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(6*Z*)-3-Diethylamino-6-(3-hydroxyanilinomethylene)cyclohexa-2,4-dien-1-one

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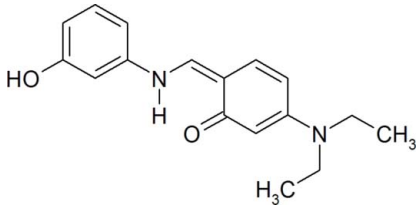
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.083; wR factor = 0.270; data-to-parameter ratio = 24.1.

In the title molecule, $C_{17}H_{20}N_2O_2$, the angle between the mean planes of the 3-hydroxyphenyl and cyclohexa-2,4-dien-1-one rings is 10.7 (7)°. Intramolecular N—H···O hydrogen bonding involving the amine H atom and the carbonyl O atom affects the conformation of the molecule. One of the ethyl arms is disordered over two conformations with occupancies of 0.766 (8) and 0.234 (8). Crystal packing is stabilized by intermolecular C—H···O hydrogen bonding between the major component of the disordered ethyl C atom and a nearby carbonyl O atom, and by O—H···O hydrogen bonding between the hydroxyl H atom and the carbonyl O atom. This links the molecules into chains in an alternate inverted pattern, parallel, oblique and diagonal to the *bc* face of the unit cell.

Related literature

For related structures, see: Nagao *et al.* (2002); Bohme & Fels (2006); Butcher *et al.* (2007); Büyükgüngör *et al.* (2007); Odabaşoğlu *et al.* (2007); Yathirajan *et al.* (2007); For details of the biological activities of Schiff base derivatives, 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).



Experimental

Crystal data

$C_{17}H_{20}N_2O_2$
M_r = 284.35
Monoclinic, $P2_1/a$
a = 7.4780 (6) Å
b = 15.822 (2) Å
c = 12.6372 (13) Å
β = 94.149 (9)°
V = 1491.3 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 296 K
0.55 × 0.43 × 0.27 mm

Data collection

Oxford Diffraction Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.827, T_{max} = 1.000 (expected range = 0.808–0.978)
13075 measured reflections
4836 independent reflections
1828 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.083
$wR(F^2)$ = 0.270
S = 1.02
4836 reflections
201 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1B···O2^{i}	0.82	1.77	2.580 (2)	172
N1—H1A···O2	0.86	1.92	2.598 (2)	135
C15A—H15C···O2^{ii}	0.96	2.53	3.422 (5)	155

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

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: SJ2389).

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supplementary materials

Acta Cryst. (2007). E**63**, o4566-o4567 [**doi:10.1107/S1600536807053652**]

(6*Z*)-3-Diethylamino-6-(3-hydroxyanilinomethylene)cyclohexa-2,4-dien-1-one

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Comment

Schiff bases are used as substrates in the preparation of number of industrial and biologically active compounds *via* ring closure, cycloaddition and replacement reactions. Some Schiff base derivatives are also known to have biological 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) and 2-{(*E*)-[(2-chloro-5-nitrophenyl)imino]methyl}-5-(diethylamino)phenol (Butcher *et al.* 2007); 6(*Z*)-((2-hydroxyphenylamino)methylene)-3-(diethylamino)cyclohexyl-2,4-dien-1-one (Bohme & Fels, 2006) and *N*-(2-hydroxybenzylidene)-4-diethylamino-2-hydroxyaniline (Nagao *et al.* 2002) have been reported previously. The title compound (6*Z*)-3-(diethylamino)-6-{[(3-hydroxyphenyl)amino]methylene} cyclohexa-2,4-dien-1-one, (I), $C_{17}H_{20}N_2O_2$ was the unexpected product of an attempt to synthesize a new Schiff base, 5-(diethylamino)-2-{(*E*)-[(3-hydroxyphenyl)imino]methyl}phenol by enolization and its crystal structure is reported here.

