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Crystal structure of 4-methyl-*N*-(4-methylbenzyl)-benzenesulfonamide

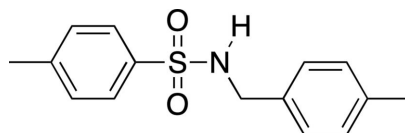
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The title compound, C₁₅H₁₇NO₂S, was synthesized *via* a substitution reaction between 4-methylbenzylamine and *p*-toluenesulfonyl chloride. In the crystal, N—H···O hydrogen bonds link the molecules, forming ribbons running along the *b*-axis direction. One of the aromatic rings hosts two intermolecular C—H··· π interactions that link these hydrogen-bonded ribbons into a three-dimensional network.

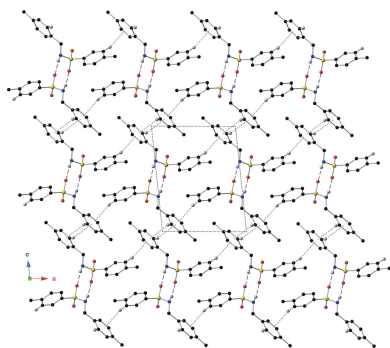
1. Chemical context

Sulfonamides, commonly referred to as ‘sulfa drugs’, are a biologically significant class of drugs. Over 70 years since its discovery, the sulfonamide moiety is frequently used in modern medicine (Zhao *et al.*, 2016). First recognized as a class of antibiotics in the 1930s, this class of drugs is used today to treat infectious diseases such as malaria, tuberculosis, HIV, and many more by targeting the dihydropteroate synthase (DHPS) pathway (Dennis *et al.*, 2018). Sulfonamides also exhibit remarkable antitumor, anticancer, and antithyroid activities among others (Scozzafava *et al.*, 2003).



The title compound, 4-methylbenzylamine-4-methylbenzenesulfonamide (I), is structurally similar to *N*-benzyl-*p*-toluene sulfonamide (BTS, Fig. 1). BTS is known to be a potent and specific inhibitor of the ATPase activity of skeletal myosin II subfragment 1 (S1) (Cheung *et al.*, 2002). The properties of BTS are significant in the study of muscle contraction (Pinniger *et al.*, 2005). In addition, the 4-methylbenzylamine-4-methylbenzenesulfonamide moiety is found in a potent and selective kappa opioid receptor (KOR) antagonist (Frankowski *et al.*, 2012; Fig. 1).

As therapeutic properties of sulfonamides continue to be discovered, it is important to synthesize these compounds efficiently. Sulfonamides are commonly synthesized by a mechanism analogous to the nucleophilic acyl-substitution reaction between an electrophile and a nucleophilic amine (Patel *et al.*, 2018). A review of the literature suggests that the most efficient method for synthesizing these compounds is by the sulfonylation of amines using either sulfonyl halides or sulfonic acids as electrophiles (Yan *et al.*, 2007; De Luca & Giacomelli, 2008). The title compound was synthesized in dichloromethane using a sulfonyl chloride, in the presence of



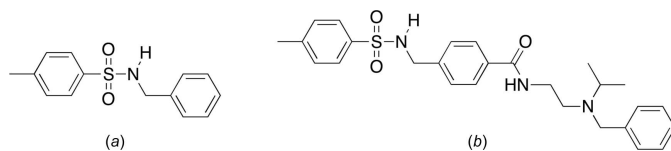


Figure 1
 (a) *N*-benzyl-*p*-toluene sulfonamide (BTS) and (b) a kappa opioid receptor (KOR) antagonist containing the 4-methylbenzylamine-4-methylbenzenesulfonamide moiety.

pyridine. The main purpose of pyridine is to act as a hydrochloric acid scavenger. However, in our ongoing efforts to produce sulfonamides, we have recently discovered an environmentally benign and facile synthesis of aryl sulfonamides. This method uses aqueous potassium carbonate in tetrahydrofuran. An increased rate of reaction and yield of sulfonamide compounds produced from a wide range of amines have been observed. We report here the synthesis of the title compound (I), as well as its molecular and crystal structures.

