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# *N*-(2-Hydroxy-1,1-dimethylethyl)-4-methylbenzenesulfonamide

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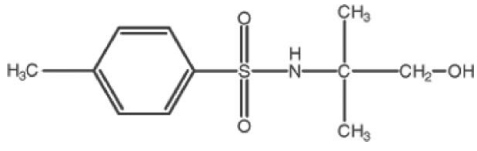
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.003 Å; disorder in main residue; $R$ factor = 0.045; $wR$ factor = 0.135; data-to-parameter ratio = 16.9.

In the title molecule, $C_{11}H_{17}NO_3S$, the S atom has a distorted tetrahedral geometry [maximum deviation: O—S—O = 119.08 (9)°]. In the crystal, molecules are connected by intermolecular N—H···O, O—H···O and C—H···O hydrogen bonds, forming layers of molecules aligned parallel to (110). The 2-methylpropan-1-ol group of the molecule is disordered over two positions with an 0.592 (4):0.408 (4) occupancy ratio.

## Related literature

For background to the biological activity of sulfonamide derivatives, see: Berredjem *et al.* (2000); Lee & Lee (2002); Soledade *et al.* (2006); Xiao & Timberlake (2000). For some of our structural studies on various sulfonamide derivatives, see: Asiri *et al.* (2009); Aziz-ur-Rehman *et al.* (2010*a*,*b*).




## Experimental

### *Crystal data*

$C_{11}H_{17}NO_3S$
$M_r$ = 243.33
Monoclinic, $P2_1/a$
$a$ = 10.4870 (3) Å
$b$ = 9.0760 (3) Å
$c$ = 13.4930 (5) Å
$\beta$ = 97.755 (2)°
$V$ = 1272.52 (7) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.25 mm$^{-1}$
$T$ = 296 K
0.27 × 0.16 × 0.11 mm

### *Data collection*

Bruker APEXII CCD diffractometer
11733 measured reflections
3116 independent reflections
2361 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.029

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.135
$S$ = 1.01
3116 reflections
184 parameters
8 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O3$A^{i}$ | 0.86 | 2.23 | 2.888 (10) | 133 |
| O3$A$—H3$A$···O1$^{ii}$ | 0.82 | 2.15 | 2.894 (12) | 151 |
| C10$A$—H10$B$···O2$^{iii}$ | 0.96 | 2.59 | 3.488 (4) | 155 |

Symmetry codes: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z$; (ii) $-x+1, -y+1, -z$; (iii) $x-\frac{1}{2}, -y+\frac{3}{2}, z$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; 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) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5093).

## References

Asiri, A. M., Akkurt, M., Khan, S. A., Arshad, M. N., Khan, I. U. & Sharif, H. M. A. (2009). *Acta Cryst.* E**65**, o1246–o1247.
Aziz-ur-Rehman, Abbas, N., Akkurt, M., Abbasi, M. A., Sharif, S. & Khan, I. U. (2010*a*). *Acta Cryst.* E**66**, o3028.
Aziz-ur-Rehman, Sajjad, M. A., Akkurt, M., Sharif, S., Abbasi, M. A. & Khan, I. U. (2010*b*). *Acta Cryst.* E**66**, o1769.
Berredjem, M., Re'gainia, Z., Djahoudi, A., Aouf, N. E., Dewinter, G. & Montero, J. L. (2000). *Phosphorus Sulfur Silicon Relat. Elem.* **165**, 249–264.
Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Lee, J. S. & Lee, C. H. (2002). *Bull. Korean Chem. Soc.* **23**, 167–169.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Soledade, M., Pedras, C. & Jha, M. (2006). *Bioorg. Med. Chem.* **14**, 4958–4979.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Xiao, Z. & Timberlake, J. W. (2000). *J. Heterocycl. Chem.* **37**, 773–777.

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# supporting information

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## *N*-(2-Hydroxy-1,1-dimethylethyl)-4-methylbenzenesulfonamide

**Aziz-ur-Rehman, Amina Yasin, Mehmet Akkurt, Nadia Abbas, Muhammad Athar Abbasi and Islam Ullah Khan**

### S1. Comment

Sulfonamide is an important functionality found in a number of synthetic as well as natural compounds and exhibiting various types of biological activity *e.g.* herbicidal, anti-malarial, anti-convulsant and anti-hypertensive (Soledade *et al.*, 2006; Xiao & Timberlake, 2000; Berredjem *et al.*, 2000; Lee & Lee, 2002) activities. As a contribution to a structural study of sulfonamide derivatives (Asiri *et al.*, 2009; Aziz-ur-Rehman *et al.*, 2010*a*,*b*;), we report here the title compound, *N*-(2-hydroxy-1,1-dimethylethyl)-4-methylbenzenesulfonamide, (I).

