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# 4-[(1-Benzyl-1*H*-1,2,3-triazol-4-yl)methyl]-2*H*-1,4-benzothiazin-3(4*H*)-one

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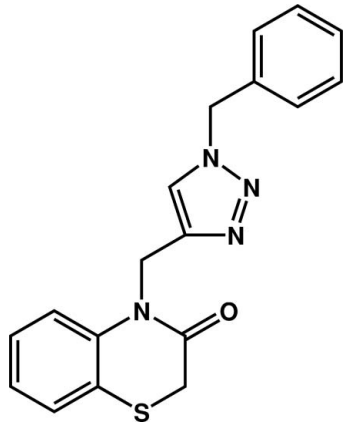
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.046; $wR$ factor = 0.149; data-to-parameter ratio = 16.2.

In the title compound, $C_{18}H_{16}N_4OS$, the six-membered heterocycle of the benzothiazine fragment exhibits a screw-boat conformation. The dihedral angles between the plane through the triazole ring and those through the fused and terminal benzene rings are 76.68 (11) and 71.0 (1)°, respectively; the benzene rings are nearly perpendicular [dihedral angle = 79.6 (1)°]. In the crystal, molecules are linked by C—H···N and C—H···O interactions, forming a three-dimensional network.

## Related literature

For the biological activity of 1,4-benzothiazin-3-one derivatives, see: Rathore & Kumar (2006); Barazarte *et al.* (2008); Chia *et al.* (2008). For related structures, see: Ouzidan *et al.* (2011); Sebbar *et al.* (2014). For puckering parameters, see: Cremer & Pople (1975).



## Experimental

### Crystal data

$C_{18}H_{16}N_4OS$
$M_r$ = 336.41
Monoclinic, $P2_1/c$
$a$ = 13.283 (2) Å
$b$ = 5.3661 (10) Å
$c$ = 23.281 (4) Å
$\beta$ = 96.633 (10)°
$V$ = 1648.3 (5) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.21 mm$^{-1}$
$T$ = 296 K
0.39 × 0.35 × 0.28 mm

### Data collection

Bruker X8 APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.649, $T_{max}$ = 0.747
15366 measured reflections
3526 independent reflections
2540 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.044

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.149
$S$ = 1.03
3526 reflections
217 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.33 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C8—H8···N2$^{i}$ | 0.93 | 2.44 | 3.344 (3) | 165 |
| C8—H8···N3$^{i}$ | 0.93 | 2.44 | 3.339 (3) | 164 |
| C5—H5···O1$^{ii}$ | 0.93 | 2.58 | 3.477 (2) | 163 |

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT-Plus* (Bruker, 2009); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

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Supporting information for this paper is available from the IUCr electronic archives (Reference: TK5287).

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# supporting information

*Acta Cryst.* (2014). E**70**, o160–o161 [doi:10.1107/S1600536814000786]

## 4-[(1-Benzyl-1*H*-1,2,3-triazol-4-yl)methyl]-2*H*-1,4-benzothiazin-3(4*H*)-one

**Nada Kheira Sebbar, Abdelfettah Zerzouf, El Mokhtar Essassi, Mohamed Saadi and Lahcen El Ammari**

### S1. Experimental

#### S1.1. Synthesis and crystallization

A mixture of 4-(prop-2-yn-1-yl)-3,4-dihydro-2*H*-1,4-benzothiazin-3-one (0.27 g, 0.35 mmol) and benzylazide (1.34 ml, 0.35 mmol) in ethanol (5 ml) was stirred at room temperature for 24 h. After cooling, the solid obtained was purified by column chromatography on silica gel with ethyl acetate-hexane (1/2) as eluent. Crystals were isolated when the solvent was allowed to evaporate.

#### S1.2. Refinement

The H atoms were located in a difference map and treated as riding with C—H = 0.93 Å (aromatic) and C—H = 0.97 Å (methylene), and with $U_{iso}$(H) = 1.2 $U_{eq}$(C).