2. Structural commentary

The crystal structure of compound (I) was solved in the Sohnke space group $P2_1$, with a Flack parameter of 0.06 (4). The molecular structure is shown in Fig. 2 along with the atom-labeling scheme. The S=O bond lengths are 1.429 (2) and 1.424 (2) Å, with S1–N1 and S1–C1 bond lengths of 1.608 (2) and 1.764 (3) Å, respectively. The aryl groups of the sulfonamide are oriented gauche to one another with a C1–S1–N1–C8 torsion angle of 57.9 (2)°. The τ_4 descriptor for fourfold coordination around the sulfur atom S1 is 0.94, indicating a slightly distorted tetrahedral geometry of the sulfonamide group (where 0.00 = square-planar, 0.85 = trigonal-pyramidal, and 1.00 = tetrahedral; Yang *et al.*, 2007). An intramolecular C–H···O contact (Sutor, 1958,1962,1963; Table 1) is present between an aromatic C–H group and an O atom of the sulfonamide moiety in a $S(5)$ motif (Table 1).

3. Supramolecular features

Molecules of compound (I) exhibit both intermolecular N–H···O hydrogen bonds and C–H··· π interactions in the crystal structure (Fig. 3). The intermolecular N1–H1···O1 hydrogen bond is of medium strength and links molecules of

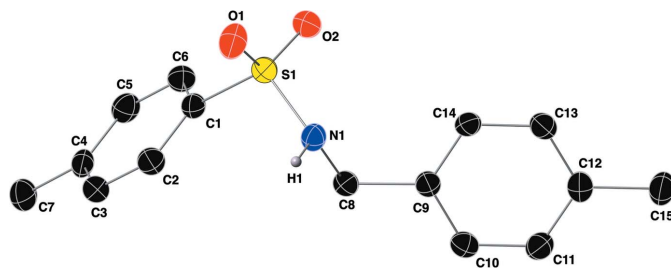


Figure 2
 The molecular structure of the title compound using standard CPK colors, showing the atom-labeling scheme. Anisotropic displacement ellipsoids are shown at the 40% probability level.

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

C_g is the centroid of the C9–C14 ring

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C6–H6···O2	0.95	2.51	2.890 (4)	104
N1–H1···O1 ⁱ	0.86 (1)	2.03 (2)	2.889 (3)	170 (3)
C5–H5··· C_g^{ii}	0.95	2.86	3.761 (3)	159
C10–H10··· C_g^{iii}	0.95	2.89	3.564 (3)	129

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

title compound into ribbons that run parallel to the b axis (Table 1, Fig. 4). The C9–C14 ring hosts two C–H··· π interactions that link the ribbons into an intricate three-dimensional network (Table 1, Fig. 5).

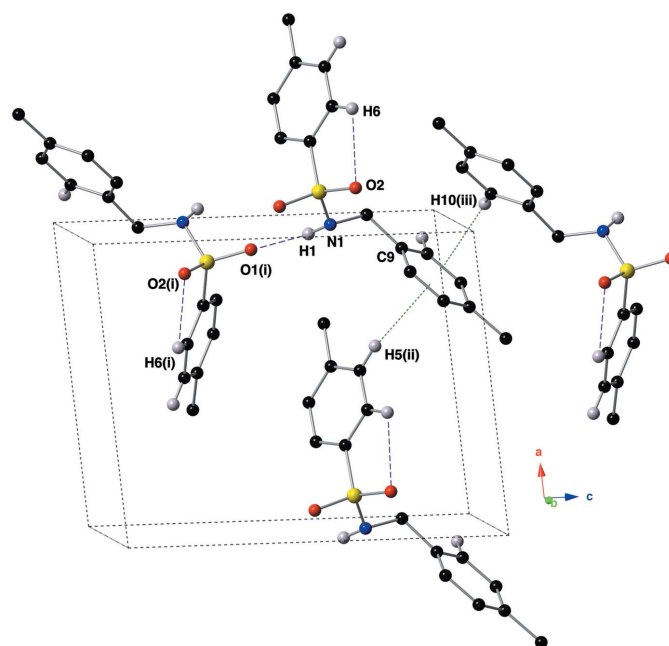


Figure 3
 Depiction of the intra- and intermolecular hydrogen bonds present in the structure of the title compound, using standard CPK colors with a ball-and-stick model. Hydrogen bonds and contacts are depicted with purple dashed lines, while C–H··· π interactions are shown with green dotted lines. [Symmetry codes: (i) $-x, -\frac{1}{2} + y, 1 - z$; (ii) $1 + x, y, z$; (iii) $-x, -\frac{1}{2} + y, 2 - z$.]

