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(2,4-Dichlorobenzylidene)[2-(1*H*-indol-3-yl)ethyl]-amine

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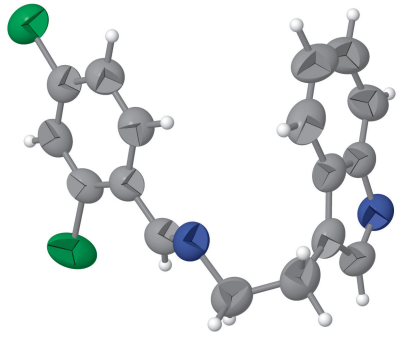
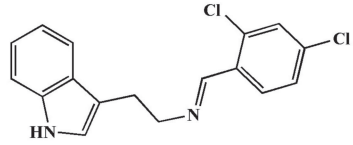
In the title compound, $C_{17}H_{14}Cl_2N_2$, the molecule exists in an *E* configuration with respect to the C=N bond of the Schiff base fragment. The dihedral angle between the indole ring system and the benzene ring is 80.86 (12)°. In the crystal, molecules are connected by N—H···N hydrogen bonds, generating a *C*(7) chain extending along the *a*-axis direction. No aromatic π–π stacking occurs but weak C—H···π interactions are observed.

3D view



Chemical scheme



Structure description

Schiff bases are widely used as catalysts, corrosion inhibitors and intermediates in organic synthesis, and also play a potential role in the development of coordination chemistry (Muralisankar *et al.*, 2016). Indole and its derivatives are useful staring compounds to derive pharmaceutical (Nalli *et al.*, 2020) and biological (Arumugam *et al.*, 2021) materials. In the present study, the hydrogen-bonding interactions and C—H···π interactions of the title compound are investigated.

The asymmetric unit of the title compound is shown in Fig. 1. The C=N double bond adopts an *E* configuration. The bond lengths and angles in the title molecule are normal and agree with those in other indole–imine compounds (*e.g.*, Suresh *et al.*, 2016; Ho *et al.*, 2006). The dihedral angle between the C1–C8/N1 indole ring system and the C12–C17 benzene ring is 80.86 (10)°.

In the extended structure, the N1—H5 group is a hydrogen-bond donor to atom N2 of the imino group (Table 1). These hydrogen bonds generate a *C*(7) chain extending along the *a*-axis direction, as shown in Fig. 2. There are no π–π interactions in this crystal structure but weak C—H···π interactions occur.

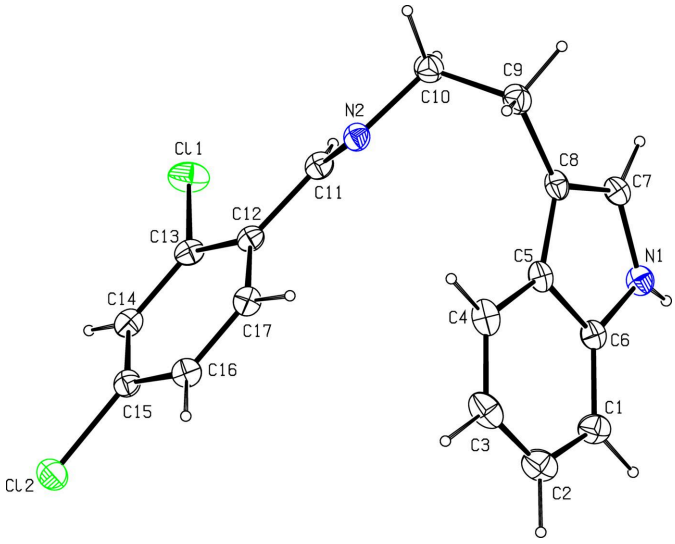


Figure 1
The molecular structure of the title compound showing 50% displacement ellipsoids.