### S2. Results and discussion

1,4-Benzothiazine derivatives have a wide spectrum of pharmaceutical and biological activities, such as anti-microbial (Rathore & Kumar, 2006); anti-malarial (Barazarte *et al.*, 2008) and anti-inflammatory (Chia *et al.*, 2008). The present work is a continuation of the investigation of the benzothiazine derivatives published recently by our team (Ouzidan *et al.*, 2011; Sebbar *et al.*, 2014). The aim of the present paper was to study the crystal structure of the recently synthesized 4-[(1-benzyl-1*H*-1,2,3-triazol-4-yl)methyl]-3,4-dihydro-2*H*-1,4-benzothiazin-3-one compound.

The molecule of the title compound is built up from two fused six-membered rings linked to a triazole ring, *via* the heterocyclic, which in turn is attached to benzene ring as shown in Fig. 1. The 1,4-thiazine ring adopts a screw boat conformation as indicated by the puckering amplitude Q = 0.6197 (17) Å, spherical polar angle $\theta$ = 64.42 (16)° and with $\varphi$ = 329.6 (2)° (Cremer & Pople, 1975). The triazole ring (N1N2N3C8C9) makes dihedral angles of 76.68 (11) and 71.0 (1)° with the benzene fused to the 1,4-thiazine ring (C11 to C16) and the other benzene ring (C1 to C6), respectively. Moreover, the two benzene rings are nearly perpendicular as indicated by the dihedral angle between them of 79.6 (1)°.

In the crystal, the molecules are linked together by a weak intermolecular C8–H8···N2, C8–H8···N3 and C5–H5···O1 interactions, to form a three-dimensional network (see Fig. 2 and Table 1).

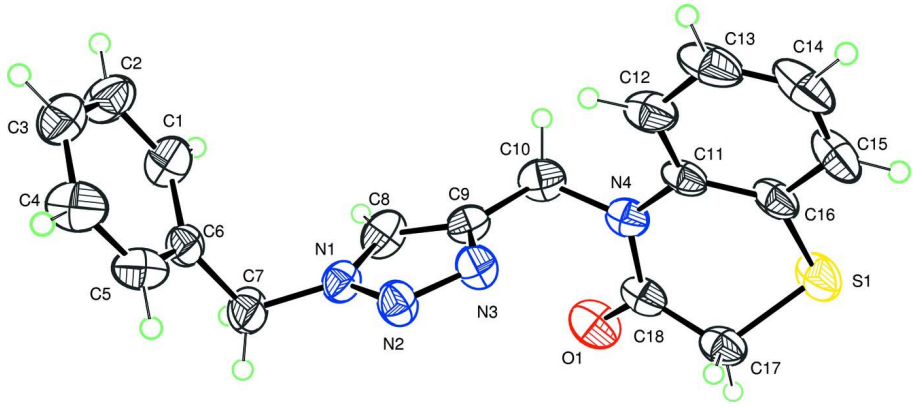


**Figure 1**

Molecular structure of the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small circles.

