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# 5-Amino-1,3,4-thiadiazol-2(3*H*)-one

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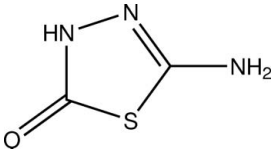
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(N–C) = 0.002 Å; $R$ factor = 0.031; $wR$ factor = 0.080; data-to-parameter ratio = 15.2.

The asymmetric unit of the title compound, $C_2H_3N_3OS$, contains three independent molecules which are essentially planar, with r.m.s. deviations of 0.011 (2)–0.027 (2) Å from the mean plane defined by the seven non-H atoms. In the crystal, N—H···N and N—H···O hydrogen bonds link the molecules into a sheet parallel to the (111) plane.

## Related literature

For the structures and reactivity of thiadiazole derivatives, see: Parkanyi *et al.* (1989); Cho, Cho *et al.* (1996); Cho, Ra *et al.* (1996). For the biological activity of thiadiazole derivatives, see: Castro *et al.* (2008); Ra, Cho & Cho (1998); Ra, Cho, Moon & Kang (1998).




## Experimental

### Crystal data

$C_2H_3N_3OS$
$M_r$ = 117.13
Triclinic, $P\overline{1}$
$a$ = 7.2860 (2) Å
$b$ = 10.2982 (3) Å
$c$ = 10.7727 (3) Å
$\alpha$ = 63.721 (3)°
$\beta$ = 73.122 (2)°
$\gamma$ = 76.737 (2)°
$V$ = 688.74 (3) Å$^3$
$Z$ = 6
Mo $K\alpha$ radiation
$\mu$ = 0.57 mm$^{-1}$
$T$ = 296 K
0.15 × 0.1 × 0.05 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min}$ = 0.93, $T_{max}$ = 0.97
23857 measured reflections
3433 independent reflections
2526 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.055

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.080
$S$ = 0.94
3433 reflections
226 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.30 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.26 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H3···N18 | 0.854 (19) | 2.004 (19) | 2.8516 (19) | 171.9 (18) |
| N7—H7$A$···O20$^{i}$ | 0.87 (2) | 2.07 (2) | 2.907 (2) | 160 (2) |
| N10—H10···N4 | 0.98 (2) | 1.88 (2) | 2.8558 (19) | 175.7 (18) |
| N14—H14$A$···O6$^{ii}$ | 0.83 (2) | 2.10 (2) | 2.897 (2) | 162 (2) |
| N17—H17···N11 | 0.88 (2) | 1.97 (2) | 2.8424 (18) | 179 (4) |
| N21—H21$A$···O13$^{iii}$ | 0.80 (3) | 2.10 (3) | 2.878 (2) | 163 (2) |

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS5096).

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# supporting information

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## 5-Amino-1,3,4-thiadiazol-2(3*H*)-one

**Sung Kwon Kang, Nam Sook Cho and Siyoung Jang**

### S1. Comment

5-Amino-2*H*-1,2,4-thiadiazolin-3-one heterocycle is an analog of cytosine (Parkanyi *et al.*, 1989). Derivatives of 5-amino-2*H*-1,2,4-thiadiazolin-3-one have recently attracted attention on the antibacterial activity, potential carcinogenicity, and kinase inhibitor activity (Castro *et al.*, 2008; Cho, Ra *et al.*, 1996; Ra, Cho, Moon & Kang, 1998). 5-Amino-3*H*-1,3,4-thiadiazolin-2-one is an isomer of 5-amino-2*H*-1,2,4-thiadiazolin-3-one, which has become an attractive moiety due to potential biological activities (Cho, Cho, Ra, Moon *et al.*, 1996; Ra, Cho & Cho 1998).

In (I), three independent but similar molecules, which are linked by the intermolecular N—H···N hydrogen bonds (Fig. 1), comprise the asymmetric unit. The 1,3,4-thiadiazolin-2-one units are almost planar with r.m.s. deviations of 0.011 (2)–0.027 (2) Å from the corresponding least-squares plane defined by the seven constituent atoms. The bond distance of N4—C5 [1.291 (2) Å; N11—C12, 1.287 (2) Å; N18—C19, 1.282 (2) Å] is shorter than that of C2—N3 [1.333 (2) Å; C9—N10, 1.336 (2) Å; C16—N17, 1.327 Å], which is consistent with double bond character. The crystal structure is stabilized by the intermolecular N—H···N and N—H···O hydrogen bonds, which link the molecules into a two-dimensional sheet parallel to the (111) plane (Table 1 and Fig. 2).

