

Crystal structure of 1-[(4-methylphenyl)sulfonyl]-2-phenylazetidine

Berthy J. Aroche, Katherine Barraza Hernandez, Zoe Y. Marr, S. Chantal E. Stieber and Taylor A. Thane*

Department of Chemistry & Biochemistry, California State Polytechnic University, Pomona, 3801 W. Temple Ave., Pomona, CA 91768, USA. *Correspondence e-mail: tathane@cpp.edu

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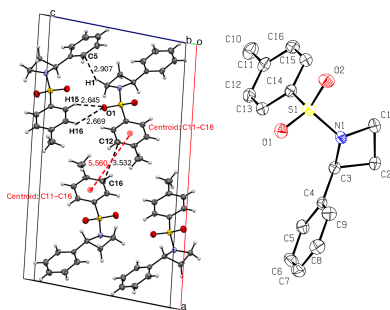
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The crystal structure of 1-[(4-methylphenyl)sulfonyl]-2-phenylazetidine, $C_{16}H_{17}NO_2S$, commonly referred to as 2-phenyl-*N*-tosylazetidine, is reported. There are three close contacts stabilizing the supramolecular structure. Two of the close contacts are between one of the O atoms on the sulfonamide moiety and two neighboring C—H bonds from the tolyl ring. The third close contact is between the H—C bond of the azetidine and a C atom on the phenyl ring. Distances between the tolyl rings are greater than the standard distance of 5 Å for π -stacking.

1. Chemical context

Azetidines, highly strained four-membered nitrogen-containing heterocycles, serve as unique linchpin motifs due to their prevalence in biologically relevant compounds and their propensity for ring-opening reaction pathways (Alberto *et al.*, 2008). As such, the synthesis of new azetidine motifs is necessary for the development of novel pharmaceutical and agrochemical compounds and has garnered a resurging interest by synthetic and medicinal chemists alike (Bauer *et al.*, 2021). This resurgence is due to unique physiochemical and pharmacokinetic properties which make them attractive targets for drug development (Cheekatla, 2026). As such, azetidines are used strategically in drug development as bioisosteres for their five- and six-membered ring counterparts, such as piperidines and pyrrolidines (Feskov *et al.*, 2019; Meanwell & Loiseleur, 2022; Kirichock *et al.*, 2024). This renewed interest in the azetidine moiety is evident by the increased number of FDA approved drugs that contain an azetidine moiety over the last ten years (Gelato *et al.*, 2026). Examples of small-molecule drugs that contain an azetidine moiety include tebanicline, a non-opioid analgesic, ximelagatran, an anti-coagulant, and delafloxacin, an antibiotic (Parmar *et al.*, 2021; Mughal & Szostak, 2021).

Efficient synthetic approaches that install the azetidine motif are required to meet the demand of medicinal chemists. The most common strategies include intramolecular nucleophilic substitution reactions and UV- or blue-light-mediated aza-Paternò–Büchi reactions (Brandi *et al.*, 2008; Richardson *et al.*, 2020). Another common approach to accessing azetidine motifs includes functionalizing 3-azetidinones which allows for a variety of functionalization reactions, such as a Wittig addition or Grignard addition at the ketone (Dejaegher *et al.*, 2002). Alternatively, 2-azetidinones, which are building blocks for β -lactams, can be reduced to yield the desired azetidine (Alcaide *et al.*, 2013). Cumulatively, these synthetic methods

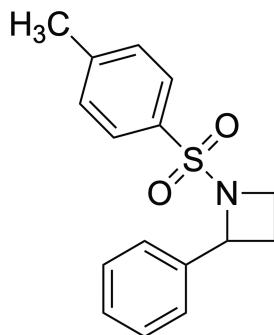


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rely on pre-functionalized starting materials and classic synthetic approaches.

Herein, we report the crystal structure of 1-[(4-methylphenyl)sulfonyl]-2-phenylazetidine (2-phenyl-*N*-tosylazetidine). 2-Phenyl-*N*-tosylazetidine was synthesized *via* a two-step synthesis from β -phenylalanine. β -Phenylalanine was subjected to a lithium aluminium hydride reduction in quantitative yield and was carried forward without further purification into an intramolecular substitution reaction which yielded the desired 2-phenyl-*N*-tosylazetidine.



