IUCrData

ISSN 2414-3146

# (*E*)-4-({[4-(Benzo[*d*]thiazol-2-yl)phenyl]imino}methyl)-*N*,*N*-diethylaniline

**Shun Yao and Xin Zhang***

Department of Chemistry, Anhui University, Hefei 230601, Peoples Republic of China and, Key Laboratory of Functional Inorganic Materials, Chemistry, Hefei 230601, People's Republic of China. *Correspondence e-mail: 329408172@qq.com

Received 24 September 2016
Accepted 12 October 2016

Edited by H. Stoeckli-Evans, University of Neuchâtel, Switzerland

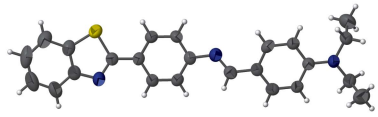
**Keywords:** crystal structure; benzothiazole; Schiff base; C—H$\cdots\pi$ interactions.

**CCDC reference**: 1509540

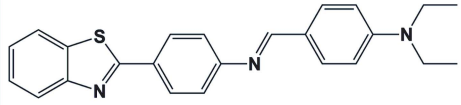
**Structural data**: full structural data are available from iucrdata.iucr.org

The title benzothiazole derivative molecule, $C_{24}H_{23}N_3S$, is almost planar with the central benzene ring being inclined to the benzothiazole ring and the diethylaniline ring by 4.05 (13) and 5.05 (13)°, respectively. The conformation about the N=C bond is *E*. In the crystal, molecules are linked by C—H$\cdots\pi$ interactions, forming layers parallel to the *ab* plane.

**3D view**



**Chemical scheme**




## Structure description

Benzothiazole derivatives are considered to be important because of their wide range of biological activities (Ali & Siddiqui, 2013). At the same time, their high electron affinity and good planarity make them appropriate building blocks for the construction of optical materials (Wang *et al.*, 2010). Herein, we report on the synthesis and crystal structure of the title compound, a new benzothiazole derivative.

The molecular structure is illustrated in Fig. 1. The molecule is almost planar with the central benzene ring (C8–C13) being inclined to the benzothiazole ring (C15–C20; r.m.s. deviation = 0.021 Å) and the diethylaniline ring (C15–C20) by 4.05 (13) and 5.05 (13)°, respectively. The conformation about the N2=C14 bond is *E*.

In the crystal, molecules are linked by C—H$\cdots\pi$ interactions forming layers parallel to the *ab* plane (Table 1 and Fig. 2).

## Synthesis and crystallization

4-(Diethylamino)salicylaldehyde (0.52 g, 2.7 mmol) was dissolved in 20 ml ethanol and added drop wise to a 20 ml ethanol solution of 4-(benzothiazol-2-yl)aniline (0.61 g, 2.7 mmol) with stirring. The mixture was stirred at room temperature, and then filtered.

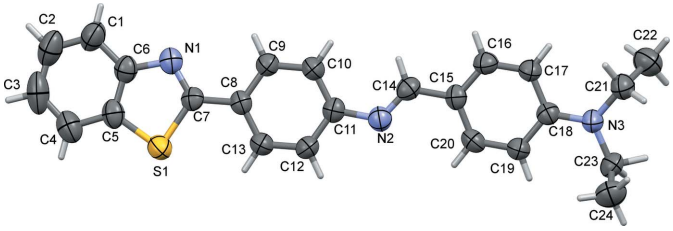



**Figure 1**
The molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids drawn at the 50% probability level.

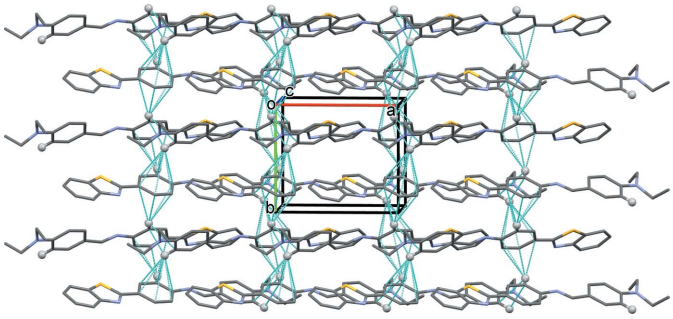



**Figure 2**
A view along the *c* axis of the crystal packing of the title compound. The C—H···$\pi$ interactions are represented by dashed lines (see Table 1), and only the H atoms (H12 and H17; grey balls) involved in these interactions have been included.

