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(*E*)-2-{[4-*tert*-Butyl-5-(2,4-dichlorobenzyl)thiazol-2-yl]iminomethyl}phenol

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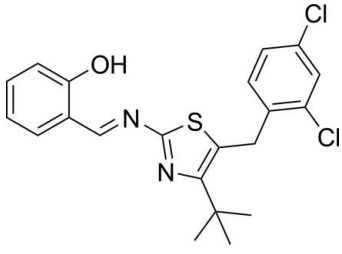
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.041; wR factor = 0.110; data-to-parameter ratio = 18.0.

Geometric parameters of the title compound, $C_{21}H_{20}Cl_2N_2OS$, a Schiff base, are in the usual ranges. The 4-hydroxyphenyl group and thiazole ring are almost coplanar, with a dihedral angle of 2.4 (1)°; the 2,4-dichlorobenzyl group is approximately perpendicular to the thiazole ring [dihedral angle = 86.6 (2)°]. The molecular conformation is stabilized by an intramolecular O—H···N hydrogen bond.

Related literature

For related literature, see: Hu *et al.* (2006).



Experimental

Crystal data

$C_{21}H_{20}Cl_2N_2OS$
M_r = 419.35
Monoclinic, $P2_1/c$
a = 8.3005 (4) Å
b = 19.0883 (10) Å
c = 13.3014 (7) Å
β = 106.1210 (10)°
V = 2024.63 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.44 mm^{-1}
T = 173 (2) K
0.48 × 0.38 × 0.33 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.818, T_{max} = 0.869
11999 measured reflections
4441 independent reflections
3382 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.110
S = 1.05
4441 reflections
248 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N2	0.84	1.87	2.611 (2)	147

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2003); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2005); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2623).

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supplementary materials

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(*E*)-2-{[4-*tert*-Butyl-5-(2,4-dichlorobenzyl)thiazol-2-yl]iminomethyl}phenol

A.-X. Hu, G. Cao and Y.-Q. Mang

Comment

In recent years, there has been considerable and increasing interest in the study of Schiff-base containing thiazole rings due to their antiviral, anticancer and antibacterial activities (Hu *et al.*, 2006). Herein we report the synthesis and crystal structure of (*E*)-2-((4-*tert*-butyl-5-(2,4-dichlorobenzyl)thiazol-2- ylimino)methyl)phenol.

A perspective view of the title compound with the labeling scheme is shown in Fig. 1 with dashed line indicateing the hydrogen bond forming a six-membered ring. The length of C=N double bond is 1.286 (2) Å. The 2,4-dichlorobenzyl is approximately perpendicular to the thiazole ring with a dihedral angle of 86.6 (2)°.

Experimental

A solution of thiourea (0.03 mol) and 2-bromo-1-(2,4-dichlorophenyl)-4,4-dimethylpentan-3-one (0.03 mol) in ethanol (70 ml) was refluxed for 9 h (monitoring by TLC). A part of the solvent was evaporated, and the precipitate formed was filtered out, dried, giving a yellowish crystalline substance which was the hydrobromide. The salt dissolved directly in ethanol and was neutralized with ammonia. The precipitate was filtered out and washed with water, dried to give 4-*tert*-butyl-5-(2,4-dichlorobenzyl)thiazol-2-amine. Then 1 mmol salicylal was dissolved in 5 ml of freshly dried alcohol and heated to 348 K, and the above-prepared alcohol solution of 4-*tert*-butyl-5-(2,4-dichlorobenzyl)thiazol-2-amine(1 mmol) was added dropwise and the resulting raction mixture was stirred at this temperature for furture 8.5 h. The mixture was then cooled, and the yellow solid was removed by filtration and recrystallized from dried alcohol to give the desired product. Yield: 75.1%. m.p. 417–418 K. Spectroscopic analysis: ^{1}H-NMR ($CDCl_3$, 400 MHz) (p.p.m.): 1.43(s, 9H, $(CH_3)_3$), 4.33(s, 2H, CH_2), 6.95(dd, J = 8.0 Hz, J = 8.0 Hz, 1H, 2-HO$C_6H_4$5-H), 7.00(d, J = 8.0 Hz, 1H, 2-HO$C_6H_4$3-H), 7.09(d, J = 8.0 Hz, 1H, 2,4-$Cl_2C_6H_3$6-H), 7.21(dd, J = 8.0 Hz, J =1.6 Hz, 1H, 2,4-$Cl_2C_6H_3$5-H), 7.40(ddd, J = 8.0 Hz, J = 8.0 Hz, J = 1.6 Hz,1*H*, 2-HO$C_6H_4$4-H), 7.43(d, J = 1.6 Hz, 1H, 2,4-$Cl_2C_6H_3$3-H), 7.44(dd, J = 8.0 Hz, J = 1.6 Hz,1*H*, 2-HO$C_6H_4$6-H), 9.06(s, 1H, N=CH), 12.28(s, 1H, OH). Crystals suitable for X-ray structure determination were obtained by slow evaporation of an ethanol solution at room temperature.

