

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

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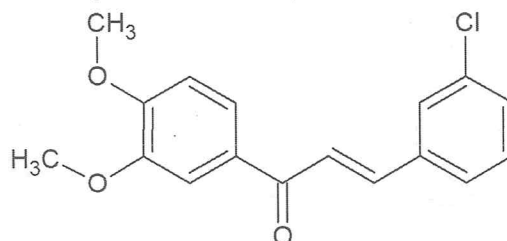
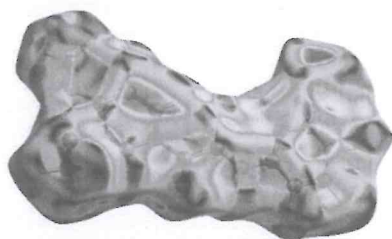
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In title compound, C₁₇H₁₅ClO₃, the dihedral angle between the benzene and chlorophenyl rings is 18.46 (7)°. In the crystal, molecules are linked by C—H...O hydrogen contacts, enclosing an R₂²(14) ring motif, and by a further C—H...O hydrogen contact, forming a two-dimensional supramolecular structure extending along the direction parallel to the *ac* plane. Hirshfeld surface analysis shows that van der Waals interactions constitute the major contribution to the intermolecular interactions, with H...H contacts accounting for 36.2% of the surface.

1. Chemical context

Materials exhibiting two photon absorption (TPA) have wide applications such as frequency-up lasing, multi-photon microscopy, three-dimensional fluorescence imaging, eye and sensor protection. Materials with potential non-linear optical (NLO) properties have significant applications in the field of photonics. Chalcone and its derivatives have attracted significant attention in the past few years because of their availability of high optical non-linearities resulting from the significant delocalization of π -conjugated electron clouds throughout the chalcone system, providing a large charge-transfer axis with appropriate substituents on the terminal aromatic rings. The second harmonic generation (SHG) efficiency of these compounds is due to the strong intermolecular electron-donor-acceptor interactions, which may also enhance the non-linear optical (NLO) properties. With the possibility of developing low-cost, large-area and flexible electronic devices, π -conjugated systems have been studied extensively for their optoelectronic properties (Chandra Shekhara Shetty *et al.*, 2016, 2017).



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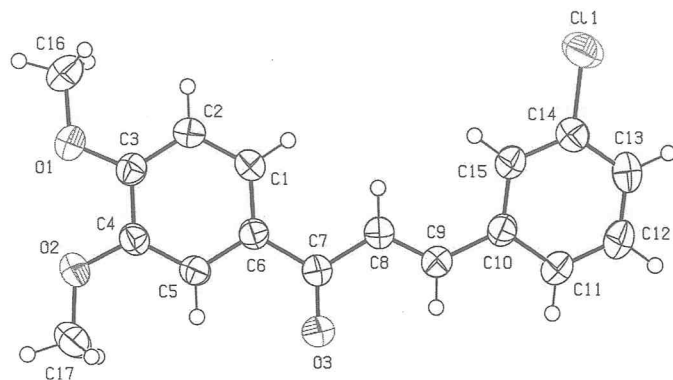


Figure 1
The molecular structure of the title compound, showing the atom labelling and displacement ellipsoids drawn at the 50% probability level.

2. Structural commentary

The molecular structure of the title compound is shown in Fig. 1. The title compound is constructed from two aromatic

