Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-[(5,5-Dimethyl-3-oxocyclohex-1-enyl)-amino]benzenesulfonamide

Mansour S. Al-Said,[a] Mostafa M. Ghorab,[a] Hazem A. Ghabbour,[b] Ching Kheng Quah[c]‡ and Hoong-Kun Fun[c]*§

[a]Medicinal, Aromatic and Poisonous Plants Research Center (MAPPRC), College of Pharmacy, King Saud University, PO Box 2457, Riyadh 11451, Saudi Arabia, [b]Department of Pharmaceutical Chemistry, College of Pharmacy, King Saud University, Riyadh 11451, Saudi Arabia, and [c]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia
Correspondence e-mail: hkfun@usm.my

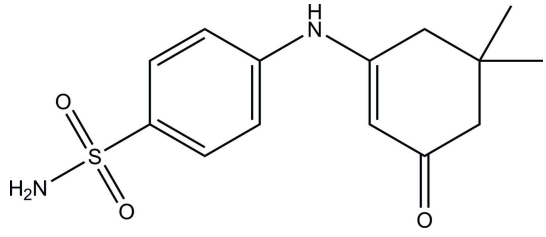
Received 28 June 2012; accepted 1 July 2012

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.044; wR factor = 0.125; data-to-parameter ratio = 14.5.

In the title compound, $C_{14}H_{18}N_2O_3S$, the cyclohexene ring exhibits a distorted half-chair conformation and its mean plane makes a dihedral angle of 46.18 (8)° with the benzene ring. In the crystal, molecules are linked *via* N—H···O, N—H···(O,O) and C—H···O hydrogen bonds, forming a three-dimensional network.

Related literature

For general background to and the pharmacological activities of related compounds, see: Drews (2000); Supuran (2008); Supuran & Scozzafava (2000); Boyd (1988); Ghorab *et al.* (2007, 2009, 2011). For standard bond-length data, see: Allen *et al.* (1987). For ring conformations, see: Cremer & Pople (1975).



Experimental

Crystal data

$C_{14}H_{18}N_2O_3S$
M_r = 294.36
Orthorhombic, *Pbca*
a = 11.0365 (3) Å
b = 13.4763 (3) Å
c = 20.0092 (6) Å
V = 2975.99 (14) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 2.02 mm^{-1}
T = 296 K
0.73 × 0.40 × 0.09 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.322, T_{max} = 0.839
10908 measured reflections
2829 independent reflections
2361 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.125
S = 1.04
2829 reflections
195 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N1···O1^{i}	0.88 (2)	2.10 (2)	2.958 (2)	166 (2)
N2—H1N2···O3^{ii}	0.89 (2)	2.02 (2)	2.900 (2)	169 (2)
N2—H2N2···O3^{iii}	0.88 (2)	2.13 (2)	2.969 (2)	159 (2)
C6—H6A···O2^{iv}	0.97	2.44	3.229 (2)	139

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

The authors are grateful for the sponsorship of the Research Center, College of Pharmacy, and the Deanship of Scientific Research, King Saud University, Riyadh, Saudi Arabia. HKF and CKQ thank Universiti Sains Malaysia (USM) for the Research University Grant No. 1001/PFIZIK/811160.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS5161).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Boyd, A. E. (1988). *Diabetes*, **37**, 847–850.
Bruker (2009). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
Drews, J. (2000). *Science*, **287**, 1960–1964.
Ghorab, M. M., Al-Said, M. S. & El- Hossary, E. M. (2011). *J. Heterocycl. Chem.* **48**, 563–571.
Ghorab, M. M., Ragab, F. A. & Hamed, M. M. (2009). *Eur. J. Med. Chem.* **44**, 4211–4217.
Ghorab, M. M., Ragab, F. A., Noaman, E., Heiba, H. I. & El-Hossary, E. M. (2007). *Arzneimittelforschung*, **57**, 795–803.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Supuran, C. T. (2008). *Nat. Rev. Drug Discov.* **7**, 168–181.
Supuran, C. T. & Scozzafava, A. (2000). *Expert Opin. Ther. Pat.* **10**, 575–600.

