

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

(E)-1-(2-Nitrobenzylidene)-4-phenylthiosemicarbazideSamaneh Feizi,^a Ali Hossein Rezayan,^b Soroush Sardari^{a*} and Behrouz Notash^c

^aDrug Design and Bioinformatics Unit, Medical Biotechnology Department, Biotechnology Research Center, Pasteur Institute, Tehran Iran13164, ^bDepartment of Life Science Engineering, Faculty of New Science and Technology, University of Tehran, Tehran, Iran, and ^cDepartment of Chemistry, Shahid Beheshti University, G. C., Evin, Tehran, 1983963113, Iran
Correspondence e-mail: ssardari@hotmail.com

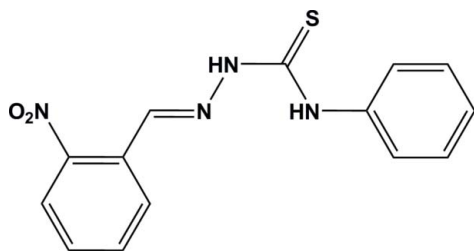
Received 23 April 2012; accepted 13 June 2012

Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.053; wR factor = 0.128; data-to-parameter ratio = 19.0.

In the title molecule, $\text{C}_{14}\text{H}_{12}\text{N}_4\text{O}_2\text{S}$, the conformation about the imine bond is *trans*. The dihedral angle between the two rings is $88.22(11)^\circ$. An intramolecular $\text{N}-\text{H}\cdots\text{N}$ contact occurs. The crystal structure features $\text{N}-\text{H}\cdots\text{S}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

For background to thiosemicarbazone derivatives, see: Shaabani *et al.* (2011); Sardari *et al.* (1999). For applications of imine bonds in synthesis, see: Plech *et al.* (2011); Tada *et al.* (2011); Sriram *et al.* (2007). For related structures, see: Jian & Li (2006a,b); Fang *et al.* (2007).



Experimental

Crystal data

$\text{C}_{14}\text{H}_{12}\text{N}_4\text{O}_2\text{S}$
 $M_r = 300.35$
Triclinic, $P\bar{1}$
 $a = 7.4050(7)$ Å

$b = 8.4239(8)$ Å
 $c = 12.2363(10)$ Å
 $\alpha = 90.382(7)^\circ$
 $\beta = 93.974(7)^\circ$

$\gamma = 110.004(8)^\circ$
 $V = 715.14(12)$ Å³
 $Z = 2$
Mo $K\alpha$ radiation

$\mu = 0.24$ mm⁻¹
 $T = 298$ K
 $0.38 \times 0.35 \times 0.32$ mm

Data collection

Stoe IPDS II diffractometer
Absorption correction: numerical
(*X-RED* and *X-SHAPE*; Stoe & Cie (2005))
 $T_{\min} = 0.910$, $T_{\max} = 0.930$

7967 measured reflections
3832 independent reflections
2715 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.043$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.053$
 $wR(F^2) = 0.128$
 $S = 1.03$
3832 reflections
202 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.26$ e Å⁻³
 $\Delta\rho_{\min} = -0.23$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|--|--------------|--------------------|-------------|----------------------|
| $\text{N3}-\text{H3B}\cdots\text{S1}^{\text{i}}$ | 0.87 (2) | 2.51 (2) | 3.3664 (18) | 168.8 (19) |
| $\text{N4}-\text{H4B}\cdots\text{N2}$ | 0.79 (3) | 2.29 (2) | 2.642 (2) | 108 (2) |
| $\text{C11}-\text{H11}\cdots\text{O1}^{\text{ii}}$ | 0.93 | 2.60 | 3.214 (3) | 125 |

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

Data collection: *X-AREA* (Stoe & Cie, 2005); cell refinement: *X-AREA*; data reduction: *X-AREA*; 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, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

We gratefully acknowledge the Pasteur Institute for grant No. 456.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5899).

