Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(4-Chlorophenyl)-1,1,1-trifluoro-*N*-(trifluoromethylsulfonyl)methanesulfonamide

Núbia Boechat,[a] Adriana dos Santos Lages,[a] Warner B. Kover,[b] Edward R. T. Tiekink,[c]* James L. Wardell[d]‡ and Solange M. S. V. Wardell[e]

[a]Fundação Oswaldo Cruz, Instituto de Tecnologia em Fármacos, Departamento de Síntese Orgânica, Manguinhos, CEP 21041250 Rio de Janeiro, RJ, Brazil, [b]Universidade Federal do Rio de Janeiro, Departamento de Química Orgânica, Instituto de Quiímica, Cidade Universitária, 21949-900 Rio de Janeiro, RJ, Brazil, [c]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia, [d]Centro de Desenvolvimento Tecnológico em Saúde (CDTS), Fundação Oswaldo Cruz (FIOCRUZ), Casa Amarela, Campus de Manguinhos, Av. Brasil 4365, 21040-900 Rio de Janeiro, RJ, Brazil, and [e]CHEMSOL, 1 Harcourt Road, Aberdeen AB15 5NY, Scotland
Correspondence e-mail: edward.tiekink@gmail.com

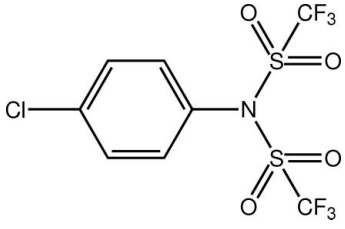
Received 26 January 2010; accepted 27 January 2010

Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.002 Å; R factor = 0.031; wR factor = 0.082; data-to-parameter ratio = 15.3.

The title molecule, also called 4-chloro-*N*,*N*-bis(trifluoromethanesulfonyl)aniline, $C_8H_4ClF_6NO_4S_2$, has non-crystallographic twofold symmetry with the pseudo-axis aligned along the Cl—C···C—N backbone of the molecule: the SO_2CF_3 residues lie to either side of the benzene ring. In the crystal, the presence of C—H···O contacts lead to the formation of a sequence of 12-membered $\{\cdots HC_2NSO\}_2$ synthons within a supramolecular chain aligned along [101].

Related literature

For uses of *N*,*N*-bis(trifluoromethanesulfonyl)aniline derivatives, see: Zeller (2001); Wulff *et al.* (1986). For general background to the synthesis, see: Deprez *et al.* (1995); Greenfield & Crosanu (2008). For a previous synthesis of the title compound, see: Laali *et al.* (2007).



Experimental

Crystal data

$C_8H_4ClF_6NO_4S_2$
M_r = 391.70
Monoclinic, $P2_1/c$
a = 11.5998 (3) Å
b = 13.4423 (4) Å
c = 9.0548 (2) Å
β = 108.014 (2)°
V = 1342.69 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.68 mm^{-1}
T = 120 K
0.40 × 0.25 × 0.25 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
T_{min} = 0.821, T_{max} = 1.000
17100 measured reflections
3047 independent reflections
2806 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.082
S = 1.04
3047 reflections
199 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 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}	0.95	2.57	3.496 (2)	164
C5—H5···O1^{ii}	0.95	2.59	3.385 (2)	141

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

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

The use of the EPSRC X-ray crystallographic service at the University of Southampton, England, and the valuable assistance of the staff there is gratefully acknowledged. JLW acknowledges support from CAPES (Brazil).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5319).

References

Brandenburg, K. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Deprez, P., Guillaume, J., Becker, R., Corbier, A., Didierlaurent, S., Fortin, M., Frechet, D., Hamon, G., Heckman, B., Heitsch, H., Kleeman, H.-W., Vevert, J. P., Vincent, J. C., Wagner, A. & Zhang, J. (1995). *J. Med. Chem.* **38**, 2357–2377.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Greenfield, L. A. & Crosanu, C. (2008). *Tetrahedron Lett.* **49**, 6300–6303.
Hooft, R. W. W. (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Laali, K. K., Okazaki, T. & Bunge, S. D. (2007). *J. Org. Chem.* **72**, 6758–6762.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.