2. Structural commentary

The structural features for 2-phenyl-*N*-tosylazetidine as shown in Fig. 1 are reported below. The bond lengths of the azetidine ring are N1—C1 = 1.500 (2) Å, N1—C3 = 1.499 (2) Å, C1—C2 = 1.539 (3) Å, and C2—C3 = 1.552 (3) Å. The bond distances within the azetidine ring are consistent with literature reports (Taggi *et al.*, 2000). A related compound, 2-(4-bromophenyl)-1-[(4-methylphenyl)sulfonyl]azetidine, reports C—N bond lengths of 1.567 and 1.488 Å, respectively, and C—C bond lengths of 1.648 and 1.474 Å, which are consistent with the title compound (Malik & Pandey, 2022). The bond

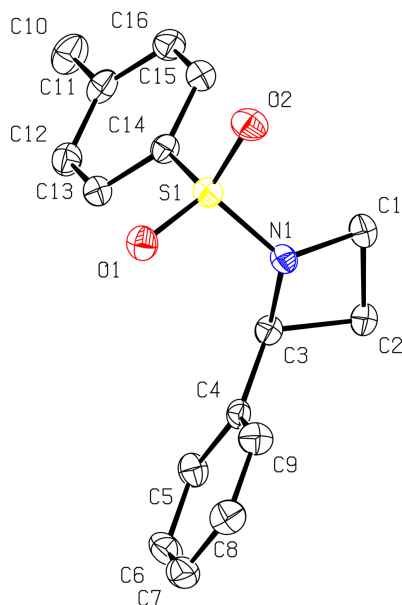


Figure 1

View of one 2-phenyl-*N*-tosylazetidine molecule drawn with 50% probability displacement ellipsoids.

lengths of the sulfonamide are N1—S1 = 1.6319 (16) Å, S1—O1 = 1.4340 (14) Å, S1—O2 = 1.4361 (14) Å, and S1—C14 = 1.761 (2) Å. The bond lengths of the S atom on the sulfonamide moiety are consistent with literature values from prior reports (Syed *et al.*, 2011). Similar bond lengths for the sulfonamide group of the related compound are reported as follows: S—N = 1.611 Å, S—C = 1.749 Å, S—O1 = 1.462 Å, and S—O2 = 1.452 Å (Malik & Pandey, 2022).

The bond angles within the azetidine ring are C3—N1—C1 = 91.48 (14)°, N1—C1—C2 = 87.70 (14)°, C1—C2—C3 = 88.04 (14)°, and N1—C3—C2 = 87.29 (13)°, which are consistent with prior reports for *N*-tosylazetidines (Taggi *et al.*, 2000). The related compound 2-(4-bromophenyl)-1-[(4-methylphenyl)sulfonyl]azetidine reports similar bond angles within the azetidine moiety, with a C—N—C bond angle of 93.21° (Malik & Pandey, 2022). The bond angles around the S atom of the sulfonamide moiety are O1—S1—O2 = 120.64 (9)°, O1—S1—N1 = 106.31 (8)°, O1—S1—C14 = 107.76 (9)°, O2—S1—N1 = 105.86 (8)°, O2—S1—C14 = 108.26 (9)°, and N1—S1—C14 = 107.25 (9)°, which are also consistent with prior reports (Syed *et al.*, 2011). Bond angles around the sulfonamide moiety of the related compound include an O—S—O angle of 121.94°, O—S—N angles of 98.82 and 112.22°, and a C—S—N angle of 107.09° which are consistent with the title compound (Malik & Pandey, 2022)

