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# 2-[(*E*)-2-(4-Methylbenzenesulfonamido)-ethyliminiomethyl]-4-nitrophenolate

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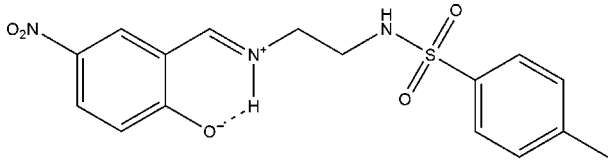
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.032; $wR$ factor = 0.094; data-to-parameter ratio = 13.9.

The molecule of the title compound, $C_{16}H_{17}N_3O_5S$, crystallizes in a zwitterionic form, with a strong intramolecular N—H···O hydrogen bond. The dihedral angle between the two benzene rings is 7.06 (9)°. In the crystal, molecules are linked into chains along the $c$ axis by intermolecular N—H···O hydrogen bonds.

## Related literature

For general background to Schiff bases, see: Calligaris *et al.* (1972); Cohen *et al.* (1964); Hadjoudis *et al.* (1987); Karabıyık *et al.* (2008). For the crystal structure of 2-[2-(1*H*-indol-3-yl)ethyliminiomethyl]-4-nitrophenolate, see: Ali *et al.* (2008). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



## Experimental

### Crystal data

$C_{16}H_{17}N_3O_5S$
$M_r$ = 363.39
Monoclinic, $P2_1/c$
$a$ = 17.915 (5) Å
$b$ = 7.342 (5) Å
$c$ = 13.055 (5) Å
$\beta$ = 103.928 (5)°
$V$ = 1666.7 (14) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.23 mm$^{-1}$
$T$ = 296 K
0.68 × 0.50 × 0.26 mm

### Data collection

Stoe IPDS-II diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{min}$ = 0.887, $T_{max}$ = 0.956
22908 measured reflections
3272 independent reflections
2845 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.024

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.094
$S$ = 1.07
3272 reflections
236 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.26 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.27 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H1···O3$^{i}$ | 0.78 (2) | 2.06 (2) | 2.833 (2) | 170 (2) |
| N2—H1*A*···O3 | 0.87 (2) | 1.94 (2) | 2.648 (2) | 137 (2) |

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

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32*; 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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2882).

## References

Ali, H. M., Mohamed Mustafa, M. I., Rizal, M. R. & Ng, S. W. (2008). *Acta Cryst.* E**64**, o913.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Calligaris, M., Nardin, G. & Randaccio, L. (1972). *Coord. Chem. Rev.* **7**, 385–403.
Cohen, M. D., Schmidt, G. M. J. & Flavian, S. (1964). *J. Chem. Soc.* pp. 2041–2051.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Hadjoudis, E., Vitterakis, M., Moustakali, I. & Mavridis, I. (1987). *Tetrahedron*, **43**, 1345–1360.
Karabıyık, H., Ocak İskeleli, N., Petek, H., Albayrak, Ç. & Ağar, E. (2008). *J. Mol. Struct.* **873**, 130–136.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Stoe & Cie (2002). *X-AREA* and *X-RED32*. Stoe & Cie, Darmstadt, Germany.

# supporting information

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## 2-[(*E*)-2-(4-Methylbenzenesulfonamido)ethyliminiomethyl]-4-nitrophenolate

**Marife Tüfekçi, Gökhan Alpaslan, Mustafa Macit and Ahmet Erdönmez**

### S1. Comment

Schiff bases have been extensively used as ligands in the field of coordination chemistry (Calligaris *et al.*, 1972). Schiff base compounds can be classified by their photochromic and thermochromic characteristics (Cohen *et al.*, 1964). These properties result from a proton transfer from the hydroxyl O atom to the imine N atom (Hadjoudis *et al.*, 1987). Schiff bases exhibit two well known tautomeric forms *viz*. OH and NH tautomers, and they also exist in zwitterionic form (Karabıyık *et al.*, 2008). Our investigations show that the title compund has a zwitterionic form with a strong intramolecular N—H···O hydrogen bond (Fig. 1).

