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# 2,2′,4,4′,6,6′-Hexamethyl-*N*-(3-phthalimidopropyl)-*N*,*N*′-(propane-1,3-diyl)dibenzenesulfonamide

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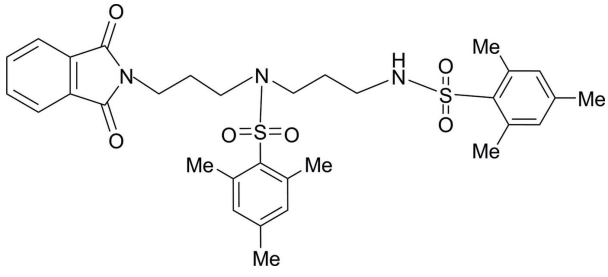
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.006 Å; $R$ factor = 0.069; $wR$ factor = 0.219; data-to-parameter ratio = 16.0.

In the title compound, $C_{32}H_{38}N_3O_6S_2$, an intermediate in the synthesis of polyamine drugs, the dihedral angle between the phenyl rings of the two 2,4,6-trimethylbenzenesulfonyl groups is 27.1 (3)°. In the crystal structure, molecules are linked by intermolecular N—H···O hydrogen bonds, thereby forming an infinite one-dimensional chain propagating along [010].

## Related literature

Polyamines are essential growth factors for cells, existing mainly as polycations at physiological pH, see: Cullis *et al.* (1999); Seiler *et al.* (1996); Tsen *et al.* (2008).



## Experimental

### Crystal data

$C_{32}H_{39}N_3O_6S_2$
$M_r$ = 625.78
Monoclinic, $C2/c$
$a$ = 32.042 (3) Å
$b$ = 9.9782 (8) Å
$c$ = 25.105 (2) Å
$\beta$ = 127.917 (1)°
$V$ = 6332.1 (9) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.22 mm$^{-1}$
$T$ = 296 (2) K
0.18 × 0.15 × 0.13 mm

### Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
$T_{min}$ = 0.962, $T_{max}$ = 0.973
17128 measured reflections
6212 independent reflections
4574 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.022

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.219
$S$ = 1.09
6212 reflections
388 parameters
44 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.80 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.57 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H3$B$···O5$^{i}$ | 0.86 | 2.53 | 3.192 (4) | 134 |

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

This work was supported by the Basic Research Foundation for Natural Science of Henan University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2835).

## References

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Tsen, C., Iltis, M., Kaur, N., Bayer, C., Dekcros, J-G., von Kalm, L. & Phanstiel IV, O. (2008). *J. Med. Chem.* **51**, 324–330.

# supporting information

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# 2,2′,4,4′,6,6′-Hexamethyl-*N*-(3-phthalimidopropyl)-*N*,*N*′-(propane-1,3-diyl)dibenzenesulfonamide

**Yu-Xia Wang, Peng-Fei Cheng and Chao-Jie Wang**

## S1. Comment

Polyamines are essential growth factors for cells, which exist mainly as polycations at physiological pH (Cullis *et al.*, 1999; Seiler *et al.*, 1996; Tsen *et al.*, 2008). As part of our studies in this area, herein we report the synthesis and structure of the title compound, (I).

The compound (I) consists of a polyamine chain with two 2,4,6-trimethylbenzenesulfonyl group acting as protecting groups (Fig. 1). In the structure of (I), the two phenyl ring of two 2,4,6-trimethylbenzenesulfonyl group are nonparallel due to steric hindrance, charactrtized by a dihedral angel of 27.1 (3) °.

In the crystal, molecules are linked through intermolecular N–H···O hydrogen bonds to construct an infinite one-dimensional chain (Fig. 2 and Table 1).

## S2. Experimental

Propane-1,3-diamine 1.85 g (25 mmol) was dissolved in 2 *M* sodium hydroxide and the solution was cooled to 0 °C, a solution of 2,4,6-trimethylbenzenesulfonyl chloride 10.9 g (50 mmol) in $CH_2Cl_2$ (25 ml) was added dropwise. The reaction mixture was then stirred at room temperture for 18 h. The organic phase was separated from the aqueous phase and washed with 0.5 *M* HCl solution and brine. The $CH_2Cl_2$ layer was dried over sodium sulfate, filtered and the solvent removed *in vacuo*, and the residue purified by chromatography.

