# organic compounds

# 4-[(2-Hydroxybenzylidene)amino]-N-(5-methylisoxazol-3-yl)benzene-sulfonamide: a monoclinic polymorph

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The title compound, $C_{17}H_{15}N_3O_4S$, is a monoclinic polymorph with space group $P2_1/c$ of the previously reported triclinic form in $P\bar{1}$ [Subashini et al. (2009). J. Chem. Crystallogr. **39**, 112–116]. In both polymorphs, intramolecular O—H···N hydrogen bonds and dimer formation via a pair of inter-molecular N—H···N hydrogen bonds with an $R_2^2(8)$ motif are observed. The two polymorphs differ in the next level of supramolecular organization involving C—H···O hydrogen bonds with varied packing and different conformations.

## Related literature

For the biological relevance of sulfonamide drugs and their Schiff base derivatives, see: Genc et al. (2008); Supuran et al. (1997). For the triclinic polymorph of the title compound, see: Subashini et al. (2009). For $R_2^2(8)$ ring motifs in sulfonamides, see: Adsmond & Grant (2001). For conformational studies on sulfonamides, see: Kálmán et al. (1981).
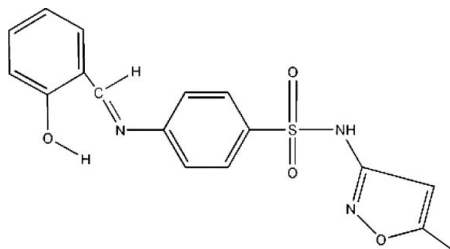


## Experimental

### Crystal data

$C_{17}H_{15}N_3O_4S$

$M_r$ = 357.39

Monoclinic, $P2_1/c$

$a$ = 7.0374 (1) Å

$b$ = 17.9244 (3) Å

$c$ = 14.5175 (3) Å

$\beta$ = 112.962 (1)°

$V$ = 1686.15 (5) Å$^3$

$Z$ = 4

Mo $K\alpha$ radiation

$\mu$ = 0.22 mm$^{-1}$

$T$ = 293 K

$0.25 \times 0.22 \times 0.20$ mm

### Data collection

Bruker SMART APEXII CCD area-detector diffractometer

Absorption correction: multi-scan (SADABS; Bruker, 2008)

$T_{min}$ = 0.947, $T_{max}$ = 0.957

14935 measured reflections

2953 independent reflections

2198 reflections with $I > 2\sigma(I)$

$R_{int}$ = 0.038

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049

$wR(F^2)$ = 0.115

$S$ = 1.06

2953 reflections

227 parameters

H-atom parameters constrained

$\Delta\rho_{max}$ = 0.25 e Å$^{-3}$

$\Delta\rho_{min}$ = −0.30 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···N1 | 0.82 | 1.88 | 2.606 (3) | 147 |
| N2—H2A···N3[i] | 0.86 | 2.24 | 2.898 (4) | 134 |
| C10—H10···O1[ii] | 0.93 | 2.53 | 3.313 (3) | 141 |

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

Data collection: APEX2 (Bruker, 2008); cell refinement: SAINT (Bruker, 2008); data reduction: SAINT; program(s) used to solve structure: SHELXS86 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: PLATON (Spek, 2009); software used to prepare material for publication: PLATON.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2595).

## References

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# supporting information

# 4-[(2-Hydroxybenzylidene)amino]-*N*-(5-methylisoxazol-3-yl)benzene-sulfonamide: a monoclinic polymorph

## Samuel Ebenezer and Packianathan Thomas Muthiah

### S1. Comment

Sulfonamide drugs are known to have antibacterial, antifungal,antimalarial and antileprotic properties (Genc *et al.*, 2008). Schiff bases derived from sulfonamide compounds also display enzymatic inhibition (Supuran *et al.*, 1997). A polymorph, I, of the title compound has been reported earlier from our group (Subashini *et al.*, 2009). In the present study we report a new dimorph, II, and its crystal structure.

The new dimorph crystallizes in monoclinic system ($P2_1/c$) which contains only one molecule in the asymmetric unit (Fig. 1). There is one N—H⋯N intermolecular hydrogen bond [N2⋯N3 = 2.899 (3) Å; Table 1], where the amido nitrogen acts as a donor and the nitrogen of the isoxazole acts as an acceptor. The donor and acceptor of one of the Schiff base molecule pair up with another inversely related molecule to form a dimer with graph set notation $R_2^2(8)$ (Fig 2). A similar type of homosynthon is also formed in the polymorph I. A recent statistical survey has shown that the absence of amino group in the sulfonamide compounds further encourages amido protons to hydrogen bond with an activated nitrogen (atom of a heterocycle that lies in conjugation with the amido nitrogen) of the heterocyclic ring to form an optimum sized $R_2^2(8)$ ring motif (Adsmond & Grant, 2001). This could be the reason why both the polymorphs form the same synthons thereby succumb to similar first order arrangement of molecules.

