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# Crystal structure of methyl (2*Z*)-2-{[*N*-(2-formylphenyl)-4-methylbenzenesulfonamido]methyl}-3-(4-methoxyphenyl)prop-2-enoate

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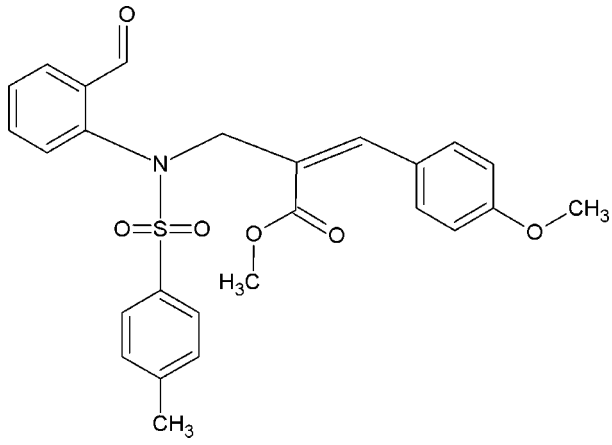
In the title compound, $C_{26}H_{25}NO_6S$, the S atom shows a distorted tetrahedral geometry, with O—S—O [119.46 (9)°] and N—S—C [107.16 (7)°] angles deviating from ideal tetrahedral values, a fact attributed to the Thorpe–Ingold effect. The sulfonyl-bound phenyl ring forms dihedral angles of 41.1 (1) and 83.3 (1)°, respectively, with the formylphenyl and phenyl rings. The dihedral angle between formylphenyl and phenyl rings is 47.6 (1)°. The crystal packing features C—H···O hydrogen-bond interactions.

**Keywords:** crystal structure; sulfonamide; Thorpe–Ingold effect.

**CCDC reference**: 1442750

## 1. Related literature

For background to the pharmacological uses of sulfonamides, see: Korolkovas *et al.* (1988); Mandell & Sande (1992). For the antifilarial activity of sulfonamide derivatives, see: Radembino *et al.* (1997); For related structures, see: Ranjith *et al.* (2009); Madhanraj *et al.* (2011). For the Thorpe–Ingold effect, see: Bassindale *et al.* (1984).



## 2. Experimental

### 2.1. Crystal data

$C_{26}H_{25}NO_6S$
$M_r$ = 479.53
Triclinic, $P\overline{1}$
$a$ = 8.3501 (2) Å
$b$ = 8.4859 (2) Å
$c$ = 17.6814 (4) Å
$\alpha$ = 84.424 (1)°
$\beta$ = 80.952 (1)°
$\gamma$ = 80.954 (1)°
$V$ = 1218.52 (5) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.17 mm$^{-1}$
$T$ = 293 K
0.25 × 0.20 × 0.20 mm

### 2.2. Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker 2004)
$T_{min}$ = 0.979, $T_{max}$ = 0.983
23816 measured reflections
5519 independent reflections
4232 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.028

### 2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.135
$S$ = 1.02
5519 reflections
314 parameters
13 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.36 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C9—H9···O1$B^{i}$ | 0.93 | 2.50 | 3.397 (7) | 162 |
| C15—H15$A$···O6 | 0.97 | 2.24 | 2.7322 (19) | 111 |
| C24—H24$A$···O4$^{ii}$ | 0.96 | 2.52 | 3.341 (3) | 143 |

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2009).

## Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: BG2572).

## References

Bassindale, A. (1984). *The Third Dimension in Organic Chemistry*, ch. 1, p. 11. New York: John Wiley and Sons.
Bruker (2004). *APEX2*, *SAINT* and *XPREP*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Korolkovas, A. (1988). *Essentials ofMedicinal Chemistry*, 2nd ed., pp. 699–716. New York: Wiley.
Madhanraj, R., Murugavel, S., Kannan, D. & Bakthadoss, M. (2011). *Acta Cryst.* E**67**, o3511.
Mandell, G. L. & Sande, M. A. (1992). In *Goodman and Gilman, The Pharmacological Basis of Therapeutics 2*, edited by A. Gilman, T. W. Rall, A. S. Nies & P. Taylor, 8th ed., pp. 1047–1057. Singapore: McGraw-Hill.
Radembino, N., Dessalles, M. C., -, C., Trouvin, J.-H., Loiseau, P. M., Gayral, P., Mahuzier, G., Rapp, M., Labarre, P., Godeneche, D., Madelmont, J.-C., Maurizis, J.-C., Veyre, A. & Chabard, J.-L. (1997). *Xenobiotica*, **27**, 73–85.
Ranjith, S., Sugumar, P., Sureshbabu, R., Mohanakrishnan, A. K. & Ponnuswamy, M. N. (2009). *Acta Cryst.* E**65**, o483.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

