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2-Amino-5-chloro-1,3-benzoxazole

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The structure of the title compound, $C_7H_5ClN_2O$, comprises a planar molecule that associates *via* N—H···N interactions to form $R_2^2(8)$ graph set hydrogen-bonded dimers, while N—H···Cl associations from the second 2-amino H atom create a two-dimensional hydrogen-bonding network containing $C_2^2(8)$ helical chains.

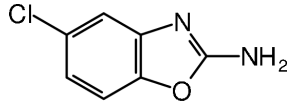
Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.002 Å
R factor = 0.029
wR factor = 0.084
Data-to-parameter ratio = 15.3

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

Comment

2-Amino-5-chloro-1,3-benzoxazole, or Zoxazolamine, (I), is a human metabolite and a centrally acting myorelaxant that was formerly used as an antispasmodic and uricosuric; current uses for the compound include as a tool for assessing hepatic cytochrome P-450 activity in rodents (The Merck Index, 2001). Chemically, (I) is a 2-aminooxazole derivative, the Cambridge Structural Database, version of April 2004 (Allen, 2002) lists 22 (in total) 2-aminooxazoles, 2-aminooxazolines, 2-aminooxadiazoles and 2-aminobenzoxazoles, four being co-crystals containing (I) (Lynch, Daly & Parsons, 2000, Lynch, Singh & Parsons, 2000). The structure of (I), reported here, consists of a planar molecule (Fig. 1) that associates *via* N—H···N interactions, forming a $R_2^2(8)$ graph set (Etter, 1990) hydrogen-bonded dimer (Fig. 2). The second 2-amino N—H donates to an adjacent Cl atom, creating a two-dimensional hydrogen-bonding network that consists of $C_2^2(8)$ helical chains. Hydrogen-bonding associations are listed in Table 1. Molecules of (I) are slip-stacked in the *b*-axis direction, 3.36 (2) Å apart.



(I)

Experimental

The title compound was purchased from Aldrich Chemical Co. and recrystallized from ethanol.

Crystal data

$C_7H_5ClN_2O$
M_r = 168.58
Monoclinic, $P2_1/n$
a = 9.4403 (19) Å
b = 3.7390 (7) Å
c = 19.737 (4) Å
β = 101.67 (3)°
V = 682.2 (2) Å^3
Z = 4
D_x = 1.641 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3789 reflections
θ = 2.9–27.5°
μ = 0.49 mm^{-1}
T = 120 (2) K
Plate, colourless
0.24 × 0.18 × 0.05 mm

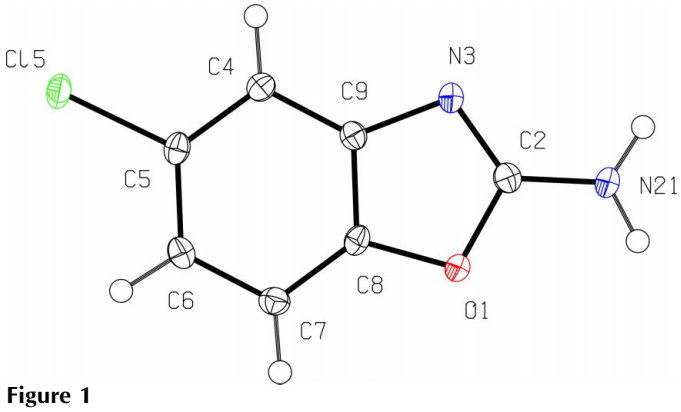


Figure 1
The molecular structure and atom-numbering scheme for (I). Displacement ellipsoids are drawn at the 50% probability level.

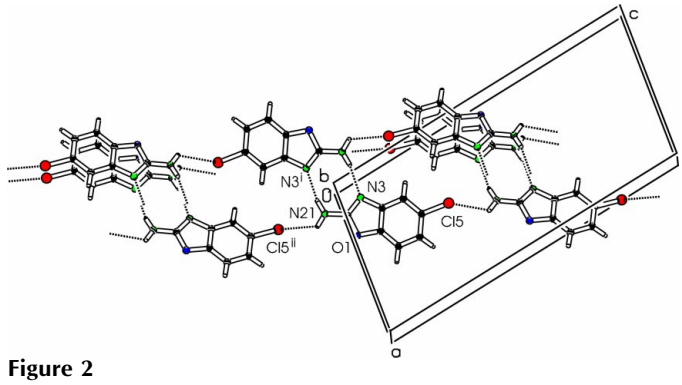


Figure 2
Packing diagram for (I). Dotted lines represent hydrogen bonds. [Symmetry codes (i) $-x, -y, -z$; (ii) $x-\frac{1}{2}, \frac{1}{2}-y, z-\frac{1}{2}$.]

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer	1526 independent reflections
φ and ω scans	1360 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)	$R_{int} = 0.032$
$T_{min} = 0.806$, $T_{max} = 0.978$	$\theta_{max} = 27.5^{\circ}$
4816 measured reflections	$h = -12 \rightarrow 12$
	$k = -4 \rightarrow 4$
	$l = -22 \rightarrow 25$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0405P)^2 + 0.2976P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.029$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.084$	$\Delta\rho_{max} = 0.31$ e Å^{-3}
$S = 1.06$	$\Delta\rho_{min} = -0.30$ e Å^{-3}
1526 reflections	
100 parameters	
H-atom parameters constrained	

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

D—H···A	D—H	H···A	D···A	D—H···A
N21—H21···N3^{i}	0.88	2.04	2.901 (2)	166
N21—H22···Cl5^{ii}	0.88	2.83	3.444 (2)	128

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

All H atoms were included in the refinement at calculated positions, in the riding-model approximation, with aromatic C—H distances of 0.95 Å and N—H distances of 0.88 Å. The isotropic displacement parameters were set equal to $1.25U_{eq}$ of the carrier atom.

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO, SCALEPACK* (Otwinowski & Minor, 1997) and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON*97 (Spek, 2003); software used to prepare material for publication: *SHELXL*97.

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References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Etter, M. C. (1990). *Acc. Chem. Res.* **23**, 120–126.
Hooft, R. W. W. (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Lynch, D. E., Daly, D. & Parsons, S. (2000). *Acta Cryst.* C**56**, 1478–1479.
Lynch, D. E., Singh, M. & Parsons, S. (2000). *Cryst. Eng.* **3**, 71–79.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr and R. M. Sweet, pp. 307–326. New York: Academic Press.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 3–17.
The Merck Index (2001). 13th ed. Whitehouse Station: Merck and Co. Inc.