Polymorph II forms an intramolecular C—H⋯O bond with a graph set notation S(6) similar to its predecessor. It is only the weaker bonds in both the polymorphs that are significantly responsible for the differences in arrangement of molecules in the crystal. In both the polymorphs the homosynthon combines with each other through a couple of weak C—H⋯O bonds (C10—H10⋯O1 in polymorph II) forming a large ring motif with graph set notation $R_4^4(12)$ and $R_4^4(14)$ for polymorphs I and II respectively. These homosynthons stretch along a particular direction linked through weak C—H⋯O interaction forming a supramolecular chain (Fig. 3).

In addition to the packing differences there are changes in the conformations of the molecules which are obvious from their torsion angles. Though there are many possible conformations in which the molecule could exist, the steric and electrostatic constraints of sulfonamides have restricted them to torsion angles between 70–120° and 60–90° for $\varepsilon1$ and $\varepsilon2$ respectively [where $\varepsilon1$ and $\varepsilon2$ are the modulus of the torsion angles along C—S and S—N bonds respectively] (Kálmán *et al.*, 1981). The angles $\varepsilon1$ and $\varepsilon2$ for polymorph II lie in the expected range. The bond lengths and the bond angles among the polymorphs are more or less close to one another but differ hugely in their torsion angles.

To conclude with, both dimorphs posses same intermolecular hydrogen bonds leading to formation of dimers through N—H⋯N hydrogen bonds, showing similar first level of organization. They differ only in the higher level supramolecular organization through C—H⋯O hydrogen bonds. A thorough inspection reveals that conformational changes in the molecule lead to the packing differences between the dimorphs.

## S2. Experimental

The base of the title compound was synthesized by refluxing ethanolic solutions of 4-amino-*N*-(5-methyl-3-isoxazolyl)
benzene sulfonamide (SMZ) (25 mg, Qualigens) with 2-hydroxy benzaldehyde (SA) (25 mg, LOBA Chemie) in an
equimolar ratio. The mixture was refluxed for up to 6 h and then transferred to a beaker which was eventually allowed to
evaporate slowly in the mother liquor. After a couple of days yellow crystals separated out. This base was characterized
using single-crystal XRD method and found to be a new polymorph.

## S3. Refinement

All hydrogen atoms were positioned geometrically and were refined using riding model. The C—H, N—H and O—H
bond lengths are 0.93–0.97, 0.86 and 0.82 Å, respectively. [$U_{iso}$(H) = 1.2$U_{eq}$(aromatic C and N) and 1.5$U_{eq}$(methyl C and
O)].
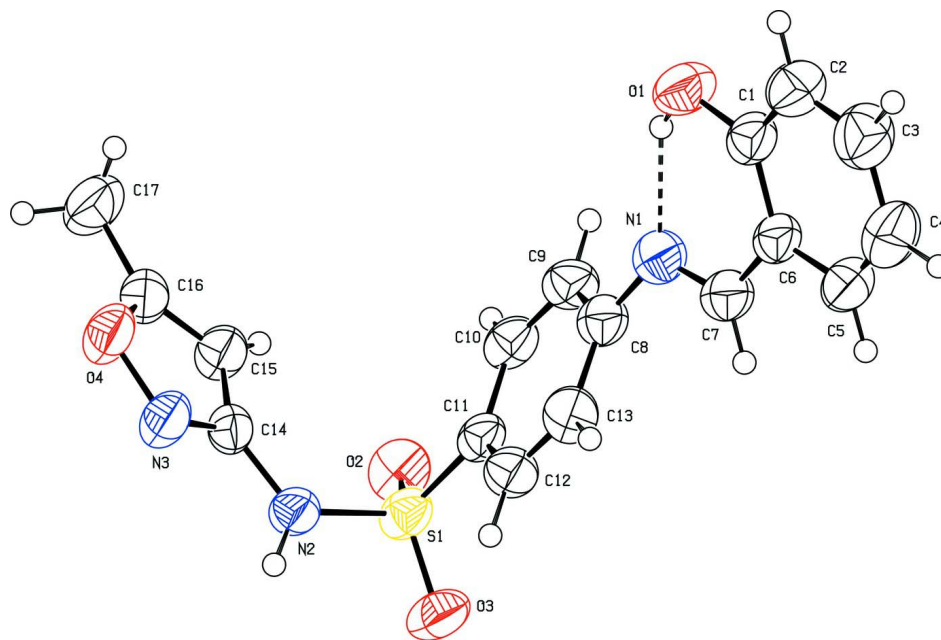


