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(3a*R*,6*S*,7a*R*)-7a-Chloro-6-methyl-2-(4-nitrophenylsulfonyl)-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindole

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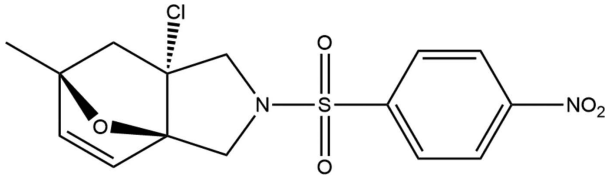
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.007 Å; R factor = 0.068; wR factor = 0.192; data-to-parameter ratio = 15.9.

In the title compound, $C_{15}H_{15}ClN_2O_5S$, the tetrahydrofuran ring adopts an envelope conformation with the O atom as the flap. The pyrrolidine ring adopts an envelope conformation with the chlorine-substituted C atom as the flap. In the crystal, two types of C—H···O hydrogen bonds generate $R_2^2(20)$ and $R_4^4(26)$ rings, with adjacent rings running parallel to *ac* plane. Further C—H···O hydrogen bonds form a $C(6)$ chain, linking the molecules in the *b*-axis direction.

Related literature

For chemical background to protecting groups, see: Greene & Wuts (1999); Romanski *et al.* (2012); Chan & White (2004); Yasushi & Higuchi (2006); Blanc & Bochet (2007); Demircan & Parsons (2002); Demirtaş *et al.* (2002); Katritzky *et al.* (2004); Merlin *et al.* (1988); Büyükgüngör *et al.* (2005); Koşar *et al.* (2006*a*,*b*); Karaarslan *et al.* (2007); Demircan *et al.* (2011); Temel *et al.* (2011, 2012). For puckering parameters, see: Cremer & Pople, (1975). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{15}H_{15}ClN_2O_5S$
M_r = 370.80
Monoclinic, $P2_1/c$
a = 8.6049 (5) Å
b = 7.1949 (3) Å
c = 26.8195 (15) Å
β = 101.186 (4)°
V = 1628.89 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.39 mm^{-1}
T = 296 K
0.48 × 0.24 × 0.02 mm

Data collection

Stoe IPDS 2 diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.894, T_{max} = 0.992
13941 measured reflections
3449 independent reflections
1564 reflections with $I > 2\sigma(I)$
R_{int} = 0.090

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.192
S = 0.89
3449 reflections
217 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O3^{i}	0.93	2.46	3.205 (6)	138
C7—H7*A*···O2^{ii}	0.97	2.51	3.219 (6)	129
C9—H9···O4^{iii}	0.93	2.52	3.388 (6)	155

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

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

The authors acknowledge the Faculty of Arts and Sciences, Ondokuz Mayıs University, Turkey, for the use of the diffractometer (purchased under grant F.279 of University Research Fund) and also The Scientific & Technological Research Council of Turkey (TÜBİTAK) for the financial support of this work (P·N.: 107 T831).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT6935).

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supporting information

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(3a*R*,6*S*,7a*R*)-7a-Chloro-6-methyl-2-(4-nitrophenylsulfonyl)-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindole

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S1. Comment

The use of protective groups has been popular in synthetic pathways (Romanski *et al.*, 2012; Chan & White, 2004; Yasushi and Higuchi, 2006; Blanc and Bochet, 2007). Many protective groups have been, developed to block other reactive sites of a molecule like NH, OH, SH, aldehyde *etc*. They should be easily removable (Greene & Wuts, 1999). Bulky protective groups on nitrogen like *tert*-butoxy carboxylate (Demircan and Parsons, 2002), the trityl group (Demirtaş *et al.*, 2002), tosyl (Katritzky *et al.*, 2004), mesyl (Merlin *et al.*, 1988) predominates in cycloaddition reactions over relatively small protective groups such as methyl, ethyl groups.

We have been working on intramolecular Diels Alder reaction (IMDAF) of compounds with a furan core using different side chains containing a heteroatom like oxygen, sulfur and nitrogen. Isoindole derivatives have been often synthesized and analyzed in our group using bulky protective groups (Büyükgüngör *et al.*, 2005; Koşar *et al.*, 2006*a*; Koşar *et al.*, 2006*b*; Karaarslan *et al.*, 2007; Demircan *et al.*, 2011). Tosyl and mesyl groups have been previously used and reported in a series of sulfonamides (Temel *et al.*, 2012; Temel *et al.*, 2011). We now here report our further finding that cycloadduct, 3 with *p*-nosyl group was generated at the intermediate *via*, 2 in aqueous condition without any other solvent system.