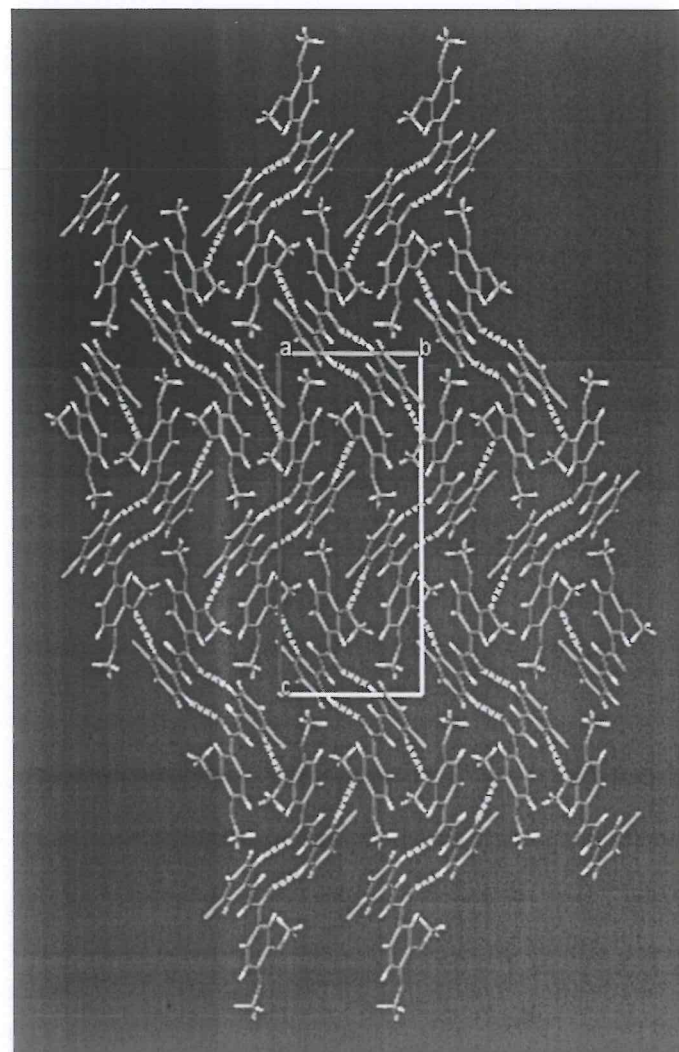


Figure 2
A view along the *a* axis of the crystal packing of the title compound. Intermolecular interactions are shown as dashed lines.

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

<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>
C11—H11A...O3 ⁱ	0.93	2.54	3.417 (2)	157
C15—H15A...O2 ⁱⁱ	0.93	2.54	3.4378 (18)	163

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

rings (chlorophenyl and terminal methoxyphenyl rings), which are linked by a C=C—C(=O)—C enone bridge. Compared to the nearly coplanar arrangement of rings in the title compound, the molecule is twisted substantially [C5—C6—C7—O3 = 3.5 (2)° and O3—C7—C8—C9 = 10.5 (2)°] about the enone bridge, which may arise from steric repulsion with the *ortho*-O2 atom. Hence, the dihedral angle between the 3,4-methoxyphenyl and chlorophenyl rings increases to 18.46 (7)°. The C atoms of the methoxy groups are close to the plane of their attached ring: deviations of C16 and C17 are 0.252 (2) and 0.038 (2) Å, respectively. The bond lengths and angles are comparable with those in the similar compounds (*E*)-3-(3,4-dimethoxyphenyl)-1-(1-hydroxynaphthalen-2yl)prop-2-en-1-one (Ezhilarasi *et al.*, 2015), (*E*)-1-(3-bromophenyl)-3-(3,4-dimethoxyphenyl)prop-2-en-1-one (Escobar *et al.*, 2012) and (*E*)-3-(2-bromophenyl)-1-(3,4-dimethoxyphenyl)prop-2-en-1-one (Li *et al.*, 2012).

3. Supramolecular features and Hirshfeld surface analysis

In the crystal, molecules are linked by C—H...O hydrogen contacts (Table 1, Fig. 2), enclosing an $R_2^2(14)$ ring motif, and by a further C—H...O hydrogen contact, forming a three-dimensional structure extending in the *a*- and *c*-axis directions.