‡ Additional correspondence author, e-mail: j.wardell@abdn.ac.uk.

Sheldrick, G. M. (2007). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *publCIF*. In preparation.
Wulff, W., Peterson, G., Bauta, W., Chan, K. S., Faron, K., Gilbertson, S., Kaesler, R., Yang, D. & Murray, C. (1986). *J. Org. Chem.* **51**, 277–279.
Zeller, W. E. (2001). In *E-EROS Encyclopedia of Reagents for Organic Synthesis*. Chichester: Wiley.

supporting information

Acta Cryst. (2010). E**66**, o506–o507 [doi:10.1107/S1600536810003326]

N-(4-Chlorophenyl)-1,1,1-trifluoro-*N*-(trifluoromethylsulfonyl)methanesulfonamide

Núbia Boechat, Adriana dos Santos Lages, Warner B. Kover, Edward R. T. Tiekink, James L. Wardell and Solange M. S. V. Wardell

S1. Comment

N,*N*-Bis(trifluoromethanesulfonyl)aniline derivatives find use in synthetic chemistry such as mild triflating reagents (Zeller, 2001; Wulff *et al.*, 1986). Following a literature procedure to *p*-$ClC_6H_4NHSO_2CF_3$, using *p*-$ClC_6H_4NH_2$, $(F_3CSO_2)O$ and Et_3N in CH_2Cl_2 at 213 K, a little of the di-substituted compound, *p*-$ClC_6H_4(NSO_2CF_3)$, (I), was isolated as a side-product (Greenfield & Crosanu, 2008; Deprez *et al.*, 1995). Compound (I) has been reported previously (Laali *et al.*, 2007) and the X-ray structure determination is reported herein.

In (I), the SO_2CF_3 groups occupy approximately orthogonal positions to either side of the aromatic ring: the C3/C4/N1/S1, S2 torsion angles are 77.44 (17) and -101.55 (15) °, respectively; the dihedral angle formed between the benzene ring and NS_2 group is 78.13 (6) °. The CF_3 groups lie to either side of the molecule and fold back over the benzene ring so that, overall, the molecule has non-crystallographic 2-fold symmetry when viewed down the Cl1–C1–C4–N1 axis.

Supramolecular aggregation in (I) is dominated by C–H···O interactions that lead to the formation of a sequence of 12-membered $\{\cdots HC_2NSO\}_2$ synthons aligned along [1 0 1], Fig. 2 and Table 1. Chains are connected into layers through the agency of C–Cl···π interactions between centrosymmetrically related residues [C1–Cl1···ring centroid(C1–C6)^{i} = 3.4592 (8) Å with angle at Cl1 = 92.46 (6) ° for i: 2-*x*, 2-*y*, 1-*z*]. The layers thus formed stack along the *b* axis with the closest contacts between successive layers being of the type C–F···π [C8–F4···ring centroid(C1–C6)^{ii} = 3.4708 (16) Å with angle at F4 = 122.83 (11) ° for *ii*: *x*, 3/2-*y*,1/2+*z*].

S2. Experimental

To a cooled (213 K) solution of *p*-$ClC_6H_4NH_2$ (11.5 g, 9.0 mmol) and triethylamine (1.50 ml; 10.8 mmol, 1.20 eq.) in CH_2Cl_2 (40 ml) was slowly added a solution of trifluoromethanesulfonic anhydride (2.40 ml; 13.5 mmol, 1.50 eq) in CH_2Cl_2 (40 ml). After the mixture was stirred at 213-223 K for 1 h, water (30 ml) was added. The mixture was allowed to warm to room temperature, and the organic layer was decanted, washed with water, dried, and evaporated. The products, *N*-(4-chlorophenyl)trifluoromethylsulfonamide and *N*-(4-chlorophenyl)-bis-trifluoromethylsulfonamide, (I), were purified by chromatography on silica gel with hexane as eluent. Products were recrystallized from hexane. Characterisation data for (I): m.pt. 346-348 K, ^{1}H-NMR (500 MHz, $CDCl_3$) δ: 7.34 (2*H*), 7.50 (2*H*) p.p.m. ^{13}C-NMR (125 MHz, $CDCl_3$) δ: 119.36 (q, ^{1}J(C,F) = 325 Hz), 125.17 (C3), 130.06, 132.18, 138.84 p.p.m. ^{19}F-NMR (376 MHz, $CDCl_3$) δ: 71.11 p.p.m.

