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1-(4-Chlorobenzyl)-2-(4-chlorophenyl)-1*H*-benzimidazole

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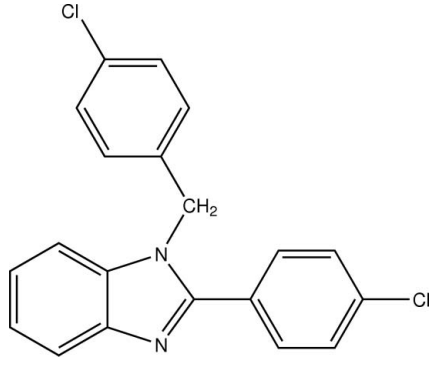
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.042; wR factor = 0.086; data-to-parameter ratio = 12.7.

In the title compound, $C_{20}H_{14}Cl_2N_2$, the dihedral angles formed by the benzimidazole ring with the benzene rings of the 4-chlorobenzyl and the 4-chlorophenyl groups are 88.15 (8) and 33.4 (1)°, respectively. The molecules are linked by C—H···Cl hydrogen bonds, forming a $C(12)$ chain along the [010] direction.

Related literature

For related literature, see: Bernstein *et al.* (1995); Ishida *et al.* (2006); Özden *et al.* (2005); Xu *et al.* (2006); Yang *et al.* (2007).



Experimental

Crystal data

$C_{20}H_{14}Cl_2N_2$
M_r = 353.23
Monoclinic, $P2_1$
a = 11.6427 (17) Å
b = 5.4420 (7) Å
c = 13.2339 (19) Å
β = 90.936 (2)°
V = 838.4 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.39 mm^{-1}
T = 298 (2) K
0.48 × 0.23 × 0.15 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.835, T_{max} = 0.944
4248 measured reflections
2749 independent reflections
1744 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.086
S = 1.02
2749 reflections
217 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Absolute structure: Flack (1983), 1102 Freidel pairs
Flack parameter: −0.01 (8)

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

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11···Cl1^{i}	0.93	2.79	3.701 (4)	167

Symmetry code: (i) $-x+1, y+\frac{3}{2}, -z+1$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); 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: AT2364).

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supplementary materials

Acta Cryst. (2007). E**63**, o3758 [**doi:10.1107/S1600536807038871**]

1-(4-Chlorobenzyl)-2-(4-chlorophenyl)-1*H*-benzimidazole

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Comment

Benzimidazole derivatives display wide-ranging biological activities, such as as inhibitors of hepatitis C virus NS5B polymerase (Ishida *et al.*, 2006) and heparanase (Xu *et al.*, 2006) and antimicrobial activities (Özden *et al.*, 2005). The crystal structures of some benzimidazole derivatives have been previously reported (Yang *et al.*, 2007). Here we report the crystal structure of a new benzimidazole derivative, 2-(4-chlorophenyl)-1-[(4-chlorophenyl)methyl]-1*H* benzimidazole, (I).

In the molecule of compound (I) (Fig. 1), the benzene ring C9—C14 is approximately perpendicular to the benzimidazole ring. The dihedral angles enclosed by the benzimidazole ring with the benzene rings C9–C14 and benzene ring C15–C20 are 88.15 (8)° and 33.4 (1)°, respectively. The geometrical parameters for (I) are normal.

In the crystal structure of (I), the C11 atom in the molecule at (*x*, *y*, *z*) acts as hydrogen-bond donor, to the Cl1 atom in the molecule at (1 − *x*, 3/2 + *y*, 1 − *z*), the molecules are linked through C—H···Cl hydrogen bonds, forming a C(12) chain (Bernstein *et al.*, 1995) along the [010] direction (Fig. 2 and Table 1).