### S2. Experimental

Synthesis of 5-amino-2-ethoxy-1,3,4-thiadiazole: Ethyl thiocarbazate (4.8 g, 0.04 mol) was dissolved in 24 ml of 2 N NaOH at 10 °C. Cyanogen bromide (4.2 g, 0.04 mol) dissolved in 20 ml of ethanol was added to the above solution keeping the temperature below 10 °C during 45 minutes. The solid product (4.1 g, 71%) was collected by filtration. To obtain the analytical sample the product was recrystallized from ethanol. m.p. 200–202 °C; IR (KBr, $cm^{-1}$) 3300 (NH), 3150 (NH), 3000 (CH), 2950 (CH), 1620 (C=O), 1580 (C=N); $^1$H NMR (DMSO-$d_6$, p.p.m.) 6.65 (2*H*, b, $NH_2$), 4.25 (2*H*, q, $CH_2$), 1.29 (3*H*, t, $CH_3$); $^{13}$C NMR (DMSO-$d_6$, p.p.m.) 164.85 (C=N), 162.18 (C—O), 67.48 ($CH_2$), 14.35 ($CH_3$); Anal. Calcd. For $C_4H_7N_3OS$: C 33.09, H 4.86, N 28.94. Found: C 33.71, H 4.94, N 28.50.

Synthesis of title compound: 5-Amino-2-ethoxy-1,3,4-thiadiazole (5 g, 34.5 mmol) was dissolved in 50 ml of dioxane and 3.5 ml of c-HCl was added. The reaction mixture was refluxed for 4.5 h. The solvent was distilled off under reduced pressure. The residue product was washed with ether (3.7 g, 92.5%). To obtain the analytical sample the product was recrystallized from water. Recrystallization from DMSO afforded the colorless crystals suitable for X-ray diffraction. m.p. 176–178 °C; IR (KBr, $cm^{-1}$) 3450 (NH), 3150 (NH), 3100, 3000, 2900 (CH), 1700 (C=O), 1610, 1500 (C=N); $^1$H NMR (DMSO-$d_6$, p.p.m.) 11.3 (1*H*, b, NH), 6.4 (2*H*, b, $NH_2$; $^{13}$C NMR (DMSO-$d_6$, p.p.m.) 169.4 (C=N), 153.0 (C=O); Anal. Calcd. For $C_2H_3N_3OS$: C 20.51, H 2.58, N 35.88, S 27.37. Found: C 20.19, H 2.65, N 34.28, S 27.22.

### S3. Refinement

H atoms of the NH and $NH_2$ groups were located in a difference Fourier map and refined freely [refined distances = 0.79 (2)–0.94 (2) Å].

