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5-Chloro-1*H*-indole-3-carbaldehyde 4-chlorobenzoylhydrazone

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.051
wR factor = 0.155
Data-to-parameter ratio = 16.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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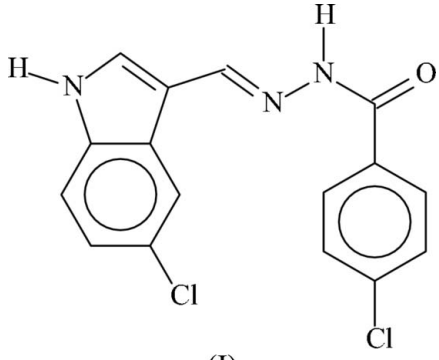
The amido O atom in the title molecule, $C_{16}H_{11}Cl_2N_3O$, is the hydrogen-bond acceptor for the amide group and amine groups of two adjacent molecules; the hydrogen-bonding interactions result in a layer motif.

Comment

The preceeding study (Ali *et al.*, 2006) describes the Schiff base derived by condensing 5-chloro-1*H*-indole-3-carbaldehyde with benzoylhydrazine. The present compound, (I) (Fig. 1), has a chloro substituent in the benzoylhydrazine unit, but it shows only minor differences in bond dimensions compared with the unsubstituted derivative.



(I)

The zigzag —C(O)—NH—N=CH— chain is coplanar with the chloroindolyl unit [dihedral angle = 10.0 (2)°], but the 4-chlorophenyl unit is twisted away from it [dihedral angle = 47.6 (1)°]. The crystal structure is stabilized by hydrogen bonding; the amide O atom is an acceptor for two donor atoms (Table 1).

Experimental

5-Chloroindole-3-carbaldehyde (0.63 g, 4.0 mmol) and 4-chlorobenzhydrazide (0.68 g, 4.0 mmol) were heated in ethanol (100 ml) for 2 h. The solvent was removed and the product recrystallized from acetonitrile.

Crystal data

$C_{16}H_{11}Cl_2N_3O$
M_r = 332.18
Monoclinic, $P2_1/n$
a = 8.7172 (8) Å
b = 8.6686 (8) Å
c = 19.960 (2) Å
β = 93.202 (1)°
V = 1505.9 (2) Å^3
Z = 4
D_x = 1.465 Mg m^{-3}
Mo *Kα* radiation
μ = 0.44 mm^{-1}
T = 295 (2) K
Irregular fragment, yellow
0.49 × 0.47 × 0.23 mm

Data collection

Bruker APEX-II area-detector diffractometer
φ and ω scans
Absorption correction: none
13557 measured reflections
3423 independent reflections
2181 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 27.5^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.155$
$S = 1.03$
3423 reflections
207 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0675P)^2 + 0.7475P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.46$ e Å^{-3}
$\Delta\rho_{min} = -0.63$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1n···O1^{i}	0.86 (1)	2.10 (1)	2.941 (3)	167 (3)
N3—H3n···O1^{ii}	0.85 (1)	2.13 (2)	2.935 (3)	157 (4)

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

The carbon-bound H atoms were placed at calculated positions (C—H = 0.93 Å) and they were included in the refinement in the riding-model approximation, with U_{iso}(H) values set at $1.2U_{eq}$(C). The amide and amine H atoms were located in a difference Fourier map and were refined with a distance restraint [N—H = 0.85 (1) Å]; their displacement parameters were refined.

Data collection: *APEXII* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *SHELXL97*.

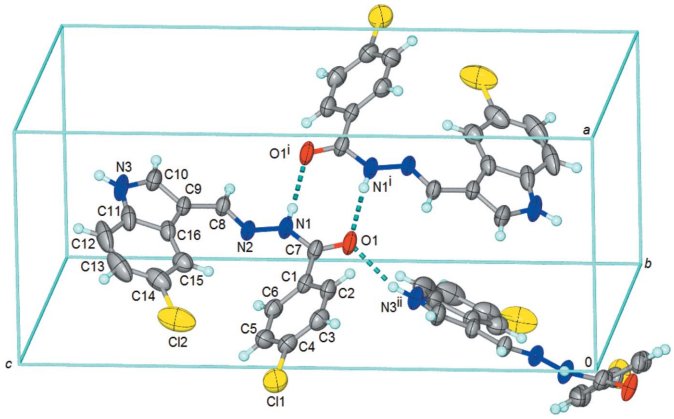


Figure 1
A partial packing diagram of (I), showing displacement ellipsoids drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii. Dashed lines represent hydrogen bonds.

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