The filtrate was allow to evaporate slowly at room temperature and after one week, yellow block-like crystals were obtained (yield 62.0%).

## Refinement

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

## Acknowledgements

This work was supported by the Graduate Students Innovative Program of Anhui University (grant Nos. J18515024, J18515019 and 201310357155).

## References

Ali, R. & Siddiqui, N. (2013). *J. Chem.* Article ID 345198, 12 pp. http://dx.doi.org/10.1155/2013/345198
Bruker (2004). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.

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

*Cg* is the centroid of the C8–C13 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C12—H12···$Cg^{i}$ | 0.93 | 2.88 | 3.577 (5) | 133 |
| C17—H17···$Cg^{ii}$ | 0.93 | 2.93 | 3.646 (4) | 135 |

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

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{24}H_{23}N_3S$ |
| $M_r$ | 385.51 |
| Crystal system, space group | Monoclinic, $P2_1$ |
| Temperature (K) | 298 |
| *a*, *b*, *c* (Å) | 8.895 (5), 7.648 (5), 15.091 (5) |
| $\beta$ (°) | 98.566 (5) |
| *V* (Å$^3$) | 1015.2 (9) |
| *Z* | 2 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.17 |
| Crystal size (mm) | 0.30 × 0.20 × 0.20 |
| | |
| Data collection | |
| Diffractometer | Bruker SMART CCD area detector |
| Absorption correction | Multi-scan (*SADABS*; Bruker, 2004) |
| $T_{min}$, $T_{max}$ | 0.950, 0.966 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 7218, 3278, 2690 |
| $R_{int}$ | 0.024 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.595 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S* | 0.044, 0.122, 1.04 |
| No. of reflections | 3278 |
| No. of parameters | 256 |
| No. of restraints | 1 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.23, −0.18 |
| Absolute structure | Flack (1983), 1363 Friedel pairs |
| Absolute structure parameter | 0.27 (10) |

Computer programs: *SMART* and *SAINT* (Bruker, 2004), *SHELXS97*, *SHELXL97* and *SHELXTL* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008) and *PLATON* (Spek, 2009).

Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Wang, H., Chen, G., Xu, X., Chen, H. & Ji, S. (2010). *Dyes Pigments*, **86**, 238–248.

# full crystallographic data

*IUCrData* (2016). **1**, x161621 [https://doi.org/10.1107/S2414314616016217]

## (*E*)-4-({[4-(Benzo[*d*]thiazol-2-yl)phenyl]imino}methyl)-*N*,*N*-diethylaniline

**Shun Yao and Xin Zhang**

**(*E*)-4-({[4-(Benzo[*d*]thiazol-2-yl)phenyl]imino}methyl)-*N*,*N*-diethylaniline**

*Crystal data*

$C_{24}H_{23}N_3S$
$M_r$ = 385.51
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a$ = 8.895 (5) Å
$b$ = 7.648 (5) Å
$c$ = 15.091 (5) Å
$\beta$ = 98.566 (5)°
$V$ = 1015.2 (9) Å$^3$
$Z$ = 2
$F(000)$ = 408
$D_x$ = 1.261 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71069 Å
Cell parameters from 2407 reflections
$\theta$ = 2.5–23.5°
$\mu$ = 0.17 mm$^{-1}$
$T$ = 298 K
Block, yellow
0.30 × 0.20 × 0.20 mm

*Data collection*

Bruker SMART CCD area detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi scans
Absorption correction: multi-scan (SADABS; Bruker, 2004)
$T_{min}$ = 0.950, $T_{max}$ = 0.966
7218 measured reflections
3278 independent reflections
2690 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.024
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 1.4°
$h$ = −10→10
$k$ = −8→9
$l$ = 0→17