The C7N2 [1.292 (2) Å] and C6—03 [1.272 (2) Å] bond distances in the title compound are comparable to those [1.292 (2) and 1.264 (2) Å] observed in a related zwitterionic structure (Ali *et al.*, 2008). The molecule adopts a folded conformation. The dihedral angle between the two benzene rings is 7.06 (9)°.

The intramolecular N2—H1A···O3 hydrogen bond generates an S(6) ring motif (Bernstein *et al.*, 1995). The molecules are linked into chains (Fig. 2) along the *c* axis by intermolecular N—H···O hydrogen bonds (Table 1).

### S2. Experimental

2-Hydroxy-5-nitrobenzaldehyde (10 mg, 5.98× $10^{-2}$ mmol) in ethanol (20 ml) was added to a solution of *N*-*p*-tolyl-sulfonylethylenediamine (12.7 mg, 5.98× $10^{-2}$ mmol) in ethanol (20 ml). The reaction mixture was stirred for 1 h under reflux. Single crystals of the title compound were obtained by slow evaporation of an ethylacetate solution (yield 55%; m.p. 446–447 K).

### S3. Refinement

Atoms H1 and H1A were located in a difference map and were refined freely. The remaining H atoms were placed in calculated positions and constrained to ride on their parent atoms, with C—H = 0.93–0.97 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C) or 1.5$U_{eq}$(methyl C).

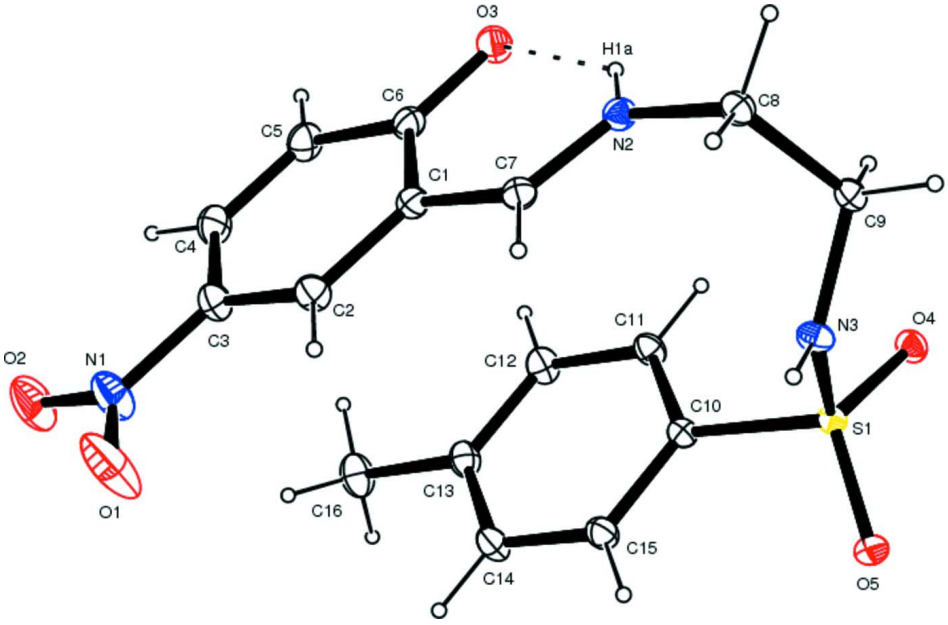


**Figure 1**

The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii. The dashed line indicates a hydrogen bond.

