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N-Cyclohexyl-4-methoxybenzenesulfonamide

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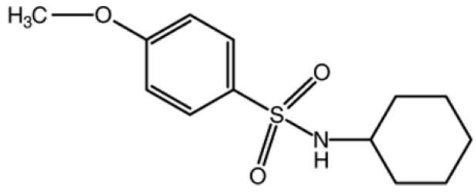
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.048; wR factor = 0.136; data-to-parameter ratio = 16.2.

In the title molecule, $C_{13}H_{19}NO_3S$, the S atom has a distorted tetrahedral geometry with an O—S—O bond angle of 120.39 (18)°. The cyclohexane ring has a chair conformation. In the crystal, molecules are connected by intermolecular N—H···O hydrogen bonds, forming zigzag hydrogen-bonded chains directed along the *c* axis.

Related literature

For background to the biological activity of sulfonamides, see: Gennarti *et al.* (1994); Hanson *et al.* (1999); Moree *et al.* (1991); Ozbek *et al.* (2007); Rough *et al.* (1998); Siddiqui *et al.* (2007). For literature on sulfonamide derivatives, see: Akkurt *et al.* (2011); Aziz-ur-Rehman, Rafique *et al.* (2010); Aziz-ur-Rehman, Sajjad *et al.* (2010); Aziz-ur-Rehman, Siddiqa *et al.* (2010); Khan, Akkurt *et al.* (2010); Khan, Sharif *et al.* (2010). For puckering parameters, see: Cremer & Pople (1975).



Experimental

Crystal data

$C_{13}H_{19}NO_3S$
M_r = 269.36
Orthorhombic, *Aba*2
a = 17.2644 (12) Å
b = 20.4707 (16) Å
c = 7.9139 (5) Å
V = 2796.9 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 296 K
0.29 × 0.12 × 0.09 mm

Data collection

Bruker APEXII CCD diffractometer
10601 measured reflections
2704 independent reflections
1945 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.136
S = 1.02
2704 reflections
167 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}
Absolute structure: Flack (1983), 829 Freidel pairs
Flack parameter: −0.05 (12)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H*N*1···O2^{i}	0.85 (3)	2.09 (3)	2.913 (4)	161 (3)

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5173).

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N-Cyclohexyl-4-methoxybenzenesulfonamide

Muneeb Hayat Khan, Islam Ullah Khan, Muhammad Nadeem Arshad, Shumaila Younas Mughal and Mehmet Akkurt

S1. Comment

Sulfonamides are familiar for their enormous potential as biologically active molecules (Hanson *et al.*, 1999; Moree *et al.*,1991; Rough *et al.*, 1998). They are being used as anti-microbial (Ozbek *et al.*, 2007), anti-convulsant (Siddiqui *et al.*, 2007), and for the treatment of inflammatory rheumatic and non-rheumatic processes including onsets and traumatologic lesions (Gennarti *et al.*, 1994). In continuation of our structural studies on various sulfonamide derivatives, herein we report the crystal structure of the title compound (I) (Akkurt *et al.*, 2011; Aziz-ur-Rehman, Rafique *et al.*, 2010; Aziz-ur-Rehman, Sajjad *et al.*, 2010; Aziz-ur-Rehman, Siddiqa *et al.*, 2010; Khan, Akkurt *et al.*, 2010; Khan, Sharif *et al.*, 2010).

As shown in Fig. 1, the S atom of the title molecule has a distorted tetrahedral coordination geometry, with S1—O1 = 1.424 (3), S1—O2 = 1.436 (3), S1— N1 = 1.586 (3), S1—C7 = 1.747 (4) Å, O1—S1—O2 = 120.39 (18), O1—S1—N1 = 108.09 (16), O1—S1—C7 = 107.08 (16), O2—S1—N1 = 105.37 (16), O2—S1—C7 = 106.18 (15) and N1— S1—C7 = 109.43 (16)°. The cyclohexane ring (C1–C6) has an almost ideal chair conformation and the ring-puckering parameters (Cremer & Pople, 1975) are Q_T = 0.559 (4) Å, θ = 1.8 (4) ° and φ = 338 (9)°.