# supporting information

*Acta Cryst.* (2015). E**71**, o1088–o1089 [https://doi.org/10.1107/S2056989015024172]

## Crystal structure of methyl (2*Z*)-2-{[*N*-(2-formylphenyl)-4-methylbenzenesulfonamido]methyl}-3-(4-methoxyphenyl)prop-2-enoate

**Ankur Trigunait, Kannan Damodharan, Bakthadoss Manickam and Gunasekaran Krishnasamy**

### S1. Comment

Sulfonamide drugs are widely used for the treatment of certain infections caused by Gram-positive and Gram-negative micro-organisms, some fungi, and certain protozoa (Korolkovas *et al.*, 1988, Mandell & Sande 1992). One of the Sulfonamide derivatives (epoxysulphonamides and ethynesulphonamides) shows anti-filarial activity (Radembino *et al.*, 1997). In view of this biological importance, the crystal structure of the title compound has been determined and the results are presented here. The molecular structure of the title compound is shown in Fig. 1.The S1 atom shows a distorted tetrahedral geometry, with O2—S1—O3 [119.4 (1)°] and N1—S1—C8 [107.1 (1)°] angles deviating from ideal tetrahedral values are attributed to the Thrope-Ingold effect (Bassindale *et al.*, 1984). The sum of bond angles around N1 (348.3°) indicates that N1 is in sp2 hybridization. The sulfonyl bound phenyl (C8–C13) ring forms dihedral angles of 41.1 (1)° and 83.3 (1)°, respectively, with the formyl phenyl (C1–C6) and phenyl (C18—C23) rings. The dihedral angle between formyl phenyl and phenyl rings is 47.6 (1)°. The geometric parameters agree well with those reported for similar structures (Ranjith *et al.*, 2009; Madhanraj *et al.*, 2011). Crystal packing is stabilized by C19—H19···O5 and C24—H24A···O4 inter molecular hydrogen bond interaction. (Shown in Fig.2).

### S2. Experimental

A solution of *N*-(formylphenyl)(4-methylbenzene)sulfonamide (1 mmol, 0.275 g) and potassium carbonate (1.5 mmol, 0.207 g) in acetonitrile solvent was stirred for 15 min at room temperature. To this solution, methyl(2*Z*)-2-(bromomethyl)-3-(4-methoxyphenyl)prop-2-enoate (1.2 mmol, 0.342 g) was added dropwise till the addition was complete. After the completion of the reaction, as indicated by TLC, acetonitrile was evaporated. EtOAc (15 ml) and water (15 ml) were added to the crude mass. The organic layer was dried over anhydrous sodium sulfate. Removal of solvent led to the crude product, which was purified through pad of silica gel (100–200mesh) using ethylacetate and hexane(1:9) as solvents. The pure title compound was obtained as a colourless solid (0.426 g, 89% yield). Recrystallization was carried out using ethylacetate as solvent.

### S3. Refinement

All H atoms were fixed and refined using a riding model with C—H ranging from 0.93 to 0.97 Å. The formylphenyl O1 (O1A, O1B) and H7 (H7A, H7B) atoms appear disordered over two sites with s.o.f 0.740 (4) and 0.260 (4), respectively. O1A and O1B were refined with restraints in their anisotropic thermal parameters and C-O distances.