Experimental

The reaction mixture containing 4-chlorobenzaldehyde (2.80 g, 20 mmol) and *o*-phenylene diamine (1.08 g, 10 mmol) was refluxed for about 4 h in ethanol (30 ml), then cooled and the product filtered off, washed with ethanol and dried. Yellow crystals of (I) suitable for X-ray structure analysis were obtained by recrystallizing the crude product from ethanol (m.p. 450–452 K).

Refinement

All H atoms were positioned geometrically and refined as riding on their parent atoms, with C—H = 0.93–0.97Å and U_{iso}(H) = 1.2U_{eq}(C) for all H atoms.

Figures

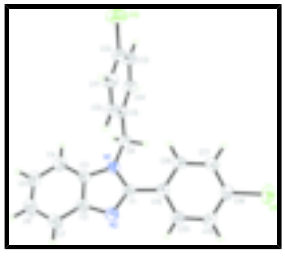

Fig. 1. The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

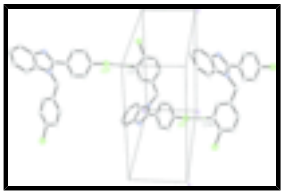

Fig. 2. Part of the crystal structure of (I), showing the formation of a C(12) chain along the [010] direction. For clarity, the H atoms not involved in the motif shown have been omitted. [Symmetry codes: (*) 1 − *x*, 3/2 + *y*, 1 − *z*; (&) 1 − *x*, −3/2 + *y*, 1 − *z*]. Dashed lines indicate hydrogen bonds.

1-(4-Chlorobenzyl)-2-(4-chlorophenyl)-1*H*-benzimidazole

Crystal data

$C_{20}H_{14}Cl_2N_2$	F_{000} = 364
M_r = 353.23	D_x = 1.399 Mg m^{-3}
Monoclinic, $P2_1$	Melting point: 450 K
Hall symbol: P 2yb	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 11.6427 (17) Å	Cell parameters from 1152 reflections
b = 5.4420 (7) Å	θ = 2.3–21.3º
c = 13.2339 (19) Å	μ = 0.39 mm^{-1}
β = 90.936 (2)º	*T* = 298 (2) K
V = 838.4 (2) Å^3	Plate, yellow
Z = 2	0.48 × 0.23 × 0.15 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	2749 independent reflections
Radiation source: fine-focus sealed tube	1744 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.029
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.5º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −10→13
T_{min} = 0.835, T_{max} = 0.944	*k* = −6→6
4248 measured reflections	*l* = −15→15

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.042	$w = 1/[\sigma^2(F_o^2) + (0.0295P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.086	$(\Delta/\sigma)_{max} < 0.001$
S = 1.02	$\Delta\rho_{max}$ = 0.23 e Å^{-3}
2749 reflections	$\Delta\rho_{min}$ = −0.18 e Å^{-3}
217 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), 1102 Freidel pairs

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Flack parameter: −0.01 (8)