Refinement

The hydroxy H atom was positioned geometrically (O—H = 0.84 Å) and refined as riding [U_{iso}(H) = 1.5 U_{eq}(O)]. Methyl H atoms were positioned geometrically (C—H = 0.98 Å) and torsion angles refined to fit the electron density [U_{iso}(H) = 1.5 U_{eq}(C)]. Other H atoms were placed in calculated positions (methylene C—H = 0.99 Å, aromatic C—H = 0.95 Å) and refined as riding [U_{iso}(H) = 1.2 U_{eq}(C)].

Figures

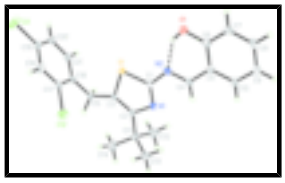

Fig. 1. The molecular structure of the title compound, with atom labels and 30% probability displacement ellipsoids for non-H atoms. the hydrogen bond is shown as a dashed line.

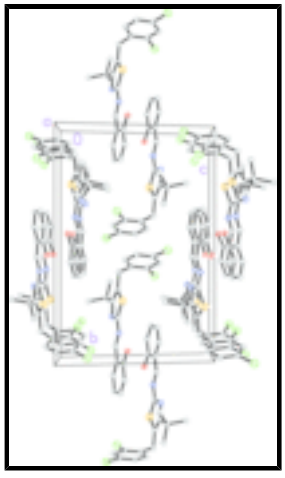

Fig. 2. The crystal packing of the title compound, with all H atoms omitted for clarity.

(*E*)-2-{[(4-*tert*-Butyl-5-(2,4-dichlorobenzyl)thiazol-2-yl]iminomethyl}phenol

Crystal data

$C_{21}H_{20}Cl_2N_2OS$	F_{000} = 872
M_r = 419.35	D_x = 1.376 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 5068 reflections
a = 8.3005 (4) Å	θ = 2.6–27.0º
b = 19.0883 (10) Å	μ = 0.44 mm^{-1}
c = 13.3014 (7) Å	T = 173 (2) K
β = 106.1210 (10)º	Block, yellow
V = 2024.63 (18) Å^3	0.48 × 0.38 × 0.33 mm
Z = 4	

Data collection

Bruker AXS SMART 1000 CCD diffractometer	4441 independent reflections
Radiation source: fine-focus sealed tube	3382 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.027
T = 173(2) K	θ_{max} = 27.1º
ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	h = −10→10

T_{min} = 0.818, T_{max} = 0.869
11999 measured reflections
k = −20→24
l = −16→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.110
S = 1.05
4441 reflections
248 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
$w = 1/[\sigma^2(F_o^2) + (0.051P)^2 + 0.8438P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 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	0.03027 (7)	0.47395 (3)	0.30136 (6)	0.0597 (2)
Cl2	0.64380 (8)	0.36001 (4)	0.37832 (4)	0.05161 (18)
S1	0.48133 (6)	0.25450 (2)	0.58721 (4)	0.02904 (13)
C1	0.5844 (2)	0.17648 (9)	0.62257 (14)	0.0254 (4)
C2	0.7997 (2)	0.24959 (10)	0.65619 (14)	0.0261 (4)
C3	0.6734 (2)	0.29737 (10)	0.62080 (14)	0.0258 (4)
C4	0.5664 (2)	0.05644 (10)	0.63223 (14)	0.0262 (4)
H4	0.6855	0.0563	0.6557	0.031*
C5	0.4777 (2)	−0.00926 (10)	0.62176 (14)	0.0265 (4)
C6	0.3014 (2)	−0.01282 (10)	0.58307 (16)	0.0309 (4)
C7	0.2203 (3)	−0.07746 (11)	0.57246 (17)	0.0377 (5)
H7	0.1016	−0.0799	0.5463	0.045*
C8	0.3135 (3)	−0.13780 (11)	0.60019 (16)	0.0365 (5)
H8	0.2577	−0.1818	0.5930	0.044*
C9	0.4859 (3)	−0.13567 (11)	0.63817 (16)	0.0350 (5)
H9	0.5480	−0.1778	0.6571	0.042*

