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# 3-(3-Methoxybenzyl)-4-(2-methoxyphenyl)-1*H*-1,2,4-triazole-5(4*H*)-thione

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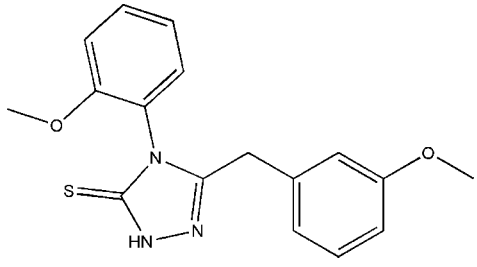
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.006 Å; $R$ factor = 0.073; $wR$ factor = 0.159; data-to-parameter ratio = 17.8.

In the title compound, $C_{17}H_{17}N_3O_2S$, the five-membered ring forms dihedral angles of 53.02 (3) and 78.57 (3)° with the 3-methoxy-substituted and 2-methoxy-substituted benzene rings, respectively. In the crystal structure, molecules are linked into centrosymmetric dimers *via* intermolecular N—H···S hydrogen bonds.

## Related literature

For background information on the biological activity of substituted triazole derivatives, see: Demirbas *et al.* (2002); Holla *et al.* (1998); Omar *et al.* (1986); Paulvannan *et al.* (2000); Turan-Zitouni *et al.* (1999); Kritsanida *et al.* (2002). For related structures, see: Öztürk *et al.* (2004*a*,*b*); Zhang *et al.* (2004). For bond-length data, see: Allen *et al.* (1987).




## Experimental

### Crystal data

$C_{17}H_{17}N_3O_2S$
$M_r$ = 327.40
Triclinic, $P\overline{1}$
$a$ = 7.3941 (3) Å
$b$ = 10.6459 (5) Å
$c$ = 12.1940 (8) Å
$\alpha$ = 68.841 (5)°
$\beta$ = 74.317 (5)°
$\gamma$ = 75.187 (5)°
$V$ = 848.37 (8) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.20 mm$^{-1}$
$T$ = 293 (2) K
0.40 × 0.24 × 0.15 mm

### Data collection

Bruker–Nonius KappaCCD area-detector diffractometer
Absorption correction: integration (Gaussian; Coppens, 1970)
$T_{min}$ = 0.946, $T_{max}$ = 0.983
10764 measured reflections
3708 independent reflections
2064 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.079

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.073
$wR(F^2)$ = 0.159
$S$ = 1.10
3708 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.24 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2···S1$^{i}$ | 0.86 | 2.42 | 3.277 (3) | 172 |

Symmetry code: (i) $-x-1, -y+1, -z+1$.

Data collection: *COLLECT* (Hooft, 1998) and *DENZO* (Otwinowski & Minor, 1997); cell refinement: *DIRAX/LSQ* (Duisenberg, 1992); data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2729).

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# supporting information

*Acta Cryst.* (2008). E**64**, o2345–o2346 [doi:10.1107/S1600536808037215]

## 3-(3-Methoxybenzyl)-4-(2-methoxyphenyl)-1*H*-1,2,4-triazole-5(4*H*)-thione

**Muhammad Hanif, Ghulam Qadeer, Nasim Hasan Rama and Ales Ruzicka**

### S1. Comment

Substituted triazole derivatives display significant biological activity including antimicrobial (Holla *et al.*, 1998), analgesic (Turan-Zitouni *et al.*, 1999), antitumor (Demirbas *et al.*, 2002), antihypertensive (Paulvannan *et al.*, 2000) and antiviral activities (Kritsanida *et al.*, 2002). The biological activity is closely related to structure, possibly being due to the presence of the —N—C=S unit (Omar *et al.*, 1986). We are interested in the synthesis and biological activity of substituted triazole derivatives and report here the synthesis and crystal structure of the title compound, (I) (Fig. 1).

