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(2*E*)-1-(2,4-Dichlorophenyl)-3-[4-(diethylamino)-2-hydroxyphenyl]prop-2-en-1-one

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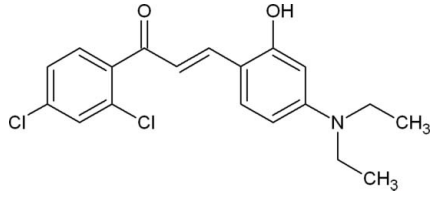
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.046; wR factor = 0.149; data-to-parameter ratio = 28.7.

In the title molecule, $C_{19}H_{19}Cl_2NO_2$, the angle between the mean planes of the 2,4-dichlorophenyl and 2-hydroxyphenyl groups is 81.8 (2)°. The ketone oxygen of the prop-2-en-1-one group is twisted in a synclinal conformation with the 2,4-dichlorophenyl group [torsion angle = −75.7 (2)°]. The two diethyl extensions from the 4-(diethylamino)-2-hydroxyphenyl group are twisted in *anti*- and *syn*-periplanar conformations. Crystal packing is stabilized by intermolecular C—H···O hydrogen bonding between the ketone O atom from the prop-2-en-1-one group and H atoms from both the 2-hydroxyphenyl ring and the hydroxy group; these hydrogen bonds link the molecules into chains along the diagonal of the *bc* face of the unit cell. The 2-hydroxyphenyl rings are stacked obliquely parallel to the *ab* face while the 2,4-dichlorophenyl rings are stacked obliquely parallel to the *bc* face of the unit cell, each in an inverted conformation. Additional intermolecular packing interactions occur between π orbitals of the 4-hydroxyphenyl ring and an H atom from a nearby 2,4-dichlorophenyl ring.

Related literature

For related structures, see: Sarojini *et al.* (2007); Yathirajan *et al.* (2007*a*,*b*,*c*,*d*,*e*). For related literature, see: Goto *et al.* (1991); Indira *et al.* (2002); Lawrence *et al.* (2001); Pandey *et al.* (2005); Sarojini *et al.* (2006).



Experimental

Crystal data

$C_{19}H_{19}Cl_2NO_2$
M_r = 364.25
Monoclinic, $P2_1/n$
a = 10.6129 (5) Å
b = 13.9570 (7) Å
c = 12.6858 (6) Å
β = 106.012 (5)°
V = 1806.17 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.37 mm^{-1}
T = 296 K
0.51 × 0.35 × 0.21 mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.721, T_{max} = 1.000 (expected range = 0.667–0.925)
19547 measured reflections
6017 independent reflections
1867 reflections with $I > 2\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.149
S = 0.83
6017 reflections
210 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

*Cg*2 is the centroid of the C10–C15 ring.

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2*A*···O1^{i}	0.82	1.94	2.751 (2)	173
C12—H12*A*···O1^{i}	0.93	2.50	3.205 (3)	132
C6—H6*A*···*Cg*2^{ii}	0.93	2.83	3.739(1)	166

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

Data collection: *CrysAlisPro* (Oxford Diffraction, 2007); cell refinement: *CrysAlisPro*; data reduction: *CrysAlisPro*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); 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: AT2413).

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supplementary materials

Acta Cryst. (2007). E**63**, o4231-o4232 [**doi:10.1107/S1600536807047666**]

(2*E*)-1-(2,4-Dichlorophenyl)-3-[4-(diethylamino)-2-hydroxyphenyl]prop-2-en-1-one