Hirshfeld surfaces and fingerprint plots were generated for the title compound based on the crystallographic information file (CIF) using *CrystalExplorer* (McKinnon *et al.*, 2007). Hirshfeld surfaces enable the visualization of intermolecular interactions by different colors and color intensity, repre-

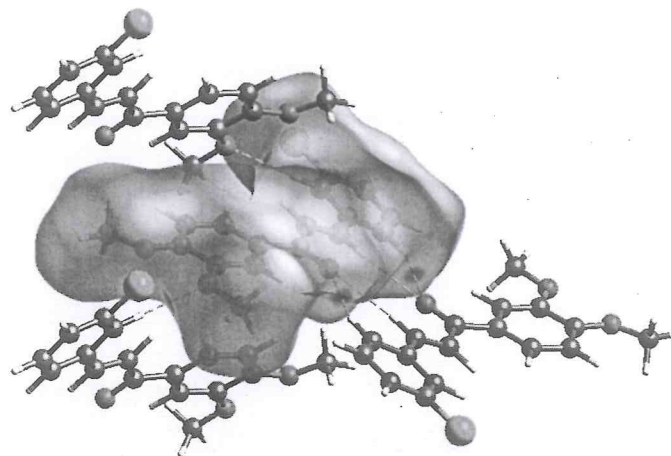


Figure 3
View of the three-dimensional Hirshfeld surface of the title compound mapped over d_{norm} .



Figure 4
Hirshfeld surface of the title complex plotted over shape-index.

Table 2

Summary of short interatomic contacts (Å) in the title compound.

Contact	Distance	Symmetry operation
Cl1...H17B	3.05	$-1 + x, 1 + y, z$
Cl1...C1	3.4666 (15)	$-x, \frac{1}{2} + y, \frac{1}{2} - z$
O2...H15A	2.54	$-x, -\frac{1}{2} + y, \frac{1}{2} - z$
O1...H17A	2.86	$-x, \frac{1}{2} + y, \frac{1}{2} - z$
H17C...C10	2.88	$1 + x, y, z$
H11A...O3	2.54	$1 - x, 1 - y, -z$
C1...Cl1	3.4666 (15)	$-x, -\frac{1}{2} + y, \frac{1}{2} - z$
H15A...O2	2.54	$-x, \frac{1}{2} + y, \frac{1}{2} - z$
C10...H17C	2.88	$-1 + x, y, z$
C13...C13	3.497 (2)	$-x, 2 - y, -z$
H13A...H16A	2.46	$-\frac{1}{2} + x, \frac{3}{2} - y, -\frac{1}{2} + z$
H16A...H13A	2.46	$+\frac{1}{2} + x, \frac{3}{2} - y, \frac{1}{2} + z$
H17A...O1	2.86	$-x, -\frac{1}{2} + y, \frac{1}{2} - z$
H17B...Cl1	3.05	$1 + x, -1 + y, z$