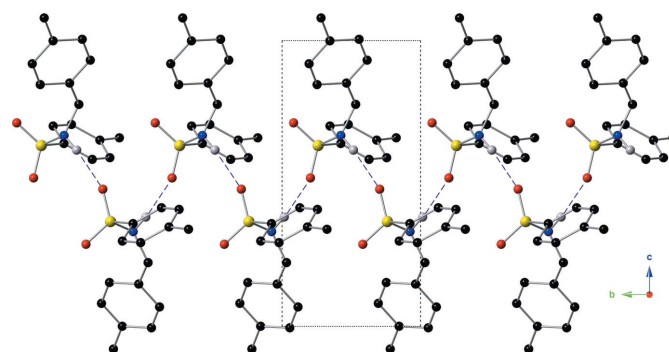


Figure 4
 Depiction of the supramolecular ribbons formed *via* intermolecular N–H···O hydrogen bonds (purple dashed lines), as viewed down the a axis.

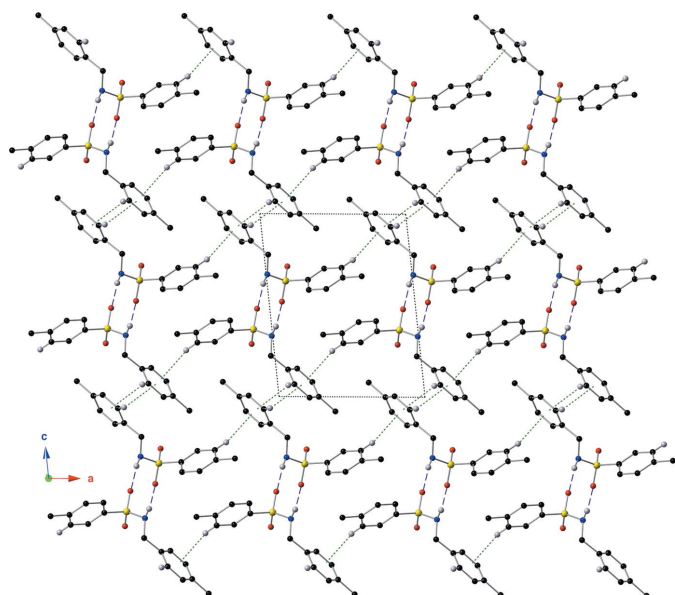


Figure 5

A view down the b axis of the crystal, showing the supramolecular interactions. Hydrogen bonds and contacts are shown with purple dashed lines, and $C-H \cdots \pi$ interactions are shown with green dotted lines. For clarity, only hydrogen atoms involved in a non-covalent interaction are shown, and the intramolecular hydrogen-bonding interactions have been omitted.

4. Database survey

The Cambridge Structural Database (CSD, Version 5.40, Aug 2019; Groom, *et al.*, 2016) contains 11 structures with the N -benzyl- p -toluene sulfonamide moiety. Included in this set is the structure of N -benzyl- p -toluene sulfonamide (BTS, Fig. 1). This structure has been deposited four times as PTSBZA–PTSBZA03 (Cameron, *et al.*, 1975; Yi-Ni, 2014; Bagchi *et al.*, 2014; Valerga & Puerta, 2016). Other structures that are closely related to the title compound are N -(2,4-dimethoxybenzyl)-4-methylbenzenesulfonamide (DERXAA; Hashmi *et al.*, 2006) and 2-(p -tosylaminomethyl)aniline (MILHIZ; Sanmartín *et al.*, 2007). All three crystal structures exhibit intramolecular $C-H \cdots O$ hydrogen bonds, and MILHIZ is the only structure that does not show $C-H \cdots \pi$ interactions.

5. Synthesis and crystallization

The title compound was prepared by the dropwise addition of p -toluenesulfonyl chloride (1.00 g, 5.25 mmol) to a stirring mixture of 4-methylbenzylamine (0.75 ml, 5.90 mmol), pyridine (0.48 ml, 5.90 mmol) and 10 ml of degassed dichloromethane under a nitrogen atmosphere. The reaction mixture was stirred at room temperature for 24 h under a nitrogen atmosphere. The mixture was acidified with 5 M HCl and diluted with 15 ml of dichloromethane. The organic phase was washed with water. The aqueous layers were combined and back extracted with dichloromethane (10 ml). The combined organic layers were dried over anhydrous sodium sulfate and evaporated to dryness. The residue was dissolved in hot ethanol and filtered. The filtrate was transferred to a scintil-