The angle between the mean planes of the planar 3-hydroxyphenyl and cyclohexa-2,4-dien-1-one groups of the title molecule is 10.7 (7)° Fig. 1). These two rings are twisted slightly about the methylene amino group with torsion angles of −9.5 (4) [C7—N1—C5—C4] and 178.9 (2) [N1—C7—C8—C9], respectively. Intramolecular N1—H1A···O2 hydrogen bonding contributes to the overall planarity of the molecule. One of the ethyl arms is disordered over two conformations which are constrained to have similar metrical parameters with occupancies of 0.234 (8) [C14A] and 0.766 (8) [C15A] respectively. Crystal packing is stabilized by intermolecular C15A—H1A···O2 and O1—H1B···O2 hydrogen bonds (Fig 2) that link the molecules into chains in an alternate inverted pattern, which is parallel and oblique to the *bc* face and diagonal to the *a* axis of the unit cell (Fig. 2).

Experimental

A mixture of 3-aminophenol (1.09 g, 0.01 mol) and 4-(diethylamino)-2-hydroxybenzaldehyde (1.92 g, 0.01 mol) in 25 ml of absolute ethanol containing 2 drops of 4 *M* sulfuric acid was refluxed for about 4 h (Fig. 3). On cooling, the solid separated was filtered and recrystallized from acetone (m.p.: 467–473 K). The expected product was 5-(diethylamino)-2-{(*E*)-[(3-hydroxyphenyl)imino]methyl}phenol, but the structure observed is that of its tautomeric form, (6*Z*)-3-(diethylamino)-6-{[(3-hydroxyphenyl)amino]methylene}cyclohexa-2,4- dien-1-one. Analysis found: C 70.73, H 7.01, N 9.78%; $C_{17}H_{20}N_2O_2$ requires: C 70.81, H 7.09, N 9.85%.

Refinement

The C14A–C15A ethyl group was disordered over two positions A and B and the occupancy factors refined to 0.766 (8) and 0.234 (8); the two components were constrained to have similar metrical parameters. Owing to the poor diffraction qualities of the crystal, the ratio of observed to unique reflelctions is low (38%).

All H atoms were placed in calculated positions except H1A and H1B which were found in a difference map. All H atoms were refined using a riding model with O—H = 0.82 Å, N—H = 0.86 Å and C—H = 0.93 to 0.97 Å, and with U_{iso}(H) = 1.0–1.5U_{eq}(C,*O*,*N*).

Figures

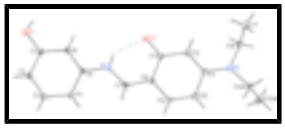

Fig. 1. Molecular structure of the title compound, showing atom labeling and 50% probability displacement ellipsoids. Only the major disorder components C14A and C15A are displayed. The dashed line indicates the intramolecular hydrogen bond.

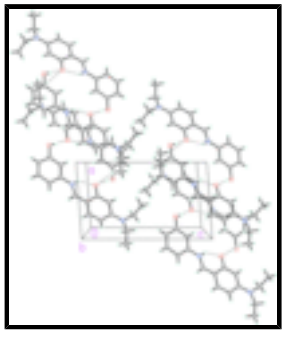

Fig. 2. Packing diagram for (I), viewed down the *b* axis with hydrogen bonds drawn as dashed lines.

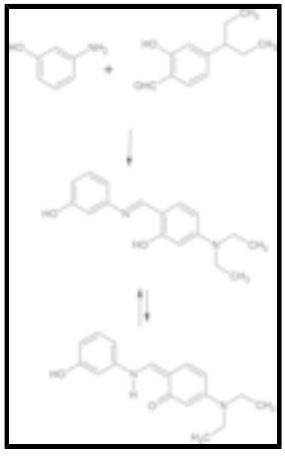

Fig. 3. Synthesis of the title compound.