S3. Refinement

The C-bound H atoms were geometrically placed (C–H = 0.95 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$.

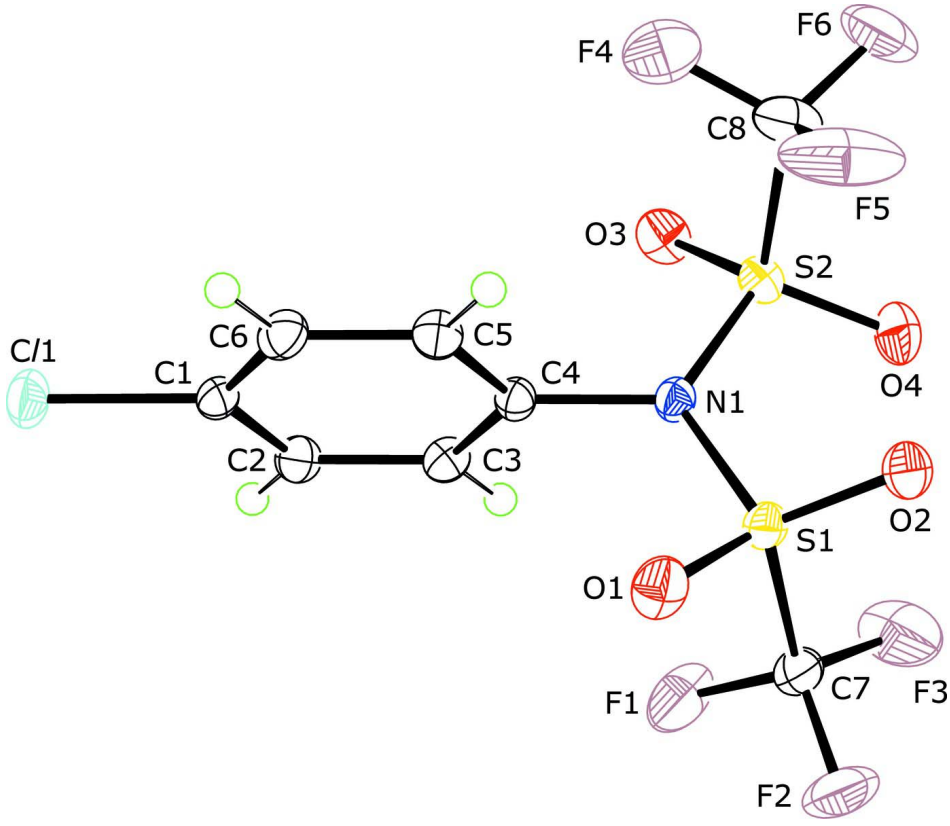


Figure 1

The molecular structure of (I) showing displacement ellipsoids at the 50% probability level.

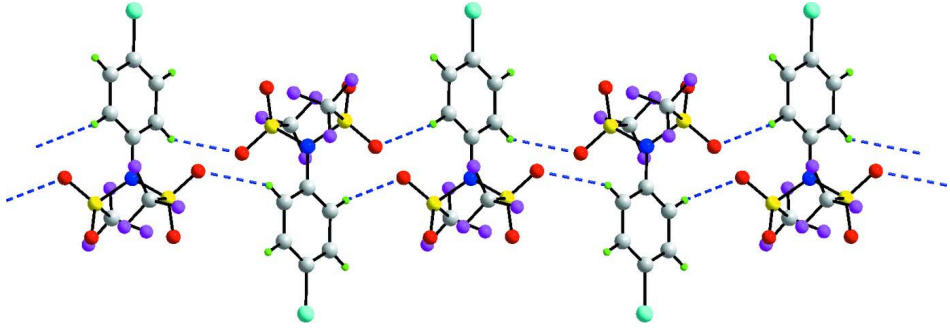


Figure 2

A view of the supramolecular chain in (I) aligned along [1 0 1] and mediated by C–H···O interactions (blue dashed lines). Colour code: Cl, cyan; S, yellow; F, pink; O, red; N, blue; C, grey; and H, green.

