# N-(2,4-Dimethylphenyl)-2,4-dimethyl-benzenesulfonamide

## P. G. Nirmala,[a] B. Thimme Gowda,[a]* Sabine Foro[b] and Hartmut Fuess[b]

[a]Department of Chemistry, Mangalore University, Mangalagangotri 574 199, Mangalore, India, and [b]Institute of Materials Science, Darmstadt University of Technology, Petersenstrasse 23, D-64287 Darmstadt, Germany
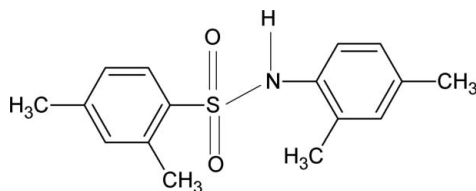Correspondence e-mail: gowdabt@yahoo.com

In the crystal structure of the title compound, $C_{16}H_{19}NO_2S$, the molecule is bent at the S atom with a $C-SO_2-NH-C$ torsion angle of 66.5 (2)°. The dihedral angle between the sulfonyl and aniline benzene rings in the molecule is 41.0 (1)°. The crystal structure features inversion dimers linked by pairs of N—H···O hydrogen bonds.

## Related literature

For the preparation of the title compound, see: Savitha & Gowda (2006). For our studies of the effect of substituents on the structures of N-(aryl)arylsulfonamides, see: Gowda *et al.* (2009a,b); Nirmala *et al.* (2010). For related structures, see: Gelbrich *et al.* (2007); Perlovich *et al.* (2006).



## Experimental

### Crystal data

$C_{16}H_{19}NO_2S$
$M_r = 289.38$
Triclinic, $P\bar{1}$
$a = 8.225$ (1) Å
$b = 8.423$ (1) Å
$c = 10.992$ (2) Å
$\alpha = 85.58$ (2)°
$\beta = 88.97$ (2)°

$\gamma = 84.43$ (1)°
$V = 755.62$ (19) Å³
$Z = 2$
Cu $K\alpha$ radiation
$\mu = 1.91$ mm$^{-1}$
$T = 299$ K
$0.40 \times 0.38 \times 0.25$ mm

### Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: $\psi$ scan (North *et al.*, 1968)
  $T_{min} = 0.516$, $T_{max} = 0.647$
2899 measured reflections

2689 independent reflections
2419 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
3 standard reflections every 120 min
  intensity decay: 1.5%

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.282$
$S = 1.36$
2689 reflections
188 parameters
1 restraint

H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.48$ e Å$^{-3}$
$\Delta\rho_{min} = -0.50$ e Å$^{-3}$

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

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---|---|---|---|---|
| N1—H1N···O1$^i$ | 0.87 (2) | 2.19 (2) | 3.024 (4) | 161 (3) |

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

Data collection: *CAD-4-PC* (Enraf–Nonius, 1996); cell refinement: *CAD-4-PC*; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

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**supplementary materials**

## *N*-(2,4-Dimethylphenyl)-2,4-dimethylbenzenesulfonamide

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### Comment

In the present work, as part of a study of substituent effects on the structures of *N*-(aryl)arylsulfonamides (Gowda *et al.*, 2009*a*,*b*; Nirmala *et al.*, 2010), the structure of 2,4-dimethyl-*N*-(2,4-dimethylphenyl)benzenesulfonamide (I) has been determined (Fig. 1). The molecule in (I) is bent at the S atom with the C—SO$_2$—NH—C torsion angle of 66.5 (2)°, compared to the values of 70.1 (2) and -66.0 (2)° in the two independent molecules of 2,4-dimethyl-*N*-(2,3-dimethylphenyl)benzenesulfonamide (II) (Nirmala *et al.*, 2010), 53.9 (2)° in 2,4-dimethyl-*N*-(3,5-dimethylphenyl)benzenesulfonamide (III) (Gowda *et al.*, 2009*b*) and 46.1 (3)° (glide image of molecule 1) and 47.7 (3)° (molecule 2) in the two independent molecules of 2,4-dimethyl-*N*-(phenyl)benzenesulfonamide (IV)(Gowda *et al.*, 2009*a*).

