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N-[3-(Benzenesulfonamido)propyl]-benzenesulfonamide

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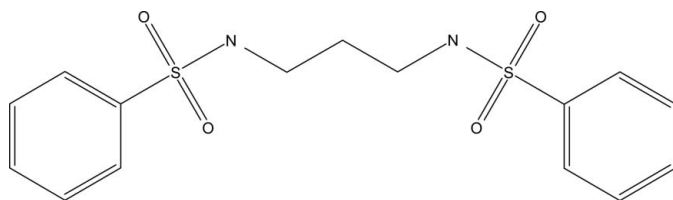
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.010$ Å; R factor = 0.069; wR factor = 0.181; data-to-parameter ratio = 15.8.

In the title compound, $\text{C}_{15}\text{H}_{18}\text{N}_2\text{O}_4\text{S}_2$, the dihedral angle between the aromatic rings is $71.8(2)^\circ$. The conformation of the central $\text{N}-\text{C}-\text{C}-\text{N}$ fragment is *gauche-gauche* [torsion angles = $72.5(5)$ and $65.7(5)^\circ$]. Both N atoms adopt pyramidal geometries. In the crystal, molecules are linked by $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds, generating (001) sheets, and weak $\text{C}-\text{H}\cdots\text{O}$ interactions consolidate the packing.

Related literature

For a related structure, see: Linden & Bienz (1999).



Experimental

Crystal data

 $\text{C}_{15}\text{H}_{18}\text{N}_2\text{O}_4\text{S}_2$
 $M_r = 354.43$ Orthorhombic, $Pbca$
 $a = 9.2650(13)$ Å $b = 16.402(2)$ Å
 $c = 22.740(3)$ Å
 $V = 3455.5(8)$ Å³
 $Z = 8$ Mo $K\alpha$ radiation
 $\mu = 0.33$ mm⁻¹
 $T = 296$ K
 $0.40 \times 0.20 \times 0.20$ mm

Data collection

Bruker APEXII CCD
diffractometer
13896 measured reflections3393 independent reflections
1607 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.091$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.069$
 $wR(F^2) = 0.181$
 $S = 1.03$
3393 reflections
215 parametersH atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.23$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.35$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|--|--------------|--------------------|-------------|----------------------|
| $\text{N1}-\text{H1}\cdots\text{O4}^{\text{i}}$ | 0.82 (4) | 2.15 (5) | 2.954 (6) | 164 (4) |
| $\text{N2}-\text{H2}\cdots\text{O3}^{\text{ii}}$ | 0.74 (4) | 2.15 (4) | 2.836 (4) | 154 (5) |
| $\text{C9}-\text{H9B}\cdots\text{O4}^{\text{iii}}$ | 0.97 | 2.51 | 3.430 (5) | 158 |
| $\text{C13}-\text{H13}\cdots\text{O1}^{\text{iv}}$ | 0.93 | 2.42 | 3.276 (8) | 153 |

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

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* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2431).

References

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supplementary materials

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***N*-[3-(Benzenesulfonamido)propyl]benzenesulfonamide**

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Comment

The title compound, (I), complements *N*-{4-[(benzenesulfonyl)amino]butyl}benzenesulfonamide, C₁₆H₂₀N₂O₄S₂ (Linden & Bienz, 1999), (II), with a propyl chain in (I) replacing the butyl chain in (II).

In (I) (Fig. 1), the dihedral angle between the aromatic rings is 71.8 (2)°. The conformation of the central N—C—C—N chain linking the two S atoms can be described as *gauche-gauche* in terms of the N1—C7—C8—C9 and C7—C8—C9—N2 torsion angles of 72.5 (5) and 65.7 (5)°, respectively. Both N atoms in (I) are clearly in pyramidal coordination geometries, implying that the lone pairs on the N atoms are not conjugated with their adjacent benzene sulfonyl groups. A similar situation was observed in (II).