C10	0.5676 (2)	−0.07210 (10)	0.64841 (15)	0.0306 (4)
H10	0.6864	−0.0707	0.6738	0.037*
C11	0.9897 (2)	0.25934 (11)	0.69580 (17)	0.0346 (5)
C12	1.0421 (3)	0.24370 (16)	0.8141 (2)	0.0601 (7)
H12A	1.1647	0.2416	0.8397	0.090*
H12B	0.9947	0.1986	0.8269	0.090*
H12C	1.0003	0.2809	0.8511	0.090*
C13	1.0742 (3)	0.20476 (14)	0.6436 (2)	0.0515 (6)
H13A	1.0452	0.2137	0.5681	0.077*
H13B	1.0355	0.1579	0.6560	0.077*
H13C	1.1961	0.2076	0.6731	0.077*
C14	1.0498 (3)	0.33084 (14)	0.6732 (3)	0.0745 (10)
H14A	1.1727	0.3315	0.6932	0.112*
H14B	1.0091	0.3664	0.7134	0.112*
H14C	1.0066	0.3410	0.5983	0.112*
C15	0.6701 (2)	0.37653 (10)	0.61058 (15)	0.0294 (4)
H15A	0.6787	0.3977	0.6798	0.035*
H15B	0.7686	0.3920	0.5881	0.035*
C16	0.5124 (2)	0.40248 (9)	0.53298 (14)	0.0267 (4)
C17	0.4866 (2)	0.39610 (10)	0.42552 (15)	0.0298 (4)
C18	0.3403 (3)	0.41804 (11)	0.35340 (17)	0.0353 (5)
H18	0.3262	0.4134	0.2803	0.042*
C19	0.2158 (2)	0.44676 (10)	0.39103 (18)	0.0367 (5)
C20	0.2354 (3)	0.45450 (11)	0.49643 (19)	0.0393 (5)
H20	0.1488	0.4747	0.5210	0.047*
C21	0.3834 (3)	0.43247 (10)	0.56634 (17)	0.0341 (5)
H21	0.3973	0.4380	0.6392	0.041*
N1	0.74610 (19)	0.18098 (8)	0.65692 (12)	0.0270 (3)
N2	0.48872 (19)	0.11518 (8)	0.61060 (12)	0.0267 (3)
O1	0.20766 (18)	0.04525 (8)	0.55414 (14)	0.0452 (4)
H1	0.2704	0.0806	0.5635	0.068*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0377 (3)	0.0436 (3)	0.0777 (5)	0.0068 (2)	−0.0176 (3)	−0.0032 (3)
Cl2	0.0522 (4)	0.0697 (4)	0.0373 (3)	0.0217 (3)	0.0197 (3)	0.0039 (3)
S1	0.0232 (2)	0.0250 (2)	0.0365 (3)	−0.00092 (18)	0.00423 (19)	0.0030 (2)
C1	0.0287 (10)	0.0234 (9)	0.0241 (9)	−0.0013 (7)	0.0073 (8)	0.0007 (7)
C2	0.0258 (9)	0.0246 (9)	0.0273 (9)	−0.0024 (7)	0.0062 (7)	0.0000 (8)
C3	0.0243 (9)	0.0249 (9)	0.0265 (9)	−0.0041 (7)	0.0044 (7)	0.0014 (7)
C4	0.0253 (9)	0.0280 (10)	0.0249 (9)	−0.0030 (7)	0.0060 (8)	0.0005 (8)
C5	0.0300 (10)	0.0261 (10)	0.0227 (9)	−0.0014 (7)	0.0063 (8)	−0.0001 (7)
C6	0.0290 (10)	0.0280 (10)	0.0343 (11)	−0.0027 (8)	0.0066 (8)	−0.0019 (8)
C7	0.0295 (11)	0.0358 (12)	0.0463 (12)	−0.0099 (9)	0.0081 (9)	−0.0037 (10)
C8	0.0458 (12)	0.0267 (10)	0.0385 (11)	−0.0121 (9)	0.0143 (10)	−0.0028 (9)
C9	0.0468 (13)	0.0247 (10)	0.0321 (11)	0.0003 (9)	0.0090 (9)	0.0022 (8)
C10	0.0301 (10)	0.0292 (10)	0.0306 (10)	−0.0007 (8)	0.0054 (8)	0.0014 (8)

