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## 4-Methyl-N-{2-[(E)-3-oxo-3-phenylprop-1-en-1-yl]phenyl}benzenesulfonamide

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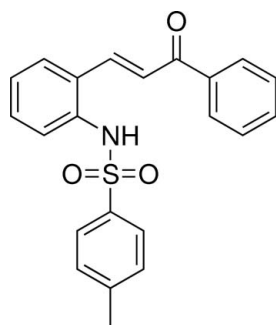
Edited by D.-J. Xu, Zhejiang University (Yuquan Campus), China

Key indicators: single-crystal X-ray study;  $T = 200$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.057;  $wR$  factor = 0.154; data-to-parameter ratio = 18.7.

In the title compound,  $\text{C}_{22}\text{H}_{19}\text{NO}_3\text{S}$ , the terminal phenyl and methylphenyl rings are twisted by 37.35 (12) and 49.08 (13)°, respectively, to the central benzene ring. In the crystal, molecules are linked by classical  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds and weak  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds into a three-dimensional supramolecular network.

## Related literature

For applications of sulfonamides in the fields of chemistry, biology and pharmacology, see: Chohan *et al.* (2010); El-Sayed *et al.* (2011); Seri *et al.* (2000); Suparan *et al.* (2000). For related structures, see: Murugavel *et al.* (2012); Zhang *et al.* (2010); Mughal *et al.* (2012).



## Experimental

## Crystal data

$\text{C}_{22}\text{H}_{19}\text{NO}_3\text{S}$   
 $M_r = 377.44$   
Monoclinic,  $P2_1/n$   
 $a = 8.9356$  (7) Å

$b = 10.8873$  (8) Å  
 $c = 19.3122$  (14) Å  
 $\beta = 99.472$  (2)°  
 $V = 1853.2$  (2) Å<sup>3</sup>

$Z = 4$   
Mo  $K\alpha$  radiation  
 $\mu = 0.20$  mm<sup>-1</sup>

$T = 200$  K  
 $0.19 \times 0.12 \times 0.06$  mm

## Data collection

Bruker SMART 1000 CCD area-detector diffractometer  
Absorption correction: multi-scan (SADABS; Bruker, 2001)  
 $T_{\min} = 0.964$ ,  $T_{\max} = 0.988$

13392 measured reflections  
4589 independent reflections  
2366 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.066$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.057$   
 $wR(F^2) = 0.154$   
 $S = 1.01$   
4589 reflections

245 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.46$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.43$  e Å<sup>-3</sup>

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

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1}\cdots\text{O1}^i$	0.88	2.24	2.839 (3)	125
$\text{C4}-\text{H4}\cdots\text{O2}^i$	0.95	2.51	3.272 (4)	137
$\text{C18}-\text{H18}\cdots\text{O3}^{ii}$	0.95	2.44	3.373 (3)	167
$\text{C22}-\text{H22B}\cdots\text{O1}^{iii}$	0.98	2.58	3.466 (4)	150

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

Data collection: SMART (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: ORTEP-3 for Windows (Farrugia, 2012); software used to prepare material for publication: SHELXTL and publCIF (Westrip, 2010).

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Supporting information for this paper is available from the IUCr electronic archives (Reference: XU5798).

## References

- Bruker (2001). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.  
Bruker (2007). *SMART* and *S SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.  
Chohan, Z. H., Moulay, H., Youssoufi, M. H., Jarrahpour, A. & Hadda, T. B. (2010). *Eur. J. Med. Chem.* **45**, 1189–1199.  
El-Sayed, N. S., El-Bendary, E. R., El-Ashry, S. M. & El-Kerdawy, M. M. (2011). *Eur. J. Med. Chem.* **46**, 3714–3720.  
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.  
Mughal, S. Y., Khan, I. U., Harrison, W. T. A., Khan, M. H. & Tahir, M. N. (2012). *Acta Cryst.* **E68**, o3013.  
Murugavel, S., Manikandan, N., Kannan, D. & Bakthadoss, M. (2012). *Acta Cryst.* **E68**, o1009–o1010.  
Seri, K., Sanai, K., Kurashima, K., Imamura, Y. & Akita, H. (2000). *Eur. J. Pharmacol.* **389**, 253–256.  
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
Suparan, C. T., Briganti, F., Tilli, S., Chegwiddden, W. R. & Scozzafava, A. (2000). *Bioorg. Med. Chem.* **9**, 703–714.  
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.  
Zhang, G.-Y., Chen, D.-J., Guo, X.-Y., Wang, S.-H. & Chang, J.-G. (2010). *Acta Cryst.* **E66**, o346.