The title compound contains epoxyisoindole and phenyl rings linked through N—S—C bridge (Fig. 2). Tetrahydrofuran rings, pyrrolidine ring and six-membered ring that generate epoxyisoindole moiety are puckered. Both tetrahydrofuran rings adopt an envelope conformation with the puckering parameters of Q=0.516 (5) Å, φ=182.8 (6)° for $O_5/C_{8–11}$ and Q=0.611 (5) Å, φ=3.5 (5)° for $O_5/C_{8,13,12,11}$, respectively. The other five-membered ring, pyrrolidine, has the puckering parameters of Q=0.288 (5) Å and φ=277.2 (9)°. The six-membered ring, $C_{8–13}$, has a boat conformation, according to the puckering parameters [Q=0.928 (5) Å, θ=87.5 (3)° and φ=180.8 (3)°] (Cremer & Pople, 1975).

The crystal packing of is stabilized by C—H···O hydrogen bonds. While the C7—H7A···O2 hydrogen bonds generate $R^2_2(20)$ rings, the combination of C7—H7A···O2 and C9—H9···O4 hydrogen bonds generate $R^4_4(26)$ rings (Fig. 4). These adjacent rings are running parallel to *ac*-plane. Additionally, C3—H3···O3 hydrogen bonds forming a C(6) chain link the molecules through *b* axis (Fig 3) (Bernstein *et al.* 1995).

S2. Experimental

2-Chloro-*N*-(furan-2-ylmethyl)prop-2-en-1-amine, 1 (0.32 g, 1.72 mmol) in water (50 ml) was added *p*-nitrobenzenesulfonyl chloride (0.45 g, 2.06 mmol) portion wise followed by potassium carbonate (0.9 g, 6.45 mol). The reaction mixture was stirred for 48 h at 369 K. Then, the reaction mixture was allowed to warm up to room temperature and NaOH 10% (35 ml) was added. The mixture was then extracted with ethyl acetate (3x35 ml) and brine (35 ml). Combined organic phases were dried over magnesium sulfate, filtered and evaporated. The purification by column

chromatography afforded colourless crystals (0.42 g, 66% yield). t.l.c., (Hexane:Ethylacetate); (8:2), Rf: 0.42). Recrystallization was performed in DCM:Hexane. Melting Point: 444–445 K.

S3. Refinement

H atoms were positioned geometrically and treated using a riding model, fixing the bond lengths at 0.97, 0.98 and 0.93 Å for CH_2, CH and CH(aromatic), respectively. The displacement parameters of the H atoms were constrained with U_{iso}(H) = 1.2U_{eq} (aromatic, methylene or methine C).

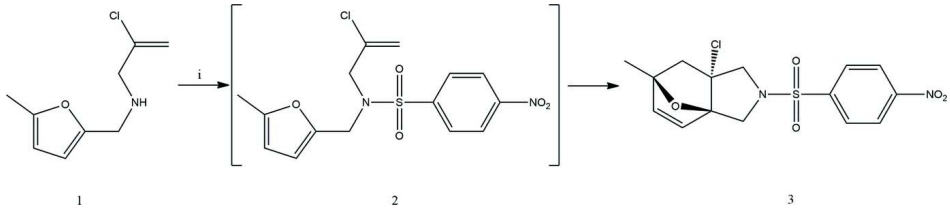

Figure 1

Synthesis of the title compound.