References

- Fang, W., Lin, L.-R., Huang, R.-B. & Zheng, L.-S. (2007). *Acta Cryst.* **E63**, o112–o113.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Jian, F.-F. & Li, Y. (2006a). *Acta Cryst.* **E62**, o2934–o2935.
Jian, F.-F. & Li, Y. (2006b). *Acta Cryst.* **E62**, o4563–o4564.
Plech, T., Wujec, M., Siwek, A., Kosikowska, U. & Malm, A. (2011). *Eur. J. Med. Chem.* **46**, 241–248.
Sardari, S., Mori, Y., Horita, K., Micetich, R. G., Nishibe, S. & Daneshtalab, M. (1999). *Bioorg. Med. Chem.* **7**, 1933–1940.
Shaabani, A., Maleki, A., Rezayan, A. H. & Sarvary, A. (2011). *Mol. Divers.* **15**, 41–68.
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
Sriram, D., Yogeewari, P., Dinakaran, M. & Thirumurugan, R. (2007). *J. Antimicrob. Chemother.* **59**, 1194–1196.
Stoe & Cie (2005). *X-AREA, X-RED* and *X-SHAPE*. Stoe & Cie, Darmstadt, Germany.
Tada, R., Chavda, N. & Shah, M. K. (2011). *J. Chem. Pharm. Res.* **3**, 290–297.

supporting information

Acta Cryst. (2012). E68, o2154 [https://doi.org/10.1107/S1600536812026803]

(E)-1-(2-Nitrobenzylidene)-4-phenylthiosemicarbazide**Samaneh Feizi, Ali Hossein Rezayan, Soroush Sardari and Behrouz Notash****S1. Comment**

Thiosemicarbazone derivatives are of special importance because of their versatile biological and pharmacological activities. Thiosemicarbazides are potent intermediates for the synthesis of pharmaceutical and bioactive materials and thus, they are used extensively in the field of medicinal chemistry. The imine bond ($-N=CH-$) in this compounds are useful intermediates in organic synthesis, in particular for the preparation of heterocycles and non-natural β -aminoacids (Plech *et al.*, 2011; Tada *et al.*, 2011; Sriram *et al.*, 2007).

In a continuation of our research on the development of synthetic methods in heterocyclic chemistry (Shaabani *et al.*, 2011; Sardari *et al.*, 1999) here we report the synthesis and structure of the title compound.

The asymmetric unit of the title compound is shown in Fig. 1. In the title molecule, the configuration is *trans* about the imine bond ($C=N$). Bond lengths and angles are in the normal ranges reported for similar structures (Jian and Li (2006a,b); Fang *et al.* (2007)). The dihedral angle between the two phenyl ring is $88.22(11)^\circ$. The crystal structure exhibits intermolecular $N-H\cdots S$ and $C-H\cdots O$ hydrogen bonds and also intramolecular $N-H\cdots O$ and $C-H\cdots N$ hydrogen bonds (Fig. 2 & Table 1).

S2. Experimental

To a magnetically stirred solution of 4-phenylthiosemicarbazide (0.167 g, 1.0 mmol) in MeOH (30 ml) in round bottom flask was added a solution of 2-nitrobenzaldehyde (0.151 g, 1 mmol) at room temperature. The mixture was stirred for 48 h. After completion of the reaction, the Precipitate product was filtered and washed with MeOH (20 ml) and dried at room temperature. The final product is a yellow solid (yield 70%).

S3. Refinement

The hydrogen atom attached to nitrogen atoms and $C-H$ of imine moiety were found in difference Fourier map and refined isotropically without restraint. Aromatic $C-H$ protons were positioned geometrically and refined as riding atoms with $C-H = 0.93 \text{ \AA}$ and $U_{iso}(H) = 1.2 U_{eq}(C)$.

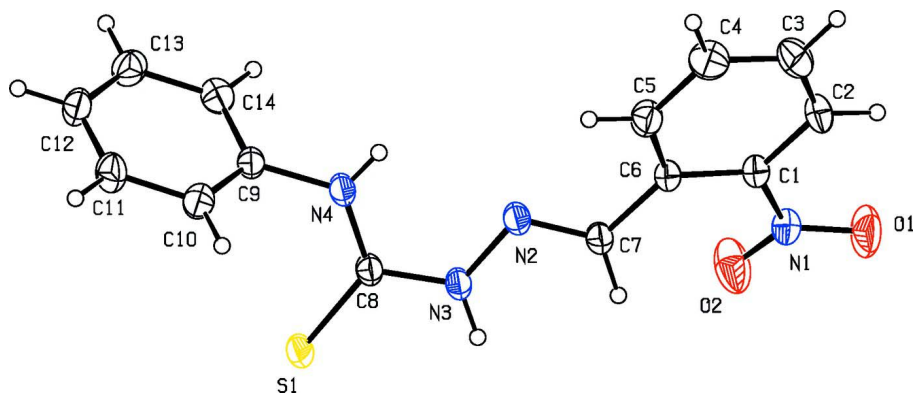


Figure 1

The asymmetric unit of the title compound with displacement ellipsoids drawn at 30% probability level.