In the crystal of (I), the molecules are linked by N—H···O hydrogen bonds (Table 1). Considered separately, the N1 bond leads to [010] C(8) chains and the N2 bond generates [100] C(4) chains. Both the acceptor O atoms are part of the same (atom S2) sulfonyl group: it is perhaps notable that these O atoms have significantly smaller U_{eq} values than the O atoms in the other (atom S1) sulfonyl group that do not accept a hydrogen bond. Overall, (001) sheets arise from the N—H···O hydrogen bonds in (I) and weak C—H···O links consolidate the packing.

The complete molecule of (II) is generated by inversion symmetry and therefore the conformation of the central alkyl chain is all-*trans* and the dihedral angle between the aromatic rings is constrained to be zero by symmetry.

Experimental

A mixture of 1,3-diaminopropane (0.0067 mol, 0.561 ml) and benzene sulfonyl chloride (0.0135 mol, 1.72 ml), was stirred in 15 ml of distilled water, while maintaining the pH of the reaction mixture at 9 using 3% sodium carbonate. The progress of the reaction was checked by TLC. On completion, the precipitate obtained was filtered, washed with water and finally dried. Colourless blocks of (I) were grown from methanol by slow evaporation.

Refinement

The N-bound H atoms were located in difference maps and their positions were freely refined with the constraint $U_{iso}(H) = 1.2U_{eq}(N)$. The C-bound H atoms were placed at idealised positions and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

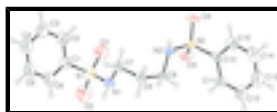


Fig. 1. The molecular structure of (I) with displacement ellipsoids drawn at the 50% probability level.

N-[3-(Benzenesulfonamido)propyl]benzenesulfonamide

Crystal data

| | |
|--------------------------------|---|
| $C_{15}H_{18}N_2O_4S_2$ | $F(000) = 1488$ |
| $M_r = 354.43$ | $D_x = 1.363 \text{ Mg m}^{-3}$ |
| Orthorhombic, <i>Pbca</i> | Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$ |
| Hall symbol: -P 2ac 2ab | Cell parameters from 2014 reflections |
| $a = 9.2650 (13) \text{ \AA}$ | $\theta = 2.6\text{--}21.2^\circ$ |
| $b = 16.402 (2) \text{ \AA}$ | $\mu = 0.33 \text{ mm}^{-1}$ |
| $c = 22.740 (3) \text{ \AA}$ | $T = 296 \text{ K}$ |
| $V = 3455.5 (8) \text{ \AA}^3$ | Prism, colourless |
| $Z = 8$ | $0.40 \times 0.20 \times 0.20 \text{ mm}$ |

Data collection

| | |
|--|--|
| Bruker APEXII CCD diffractometer | 1607 reflections with $I > 2\sigma(I)$ |
| Radiation source: fine-focus sealed tube | $R_{\text{int}} = 0.091$ |
| graphite | $\theta_{\text{max}} = 26.0^\circ$, $\theta_{\text{min}} = 2.5^\circ$ |
| ω scans | $h = -5 \rightarrow 11$ |
| 13896 measured reflections | $k = -18 \rightarrow 20$ |
| 3393 independent reflections | $l = -28 \rightarrow 27$ |

Refinement

| | |
|---------------------------------|--|
| Refinement on F^2 | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.069$ | Hydrogen site location: difmap (N-H) and geom (C-H) |
| $wR(F^2) = 0.181$ | H atoms treated by a mixture of independent and constrained refinement |
| $S = 1.03$ | $w = 1/[\sigma^2(F_o^2) + (0.0722P)^2 + 0.3591P]$ |
| 3393 reflections | where $P = (F_o^2 + 2F_c^2)/3$ |
| 215 parameters | $(\Delta/\sigma)_{\text{max}} < 0.001$ |
| 0 restraints | $\Delta\rho_{\text{max}} = 0.23 \text{ e \AA}^{-3}$ |
| | $\Delta\rho_{\text{min}} = -0.35 \text{ e \AA}^{-3}$ |