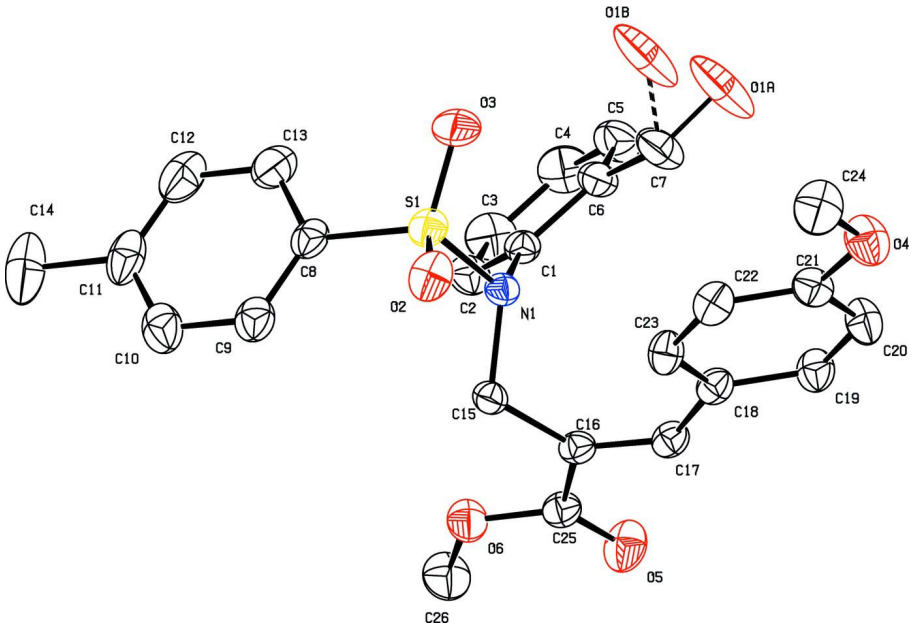


**Figure 1**

The molecular structure of the title compound showing 30% probability displacement ellipsoids for non-H atoms

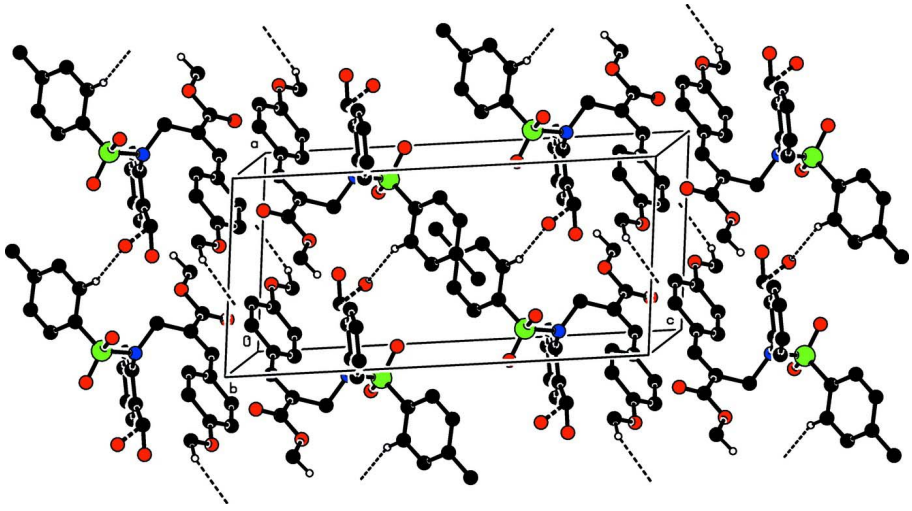

**Figure 2**

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

**Methyl (2*Z*)-2-{[*N*-(2-formylphenyl)-4-methylbenzenesulfonamido]methyl}-3-(4-methoxyphenyl)prop-2-enoate**

*Crystal data*

$C_{26}H_{25}NO_6S$
$M_r = 479.53$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.3501$ (2) Å
$b = 8.4859$ (2) Å
$c = 17.6814$ (4) Å
$\alpha = 84.424$ (1)°
$\beta = 80.952$ (1)°
$\gamma = 80.954$ (1)°
$V = 1218.52$ (5) Å$^3$
$Z = 2$
$F(000) = 504$
$D_x = 1.307$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8834 reflections

$\theta$ = 2.6–31.2°
$\mu$ = 0.17 mm$^{-1}$
$T$ = 293 K

Block, colourless
0.25 × 0.20 × 0.20 mm

*Data collection*

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ and $\varphi$ scan
Absorption correction: multi-scan (*SADABS*; Bruker 2004)
$T_{min}$ = 0.979, $T_{max}$ = 0.983

23816 measured reflections
5519 independent reflections
4232 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.028
$\theta_{max}$ = 27.5°, $\theta_{min}$ = 2.3°
$h$ = −10→10
$k$ = −11→11
$l$ = −22→22

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.135
$S$ = 1.02
5519 reflections
314 parameters
13 restraints

Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0713P)^2 + 0.275P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.34 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.36 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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| S1 | 0.89631 (5) | 0.51292 (5) | 0.33325 (2) | 0.04835 (15) | |
| O1A | 1.4384 (2) | 0.5552 (4) | 0.2246 (2) | 0.1151 (13) | 0.740 (4) |
| H7A | 1.2277 | 0.5012 | 0.2267 | 0.080* | 0.740 (4) |
| O1B | 1.3729 (9) | 0.4953 (8) | 0.2764 (4) | 0.1151 (13) | 0.260 (4) |
| H7B | 1.2365 | 0.5460 | 0.1946 | 0.080* | 0.260 (4) |
| O2 | 0.82045 (18) | 0.40111 (14) | 0.30104 (8) | 0.0609 (4) | |
| O3 | 1.04550 (18) | 0.46004 (16) | 0.36347 (8) | 0.0696 (4) | |
| O4 | 1.35510 (18) | 0.15273 (16) | 0.03718 (9) | 0.0700 (4) | |
| O5 | 0.83811 (19) | 1.06484 (15) | 0.08082 (8) | 0.0693 (4) | |
| O6 | 0.66997 (15) | 1.02738 (14) | 0.18898 (7) | 0.0565 (3) | |
| N1 | 0.93431 (15) | 0.65272 (14) | 0.26408 (7) | 0.0379 (3) | |
| C1 | 1.03147 (19) | 0.76893 (18) | 0.27928 (9) | 0.0396 (3) | |
| C2 | 0.9569 (2) | 0.9142 (2) | 0.30551 (11) | 0.0525 (4) | |
| H2 | 0.8432 | 0.9362 | 0.3149 | 0.063* | |
| C3 | 1.0505 (3) | 1.0272 (2) | 0.31794 (13) | 0.0677 (6) | |