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	0.33404 (9)	0.0815 (2)	0.63346 (7)	0.0884 (4)
Cl2	0.75909 (8)	1.0489 (3)	0.12846 (9)	0.1146 (5)
N1	0.2015 (2)	0.8712 (5)	0.24471 (19)	0.0480 (7)
N2	0.0955 (2)	1.0188 (6)	0.3711 (2)	0.0587 (8)
C1	0.1724 (3)	0.8546 (7)	0.3452 (2)	0.0481 (9)
C2	0.0722 (3)	1.1501 (6)	0.2833 (3)	0.0549 (10)
C3	0.1370 (2)	1.0590 (7)	0.2042 (2)	0.0499 (8)
C4	0.1289 (3)	1.1528 (7)	0.1067 (3)	0.0618 (10)
H4	0.1722	1.0892	0.0543	0.074*
C5	0.0540 (3)	1.3436 (8)	0.0918 (3)	0.0710 (12)
H5	0.0457	1.4107	0.0274	0.085*
C6	−0.0100 (3)	1.4397 (8)	0.1699 (4)	0.0788 (13)
H6	−0.0592	1.5710	0.1568	0.095*
C7	−0.0027 (3)	1.3453 (8)	0.2671 (3)	0.0698 (11)
H7	−0.0460	1.4099	0.3192	0.084*
C8	0.2738 (3)	0.7104 (6)	0.1855 (2)	0.0545 (9)
H8A	0.2384	0.6883	0.1193	0.065*
H8B	0.2772	0.5507	0.2180	0.065*
C9	0.3948 (3)	0.8033 (6)	0.1723 (2)	0.0439 (8)
C10	0.4364 (3)	1.0114 (7)	0.2183 (2)	0.0596 (10)
H10	0.3889	1.1036	0.2595	0.071*
C11	0.5489 (3)	1.0852 (8)	0.2038 (3)	0.0680 (10)
H11	0.5764	1.2271	0.2350	0.082*
C12	0.6190 (3)	0.9516 (8)	0.1443 (3)	0.0657 (11)
C13	0.5794 (3)	0.7433 (8)	0.0987 (3)	0.0681 (11)
H13	0.6278	0.6500	0.0587	0.082*
C14	0.4680 (3)	0.6721 (6)	0.1120 (2)	0.0579 (10)
H14	0.4410	0.5315	0.0795	0.069*
C15	0.2178 (3)	0.6688 (6)	0.4160 (2)	0.0506 (9)
C16	0.3296 (3)	0.5778 (8)	0.4130 (2)	0.0588 (9)

H16	0.3803	0.6379	0.3653	0.071*
C17	0.3657 (3)	0.3989 (7)	0.4805 (3)	0.0642 (11)
H17	0.4397	0.3357	0.4772	0.077*
C18	0.2917 (3)	0.3150 (7)	0.5521 (2)	0.0579 (10)
C19	0.1828 (3)	0.4092 (7)	0.5594 (3)	0.0609 (10)
H19	0.1339	0.3547	0.6096	0.073*
C20	0.1469 (3)	0.5865 (8)	0.4911 (2)	0.0587 (9)
H20	0.0734	0.6515	0.4959	0.070*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1053 (8)	0.0830 (8)	0.0764 (6)	0.0009 (8)	−0.0143 (6)	0.0255 (6)
Cl2	0.0583 (6)	0.1482 (13)	0.1377 (9)	−0.0234 (9)	0.0129 (6)	0.0186 (10)
N1	0.0442 (16)	0.049 (2)	0.0513 (17)	−0.0001 (15)	−0.0003 (13)	0.0016 (16)
N2	0.0527 (17)	0.062 (2)	0.0609 (18)	0.0069 (18)	0.0037 (15)	−0.0004 (17)
C1	0.041 (2)	0.052 (2)	0.051 (2)	−0.0077 (19)	0.0021 (17)	0.0018 (19)
C2	0.042 (2)	0.055 (3)	0.067 (2)	−0.0033 (19)	−0.0052 (19)	−0.001 (2)
C3	0.0389 (18)	0.048 (2)	0.063 (2)	−0.006 (2)	−0.0093 (17)	0.002 (2)
C4	0.056 (2)	0.065 (3)	0.064 (2)	−0.012 (2)	−0.0116 (18)	0.007 (2)
C5	0.062 (3)	0.066 (3)	0.084 (3)	−0.012 (2)	−0.022 (2)	0.019 (3)
C6	0.057 (3)	0.061 (3)	0.118 (4)	−0.002 (2)	−0.027 (3)	0.014 (3)
C7	0.054 (2)	0.063 (3)	0.092 (3)	0.006 (2)	−0.002 (2)	−0.005 (2)
C8	0.060 (2)	0.050 (2)	0.053 (2)	−0.006 (2)	−0.0035 (18)	−0.0054 (18)
C9	0.048 (2)	0.043 (2)	0.0409 (18)	−0.0019 (18)	−0.0019 (16)	0.0008 (17)
C10	0.059 (2)	0.052 (3)	0.068 (2)	−0.004 (2)	0.0028 (19)	−0.013 (2)
C11	0.062 (2)	0.055 (3)	0.086 (3)	−0.022 (2)	−0.004 (2)	−0.010 (2)
C12	0.052 (2)	0.080 (3)	0.065 (3)	−0.002 (2)	0.004 (2)	0.013 (2)
C13	0.067 (3)	0.074 (3)	0.063 (2)	0.008 (2)	0.013 (2)	−0.003 (2)
C14	0.069 (2)	0.054 (3)	0.051 (2)	−0.003 (2)	0.0039 (19)	−0.0112 (18)
C15	0.052 (2)	0.054 (3)	0.0457 (19)	−0.0022 (19)	−0.0030 (17)	−0.0044 (18)
C16	0.048 (2)	0.067 (3)	0.061 (2)	0.001 (2)	0.0053 (17)	0.012 (2)
C17	0.054 (2)	0.069 (3)	0.069 (2)	0.009 (2)	−0.002 (2)	0.005 (2)
C18	0.066 (2)	0.058 (3)	0.049 (2)	−0.004 (2)	−0.0115 (19)	0.005 (2)
C19	0.061 (2)	0.069 (3)	0.052 (2)	−0.010 (2)	0.0045 (19)	0.003 (2)
C20	0.050 (2)	0.073 (3)	0.053 (2)	0.003 (2)	0.0017 (17)	0.005 (2)

