Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-(4-Chlorophenylsulfonyl)-8-methyl-1,3-diazaspiro[4.5]decane-2,4-dione

M. Kalim Kashif,[a] M. Khawar Rauf,[a] Michael Bolte[b] and Shahid Hameed[a]*

[a]Department of Chemistry, Quaid-i-Azam University, Islamabad 45320, Pakistan, and [b]Institut für Anorganische Chemie, J. W. Goethe-Universität Frankfurt, Max-von-Laue-Strasse 7, 60438 Frankfurt/Main, Germany
Correspondence e-mail: shameed@qau.edu.pk

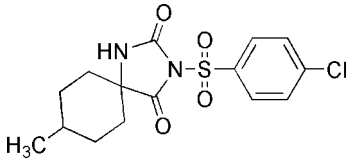
Received 9 July 2009; accepted 13 July 2009

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.030; wR factor = 0.081; data-to-parameter ratio = 15.0.

In the title compound, $C_{15}H_{17}ClN_2O_4S$, the atoms in the hydantoin ring are coplanar (r.m.s. deviation = 0.006 Å). The crystal structure is stabilized by intermolecular N—H···O hydrogen bonds which link the molecules into centrosymmetric dimers. The dihedral angle subtended by the 4-chlorophenyl group with the plane passing through the hydantoin unit is 82.98 (4)°. The cyclohexyl ring adopts an ideal chair conformation.

Related literature

For background to diabetes and its treatment, see: Tiwari & Rao (2002); DeFronzo (1999); Feinglos & Bethel (1998); Murakami *et al.*, (1997). We have synthesized a number of *N*-arylsulfonylimidazolidine-2,4-diones and evaluated their antidiabetic activity, see: Hussain *et al.* (2009*a*,*b*); Kashif, Ahmad *et al.* (2008); Kashif, Hussain *et al.* (2008); For related structures, see: Gauthier *et al.* (1997); Kashif, Hussain *et al.* (2008).



Experimental

Crystal data

$C_{15}H_{17}ClN_2O_4S$
M_r = 356.82
Monoclinic, $P2_1/c$
a = 6.1722 (4) Å
b = 17.4561 (12) Å
c = 15.1355 (9) Å
β = 94.460 (5)°
V = 1625.80 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.38 mm^{-1}
T = 173 K
0.38 × 0.36 × 0.33 mm

Data collection

Stoe IPDS-II two-circle diffractometer
Absorption correction: multi-scan (*MULABS*; Spek, 2009; Blessing, 1995)
T_{min} = 0.868, T_{max} = 0.884
19365 measured reflections
3203 independent reflections
2983 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.081
S = 1.04
3203 reflections
213 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O4^{i}	0.84 (2)	2.04 (2)	2.8763 (15)	171.5 (19)

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

MKR is grateful to the HEC-Pakistan for financial support for a PhD program under scholarship No. [ILC–0363104].

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2537).

References

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
DeFronzo, R. A. (1999). *Ann. Intern. Med.* **131**, 281–303.
Feinglos, M. N. & Bethel, M. A. (1998). *Med. Clin. North Am.* **82**, 757–790.
Gauthier, T. J., Yokum, T. S., Morales, G. A., McLaughlin, M. L., Liu, Y.-H. & Fronczek, F. R. (1997). *Acta Cryst.* C**53**, 1659–1661.
Hussain, A., Hameed, S. & Stoeckli-Evans, H. (2009*a*). *Acta Cryst.* E**65**, o858–o859.
Hussain, A., Hameed, S. & Stoeckli-Evans, H. (2009*b*). *Acta Cryst.* E**65**, o1207–o1208.
Kashif, M. K., Ahmad, I. & Hameed, S. (2008). *ARKIVOC*, **x**vi, 311–317.
Kashif, M. K., Hussain, A., Khawar Rauf, M., Ebihara, M. & Hameed, S. (2008). *Acta Cryst.* E**64**, o444.
Murakami, N., Ohta, M., Kato, K., Nakayama, K., Mizota, M., Miwa, I. & Okuda, J. (1997). *Arzneim. Forsch.* **47**, 1222–1225.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Stoe & Cie (2001). *X-AREA*. Stoe & Cie, Darmstadt, Germany.
Tiwari, A. K. & Rao, J. M. (2002). *Curr. Sci.* **83**, 30–38.