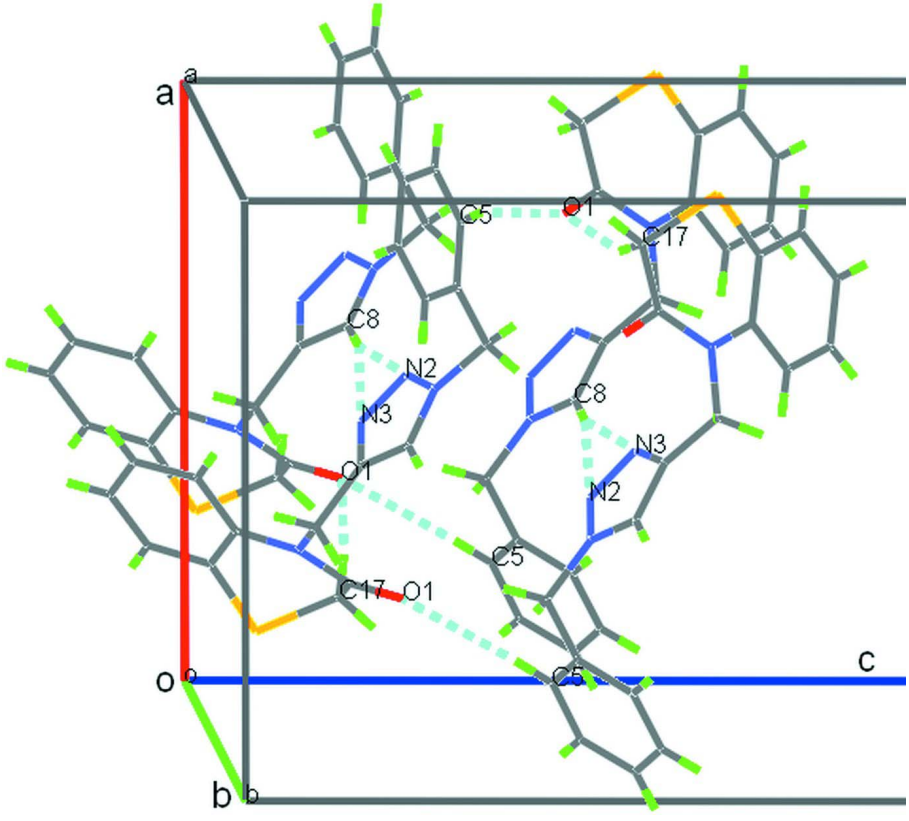


**Figure 2**

Partial three dimensional plot of the title compound, showing molecules linked through C8–H8···N2, C8–H8···N3 and C5–H5···O1 hydrogen bonds (dashed lines).

## 4-[(1-Benzyl-1*H*-1,2,3-triazol-4-yl)methyl]-2*H*-1,4-benzothiazin-3(4*H*)-one

*Crystal data*

$C_{18}H_{16}N_4OS$
$M_r = 336.41$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 13.283$ (2) Å
$b = 5.3661$ (10) Å
$c = 23.281$ (4) Å
$\beta = 96.633$ (10)°
$V = 1648.3$ (5) Å$^3$
$Z = 4$
$F(000) = 704$
$D_x = 1.356$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3526 reflections
$\theta = 1.8$–27.1°
$\mu = 0.21$ mm$^{-1}$
$T = 296$ K
Block, colourless
0.39 × 0.35 × 0.28 mm

*Data collection*

Bruker X8 APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.649$, $T_{max} = 0.747$
15366 measured reflections
3526 independent reflections
2540 reflections with $I > 2\sigma(I)$
$R_{int} = 0.044$
$\theta_{max} = 27.1°$, $\theta_{min} = 1.8°$
$h = -16\rightarrow17$
$k = -6\rightarrow5$
$l = -29\rightarrow29$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.149$
$S = 1.03$
3526 reflections
217 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
$w = 1/[\sigma^2(F_o^2) + (0.087P)^2 + 0.1602P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.22$ e Å$^{-3}$
$\Delta\rho_{min} = -0.33$ e Å$^{-3}$

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'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 $F^2 > \sigma(F^2)$ 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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.22144 (17) | 1.2104 (4) | 0.32721 (9) | 0.0608 (6) |
| H1 | 0.2703 | 1.3328 | 0.3361 | 0.073* |
| C2 | 0.13131 (19) | 1.2201 (4) | 0.35176 (10) | 0.0663 (6) |
| H2 | 0.1207 | 1.3471 | 0.3776 | 0.080* |