## supporting information

*Acta Cryst.* (2014). E70, o851 [doi:10.1107/S1600536814015311]

## 4-Methyl-*N*-{2-[(*E*)-3-oxo-3-phenylprop-1-en-1-yl]phenyl}benzenesulfonamide

Sung-Gon Kim

### 1. Chemical context

### 2. Structural commentary

For related structures, see: Murugavel *et al.* (2012); Zhang *et al.* (2010). Sulfonamides, which are already known as sulfa drugs, are an important class of compounds in the field of chemistry, biology and pharmacology. Several sulfonamide derivatives are used as chemotherapeutic agents for their antibacterial, antifungal, antitumor and hypoglycemic (Chohan *et al.*, 2010; El-Sayed *et al.*, 2011; Seri *et al.*, 2000). In addition, some sulfonamide derivatives have been shown to inhibit on carbonic anhydrases (Suparan *et al.*, 2000). In view of these potential applications and in continuation of our work, the structure of the title compound has been carried out and the results are presented here.

X-ray analysis confirms the molecular structure and atom connectivity as illustrated in Fig. 1. The geometry around atoms S and N are distorted tetrahedral and planar trigonal, respectively. The average S—O bond length is 1.427 (2) Å, while the S—N and S—C bond lengths are 1.638 (3) and 1.757 (3), respectively. The dihedral angle between the vinyl-phenyl ring (C1—C6) and the methylphenyl ring (C16—C21) is 49.08 (13)°, and the dihedral angle between the vinyl-phenyl ring (C1—C6) and ketophenyl (C10—C15) ring is 37.35 (12)°. The sulfonamide torsion angle is 64.0 (2)° for C2—N1—S1—C16. The C=C double bond is in an *E* conformation and the vinylcarbonyl groups adopt extended conformations.

