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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.

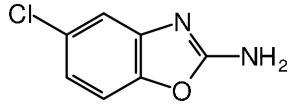
Key indicators

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

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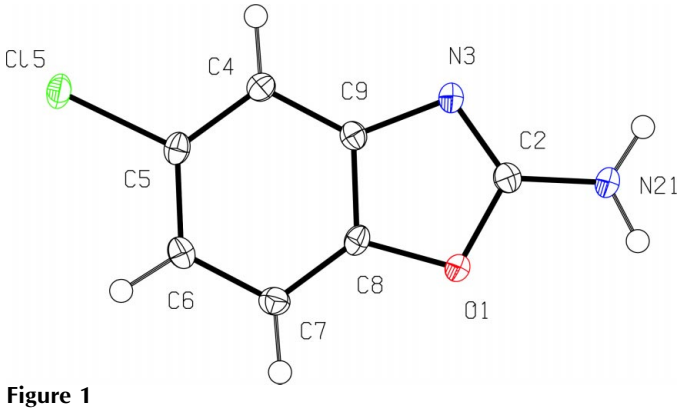

Figure 1
The molecular structure and atom-numbering scheme for (I). Displacement ellipsoids are drawn at the 50% probability level.

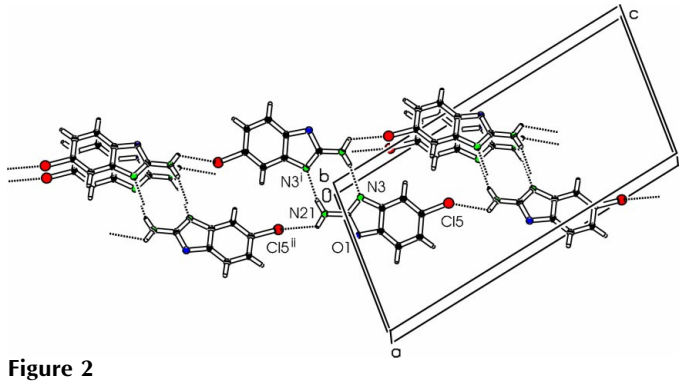

Figure 2
Packing diagram for (I). Dotted lines represent hydrogen bonds. [Symmetry codes (i) $-x, -y, -z$; (ii) $x-\frac{1}{2}, \frac{1}{2}-y, z-\frac{1}{2}$.]

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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$c = 19.737$ (4) Å
$\beta = 101.67$ (3)°
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$Z = 4$
$F(000) = 344$
$D_x = 1.641$ Mg m^{-3}
Melting point = 458–458.5 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3789 reflections
$\theta = 2.9$–27.5°
$\mu = 0.49$ mm^{-1}
$T = 120$ K
Plate, colourless
0.24 × 0.18 × 0.05 mm

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer
Radiation source: Bruker–Nonius FR591 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SORTAV; Blessing, 1995)
$T_{min} = 0.806$, $T_{max} = 0.978$
4816 measured reflections
1526 independent reflections
1360 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.5°$
$h = -12 \rightarrow 12$
$k = -4 \rightarrow 4$
$l = -22 \rightarrow 25$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.084$
$S = 1.06$
1526 reflections
100 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0405P)^2 + 0.2976P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.35183 (11)	0.2435 (3)	0.01453 (5)	0.0168 (2)
C2	0.21001 (15)	0.1379 (4)	0.00663 (7)	0.0168 (3)

