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2-[(*Z*)-(2,5-Dichlorophenyl)iminomethyl]-5-(diethylamino)phenol

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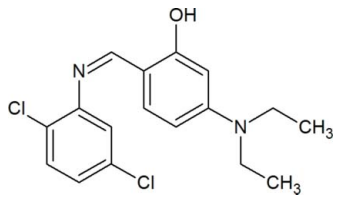
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.120; data-to-parameter ratio = 27.2.

In the title molecule, $C_{17}H_{18}Cl_2N_2O$, the angle between the mean planes of the 2,5-dichlorophenylimino and phenol groups is 19.5 (5)°. The two ethyl groups adopt a synclinal conformation. The crystal structure is stabilized by intermolecular π–π stacking interactions between adjacent 2,5-dichlorophenyl rings, the distance between the centroids of interacting rings being 3.860 (8) Å. The molecules are stacked parallel to the *a* axis. In addition, an O—H···N intramolecular hydrogen-bonding interaction between the phenol H atom and imino N atom is observed.

Related literature

For related structures, see: Büyükgüngör *et al.* (2007); Odabaşoğlu *et al.* (2007); Yathirajan *et al.* (2007); Butcher *et al.* (2007). For related literature, see: Hodnett & Dunn (1970); Misra *et al.* (1981); Agarwal *et al.* (1983); Varma *et al.* (1986); Singh & Dash (1988); Pandey *et al.* (1999); El-Masry *et al.* (2000); Samadhiya & Halve (2001); Siddiqui *et al.* (2006).



Experimental

Crystal data

$C_{17}H_{18}Cl_2N_2O$
M_r = 337.23
Monoclinic, $P2_1/c$
a = 7.1729 (2) Å
b = 18.6396 (6) Å
c = 12.6378 (4) Å
β = 104.157 (3)°
V = 1638.36 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.40 mm^{-1}
T = 296 K
0.53 × 0.25 × 0.19 mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.720, T_{max} = 0.927
17605 measured reflections
5491 independent reflections
2626 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.120
S = 0.98
5491 reflections
202 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1O···N1	0.82	1.89	2.6139 (16)	147

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: FJ2061).

References

Agarwal, R., Chaudhary, K. C. & Misra, V. S. (1983). *Indian J. Chem. Sect. B*, **22**, 308–310.
Bruker (2000). *SHELXTL*. Version 6.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Butcher, R. J., Jasinski, J. P., Yathirajan, H. S., Vijesh, A. M. & Narayana, B. (2007). *Acta Cryst.* E**63**, o3748.
Büyükgüngör, O., Odabaşoğlu, M., Narayana, B., Vijesh, A. M. & Yathirajan, H. S. (2007). *Acta Cryst.* E**63**, o1996–o1998.
El-Masry, A. H., Fahmy, H. H. & Abdelwahed, S. H. A. (2000). *Molecules*, **5**, 1429–1438.
Hodnett, E. M. & Dunn, W. J. (1970). *J. Med. Chem.* **13**, 768–770.
Misra, V. S., Singh, S., Agarwal, R. & Chaudhary, K. C. (1981). *J. Chem. Soc. Pak.* **3**, 209–213.
Odabaşoğlu, M., Büyükgüngör, O., Narayana, B., Vijesh, A. M. & Yathirajan, H. S. (2007). *Acta Cryst.* E**63**, o1916–o1918.
Oxford Diffraction (2007). *CrysAlisPro* (Version 171.31.8) and *CrysAlis RED* (Version 1.171.31.8). Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
Pandey, S. N., Sriram, D., Nath, G. & De Clercq, E. (1999). *Il Farmaco*, **54**, 624–628.
Samadhiya, S. & Halve, A. (2001). *Orient. J. Chem.* **17**, 119–122.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Siddiqui, H. L., Iqbal, A., Ahmad, S. & Weaver, G. W. (2006). *Molecules*, **11**, 206–211.

