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2-(2-Amino-1,3-thiazol-4-yl)acetohydrazide

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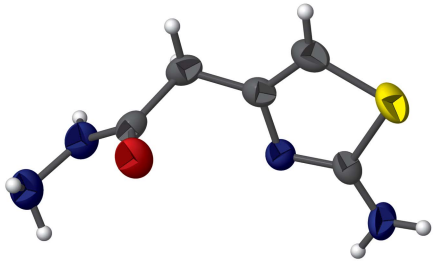
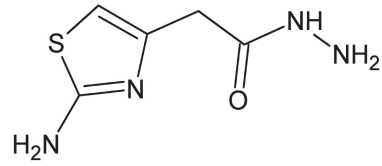
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_5H_8N_4OS$, the dihedral angle between the acetohydrazide moiety and the thiazole ring is 80.96 (8)°. In the crystal, molecules are linked by N—H···O and N—H···N hydrogen bonds generating (010) sheets.

3D view



Chemical scheme



Structure description

2-Aminothiazole is an important and versatile five-membered heterocyclic scaffold which is applied extensively in various branches of chemistry including dyes and pharmaceutical industries. Derivatives of 2-aminothiazoles are used widely by medicinal chemists in drug discovery research: Famotidine is used in the treatment of peptic ulcers and controls gastroesophageal reflux, Abafungin is an antimicrobial agent used for the treatment of dermatomycoses and Cefdinir is used for the treatment of pneumonia, chronic bronchitis, sinusitis, pharyngitis and tonsillitis. Non-steroidal anti-inflammatory drugs (NSAIDs) such as Sudoxicam and Meloxicam are used in arthritis, dysmenorrhea and fever while Pramipexole (Mirapex) has been evaluated as a selective serotonin reuptake inhibitor (SSRI) antidepressant and demonstrated in a placebo-controlled proof of concept study in bipolar disorder which have been reviewed (Das *et al.* 2016).

The crystal structure of the title compound (Fig. 1) reveals an L-shaped conformation for the molecule: the dihedral angle between the acetohydrazide moiety and the thiazole ring (r.m.s. deviation = 0.011 Å) is 80.96 (8)°. The C2—S1—C1 bond angle of 88.76 (8)° reflects the presence of an un-delocalized lone pair of electrons and is similar to that observed in other thiazoles.

The crystal structure features N—H···O and N—H···N hydrogen bonds, which link the molecules into (010) sheets (Fig. 2, Table 1).

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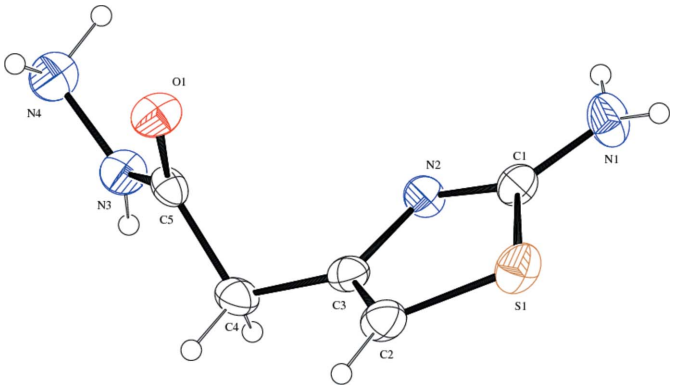

Figure 1
The molecular structure of the title compound, showing 40% probability displacement ellipsoids.

Synthesis and crystallization

A solution of (2-amino-thiazol-4-yl)-acetic acid ethyl ester (0.0116 mol) was refluxed with hydrazine hydrate (Hardy *et al.* 1984) (0.035 mol) in absolute ethanol for 24 h (the completion of the reaction was monitored by thin-layer chromatography). The reaction mixture was concentrated *in vacuo* to obtain the crude product, which was filtered and washed with cold methanol to remove any traces of impurities of hydrazine. Brown blocks of the title compound were obtained by recrystallization from an ethanol and ethyl acetate solvent mixture by slow evaporation

