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4-Chlorobenzaldehyde (pyrazin-2-ylcarbonyl)-hydrazone

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The title compound, $C_{12}H_9ClN_4O$, was prepared by the reaction of pyrazine-2-carboxylic acid hydrazide and 4-chlorobenzaldehyde in methanol. In the crystal structure, there is an intramolecular N—H···N hydrogen bond, forming a five-membered ring, and an intermolecular C—H···O hydrogen bond, resulting in a one-dimensional infinite chain along the *a* axis. Weak face-to-face π–π stacking interactions are also observed between two antiparallel molecules. These π–π stacking interactions further join the molecules into a three-dimensional structure.

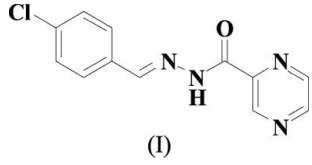
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.039
wR factor = 0.107
Data-to-parameter ratio = 12.4

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

Comment

Pyrazinyl hydrazonecarbonyl compounds (Edwards *et al.*, 1975; Kushner *et al.*, 1952) have many applications in the treatment of tuberculosis and also exhibit fungicidal activity. Two related hydrazone complexes have been investigated previously (Pan & Yang, 2005*a*,*b*). This kind of Schiff base possesses pharmacological activity (Parashar *et al.*, 1988) and photochromic properties (Hadjoudis *et al.*, 1987). Here we report the crystal structure of 4-chlorobenzaldehyde (pyrazine-2-carbonyl)hydrazone, (I).



(I)

Compound (I) adopts a nearly planar conformation, with an r.m.s. deviation of 0.0985 Å for all atoms. In the crystal structure, there is an intramolecular N—H···N hydrogen bond forming a five-membered ring (Table 2) and also an intermolecular C—H···O hydrogen bond between the O atom of the carbonyl group and C6, resulting in a one-dimensional infinite chain along the *a* axis (Fig. 2). There are weak face-to-face π–π stacking interactions between two antiparallel molecules, with the centroids of the benzene and pyrazine rings separated by 3.830 (3) and 4.017 (3) Å.

Experimental

The title compound was synthesized by the reaction of pyrazine-2-carboxylic acid hydrazide (1.3 g, 5 mmol) and 4-chlorobenzaldehyde (0.7 g, 5 mmol) in methanol (60 ml). Single crystals suitable for X-ray analysis were obtained by slow evaporation of a methanol solution (yield 88%, m.p. 479–480 K).

Crystal data

$C_{12}H_9ClN_4O$
$M_r = 260.68$
Triclinic, $P\overline{1}$
$a = 5.8860\ (16)$ Å
$b = 7.818\ (2)$ Å
$c = 13.500\ (4)$ Å
$\alpha = 84.883\ (5)^\circ$
$\beta = 80.500\ (5)^\circ$
$\gamma = 73.769\ (4)^\circ$
$V = 587.7\ (3)$ Å^3
$Z = 2$
$D_x = 1.473$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.32$ mm^{-1}
$T = 293\ (2)$ K
Block, colourless
0.22 × 0.18 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.925$, $T_{max} = 0.969$
3000 measured reflections
2055 independent reflections
1350 reflections with $I > 2\sigma(I)$
$R_{int} = 0.015$
$\theta_{max} = 25.0^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.107$
$S = 1.02$
2055 reflections
166 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.044P)^2 + 0.1868P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···N2	0.83 (3)	2.27 (3)	2.689 (3)	111 (2)
C6—H6···O1^{i}	0.93	2.24 (3)	3.133 (3)	160 (2)

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

All H atoms were initially located in a difference Fourier map. The C—H atoms were then constrained to an ideal geometry, with methyl C—H = 0.96 Å, aromatic C—H = 0.93 Å, and refined as riding with U_{iso}(H) = 1.2U_{eq}(C). The coordinates of the amino H atom were refined freely, with U_{iso}(H) = 1.2U_{eq}(N).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

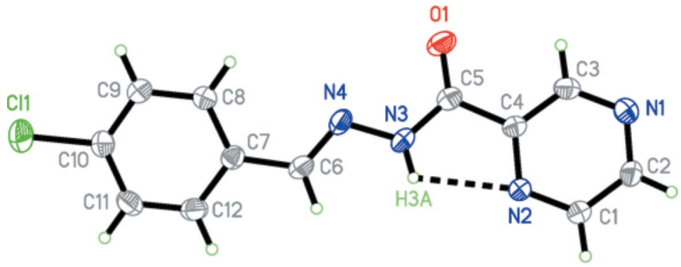


Figure 1
The structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are shown as small spheres of arbitrary radii. The intramolecular hydrogen bond is shown as a dashed line.

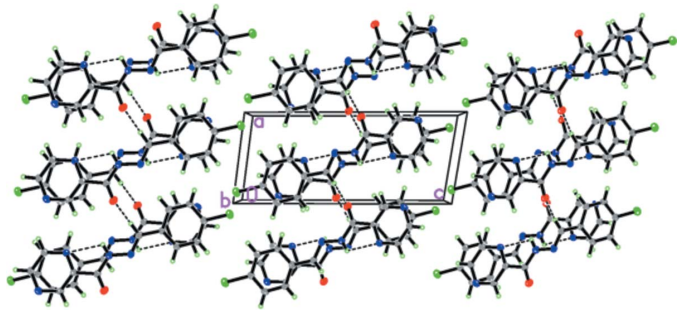


Figure 2
The molecular packing of (I), viewed along the b axis. Hydrogen bonds are shown as dashed lines.

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