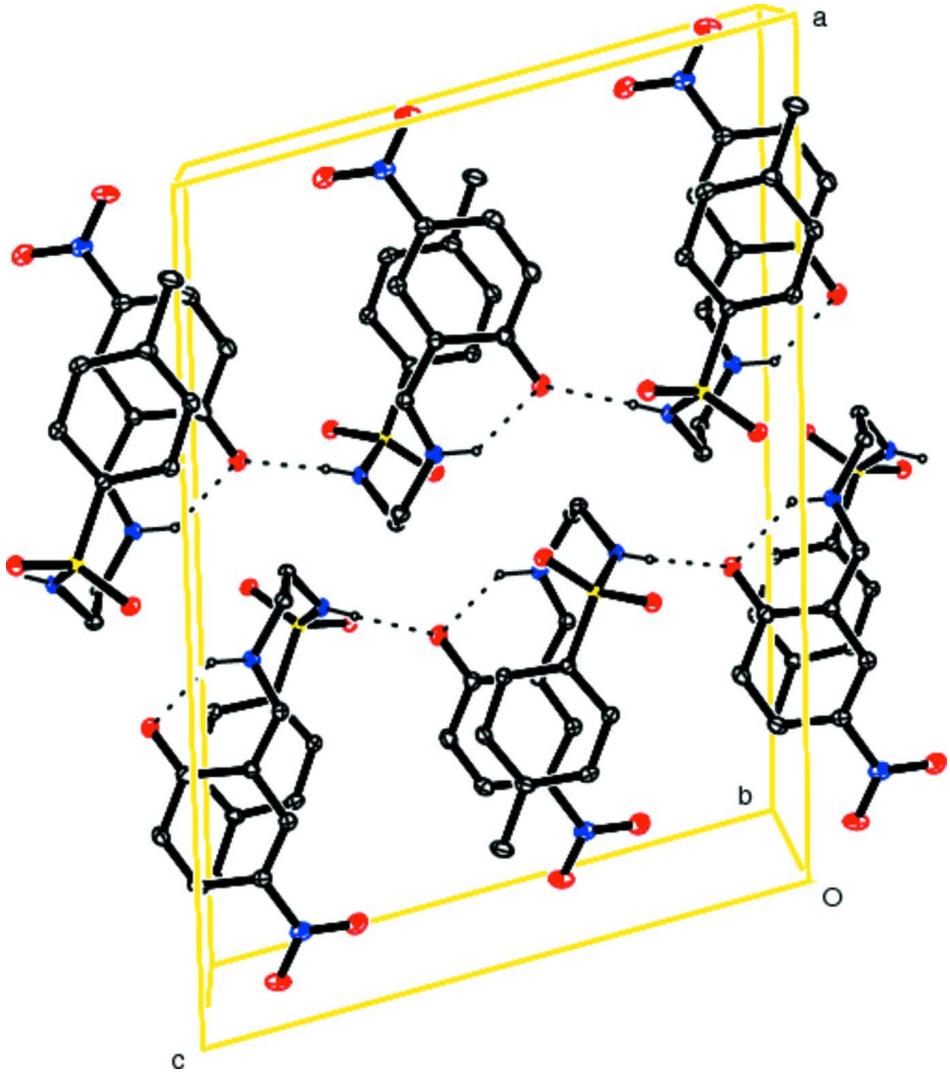


**Figure 2**

A packing diagram for (I). H atoms not involved in hydrogen bonding (dashed lines) have been omitted for clarity.

**2-[(*E*)-2-(4-Methylbenzenesulfonamido)ethyliminiomethyl]-4-nitrophenolate**

*Crystal data*

$C_{16}H_{17}N_3O_5S$
$M_r = 363.39$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 17.915\ (5)$ Å
$b = 7.342\ (5)$ Å
$c = 13.055\ (5)$ Å
$\beta = 103.928\ (5)°$
$V = 1666.7\ (14)$ Å$^3$
$Z = 4$

$F(000) = 760$
$D_x = 1.448$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 37649 reflections
$\theta = 1.6–28.0°$
$\mu = 0.23$ mm$^{-1}$
$T = 296$ K
Block, yellow
0.68 × 0.50 × 0.26 mm

*Data collection*

Stoe IPDS-II diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 6.67 pixels $mm^{-1}$
$\omega$ scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{min}$ = 0.887, $T_{max}$ = 0.956

22908 measured reflections
3272 independent reflections
2845 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.024
$\theta_{max}$ = 26.0°, $\theta_{min}$ = 2.3°
$h = -22 \rightarrow 22$
$k = -9 \rightarrow 9$
$l = -16 \rightarrow 15$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.094
$S$ = 1.07
3272 reflections
236 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
$w = 1/[\sigma^2(F_o^2) + (0.0542P)^2 + 0.2378P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 0.26 e $Å^{-3}$
$\Delta\rho_{min}$ = −0.27 e $Å^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0025 (8)