J. P. Jasinski, R. J. Butcher, A. N. Mayekar, B. Narayana and H. S. Yathirajan

Comment

Chalcones are a class of naturally occurring compounds with various biological activities. They are known as the precursors of all flavonoid type natural products in biosynthesis. Chalcones can be easily obtained from the aldol condensation of aromatic aldehydes and aromatic ketones. This class of compounds presents interesting biological properties such as cytotoxicity (Pandey *et al.* 2005), antiherpes, and antitumour activity and may be useful for the chemotherapy of leishmaniasis among others (Lawrence *et al.* 2001). Chalcone derivatives are recognized for NLO properties and have good crystallization ability (Goto *et al.* 1991; Indira *et al.* 2002; Sarojini *et al.* 2006). Structures of few dichloro substituted chalcones *viz*., (2E)-1-(2,4-dichlorophenyl)-3-(quinolin-8-yl)prop-2-en-1-one (Sarojini *et al.* 2007), (2E)-1-(2,4-dichlorophenyl)-3-(4,5-dimethoxy-2-nitrophenyl) prop-2-en-1-one (Yathirajan *et al.* 2007*a*), (2E)-1-(2,4-dichlorophenyl)-3-(6-methoxy-2-naphthyl)prop-2-en-1-one (Yathirajan *et al.* 2007*b*), (2E)-1-(2,4-dichlorophenyl)-3-(2-hydroxy-3-methoxyphenyl) prop-2-en-1-one (Yathirajan *et al.* 2007*c*), (2E)-1-(2,4-dichlorophenyl)-3-(4-nitrophenyl)prop-2-en-1-one (Yathirajan *et al.* 2007 d), (2E)-1-(2,4-dichlorophenyl)-3-(2-hydroxyphenyl)prop-2-en-1-one (Yathirajan *et al.* 2007 e) have been published. In continuation of our work on chalcones, a new chalcone, (I), $C_{19}H_{19}Cl_4O_2$ has been synthesized and its crystal structure is reported.

The angle between the mean planes of the 2,4-dichlorolphenyl and 2-hydroxyphenyl groups is 81.8 (2)° (Fig. 1). The ketone oxygen of the prop-2-en-1-one group is twisted in a *syn*-clinal conformation with the 2,4-dichlorophenyl group [C2–C1–C7–O1 torsion angle = −75.7 (2)°]. The two diethyl extensions from the 4-(diethylamino)-2-hydroxyphenyl group are twisted in an *anti*- [C12–C13–N–C18 = −174.65 (17)°] and *syn*- [C2–C13—N–C16 = 3.3 (3)°] periplanar conformation. Crystal packing is stabilized by intermolecular C—H···O hydrogen bonding between the ketone oxygen (O1) from the prop-2-en-1-one group and hydrogen atoms from both the 2-hydroxyl phenyl ring (H12A) and the hydroxyl group (H2A) which link the molecules into chains diagonal along the *bc* face of the unit cell (Fig. 2). The 2-hydroxypheny rings are stacked obliquely parallel to the *ab* face while the 2,4-dichlorolphenyl rings are stacked obliquely parallel to the *bc* face, respectively, of the unit cell, each in an inverted conformation. Additional intermolecular packing interactions occur between *Cg*2-π orbitals of the 4-hydroxyphenyl ring and H6A from a nearby 2,4-dichlorolphenyl ring. [*Cg*2 - center of gravity, C10–C15; C6–H6A···*Cg*(2) = 2.83Å (1 − *x*, 1 − *y*, 1 − *z*)].

Experimental

4-(Diethylamino)-2-hydroxybenzaldehyde (1.93 g, 0.01 mol) in ethanol (25 ml) was mixed with 1-(2,4-dichlorophenyl)ethanone (1.89 g, 0.01 mol) in ethanol (25 ml) and the mixture was treated with 10 ml of 10% KOH solution (Fig. 3). The reaction mixture was then kept for constant stirring. The solid precipitate obtained was filtered, washed with ethanol and dried. Crystal growth was carried out from a 1:1 mixture of acetone and toluene by the slow evaporation technique (m.p.: 427–429 K). Analysis found: C 62.58, H 5.22, N 3.18%; $C_{19}H_{19}Cl_4O_2$ requires: C 62.65, H 5.26, N 3.85%.

Refinement

The hydroxyl atom (H2A) was located in a difference Fourier map and along with all other all other H atoms placed in their calculated positions were then refined using the riding model with O—H = 0.82Å and C—H = 0.93 to 0.97 Å, and with U_{iso}(H) = 1.19–1.50U_{eq}(C, O).

Figures

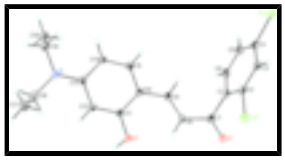

Fig. 1. Molecular structure of the title compound, showing atom labeling and 50% probability displacement ellipsoids.