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

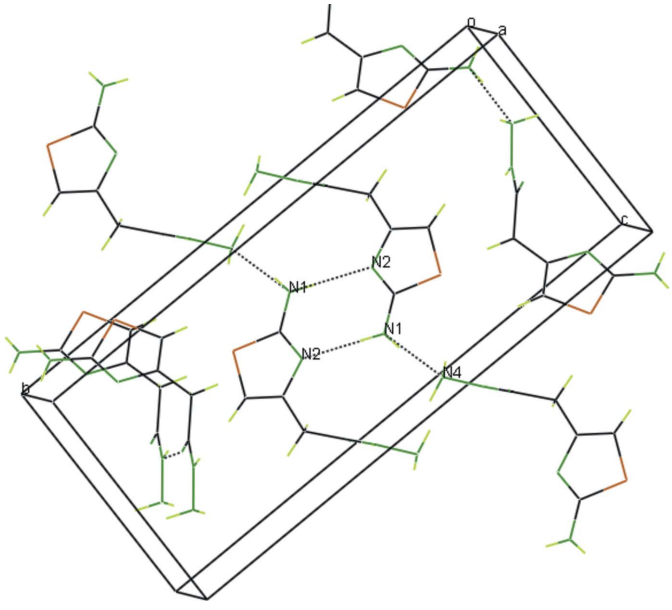

Figure 2
The crystal packing diagram of the title compound. The dotted lines indicate intermolecular hydrogen bonds. All H atoms which are not involved in these interactions have been omitted for clarity.

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···N2^{i}	0.84 (2)	2.14 (2)	2.976 (2)	171 (2)
N1—H1B···N4^{ii}	0.82 (3)	2.21 (2)	3.023 (2)	172 (2)
N3—H3···O1^{iii}	0.84 (2)	1.99 (2)	2.8027 (18)	160.9 (17)
N4—H4C···N1^{iv}	0.83 (2)	2.60 (2)	3.300 (2)	144 (2)
N4—H4D···O1^{v}	0.91 (3)	2.26 (3)	3.148 (2)	164 (2)

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x+1, y, z+1$; (iii) $x-1, y, z$; (iv) $x, y, z-1$; (v) $-x+1, -y+1, -z$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_5H_8N_4OS$
M_r	172.21
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, b, c (Å)	4.9685 (1), 18.8795 (5), 8.2913 (2)
β (°)	91.448 (2)
V (Å^3)	777.50 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.36
Crystal size (mm)	0.3 × 0.2 × 0.2
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.917, 0.930
No. of measured, independent and observed [$I \geq 2u(I)$] reflections	1364, 1364, 1262
R_{int}	0.020
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.030, 0.079, 1.09
No. of reflections	1364
No. of parameters	131
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.28, −0.27

Computer programs: *APEX2*and *SAINT* (Bruker, 2004), *OLEX2* (Dolomanov *et al.*, 2009) and *olex2.refine* (Bourhis *et al.*, 2015).

Acknowledgements

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full crystallographic data

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2-(2-Amino-1,3-thiazol-4-yl)acetohydrazide

Crystal data

$C_5H_8N_4OS$
M_r = 172.21
Monoclinic, $P2_1/c$
a = 4.9685 (1) Å
b = 18.8795 (5) Å
c = 8.2913 (2) Å
β = 91.448 (2)°
V = 777.50 (3) Å^3
Z = 4
$F(000)$ = 360.5934
D_x = 1.471 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4593 reflections
θ = 2.5–30.2°
μ = 0.36 mm^{-1}
T = 293 K
Block, brown
0.3 × 0.2 × 0.2 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
ω and φ scan
Absorption correction: multi-scan (SADABS; Bruker, 2004)
T_{min} = 0.917, T_{max} = 0.930
1364 measured reflections
1364 independent reflections
1262 reflections with $I \geq 2u(I)$
R_{int} = 0.020
θ_{max} = 25.0°, θ_{min} = 2.2°
h = −5→5
k = 0→22
l = 0→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.079
S = 1.09
1364 reflections
131 parameters
0 restraints
0 constraints
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0366P)^2 + 0.2878P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.0002
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Special details