### 3. Supramolecular features

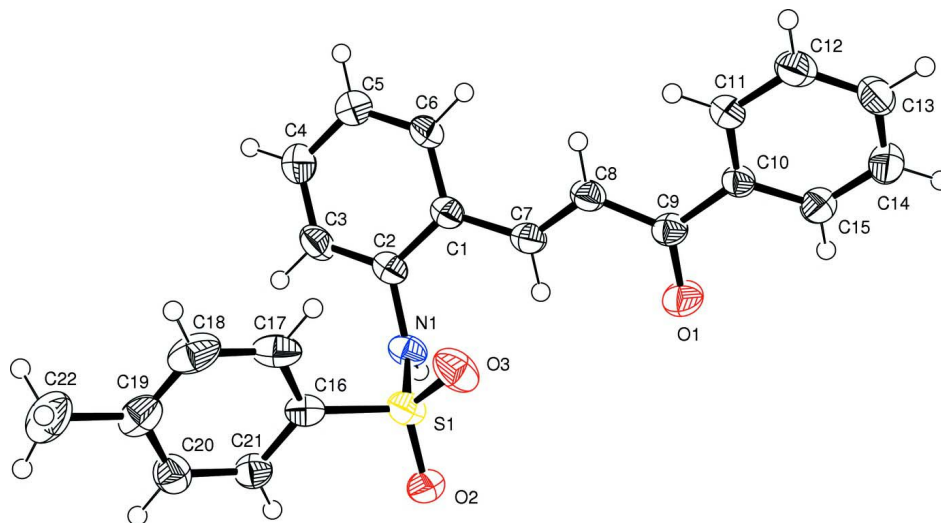
### 4. Database survey

### 5. Synthesis and crystallization

A solution of 4 M Na<sub>2</sub>CO<sub>3</sub> in water (10 mL) was added to a solution of 2-aminobenzyl alcohol (5.0 mmol) and *p*-toluenesulfonyl chloride (5.5 mmol) in THF (10 mL). After stirring at room temperature for 24 h, the reaction mixture was poured into cold water and extracted with EtOAc. The resultant organic layer was washed with brine and dried over MgSO<sub>4</sub>. The resulting residue was purified by silica gel chromatography to afford 2-(toluenesulfonylamino)benzyl alcohol. Next, to solution of 2-(toluenesulfonylamino)benzyl alcohol (3.0 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (10 mL) was added excess MnO<sub>2</sub> (15 mmol). After stirring for at room temperature for 36 h, the reaction mixture was filtered under celite pad and purified by silica gel chromatography to afford 2-(toluenesulfonylamino)benzaldehyde. To a solution of phenacyltriphenylphosphonium bromide (1.1 mmol) in toluene (5 mL) was added NaH (1.2 mmol) at 273 K. After stirring at 273 K for 1 h, to the reactin mixture, 2-(toluenesulfonylamino)benzaldehyde (1.0 mmol) was added. After stirring at room temperature for 24 h, the reaction mixture was poured into water and extracted with EtOAc. The resultant organic layer was washed with brine and dried over MgSO<sub>4</sub>. Theresulting residue was purified by silica gel chromatography to afford the title compound. Crystals suitable for X-ray analysis were obtained by recryatallization from an n-hexane/CH<sub>2</sub>Cl<sub>2</sub> solution.

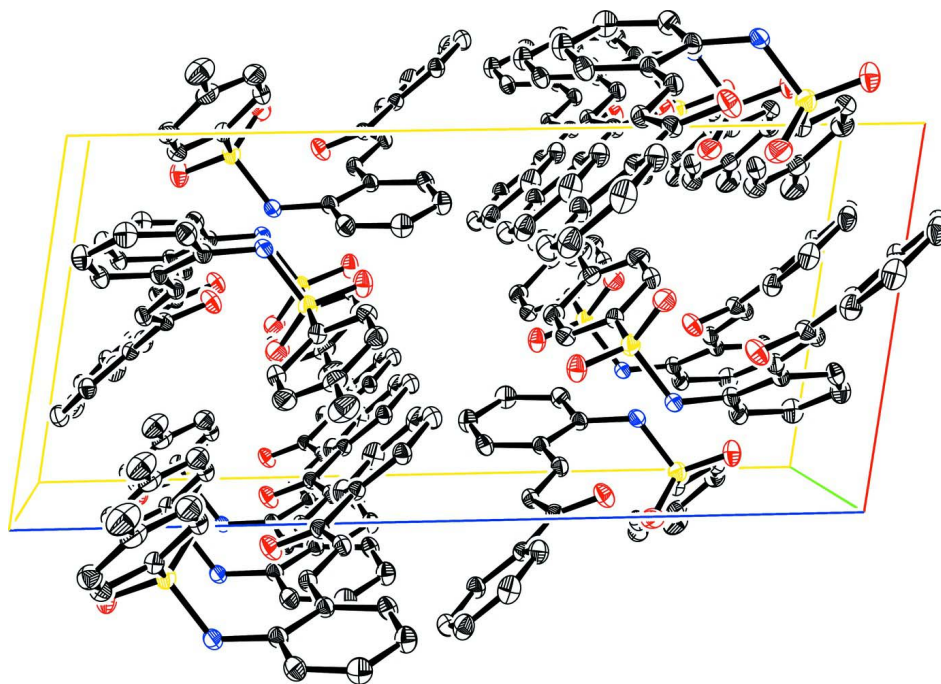
## 6. Refinement

All H atoms were positioned geometrically, ( $C-H = 0.95-0.96 \text{ \AA}$ ) and constrained to ride on their parent atoms, with  $U_{iso}(H) = xU_{eq}(C)$ , where  $x = 1.2$  for all other H atoms.



**Figure 1**

A view of the molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.



**Figure 2**

A partial view of the crystal packing of the title compound. Hydrogen atoms have been omitted for clarity.