A search of the Cambridge Structural Database (Version 5.43, update November 2022; Groom *et al.*, 2016) for the benzylidene)-[2-(1*H*-indol-3-yl)-ethyl]-amine skeleton yielded the hits 1-(anthracen-9-yl)-*N*-[2-(1*H*- indol-3-yl)ethyl]methanimine (CSD refcode TEGJIB; Faizi *et al.*, 2017), 2-[2-(1*H*-indol-3-ylethyliminomethyl)]-5-methylphenol (PEVXEW; Brink *et al.*, 2018), *rac*-4-{(*E*)-[1-cyano-1-cyclohexyl-2-(1*H*-indol-yl)ethyl]iminomethyl} benzonitrile (OCEWIE; Letessier *et al.*, 2011), 1*H*-indole-3-ethylenesalicylaldimine (FAJVIV; Rodriguez *et al.*, 1987) and 1-(4-chlorophenyl)-2-{[2-(1*H*-indol-3-yl) ethyl]imino}-2-(4-methoxyphenyl)ethan-1-one (AZUYUS; Li *et al.*, 2021).

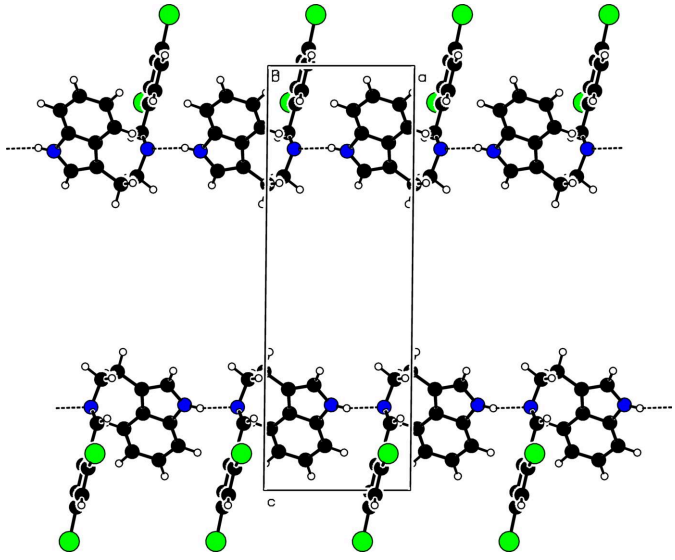


Figure 2
Partial packing diagram for the title compound showing the formation of [100] hydrogen-bonded chains.

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H5···N2^{i}	0.83 (3)	2.17 (3)	2.971 (3)	163 (2)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{14}Cl_2N_2$
M_r	317.20
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	296
a, b, c (Å)	7.2107 (8), 10.2179 (13), 20.863 (3)
β (°)	90.562 (4)
V (Å^3)	1537.1 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.42
Crystal size (mm)	0.52 × 0.34 × 0.13
Data collection	
Diffractometer	Agilent Xcalibur, Atlas, Gemini
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.631, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	68672, 3872, 1946
R_{int}	0.091
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.671
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.048, 0.134, 1.01
No. of reflections	3872
No. of parameters	246
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.20, −0.27

Computer programs: *CrysAlis PRO* and *CrysAlis RED* (Agilent, 2012), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*) and *PLATON* (Spek, 2020).

Synthesis and crystallization

The title compound was synthesized by condensing tryptamine, 2-(1*H*-indol-3-yl)ethan-1-amine (0.01 mmol) and 2,4-dichlorobenzaldehyde (0.01 mmol), which were taken separately, dissolved in 40 ml of ethanol, then mixed, and heated on a water bath for one h, then kept for crystallization. After a few days, colourless plate-shaped crystals were obtained.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

IUCrData (2023). **8**, x230780 [https://doi.org/10.1107/S2414314623007800]

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Crystal data

$C_{17}H_{14}Cl_2N_2$
M_r = 317.20
Monoclinic, $P2_1/n$
a = 7.2107 (8) Å
b = 10.2179 (13) Å
c = 20.863 (3) Å
β = 90.562 (4)°
V = 1537.1 (3) Å^3
Z = 4
$F(000)$ = 656
D_x = 1.371 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3778 reflections
θ = 2.6–29.9°
μ = 0.42 mm^{-1}
T = 296 K
Plate, colourless
0.52 × 0.34 × 0.13 mm

Data collection

Agilent Xcalibur, Atlas, Gemini diffractometer
Radiation source: fine-focus sealed tube
ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.631, T_{max} = 0.746
68672 measured reflections
3872 independent reflections
1946 reflections with $I > 2\sigma(I)$
R_{int} = 0.091
θ_{max} = 28.5°, θ_{min} = 2.0°
h = −9→9
k = −13→13
l = −27→27

