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2-(1,3-Benzothiazol-2-yl)guanidine

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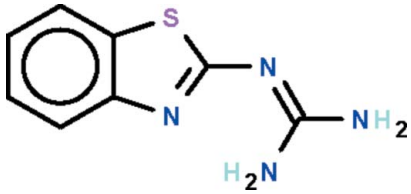
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.039; wR factor = 0.111; data-to-parameter ratio = 15.0.

In the title comound, $C_8H_8N_4S$, one of the two independent molecules is essentially planar (r.m.s. deviation = 0.025 Å), while the other is slightly buckled (r.m.s. deviation = 0.131 Å) with the guanidine unit bent out of the plane of the fused-ring system by 16.8 (1)°. In the crystal, intermolecular N—H···N hydrogen bonds between the two independent molecules give rise to a hydrogen-bonded dimer. Addtional weak intermolecular N—H···N hydrogen bonds connect these dimers into chains along [010]. An intramolecular N—H···N hydrogen bond is also observed in each independent molecule.

Related literature

For the synthesis, see: Dolzhenko *et al.* (2006).



Experimental

Crystal data

$C_8H_8N_4S$
M_r = 192.24
Orthorhombic, *Pbca*
a = 10.2970 (3) Å
b = 10.0817 (3) Å
c = 33.5158 (11) Å
V = 3479.32 (18) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 0.33 mm^{-1}
T = 295 K
0.30 × 0.30 × 0.30 mm

Data collection

Bruker APEXII diffractometer
35704 measured reflections
3996 independent reflections
3345 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.111
S = 1.13
3996 reflections
267 parameters
8 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H31···N1	0.86 (1)	2.00 (2)	2.679 (2)	134 (2)
N3—H32···N2^{i}	0.86 (1)	2.40 (2)	3.228 (2)	161 (2)
N4—H41···N6	0.86 (1)	2.25 (1)	3.084 (3)	165 (3)
N4—H42···N8^{i}	0.86 (1)	2.50 (2)	3.350 (3)	176 (2)
N7—H71···N5	0.86 (1)	2.03 (2)	2.717 (3)	136 (2)
N8—H81···N2	0.86 (1)	2.24 (1)	3.096 (3)	177 (2)

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5214).

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supporting information

Acta Cryst. (2011). E**67**, o786 [doi:10.1107/S160053681100732X]

2-(1,3-Benzothiazol-2-yl)guanidine

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S1. Comment

The title compound was synthesized as an intermediate for the synthesis of other heterocyclic compounds (Dolzhenko *et al.*, 2006). In the title comound, $C_8H_8N_4$, one of the two independent molecules of is essentially planar (r.m.s. deviation 0.025 Å) while the other is slightly buckled (r.m.s. deviation 0.131 Å) with the guanidine unit bent out of the plane of the fused-ring system by 16.8 (1) °. In the crystal a pair of intermolecular N-H···N hydrogen bonds between the two independent molecules give rise to a hydrogen-bonded dimer (Fig. 1). Addtional weak intermolecular N-H···N hydrogen bonds connect these dimers into one-dimensional chains along [010].

S2. Experimental

2-Aminothiophenol (0.050 mol) was dissolved in 10% sulfuric acid (50 ml) and to the solution was added cyano-duanidine (0.075 mol). The mixture was heated to give a clear solution. To the cool solution was added 50% sodium hydroxide (10 mol) to precipitate the product. X-ray quality crystals were recrystallized from ethanol in 90% yield. The synthesis was based on a reported procedure (Dolzhenko *et al.*, 2006).

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions [C–H 0.93 Å; U_{iso}(H) 1.2U_{eq}(C)] and were included in the refinement in a riding-model approximation. The amino H-atoms were located in a difference Fourier map, and were refined with a distance restraint of N–H 0.86±0.01 Å; the U_{iso}(H) values were refined.