A mixture of $N^1$,$N^3$—Bis(mesitylenesulfonyl)-1,3-propyl-diamine 1.05 g (2.33 mmol) and 60% NaH (5.35 mmol, 0.22 g) in DMF 20 ml was stirred at 0 °C for 0.5 h, then warmed to room temperature for 0.5 h. *N*-(3-bromopropyl)-phthalimide 1.57 g (5.82 mmol) was added and the reaction mixture was stirred at 40 °C for 4 h, then EtoH (2.5 ml) and water (5 ml) were added, the solvent was removed *in vacuo* at 80 °C, the residue was dissolved in $CHCl_3$ and washed with water, the organic layer was dried over anhydrous sodium sulfate and filtered, then concentrated *in vacuo*, the residue was purified by chromatography. Colorless rod crystal of (I) were obtained.

## S3. Refinement

The H atoms were positioned geogmetrically (N—H = 0.86 Å, C—H = 0.93–0.97Å) and refined as riding with $U_{iso}(H)$=1.2$U_{eq}$(carrier) or $U_{iso}(H)$=1.5$U_{eq}$(methyl-C).

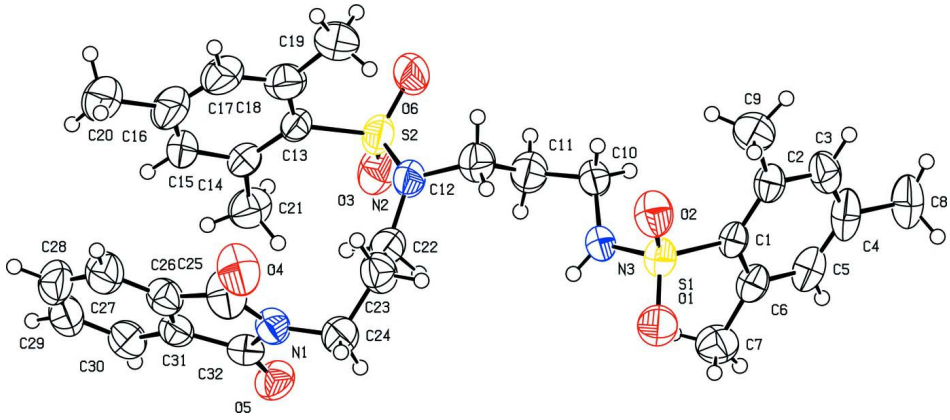


**Figure 1**

The molecular structure of (I). Displacement ellipsoids for the non-hydrogen atoms are drawn at the 50% probability level.

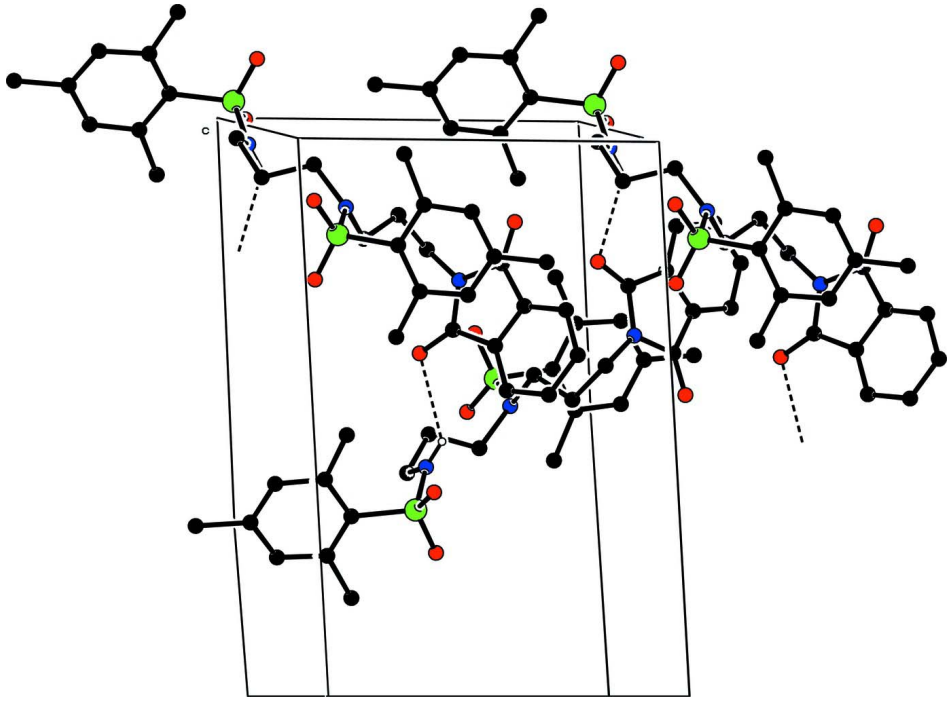


**Figure 2**

One-dimensional structure of (I), Hydrogen bonds are shown as dashed lines. For clarity, H atoms not involved in hydrogen bonds are omitted.