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Singh, W. M. & Dash, B. C. (1988). *Pesticides*, **22**, 33–37.
Varma, R. S., Prakash, R., Khan, M. M. & Ali, A. (1986). *Indian Drugs*, **23**, 345–349.
Yathirajan, H. S., Vijesh, A. M., Narayana, B., Sarojini, B. K. & Bolte, M. (2007). *Acta Cryst.* E**63**, o936–o938.

supplementary materials

Acta Cryst. (2007). E**63**, o4592-o4593 [**doi:10.1107/S1600536807055791**]

2-[(*Z*)-(2,5-Dichlorophenyl)iminomethyl]-5-(diethylamino)phenol

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Comment

Schiff bases are synthesized from an aromatic amine and a carbonyl compound by a nucleophilic addition reaction. They are used as substrates in the preparation of number of biologically active compounds (Siddiqui *et al.*, 2006). Some Schiff base derivatives are also known to have activities such as antimicrobial (El-Masry *et al.*, 2000; Pandey *et al.*, 1999), antifungal (Singh & Dash, 1988; Varma *et al.*, 1986), antitumor (Hodnett & Dunn, 1970; Misra *et al.*, 1981; Agarwal *et al.*, 1983) and as herbicides (Samadhiya & Halve, 2001). The crystal structures of (*E*)-2-hydroxy-5-methyl-3-[(4-methyl-2 pyridyl)iminomethyl] benzaldehyde (Büyükgüngör *et al.*, 2007), (*E*)-2-hydroxy-5-methyl-3-[(2-pyridylimino) methyl]benzaldehyde (Odabaşoğlu *et al.*, 2007), 1-(4-{[(*E*)-(4-diethylamino-2-hydroxy phenyl)methylene]amino} phenyl)ethanone (Yathirajan *et al.*, (2007), 2-{(*E*)-[(2-chloro-5-nitrophenyl)imino]methyl}-5-(diethylamino)phenol (Butcher *et al.*, 2007) have been reported. A new Schiff base, (I), $C_{17}H_{18}Cl_2N_2O$ is prepared and its crystal structure is reported.

The angle between the mean planes of the 2,5-dichlorophenyl-imino and phenol groups is 19.5 (5)° Fig. 1). The two ethyl groups adopt a *syn*-clinal conformation [C11—N2—C14—C15 = −87.9 (2)°; C11—N2—C16—C17 = −87.58 (19)°]. Crystal packing is stabilized by intermolecular π stacking interactions between $Cg1^{i}$-π orbitals of nearby 2,5-dichlorolphenyl rings [*Cg*1···*Cg*1 = 3.860 (8) Å; *Cg*1 = center of gravity of the 2,5-dichlorophenyl ring (Fig. 2)]. The molecules are aligned in an inverted pattern along the *c* axis with the with the 2,5-dichlorophenyl rings stacked obliquely parallel to the *ac* face of the unit cell (Fig. 3). Intramolecular hydrogen bonding interactions [O1—H10···N1] between the phenol hydrogen atom and imino nitrogen atom provides additional crystal stability within the asymmetric unit. [i = 2 − *x*, −*y*, 2 − *z*].

Experimental

A mixture of 2,5-dichloroaniline (1.62 g, 0.01 mol) and 4-(diethylamino)-2-hydroxybenzaldehyde (1.93 g, 0.01 mol) in 30 ml of ethanol containing 2 drops of 4 *M* sulfuric acid was refluxed for about 7 h (Fig. 4). On cooling, the solid separated was filtered and recrystallized from acetone (m.p.: 397–401 K). Analysis found: C 60.46, H 5.32, N 8.24%; $C_{17}H_{18}Cl_2N_2O$ requires: C 60.54, H 5.38, N 8.31%.

Refinement

The hydroxyl atom (H10) was located in a difference Fourier map and along with all other H atoms were placed in their calculated positions and then refined using the riding model with O—H = 0.82 Å and C—H = 0.93 to 0.97 Å, and with U_{iso}(H) = 1.19–1.49U_{eq}(C, O).

Figures

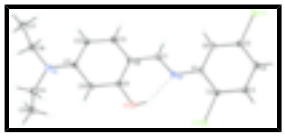

Fig. 1. Molecular structure of the title compound, showing atom labeling and 50% probability displacement ellipsoids. The dashed line indicates the intramolecular O—H···N hydrogen bond.