**Figure 1**

An *ORTEP* view of new dimorph showing 50% probability displacement ellipsoids.
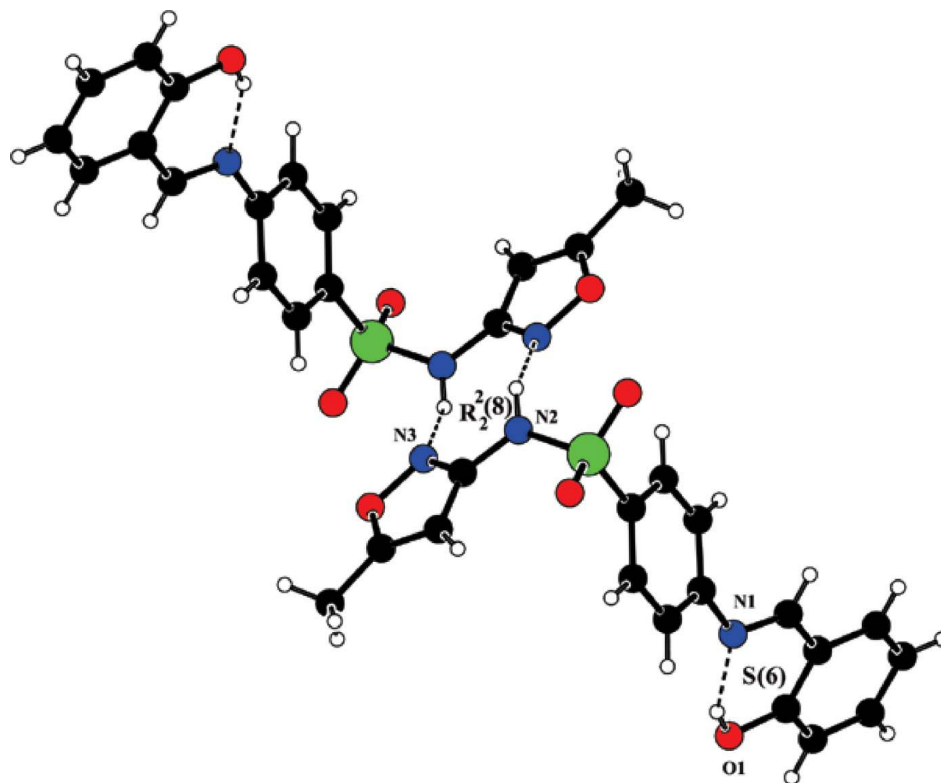
**Figure 2**

Two inversely related molecules form dimer through $R_2^2(8)$ motif. [Symmetry code: (i) -*x* + 2, -*y* + 1, -*z* + 2.]
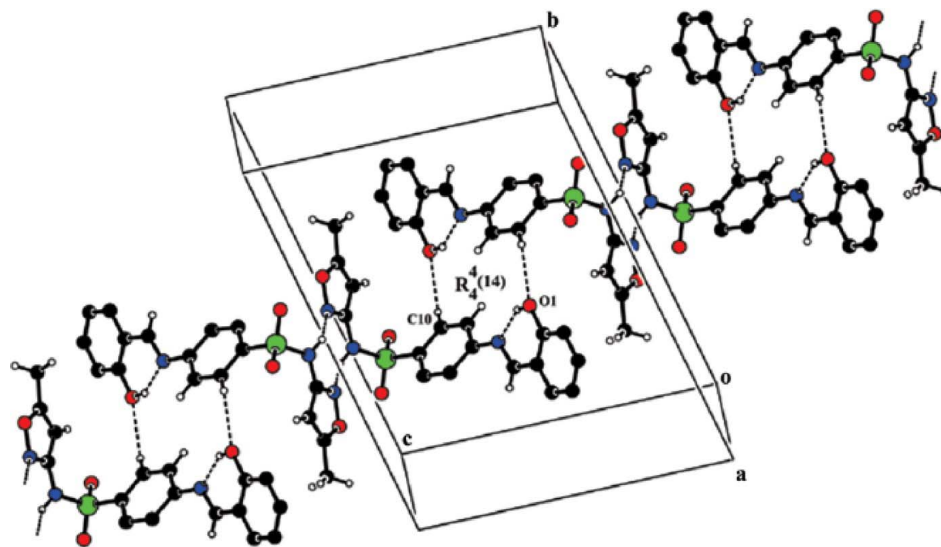


**Figure 3**

View of supramolecular chain formed through the dimers *via* weak C—H···O interactions.