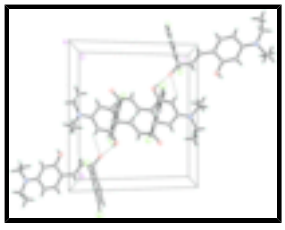

Fig. 2. Packing diagram of the title compound, viewed down the *b* axis.

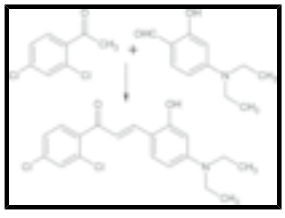

Fig. 3. Synthetic scheme for $C_{19}H_{19}Cl_4O_2$.

(2E)-1-(2,4-Dichlorophenyl)-3-[4-(diethylamino)-2-hydroxyphenyl]prop-2-en-1-one

Crystal data

$C_{19}H_{19}Cl_2NO_2$	F_{000} = 760
M_r = 364.25	D_x = 1.340 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 3455 reflections
a = 10.6129 (5) Å	θ = 4.6–32.5º
b = 13.9570 (7) Å	μ = 0.37 mm^{-1}
c = 12.6858 (6) Å	*T* = 296 K
β = 106.012 (5)º	Chunk, yellow
V = 1806.17 (15) Å^3	0.51 × 0.35 × 0.21 mm
Z = 4	

Data collection

Oxford Diffraction Gemini R CCD diffractometer	6017 independent reflections

Radiation source: fine-focus sealed tube
Monochromator: graphite
Detector resolution: 10.5081 pixels mm^{-1}
T = 296 K
φ and ω scans
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)
T_{min} = 0.721, T_{max} = 1.000
19547 measured reflections
1867 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
θ_{max} = 32.5º
θ_{min} = 4.6º
h = −15→13
k = −20→12
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.149
S = 0.83
6017 reflections
210 parameters
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
$w = 1/[\sigma^2(F_o^2) + (0.0576P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.34 e $Å^{-3}$
$\Delta\rho_{min}$ = −0.27 e $Å^{-3}$
Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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 ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.45137 (6)	0.16227 (5)	0.89389 (6)	0.0833 (2)
Cl2	0.34504 (7)	−0.20410 (5)	0.78456 (5)	0.0877 (3)
O1	0.70872 (15)	0.19447 (12)	0.79693 (12)	0.0708 (5)
O2	1.01216 (14)	0.20094 (11)	1.15772 (12)	0.0671 (4)
H2A	1.0729	0.2332	1.1947	0.081*
N	1.15746 (18)	−0.00593 (14)	1.46912 (14)	0.0704 (6)
C1	0.62657 (19)	0.04520 (16)	0.83812 (14)	0.0521 (5)
C2	0.5016 (2)	0.05425 (16)	0.85143 (15)	0.0546 (5)
C3	0.4148 (2)	−0.02179 (16)	0.83333 (16)	0.0597 (6)

