Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-Chloro-2-[1-(5-chloro-2-hydroxybenzyl)-1*H*-benzimidazol-2-yl]phenol

Xiao-Niu Fang,* Li-Min Liu, Gan-Sheng Huang and Ping Hu

College of Chemistry & Chemical Engineering, JingGangShan University, 343009 Ji'an, JiangXi, People's Republic of China
Correspondence e-mail: fangxiaoniu@163.com

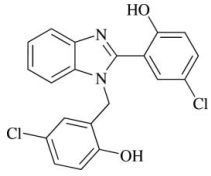
Received 14 November 2007; accepted 17 November 2007

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.067; wR factor = 0.211; data-to-parameter ratio = 18.7.

The title compound, $C_{20}H_{14}Cl_2N_2O_2$, was prepared by the one-step condensation of *o*-phenylenediamine with 5-chloro-2-hydroxybenzaldehyde. The dihedral angles between the benzimidaloe ring system and the benzene rings are 77.2 (2) and 87.1 (2)° Molecules are linked by O—H···N intermolecular hydrogen bonds, forming one-dimensional infinite chains, and the chains are linked by C—Cl···π(Ar) interactions, forming a two-dimensional network.

Related literature

For related literature, see: Boiani & Gonzalez (2005); Eltayeb *et al.* (2007); Jian *et al.* (2006); Sheikhshoaie *et al.* (2006); Spek (2003, 2005); Yang *et al.* (2004, 2006, 2007*a*,*b*); Yang, Han *et al.* (2007); Yang, Wang *et al.* (2007); Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{20}H_{14}Cl_2N_2O_2$
M_r = 385.23
Monoclinic, $P2_1/c$
a = 13.439 (2) Å
b = 8.9757 (7) Å
c = 18.811 (2) Å
β = 95.033 (1)°
V = 2260.4 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.30 mm^{-1}
T = 296 (2) K
0.25 × 0.20 × 0.13 mm

Data collection

Bruker APEX-II area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.92, T_{max} = 0.96
15245 measured reflections
4432 independent reflections
2296 reflections with $I > 2\sigma(I)$
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.211
S = 1.00
4432 reflections
237 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···N1^{i}	0.82	1.86	2.671 (3)	169
C20—H20···N2	0.93	2.62	2.923 (4)	100
C14—H14*B*···O2	0.97	2.38	2.723 (3)	100

Symmetry code: (i) $x, y+1, z$.

Table 2
C—Cl···π(Ar) interaction (Å, °).

C—Cl···π(Ar)	C—Cl	Cl···π(Ar)	C···π(Ar)	C—Cl···π(Ar)
C12—Cl1···*Cg*^{ii}	1.737 (4)	3.607 (2)	5.026 (4)	137.4 (2)

Symmetry codes: (ii) $x, \frac{3}{2}-y, \frac{1}{2}+z$. *Cg* is the centroid of atoms C1–C6.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *APEX2*; software used to prepare material for publication: *APEX2* and *publCIF* (Westrip, 2007).

The authors are grateful for the support of this work by the Natural Science Foundation of Jiangxi Province (No. 0620029).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2495).

References

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Boiani, M. & Gonzalez, M. (2005). *Mini Rev. Med. Chem.* **5**, 409–425.
Bruker (2004). *APEX2*. Version 1.22. Bruker AXS Inc., Madison, Wisconsin, USA.
Eltayeb, N. E., Teoh, S. G., Teh, J. B.-J., Fun, H.-K. & Ibrahim, K. (2007). *Acta Cryst.* E**63**, o465–o467.
Jian, F.-F., Yu, H.-Q., Qiao, Y.-B., Zhao, P.-S. & Xiao, H.-L. (2006). *Acta Cryst.* E**62**, o3608–o3609.
Sheikhshoaie, I., Belaj, F. & Fabian, W. M. F. (2006). *J. Mol. Struct.* **794**, 244–250.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Westrip, S. P. (2007). *publCIF*. Version 1.9.0_c. In preparation
Yang, S.-P., Han, L.-J., Wang, D.-Q. & Ding, T.-Z. (2007). *Acta Cryst.* E**63**, o365–o367.
Yang, X., Jones, R. A., Lai, R. J., waheed, A., Oye, M. M. & Holmes, A. L. (2006). *Polyhedron*, **25**, 881–887.
Yang, S.-P., Wang, D.-Q., Han, L.-J. & Xia, H.-T. (2007). *Acta Cryst.* E**63**, o3758.
Yang, H.-W., Yue, F., Feng, S., Wang, J.-D., Liu, A.-H., Chen, H.-M. & Yu, K.-B. (2004). *Chin. J. Org. Chem.* **24**, 792–796.