Geometric parameters (Å, °)

Cl1—C18	1.732 (4)	C9—C10	1.371 (4)
Cl2—C12	1.731 (4)	C9—C14	1.377 (4)
N1—C3	1.373 (4)	C10—C11	1.387 (4)
N1—C1	1.381 (3)	C10—H10	0.9300
N1—C8	1.453 (4)	C11—C12	1.354 (5)
N2—C1	1.314 (4)	C11—H11	0.9300
N2—C2	1.387 (4)	C12—C13	1.361 (5)
C1—C15	1.471 (4)	C13—C14	1.368 (4)
C2—C7	1.388 (5)	C13—H13	0.9300
C2—C3	1.392 (4)	C14—H14	0.9300

C3—C4	1.389 (4)	C15—C20	1.376 (4)
C4—C5	1.369 (5)	C15—C16	1.394 (4)
C4—H4	0.9300	C16—C17	1.382 (5)
C5—C6	1.387 (5)	C16—H16	0.9300
C5—H5	0.9300	C17—C18	1.369 (4)
C6—C7	1.386 (5)	C17—H17	0.9300
C6—H6	0.9300	C18—C19	1.373 (4)
C7—H7	0.9300	C19—C20	1.382 (5)
C8—C9	1.509 (4)	C19—H19	0.9300
C8—H8A	0.9700	C20—H20	0.9300
C8—H8B	0.9700		
C3—N1—C1	106.5 (3)	C9—C10—C11	120.4 (3)
C3—N1—C8	123.8 (3)	C9—C10—H10	119.8
C1—N1—C8	129.3 (3)	C11—C10—H10	119.8
C1—N2—C2	104.9 (3)	C12—C11—C10	120.3 (4)
N2—C1—N1	112.7 (3)	C12—C11—H11	119.8
N2—C1—C15	122.8 (3)	C10—C11—H11	119.8
N1—C1—C15	124.5 (3)	C11—C12—C13	120.1 (4)
N2—C2—C7	129.6 (4)	C11—C12—Cl2	119.0 (4)
N2—C2—C3	110.2 (3)	C13—C12—Cl2	120.9 (3)
C7—C2—C3	120.2 (3)	C12—C13—C14	119.6 (4)
N1—C3—C4	131.7 (3)	C12—C13—H13	120.2
N1—C3—C2	105.7 (3)	C14—C13—H13	120.2
C4—C3—C2	122.6 (4)	C13—C14—C9	121.7 (3)
C5—C4—C3	116.5 (4)	C13—C14—H14	119.2
C5—C4—H4	121.8	C9—C14—H14	119.2
C3—C4—H4	121.8	C20—C15—C16	118.4 (3)
C4—C5—C6	121.9 (4)	C20—C15—C1	118.0 (3)
C4—C5—H5	119.1	C16—C15—C1	123.5 (3)
C6—C5—H5	119.1	C17—C16—C15	120.4 (3)
C7—C6—C5	121.7 (4)	C17—C16—H16	119.8
C7—C6—H6	119.1	C15—C16—H16	119.8
C5—C6—H6	119.1	C18—C17—C16	119.6 (3)
C6—C7—C2	117.2 (4)	C18—C17—H17	120.2
C6—C7—H7	121.4	C16—C17—H17	120.2
C2—C7—H7	121.4	C17—C18—C19	121.1 (3)