‡ Thomson Reuters ResearcherID: A-5525-2009.
§ Thomson Reuters ResearcherID: A-3561-2009.

supplementary materials

Acta Cryst. (2012). E**68**, o2370 [doi:10.1107/S1600536812029996]

4-[(5,5-Dimethyl-3-oxocyclohex-1-enyl)amino]benzenesulfonamide

Mansour S. Al-Said, Mostafa M. Ghorab, Hazem A. Ghabbour, Ching Kheng Quah and Hoong-Kun Fun

Comment

From literature survey, it was found that sulfonamides constitute an important class of drugs with several types of pharmacological activities including antibacterial (Drews, 2000), anti-carbonic anhydrase (Supuran, 2008), diuretic (Supuran & Scozzafava, 2000) and hypoglycemic (Boyd, 1988) properties. Also, some structurally novel sulfonamide derivatives have recently been reported to show substantial antitumor activity (Ghorab *et al.*, 2011). Based on the above informations and due to our interest in the synthesizing novel sulfonamides (Ghorab *et al.*, 2009), the present investigation deals with the design and synthesis of a novel 4-(5,5-dimethyl-3- oxocyclohex-1-enylamino) carrying a biologically active sulfonamide moiety for evaluation as an anticancer agent.

In the title molecule (Fig. 1), the cyclohexene ring (C1–C6) exhibits a distorted half-chair conformation with puckering parameters (Cremer & Pople, 1975) Q = 0.4561 (19) Å, Θ = 52.5 (2)° and φ = 210.9 (3) Å, and its least square plane makes a dihedral angle of 46.18 (8)° with the benzene ring (C9–C14). Bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. In the crystal (Fig. 2), molecules are linked *via* intermolecular N1—H1N1···O1, N2—H1N2···O3, N2—H2N2···O3 and C6—H6A···O2 hydrogen bonds (Table 1), forming a three-dimensional network.

Experimental

4-(5,5-Dimethyl-3-oxocyclohex-1-enylamino)benzenesulfonamide was prepared according to the previously reported procedure (Ghorab *et al.*, 2007). Single crystals suitable for an X-ray structural analysis was obtained by slow evaporation from ethanol at room temperature.

Refinement

The N-bound hydrogen atoms was located in a difference Fourier map and refined freely [N—H = 0.88 (2)–0.89 (2) Å]. The remaining hydrogen atoms were positioned geometrically (C—H = 0.96–0.97 Å) and were refined using a riding model, with U_{iso}(H) = 1.2 or 1.5U_{eq}(C). A rotating group model was applied to the methyl groups.

Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

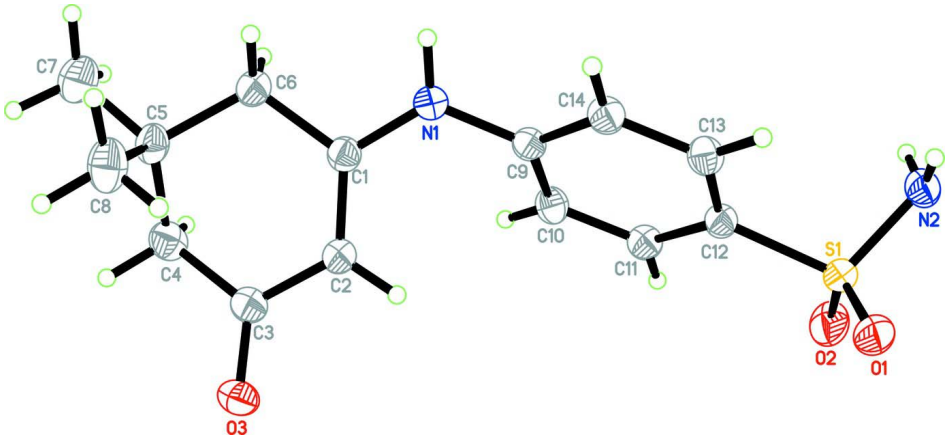


Figure 1

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

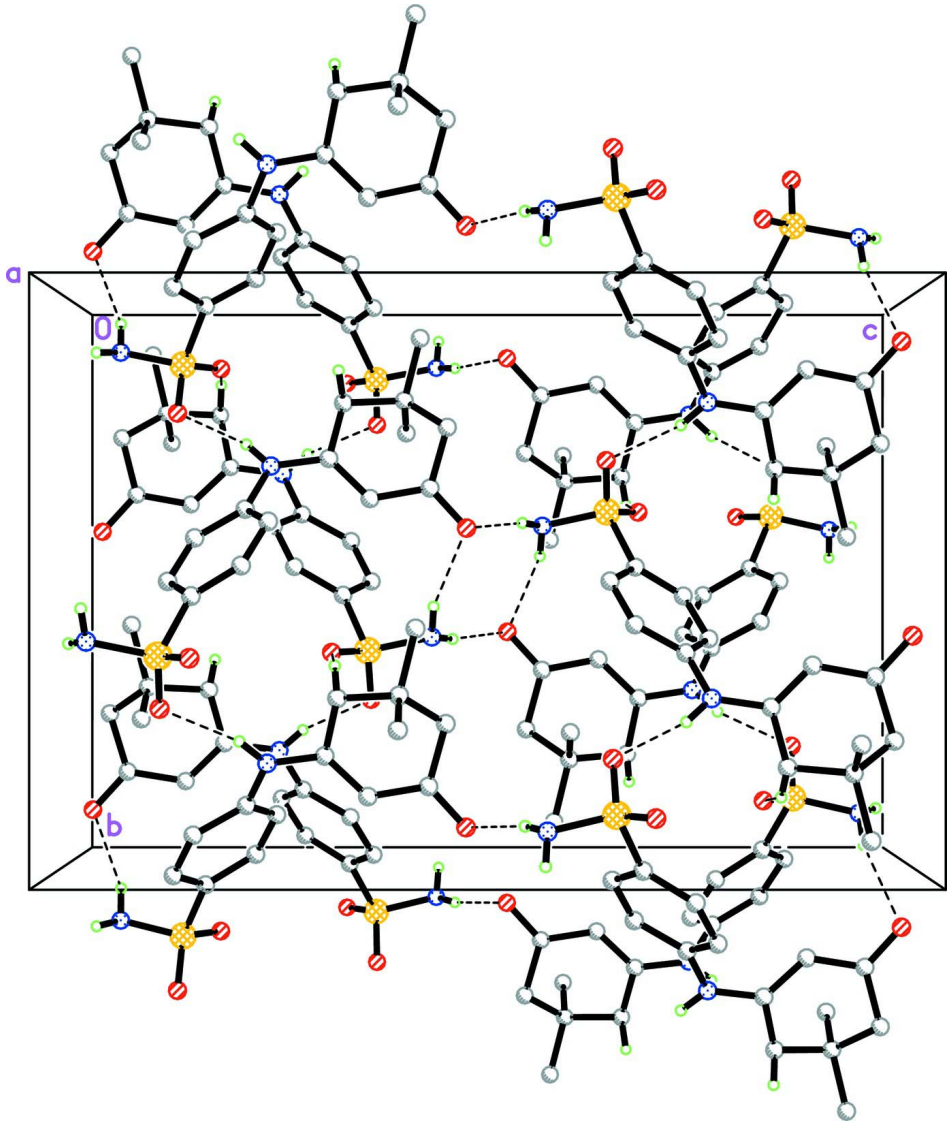


Figure 2

The crystal structure of the title compound, viewed along the *a* axis. H atoms not involved in hydrogen bonds (dashed lines) have been omitted for clarity.

4-[(5,5-Dimethyl-3-oxocyclohex-1-enyl)amino]benzenesulfonamide

Crystal data

$C_{14}H_{18}N_2O_3S$
$M_r = 294.36$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 11.0365$ (3) Å
$b = 13.4763$ (3) Å
$c = 20.0092$ (6) Å
$V = 2975.99$ (14) Å^3
$Z = 8$