N21	0.12672 (14)	0.1887 (4)	−0.05575 (6)	0.0234 (3)
H21	0.0359	0.1183	−0.0641	0.029*
H22	0.1626	0.2926	−0.0886	0.029*
N3	0.17429 (12)	−0.0105 (3)	0.06061 (6)	0.0165 (3)
C4	0.33211 (14)	−0.1232 (4)	0.17882 (7)	0.0146 (3)
H4	0.2601	−0.2295	0.1997	0.018*
C5	0.47302 (15)	−0.0765 (4)	0.21461 (7)	0.0148 (3)
Cl5	0.51663 (4)	−0.21998 (9)	0.300743 (16)	0.01855 (14)
C6	0.58231 (15)	0.0731 (4)	0.18576 (7)	0.0163 (3)
H6	0.6775	0.0948	0.2127	0.020*
C7	0.55165 (15)	0.1915 (4)	0.11709 (8)	0.0167 (3)
H7	0.6235	0.2957	0.0959	0.021*
C8	0.41178 (15)	0.1480 (4)	0.08232 (7)	0.0147 (3)
C9	0.30223 (14)	−0.0054 (4)	0.11057 (7)	0.0137 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0157 (5)	0.0231 (6)	0.0112 (5)	−0.0035 (4)	0.0015 (4)	0.0023 (4)
C2	0.0164 (7)	0.0184 (7)	0.0149 (7)	−0.0024 (6)	0.0015 (5)	−0.0012 (5)
N21	0.0190 (7)	0.0374 (8)	0.0123 (6)	−0.0066 (5)	−0.0008 (5)	0.0067 (5)
N3	0.0158 (6)	0.0203 (6)	0.0123 (5)	−0.0015 (5)	0.0001 (4)	0.0014 (5)
C4	0.0159 (7)	0.0140 (7)	0.0142 (7)	0.0004 (5)	0.0038 (5)	−0.0002 (5)
C5	0.0190 (7)	0.0126 (7)	0.0121 (6)	0.0012 (5)	0.0012 (5)	−0.0010 (5)
Cl5	0.0210 (2)	0.0211 (2)	0.0118 (2)	0.00004 (13)	−0.00093 (15)	0.00199 (12)
C6	0.0147 (7)	0.0161 (7)	0.0166 (6)	−0.0005 (5)	−0.0001 (5)	−0.0017 (5)
C7	0.0161 (7)	0.0173 (7)	0.0172 (7)	−0.0026 (5)	0.0045 (6)	−0.0015 (5)
C8	0.0184 (7)	0.0151 (7)	0.0102 (6)	0.0000 (6)	0.0023 (5)	−0.0004 (5)
C9	0.0139 (6)	0.0131 (7)	0.0137 (6)	−0.0003 (5)	0.0017 (5)	−0.0021 (5)

Geometric parameters (Å, º)

O1—C2	1.3742 (17)	C4—H4	0.95
O1—C8	1.3898 (17)	C5—C6	1.3926 (19)
C2—N3	1.3045 (18)	C5—Cl5	1.7504 (14)
C2—N21	1.3335 (19)	C6—C7	1.399 (2)
N21—H21	0.88	C6—H6	0.95
N21—H22	0.88	C7—C8	1.369 (2)
N3—C9	1.3962 (18)	C7—H7	0.95
C4—C5	1.385 (2)	C8—C9	1.3937 (19)
C4—C9	1.3908 (19)		
C2—O1—C8	103.47 (11)	C6—C5—Cl5	118.17 (11)
N3—C2—N21	127.81 (13)	C5—C6—C7	119.86 (13)
N3—C2—O1	115.88 (13)	C5—C6—H6	120.1
N21—C2—O1	116.28 (12)	C7—C6—H6	120.1
C2—N21—H21	120.0	C8—C7—C6	115.94 (13)
C2—N21—H22	120.0	C8—C7—H7	122.0

H21—N21—H22	120.0	C6—C7—H7	122.0
C2—N3—C9	103.97 (11)	C7—C8—O1	127.99 (12)
C5—C4—C9	116.09 (12)	C7—C8—C9	124.53 (13)
C5—C4—H4	122.0	O1—C8—C9	107.47 (12)
C9—C4—H4	122.0	C4—C9—C8	119.75 (13)
C4—C5—C6	123.82 (13)	C4—C9—N3	131.05 (12)
C4—C5—Cl5	118.01 (10)	C8—C9—N3	109.21 (12)
C8—O1—C2—N3	−0.01 (16)	C2—O1—C8—C7	179.64 (14)
C8—O1—C2—N21	−177.95 (13)	C2—O1—C8—C9	−0.43 (14)
N21—C2—N3—C9	178.10 (15)	C5—C4—C9—C8	0.2 (2)
O1—C2—N3—C9	0.43 (16)	C5—C4—C9—N3	−179.91 (13)
C9—C4—C5—C6	−1.0 (2)	C7—C8—C9—C4	0.6 (2)
C9—C4—C5—Cl5	179.99 (10)	O1—C8—C9—C4	−179.34 (11)
C4—C5—C6—C7	1.0 (2)	C7—C8—C9—N3	−179.36 (13)
Cl5—C5—C6—C7	−179.90 (11)	O1—C8—C9—N3	0.71 (15)
C5—C6—C7—C8	−0.3 (2)	C2—N3—C9—C4	179.37 (14)
C6—C7—C8—O1	179.40 (13)	C2—N3—C9—C8	−0.68 (15)
C6—C7—C8—C9	−0.5 (2)		

Hydrogen-bond geometry (Å, º)

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*−1/2, −*y*+1/2, *z*−1/2.