In the title molecule (I), (Fig. 1), the S atom has a distorted tetrahedral geometry [maximum deviation: O1—S1—O2 = 119.08 (9)°]. The molecule is twisted at the S atom, with a C1—S1—N1—C8 torsion angle of 68.22 (15)°.

The crystal packing is stabilized by intermolecular N—H···O and C—H···O hydrogen bonds, forming layers of molecules aligned parallel to the (110) lattice plane. (Table 1, Fig. 2).

### S2. Experimental

A mixture of 4-methyl benzene sulfonyl chloride (10.0 mmoles; 1.90 g), 2-amino-2-methyl propanol (10.0 mmoles; 0.95 ml), aqueous sodium carbonate (10%; 10.0 ml) and water (25 ml) was stirred for half an hour at room temperature. The crude mixture was washed with water and dried. Product was dissolved in methanol and crystallized by slow evaporation of the solvent. Yield 76%.

### S3. Refinement

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with N—H = 0.86, O—H = 0.82 and C—H = 0.93–0.97 Å and allowed to ride on their parent atoms, with $U_{iso}$(H) = 1.2$U_{eq}$(C,*N*) for CH, $CH_2$ and NH groups and 1.5$U_{eq}$(C,*O*) for OH and $CH_3$ groups. Disorder was observed with the 2-methylpropan-1-ol group of the title molecule, which was modeled in two positions with with an occupancy ratio of 0.592 (4):0.408 (4).

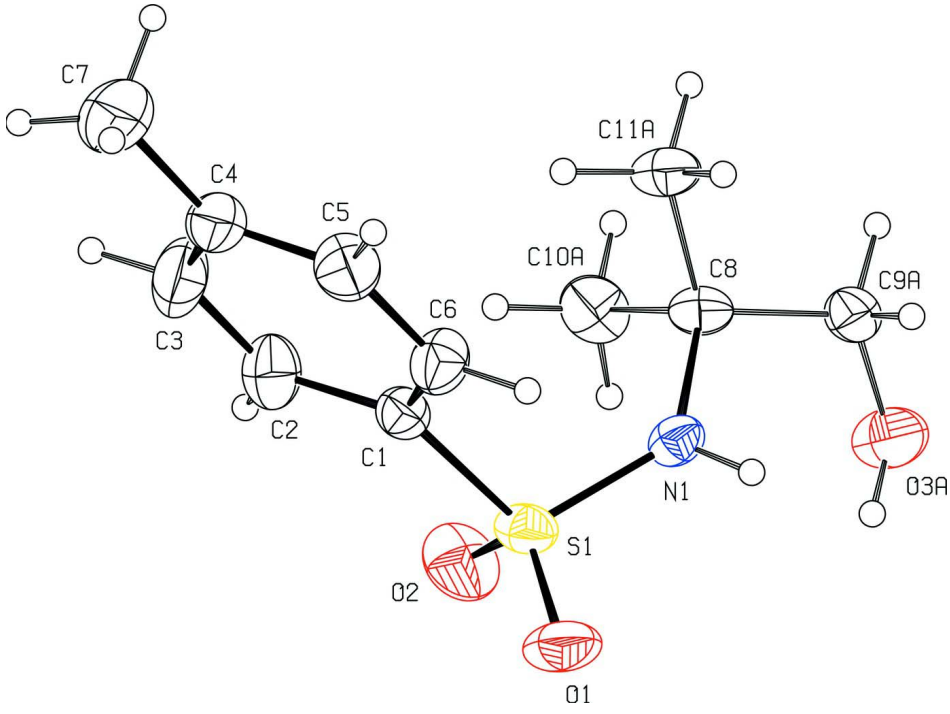


**Figure 1**

View of the major component of the disordered molecule shown with 30% probability displacement ellipsoids.

