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4-(Pyridin-2-yl)thiazol-2-ylamine

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
R factor = 0.034
wR factor = 0.083
Data-to-parameter ratio = 20.1

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

At 150 K, the asymmetric unit of the crystal structure of the title compound, $C_8H_7N_3S$, comprises three molecules. All the amine N—H groups and heterocyclic N atoms are involved in intermolecular hydrogen bonding.

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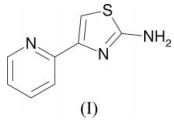
Comment

The title compound, (I), crystallizes with three molecules in the asymmetric unit. The dihedral angles between the least-squares planes of the two heterocyclic rings in molecules 1 (S1, *etc.*), 2 (S2, *etc.*) and 3 (S3, *etc.*) are 22.23 (4), 14.02 (4) and 21.08 (4)°, respectively. All three molecules form doubly intermolecularly hydrogen-bonded dimers through pairs of intermolecular hydrogen bonds, molecule 1 with molecule 2 (Fig. 1), and molecule 3 with a centrosymmetrically related partner (Fig. 2). The outwardly directed N—H bonds of these dimers are hydrogen bonded to pyridine N atoms of neighbouring dimers (Table 3).



(I)

Experimental

The title compound, (I), was prepared according to the methods of Brown *et al.* (1980) and Taurins & Blaga (1970). Suitable crystals were grown by recrystallization from acetonitrile.

Crystal data

$C_8H_7N_3S$
M_r = 177.23
Monoclinic, $P2_1/c$
a = 13.2392 (10) Å
b = 13.7499 (9) Å
c = 14.1126 (12) Å
β = 109.268 (6)°
V = 2425.1 (3) Å^3
Z = 12
D_x = 1.456 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 22342 reflections
θ = 2.1–30.0°
μ = 0.34 mm^{-1}
T = 150 (2) K
Block, colourless
0.60 × 0.55 × 0.50 mm

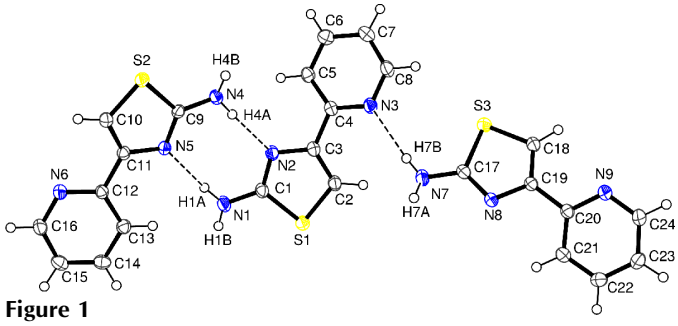


Figure 1
View of the three independent molecules of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are represented by circles of arbitrary size. Hydrogen bonds are indicated by dashed lines.

Data collection

Stoe IPDS II area-detector diffractometer
ω scans
Absorption correction: none
25877 measured reflections
7032 independent reflections
5224 reflections with $I > 2\sigma(I)$
$R_{int} = 0.077$
$\theta_{max} = 30.0°$
$h = -17 \rightarrow 18$
$k = -17 \rightarrow 19$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.084$
$S = 0.90$
7032 reflections
349 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0456P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C2	1.7265 (13)	N6—C16	1.3368 (17)
S1—C1	1.7557 (13)	N6—C12	1.3539 (15)
S2—C10	1.7247 (13)	N7—C17	1.3503 (17)
S2—C9	1.7595 (12)	N8—C17	1.3102 (17)
S3—C18	1.7294 (13)	N8—C19	1.3915 (15)
S3—C17	1.7523 (13)	N9—C24	1.3402 (18)
N1—C1	1.3452 (17)	N9—C20	1.3451 (16)
N2—C1	1.3104 (17)	C2—C3	1.3553 (18)
N2—C3	1.3894 (15)	C3—C4	1.4712 (17)
N3—C8	1.3419 (18)	C10—C11	1.3607 (17)
N3—C4	1.3497 (16)	C11—C12	1.4722 (17)
N4—C9	1.3446 (16)	C18—C19	1.3527 (19)
N5—C9	1.3113 (16)	C19—C20	1.4731 (17)
N5—C11	1.3928 (15)		
C2—S1—C1	89.27 (6)	N5—C9—N4	124.81 (11)
C10—S2—C9	89.04 (6)	N5—C9—S2	114.43 (9)
C18—S3—C17	89.04 (6)	N4—C9—S2	120.74 (10)
N2—C1—N1	124.34 (12)	N8—C17—N7	124.31 (13)
N2—C1—S1	114.13 (9)	N8—C17—S3	114.53 (9)
N1—C1—S1	121.49 (11)	N7—C17—S3	121.16 (11)

Table 2
Contact distances (Å).

N2···C23^{i}	3.396 (2)	C6···C11^{iii}	3.276 (2)
C1···C23^{i}	3.367 (2)	N3···C22^{ii}	3.4973 (17)
C2···C20^{ii}	3.3936 (16)	N3···C23^{ii}	3.3729 (18)
C2···C21^{ii}	3.346 (2)	C14···N8^{iv}	3.2414 (16)
C5···C9^{iii}	3.489 (2)	C14···C19^{iv}	3.4051 (16)
C6···N5^{iii}	3.2952 (19)		

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

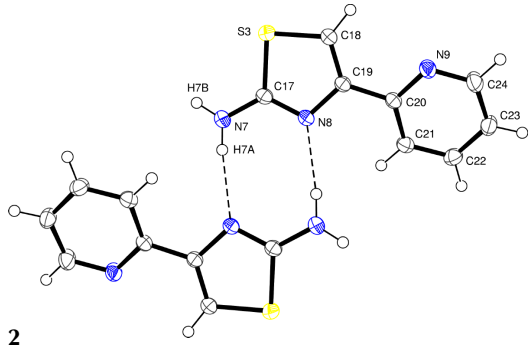


Figure 2
View of the centrosymmetric hydrogen-bonded dimer of molecule 3.

Table 3
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···N5	0.90 (2)	2.33 (2)	3.1852 (17)	159.1 (18)
N1—H1B···N9^{iv}	0.82 (2)	2.19 (2)	3.0077 (19)	170.1 (17)
N4—H4A···N2	0.889 (18)	2.101 (18)	2.9893 (17)	177.0 (15)
N4—H4B···N6^{v}	0.838 (19)	2.207 (19)	3.0320 (18)	168.1 (18)
N7—H7A···N8^{i}	0.88 (2)	2.21 (2)	3.0828 (19)	172.2 (19)
N7—H7B···N3	0.86 (2)	2.38 (2)	3.2249 (19)	169.1 (17)

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

All H atoms were initially located in a difference Fourier map. The amine H-atom positional parameters were refined freely, along with an isotropic displacement parameter. All C—H atoms were placed in geometrically idealized positions, with C—H distances of 0.95 Å. U_{iso}(H) values were set at 1.2U_{eq}(C) for all H atoms.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-RED* (Stoe & Cie, 2001); data reduction: *X-RED*; program(s) used to solve structure: *X-STEP*32 (Stoe & Cie, 2001) and *WinGX* (Farrugia, 1999); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX*.

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