supporting information

Acta Cryst. (2009). E**65**, o1893 [doi:10.1107/S1600536809027482]

3-(4-Chlorophenylsulfonyl)-8-methyl-1,3-diazaspiro[4.5]decane-2,4-dione

M. Kalim Kashif, M. Khawar Rauf, Michael Bolte and Shahid Hameed

S1. Comment

Diabetes is one of the major causes of disease related deaths in these modern times and the people in South-east Asia and Western Pacific are being the most at risk (Tiwari *et al.*, 2002). To cure the disease sulfonyl ureas are the most frequently used antidiabetic drugs (DeFronzo, 1999; Feinglos & Bethel, 1998). An important complication related to this disease is the cataract formation and imidazolidine-2,4-diones have been found as aldose reductase inhibitors (Murakami *et al.*, 1997). The combination of the two scaffolds, *i.e.* the sulfonyl urea and the imidazolidine-2,4-dione, in one molecule may be a useful combination to cure the disease and associated complications, especially the cataract formation. With this hypothesis in mind, we synthesized a number of *N*-arylsulfonylimidazolidine-2,4-diones and evaluated their antidiabetic activity (Hussain *et al.*, 2009*a*,*b*; Kashif, Ahmad *et al.*, 2008; Kashif, Hussain *et al.*, 2008). In the present paper, we report the synthesis and crystal structure of the title compound. The bond lengths and angles within the hydantoin (2,4-imidazolidenedione) moiety are normal, typical of those observed in cyclohexanespiro-5′-hydantoin (Gauthier *et al.*, 1997; Kashif & Hussain *et al.*, 2008). The hydantoin unit is exactly planar (r.m.s. deviation 0.006 Å). The cyclohexane ring has adopted chair conformation, with endocyclic torsion-angle magnitudes of 54.87 (16)–56.26 (16)°. The C1—O3 and C3—O4 bond lengths are 1.1985 (17) and 1.2242 (16) Å, respectively, which are close to the standard value for CO(1.20 Å). The dihedral angle subtended by the *p*-chlorophenyl group with the plane passing through the hydantoin moiety is 82.98 (4)°. Intermolecular N—H···O hydrogen bonds link the molecules to form centrosymmetric dimers.

S2. Experimental

Substituted cyclohexanone (0.1 mol) and ammonium carbonate (0.6 mol) were placed in a 100 ml round bottom flask. Potassium cyanide (0.1 mol) was dissolved in aqueous ethanol (60%) and added to the reaction flask. The mixture was heated on an oil bath at 328–333 K until the reaction was complete (monitored by *TLC*). After cooling to room temperature, the reaction mixture was concentrated and acidified using conc. HCl. The resulting precipitates were filtered, dissolved in saturated $NaOH_{(aq)}$ solution and extracted with diethyl ether (2 × 25 ml). The aqueous layer was acidified to precipitate 8-substituted-1,3-diazaspiro[4.5]decane-2,4-dione, which was filtered and recrystallized from ethanol/water. 8-substituted-1,3-diazaspiro[4.5]decane-2,4-dione (4.8 mmol) in CH_2Cl_2 (20 ml) was stirred with triethyl amine (4.8 mmol) and catalytic amounts of DMAP. The aryl sulfonyl chloride (5.8 mmol) in CH_2Cl_2 (10 ml) was added drop wise and the reaction mixture stirred at room temperature. After completion of the reaction (*TLC*), the mixture was diluted with 1 *M* HCl (20 ml) and extracted with CH_2Cl_2 (3 × 25 ml). The organic layer was dried over anhydrous sodium sulfate and concentrated under reduced pressure. Recrystallization of the residue from ethyl acetate afforded the colourless plate-like crystals, suitable for X-ray analysis.