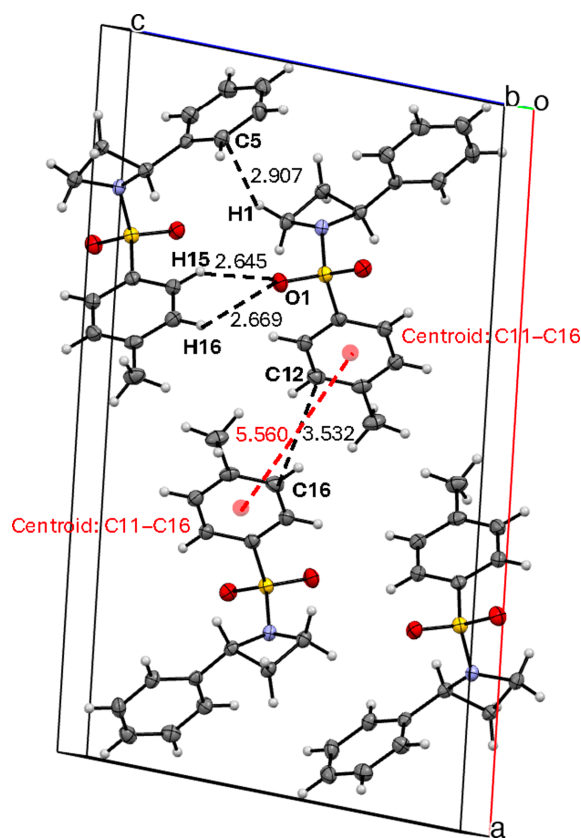


Figure 2

The unit cell with 50% probability displacement ellipsoids shows four 2-phenyl-*N*-tosylazetidine molecules. Molecular distances and close contacts (Å) are represented in black. Distances between centroids (red circles) are calculated.

3. Supramolecular features

Four 2-phenyl-*N*-tosylazetidine molecules are shown in the unit cell (Fig. 2). Three H...*X* bonds stabilize the supramolecular structure, with the corresponding distances indicating hydrogen-bonding interactions. The H15...O1 interaction is at a distance of 2.645 Å, the H16...O1 interaction is at a distance of 2.669 Å, and the H1...C5 interaction is at a distance of 2.907 Å. Additionally, there is a relatively close C12...C13 distance of 3.532 Å. The distance between the centroid of the C11–C16 aryl ring and another C11–C16 centroid on a neighboring molecule is 5.560 Å, which is outside the range expected for π -stacking (Janiak, 2000). The centroid algorithm in the program *Mercury* was used to place the centroids resulting in the measured distance (Macrae *et al.*, 2020).

4. Database survey

A database search in the Cambridge Structural Database (WebCSD, Version of 2026) on 15 June 2026 produced no structural results (Groom *et al.*, 2016). Additionally, a search in *Scifinder* (Scifinder, 2026) yielded a compound match for the racemic compound 1-[(4-methylphenyl)sulfonyl]-2-phenylazetidine (code 38455-36-6). Matches for both the *S* and *R* enantiomers, (2*S*)-1-[(4-methylphenyl)sulfonyl]-2-phenylazetidine (code 936011-91-5) and (2*R*)-1-[(4-methylphenyl)sulfonyl]-2-phenylazetidine (code 1079366-88-3), were also found. While both racemic and enantiopure forms of the structure have been synthesized and characterized, no structural data has been reported. However, a related compound, 2-(4-bromophenyl)-1-[(4-methylphenyl)sulfonyl]azetidine, has been reported with bond angles and bond lengths similar to those determined for the title azetidine, 2-phenyl-*N*-tosylazetidine (deposition No. 762724; Malik & Pandey, 2022).

5. Synthesis and crystallization

2-Phenyl-*N*-tosylazetidine was synthesized in two steps (Fig. 3). The first step was a lithium aluminium hydride reduction of β -phenylalanine that was modified from the literature (Sanford *et al.*, 2020). A flame-dried round-bottomed flask equipped with a stir bar was charged with β -phenylalanine (3.31 g, 20.0 mmol, 1.00 equiv.) and tetrahydrofuran (THF; 100 ml, 0.2 *M* in substrate). The reaction flask was cooled to 0 °C and lithium aluminium hydride (16.5 ml, 66.0 mmol, 3.30 equiv., 4.00 *M* solution in THF) was added dropwise. The reaction flask was warmed to room temperature and stirred overnight. The reaction was worked

up according to the Fieser workup, where *X* ml is equal to *X* grams of LiAlH₄ used (Chandra & Zebrowski, 2024). For example, in this reaction, *X* grams of lithium aluminium hydride equals 2.5 g (66 mmol), so 2.5 ml of water (*X* ml), 2.5 ml of 15% aqueous NaOH solution (*X* ml), and 7.5 ml of water (3*X* ml) were added respectively as described below. The reaction was diluted with neat Et₂O and cooled to 0 °C. Water (2.5 ml, *X* ml) was added slowly, followed by the addition of 15% aqueous NaOH (2.5 ml, *X* ml) and then by a second slow addition of water (7.5 ml, 3*X* ml). The reaction was allowed to warm to room temperature and left to stir for 15 min. MgSO₄ was then added to the reaction mixture and left to stir for an additional 15 min. The precipitates were removed by vacuum filtration and the filtrate was concentrated *in vacuo*. The white solid, γ -aminobenzenepropanol, was carried forward without further purification (2.68 g, 17.8 mmol, 89% yield). ¹H NMR analysis is consistent with literature reports (Torre *et al.*, 2006).