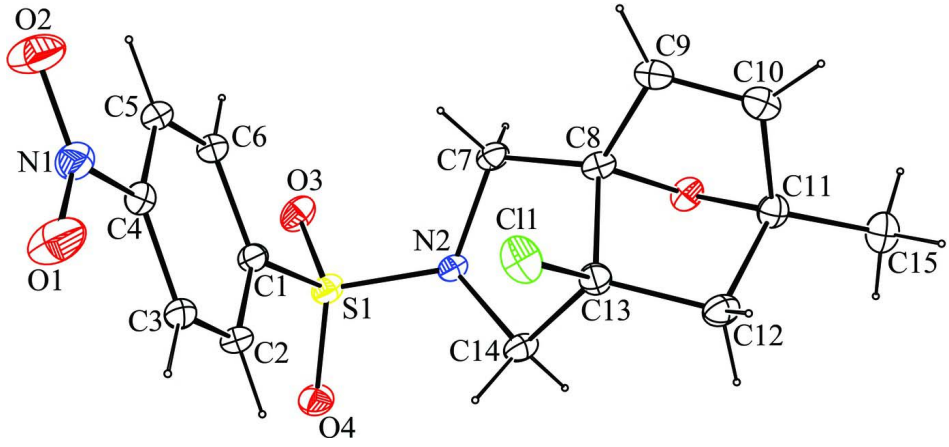

Figure 2

The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level.

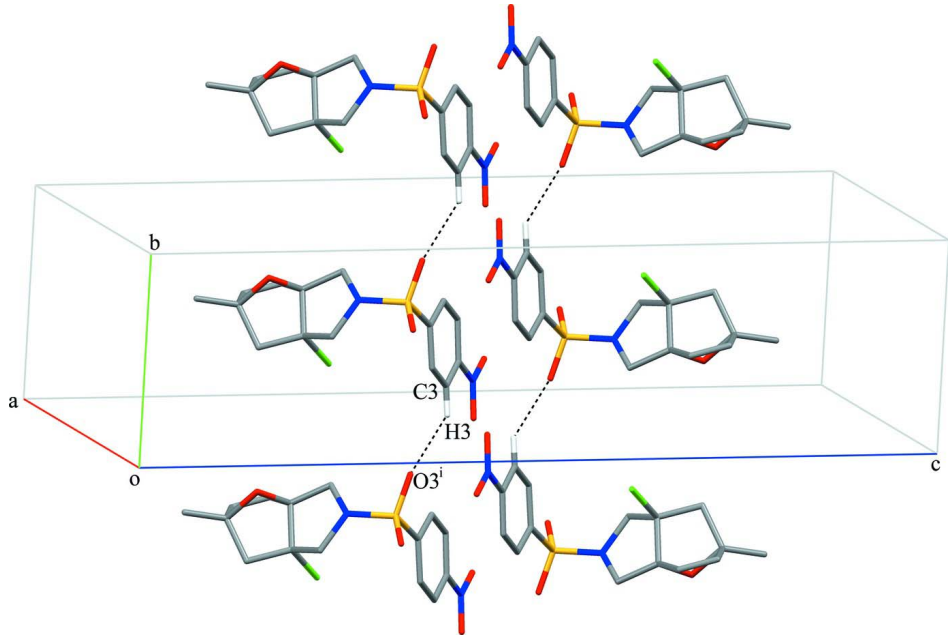

Figure 3

Part of the crystal structure of the title compound, showing the formation of C(6) chain.