S3. Refinement

H atom on the N atom was refined isotropically. Other H atoms were placed in idealized positions and treated as riding atoms with C—H distance in the range 0.95–1.00 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C_{methyl}).

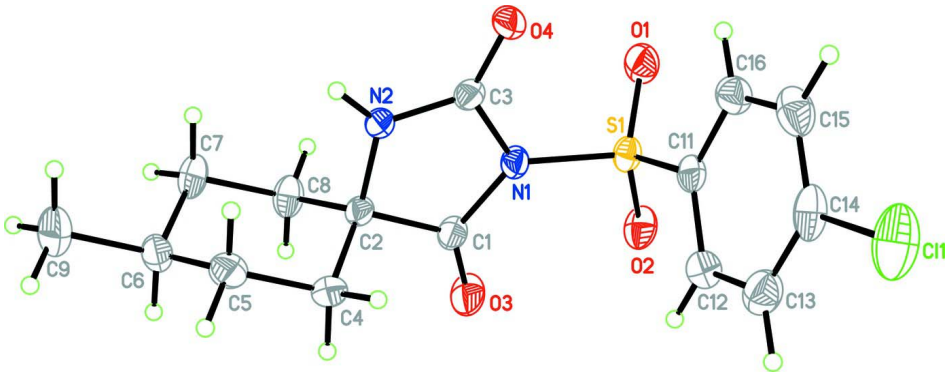


Figure 1

Molecular structure of the title compound with displacement ellipsoids at the 50% probability level showing atom-labelling scheme.

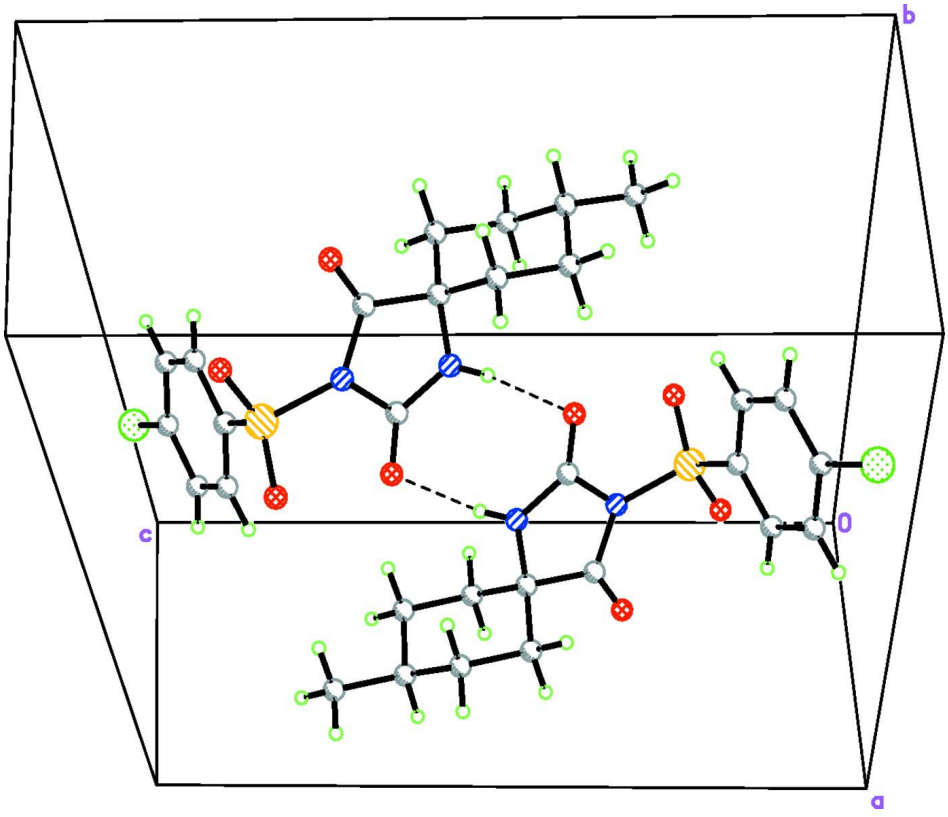


Figure 2

Partial packing diagram of (I) with view onto the *ac* plane. Hydrogen bonds shown as dashed lines.