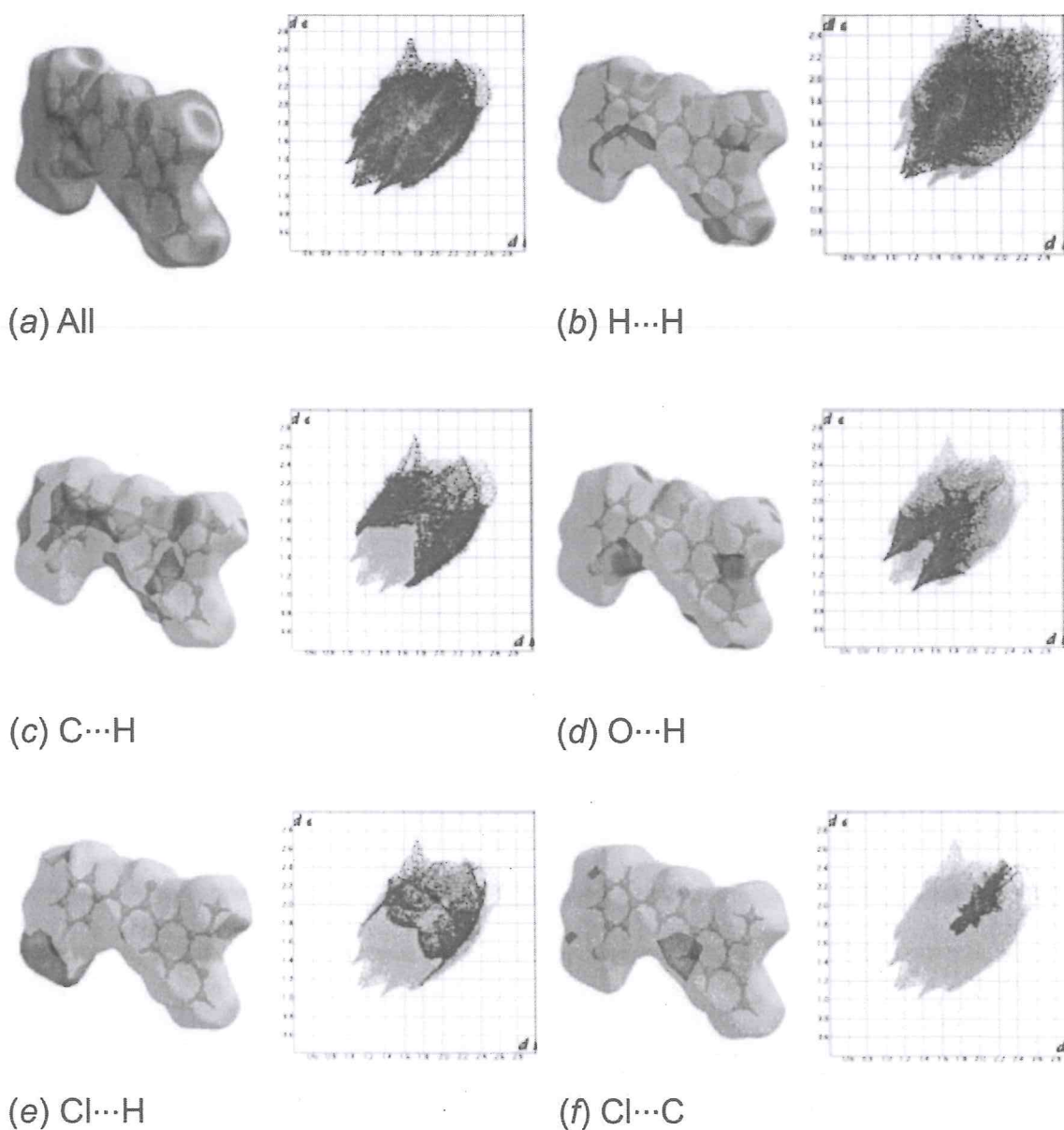


Figure 5

The two-dimensional fingerprint plots of the title compound, showing (a) all interactions, and delineated into (b) H...H, (c) C...H, (d) O...H, (e) Cl...H and (f) Cl...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].

Table 3
Experimental details.

Crystal data	
Chemical formula	C ₁₇ H ₁₅ ClO ₃
<i>M_r</i>	302.74
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>n</i>
Temperature (K)	294
<i>a</i> , <i>b</i> , <i>c</i> (Å)	9.0491 (4), 8.3257 (4), 20.2857 (9)
β (°)	99.484 (1)
<i>V</i> (Å ³)	1507.44 (12)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.26
Crystal size (mm)	0.40 × 0.24 × 0.19
Data collection	
Diffractometer	Bruker APEXII CCD
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	39332, 5506, 3732
<i>R</i> _{int}	0.036
(sin θ/λ) _{max} (Å ⁻¹)	0.758
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.049, 0.158, 1.01
No. of reflections	5506
No. of parameters	190
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.31, -0.43

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

sending short or long contacts and indicating the relative strength of the interactions. Figs. 3 and 4 show the Hirshfeld surfaces mapped over *d*_{norm} (−0.16 to 1.25 a.u.) and shape-index (−1.0 to 1.0 a.u.).