In the crystal structure, adjacent molecules form zigzag hydrogen-bonded chains directed along the *c* axis, linking by intermolecular N—H···O hydrogen bonds (Table 1). The packing and hydrogen bonding of (I) are viewed down a, b and c axes, respectively, in Figs. 2, 3 and 4.

S2. Experimental

Cylcohexylamine (0.5 g, 6.494 mmol) was taken in 50 ml round bottom flask and added 10 ml of distilled water. After 5 minutes stirring at room temperature 4-methoxy benzene sulfonyl chloride was carefully added. The pH of the reaction mixture was maintained at 8 with 10% Na_2CO_3 solution. After 6 h of stirring at room temperature the TLC check confirmed the completion of the reaction. The reaction mixture pH was reduced to 3 with 3 M HCl, product precipitated out was filtered and dried. Dried precipitates were dissolved in methanol for crystallization (yield: 87%).

S3. Refinement

In the last cycles of the refinement, 3 reflections (2 0 0), (1 2 0) and (0 2 0) were eliminated due to being poorly measured in the vicinity of the beam stop. The H atom of the NH group of the title compound was located in a difference map and refined with the distance restraint N—H = 0.86 (2) Å; its isotropic displacement parameter was set to be 1.2U_{eq}(N). The aromatic, methine, methylene and methyl H atoms were positioned geometrically with C—H = 0.93 - 0.98 Å, and allowed to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C) for aromatic, methylene and methine, and 1.5U_{eq}(C) for methyl.

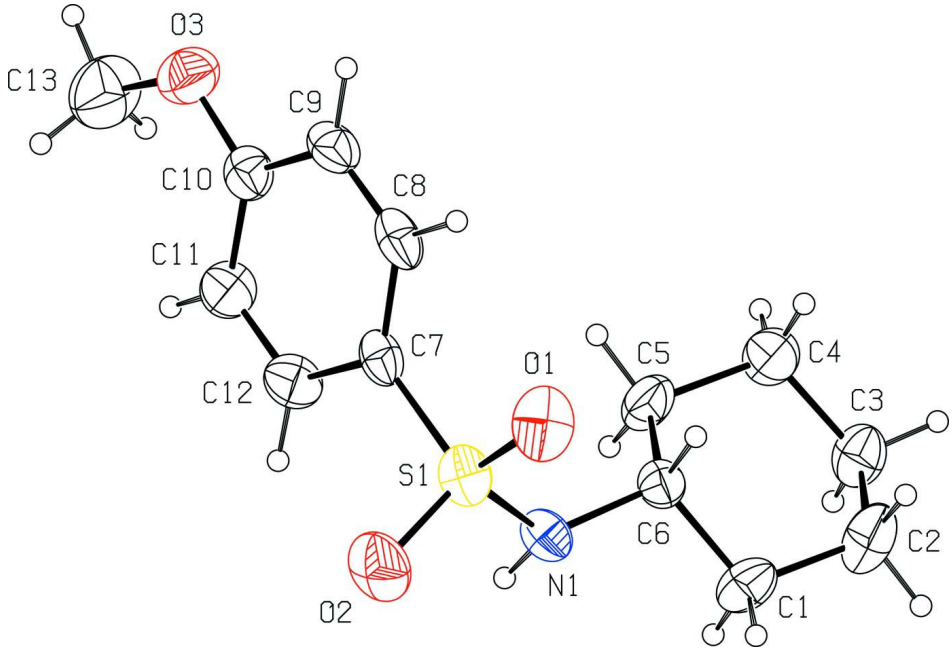

Figure 1

View of the title molecule, with atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level.