| | | | | |
|---|---|---|---|---|
| C3 | 0.05772 (18) | 1.0436 (4) | 0.33828 (10) | 0.0620 (6) |
| H3 | −0.0028 | 1.0501 | 0.3547 | 0.074* |
| C4 | 0.07467 (19) | 0.8572 (5) | 0.30010 (9) | 0.0675 (7) |
| H4 | 0.0246 | 0.7387 | 0.2901 | 0.081* |
| C5 | 0.16506 (19) | 0.8438 (4) | 0.27650 (8) | 0.0577 (6) |
| H5 | 0.1759 | 0.7140 | 0.2515 | 0.069* |
| C6 | 0.23928 (15) | 1.0199 (4) | 0.28950 (7) | 0.0457 (4) |
| C7 | 0.33713 (17) | 1.0077 (4) | 0.26263 (8) | 0.0597 (6) |
| H7A | 0.3309 | 0.8829 | 0.2323 | 0.072* |
| H7B | 0.3490 | 1.1673 | 0.2450 | 0.072* |
| C8 | 0.48825 (17) | 1.0970 (4) | 0.33613 (9) | 0.0545 (5) |
| H8 | 0.4885 | 1.2703 | 0.3354 | 0.065* |
| C9 | 0.55342 (15) | 0.9457 (3) | 0.36961 (7) | 0.0424 (4) |
| C10 | 0.64140 (18) | 1.0099 (4) | 0.41219 (9) | 0.0555 (5) |
| H10A | 0.6711 | 1.1646 | 0.4006 | 0.067* |
| H10B | 0.6181 | 1.0363 | 0.4497 | 0.067* |
| C11 | 0.72308 (14) | 0.6346 (4) | 0.46251 (7) | 0.0438 (4) |
| C12 | 0.64100 (17) | 0.6069 (5) | 0.49446 (8) | 0.0581 (6) |
| H12 | 0.5823 | 0.6994 | 0.4847 | 0.070* |
| C13 | 0.6465 (2) | 0.4417 (5) | 0.54082 (8) | 0.0727 (8) |
| H13 | 0.5923 | 0.4296 | 0.5627 | 0.087* |
| C14 | 0.7301 (2) | 0.2979 (6) | 0.55454 (8) | 0.0780 (8) |
| H14 | 0.7327 | 0.1873 | 0.5854 | 0.094* |
| C15 | 0.81136 (19) | 0.3164 (5) | 0.52239 (8) | 0.0683 (7) |
| H15 | 0.8680 | 0.2154 | 0.5311 | 0.082* |
| C16 | 0.80820 (15) | 0.4867 (4) | 0.47686 (7) | 0.0499 (5) |
| C17 | 0.84430 (15) | 0.5783 (4) | 0.36944 (7) | 0.0526 (5) |
| H17A | 0.8910 | 0.6067 | 0.3410 | 0.063* |
| H17B | 0.8032 | 0.4341 | 0.3572 | 0.063* |
| C18 | 0.77735 (15) | 0.8007 (4) | 0.37190 (7) | 0.0480 (5) |
| N1 | 0.42420 (12) | 0.9464 (3) | 0.30471 (6) | 0.0442 (4) |
| N2 | 0.44742 (13) | 0.7078 (3) | 0.31697 (6) | 0.0482 (4) |
| N3 | 0.52629 (12) | 0.7072 (3) | 0.35664 (6) | 0.0461 (4) |
| N4 | 0.71926 (12) | 0.8149 (3) | 0.41721 (6) | 0.0451 (4) |
| O1 | 0.77092 (14) | 0.9600 (3) | 0.33403 (6) | 0.0689 (5) |
| S1 | 0.91484 (4) | 0.51598 (14) | 0.43858 (2) | 0.0692 (2) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0529 (13) | 0.0505 (13) | 0.0794 (14) | −0.0036 (10) | 0.0088 (11) | −0.0073 (10) |
| C2 | 0.0640 (15) | 0.0553 (13) | 0.0817 (14) | 0.0067 (11) | 0.0168 (12) | −0.0186 (11) |
| C3 | 0.0530 (13) | 0.0659 (14) | 0.0694 (13) | 0.0021 (11) | 0.0169 (11) | 0.0023 (11) |
| C4 | 0.0738 (16) | 0.0651 (15) | 0.0658 (12) | −0.0245 (12) | 0.0177 (12) | −0.0075 (11) |
| C5 | 0.0784 (16) | 0.0501 (12) | 0.0461 (9) | −0.0030 (11) | 0.0137 (10) | −0.0047 (9) |
| C6 | 0.0480 (11) | 0.0503 (11) | 0.0385 (8) | 0.0108 (9) | 0.0041 (7) | 0.0125 (8) |