**4-[(2-Hydroxybenzylidene)amino]-*N*-(5-methylisoxazol-3- yl)benzenesulfonamide**

*Crystal data*

| | |
|---|---|
| $C_{17}H_{15}N_3O_4S$ | $F(000) = 744$ |
| $M_r = 357.39$ | $D_x = 1.408$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2ybc | Cell parameters from 2953 reflections |
| $a = 7.0374$ (1) Å | $\theta = 1.9–25.0°$ |
| $b = 17.9244$ (3) Å | $\mu = 0.22$ mm$^{-1}$ |
| $c = 14.5175$ (3) Å | $T = 293$ K |
| $\beta = 112.962$ (1)° | PRISM, yellow |
| $V = 1686.15$ (5) Å$^3$ | $0.25 \times 0.22 \times 0.20$ mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART APEXII CCD area-detector diffractometer | 14935 measured reflections |
| Radiation source: fine-focus sealed tube | 2953 independent reflections |
| Graphite monochromator | 2198 reflections with $I > 2\sigma(I)$ |
| $\varphi$ and $\omega$ scans | $R_{int} = 0.038$ |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2008) | $\theta_{max} = 25.0°$, $\theta_{min} = 1.9°$ |
| $T_{min} = 0.947$, $T_{max} = 0.957$ | $h = -7 \rightarrow 8$ |
| | $k = -19 \rightarrow 21$ |
| | $l = -17 \rightarrow 17$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.049$ | |
| $wR(F^2) = 0.115$ | H-atom parameters constrained |
| $S = 1.06$ | $w = 1/[\sigma^2(F_o^2) + (0.040P)^2 + 0.9817P]$ |
| 2953 reflections | where $P = (F_o^2 + 2F_c^2)/3$ |
| 227 parameters | $(\Delta/\sigma)_{max} < 0.001$ |
| 0 restraints | $\Delta\rho_{max} = 0.25$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{min} = -0.30$ e Å$^{-3}$ |

*Special details*

**Geometry**. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**Refinement**. Refinement on $F^2$ for ALL reflections except those flagged by the user for potential systematic errors. Weighted $R$-factors $wR$ and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -$R$-factor-obs *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* | $U_{iso}*/U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.61583 (11) | 0.37355 (3) | 0.87561 (5) | 0.0507 (3) |
| O1 | 0.8540 (3) | 0.47399 (10) | 0.37502 (16) | 0.0676 (8) |
| O2 | 0.3998 (3) | 0.38398 (10) | 0.84707 (15) | 0.0625 (7) |
| O3 | 0.7159 (3) | 0.30911 (10) | 0.93038 (15) | 0.0667 (8) |