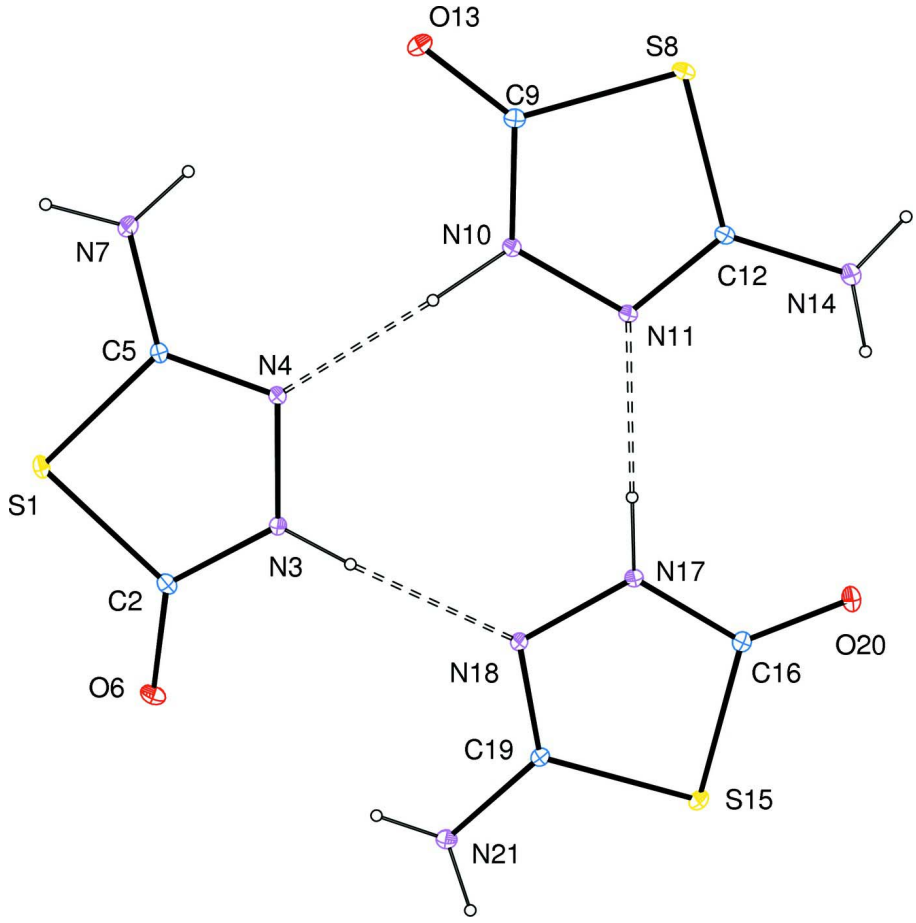


**Figure 1**

Molecular structure of the title compound, showing the atom-numbering scheme and 30% probability ellipsoids. Intermolecular N—H···N hydrogen bonds are indicated by dashed lines.

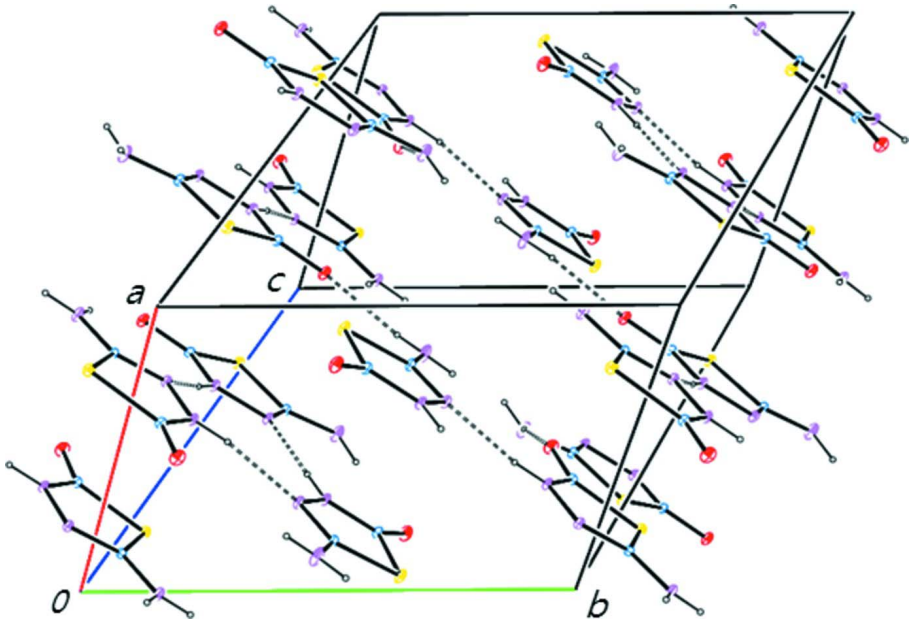


**Figure 2**

Part of the crystal structure of the title compound, showing molecules linked by intermolecular N—H···N and N—H···O hydrogen bonds (dashed lines).