Table 2

Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{17}NO_2S$
M_r	275.35
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	173
a, b, c (Å)	9.655 (2), 5.8820 (15), 12.180 (3)
β (°)	96.275 (3)
V (Å ³)	687.5 (3)
Z	2
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	0.23
Crystal size (mm)	0.49 × 0.22 × 0.16
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
T_{\min} , T_{\max}	0.474, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10794, 2811, 2619
R_{int}	0.047
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.035, 0.092, 1.04
No. of reflections	2811
No. of parameters	178
No. of restraints	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.35, -0.21
Absolute structure	Flack x determined using 1114 quotients $[(I^+) - (I^-)] / [(I^+) + (I^-)]$ (Parsons <i>et al.</i> , 2013)
Absolute structure parameter	0.06 (4)

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXS* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009; Bourhis *et al.*, 2015) and *CrystalMaker* (Palmer, 2007).

lation vial and, upon standing for 24 h, crystallized to afford pale-yellow crystals that were filtered from the mother liquor (42%; m.p. 376–378 K).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All hydrogen atoms bonded to carbon atoms were placed in calculated positions and refined as riding: $C-H = 0.95-1.00$ Å with $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$ for methylene groups and aromatic hydrogen atoms, and $U_{\text{iso}}(H) = 1.5U_{\text{eq}}(C)$ for methyl groups. The hydrogen atom bonded to the nitrogen atom (H1) was located using electron-density difference maps. The N1–H1 bond distance was restrained using *DFIX* instructions in *SHELXL* (Sheldrick, 2015) at 0.88 Å to agree with the known value.

Acknowledgements

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Crystal structure of 4-methyl-*N*-(4-methylbenzyl)benzenesulfonamide

Brock A. Stenfors, Richard J. Staples, Shannon M. Biros and Felix N. Ngassa

Computing details

Data collection: *APEX2* (Bruker, 2013); cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT* (Bruker, 2013); program(s) used to solve structure: *SHELXS* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009; Bourhis *et al.*, 2015); software used to prepare material for publication: *CrystalMaker* (Palmer, 2007).

4-Methyl-*N*-(4-methylbenzyl)benzenesulfonamide

Crystal data

$C_{15}H_{17}NO_2S$

$M_r = 275.35$

Monoclinic, $P2_1$

$a = 9.655$ (2) Å

$b = 5.8820$ (15) Å

$c = 12.180$ (3) Å

$\beta = 96.275$ (3)°

$V = 687.5$ (3) Å³

$Z = 2$

$F(000) = 292$

$D_x = 1.330$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 6778 reflections

$\theta = 2.6$ – 26.4 °

$\mu = 0.23$ mm⁻¹

$T = 173$ K

Block, pale yellow

$0.49 \times 0.22 \times 0.16$ mm

Data collection

Bruker APEXII CCD
diffractometer

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Krause *et al.*, 2015)

$T_{\min} = 0.474$, $T_{\max} = 0.745$

10794 measured reflections

2811 independent reflections

2619 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.047$

$\theta_{\max} = 26.4$ °, $\theta_{\min} = 1.7$ °

$h = -12 \rightarrow 12$

$k = -7 \rightarrow 7$

$l = -15 \rightarrow 15$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.035$

$wR(F^2) = 0.092$

$S = 1.04$

2811 reflections

178 parameters

2 restraints

Primary atom site location: structure-invariant
direct methods

Hydrogen site location: mixed

H atoms treated by a mixture of independent
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0564P)^2 + 0.0356P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.35$ e Å⁻³

$\Delta\rho_{\min} = -0.21$ e Å⁻³

Absolute structure: Flack x determined using

1114 quotients $[(I^+) - (I^-)] / [(I^+) + (I^-)]$ (Parsons *et al.*, 2013)