$F(000) = 1248$
$D_x = 1.314$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 2253 reflections
$\theta = 4.4$–$70.1°$
$\mu = 2.02$ mm^{-1}
$T = 296$ K
Plate, colourless
0.73 × 0.40 × 0.09 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.322, T_{max} = 0.839
10908 measured reflections
2829 independent reflections
2361 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 72.0°, θ_{min} = 4.4°
h = −11→13
k = −16→10
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.125
S = 1.04
2829 reflections
195 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0919P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 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 $F^2 > 2$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}
S1	−0.00703 (4)	0.12128 (3)	0.35905 (2)	0.04078 (17)
N1	0.30747 (13)	−0.19577 (10)	0.24788 (7)	0.0409 (3)
N2	−0.04392 (17)	0.09709 (12)	0.43487 (8)	0.0470 (4)
O1	0.06697 (14)	0.20885 (9)	0.36157 (7)	0.0578 (4)
O2	−0.11492 (13)	0.12253 (11)	0.31954 (8)	0.0628 (4)
O3	0.33684 (13)	−0.09069 (10)	0.02398 (6)	0.0542 (4)
C1	0.33333 (14)	−0.20944 (11)	0.18227 (8)	0.0371 (3)
C2	0.31006 (16)	−0.14052 (12)	0.13444 (8)	0.0411 (4)
H2A	0.2760	−0.0801	0.1467	0.049*
C3	0.33664 (15)	−0.15894 (12)	0.06597 (9)	0.0419 (4)
C4	0.36612 (17)	−0.26403 (13)	0.04640 (9)	0.0480 (4)
H4A	0.4044	−0.2642	0.0028	0.058*
H4B	0.2917	−0.3020	0.0432	0.058*
C5	0.45074 (16)	−0.31347 (13)	0.09715 (9)	0.0440 (4)
C6	0.39348 (16)	−0.30700 (12)	0.16681 (9)	0.0429 (4)
H6A	0.3338	−0.3594	0.1711	0.052*

H6B	0.4560	−0.3190	0.1999	0.052*
C7	0.4679 (2)	−0.42291 (16)	0.07882 (12)	0.0677 (6)
H7A	0.5099	−0.4277	0.0369	0.102*
H7B	0.3902	−0.4544	0.0751	0.102*
H7C	0.5145	−0.4553	0.1130	0.102*
C8	0.57395 (17)	−0.26183 (16)	0.09661 (12)	0.0615 (5)
H8A	0.6078	−0.2649	0.0525	0.092*
H8B	0.6273	−0.2945	0.1275	0.092*
H8C	0.5641	−0.1937	0.1096	0.092*
C9	0.23173 (14)	−0.12110 (11)	0.27412 (8)	0.0356 (3)
C10	0.12181 (15)	−0.09880 (12)	0.24388 (8)	0.0402 (4)
H10A	0.0975	−0.1328	0.2057	0.048*
C11	0.04870 (14)	−0.02559 (12)	0.27089 (8)	0.0392 (4)
H11A	−0.0248	−0.0100	0.2507	0.047*
C12	0.08487 (14)	0.02434 (11)	0.32787 (8)	0.0365 (3)
C13	0.19250 (15)	0.00026 (12)	0.35958 (8)	0.0400 (4)
H13A	0.2153	0.0332	0.3984	0.048*
C14	0.26572 (15)	−0.07305 (12)	0.33301 (8)	0.0401 (4)
H14A	0.3375	−0.0903	0.3544	0.048*
H1N1	0.3431 (18)	−0.2337 (16)	0.2774 (11)	0.058 (6)*
H1N2	0.024 (2)	0.1016 (15)	0.4588 (12)	0.053 (6)*
H2N2	−0.090 (2)	0.0441 (18)	0.4374 (12)	0.070 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0482 (3)	0.0360 (3)	0.0381 (3)	0.00670 (16)	0.00260 (16)	0.00170 (14)
N1	0.0455 (7)	0.0400 (7)	0.0372 (7)	0.0075 (6)	0.0036 (6)	0.0035 (6)
N2	0.0552 (10)	0.0451 (8)	0.0408 (8)	−0.0019 (7)	0.0078 (7)	−0.0014 (6)
O1	0.0801 (10)	0.0362 (6)	0.0572 (8)	−0.0043 (6)	0.0143 (7)	0.0014 (5)
O2	0.0568 (8)	0.0722 (9)	0.0595 (9)	0.0265 (7)	−0.0102 (7)	−0.0065 (7)
O3	0.0713 (9)	0.0505 (7)	0.0409 (7)	0.0019 (6)	0.0039 (6)	0.0088 (5)
C1	0.0363 (8)	0.0355 (8)	0.0394 (8)	−0.0015 (6)	0.0039 (6)	−0.0001 (6)
C2	0.0468 (9)	0.0351 (8)	0.0414 (8)	0.0041 (7)	0.0056 (7)	0.0007 (6)
C3	0.0419 (8)	0.0429 (9)	0.0408 (8)	−0.0026 (7)	0.0013 (7)	0.0026 (7)
C4	0.0592 (11)	0.0442 (9)	0.0408 (8)	−0.0062 (8)	−0.0010 (8)	−0.0059 (7)
C5	0.0474 (9)	0.0390 (8)	0.0456 (9)	0.0014 (7)	0.0044 (7)	−0.0092 (7)
C6	0.0458 (9)	0.0373 (8)	0.0457 (9)	0.0044 (7)	0.0046 (7)	0.0002 (7)
C7	0.0897 (16)	0.0462 (11)	0.0673 (13)	0.0112 (11)	0.0052 (12)	−0.0157 (10)
C8	0.0440 (10)	0.0679 (12)	0.0724 (13)	−0.0023 (9)	0.0105 (9)	−0.0133 (10)
C9	0.0369 (8)	0.0343 (8)	0.0357 (8)	−0.0009 (6)	0.0055 (6)	0.0031 (5)
C10	0.0407 (8)	0.0431 (8)	0.0368 (8)	−0.0027 (7)	−0.0003 (6)	−0.0054 (6)
C11	0.0358 (8)	0.0425 (8)	0.0392 (8)	0.0002 (7)	−0.0021 (6)	0.0007 (6)
C12	0.0382 (8)	0.0346 (7)	0.0366 (8)	−0.0002 (6)	0.0042 (6)	0.0002 (6)
C13	0.0398 (8)	0.0424 (8)	0.0379 (8)	−0.0020 (7)	−0.0023 (6)	−0.0043 (6)
C14	0.0358 (8)	0.0458 (9)	0.0386 (8)	0.0011 (7)	−0.0021 (6)	0.0004 (6)