In the molecluar structure of (I), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987) and comparable with those observed in related structures (Öztürk *et al.*, 2004*a*,b). The C7-S1 bond length [1.679 (3) A °] compares with 1.6773 (19) A ° in 4-(4-chlorophenyl)-3-(furan-2-yl)-1*H*-1,2,4-triazole-5(4*H*)-thione (Ozturk *et al.*, 2004*a*) and 1.668 (5) A ° in 4-amino-3-(1,2,3,4,5- pentahydroxypentyl)-1*H*-1,2,4-triazole-5(4*H*)-thione (Zhang *et al.*, 2004). In the triazole ring, the N3-C8 bond [1.294 (4)] bond shows the expected double bond character.

The rings A (N1—N3/C7/C8), B (C1—C6) and C (C10—C15) are eesentially planar and dihedral angles between them are A/B = 78.57 (3)°, A/C = 53.02 (3)° and B/C = 16.23 (3)°. In the crystal structure, molecules are linked into centrosymmetric dimers via intermolecular N–H···S hydrogen bonds.

### S2. Experimental

The synthesis of the title compound was carried out by refluxing a solution of 4-(2-methoxyphenyl)-1-(2-(3-methoxyphenyl)acetyl)thiosemicarbazide (3.45 g, 10 mmol) in 2 *M* NaOH for 5 h. Single crystals suitable for X-ray measurements were obtained by recrystallization from an aqeous ethanol solution at room temperature (yield: 75%; m.p. 469–470 K).

### S3. Refinement

H atoms were placed in calculated positions with C-H = 0.93-0.97Å and N-H = 0.86Å and included in the refinement with $U_{iso}(H) = 1.2U_{eq}(C,N)$. Although the atoms of substituted methoxy have larger than normal anisotropic displacement parameters, attempts to create disorder models did not improve the precision of the structure.

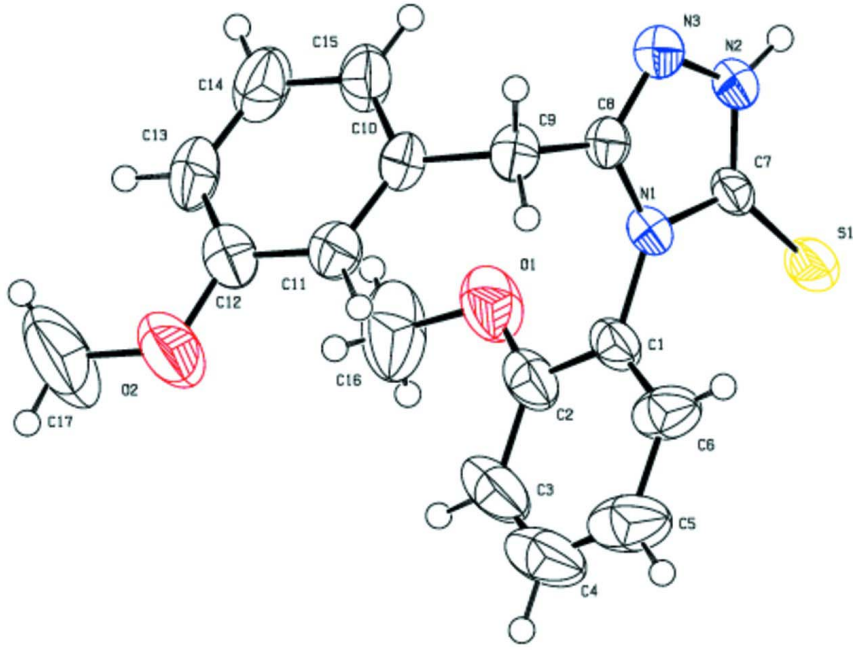


**Figure 1**

The molecular structure of (I) with 50% probability displacement ellipsoids (arbitrary spheres for H atoms).