supplementary materials

Acta Cryst. (2007). E**63**, o4881 [**doi:10.1107/S160053680706014X**]

4-Chloro-2-[1-(5-chloro-2-hydroxybenzyl)-1*H*-benzimidazol-2-yl]phenol

X.-N. Fang, L.-M. Liu, G.-S. Huang and P. Hu

Comment

Benzimidazole derivatives and their metal complexes display wide-ranging biological activities in chemical and biological profiles, for example as antitumoral, antiparasitic, antifungal, anti-HIV, anticancer, antiviral and antimicrobial agents (Boiani *et al.*, 2005; Eltayeb *et al.* 2007). The benzimidazole derivatives can be prepared by one-step condensation of *o*-phenylenediamine with relative aromatic aldehyde (Yang *et al.*, 2004). Some similar structures have been reported previously for the derivatives of 2-chlorobenzaldehyde (Jian *et al.*, 2006), 4-chlorobenzaldehyde (Yang *et al.*, 2007*a*), 4-(dimethylamino)benzaldehyde (Sheikhshoaie *et al.*, 2006; Yang *et al.*, 2007*b*), 5-bromo-2-hydroxy-3-methoxybenzaldehyde (Yang *et al.*, 2006) and 8-methoxy-1-naphthaldehyde (Eltayeb *et al.*, 2007). Considering the biological importance of benzimidazole derivatives, we present here the crystal structure of the title compound (I).

In the crystal structure of (I) (Fig. 1), the C—C and C—N bond lengths are within normal ranges and comparable to values found by Yang *et al.* (2006). The benzimidazole system is essentially planar and well conjugated, with a dihedral angle of 0.6 (2)° between the planes of the benzene ring and its fused imidazole ring. The conformation of the overall molecule can be described by dihedral angles between the benzimidazole-ring and C8—C13 ring systems of 77.7 (2)°, and between the benzimidazole-ring and C15—C20 ring systems of 87.1 (2)°. The 5-chloro-2-hydroxybenzyl and 5-chloro-2-hydroxyphenyl groups make an angle of 86.7 (2)° with each other.

There are two kinds of weak intramolecular hydrogen bonds, C—H···O and C—H···N, which generate two *S*(5) ring motif (Bernstein *et al.*, 1995) in the molecule. The molecules of the title compound are linked by O2—H···N1^{i} hydrogen bonds, forming an one-dimensional infinite chains along the [010] direction (Fig. 2) [symmetry code: (i) *x*, *y* + 1, *z*]. No π-π interaction is found in the structure, whereas the chains are linked by C12—Cl1···π(Ar, the centroid^{ii} of C1—C6 ring) interaction to form two-dimensional networks (Fig. 3) [the distance of Cl···*Cg* is 3.6.7 (2)Å and the angle of C—Cl···*Cg* is 137.4 (2)°] [symmetry code: (ii) *x*, 1.5 − *y*, 1/2 + *z*]. The packing is further stabilized by van der Waals forces.

Experimental

A solution of 0.108 g (1 m mol) *o*-phenylenediamine, 0.313 g (2 m mol) 5-chloro-2-hydroxybenzaldehyde and 20 ml me thonal was heated for 1 h under reflux and ultrasonic radiation. The reaction mixture was then cooled and the pale yellow precipitate that had formed was filtered off with yield of 67%. Recrystallization of the crude product from ethanol solution resulted in single crystals of (I) suitable for X-ray diffraction analysis after several days.