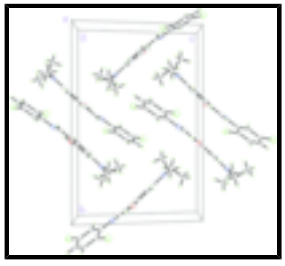

Fig. 2. Packing diagram of the title compound, viewed down the *a* axis.

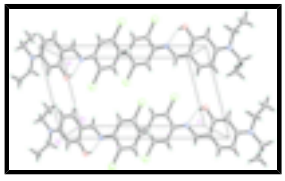

Fig. 3. Packing diagram of the title compound, viewed down the *b* axis. Dashed lines indicate intramolecular O—H···N hydrogen bonds.

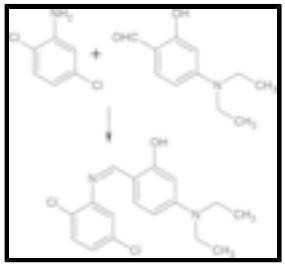

Fig. 4. Synthetic scheme for $C_{17}H_{18}Cl_2N_2O$.

2-[(*Z*)-(2,5-Dichlorophenyl)iminomethyl]-5-(diethylamino)phenol

Crystal data

$C_{17}H_{18}Cl_2N_2O$	F_{000} = 704
M_r = 337.23	D_x = 1.367 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 4869 reflections
a = 7.1729 (2) Å	θ = 4.7–32.5º
b = 18.6396 (6) Å	μ = 0.40 mm^{-1}
c = 12.6378 (4) Å	T = 296 K
β = 104.157 (3)º	Thick needle, pale yellow
V = 1638.36 (9) Å^3	0.53 × 0.25 × 0.19 mm
Z = 4	

Data collection

Oxford Diffraction Gemini R CCD diffractometer	5491 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} = 0.720, T_{max} = 0.927
17605 measured reflections
2626 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 32.5º
θ_{min} = 4.7º
$h = -10 \rightarrow 10$
$k = -27 \rightarrow 27$
$l = -18 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.120
S = 0.98
5491 reflections
202 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
$w = 1/[\sigma^2(F_o^2) + (0.055P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.28 e $Å^{-3}$
$\Delta\rho_{min}$ = −0.31 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	0.43274 (6)	0.45456 (3)	0.77923 (4)	0.06735 (16)
Cl2	−0.37011 (6)	0.41423 (3)	0.46310 (4)	0.06539 (16)
O1	0.30792 (15)	0.59856 (7)	0.95939 (10)	0.0573 (3)
H1O	0.2780	0.5722	0.9060	0.069*
N1	0.07935 (18)	0.52207 (6)	0.80838 (10)	0.0435 (3)
N2	0.0292 (2)	0.73892 (7)	1.19527 (11)	0.0532 (3)
C1	0.0490 (2)	0.47783 (7)	0.71617 (12)	0.0398 (3)
C2	0.2079 (2)	0.44459 (8)	0.69148 (13)	0.0443 (4)
C3	0.1895 (3)	0.40261 (9)	0.59958 (14)	0.0547 (4)