| | | | | |
|---|---|---|---|---|
| H3 | 0.9996 | 1.1253 | 0.3352 | 0.081* |
| C4 | 1.2173 (3) | 0.9952 (3) | 0.30501 (14) | 0.0720 (6) |
| H4 | 1.2801 | 1.0710 | 0.3139 | 0.086* |
| C5 | 1.2920 (2) | 0.8516 (3) | 0.27898 (12) | 0.0651 (5) |
| H5 | 1.4059 | 0.8307 | 0.2703 | 0.078* |
| C6 | 1.2016 (2) | 0.7363 (2) | 0.26528 (10) | 0.0494 (4) |
| C7 | 1.2889 (2) | 0.5845 (3) | 0.23465 (13) | 0.0674 (6) |
| C8 | 0.7539 (2) | 0.6044 (2) | 0.40537 (9) | 0.0493 (4) |
| C9 | 0.5901 (2) | 0.6237 (2) | 0.39958 (11) | 0.0587 (5) |
| H9 | 0.5535 | 0.5855 | 0.3588 | 0.070* |
| C10 | 0.4797 (3) | 0.7018 (3) | 0.45622 (13) | 0.0703 (6) |
| H10 | 0.3682 | 0.7165 | 0.4528 | 0.084* |
| C11 | 0.5324 (3) | 0.7579 (2) | 0.51727 (12) | 0.0702 (6) |
| C12 | 0.6966 (4) | 0.7339 (3) | 0.52188 (13) | 0.0793 (7) |
| H12 | 0.7333 | 0.7691 | 0.5634 | 0.095* |
| C13 | 0.8076 (3) | 0.6594 (3) | 0.46667 (11) | 0.0678 (6) |
| H13 | 0.9190 | 0.6457 | 0.4703 | 0.081* |
| C14 | 0.4101 (4) | 0.8423 (3) | 0.57835 (16) | 0.1047 (10) |
| H14A | 0.3053 | 0.8683 | 0.5608 | 0.157* |
| H14B | 0.4473 | 0.9388 | 0.5882 | 0.157* |
| H14C | 0.4002 | 0.7734 | 0.6247 | 0.157* |
| C15 | 0.79663 (18) | 0.71501 (18) | 0.22006 (9) | 0.0401 (3) |
| H15A | 0.7147 | 0.7856 | 0.2509 | 0.048* |
| H15B | 0.7455 | 0.6265 | 0.2089 | 0.048* |
| C16 | 0.85673 (19) | 0.80473 (18) | 0.14613 (9) | 0.0392 (3) |
| C17 | 0.9703 (2) | 0.74544 (19) | 0.08975 (9) | 0.0430 (4) |
| H17 | 0.9941 | 0.8196 | 0.0488 | 0.052* |
| C18 | 1.0633 (2) | 0.58688 (19) | 0.08059 (9) | 0.0424 (4) |
| C19 | 1.2034 (2) | 0.5730 (2) | 0.02594 (10) | 0.0524 (4) |
| H19 | 1.2334 | 0.6645 | −0.0027 | 0.063* |
| C20 | 1.2982 (2) | 0.4287 (2) | 0.01316 (12) | 0.0587 (5) |
| H20 | 1.3920 | 0.4232 | −0.0232 | 0.070* |
| C21 | 1.2547 (2) | 0.2907 (2) | 0.05425 (11) | 0.0507 (4) |
| C22 | 1.1149 (2) | 0.2998 (2) | 0.10759 (10) | 0.0521 (4) |
| H22 | 1.0840 | 0.2076 | 0.1351 | 0.062* |
| C23 | 1.0211 (2) | 0.4462 (2) | 0.12001 (10) | 0.0489 (4) |
| H23 | 0.9265 | 0.4510 | 0.1559 | 0.059* |
| C24 | 1.3116 (3) | 0.0075 (2) | 0.07567 (14) | 0.0790 (7) |
| H24A | 1.3916 | −0.0803 | 0.0580 | 0.119* |
| H24B | 1.2059 | −0.0071 | 0.0650 | 0.119* |
| H24C | 1.3080 | 0.0117 | 0.1300 | 0.119* |
| C25 | 0.7907 (2) | 0.97716 (19) | 0.13359 (9) | 0.0445 (4) |
| C26 | 0.6048 (3) | 1.1955 (2) | 0.18269 (14) | 0.0693 (6) |
| H26A | 0.5197 | 1.2190 | 0.2250 | 0.104* |
| H26B | 0.5607 | 1.2211 | 0.1353 | 0.104* |
| H26C | 0.6908 | 1.2579 | 0.1836 | 0.104* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0578 (3) | 0.0350 (2) | 0.0469 (2) | 0.00262 (17) | −0.00629 (19) | 0.00590 (16) |
| O1A | 0.0336 (12) | 0.118 (2) | 0.199 (3) | 0.0111 (12) | −0.0125 (15) | −0.082 (2) |
| O1B | 0.0336 (12) | 0.118 (2) | 0.199 (3) | 0.0111 (12) | −0.0125 (15) | −0.082 (2) |
| O2 | 0.0854 (10) | 0.0349 (6) | 0.0604 (8) | −0.0140 (6) | −0.0004 (7) | −0.0018 (5) |
| O3 | 0.0716 (9) | 0.0610 (8) | 0.0674 (8) | 0.0168 (7) | −0.0208 (7) | 0.0137 (7) |
| O4 | 0.0663 (9) | 0.0500 (7) | 0.0866 (10) | 0.0013 (6) | 0.0017 (8) | −0.0059 (7) |
| O5 | 0.0902 (10) | 0.0450 (7) | 0.0628 (8) | −0.0074 (7) | 0.0068 (7) | 0.0127 (6) |
| O6 | 0.0576 (8) | 0.0441 (6) | 0.0602 (8) | 0.0031 (5) | −0.0009 (6) | 0.0047 (6) |
| N1 | 0.0368 (7) | 0.0346 (6) | 0.0406 (7) | −0.0006 (5) | −0.0064 (5) | 0.0006 (5) |
| C1 | 0.0417 (8) | 0.0379 (7) | 0.0383 (8) | −0.0002 (6) | −0.0089 (6) | −0.0023 (6) |
| C2 | 0.0524 (10) | 0.0443 (9) | 0.0589 (11) | 0.0044 (7) | −0.0095 (8) | −0.0106 (8) |
| C3 | 0.0856 (16) | 0.0428 (10) | 0.0773 (14) | −0.0027 (9) | −0.0198 (12) | −0.0158 (9) |
| C4 | 0.0803 (16) | 0.0650 (13) | 0.0815 (15) | −0.0261 (11) | −0.0252 (12) | −0.0128 (11) |
| C5 | 0.0493 (11) | 0.0781 (14) | 0.0737 (13) | −0.0138 (10) | −0.0171 (10) | −0.0125 (11) |
| C6 | 0.0417 (9) | 0.0550 (10) | 0.0522 (10) | 0.0012 (7) | −0.0134 (8) | −0.0104 (8) |
| C7 | 0.0425 (10) | 0.0754 (13) | 0.0857 (15) | 0.0117 (9) | −0.0194 (10) | −0.0296 (11) |
| C8 | 0.0617 (11) | 0.0423 (8) | 0.0395 (9) | −0.0038 (7) | −0.0039 (8) | 0.0074 (7) |
| C9 | 0.0653 (12) | 0.0546 (10) | 0.0525 (10) | −0.0110 (9) | −0.0007 (9) | 0.0058 (8) |
| C10 | 0.0643 (13) | 0.0620 (12) | 0.0742 (14) | −0.0079 (10) | 0.0090 (11) | 0.0136 (10) |
| C11 | 0.0995 (18) | 0.0490 (10) | 0.0504 (11) | −0.0066 (11) | 0.0152 (11) | 0.0061 (9) |
| C12 | 0.111 (2) | 0.0733 (14) | 0.0500 (12) | −0.0041 (13) | −0.0071 (12) | −0.0084 (10) |
| C13 | 0.0805 (15) | 0.0700 (13) | 0.0512 (11) | −0.0029 (11) | −0.0138 (10) | −0.0026 (10) |
| C14 | 0.134 (2) | 0.0742 (16) | 0.0836 (17) | −0.0069 (16) | 0.0461 (17) | −0.0058 (14) |
| C15 | 0.0339 (8) | 0.0409 (8) | 0.0436 (8) | −0.0044 (6) | −0.0060 (6) | 0.0047 (6) |
| C16 | 0.0403 (8) | 0.0395 (8) | 0.0402 (8) | −0.0108 (6) | −0.0108 (7) | 0.0022 (6) |
| C17 | 0.0499 (9) | 0.0417 (8) | 0.0394 (8) | −0.0138 (7) | −0.0086 (7) | 0.0019 (6) |
| C18 | 0.0479 (9) | 0.0440 (8) | 0.0383 (8) | −0.0126 (7) | −0.0085 (7) | −0.0042 (6) |
| C19 | 0.0540 (10) | 0.0483 (9) | 0.0529 (10) | −0.0127 (8) | 0.0003 (8) | 0.0023 (8) |
| C20 | 0.0481 (10) | 0.0584 (11) | 0.0652 (12) | −0.0090 (8) | 0.0068 (9) | −0.0041 (9) |
| C21 | 0.0499 (10) | 0.0464 (9) | 0.0566 (10) | −0.0042 (7) | −0.0105 (8) | −0.0086 (8) |
| C22 | 0.0659 (12) | 0.0416 (8) | 0.0501 (10) | −0.0156 (8) | −0.0054 (8) | −0.0033 (7) |
| C23 | 0.0554 (10) | 0.0464 (9) | 0.0452 (9) | −0.0158 (7) | 0.0026 (8) | −0.0075 (7) |
| C24 | 0.0998 (18) | 0.0466 (11) | 0.0829 (15) | −0.0004 (11) | 0.0001 (13) | −0.0043 (10) |
| C25 | 0.0486 (9) | 0.0414 (8) | 0.0442 (9) | −0.0079 (7) | −0.0102 (7) | 0.0013 (7) |
| C26 | 0.0743 (14) | 0.0447 (10) | 0.0818 (14) | 0.0054 (9) | −0.0061 (11) | −0.0011 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—O3 | 1.4233 (14) | C11—C12 | 1.368 (3) |
| S1—O2 | 1.4259 (14) | C11—C14 | 1.515 (3) |
| S1—N1 | 1.6486 (13) | C12—C13 | 1.365 (3) |
| S1—C8 | 1.7517 (18) | C12—H12 | 0.9300 |
| O1A—C7 | 1.222 (3) | C13—H13 | 0.9300 |
| O1B—C7 | 1.223 (3) | C14—H14A | 0.9600 |
| O4—C21 | 1.359 (2) | C14—H14B | 0.9600 |