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 $F^2 > 2\sigma(F^2)$ 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)

| | x | y | z | U_{iso}^*/U_{eq} |
|-----|--------------|--------------|--------------|--------------------|
| C1 | 0.1983 (7) | 0.4365 (4) | 0.3462 (2) | 0.0749 (16) |
| C2 | 0.0703 (9) | 0.4669 (4) | 0.3255 (3) | 0.102 (2) |
| H2A | 0.0580 | 0.5230 | 0.3219 | 0.123* |
| C3 | -0.0417 (9) | 0.4144 (6) | 0.3098 (3) | 0.124 (3) |
| H3A | -0.1276 | 0.4354 | 0.2950 | 0.148* |
| C4 | -0.0255 (10) | 0.3346 (5) | 0.3158 (3) | 0.118 (3) |
| H4A | -0.1004 | 0.2997 | 0.3053 | 0.141* |
| C5 | 0.0988 (12) | 0.3034 (4) | 0.3372 (3) | 0.118 (3) |
| H5 | 0.1090 | 0.2473 | 0.3414 | 0.142* |
| C6 | 0.2110 (8) | 0.3546 (4) | 0.3528 (3) | 0.102 (2) |
| H6 | 0.2958 | 0.3327 | 0.3679 | 0.123* |
| C7 | 0.1906 (5) | 0.5379 (3) | 0.4664 (2) | 0.0624 (13) |
| H7A | 0.1191 | 0.4948 | 0.4645 | 0.075* |
| H7B | 0.1539 | 0.5845 | 0.4447 | 0.075* |
| C8 | 0.2153 (5) | 0.5616 (3) | 0.5296 (2) | 0.0603 (13) |
| H8A | 0.1224 | 0.5666 | 0.5489 | 0.072* |
| H8B | 0.2677 | 0.5179 | 0.5489 | 0.072* |
| C9 | 0.2973 (4) | 0.6398 (2) | 0.5381 (2) | 0.0556 (12) |
| H9A | 0.3180 | 0.6476 | 0.5795 | 0.067* |
| H9B | 0.3883 | 0.6371 | 0.5171 | 0.067* |
| C10 | 0.3019 (4) | 0.8225 (2) | 0.5942 (2) | 0.0490 (11) |
| C11 | 0.4299 (5) | 0.7968 (3) | 0.6201 (2) | 0.0680 (14) |
| H11 | 0.5002 | 0.7705 | 0.5980 | 0.082* |
| C12 | 0.4507 (8) | 0.8108 (4) | 0.6785 (3) | 0.096 (2) |
| H12 | 0.5355 | 0.7930 | 0.6963 | 0.116* |
| C13 | 0.3495 (10) | 0.8504 (5) | 0.7115 (3) | 0.106 (2) |
| H13 | 0.3650 | 0.8589 | 0.7514 | 0.128* |
| C14 | 0.2258 (8) | 0.8775 (3) | 0.6857 (3) | 0.095 (2) |
| H14 | 0.1585 | 0.9061 | 0.7079 | 0.114* |
| C15 | 0.1992 (6) | 0.8627 (3) | 0.6261 (3) | 0.0738 (15) |
| H15 | 0.1136 | 0.8798 | 0.6087 | 0.089* |
| S1 | 0.33690 (18) | 0.50195 (11) | 0.36927 (6) | 0.0851 (5) |
| S2 | 0.27067 (10) | 0.79981 (7) | 0.52013 (5) | 0.0495 (4) |
| N1 | 0.3261 (4) | 0.5097 (3) | 0.43942 (19) | 0.0622 (12) |
| H1 | 0.349 (5) | 0.466 (3) | 0.455 (2) | 0.064 (17)* |
| N2 | 0.2115 (3) | 0.7085 (2) | 0.51605 (18) | 0.0547 (10) |
| H2 | 0.135 (5) | 0.708 (3) | 0.525 (2) | 0.066* |
| O1 | 0.3051 (5) | 0.5811 (3) | 0.34561 (18) | 0.1226 (17) |
| O2 | 0.4721 (5) | 0.4642 (3) | 0.35702 (17) | 0.1228 (17) |
| O3 | 0.4064 (3) | 0.8029 (2) | 0.49056 (13) | 0.0654 (9) |

supplementary materials

O4 0.1556 (3) 0.85005 (18) 0.49911 (14) 0.0637 (9)