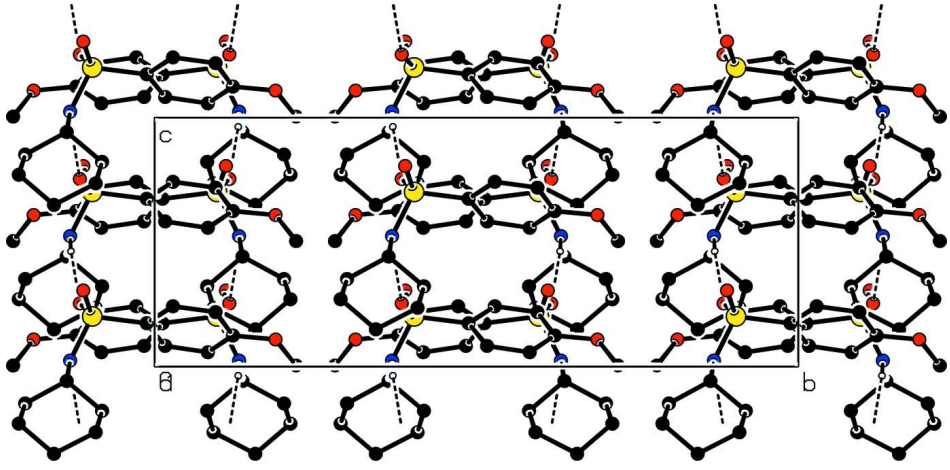

Figure 2

The packing and hydrogen bonding of (I) viewed down *a* axis. Hydrogen atoms that not involved in the hydrogen-bonding (dashed lines) have been omitted for clarity.

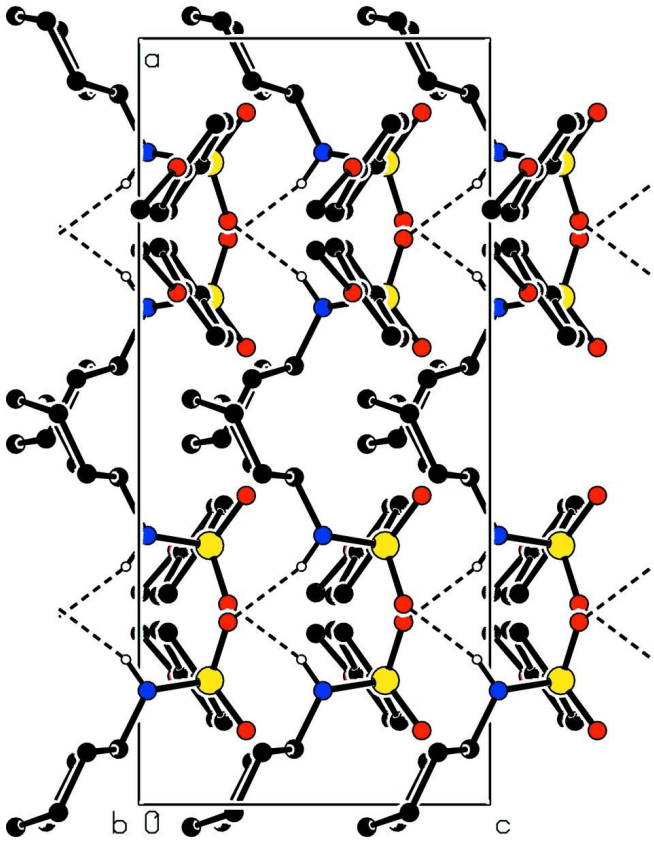

Figure 3

The packing and hydrogen bonding of (I) viewed down *b* axis. Hydrogen atoms that not involved in the hydrogen-bonding (dashed lines) have been omitted for clarity.