Refinement

Some residual electron density in the accesible voids of the structure was difficult to model. The deepest hole in the final Fourier map is 3.81 Å from atom H14A. Therefore the SQUEEZE function of *PLATON* (Spek, 2003) was used to eliminate the contribution of the electron density in the solvent region from the intensity data, and the solvent-free model was employed

for the final refinement. The volume which is accessible for potential solvent molecules was calculated to be 643.0 A^3 and the total electron count per cell was calculated to be 106. Note that the calculated density, the F(000) value, the molecular weight and the formula are given without taking into account the results obtained with the SQUEEZE option in *PLATON* (Spek, 2003). All the H atoms were positioned in idealized locations and refined as riding on their carrier atoms, with O—H distances of 0.82 (hydroxyl), C—H distances of 0.93 (aryl) and 0.97Å (methylene) with $U_{iso}(H) = 1.5U_{eq}(O)$ for hydroxyl, $U_{iso}(H) = 1.2U_{eq}(C)$ for the other atoms.

Figures

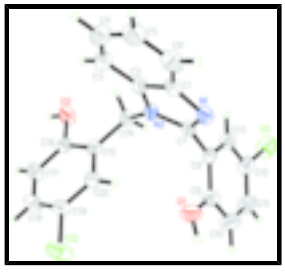


Fig. 1. Molecular structure of (I), showing 25% probability displacement ellipsoids.

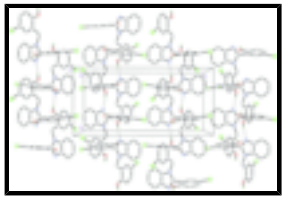


Fig. 2. The packing diagram of (I), viewed down the *a* axis, All the non-hydroxyl H atoms have been omitted for clarity.

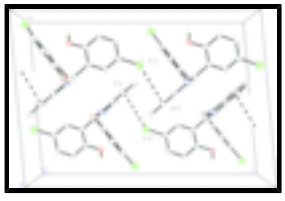


Fig. 3. The C—Cl···π(Ar) interaction in the packing of (I), viewed down the *b* axis., All the non-hydroxyl H atoms have been omitted for clarity.

4-Chloro-2-[1-(5-chloro-2-hydroxybenzyl)-1*H*-benzimidazol-2-yl]phenol

Crystal data

$C_{20}H_{14}Cl_2N_2O_2$	F_{000} = 792
M_r = 385.23	D_x = 1.132 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1705 reflections
a = 13.4393 (11) Å	θ = 2.2–18.8º
b = 8.9757 (7) Å	μ = 0.30 mm^{-1}
c = 18.8114 (15) Å	T = 296 (2) K
β = 95.0330 (10)º	Block, pale yellow
V = 2260.4 (3) $Å^3$	0.25 × 0.20 × 0.13 mm
Z = 4	

Data collection

Bruker APEX-II area-detector diffractometer	4432 independent reflections
Radiation source: fine-focus sealed tube	2296 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.052$
$T = 296(2)$ K	$\theta_{max} = 26.0°$
φ and ω scan	$\theta_{min} = 2.2°$
Absorption correction: multi-scan (SADABS; Bruker, 2004)	$h = -16\rightarrow16$
$T_{min} = 0.92$, $T_{max} = 0.96$	$k = -11\rightarrow11$
15245 measured reflections	$l = -23\rightarrow22$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.067$	H-atom parameters constrained
$wR(F^2) = 0.211$	$w = 1/[\sigma^2(F_o^2) + (0.1107P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} < 0.001$
4432 reflections	$\Delta\rho_{max} = 0.44$ e Å^{-3}
237 parameters	$\Delta\rho_{min} = -0.28$ 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}
C1	0.5263 (2)	0.6889 (4)	0.13250 (17)	0.0565 (8)
C2	0.5229 (2)	0.8419 (3)	0.13514 (17)	0.0555 (8)
C3	0.4650 (3)	0.9273 (5)	0.0858 (2)	0.0778 (11)
H3	0.4635	1.0308	0.0876	0.093*
C4	0.4096 (3)	0.8459 (7)	0.0334 (3)	0.1001 (15)