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|--------------|-------------|
| C1 | 0.106 (5) | 0.064 (4) | 0.054 (3) | -0.007 (3) | 0.002 (3) | 0.011 (3) |
| C2 | 0.140 (6) | 0.064 (4) | 0.104 (5) | -0.017 (4) | -0.029 (5) | 0.018 (3) |
| C3 | 0.137 (7) | 0.110 (7) | 0.125 (6) | -0.012 (5) | -0.049 (5) | -0.002 (5) |
| C4 | 0.170 (8) | 0.086 (6) | 0.097 (5) | -0.031 (6) | -0.025 (5) | -0.008 (4) |
| C5 | 0.202 (9) | 0.059 (5) | 0.093 (5) | -0.010 (6) | -0.022 (6) | -0.010 (4) |
| C6 | 0.144 (6) | 0.072 (5) | 0.090 (4) | 0.001 (5) | -0.016 (4) | -0.009 (4) |
| C7 | 0.051 (3) | 0.048 (3) | 0.088 (4) | -0.005 (2) | -0.003 (3) | -0.006 (3) |
| C8 | 0.053 (3) | 0.045 (3) | 0.083 (4) | -0.003 (2) | 0.002 (3) | 0.005 (2) |
| C9 | 0.044 (2) | 0.046 (3) | 0.077 (3) | 0.005 (2) | -0.013 (2) | 0.000 (2) |
| C10 | 0.045 (3) | 0.033 (2) | 0.068 (3) | 0.0005 (19) | 0.009 (2) | 0.000 (2) |
| C11 | 0.055 (3) | 0.067 (4) | 0.082 (4) | 0.005 (3) | -0.008 (3) | -0.011 (3) |
| C12 | 0.103 (5) | 0.098 (5) | 0.088 (5) | -0.012 (4) | -0.021 (4) | -0.020 (4) |
| C13 | 0.144 (7) | 0.089 (5) | 0.086 (5) | -0.015 (5) | -0.001 (5) | -0.005 (4) |
| C14 | 0.122 (6) | 0.063 (4) | 0.099 (5) | -0.010 (4) | 0.045 (5) | -0.017 (4) |
| C15 | 0.069 (4) | 0.055 (4) | 0.098 (4) | 0.001 (3) | 0.017 (3) | 0.006 (3) |
| S1 | 0.0949 (12) | 0.0843 (12) | 0.0762 (10) | -0.0253 (10) | 0.0100 (8) | 0.0154 (9) |
| S2 | 0.0281 (5) | 0.0490 (7) | 0.0714 (8) | 0.0022 (5) | 0.0015 (5) | 0.0115 (6) |
| N1 | 0.062 (3) | 0.049 (3) | 0.075 (3) | -0.004 (2) | -0.002 (2) | 0.005 (2) |
| N2 | 0.0289 (17) | 0.048 (2) | 0.087 (3) | 0.0049 (18) | -0.001 (2) | 0.007 (2) |
| O1 | 0.176 (5) | 0.095 (3) | 0.098 (3) | -0.049 (3) | -0.024 (3) | 0.050 (3) |
| O2 | 0.091 (3) | 0.169 (5) | 0.108 (3) | -0.015 (3) | 0.045 (3) | -0.021 (3) |
| O3 | 0.0318 (15) | 0.090 (2) | 0.075 (2) | -0.0012 (16) | 0.0080 (15) | 0.0128 (18) |
| O4 | 0.0395 (16) | 0.057 (2) | 0.095 (2) | 0.0091 (15) | -0.0078 (16) | 0.0255 (17) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|--------|-----------|---------|-----------|
| C1—C6 | 1.357 (7) | C9—H9B | 0.9700 |
| C1—C2 | 1.370 (8) | C10—C15 | 1.368 (6) |
| C1—S1 | 1.754 (6) | C10—C11 | 1.390 (6) |
| C2—C3 | 1.395 (9) | C10—S2 | 1.748 (5) |
| C2—H2A | 0.9300 | C11—C12 | 1.362 (7) |
| C3—C4 | 1.325 (9) | C11—H11 | 0.9300 |
| C3—H3A | 0.9300 | C12—C13 | 1.365 (9) |
| C4—C5 | 1.351 (9) | C12—H12 | 0.9300 |
| C4—H4A | 0.9300 | C13—C14 | 1.362 (9) |
| C5—C6 | 1.382 (9) | C13—H13 | 0.9300 |
| C5—H5 | 0.9300 | C14—C15 | 1.398 (7) |
| C6—H6 | 0.9300 | C14—H14 | 0.9300 |
| C7—N1 | 1.471 (6) | C15—H15 | 0.9300 |
| C7—C8 | 1.506 (6) | S1—O2 | 1.424 (4) |
| C7—H7A | 0.9700 | S1—O1 | 1.435 (4) |
| C7—H7B | 0.9700 | S1—N1 | 1.603 (4) |
| C8—C9 | 1.503 (6) | S2—O3 | 1.427 (3) |
| C8—H8A | 0.9700 | S2—O4 | 1.430 (3) |