The sulfonyl and the anilino benzene rings in (I) are tilted relative to each other by 41.0 (1)°, compared to the values of 41.5 (1) and 43.8 (1)° in the two molecules of (II), 82.1 (1)° in (III) and 67.5 (1)° (molecule 1) and 72.9 (1)° (molecule 2) in (IV),

The remaining bond parameters in (I) are similar to those observed in (II), (III), (IV) and other aryl sulfonamides (Perlovich *et al.*, 2006; Gelbrich *et al.*, 2007). The crystal packing of molecules in (I) through pairs of N—H···O(S) hydrogen bonds (Table 1) is shown in Fig. 2.

### Experimental

The solution of *m*-xylene (10 ml) in chloroform (40 ml) was treated dropwise with chlorosulfonic acid (25 ml) at 0° C. After the initial evolution of hydrogen chloride subsided, the reaction mixture was brought to room temperature and poured into crushed ice in a beaker. The chloroform layer was separated, washed with cold water and allowed to evaporate slowly. The residual 2,4-dimethylbenzenesulfonylchloride was treated with 2,4-dimethylaniline in the stoichiometric ratio and boiled for ten minutes. The reaction mixture was then cooled to room temperature and added to ice cold water (100 ml). The resultant solid 2,4-dimethyl-*N*-(2,4-dimethylphenyl)benzenesulfonamide was filtered under suction and washed thoroughly with cold water. It was then recrystallized to constant melting point from dilute ethanol. The purity of the compound was checked and characterized by recording its infrared and NMR spectra (Savitha & Gowda, 2006). Prism like brown single crystals used in X-ray diffraction studies were grown in ethanolic solution by slow evaporation at room temperature.

### Refinement

The H atom of the NH group was located in a difference map and later restrained to N—H = 0.86 (2) Å. The other H atoms were positioned with idealized geometry using a riding model [C—H = 0.93–0.96 Å]. All H atoms were refined with isotropic displacement parameters (set to 1.2 times of the $U_{eq}$ of the parent atom).
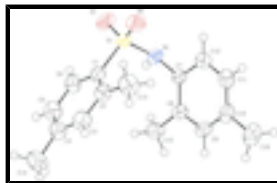
# supplementary materials

**Figures**



Fig. 1. Molecular structure of (I), showing the atom-labelling scheme and displacement ellipsoids are drawn at the 50% probability level.
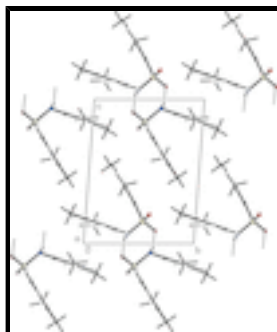


Fig. 2. Molecular packing of (I), with hydrogen bonding shown as dashed lines.