### 2,2′,4,4′,6,6′-Hexamethyl-N-(3-phthalimidopropyl)-N,N′- (propane-1,3-diyl)dibenzenesulfonamide

*Crystal data*

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$M_r = 625.78$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 32.042\ (3)$ Å
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$c = 25.105\ (2)$ Å
$\beta = 127.917\ (1)°$
$V = 6332.1\ (9)$ Å$^3$
$Z = 8$
$F(000) = 2656$
$D_x = 1.313$ Mg m$^{-3}$

Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 6528 reflections
$\theta$ = 2.4–28.1°
$\mu$ = 0.22 mm$^{-1}$
$T$ = 296 K
Block, colourless
0.18 × 0.15 × 0.13 mm

*Data collection*

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
$T_{min}$ = 0.962, $T_{max}$ = 0.973
17128 measured reflections
6212 independent reflections
4574 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.022
$\theta_{max}$ = 26.0°, $\theta_{min}$ = 2.1°
$h$ = −25→39
$k$ = −12→11
$l$ = −30→21

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.219
$S$ = 1.10
6212 reflections
388 parameters
44 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
$w = 1/[\sigma^2(F_o^2) + (0.1169P)^2 + 7.2057P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.80 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.57 e Å$^{-3}$

*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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.15326 (3) | 0.47012 (8) | 0.46771 (4) | 0.0531 (3) |
| S2 | 0.06920 (4) | 0.72487 (9) | 0.64731 (6) | 0.0655 (3) |
| C1 | 0.14805 (12) | 0.2922 (3) | 0.45787 (15) | 0.0464 (7) |
| C2 | 0.10216 (14) | 0.2310 (3) | 0.40203 (16) | 0.0539 (8) |
| C3 | 0.10074 (16) | 0.0918 (4) | 0.39911 (18) | 0.0635 (9) |
| H3A | 0.0703 | 0.0502 | 0.3626 | 0.076* |
| C4 | 0.1424 (2) | 0.0131 (4) | 0.4479 (2) | 0.0757 (9) |
| C5 | 0.18654 (16) | 0.0764 (4) | 0.50242 (19) | 0.0637 (9) |
| H5A | 0.2148 | 0.0242 | 0.5361 | 0.076* |
| C6 | 0.19082 (13) | 0.2140 (3) | 0.50937 (17) | 0.0546 (8) |
| C7 | 0.24128 (15) | 0.2685 (4) | 0.57208 (19) | 0.0734 (10) |
| H7A | 0.2644 | 0.1956 | 0.5992 | 0.110* |