*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 | 0.73857 (9) | 0.1439 (2) | 0.58535 (12) | 0.0464 (3) |
| C2 | 0.81399 (10) | 0.1345 (2) | 0.64584 (14) | 0.0559 (4) |
| H2 | 0.8238 | 0.1405 | 0.7190 | 0.067* |
| C3 | 0.87338 (10) | 0.1163 (3) | 0.59823 (15) | 0.0604 (4) |
| C4 | 0.86008 (11) | 0.1075 (3) | 0.48830 (16) | 0.0648 (5) |
| H4 | 0.9012 | 0.0958 | 0.4567 | 0.078* |
| C5 | 0.78743 (11) | 0.1160 (3) | 0.42812 (15) | 0.0642 (5) |
| H5 | 0.7796 | 0.1093 | 0.3552 | 0.077* |
| C6 | 0.72214 (10) | 0.1346 (2) | 0.47198 (13) | 0.0523 (4) |
| C7 | 0.67882 (9) | 0.1617 (2) | 0.63841 (13) | 0.0463 (3) |
| H7 | 0.6925 | 0.1648 | 0.7118 | 0.056* |
| C8 | 0.54749 (9) | 0.1973 (2) | 0.65034 (13) | 0.0466 (4) |
| H8A | 0.5661 | 0.1505 | 0.7214 | 0.056* |
| H8B | 0.5024 | 0.1275 | 0.6162 | 0.056* |