H3A	0.2976	0.3812	0.5849	0.066*
C4	0.0108 (3)	0.39229 (9)	0.52911 (14)	0.0539 (4)
H4A	−0.0033	0.3636	0.4674	0.065*
C5	−0.1452 (2)	0.42544 (8)	0.55252 (12)	0.0458 (4)
C6	−0.1297 (2)	0.46767 (8)	0.64337 (12)	0.0433 (3)
H6A	−0.2385	0.4895	0.6564	0.052*
C7	−0.0578 (2)	0.53797 (8)	0.85377 (12)	0.0441 (4)
H7A	−0.1774	0.5166	0.8277	0.053*
C8	−0.0324 (2)	0.58710 (8)	0.94251 (12)	0.0411 (3)
C9	0.1485 (2)	0.61728 (8)	0.99181 (12)	0.0422 (3)
C10	0.1682 (2)	0.66657 (8)	1.07560 (13)	0.0474 (4)
H10A	0.2889	0.6856	1.1070	0.057*
C11	0.0095 (2)	0.68848 (8)	1.11419 (12)	0.0439 (4)
C12	−0.1712 (2)	0.65751 (8)	1.06588 (13)	0.0484 (4)
H12A	−0.2790	0.6707	1.0899	0.058*
C13	−0.1882 (2)	0.60832 (8)	0.98419 (13)	0.0474 (4)
H13A	−0.3081	0.5880	0.9548	0.057*
C14	0.2107 (3)	0.77568 (9)	1.24016 (14)	0.0550 (4)
H14A	0.1839	0.8229	1.2650	0.066*
H14B	0.2776	0.7820	1.1828	0.066*
C15	0.3403 (3)	0.73581 (11)	1.33400 (16)	0.0708 (5)
H15A	0.4551	0.7632	1.3618	0.106*
H15B	0.3737	0.6901	1.3090	0.106*
H15C	0.2746	0.7288	1.3909	0.106*
C16	−0.1285 (3)	0.75621 (9)	1.24523 (14)	0.0548 (4)
H16A	−0.0757	0.7719	1.3197	0.066*
H16B	−0.2035	0.7132	1.2477	0.066*
C17	−0.2591 (3)	0.81395 (10)	1.18432 (16)	0.0647 (5)
H17A	−0.3574	0.8245	1.2217	0.097*
H17B	−0.3177	0.7976	1.1117	0.097*
H17C	−0.1855	0.8565	1.1807	0.097*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0356 (2)	0.1007 (4)	0.0625 (3)	0.0009 (2)	0.00571 (19)	−0.0005 (2)
Cl2	0.0521 (3)	0.0786 (3)	0.0573 (3)	−0.0096 (2)	−0.0023 (2)	−0.0120 (2)
O1	0.0354 (6)	0.0763 (8)	0.0580 (8)	0.0022 (5)	0.0073 (5)	−0.0187 (6)
N1	0.0392 (7)	0.0453 (7)	0.0430 (7)	0.0010 (6)	0.0047 (5)	−0.0007 (5)
N2	0.0458 (8)	0.0567 (8)	0.0551 (9)	0.0044 (6)	0.0086 (6)	−0.0122 (6)
C1	0.0394 (8)	0.0400 (7)	0.0390 (8)	−0.0030 (6)	0.0077 (6)	0.0033 (6)
C2	0.0343 (8)	0.0548 (9)	0.0433 (9)	−0.0019 (7)	0.0088 (6)	0.0063 (7)
C3	0.0462 (10)	0.0688 (11)	0.0533 (10)	0.0061 (8)	0.0202 (8)	0.0015 (8)
C4	0.0577 (11)	0.0601 (10)	0.0461 (10)	−0.0042 (9)	0.0170 (8)	−0.0085 (7)
C5	0.0420 (9)	0.0507 (9)	0.0420 (9)	−0.0074 (7)	0.0048 (7)	0.0000 (7)
C6	0.0381 (8)	0.0455 (8)	0.0455 (9)	0.0012 (7)	0.0088 (6)	0.0006 (6)
C7	0.0380 (8)	0.0453 (8)	0.0455 (9)	−0.0056 (7)	0.0038 (6)	0.0021 (7)
C8	0.0370 (8)	0.0433 (8)	0.0412 (8)	−0.0031 (6)	0.0065 (6)	0.0035 (6)

C9	0.0349 (8)	0.0453 (8)	0.0436 (8)	0.0038 (7)	0.0043 (6)	0.0028 (6)
C10	0.0358 (8)	0.0533 (9)	0.0486 (9)	−0.0021 (7)	0.0017 (7)	−0.0024 (7)
C11	0.0425 (9)	0.0440 (8)	0.0424 (9)	0.0035 (7)	0.0048 (7)	0.0021 (6)
C12	0.0396 (9)	0.0541 (9)	0.0526 (10)	0.0017 (7)	0.0134 (7)	0.0006 (7)
C13	0.0382 (8)	0.0518 (9)	0.0518 (10)	−0.0090 (7)	0.0103 (7)	−0.0022 (7)
C14	0.0587 (11)	0.0498 (9)	0.0528 (10)	−0.0009 (8)	0.0065 (8)	−0.0075 (7)
C15	0.0641 (12)	0.0752 (12)	0.0644 (12)	0.0043 (10)	−0.0014 (10)	−0.0011 (10)
C16	0.0593 (11)	0.0566 (10)	0.0490 (10)	0.0041 (8)	0.0144 (8)	−0.0022 (7)
C17	0.0571 (11)	0.0673 (11)	0.0693 (12)	0.0124 (9)	0.0149 (9)	0.0008 (9)