| | | | | |
|---|---|---|---|---|
| H7B | 0.2334 | 0.3194 | 0.5974 | 0.110* |
| H7C | 0.2583 | 0.3253 | 0.5597 | 0.110* |
| C8 | 0.1398 (2) | −0.1383 (4) | 0.4422 (2) | 0.0849 (10) |
| H8A | 0.1062 | −0.1645 | 0.4014 | 0.127* |
| H8B | 0.1439 | −0.1763 | 0.4803 | 0.127* |
| H8C | 0.1676 | −0.1700 | 0.4413 | 0.127* |
| C9 | 0.05315 (15) | 0.3038 (5) | 0.34304 (18) | 0.0761 (11) |
| H9A | 0.0273 | 0.2393 | 0.3114 | 0.114* |
| H9B | 0.0627 | 0.3598 | 0.3210 | 0.114* |
| H9C | 0.0385 | 0.3580 | 0.3595 | 0.114* |
| C10 | 0.10008 (13) | 0.4624 (3) | 0.51695 (17) | 0.0581 (8) |
| H10A | 0.0998 | 0.3656 | 0.5203 | 0.070* |
| H10B | 0.0691 | 0.4888 | 0.4724 | 0.070* |
| C11 | 0.09849 (17) | 0.5273 (4) | 0.5705 (2) | 0.0732 (10) |
| H11A | 0.0740 | 0.4792 | 0.5740 | 0.088* |
| H11B | 0.1333 | 0.5236 | 0.6140 | 0.088* |
| C12 | 0.08133 (16) | 0.6696 (4) | 0.55154 (18) | 0.0698 (10) |
| H12A | 0.0432 | 0.6719 | 0.5171 | 0.084* |
| H12B | 0.0972 | 0.7070 | 0.5321 | 0.084* |
| C13 | 0.05511 (12) | 0.8878 (3) | 0.66060 (17) | 0.0512 (7) |
| C14 | 0.08566 (13) | 0.9494 (4) | 0.72467 (17) | 0.0554 (8) |
| C15 | 0.07141 (15) | 1.0790 (4) | 0.7284 (2) | 0.0718 (10) |
| H15A | 0.0910 | 1.1211 | 0.7702 | 0.086* |
| C16 | 0.03042 (19) | 1.1470 (5) | 0.6740 (3) | 0.1001 (12) |
| C17 | 0.00179 (16) | 1.0841 (4) | 0.6122 (2) | 0.0822 (12) |
| H17A | −0.0259 | 1.1306 | 0.5745 | 0.099* |
| C18 | 0.01232 (15) | 0.9547 (5) | 0.6035 (2) | 0.0743 (9) |
| C19 | −0.02361 (16) | 0.8980 (5) | 0.5329 (2) | 0.0848 (10) |
| H19A | −0.0494 | 0.9641 | 0.5028 | 0.127* |
| H19B | −0.0413 | 0.8201 | 0.5326 | 0.127* |
| H19C | −0.0030 | 0.8737 | 0.5185 | 0.127* |
| C20 | 0.0171 (2) | 1.2887 (5) | 0.6807 (3) | 0.1087 (13) |
| H20A | 0.0404 | 1.3153 | 0.7273 | 0.163* |
| H20B | −0.0188 | 1.2922 | 0.6646 | 0.163* |
| H20C | 0.0215 | 1.3484 | 0.6545 | 0.163* |
| C21 | 0.13243 (15) | 0.8889 (5) | 0.78906 (18) | 0.0743 (11) |
| H21A | 0.1462 | 0.9517 | 0.8253 | 0.111* |
| H21B | 0.1593 | 0.8679 | 0.7844 | 0.111* |
| H21C | 0.1217 | 0.8085 | 0.7987 | 0.111* |
| C22 | 0.14972 (14) | 0.8142 (4) | 0.65501 (19) | 0.0644 (9) |
| H22A | 0.1754 | 0.7424 | 0.6717 | 0.077* |
| H22B | 0.1547 | 0.8552 | 0.6936 | 0.077* |
| C23 | 0.16017 (16) | 0.9152 (4) | 0.62171 (19) | 0.0692 (10) |
| H23A | 0.1295 | 0.9732 | 0.5946 | 0.083* |
| H23B | 0.1647 | 0.8699 | 0.5914 | 0.083* |
| C24 | 0.20845 (15) | 1.0008 (4) | 0.67022 (18) | 0.0644 (9) |
| H24A | 0.2389 | 0.9430 | 0.6991 | 0.077* |
| H24B | 0.2152 | 1.0570 | 0.6447 | 0.077* |