## 4-Methyl-N-{2-[(E)-3-oxo-3-phenylprop-1-en-1-yl]phenyl}benzenesulfonamide

## Crystal data

C<sub>22</sub>H<sub>19</sub>NO<sub>3</sub>S $M_r = 377.44$ Monoclinic,  $P2_1/n$ 

Hall symbol: -P 2yn

 $a = 8.9356$  (7) Å $b = 10.8873$  (8) Å $c = 19.3122$  (14) Å $\beta = 99.472$  (2)° $V = 1853.2$  (2) Å<sup>3</sup> $Z = 4$  $F(000) = 792$  $D_x = 1.353$  Mg m<sup>-3</sup>Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 2689 reflections

 $\theta = 2.4$ – $26.1$ ° $\mu = 0.20$  mm<sup>-1</sup> $T = 200$  K

Rod, colorless

 $0.19 \times 0.12 \times 0.06$  mm

## Data collection

Bruker SMART 1000 CCD area-detector  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 $\phi$  and  $\omega$  scansAbsorption correction: multi-scan  
(SADABS; Bruker, 2001) $T_{\min} = 0.964$ ,  $T_{\max} = 0.988$ 

13392 measured reflections

4589 independent reflections

2366 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.066$  $\theta_{\text{max}} = 28.3$ °,  $\theta_{\text{min}} = 2.1$ ° $h = -11 \rightarrow 11$  $k = -14 \rightarrow 13$  $l = -25 \rightarrow 24$ 

## Refinement

Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.057$  $wR(F^2) = 0.154$  $S = 1.01$ 

4589 reflections

245 parameters

0 restraints

Primary atom site location: structure-invariant  
direct methodsSecondary atom site location: difference Fourier  
mapHydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0583P)^2]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\text{max}} < 0.001$  $\Delta\rho_{\text{max}} = 0.46$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -0.43$  e Å<sup>-3</sup>

## 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 (Å<sup>2</sup>)

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	1.1405 (3)	0.4390 (2)	0.37034 (13)	0.0321 (6)
C2	1.1969 (3)	0.5180 (3)	0.32288 (13)	0.0340 (6)
C3	1.2509 (3)	0.6334 (3)	0.34430 (14)	0.0407 (7)
H3	1.2877	0.6861	0.3117	0.049*

C4	1.2520 (3)	0.6731 (3)	0.41228 (15)	0.0459 (8)
H4	1.2912	0.7518	0.4267	0.055*
C5	1.1952 (3)	0.5965 (3)	0.45938 (15)	0.0439 (8)
H5	1.1947	0.6233	0.5062	0.053*
C6	1.1398 (3)	0.4822 (3)	0.43849 (13)	0.0372 (7)
H6	1.1001	0.4314	0.4711	0.045*
C7	1.0964 (3)	0.3133 (2)	0.35017 (13)	0.0336 (6)
H7	1.1236	0.2853	0.3073	0.040*
C8	1.0229 (3)	0.2331 (2)	0.38424 (13)	0.0335 (6)
H8	0.9856	0.2581	0.4253	0.040*
C9	0.9987 (3)	0.1067 (2)	0.35913 (14)	0.0326 (6)
O1	1.0479 (2)	0.07285 (18)	0.30617 (10)	0.0461 (5)
C10	0.9149 (3)	0.0178 (2)	0.39676 (13)	0.0300 (6)
C11	0.8184 (3)	0.0538 (3)	0.44267 (13)	0.0355 (7)
H11	0.8081	0.1386	0.4526	0.043*
C12	0.7373 (3)	-0.0321 (3)	0.47403 (14)	0.0426 (7)
H12	0.6711	-0.0066	0.5050	0.051*
C13	0.7536 (4)	-0.1553 (3)	0.45992 (14)	0.0470 (8)
H13	0.6968	-0.2146	0.4807	0.056*
C14	0.8511 (4)	-0.1927 (3)	0.41609 (15)	0.0493 (8)
H14	0.8632	-0.2778	0.4076	0.059*
C15	0.9315 (3)	-0.1073 (3)	0.38437 (14)	0.0400 (7)
H15	0.9986	-0.1337	0.3540	0.048*
N1	1.2050 (2)	0.4787 (2)	0.25294 (10)	0.0350 (6)
H1	1.2927	0.4543	0.2427	0.042*
S1	1.05508 (8)	0.47777 (7)	0.19146 (4)	0.0388 (2)
O2	1.1089 (2)	0.43544 (17)	0.13014 (9)	0.0465 (5)
O3	0.9384 (2)	0.41316 (19)	0.21857 (10)	0.0520 (6)
C16	0.9960 (3)	0.6311 (3)	0.17777 (13)	0.0359 (7)
C17	0.8957 (3)	0.6821 (3)	0.21770 (14)	0.0464 (8)
H17	0.8601	0.6346	0.2529	0.056*
C18	0.8480 (3)	0.8018 (3)	0.20592 (16)	0.0533 (9)
H18	0.7802	0.8365	0.2336	0.064*
C19	0.8975 (3)	0.8729 (3)	0.15412 (16)	0.0455 (8)
C20	0.9965 (3)	0.8202 (3)	0.11462 (15)	0.0423 (7)
H20	1.0310	0.8672	0.0789	0.051*
C21	1.0464 (3)	0.7003 (3)	0.12619 (14)	0.0360 (7)
H21	1.1150	0.6658	0.0988	0.043*
C22	0.8426 (4)	1.0035 (3)	0.14254 (18)	0.0638 (10)
H22A	0.8766	1.0368	0.1006	0.096*
H22B	0.8840	1.0535	0.1834	0.096*
H22C	0.7315	1.0051	0.1361	0.096*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0322 (15)	0.0345 (16)	0.0305 (14)	0.0012 (12)	0.0077 (12)	0.0040 (12)
C2	0.0333 (16)	0.0384 (17)	0.0312 (14)	0.0015 (13)	0.0079 (12)	0.0065 (13)