H3A	0.3315	−0.0143	0.8427	0.072*
C4	0.4530 (2)	−0.10837 (16)	0.80141 (16)	0.0600 (6)
C5	0.5745 (2)	−0.11972 (18)	0.78363 (17)	0.0681 (7)
H5A	0.5984	−0.1778	0.7589	0.082*
C6	0.6597 (2)	−0.04327 (18)	0.80330 (17)	0.0662 (7)
H6A	0.7425	−0.0511	0.7929	0.079*
C7	0.7233 (2)	0.12748 (16)	0.86219 (17)	0.0544 (5)
C8	0.8254 (2)	0.12713 (16)	0.96368 (16)	0.0563 (6)
H8A	0.8793	0.1807	0.9817	0.068*
C9	0.84670 (18)	0.05259 (16)	1.03407 (15)	0.0518 (5)
H9A	0.7955	−0.0010	1.0082	0.062*
C10	0.93474 (17)	0.04148 (15)	1.14228 (15)	0.0496 (5)
C11	1.01176 (18)	0.11466 (14)	1.20542 (16)	0.0469 (5)
C12	1.08461 (18)	0.09849 (15)	1.31272 (16)	0.0541 (5)
H12A	1.1324	0.1487	1.3528	0.065*
C13	1.08816 (19)	0.00860 (16)	1.36241 (16)	0.0563 (6)
C14	1.0175 (2)	−0.06473 (16)	1.29886 (18)	0.0608 (6)
H14A	1.0213	−0.1262	1.3279	0.073*
C15	0.94212 (19)	−0.04778 (16)	1.19390 (17)	0.0577 (5)
H15A	0.8934	−0.0982	1.1550	0.069*
C16	1.2275 (3)	0.0739 (2)	1.5403 (2)	0.0884 (8)
H16A	1.1798	0.1332	1.5188	0.106*
H16B	1.2302	0.0608	1.6160	0.106*
C17	1.3600 (3)	0.0848 (2)	1.5315 (3)	0.1107 (10)*
H17A	1.4006	0.1389	1.5743	0.166*
H17B	1.3577	0.0948	1.4561	0.166*
H17C	1.4094	0.0279	1.5582	0.166*
C18	1.1709 (3)	−0.10152 (18)	1.51721 (19)	0.0753 (7)
H18A	1.0860	−0.1328	1.4957	0.090*
H18B	1.1961	−0.0952	1.5964	0.090*
C19	1.2693 (3)	−0.1652 (2)	1.4854 (2)	0.0872 (8)*
H19A	1.2676	−0.2277	1.5165	0.131*
H19B	1.3554	−0.1382	1.5126	0.131*
H19C	1.2476	−0.1701	1.4070	0.131*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0783 (4)	0.0719 (5)	0.1067 (5)	0.0181 (3)	0.0374 (4)	−0.0113 (4)
Cl2	0.0944 (5)	0.0696 (5)	0.0860 (5)	−0.0061 (3)	0.0031 (4)	0.0063 (3)
O1	0.0686 (10)	0.0764 (11)	0.0587 (9)	0.0064 (8)	0.0028 (7)	0.0122 (8)
O2	0.0614 (10)	0.0628 (10)	0.0622 (9)	−0.0036 (7)	−0.0081 (7)	0.0075 (8)
N	0.0764 (13)	0.0731 (14)	0.0481 (11)	−0.0049 (10)	−0.0053 (9)	0.0078 (9)
C1	0.0424 (11)	0.0711 (15)	0.0395 (10)	0.0132 (10)	0.0058 (8)	−0.0009 (10)
C2	0.0569 (13)	0.0585 (14)	0.0441 (11)	0.0119 (11)	0.0069 (9)	−0.0005 (9)
C3	0.0518 (12)	0.0699 (17)	0.0556 (13)	0.0125 (12)	0.0121 (10)	0.0092 (11)
C4	0.0647 (15)	0.0605 (15)	0.0459 (11)	0.0129 (11)	0.0001 (10)	0.0009 (10)
C5	0.0715 (17)	0.0655 (16)	0.0595 (14)	0.0177 (13)	0.0053 (11)	−0.0137 (11)

C6	0.0522 (13)	0.0813 (18)	0.0622 (14)	0.0261 (12)	0.0110 (11)	−0.0120 (12)
C7	0.0459 (12)	0.0675 (15)	0.0477 (12)	0.0085 (10)	0.0096 (9)	−0.0007 (11)
C8	0.0472 (12)	0.0684 (15)	0.0486 (12)	0.0012 (10)	0.0055 (9)	−0.0015 (10)
C9	0.0408 (11)	0.0612 (14)	0.0506 (12)	0.0021 (9)	0.0078 (9)	−0.0052 (10)
C10	0.0381 (10)	0.0568 (14)	0.0498 (12)	0.0081 (9)	0.0052 (9)	−0.0019 (10)
C11	0.0389 (10)	0.0479 (13)	0.0514 (11)	0.0088 (9)	0.0081 (9)	0.0030 (9)
C12	0.0459 (12)	0.0616 (15)	0.0497 (12)	0.0006 (10)	0.0048 (9)	−0.0018 (10)
C13	0.0492 (12)	0.0661 (15)	0.0487 (12)	0.0041 (10)	0.0054 (9)	0.0054 (10)
C14	0.0578 (13)	0.0545 (14)	0.0623 (13)	0.0012 (11)	0.0035 (11)	0.0120 (11)
C15	0.0489 (12)	0.0561 (14)	0.0624 (13)	0.0016 (10)	0.0059 (10)	−0.0007 (11)
C16	0.0817 (19)	0.108 (2)	0.0698 (16)	0.0169 (16)	0.0122 (14)	0.0233 (15)
C18	0.0792 (17)	0.0818 (19)	0.0589 (14)	0.0060 (13)	0.0091 (12)	0.0192 (12)

