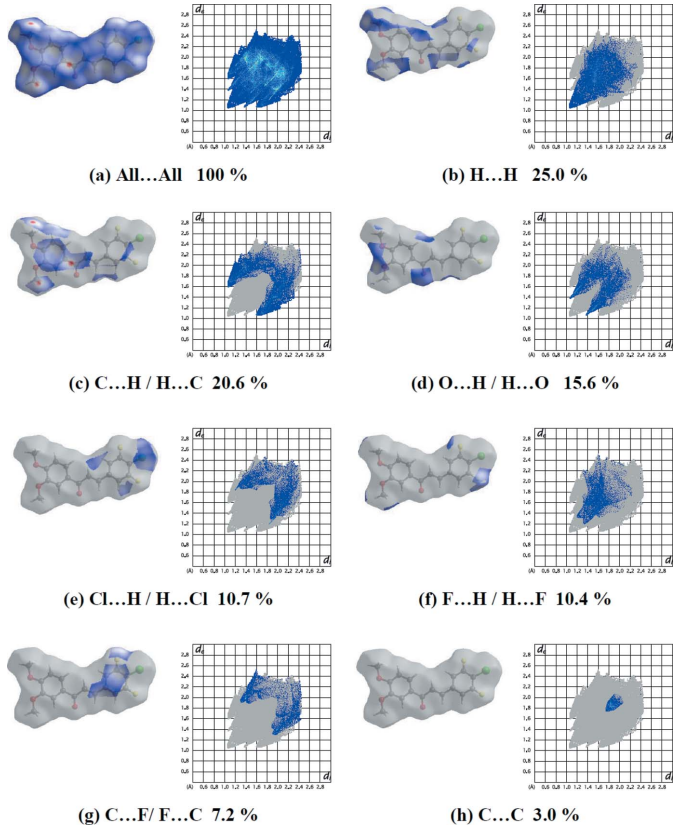

Figure 5
Hirshfeld surface representations and the overall two-dimensional fingerprint plots of the title compound, showing (*a*) all interactions, and delineated into (*b*) H···H, (*c*) C···H/H···C, (*d*) O···H/H···O, (*e*) Cl···H/H···Cl, (*f*) F···H/H···F, (*g*) F···C/C···F and (*h*) C···C interactions [d_e and d_i represent the distances from a point on the Hirshfeld surface to the nearest atoms outside (external) and inside (internal) the surface, respectively].

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The C-bound H atoms were positioned geometrically (C—H = 0.93 or 0.96 Å) and refined using a riding model, with $U_{iso}(H) = 1.2$ or $1.5U_{eq}(C)$. The 4-chloro-3-fluorophenyl fragment was found to be disordered in a difference-Fourier map, and the F and H atoms at the *meta* positions of the benzene ring were treated as disordered over two sites with an occupancy ratio of 0.785 (3):0.215 (3).

Acknowledgements

The authors extend their appreciation to the Vidya Vikas Research & Development Centre for the facilities and encouragement.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{14}ClFO_3$
M_r	320.73
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	294
a, b, c (Å)	14.9088 (13), 5.7669 (5), 17.9074 (15)
β (°)	104.491 (2)
V (Å^3)	1490.7 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.28
Crystal size (mm)	0.45 × 0.37 × 0.30
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Sheldrick, 2007)
T_{min}, T_{max}	0.884, 0.921
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	16268, 4334, 3195
R_{int}	0.024
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.704
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.047, 0.143, 1.05
No. of reflections	4334
No. of parameters	211
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.33, −0.36

Computer programs: *APEX2* and *SAINT* (Bruker, 2007), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009).

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supporting information

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Computing details

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2009).