Experimental. Absorption correction: SADABS-2004/1 (Bruker,2004) was used for absorption correction. R(int) was 0.0304 before and 0.0203 after correction. The Ratio of minimum to maximum transmission is 0.8035. The $\lambda/2$ correction factor is 0.0015.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.7239 (3)	0.40966 (9)	0.56391 (19)	0.0381 (4)
C2	0.7249 (4)	0.29205 (10)	0.4459 (2)	0.0468 (4)
H2	0.755 (4)	0.2469 (13)	0.416 (3)	0.066 (6)*
C3	0.5557 (3)	0.33835 (8)	0.3747 (2)	0.0376 (4)
C4	0.3736 (4)	0.32468 (9)	0.2323 (2)	0.0422 (4)
H4a	0.403 (4)	0.2776 (11)	0.190 (2)	0.055 (6)*
H4b	0.197 (4)	0.3273 (9)	0.259 (2)	0.045 (5)*
C5	0.4288 (3)	0.37505 (8)	0.09570 (18)	0.0340 (4)
N1	0.7600 (4)	0.46674 (9)	0.6572 (2)	0.0529 (4)
N2	0.5537 (3)	0.40546 (7)	0.44149 (16)	0.0386 (3)
N3	0.2152 (3)	0.40373 (8)	0.02335 (18)	0.0441 (4)
N4	0.2344 (3)	0.44932 (11)	−0.1106 (2)	0.0515 (4)
S1	0.89807 (10)	0.33134 (2)	0.60529 (5)	0.05055 (19)
O1	0.6576 (2)	0.38824 (7)	0.05292 (15)	0.0462 (3)
H1a	0.687 (4)	0.5046 (12)	0.625 (2)	0.054 (6)*
H1b	0.883 (5)	0.4656 (12)	0.725 (3)	0.064 (7)*
H3	0.058 (4)	0.3921 (10)	0.049 (2)	0.049 (5)*
H4c	0.358 (5)	0.4329 (13)	−0.164 (3)	0.069 (8)*
H4d	0.276 (5)	0.4936 (15)	−0.073 (3)	0.082 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0376 (9)	0.0405 (9)	0.0361 (8)	0.0058 (7)	−0.0014 (7)	0.0067 (7)
C2	0.0588 (11)	0.0353 (9)	0.0467 (10)	0.0063 (8)	0.0089 (8)	0.0049 (7)
C3	0.0378 (9)	0.0358 (8)	0.0397 (8)	−0.0034 (6)	0.0082 (7)	0.0037 (7)
C4	0.0360 (9)	0.0417 (9)	0.0492 (10)	−0.0106 (7)	0.0057 (7)	−0.0040 (7)
C5	0.0245 (8)	0.0383 (8)	0.0391 (8)	−0.0036 (6)	0.0004 (6)	−0.0091 (6)
N1	0.0611 (11)	0.0479 (9)	0.0484 (9)	0.0124 (8)	−0.0243 (8)	−0.0043 (7)
N2	0.0381 (7)	0.0361 (7)	0.0411 (7)	0.0034 (6)	−0.0051 (6)	0.0010 (6)
N3	0.0218 (7)	0.0591 (9)	0.0513 (9)	−0.0037 (6)	−0.0007 (6)	0.0029 (7)
N4	0.0340 (8)	0.0659 (11)	0.0542 (10)	−0.0007 (8)	−0.0079 (7)	0.0077 (8)
S1	0.0572 (3)	0.0499 (3)	0.0443 (3)	0.0186 (2)	−0.0035 (2)	0.01077 (19)
O1	0.0215 (6)	0.0620 (8)	0.0551 (7)	−0.0016 (5)	0.0026 (5)	0.0102 (6)

Geometric parameters (Å, º)

C1—N1	1.336 (2)	C4—C5	1.509 (2)
C1—N2	1.307 (2)	C5—N3	1.322 (2)
C1—S1	1.7431 (16)	C5—O1	1.2254 (18)
C2—H2	0.90 (2)	N1—H1a	0.84 (2)
C2—C3	1.339 (3)	N1—H1b	0.82 (2)
C2—S1	1.726 (2)	N3—N4	1.411 (2)
C3—C4	1.492 (2)	N3—H3	0.84 (2)
C3—N2	1.383 (2)	N4—H4c	0.83 (3)

C4—H4a	0.97 (2)	N4—H4d	0.91 (3)
C4—H4b	0.91 (2)		
N2—C1—N1	125.00 (15)	N3—C5—C4	116.10 (14)
S1—C1—N1	120.76 (13)	O1—C5—C4	122.19 (15)
S1—C1—N2	114.18 (13)	O1—C5—N3	121.71 (16)
C3—C2—H2	127.3 (14)	H1a—N1—C1	117.0 (14)
S1—C2—H2	122.1 (14)	H1b—N1—C1	117.5 (16)
S1—C2—C3	110.60 (14)	H1b—N1—H1a	123 (2)
C4—C3—C2	126.66 (16)	C3—N2—C1	110.83 (14)
N2—C3—C2	115.62 (16)	N4—N3—C5	122.56 (15)
N2—C3—C4	117.72 (14)	H3—N3—C5	121.2 (13)
H4a—C4—C3	110.4 (12)	H3—N3—N4	116.0 (13)
H4b—C4—C3	111.3 (12)	H4c—N4—N3	105.0 (17)
H4b—C4—H4a	107.0 (16)	H4d—N4—N3	108.0 (17)
C5—C4—C3	111.54 (13)	H4d—N4—H4c	111 (2)
C5—C4—H4a	106.1 (12)	C2—S1—C1	88.76 (8)
C5—C4—H4b	110.1 (12)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···N2^{i}	0.84 (2)	2.14 (2)	2.976 (2)	171 (2)
N1—H1B···N4^{ii}	0.82 (3)	2.21 (2)	3.023 (2)	172 (2)
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N4—H4D···O1^{v}	0.91 (3)	2.26 (3)	3.148 (2)	164 (2)

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