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.134
S = 1.01
3872 reflections
246 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0498P)^2 + 0.4436P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. All the H atoms were located in a difference Fourier map and allowed to refine freely (C—H = 0.93–0.96 and N—H = 0.83 Å).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl2	0.82313 (10)	0.46440 (8)	0.37941 (3)	0.0896 (3)
Cl1	0.65404 (13)	0.74406 (7)	0.58638 (4)	0.1034 (3)
N2	0.6843 (2)	0.3930 (2)	0.69593 (9)	0.0656 (5)
N1	0.0458 (3)	0.2537 (2)	0.70118 (10)	0.0701 (6)
C5	0.3287 (3)	0.1772 (2)	0.68119 (11)	0.0628 (6)
C8	0.3389 (3)	0.2540 (2)	0.73804 (11)	0.0648 (6)
C6	0.1440 (3)	0.1792 (2)	0.65910 (11)	0.0631 (6)
C12	0.6934 (3)	0.4814 (2)	0.58989 (12)	0.0593 (6)
C7	0.1639 (3)	0.2993 (3)	0.74787 (13)	0.0680 (7)
C13	0.6992 (3)	0.5929 (2)	0.55222 (12)	0.0641 (6)
C14	0.7393 (3)	0.5892 (3)	0.48855 (14)	0.0683 (7)
C15	0.7767 (3)	0.4709 (3)	0.46026 (12)	0.0648 (6)
C17	0.7315 (3)	0.3640 (3)	0.55950 (14)	0.0675 (7)
C11	0.6416 (3)	0.4833 (3)	0.65769 (13)	0.0661 (7)
C16	0.7732 (3)	0.3571 (3)	0.49571 (14)	0.0707 (7)
C4	0.4574 (4)	0.1057 (3)	0.64506 (16)	0.0818 (8)
C10	0.6134 (4)	0.4015 (3)	0.76114 (14)	0.0785 (8)
C1	0.0861 (5)	0.1121 (3)	0.60482 (14)	0.0836 (8)
C3	0.4003 (6)	0.0415 (3)	0.59108 (17)	0.0979 (11)
C9	0.5055 (4)	0.2801 (3)	0.77920 (14)	0.0796 (8)
C2	0.2174 (6)	0.0439 (3)	0.57140 (17)	0.0972 (10)
H12	0.720 (3)	0.289 (3)	0.5830 (12)	0.082 (8)*
H11	0.573 (3)	0.556 (2)	0.6692 (10)	0.065 (7)*
H10	0.543 (4)	0.476 (3)	0.7641 (12)	0.081 (9)*
H9	0.726 (4)	0.407 (3)	0.7916 (13)	0.099 (9)*
H8	0.586 (4)	0.201 (3)	0.7761 (12)	0.091 (9)*
H4	0.579 (4)	0.105 (3)	0.6598 (12)	0.083 (9)*
H13	0.797 (3)	0.275 (3)	0.4752 (12)	0.076 (8)*
H14	0.743 (3)	0.663 (3)	0.4649 (12)	0.082 (8)*
H7	0.470 (3)	0.290 (2)	0.8258 (12)	0.078 (7)*
H6	0.126 (3)	0.357 (2)	0.7814 (10)	0.068 (7)*
H1	−0.045 (4)	0.108 (3)	0.5888 (13)	0.106 (10)*
H3	0.489 (4)	−0.005 (3)	0.5634 (15)	0.119 (11)*
H2	0.177 (5)	−0.006 (4)	0.5331 (17)	0.132 (13)*
H5	−0.060 (4)	0.282 (3)	0.6933 (12)	0.082 (9)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl2	0.0795 (5)	0.1146 (6)	0.0746 (5)	0.0090 (4)	0.0029 (3)	0.0035 (4)
Cl1	0.1558 (8)	0.0600 (4)	0.0939 (6)	0.0151 (4)	−0.0242 (5)	−0.0064 (4)
N2	0.0525 (11)	0.0758 (14)	0.0685 (13)	0.0038 (10)	−0.0010 (9)	0.0048 (11)
N1	0.0601 (13)	0.0747 (15)	0.0757 (15)	0.0114 (12)	0.0050 (11)	0.0011 (11)
C5	0.0652 (15)	0.0551 (14)	0.0681 (15)	0.0121 (11)	0.0125 (11)	0.0153 (12)
C8	0.0605 (14)	0.0739 (16)	0.0602 (14)	0.0068 (12)	0.0087 (11)	0.0181 (13)