Geometric parameters (Å, °)

Cl1—C2	1.734 (2)	C9—H9A	0.9300
Cl2—C4	1.734 (2)	C10—C15	1.400 (3)
O1—C7	1.230 (2)	C10—C11	1.411 (3)
O2—C11	1.348 (2)	C11—C12	1.386 (3)
O2—H2A	0.8200	C12—C13	1.400 (3)
N—C13	1.366 (2)	C12—H12A	0.9300
N—C18	1.458 (3)	C13—C14	1.388 (3)
N—C16	1.496 (3)	C14—C15	1.371 (3)
C1—C2	1.388 (3)	C14—H14A	0.9300
C1—C6	1.389 (3)	C15—H15A	0.9300
C1—C7	1.514 (3)	C16—C17	1.448 (4)
C2—C3	1.382 (3)	C16—H16A	0.9700
C3—C4	1.371 (3)	C16—H16B	0.9700
C3—H3A	0.9300	C17—H17A	0.9600
C4—C5	1.378 (3)	C17—H17B	0.9600
C5—C6	1.377 (3)	C17—H17C	0.9600
C5—H5A	0.9300	C18—C19	1.508 (3)
C6—H6A	0.9300	C18—H18A	0.9700
C7—C8	1.436 (3)	C18—H18B	0.9700
C8—C9	1.349 (3)	C19—H19A	0.9600
C8—H8A	0.9300	C19—H19B	0.9600
C9—C10	1.440 (3)	C19—H19C	0.9600
C11—O2—H2A	109.5	C11—C12—C13	121.78 (19)
C13—N—C18	120.97 (19)	C11—C12—H12A	119.1
C13—N—C16	121.99 (19)	C13—C12—H12A	119.1
C18—N—C16	116.99 (18)	N—C13—C14	121.5 (2)
C2—C1—C6	117.0 (2)	N—C13—C12	121.31 (19)
C2—C1—C7	121.58 (19)	C14—C13—C12	117.15 (18)
C6—C1—C7	121.43 (19)	C15—C14—C13	120.9 (2)
C3—C2—C1	121.7 (2)	C15—C14—H14A	119.5
C3—C2—Cl1	118.13 (17)	C13—C14—H14A	119.5
C1—C2—Cl1	120.19 (17)	C14—C15—C10	123.4 (2)
C4—C3—C2	119.2 (2)	C14—C15—H15A	118.3
C4—C3—H3A	120.4	C10—C15—H15A	118.3