| | | | | |
|---|---|---|---|---|
| O4 | 0.7150 (3) | 0.63662 (10) | 0.93497 (15) | 0.0658 (7) |
| N1 | 0.8210 (4) | 0.39344 (12) | 0.51746 (17) | 0.0551 (8) |
| N2 | 0.7352 (3) | 0.44313 (11) | 0.94686 (16) | 0.0501 (8) |
| N3 | 0.8188 (4) | 0.56808 (12) | 0.96244 (18) | 0.0594 (9) |
| C1 | 0.9847 (4) | 0.42129 (14) | 0.3684 (2) | 0.0528 (10) |
| C2 | 1.0800 (5) | 0.43213 (17) | 0.3024 (2) | 0.0664 (11) |
| C3 | 1.2136 (6) | 0.38013 (19) | 0.2939 (3) | 0.0770 (14) |
| C4 | 1.2539 (6) | 0.31558 (19) | 0.3500 (3) | 0.0787 (16) |
| C5 | 1.1614 (5) | 0.30449 (15) | 0.4157 (2) | 0.0650 (11) |
| C6 | 1.0262 (4) | 0.35658 (13) | 0.4270 (2) | 0.0495 (9) |
| C7 | 0.9426 (4) | 0.34594 (15) | 0.5023 (2) | 0.0549 (10) |
| C8 | 0.7705 (4) | 0.38551 (14) | 0.6022 (2) | 0.0506 (9) |
| C9 | 0.5773 (4) | 0.40732 (14) | 0.5957 (2) | 0.0544 (10) |
| C10 | 0.5264 (4) | 0.40347 (14) | 0.6783 (2) | 0.0511 (10) |
| C11 | 0.6728 (4) | 0.37909 (13) | 0.7690 (2) | 0.0459 (8) |
| C12 | 0.8681 (4) | 0.35926 (15) | 0.7762 (2) | 0.0544 (10) |
| C13 | 0.9170 (4) | 0.36252 (15) | 0.6943 (2) | 0.0561 (10) |
| C14 | 0.6769 (4) | 0.51741 (13) | 0.92693 (19) | 0.0447 (9) |
| C15 | 0.4810 (4) | 0.54900 (15) | 0.8754 (2) | 0.0543 (10) |
| C16 | 0.5134 (4) | 0.62267 (15) | 0.8831 (2) | 0.0551 (10) |
| C17 | 0.3782 (5) | 0.68894 (17) | 0.8475 (3) | 0.0798 (13) |
| H1 | 0.81330 | 0.46250 | 0.41890 | 0.1010* |
| H2 | 1.05290 | 0.47510 | 0.26360 | 0.0800* |
| H2A | 0.84130 | 0.43320 | 1.00030 | 0.0600* |
| H3 | 1.27820 | 0.38830 | 0.24980 | 0.0920* |
| H4 | 1.34340 | 0.27990 | 0.34300 | 0.0940* |
| H5 | 1.18960 | 0.26110 | 0.45380 | 0.0780* |
| H7 | 0.97800 | 0.30310 | 0.54140 | 0.0660* |
| H9 | 0.48080 | 0.42480 | 0.53520 | 0.0650* |
| H10 | 0.39510 | 0.41710 | 0.67330 | 0.0610* |
| H12 | 0.96640 | 0.34360 | 0.83730 | 0.0650* |
| H13 | 1.04890 | 0.34940 | 0.69990 | 0.0670* |
| H15 | 0.35650 | 0.52420 | 0.84310 | 0.0650* |
| H17A | 0.39730 | 0.71040 | 0.79110 | 0.1200* |
| H17B | 0.41320 | 0.72510 | 0.90030 | 0.1200* |
| H17C | 0.23670 | 0.67420 | 0.82810 | 0.1200* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0458 (4) | 0.0386 (4) | 0.0611 (5) | −0.0045 (3) | 0.0136 (3) | 0.0006 (3) |
| O1 | 0.0703 (14) | 0.0556 (12) | 0.0757 (14) | 0.0180 (10) | 0.0273 (12) | 0.0130 (10) |
| O2 | 0.0397 (11) | 0.0645 (12) | 0.0791 (14) | −0.0079 (9) | 0.0186 (10) | −0.0030 (10) |
| O3 | 0.0735 (14) | 0.0420 (10) | 0.0787 (15) | 0.0032 (10) | 0.0233 (12) | 0.0149 (10) |
| O4 | 0.0604 (13) | 0.0418 (10) | 0.0777 (14) | 0.0020 (9) | 0.0081 (11) | −0.0114 (10) |
| N1 | 0.0494 (14) | 0.0503 (13) | 0.0569 (15) | −0.0036 (11) | 0.0112 (12) | −0.0023 (11) |
| N2 | 0.0453 (13) | 0.0437 (12) | 0.0482 (14) | 0.0015 (10) | 0.0040 (10) | 0.0004 (10) |