| | | | | |
|---|---|---|---|---|
| C9 | 0.52559 (8) | 0.3947 (2) | 0.65549 (12) | 0.0438 (3) |
| H9A | 0.5085 | 0.4419 | 0.5843 | 0.053* |
| H9B | 0.4829 | 0.4035 | 0.6889 | 0.053* |
| C10 | 0.69671 (8) | 0.65737 (19) | 0.62312 (11) | 0.0400 (3) |
| C11 | 0.69016 (9) | 0.6244 (2) | 0.51721 (12) | 0.0495 (4) |
| H11 | 0.6420 | 0.6182 | 0.4705 | 0.059* |
| C12 | 0.75608 (10) | 0.6008 (3) | 0.48147 (13) | 0.0571 (4) |
| H12 | 0.7515 | 0.5781 | 0.4102 | 0.068* |
| C13 | 0.82838 (10) | 0.6100 (2) | 0.54833 (15) | 0.0553 (4) |
| C14 | 0.83365 (10) | 0.6421 (3) | 0.65479 (15) | 0.0601 (4) |
| H14 | 0.8818 | 0.6474 | 0.7015 | 0.072* |
| C15 | 0.76879 (9) | 0.6661 (2) | 0.69225 (13) | 0.0522 (4) |
| H15 | 0.7733 | 0.6882 | 0.7636 | 0.063* |
| C16 | 0.89969 (12) | 0.5917 (3) | 0.50703 (19) | 0.0795 (6) |
| H16A | 0.8863 | 0.5403 | 0.4374 | 0.119* |
| H16B | 0.9359 | 0.5136 | 0.5529 | 0.119* |
| H16C | 0.9223 | 0.7097 | 0.5045 | 0.119* |
| N1 | 0.95110 (10) | 0.1062 (3) | 0.66326 (18) | 0.0917 (6) |
| N2 | 0.60663 (7) | 0.17413 (18) | 0.59235 (11) | 0.0456 (3) |
| N3 | 0.58876 (7) | 0.50612 (18) | 0.71366 (10) | 0.0448 (3) |
| O1 | 0.96069 (10) | 0.1084 (5) | 0.75840 (16) | 0.1571 (12) |
| O2 | 1.00420 (9) | 0.0954 (4) | 0.62016 (16) | 0.1183 (7) |
| O3 | 0.65360 (7) | 0.1427 (2) | 0.41569 (9) | 0.0669 (4) |
| O4 | 0.55334 (6) | 0.75149 (15) | 0.58460 (9) | 0.0479 (3) |
| O5 | 0.63776 (6) | 0.81294 (15) | 0.76080 (9) | 0.0522 (3) |
| S1 | 0.614192 (19) | 0.69488 (5) | 0.67146 (3) | 0.03887 (13) |
| H1 | 0.6088 (10) | 0.478 (2) | 0.7710 (14) | 0.048 (5)* |
| H1A | 0.5970 (12) | 0.176 (3) | 0.5235 (17) | 0.067 (6)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0470 (8) | 0.0456 (8) | 0.0471 (8) | −0.0002 (6) | 0.0121 (7) | −0.0028 (7) |
| C2 | 0.0522 (9) | 0.0660 (10) | 0.0494 (9) | −0.0005 (8) | 0.0124 (7) | 0.0003 (8) |
| C3 | 0.0452 (9) | 0.0709 (11) | 0.0658 (11) | 0.0025 (8) | 0.0148 (8) | 0.0017 (9) |
| C4 | 0.0601 (11) | 0.0720 (12) | 0.0701 (12) | 0.0056 (9) | 0.0307 (9) | −0.0012 (10) |
| C5 | 0.0709 (12) | 0.0753 (12) | 0.0507 (9) | 0.0086 (10) | 0.0232 (9) | −0.0062 (9) |
| C6 | 0.0568 (10) | 0.0516 (9) | 0.0487 (9) | 0.0038 (7) | 0.0130 (7) | −0.0072 (7) |
| C7 | 0.0505 (9) | 0.0449 (8) | 0.0432 (8) | −0.0021 (6) | 0.0107 (7) | −0.0007 (6) |
| C8 | 0.0438 (8) | 0.0475 (8) | 0.0502 (9) | −0.0058 (6) | 0.0147 (7) | 0.0030 (7) |
| C9 | 0.0348 (7) | 0.0498 (8) | 0.0472 (8) | −0.0037 (6) | 0.0109 (6) | 0.0008 (7) |
| C10 | 0.0389 (7) | 0.0409 (7) | 0.0399 (7) | −0.0016 (6) | 0.0089 (6) | 0.0033 (6) |
| C11 | 0.0425 (8) | 0.0643 (10) | 0.0407 (8) | −0.0008 (7) | 0.0079 (6) | 0.0049 (7) |
| C12 | 0.0556 (10) | 0.0750 (12) | 0.0440 (9) | 0.0037 (8) | 0.0185 (7) | 0.0086 (8) |
| C13 | 0.0469 (9) | 0.0583 (10) | 0.0651 (11) | 0.0003 (7) | 0.0222 (8) | 0.0094 (8) |
| C14 | 0.0378 (8) | 0.0749 (12) | 0.0637 (11) | −0.0013 (8) | 0.0044 (7) | 0.0005 (9) |
| C15 | 0.0444 (8) | 0.0643 (10) | 0.0450 (8) | 0.0001 (7) | 0.0054 (7) | −0.0027 (7) |
| C16 | 0.0553 (11) | 0.0987 (16) | 0.0943 (15) | 0.0034 (11) | 0.0372 (11) | 0.0117 (13) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N1 | 0.0490 (9) | 0.1412 (19) | 0.0847 (13) | 0.0029 (11) | 0.0154 (9) | 0.0064 (13) |
| N2 | 0.0471 (7) | 0.0463 (7) | 0.0444 (7) | −0.0015 (5) | 0.0131 (6) | −0.0026 (6) |
| N3 | 0.0466 (7) | 0.0521 (8) | 0.0328 (7) | −0.0071 (6) | 0.0041 (5) | 0.0045 (6) |
| O1 | 0.0575 (10) | 0.327 (4) | 0.0791 (12) | 0.0105 (15) | 0.0021 (9) | 0.0096 (18) |
| O2 | 0.0494 (8) | 0.195 (2) | 0.1165 (14) | 0.0089 (11) | 0.0310 (9) | −0.0005 (14) |
| O3 | 0.0600 (8) | 0.0888 (9) | 0.0472 (7) | 0.0093 (7) | 0.0038 (6) | −0.0159 (6) |
| O4 | 0.0417 (5) | 0.0488 (6) | 0.0494 (6) | 0.0043 (4) | 0.0034 (5) | 0.0055 (5) |
| O5 | 0.0512 (6) | 0.0543 (6) | 0.0504 (6) | −0.0036 (5) | 0.0108 (5) | −0.0159 (5) |
| S1 | 0.03696 (19) | 0.0403 (2) | 0.0382 (2) | 0.00009 (14) | 0.00693 (14) | −0.00238 (14) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.393 (2) | C10—C15 | 1.387 (2) |
| C1—C7 | 1.414 (2) | C10—S1 | 1.7631 (15) |
| C1—C6 | 1.440 (2) | C11—C12 | 1.381 (2) |
| C2—C3 | 1.362 (2) | C11—H11 | 0.93 |
| C2—H2 | 0.93 | C12—C13 | 1.378 (3) |
| C3—C4 | 1.399 (3) | C12—H12 | 0.93 |
| C3—N1 | 1.448 (3) | C13—C14 | 1.390 (3) |
| C4—C5 | 1.350 (3) | C13—C16 | 1.507 (2) |
| C4—H4 | 0.93 | C14—C15 | 1.376 (2) |
| C5—C6 | 1.427 (2) | C14—H14 | 0.93 |
| C5—H5 | 0.93 | C15—H15 | 0.93 |
| C6—O3 | 1.272 (2) | C16—H16A | 0.96 |
| C7—N2 | 1.292 (2) | C16—H16B | 0.96 |
| C7—H7 | 0.93 | C16—H16C | 0.96 |
| C8—N2 | 1.4529 (19) | N1—O1 | 1.212 (3) |
| C8—C9 | 1.507 (2) | N1—O2 | 1.219 (2) |
| C8—H8A | 0.97 | N2—H1A | 0.87 (2) |
| C8—H8B | 0.97 | N3—S1 | 1.5976 (16) |
| C9—N3 | 1.4537 (19) | N3—H1 | 0.777 (18) |
| C9—H9A | 0.97 | O4—S1 | 1.4325 (11) |
| C9—H9B | 0.97 | O5—S1 | 1.4329 (12) |
| C10—C11 | 1.381 (2) | | |
| | | | |
| C2—C1—C7 | 118.18 (15) | C10—C11—C12 | 119.13 (15) |
| C2—C1—C6 | 120.72 (15) | C10—C11—H11 | 120.4 |
| C7—C1—C6 | 121.10 (15) | C12—C11—H11 | 120.4 |
| C3—C2—C1 | 120.26 (16) | C13—C12—C11 | 121.97 (16) |
| C3—C2—H2 | 119.9 | C13—C12—H12 | 119.0 |
| C1—C2—H2 | 119.9 | C11—C12—H12 | 119.0 |
| C2—C3—C4 | 120.93 (17) | C12—C13—C14 | 117.95 (15) |
| C2—C3—N1 | 118.96 (18) | C12—C13—C16 | 121.15 (18) |
| C4—C3—N1 | 120.11 (17) | C14—C13—C16 | 120.87 (17) |
| C5—C4—C3 | 119.81 (16) | C15—C14—C13 | 121.12 (16) |
| C5—C4—H4 | 120.1 | C15—C14—H14 | 119.4 |
| C3—C4—H4 | 120.1 | C13—C14—H14 | 119.4 |
| C4—C5—C6 | 122.64 (17) | C14—C15—C10 | 119.75 (16) |