In Fig. 3, the spots near atoms O2 and O3 result from the C15—H15A...O2ⁱⁱ and C11—H11A...O3ⁱ interactions significant in the molecule packing of the title compound (Table 1). Some of the short intermolecular contacts for the title compound are listed in Table 2. The Hirshfeld surfaces illustrated in Fig. 3 also reflect the involvement of different atoms in the intermolecular interactions through the appearance of blue and red regions around the participating atoms, which correspond to positive and negative electrostatic potential, respectively.

The overall two-dimensional fingerprint plot for the title compound and those delineated into H...H, C...H/H...C, H...O/O...H, Cl...H/H...Cl and Cl...C/C...Cl contacts are illustrated in Fig. 5; the percentage contributions from the different interatomic contacts to the Hirshfeld surfaces are as follows: H...H (36.2%), C...H/H...C (24.6%), H...O/O...H (19.2%), Cl...H/H...Cl (10.5%), Cl...C/C...Cl (5.8%), C...C (3.3%), Cl...O/O...Cl (0.3%) and O...C/C...O (0.2%), as shown in the two-dimensional fingerprint plots in Fig. 4.

4. Synthesis and crystallization

The reagents and solvents for the synthesis were obtained from the Aldrich Chemical Co. and were used without additional purification. 1-(3,4-Dimethoxyphenyl) ethanone (0.01 mol) and 3-chlorobenzaldehyde (0.01 mol) were dissolved in 20 ml methanol. A catalytic amount of NaOH was added to the solution dropwise with vigorous stirring. The reaction mixture was stirred for about 5–6 h at room temperature. The progress of the reaction was monitored by TLC. The formed crude products were filtered, washed successively with distilled water and recrystallized from ethanol to get the title chalcone. Crystals suitable for X-ray diffraction studies were obtained from acetone solution by slow evaporation at room temperature. The melting point (371–373 K) was determined by a Stuart Scientific (UK) apparatus. The purity of the compound was confirmed by thin layer chromatography using Merck silica gel 60 F254 coated aluminum plates.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. C-bound H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å and *U*_{iso}(H) = 1.2*U*_{eq}(C) for C—H and C—H = 0.96 Å and *U*_{iso}(H) = 1.5*U*_{eq}(C) for methyl H atoms.

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

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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-(3-Chlorophenyl)-1-(3,4-dimethoxyphenyl)prop-2-en-1-one

Crystal data

$C_{17}H_{15}ClO_3$
 $M_r = 302.74$
 Monoclinic, $P2_1/n$
 Hall symbol: $-P\ 2_1/n$
 $a = 9.0491\ (4)\ \text{\AA}$
 $b = 8.3257\ (4)\ \text{\AA}$
 $c = 20.2857\ (9)\ \text{\AA}$
 $\beta = 99.484\ (1)^\circ$
 $V = 1507.44\ (12)\ \text{\AA}^3$
 $Z = 4$

$F(000) = 632$
 $D_x = 1.334\ \text{Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$
 Cell parameters from 8862 reflections
 $\theta = 2.7\text{--}30.8^\circ$
 $\mu = 0.26\ \text{mm}^{-1}$
 $T = 294\ \text{K}$
 Block, yellow
 $0.40 \times 0.24 \times 0.19\ \text{mm}$

Data collection

Bruker APEXII CCD
 diffractometer
 φ and ω scans
 39332 measured reflections
 5506 independent reflections
 3732 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.036$
 $\theta_{\text{max}} = 32.6^\circ$, $\theta_{\text{min}} = 2.0^\circ$
 $h = -13 \rightarrow 13$
 $k = -12 \rightarrow 12$
 $l = -30 \rightarrow 30$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.049$
 $wR(F^2) = 0.158$
 $S = 1.01$
 5506 reflections
 190 parameters
 0 restraints

Hydrogen site location: inferred from neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0758P)^2 + 0.3034P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.31\ \text{e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.43\ \text{e \AA}^{-3}$