| C7 | 0.0553 (13) | 0.0785 (16) | 0.0465 (10) | 0.0182 (11) | 0.0108 (9) | 0.0225 (10) |
| C8 | 0.0598 (13) | 0.0292 (9) | 0.0759 (13) | 0.0004 (9) | 0.0141 (11) | 0.0046 (9) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C9 | 0.0480 (11) | 0.0325 (9) | 0.0483 (9) | −0.0044 (8) | 0.0125 (8) | −0.0029 (7) |
| C10 | 0.0621 (13) | 0.0426 (11) | 0.0615 (11) | −0.0112 (10) | 0.0064 (10) | −0.0110 (9) |
| C11 | 0.0433 (10) | 0.0563 (11) | 0.0312 (7) | −0.0180 (9) | 0.0015 (7) | −0.0067 (7) |
| C12 | 0.0483 (12) | 0.0824 (15) | 0.0449 (10) | −0.0193 (11) | 0.0101 (9) | −0.0094 (10) |
| C13 | 0.0673 (16) | 0.114 (2) | 0.0379 (9) | −0.0397 (15) | 0.0129 (10) | −0.0035 (11) |
| C14 | 0.0828 (19) | 0.110 (2) | 0.0378 (9) | −0.0344 (16) | −0.0084 (10) | 0.0178 (11) |
| C15 | 0.0655 (15) | 0.0909 (18) | 0.0437 (10) | −0.0127 (13) | −0.0145 (9) | 0.0138 (11) |
| C16 | 0.0410 (10) | 0.0736 (14) | 0.0332 (8) | −0.0165 (10) | −0.0039 (7) | −0.0012 (8) |
| C17 | 0.0461 (11) | 0.0736 (14) | 0.0391 (8) | −0.0139 (10) | 0.0094 (8) | −0.0017 (9) |
| C18 | 0.0469 (11) | 0.0581 (12) | 0.0387 (8) | −0.0221 (9) | 0.0036 (7) | −0.0004 (8) |
| N1 | 0.0450 (9) | 0.0419 (9) | 0.0469 (8) | 0.0054 (7) | 0.0102 (7) | 0.0093 (6) |
| N2 | 0.0531 (10) | 0.0375 (9) | 0.0513 (8) | 0.0015 (7) | −0.0049 (7) | 0.0012 (7) |
| N3 | 0.0538 (10) | 0.0318 (8) | 0.0503 (8) | −0.0042 (7) | −0.0035 (7) | −0.0009 (6) |
| N4 | 0.0435 (9) | 0.0497 (9) | 0.0419 (7) | −0.0123 (7) | 0.0044 (6) | −0.0033 (7) |
| O1 | 0.0803 (12) | 0.0684 (10) | 0.0588 (8) | −0.0190 (8) | 0.0122 (8) | 0.0172 (7) |
| S1 | 0.0364 (3) | 0.1170 (6) | 0.0528 (3) | −0.0050 (3) | −0.0005 (2) | 0.0036 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C6 | 1.385 (3) | C10—H10B | 0.9700 |
| C1—C2 | 1.386 (3) | C11—C16 | 1.390 (3) |
| C1—H1 | 0.9300 | C11—C12 | 1.397 (3) |
| C2—C3 | 1.371 (3) | C11—N4 | 1.428 (2) |
| C2—H2 | 0.9300 | C12—C13 | 1.392 (3) |
| C3—C4 | 1.374 (3) | C12—H12 | 0.9300 |
| C3—H3 | 0.9300 | C13—C14 | 1.360 (4) |
| C4—C5 | 1.379 (3) | C13—H13 | 0.9300 |
| C4—H4 | 0.9300 | C14—C15 | 1.387 (4) |
| C5—C6 | 1.374 (3) | C14—H14 | 0.9300 |
| C5—H5 | 0.9300 | C15—C16 | 1.396 (3) |
| C6—C7 | 1.508 (3) | C15—H15 | 0.9300 |
| C7—N1 | 1.464 (3) | C16—S1 | 1.766 (2) |
| C7—H7A | 0.9700 | C17—C18 | 1.493 (3) |
| C7—H7B | 0.9700 | C17—S1 | 1.798 (2) |
| C8—N1 | 1.330 (3) | C17—H17A | 0.9700 |
| C8—C9 | 1.364 (3) | C17—H17B | 0.9700 |
| C8—H8 | 0.9300 | C18—O1 | 1.224 (2) |
| C9—N3 | 1.354 (2) | C18—N4 | 1.379 (2) |
| C9—C10 | 1.483 (3) | N1—N2 | 1.340 (2) |
| C10—N4 | 1.466 (3) | N2—N3 | 1.314 (2) |
| C10—H10A | 0.9700 | | |