| | | | |
|---|---|---|---|
| C4—C5—H5 | 118.7 | C14—C15—H15 | 120.1 |
| C6—C5—H5 | 118.7 | C10—C15—H15 | 120.1 |
| O3—C6—C5 | 122.91 (16) | C13—C16—H16A | 109.5 |
| O3—C6—C1 | 121.46 (15) | C13—C16—H16B | 109.5 |
| C5—C6—C1 | 115.63 (16) | H16A—C16—H16B | 109.5 |
| N2—C7—C1 | 124.73 (15) | C13—C16—H16C | 109.5 |
| N2—C7—H7 | 117.6 | H16A—C16—H16C | 109.5 |
| C1—C7—H7 | 117.6 | H16B—C16—H16C | 109.5 |
| N2—C8—C9 | 111.47 (12) | O1—N1—O2 | 122.7 (2) |
| N2—C8—H8A | 109.3 | O1—N1—C3 | 118.65 (18) |
| C9—C8—H8A | 109.3 | O2—N1—C3 | 118.7 (2) |
| N2—C8—H8B | 109.3 | C7—N2—C8 | 122.67 (14) |
| C9—C8—H8B | 109.3 | C7—N2—H1A | 114.1 (14) |
| H8A—C8—H8B | 108.0 | C8—N2—H1A | 123.0 (14) |
| N3—C9—C8 | 112.72 (13) | C9—N3—S1 | 123.98 (11) |
| N3—C9—H9A | 109.0 | C9—N3—H1 | 118.3 (13) |
| C8—C9—H9A | 109.0 | S1—N3—H1 | 117.4 (13) |
| N3—C9—H9B | 109.0 | O4—S1—O5 | 119.20 (8) |
| C8—C9—H9B | 109.0 | O4—S1—N3 | 107.39 (7) |
| H9A—C9—H9B | 107.8 | O5—S1—N3 | 107.26 (8) |
| C11—C10—C15 | 120.07 (14) | O4—S1—C10 | 107.82 (7) |
| C11—C10—S1 | 120.62 (11) | O5—S1—C10 | 106.12 (7) |
| C15—C10—S1 | 119.29 (12) | N3—S1—C10 | 108.74 (7) |