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > 2\sigma(F^2)$ is used only for calculating -R-factor-obs 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	-0.02901 (5)	1.02517 (6)	0.15452 (2)	0.0710 (2)
O1	1.07019 (12)	0.65283 (15)	0.35402 (5)	0.0576 (3)
O2	1.13649 (12)	0.52216 (16)	0.24887 (6)	0.0634 (4)
O3	0.67255 (12)	0.57110 (17)	0.07167 (5)	0.0632 (4)
C1	0.72153 (15)	0.73479 (17)	0.23869 (7)	0.0458 (4)
C2	0.82535 (15)	0.73642 (17)	0.29717 (7)	0.0463 (4)
C3	0.96267 (14)	0.66310 (15)	0.29901 (6)	0.0420 (3)
C4	0.99836 (14)	0.59071 (16)	0.24086 (6)	0.0415 (3)
C5	0.89499 (14)	0.59023 (15)	0.18335 (6)	0.0405 (3)
C6	0.75372 (13)	0.66142 (14)	0.18154 (6)	0.0394 (3)
C7	0.64331 (14)	0.64884 (17)	0.11929 (7)	0.0444 (4)
C8	0.49469 (15)	0.72588 (18)	0.11575 (7)	0.0495 (4)
C9	0.38379 (15)	0.69300 (18)	0.06640 (6)	0.0452 (4)
C10	0.22936 (14)	0.75164 (16)	0.05882 (6)	0.0424 (3)
C11	0.12555 (17)	0.69543 (19)	0.00574 (7)	0.0525 (4)
C12	-0.02283 (18)	0.7421 (2)	-0.00148 (8)	0.0610 (5)
C13	-0.07040 (16)	0.8446 (2)	0.04383 (8)	0.0564 (5)
C14	0.03261 (16)	0.90063 (17)	0.09633 (7)	0.0470 (4)
C15	0.18120 (15)	0.85720 (16)	0.10468 (7)	0.0447 (3)
C16	1.0326 (2)	0.7046 (3)	0.41599 (8)	0.0826 (7)
C17	1.1814 (2)	0.4431 (2)	0.19409 (9)	0.0669 (6)
H1A	0.62888	0.78375	0.23788	0.0550*
H2A	0.80242	0.78689	0.33512	0.0560*
H5A	0.91867	0.54216	0.14504	0.0490*
H8A	0.47900	0.79854	0.14872	0.0590*
H9A	0.40642	0.62539	0.03295	0.0540*
H11A	0.15612	0.62577	-0.02523	0.0630*
H12A	-0.09113	0.70376	-0.03734	0.0730*
H13A	-0.17036	0.87545	0.03911	0.0680*
H15A	0.24886	0.89746	0.14035	0.0540*
H16A	1.11764	0.69130	0.45069	0.1240*
H16B	1.00432	0.81587	0.41282	0.1240*
H16C	0.95044	0.64175	0.42628	0.1240*
H17A	1.28064	0.40096	0.20705	0.1000*
H17B	1.11330	0.35669	0.17988	0.1000*