3-(4-Chlorophenylsulfonyl)-8-methyl-1,3-diazaspiro[4.5]decane-2,4-dione

Crystal data

$C_{15}H_{17}ClN_2O_4S$
$M_r = 356.82$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 6.1722$ (4) Å
$b = 17.4561$ (12) Å
$c = 15.1355$ (9) Å
$\beta = 94.460$ (5)°
$V = 1625.80$ (18) Å^3
$Z = 4$
$F(000) = 744$
$D_x = 1.458$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 15156 reflections
$\theta = 3.0$–$26.3°$
$\mu = 0.38$ mm^{-1}
$T = 173$ K
Block, colourless
0.38 × 0.36 × 0.33 mm

Data collection

Stoe IPDS-II two-circle diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 2009; Blessing, 1995)
$T_{min} = 0.868$, $T_{max} = 0.884$
19365 measured reflections
3203 independent reflections
2983 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.9°$
$h = -7 \rightarrow 7$
$k = -21 \rightarrow 21$
$l = -16 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.081$
$S = 1.04$
3203 reflections
213 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
$w = 1/[\sigma^2(F_o^2) + (0.038P)^2 + 0.7834P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.38$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0255 (15)

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^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.36511 (5)	0.371795 (19)	0.23107 (2)	0.02303 (12)
Cl1	0.79176 (9)	0.63621 (3)	0.02791 (3)	0.05300 (16)
N1	0.50643 (18)	0.37056 (6)	0.33214 (7)	0.0219 (2)