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|---|---|---|---|
| O4—C24 | 1.419 (3) | C14—H14C | 0.9600 |
| O5—C25 | 1.193 (2) | C15—C16 | 1.504 (2) |
| O6—C25 | 1.339 (2) | C15—H15A | 0.9700 |
| O6—C26 | 1.445 (2) | C15—H15B | 0.9700 |
| N1—C1 | 1.440 (2) | C16—C17 | 1.340 (2) |
| N1—C15 | 1.4891 (18) | C16—C25 | 1.489 (2) |
| C1—C2 | 1.379 (2) | C17—C18 | 1.454 (2) |
| C1—C6 | 1.391 (2) | C17—H17 | 0.9300 |
| C2—C3 | 1.382 (3) | C18—C23 | 1.389 (2) |
| C2—H2 | 0.9300 | C18—C19 | 1.392 (2) |
| C3—C4 | 1.363 (3) | C19—C20 | 1.368 (3) |
| C3—H3 | 0.9300 | C19—H19 | 0.9300 |
| C4—C5 | 1.366 (3) | C20—C21 | 1.384 (3) |
| C4—H4 | 0.9300 | C20—H20 | 0.9300 |
| C5—C6 | 1.386 (3) | C21—C22 | 1.377 (3) |
| C5—H5 | 0.9300 | C22—C23 | 1.378 (2) |
| C6—C7 | 1.483 (3) | C22—H22 | 0.9300 |
| C7—H7A | 0.9672 | C23—H23 | 0.9300 |
| C7—H7B | 0.9933 | C24—H24A | 0.9600 |
| C8—C9 | 1.371 (3) | C24—H24B | 0.9600 |
| C8—C13 | 1.383 (3) | C24—H24C | 0.9600 |
| C9—C10 | 1.392 (3) | C26—H26A | 0.9600 |
| C9—H9 | 0.9300 | C26—H26B | 0.9600 |
| C10—C11 | 1.378 (3) | C26—H26C | 0.9600 |
| C10—H10 | 0.9300 | | |