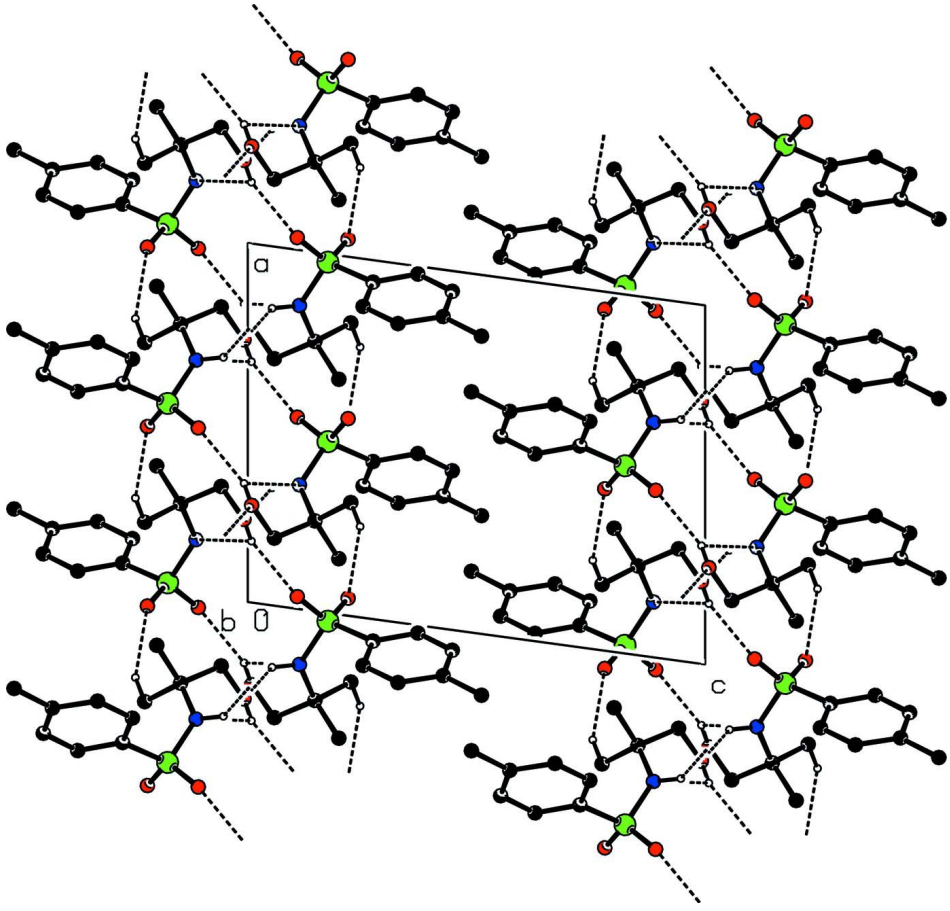


**Figure 2**

View of the packing and hydrogen bonding of (I) down the *b* axis. H atoms not involved in hydrogen bonding have been omitted for clarity and only the major component of the disorder is shown.

### *N*-(2-Hydroxy-1,1-dimethylethyl)-4-methylbenzenesulfonamide

*Crystal data*

$C_{11}H_{17}NO_3S$
$M_r = 243.33$
Monoclinic, $P2_1/a$
Hall symbol: -P 2yab
$a = 10.4870\ (3)$ Å
$b = 9.0760\ (3)$ Å
$c = 13.4930\ (5)$ Å
$\beta = 97.755\ (2)°$
$V = 1272.52\ (7)$ Å$^3$
$Z = 4$

$F(000) = 520$
$D_x = 1.270$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3805 reflections
$\theta = 2.7–28.1°$
$\mu = 0.25$ mm$^{-1}$
$T = 296$ K
Needle, colourless
0.27 × 0.16 × 0.11 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans

11733 measured reflections
3116 independent reflections
2361 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 28.3°$, $\theta_{min} = 3.2°$