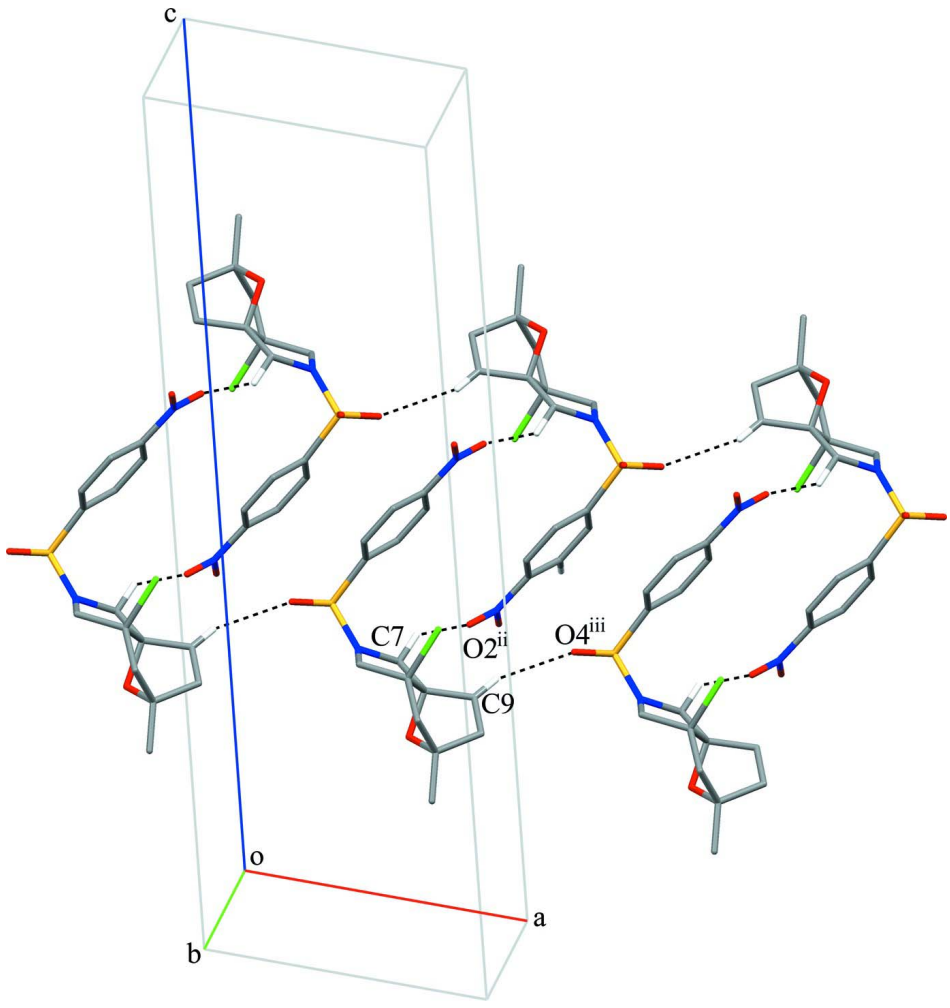

Figure 4

Part of the crystal structure of the title compound, showing the formation of $R^2_2(10)$ and $R^4_4(26)$ rings.

(3a*R*,6*S*,7a*R*)-7a-Chloro-6-methyl-2-(4-nitrophenylsulfonyl)-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindole

Crystal data

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Monoclinic, $P2_1/c$
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$a = 8.6049$ (5) Å
$b = 7.1949$ (3) Å
$c = 26.8195$ (15) Å
$\beta = 101.186$ (4)°
$V = 1628.89$ (15) Å^3
$Z = 4$
$F(000) = 768$
$D_x = 1.512$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 13941 reflections
$\theta = 1.6$–27.2°
$\mu = 0.39$ mm^{-1}
$T = 296$ K
Plate, colorless
0.48 × 0.24 × 0.02 mm

Data collection

Stoe IPDS 2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
rotation method scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{min} = 0.894$, $T_{max} = 0.992$

13941 measured reflections
3449 independent reflections
1564 reflections with $I > 2\sigma(I)$
$R_{int} = 0.090$
$\theta_{max} = 26.8°$, $\theta_{min} = 1.6°$
$h = -10 \rightarrow 10$
$k = -9 \rightarrow 9$
$l = -33 \rightarrow 33$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.068$
$wR(F^2) = 0.192$
$S = 0.89$
3449 reflections
217 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1022P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.12$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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}
C1	0.5887 (5)	0.4475 (7)	0.44296 (17)	0.0556 (12)
C2	0.5543 (5)	0.2605 (7)	0.44330 (18)	0.0618 (13)
H2	0.4667	0.2139	0.4209	0.074*
C3	0.6482 (6)	0.1425 (7)	0.47633 (17)	0.0616 (13)
H3	0.6257	0.0161	0.4764	0.074*
C4	0.7759 (5)	0.2143 (7)	0.50928 (17)	0.0579 (12)
C5	0.8113 (5)	0.4015 (8)	0.51046 (17)	0.0630 (13)
H5	0.8979	0.4474	0.5334	0.076*
C6	0.7182 (5)	0.5177 (7)	0.47768 (18)	0.0608 (13)
H6	0.7405	0.6443	0.4783	0.073*
C7	0.7168 (6)	0.6656 (7)	0.34900 (18)	0.0594 (12)
H7A	0.7832	0.6501	0.3824	0.071*
H7B	0.7080	0.7971	0.3410	0.071*
C8	0.7840 (5)	0.5617 (6)	0.30954 (17)	0.0573 (12)
C9	0.9556 (6)	0.5353 (7)	0.3091 (2)	0.0727 (15)
H9	1.0398	0.5502	0.3363	0.087*
C10	0.9638 (6)	0.4871 (8)	0.2628 (2)	0.0741 (15)
H10	1.0550	0.4557	0.2510	0.089*
C11	0.7968 (6)	0.4919 (7)	0.23212 (18)	0.0599 (12)
C12	0.7102 (6)	0.3187 (7)	0.2476 (2)	0.0691 (14)
H12A	0.6075	0.3012	0.2257	0.083*