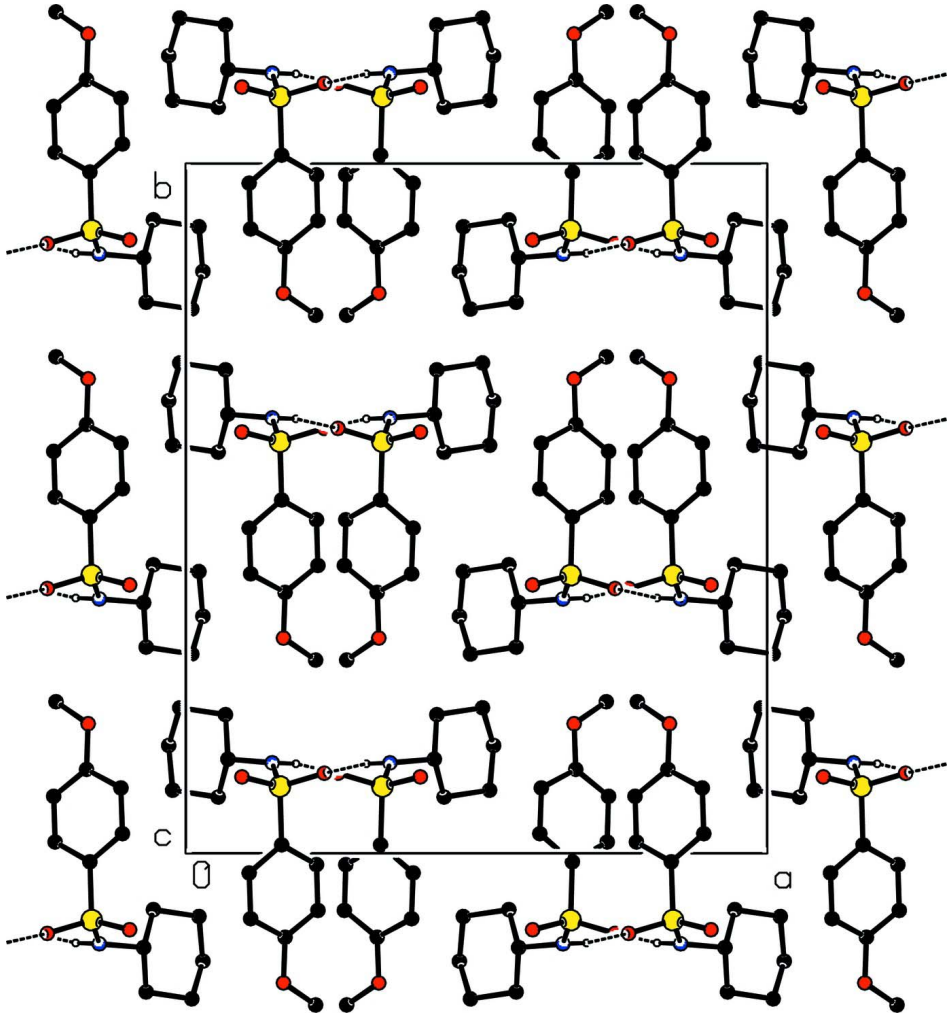

Figure 4

The packing and hydrogen bonding of (I) viewed down *c* axis. Hydrogen atoms that not involved in the hydrogen-bonding (dashed lines) have been omitted for clarity.

N-Cyclohexyl-4-methoxybenzenesulfonamide

Crystal data

$C_{13}H_{19}NO_3S$
$M_r = 269.36$
Orthorhombic, *Aba*2
Hall symbol: A 2 -2ac
$a = 17.2644\ (12)$ Å
$b = 20.4707\ (16)$ Å
$c = 7.9139\ (5)$ Å
$V = 2796.9\ (3)$ Å^3
$Z = 8$
$F(000) = 1152$
$D_x = 1.279$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3418 reflections
$\theta = 2.3–24.7°$
$\mu = 0.23$ mm^{-1}
$T = 296$ K
Prism, light brown
0.29 × 0.12 × 0.09 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
10601 measured reflections
2704 independent reflections
1945 reflections with $I > 2\sigma(I)$
$R_{int} = 0.047$
$\theta_{max} = 28.3°$, $\theta_{min} = 3.0°$
$h = -23 \rightarrow 23$
$k = -23 \rightarrow 27$
$l = -10 \rightarrow 6$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.136$
$S = 1.02$
2704 reflections
167 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0633P)^2 + 1.387P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}
Absolute structure: Flack (1983), 829 Freidel pairs
Absolute structure parameter: −0.05 (12)