$h = -13 \rightarrow 13$
$k = -11 \rightarrow 12$
$l = -18 \rightarrow 17$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.135$
$S = 1.01$
3116 reflections
184 parameters
8 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
$w = 1/[\sigma^2(F_o^2) + (0.0748P)^2 + 0.2304P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.37$ e Å$^{-3}$
$\Delta\rho_{min} = -0.31$ 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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| S1 | 0.47716 (4) | 0.43875 (5) | 0.17517 (3) | 0.0489 (2) | |
| O1 | 0.53388 (14) | 0.34471 (17) | 0.10820 (12) | 0.0738 (6) | |
| O2 | 0.54916 (15) | 0.56058 (18) | 0.21936 (14) | 0.0805 (6) | |
| O3A | 0.2711 (12) | 0.7568 (11) | 0.0084 (7) | 0.086 (3) | 0.592 (4) |
| N1 | 0.34572 (13) | 0.49570 (15) | 0.11298 (10) | 0.0417 (4) | |
| C1 | 0.43891 (15) | 0.32645 (19) | 0.27376 (12) | 0.0430 (5) | |
| C2 | 0.4783 (2) | 0.3647 (2) | 0.37187 (15) | 0.0639 (7) | |
| C3 | 0.4433 (3) | 0.2773 (3) | 0.44705 (16) | 0.0779 (9) | |
| C4 | 0.3693 (2) | 0.1524 (3) | 0.42712 (16) | 0.0672 (7) | |
| C5 | 0.3328 (2) | 0.1157 (3) | 0.32844 (17) | 0.0669 (7) | |
| C6 | 0.36707 (19) | 0.2008 (2) | 0.25219 (14) | 0.0571 (6) | |
| C7 | 0.3293 (3) | 0.0610 (4) | 0.5110 (2) | 0.1129 (14) | |
| C8 | 0.25142 (16) | 0.6009 (2) | 0.14690 (13) | 0.0469 (5) | |
| C9A | 0.1880 (3) | 0.6689 (4) | 0.0581 (2) | 0.0521 (10) | 0.592 (4) |
| C10A | 0.3165 (3) | 0.7094 (4) | 0.2253 (3) | 0.0617 (11) | 0.592 (4) |
| C11A | 0.1552 (3) | 0.5071 (4) | 0.1991 (3) | 0.0551 (11) | 0.592 (4) |
| C9B | 0.2902 (5) | 0.7615 (5) | 0.1091 (4) | 0.0577 (16) | 0.408 (4) |
| C10B | 0.1167 (5) | 0.5723 (7) | 0.0779 (5) | 0.078 (2) | 0.408 (4) |
| O3B | 0.2923 (17) | 0.7726 (13) | 0.0068 (8) | 0.060 (3) | 0.408 (4) |
| C11B | 0.2318 (7) | 0.6089 (7) | 0.2491 (4) | 0.078 (2) | 0.408 (4) |
| H1 | 0.32740 | 0.46180 | 0.05320 | 0.0500* | |
| H9A1 | 0.15060 | 0.59280 | 0.01270 | 0.0620* | 0.592 (4) |