N1—C8—C9	114.2 (3)	C17—C18—Cl1	119.9 (3)
N1—C8—H8A	108.7	C19—C18—Cl1	118.9 (3)
C9—C8—H8A	108.7	C18—C19—C20	118.9 (3)
N1—C8—H8B	108.7	C18—C19—H19	120.5
C9—C8—H8B	108.7	C20—C19—H19	120.5
H8A—C8—H8B	107.6	C15—C20—C19	121.4 (3)
C10—C9—C14	117.9 (3)	C15—C20—H20	119.3
C10—C9—C8	123.4 (3)	C19—C20—H20	119.3
C14—C9—C8	118.7 (3)		
C2—N2—C1—N1	0.3 (4)	N1—C8—C9—C14	−175.9 (3)
C2—N2—C1—C15	−177.5 (3)	C14—C9—C10—C11	0.1 (5)
C3—N1—C1—N2	−0.6 (3)	C8—C9—C10—C11	179.3 (3)

C8—N1—C1—N2	−173.5 (3)	C9—C10—C11—C12	−0.4 (5)
C3—N1—C1—C15	177.1 (3)	C10—C11—C12—C13	−0.2 (5)
C8—N1—C1—C15	4.3 (5)	C10—C11—C12—Cl2	−179.7 (3)
C1—N2—C2—C7	180.0 (3)	C11—C12—C13—C14	1.0 (6)
C1—N2—C2—C3	0.2 (4)	Cl2—C12—C13—C14	−179.5 (3)
C1—N1—C3—C4	−178.3 (3)	C12—C13—C14—C9	−1.3 (5)
C8—N1—C3—C4	−5.0 (5)	C10—C9—C14—C13	0.8 (5)
C1—N1—C3—C2	0.7 (3)	C8—C9—C14—C13	−178.5 (3)
C8—N1—C3—C2	174.0 (3)	N2—C1—C15—C20	30.5 (5)
N2—C2—C3—N1	−0.6 (3)	N1—C1—C15—C20	−147.0 (3)
C7—C2—C3—N1	179.6 (3)	N2—C1—C15—C16	−147.4 (3)
N2—C2—C3—C4	178.5 (3)	N1—C1—C15—C16	35.1 (5)
C7—C2—C3—C4	−1.3 (5)	C20—C15—C16—C17	3.7 (5)
N1—C3—C4—C5	179.5 (3)	C1—C15—C16—C17	−178.4 (3)
C2—C3—C4—C5	0.6 (5)	C15—C16—C17—C18	−1.5 (5)
C3—C4—C5—C6	0.4 (5)	C16—C17—C18—C19	−1.3 (5)
C4—C5—C6—C7	−0.9 (6)	C16—C17—C18—Cl1	177.3 (3)
C5—C6—C7—C2	0.3 (5)	C17—C18—C19—C20	1.9 (5)
N2—C2—C7—C6	−179.0 (3)	Cl1—C18—C19—C20	−176.7 (3)
C3—C2—C7—C6	0.8 (5)	C16—C15—C20—C19	−3.1 (5)
C3—N1—C8—C9	88.7 (3)	C1—C15—C20—C19	178.9 (3)
C1—N1—C8—C9	−99.6 (4)	C18—C19—C20—C15	0.3 (5)
N1—C8—C9—C10	4.8 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···Cl1^{i}	0.93	2.79	3.701 (4)	167

Symmetry codes: (i) −*x*+1, *y*+3/2, −*z*+1.