Geometric parameters (Å, °)

Cl1—C2	1.7293 (16)	C8—C9	1.411 (2)
Cl2—C5	1.7412 (16)	C9—C10	1.383 (2)
O1—C9	1.3516 (17)	C10—C11	1.404 (2)
O1—H1O	0.8200	C10—H10A	0.9300
N1—C7	1.2885 (19)	C11—C12	1.414 (2)
N1—C1	1.4005 (18)	C12—C13	1.364 (2)
N2—C11	1.372 (2)	C12—H12A	0.9300
N2—C14	1.457 (2)	C13—H13A	0.9300
N2—C16	1.461 (2)	C14—C15	1.511 (2)
C1—C6	1.396 (2)	C14—H14A	0.9700
C1—C2	1.398 (2)	C14—H14B	0.9700
C2—C3	1.380 (2)	C15—H15A	0.9600
C3—C4	1.384 (2)	C15—H15B	0.9600
C3—H3A	0.9300	C15—H15C	0.9600
C4—C5	1.372 (2)	C16—C17	1.508 (2)
C4—H4A	0.9300	C16—H16A	0.9700
C5—C6	1.374 (2)	C16—H16B	0.9700
C6—H6A	0.9300	C17—H17A	0.9600
C7—C8	1.425 (2)	C17—H17B	0.9600
C7—H7A	0.9300	C17—H17C	0.9600
C8—C13	1.404 (2)		
C9—O1—H1O	109.5	C11—C10—H10A	119.4
C7—N1—C1	121.73 (13)	N2—C11—C10	120.95 (14)
C11—N2—C14	122.14 (14)	N2—C11—C12	121.22 (14)
C11—N2—C16	121.65 (14)	C10—C11—C12	117.83 (14)
C14—N2—C16	116.15 (14)	C13—C12—C11	120.25 (15)
C6—C1—C2	117.40 (14)	C13—C12—H12A	119.9
C6—C1—N1	123.98 (13)	C11—C12—H12A	119.9
C2—C1—N1	118.53 (13)	C12—C13—C8	122.81 (15)
C3—C2—C1	121.60 (15)	C12—C13—H13A	118.6
C3—C2—Cl1	118.88 (12)	C8—C13—H13A	118.6
C1—C2—Cl1	119.51 (12)	N2—C14—C15	113.20 (15)
C2—C3—C4	120.22 (15)	N2—C14—H14A	108.9
C2—C3—H3A	119.9	C15—C14—H14A	108.9
C4—C3—H3A	119.9	N2—C14—H14B	108.9
C5—C4—C3	118.33 (15)	C15—C14—H14B	108.9
C5—C4—H4A	120.8	H14A—C14—H14B	107.8