## *N*-(2,4-Dimethylphenyl)-2,4-dimethylbenzenesulfonamide

*Crystal data*

| | |
|---|---|
| $C_{16}H_{19}NO_2S$ | $Z = 2$ |
| $M_r = 289.38$ | $F(000) = 308$ |
| Triclinic, $P\bar{1}$ | $D_x = 1.272$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Cu $K\alpha$ radiation, $\lambda = 1.54180$ Å |
| $a = 8.225$ (1) Å | Cell parameters from 25 reflections |
| $b = 8.423$ (1) Å | $\theta = 7.8–18.8°$ |
| $c = 10.992$ (2) Å | $\mu = 1.91$ mm$^{-1}$ |
| $\alpha = 85.58$ (2)° | $T = 299$ K |
| $\beta = 88.97$ (2)° | Prism, brown |
| $\gamma = 84.43$ (1)° | $0.40 \times 0.38 \times 0.25$ mm |
| $V = 755.62$ (19) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Enraf–Nonius CAD-4 diffractometer | 2419 reflections with $I > 2\sigma(I)$ |
| Radiation source: fine-focus sealed tube | $R_{int} = 0.026$ |
| graphite | $\theta_{max} = 67.1°$, $\theta_{min} = 4.0°$ |
| $\omega/2\theta$ scans | $h = -9 \rightarrow 9$ |
| Absorption correction: $\psi$ scan (North *et al.*, 1968) | $k = -10 \rightarrow 10$ |
| $T_{min} = 0.516$, $T_{max} = 0.647$ | $l = -13 \rightarrow 1$ |
| 2899 measured reflections | 3 standard reflections every 120 min |
| 2689 independent reflections | intensity decay: 1.5% |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.058$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.282$ | H atoms treated by a mixture of independent and constrained refinement |
| $S = 1.36$ | $w = 1/[\sigma^2(F_o^2) + (0.2P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 2689 reflections | $(\Delta/\sigma)_{max} = 0.002$ |
| 188 parameters | $\Delta\rho_{max} = 0.48$ e Å$^{-3}$ |
| 1 restraint | $\Delta\rho_{min} = -0.50$ e Å$^{-3}$ |

*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 $F^2 > \sigma(F^2)$ 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 | 0.4299 (4) | 0.5647 (3) | 0.7203 (3) | 0.0402 (7) |
| C2 | 0.3552 (4) | 0.6498 (4) | 0.6195 (3) | 0.0452 (8) |
| C3 | 0.4587 (5) | 0.7247 (5) | 0.5349 (3) | 0.0558 (9) |
| H3 | 0.4125 | 0.7809 | 0.4658 | 0.067* |
| C4 | 0.6233 (5) | 0.7190 (5) | 0.5491 (3) | 0.0544 (9) |
| C5 | 0.6937 (5) | 0.6310 (5) | 0.6489 (3) | 0.0555 (9) |
| H5 | 0.8064 | 0.6230 | 0.6586 | 0.067* |
| C6 | 0.5975 (4) | 0.5549 (4) | 0.7343 (3) | 0.0482 (8) |
| H6 | 0.6455 | 0.4965 | 0.8019 | 0.058* |
| C7 | 0.1553 (3) | 0.7468 (3) | 0.9002 (2) | 0.0349 (7) |
| C8 | 0.2064 (4) | 0.8968 (3) | 0.8660 (3) | 0.0376 (7) |
| C9 | 0.0873 (4) | 1.0200 (4) | 0.8323 (3) | 0.0440 (7) |
| H9 | 0.1186 | 1.1217 | 0.8109 | 0.053* |
| C10 | −0.0762 (4) | 0.9960 (4) | 0.8295 (3) | 0.0466 (8) |
| C11 | −0.1231 (4) | 0.8477 (4) | 0.8650 (3) | 0.0507 (8) |
| H11 | −0.2332 | 0.8310 | 0.8649 | 0.061* |
| C12 | −0.0100 (4) | 0.7242 (4) | 0.9006 (3) | 0.0462 (8) |