(6*Z*)-3-Diethylamino-6-(3-hydroxyanilinomethylene)cyclohexa-2,4-dien-1-one

Crystal data

$C_{17}H_{20}N_2O_2$	F_{000} = 608
M_r = 284.35	D_x = 1.266 Mg m^{-3}

Monoclinic, $P2_1/a$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2yab	Cell parameters from 3116 reflections
$a = 7.4780$ (6) Å	$\theta = 4.8–32.5°$
$b = 15.822$ (2) Å	$\mu = 0.08$ mm^{-1}
$c = 12.6372$ (13) Å	$T = 296$ K
$\beta = 94.149$ (9)°	Chunk, pale yellow
$V = 1491.3$ (3) Å^3	0.55 × 0.43 × 0.27 mm
$Z = 4$	

Data collection

Oxford Diffraction Gemini diffractometer	4836 independent reflections
Radiation source: fine-focus sealed tube	1828 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.058$
$T = 296$ K	$\theta_{max} = 32.6°$
φ and ω scans	$\theta_{min} = 4.8°$
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)	$h = -11\rightarrow11$
$T_{min} = 0.827$, $T_{max} = 1.000$	$k = -22\rightarrow22$
13075 measured reflections	$l = -19\rightarrow19$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.083$	H-atom parameters constrained
$wR(F^2) = 0.270$	$w = 1/[\sigma^2(F_o^2) + (0.1294P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.004$
4836 reflections	$\Delta\rho_{max} = 0.37$ e Å^{-3}
201 parameters	$\Delta\rho_{min} = -0.19$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	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}	Occ. (<1)
O1	−0.7397 (2)	0.07199 (13)	1.24994 (15)	0.0716 (6)	
H1B	−0.7597	0.0388	1.2007	0.107*	
O2	−0.17605 (19)	0.04039 (11)	0.89295 (12)	0.0577 (5)	
N1	−0.1930 (2)	0.10814 (12)	1.07924 (14)	0.0480 (5)	
H1A	−0.2386	0.0746	1.0310	0.058*	
N2	0.3053 (3)	0.11735 (17)	0.68516 (17)	0.0750 (7)	
C1	−0.5685 (3)	0.09987 (15)	1.25042 (18)	0.0511 (6)	
C2	−0.4974 (3)	0.14220 (17)	1.3390 (2)	0.0617 (7)	
H2A	−0.5665	0.1500	1.3965	0.074*	
C3	−0.3255 (3)	0.17289 (19)	1.3430 (2)	0.0713 (8)	
H3A	−0.2794	0.2013	1.4034	0.086*	
C4	−0.2198 (3)	0.16219 (19)	1.2589 (2)	0.0655 (7)	
H4A	−0.1033	0.1831	1.2620	0.079*	
C5	−0.2913 (3)	0.11953 (14)	1.16938 (17)	0.0451 (5)	
C6	−0.4639 (3)	0.08804 (14)	1.16547 (17)	0.0474 (6)	
H6A	−0.5101	0.0589	1.1057	0.057*	
C7	−0.0377 (3)	0.14383 (15)	1.06111 (18)	0.0496 (6)	
H7A	0.0181	0.1776	1.1139	0.060*	
C8	0.0459 (3)	0.13346 (14)	0.96764 (17)	0.0456 (5)	
C9	0.2103 (3)	0.17529 (17)	0.9547 (2)	0.0616 (7)	
H9A	0.2616	0.2076	1.0104	0.074*	
C10	0.2951 (3)	0.16995 (19)	0.8644 (2)	0.0684 (8)	
H10A	0.4025	0.1987	0.8589	0.082*	
C11	0.2219 (3)	0.12066 (16)	0.77704 (18)	0.0533 (6)	
C12	0.0630 (3)	0.07688 (15)	0.78963 (17)	0.0499 (6)	
H12A	0.0153	0.0433	0.7341	0.060*	
C13	−0.0277 (3)	0.08148 (14)	0.88289 (17)	0.0451 (5)	
C14A	0.4495 (4)	0.1786 (2)	0.6598 (3)	0.0623 (12)	0.766 (8)
H14A	0.4271	0.1989	0.5876	0.075*	0.766 (8)
H14B	0.4483	0.2268	0.7072	0.075*	0.766 (8)
C15A	0.6271 (5)	0.1367 (4)	0.6718 (4)	0.1014 (19)	0.766 (8)
H15A	0.7188	0.1767	0.6574	0.152*	0.766 (8)
H15B	0.6294	0.0905	0.6228	0.152*	0.766 (8)
H15C	0.6480	0.1159	0.7430	0.152*	0.766 (8)
C14B	0.5209 (15)	0.1174 (9)	0.6931 (10)	0.0623 (12)	0.234 (8)
H14C	0.5708	0.1167	0.7661	0.075*	0.234 (8)
H14D	0.5689	0.0704	0.6548	0.075*	0.234 (8)
C15B	0.5501 (19)	0.1965 (12)	0.6427 (15)	0.1014 (19)	0.234 (8)
H15D	0.6761	0.2040	0.6356	0.152*	0.234 (8)
H15E	0.5066	0.2415	0.6848	0.152*	0.234 (8)
H15F	0.4873	0.1971	0.5737	0.152*	0.234 (8)
C16	0.2402 (3)	0.06431 (19)	0.5966 (2)	0.0686 (8)	
H16A	0.1915	0.0126	0.6240	0.082*	
H16B	0.3401	0.0492	0.5556	0.082*	
C17	0.0984 (4)	0.1068 (2)	0.5251 (2)	0.0825 (9)	