The second step, an intramolecular substitution of γ -aminobenzenepropanol, was also adapted from prior reports (Wang *et al.*, 2026). To a flame-dried round-bottomed flask equipped with a stir bar, NaOH (0.48 g, 12 mmol, 3.0 equiv.) and THF (6 ml, 2 *M* in NaOH) were added. In a separate flame-dried round-bottomed flask, a solution of γ -aminobenzenepropanol (0.61 g, 4.0 mmol, 1.0 equiv.) was dissolved in THF (10 ml, 0.4 *M* in γ -aminobenzenepropanol) and added to the reaction mixture dropwise at room temperature. Next, toluenesulfonic acid (0.84 g, 4.4 mmol, 1.1 equiv.) was added to the reaction mixture in portions. The reaction mixture was then heated to reflux and allowed to stir for 3 h. After completion, the reaction mixture was diluted with cold deionized water (30 ml) and extracted with EtOAc ($\times 3$). The combined organic layers were washed with brine, dried over Na₂SO₄, and concentrated *in vacuo*. The resulting oil was purified by flash column chromatography (0–25% EtOAc/hexanes) to afford a white solid (0.398 g, 1.39 mmol, 35% yield). ¹H NMR analysis is consistent with literature reports (Prasad *et al.*, 2004). The melting-point range was 103–105 °C. A singular crystal was grown *via* vapor diffusion by dissolving 10 mg of 2-phenyl-*N*-tosylazetidine in 0.5 ml of ethyl acetate. Ethyl acetate was used as the solvent and hexanes as the anti-solvent.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. H atoms that were tertiary CH and secondary CH₂ were refined using a riding model. The methyl group was refined as an idealized rotating methyl group. Fixed

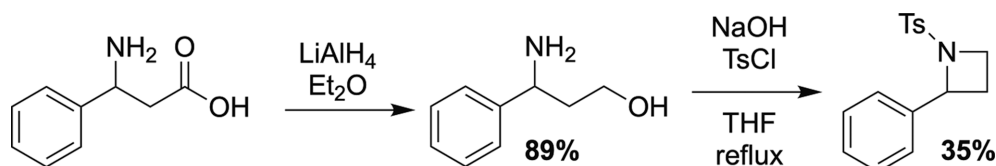


Figure 3
The synthesis of 2-phenyl-*N*-tosylazetidine.

Table 1

Experimental details.

Crystal data	
Chemical formula	C ₁₆ H ₁₇ NO ₂ S
<i>M_r</i>	287.36
Crystal system, space group	Monoclinic, <i>P</i> ₂ /c
Temperature (K)	127
<i>a</i> , <i>b</i> , <i>c</i> (Å)	21.3441 (12), 5.5024 (3), 12.1775 (6)
β (°)	97.856 (2)
<i>V</i> (Å ³)	1416.75 (13)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ^{−1})	0.23
Crystal size (mm)	0.13 × 0.10 × 0.02
Data collection	
Diffractionmeter	Bruker APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; (Bruker, 2016)
<i>T</i> _{min} , <i>T</i> _{max}	0.667, 0.746
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	42002, 3588, 2531
<i>R</i> _{int}	0.114
(sin θ/λ) _{max} (Å ^{−1})	0.671
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.044, 0.112, 1.05
No. of reflections	3588
No. of parameters	182
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ^{−3})	0.24, −0.47

Computer programs: *APEX2* (Bruker, 2019), *SAINT* (Bruker, 2019), *SHELXT2018* (Sheldrick, 2015a), *SHELXL2019* (Sheldrick, 2015b), and *OLEX2* (Dolomanov *et al.*, 2009).

atomic displacement parameters [*U*_{iso}(H)] were set at 1.2 times *U*_{iso}(C) for all CH and CH₂ groups, and 1.5 times for all CH₃ groups.