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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	0.16185 (4)	0.09694 (5)	0.20157 (12)	0.0614 (3)
O1	0.09659 (16)	0.11080 (14)	0.3056 (4)	0.0832 (11)
O2	0.23822 (17)	0.11611 (14)	0.2537 (4)	0.0901 (11)
O3	0.16806 (14)	−0.18793 (14)	0.1087 (4)	0.0822 (11)
N1	0.14869 (13)	0.13120 (14)	0.0241 (4)	0.0556 (10)
C1	0.0682 (2)	0.20104 (16)	−0.1482 (5)	0.0697 (15)
C2	−0.0103 (3)	0.21102 (18)	−0.2295 (6)	0.0850 (16)
C3	−0.0294 (2)	0.15634 (19)	−0.3505 (5)	0.0710 (16)
C4	−0.0226 (2)	0.09157 (18)	−0.2642 (6)	0.0783 (16)
C5	0.0557 (2)	0.08162 (16)	−0.1777 (6)	0.0724 (13)
C6	0.07253 (15)	0.13658 (15)	−0.0581 (4)	0.0501 (10)
C7	0.16495 (15)	0.01229 (17)	0.1741 (4)	0.0515 (10)
C8	0.10900 (15)	−0.0285 (2)	0.2421 (4)	0.0613 (13)
C9	0.11159 (16)	−0.09474 (19)	0.2187 (5)	0.0621 (11)
C10	0.17072 (17)	−0.12166 (19)	0.1247 (5)	0.0576 (11)