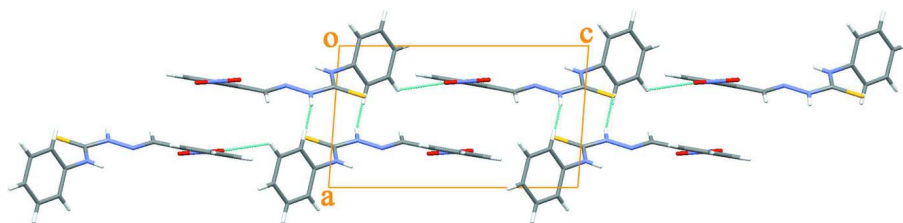


Figure 2

The packing diagram of the title compound. The intermolecular N—H...S and C—H...O hydrogen bonds are shown as blue dashed lines.

(*E*)-1-(2-Nitrobenzylidene)-4-phenylthiosemicarbazide

Crystal data

$C_{14}H_{12}N_4O_2S$

$M_r = 300.35$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 7.4050$ (7) Å

$b = 8.4239$ (8) Å

$c = 12.2363$ (10) Å

$\alpha = 90.382$ (7)°

$\beta = 93.974$ (7)°

$\gamma = 110.004$ (8)°

$V = 715.14$ (12) Å³

$Z = 2$

$F(000) = 312$

$D_x = 1.395$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 7967 reflections

$\theta = 2.6$ – 29.2 °

$\mu = 0.24$ mm⁻¹

$T = 298$ K

Prism, yellow

$0.38 \times 0.35 \times 0.32$ mm

Data collection

Stoe IPDS II

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 0.15 mm pixels mm⁻¹

rotation method scans

Absorption correction: numerical

(*X-RED* and *X-SHAPE*; Stoe & Cie (2005))

$T_{\min} = 0.910$, $T_{\max} = 0.930$

7967 measured reflections

3832 independent reflections

2715 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.043$

$\theta_{\max} = 29.2$ °, $\theta_{\min} = 2.6$ °

$h = -10 \rightarrow 10$

$k = -11 \rightarrow 10$

$l = -15 \rightarrow 16$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.053$
 $wR(F^2) = 0.128$
 $S = 1.03$
 3832 reflections
 202 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 atoms treated by a mixture of independent
 and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0528P)^2 + 0.223P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.005$
 $\Delta\rho_{\max} = 0.26 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.23 \text{ e } \text{\AA}^{-3}$

Special details

Experimental. shape of crystal determined optically

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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|-------------|------------|--------------|----------------------------------|
| C1 | 0.2544 (3) | 0.5115 (3) | 0.51143 (14) | 0.0381 (4) |
| C2 | 0.2249 (3) | 0.5628 (3) | 0.40645 (15) | 0.0509 (5) |
| H2 | 0.2076 | 0.4892 | 0.3465 | 0.061* |
| C3 | 0.2213 (4) | 0.7226 (3) | 0.39147 (18) | 0.0609 (6) |
| H3 | 0.2007 | 0.7575 | 0.3212 | 0.073* |
| C4 | 0.2482 (4) | 0.8319 (3) | 0.48040 (19) | 0.0597 (6) |
| H4 | 0.2457 | 0.9404 | 0.4700 | 0.072* |
| C5 | 0.2790 (3) | 0.7805 (3) | 0.58510 (17) | 0.0479 (5) |
| H5 | 0.2977 | 0.8559 | 0.6442 | 0.057* |
| C6 | 0.2826 (3) | 0.6186 (2) | 0.60429 (14) | 0.0366 (4) |
| C7 | 0.3227 (3) | 0.5732 (3) | 0.71685 (14) | 0.0406 (4) |
| H7 | 0.388 (3) | 0.492 (3) | 0.7285 (18) | 0.052 (6)* |
| C8 | 0.2886 (3) | 0.6664 (2) | 0.99057 (14) | 0.0372 (4) |
| C9 | 0.1339 (3) | 0.8556 (2) | 1.06241 (14) | 0.0375 (4) |
| C10 | 0.2729 (3) | 0.9819 (3) | 1.12422 (16) | 0.0469 (5) |
| H10 | 0.4023 | 1.0094 | 1.1118 | 0.056* |
| C11 | 0.2178 (4) | 1.0678 (3) | 1.20523 (17) | 0.0530 (5) |
| H11 | 0.3108 | 1.1530 | 1.2475 | 0.064* |
| C12 | 0.0278 (4) | 1.0282 (3) | 1.22337 (17) | 0.0517 (5) |
| H12 | -0.0080 | 1.0859 | 1.2782 | 0.062* |
| C13 | -0.1108 (3) | 0.9032 (3) | 1.16084 (18) | 0.0514 (5) |
| H13 | -0.2402 | 0.8768 | 1.1732 | 0.062* |
| C14 | -0.0578 (3) | 0.8164 (3) | 1.07917 (16) | 0.0441 (5) |