| | | | | |
|---|---|---|---|---|
| H12 | −0.0436 | 0.6243 | 0.9253 | 0.055* |
| C13 | 0.1763 (5) | 0.6667 (6) | 0.5928 (4) | 0.0643 (10) |
| H13A | 0.1163 | 0.7044 | 0.6623 | 0.077* |
| H13B | 0.1430 | 0.5648 | 0.5755 | 0.077* |
| H13C | 0.1549 | 0.7419 | 0.5235 | 0.077* |
| C14 | 0.7272 (7) | 0.8078 (6) | 0.4575 (4) | 0.0820 (14) |
| H14A | 0.6587 | 0.8646 | 0.3956 | 0.098* |
| H14B | 0.8048 | 0.7329 | 0.4206 | 0.098* |
| H14C | 0.7843 | 0.8823 | 0.4981 | 0.098* |
| C15 | 0.3816 (4) | 0.9290 (4) | 0.8660 (3) | 0.0517 (9) |
| H15A | 0.4333 | 0.8978 | 0.7913 | 0.062* |
| H15B | 0.4356 | 0.8689 | 0.9339 | 0.062* |
| H15C | 0.3887 | 1.0411 | 0.8725 | 0.062* |
| C16 | −0.1989 (5) | 1.1362 (5) | 0.7893 (4) | 0.0717 (12) |
| H16A | −0.1420 | 1.2219 | 0.7519 | 0.086* |
| H16B | −0.2595 | 1.1723 | 0.8591 | 0.086* |
| H16C | −0.2726 | 1.1029 | 0.7317 | 0.086* |
| N1 | 0.2700 (3) | 0.6121 (3) | 0.9369 (2) | 0.0397 (7) |
| H1N | 0.363 (3) | 0.632 (4) | 0.966 (3) | 0.048* |
| O1 | 0.4329 (3) | 0.3611 (3) | 0.9106 (2) | 0.0548 (7) |
| O2 | 0.1751 (3) | 0.4227 (3) | 0.7989 (2) | 0.0556 (7) |
| S1 | 0.32074 (8) | 0.47490 (7) | 0.84308 (6) | 0.0403 (4) |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0449 (16) | 0.0342 (15) | 0.0406 (15) | 0.0018 (12) | 0.0016 (12) | −0.0038 (12) |
| C2 | 0.0482 (17) | 0.0451 (17) | 0.0413 (16) | 0.0014 (13) | −0.0062 (13) | −0.0042 (13) |
| C3 | 0.068 (2) | 0.059 (2) | 0.0377 (16) | 0.0034 (17) | −0.0005 (15) | 0.0034 (14) |
| C4 | 0.059 (2) | 0.059 (2) | 0.0459 (17) | −0.0082 (16) | 0.0117 (15) | −0.0051 (15) |
| C5 | 0.0485 (18) | 0.063 (2) | 0.055 (2) | −0.0048 (16) | 0.0004 (15) | −0.0073 (17) |
| C6 | 0.0426 (16) | 0.054 (2) | 0.0461 (17) | 0.0023 (13) | −0.0020 (13) | −0.0024 (14) |
| C7 | 0.0395 (14) | 0.0278 (13) | 0.0361 (14) | 0.0007 (10) | −0.0008 (11) | 0.0006 (10) |
| C8 | 0.0445 (16) | 0.0305 (14) | 0.0379 (14) | −0.0048 (11) | −0.0019 (11) | −0.0021 (11) |
| C9 | 0.0565 (18) | 0.0344 (15) | 0.0394 (15) | −0.0006 (13) | −0.0021 (13) | 0.0030 (12) |
| C10 | 0.0490 (17) | 0.0496 (18) | 0.0382 (15) | 0.0114 (14) | −0.0028 (13) | −0.0039 (13) |
| C11 | 0.0373 (15) | 0.060 (2) | 0.0546 (19) | −0.0009 (14) | 0.0004 (13) | −0.0073 (15) |
| C12 | 0.0450 (17) | 0.0396 (16) | 0.0548 (18) | −0.0091 (13) | 0.0068 (14) | −0.0035 (13) |
| C13 | 0.051 (2) | 0.083 (3) | 0.057 (2) | 0.0006 (18) | −0.0143 (16) | 0.0042 (19) |
| C14 | 0.093 (3) | 0.085 (3) | 0.068 (3) | −0.021 (3) | 0.028 (2) | 0.003 (2) |
| C15 | 0.0484 (18) | 0.0418 (18) | 0.066 (2) | −0.0129 (14) | −0.0079 (15) | 0.0005 (15) |