| N3 | 0.0514 (15) | 0.0416 (13) | 0.0701 (17) | 0.0036 (11) | 0.0072 (12) | −0.0079 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C1 | 0.0501 (17) | 0.0427 (15) | 0.0569 (18) | −0.0005 (13) | 0.0115 (14) | −0.0037 (13) |
| C2 | 0.075 (2) | 0.0521 (18) | 0.072 (2) | −0.0019 (16) | 0.0286 (18) | 0.0057 (15) |
| C3 | 0.093 (3) | 0.070 (2) | 0.081 (2) | 0.0014 (19) | 0.048 (2) | −0.0028 (18) |
| C4 | 0.086 (3) | 0.063 (2) | 0.092 (3) | 0.0162 (18) | 0.040 (2) | −0.0062 (19) |
| C5 | 0.074 (2) | 0.0438 (16) | 0.066 (2) | 0.0054 (15) | 0.0150 (17) | −0.0016 (14) |
| C6 | 0.0493 (16) | 0.0375 (14) | 0.0508 (17) | −0.0035 (12) | 0.0077 (13) | −0.0032 (12) |
| C7 | 0.0539 (18) | 0.0430 (15) | 0.0542 (18) | −0.0101 (13) | 0.0062 (14) | −0.0002 (13) |
| C8 | 0.0494 (17) | 0.0421 (14) | 0.0530 (18) | −0.0076 (12) | 0.0120 (14) | −0.0018 (13) |
| C9 | 0.0432 (17) | 0.0520 (16) | 0.0547 (18) | 0.0016 (13) | 0.0048 (14) | 0.0039 (13) |
| C10 | 0.0371 (15) | 0.0427 (15) | 0.066 (2) | 0.0016 (12) | 0.0121 (14) | 0.0005 (13) |
| C11 | 0.0417 (15) | 0.0334 (13) | 0.0529 (16) | −0.0021 (11) | 0.0080 (13) | −0.0019 (12) |
| C12 | 0.0446 (17) | 0.0538 (16) | 0.0513 (18) | 0.0040 (13) | 0.0042 (14) | 0.0002 (13) |
| C13 | 0.0401 (16) | 0.0588 (18) | 0.061 (2) | 0.0018 (13) | 0.0105 (14) | −0.0047 (14) |
| C14 | 0.0452 (16) | 0.0420 (14) | 0.0426 (16) | 0.0005 (12) | 0.0125 (13) | −0.0054 (12) |
| C15 | 0.0433 (16) | 0.0483 (16) | 0.0607 (19) | 0.0027 (12) | 0.0087 (14) | −0.0045 (13) |
| C16 | 0.0545 (18) | 0.0513 (17) | 0.0512 (17) | 0.0068 (14) | 0.0115 (14) | −0.0074 (13) |
| C17 | 0.078 (2) | 0.0523 (18) | 0.090 (3) | 0.0170 (16) | 0.012 (2) | −0.0013 (17) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—O2 | 1.424 (2) | C8—C9 | 1.382 (4) |
| S1—O3 | 1.423 (2) | C9—C10 | 1.381 (4) |
| S1—N2 | 1.629 (2) | C10—C11 | 1.388 (4) |
| S1—C11 | 1.747 (3) | C11—C12 | 1.384 (4) |
| O1—C1 | 1.348 (3) | C12—C13 | 1.362 (4) |
| O4—N3 | 1.405 (3) | C14—C15 | 1.406 (4) |
| O4—C16 | 1.345 (4) | C15—C16 | 1.337 (4) |
| O1—H1 | 0.8200 | C16—C17 | 1.483 (4) |
| N1—C7 | 1.286 (4) | C2—H2 | 0.9300 |
| N1—C8 | 1.415 (4) | C3—H3 | 0.9300 |
| N2—C14 | 1.390 (3) | C4—H4 | 0.9300 |
| N3—C14 | 1.299 (4) | C5—H5 | 0.9300 |
| N2—H2A | 0.8600 | C7—H7 | 0.9300 |
| C1—C2 | 1.381 (4) | C9—H9 | 0.9300 |
| C1—C6 | 1.400 (4) | C10—H10 | 0.9300 |
| C2—C3 | 1.363 (5) | C12—H12 | 0.9300 |
| C3—C4 | 1.379 (5) | C13—H13 | 0.9300 |
| C4—C5 | 1.363 (5) | C15—H15 | 0.9300 |
| C5—C6 | 1.388 (4) | C17—H17A | 0.9600 |
| C6—C7 | 1.442 (4) | C17—H17B | 0.9600 |
| C8—C13 | 1.395 (4) | C17—H17C | 0.9600 |
| | | | |
| S1···H15 | 3.1900 | C2···H15ii | 3.0700 |
| O1···N1 | 2.606 (3) | C5···H12ix | 3.0000 |
| O1···N1i | 3.245 (3) | C7···H13 | 2.6700 |
| O1···C10ii | 3.313 (3) | C7···H1 | 2.4100 |
| O2···C13iii | 3.276 (4) | C13···H7 | 2.6400 |
| O2···C15 | 3.010 (3) | C13···H2i | 2.9600 |