Fig. 1

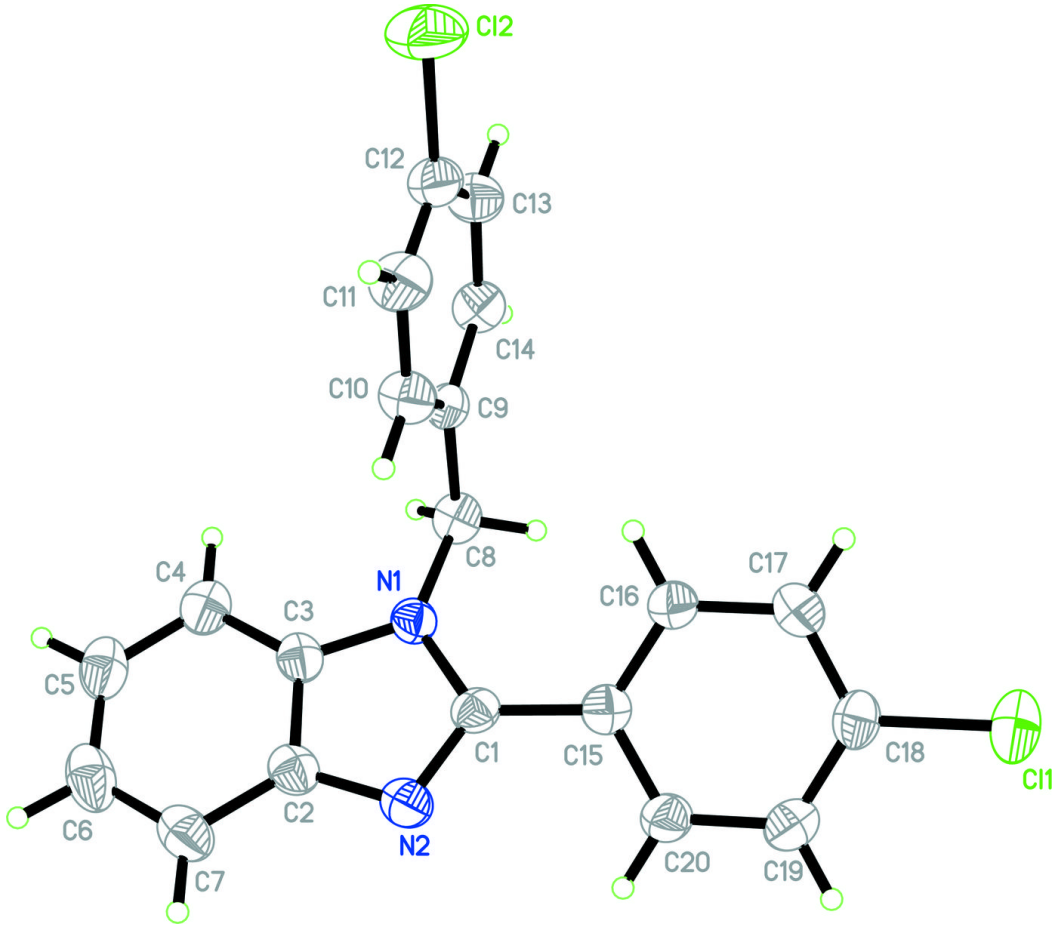
Cl2
C12
C13
C11
C14
C10
C9
C8
N1
C4
C3
C5
C1
C15
C16
C17
C18
Cl1
C6
C2
N2
C7
C20
C19

Fig. 2