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Computing details

1-[(4-Methylphenyl)sulfonyl]-2-phenylazetidine

Crystal data

$C_{16}H_{17}NO_2S$

$M_r = 287.36$

Monoclinic, $P2_1/c$

$a = 21.3441$ (12) Å

$b = 5.5024$ (3) Å

$c = 12.1775$ (6) Å

$\beta = 97.856$ (2)°

$V = 1416.75$ (13) Å³

$Z = 4$

$F(000) = 608$

$D_x = 1.347$ Mg m⁻³

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

Cell parameters from 4338 reflections

$\theta = 2.9$ – 26.2°

$\mu = 0.23$ mm⁻¹

$T = 127$ K

Plate, colourless

$0.13 \times 0.10 \times 0.02$ mm

Data collection

Bruker APEXII CCD

diffractometer

φ and ω scans

Absorption correction: multi-scan

(SADABS; (Bruker, 2016))

$T_{\min} = 0.667$, $T_{\max} = 0.746$

42002 measured reflections

3588 independent reflections

2531 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.114$

$\theta_{\max} = 28.5^\circ$, $\theta_{\min} = 2.9^\circ$

$h = -28 \rightarrow 28$

$k = -7 \rightarrow 7$

$l = -16 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.044$

$wR(F^2) = 0.112$

$S = 1.05$

3588 reflections

182 parameters

0 restraints

Primary atom site location: dual

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0334P)^2 + 1.1271P]$

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

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

$\Delta\rho_{\max} = 0.24$ e Å⁻³

$\Delta\rho_{\min} = -0.47$ 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.27972 (2)	0.88010 (8)	0.42309 (4)	0.02094 (13)
O1	0.26099 (7)	1.0097 (2)	0.32175 (11)	0.0257 (3)
O2	0.30263 (7)	1.0082 (3)	0.52331 (11)	0.0289 (3)
N1	0.21746 (7)	0.7304 (3)	0.44931 (12)	0.0200 (3)
C1	0.21859 (10)	0.5633 (4)	0.54692 (16)	0.0239 (4)
H1A	0.203627	0.639064	0.612336	0.029*
H1B	0.259478	0.479016	0.567666	0.029*
C2	0.16829 (9)	0.4087 (4)	0.47600 (15)	0.0228 (4)
H2A	0.124461	0.441139	0.490053	0.027*
H2B	0.177494	0.232241	0.478166	0.027*
C3	0.18662 (9)	0.5398 (3)	0.37217 (15)	0.0196 (4)
H3	0.219346	0.444061	0.339458	0.024*
C4	0.13608 (9)	0.6240 (3)	0.28295 (15)	0.0195 (4)
C5	0.12295 (10)	0.4868 (4)	0.18672 (16)	0.0245 (4)
H5	0.146691	0.343721	0.178011	0.029*
C6	0.07557 (11)	0.5567 (4)	0.10338 (17)	0.0307 (5)
H6	0.066834	0.460759	0.038214	0.037*
C7	0.04093 (10)	0.7656 (4)	0.11469 (17)	0.0297 (5)
H7	0.008537	0.813451	0.057377	0.036*
C8	0.05369 (10)	0.9048 (4)	0.20987 (18)	0.0293 (5)
H8	0.030168	1.048721	0.217865	0.035*
C9	0.10075 (10)	0.8338 (4)	0.29336 (17)	0.0262 (4)
H9	0.109089	0.929486	0.358671	0.031*
C10	0.46824 (11)	0.1036 (4)	0.3375 (2)	0.0353 (5)
H10A	0.508539	0.127096	0.385503	0.053*
H10B	0.475353	0.108096	0.259753	0.053*
H10C	0.450226	−0.054081	0.353719	0.053*
C11	0.42296 (9)	0.3035 (4)	0.35857 (18)	0.0261 (4)
C12	0.38082 (10)	0.3990 (4)	0.27229 (17)	0.0258 (4)
H12	0.381427	0.340038	0.199118	0.031*
C13	0.33794 (9)	0.5783 (4)	0.29077 (16)	0.0236 (4)
H13	0.309414	0.641763	0.230925	0.028*
C14	0.33712 (9)	0.6646 (3)	0.39812 (16)	0.0217 (4)
C15	0.37905 (9)	0.5731 (4)	0.48549 (16)	0.0251 (4)
H15	0.378530	0.632727	0.558586	0.030*
C16	0.42172 (10)	0.3940 (4)	0.46518 (17)	0.0284 (5)
H16	0.450587	0.331957	0.524898	0.034*