| | | | | |
|-----|--------------|-------------|--------------|--------------|
| H14 | -0.1512 | 0.7325 | 1.0362 | 0.053* |
| O1 | 0.2599 (4) | 0.2612 (3) | 0.43801 (14) | 0.0824 (6) |
| O2 | 0.2395 (4) | 0.2728 (2) | 0.60884 (14) | 0.0829 (6) |
| N1 | 0.2507 (3) | 0.3363 (2) | 0.52080 (13) | 0.0453 (4) |
| N2 | 0.2793 (2) | 0.6465 (2) | 0.79714 (12) | 0.0395 (4) |
| N3 | 0.3341 (3) | 0.6036 (2) | 0.89882 (12) | 0.0433 (4) |
| H3B | 0.411 (3) | 0.546 (3) | 0.9056 (18) | 0.042 (6)* |
| N4 | 0.1877 (3) | 0.7690 (2) | 0.97626 (13) | 0.0469 (4) |
| H4B | 0.150 (3) | 0.782 (3) | 0.916 (2) | 0.053 (7)* |
| S1 | 0.35639 (10) | 0.60896 (8) | 1.11356 (4) | 0.05372 (19) |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|-------------|-------------|-------------|
| C1 | 0.0429 (10) | 0.0444 (11) | 0.0292 (8) | 0.0173 (9) | 0.0053 (7) | -0.0006 (7) |
| C2 | 0.0620 (14) | 0.0657 (15) | 0.0267 (8) | 0.0237 (12) | 0.0059 (8) | 0.0002 (9) |
| C3 | 0.0796 (17) | 0.0730 (17) | 0.0355 (10) | 0.0323 (14) | 0.0075 (10) | 0.0168 (10) |
| C4 | 0.0784 (17) | 0.0517 (13) | 0.0568 (13) | 0.0310 (13) | 0.0111 (12) | 0.0180 (11) |
| C5 | 0.0622 (14) | 0.0456 (12) | 0.0411 (10) | 0.0246 (11) | 0.0072 (9) | 0.0003 (9) |
| C6 | 0.0413 (10) | 0.0440 (10) | 0.0278 (8) | 0.0185 (9) | 0.0049 (7) | -0.0004 (7) |
| C7 | 0.0536 (12) | 0.0448 (11) | 0.0295 (8) | 0.0255 (10) | -0.0008 (8) | -0.0045 (7) |
| C8 | 0.0494 (11) | 0.0370 (10) | 0.0281 (8) | 0.0190 (9) | 0.0010 (7) | -0.0027 (7) |
| C9 | 0.0547 (12) | 0.0367 (10) | 0.0281 (8) | 0.0247 (9) | 0.0037 (7) | 0.0017 (7) |
| C10 | 0.0467 (12) | 0.0527 (13) | 0.0433 (10) | 0.0194 (10) | 0.0061 (9) | -0.0046 (9) |
| C11 | 0.0640 (15) | 0.0501 (13) | 0.0444 (11) | 0.0199 (11) | 0.0005 (10) | -0.0139 (9) |
| C12 | 0.0698 (15) | 0.0571 (13) | 0.0395 (10) | 0.0352 (12) | 0.0114 (10) | -0.0032 (9) |
| C13 | 0.0521 (13) | 0.0590 (14) | 0.0493 (11) | 0.0248 (11) | 0.0152 (10) | 0.0095 (10) |
| C14 | 0.0541 (12) | 0.0363 (10) | 0.0407 (10) | 0.0147 (9) | 0.0008 (9) | 0.0021 (8) |
| O1 | 0.1373 (19) | 0.0725 (12) | 0.0507 (10) | 0.0532 (13) | 0.0082 (10) | -0.0205 (9) |
| O2 | 0.155 (2) | 0.0529 (11) | 0.0455 (9) | 0.0410 (12) | 0.0083 (11) | 0.0041 (8) |
| N1 | 0.0516 (10) | 0.0481 (10) | 0.0377 (8) | 0.0193 (8) | 0.0037 (7) | -0.0076 (7) |
| N2 | 0.0534 (10) | 0.0419 (9) | 0.0275 (7) | 0.0222 (8) | 0.0021 (6) | -0.0007 (6) |
| N3 | 0.0664 (12) | 0.0493 (10) | 0.0259 (7) | 0.0359 (10) | -0.0009 (7) | -0.0034 (6) |
| N4 | 0.0751 (13) | 0.0546 (11) | 0.0257 (7) | 0.0425 (10) | -0.0017 (7) | -0.0034 (7) |
| S1 | 0.0844 (4) | 0.0706 (4) | 0.0259 (2) | 0.0526 (3) | 0.0011 (2) | 0.0008 (2) |