(2*E*)-3-(4-Chloro-3-fluorophenyl)-1-(3,4-dimethoxyphenyl)prop-2-en-1-one

Crystal data

$C_{17}H_{14}ClFO_3$
M_r = 320.73
Monoclinic, $P2_1/n$
a = 14.9088 (13) Å
b = 5.7669 (5) Å
c = 17.9074 (15) Å
β = 104.491 (2)°
V = 1490.7 (2) Å^3
Z = 4
F(000) = 664
D_x = 1.429 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5099 reflections
θ = 2.4–29.4°
μ = 0.28 mm^{-1}
T = 294 K
Block, colourless
0.45 × 0.37 × 0.30 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2007)
T_{min} = 0.884, T_{max} = 0.921
16268 measured reflections
4334 independent reflections
3195 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 30.0°, θ_{min} = 1.6°
$h = -19 \rightarrow 20$
$k = -8 \rightarrow 7$
$l = -25 \rightarrow 25$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.143
S = 1.05
4334 reflections
211 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0736P)^2 + 0.2421P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cl1	0.36793 (3)	0.45137 (9)	0.15399 (3)	0.06876 (17)	
F1	0.34304 (9)	0.0254 (3)	0.06801 (10)	0.0765 (6)	0.785 (3)
F1A	0.1946 (4)	0.5065 (11)	0.2007 (4)	0.094 (2)	0.215 (3)
O1	−0.44876 (7)	−0.2364 (2)	0.18315 (7)	0.0525 (3)	
O2	−0.42868 (8)	−0.5737 (2)	0.09682 (7)	0.0534 (3)	
O3	−0.11186 (9)	−0.4829 (2)	0.04648 (8)	0.0690 (4)	
C1	−0.21547 (10)	−0.0994 (3)	0.16131 (8)	0.0438 (3)	
H1	−0.168526	0.009416	0.177135	0.053*	
C2	−0.29625 (10)	−0.0816 (3)	0.18676 (8)	0.0439 (3)	
H2	−0.302640	0.038463	0.219715	0.053*	
C3	−0.36666 (9)	−0.2405 (2)	0.16343 (8)	0.0388 (3)	
C4	−0.35591 (9)	−0.4244 (2)	0.11467 (7)	0.0392 (3)	
C5	−0.27631 (10)	−0.4408 (2)	0.08964 (8)	0.0412 (3)	
H5	−0.269807	−0.561469	0.056957	0.049*	
C6	−0.20461 (9)	−0.2784 (2)	0.11254 (8)	0.0400 (3)	
C7	−0.11934 (10)	−0.3123 (3)	0.08476 (9)	0.0462 (3)	
C8	−0.04346 (11)	−0.1412 (3)	0.10561 (9)	0.0514 (4)	
H8	−0.050846	−0.012603	0.134851	0.062*	
C9	0.03440 (10)	−0.1648 (3)	0.08409 (9)	0.0468 (3)	
H9	0.038821	−0.294198	0.054228	0.056*	
C10	0.11470 (10)	−0.0096 (3)	0.10207 (8)	0.0437 (3)	
C11	0.19219 (11)	−0.0652 (3)	0.07626 (9)	0.0495 (4)	
H11	0.192714	−0.199152	0.047458	0.059*	
C12	0.26843 (10)	0.0782 (3)	0.09329 (9)	0.0503 (4)	
H12A	0.319949	0.038662	0.075551	0.060*	0.215 (3)
C13	0.27083 (10)	0.2763 (3)	0.13536 (9)	0.0484 (3)	
C14	0.19390 (13)	0.3344 (3)	0.16078 (11)	0.0613 (4)	
H14	0.194093	0.469027	0.189426	0.074*	0.785 (3)
C15	0.11650 (12)	0.1938 (3)	0.14396 (11)	0.0597 (4)	
H15	0.064721	0.235966	0.160943	0.072*	
C16	−0.46843 (13)	−0.0410 (3)	0.22426 (11)	0.0599 (4)	
H16A	−0.531649	−0.047899	0.227596	0.090*	
H16B	−0.458981	0.098166	0.197789	0.090*	
H16C	−0.428007	−0.040654	0.275248	0.090*	
C17	−0.43044 (13)	−0.7381 (3)	0.03698 (10)	0.0576 (4)	
H17A	−0.487558	−0.823211	0.026665	0.086*	
H17B	−0.379347	−0.843355	0.052900	0.086*	
H17C	−0.425610	−0.658282	−0.008901	0.086*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0483 (3)	0.0636 (3)	0.0962 (4)	−0.01829 (19)	0.0215 (2)	−0.0083 (2)
F1	0.0457 (8)	0.0828 (11)	0.1146 (12)	−0.0100 (6)	0.0454 (8)	−0.0308 (8)
F1A	0.075 (4)	0.081 (4)	0.137 (5)	−0.023 (3)	0.048 (4)	−0.061 (4)
O1	0.0380 (5)	0.0559 (7)	0.0690 (7)	−0.0088 (5)	0.0234 (5)	−0.0118 (5)
O2	0.0445 (6)	0.0533 (7)	0.0650 (6)	−0.0199 (5)	0.0186 (5)	−0.0151 (5)
O3	0.0533 (7)	0.0692 (8)	0.0944 (9)	−0.0154 (6)	0.0372 (7)	−0.0334 (7)
C1	0.0334 (7)	0.0433 (7)	0.0550 (8)	−0.0086 (5)	0.0120 (6)	−0.0064 (6)
C2	0.0380 (7)	0.0425 (7)	0.0519 (7)	−0.0042 (6)	0.0128 (6)	−0.0098 (6)
C3	0.0314 (6)	0.0423 (7)	0.0430 (6)	−0.0021 (5)	0.0101 (5)	0.0017 (5)
C4	0.0337 (6)	0.0398 (7)	0.0429 (6)	−0.0075 (5)	0.0075 (5)	−0.0002 (5)
C5	0.0388 (7)	0.0416 (7)	0.0441 (7)	−0.0053 (5)	0.0120 (6)	−0.0054 (5)
C6	0.0333 (6)	0.0432 (7)	0.0442 (6)	−0.0045 (5)	0.0111 (5)	−0.0013 (5)
C7	0.0371 (7)	0.0517 (8)	0.0523 (7)	−0.0063 (6)	0.0158 (6)	−0.0053 (6)
C8	0.0404 (7)	0.0550 (9)	0.0635 (9)	−0.0096 (7)	0.0215 (7)	−0.0107 (7)
C9	0.0376 (7)	0.0530 (9)	0.0522 (7)	−0.0065 (6)	0.0159 (6)	−0.0045 (6)
C10	0.0359 (7)	0.0507 (8)	0.0471 (7)	−0.0039 (6)	0.0153 (6)	−0.0011 (6)
C11	0.0406 (8)	0.0534 (9)	0.0586 (8)	−0.0035 (6)	0.0197 (6)	−0.0116 (7)
C12	0.0349 (7)	0.0591 (9)	0.0614 (8)	−0.0020 (6)	0.0206 (6)	−0.0032 (7)
C13	0.0387 (7)	0.0510 (8)	0.0569 (8)	−0.0088 (6)	0.0147 (6)	−0.0008 (6)
C14	0.0558 (10)	0.0581 (10)	0.0773 (11)	−0.0098 (8)	0.0305 (9)	−0.0195 (9)
C15	0.0465 (9)	0.0625 (10)	0.0807 (11)	−0.0084 (7)	0.0360 (8)	−0.0177 (8)
C16	0.0514 (9)	0.0636 (11)	0.0738 (11)	−0.0024 (8)	0.0328 (8)	−0.0113 (8)
C17	0.0550 (9)	0.0507 (9)	0.0636 (9)	−0.0141 (7)	0.0082 (7)	−0.0145 (7)