C11	0.0229 (9)	0.0325 (11)	0.0445 (12)	−0.0022 (8)	0.0024 (9)	0.0002 (9)
C12	0.0365 (13)	0.087 (2)	0.0478 (15)	0.0051 (13)	−0.0041 (11)	−0.0078 (14)
C13	0.0311 (12)	0.0542 (15)	0.0726 (17)	−0.0014 (10)	0.0200 (12)	−0.0005 (13)
C14	0.0275 (12)	0.0427 (15)	0.139 (3)	−0.0083 (10)	−0.0015 (15)	0.0170 (17)
C15	0.0311 (10)	0.0249 (10)	0.0300 (10)	−0.0023 (8)	0.0047 (8)	0.0006 (8)
C16	0.0299 (10)	0.0206 (9)	0.0291 (10)	−0.0025 (7)	0.0072 (8)	0.0037 (8)
C17	0.0323 (10)	0.0249 (10)	0.0329 (10)	0.0020 (8)	0.0098 (9)	0.0025 (8)
C18	0.0385 (12)	0.0299 (11)	0.0333 (11)	−0.0010 (9)	0.0032 (9)	0.0000 (9)
C19	0.0277 (10)	0.0232 (10)	0.0504 (13)	−0.0009 (8)	−0.0037 (9)	0.0032 (9)
C20	0.0308 (11)	0.0320 (11)	0.0564 (14)	0.0034 (9)	0.0143 (10)	0.0001 (10)
C21	0.0390 (12)	0.0288 (10)	0.0366 (11)	0.0017 (8)	0.0141 (9)	0.0009 (8)
N1	0.0259 (8)	0.0240 (8)	0.0301 (8)	−0.0020 (6)	0.0059 (7)	0.0009 (6)
N2	0.0262 (8)	0.0240 (8)	0.0289 (8)	−0.0035 (6)	0.0060 (7)	0.0010 (6)
O1	0.0271 (8)	0.0296 (8)	0.0722 (11)	−0.0007 (6)	0.0024 (7)	0.0017 (8)

Geometric parameters (Å, °)

Cl1—C19	1.745 (2)	C11—C13	1.527 (3)
Cl2—C17	1.740 (2)	C11—C12	1.541 (3)
S1—C1	1.7168 (19)	C12—H12A	0.9800
S1—C3	1.7367 (18)	C12—H12B	0.9800
C1—N1	1.295 (2)	C12—H12C	0.9800
C1—N2	1.398 (2)	C13—H13A	0.9800
C2—C3	1.370 (3)	C13—H13B	0.9800
C2—N1	1.384 (2)	C13—H13C	0.9800
C2—C11	1.529 (3)	C14—H14A	0.9800
C3—C15	1.517 (3)	C14—H14B	0.9800
C4—N2	1.286 (2)	C14—H14C	0.9800
C4—C5	1.442 (3)	C15—C16	1.507 (3)
C4—H4	0.9500	C15—H15A	0.9900
C5—C10	1.405 (3)	C15—H15B	0.9900
C5—C6	1.411 (3)	C16—C17	1.391 (3)
C6—O1	1.348 (2)	C16—C21	1.391 (3)
C6—C7	1.394 (3)	C17—C18	1.387 (3)
C7—C8	1.379 (3)	C18—C19	1.381 (3)
C7—H7	0.9500	C18—H18	0.9500
C8—C9	1.380 (3)	C19—C20	1.374 (3)
C8—H8	0.9500	C20—C21	1.384 (3)
C9—C10	1.378 (3)	C20—H20	0.9500
C9—H9	0.9500	C21—H21	0.9500
C10—H10	0.9500	O1—H1	0.8400
C11—C14	1.512 (3)		
C1—S1—C3	89.22 (9)	H12A—C12—H12C	109.5
N1—C1—N2	126.57 (17)	H12B—C12—H12C	109.5
N1—C1—S1	115.33 (14)	C11—C13—H13A	109.5
N2—C1—S1	118.10 (13)	C11—C13—H13B	109.5
C3—C2—N1	114.54 (16)	H13A—C13—H13B	109.5
C3—C2—C11	130.90 (17)	C11—C13—H13C	109.5
N1—C2—C11	114.57 (16)	H13A—C13—H13C	109.5