H4	0.3701	0.8976	−0.0014	0.120*
C5	0.4101 (3)	0.6935 (6)	0.0304 (2)	0.0961 (14)
H5	0.3702	0.6452	−0.0053	0.115*
C6	0.4682 (3)	0.6112 (5)	0.0790 (2)	0.0787 (11)
H6	0.4692	0.5077	0.0768	0.094*
C7	0.6265 (2)	0.7535 (3)	0.22244 (17)	0.0496 (8)
C8	0.6978 (2)	0.7501 (3)	0.28621 (19)	0.0553 (8)
C9	0.7996 (3)	0.7232 (4)	0.2781 (2)	0.0681 (9)
C10	0.8665 (3)	0.7139 (5)	0.3379 (3)	0.0919 (13)
H10	0.9334	0.6940	0.3328	0.110*
C11	0.8351 (4)	0.7338 (5)	0.4053 (2)	0.0891 (13)
H11	0.8810	0.7299	0.4452	0.107*
C12	0.7351 (3)	0.7595 (4)	0.4129 (2)	0.0746 (11)
C13	0.6678 (3)	0.7696 (3)	0.35376 (19)	0.0640 (9)
H13	0.6011	0.7898	0.3594	0.077*
C14	0.6075 (2)	1.0372 (3)	0.21725 (18)	0.0586 (8)
H14A	0.6327	1.0355	0.2672	0.070*
H14B	0.5449	1.0917	0.2136	0.070*
C15	0.6809 (2)	1.1189 (3)	0.17565 (15)	0.0507 (8)
C16	0.6782 (2)	1.2735 (3)	0.17478 (18)	0.0558 (8)
C17	0.7485 (3)	1.3551 (4)	0.14095 (19)	0.0702 (10)
H17	0.7477	1.4587	0.1419	0.084*
C18	0.8192 (3)	1.2801 (4)	0.1061 (2)	0.0731 (10)
H18	0.8658	1.3337	0.0827	0.088*
C19	0.8219 (2)	1.1288 (4)	0.10552 (18)	0.0643 (9)
C20	0.7541 (2)	1.0472 (4)	0.14033 (17)	0.0589 (8)
H20	0.7572	0.9437	0.1402	0.071*
Cl1	0.69503 (11)	0.78143 (16)	0.49766 (6)	0.1145 (5)
Cl2	0.91134 (8)	1.03568 (13)	0.06080 (7)	0.1035 (5)
N1	0.59146 (19)	0.6339 (3)	0.18823 (14)	0.0554 (7)
N2	0.58792 (18)	0.8822 (3)	0.19284 (13)	0.0505 (6)
O1	0.82533 (19)	0.7035 (3)	0.21081 (14)	0.0859 (8)
H1	0.8828	0.6724	0.2121	0.129*
O2	0.60531 (19)	1.3402 (2)	0.20982 (14)	0.0739 (7)
H2	0.6091	1.4309	0.2055	0.111*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.059 (2)	0.0566 (19)	0.056 (2)	−0.0079 (15)	0.0133 (17)	0.0022 (16)
C2	0.059 (2)	0.0490 (19)	0.059 (2)	−0.0008 (15)	0.0104 (17)	0.0079 (15)
C3	0.082 (3)	0.082 (3)	0.068 (2)	0.003 (2)	0.001 (2)	0.017 (2)
C4	0.078 (3)	0.136 (4)	0.083 (3)	−0.004 (3)	−0.011 (2)	0.032 (3)
C5	0.090 (3)	0.127 (4)	0.068 (3)	−0.031 (3)	−0.013 (2)	0.005 (3)
C6	0.087 (3)	0.081 (3)	0.068 (3)	−0.023 (2)	0.012 (2)	−0.016 (2)
C7	0.0498 (17)	0.0387 (16)	0.062 (2)	0.0024 (13)	0.0130 (15)	0.0054 (14)
C8	0.059 (2)	0.0398 (16)	0.067 (2)	0.0034 (14)	0.0061 (17)	0.0029 (14)
C9	0.064 (2)	0.072 (2)	0.070 (2)	0.0080 (18)	0.0109 (19)	0.0053 (18)