Absolute structure parameter: 0.06 (4)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.12783 (6)	0.74015 (12)	0.63296 (5)	0.03224 (19)
O1	0.0878 (2)	0.7954 (4)	0.51967 (17)	0.0460 (6)
O2	0.1502 (2)	0.9174 (4)	0.71256 (18)	0.0414 (5)
N1	0.0070 (2)	0.5761 (4)	0.66826 (19)	0.0323 (5)
H1	-0.028 (3)	0.485 (5)	0.617 (2)	0.040 (9)*
C1	0.2818 (3)	0.5768 (5)	0.6401 (2)	0.0307 (6)
C2	0.2808 (3)	0.3720 (5)	0.5847 (2)	0.0344 (6)
H2	0.1980	0.3194	0.5432	0.041*
C3	0.4009 (3)	0.2447 (6)	0.5903 (2)	0.0352 (6)
H3	0.4007	0.1047	0.5514	0.042*
C4	0.5223 (3)	0.3174 (5)	0.6518 (2)	0.0323 (6)
C5	0.5210 (3)	0.5225 (6)	0.7066 (2)	0.0381 (7)
H5	0.6036	0.5745	0.7486	0.046*
C6	0.4011 (3)	0.6544 (5)	0.7014 (2)	0.0358 (6)
H6	0.4012	0.7955	0.7394	0.043*
C7	0.6530 (3)	0.1762 (6)	0.6601 (3)	0.0434 (8)
H7A	0.6287	0.0170	0.6440	0.065*
H7B	0.7013	0.1882	0.7349	0.065*
H7C	0.7141	0.2316	0.6067	0.065*
C8	0.0272 (3)	0.4685 (5)	0.7768 (2)	0.0334 (6)
H8A	0.1206	0.5097	0.8131	0.040*
H8B	0.0248	0.3014	0.7671	0.040*
C9	-0.0812 (3)	0.5358 (5)	0.8516 (2)	0.0298 (6)
C10	-0.1137 (3)	0.3858 (5)	0.9318 (2)	0.0340 (6)
H10	-0.0709	0.2403	0.9371	0.041*
C11	-0.2081 (3)	0.4445 (5)	1.0049 (2)	0.0370 (6)
H11	-0.2292	0.3385	1.0595	0.044*
C12	-0.2721 (3)	0.6552 (5)	0.9995 (2)	0.0351 (6)
C13	-0.2383 (3)	0.8054 (5)	0.9192 (2)	0.0343 (6)
H13	-0.2810	0.9511	0.9139	0.041*
C14	-0.1435 (2)	0.7477 (6)	0.8463 (2)	0.0321 (5)
H14	-0.1212	0.8544	0.7924	0.038*
C15	-0.3752 (3)	0.7190 (7)	1.0793 (2)	0.0451 (7)
H15A	-0.4628	0.6372	1.0597	0.068*
H15B	-0.3925	0.8831	1.0753	0.068*
H15C	-0.3370	0.6779	1.1545	0.068*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0313 (3)	0.0305 (3)	0.0357 (3)	0.0031 (3)	0.0072 (2)	0.0024 (3)
O1	0.0453 (11)	0.0546 (16)	0.0393 (11)	0.0127 (10)	0.0100 (9)	0.0138 (10)
O2	0.0414 (11)	0.0331 (11)	0.0510 (13)	0.0007 (9)	0.0112 (9)	-0.0031 (10)
N1	0.0286 (11)	0.0358 (13)	0.0332 (12)	-0.0018 (10)	0.0060 (9)	-0.0034 (10)
C1	0.0282 (12)	0.0313 (14)	0.0334 (14)	0.0010 (10)	0.0076 (10)	0.0040 (12)
C2	0.0310 (13)	0.0343 (16)	0.0375 (15)	-0.0029 (11)	0.0023 (11)	-0.0027 (13)
C3	0.0380 (13)	0.0316 (13)	0.0369 (13)	0.0002 (14)	0.0076 (10)	-0.0011 (14)
C4	0.0288 (12)	0.0387 (15)	0.0310 (13)	0.0007 (11)	0.0103 (10)	0.0058 (11)
C5	0.0307 (13)	0.0430 (17)	0.0406 (16)	-0.0066 (12)	0.0041 (11)	-0.0015 (14)
C6	0.0357 (14)	0.0334 (14)	0.0387 (15)	-0.0054 (12)	0.0059 (11)	-0.0037 (12)
C7	0.0346 (14)	0.0469 (19)	0.0500 (17)	0.0068 (13)	0.0103 (12)	0.0019 (14)
C8	0.0310 (12)	0.0303 (14)	0.0397 (15)	0.0033 (11)	0.0079 (11)	0.0023 (12)
C9	0.0259 (12)	0.0294 (14)	0.0339 (14)	-0.0035 (10)	0.0030 (10)	-0.0044 (11)
C10	0.0332 (13)	0.0307 (14)	0.0375 (15)	0.0025 (11)	0.0013 (11)	0.0007 (12)
C11	0.0386 (14)	0.0362 (16)	0.0369 (15)	-0.0014 (12)	0.0072 (12)	0.0041 (12)
C12	0.0302 (13)	0.0417 (16)	0.0334 (14)	-0.0010 (12)	0.0037 (10)	-0.0062 (12)
C13	0.0285 (12)	0.0301 (15)	0.0443 (16)	-0.0001 (10)	0.0037 (11)	-0.0047 (12)
C14	0.0292 (11)	0.0284 (13)	0.0394 (13)	-0.0022 (13)	0.0068 (10)	0.0027 (15)
C15	0.0401 (14)	0.052 (2)	0.0458 (16)	0.0010 (16)	0.0152 (12)	-0.0031 (18)