Geometric parameters (Å, º)

S1—O2	1.4294 (15)	C5—C6	1.533 (2)
S1—O1	1.4360 (14)	C6—H6A	0.9700
S1—N2	1.6044 (15)	C6—H6B	0.9700
S1—C12	1.7677 (15)	C7—H7A	0.9600
N1—C1	1.356 (2)	C7—H7B	0.9600
N1—C9	1.410 (2)	C7—H7C	0.9600
N1—H1N1	0.88 (2)	C8—H8A	0.9600
N2—H1N2	0.89 (2)	C8—H8B	0.9600
N2—H2N2	0.88 (2)	C8—H8C	0.9600
O3—C3	1.246 (2)	C9—C10	1.389 (2)
C1—C2	1.358 (2)	C9—C14	1.396 (2)
C1—C6	1.505 (2)	C10—C11	1.384 (2)
C2—C3	1.423 (2)	C10—H10A	0.9300
C2—H2A	0.9300	C11—C12	1.383 (2)
C3—C4	1.505 (2)	C11—H11A	0.9300
C4—C5	1.532 (2)	C12—C13	1.385 (2)
C4—H4A	0.9700	C13—C14	1.383 (2)
C4—H4B	0.9700	C13—H13A	0.9300
C5—C8	1.528 (3)	C14—H14A	0.9300
C5—C7	1.532 (2)		
O2—S1—O1	118.92 (9)	C5—C6—H6A	108.6
O2—S1—N2	108.30 (10)	C1—C6—H6B	108.6
O1—S1—N2	106.15 (9)	C5—C6—H6B	108.6
O2—S1—C12	106.95 (8)	H6A—C6—H6B	107.6
O1—S1—C12	107.06 (8)	C5—C7—H7A	109.5
N2—S1—C12	109.21 (8)	C5—C7—H7B	109.5
C1—N1—C9	125.62 (14)	H7A—C7—H7B	109.5
C1—N1—H1N1	118.7 (14)	C5—C7—H7C	109.5
C9—N1—H1N1	115.6 (14)	H7A—C7—H7C	109.5
S1—N2—H1N2	106.5 (15)	H7B—C7—H7C	109.5
S1—N2—H2N2	111.5 (16)	C5—C8—H8A	109.5
H1N2—N2—H2N2	121 (2)	C5—C8—H8B	109.5
N1—C1—C2	123.34 (15)	H8A—C8—H8B	109.5
N1—C1—C6	114.23 (14)	C5—C8—H8C	109.5
C2—C1—C6	122.41 (15)	H8A—C8—H8C	109.5
C1—C2—C3	121.35 (15)	H8B—C8—H8C	109.5
C1—C2—H2A	119.3	C10—C9—C14	120.15 (14)
C3—C2—H2A	119.3	C10—C9—N1	120.67 (14)
O3—C3—C2	121.40 (16)	C14—C9—N1	119.09 (15)
O3—C3—C4	121.27 (16)	C11—C10—C9	119.55 (15)
C2—C3—C4	117.33 (15)	C11—C10—H10A	120.2
C3—C4—C5	111.63 (14)	C9—C10—H10A	120.2
C3—C4—H4A	109.3	C12—C11—C10	120.03 (15)
C5—C4—H4A	109.3	C12—C11—H11A	120.0
C3—C4—H4B	109.3	C10—C11—H11A	120.0
C5—C4—H4B	109.3	C11—C12—C13	120.75 (14)
H4A—C4—H4B	108.0	C11—C12—S1	119.01 (12)