C2—C3—H3A	120.4	C17—C16—N	111.3 (2)
C3—C4—C5	121.0 (2)	C17—C16—H16A	109.4
C3—C4—Cl2	118.46 (19)	N—C16—H16A	109.4
C5—C4—Cl2	120.49 (18)	C17—C16—H16B	109.4
C6—C5—C4	118.6 (2)	N—C16—H16B	109.4
C6—C5—H5A	120.7	H16A—C16—H16B	108.0
C4—C5—H5A	120.7	C16—C17—H17A	109.5
C5—C6—C1	122.4 (2)	C16—C17—H17B	109.5
C5—C6—H6A	118.8	H17A—C17—H17B	109.5
C1—C6—H6A	118.8	C16—C17—H17C	109.5
O1—C7—C8	122.0 (2)	H17A—C17—H17C	109.5
O1—C7—C1	119.24 (17)	H17B—C17—H17C	109.5
C8—C7—C1	118.71 (19)	N—C18—C19	115.0 (2)
C9—C8—C7	122.9 (2)	N—C18—H18A	108.5
C9—C8—H8A	118.6	C19—C18—H18A	108.5
C7—C8—H8A	118.6	N—C18—H18B	108.5
C8—C9—C10	131.3 (2)	C19—C18—H18B	108.5
C8—C9—H9A	114.3	H18A—C18—H18B	107.5
C10—C9—H9A	114.3	C18—C19—H19A	109.5
C15—C10—C11	115.45 (17)	C18—C19—H19B	109.5
C15—C10—C9	118.67 (19)	H19A—C19—H19B	109.5
C11—C10—C9	125.80 (19)	C18—C19—H19C	109.5
O2—C11—C12	121.08 (18)	H19A—C19—H19C	109.5
O2—C11—C10	117.69 (16)	H19B—C19—H19C	109.5
C12—C11—C10	121.22 (19)		
C6—C1—C2—C3	1.4 (3)	C15—C10—C11—O2	177.35 (18)
C7—C1—C2—C3	−177.62 (18)	C9—C10—C11—O2	−5.9 (3)
C6—C1—C2—Cl1	−179.63 (15)	C15—C10—C11—C12	−2.6 (3)
C7—C1—C2—Cl1	1.3 (3)	C9—C10—C11—C12	174.15 (19)
C1—C2—C3—C4	0.0 (3)	O2—C11—C12—C13	−178.17 (19)
Cl1—C2—C3—C4	−178.97 (15)	C10—C11—C12—C13	1.8 (3)
C2—C3—C4—C5	−2.2 (3)	C18—N—C13—C14	6.4 (3)
C2—C3—C4—Cl2	177.41 (15)	C16—N—C13—C14	−176.3 (2)
C3—C4—C5—C6	2.9 (3)	C18—N—C13—C12	−174.1 (2)
Cl2—C4—C5—C6	−176.74 (16)	C16—N—C13—C12	3.1 (3)
C4—C5—C6—C1	−1.4 (3)	C11—C12—C13—N	−178.2 (2)
C2—C1—C6—C5	−0.7 (3)	C11—C12—C13—C14	1.3 (3)
C7—C1—C6—C5	178.32 (19)	N—C13—C14—C15	176.1 (2)
C2—C1—C7—O1	−75.2 (3)	C12—C13—C14—C15	−3.4 (3)
C6—C1—C7—O1	105.8 (2)	C13—C14—C15—C10	2.6 (4)
C2—C1—C7—C8	101.6 (2)	C11—C10—C15—C14	0.5 (3)
C6—C1—C7—C8	−77.4 (3)	C9—C10—C15—C14	−176.5 (2)
O1—C7—C8—C9	−177.0 (2)	C13—N—C16—C17	−88.9 (3)
C1—C7—C8—C9	6.3 (3)	C18—N—C16—C17	88.5 (3)
C7—C8—C9—C10	−173.9 (2)	C13—N—C18—C19	77.2 (3)
C8—C9—C10—C15	−175.7 (2)	C16—N—C18—C19	−100.2 (3)
C8—C9—C10—C11	7.7 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2A···O1^{i}	0.82	1.94	2.751 (2)	173
C12—H12A···O1^{i}	0.93	2.50	3.205 (3)	132