Geometric parameters (Å, º)

Cl1—C13	1.7278 (15)	C8—H8	0.9300
F1—C12	1.3367 (18)	C9—C10	1.465 (2)
F1A—C14	1.222 (5)	C9—H9	0.9300
O1—C3	1.3565 (16)	C10—C11	1.3851 (19)
O1—C16	1.416 (2)	C10—C15	1.389 (2)
O2—C4	1.3590 (16)	C11—C12	1.376 (2)
O2—C17	1.4259 (19)	C11—H11	0.9300
O3—C7	1.2202 (19)	C12—C13	1.364 (2)
C1—C6	1.3876 (19)	C12—H12A	0.9300
C1—C2	1.3940 (19)	C13—C14	1.377 (2)
C1—H1	0.9300	C14—C15	1.381 (2)
C2—C3	1.3772 (19)	C14—H14	0.9300
C2—H2	0.9300	C15—H15	0.9300
C3—C4	1.4082 (19)	C16—H16A	0.9600
C4—C5	1.3727 (19)	C16—H16B	0.9600
C5—C6	1.4028 (19)	C16—H16C	0.9600
C5—H5	0.9300	C17—H17A	0.9600
C6—C7	1.4893 (19)	C17—H17B	0.9600
C7—C8	1.477 (2)	C17—H17C	0.9600

C8—C9	1.319 (2)