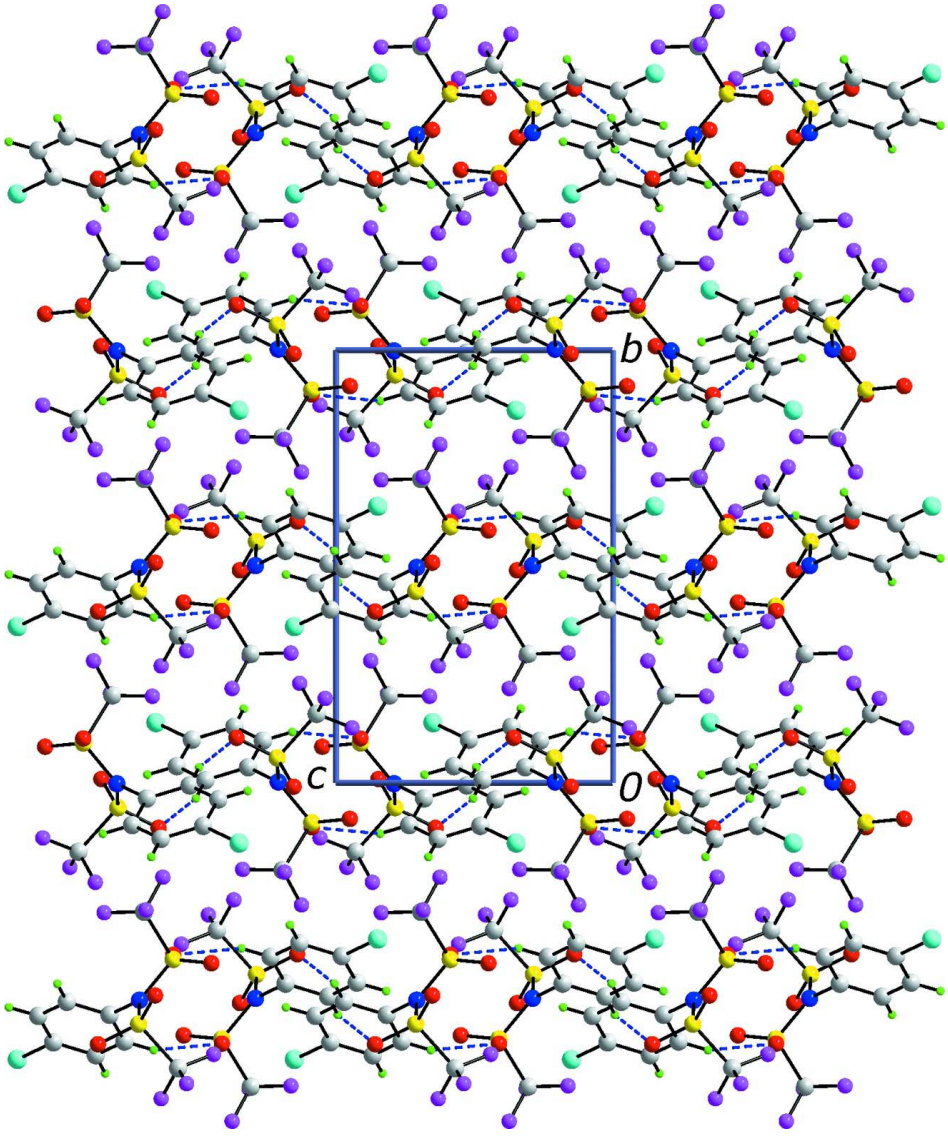


Figure 3

View of the stacking of layers in (I). The C–H···O interactions are shown as blue dashed lines. Colour code: Cl, cyan; S, yellow; F, pink; O, red; N, blue; C, grey; and H, green.