C2—C3—C15	133.40 (17)	H13B—C13—H13C	109.5
C2—C3—S1	109.57 (14)	C11—C14—H14A	109.5
C15—C3—S1	116.97 (14)	C11—C14—H14B	109.5
N2—C4—C5	121.73 (17)	H14A—C14—H14B	109.5
N2—C4—H4	119.1	C11—C14—H14C	109.5
C5—C4—H4	119.1	H14A—C14—H14C	109.5
C10—C5—C6	118.38 (17)	H14B—C14—H14C	109.5
C10—C5—C4	119.79 (17)	C16—C15—C3	112.31 (16)
C6—C5—C4	121.82 (17)	C16—C15—H15A	109.1
O1—C6—C7	118.32 (18)	C3—C15—H15A	109.1
O1—C6—C5	121.51 (17)	C16—C15—H15B	109.1
C7—C6—C5	120.16 (19)	C3—C15—H15B	109.1
C8—C7—C6	119.5 (2)	H15A—C15—H15B	107.9
C8—C7—H7	120.2	C17—C16—C21	116.82 (18)
C6—C7—H7	120.2	C17—C16—C15	122.14 (17)
C7—C8—C9	121.40 (19)	C21—C16—C15	121.02 (18)
C7—C8—H8	119.3	C18—C17—C16	122.69 (18)
C9—C8—H8	119.3	C18—C17—Cl2	118.06 (16)
C10—C9—C8	119.60 (19)	C16—C17—Cl2	119.24 (15)
C10—C9—H9	120.2	C19—C18—C17	117.96 (19)
C8—C9—H9	120.2	C19—C18—H18	121.0
C9—C10—C5	120.95 (19)	C17—C18—H18	121.0
C9—C10—H10	119.5	C20—C19—C18	121.62 (19)
C5—C10—H10	119.5	C20—C19—Cl1	119.84 (17)
C14—C11—C13	107.9 (2)	C18—C19—Cl1	118.54 (17)
C14—C11—C2	114.02 (17)	C19—C20—C21	119.0 (2)
C13—C11—C2	108.69 (17)	C19—C20—H20	120.5
C14—C11—C12	111.3 (2)	C21—C20—H20	120.5
C13—C11—C12	107.29 (19)	C20—C21—C16	121.9 (2)
C2—C11—C12	107.46 (17)	C20—C21—H21	119.0
C11—C12—H12A	109.5	C16—C21—H21	119.0
C11—C12—H12B	109.5	C1—N1—C2	111.35 (15)
H12A—C12—H12B	109.5	C4—N2—C1	118.08 (16)
C11—C12—H12C	109.5	C6—O1—H1	109.5
C3—S1—C1—N1	0.42 (15)	N1—C2—C11—C12	−68.7 (2)
C3—S1—C1—N2	−178.71 (15)	C2—C3—C15—C16	159.3 (2)
N1—C2—C3—C15	176.90 (19)	S1—C3—C15—C16	−23.9 (2)
C11—C2—C3—C15	−2.5 (4)	C3—C15—C16—C17	−75.0 (2)
N1—C2—C3—S1	−0.1 (2)	C3—C15—C16—C21	103.3 (2)
C11—C2—C3—S1	−179.56 (17)	C21—C16—C17—C18	−0.1 (3)
C1—S1—C3—C2	−0.15 (14)	C15—C16—C17—C18	178.22 (18)
C1—S1—C3—C15	−177.72 (15)	C21—C16—C17—Cl2	179.24 (15)
N2—C4—C5—C10	−178.66 (18)	C15—C16—C17—Cl2	−2.4 (3)
N2—C4—C5—C6	2.7 (3)	C16—C17—C18—C19	−0.5 (3)
C10—C5—C6—O1	−178.73 (19)	Cl2—C17—C18—C19	−179.90 (16)
C4—C5—C6—O1	−0.1 (3)	C17—C18—C19—C20	0.8 (3)
C10—C5—C6—C7	0.3 (3)	C17—C18—C19—Cl1	−179.47 (15)
C4—C5—C6—C7	178.96 (18)	C18—C19—C20—C21	−0.4 (3)
O1—C6—C7—C8	179.2 (2)	Cl1—C19—C20—C21	179.86 (16)