### 5-Amino-1,3,4-thiadiazol-2(3*H*)-one

*Crystal data*

$C_2H_3N_3OS$
$M_r$ = 117.13
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a$ = 7.2860 (2) Å
$b$ = 10.2982 (3) Å
$c$ = 10.7727 (3) Å
$\alpha$ = 63.721 (3)°
$\beta$ = 73.122 (2)°
$\gamma$ = 76.737 (2)°
$V$ = 688.74 (3) Å$^3$
$Z$ = 6
$F(000)$ = 360
$D_x$ = 1.694 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 5437 reflections
$\theta$ = 2.2–26.1°
$\mu$ = 0.57 mm$^{-1}$
$T$ = 296 K
Block, colourless
0.15 × 0.1 × 0.05 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min}$ = 0.93, $T_{max}$ = 0.97
23857 measured reflections
3433 independent reflections
2526 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.055
$\theta_{max}$ = 28.3°, $\theta_{min}$ = 2.2°
$h$ = −9→9
$k$ = −13→13
$l$ = −14→14

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.080$
$S = 0.94$
3433 reflections
226 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
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0423P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.30$ e Å$^{-3}$
$\Delta\rho_{min} = -0.26$ e Å$^{-3}$

*Special details*

**Geometry**. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on $F^2$, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative $F^2$. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.86165 (6) | −0.07773 (5) | −0.06572 (4) | 0.03647 (13) |
| C2 | 0.7587 (2) | 0.10880 (18) | −0.13554 (16) | 0.0339 (4) |
| N3 | 0.6466 (2) | 0.13649 (15) | −0.02585 (14) | 0.0329 (3) |
| H3 | 0.580 (3) | 0.219 (2) | −0.0362 (19) | 0.044 (5)* |
| N4 | 0.62764 (19) | 0.02538 (14) | 0.10886 (13) | 0.0303 (3) |
| C5 | 0.7333 (2) | −0.09181 (17) | 0.10313 (16) | 0.0289 (3) |
| O6 | 0.7853 (2) | 0.19397 (15) | −0.26078 (12) | 0.0517 (4) |
| N7 | 0.7416 (3) | −0.21857 (17) | 0.21825 (17) | 0.0472 (4) |
| H7A | 0.825 (3) | −0.291 (3) | 0.210 (2) | 0.072 (7)* |
| H7B | 0.672 (3) | −0.224 (2) | 0.297 (2) | 0.052 (6)* |
| S8 | 0.15828 (7) | 0.02436 (5) | 0.59226 (4) | 0.03889 (13) |
| C9 | 0.3260 (2) | −0.05097 (18) | 0.47618 (16) | 0.0338 (4) |
| N10 | 0.3484 (2) | 0.05559 (15) | 0.34594 (14) | 0.0353 (3) |
| H10 | 0.439 (3) | 0.047 (2) | 0.262 (2) | 0.065 (6)* |
| N11 | 0.2481 (2) | 0.19183 (14) | 0.32756 (13) | 0.0354 (3) |
| C12 | 0.1437 (2) | 0.19073 (18) | 0.44702 (16) | 0.0348 (4) |
| O13 | 0.40594 (19) | −0.17651 (13) | 0.51031 (13) | 0.0485 (3) |
| N14 | 0.0375 (3) | 0.3114 (2) | 0.4619 (2) | 0.0592 (5) |
| H14A | −0.048 (3) | 0.297 (2) | 0.536 (3) | 0.070 (7)* |
| H14B | 0.019 (3) | 0.387 (2) | 0.386 (2) | 0.050 (6)* |
| S15 | 0.23799 (7) | 0.66689 (5) | −0.15169 (5) | 0.04302 (14) |
| C16 | 0.1723 (2) | 0.55543 (18) | 0.03347 (17) | 0.0363 (4) |
| N17 | 0.2688 (2) | 0.42407 (15) | 0.05437 (15) | 0.0353 (3) |
| H17 | 0.262 (3) | 0.352 (2) | 0.138 (2) | 0.053 (6)* |
| N18 | 0.3933 (2) | 0.40035 (14) | −0.06009 (13) | 0.0354 (3) |