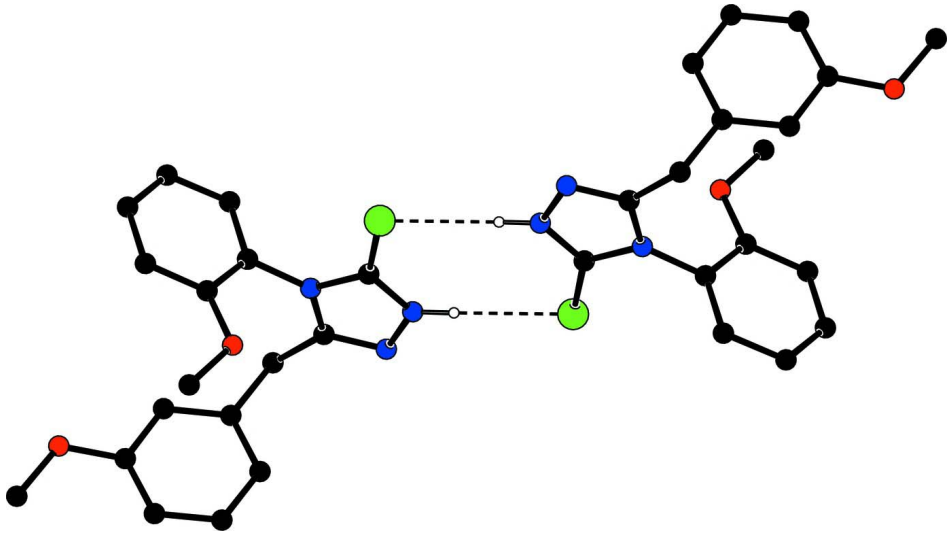

**Figure 2**

Part of the crystal structure of (I) showing hydrogen bonds as dashed lines.

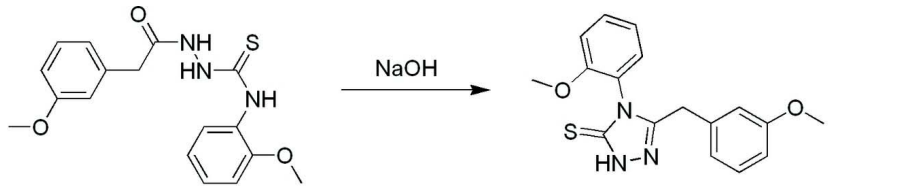


**Figure 3**

The reaction scheme.

### 3-(3-Methoxybenzyl)-4-(2-methoxyphenyl)-1*H*-1,2,4-triazole-5(4*H*)- thione

*Crystal data*

$C_{17}H_{17}N_3O_2S$
$M_r = 327.40$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.3941\ (3)$ Å
$b = 10.6459\ (5)$ Å
$c = 12.1940\ (8)$ Å
$\alpha = 68.841\ (5)°$
$\beta = 74.317\ (5)°$
$\gamma = 75.187\ (5)°$
$V = 848.37\ (8)$ Å$^3$
$Z = 2$
$F(000) = 344$
$D_x = 1.282$ Mg m$^{-3}$
Melting point: 469(1) K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 10808 reflections
$\theta = 1–27.5°$
$\mu = 0.20$ mm$^{-1}$
$T = 293$ K
Plate, colourless
0.40 × 0.24 × 0.15 mm