N-(4-Chlorophenyl)-1,1,1-trifluoro-*N*- (trifluoromethylsulfonyl)methanesulfonamide

Crystal data

$C_8H_4ClF_6NO_4S_2$
$M_r = 391.70$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 11.5998$ (3) Å
$b = 13.4423$ (4) Å
$c = 9.0548$ (2) Å
$\beta = 108.014$ (2)°
$V = 1342.69$ (6) Å^3
$Z = 4$
$F(000) = 776$
$D_x = 1.938$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2983 reflections
$\theta = 2.9$–27.5°
$\mu = 0.68$ mm^{-1}
$T = 120$ K
Block, colourless
0.40 × 0.25 × 0.25 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Radiation source: Enraf Nonius FR591 rotating anode
10 cm confocal mirrors monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
T_{min} = 0.821, T_{max} = 1.000
17100 measured reflections
3047 independent reflections
2806 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 27.5°, θ_{min} = 2.9°
h = −15→15
k = −17→17
l = −11→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.082
S = 1.04
3047 reflections
199 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
$w = 1/[\sigma^2(F_o^2) + (0.0407P)^2 + 1.1662P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
Cl1	0.97286 (4)	0.86092 (3)	0.34987 (5)	0.02733 (12)
S1	0.78053 (4)	1.09197 (3)	0.91222 (4)	0.01889 (11)
S2	0.59031 (4)	0.94255 (3)	0.78741 (5)	0.01943 (11)
F1	0.70006 (16)	1.20000 (9)	0.66292 (14)	0.0497 (4)
F2	0.75847 (13)	1.28200 (9)	0.87505 (16)	0.0449 (3)
F3	0.58975 (12)	1.20628 (11)	0.8139 (2)	0.0551 (4)
F4	0.69058 (14)	0.77016 (10)	0.86879 (18)	0.0525 (4)
F5	0.71980 (16)	0.87281 (11)	1.05802 (17)	0.0663 (5)
F6	0.54674 (13)	0.80495 (10)	0.96076 (16)	0.0478 (3)
O1	0.90194 (11)	1.10259 (10)	0.91208 (15)	0.0280 (3)
O2	0.74816 (13)	1.08338 (10)	1.04986 (15)	0.0293 (3)
O3	0.54372 (11)	0.89593 (10)	0.64061 (14)	0.0254 (3)
O4	0.52094 (12)	1.00882 (11)	0.84680 (16)	0.0308 (3)
N1	0.72049 (12)	0.99798 (10)	0.79108 (15)	0.0167 (3)
C1	0.89885 (15)	0.90047 (12)	0.4795 (2)	0.0192 (3)
C2	0.79853 (15)	0.96166 (12)	0.42518 (19)	0.0201 (3)