C3	0.0464 (18)	0.0390 (18)	0.0379 (16)	-0.0060 (14)	0.0108 (14)	0.0105 (14)
C4	0.054 (2)	0.0364 (18)	0.0481 (18)	-0.0060 (15)	0.0094 (15)	0.0004 (15)
C5	0.054 (2)	0.0407 (18)	0.0376 (16)	-0.0011 (15)	0.0102 (14)	-0.0026 (14)
C6	0.0447 (18)	0.0358 (16)	0.0336 (15)	-0.0023 (14)	0.0144 (13)	0.0054 (13)
C7	0.0361 (16)	0.0382 (17)	0.0275 (14)	0.0048 (13)	0.0078 (12)	0.0029 (12)
C8	0.0359 (16)	0.0367 (16)	0.0296 (14)	0.0006 (12)	0.0103 (12)	0.0025 (12)
C9	0.0310 (15)	0.0357 (16)	0.0321 (14)	0.0045 (12)	0.0081 (12)	-0.0012 (13)
O1	0.0521 (13)	0.0464 (13)	0.0453 (12)	0.0009 (10)	0.0245 (10)	-0.0084 (10)
C10	0.0316 (15)	0.0308 (15)	0.0268 (13)	-0.0004 (12)	0.0024 (11)	0.0014 (12)
C11	0.0415 (17)	0.0350 (17)	0.0310 (14)	-0.0024 (13)	0.0085 (13)	0.0031 (12)
C12	0.0448 (18)	0.050 (2)	0.0348 (15)	-0.0050 (15)	0.0106 (13)	0.0025 (15)
C13	0.061 (2)	0.044 (2)	0.0353 (16)	-0.0149 (16)	0.0037 (15)	0.0074 (15)
C14	0.069 (2)	0.0337 (18)	0.0433 (18)	-0.0035 (16)	0.0036 (16)	0.0000 (14)
C15	0.0487 (19)	0.0356 (17)	0.0356 (15)	0.0025 (14)	0.0065 (14)	-0.0013 (13)
N1	0.0308 (13)	0.0458 (14)	0.0300 (11)	0.0047 (11)	0.0092 (10)	0.0054 (11)
S1	0.0408 (4)	0.0434 (5)	0.0324 (4)	-0.0028 (3)	0.0070 (3)	0.0039 (3)
O2	0.0667 (15)	0.0398 (12)	0.0338 (10)	0.0078 (10)	0.0112 (10)	-0.0038 (9)
O3	0.0428 (13)	0.0633 (15)	0.0489 (12)	-0.0159 (11)	0.0043 (10)	0.0154 (11)
C16	0.0346 (16)	0.0450 (18)	0.0279 (14)	-0.0004 (13)	0.0047 (12)	-0.0019 (13)
C17	0.0419 (18)	0.069 (2)	0.0302 (15)	0.0050 (16)	0.0111 (13)	-0.0014 (15)
C18	0.0402 (19)	0.072 (3)	0.0471 (19)	0.0184 (17)	0.0051 (15)	-0.0167 (18)
C19	0.0378 (18)	0.050 (2)	0.0449 (18)	0.0093 (15)	-0.0058 (14)	-0.0130 (16)
C20	0.0419 (18)	0.0417 (18)	0.0423 (17)	0.0013 (14)	0.0039 (14)	0.0037 (14)
C21	0.0328 (16)	0.0405 (17)	0.0355 (15)	0.0025 (13)	0.0078 (12)	-0.0018 (13)
C22	0.062 (2)	0.056 (2)	0.068 (2)	0.0236 (18)	-0.0084 (18)	-0.0161 (19)