N2	0.62920 (18)	0.41517 (6)	0.46472 (7)	0.0220 (2)
H2	0.641 (3)	0.4423 (11)	0.5109 (14)	0.042 (5)*
O1	0.14563 (16)	0.39092 (7)	0.24485 (7)	0.0341 (3)
O2	0.41742 (18)	0.30140 (6)	0.19042 (7)	0.0313 (2)
O3	0.7072 (2)	0.25599 (6)	0.33154 (7)	0.0384 (3)
O4	0.37659 (16)	0.48815 (6)	0.38160 (6)	0.0289 (2)
C1	0.6589 (2)	0.31459 (8)	0.36628 (9)	0.0234 (3)
C2	0.7484 (2)	0.34352 (7)	0.45728 (8)	0.0200 (3)
C3	0.4938 (2)	0.43204 (7)	0.39448 (8)	0.0212 (3)
C4	0.9937 (2)	0.35863 (9)	0.45695 (9)	0.0277 (3)
H4A	1.0689	0.3109	0.4417	0.033*
H4B	1.0202	0.3976	0.4115	0.033*
C5	1.0850 (2)	0.38688 (9)	0.54830 (10)	0.0303 (3)
H5A	1.2440	0.3940	0.5478	0.036*
H5B	1.0198	0.4372	0.5605	0.036*
C6	1.0389 (2)	0.33104 (9)	0.62226 (10)	0.0313 (3)
H6	1.1136	0.2816	0.6107	0.038*
C7	0.7954 (3)	0.31502 (9)	0.62127 (9)	0.0302 (3)
H7A	0.7193	0.3625	0.6368	0.036*
H7B	0.7699	0.2760	0.6668	0.036*
C8	0.7004 (2)	0.28651 (8)	0.53063 (9)	0.0284 (3)
H8A	0.5413	0.2800	0.5317	0.034*
H8B	0.7641	0.2360	0.5179	0.034*
C9	1.1307 (3)	0.36103 (12)	0.71245 (12)	0.0472 (4)
H9A	1.2869	0.3704	0.7109	0.071*
H9B	1.1067	0.3229	0.7583	0.071*
H9C	1.0573	0.4089	0.7260	0.071*
C11	0.4850 (2)	0.44792 (8)	0.17624 (8)	0.0228 (3)
C12	0.6817 (2)	0.43427 (8)	0.13975 (9)	0.0286 (3)
H12	0.7502	0.3856	0.1460	0.034*
C13	0.7761 (2)	0.49288 (10)	0.09407 (10)	0.0340 (3)
H13	0.9109	0.4851	0.0691	0.041*
C14	0.6711 (3)	0.56299 (9)	0.08531 (9)	0.0332 (3)
C15	0.4758 (3)	0.57708 (9)	0.12184 (10)	0.0352 (3)
H15	0.4075	0.6257	0.1152	0.042*
C16	0.3816 (2)	0.51863 (8)	0.16838 (10)	0.0295 (3)
H16	0.2484	0.5269	0.1944	0.035*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.02463 (19)	0.02646 (19)	0.01742 (17)	−0.00340 (12)	−0.00210 (12)	−0.00176 (12)
Cl1	0.0750 (3)	0.0439 (3)	0.0392 (2)	−0.0247 (2)	−0.0012 (2)	0.01235 (18)
N1	0.0264 (6)	0.0221 (6)	0.0168 (5)	0.0020 (4)	−0.0016 (4)	−0.0026 (4)
N2	0.0249 (6)	0.0227 (6)	0.0179 (5)	0.0060 (4)	−0.0015 (4)	−0.0051 (4)
O1	0.0235 (5)	0.0503 (7)	0.0281 (5)	−0.0030 (5)	−0.0013 (4)	0.0017 (5)
O2	0.0438 (6)	0.0258 (5)	0.0233 (5)	−0.0057 (4)	−0.0036 (4)	−0.0056 (4)
O3	0.0607 (7)	0.0273 (5)	0.0261 (5)	0.0145 (5)	−0.0041 (5)	−0.0077 (4)

O4	0.0328 (5)	0.0288 (5)	0.0241 (5)	0.0120 (4)	−0.0042 (4)	−0.0049 (4)
C1	0.0301 (7)	0.0215 (7)	0.0187 (6)	0.0018 (5)	0.0021 (5)	0.0001 (5)
C2	0.0242 (6)	0.0185 (6)	0.0173 (6)	0.0032 (5)	0.0017 (5)	−0.0010 (5)
C3	0.0215 (6)	0.0236 (6)	0.0186 (6)	0.0005 (5)	0.0019 (5)	−0.0032 (5)
C4	0.0232 (7)	0.0355 (8)	0.0250 (7)	0.0049 (6)	0.0062 (5)	0.0005 (6)
C5	0.0192 (6)	0.0401 (8)	0.0314 (8)	−0.0007 (6)	0.0011 (5)	−0.0038 (6)
C6	0.0346 (8)	0.0340 (8)	0.0239 (7)	0.0101 (6)	−0.0063 (6)	−0.0037 (6)
C7	0.0417 (8)	0.0309 (8)	0.0178 (6)	−0.0053 (6)	0.0005 (6)	0.0042 (5)
C8	0.0377 (8)	0.0253 (7)	0.0218 (7)	−0.0070 (6)	−0.0008 (6)	0.0038 (5)
C9	0.0475 (10)	0.0605 (11)	0.0313 (9)	0.0052 (8)	−0.0122 (7)	−0.0098 (8)
C11	0.0258 (6)	0.0246 (6)	0.0171 (6)	−0.0014 (5)	−0.0033 (5)	−0.0012 (5)
C12	0.0291 (7)	0.0298 (7)	0.0266 (7)	0.0025 (6)	0.0008 (6)	0.0016 (6)
C13	0.0325 (8)	0.0411 (9)	0.0286 (8)	−0.0050 (6)	0.0035 (6)	0.0022 (6)
C14	0.0457 (9)	0.0315 (8)	0.0210 (7)	−0.0122 (6)	−0.0068 (6)	0.0032 (6)
C15	0.0470 (9)	0.0254 (7)	0.0313 (8)	0.0018 (6)	−0.0079 (7)	0.0004 (6)
C16	0.0316 (7)	0.0301 (7)	0.0263 (7)	0.0044 (6)	−0.0023 (6)	−0.0029 (6)