| | | | | |
|---|---|---|---|---|
| C25 | 0.16924 (18) | 1.1983 (4) | 0.68724 (19) | 0.0795 (9) |
| C26 | 0.17520 (14) | 1.2568 (3) | 0.74571 (17) | 0.0596 (8) |
| C27 | 0.15189 (16) | 1.3666 (4) | 0.7500 (2) | 0.0748 (11) |
| H27A | 0.1280 | 1.4190 | 0.7123 | 0.090* |
| C28 | 0.16498 (18) | 1.3968 (4) | 0.8121 (2) | 0.0789 (11) |
| H28A | 0.1497 | 1.4712 | 0.8162 | 0.095* |
| C29 | 0.20005 (17) | 1.3201 (4) | 0.8680 (2) | 0.0719 (10) |
| H29A | 0.2080 | 1.3429 | 0.9093 | 0.086* |
| C30 | 0.22369 (14) | 1.2090 (4) | 0.86355 (18) | 0.0636 (9) |
| H30A | 0.2474 | 1.1565 | 0.9013 | 0.076* |
| C31 | 0.21105 (12) | 1.1789 (3) | 0.80191 (16) | 0.0528 (7) |
| C32 | 0.22889 (12) | 1.0682 (3) | 0.78088 (16) | 0.0522 (7) |
| O1 | 0.20542 (11) | 0.5116 (3) | 0.49361 (14) | 0.0727 (7) |
| O2 | 0.11048 (11) | 0.5309 (3) | 0.40790 (13) | 0.0741 (7) |
| O3 | 0.10576 (13) | 0.6647 (3) | 0.71039 (18) | 0.0900 (9) |
| O4 | 0.14220 (13) | 1.2330 (3) | 0.62932 (13) | 0.0890 (8) |
| O5 | 0.26026 (10) | 0.9802 (3) | 0.81456 (12) | 0.0691 (7) |
| O6 | 0.02164 (12) | 0.6529 (3) | 0.59969 (18) | 0.0939 (10) |
| N1 | 0.20210 (11) | 1.0851 (3) | 0.71198 (13) | 0.0566 (7) |
| N2 | 0.09614 (12) | 0.7566 (3) | 0.61035 (16) | 0.0662 (8) |
| N3 | 0.14813 (10) | 0.5046 (3) | 0.52664 (13) | 0.0523 (6) |
| H3B | 0.1729 | 0.5466 | 0.5626 | 0.063* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0687 (5) | 0.0447 (4) | 0.0570 (5) | 0.0021 (4) | 0.0443 (4) | 0.0024 (3) |
| S2 | 0.0762 (6) | 0.0477 (5) | 0.0974 (7) | −0.0042 (4) | 0.0659 (6) | −0.0118 (5) |
| C1 | 0.0573 (17) | 0.0451 (15) | 0.0488 (16) | 0.0052 (13) | 0.0387 (15) | 0.0006 (13) |
| C2 | 0.0663 (19) | 0.0585 (19) | 0.0489 (16) | 0.0028 (15) | 0.0414 (16) | −0.0046 (14) |
| C3 | 0.082 (2) | 0.061 (2) | 0.0574 (19) | −0.0106 (18) | 0.0483 (19) | −0.0156 (16) |
| C4 | 0.127 (3) | 0.0491 (15) | 0.094 (2) | 0.0034 (17) | 0.089 (2) | −0.0075 (15) |
| C5 | 0.085 (2) | 0.0552 (19) | 0.068 (2) | 0.0204 (18) | 0.056 (2) | 0.0112 (17) |
| C6 | 0.0643 (19) | 0.0556 (18) | 0.0589 (18) | 0.0071 (15) | 0.0454 (17) | 0.0024 (15) |
| C7 | 0.060 (2) | 0.078 (3) | 0.062 (2) | 0.0080 (19) | 0.0281 (18) | 0.0070 (19) |
| C8 | 0.131 (3) | 0.0509 (15) | 0.098 (2) | 0.0032 (17) | 0.083 (2) | −0.0078 (15) |
| C9 | 0.064 (2) | 0.090 (3) | 0.054 (2) | 0.005 (2) | 0.0263 (18) | −0.0025 (19) |
| C10 | 0.0620 (19) | 0.0545 (18) | 0.0641 (19) | −0.0097 (15) | 0.0420 (17) | −0.0172 (15) |
| C11 | 0.079 (2) | 0.067 (2) | 0.087 (3) | −0.0039 (19) | 0.058 (2) | −0.010 (2) |
| C12 | 0.069 (2) | 0.076 (2) | 0.065 (2) | 0.0016 (19) | 0.0412 (19) | −0.0101 (16) |
| C13 | 0.0510 (16) | 0.0481 (16) | 0.0657 (19) | 0.0003 (13) | 0.0415 (16) | −0.0056 (14) |
| C14 | 0.0531 (17) | 0.062 (2) | 0.0628 (19) | 0.0002 (15) | 0.0417 (16) | −0.0057 (16) |
| C15 | 0.067 (2) | 0.069 (2) | 0.089 (3) | −0.0076 (18) | 0.053 (2) | −0.029 (2) |
| C16 | 0.083 (2) | 0.068 (2) | 0.151 (3) | 0.0135 (17) | 0.073 (2) | −0.015 (2) |
| C17 | 0.061 (2) | 0.074 (2) | 0.098 (3) | 0.0204 (19) | 0.042 (2) | 0.009 (2) |
| C18 | 0.0549 (15) | 0.093 (2) | 0.0681 (17) | 0.0012 (15) | 0.0343 (14) | −0.0060 (16) |
| C19 | 0.0613 (16) | 0.097 (2) | 0.0718 (17) | 0.0007 (15) | 0.0288 (14) | −0.0062 (16) |
| C20 | 0.088 (2) | 0.070 (2) | 0.155 (3) | 0.0145 (17) | 0.069 (2) | −0.015 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C21 | 0.070 (2) | 0.099 (3) | 0.059 (2) | 0.007 (2) | 0.0428 (19) | 0.004 (2) |
| C22 | 0.065 (2) | 0.062 (2) | 0.077 (2) | 0.0052 (17) | 0.0488 (19) | −0.0013 (18) |
| C23 | 0.079 (2) | 0.071 (2) | 0.069 (2) | −0.0127 (19) | 0.051 (2) | −0.0134 (18) |
| C24 | 0.068 (2) | 0.071 (2) | 0.067 (2) | −0.0084 (18) | 0.0480 (19) | −0.0093 (18) |
| C25 | 0.1013 (19) | 0.0670 (16) | 0.0558 (13) | 0.0131 (14) | 0.0410 (14) | 0.0110 (12) |
| C26 | 0.0613 (19) | 0.0478 (17) | 0.0597 (19) | −0.0017 (15) | 0.0321 (17) | 0.0019 (14) |
| C27 | 0.077 (2) | 0.054 (2) | 0.082 (3) | 0.0068 (18) | 0.043 (2) | 0.0018 (18) |
| C28 | 0.094 (3) | 0.051 (2) | 0.108 (3) | 0.002 (2) | 0.070 (3) | −0.009 (2) |
| C29 | 0.087 (3) | 0.063 (2) | 0.081 (3) | −0.018 (2) | 0.059 (2) | −0.020 (2) |
| C30 | 0.064 (2) | 0.065 (2) | 0.0557 (19) | −0.0042 (17) | 0.0340 (17) | −0.0022 (16) |
| C31 | 0.0471 (16) | 0.0491 (17) | 0.0546 (17) | −0.0055 (13) | 0.0274 (14) | −0.0026 (14) |
| C32 | 0.0422 (15) | 0.0573 (18) | 0.0510 (16) | −0.0027 (14) | 0.0255 (14) | 0.0013 (14) |
| O1 | 0.0816 (17) | 0.0666 (16) | 0.0918 (18) | −0.0112 (13) | 0.0644 (15) | −0.0050 (14) |
| O2 | 0.0906 (18) | 0.0586 (15) | 0.0659 (15) | 0.0090 (13) | 0.0444 (14) | 0.0070 (12) |
| O3 | 0.115 (2) | 0.0606 (16) | 0.125 (3) | 0.0143 (16) | 0.090 (2) | 0.0101 (17) |
| O4 | 0.1081 (18) | 0.0715 (15) | 0.0585 (12) | 0.0151 (13) | 0.0364 (13) | 0.0111 (11) |
| O5 | 0.0614 (14) | 0.0711 (16) | 0.0638 (14) | 0.0187 (12) | 0.0329 (12) | 0.0094 (12) |
| O6 | 0.096 (2) | 0.0750 (18) | 0.146 (3) | −0.0360 (16) | 0.092 (2) | −0.0488 (19) |
| N1 | 0.0579 (15) | 0.0545 (15) | 0.0524 (15) | −0.0013 (12) | 0.0314 (13) | −0.0031 (12) |
| N2 | 0.0697 (18) | 0.0615 (17) | 0.088 (2) | −0.0128 (14) | 0.0592 (17) | −0.0233 (14) |
| N3 | 0.0554 (15) | 0.0481 (14) | 0.0540 (14) | −0.0052 (11) | 0.0339 (13) | −0.0116 (11) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—O2 | 1.404 (3) | C15—H15A | 0.9300 |
| S1—O1 | 1.432 (3) | C16—C17 | 1.375 (7) |
| S1—N3 | 1.623 (3) | C16—C20 | 1.516 (6) |
| S1—C1 | 1.786 (3) | C17—C18 | 1.385 (6) |
| S2—O3 | 1.400 (3) | C17—H17A | 0.9300 |
| S2—O6 | 1.424 (3) | C18—C19 | 1.510 (5) |
| S2—N2 | 1.640 (3) | C19—H19A | 0.9600 |
| S2—C13 | 1.773 (3) | C19—H19B | 0.9600 |
| C1—C2 | 1.403 (5) | C19—H19C | 0.9600 |
| C1—C6 | 1.408 (4) | C20—H20A | 0.9600 |
| C2—C3 | 1.390 (5) | C20—H20B | 0.9600 |
| C2—C9 | 1.526 (5) | C20—H20C | 0.9600 |
| C3—C4 | 1.374 (6) | C21—H21A | 0.9600 |
| C3—H3A | 0.9300 | C21—H21B | 0.9600 |
| C4—C5 | 1.377 (6) | C21—H21C | 0.9600 |
| C4—C8 | 1.515 (5) | C22—N2 | 1.473 (5) |
| C5—C6 | 1.379 (5) | C22—C23 | 1.474 (5) |
| C5—H5A | 0.9300 | C22—H22A | 0.9700 |
| C6—C7 | 1.503 (5) | C22—H22B | 0.9700 |
| C7—H7A | 0.9600 | C23—C24 | 1.513 (5) |
| C7—H7B | 0.9600 | C23—H23A | 0.9700 |
| C7—H7C | 0.9600 | C23—H23B | 0.9700 |
| C8—H8A | 0.9600 | C24—N1 | 1.453 (4) |
| C8—H8B | 0.9600 | C24—H24A | 0.9700 |