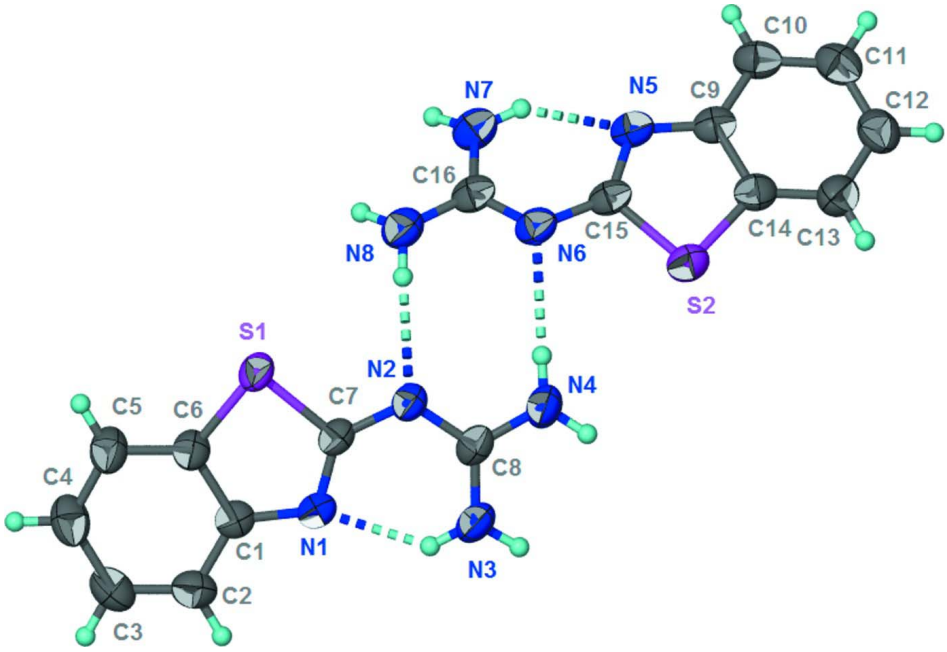

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of the two independent molecules of $C_8H_8N_4$ with displacement ellipsoids drawn at the 50% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius. Hydrogen bonds are denoted by dashed lines.

2-(1,3-Benzothiazol-2-yl)guanidine

Crystal data

$C_8H_8N_4S$
$M_r = 192.24$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 10.2970\ (3)$ Å
$b = 10.0817\ (3)$ Å
$c = 33.5158\ (11)$ Å
$V = 3479.32\ (18)$ Å^3
$Z = 16$
$F(000) = 1600$
$D_x = 1.468$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9882 reflections
$\theta = 2.3$–$27.7°$
$\mu = 0.33$ mm^{-1}
$T = 295$ K
Prism, colorless
0.30 × 0.30 × 0.30 mm

Data collection

Bruker APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
35704 measured reflections
3996 independent reflections
3345 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.3°$
$h = -13\rightarrow13$
$k = -13\rightarrow13$
$l = -43\rightarrow43$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.111$
$S = 1.13$
3996 reflections
267 parameters
8 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0453P)^2 + 1.2618P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.48382 (5)	0.66100 (5)	0.659730 (17)	0.05839 (16)
S2	0.84372 (5)	0.47427 (6)	0.472576 (17)	0.06418 (17)
N1	0.55487 (14)	0.42140 (14)	0.67760 (4)	0.0474 (3)
N2	0.64035 (14)	0.51382 (15)	0.61637 (5)	0.0485 (3)
N3	0.71411 (18)	0.29516 (18)	0.62708 (6)	0.0605 (4)
H31	0.6709 (19)	0.293 (2)	0.6491 (4)	0.064 (7)*
H32	0.756 (2)	0.2272 (16)	0.6184 (7)	0.073 (7)*
N4	0.77196 (19)	0.4128 (2)	0.57119 (5)	0.0649 (5)
H41	0.753 (3)	0.4781 (19)	0.5560 (6)	0.087 (9)*
H42	0.8259 (19)	0.3507 (18)	0.5657 (7)	0.071 (7)*
N5	0.67826 (16)	0.63000 (15)	0.43811 (5)	0.0537 (4)
N6	0.66455 (16)	0.61327 (15)	0.51004 (5)	0.0534 (4)
N7	0.47131 (19)	0.70197 (19)	0.48350 (6)	0.0612 (4)
H71	0.505 (2)	0.692 (3)	0.4602 (4)	0.079 (9)*
H72	0.3919 (12)	0.722 (2)	0.4882 (7)	0.074 (7)*
N8	0.5036 (2)	0.68148 (19)	0.55135 (6)	0.0649 (5)
H81	0.539 (2)	0.635 (2)	0.5699 (5)	0.066 (7)*
H82	0.4247 (12)	0.706 (3)	0.5554 (7)	0.082 (8)*
C1	0.47271 (17)	0.46403 (18)	0.70777 (6)	0.0477 (4)
C2	0.4344 (2)	0.3899 (2)	0.74069 (6)	0.0609 (5)
H2	0.4661	0.3043	0.7443	0.073*
C3	0.3497 (2)	0.4436 (3)	0.76785 (7)	0.0682 (6)
H3	0.3247	0.3939	0.7899	0.082*
C4	0.3009 (2)	0.5704 (2)	0.76293 (7)	0.0690 (6)
H4	0.2434	0.6047	0.7817	0.083*
C5	0.3367 (2)	0.6461 (2)	0.73061 (7)	0.0626 (5)
H5	0.3037	0.7312	0.7272	0.075*
C6	0.42309 (18)	0.59256 (18)	0.70318 (6)	0.0504 (4)
C7	0.56907 (17)	0.51333 (16)	0.65055 (5)	0.0448 (4)
C8	0.70785 (17)	0.40623 (18)	0.60589 (6)	0.0488 (4)
C9	0.75591 (18)	0.57694 (17)	0.40817 (5)	0.0495 (4)
C10	0.7460 (2)	0.6048 (2)	0.36749 (6)	0.0604 (5)
H10	0.6833	0.6637	0.3582	0.072*