C11	0.22723 (18)	−0.08270 (18)	0.0575 (6)	0.0693 (16)
C12	0.22479 (17)	−0.01640 (19)	0.0830 (5)	0.0694 (15)
C13	0.2233 (3)	−0.2198 (2)	0.0041 (8)	0.111 (2)
HN1	0.1894 (15)	0.1299 (18)	−0.037 (4)	0.0740*
H1A	0.10810	0.20280	−0.23440	0.0840*
H1B	0.07780	0.23610	−0.06840	0.0840*
H2A	−0.04970	0.21310	−0.14230	0.1020*
H2B	−0.01050	0.25220	−0.29000	0.1020*
H3A	−0.08170	0.16190	−0.39270	0.0860*
H3B	0.00570	0.15780	−0.44610	0.0860*
H4A	−0.03020	0.05720	−0.34680	0.0940*
H4B	−0.06340	0.08780	−0.18040	0.0940*
H5A	0.05530	0.04060	−0.11610	0.0870*
H5B	0.09620	0.07930	−0.26240	0.0870*
H6	0.03280	0.13630	0.03040	0.0600*
H8	0.06880	−0.01050	0.30500	0.0740*
H9	0.07370	−0.12140	0.26590	0.0750*
H11	0.26720	−0.10110	−0.00540	0.0830*
H12	0.26380	0.00980	0.03860	0.0830*
H13A	0.22010	−0.20250	−0.10840	0.1670*
H13B	0.21260	−0.26580	0.00190	0.1670*
H13C	0.27430	−0.21260	0.04830	0.1670*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0628 (4)	0.0785 (6)	0.0429 (4)	0.0052 (4)	−0.0071 (4)	−0.0091 (5)
O1	0.0961 (19)	0.106 (2)	0.0476 (16)	0.0250 (15)	0.0154 (14)	−0.0076 (15)
O2	0.0793 (17)	0.107 (2)	0.084 (2)	−0.0051 (15)	−0.0333 (15)	−0.0189 (17)
O3	0.0877 (18)	0.0690 (18)	0.090 (2)	−0.0011 (13)	0.0110 (15)	0.0140 (15)
N1	0.0457 (13)	0.0707 (19)	0.0503 (17)	−0.0032 (12)	0.0027 (11)	−0.0033 (14)
C1	0.096 (3)	0.0442 (18)	0.069 (3)	−0.0004 (17)	−0.0043 (19)	−0.0053 (19)
C2	0.110 (3)	0.066 (2)	0.079 (3)	0.024 (2)	−0.020 (2)	0.002 (2)
C3	0.082 (2)	0.074 (3)	0.057 (3)	0.0093 (19)	−0.0133 (18)	0.0056 (19)
C4	0.082 (2)	0.064 (2)	0.089 (4)	−0.0068 (18)	−0.033 (2)	0.000 (2)
C5	0.086 (2)	0.0413 (18)	0.090 (3)	0.0029 (17)	−0.028 (2)	−0.0018 (19)
C6	0.0466 (14)	0.057 (2)	0.0467 (18)	0.0002 (12)	0.0011 (13)	0.0052 (14)
C7	0.0403 (13)	0.075 (2)	0.0391 (19)	0.0071 (13)	−0.0031 (12)	0.0041 (15)
C8	0.0380 (14)	0.098 (3)	0.048 (2)	0.0078 (15)	0.0035 (13)	0.0058 (18)
C9	0.0442 (14)	0.084 (2)	0.058 (2)	−0.0074 (15)	0.0043 (16)	0.016 (2)
C10	0.0542 (18)	0.070 (2)	0.0487 (19)	0.0028 (16)	−0.0023 (15)	0.0097 (17)
C11	0.064 (2)	0.074 (3)	0.070 (3)	0.0076 (17)	0.0265 (19)	0.007 (2)
C12	0.0581 (19)	0.082 (3)	0.068 (3)	−0.0029 (16)	0.0222 (17)	0.009 (2)
C13	0.122 (4)	0.091 (3)	0.121 (5)	0.019 (3)	0.035 (3)	−0.009 (3)

Geometric parameters (Å, º)

S1—O1	1.424 (3)	C11—C12	1.373 (5)
S1—O2	1.436 (3)	C1—H1A	0.9700
S1—N1	1.586 (3)	C1—H1B	0.9700
S1—C7	1.747 (4)	C2—H2A	0.9700
O3—C10	1.363 (5)	C2—H2B	0.9700
O3—C13	1.421 (6)	C3—H3A	0.9700
N1—C6	1.471 (4)	C3—H3B	0.9700
N1—HN1	0.85 (3)	C4—H4A	0.9700
C1—C2	1.514 (6)	C4—H4B	0.9700
C1—C6	1.502 (5)	C5—H5A	0.9700
C2—C3	1.510 (6)	C5—H5B	0.9700
C3—C4	1.496 (6)	C6—H6	0.9800
C4—C5	1.529 (5)	C8—H8	0.9300
C5—C6	1.499 (5)	C9—H9	0.9300
C7—C12	1.390 (4)	C11—H11	0.9300
C7—C8	1.386 (4)	C12—H12	0.9300
C8—C9	1.369 (6)	C13—H13A	0.9600
C9—C10	1.378 (5)	C13—H13B	0.9600
C10—C11	1.368 (5)	C13—H13C	0.9600
O1—S1—O2	120.39 (18)	C3—C2—H2A	109.00
O1—S1—N1	108.09 (16)	C3—C2—H2B	109.00
O1—S1—C7	107.08 (16)	H2A—C2—H2B	108.00
O2—S1—N1	105.37 (16)	C2—C3—H3A	110.00
O2—S1—C7	106.18 (15)	C2—C3—H3B	110.00
N1—S1—C7	109.43 (16)	C4—C3—H3A	110.00
C10—O3—C13	119.2 (3)	C4—C3—H3B	110.00
S1—N1—C6	123.6 (2)	H3A—C3—H3B	108.00
S1—N1—HN1	112 (2)	C3—C4—H4A	109.00
C6—N1—HN1	119 (2)	C3—C4—H4B	109.00
C2—C1—C6	111.4 (3)	C5—C4—H4A	109.00
C1—C2—C3	111.4 (3)	C5—C4—H4B	109.00
C2—C3—C4	110.5 (3)	H4A—C4—H4B	108.00
C3—C4—C5	113.1 (3)	C4—C5—H5A	109.00
C4—C5—C6	110.7 (3)	C4—C5—H5B	110.00
N1—C6—C5	113.4 (3)	C6—C5—H5A	109.00
C1—C6—C5	110.5 (3)	C6—C5—H5B	109.00
N1—C6—C1	108.7 (2)	H5A—C5—H5B	108.00
C8—C7—C12	117.7 (3)	N1—C6—H6	108.00
S1—C7—C8	121.9 (2)	C1—C6—H6	108.00
S1—C7—C12	120.4 (3)	C5—C6—H6	108.00
C7—C8—C9	121.4 (3)	C7—C8—H8	119.00
C8—C9—C10	119.6 (3)	C9—C8—H8	119.00
O3—C10—C11	124.6 (3)	C8—C9—H9	120.00
O3—C10—C9	115.0 (3)	C10—C9—H9	120.00
C9—C10—C11	120.3 (4)	C10—C11—H11	120.00