| | | | | | |
|---|---|---|---|---|---|
| H5 | 0.28380 | 0.03130 | 0.31310 | 0.0800* | |
| H6 | 0.34180 | 0.17360 | 0.18600 | 0.0680* | |
| H7A | 0.38440 | 0.08280 | 0.57200 | 0.1690* | |
| H7B | 0.33600 | −0.04170 | 0.49540 | 0.1690* | |
| H7C | 0.24180 | 0.08370 | 0.51900 | 0.1690* | |
| H10A | 0.35700 | 0.65560 | 0.28230 | 0.0920* | 0.592 (4) |
| H10B | 0.25290 | 0.77470 | 0.24570 | 0.0920* | 0.592 (4) |
| H10C | 0.38010 | 0.76560 | 0.19680 | 0.0920* | 0.592 (4) |
| H11A | 0.19980 | 0.46320 | 0.25860 | 0.0830* | 0.592 (4) |
| H11B | 0.11900 | 0.43110 | 0.15440 | 0.0830* | 0.592 (4) |
| H11C | 0.08760 | 0.56940 | 0.21640 | 0.0830* | 0.592 (4) |
| H2 | 0.52800 | 0.44860 | 0.38710 | 0.0770* | |
| H9A2 | 0.11830 | 0.72980 | 0.07540 | 0.0620* | 0.592 (4) |
| H3 | 0.47040 | 0.30320 | 0.51320 | 0.0940* | |
| H3A | 0.32910 | 0.70550 | −0.00800 | 0.1290* | 0.592 (4) |
| H9B1 | 0.22970 | 0.83320 | 0.12860 | 0.0690* | 0.408 (4) |
| H3B | 0.34680 | 0.71640 | −0.00990 | 0.0900* | 0.408 (4) |
| H9B2 | 0.37480 | 0.78700 | 0.14320 | 0.0690* | 0.408 (4) |
| H10D | 0.13040 | 0.56780 | 0.00910 | 0.1180* | 0.408 (4) |
| H10E | 0.05830 | 0.65120 | 0.08680 | 0.1180* | 0.408 (4) |
| H10F | 0.08080 | 0.48070 | 0.09670 | 0.1180* | 0.408 (4) |
| H11D | 0.20820 | 0.51350 | 0.27130 | 0.1180* | 0.408 (4) |
| H11E | 0.16430 | 0.67800 | 0.25610 | 0.1180* | 0.408 (4) |
| H11F | 0.30980 | 0.64070 | 0.28890 | 0.1180* | 0.408 (4) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0392 (2) | 0.0492 (3) | 0.0606 (3) | −0.0009 (2) | 0.0154 (2) | 0.0076 (2) |
| O1 | 0.0678 (9) | 0.0802 (10) | 0.0825 (10) | 0.0284 (8) | 0.0431 (8) | 0.0209 (8) |
| O2 | 0.0622 (9) | 0.0712 (10) | 0.1048 (13) | −0.0276 (7) | −0.0005 (8) | 0.0140 (9) |
| O3A | 0.084 (4) | 0.093 (5) | 0.089 (4) | 0.048 (4) | 0.042 (3) | 0.051 (3) |
| N1 | 0.0492 (7) | 0.0395 (7) | 0.0386 (7) | 0.0052 (6) | 0.0139 (5) | 0.0000 (6) |
| C1 | 0.0384 (7) | 0.0445 (9) | 0.0460 (8) | 0.0031 (6) | 0.0056 (6) | 0.0023 (7) |
| C2 | 0.0726 (12) | 0.0601 (12) | 0.0549 (11) | −0.0001 (10) | −0.0058 (9) | −0.0051 (9) |
| C3 | 0.0952 (17) | 0.0927 (18) | 0.0427 (10) | 0.0160 (15) | −0.0024 (10) | 0.0014 (11) |
| C4 | 0.0581 (11) | 0.0864 (16) | 0.0589 (11) | 0.0148 (11) | 0.0144 (9) | 0.0258 (11) |
| C5 | 0.0592 (11) | 0.0678 (13) | 0.0730 (13) | −0.0125 (10) | 0.0064 (10) | 0.0181 (11) |
| C6 | 0.0628 (11) | 0.0592 (11) | 0.0482 (9) | −0.0139 (9) | 0.0038 (8) | 0.0030 (8) |
| C7 | 0.100 (2) | 0.155 (3) | 0.0892 (19) | 0.022 (2) | 0.0323 (17) | 0.066 (2) |
| C8 | 0.0437 (8) | 0.0455 (9) | 0.0548 (10) | 0.0037 (7) | 0.0184 (7) | −0.0045 (7) |
| C9A | 0.0461 (16) | 0.0575 (19) | 0.0534 (16) | 0.0148 (14) | 0.0098 (12) | 0.0115 (14) |