C11	0.8292 (2)	0.5445 (2)	0.34137 (7)	0.0640 (6)
H11	0.8221	0.5624	0.3142	0.077*
C12	0.9238 (2)	0.4574 (2)	0.35448 (7)	0.0685 (6)
H12	0.9791	0.4175	0.3361	0.082*
C13	0.9367 (2)	0.4293 (2)	0.39439 (7)	0.0697 (6)
H13	1.0006	0.3712	0.4033	0.084*
C14	0.85219 (19)	0.48948 (19)	0.42113 (6)	0.0545 (5)
C15	0.71308 (18)	0.58623 (17)	0.47312 (6)	0.0494 (4)
C16	0.5469 (2)	0.66392 (17)	0.51381 (6)	0.0529 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0643 (3)	0.0367 (2)	0.0742 (3)	0.0069 (2)	0.0233 (2)	0.0041 (2)
S2	0.0636 (3)	0.0691 (3)	0.0598 (3)	0.0202 (3)	−0.0057 (2)	0.0084 (2)
N1	0.0456 (8)	0.0428 (7)	0.0537 (8)	0.0032 (6)	−0.0053 (6)	0.0014 (6)
N2	0.0488 (8)	0.0429 (8)	0.0537 (8)	0.0055 (6)	0.0022 (7)	−0.0031 (6)
N3	0.0647 (11)	0.0507 (9)	0.0660 (11)	0.0193 (8)	−0.0024 (9)	−0.0044 (8)
N4	0.0678 (11)	0.0718 (12)	0.0551 (10)	0.0255 (10)	0.0021 (8)	−0.0080 (9)
N5	0.0621 (9)	0.0436 (8)	0.0554 (9)	0.0028 (7)	−0.0127 (7)	−0.0002 (7)
N6	0.0627 (10)	0.0432 (8)	0.0544 (9)	0.0061 (7)	−0.0108 (7)	−0.0043 (7)
N7	0.0544 (10)	0.0582 (10)	0.0710 (12)	0.0035 (8)	−0.0113 (9)	−0.0030 (9)
N8	0.0742 (13)	0.0538 (10)	0.0667 (12)	0.0118 (9)	−0.0006 (10)	−0.0019 (8)
C1	0.0418 (9)	0.0473 (9)	0.0539 (10)	−0.0037 (7)	−0.0055 (7)	−0.0004 (8)
C2	0.0602 (12)	0.0626 (12)	0.0601 (12)	−0.0020 (10)	−0.0054 (9)	0.0120 (9)
C3	0.0689 (14)	0.0793 (15)	0.0564 (12)	−0.0138 (12)	0.0052 (10)	0.0083 (11)
C4	0.0622 (12)	0.0731 (14)	0.0716 (14)	−0.0145 (11)	0.0189 (11)	−0.0118 (11)
C5	0.0596 (12)	0.0514 (11)	0.0768 (14)	−0.0064 (9)	0.0183 (10)	−0.0085 (10)
C6	0.0478 (9)	0.0437 (9)	0.0596 (11)	−0.0064 (8)	0.0075 (8)	−0.0032 (8)
C7	0.0410 (8)	0.0382 (8)	0.0551 (10)	0.0016 (7)	−0.0019 (7)	−0.0037 (7)
C8	0.0435 (9)	0.0503 (10)	0.0526 (10)	0.0070 (8)	−0.0115 (8)	−0.0111 (8)
C9	0.0520 (10)	0.0376 (8)	0.0588 (10)	−0.0089 (8)	−0.0089 (8)	0.0002 (8)
C10	0.0686 (12)	0.0525 (11)	0.0602 (11)	−0.0076 (10)	−0.0137 (10)	0.0056 (9)
C11	0.0776 (14)	0.0571 (12)	0.0571 (12)	−0.0192 (11)	−0.0018 (10)	0.0028 (9)
C12	0.0769 (15)	0.0618 (12)	0.0669 (13)	−0.0092 (11)	0.0149 (11)	0.0024 (10)
C13	0.0686 (13)	0.0658 (13)	0.0748 (14)	0.0097 (11)	0.0105 (11)	0.0092 (11)
C14	0.0559 (11)	0.0475 (10)	0.0600 (11)	−0.0040 (8)	−0.0032 (9)	0.0054 (8)
C15	0.0543 (10)	0.0355 (8)	0.0583 (10)	−0.0008 (7)	−0.0134 (8)	−0.0021 (7)
C16	0.0625 (11)	0.0325 (8)	0.0637 (11)	−0.0023 (8)	−0.0099 (9)	−0.0051 (8)