*Data collection*

Bruker–Nonius KappaCCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 9.091 pixels mm$^{-1}$
$\varphi$ and $\omega$ scans to fill the Ewald sphere
Absorption correction: integration (Gaussian; Coppens, 1970)
$T_{min} = 0.946$, $T_{max} = 0.983$
10764 measured reflections
3708 independent reflections
2064 reflections with $I > 2\sigma(I)$
$R_{int} = 0.079$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.8°$
$h = -9\rightarrow9$
$k = -13\rightarrow13$
$l = -15\rightarrow15$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.073$
$wR(F^2) = 0.159$
$S = 1.10$
3708 reflections
208 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
$w = 1/[\sigma^2(F_o^2) + (0.0364P)^2 + 0.6393P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.32$ e Å$^{-3}$
$\Delta\rho_{min} = -0.24$ 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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | −0.37112 (12) | 0.55979 (11) | 0.30006 (8) | 0.0515 (3) |
| N2 | −0.2330 (4) | 0.4093 (3) | 0.5026 (2) | 0.0410 (7) |
| H2 | −0.3425 | 0.4150 | 0.5499 | 0.049* |
| N1 | −0.0166 (3) | 0.4302 (3) | 0.3462 (2) | 0.0379 (6) |
| N3 | −0.0666 (4) | 0.3402 (3) | 0.5425 (2) | 0.0444 (7) |
| C7 | −0.2087 (4) | 0.4659 (3) | 0.3847 (3) | 0.0362 (7) |
| C10 | 0.3280 (4) | 0.1679 (3) | 0.4006 (3) | 0.0416 (8) |
| C1 | 0.0831 (4) | 0.4687 (4) | 0.2239 (3) | 0.0460 (9) |
| C8 | 0.0625 (4) | 0.3535 (3) | 0.4452 (3) | 0.0374 (7) |
| C11 | 0.4677 (5) | 0.1629 (4) | 0.3017 (3) | 0.0535 (9) |
| H11 | 0.5259 | 0.2385 | 0.2566 | 0.064* |
| O1 | 0.0235 (4) | 0.2702 (3) | 0.2152 (3) | 0.0745 (8) |
| C14 | 0.2995 (6) | −0.0616 (4) | 0.4330 (4) | 0.0700 (12) |
| H14 | 0.2433 | −0.1380 | 0.4789 | 0.084* |
| C9 | 0.2686 (4) | 0.2945 (3) | 0.4391 (3) | 0.0446 (8) |
| H9A | 0.2988 | 0.2723 | 0.5173 | 0.054* |
| H9B | 0.3424 | 0.3630 | 0.3829 | 0.054* |
| C15 | 0.2434 (5) | 0.0546 (4) | 0.4662 (4) | 0.0591 (11) |
| H15 | 0.1477 | 0.0574 | 0.5333 | 0.071* |
| C2 | 0.1052 (5) | 0.3814 (5) | 0.1581 (3) | 0.0543 (10) |
| C3 | 0.2031 (6) | 0.4167 (6) | 0.0396 (4) | 0.0767 (15) |
| H3 | 0.2209 | 0.3601 | −0.0067 | 0.092* |
| C13 | 0.4385 (6) | −0.0674 (4) | 0.3336 (4) | 0.0634 (11) |
| H13 | 0.4743 | −0.1460 | 0.3107 | 0.076* |
| C6 | 0.1539 (5) | 0.5894 (4) | 0.1775 (3) | 0.0605 (11) |
| H6 | 0.1374 | 0.6459 | 0.2237 | 0.073* |
| C12 | 0.5230 (6) | 0.0434 (4) | 0.2686 (4) | 0.0639 (11) |
| C5 | 0.2519 (6) | 0.6227 (6) | 0.0573 (4) | 0.0808 (15) |
| H5 | 0.3011 | 0.7034 | 0.0217 | 0.097* |
| O2 | 0.6618 (5) | 0.0512 (4) | 0.1674 (3) | 0.1103 (13) |
| C16 | 0.0674 (8) | 0.1673 (6) | 0.1580 (5) | 0.106 (2) |
| H16A | 0.0231 | 0.2046 | 0.0837 | 0.127* |
| H16B | 0.0055 | 0.0915 | 0.2094 | 0.127* |
| H16C | 0.2029 | 0.1366 | 0.1426 | 0.127* |
| C4 | 0.2727 (6) | 0.5350 (7) | −0.0064 (4) | 0.0838 (17) |