| C10A | 0.0620 (19) | 0.0518 (19) | 0.070 (2) | 0.0075 (15) | 0.0041 (16) | −0.0229 (16) |
| C11A | 0.0508 (17) | 0.0559 (19) | 0.064 (2) | 0.0055 (14) | 0.0272 (14) | 0.0030 (15) |
| C9B | 0.067 (3) | 0.043 (2) | 0.067 (3) | 0.011 (2) | 0.023 (2) | 0.005 (2) |
| C10B | 0.044 (3) | 0.084 (4) | 0.106 (5) | 0.012 (3) | 0.007 (3) | 0.012 (3) |
| O3B | 0.086 (6) | 0.044 (3) | 0.056 (4) | 0.021 (3) | 0.034 (3) | 0.010 (3) |
| C11B | 0.103 (5) | 0.078 (4) | 0.063 (3) | 0.039 (4) | 0.044 (3) | 0.018 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—O1 | 1.4297 (16) | C2—H2 | 0.9300 |
| S1—O2 | 1.4237 (17) | C3—H3 | 0.9300 |
| S1—N1 | 1.5997 (14) | C5—H5 | 0.9300 |
| S1—C1 | 1.7645 (17) | C6—H6 | 0.9300 |
| O3A—C9A | 1.415 (12) | C7—H7A | 0.9600 |
| O3B—C9B | 1.387 (12) | C7—H7C | 0.9600 |
| O3A—H3A | 0.8200 | C7—H7B | 0.9600 |
| O3B—H3B | 0.8200 | C9A—H9A1 | 0.9700 |
| N1—C8 | 1.490 (2) | C9A—H9A2 | 0.9700 |
| N1—H1 | 0.8600 | C9B—H9B2 | 0.9700 |
| C1—C2 | 1.377 (3) | C9B—H9B1 | 0.9700 |
| C1—C6 | 1.376 (3) | C10A—H10C | 0.9600 |
| C2—C3 | 1.376 (3) | C10A—H10A | 0.9600 |
| C3—C4 | 1.380 (4) | C10A—H10B | 0.9600 |
| C4—C5 | 1.376 (3) | C10B—H10E | 0.9600 |
| C4—C7 | 1.508 (4) | C10B—H10F | 0.9600 |
| C5—C6 | 1.373 (3) | C10B—H10D | 0.9600 |
| C8—C10B | 1.605 (6) | C11A—H11C | 0.9600 |
| C8—C11B | 1.423 (6) | C11A—H11A | 0.9600 |
| C8—C9B | 1.614 (5) | C11A—H11B | 0.9600 |
| C8—C9A | 1.430 (3) | C11B—H11D | 0.9600 |
| C8—C10A | 1.536 (4) | C11B—H11E | 0.9600 |
| C8—C11A | 1.559 (4) | C11B—H11F | 0.9600 |
| | | | |
| S1···H10A | 2.8400 | H1···H3A | 2.3600 |
| S1···H10C | 3.1600 | H1···C9B$^{i}$ | 2.9800 |
| S1···H11F | 3.0900 | H9A1···H1 | 2.2100 |
| O1···C9A$^{i}$ | 3.404 (3) | H9A1···H11B | 2.4700 |
| O1···O3A$^{ii}$ | 2.894 (12) | H2···O2 | 2.5200 |
| O1···O3B$^{ii}$ | 2.762 (15) | H9A2···H11C | 2.4500 |
| O2···C10A | 2.799 (4) | H9A2···O2$^{ix}$ | 2.8800 |
| O3A···N1 | 2.815 (10) | H9A2···H10B | 2.5600 |
| O3A···N1$^{iii}$ | 2.888 (10) | H3···H7A | 2.3700 |
| O3A···O1$^{ii}$ | 2.894 (12) | H9B1···H10E | 2.4500 |
| O3B···O1$^{ii}$ | 2.762 (15) | H9B1···H11E | 2.3900 |
| O3B···N1$^{iii}$ | 2.859 (13) | H9B1···O2$^{ix}$ | 2.5800 |
| O3B···C10B$^{iii}$ | 3.148 (14) | H3A···N1 | 2.5000 |
| O3B···N1 | 2.910 (12) | H3A···H1 | 2.3600 |
| O1···H3B$^{ii}$ | 2.0200 | H3A···O1$^{ii}$ | 2.1500 |
| O1···H3A$^{ii}$ | 2.1500 | H3B···N1 | 2.6000 |
| O1···H6 | 2.8500 | H3B···H1 | 2.4800 |
| O1···H11B$^{iv}$ | 2.7000 | H3B···O1$^{ii}$ | 2.0200 |
| O2···H2 | 2.5200 | H9B2···O2 | 2.8500 |
| O2···H10C | 2.5600 | H9B2···H11F | 2.5400 |
| O2···H11E$^{v}$ | 2.6800 | H9B2···H10E$^{v}$ | 2.2300 |
| O2···H9B2 | 2.8500 | H9B2···C10B$^{v}$ | 3.0700 |