C3—C4—H4A	120.8	C14—C15—H15A	109.5
C4—C5—C6	122.32 (15)	C14—C15—H15B	109.5
C4—C5—Cl2	118.75 (13)	H15A—C15—H15B	109.5
C6—C5—Cl2	118.93 (12)	C14—C15—H15C	109.5
C5—C6—C1	120.12 (14)	H15A—C15—H15C	109.5
C5—C6—H6A	119.9	H15B—C15—H15C	109.5
C1—C6—H6A	119.9	N2—C16—C17	112.77 (14)
N1—C7—C8	122.27 (14)	N2—C16—H16A	109.0
N1—C7—H7A	118.9	C17—C16—H16A	109.0
C8—C7—H7A	118.9	N2—C16—H16B	109.0
C13—C8—C9	116.88 (14)	C17—C16—H16B	109.0
C13—C8—C7	121.09 (14)	H16A—C16—H16B	107.8
C9—C8—C7	122.03 (14)	C16—C17—H17A	109.5
O1—C9—C10	117.90 (13)	C16—C17—H17B	109.5
O1—C9—C8	121.19 (13)	H17A—C17—H17B	109.5
C10—C9—C8	120.91 (14)	C16—C17—H17C	109.5
C9—C10—C11	121.29 (14)	H17A—C17—H17C	109.5
C9—C10—H10A	119.4	H17B—C17—H17C	109.5
C7—N1—C1—C6	23.4 (2)	C13—C8—C9—C10	−1.4 (2)
C7—N1—C1—C2	−160.16 (14)	C7—C8—C9—C10	177.95 (14)
C6—C1—C2—C3	−0.7 (2)	O1—C9—C10—C11	−179.71 (14)
N1—C1—C2—C3	−177.40 (14)	C8—C9—C10—C11	−0.2 (2)
C6—C1—C2—Cl1	−179.43 (11)	C14—N2—C11—C10	4.2 (2)
N1—C1—C2—Cl1	3.92 (18)	C16—N2—C11—C10	−172.72 (15)
C1—C2—C3—C4	−0.2 (2)	C14—N2—C11—C12	−175.03 (15)
Cl1—C2—C3—C4	178.53 (13)	C16—N2—C11—C12	8.0 (2)
C2—C3—C4—C5	0.8 (2)	C9—C10—C11—N2	−178.16 (14)
C3—C4—C5—C6	−0.5 (2)	C9—C10—C11—C12	1.1 (2)
C3—C4—C5—Cl2	178.80 (12)	N2—C11—C12—C13	178.94 (15)
C4—C5—C6—C1	−0.4 (2)	C10—C11—C12—C13	−0.3 (2)
Cl2—C5—C6—C1	−179.72 (11)	C11—C12—C13—C8	−1.4 (2)
C2—C1—C6—C5	1.0 (2)	C9—C8—C13—C12	2.2 (2)
N1—C1—C6—C5	177.46 (13)	C7—C8—C13—C12	−177.13 (15)
C1—N1—C7—C8	−175.23 (13)	C11—N2—C14—C15	−87.9 (2)
N1—C7—C8—C13	174.32 (14)	C16—N2—C14—C15	89.23 (18)
N1—C7—C8—C9	−5.0 (2)	C11—N2—C16—C17	−87.58 (19)
C13—C8—C9—O1	178.08 (14)	C14—N2—C16—C17	95.31 (19)
C7—C8—C9—O1	−2.6 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1O···N1	0.82	1.89	2.6139 (16)	147

Fig. 1

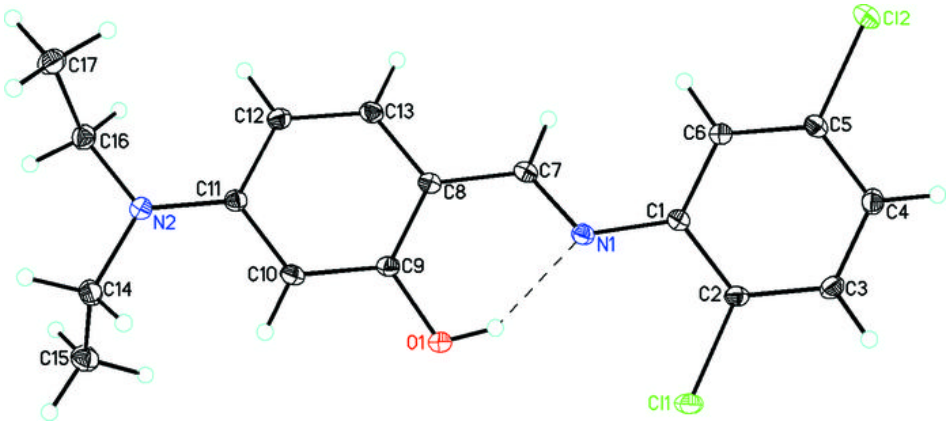
Cl2
C17
C16
C12
C13
C6
C5
C11
C8
C7
C1
C4
N2
N1
C10
C9
C14
C2
C3
O1
C15
Cl1