H17C 1.18073 0.51778 0.15799 0.1000*

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

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0650 (3)	0.0704 (3)	0.0809 (3)	0.0083 (2)	0.0216 (2)	−0.0176 (2)
O1	0.0518 (6)	0.0735 (7)	0.0440 (5)	0.0124 (5)	−0.0028 (4)	−0.0031 (5)
O2	0.0487 (6)	0.0881 (8)	0.0518 (6)	0.0278 (5)	0.0039 (4)	−0.0044 (5)
O3	0.0479 (6)	0.0898 (8)	0.0505 (6)	0.0088 (5)	0.0038 (4)	−0.0226 (6)
C1	0.0400 (6)	0.0500 (7)	0.0472 (7)	0.0080 (5)	0.0064 (5)	−0.0052 (5)
C2	0.0462 (7)	0.0506 (7)	0.0420 (6)	0.0063 (5)	0.0074 (5)	−0.0069 (5)
C3	0.0425 (6)	0.0424 (6)	0.0398 (6)	0.0012 (5)	0.0028 (5)	0.0021 (5)
C4	0.0382 (6)	0.0423 (6)	0.0441 (6)	0.0057 (5)	0.0073 (5)	0.0033 (5)
C5	0.0404 (6)	0.0425 (6)	0.0396 (6)	0.0032 (5)	0.0093 (5)	−0.0010 (5)
C6	0.0382 (6)	0.0393 (5)	0.0403 (6)	0.0007 (4)	0.0057 (4)	−0.0005 (4)
C7	0.0384 (6)	0.0510 (7)	0.0434 (6)	0.0014 (5)	0.0055 (5)	−0.0046 (5)
C8	0.0426 (6)	0.0562 (8)	0.0476 (7)	0.0070 (6)	0.0014 (5)	−0.0090 (6)
C9	0.0424 (6)	0.0539 (7)	0.0388 (6)	0.0028 (5)	0.0050 (5)	−0.0017 (5)
C10	0.0401 (6)	0.0469 (6)	0.0384 (6)	−0.0001 (5)	0.0011 (5)	0.0006 (5)
C11	0.0493 (7)	0.0603 (8)	0.0449 (7)	0.0006 (6)	−0.0014 (6)	−0.0093 (6)
C12	0.0468 (8)	0.0733 (10)	0.0568 (8)	−0.0030 (7)	−0.0092 (6)	−0.0092 (7)
C13	0.0379 (6)	0.0642 (9)	0.0643 (9)	0.0002 (6)	−0.0002 (6)	0.0022 (7)
C14	0.0452 (7)	0.0445 (6)	0.0519 (7)	−0.0005 (5)	0.0094 (5)	0.0004 (5)
C15	0.0419 (6)	0.0476 (6)	0.0427 (6)	−0.0022 (5)	0.0016 (5)	−0.0030 (5)
C16	0.0814 (12)	0.1149 (17)	0.0452 (8)	0.0267 (12)	−0.0080 (8)	−0.0161 (10)
C17	0.0583 (9)	0.0781 (11)	0.0673 (10)	0.0238 (8)	0.0189 (8)	−0.0001 (8)

Geometric parameters ($\text{\AA}$, $^\circ$)

C11—C14	1.7310 (15)	C12—C13	1.374 (2)
O1—C3	1.3570 (16)	C13—C14	1.376 (2)
O1—C16	1.422 (2)	C14—C15	1.376 (2)
O2—C4	1.3593 (17)	C1—H1A	0.9300
O2—C17	1.408 (2)	C2—H2A	0.9300
O3—C7	1.2273 (18)	C5—H5A	0.9300
C1—C2	1.387 (2)	C8—H8A	0.9300
C1—C6	1.3832 (18)	C9—H9A	0.9300
C2—C3	1.3794 (19)	C11—H11A	0.9300
C3—C4	1.4088 (17)	C12—H12A	0.9300
C4—C5	1.3698 (17)	C13—H13A	0.9300
C5—C6	1.4041 (17)	C15—H15A	0.9300
C6—C7	1.4792 (18)	C16—H16A	0.9600
C7—C8	1.4810 (19)	C16—H16B	0.9600
C8—C9	1.3241 (19)	C16—H16C	0.9600
C9—C10	1.4643 (19)	C17—H17A	0.9600
C10—C11	1.3884 (19)	C17—H17B	0.9600
C10—C15	1.4005 (19)	C17—H17C	0.9600
C11—C12	1.382 (2)		