C6	0.0695 (15)	0.0528 (14)	0.0671 (15)	0.0071 (12)	0.0078 (12)	0.0093 (12)
C12	0.0467 (12)	0.0621 (15)	0.0690 (15)	0.0059 (11)	−0.0094 (10)	−0.0004 (12)
C7	0.0707 (16)	0.0718 (17)	0.0617 (15)	0.0074 (13)	0.0119 (13)	0.0002 (13)
C13	0.0644 (14)	0.0555 (15)	0.0721 (16)	0.0053 (11)	−0.0151 (12)	0.0018 (13)
C14	0.0659 (16)	0.0587 (16)	0.0800 (19)	−0.0008 (12)	−0.0136 (13)	0.0104 (15)
C15	0.0478 (13)	0.0780 (18)	0.0684 (15)	0.0042 (12)	−0.0071 (10)	0.0065 (14)
C17	0.0659 (15)	0.0596 (16)	0.0769 (18)	0.0066 (12)	−0.0027 (12)	0.0089 (14)
C11	0.0534 (14)	0.0663 (17)	0.0783 (18)	0.0082 (12)	−0.0057 (12)	−0.0042 (14)
C16	0.0676 (16)	0.0640 (17)	0.0803 (19)	0.0123 (13)	−0.0014 (13)	−0.0037 (15)
C4	0.079 (2)	0.0709 (18)	0.096 (2)	0.0228 (15)	0.0201 (17)	0.0209 (17)
C10	0.0702 (18)	0.096 (2)	0.0690 (18)	0.0042 (17)	−0.0010 (14)	−0.0028 (16)
C1	0.102 (2)	0.0655 (17)	0.083 (2)	0.0028 (17)	−0.0044 (17)	−0.0025 (16)
C3	0.138 (3)	0.0652 (19)	0.091 (2)	0.031 (2)	0.032 (2)	−0.0007 (17)
C9	0.0741 (18)	0.098 (2)	0.0663 (18)	0.0031 (16)	−0.0018 (14)	0.0154 (16)
C2	0.137 (3)	0.0653 (19)	0.090 (2)	0.010 (2)	0.006 (2)	−0.0077 (17)

Geometric parameters (Å, º)

Cl2—C15	1.724 (3)	C14—H14	0.90 (3)
Cl1—C13	1.733 (2)	C15—C16	1.378 (4)
N2—C11	1.256 (3)	C17—C16	1.369 (4)
N2—C10	1.461 (3)	C17—H12	0.92 (3)
N1—C6	1.365 (3)	C11—H11	0.92 (2)
N1—C7	1.369 (3)	C16—H13	0.95 (3)
N1—H5	0.83 (3)	C4—C3	1.364 (5)
C5—C6	1.405 (3)	C4—H4	0.93 (3)
C5—C4	1.406 (4)	C10—C9	1.514 (4)
C5—C8	1.424 (3)	C10—H10	0.92 (3)
C8—C7	1.362 (3)	C10—H9	1.03 (3)
C8—C9	1.494 (4)	C1—C2	1.371 (4)
C6—C1	1.385 (4)	C1—H1	1.00 (3)
C12—C13	1.385 (3)	C3—C2	1.377 (5)
C12—C17	1.386 (3)	C3—H3	0.99 (3)
C12—C11	1.467 (3)	C9—H8	1.00 (3)
C7—H6	0.96 (2)	C9—H7	1.01 (2)
C13—C14	1.363 (4)	C2—H2	0.99 (4)
C14—C15	1.373 (4)		
C11—N2—C10	117.5 (2)	N2—C11—C12	122.7 (2)
C6—N1—C7	108.9 (2)	N2—C11—H11	123.5 (14)
C6—N1—H5	123.4 (18)	C12—C11—H11	113.8 (14)
C7—N1—H5	125.7 (19)	C17—C16—C15	118.9 (3)
C6—C5—C4	117.4 (3)	C17—C16—H13	121.4 (15)
C6—C5—C8	107.8 (2)	C15—C16—H13	119.6 (15)
C4—C5—C8	134.7 (3)	C3—C4—C5	119.8 (3)
C7—C8—C5	105.8 (2)	C3—C4—H4	123.2 (17)
C7—C8—C9	126.5 (3)	C5—C4—H4	117.0 (17)
C5—C8—C9	127.7 (2)	N2—C10—C9	111.6 (3)