| | | | | |
|---|---|---|---|---|
| H4 | 0.3387 | 0.5582 | −0.0855 | 0.101* |
| C17 | 0.7351 (12) | −0.0684 (7) | 0.1341 (7) | 0.181 (4) |
| H17A | 0.7803 | −0.1401 | 0.2007 | 0.217* |
| H17B | 0.8390 | −0.0520 | 0.0666 | 0.217* |
| H17C | 0.6375 | −0.0952 | 0.1134 | 0.217* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0403 (5) | 0.0619 (7) | 0.0415 (5) | 0.0027 (4) | −0.0018 (4) | −0.0162 (4) |
| N2 | 0.0386 (15) | 0.0399 (17) | 0.0390 (16) | −0.0030 (12) | 0.0016 (12) | −0.0155 (13) |
| N1 | 0.0363 (14) | 0.0392 (17) | 0.0346 (15) | −0.0026 (12) | 0.0005 (11) | −0.0154 (13) |
| N3 | 0.0486 (16) | 0.0385 (17) | 0.0425 (17) | −0.0052 (13) | −0.0046 (13) | −0.0135 (14) |
| C7 | 0.0415 (17) | 0.0327 (19) | 0.0339 (17) | −0.0070 (14) | 0.0042 (13) | −0.0180 (15) |
| C10 | 0.0378 (17) | 0.035 (2) | 0.052 (2) | 0.0009 (14) | −0.0134 (15) | −0.0141 (16) |
| C1 | 0.0340 (17) | 0.059 (2) | 0.0374 (18) | 0.0044 (16) | −0.0034 (14) | −0.0182 (18) |
| C8 | 0.0442 (18) | 0.0298 (18) | 0.0399 (19) | −0.0055 (14) | −0.0060 (15) | −0.0152 (15) |
| C11 | 0.063 (2) | 0.039 (2) | 0.054 (2) | −0.0098 (17) | −0.0022 (18) | −0.0157 (18) |
| O1 | 0.086 (2) | 0.076 (2) | 0.076 (2) | −0.0040 (17) | −0.0174 (16) | −0.0474 (18) |
| C14 | 0.062 (2) | 0.041 (2) | 0.099 (3) | −0.0095 (19) | −0.010 (2) | −0.017 (2) |
| C9 | 0.0454 (19) | 0.039 (2) | 0.050 (2) | −0.0018 (15) | −0.0128 (16) | −0.0164 (17) |
| C15 | 0.046 (2) | 0.044 (2) | 0.077 (3) | −0.0036 (18) | 0.0007 (19) | −0.020 (2) |
| C2 | 0.040 (2) | 0.075 (3) | 0.047 (2) | 0.0079 (19) | −0.0101 (16) | −0.030 (2) |
| C3 | 0.049 (2) | 0.124 (5) | 0.050 (3) | 0.015 (3) | −0.007 (2) | −0.041 (3) |
| C13 | 0.072 (3) | 0.040 (2) | 0.082 (3) | 0.003 (2) | −0.022 (2) | −0.029 (2) |
| C6 | 0.041 (2) | 0.068 (3) | 0.053 (2) | −0.0121 (19) | −0.0062 (17) | 0.003 (2) |
| C12 | 0.066 (3) | 0.057 (3) | 0.062 (3) | −0.002 (2) | 0.000 (2) | −0.027 (2) |
| C5 | 0.052 (2) | 0.102 (4) | 0.061 (3) | −0.021 (2) | −0.005 (2) | 0.007 (3) |
| O2 | 0.142 (3) | 0.076 (2) | 0.094 (3) | −0.024 (2) | 0.042 (2) | −0.049 (2) |
| C16 | 0.129 (5) | 0.094 (4) | 0.130 (5) | 0.021 (3) | −0.062 (4) | −0.077 (4) |
| C4 | 0.047 (2) | 0.137 (5) | 0.047 (3) | −0.002 (3) | 0.000 (2) | −0.020 (3) |
| C17 | 0.222 (8) | 0.116 (6) | 0.175 (7) | −0.045 (5) | 0.100 (6) | −0.102 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—C7 | 1.679 (3) | C9—H9A | 0.9700 |
| N2—C7 | 1.324 (4) | C9—H9B | 0.9700 |
| N2—N3 | 1.377 (4) | C15—H15 | 0.9300 |
| N2—H2 | 0.8600 | C2—C3 | 1.390 (6) |
| N1—C7 | 1.369 (4) | C3—C4 | 1.353 (7) |
| N1—C8 | 1.375 (4) | C3—H3 | 0.9300 |
| N1—C1 | 1.434 (4) | C13—C12 | 1.358 (6) |
| N3—C8 | 1.294 (4) | C13—H13 | 0.9300 |
| C10—C11 | 1.367 (5) | C6—C5 | 1.407 (6) |
| C10—C15 | 1.380 (5) | C6—H6 | 0.9300 |
| C10—C9 | 1.507 (5) | C12—O2 | 1.366 (5) |
| C1—C6 | 1.380 (5) | C5—C4 | 1.372 (7) |
| C1—C2 | 1.387 (5) | C5—H5 | 0.9300 |