H2	0.7706	0.9812	0.3192	0.024*
C3	0.73954 (14)	0.99385 (12)	0.52852 (18)	0.0182 (3)
H3	0.6704	1.0358	0.4943	0.022*
C4	0.78292 (14)	0.96396 (12)	0.68241 (18)	0.0162 (3)
C5	0.88287 (15)	0.90243 (12)	0.73621 (19)	0.0198 (3)
H5	0.9106	0.8824	0.8420	0.024*
C6	0.94185 (15)	0.87055 (12)	0.6327 (2)	0.0218 (3)
H6	1.0110	0.8286	0.6668	0.026*
C7	0.70024 (18)	1.20199 (13)	0.8072 (2)	0.0258 (4)
C8	0.64203 (18)	0.84073 (14)	0.9298 (2)	0.0301 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0291 (2)	0.0285 (2)	0.0294 (2)	−0.00347 (16)	0.01644 (18)	−0.01089 (17)
S1	0.0231 (2)	0.0187 (2)	0.01481 (19)	−0.00119 (14)	0.00583 (15)	−0.00231 (13)
S2	0.0178 (2)	0.0220 (2)	0.0187 (2)	−0.00101 (14)	0.00585 (15)	0.00126 (14)
F1	0.0996 (12)	0.0286 (6)	0.0236 (6)	0.0191 (7)	0.0229 (7)	0.0060 (5)
F2	0.0691 (9)	0.0188 (5)	0.0461 (7)	−0.0062 (6)	0.0167 (7)	−0.0067 (5)
F3	0.0402 (7)	0.0402 (7)	0.0918 (12)	0.0177 (6)	0.0303 (8)	0.0267 (7)
F4	0.0650 (9)	0.0347 (7)	0.0620 (9)	0.0206 (7)	0.0257 (8)	0.0194 (6)
F5	0.0872 (11)	0.0427 (8)	0.0367 (7)	−0.0277 (8)	−0.0281 (7)	0.0189 (6)
F6	0.0593 (9)	0.0433 (7)	0.0469 (8)	−0.0179 (6)	0.0252 (7)	0.0100 (6)
O1	0.0216 (6)	0.0317 (7)	0.0290 (7)	−0.0046 (5)	0.0053 (5)	−0.0099 (5)
O2	0.0462 (8)	0.0276 (7)	0.0174 (6)	−0.0026 (6)	0.0146 (6)	−0.0025 (5)
O3	0.0211 (6)	0.0313 (7)	0.0216 (6)	−0.0065 (5)	0.0032 (5)	−0.0025 (5)
O4	0.0267 (7)	0.0358 (7)	0.0357 (7)	0.0025 (6)	0.0182 (6)	−0.0020 (6)
N1	0.0178 (6)	0.0171 (6)	0.0158 (6)	−0.0006 (5)	0.0060 (5)	−0.0025 (5)
C1	0.0216 (8)	0.0159 (7)	0.0226 (8)	−0.0044 (6)	0.0105 (6)	−0.0059 (6)
C2	0.0241 (8)	0.0204 (8)	0.0152 (7)	−0.0020 (6)	0.0055 (6)	−0.0020 (6)
C3	0.0182 (7)	0.0175 (7)	0.0171 (7)	0.0018 (6)	0.0027 (6)	0.0002 (6)
C4	0.0163 (7)	0.0166 (7)	0.0160 (7)	−0.0004 (6)	0.0055 (6)	−0.0015 (6)
C5	0.0197 (8)	0.0207 (8)	0.0176 (8)	0.0021 (6)	0.0038 (6)	0.0024 (6)
C6	0.0190 (8)	0.0193 (8)	0.0269 (8)	0.0029 (6)	0.0069 (7)	−0.0003 (6)
C7	0.0371 (10)	0.0185 (8)	0.0244 (9)	0.0017 (7)	0.0134 (7)	0.0002 (6)
C8	0.0360 (10)	0.0247 (9)	0.0258 (9)	−0.0082 (7)	0.0040 (8)	0.0053 (7)

Geometric parameters (Å, º)

Cl1—C1	1.7380 (16)	F5—C8	1.304 (2)
S1—O2	1.4131 (13)	F6—C8	1.313 (2)
S1—O1	1.4160 (13)	N1—C4	1.4637 (19)
S1—N1	1.6769 (13)	C1—C6	1.381 (2)
S1—C7	1.8470 (18)	C1—C2	1.385 (2)
S2—O4	1.4135 (13)	C2—C3	1.388 (2)
S2—O3	1.4168 (13)	C2—H2	0.9500
S2—N1	1.6749 (14)	C3—C4	1.387 (2)
S2—C8	1.8483 (19)	C3—H3	0.9500