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

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0236 (2)	0.0173 (2)	0.0216 (2)	−0.0011 (2)	0.00212 (18)	−0.00076 (19)
O1	0.0297 (8)	0.0205 (7)	0.0271 (8)	0.0012 (6)	0.0047 (6)	0.0052 (6)
O2	0.0332 (8)	0.0251 (8)	0.0272 (8)	−0.0047 (6)	−0.0002 (6)	−0.0081 (6)
N1	0.0232 (8)	0.0200 (8)	0.0169 (8)	−0.0003 (7)	0.0029 (6)	−0.0011 (6)

C1	0.0285 (11)	0.0234 (10)	0.0205 (10)	0.0017 (8)	0.0054 (8)	0.0024 (8)
C2	0.0244 (10)	0.0221 (9)	0.0228 (10)	−0.0013 (8)	0.0069 (8)	0.0015 (8)
C3	0.0216 (10)	0.0170 (8)	0.0209 (9)	−0.0008 (7)	0.0053 (8)	−0.0034 (7)
C4	0.0214 (9)	0.0199 (9)	0.0182 (9)	−0.0037 (8)	0.0058 (7)	0.0013 (8)
C5	0.0300 (11)	0.0221 (10)	0.0222 (10)	0.0009 (8)	0.0059 (8)	−0.0024 (8)
C6	0.0371 (12)	0.0341 (12)	0.0196 (10)	−0.0042 (10)	−0.0004 (9)	−0.0029 (9)
C7	0.0294 (11)	0.0317 (11)	0.0265 (11)	−0.0032 (9)	−0.0011 (9)	0.0076 (9)
C8	0.0286 (11)	0.0244 (10)	0.0345 (12)	0.0022 (9)	0.0035 (9)	0.0022 (9)
C9	0.0273 (11)	0.0232 (10)	0.0278 (11)	0.0018 (8)	0.0028 (9)	−0.0044 (8)
C10	0.0289 (12)	0.0323 (12)	0.0465 (14)	0.0067 (10)	0.0119 (10)	0.0065 (11)
C11	0.0215 (10)	0.0238 (10)	0.0345 (11)	−0.0008 (8)	0.0089 (9)	0.0046 (9)
C12	0.0257 (10)	0.0272 (10)	0.0255 (10)	−0.0010 (9)	0.0068 (8)	−0.0009 (9)
C13	0.0229 (10)	0.0264 (10)	0.0214 (10)	−0.0005 (8)	0.0031 (8)	0.0022 (8)
C14	0.0210 (10)	0.0216 (9)	0.0228 (10)	−0.0027 (8)	0.0035 (8)	0.0011 (8)
C15	0.0242 (10)	0.0289 (11)	0.0221 (10)	−0.0010 (8)	0.0028 (8)	0.0019 (8)
C16	0.0229 (10)	0.0327 (11)	0.0289 (11)	0.0016 (9)	0.0013 (8)	0.0082 (9)

Geometric parameters (Å, °)

S1—O1	1.4340 (14)	C7—H7	0.9500
S1—O2	1.4361 (14)	C7—C8	1.385 (3)
S1—N1	1.6319 (16)	C8—H8	0.9500
S1—C14	1.761 (2)	C8—C9	1.384 (3)
N1—C1	1.500 (2)	C9—H9	0.9500
N1—C3	1.499 (2)	C10—H10A	0.9800
C1—H1A	0.9900	C10—H10B	0.9800
C1—H1B	0.9900	C10—H10C	0.9800
C1—C2	1.539 (3)	C10—C11	1.509 (3)
C2—H2A	0.9900	C11—C12	1.390 (3)
C2—H2B	0.9900	C11—C16	1.394 (3)
C2—C3	1.552 (3)	C12—H12	0.9500
C3—H3	1.0000	C12—C13	1.385 (3)
C3—C4	1.496 (3)	C13—H13	0.9500
C4—C5	1.390 (3)	C13—C14	1.393 (3)
C4—C9	1.394 (3)	C14—C15	1.388 (3)
C5—H5	0.9500	C15—H15	0.9500
C5—C6	1.386 (3)	C15—C16	1.387 (3)
C6—H6	0.9500	C16—H16	0.9500
C6—C7	1.384 (3)		
O1—S1—O2	120.64 (9)	C7—C6—H6	119.9
O1—S1—N1	106.31 (8)	C6—C7—H7	120.1
O1—S1—C14	107.76 (9)	C6—C7—C8	119.7 (2)
O2—S1—N1	105.86 (8)	C8—C7—H7	120.1
O2—S1—C14	108.26 (9)	C7—C8—H8	120.0
N1—S1—C14	107.35 (9)	C9—C8—C7	119.9 (2)
C1—N1—S1	122.62 (13)	C9—C8—H8	120.0
C3—N1—S1	122.02 (12)	C4—C9—H9	119.5