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| O3—S1—O2 | 119.46 (9) | C8—C13—H13 | 120.1 |
| O3—S1—N1 | 106.81 (8) | C11—C14—H14A | 109.5 |
| O2—S1—N1 | 106.18 (7) | C11—C14—H14B | 109.5 |
| O3—S1—C8 | 108.18 (9) | H14A—C14—H14B | 109.5 |
| O2—S1—C8 | 108.44 (9) | C11—C14—H14C | 109.5 |
| N1—S1—C8 | 107.16 (7) | H14A—C14—H14C | 109.5 |
| C21—O4—C24 | 117.95 (16) | H14B—C14—H14C | 109.5 |
| C25—O6—C26 | 116.06 (14) | N1—C15—C16 | 110.86 (12) |
| C1—N1—C15 | 116.00 (11) | N1—C15—H15A | 109.5 |
| C1—N1—S1 | 116.79 (10) | C16—C15—H15A | 109.5 |
| C15—N1—S1 | 115.48 (10) | N1—C15—H15B | 109.5 |
| C2—C1—C6 | 119.77 (16) | C16—C15—H15B | 109.5 |
| C2—C1—N1 | 120.41 (14) | H15A—C15—H15B | 108.1 |
| C6—C1—N1 | 119.79 (14) | C17—C16—C25 | 115.34 (14) |
| C1—C2—C3 | 120.25 (18) | C17—C16—C15 | 126.06 (14) |
| C1—C2—H2 | 119.9 | C25—C16—C15 | 118.56 (14) |
| C3—C2—H2 | 119.9 | C16—C17—C18 | 132.06 (14) |
| C4—C3—C2 | 120.22 (18) | C16—C17—H17 | 114.0 |
| C4—C3—H3 | 119.9 | C18—C17—H17 | 114.0 |
| C2—C3—H3 | 119.9 | C23—C18—C19 | 116.85 (15) |
| C3—C4—C5 | 119.86 (19) | C23—C18—C17 | 125.39 (15) |
| C3—C4—H4 | 120.1 | C19—C18—C17 | 117.72 (15) |

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| C5—C4—H4 | 120.1 | C20—C19—C18 | 121.79 (16) |
| C4—C5—C6 | 121.33 (19) | C20—C19—H19 | 119.1 |
| C4—C5—H5 | 119.3 | C18—C19—H19 | 119.1 |
| C6—C5—H5 | 119.3 | C19—C20—C21 | 120.10 (17) |
| C5—C6—C1 | 118.57 (16) | C19—C20—H20 | 119.9 |
| C5—C6—C7 | 119.11 (17) | C21—C20—H20 | 119.9 |
| C1—C6—C7 | 122.31 (16) | O4—C21—C22 | 124.42 (17) |
| O1A—C7—C6 | 121.8 (2) | O4—C21—C20 | 115.99 (17) |
| O1B—C7—C6 | 117.2 (4) | C22—C21—C20 | 119.57 (16) |
| O1A—C7—H7A | 118.0 | C21—C22—C23 | 119.62 (16) |
| C6—C7—H7A | 120.0 | C21—C22—H22 | 120.2 |
| O1B—C7—H7B | 123.3 | C23—C22—H22 | 120.2 |
| C6—C7—H7B | 114.0 | C22—C23—C18 | 122.03 (16) |
| C9—C8—C13 | 120.62 (18) | C22—C23—H23 | 119.0 |
| C9—C8—S1 | 119.52 (15) | C18—C23—H23 | 119.0 |
| C13—C8—S1 | 119.85 (16) | O4—C24—H24A | 109.5 |
| C8—C9—C10 | 118.4 (2) | O4—C24—H24B | 109.5 |
| C8—C9—H9 | 120.8 | H24A—C24—H24B | 109.5 |
| C10—C9—H9 | 120.8 | O4—C24—H24C | 109.5 |
| C11—C10—C9 | 121.3 (2) | H24A—C24—H24C | 109.5 |
| C11—C10—H10 | 119.4 | H24B—C24—H24C | 109.5 |
| C9—C10—H10 | 119.4 | O5—C25—O6 | 122.00 (15) |
| C12—C11—C10 | 118.6 (2) | O5—C25—C16 | 125.15 (16) |
| C12—C11—C14 | 121.0 (2) | O6—C25—C16 | 112.85 (13) |
| C10—C11—C14 | 120.4 (3) | O6—C26—H26A | 109.5 |
| C13—C12—C11 | 121.3 (2) | O6—C26—H26B | 109.5 |
| C13—C12—H12 | 119.4 | H26A—C26—H26B | 109.5 |
| C11—C12—H12 | 119.4 | O6—C26—H26C | 109.5 |
| C12—C13—C8 | 119.7 (2) | H26A—C26—H26C | 109.5 |
| C12—C13—H13 | 120.1 | H26B—C26—H26C | 109.5 |