Geometric parameters (Å, °)

| | | | |
|-------|-----------|---------|-----------|
| C1—C2 | 1.385 (3) | C9—C14 | 1.374 (3) |
| C1—C6 | 1.405 (2) | C9—C10 | 1.377 (3) |
| C1—N1 | 1.472 (3) | C9—N4 | 1.432 (2) |
| C2—C3 | 1.369 (3) | C10—C11 | 1.386 (3) |
| C2—H2 | 0.9300 | C10—H10 | 0.9300 |
| C3—C4 | 1.379 (3) | C11—C12 | 1.365 (3) |
| C3—H3 | 0.9300 | C11—H11 | 0.9300 |
| C4—C5 | 1.384 (3) | C12—C13 | 1.374 (3) |
| C4—H4 | 0.9300 | C12—H12 | 0.9300 |
| C5—C6 | 1.394 (3) | C13—C14 | 1.389 (3) |

| | | | |
|-------------|--------------|-----------------|--------------|
| C5—H5 | 0.9300 | C13—H13 | 0.9300 |
| C6—C7 | 1.470 (2) | C14—H14 | 0.9300 |
| C7—N2 | 1.273 (2) | O1—N1 | 1.209 (2) |
| C7—H7 | 0.97 (2) | O2—N1 | 1.202 (2) |
| C8—N4 | 1.327 (2) | N2—N3 | 1.371 (2) |
| C8—N3 | 1.349 (2) | N3—H3B | 0.87 (2) |
| C8—S1 | 1.6799 (18) | N4—H4B | 0.79 (3) |
| | | | |
| C2—C1—C6 | 122.28 (19) | C10—C9—N4 | 120.05 (19) |
| C2—C1—N1 | 116.16 (17) | C9—C10—C11 | 119.3 (2) |
| C6—C1—N1 | 121.55 (16) | C9—C10—H10 | 120.4 |
| C3—C2—C1 | 119.5 (2) | C11—C10—H10 | 120.4 |
| C3—C2—H2 | 120.2 | C12—C11—C10 | 120.4 (2) |
| C1—C2—H2 | 120.2 | C12—C11—H11 | 119.8 |
| C2—C3—C4 | 120.11 (19) | C10—C11—H11 | 119.8 |
| C2—C3—H3 | 119.9 | C11—C12—C13 | 120.19 (19) |
| C4—C3—H3 | 119.9 | C11—C12—H12 | 119.9 |
| C3—C4—C5 | 120.2 (2) | C13—C12—H12 | 119.9 |
| C3—C4—H4 | 119.9 | C12—C13—C14 | 120.0 (2) |
| C5—C4—H4 | 119.9 | C12—C13—H13 | 120.0 |
| C4—C5—C6 | 121.7 (2) | C14—C13—H13 | 120.0 |
| C4—C5—H5 | 119.1 | C9—C14—C13 | 119.4 (2) |
| C6—C5—H5 | 119.1 | C9—C14—H14 | 120.3 |
| C5—C6—C1 | 116.22 (17) | C13—C14—H14 | 120.3 |
| C5—C6—C7 | 119.24 (17) | O2—N1—O1 | 122.1 (2) |
| C1—C6—C7 | 124.48 (17) | O2—N1—C1 | 119.95 (16) |
| N2—C7—C6 | 119.59 (17) | O1—N1—C1 | 117.90 (18) |
| N2—C7—H7 | 121.3 (13) | C7—N2—N3 | 115.10 (15) |