C3—N1—C1	91.48 (14)	C8—C9—C4	120.92 (19)
N1—C1—H1A	114.0	C8—C9—H9	119.5
N1—C1—H1B	114.0	H10A—C10—H10B	109.5
N1—C1—C2	87.70 (14)	H10A—C10—H10C	109.5
H1A—C1—H1B	111.2	H10B—C10—H10C	109.5
C2—C1—H1A	114.0	C11—C10—H10A	109.5
C2—C1—H1B	114.0	C11—C10—H10B	109.5
C1—C2—H2A	114.0	C11—C10—H10C	109.5
C1—C2—H2B	114.0	C12—C11—C10	120.71 (19)
C1—C2—C3	88.04 (14)	C12—C11—C16	118.45 (19)
H2A—C2—H2B	111.2	C16—C11—C10	120.83 (19)
C3—C2—H2A	114.0	C11—C12—H12	119.3
C3—C2—H2B	114.0	C13—C12—C11	121.36 (19)
N1—C3—C2	87.29 (13)	C13—C12—H12	119.3
N1—C3—H3	110.3	C12—C13—H13	120.4
C2—C3—H3	110.3	C12—C13—C14	119.25 (18)
C4—C3—N1	116.72 (15)	C14—C13—H13	120.4
C4—C3—C2	119.91 (16)	C13—C14—S1	119.32 (15)
C4—C3—H3	110.3	C15—C14—S1	120.18 (15)
C5—C4—C3	119.08 (17)	C15—C14—C13	120.43 (19)
C5—C4—C9	118.51 (18)	C14—C15—H15	120.3
C9—C4—C3	122.40 (17)	C16—C15—C14	119.42 (19)
C4—C5—H5	119.7	C16—C15—H15	120.3
C6—C5—C4	120.64 (19)	C11—C16—H16	119.5
C6—C5—H5	119.7	C15—C16—C11	121.09 (19)
C5—C6—H6	119.9	C15—C16—H16	119.5
C7—C6—C5	120.26 (19)		
S1—N1—C1—C2	−148.20 (13)	C2—C3—C4—C9	77.7 (2)
S1—N1—C3—C2	148.51 (13)	C3—N1—C1—C2	−17.94 (14)
S1—N1—C3—C4	−89.15 (19)	C3—C4—C5—C6	178.66 (18)
S1—C14—C15—C16	176.57 (16)	C3—C4—C9—C8	−179.05 (19)
O1—S1—N1—C1	177.47 (14)	C4—C5—C6—C7	0.5 (3)
O1—S1—N1—C3	61.59 (16)	C5—C4—C9—C8	−0.1 (3)
O1—S1—C14—C13	−25.47 (18)	C5—C6—C7—C8	−0.1 (3)
O1—S1—C14—C15	157.66 (15)	C6—C7—C8—C9	−0.3 (3)
O2—S1—N1—C1	−53.09 (16)	C7—C8—C9—C4	0.4 (3)
O2—S1—N1—C3	−168.98 (14)	C9—C4—C5—C6	−0.3 (3)
O2—S1—C14—C13	−157.47 (15)	C10—C11—C12—C13	178.42 (19)
O2—S1—C14—C15	25.65 (19)	C10—C11—C16—C15	−178.3 (2)
N1—S1—C14—C13	88.67 (17)	C11—C12—C13—C14	0.0 (3)
N1—S1—C14—C15	−88.21 (17)	C12—C11—C16—C15	0.8 (3)
N1—C1—C2—C3	17.31 (14)	C12—C13—C14—S1	−176.44 (15)
N1—C3—C4—C5	155.55 (17)	C12—C13—C14—C15	0.4 (3)
N1—C3—C4—C9	−25.5 (3)	C13—C14—C15—C16	−0.3 (3)
C1—N1—C3—C2	17.79 (14)	C14—S1—N1—C1	62.37 (16)
C1—N1—C3—C4	140.14 (16)	C14—S1—N1—C3	−53.52 (16)
C1—C2—C3—N1	−17.33 (14)	C14—C15—C16—C11	−0.3 (3)

C1—C2—C3—C4	−136.81 (17)	C16—C11—C12—C13	−0.6 (3)
C2—C3—C4—C5	−101.2 (2)		