| | | | |
|---|---|---|---|
| C7—C1—C2—C3 | 179.67 (16) | C12—C13—C14—C15 | −0.7 (3) |
| C6—C1—C2—C3 | 0.0 (3) | C16—C13—C14—C15 | 177.35 (18) |
| C1—C2—C3—C4 | 0.2 (3) | C13—C14—C15—C10 | 0.3 (3) |
| C1—C2—C3—N1 | −179.76 (18) | C11—C10—C15—C14 | 0.1 (3) |
| C2—C3—C4—C5 | −0.4 (3) | S1—C10—C15—C14 | −178.20 (13) |
| N1—C3—C4—C5 | 179.6 (2) | C2—C3—N1—O1 | 2.3 (4) |
| C3—C4—C5—C6 | 0.3 (3) | C4—C3—N1—O1 | −177.7 (3) |
| C4—C5—C6—O3 | 180.00 (19) | C2—C3—N1—O2 | −177.8 (2) |
| C4—C5—C6—C1 | 0.0 (3) | C4—C3—N1—O2 | 2.2 (4) |
| C2—C1—C6—O3 | 179.83 (16) | C1—C7—N2—C8 | −178.27 (14) |
| C7—C1—C6—O3 | 0.2 (3) | C9—C8—N2—C7 | 96.71 (17) |
| C2—C1—C6—C5 | −0.1 (2) | C8—C9—N3—S1 | 131.22 (13) |
| C7—C1—C6—C5 | −179.75 (16) | C9—N3—S1—O4 | 14.65 (14) |
| C2—C1—C7—N2 | 179.17 (15) | C9—N3—S1—O5 | 143.88 (12) |
| C6—C1—C7—N2 | −1.2 (3) | C9—N3—S1—C10 | −101.76 (13) |
| N2—C8—C9—N3 | −63.94 (17) | C11—C10—S1—O4 | −21.41 (15) |
| C15—C10—C11—C12 | −0.1 (2) | C15—C10—S1—O4 | 156.87 (13) |
| S1—C10—C11—C12 | 178.14 (13) | C11—C10—S1—O5 | −150.18 (13) |
| C10—C11—C12—C13 | −0.3 (3) | C15—C10—S1—O5 | 28.09 (15) |
| C11—C12—C13—C14 | 0.7 (3) | C11—C10—S1—N3 | 94.72 (14) |
| C11—C12—C13—C16 | −177.38 (18) | C15—C10—S1—N3 | −87.00 (14) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H1···O3$^{i}$ | 0.78 (2) | 2.06 (2) | 2.833 (2) | 170 (2) |
| N2—H1*A*···O3 | 0.87 (2) | 1.94 (2) | 2.648 (2) | 137 (2) |

Symmetry code: (i) $x$, $-y+1/2$, $z+1/2$.