| | | | |
|---|---|---|---|
| O2···H11F | 2.8900 | H5···H10B$^{x}$ | 2.5100 |
| O2···H5$^{iv}$ | 2.7400 | H5···O2$^{xi}$ | 2.7400 |
| O2···H10B$^{v}$ | 2.5900 | H5···H7B | 2.5300 |
| O2···H10A | 2.4500 | H6···O3A$^{i}$ | 2.8300 |
| O2···H9A2$^{v}$ | 2.8800 | H6···O1 | 2.8500 |
| O2···H9B1$^{v}$ | 2.5800 | H7A···H3 | 2.3700 |
| O3A···H10C | 2.6400 | H7A···H11E$^{vi}$ | 2.5900 |
| O3A···H6$^{iii}$ | 2.8300 | H7A···C11B$^{vi}$ | 2.8600 |
| O3A···H1 | 2.7900 | H7A···H11D$^{vi}$ | 2.5200 |
| O3A···H1$^{iii}$ | 2.2300 | H7B···H5 | 2.5300 |
| O3B···H10D$^{iii}$ | 2.8200 | H10A···S1 | 2.8400 |
| O3B···H10D | 2.5200 | H10A···H11A | 2.3900 |
| O3B···H1$^{iii}$ | 2.2100 | H10A···O2 | 2.4500 |
| O3B···H10F$^{iii}$ | 2.7900 | H10B···H9A2 | 2.5600 |
| O3B···H1 | 2.9000 | H10B···O2$^{ix}$ | 2.5900 |
| N1···O3B | 2.910 (12) | H10B···H5$^{xii}$ | 2.5100 |
| N1···O3A | 2.815 (10) | H10B···H11C | 2.5400 |
| N1···O3B$^{i}$ | 2.859 (13) | H10C···S1 | 3.1600 |
| N1···O3A$^{i}$ | 2.888 (10) | H10C···O3A | 2.6400 |
| N1···H3A | 2.5000 | H10C···O2 | 2.5600 |
| N1···H3B | 2.6000 | H10D···O3B | 2.5200 |
| C1···C11B | 3.347 (7) | H10D···H1 | 2.2800 |
| C1···C11A | 3.427 (4) | H10D···O3B$^{i}$ | 2.8200 |
| C6···C11A | 3.571 (4) | H10D···C10B$^{vii}$ | 2.9800 |
| C7···C11B$^{vi}$ | 3.411 (6) | H10D···H10F$^{vii}$ | 2.5100 |
| C9A···O1$^{iii}$ | 3.404 (3) | H10E···H9B1 | 2.4500 |
| C10A···O2 | 2.799 (4) | H10E···H11E | 2.4100 |
| C10B···C10B$^{vii}$ | 3.278 (9) | H10E···C9B$^{ix}$ | 2.9800 |
| C10B···O3B$^{i}$ | 3.148 (14) | H10E···H9B2$^{ix}$ | 2.2300 |
| C11A···C6 | 3.571 (4) | H10F···O3B$^{i}$ | 2.7900 |
| C11A···C1 | 3.427 (4) | H10F···C10B$^{vii}$ | 2.9600 |
| C11B···C1 | 3.347 (7) | H10F···H10D$^{vii}$ | 2.5100 |
| C11B···C7$^{viii}$ | 3.411 (6) | H10F···H11D | 2.5600 |
| C1···H11D | 2.9500 | H11A···H10A | 2.3900 |
| C1···H11A | 2.7800 | H11A···C1 | 2.7800 |
| C6···H11A | 2.9700 | H11A···C6 | 2.9700 |
| C7···H11D$^{vi}$ | 3.0500 | H11B···O1$^{xi}$ | 2.7000 |
| C9A···H1$^{iii}$ | 3.0500 | H11B···H9A1 | 2.4700 |
| C9B···H10E$^{v}$ | 2.9800 | H11C···H9A2 | 2.4500 |
| C9B···H1$^{iii}$ | 2.9800 | H11C···H10B | 2.5400 |
| C10B···H10D$^{vii}$ | 2.9800 | H11D···C1 | 2.9500 |
| C10B···H10F$^{vii}$ | 2.9600 | H11D···H10F | 2.5600 |
| C10B···H9B2$^{ix}$ | 3.0700 | H11D···C7$^{viii}$ | 3.0500 |
| C11B···H7A$^{viii}$ | 2.8600 | H11D···H7A$^{viii}$ | 2.5200 |
| H1···H3B | 2.4800 | H11E···H9B1 | 2.3900 |
| H1···H10D | 2.2800 | H11E···H10E | 2.4100 |
| H1···O3B | 2.9000 | H11E···H7A$^{viii}$ | 2.5900 |
| H1···C9A$^{i}$ | 3.0500 | H11E···O2$^{ix}$ | 2.6800 |