| C16 | 0.066 (2) | 0.071 (3) | 0.069 (2) | 0.027 (2) | −0.0035 (19) | 0.011 (2) |
| N1 | 0.0447 (14) | 0.0315 (13) | 0.0412 (13) | 0.0011 (11) | −0.0033 (10) | 0.0035 (10) |
| O1 | 0.0646 (15) | 0.0334 (12) | 0.0617 (15) | 0.0110 (11) | −0.0033 (12) | 0.0080 (10) |
| O2 | 0.0544 (14) | 0.0451 (13) | 0.0700 (16) | −0.0142 (11) | −0.0020 (11) | −0.0086 (11) |
| S1 | 0.0460 (6) | 0.0271 (6) | 0.0469 (6) | −0.0010 (3) | −0.0018 (4) | 0.0014 (3) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—C6 | 1.384 (4) | C10—C16 | 1.520 (4) |
| C1—C2 | 1.391 (4) | C11—C12 | 1.365 (5) |
| C1—S1 | 1.769 (3) | C11—H11 | 0.9300 |
| C2—C3 | 1.404 (5) | C12—H12 | 0.9300 |
| C2—C13 | 1.497 (5) | C13—H13A | 0.9600 |
| C3—C4 | 1.362 (6) | C13—H13B | 0.9600 |
| C3—H3 | 0.9300 | C13—H13C | 0.9600 |
| C4—C5 | 1.380 (5) | C14—H14A | 0.9600 |
| C4—C14 | 1.510 (5) | C14—H14B | 0.9600 |
| C5—C6 | 1.378 (5) | C14—H14C | 0.9600 |
| C5—H5 | 0.9300 | C15—H15A | 0.9600 |
| C6—H6 | 0.9300 | C15—H15B | 0.9600 |
| C7—C12 | 1.390 (4) | C15—H15C | 0.9600 |
| C7—C8 | 1.392 (4) | C16—H16A | 0.9600 |
| C7—N1 | 1.441 (3) | C16—H16B | 0.9600 |
| C8—C9 | 1.389 (4) | C16—H16C | 0.9600 |
| C8—C15 | 1.492 (4) | N1—S1 | 1.627 (3) |
| C9—C10 | 1.380 (5) | N1—H1N | 0.869 (19) |
| C9—H9 | 0.9300 | O1—S1 | 1.436 (2) |
| C10—C11 | 1.369 (5) | O2—S1 | 1.421 (3) |
| C6—C1—C2 | 121.0 (3) | C7—C12—H12 | 119.8 |
| C6—C1—S1 | 115.3 (2) | C2—C13—H13A | 109.5 |
| C2—C1—S1 | 123.6 (2) | C2—C13—H13B | 109.5 |
| C1—C2—C3 | 116.4 (3) | H13A—C13—H13B | 109.5 |
| C1—C2—C13 | 126.0 (3) | C2—C13—H13C | 109.5 |
| C3—C2—C13 | 117.6 (3) | H13A—C13—H13C | 109.5 |
| C4—C3—C2 | 123.2 (3) | H13B—C13—H13C | 109.5 |
| C4—C3—H3 | 118.4 | C4—C14—H14A | 109.5 |
| C2—C3—H3 | 118.4 | C4—C14—H14B | 109.5 |
| C3—C4—C5 | 118.8 (3) | H14A—C14—H14B | 109.5 |
| C3—C4—C14 | 120.7 (4) | C4—C14—H14C | 109.5 |
| C5—C4—C14 | 120.5 (4) | H14A—C14—H14C | 109.5 |
| C6—C5—C4 | 120.2 (3) | H14B—C14—H14C | 109.5 |
| C6—C5—H5 | 119.9 | C8—C15—H15A | 109.5 |
| C4—C5—H5 | 119.9 | C8—C15—H15B | 109.5 |
| C5—C6—C1 | 120.4 (3) | H15A—C15—H15B | 109.5 |
| C5—C6—H6 | 119.8 | C8—C15—H15C | 109.5 |
| C1—C6—H6 | 119.8 | H15A—C15—H15C | 109.5 |
| C12—C7—C8 | 120.2 (3) | H15B—C15—H15C | 109.5 |
| C12—C7—N1 | 118.3 (3) | C10—C16—H16A | 109.5 |
| C8—C7—N1 | 121.5 (3) | C10—C16—H16B | 109.5 |
| C9—C8—C7 | 117.7 (3) | H16A—C16—H16B | 109.5 |
| C9—C8—C15 | 119.7 (3) | C10—C16—H16C | 109.5 |
| C7—C8—C15 | 122.6 (3) | H16A—C16—H16C | 109.5 |
| C10—C9—C8 | 122.0 (3) | H16B—C16—H16C | 109.5 |
| C10—C9—H9 | 119.0 | C7—N1—S1 | 120.14 (19) |