H12B	0.7730	0.2068	0.2476	0.083*
C13	0.6946 (6)	0.3746 (6)	0.30125 (18)	0.0594 (12)
C14	0.5329 (5)	0.4221 (7)	0.31263 (18)	0.0613 (12)
H14A	0.4592	0.4537	0.2816	0.074*
H14B	0.4906	0.3178	0.3286	0.074*
C15	0.7767 (7)	0.5299 (9)	0.1765 (2)	0.0832 (17)
H15A	0.8270	0.6456	0.1714	0.100*
H15B	0.6659	0.5372	0.1618	0.100*
H15C	0.8244	0.4314	0.1605	0.100*
N1	0.8795 (6)	0.0885 (8)	0.54414 (17)	0.0793 (13)
N2	0.5591 (4)	0.5831 (5)	0.34738 (13)	0.0522 (9)
O1	0.8474 (6)	−0.0760 (7)	0.54284 (18)	0.1241 (18)
O2	0.9903 (6)	0.1529 (6)	0.57330 (19)	0.1193 (17)
O3	0.4999 (4)	0.7806 (5)	0.41540 (13)	0.0780 (10)
O4	0.3234 (4)	0.5168 (6)	0.38233 (13)	0.0780 (11)
O5	0.7281 (4)	0.6367 (4)	0.25862 (11)	0.0637 (9)
S1	0.47826 (14)	0.59405 (19)	0.39663 (5)	0.0621 (4)
Cl1	0.79058 (18)	0.2099 (2)	0.34891 (6)	0.0899 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.050 (2)	0.063 (3)	0.052 (3)	−0.006 (2)	0.007 (2)	−0.009 (2)
C2	0.055 (3)	0.072 (4)	0.054 (3)	−0.019 (2)	0.002 (2)	−0.012 (2)
C3	0.072 (3)	0.059 (3)	0.053 (3)	−0.020 (2)	0.011 (2)	−0.006 (2)
C4	0.058 (3)	0.066 (3)	0.048 (3)	−0.005 (2)	0.007 (2)	0.003 (2)
C5	0.057 (3)	0.079 (4)	0.049 (3)	−0.017 (3)	0.001 (2)	−0.004 (3)
C6	0.062 (3)	0.064 (3)	0.055 (3)	−0.015 (2)	0.009 (2)	−0.009 (2)
C7	0.067 (3)	0.049 (3)	0.058 (3)	−0.011 (2)	0.001 (2)	−0.006 (2)
C8	0.054 (3)	0.052 (3)	0.061 (3)	−0.002 (2)	−0.002 (2)	−0.004 (2)
C9	0.057 (3)	0.073 (4)	0.086 (4)	−0.014 (3)	0.007 (3)	0.000 (3)
C10	0.065 (3)	0.069 (4)	0.090 (4)	−0.007 (3)	0.018 (3)	0.001 (3)
C11	0.069 (3)	0.050 (3)	0.061 (3)	0.005 (2)	0.014 (2)	−0.003 (2)
C12	0.066 (3)	0.060 (3)	0.079 (4)	−0.002 (3)	0.007 (3)	−0.018 (3)
C13	0.070 (3)	0.045 (3)	0.066 (3)	−0.004 (2)	0.018 (2)	−0.004 (2)
C14	0.058 (3)	0.056 (3)	0.066 (3)	−0.002 (2)	0.000 (2)	−0.018 (2)
C15	0.100 (4)	0.081 (4)	0.071 (4)	0.009 (3)	0.022 (3)	0.002 (3)
N1	0.085 (3)	0.083 (4)	0.064 (3)	−0.015 (3)	−0.001 (2)	0.008 (3)
N2	0.0494 (19)	0.054 (2)	0.050 (2)	−0.0019 (18)	0.0006 (16)	−0.0083 (18)
O1	0.158 (4)	0.077 (3)	0.110 (4)	−0.019 (3)	−0.042 (3)	0.016 (3)
O2	0.111 (3)	0.097 (3)	0.122 (4)	−0.026 (3)	−0.047 (3)	0.024 (3)
O3	0.084 (2)	0.073 (2)	0.073 (2)	0.0175 (19)	0.0053 (18)	−0.0221 (19)
O4	0.0455 (18)	0.107 (3)	0.078 (2)	0.0014 (18)	0.0031 (16)	−0.012 (2)
O5	0.076 (2)	0.054 (2)	0.0566 (19)	0.0075 (16)	0.0016 (16)	0.0036 (15)
S1	0.0529 (7)	0.0696 (9)	0.0603 (7)	0.0052 (6)	0.0027 (5)	−0.0132 (7)
Cl1	0.1013 (11)	0.0687 (9)	0.1046 (12)	0.0213 (8)	0.0322 (9)	0.0296 (8)