C10—C11—C12	119.8 (3)	C12—C11—H11	120.00
C7—C12—C11	121.1 (3)	C7—C12—H12	119.00
C2—C1—H1A	109.00	C11—C12—H12	120.00
C2—C1—H1B	109.00	O3—C13—H13A	109.00
C6—C1—H1A	109.00	O3—C13—H13B	109.00
C6—C1—H1B	109.00	O3—C13—H13C	109.00
H1A—C1—H1B	108.00	H13A—C13—H13B	110.00
C1—C2—H2A	109.00	H13A—C13—H13C	110.00
C1—C2—H2B	109.00	H13B—C13—H13C	110.00

O1—S1—N1—C6	−36.4 (3)	C1—C2—C3—C4	54.1 (4)
O2—S1—N1—C6	−166.3 (3)	C2—C3—C4—C5	−53.2 (5)
C7—S1—N1—C6	79.9 (3)	C3—C4—C5—C6	54.4 (5)
N1—S1—C7—C12	65.7 (3)	C4—C5—C6—N1	−177.6 (3)
O2—S1—C7—C8	132.0 (3)	C4—C5—C6—C1	−55.4 (4)
N1—S1—C7—C8	−114.7 (3)	S1—C7—C12—C11	−178.7 (3)
O1—S1—C7—C8	2.2 (3)	C8—C7—C12—C11	1.7 (5)
O2—S1—C7—C12	−47.6 (3)	S1—C7—C8—C9	179.5 (3)
O1—S1—C7—C12	−177.4 (3)	C12—C7—C8—C9	−1.0 (5)
C13—O3—C10—C11	−5.6 (6)	C7—C8—C9—C10	−0.4 (5)
C13—O3—C10—C9	175.5 (4)	C8—C9—C10—C11	1.1 (6)
S1—N1—C6—C1	144.0 (3)	C8—C9—C10—O3	−179.9 (3)
S1—N1—C6—C5	−92.7 (3)	O3—C10—C11—C12	−179.2 (4)
C2—C1—C6—N1	−177.5 (3)	C9—C10—C11—C12	−0.4 (6)
C6—C1—C2—C3	−57.0 (4)	C10—C11—C12—C7	−1.1 (6)
C2—C1—C6—C5	57.5 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···O2^{i}	0.85 (3)	2.09 (3)	2.913 (4)	161 (3)

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