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

S1—O1	1.429 (2)	C7—H7C	0.9800
S1—O2	1.424 (2)	C8—H8A	0.9900
S1—N1	1.608 (2)	C8—H8B	0.9900
S1—C1	1.764 (3)	C8—C9	1.513 (4)
N1—H1	0.865 (13)	C9—C10	1.378 (4)
N1—C8	1.460 (4)	C9—C14	1.382 (4)
C1—C2	1.380 (4)	C10—H10	0.9500
C1—C6	1.380 (4)	C10—C11	1.385 (4)
C2—H2	0.9500	C11—H11	0.9500
C2—C3	1.375 (4)	C11—C12	1.383 (4)
C3—H3	0.9500	C12—C13	1.383 (4)
C3—C4	1.388 (4)	C12—C15	1.513 (4)
C4—C5	1.379 (4)	C13—H13	0.9500
C4—C7	1.504 (4)	C13—C14	1.385 (4)
C5—H5	0.9500	C14—H14	0.9500
C5—C6	1.389 (4)	C15—H15A	0.9800
C6—H6	0.9500	C15—H15B	0.9800
C7—H7A	0.9800	C15—H15C	0.9800
C7—H7B	0.9800		
O1—S1—N1	105.50 (13)	H7B—C7—H7C	109.5
O1—S1—C1	108.00 (12)	N1—C8—H8A	108.9
O2—S1—O1	119.71 (14)	N1—C8—H8B	108.9

O2—S1—N1	108.51 (12)	N1—C8—C9	113.5 (2)
O2—S1—C1	107.52 (13)	H8A—C8—H8B	107.7
N1—S1—C1	106.98 (13)	C9—C8—H8A	108.9
S1—N1—H1	115 (2)	C9—C8—H8B	108.9
C8—N1—S1	118.26 (18)	C10—C9—C8	119.1 (2)
C8—N1—H1	113 (2)	C10—C9—C14	118.6 (2)
C2—C1—S1	119.3 (2)	C14—C9—C8	122.3 (2)
C6—C1—S1	119.7 (2)	C9—C10—H10	119.6
C6—C1—C2	121.0 (3)	C9—C10—C11	120.9 (3)
C1—C2—H2	120.3	C11—C10—H10	119.6
C3—C2—C1	119.3 (3)	C10—C11—H11	119.5
C3—C2—H2	120.3	C12—C11—C10	120.9 (3)
C2—C3—H3	119.4	C12—C11—H11	119.5
C2—C3—C4	121.1 (3)	C11—C12—C15	120.9 (3)
C4—C3—H3	119.4	C13—C12—C11	117.9 (3)
C3—C4—C7	121.3 (3)	C13—C12—C15	121.2 (3)
C5—C4—C3	118.6 (3)	C12—C13—H13	119.3
C5—C4—C7	120.2 (3)	C12—C13—C14	121.3 (3)
C4—C5—H5	119.4	C14—C13—H13	119.3
C4—C5—C6	121.2 (3)	C9—C14—C13	120.4 (3)
C6—C5—H5	119.4	C9—C14—H14	119.8
C1—C6—C5	118.8 (3)	C13—C14—H14	119.8
C1—C6—H6	120.6	C12—C15—H15A	109.5
C5—C6—H6	120.6	C12—C15—H15B	109.5
C4—C7—H7A	109.5	C12—C15—H15C	109.5
C4—C7—H7B	109.5	H15A—C15—H15B	109.5
C4—C7—H7C	109.5	H15A—C15—H15C	109.5
H7A—C7—H7B	109.5	H15B—C15—H15C	109.5
H7A—C7—H7C	109.5		

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

Cg is the centroid of the C9–C14 ring

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C6—H6 \cdots O2	0.95	2.51	2.890 (4)	104
N1—H1 \cdots O1 ⁱ	0.86 (1)	2.03 (2)	2.889 (3)	170 (3)
C5—H5 \cdots Cg ⁱⁱ	0.95	2.86	3.761 (3)	159
C10—H10 \cdots Cg ⁱⁱⁱ	0.95	2.89	3.564 (3)	129

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