Geometric parameters (Å, º)

C1—C2	1.378 (7)	C10—C11	1.512 (7)
C1—C6	1.401 (6)	C10—H10	0.9300
C1—S1	1.761 (5)	C11—O5	1.450 (5)
C2—C3	1.372 (7)	C11—C15	1.494 (7)
C2—H2	0.9300	C11—C12	1.549 (7)
C3—C4	1.371 (6)	C12—C13	1.524 (7)
C3—H3	0.9300	C12—H12A	0.9700
C4—C5	1.380 (7)	C12—H12B	0.9700
C4—N1	1.471 (7)	C13—C14	1.520 (6)
C5—C6	1.357 (7)	C13—Cl1	1.819 (5)
C5—H5	0.9300	C14—N2	1.476 (5)
C6—H6	0.9300	C14—H14A	0.9700
C7—N2	1.474 (6)	C14—H14B	0.9700
C7—C8	1.500 (7)	C15—H15A	0.9600
C7—H7A	0.9700	C15—H15B	0.9600
C7—H7B	0.9700	C15—H15C	0.9600
C8—O5	1.460 (5)	N1—O2	1.202 (6)
C8—C9	1.492 (7)	N1—O1	1.214 (6)
C8—C13	1.545 (6)	N2—S1	1.610 (4)
C9—C10	1.302 (7)	O3—S1	1.433 (4)
C9—H9	0.9300	O4—S1	1.426 (3)
C2—C1—C6	119.5 (4)	C15—C11—C12	116.5 (4)
C2—C1—S1	120.1 (3)	C10—C11—C12	107.0 (4)
C6—C1—S1	120.3 (4)	C13—C12—C11	100.1 (4)
C3—C2—C1	120.5 (4)	C13—C12—H12A	111.7
C3—C2—H2	119.7	C11—C12—H12A	111.7
C1—C2—H2	119.7	C13—C12—H12B	111.7
C4—C3—C2	118.8 (5)	C11—C12—H12B	111.7
C4—C3—H3	120.6	H12A—C12—H12B	109.5
C2—C3—H3	120.6	C14—C13—C12	120.0 (4)
C3—C4—C5	121.9 (5)	C14—C13—C8	103.0 (4)
C3—C4—N1	119.3 (5)	C12—C13—C8	103.5 (4)
C5—C4—N1	118.8 (4)	C14—C13—Cl1	108.3 (3)
C6—C5—C4	119.1 (4)	C12—C13—Cl1	112.4 (3)
C6—C5—H5	120.4	C8—C13—Cl1	108.7 (3)
C4—C5—H5	120.4	N2—C14—C13	105.7 (4)
C5—C6—C1	120.2 (5)	N2—C14—H14A	110.6
C5—C6—H6	119.9	C13—C14—H14A	110.6
C1—C6—H6	119.9	N2—C14—H14B	110.6
N2—C7—C8	104.9 (3)	C13—C14—H14B	110.6
N2—C7—H7A	110.8	H14A—C14—H14B	108.7
C8—C7—H7A	110.8	C11—C15—H15A	109.5
N2—C7—H7B	110.8	C11—C15—H15B	109.5
C8—C7—H7B	110.8	H15A—C15—H15B	109.5
H7A—C7—H7B	108.8	C11—C15—H15C	109.5