F1—C7	1.306 (2)	C4—C5	1.384 (2)
F2—C7	1.317 (2)	C5—C6	1.388 (2)
F3—C7	1.303 (2)	C5—H5	0.9500
F4—C8	1.309 (3)	C6—H6	0.9500
O2—S1—O1	123.00 (9)	C2—C3—H3	120.5
O2—S1—N1	110.21 (8)	C5—C4—C3	122.06 (15)
O1—S1—N1	106.70 (7)	C5—C4—N1	119.00 (14)
O2—S1—C7	106.88 (8)	C3—C4—N1	118.94 (14)
O1—S1—C7	105.19 (9)	C4—C5—C6	118.75 (15)
N1—S1—C7	103.02 (8)	C4—C5—H5	120.6
O4—S2—O3	122.60 (8)	C6—C5—H5	120.6
O4—S2—N1	109.14 (8)	C1—C6—C5	119.21 (15)
O3—S2—N1	107.18 (7)	C1—C6—H6	120.4
O4—S2—C8	107.55 (9)	C5—C6—H6	120.4
O3—S2—C8	105.91 (8)	F3—C7—F1	110.51 (18)
N1—S2—C8	102.67 (8)	F3—C7—F2	108.18 (16)
C4—N1—S2	118.56 (10)	F1—C7—F2	109.00 (16)
C4—N1—S1	118.91 (10)	F3—C7—S1	110.98 (13)
S2—N1—S1	122.53 (8)	F1—C7—S1	110.08 (12)
C6—C1—C2	122.17 (15)	F2—C7—S1	108.03 (13)
C6—C1—Cl1	119.27 (13)	F5—C8—F4	110.23 (19)
C2—C1—Cl1	118.56 (13)	F5—C8—F6	109.09 (18)
C1—C2—C3	118.74 (15)	F4—C8—F6	108.97 (16)
C1—C2—H2	120.6	F5—C8—S2	111.24 (13)
C3—C2—H2	120.6	F4—C8—S2	109.37 (13)
C4—C3—C2	119.07 (15)	F6—C8—S2	107.89 (14)
C4—C3—H3	120.5		
O4—S2—N1—C4	−155.34 (12)	N1—C4—C5—C6	−179.88 (14)
O3—S2—N1—C4	−20.57 (14)	C2—C1—C6—C5	0.1 (3)
C8—S2—N1—C4	90.75 (13)	Cl1—C1—C6—C5	179.81 (13)
O4—S2—N1—S1	23.61 (12)	C4—C5—C6—C1	−0.4 (2)
O3—S2—N1—S1	158.38 (9)	O2—S1—C7—F3	−40.94 (16)
C8—S2—N1—S1	−90.29 (11)	O1—S1—C7—F3	−173.17 (14)
O2—S1—N1—C4	−151.50 (12)	N1—S1—C7—F3	75.21 (15)
O1—S1—N1—C4	−15.75 (14)	O2—S1—C7—F1	−163.59 (14)
C7—S1—N1—C4	94.75 (13)	O1—S1—C7—F1	64.17 (16)
O2—S1—N1—S2	29.55 (12)	N1—S1—C7—F1	−47.44 (16)
O1—S1—N1—S2	165.30 (9)	O2—S1—C7—F2	77.50 (14)
C7—S1—N1—S2	−84.20 (11)	O1—S1—C7—F2	−54.73 (14)
C6—C1—C2—C3	0.0 (2)	N1—S1—C7—F2	−166.35 (12)
Cl1—C1—C2—C3	−179.66 (12)	O4—S2—C8—F5	−67.64 (18)
C1—C2—C3—C4	0.1 (2)	O3—S2—C8—F5	159.68 (16)
C2—C3—C4—C5	−0.4 (2)	N1—S2—C8—F5	47.42 (18)
C2—C3—C4—N1	−179.97 (14)	O4—S2—C8—F4	170.36 (13)
S2—N1—C4—C5	−102.12 (15)	O3—S2—C8—F4	37.69 (16)
S1—N1—C4—C5	78.89 (17)	N1—S2—C8—F4	−74.58 (15)

S2—N1—C4—C3	77.44 (17)	O4—S2—C8—F6	51.97 (16)
S1—N1—C4—C3	−101.55 (15)	O3—S2—C8—F6	−80.71 (15)
C3—C4—C5—C6	0.6 (2)	N1—S2—C8—F6	167.02 (13)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O3^{i}	0.95	2.57	3.496 (2)	164
C5—H5···O1^{ii}	0.95	2.59	3.385 (2)	141

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