H17A	0.0794	0.0752	0.4604	0.124*
H17B	0.1366	0.1631	0.5092	0.124*
H17C	−0.0114	0.1094	0.5599	0.124*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0535 (10)	0.0900 (15)	0.0739 (12)	−0.0143 (9)	0.0228 (8)	−0.0231 (10)
O2	0.0493 (9)	0.0725 (12)	0.0530 (9)	−0.0226 (8)	0.0151 (7)	−0.0032 (8)
N1	0.0441 (9)	0.0575 (12)	0.0431 (10)	−0.0080 (9)	0.0086 (7)	−0.0054 (9)
N2	0.0532 (11)	0.1144 (19)	0.0599 (13)	−0.0330 (12)	0.0211 (9)	−0.0154 (13)
C1	0.0454 (12)	0.0495 (14)	0.0588 (14)	−0.0043 (10)	0.0067 (10)	−0.0068 (11)
C2	0.0662 (16)	0.0635 (17)	0.0575 (14)	0.0039 (13)	0.0194 (12)	−0.0164 (13)
C3	0.0636 (16)	0.091 (2)	0.0596 (15)	−0.0096 (14)	0.0055 (12)	−0.0296 (15)
C4	0.0516 (13)	0.0794 (19)	0.0659 (15)	−0.0145 (13)	0.0072 (11)	−0.0186 (14)
C5	0.0497 (11)	0.0401 (12)	0.0461 (11)	−0.0013 (10)	0.0069 (9)	−0.0014 (10)
C6	0.0493 (11)	0.0503 (13)	0.0436 (11)	−0.0060 (10)	0.0110 (9)	−0.0108 (10)
C7	0.0440 (12)	0.0531 (14)	0.0511 (12)	−0.0028 (10)	0.0000 (9)	0.0023 (11)
C8	0.0378 (10)	0.0518 (13)	0.0474 (12)	−0.0039 (10)	0.0053 (9)	0.0050 (10)
C9	0.0496 (13)	0.0783 (18)	0.0561 (14)	−0.0193 (13)	−0.0019 (11)	−0.0089 (13)
C10	0.0446 (12)	0.093 (2)	0.0675 (16)	−0.0293 (13)	0.0037 (11)	0.0005 (15)
C11	0.0409 (11)	0.0651 (16)	0.0542 (13)	−0.0123 (11)	0.0059 (9)	0.0013 (12)
C12	0.0433 (11)	0.0593 (15)	0.0477 (12)	−0.0139 (10)	0.0079 (9)	−0.0013 (11)
C13	0.0366 (10)	0.0475 (13)	0.0513 (12)	−0.0020 (9)	0.0048 (9)	0.0075 (10)
C14A	0.046 (2)	0.075 (3)	0.068 (2)	−0.0068 (16)	0.0144 (15)	0.0042 (17)
C15A	0.037 (2)	0.122 (4)	0.145 (4)	−0.001 (2)	0.008 (2)	0.017 (3)
C14B	0.046 (2)	0.075 (3)	0.068 (2)	−0.0068 (16)	0.0144 (15)	0.0042 (17)
C15B	0.037 (2)	0.122 (4)	0.145 (4)	−0.001 (2)	0.008 (2)	0.017 (3)
C16	0.0639 (15)	0.077 (2)	0.0674 (17)	−0.0133 (14)	0.0226 (13)	−0.0083 (15)
C17	0.0799 (19)	0.095 (2)	0.0738 (19)	−0.0132 (17)	0.0118 (15)	−0.0002 (17)