| | | | |
|---|---|---|---|
| C8—C9—H9 | 119.0 | C7—N1—H1N | 118 (3) |
| C11—C10—C9 | 119.0 (3) | S1—N1—H1N | 103 (2) |
| C11—C10—C16 | 122.1 (3) | O2—S1—O1 | 118.85 (15) |
| C9—C10—C16 | 118.9 (3) | O2—S1—N1 | 108.21 (14) |
| C12—C11—C10 | 120.7 (3) | O1—S1—N1 | 104.49 (13) |
| C12—C11—H11 | 119.6 | O2—S1—C1 | 109.49 (15) |
| C10—C11—H11 | 119.6 | O1—S1—C1 | 107.90 (14) |
| C11—C12—C7 | 120.4 (3) | N1—S1—C1 | 107.29 (13) |
| C11—C12—H12 | 119.8 | | |
| C6—C1—C2—C3 | −0.4 (5) | C8—C9—C10—C11 | 2.3 (5) |
| S1—C1—C2—C3 | 174.9 (2) | C8—C9—C10—C16 | −178.9 (3) |
| C6—C1—C2—C13 | 178.8 (3) | C9—C10—C11—C12 | −1.2 (5) |
| S1—C1—C2—C13 | −5.9 (5) | C16—C10—C11—C12 | −180.0 (3) |
| C1—C2—C3—C4 | −1.1 (5) | C10—C11—C12—C7 | −0.6 (5) |
| C13—C2—C3—C4 | 179.6 (4) | C8—C7—C12—C11 | 1.5 (5) |
| C2—C3—C4—C5 | 2.4 (6) | N1—C7—C12—C11 | −179.1 (3) |
| C2—C3—C4—C14 | −177.4 (3) | C12—C7—N1—S1 | 77.6 (3) |
| C3—C4—C5—C6 | −2.1 (6) | C8—C7—N1—S1 | −103.0 (3) |
| C14—C4—C5—C6 | 177.7 (4) | C7—N1—S1—O2 | −51.5 (3) |
| C4—C5—C6—C1 | 0.6 (5) | C7—N1—S1—O1 | −179.1 (2) |
| C2—C1—C6—C5 | 0.7 (5) | C7—N1—S1—C1 | 66.5 (2) |
| S1—C1—C6—C5 | −175.0 (2) | C6—C1—S1—O2 | −151.7 (3) |
| C12—C7—C8—C9 | −0.4 (4) | C2—C1—S1—O2 | 32.7 (3) |
| N1—C7—C8—C9 | −179.8 (2) | C6—C1—S1—O1 | −21.0 (3) |
| C12—C7—C8—C15 | 178.9 (3) | C2—C1—S1—O1 | 163.4 (3) |
| N1—C7—C8—C15 | −0.6 (4) | C6—C1—S1—N1 | 91.0 (3) |
| C7—C8—C9—C10 | −1.5 (4) | C2—C1—S1—N1 | −84.5 (3) |
| C15—C8—C9—C10 | 179.2 (3) | | |

*Hydrogen-bond geometry (Å, °)*

| D—H···A | D—H | H···A | D···A | D—H···A |
|---|---|---|---|---|
| N1—H1N···O1<sup>i</sup> | 0.87 (2) | 2.19 (2) | 3.024 (4) | 161 (3) |

Symmetry codes: (i) −x+1, −y+1, −z+2.

**Fig. 1**

**Fig. 2**