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|---|---|---|---|
| O3—S1—N1—C1 | −43.28 (13) | C9—C10—C11—C12 | −0.7 (3) |
| O2—S1—N1—C1 | −171.79 (11) | C9—C10—C11—C14 | −179.89 (19) |
| C8—S1—N1—C1 | 72.47 (13) | C10—C11—C12—C13 | 1.5 (3) |
| O3—S1—N1—C15 | 175.04 (11) | C14—C11—C12—C13 | −179.3 (2) |
| O2—S1—N1—C15 | 46.53 (13) | C11—C12—C13—C8 | −1.1 (3) |
| C8—S1—N1—C15 | −69.21 (13) | C9—C8—C13—C12 | −0.1 (3) |
| C15—N1—C1—C2 | 45.8 (2) | S1—C8—C13—C12 | 178.51 (16) |
| S1—N1—C1—C2 | −95.71 (16) | C1—N1—C15—C16 | 54.01 (17) |
| C15—N1—C1—C6 | −132.35 (15) | S1—N1—C15—C16 | −164.00 (11) |
| S1—N1—C1—C6 | 86.17 (16) | N1—C15—C16—C17 | 58.9 (2) |
| C6—C1—C2—C3 | 0.0 (3) | N1—C15—C16—C25 | −118.85 (15) |
| N1—C1—C2—C3 | −178.15 (16) | C25—C16—C17—C18 | 179.51 (16) |
| C1—C2—C3—C4 | −0.6 (3) | C15—C16—C17—C18 | 1.7 (3) |
| C2—C3—C4—C5 | 0.6 (4) | C16—C17—C18—C23 | 19.7 (3) |
| C3—C4—C5—C6 | 0.0 (4) | C16—C17—C18—C19 | −162.71 (17) |
| C4—C5—C6—C1 | −0.6 (3) | C23—C18—C19—C20 | −2.0 (3) |
| C4—C5—C6—C7 | 178.0 (2) | C17—C18—C19—C20 | −179.77 (17) |

| | | | |
|---|---|---|---|
| C2—C1—C6—C5 | 0.6 (3) | C18—C19—C20—C21 | 0.9 (3) |
| N1—C1—C6—C5 | 178.73 (16) | C24—O4—C21—C22 | 1.3 (3) |
| C2—C1—C6—C7 | −177.97 (18) | C24—O4—C21—C20 | −177.5 (2) |
| N1—C1—C6—C7 | 0.2 (3) | C19—C20—C21—O4 | 179.36 (18) |
| C5—C6—C7—O1A | 3.6 (4) | C19—C20—C21—C22 | 0.5 (3) |
| C1—C6—C7—O1A | −177.9 (3) | O4—C21—C22—C23 | −179.51 (17) |
| C5—C6—C7—O1B | 66.3 (5) | C20—C21—C22—C23 | −0.7 (3) |
| C1—C6—C7—O1B | −115.1 (5) | C21—C22—C23—C18 | −0.4 (3) |
| O3—S1—C8—C9 | −161.09 (14) | C19—C18—C23—C22 | 1.7 (3) |
| O2—S1—C8—C9 | −30.16 (15) | C17—C18—C23—C22 | 179.32 (16) |
| N1—S1—C8—C9 | 84.07 (15) | C26—O6—C25—O5 | −2.3 (3) |
| O3—S1—C8—C13 | 20.28 (17) | C26—O6—C25—C16 | 177.19 (15) |
| O2—S1—C8—C13 | 151.21 (15) | C17—C16—C25—O5 | −4.8 (3) |
| N1—S1—C8—C13 | −94.56 (15) | C15—C16—C25—O5 | 173.22 (17) |
| C13—C8—C9—C10 | 0.9 (3) | C17—C16—C25—O6 | 175.70 (14) |
| S1—C8—C9—C10 | −177.74 (13) | C15—C16—C25—O6 | −6.3 (2) |
| C8—C9—C10—C11 | −0.5 (3) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C9—H9···O1*B*$^{i}$ | 0.93 | 2.50 | 3.397 (7) | 162 |
| C15—H15*A*···O6 | 0.97 | 2.24 | 2.7322 (19) | 111 |
| C24—H24*A*···O4$^{ii}$ | 0.96 | 2.52 | 3.341 (3) | 143 |

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