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3-[(2-Chlorophenyl)methylenehydrazinocarbonyl]-1*H*-1,2,4-triazole

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The title compound, $C_{10}H_8ClN_5O$, was synthesized by the reaction of 3-hydrazino-1*H*-1,2,4-triazole with 2-chlorobenzaldehyde in ethanol. The molecule is nearly planar. In the crystal structure, screw-related molecules form N—H···O and N—H···N hydrogen bonded chains along the *b* axis.

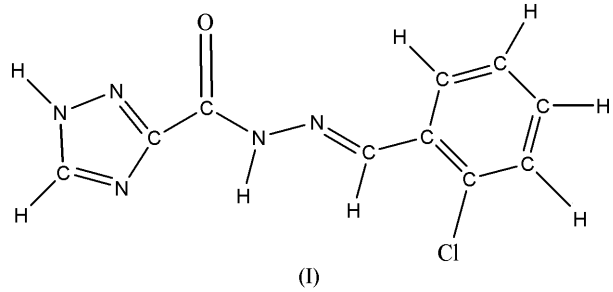
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.060
wR factor = 0.138
Data-to-parameter ratio = 12.6

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

Comment

Azole derivatives, such as derivatives of pyrazole, imidazole, triazole (including benzotriazole), tetrazole, indole, *etc*., exhibit extensive biological activities. They have become a central focus in the study of agricultural chemicals, medicine, adjustment reagents for plant growth, and so on (Ernest & William, 1982). A Schiff base is a good type of biologically active substructure and a study of a type of triazole Schiff base has been reported (Sauter *et al.*, 1991). The hydrazinocarbonyl grouping has also been shown to be bioactive (Zhi *et al.*, 2003). However, the structure of a triazole compound containing the hydrazinocarbonyl group has never been reported. In a search for more effective antibacterial medicines, we have synthesized the title compound, (I).



(I)

The title molecule is almost planar (Fig. 1). The dihedral angle between the planes of the triazole and benzene fragments is 14.1 (1)°. The bond lengths and angles (Table 1)

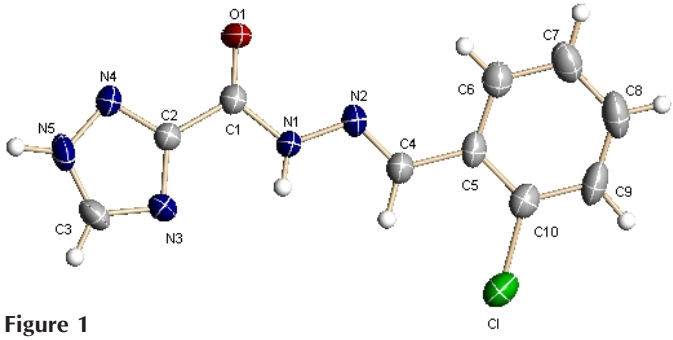


Figure 1
The structure of (I), showing the atomic numbering. Displacement ellipsoids are drawn at the 30% probability level.

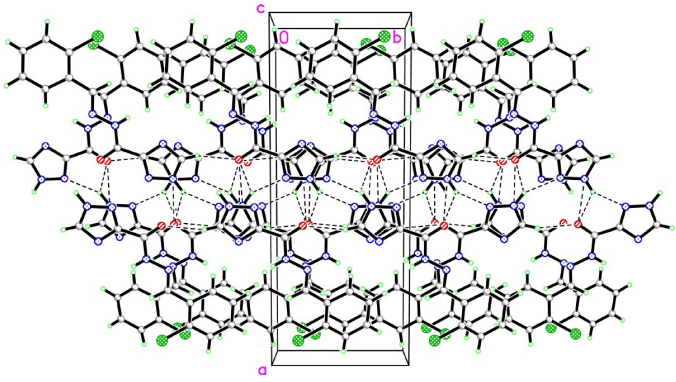


Figure 2
The crystal packing of (I), viewed down the *c* axis. Hydrogen bonds are shown as dashed lines.

observed in the title structure agree with values reported for similar compounds (Allen *et al.*, 1987). In the crystal structure, screw-related molecules are linked by N—H···O and N—H···N hydrogen bonds to form a chain along the *b* axis (Table 2). These hydrogen bonds, involving the ring NH group of one molecule and the keto group and ring N atom of an adjacent molecule, form a five-membered ring (Fig. 2).

Experimental

3–Hydrazino-1*H*-1,2,4-triazole (0.02 mol, 2.54 g) was dissolved in anhydrous ethanol (50 ml) at room temperature. 2-Chlorobenzaldehyde (0.02 mol, 2.81 g) was added to the solution and the mixture was refluxed for 2 h. The resulting precipitate was collected by filtration and washed with ethanol. The product was recrystallized from ethanol and dried under reduced pressure to obtain the title compound, (I), of which 2.5 mmol (0.62 g) was dissolved in DMF (30 ml) and kept at room temperature. Colourless single crystals were formed after 30 d and were washed with distilled water.

Crystal data

$C_{10}H_8ClN_5O$
M_r = 249.66
Monoclinic, $P2_1/c$
a = 19.395 (3) Å
b = 7.5786 (11) Å
c = 7.3930 (11) Å
β = 98.607 (3)°
V = 1074.4 (3) Å^3
Z = 4
D_x = 1.543 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1143 reflections
θ = 5.8–45.8°
μ = 0.35 mm^{-1}
T = 293 (2) K
Block, colourless
0.52 × 0.18 × 0.08 mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.508, T_{max} = 1.000
6121 measured reflections
2340 independent reflections
1504 reflections with $I > 2\sigma(I)$
R_{int} = 0.077
θ_{max} = 27.0°
$h = -24 \rightarrow 23$
$k = -9 \rightarrow 8$
$l = -9 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.138
S = 1.00
2340 reflections
186 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0565P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.207 (3)	N3—C2	1.357 (3)
N1—C1	1.357 (3)	N4—C2	1.318 (3)
N1—N2	1.358 (3)	N4—N5	1.337 (3)
N2—C4	1.263 (4)	N5—C3	1.312 (4)
N3—C3	1.336 (4)		
C1—N1—N2—C4	−175.4 (3)	N2—C4—C5—C10	−176.4 (3)
N1—N2—C4—C5	−176.2 (3)	N2—C4—C5—C6	6.8 (5)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5···O1^{i}	0.95 (4)	2.23 (4)	2.946 (3)	131 (3)
N5—H5···N4^{i}	0.95 (4)	2.20 (4)	3.057 (3)	150 (3)

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

All H atoms were located in a difference map and were isotropically refined. The N—H distances are 0.81 (3) and 0.95 (4) Å, and the C—H distances lie in the range 0.89 (2)–0.99 (3) Å.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2002); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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