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.122
$S$ = 1.04
3278 reflections
256 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0719P)^2 + 0.0425P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.23 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 e Å$^{-3}$
Absolute structure: Flack (1983), 1363 Friedel pairs
Absolute structure parameter: 0.27 (10)

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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 | 1.41511 (8) | 0.16492 (14) | 1.18673 (5) | 0.0654 (3) |
| N1 | 1.2597 (3) | 0.3273 (4) | 1.29530 (16) | 0.0583 (6) |
| N2 | 0.7097 (3) | 0.2212 (3) | 0.96102 (15) | 0.0578 (7) |
| N3 | 0.0747 (3) | 0.2513 (4) | 0.69361 (15) | 0.0600 (6) |
| C1 | 1.4589 (4) | 0.3630 (6) | 1.4264 (2) | 0.0781 (11) |
| H1 | 1.3944 | 0.4240 | 1.4586 | 0.094* |
| C2 | 1.6035 (5) | 0.3290 (7) | 1.4630 (2) | 0.0928 (13) |
| H2 | 1.6383 | 0.3681 | 1.5207 | 0.111* |
| C3 | 1.7014 (4) | 0.2380 (6) | 1.4172 (3) | 0.0945 (14) |
| H3 | 1.7999 | 0.2151 | 1.4451 | 0.113* |
| C4 | 1.6555 (3) | 0.1801 (6) | 1.3303 (2) | 0.0773 (10) |
| H4 | 1.7214 | 0.1199 | 1.2988 | 0.093* |
| C5 | 1.5068 (3) | 0.2160 (4) | 1.2925 (2) | 0.0602 (8) |
| C6 | 1.4073 (3) | 0.3051 (4) | 1.33936 (19) | 0.0588 (8) |
| C7 | 1.2487 (3) | 0.2597 (4) | 1.21464 (17) | 0.0483 (6) |
| C8 | 1.1075 (3) | 0.2557 (4) | 1.15066 (17) | 0.0462 (6) |
| C9 | 0.9747 (3) | 0.3337 (4) | 1.17029 (18) | 0.0536 (7) |
| H9 | 0.9753 | 0.3904 | 1.2249 | 0.064* |
| C10 | 0.8426 (3) | 0.3278 (4) | 1.10960 (18) | 0.0560 (7) |
| H10 | 0.7556 | 0.3824 | 1.1233 | 0.067* |
| C11 | 0.8375 (3) | 0.2414 (4) | 1.02829 (17) | 0.0490 (6) |
| C12 | 0.9689 (3) | 0.1634 (5) | 1.00924 (17) | 0.0541 (7) |
| H12 | 0.9677 | 0.1055 | 0.9550 | 0.065* |
| C13 | 1.1012 (3) | 0.1698 (5) | 1.06886 (17) | 0.0562 (7) |
| H13 | 1.1881 | 0.1159 | 1.0544 | 0.067* |
| C14 | 0.5823 (3) | 0.2863 (4) | 0.96753 (18) | 0.0551 (7) |
| H14 | 0.5718 | 0.3493 | 1.0190 | 0.066* |
| C15 | 0.4502 (3) | 0.2683 (4) | 0.89868 (17) | 0.0470 (6) |
| C16 | 0.3150 (3) | 0.3497 (4) | 0.90676 (19) | 0.0567 (7) |
| H16 | 0.3071 | 0.4113 | 0.9590 | 0.068* |
| C17 | 0.1925 (3) | 0.3434 (4) | 0.84128 (18) | 0.0530 (7) |
| H17 | 0.1032 | 0.3998 | 0.8500 | 0.064* |
| C18 | 0.1979 (3) | 0.2539 (4) | 0.76100 (17) | 0.0482 (6) |
| C19 | 0.3333 (3) | 0.1671 (5) | 0.75167 (17) | 0.0532 (6) |
| H19 | 0.3405 | 0.1053 | 0.6994 | 0.064* |