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|---|---|---|---|
| C8—H8C | 0.9600 | C24—H24B | 0.9700 |
| C9—H9A | 0.9600 | C25—O4 | 1.199 (4) |
| C9—H9B | 0.9600 | C25—N1 | 1.402 (5) |
| C9—H9C | 0.9600 | C25—C26 | 1.479 (6) |
| C10—N3 | 1.465 (4) | C26—C27 | 1.367 (5) |
| C10—C11 | 1.520 (5) | C26—C31 | 1.386 (5) |
| C10—H10A | 0.9700 | C27—C28 | 1.375 (6) |
| C10—H10B | 0.9700 | C27—H27A | 0.9300 |
| C11—C12 | 1.491 (6) | C28—C29 | 1.371 (6) |
| C11—H11A | 0.9700 | C28—H28A | 0.9300 |
| C11—H11B | 0.9700 | C29—C30 | 1.385 (5) |
| C12—N2 | 1.516 (4) | C29—H29A | 0.9300 |
| C12—H12A | 0.9700 | C30—C31 | 1.371 (5) |
| C12—H12B | 0.9700 | C30—H30A | 0.9300 |
| C13—C18 | 1.402 (5) | C31—C32 | 1.482 (5) |
| C13—C14 | 1.410 (5) | C32—O5 | 1.205 (4) |
| C14—C15 | 1.393 (5) | C32—N1 | 1.390 (4) |
| C14—C21 | 1.498 (5) | N3—H3B | 0.8600 |
| C15—C16 | 1.359 (7) | | |