Geometric parameters (Å, °)

O1—C1	1.353 (3)	C9—H9A	0.9300
O1—H1B	0.8200	C10—C11	1.428 (3)
O2—C13	1.300 (2)	C10—H10A	0.9300
N1—C7	1.326 (3)	C11—C12	1.394 (3)
N1—C5	1.411 (3)	C12—C13	1.404 (3)
N1—H1A	0.8600	C12—H12A	0.9300
N2—C11	1.358 (3)	C14A—C15A	1.482 (5)
N2—C16	1.454 (3)	C14A—H14A	0.9700
N2—C14A	1.502 (4)	C14A—H14B	0.9700
N2—C14B	1.609 (11)	C15A—H15A	0.9600
C1—C2	1.378 (3)	C15A—H15B	0.9600
C1—C6	1.386 (3)	C15A—H15C	0.9600
C2—C3	1.372 (3)	C14B—C15B	1.43 (2)
C2—H2A	0.9300	C14B—H14C	0.9700
C3—C4	1.381 (3)	C14B—H14D	0.9700
C3—H3A	0.9300	C15B—H15D	0.9600

C4—C5	1.390 (3)	C15B—H15E	0.9600
C4—H4A	0.9300	C15B—H15F	0.9600
C5—C6	1.382 (3)	C16—C17	1.502 (4)
C6—H6A	0.9300	C16—H16A	0.9700
C7—C8	1.386 (3)	C16—H16B	0.9700
C7—H7A	0.9300	C17—H17A	0.9600
C8—C9	1.416 (3)	C17—H17B	0.9600
C8—C13	1.429 (3)	C17—H17C	0.9600
C9—C10	1.347 (3)		
C1—O1—H1B	109.5	N2—C11—C12	121.7 (2)
C7—N1—C5	126.78 (19)	N2—C11—C10	120.52 (19)
C7—N1—H1A	116.6	C12—C11—C10	117.7 (2)
C5—N1—H1A	116.6	C11—C12—C13	122.5 (2)
C11—N2—C16	122.10 (19)	C11—C12—H12A	118.7
C11—N2—C14A	122.6 (2)	C13—C12—H12A	118.7
C16—N2—C14A	114.5 (2)	O2—C13—C12	121.6 (2)
C11—N2—C14B	117.8 (5)	O2—C13—C8	120.00 (19)
C16—N2—C14B	109.1 (5)	C12—C13—C8	118.40 (18)
O1—C1—C2	118.1 (2)	C15A—C14A—N2	109.9 (3)
O1—C1—C6	122.6 (2)	C15A—C14A—H14A	109.7
C2—C1—C6	119.3 (2)	N2—C14A—H14A	109.7
C3—C2—C1	120.5 (2)	C15A—C14A—H14B	109.7
C3—C2—H2A	119.7	N2—C14A—H14B	109.7
C1—C2—H2A	119.7	H14A—C14A—H14B	108.2
C2—C3—C4	121.0 (2)	C15B—C14B—N2	99.1 (10)
C2—C3—H3A	119.5	C15B—C14B—H14C	112.0
C4—C3—H3A	119.5	N2—C14B—H14C	112.0
C3—C4—C5	118.6 (2)	C15B—C14B—H14D	112.0
C3—C4—H4A	120.7	N2—C14B—H14D	112.0
C5—C4—H4A	120.7	H14C—C14B—H14D	109.6
C6—C5—C4	120.49 (19)	C14B—C15B—H15D	109.5
C6—C5—N1	117.71 (18)	C14B—C15B—H15E	109.5
C4—C5—N1	121.78 (19)	H15D—C15B—H15E	109.5
C5—C6—C1	120.1 (2)	C14B—C15B—H15F	109.5
C5—C6—H6A	119.9	H15D—C15B—H15F	109.5
C1—C6—H6A	119.9	H15E—C15B—H15F	109.5
N1—C7—C8	123.5 (2)	N2—C16—C17	112.8 (2)
N1—C7—H7A	118.3	N2—C16—H16A	109.0
C8—C7—H7A	118.3	C17—C16—H16A	109.0
C7—C8—C9	119.5 (2)	N2—C16—H16B	109.0
C7—C8—C13	122.26 (19)	C17—C16—H16B	109.0
C9—C8—C13	118.24 (19)	H16A—C16—H16B	107.8
C10—C9—C8	122.3 (2)	C16—C17—H17A	109.5
C10—C9—H9A	118.9	C16—C17—H17B	109.5
C8—C9—H9A	118.9	H17A—C17—H17B	109.5
C9—C10—C11	120.7 (2)	C16—C17—H17C	109.5
C9—C10—H10A	119.6	H17A—C17—H17C	109.5
C11—C10—H10A	119.6	H17B—C17—H17C	109.5