Fig. 2

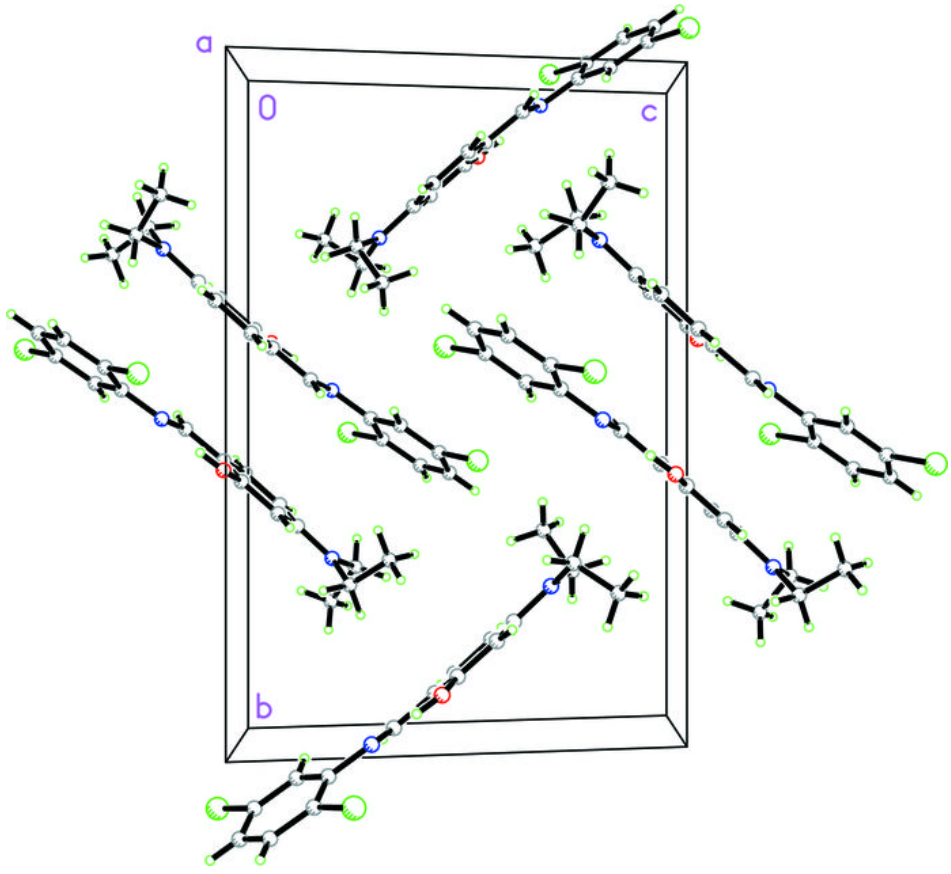

Fig. 3

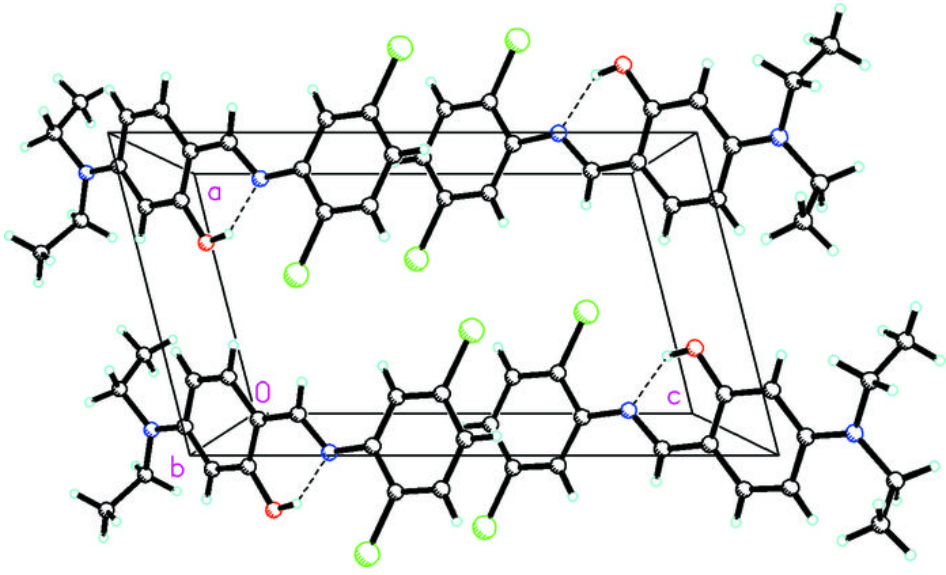

Fig. 4