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|---|---|---|---|
| O2—S1—O1 | 117.42 (17) | C17—C16—C20 | 120.9 (5) |
| O2—S1—N3 | 107.70 (16) | C16—C17—C18 | 123.0 (4) |
| O1—S1—N3 | 105.58 (15) | C16—C17—H17A | 118.5 |
| O2—S1—C1 | 109.56 (15) | C18—C17—H17A | 118.5 |
| O1—S1—C1 | 109.49 (15) | C17—C18—C13 | 117.6 (4) |
| N3—S1—C1 | 106.49 (14) | C17—C18—C19 | 116.8 (4) |
| O3—S2—O6 | 116.9 (2) | C13—C18—C19 | 125.6 (4) |
| O3—S2—N2 | 110.94 (18) | C18—C19—H19A | 109.5 |
| O6—S2—N2 | 106.63 (18) | C18—C19—H19B | 109.5 |
| O3—S2—C13 | 108.23 (17) | H19A—C19—H19B | 109.5 |
| O6—S2—C13 | 110.82 (17) | C18—C19—H19C | 109.5 |
| N2—S2—C13 | 102.29 (16) | H19A—C19—H19C | 109.5 |
| C2—C1—C6 | 120.5 (3) | H19B—C19—H19C | 109.5 |
| C2—C1—S1 | 121.5 (2) | C16—C20—H20A | 109.5 |
| C6—C1—S1 | 118.0 (2) | C16—C20—H20B | 109.5 |
| C3—C2—C1 | 117.9 (3) | H20A—C20—H20B | 109.5 |
| C3—C2—C9 | 116.3 (3) | C16—C20—H20C | 109.5 |
| C1—C2—C9 | 125.8 (3) | H20A—C20—H20C | 109.5 |
| C4—C3—C2 | 122.8 (4) | H20B—C20—H20C | 109.5 |
| C4—C3—H3A | 118.6 | C14—C21—H21A | 109.5 |
| C2—C3—H3A | 118.6 | C14—C21—H21B | 109.5 |
| C3—C4—C5 | 117.7 (3) | H21A—C21—H21B | 109.5 |
| C3—C4—C8 | 121.3 (4) | C14—C21—H21C | 109.5 |
| C5—C4—C8 | 121.0 (4) | H21A—C21—H21C | 109.5 |
| C4—C5—C6 | 123.0 (3) | H21B—C21—H21C | 109.5 |
| C4—C5—H5A | 118.5 | N2—C22—C23 | 113.6 (3) |
| C6—C5—H5A | 118.5 | N2—C22—H22A | 108.9 |
| C5—C6—C1 | 118.1 (3) | C23—C22—H22A | 108.9 |