C3—O1—C16	117.83 (12)	C12—C11—C10	119.90 (14)
C4—O2—C17	117.47 (12)	C12—C11—H11	120.1
C6—C1—C2	120.47 (13)	C10—C11—H11	120.1
C6—C1—H1	119.8	F1—C12—C13	117.94 (14)
C2—C1—H1	119.8	F1—C12—C11	119.95 (15)
C3—C2—C1	120.46 (13)	C13—C12—C11	122.11 (14)
C3—C2—H2	119.8	C13—C12—H12A	118.9
C1—C2—H2	119.8	C11—C12—H12A	118.9
O1—C3—C2	125.34 (13)	C12—C13—C14	118.53 (14)
O1—C3—C4	115.13 (12)	C12—C13—Cl1	120.07 (12)
C2—C3—C4	119.53 (12)	C14—C13—Cl1	121.38 (13)
O2—C4—C5	125.75 (13)	F1A—C14—C13	120.4 (3)
O2—C4—C3	114.52 (12)	F1A—C14—C15	119.3 (3)
C5—C4—C3	119.73 (12)	C13—C14—C15	120.31 (16)
C4—C5—C6	121.10 (13)	C13—C14—H14	119.8
C4—C5—H5	119.5	C15—C14—H14	119.8
C6—C5—H5	119.5	C14—C15—C10	121.06 (14)
C1—C6—C5	118.69 (12)	C14—C15—H15	119.5
C1—C6—C7	123.47 (12)	C10—C15—H15	119.5
C5—C6—C7	117.82 (12)	O1—C16—H16A	109.5
O3—C7—C8	120.58 (13)	O1—C16—H16B	109.5
O3—C7—C6	119.93 (13)	H16A—C16—H16B	109.5
C8—C7—C6	119.47 (13)	O1—C16—H16C	109.5
C9—C8—C7	122.13 (15)	H16A—C16—H16C	109.5
C9—C8—H8	118.9	H16B—C16—H16C	109.5
C7—C8—H8	118.9	O2—C17—H17A	109.5
C8—C9—C10	127.13 (15)	O2—C17—H17B	109.5
C8—C9—H9	116.4	H17A—C17—H17B	109.5
C10—C9—H9	116.4	O2—C17—H17C	109.5
C11—C10—C15	118.09 (14)	H17A—C17—H17C	109.5
C11—C10—C9	119.29 (14)	H17B—C17—H17C	109.5
C15—C10—C9	122.62 (13)		

C6—C1—C2—C3	−0.4 (2)	O3—C7—C8—C9	0.0 (3)
C16—O1—C3—C2	7.1 (2)	C6—C7—C8—C9	178.49 (15)
C16—O1—C3—C4	−172.50 (14)	C7—C8—C9—C10	−179.00 (15)
C1—C2—C3—O1	−178.37 (14)	C8—C9—C10—C11	178.22 (17)
C1—C2—C3—C4	1.2 (2)	C8—C9—C10—C15	−2.1 (3)
C17—O2—C4—C5	−11.5 (2)	C15—C10—C11—C12	0.9 (3)
C17—O2—C4—C3	168.72 (13)	C9—C10—C11—C12	−179.46 (15)
O1—C3—C4—O2	−1.91 (18)	C10—C11—C12—F1	−179.59 (16)
C2—C3—C4—O2	178.50 (13)	C10—C11—C12—C13	0.0 (3)
O1—C3—C4—C5	178.26 (13)	F1—C12—C13—C14	179.06 (17)
C2—C3—C4—C5	−1.3 (2)	C11—C12—C13—C14	−0.6 (3)
O2—C4—C5—C6	−179.07 (13)	F1—C12—C13—Cl1	0.4 (2)
C3—C4—C5—C6	0.7 (2)	C11—C12—C13—Cl1	−179.23 (14)

C2—C1—C6—C5	−0.2 (2)	C12—C13—C14—F1A	177.6 (5)
C2—C1—C6—C7	−178.27 (14)	Cl1—C13—C14—F1A	−3.8 (5)
C4—C5—C6—C1	0.0 (2)	C12—C13—C14—C15	0.2 (3)
C4—C5—C6—C7	178.21 (13)	Cl1—C13—C14—C15	178.81 (15)
C1—C6—C7—O3	174.71 (16)	F1A—C14—C15—C10	−176.7 (5)
C5—C6—C7—O3	−3.4 (2)	C13—C14—C15—C10	0.8 (3)
C1—C6—C7—C8	−3.8 (2)	C11—C10—C15—C14	−1.3 (3)
C5—C6—C7—C8	178.12 (14)	C9—C10—C15—C14	179.08 (17)

Hydrogen-bond geometry (Å, º)

*Cg*1 is the centroid of the C1–C6 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···O3^{i}	0.93	2.57	3.426 (2)	152
C2—H2···*Cg*1^{ii}	0.93	2.81	3.5832 (16)	142

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