*Geometric parameters (Å, °)*

C1—C6	1.399 (3)	C13—C14	1.373 (4)
C1—C2	1.409 (3)	C13—H13	0.9500
C1—C7	1.459 (4)	C14—C15	1.379 (4)
C2—C3	1.384 (4)	C14—H14	0.9500
C2—N1	1.430 (3)	C15—H15	0.9500
C3—C4	1.380 (4)	N1—S1	1.638 (2)
C3—H3	0.9500	N1—H1	0.8800
C4—C5	1.390 (4)	S1—O2	1.4259 (19)
C4—H4	0.9500	S1—O3	1.427 (2)
C5—C6	1.375 (4)	S1—C16	1.757 (3)
C5—H5	0.9500	C16—C21	1.382 (4)
C6—H6	0.9500	C16—C17	1.391 (4)
C7—C8	1.330 (3)	C17—C18	1.379 (4)
C7—H7	0.9500	C17—H17	0.9500
C8—C9	1.463 (4)	C18—C19	1.393 (4)
C8—H8	0.9500	C18—H18	0.9500
C9—O1	1.234 (3)	C19—C20	1.384 (4)
C9—C10	1.484 (4)	C19—C22	1.509 (4)
C10—C11	1.391 (4)	C20—C21	1.386 (4)
C10—C15	1.395 (4)	C20—H20	0.9500

C11—C12	1.383 (4)	C21—H21	0.9500
C11—H11	0.9500	C22—H22A	0.9800
C12—C13	1.381 (4)	C22—H22B	0.9800
C12—H12	0.9500	C22—H22C	0.9800
C6—C1—C2	117.7 (2)	C13—C14—C15	120.3 (3)
C6—C1—C7	121.6 (2)	C13—C14—H14	119.9
C2—C1—C7	120.6 (2)	C15—C14—H14	119.9
C3—C2—C1	120.3 (2)	C14—C15—C10	120.3 (3)
C3—C2—N1	119.0 (2)	C14—C15—H15	119.9
C1—C2—N1	120.7 (2)	C10—C15—H15	119.9
C4—C3—C2	121.1 (3)	C2—N1—S1	121.59 (18)
C4—C3—H3	119.5	C2—N1—H1	119.2
C2—C3—H3	119.5	S1—N1—H1	119.2
C3—C4—C5	119.2 (3)	O2—S1—O3	120.81 (13)
C3—C4—H4	120.4	O2—S1—N1	104.87 (12)
C5—C4—H4	120.4	O3—S1—N1	107.27 (12)
C6—C5—C4	120.2 (3)	O2—S1—C16	108.42 (12)
C6—C5—H5	119.9	O3—S1—C16	107.69 (13)
C4—C5—H5	119.9	N1—S1—C16	107.05 (12)
C5—C6—C1	121.5 (3)	C21—C16—C17	119.9 (3)
C5—C6—H6	119.2	C21—C16—S1	120.1 (2)
C1—C6—H6	119.2	C17—C16—S1	120.1 (2)
C8—C7—C1	128.1 (2)	C18—C17—C16	119.7 (3)
C8—C7—H7	115.9	C18—C17—H17	120.1
C1—C7—H7	115.9	C16—C17—H17	120.1
C7—C8—C9	120.8 (2)	C17—C18—C19	121.2 (3)
C7—C8—H8	119.6	C17—C18—H18	119.4
C9—C8—H8	119.6	C19—C18—H18	119.4
O1—C9—C8	120.1 (2)	C20—C19—C18	118.2 (3)
O1—C9—C10	119.2 (2)	C20—C19—C22	122.0 (3)
C8—C9—C10	120.6 (2)	C18—C19—C22	119.7 (3)
C11—C10—C15	118.6 (2)	C19—C20—C21	121.3 (3)
C11—C10—C9	123.0 (2)	C19—C20—H20	119.4
C15—C10—C9	118.4 (2)	C21—C20—H20	119.4
C12—C11—C10	120.9 (3)	C16—C21—C20	119.7 (3)
C12—C11—H11	119.6	C16—C21—H21	120.1
C10—C11—H11	119.6	C20—C21—H21	120.1
C13—C12—C11	119.4 (3)	C19—C22—H22A	109.5
C13—C12—H12	120.3	C19—C22—H22B	109.5
C11—C12—H12	120.3	H22A—C22—H22B	109.5
C14—C13—C12	120.5 (3)	C19—C22—H22C	109.5
C14—C13—H13	119.8	H22A—C22—H22C	109.5
C12—C13—H13	119.8	H22B—C22—H22C	109.5
C6—C1—C2—C3	0.8 (4)	C13—C14—C15—C10	0.2 (4)
C7—C1—C2—C3	-174.3 (3)	C11—C10—C15—C14	1.3 (4)
C6—C1—C2—N1	178.2 (2)	C9—C10—C15—C14	-177.4 (3)