O1—C1—C2—C3	−179.0 (2)	C14A—N2—C11—C10	−14.6 (4)
C6—C1—C2—C3	0.4 (4)	C14B—N2—C11—C10	36.5 (7)
C1—C2—C3—C4	0.0 (4)	C9—C10—C11—N2	178.2 (3)
C2—C3—C4—C5	0.0 (4)	C9—C10—C11—C12	−1.6 (4)
C3—C4—C5—C6	−0.5 (4)	N2—C11—C12—C13	−178.1 (2)
C3—C4—C5—N1	178.3 (2)	C10—C11—C12—C13	1.6 (4)
C7—N1—C5—C6	169.4 (2)	C11—C12—C13—O2	179.8 (2)
C7—N1—C5—C4	−9.5 (4)	C11—C12—C13—C8	0.3 (3)
C4—C5—C6—C1	1.0 (4)	C7—C8—C13—O2	−1.6 (3)
N1—C5—C6—C1	−177.9 (2)	C9—C8—C13—O2	178.3 (2)
O1—C1—C6—C5	178.5 (2)	C7—C8—C13—C12	177.9 (2)
C2—C1—C6—C5	−0.9 (4)	C9—C8—C13—C12	−2.3 (3)
C5—N1—C7—C8	−176.0 (2)	C11—N2—C14A—C15A	105.3 (4)
N1—C7—C8—C9	178.9 (2)	C16—N2—C14A—C15A	−85.1 (4)
N1—C7—C8—C13	−1.3 (3)	C14B—N2—C14A—C15A	7.5 (7)
C7—C8—C9—C10	−177.8 (3)	C11—N2—C14B—C15B	−115.0 (10)
C13—C8—C9—C10	2.4 (4)	C16—N2—C14B—C15B	100.1 (10)
C8—C9—C10—C11	−0.4 (4)	C14A—N2—C14B—C15B	−5.7 (8)
C16—N2—C11—C12	−3.6 (4)	C11—N2—C16—C17	85.9 (3)
C14A—N2—C11—C12	165.2 (3)	C14A—N2—C16—C17	−83.8 (3)
C14B—N2—C11—C12	−143.7 (6)	C14B—N2—C16—C17	−131.0 (5)
C16—N2—C11—C10	176.6 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1B···O2^{i}	0.82	1.77	2.580 (2)	172
N1—H1A···O2	0.86	1.92	2.598 (2)	135
C15A—H15C···O2^{ii}	0.96	2.53	3.422 (5)	155

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

Fig. 1

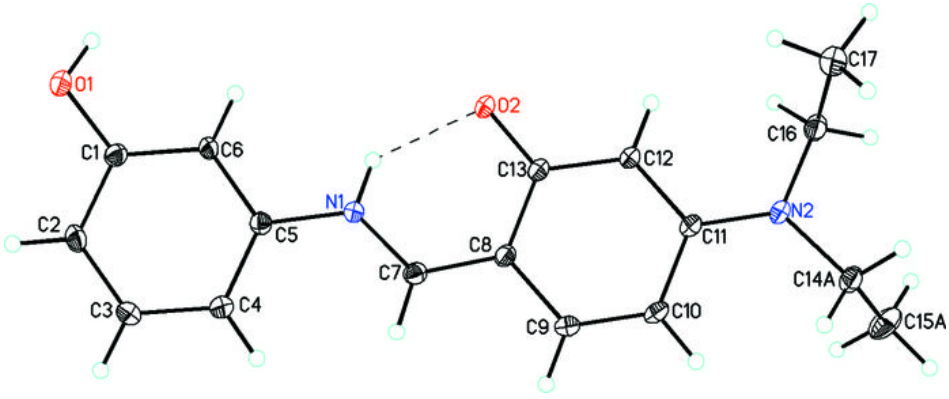
O1
C1
C6
C2
C5
N1
O2
C13
C12
C16
C17
N2
C11
C8
C7
C14A
C3
C4
C9
C10
C15A