| | | | | |
|---|---|---|---|---|
| C20 | 0.4569 (3) | 0.1725 (5) | 0.81967 (18) | 0.0548 (7) |
| H20 | 0.5452 | 0.1120 | 0.8130 | 0.066* |
| C21 | −0.0560 (3) | 0.3699 (5) | 0.6928 (2) | 0.0655 (9) |
| H21A | −0.0899 | 0.4077 | 0.6318 | 0.079* |
| H21B | −0.0234 | 0.4729 | 0.7281 | 0.079* |
| C22 | −0.1861 (4) | 0.2892 (6) | 0.7288 (2) | 0.0884 (12) |
| H22A | −0.2191 | 0.1870 | 0.6944 | 0.133* |
| H22B | −0.2682 | 0.3716 | 0.7251 | 0.133* |
| H22C | −0.1550 | 0.2568 | 0.7903 | 0.133* |
| C23 | 0.0718 (3) | 0.1430 (5) | 0.61427 (18) | 0.0647 (9) |
| H23A | −0.0327 | 0.1119 | 0.5921 | 0.078* |
| H23B | 0.1269 | 0.0356 | 0.6309 | 0.078* |
| C24 | 0.1398 (4) | 0.2295 (6) | 0.5403 (2) | 0.0914 (13) |
| H24A | 0.0835 | 0.3337 | 0.5217 | 0.137* |
| H24B | 0.1355 | 0.1508 | 0.4905 | 0.137* |
| H24C | 0.2437 | 0.2595 | 0.5614 | 0.137* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0536 (4) | 0.0666 (5) | 0.0750 (5) | 0.0054 (4) | 0.0065 (3) | −0.0112 (5) |
| N1 | 0.0498 (14) | 0.0609 (16) | 0.0624 (14) | −0.0015 (12) | 0.0022 (11) | 0.0012 (12) |
| N2 | 0.0528 (14) | 0.0632 (19) | 0.0567 (14) | 0.0001 (12) | 0.0060 (10) | 0.0011 (12) |
| N3 | 0.0488 (13) | 0.0723 (17) | 0.0558 (13) | 0.0090 (13) | −0.0018 (10) | −0.0137 (13) |
| C1 | 0.074 (2) | 0.099 (3) | 0.0584 (19) | −0.017 (2) | −0.0003 (16) | −0.0030 (18) |
| C2 | 0.097 (3) | 0.109 (3) | 0.064 (2) | −0.024 (3) | −0.016 (2) | 0.011 (2) |
| C3 | 0.062 (2) | 0.095 (3) | 0.114 (3) | −0.016 (2) | −0.027 (2) | 0.038 (3) |
| C4 | 0.0561 (18) | 0.071 (2) | 0.103 (3) | 0.000 (2) | 0.0046 (17) | 0.008 (2) |
| C5 | 0.0527 (16) | 0.052 (2) | 0.0737 (19) | −0.0072 (14) | 0.0014 (14) | 0.0095 (14) |
| C6 | 0.0565 (17) | 0.060 (2) | 0.0586 (16) | −0.0093 (15) | 0.0049 (13) | 0.0057 (15) |
| C7 | 0.0511 (15) | 0.0399 (15) | 0.0534 (15) | −0.0045 (13) | 0.0058 (12) | −0.0006 (13) |
| C8 | 0.0434 (14) | 0.0407 (15) | 0.0537 (14) | −0.0021 (13) | 0.0047 (11) | 0.0032 (13) |
| C9 | 0.0520 (16) | 0.0570 (18) | 0.0510 (15) | 0.0000 (14) | 0.0046 (12) | −0.0054 (14) |
| C10 | 0.0467 (15) | 0.062 (2) | 0.0584 (16) | 0.0064 (14) | 0.0067 (13) | −0.0047 (15) |
| C11 | 0.0504 (15) | 0.0471 (16) | 0.0485 (14) | −0.0050 (13) | 0.0035 (11) | 0.0045 (13) |
| C12 | 0.0539 (15) | 0.0604 (17) | 0.0473 (13) | −0.0001 (17) | 0.0048 (11) | −0.0094 (15) |
| C13 | 0.0511 (14) | 0.0612 (17) | 0.0563 (15) | 0.0068 (17) | 0.0082 (11) | −0.0067 (17) |
| C14 | 0.0623 (19) | 0.0495 (19) | 0.0526 (15) | −0.0010 (15) | 0.0057 (13) | −0.0013 (14) |
| C15 | 0.0484 (15) | 0.0424 (16) | 0.0499 (14) | −0.0065 (13) | 0.0060 (11) | 0.0007 (13) |
| C16 | 0.0598 (18) | 0.0551 (19) | 0.0555 (16) | 0.0039 (15) | 0.0098 (13) | −0.0068 (14) |
| C17 | 0.0475 (15) | 0.0539 (18) | 0.0572 (16) | 0.0046 (14) | 0.0061 (13) | −0.0097 (15) |
| C18 | 0.0488 (15) | 0.0451 (15) | 0.0508 (15) | −0.0004 (13) | 0.0074 (11) | 0.0000 (14) |
| C19 | 0.0498 (14) | 0.0565 (16) | 0.0532 (14) | 0.0034 (17) | 0.0076 (11) | −0.0069 (16) |
| C20 | 0.0428 (13) | 0.0542 (16) | 0.0693 (17) | 0.0049 (15) | 0.0146 (12) | 0.0076 (17) |
| C21 | 0.0592 (19) | 0.069 (2) | 0.0660 (19) | 0.0069 (17) | 0.0019 (15) | −0.0037 (16) |
| C22 | 0.072 (2) | 0.100 (3) | 0.097 (3) | −0.003 (2) | 0.0224 (19) | −0.009 (2) |
| C23 | 0.0601 (17) | 0.074 (2) | 0.0579 (16) | 0.0041 (18) | 0.0008 (13) | −0.0168 (18) |
| C24 | 0.100 (3) | 0.113 (4) | 0.064 (2) | 0.003 (3) | 0.0193 (19) | −0.004 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—C5 | 1.725 (3) | C12—C13 | 1.372 (3) |
| S1—C7 | 1.755 (3) | C12—H12 | 0.9300 |
| N1—C7 | 1.313 (4) | C13—H13 | 0.9300 |
| N1—C6 | 1.390 (4) | C14—C15 | 1.454 (4) |
| N2—C14 | 1.255 (4) | C14—H14 | 0.9300 |
| N2—C11 | 1.415 (3) | C15—C16 | 1.376 (4) |
| N3—C18 | 1.379 (3) | C15—C20 | 1.408 (4) |
| N3—C23 | 1.453 (4) | C16—C17 | 1.358 (4) |
| N3—C21 | 1.474 (4) | C16—H16 | 0.9300 |
| C1—C2 | 1.348 (5) | C17—C18 | 1.398 (4) |
| C1—C6 | 1.397 (4) | C17—H17 | 0.9300 |
| C1—H1 | 0.9300 | C18—C19 | 1.401 (4) |
| C2—C3 | 1.377 (6) | C19—C20 | 1.388 (3) |
| C2—H2 | 0.9300 | C19—H19 | 0.9300 |
| C3—C4 | 1.387 (5) | C20—H20 | 0.9300 |
| C3—H3 | 0.9300 | C21—C22 | 1.483 (5) |
| C4—C5 | 1.388 (4) | C21—H21A | 0.9700 |
| C4—H4 | 0.9300 | C21—H21B | 0.9700 |
| C5—C6 | 1.391 (4) | C22—H22A | 0.9600 |
| C7—C8 | 1.466 (4) | C22—H22B | 0.9600 |
| C8—C13 | 1.392 (4) | C22—H22C | 0.9600 |
| C8—C9 | 1.394 (4) | C23—C24 | 1.500 (5) |
| C9—C10 | 1.379 (4) | C23—H23A | 0.9700 |
| C9—H9 | 0.9300 | C23—H23B | 0.9700 |
| C10—C11 | 1.388 (4) | C24—H24A | 0.9600 |
| C10—H10 | 0.9300 | C24—H24B | 0.9600 |
| C11—C12 | 1.380 (4) | C24—H24C | 0.9600 |
| | | | |
| C5—S1—C7 | 89.09 (14) | N2—C14—C15 | 123.3 (3) |
| C7—N1—C6 | 109.3 (2) | N2—C14—H14 | 118.3 |
| C14—N2—C11 | 122.6 (2) | C15—C14—H14 | 118.3 |
| C18—N3—C23 | 122.0 (2) | C16—C15—C20 | 117.3 (2) |
| C18—N3—C21 | 122.4 (2) | C16—C15—C14 | 121.2 (3) |
| C23—N3—C21 | 115.3 (2) | C20—C15—C14 | 121.5 (2) |
| C2—C1—C6 | 118.9 (4) | C17—C16—C15 | 122.5 (3) |
| C2—C1—H1 | 120.5 | C17—C16—H16 | 118.8 |
| C6—C1—H1 | 120.5 | C15—C16—H16 | 118.8 |
| C1—C2—C3 | 121.9 (4) | C16—C17—C18 | 121.3 (3) |
| C1—C2—H2 | 119.1 | C16—C17—H17 | 119.3 |
| C3—C2—H2 | 119.1 | C18—C17—H17 | 119.3 |
| C2—C3—C4 | 121.1 (3) | N3—C18—C17 | 121.3 (2) |
| C2—C3—H3 | 119.5 | N3—C18—C19 | 121.3 (2) |
| C4—C3—H3 | 119.5 | C17—C18—C19 | 117.4 (2) |
| C3—C4—C5 | 117.0 (4) | C20—C19—C18 | 120.7 (3) |
| C3—C4—H4 | 121.5 | C20—C19—H19 | 119.7 |
| C5—C4—H4 | 121.5 | C18—C19—H19 | 119.7 |