| | | | |
|---|---|---|---|
| C8—C9 | 1.485 (4) | O2—C17 | 1.407 (6) |
| C11—C12 | 1.402 (5) | C16—H16A | 0.9599 |
| C11—H11 | 0.9300 | C16—H16B | 0.9601 |
| O1—C2 | 1.340 (5) | C16—H16C | 0.9600 |
| O1—C16 | 1.428 (5) | C4—H4 | 0.9300 |
| C14—C15 | 1.370 (5) | C17—H17A | 0.9600 |
| C14—C13 | 1.370 (6) | C17—H17B | 0.9600 |
| C14—H14 | 0.9299 | C17—H17C | 0.9599 |
| | | | |
| C7—N2—N3 | 113.7 (3) | O1—C2—C1 | 115.7 (3) |
| C7—N2—H2 | 123.2 | O1—C2—C3 | 125.5 (4) |
| N3—N2—H2 | 123.1 | C1—C2—C3 | 118.7 (5) |
| C7—N1—C8 | 108.1 (2) | C4—C3—C2 | 118.4 (5) |
| C7—N1—C1 | 125.4 (3) | C4—C3—H3 | 120.8 |
| C8—N1—C1 | 126.5 (2) | C2—C3—H3 | 120.8 |
| C8—N3—N2 | 103.9 (3) | C12—C13—C14 | 119.2 (4) |
| N2—C7—N1 | 103.5 (3) | C12—C13—H13 | 120.3 |
| N2—C7—S1 | 129.2 (2) | C14—C13—H13 | 120.5 |
| N1—C7—S1 | 127.3 (2) | C1—C6—C5 | 116.9 (5) |
| C11—C10—C15 | 119.2 (3) | C1—C6—H6 | 121.3 |
| C11—C10—C9 | 120.7 (3) | C5—C6—H6 | 121.7 |
| C15—C10—C9 | 120.1 (3) | C13—C12—O2 | 124.9 (4) |
| C6—C1—C2 | 123.1 (4) | C13—C12—C11 | 120.6 (4) |
| C6—C1—N1 | 118.8 (3) | O2—C12—C11 | 114.5 (4) |
| C2—C1—N1 | 118.1 (4) | C4—C5—C6 | 119.1 (5) |
| N3—C8—N1 | 110.8 (3) | C4—C5—H5 | 120.7 |
| N3—C8—C9 | 125.4 (3) | C6—C5—H5 | 120.1 |
| N1—C8—C9 | 123.8 (3) | C12—O2—C17 | 117.6 (4) |
| C10—C11—C12 | 119.8 (4) | O1—C16—H16A | 109.5 |
| C10—C11—H11 | 120.1 | O1—C16—H16B | 109.4 |
| C12—C11—H11 | 120.1 | H16A—C16—H16B | 109.5 |
| C2—O1—C16 | 117.5 (4) | O1—C16—H16C | 109.5 |
| C15—C14—C13 | 120.9 (4) | H16A—C16—H16C | 109.5 |
| C15—C14—H14 | 119.6 | H16B—C16—H16C | 109.5 |
| C13—C14—H14 | 119.5 | C3—C4—C5 | 123.7 (5) |
| C8—C9—C10 | 113.6 (3) | C3—C4—H4 | 118.3 |
| C8—C9—H9A | 108.9 | C5—C4—H4 | 118.1 |
| C10—C9—H9A | 108.9 | O2—C17—H17A | 108.6 |
| C8—C9—H9B | 108.8 | O2—C17—H17B | 109.5 |
| C10—C9—H9B | 108.7 | H17A—C17—H17B | 109.5 |
| H9A—C9—H9B | 107.7 | O2—C17—H17C | 110.4 |
| C14—C15—C10 | 120.4 (4) | H17A—C17—H17C | 109.5 |
| C14—C15—H15 | 119.9 | H17B—C17—H17C | 109.5 |
| C10—C15—H15 | 119.7 | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2···S1$^{i}$ | 0.86 | 2.42 | 3.277 (3) | 172 |

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