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| C5—C6—C7 | 116.9 (3) | N2—C22—H22B | 108.9 |
| C1—C6—C7 | 125.1 (3) | C23—C22—H22B | 108.9 |
| C6—C7—H7A | 109.5 | H22A—C22—H22B | 107.7 |
| C6—C7—H7B | 109.5 | C22—C23—C24 | 113.9 (3) |
| H7A—C7—H7B | 109.5 | C22—C23—H23A | 108.8 |
| C6—C7—H7C | 109.5 | C24—C23—H23A | 108.8 |
| H7A—C7—H7C | 109.5 | C22—C23—H23B | 108.8 |
| H7B—C7—H7C | 109.5 | C24—C23—H23B | 108.8 |
| C4—C8—H8A | 109.5 | H23A—C23—H23B | 107.7 |
| C4—C8—H8B | 109.5 | N1—C24—C23 | 112.4 (3) |
| H8A—C8—H8B | 109.5 | N1—C24—H24A | 109.1 |
| C4—C8—H8C | 109.5 | C23—C24—H24A | 109.1 |
| H8A—C8—H8C | 109.5 | N1—C24—H24B | 109.1 |
| H8B—C8—H8C | 109.5 | C23—C24—H24B | 109.1 |
| C2—C9—H9A | 109.5 | H24A—C24—H24B | 107.9 |
| C2—C9—H9B | 109.5 | O4—C25—N1 | 123.8 (4) |
| H9A—C9—H9B | 109.5 | O4—C25—C26 | 130.2 (4) |
| C2—C9—H9C | 109.5 | N1—C25—C26 | 105.9 (3) |
| H9A—C9—H9C | 109.5 | C27—C26—C31 | 121.3 (4) |
| H9B—C9—H9C | 109.5 | C27—C26—C25 | 130.6 (3) |
| N3—C10—C11 | 109.5 (3) | C31—C26—C25 | 108.0 (3) |
| N3—C10—H10A | 109.8 | C26—C27—C28 | 117.7 (4) |
| C11—C10—H10A | 109.8 | C26—C27—H27A | 121.2 |
| N3—C10—H10B | 109.8 | C28—C27—H27A | 121.2 |
| C11—C10—H10B | 109.8 | C29—C28—C27 | 121.6 (4) |
| H10A—C10—H10B | 108.2 | C29—C28—H28A | 119.2 |
| C12—C11—C10 | 109.3 (3) | C27—C28—H28A | 119.2 |
| C12—C11—H11A | 109.8 | C28—C29—C30 | 120.6 (4) |
| C10—C11—H11A | 109.8 | C28—C29—H29A | 119.7 |
| C12—C11—H11B | 109.8 | C30—C29—H29A | 119.7 |
| C10—C11—H11B | 109.8 | C31—C30—C29 | 118.0 (3) |
| H11A—C11—H11B | 108.3 | C31—C30—H30A | 121.0 |
| C11—C12—N2 | 113.7 (3) | C29—C30—H30A | 121.0 |
| C11—C12—H12A | 108.8 | C30—C31—C26 | 120.8 (3) |
| N2—C12—H12A | 108.8 | C30—C31—C32 | 130.9 (3) |
| C11—C12—H12B | 108.8 | C26—C31—C32 | 108.4 (3) |
| N2—C12—H12B | 108.8 | O5—C32—N1 | 124.9 (3) |
| H12A—C12—H12B | 107.7 | O5—C32—C31 | 129.1 (3) |
| C18—C13—C14 | 121.0 (3) | N1—C32—C31 | 105.9 (3) |
| C18—C13—S2 | 116.5 (3) | C32—N1—C25 | 111.7 (3) |
| C14—C13—S2 | 122.4 (3) | C32—N1—C24 | 125.1 (3) |
| C15—C14—C13 | 117.0 (3) | C25—N1—C24 | 123.2 (3) |
| C15—C14—C21 | 116.9 (3) | C22—N2—C12 | 119.1 (3) |
| C13—C14—C21 | 126.0 (3) | C22—N2—S2 | 114.7 (2) |
| C16—C15—C14 | 123.4 (4) | C12—N2—S2 | 118.8 (2) |
| C16—C15—H15A | 118.3 | C10—N3—S1 | 118.2 (2) |
| C14—C15—H15A | 118.3 | C10—N3—H3B | 120.9 |
| C15—C16—C17 | 117.9 (4) | S1—N3—H3B | 120.9 |

| | |
|---|---|
| C15—C16—C20 | 121.2 (5) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H3*B*···O5$^{i}$ | 0.86 | 2.53 | 3.192 (4) | 134 |

Symmetry code: (i) −*x*+1/2, *y*−1/2, −*z*+3/2.