| | | | |
|---|---|---|---|
| C4—C5—C6 | 121.8 (3) | C19—C20—C15 | 120.8 (3) |
| C4—C5—S1 | 128.8 (3) | C19—C20—H20 | 119.6 |
| C6—C5—S1 | 109.4 (2) | C15—C20—H20 | 119.6 |
| N1—C6—C5 | 116.3 (3) | N3—C21—C22 | 113.5 (3) |
| N1—C6—C1 | 124.4 (3) | N3—C21—H21A | 108.9 |
| C5—C6—C1 | 119.2 (3) | C22—C21—H21A | 108.9 |
| N1—C7—C8 | 123.9 (2) | N3—C21—H21B | 108.9 |
| N1—C7—S1 | 115.9 (2) | C22—C21—H21B | 108.9 |
| C8—C7—S1 | 120.3 (2) | H21A—C21—H21B | 107.7 |
| C13—C8—C9 | 117.9 (2) | C21—C22—H22A | 109.5 |
| C13—C8—C7 | 120.7 (2) | C21—C22—H22B | 109.5 |
| C9—C8—C7 | 121.4 (2) | H22A—C22—H22B | 109.5 |
| C10—C9—C8 | 120.7 (3) | C21—C22—H22C | 109.5 |
| C10—C9—H9 | 119.7 | H22A—C22—H22C | 109.5 |
| C8—C9—H9 | 119.7 | H22B—C22—H22C | 109.5 |
| C9—C10—C11 | 121.0 (3) | N3—C23—C24 | 113.7 (3) |
| C9—C10—H10 | 119.5 | N3—C23—H23A | 108.8 |
| C11—C10—H10 | 119.5 | C24—C23—H23A | 108.8 |
| C12—C11—C10 | 118.2 (2) | N3—C23—H23B | 108.8 |
| C12—C11—N2 | 114.7 (2) | C24—C23—H23B | 108.8 |
| C10—C11—N2 | 127.1 (3) | H23A—C23—H23B | 107.7 |
| C13—C12—C11 | 121.2 (3) | C23—C24—H24A | 109.5 |
| C13—C12—H12 | 119.4 | C23—C24—H24B | 109.5 |
| C11—C12—H12 | 119.4 | H24A—C24—H24B | 109.5 |
| C12—C13—C8 | 121.0 (3) | C23—C24—H24C | 109.5 |
| C12—C13—H13 | 119.5 | H24A—C24—H24C | 109.5 |
| C8—C13—H13 | 119.5 | H24B—C24—H24C | 109.5 |