Geometric parameters (Å, º)

S1—O2	1.4225 (11)	C6—C7	1.528 (2)
S1—O1	1.4262 (11)	C6—C9	1.529 (2)
S1—N1	1.7011 (11)	C6—H6	1.0000
S1—C11	1.7602 (14)	C7—C8	1.5325 (19)
Cl1—C14	1.7447 (15)	C7—H7A	0.9900
N1—C1	1.4251 (17)	C7—H7B	0.9900
N1—C3	1.4352 (16)	C8—H8A	0.9900
N2—C3	1.3331 (17)	C8—H8B	0.9900
N2—C2	1.4599 (16)	C9—H9A	0.9800
N2—H2	0.84 (2)	C9—H9B	0.9800
O3—C1	1.1985 (17)	C9—H9C	0.9800
O4—C3	1.2242 (16)	C11—C16	1.390 (2)
C1—C2	1.5294 (18)	C11—C12	1.393 (2)
C2—C8	1.5369 (18)	C12—C13	1.388 (2)
C2—C4	1.5373 (18)	C12—H12	0.9500
C4—C5	1.533 (2)	C13—C14	1.386 (2)
C4—H4A	0.9900	C13—H13	0.9500
C4—H4B	0.9900	C14—C15	1.387 (2)
C5—C6	1.528 (2)	C15—C16	1.393 (2)
C5—H5A	0.9900	C15—H15	0.9500
C5—H5B	0.9900	C16—H16	0.9500
O2—S1—O1	121.04 (7)	C5—C6—H6	107.9
O2—S1—N1	105.08 (6)	C7—C6—H6	107.9
O1—S1—N1	107.33 (6)	C9—C6—H6	107.9
O2—S1—C11	109.29 (6)	C6—C7—C8	112.07 (12)
O1—S1—C11	109.35 (7)	C6—C7—H7A	109.2
N1—S1—C11	103.21 (6)	C8—C7—H7A	109.2
C1—N1—C3	110.02 (10)	C6—C7—H7B	109.2

C1—N1—S1	127.78 (9)	C8—C7—H7B	109.2
C3—N1—S1	122.10 (9)	H7A—C7—H7B	107.9
C3—N2—C2	114.60 (11)	C7—C8—C2	110.76 (11)
C3—N2—H2	123.2 (13)	C7—C8—H8A	109.5
C2—N2—H2	122.2 (13)	C2—C8—H8A	109.5
O3—C1—N1	127.29 (12)	C7—C8—H8B	109.5
O3—C1—C2	126.30 (12)	C2—C8—H8B	109.5
N1—C1—C2	106.40 (10)	H8A—C8—H8B	108.1
N2—C2—C1	101.73 (10)	C6—C9—H9A	109.5
N2—C2—C8	111.87 (11)	C6—C9—H9B	109.5
C1—C2—C8	111.12 (11)	H9A—C9—H9B	109.5
N2—C2—C4	110.84 (11)	C6—C9—H9C	109.5
C1—C2—C4	109.93 (11)	H9A—C9—H9C	109.5
C8—C2—C4	111.02 (11)	H9B—C9—H9C	109.5
O4—C3—N2	129.04 (12)	C16—C11—C12	121.78 (13)
O4—C3—N1	123.73 (12)	C16—C11—S1	120.22 (11)
N2—C3—N1	107.24 (11)	C12—C11—S1	117.98 (11)
C5—C4—C2	110.19 (11)	C13—C12—C11	118.93 (14)
C5—C4—H4A	109.6	C13—C12—H12	120.5
C2—C4—H4A	109.6	C11—C12—H12	120.5
C5—C4—H4B	109.6	C14—C13—C12	119.16 (14)
C2—C4—H4B	109.6	C14—C13—H13	120.4
H4A—C4—H4B	108.1	C12—C13—H13	120.4
C6—C5—C4	112.28 (12)	C13—C14—C15	122.20 (14)
C6—C5—H5A	109.1	C13—C14—Cl1	118.69 (13)
C4—C5—H5A	109.1	C15—C14—Cl1	119.11 (12)
C6—C5—H5B	109.1	C14—C15—C16	118.80 (14)
C4—C5—H5B	109.1	C14—C15—H15	120.6
H5A—C5—H5B	107.9	C16—C15—H15	120.6
C5—C6—C7	110.42 (11)	C11—C16—C15	119.12 (14)
C5—C6—C9	111.01 (14)	C11—C16—H16	120.4
C7—C6—C9	111.56 (13)	C15—C16—H16	120.4