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

Fig. 1

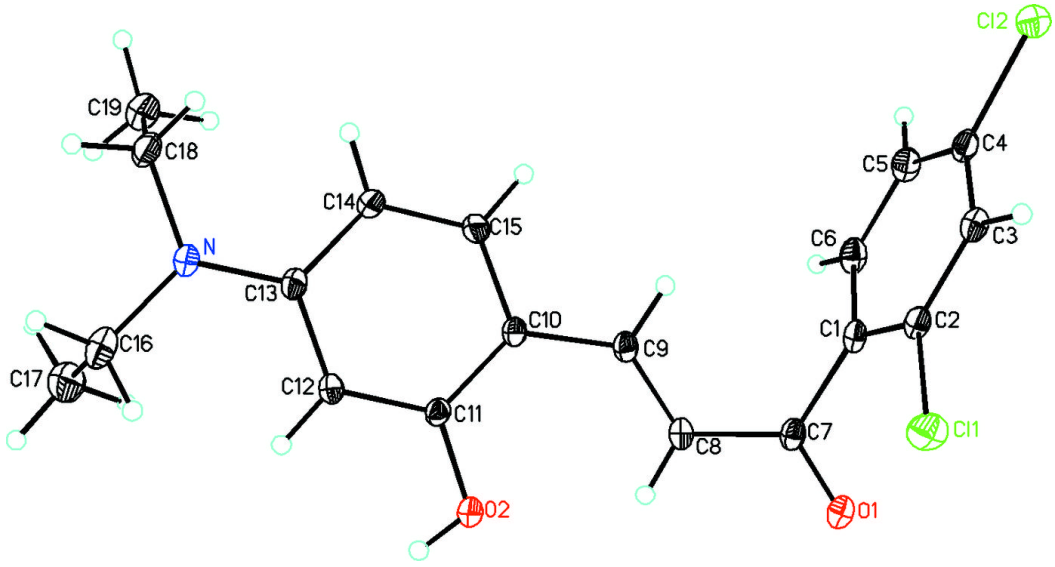
Cl2
C19
C18
C4
C5
C14
C15
C3
C6
N
C13
C10
C9
C1
C2
C16
C17
C12
C11
C8
C7
Cl1
O2
O1

Fig. 2

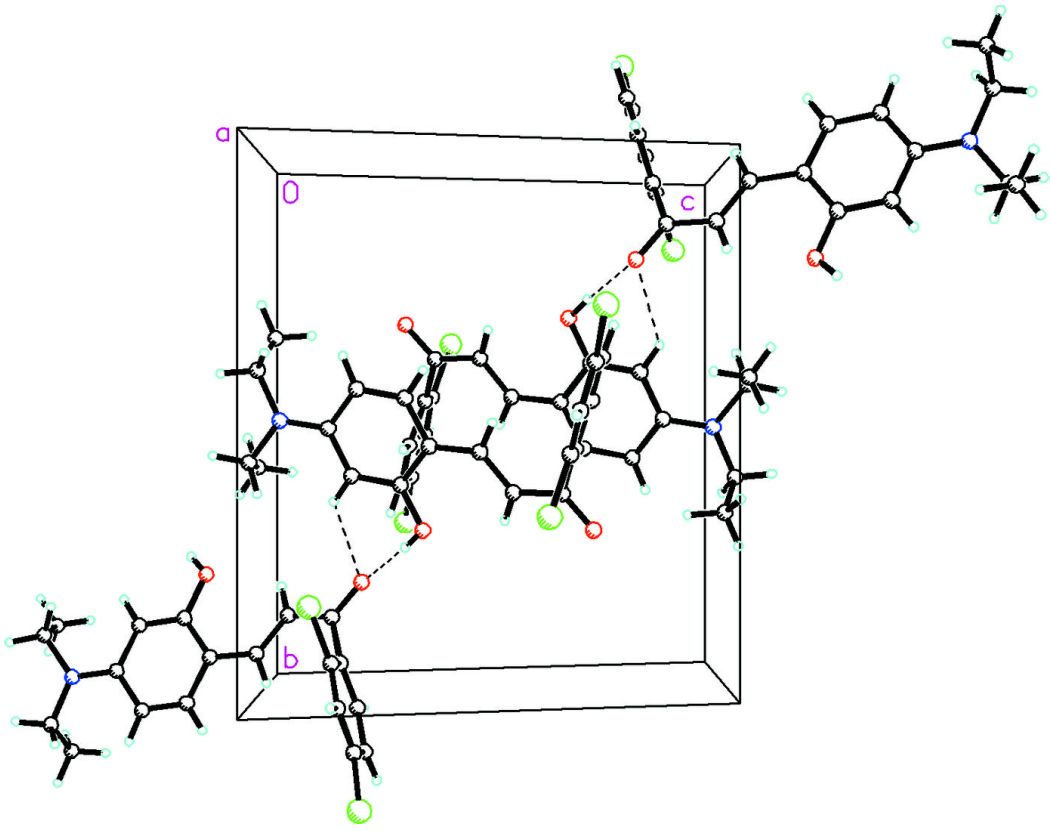

Fig. 3