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4-Chlorobenzohydrazide

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.061
wR factor = 0.143
Data-to-parameter ratio = 12.3

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

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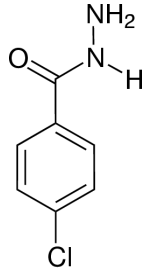
The crystal structure of the title compound, $C_7H_7N_2OCl$, has been determined in the monoclinic space group $P2_1/c$ at room temperature. The structure is stabilized by intermolecular N—H···O and N—H···N hydrogen bonds.

Comment

The title compound, (I), was tested for its activity against tuberculosis *in vitro* (Bew-Hol *et al.*, 1952), and was found to be inactive at a concentration of 10 µg ml^{-1} of the culture medium. Compound (I) was also used as a starting material for the synthesis of α-methyl-substituted or unsubstituted [(4-phenyl/ethyl-5-*p*-chlorophenyl-4*H*-1,2,4-triazol-3-yl)thio]-acetic acids, which have been found to possess good anti-inflammatory activity (Sung & Lee, 1992).



(I)

The orientations of the carbonyl and hydrazide groups with respect to the aromatic ring are defined by the torsion angles C5—C4—C7—O1 31.9 (4)° and C5—C4—C7—N1 −148.3 (3)°. The crystal structure is held together by two intermolecular hydrogen bonds, N1—H1···N2^{i} and N2—H2N···O1^{ii} (symmetry codes as in Table 1).

Experimental

The title compound was synthesized from 4-chlorobenzoic acid by refluxing it with anhydrous ethanol and concentrated sulfuric acid for 3 h to obtain ethyl 4-chlorobenzoate. This, on further reaction with hydrazine hydrate in ethanol under reflux conditions for 6 h, yielded 4-chlorobenzohydrazide. Crystallization from ethanol yielded colorless crystals (Saikachi *et al.*, 1955).

Crystal data

$C_7H_7ClN_2O$
M_r = 170.60
Monoclinic, $P2_1/c$
a = 15.945 (7) Å
b = 3.8449 (16) Å
c = 12.389 (5) Å
β = 99.664 (7)°
V = 748.7 (5) Å^3
Z = 4
D_x = 1.513 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2013 reflections
θ = 2.6–27.9°
μ = 0.45 mm^{-1}
T = 293 (2) K
Rod, colorless
0.20 × 0.18 × 0.05 mm

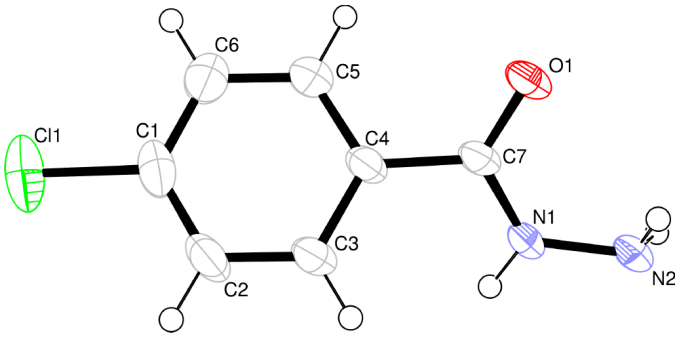


Figure 1
Molecular structure of the title compound with the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radii.

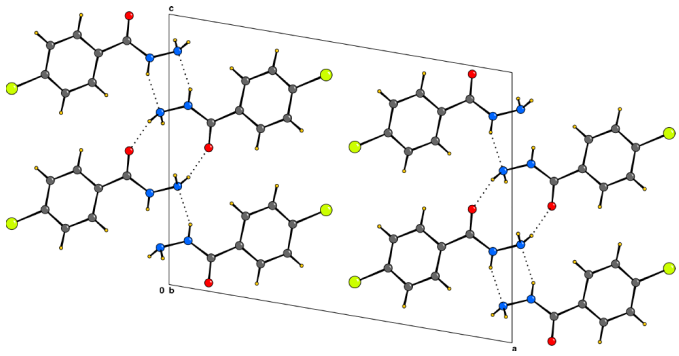


Figure 2
Packing diagram of the title compound, viewed down the *b* axis. N—H···O and N—H···N hydrogen bonds are shown as dotted lines.

Data collection

Bruker SMART CCD area-detector diffractometer	981 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.049$
Absorption correction: none	$\theta_{max} = 25.0^\circ$
4456 measured reflections	$h = -18 \rightarrow 18$
1329 independent reflections	$k = -4 \rightarrow 4$
	$l = -13 \rightarrow 14$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.1534P)^2 + 0.0248P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.061$	$(\Delta/\sigma)_{max} = 0.010$
$wR(F^2) = 0.143$	$\Delta\rho_{max} = 0.38$ e Å^{-3}
$S = 1.03$	$\Delta\rho_{min} = -0.35$ e Å^{-3}
1329 reflections	
108 parameters	
H atoms treated by a mixture of independent and constrained refinement	

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N2^{i}	0.86	2.10	2.911 (4)	157
N2—H2N···O1^{ii}	0.86 (3)	2.22 (4)	3.046 (4)	168 (3)

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

The H atoms on N2, *viz*. H1N and H2N, were located in a difference Fourier map and refined freely. All other atoms were positioned geometrically and allowed to ride on their parent atoms, with U_{iso}(H) = U_{eq} of the parent atom.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 for Windows (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *PLATON* (Spek, 1990).

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