| | | | |
|---|---|---|---|
| O3···C7[iv] | 3.172 (3) | C16···H3[i] | 2.8500 |
| O1···H10[ii] | 2.5300 | H1···N1 | 1.8800 |
| O2···H10 | 2.5800 | H1···C7 | 2.4100 |
| O2···H15 | 2.5300 | H2···C13[i] | 2.9600 |
| O2···H13[iii] | 2.6300 | H2A···N3[vii] | 2.2400 |
| O3···H12 | 2.6800 | H3···O4[i] | 2.7400 |
| O3···H4[v] | 2.9000 | H3···C16[i] | 2.8500 |
| O3···H7[iv] | 2.7800 | H4···O3[x] | 2.9000 |
| O4···H5[vi] | 2.6800 | H5···H7 | 2.4200 |
| O4···H3[i] | 2.7400 | H5···O4[xi] | 2.6800 |
| N1···O1 | 2.606 (3) | H7···C13 | 2.6400 |
| N1···O1[i] | 3.245 (3) | H7···H5 | 2.4200 |
| N2···N3[vii] | 2.898 (4) | H7···H13 | 2.3100 |
| N3···N2[vii] | 2.898 (4) | H7···O3[ix] | 2.7800 |
| N1···H1 | 1.8800 | H10···O2 | 2.5800 |
| N3···H2A[vii] | 2.2400 | H10···O1[ii] | 2.5300 |
| C2···C8[i] | 3.546 (4) | H12···O3 | 2.6800 |
| C5···C9[viii] | 3.581 (4) | H12···C5[iv] | 3.0000 |
| C7···O3[ix] | 3.172 (3) | H13···O2[viii] | 2.6300 |
| C8···C2[i] | 3.546 (4) | H13···C7 | 2.6700 |
| C9···C5[iii] | 3.581 (4) | H13···H7 | 2.3100 |
| C10···O1[ii] | 3.313 (3) | H15···S1 | 3.1900 |
| C13···O2[viii] | 3.276 (4) | H15···O2 | 2.5300 |
| C15···O2 | 3.010 (3) | H15···C2[ii] | 3.0700 |
| C2···H17C[ii] | 2.9800 | H17C···C2[ii] | 2.9800 |
| | | | |
| O2—S1—O3 | 120.58 (13) | N3—C14—C15 | 111.9 (2) |
| O2—S1—N2 | 108.18 (12) | N2—C14—N3 | 117.9 (3) |
| O2—S1—C11 | 108.84 (13) | N2—C14—C15 | 130.2 (2) |
| O3—S1—N2 | 104.27 (12) | C14—C15—C16 | 104.7 (2) |
| O3—S1—C11 | 107.86 (13) | O4—C16—C15 | 109.8 (2) |
| N2—S1—C11 | 106.23 (12) | O4—C16—C17 | 116.1 (2) |
| N3—O4—C16 | 108.3 (2) | C15—C16—C17 | 134.1 (3) |
| C1—O1—H1 | 110.00 | C1—C2—H2 | 120.00 |
| C7—N1—C8 | 119.5 (2) | C3—C2—H2 | 120.00 |
| S1—N2—C14 | 124.33 (18) | C2—C3—H3 | 120.00 |
| O4—N3—C14 | 105.4 (2) | C4—C3—H3 | 120.00 |
| S1—N2—H2A | 118.00 | C3—C4—H4 | 120.00 |
| C14—N2—H2A | 118.00 | C5—C4—H4 | 120.00 |
| C2—C1—C6 | 119.7 (3) | C4—C5—H5 | 119.00 |
| O1—C1—C6 | 121.6 (3) | C6—C5—H5 | 119.00 |
| O1—C1—C2 | 118.7 (2) | N1—C7—H7 | 119.00 |
| C1—C2—C3 | 120.4 (3) | C6—C7—H7 | 119.00 |
| C2—C3—C4 | 120.7 (4) | C8—C9—H9 | 120.00 |
| C3—C4—C5 | 119.4 (4) | C10—C9—H9 | 120.00 |
| C4—C5—C6 | 121.4 (3) | C9—C10—H10 | 120.00 |
| C5—C6—C7 | 120.1 (2) | C11—C10—H10 | 120.00 |
| C1—C6—C5 | 118.4 (3) | C11—C12—H12 | 120.00 |