C3—O1—C16	117.66 (12)	C6—C1—H1A	120.00
C4—O2—C17	118.77 (12)	C1—C2—H2A	120.00
C2—C1—C6	120.98 (13)	C3—C2—H2A	120.00
C1—C2—C3	119.94 (13)	C4—C5—H5A	120.00
O1—C3—C2	124.80 (12)	C6—C5—H5A	120.00
O1—C3—C4	115.43 (11)	C7—C8—H8A	119.00
C2—C3—C4	119.77 (12)	C9—C8—H8A	119.00
O2—C4—C3	114.38 (11)	C8—C9—H9A	116.00
O2—C4—C5	125.88 (12)	C10—C9—H9A	117.00
C3—C4—C5	119.72 (12)	C10—C11—H11A	120.00
C4—C5—C6	120.80 (11)	C12—C11—H11A	120.00
C1—C6—C5	118.76 (11)	C11—C12—H12A	120.00
C1—C6—C7	122.74 (11)	C13—C12—H12A	120.00
C5—C6—C7	118.45 (11)	C12—C13—H13A	121.00
O3—C7—C6	120.42 (12)	C14—C13—H13A	121.00
O3—C7—C8	120.14 (13)	C10—C15—H15A	120.00
C6—C7—C8	119.40 (12)	C14—C15—H15A	120.00
C7—C8—C9	121.08 (13)	O1—C16—H16A	109.00
C8—C9—C10	127.00 (13)	O1—C16—H16B	109.00
C9—C10—C11	118.76 (12)	O1—C16—H16C	109.00
C9—C10—C15	122.38 (12)	H16A—C16—H16B	109.00
C11—C10—C15	118.81 (12)	H16A—C16—H16C	109.00
C10—C11—C12	120.58 (14)	H16B—C16—H16C	109.00
C11—C12—C13	120.63 (15)	O2—C17—H17A	109.00
C12—C13—C14	118.77 (14)	O2—C17—H17B	109.00
C11—C14—C13	118.53 (11)	O2—C17—H17C	109.00
C11—C14—C15	119.45 (11)	H17A—C17—H17B	109.00
C13—C14—C15	122.00 (13)	H17A—C17—H17C	110.00
C10—C15—C14	119.21 (13)	H17B—C17—H17C	109.00
C2—C1—H1A	120.00		
C16—O1—C3—C2	7.7 (2)	C1—C6—C7—C8	3.84 (19)
C16—O1—C3—C4	-171.77 (15)	C5—C6—C7—O3	3.5 (2)
C17—O2—C4—C3	178.44 (13)	C5—C6—C7—C8	-178.75 (12)
C17—O2—C4—C5	0.3 (2)	O3—C7—C8—C9	10.5 (2)
C6—C1—C2—C3	-0.5 (2)	C6—C7—C8—C9	-167.28 (13)
C2—C1—C6—C5	-1.0 (2)	C7—C8—C9—C10	175.76 (13)
C2—C1—C6—C7	176.44 (13)	C8—C9—C10—C11	-175.75 (15)
C1—C2—C3—O1	-177.65 (13)	C8—C9—C10—C15	1.6 (2)
C1—C2—C3—C4	1.8 (2)	C9—C10—C11—C12	177.04 (14)
O1—C3—C4—O2	-0.40 (17)	C15—C10—C11—C12	-0.4 (2)
O1—C3—C4—C5	177.86 (12)	C9—C10—C15—C14	-176.57 (13)
C2—C3—C4—O2	-179.87 (12)	C11—C10—C15—C14	0.8 (2)
C2—C3—C4—C5	-1.60 (19)	C10—C11—C12—C13	-0.2 (2)
O2—C4—C5—C6	178.20 (13)	C11—C12—C13—C14	0.4 (2)
C3—C4—C5—C6	0.2 (2)	C12—C13—C14—C11	-178.21 (12)
C4—C5—C6—C1	1.13 (19)	C12—C13—C14—C15	0.0 (2)

C4—C5—C6—C7	-176.39 (12)	C11—C14—C15—C10	177.64 (10)
C1—C6—C7—O3	-173.88 (14)	C13—C14—C15—C10	-0.6 (2)

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<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>
C9—H9 <i>A</i> $\cdots$ O3	0.93	2.45	2.7888 (18)	102
C11—H11 <i>A</i> $\cdots$ O3 ⁱ	0.93	2.54	3.417 (2)	157
C15—H15 <i>A</i> $\cdots$ O2 ⁱⁱ	0.93	2.54	3.4378 (18)	163

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

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