| | | | |
|---|---|---|---|
| C6—C1—C2 | 120.5 (2) | C16—C11—C12 | 118.32 (18) |
| C6—C1—H1 | 119.7 | C16—C11—N4 | 121.53 (16) |
| C2—C1—H1 | 119.7 | C12—C11—N4 | 120.14 (19) |
| C3—C2—C1 | 120.5 (2) | C13—C12—C11 | 120.4 (2) |
| C3—C2—H2 | 119.8 | C13—C12—H12 | 119.8 |
| C1—C2—H2 | 119.8 | C11—C12—H12 | 119.8 |

| | | | |
|---|---|---|---|
| C2—C3—C4 | 119.0 (2) | C14—C13—C12 | 120.8 (2) |
| C2—C3—H3 | 120.5 | C14—C13—H13 | 119.6 |
| C4—C3—H3 | 120.5 | C12—C13—H13 | 119.6 |
| C3—C4—C5 | 120.7 (2) | C13—C14—C15 | 119.9 (2) |
| C3—C4—H4 | 119.6 | C13—C14—H14 | 120.1 |
| C5—C4—H4 | 119.6 | C15—C14—H14 | 120.1 |
| C6—C5—C4 | 120.80 (19) | C14—C15—C16 | 120.0 (2) |
| C6—C5—H5 | 119.6 | C14—C15—H15 | 120.0 |
| C4—C5—H5 | 119.6 | C16—C15—H15 | 120.0 |
| C5—C6—C1 | 118.43 (18) | C11—C16—C15 | 120.55 (19) |
| C5—C6—C7 | 120.64 (18) | C11—C16—S1 | 120.37 (14) |
| C1—C6—C7 | 120.92 (19) | C15—C16—S1 | 119.07 (18) |
| N1—C7—C6 | 112.60 (14) | C18—C17—S1 | 111.42 (13) |
| N1—C7—H7A | 109.1 | C18—C17—H17A | 109.3 |
| C6—C7—H7A | 109.1 | S1—C17—H17A | 109.3 |
| N1—C7—H7B | 109.1 | C18—C17—H17B | 109.3 |
| C6—C7—H7B | 109.1 | S1—C17—H17B | 109.3 |
| H7A—C7—H7B | 107.8 | H17A—C17—H17B | 108.0 |
| N1—C8—C9 | 106.02 (17) | O1—C18—N4 | 120.9 (2) |
| N1—C8—H8 | 127.0 | O1—C18—C17 | 121.52 (17) |
| C9—C8—H8 | 127.0 | N4—C18—C17 | 117.51 (16) |
| N3—C9—C8 | 107.47 (18) | C8—N1—N2 | 110.29 (16) |
| N3—C9—C10 | 122.51 (17) | C8—N1—C7 | 129.57 (18) |
| C8—C9—C10 | 130.00 (18) | N2—N1—C7 | 120.13 (17) |
| N4—C10—C9 | 112.43 (15) | N3—N2—N1 | 107.31 (15) |
| N4—C10—H10A | 109.1 | N2—N3—C9 | 108.92 (15) |
| C9—C10—H10A | 109.1 | C18—N4—C11 | 123.52 (17) |
| N4—C10—H10B | 109.1 | C18—N4—C10 | 115.48 (16) |
| C9—C10—H10B | 109.1 | C11—N4—C10 | 120.46 (15) |
| H10A—C10—H10B | 107.8 | C16—S1—C17 | 95.91 (9) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C8—H8···N2$^{i}$ | 0.93 | 2.44 | 3.344 (3) | 165 |
| C8—H8···N3$^{i}$ | 0.93 | 2.44 | 3.339 (3) | 164 |
| C5—H5···O1$^{ii}$ | 0.93 | 2.58 | 3.477 (2) | 163 |

Symmetry codes: (i) $x$, $y$+1, $z$; (ii) −$x$+1, $y$−1/2, −$z$+1/2.