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| C1—C6—C7 | 121.3 (2) | C13—C12—H12 | 120.00 |
| N1—C7—C6 | 122.5 (2) | C8—C13—H13 | 120.00 |
| N1—C8—C9 | 119.1 (2) | C12—C13—H13 | 120.00 |
| N1—C8—C13 | 121.4 (3) | C14—C15—H15 | 128.00 |
| C9—C8—C13 | 119.3 (3) | C16—C15—H15 | 128.00 |
| C8—C9—C10 | 120.5 (3) | C16—C17—H17A | 109.00 |
| C9—C10—C11 | 119.4 (3) | C16—C17—H17B | 109.00 |
| S1—C11—C12 | 118.9 (2) | C16—C17—H17C | 109.00 |
| S1—C11—C10 | 121.1 (2) | H17A—C17—H17B | 109.00 |
| C10—C11—C12 | 120.0 (3) | H17A—C17—H17C | 110.00 |
| C11—C12—C13 | 120.3 (3) | H17B—C17—H17C | 109.00 |
| C8—C13—C12 | 120.4 (3) | | |
| | | | |
| O2—S1—N2—C14 | −44.7 (3) | C2—C1—C6—C5 | −0.8 (4) |
| O3—S1—N2—C14 | −174.2 (2) | C2—C1—C6—C7 | 175.1 (3) |
| C11—S1—N2—C14 | 72.0 (3) | C1—C2—C3—C4 | 0.8 (5) |
| O2—S1—C11—C10 | 10.4 (2) | C2—C3—C4—C5 | −1.1 (6) |
| O2—S1—C11—C12 | −170.1 (2) | C3—C4—C5—C6 | 0.4 (5) |
| O3—S1—C11—C10 | 142.8 (2) | C4—C5—C6—C1 | 0.5 (5) |
| O3—S1—C11—C12 | −37.7 (2) | C4—C5—C6—C7 | −175.4 (3) |
| N2—S1—C11—C10 | −105.9 (2) | C1—C6—C7—N1 | 2.4 (4) |
| N2—S1—C11—C12 | 73.6 (2) | C5—C6—C7—N1 | 178.2 (3) |
| C16—O4—N3—C14 | −0.4 (3) | N1—C8—C9—C10 | −177.1 (2) |
| N3—O4—C16—C15 | −0.1 (3) | C13—C8—C9—C10 | −2.7 (4) |
| N3—O4—C16—C17 | −180.0 (3) | N1—C8—C13—C12 | 176.3 (2) |
| C8—N1—C7—C6 | −170.2 (3) | C9—C8—C13—C12 | 2.1 (4) |
| C7—N1—C8—C9 | −147.2 (3) | C8—C9—C10—C11 | 1.5 (4) |
| C7—N1—C8—C13 | 38.6 (4) | C9—C10—C11—S1 | 179.81 (19) |
| S1—N2—C14—N3 | −152.9 (2) | C9—C10—C11—C12 | 0.3 (4) |
| S1—N2—C14—C15 | 29.5 (4) | S1—C11—C12—C13 | 179.6 (2) |
| O4—N3—C14—N2 | −177.3 (2) | C10—C11—C12—C13 | −0.9 (4) |
| O4—N3—C14—C15 | 0.7 (3) | C11—C12—C13—C8 | −0.3 (4) |
| O1—C1—C2—C3 | 179.8 (3) | N2—C14—C15—C16 | 177.0 (3) |
| C6—C1—C2—C3 | 0.2 (5) | N3—C14—C15—C16 | −0.7 (3) |
| O1—C1—C6—C5 | 179.6 (3) | C14—C15—C16—O4 | 0.4 (3) |
| O1—C1—C6—C7 | −4.6 (4) | C14—C15—C16—C17 | −179.7 (3) |

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*−1, *y*, *z*; (iv) *x*, −*y*+1/2, *z*+1/2; (v) *x*−1, −*y*+1/2, *z*+1/2; (vi) −*x*+2, *y*+1/2, −*z*+3/2; (vii) −*x*+2, −*y*+1, −*z*+2; (viii) *x*+1, *y*, *z*; (ix) *x*, −*y*+1/2, *z*−1/2; (x) *x*+1, −*y*+1/2, *z*−1/2; (xi) −*x*+2, *y*−1/2, −*z*+3/2.

*Hydrogen-bond geometry (Å, °)*

| D—H···A | D—H | H···A | D···A | D—H···A |
|---|---|---|---|---|
| O1—H1···N1 | 0.82 | 1.88 | 2.606 (3) | 147 |
| N2—H2*A*···N3vii | 0.86 | 2.24 | 2.898 (4) | 134 |
| C10—H10···O1ii | 0.93 | 2.53 | 3.313 (3) | 141 |
| C15—H15···O2 | 0.93 | 2.53 | 3.010 (3) | 112 |

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