| | | | |
|---|---|---|---|
| C6—C1—C2—C3 | −0.4 (6) | C14—N2—C11—C12 | −179.0 (3) |
| C1—C2—C3—C4 | 1.2 (7) | C14—N2—C11—C10 | 1.9 (5) |
| C2—C3—C4—C5 | −0.8 (6) | C10—C11—C12—C13 | 0.3 (5) |
| C3—C4—C5—C6 | −0.4 (5) | N2—C11—C12—C13 | −178.9 (3) |
| C3—C4—C5—S1 | 179.3 (3) | C11—C12—C13—C8 | −0.1 (6) |
| C7—S1—C5—C4 | 178.3 (3) | C9—C8—C13—C12 | 0.5 (5) |
| C7—S1—C5—C6 | −2.0 (2) | C7—C8—C13—C12 | 179.1 (3) |
| C7—N1—C6—C5 | −1.7 (4) | C11—N2—C14—C15 | 179.4 (3) |
| C7—N1—C6—C1 | 179.5 (3) | N2—C14—C15—C16 | −176.6 (3) |
| C4—C5—C6—N1 | −177.7 (3) | N2—C14—C15—C20 | 1.0 (5) |
| S1—C5—C6—N1 | 2.6 (3) | C20—C15—C16—C17 | −1.6 (5) |
| C4—C5—C6—C1 | 1.2 (5) | C14—C15—C16—C17 | 176.1 (3) |
| S1—C5—C6—C1 | −178.6 (3) | C15—C16—C17—C18 | −0.5 (5) |
| C2—C1—C6—N1 | 178.0 (4) | C23—N3—C18—C17 | −172.8 (3) |
| C2—C1—C6—C5 | −0.8 (5) | C21—N3—C18—C17 | 13.3 (5) |
| C6—N1—C7—C8 | 178.2 (3) | C23—N3—C18—C19 | 7.3 (5) |
| C6—N1—C7—S1 | 0.1 (3) | C21—N3—C18—C19 | −166.7 (3) |
| C5—S1—C7—N1 | 1.2 (3) | C16—C17—C18—N3 | −178.3 (3) |
| C5—S1—C7—C8 | −177.0 (2) | C16—C17—C18—C19 | 1.6 (5) |
| N1—C7—C8—C13 | −175.0 (3) | N3—C18—C19—C20 | 179.3 (3) |