| | | | | |
|---|---|---|---|---|
| C19 | 0.3895 (2) | 0.51734 (17) | −0.17336 (17) | 0.0356 (4) |
| O20 | 0.0594 (2) | 0.59341 (14) | 0.12439 (14) | 0.0537 (4) |
| N21 | 0.4930 (3) | 0.5249 (2) | −0.30232 (18) | 0.0651 (6) |
| H21A | 0.492 (4) | 0.606 (3) | −0.363 (3) | 0.081 (8)* |
| H21B | 0.566 (3) | 0.455 (3) | −0.304 (2) | 0.071 (8)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0365 (2) | 0.0374 (2) | 0.0315 (2) | 0.00386 (18) | 0.00096 (17) | −0.01947 (18) |
| C2 | 0.0319 (9) | 0.0371 (9) | 0.0289 (8) | −0.0040 (7) | −0.0003 (7) | −0.0139 (7) |
| N3 | 0.0386 (8) | 0.0250 (7) | 0.0254 (6) | 0.0032 (6) | −0.0008 (6) | −0.0089 (6) |
| N4 | 0.0345 (7) | 0.0262 (7) | 0.0233 (6) | 0.0000 (6) | −0.0004 (5) | −0.0091 (5) |
| C5 | 0.0290 (8) | 0.0292 (8) | 0.0274 (7) | −0.0007 (7) | −0.0024 (6) | −0.0139 (7) |
| O6 | 0.0631 (9) | 0.0485 (8) | 0.0246 (6) | −0.0049 (7) | 0.0027 (6) | −0.0064 (6) |
| N7 | 0.0625 (12) | 0.0306 (9) | 0.0324 (8) | 0.0104 (8) | −0.0046 (8) | −0.0096 (7) |
| S8 | 0.0458 (3) | 0.0368 (2) | 0.02102 (19) | −0.00454 (19) | 0.00086 (17) | −0.00531 (17) |
| C9 | 0.0375 (9) | 0.0317 (9) | 0.0270 (8) | −0.0028 (7) | −0.0059 (7) | −0.0084 (7) |
| N10 | 0.0412 (8) | 0.0293 (7) | 0.0241 (6) | 0.0039 (6) | −0.0013 (6) | −0.0080 (6) |
| N11 | 0.0412 (8) | 0.0276 (7) | 0.0224 (6) | 0.0029 (6) | 0.0011 (6) | −0.0052 (6) |
| C12 | 0.0366 (9) | 0.0310 (9) | 0.0261 (8) | −0.0022 (7) | 0.0009 (7) | −0.0078 (7) |
| O13 | 0.0601 (9) | 0.0290 (7) | 0.0423 (7) | 0.0049 (6) | −0.0128 (6) | −0.0056 (6) |
| N14 | 0.0692 (13) | 0.0386 (10) | 0.0393 (10) | 0.0088 (9) | 0.0126 (9) | −0.0111 (8) |
| S15 | 0.0533 (3) | 0.0232 (2) | 0.0365 (2) | 0.00734 (19) | −0.0052 (2) | −0.00628 (18) |
| C16 | 0.0386 (10) | 0.0298 (9) | 0.0342 (9) | 0.0008 (7) | −0.0040 (7) | −0.0121 (7) |
| N17 | 0.0417 (9) | 0.0258 (7) | 0.0255 (7) | 0.0029 (6) | −0.0009 (6) | −0.0061 (6) |
| N18 | 0.0423 (8) | 0.0241 (7) | 0.0267 (7) | 0.0036 (6) | 0.0006 (6) | −0.0074 (6) |
| C19 | 0.0428 (10) | 0.0240 (8) | 0.0305 (8) | 0.0000 (7) | −0.0020 (7) | −0.0083 (7) |
| O20 | 0.0561 (9) | 0.0453 (8) | 0.0474 (7) | 0.0072 (6) | 0.0046 (6) | −0.0238 (6) |
| N21 | 0.0938 (16) | 0.0328 (10) | 0.0314 (9) | 0.0067 (10) | 0.0134 (9) | −0.0036 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—C5 | 1.7449 (15) | N10—H10 | 0.98 (2) |
| S1—C2 | 1.7905 (17) | N11—C12 | 1.2874 (19) |
| C2—O6 | 1.2270 (19) | C12—N14 | 1.354 (2) |
| C2—N3 | 1.333 (2) | N14—H14A | 0.83 (2) |
| N3—N4 | 1.3857 (18) | N14—H14B | 0.86 (2) |
| N3—H3 | 0.854 (19) | S15—C19 | 1.7419 (17) |
| N4—C5 | 1.2905 (19) | S15—C16 | 1.7876 (17) |
| C5—N7 | 1.349 (2) | C16—O20 | 1.2298 (19) |
| N7—H7A | 0.87 (2) | C16—N17 | 1.327 (2) |
| N7—H7B | 0.84 (2) | N17—N18 | 1.3853 (18) |
| S8—C12 | 1.7419 (16) | N17—H17 | 0.88 (2) |
| S8—C9 | 1.7874 (17) | N18—C19 | 1.2821 (19) |
| C9—O13 | 1.2264 (19) | C19—N21 | 1.352 (2) |
| C9—N10 | 1.336 (2) | N21—H21A | 0.80 (3) |
| N10—N11 | 1.3817 (18) | N21—H21B | 0.79 (2) |