C10	0.063 (3)	0.122 (4)	0.089 (3)	0.017 (2)	−0.003 (2)	0.009 (3)
C11	0.088 (3)	0.106 (3)	0.070 (3)	0.013 (2)	−0.015 (2)	0.008 (2)
C12	0.085 (3)	0.074 (2)	0.064 (2)	0.014 (2)	0.003 (2)	0.0025 (18)
C13	0.070 (2)	0.057 (2)	0.065 (2)	0.0086 (16)	0.0091 (19)	0.0035 (16)
C14	0.066 (2)	0.0409 (18)	0.071 (2)	0.0042 (14)	0.0166 (17)	−0.0015 (14)
C15	0.0566 (19)	0.0449 (18)	0.0500 (18)	−0.0037 (14)	0.0006 (15)	−0.0015 (13)
C16	0.055 (2)	0.052 (2)	0.061 (2)	0.0017 (15)	0.0071 (16)	−0.0013 (15)
C17	0.081 (3)	0.055 (2)	0.077 (2)	−0.0106 (18)	0.016 (2)	−0.0008 (17)
C18	0.065 (2)	0.079 (3)	0.078 (3)	−0.0224 (19)	0.018 (2)	−0.0074 (19)
C19	0.051 (2)	0.070 (2)	0.073 (2)	−0.0088 (17)	0.0127 (17)	−0.0137 (17)
C20	0.058 (2)	0.0500 (19)	0.069 (2)	−0.0010 (15)	0.0065 (17)	−0.0065 (15)
Cl1	0.1381 (11)	0.1426 (11)	0.0631 (7)	0.0356 (8)	0.0100 (7)	0.0012 (6)
Cl2	0.0804 (7)	0.1029 (9)	0.1341 (10)	−0.0098 (6)	0.0470 (7)	−0.0360 (7)
N1	0.0611 (16)	0.0391 (14)	0.0673 (17)	−0.0018 (12)	0.0122 (14)	−0.0035 (12)
N2	0.0555 (15)	0.0396 (14)	0.0567 (16)	−0.0010 (11)	0.0069 (13)	0.0048 (11)
O1	0.0631 (16)	0.116 (2)	0.0796 (19)	0.0126 (15)	0.0140 (14)	0.0064 (15)
O2	0.0855 (17)	0.0362 (12)	0.1045 (19)	0.0031 (11)	0.0339 (15)	−0.0008 (12)

Geometric parameters (Å, °)

C1—C2	1.375 (5)	C11—H11	0.9300
C1—N1	1.396 (4)	C12—C13	1.374 (5)
C1—C6	1.404 (5)	C12—Cl1	1.737 (4)
C2—N2	1.381 (4)	C13—H13	0.9300
C2—C3	1.389 (5)	C14—N2	1.482 (4)
C3—C4	1.388 (6)	C14—C15	1.503 (4)
C3—H3	0.9300	C14—H14A	0.9700
C4—C5	1.369 (7)	C14—H14B	0.9700
C4—H4	0.9300	C15—C16	1.388 (4)
C5—C6	1.366 (6)	C15—C20	1.392 (4)
C5—H5	0.9300	C16—O2	1.367 (4)
C6—H6	0.9300	C16—C17	1.392 (4)
C7—N1	1.317 (4)	C17—C18	1.376 (5)
C7—N2	1.365 (4)	C17—H17	0.9300
C7—C8	1.468 (5)	C18—C19	1.359 (5)
C8—C13	1.378 (5)	C18—H18	0.9300
C8—C9	1.411 (5)	C19—C20	1.379 (4)
C9—O1	1.353 (4)	C19—Cl2	1.740 (3)
C9—C10	1.379 (5)	C20—H20	0.9300
C10—C11	1.382 (6)	O1—H1	0.8200
C10—H10	0.9300	O2—H2	0.8200
C11—C12	1.384 (6)		
C2—C1—N1	110.3 (3)	C13—C12—Cl1	120.0 (3)
C2—C1—C6	120.3 (3)	C11—C12—Cl1	119.8 (3)
N1—C1—C6	129.4 (3)	C12—C13—C8	120.9 (4)
C1—C2—N2	105.6 (3)	C12—C13—H13	119.5
C1—C2—C3	123.1 (3)	C8—C13—H13	119.5
N2—C2—C3	131.3 (3)	N2—C14—C15	113.8 (2)
C4—C3—C2	114.7 (4)	N2—C14—H14A	108.8