C7—C1—C2—N1	3.1 (4)	C3—C2—N1—S1	-103.3 (3)
C1—C2—C3—C4	0.6 (4)	C1—C2—N1—S1	79.2 (3)
N1—C2—C3—C4	-176.9 (3)	C2—N1—S1—O2	179.0 (2)
C2—C3—C4—C5	-1.2 (4)	C2—N1—S1—O3	-51.4 (2)
C3—C4—C5—C6	0.5 (5)	C2—N1—S1—C16	64.0 (2)
C4—C5—C6—C1	0.8 (5)	O2—S1—C16—C21	-19.3 (3)
C2—C1—C6—C5	-1.5 (4)	O3—S1—C16—C21	-151.6 (2)
C7—C1—C6—C5	173.6 (3)	N1—S1—C16—C21	93.3 (2)
C6—C1—C7—C8	15.1 (4)	O2—S1—C16—C17	159.2 (2)
C2—C1—C7—C8	-170.0 (3)	O3—S1—C16—C17	26.9 (3)
C1—C7—C8—C9	-174.9 (2)	N1—S1—C16—C17	-88.2 (2)
C7—C8—C9—O1	0.7 (4)	C21—C16—C17—C18	-0.5 (4)
C7—C8—C9—C10	-179.2 (2)	S1—C16—C17—C18	-179.0 (2)
O1—C9—C10—C11	-160.3 (2)	C16—C17—C18—C19	0.6 (5)
C8—C9—C10—C11	19.6 (4)	C17—C18—C19—C20	-0.2 (4)
O1—C9—C10—C15	18.4 (4)	C17—C18—C19—C22	179.8 (3)
C8—C9—C10—C15	-161.7 (2)	C18—C19—C20—C21	-0.3 (4)
C15—C10—C11—C12	-1.7 (4)	C22—C19—C20—C21	179.7 (3)
C9—C10—C11—C12	177.0 (2)	C17—C16—C21—C20	0.0 (4)
C10—C11—C12—C13	0.5 (4)	S1—C16—C21—C20	178.5 (2)
C11—C12—C13—C14	1.1 (4)	C19—C20—C21—C16	0.4 (4)
C12—C13—C14—C15	-1.5 (4)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N1—H1...O1 <sup>i</sup>	0.88	2.24	2.839 (3)	125
C4—H4...O2 <sup>i</sup>	0.95	2.51	3.272 (4)	137
C18—H18...O3 <sup>ii</sup>	0.95	2.44	3.373 (3)	167
C22—H22 <i>B</i> ...O1 <sup>iii</sup>	0.98	2.58	3.466 (4)	150

Symmetry codes: (i)  $-x+5/2, y+1/2, -z+1/2$ ; (ii)  $-x+3/2, y+1/2, -z+1/2$ ; (iii)  $x, y+1, z$ .