O5—C8—C9	100.7 (4)	H15A—C15—H15C	109.5
O5—C8—C7	111.9 (4)	H15B—C15—H15C	109.5
C9—C8—C7	126.0 (4)	O2—N1—O1	122.8 (5)
O5—C8—C13	97.0 (3)	O2—N1—C4	118.9 (5)
C9—C8—C13	110.7 (4)	O1—N1—C4	118.4 (4)
C7—C8—C13	106.6 (4)	C7—N2—C14	111.2 (3)
C10—C9—C8	106.2 (5)	C7—N2—S1	119.9 (3)
C10—C9—H9	126.9	C14—N2—S1	121.3 (3)
C8—C9—H9	126.9	C11—O5—C8	95.8 (3)
C9—C10—C11	107.0 (5)	O4—S1—O3	120.7 (2)
C9—C10—H10	126.5	O4—S1—N2	106.86 (19)
C11—C10—H10	126.5	O3—S1—N2	106.7 (2)
O5—C11—C15	112.3 (4)	O4—S1—C1	107.7 (2)
O5—C11—C10	100.6 (4)	O3—S1—C1	107.3 (2)
C15—C11—C10	117.5 (4)	N2—S1—C1	106.8 (2)
O5—C11—C12	100.6 (4)		

C6—C1—C2—C3	−1.8 (7)	O5—C8—C13—Cl1	159.5 (3)
S1—C1—C2—C3	174.2 (4)	C9—C8—C13—Cl1	55.2 (5)
C1—C2—C3—C4	0.6 (7)	C7—C8—C13—Cl1	−85.1 (4)
C2—C3—C4—C5	0.7 (7)	C12—C13—C14—N2	−139.8 (4)
C2—C3—C4—N1	−178.7 (4)	C8—C13—C14—N2	−25.7 (5)
C3—C4—C5—C6	−0.8 (7)	Cl1—C13—C14—N2	89.3 (4)
N1—C4—C5—C6	178.6 (4)	C3—C4—N1—O2	−179.2 (5)
C4—C5—C6—C1	−0.4 (7)	C5—C4—N1—O2	1.4 (8)
C2—C1—C6—C5	1.7 (7)	C3—C4—N1—O1	−0.6 (8)
S1—C1—C6—C5	−174.3 (4)	C5—C4—N1—O1	180.0 (5)
N2—C7—C8—O5	83.0 (4)	C8—C7—N2—C14	5.6 (5)
N2—C7—C8—C9	−154.3 (4)	C8—C7—N2—S1	155.4 (3)
N2—C7—C8—C13	−21.9 (5)	C13—C14—N2—C7	13.2 (5)
O5—C8—C9—C10	−34.8 (5)	C13—C14—N2—S1	−136.2 (3)
C7—C8—C9—C10	−162.2 (5)	C15—C11—O5—C8	−174.7 (4)
C13—C8—C9—C10	67.1 (5)	C10—C11—O5—C8	−48.9 (4)
C8—C9—C10—C11	2.9 (6)	C12—C11—O5—C8	60.7 (4)
C9—C10—C11—O5	30.0 (5)	C9—C8—O5—C11	51.2 (4)
C9—C10—C11—C15	152.2 (5)	C7—C8—O5—C11	−172.7 (4)
C9—C10—C11—C12	−74.5 (5)	C13—C8—O5—C11	−61.6 (4)
O5—C11—C12—C13	−33.9 (4)	C7—N2—S1—O4	175.4 (3)
C15—C11—C12—C13	−155.5 (4)	C14—N2—S1—O4	−37.8 (4)
C10—C11—C12—C13	70.7 (5)	C7—N2—S1—O3	45.1 (4)
C11—C12—C13—C14	110.0 (5)	C14—N2—S1—O3	−168.1 (3)
C11—C12—C13—C8	−3.9 (5)	C7—N2—S1—C1	−69.4 (4)
C11—C12—C13—Cl1	−121.0 (4)	C14—N2—S1—C1	77.3 (4)
O5—C8—C13—C14	−85.8 (4)	C2—C1—S1—O4	28.7 (5)
C9—C8—C13—C14	169.9 (4)	C6—C1—S1—O4	−155.3 (4)
C7—C8—C13—C14	29.7 (5)	C2—C1—S1—O3	160.1 (4)
O5—C8—C13—C12	39.9 (4)	C6—C1—S1—O3	−23.9 (4)
C9—C8—C13—C12	−64.4 (5)	C2—C1—S1—N2	−85.8 (4)

C7—C8—C13—C12	155.3 (4)	C6—C1—S1—N2	90.2 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O3^{i}	0.93	2.46	3.205 (6)	138
C7—H7*A*···O2^{ii}	0.97	2.51	3.219 (6)	129
C9—H9···O4^{iii}	0.93	2.52	3.388 (6)	155

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