Geometric parameters (Å, º)

S1—C6	1.7285 (19)	N8—H81	0.860 (10)
S1—C7	1.7555 (17)	N8—H82	0.861 (10)
S2—C14	1.733 (2)	C1—C2	1.390 (3)
S2—C15	1.7562 (19)	C1—C6	1.401 (3)
N1—C7	1.305 (2)	C2—C3	1.372 (3)
N1—C1	1.387 (2)	C2—H2	0.9300

N2—C8	1.335 (2)	C3—C4	1.383 (3)
N2—C7	1.360 (2)	C3—H3	0.9300
N3—C8	1.328 (3)	C4—C5	1.375 (3)
N3—H31	0.863 (9)	C4—H4	0.9300
N3—H32	0.860 (10)	C5—C6	1.389 (3)
N4—C8	1.339 (3)	C5—H5	0.9300
N4—H41	0.855 (10)	C9—C10	1.396 (3)
N4—H42	0.857 (10)	C9—C14	1.396 (3)
N5—C15	1.304 (2)	C10—C11	1.368 (3)
N5—C9	1.390 (3)	C10—H10	0.9300
N6—C16	1.321 (3)	C11—C12	1.382 (3)
N6—C15	1.362 (2)	C11—H11	0.9300
N7—C16	1.336 (3)	C12—C13	1.374 (3)
N7—H71	0.862 (10)	C12—H12	0.9300
N7—H72	0.856 (10)	C13—C14	1.388 (3)
N8—C16	1.347 (3)	C13—H13	0.9300

C6—S1—C7	89.43 (9)	C5—C6—C1	121.36 (18)
C14—S2—C15	89.54 (9)	C5—C6—S1	129.38 (16)
C7—N1—C1	110.79 (15)	C1—C6—S1	109.25 (14)
C8—N2—C7	119.96 (16)	N1—C7—N2	130.40 (16)
C8—N3—H31	117.0 (16)	N1—C7—S1	115.11 (13)
C8—N3—H32	121.0 (16)	N2—C7—S1	114.48 (12)
H31—N3—H32	122 (2)	N3—C8—N2	124.73 (18)
C8—N4—H41	116.5 (19)	N3—C8—N4	118.86 (18)
C8—N4—H42	118.1 (17)	N2—C8—N4	116.41 (18)
H41—N4—H42	125 (2)	N5—C9—C10	125.84 (18)
C15—N5—C9	111.18 (16)	N5—C9—C14	115.27 (17)
C16—N6—C15	120.07 (16)	C10—C9—C14	118.89 (19)
C16—N7—H71	115.0 (18)	C11—C10—C9	119.3 (2)
C16—N7—H72	118.9 (17)	C11—C10—H10	120.3
H71—N7—H72	125 (2)	C9—C10—H10	120.3
C16—N8—H81	117.6 (16)	C10—C11—C12	121.4 (2)
C16—N8—H82	119.8 (17)	C10—C11—H11	119.3
H81—N8—H82	116 (2)	C12—C11—H11	119.3
N1—C1—C2	125.81 (18)	C13—C12—C11	120.6 (2)
N1—C1—C6	115.41 (16)	C13—C12—H12	119.7
C2—C1—C6	118.76 (18)	C11—C12—H12	119.7
C3—C2—C1	119.6 (2)	C12—C13—C14	118.5 (2)
C3—C2—H2	120.2	C12—C13—H13	120.7
C1—C2—H2	120.2	C14—C13—H13	120.7
C2—C3—C4	121.1 (2)	C13—C14—C9	121.3 (2)
C2—C3—H3	119.5	C13—C14—S2	129.41 (17)
C4—C3—H3	119.5	C9—C14—S2	109.25 (15)
C5—C4—C3	120.6 (2)	N5—C15—N6	130.46 (18)
C5—C4—H4	119.7	N5—C15—S2	114.76 (15)
C3—C4—H4	119.7	N6—C15—S2	114.79 (13)
C4—C5—C6	118.5 (2)	N6—C16—N7	124.9 (2)