| | | | |
|---|---|---|---|
| S1—C7—C8—C13 | 3.1 (4) | C17—C18—C19—C20 | −0.7 (5) |
| N1—C7—C8—C9 | 3.5 (4) | C18—C19—C20—C15 | −1.4 (5) |
| S1—C7—C8—C9 | −178.4 (2) | C16—C15—C20—C19 | 2.5 (5) |
| C13—C8—C9—C10 | −1.0 (4) | C14—C15—C20—C19 | −175.2 (3) |
| C7—C8—C9—C10 | −179.6 (3) | C18—N3—C21—C22 | −97.4 (4) |
| C8—C9—C10—C11 | 1.2 (5) | C23—N3—C21—C22 | 88.3 (3) |
| C9—C10—C11—C12 | −0.8 (5) | C18—N3—C23—C24 | −87.5 (4) |
| C9—C10—C11—N2 | 178.3 (3) | C21—N3—C23—C24 | 86.9 (3) |

*Hydrogen-bond geometry (Å, º)*

Cg is the centroid of the C8–C13 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C12—H12···*Cg*$^{i}$ | 0.93 | 2.88 | 3.577 (5) | 133 |
| C17—H17···*Cg*$^{ii}$ | 0.93 | 2.93 | 3.646 (4) | 135 |

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