| C6—C7—H7 | 119.1 (13) | C8—N3—N2 | 120.88 (16) |
| N4—C8—N3 | 116.38 (16) | C8—N3—H3B | 118.3 (14) |
| N4—C8—S1 | 124.22 (13) | N2—N3—H3B | 120.3 (14) |
| N3—C8—S1 | 119.39 (14) | C8—N4—C9 | 125.10 (16) |
| C14—C9—C10 | 120.63 (17) | C8—N4—H4B | 118.8 (17) |
| C14—C9—N4 | 119.25 (19) | C9—N4—H4B | 116.1 (17) |
| | | | |
| C6—C1—C2—C3 | -0.5 (3) | C11—C12—C13—C14 | 0.2 (3) |
| N1—C1—C2—C3 | 178.3 (2) | C10—C9—C14—C13 | -1.3 (3) |
| C1—C2—C3—C4 | 0.4 (4) | N4—C9—C14—C13 | -178.36 (18) |
| C2—C3—C4—C5 | 0.0 (4) | C12—C13—C14—C9 | 0.6 (3) |
| C3—C4—C5—C6 | -0.4 (4) | C2—C1—N1—O2 | -166.3 (2) |
| C4—C5—C6—C1 | 0.4 (3) | C6—C1—N1—O2 | 12.5 (3) |
| C4—C5—C6—C7 | 177.9 (2) | C2—C1—N1—O1 | 14.0 (3) |
| C2—C1—C6—C5 | 0.1 (3) | C6—C1—N1—O1 | -167.2 (2) |
| N1—C1—C6—C5 | -178.62 (18) | C6—C7—N2—N3 | -175.80 (18) |
| C2—C1—C6—C7 | -177.3 (2) | N4—C8—N3—N2 | 0.6 (3) |
| N1—C1—C6—C7 | 4.0 (3) | S1—C8—N3—N2 | 179.32 (15) |
| C5—C6—C7—N2 | 27.7 (3) | C7—N2—N3—C8 | -176.8 (2) |
| C1—C6—C7—N2 | -155.0 (2) | N3—C8—N4—C9 | -176.5 (2) |

| | | | |
|-----------------|-------------|--------------|------------|
| C14—C9—C10—C11 | 1.1 (3) | S1—C8—N4—C9 | 4.9 (3) |
| N4—C9—C10—C11 | 178.15 (19) | C14—C9—N4—C8 | -115.2 (2) |
| C9—C10—C11—C12 | -0.2 (3) | C10—C9—N4—C8 | 67.7 (3) |
| C10—C11—C12—C13 | -0.4 (4) | | |

Hydrogen-bond geometry (Å, °)

| <i>D</i> —H... <i>A</i> | <i>D</i> —H | H... <i>A</i> | <i>D</i> ... <i>A</i> | <i>D</i> —H... <i>A</i> |
|-----------------------------------|-------------|---------------|-----------------------|-------------------------|
| N3—H3 <i>B</i> ...S1 ⁱ | 0.87 (2) | 2.51 (2) | 3.3664 (18) | 168.8 (19) |
| N4—H4 <i>B</i> ...N2 | 0.79 (3) | 2.29 (2) | 2.642 (2) | 108 (2) |
| C7—H7...O2 | 0.97 (2) | 2.26 (2) | 2.703 (3) | 106.5 (16) |
| C11—H11...O1 ⁱⁱ | 0.93 | 2.60 | 3.214 (3) | 125 |

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