N1—C6—C1	130.4 (3)	N2—C10—H10	108.1 (16)
N1—C6—C5	107.1 (2)	C9—C10—H10	112.3 (17)
C1—C6—C5	122.5 (2)	N2—C10—H9	107.3 (15)
C13—C12—C17	116.5 (2)	C9—C10—H9	107.4 (16)
C13—C12—C11	123.1 (2)	H10—C10—H9	110 (2)
C17—C12—C11	120.4 (2)	C2—C1—C6	117.6 (3)
C8—C7—N1	110.4 (2)	C2—C1—H1	117.6 (17)
C8—C7—H6	126.3 (14)	C6—C1—H1	124.7 (17)
N1—C7—H6	123.3 (13)	C4—C3—C2	121.2 (3)
C14—C13—C12	122.5 (2)	C4—C3—H3	121.5 (19)
C14—C13—Cl1	117.9 (2)	C2—C3—H3	117.2 (19)
C12—C13—Cl1	119.5 (2)	C8—C9—C10	114.6 (2)
C13—C14—C15	119.2 (3)	C8—C9—H8	106.5 (16)
C13—C14—H14	121.4 (17)	C10—C9—H8	110.3 (15)
C15—C14—H14	119.4 (17)	C8—C9—H7	111.0 (13)
C14—C15—C16	120.5 (3)	C10—C9—H7	107.0 (14)
C14—C15—Cl2	119.7 (2)	H8—C9—H7	107 (2)
C16—C15—Cl2	119.8 (2)	C1—C2—C3	121.4 (3)
C16—C17—C12	122.4 (3)	C1—C2—H2	118 (2)
C16—C17—H12	120.0 (17)	C3—C2—H2	121 (2)
C12—C17—H12	117.5 (16)		

C6—C5—C8—C7	−0.3 (3)	C13—C14—C15—Cl2	178.70 (17)
C4—C5—C8—C7	179.1 (3)	C13—C12—C17—C16	0.2 (3)
C6—C5—C8—C9	179.4 (2)	C11—C12—C17—C16	177.4 (2)
C4—C5—C8—C9	−1.1 (4)	C10—N2—C11—C12	−175.7 (2)
C7—N1—C6—C1	179.5 (3)	C13—C12—C11—N2	−159.7 (2)
C7—N1—C6—C5	0.9 (3)	C17—C12—C11—N2	23.3 (4)
C4—C5—C6—N1	−179.9 (2)	C12—C17—C16—C15	−0.3 (4)
C8—C5—C6—N1	−0.4 (3)	C14—C15—C16—C17	0.1 (4)
C4—C5—C6—C1	1.4 (4)	Cl2—C15—C16—C17	−178.35 (18)
C8—C5—C6—C1	−179.1 (2)	C6—C5—C4—C3	−0.3 (4)
C5—C8—C7—N1	0.9 (3)	C8—C5—C4—C3	−179.7 (3)
C9—C8—C7—N1	−178.9 (2)	C11—N2—C10—C9	124.4 (3)
C6—N1—C7—C8	−1.1 (3)	N1—C6—C1—C2	−179.7 (3)
C17—C12—C13—C14	0.2 (3)	C5—C6—C1—C2	−1.4 (4)
C11—C12—C13—C14	−176.9 (2)	C5—C4—C3—C2	−0.7 (5)
C17—C12—C13—Cl1	−179.82 (17)	C7—C8—C9—C10	−89.3 (3)
C11—C12—C13—Cl1	3.1 (3)	C5—C8—C9—C10	91.0 (3)
C12—C13—C14—C15	−0.4 (4)	N2—C10—C9—C8	−60.8 (4)
Cl1—C13—C14—C15	179.62 (17)	C6—C1—C2—C3	0.3 (5)
C13—C14—C15—C16	0.2 (4)	C4—C3—C2—C1	0.8 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

N1—H5···N2^{i}	0.83 (3)	2.17 (3)	2.971 (3)	163 (2)

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