| | | | |
|---|---|---|---|
| H1···O3B$^{i}$ | 2.2100 | H11F···S1 | 3.0900 |
| H1···O3A$^{i}$ | 2.2300 | H11F···O2 | 2.8900 |
| H1···O3A | 2.7900 | H11F···H9B2 | 2.5400 |
| H1···H9A1 | 2.2100 | | |

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|---|---|---|---|
| O1—S1—O2 | 119.08 (9) | C1—C6—H6 | 120.00 |
| O1—S1—N1 | 105.30 (8) | C4—C7—H7A | 110.00 |
| O1—S1—C1 | 106.74 (9) | C4—C7—H7C | 109.00 |
| O2—S1—N1 | 109.85 (9) | H7A—C7—H7B | 110.00 |
| O2—S1—C1 | 107.13 (9) | H7A—C7—H7C | 109.00 |
| N1—S1—C1 | 108.34 (7) | H7B—C7—H7C | 109.00 |
| C9A—O3A—H3A | 110.00 | C4—C7—H7B | 109.00 |
| C9B—O3B—H3B | 109.00 | O3A—C9A—H9A1 | 109.00 |
| S1—N1—C8 | 127.33 (11) | O3A—C9A—H9A2 | 109.00 |
| S1—N1—H1 | 116.00 | C8—C9A—H9A2 | 109.00 |
| C8—N1—H1 | 116.00 | H9A1—C9A—H9A2 | 108.00 |
| S1—C1—C2 | 120.66 (14) | C8—C9A—H9A1 | 109.00 |
| S1—C1—C6 | 119.53 (13) | O3B—C9B—H9B1 | 109.00 |
| C2—C1—C6 | 119.80 (16) | O3B—C9B—H9B2 | 109.00 |
| C1—C2—C3 | 119.22 (19) | C8—C9B—H9B1 | 109.00 |
| C2—C3—C4 | 121.9 (2) | C8—C9B—H9B2 | 109.00 |
| C3—C4—C7 | 120.8 (2) | H9B1—C9B—H9B2 | 108.00 |
| C5—C4—C7 | 121.6 (2) | H10A—C10A—H10B | 109.00 |
| C3—C4—C5 | 117.6 (2) | H10A—C10A—H10C | 110.00 |
| C4—C5—C6 | 121.5 (2) | C8—C10A—H10A | 109.00 |
| C1—C6—C5 | 119.94 (18) | C8—C10A—H10B | 109.00 |
| N1—C8—C9B | 106.0 (2) | C8—C10A—H10C | 109.00 |
| N1—C8—C11B | 121.3 (3) | H10B—C10A—H10C | 110.00 |
| C9A—C8—C10A | 114.4 (2) | C8—C10B—H10D | 109.00 |
| N1—C8—C10B | 106.7 (3) | H10D—C10B—H10E | 110.00 |
| C10A—C8—C11A | 107.1 (2) | H10D—C10B—H10F | 110.00 |
| C9B—C8—C10B | 101.7 (3) | H10E—C10B—H10F | 109.00 |
| C9B—C8—C11B | 109.6 (3) | C8—C10B—H10E | 109.00 |
| C10B—C8—C11B | 109.8 (4) | C8—C10B—H10F | 109.00 |
| N1—C8—C9A | 105.79 (18) | H11B—C11A—H11C | 109.00 |
| N1—C8—C10A | 111.75 (17) | H11A—C11A—H11B | 110.00 |
| C9A—C8—C11A | 111.0 (2) | H11A—C11A—H11C | 109.00 |
| N1—C8—C11A | 106.60 (18) | C8—C11A—H11A | 109.00 |
| O3A—C9A—C8 | 113.2 (5) | C8—C11A—H11B | 109.00 |
| O3B—C9B—C8 | 114.7 (6) | C8—C11A—H11C | 109.00 |
| C3—C2—H2 | 120.00 | C8—C11B—H11D | 109.00 |
| C1—C2—H2 | 120.00 | C8—C11B—H11E | 109.00 |
| C4—C3—H3 | 119.00 | C8—C11B—H11F | 109.00 |
| C2—C3—H3 | 119.00 | H11D—C11B—H11E | 110.00 |
| C4—C5—H5 | 119.00 | H11D—C11B—H11F | 109.00 |
| C6—C5—H5 | 119.00 | H11E—C11B—H11F | 109.00 |
| C5—C6—H6 | 120.00 | | |

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|---|---|---|---|
| O1—S1—N1—C8 | −177.87 (14) | C6—C1—C2—C3 | −1.0 (3) |
| O2—S1—N1—C8 | −48.49 (17) | S1—C1—C6—C5 | −177.58 (16) |
| C1—S1—N1—C8 | 68.22 (15) | C2—C1—C6—C5 | 1.3 (3) |
| O1—S1—C1—C2 | 128.69 (16) | C1—C2—C3—C4 | −0.3 (4) |
| O1—S1—C1—C6 | −52.45 (17) | C2—C3—C4—C5 | 1.1 (4) |
| O2—S1—C1—C2 | 0.09 (18) | C2—C3—C4—C7 | −178.3 (3) |
| O2—S1—C1—C6 | 178.96 (15) | C3—C4—C5—C6 | −0.8 (4) |
| N1—S1—C1—C2 | −118.36 (15) | C7—C4—C5—C6 | 178.6 (2) |
| N1—S1—C1—C6 | 60.50 (16) | C4—C5—C6—C1 | −0.4 (3) |
| S1—N1—C8—C9A | 153.47 (18) | N1—C8—C9A—O3A | −65.4 (5) |
| S1—N1—C8—C10A | 28.3 (2) | C10A—C8—C9A—O3A | 58.1 (5) |
| S1—N1—C8—C11A | −88.3 (2) | C11A—C8—C9A—O3A | 179.4 (5) |
| S1—C1—C2—C3 | 177.89 (18) | | |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O3*A*$^{i}$ | 0.86 | 2.23 | 2.888 (10) | 133 |
| O3*A*—H3*A*···N1 | 0.82 | 2.50 | 2.815 (10) | 104 |
| O3*A*—H3*A*···O1$^{ii}$ | 0.82 | 2.15 | 2.894 (12) | 151 |
| C2—H2···O2 | 0.93 | 2.52 | 2.891 (3) | 104 |
| C10*A*—H10*A*···O2 | 0.96 | 2.45 | 2.799 (4) | 101 |
| C10*A*—H10*B*···O2$^{ix}$ | 0.96 | 2.59 | 3.488 (4) | 155 |

Symmetry codes: (i) −*x*+1/2, *y*−1/2, −*z*; (ii) −*x*+1, −*y*+1, −*z*; (ix) *x*−1/2, −*y*+3/2, *z*.