| | | | |
|-------------|------------|---------------|-------------|
| C8—H8B | 0.9700 | S2—N2 | 1.597 (4) |
| C9—N2 | 1.468 (5) | N1—H1 | 0.82 (4) |
| C9—H9A | 0.9700 | N2—H2 | 0.74 (4) |
| C6—C1—C2 | 118.3 (6) | C15—C10—C11 | 120.9 (5) |
| C6—C1—S1 | 120.7 (5) | C15—C10—S2 | 120.0 (4) |
| C2—C1—S1 | 120.9 (5) | C11—C10—S2 | 119.1 (4) |
| C1—C2—C3 | 120.4 (6) | C12—C11—C10 | 118.9 (5) |
| C1—C2—H2A | 119.8 | C12—C11—H11 | 120.5 |
| C3—C2—H2A | 119.8 | C10—C11—H11 | 120.5 |
| C4—C3—C2 | 120.0 (8) | C11—C12—C13 | 121.2 (6) |
| C4—C3—H3A | 120.0 | C11—C12—H12 | 119.4 |
| C2—C3—H3A | 120.0 | C13—C12—H12 | 119.4 |
| C3—C4—C5 | 120.5 (8) | C14—C13—C12 | 119.8 (6) |
| C3—C4—H4A | 119.7 | C14—C13—H13 | 120.1 |
| C5—C4—H4A | 119.7 | C12—C13—H13 | 120.1 |
| C4—C5—C6 | 120.3 (7) | C13—C14—C15 | 120.6 (6) |
| C4—C5—H5 | 119.9 | C13—C14—H14 | 119.7 |
| C6—C5—H5 | 119.9 | C15—C14—H14 | 119.7 |
| C1—C6—C5 | 120.5 (7) | C10—C15—C14 | 118.4 (5) |
| C1—C6—H6 | 119.7 | C10—C15—H15 | 120.8 |
| C5—C6—H6 | 119.7 | C14—C15—H15 | 120.8 |
| N1—C7—C8 | 110.4 (4) | O2—S1—O1 | 120.0 (3) |
| N1—C7—H7A | 109.6 | O2—S1—N1 | 106.5 (3) |
| C8—C7—H7A | 109.6 | O1—S1—N1 | 106.8 (3) |
| N1—C7—H7B | 109.6 | O2—S1—C1 | 108.6 (3) |
| C8—C7—H7B | 109.6 | O1—S1—C1 | 106.9 (3) |
| H7A—C7—H7B | 108.1 | N1—S1—C1 | 107.4 (2) |
| C9—C8—C7 | 114.8 (4) | O3—S2—O4 | 118.66 (18) |
| C9—C8—H8A | 108.6 | O3—S2—N2 | 107.9 (2) |
| C7—C8—H8A | 108.6 | O4—S2—N2 | 105.36 (18) |
| C9—C8—H8B | 108.6 | O3—S2—C10 | 107.48 (19) |
| C7—C8—H8B | 108.6 | O4—S2—C10 | 108.8 (2) |
| H8A—C8—H8B | 107.6 | N2—S2—C10 | 108.2 (2) |
| N2—C9—C8 | 109.8 (3) | C7—N1—S1 | 119.5 (4) |
| N2—C9—H9A | 109.7 | C7—N1—H1 | 108 (3) |
| C8—C9—H9A | 109.7 | S1—N1—H1 | 110 (3) |
| N2—C9—H9B | 109.7 | C9—N2—S2 | 121.0 (3) |
| C8—C9—H9B | 109.7 | C9—N2—H2 | 115 (4) |
| H9A—C9—H9B | 108.2 | S2—N2—H2 | 109 (4) |
| C6—C1—C2—C3 | -2.1 (9) | C2—C1—S1—O2 | -147.7 (5) |
| S1—C1—C2—C3 | -177.1 (5) | C6—C1—S1—O1 | 168.2 (5) |
| C1—C2—C3—C4 | 1.2 (11) | C2—C1—S1—O1 | -16.9 (6) |
| C2—C3—C4—C5 | 0.0 (12) | C6—C1—S1—N1 | -77.5 (5) |
| C3—C4—C5—C6 | -0.2 (12) | C2—C1—S1—N1 | 97.4 (5) |
| C2—C1—C6—C5 | 1.9 (9) | C15—C10—S2—O3 | 147.5 (4) |
| S1—C1—C6—C5 | 176.9 (5) | C11—C10—S2—O3 | -34.5 (4) |
| C4—C5—C6—C1 | -0.8 (10) | C15—C10—S2—O4 | 17.8 (4) |
| N1—C7—C8—C9 | 72.5 (5) | C11—C10—S2—O4 | -164.2 (3) |