C4—C3—H3	122.6	C15—C14—H14A	108.8
C2—C3—H3	122.6	N2—C14—H14B	108.8
C5—C4—C3	123.4 (4)	C15—C14—H14B	108.8
C5—C4—H4	118.3	H14A—C14—H14B	107.7
C3—C4—H4	118.3	C16—C15—C20	118.4 (3)
C6—C5—C4	121.2 (4)	C16—C15—C14	118.4 (3)
C6—C5—H5	119.4	C20—C15—C14	123.1 (3)
C4—C5—H5	119.4	O2—C16—C15	116.8 (3)
C5—C6—C1	117.4 (4)	O2—C16—C17	122.3 (3)
C5—C6—H6	121.3	C15—C16—C17	120.9 (3)
C1—C6—H6	121.3	C18—C17—C16	119.0 (3)
N1—C7—N2	112.6 (3)	C18—C17—H17	120.5
N1—C7—C8	124.2 (3)	C16—C17—H17	120.5
N2—C7—C8	123.2 (3)	C19—C18—C17	120.9 (3)
C13—C8—C9	119.1 (3)	C19—C18—H18	119.6
C13—C8—C7	121.9 (3)	C17—C18—H18	119.6
C9—C8—C7	119.0 (3)	C18—C19—C20	120.5 (3)
O1—C9—C10	123.6 (4)	C18—C19—Cl2	120.3 (3)
O1—C9—C8	116.9 (3)	C20—C19—Cl2	119.2 (3)
C10—C9—C8	119.4 (4)	C19—C20—C15	120.3 (3)
C9—C10—C11	120.7 (4)	C19—C20—H20	119.8
C9—C10—H10	119.6	C15—C20—H20	119.8
C11—C10—H10	119.6	C7—N1—C1	104.6 (2)
C10—C11—C12	119.6 (4)	C7—N2—C2	106.9 (2)
C10—C11—H11	120.2	C7—N2—C14	128.1 (3)
C12—C11—H11	120.2	C2—N2—C14	124.9 (3)
C13—C12—C11	120.2 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···N1^{i}	0.82	1.86	2.671 (3)	169
C20—H20···N2	0.93	2.62	2.923 (4)	100
C14—H14B···O2	0.97	2.38	2.723 (3)	100

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

C—Cl···π(Ar) interaction (Å, °)

C—Cl···π(Ar)	C—Cl	Cl···π(Ar)	C···π(Ar)	C—Cl···π(Ar)
C12—Cl1··· *Cg*^{ii}	1.737 (4)	3.607 (2)	5.026 (4)	137.4 (2)

Symmetry codes: (ii) *x*, 3/2 − *y*, 1/2 + *z*. *Cg* is the centroid of atoms C1–C6.