C4—C5—H5	120.7	N6—C16—N8	116.38 (18)
C6—C5—H5	120.7	N7—C16—N8	118.7 (2)
C7—N1—C1—C2	178.46 (18)	C15—N5—C9—C10	−178.95 (18)
C7—N1—C1—C6	0.1 (2)	C15—N5—C9—C14	0.4 (2)
N1—C1—C2—C3	−178.35 (19)	N5—C9—C10—C11	−179.80 (18)
C6—C1—C2—C3	−0.1 (3)	C14—C9—C10—C11	0.9 (3)
C1—C2—C3—C4	0.4 (3)	C9—C10—C11—C12	−0.6 (3)
C2—C3—C4—C5	−0.2 (4)	C10—C11—C12—C13	−0.1 (3)
C3—C4—C5—C6	−0.2 (3)	C11—C12—C13—C14	0.5 (4)
C4—C5—C6—C1	0.5 (3)	C12—C13—C14—C9	−0.1 (3)
C4—C5—C6—S1	178.91 (17)	C12—C13—C14—S2	179.90 (18)
N1—C1—C6—C5	178.08 (17)	N5—C9—C14—C13	−179.97 (19)
C2—C1—C6—C5	−0.4 (3)	C10—C9—C14—C13	−0.6 (3)
N1—C1—C6—S1	−0.6 (2)	N5—C9—C14—S2	0.0 (2)
C2—C1—C6—S1	−179.04 (15)	C10—C9—C14—S2	179.40 (14)
C7—S1—C6—C5	−177.9 (2)	C15—S2—C14—C13	179.7 (2)
C7—S1—C6—C1	0.65 (14)	C15—S2—C14—C9	−0.30 (14)
C1—N1—C7—N2	179.79 (18)	C9—N5—C15—N6	179.41 (18)
C1—N1—C7—S1	0.39 (19)	C9—N5—C15—S2	−0.6 (2)
C8—N2—C7—N1	1.6 (3)	C16—N6—C15—N5	19.2 (3)
C8—N2—C7—S1	−178.99 (13)	C16—N6—C15—S2	−160.82 (14)
C6—S1—C7—N1	−0.63 (15)	C14—S2—C15—N5	0.53 (15)
C6—S1—C7—N2	179.88 (14)	C14—S2—C15—N6	−179.47 (15)
C7—N2—C8—N3	−1.5 (3)	C15—N6—C16—N7	−5.5 (3)
C7—N2—C8—N4	177.80 (17)	C15—N6—C16—N8	176.74 (17)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H31···N1	0.86 (1)	2.00 (2)	2.679 (2)	134 (2)
N3—H32···N2^{i}	0.86 (1)	2.40 (2)	3.228 (2)	161 (2)
N4—H41···N6	0.86 (1)	2.25 (1)	3.084 (3)	165 (3)
N4—H42···N8^{i}	0.86 (1)	2.50 (2)	3.350 (3)	176 (2)
N7—H71···N5	0.86 (1)	2.03 (2)	2.717 (3)	136 (2)
N8—H81···N2	0.86 (1)	2.24 (1)	3.096 (3)	177 (2)

Symmetry code: (i) −*x*+3/2, *y*−1/2, *z*.