supplementary materials

| | | | |
|-----------------|------------|---------------|------------|
| C7—C8—C9—N2 | 65.7 (5) | C15—C10—S2—N2 | -96.2 (4) |
| C15—C10—C11—C12 | 1.4 (7) | C11—C10—S2—N2 | 81.8 (4) |
| S2—C10—C11—C12 | -176.6 (4) | C8—C7—N1—S1 | -165.2 (3) |
| C10—C11—C12—C13 | -1.0 (9) | O2—S1—N1—C7 | -173.0 (4) |
| C11—C12—C13—C14 | -0.8 (10) | O1—S1—N1—C7 | 57.7 (4) |
| C12—C13—C14—C15 | 2.2 (10) | C1—S1—N1—C7 | -56.7 (4) |
| C11—C10—C15—C14 | 0.0 (7) | C8—C9—N2—S2 | 179.2 (3) |
| S2—C10—C15—C14 | 178.0 (4) | O3—S2—N2—C9 | 56.7 (4) |
| C13—C14—C15—C10 | -1.8 (8) | O4—S2—N2—C9 | -175.6 (3) |
| C6—C1—S1—O2 | 37.4 (5) | C10—S2—N2—C9 | -59.3 (4) |

Hydrogen-bond geometry (\AA , $^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-----------------------------------|----------|-------------|-------------|---------------|
| N1—H1 \cdots O4 ⁱ | 0.82 (4) | 2.15 (5) | 2.954 (6) | 164 (4) |
| N2—H2 \cdots O3 ⁱⁱ | 0.74 (4) | 2.15 (4) | 2.836 (4) | 154 (5) |
| C9—H9B \cdots O4 ⁱⁱⁱ | 0.97 | 2.51 | 3.430 (5) | 158 |
| C13—H13 \cdots O1 ^{iv} | 0.93 | 2.42 | 3.276 (8) | 153 |

Symmetry codes: (i) $-x+1/2, y-1/2, z$; (ii) $x-1/2, -y+3/2, -z+1$; (iii) $x+1/2, -y+3/2, -z+1$; (iv) $x, -y+3/2, z+1/2$.

Fig. 1