| | | | |
|---|---|---|---|
| C5—S1—C2 | 88.70 (7) | C12—N11—N10 | 110.16 (13) |
| O6—C2—N3 | 126.79 (16) | N11—C12—N14 | 123.00 (15) |
| O6—C2—S1 | 126.30 (13) | N11—C12—S8 | 115.37 (12) |
| N3—C2—S1 | 106.90 (12) | N14—C12—S8 | 121.53 (13) |
| C2—N3—N4 | 119.16 (14) | C12—N14—H14A | 116.1 (16) |
| C2—N3—H3 | 122.2 (13) | C12—N14—H14B | 117.8 (13) |
| N4—N3—H3 | 118.5 (13) | H14A—N14—H14B | 118 (2) |
| C5—N4—N3 | 109.74 (12) | C19—S15—C16 | 88.49 (8) |
| N4—C5—N7 | 122.96 (15) | O20—C16—N17 | 126.47 (16) |
| N4—C5—S1 | 115.48 (12) | O20—C16—S15 | 126.48 (13) |
| N7—C5—S1 | 121.54 (12) | N17—C16—S15 | 107.05 (12) |
| C5—N7—H7A | 118.8 (15) | C16—N17—N18 | 119.02 (14) |
| C5—N7—H7B | 119.4 (14) | C16—N17—H17 | 122.9 (13) |
| H7A—N7—H7B | 122 (2) | N18—N17—H17 | 118.0 (13) |
| C12—S8—C9 | 88.73 (7) | C19—N18—N17 | 109.75 (13) |
| O13—C9—N10 | 126.70 (16) | N18—C19—N21 | 122.74 (16) |
| O13—C9—S8 | 126.29 (13) | N18—C19—S15 | 115.68 (12) |
| N10—C9—S8 | 107.01 (12) | N21—C19—S15 | 121.57 (13) |
| C9—N10—N11 | 118.72 (13) | C19—N21—H21A | 113.9 (17) |
| C9—N10—H10 | 125.0 (12) | C19—N21—H21B | 116.2 (17) |
| N11—N10—H10 | 116.1 (12) | H21A—N21—H21B | 128 (2) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H3···N18 | 0.854 (19) | 2.004 (19) | 2.8516 (19) | 171.9 (18) |
| N7—H7*A*···O20$^{i}$ | 0.87 (2) | 2.07 (2) | 2.907 (2) | 160 (2) |
| N10—H10···N4 | 0.98 (2) | 1.88 (2) | 2.8558 (19) | 175.7 (18) |
| N14—H14*A*···O6$^{ii}$ | 0.83 (2) | 2.10 (2) | 2.897 (2) | 162 (2) |
| N17—H17···N11 | 0.88 (2) | 1.97 (2) | 2.8424 (18) | 179 (4) |
| N21—H21*A*···O13$^{iii}$ | 0.80 (3) | 2.10 (3) | 2.878 (2) | 163 (2) |

Symmetry codes: (i) *x*+1, *y*−1, *z*; (ii) *x*−1, *y*, *z*+1; (iii) *x*, *y*+1, *z*−1.