C5—C6—C7—C8	0.1 (3)	C19—C20—C21—C16	−0.3 (3)
C6—C7—C8—C9	−0.1 (3)	C17—C16—C21—C20	0.5 (3)
C7—C8—C9—C10	−0.3 (3)	C15—C16—C21—C20	−177.82 (18)
C8—C9—C10—C5	0.7 (3)	N2—C1—N1—C2	178.49 (17)
C6—C5—C10—C9	−0.7 (3)	S1—C1—N1—C2	−0.6 (2)
C4—C5—C10—C9	−179.37 (18)	C3—C2—N1—C1	0.4 (2)
C3—C2—C11—C14	−13.1 (3)	C11—C2—N1—C1	179.96 (16)
N1—C2—C11—C14	167.5 (2)	C5—C4—N2—C1	−179.79 (16)
C3—C2—C11—C13	−133.5 (2)	N1—C1—N2—C4	−2.4 (3)
N1—C2—C11—C13	47.1 (2)	S1—C1—N2—C4	176.66 (14)
C3—C2—C11—C12	110.7 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2	0.84	1.87	2.611 (2)	147

Fig. 1

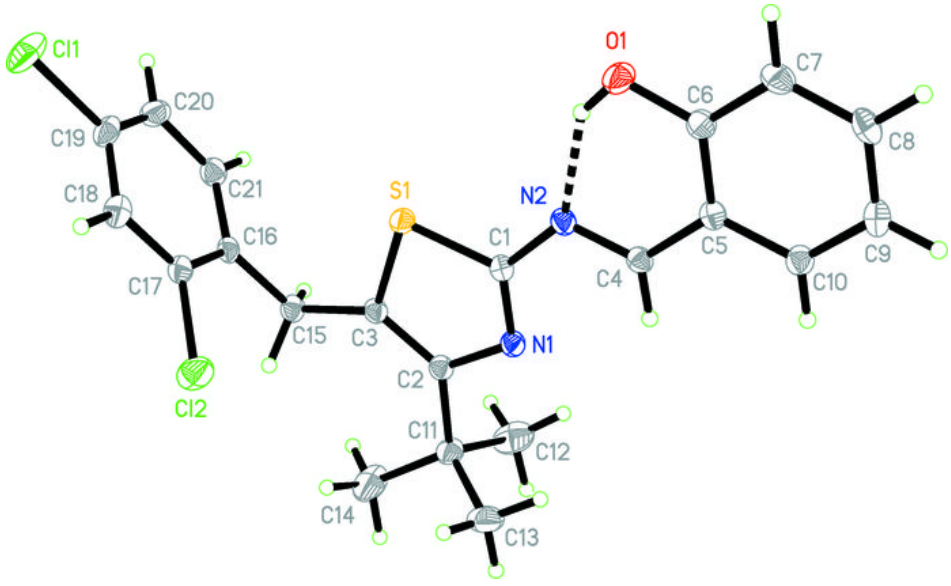
Cl1
C20
C19
C18
C21
C16
C17
Cl2
C15
C3
S1
C1
N2
O1
C6
C7
C8
C5
C9
C4
C10
N1
C2
C11
C12
C14
C13

Fig. 2