Fig. 2

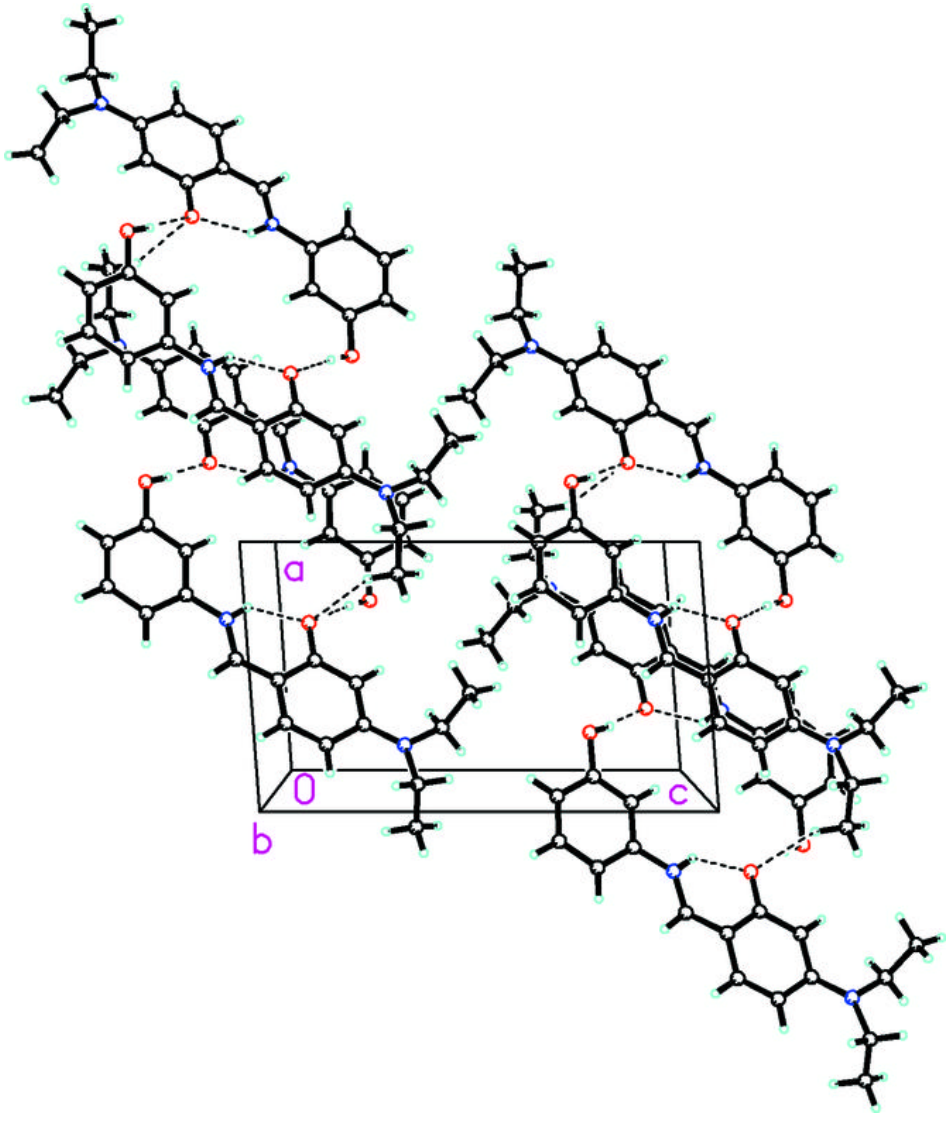

Fig. 3