Fig. 1

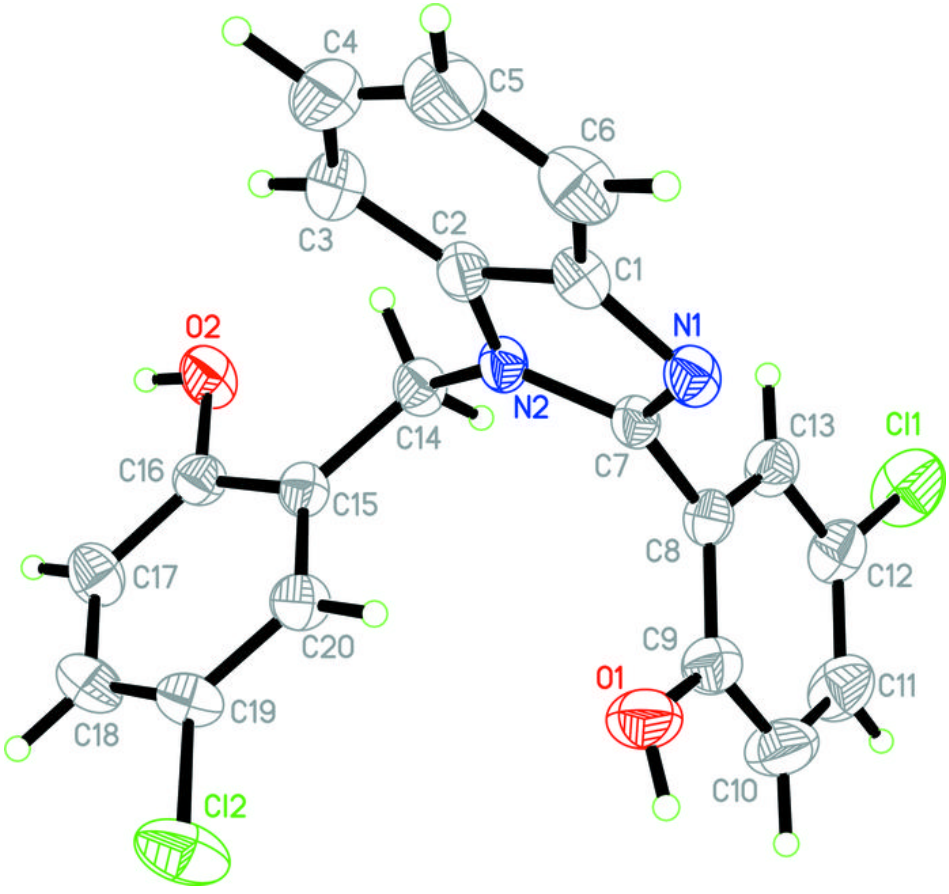

C4
C5
C6
C3
C2
C1
O2
N1
N2
C14
C7
C13
Cl1
C16
C15
C8
C12
C17
C20
C9
O1
C11
C19
C18
C10
Cl2

Fig. 2

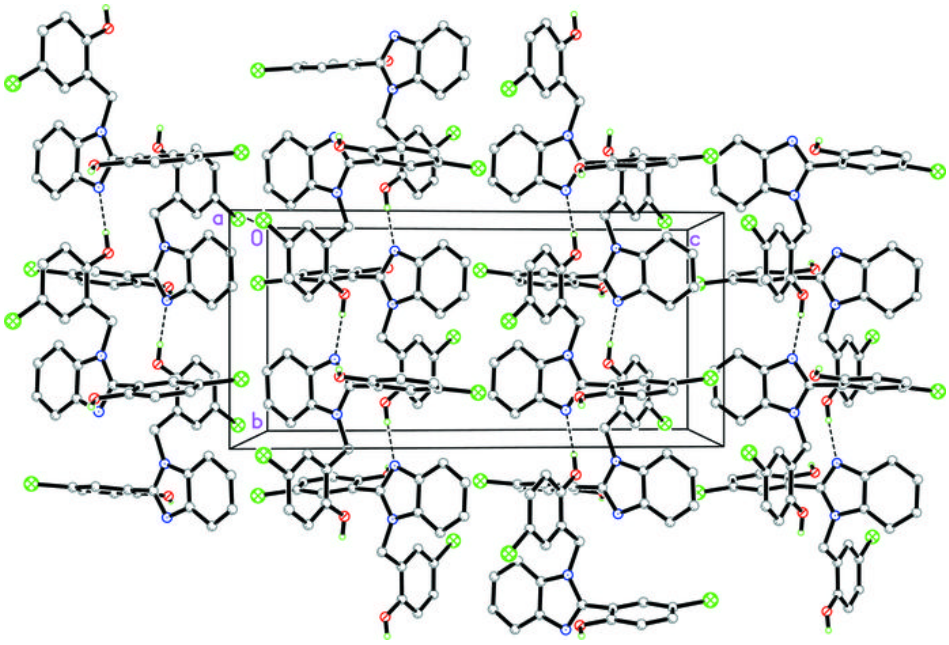


Fig. 3