O2—S1—N1—C1	4.87 (13)	C8—C2—C4—C5	−56.08 (15)
O1—S1—N1—C1	134.92 (12)	C2—C4—C5—C6	56.26 (16)
C11—S1—N1—C1	−109.63 (12)	C4—C5—C6—C7	−55.42 (16)
O2—S1—N1—C3	−179.06 (10)	C4—C5—C6—C9	−179.68 (13)
O1—S1—N1—C3	−49.01 (12)	C5—C6—C7—C8	54.87 (16)
C11—S1—N1—C3	66.44 (11)	C9—C6—C7—C8	178.81 (13)
C3—N1—C1—O3	179.43 (14)	C6—C7—C8—C2	−55.61 (16)
S1—N1—C1—O3	−4.1 (2)	N2—C2—C8—C7	−68.41 (15)
C3—N1—C1—C2	0.01 (14)	C1—C2—C8—C7	178.65 (12)
S1—N1—C1—C2	176.48 (9)	C4—C2—C8—C7	55.99 (15)
C3—N2—C2—C1	−1.17 (14)	O2—S1—C11—C16	146.70 (11)
C3—N2—C2—C8	−119.84 (12)	O1—S1—C11—C16	12.12 (13)
C3—N2—C2—C4	115.67 (12)	N1—S1—C11—C16	−101.87 (11)
O3—C1—C2—N2	−178.79 (14)	O2—S1—C11—C12	−31.78 (12)
N1—C1—C2—N2	0.63 (13)	O1—S1—C11—C12	−166.36 (11)

O3—C1—C2—C8	−59.59 (19)	N1—S1—C11—C12	79.64 (11)
N1—C1—C2—C8	119.83 (12)	C16—C11—C12—C13	−0.2 (2)
O3—C1—C2—C4	63.71 (18)	S1—C11—C12—C13	178.21 (11)
N1—C1—C2—C4	−116.87 (12)	C11—C12—C13—C14	−0.6 (2)
C2—N2—C3—O4	−178.83 (13)	C12—C13—C14—C15	1.0 (2)
C2—N2—C3—N1	1.22 (15)	C12—C13—C14—Cl1	179.88 (11)
C1—N1—C3—O4	179.32 (13)	C13—C14—C15—C16	−0.4 (2)
S1—N1—C3—O4	2.62 (18)	Cl1—C14—C15—C16	−179.32 (11)
C1—N1—C3—N2	−0.73 (14)	C12—C11—C16—C15	0.8 (2)
S1—N1—C3—N2	−177.43 (9)	S1—C11—C16—C15	−177.62 (11)
N2—C2—C4—C5	68.89 (14)	C14—C15—C16—C11	−0.5 (2)
C1—C2—C4—C5	−179.43 (11)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O4^{i}	0.84 (2)	2.04 (2)	2.8763 (15)	171.5 (19)

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