C8—C5—C7	109.08 (17)	C13—C12—S1	120.24 (12)
C8—C5—C4	109.87 (17)	C14—C13—C12	119.51 (14)
C7—C5—C4	109.60 (16)	C14—C13—H13A	120.2
C8—C5—C6	110.33 (15)	C12—C13—H13A	120.2
C7—C5—C6	108.87 (15)	C13—C14—C9	119.93 (15)
C4—C5—C6	109.06 (14)	C13—C14—H14A	120.0
C1—C6—C5	114.73 (14)	C9—C14—H14A	120.0
C1—C6—H6A	108.6		

C9—N1—C1—C2	14.4 (3)	C1—N1—C9—C14	−139.55 (17)
C9—N1—C1—C6	−167.16 (15)	C14—C9—C10—C11	2.8 (2)
N1—C1—C2—C3	−178.77 (15)	N1—C9—C10—C11	179.57 (14)
C6—C1—C2—C3	2.9 (3)	C9—C10—C11—C12	−0.4 (2)
C1—C2—C3—O3	−166.50 (17)	C10—C11—C12—C13	−1.7 (2)
C1—C2—C3—C4	12.7 (3)	C10—C11—C12—S1	177.15 (12)
O3—C3—C4—C5	136.43 (17)	O2—S1—C12—C11	5.87 (16)
C2—C3—C4—C5	−42.8 (2)	O1—S1—C12—C11	−122.63 (13)
C3—C4—C5—C8	−65.7 (2)	N2—S1—C12—C11	122.86 (14)
C3—C4—C5—C7	174.46 (16)	O2—S1—C12—C13	−175.28 (13)
C3—C4—C5—C6	55.35 (19)	O1—S1—C12—C13	56.22 (15)
N1—C1—C6—C5	−165.84 (15)	N2—S1—C12—C13	−58.29 (15)
C2—C1—C6—C5	12.6 (2)	C11—C12—C13—C14	1.4 (2)
C8—C5—C6—C1	79.9 (2)	S1—C12—C13—C14	−177.40 (12)
C7—C5—C6—C1	−160.42 (16)	C12—C13—C14—C9	1.0 (2)
C4—C5—C6—C1	−40.9 (2)	C10—C9—C14—C13	−3.1 (2)
C1—N1—C9—C10	43.7 (2)	N1—C9—C14—C13	−179.88 (14)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*1···O1^{i}	0.88 (2)	2.10 (2)	2.958 (2)	166 (2)
N2—H1*N*2···O3^{ii}	0.89 (2)	2.02 (2)	2.900 (2)	169 (2)
N2—H2*N*2···O3^{iii}	0.88 (2)	2.13 (2)	2.969 (2)	159 (2)
C6—H6*A*···O2^{iv}	0.97	2.44	3.229 (2)	139

Symmetry codes: (i) −*x*+1/2, *y*−1/2, *z*; (ii) −*x*+1/2, −*y*, *z*+1/2; (iii) *x*−1/2, *y*, −*z*+1/2; (iv) −*x*, *y*−1/2, −*z*+1/2.