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Hydrogen-bonding patterns in 4-[(5-methylisoxazol-3-yl)amino-sulfonyl]anilinium chloride

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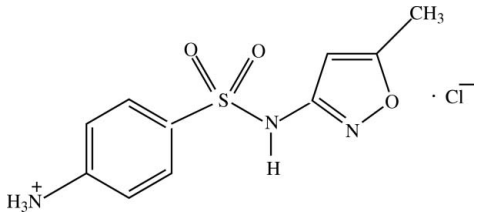
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.037; wR factor = 0.071; data-to-parameter ratio = 12.1.

In the title compound, $C_{10}H_{12}O_3N_3S^+\cdot Cl^-$, 4-amino-*N*-(5-methyl-3-isoxazolyl)benzenesulfonamide is protonated on the amine N atom which is connected to the benzene ring. The geometry around the S atom is considerably distorted from ideal tetrahedral geometry. The crystal packing is stabilized by intermolecular N—H···N, N—H···Cl, N—H···O and C—H···O hydrogen bonds.

Related literature

For related literature, see: Abramenko & Sergienko (2002); Bettinetti *et al.* (1982); Chatterjee *et al.* (1982); Ghosh *et al.* (1991); Haridas *et al.* (1984); Johnson (1976); Kálmán *et al.* (1981); Kendi *et al.* (2000); Özbey *et al.* (2005); Singh *et al.* (1984); Takasuka & Nakai (2001).



Experimental

Crystal data

$C_{10}H_{12}N_3O_3S^+\cdot Cl^-$
M_r = 289.75
Monoclinic, *Cc*
a = 8.677 (2) Å
b = 15.615 (3) Å
c = 10.435 (2) Å
β = 111.29 (2)°
V = 1317.4 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.45 mm^{-1}
T = 293 K
0.15 × 0.14 × 0.13 mm

Data collection

Philips PW 1100 diffractometer
Absorption correction: none
2021 measured reflections
2021 independent reflections
1318 reflections with $I > 2\sigma(I)$
1 standard reflection
every 100 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.071
S = 0.90
2021 reflections
167 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Absolute structure: Flack (1983), 89 Friedel pairs
Flack parameter: −0.05 (7)

Table 1
Selected geometric parameters (Å, °).

S1—O1	1.429 (2)	S1—N7	1.631 (3)
S1—O2	1.433 (2)	S1—C1	1.775 (3)
O1—S1—O2	120.92 (17)	N7—S1—C1	106.01 (15)
O1—S1—N7	104.98 (16)	S1—N7—C8	124.0 (2)
O1—S1—C1	108.03 (15)	S1—C1—C2	120.3 (3)
O2—S1—N7	107.48 (15)	S1—C1—C6	119.4 (2)
O2—S1—C1	108.47 (16)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4A···N8^{i}	0.92	1.93	2.843 (4)	170
N4—H4B···Cl1^{ii}	0.98	2.20	3.177 (3)	175
N4—H4C···Cl1^{iii}	0.86	2.24	3.093 (3)	169
N7—H7···Cl1	0.86	2.55	3.094 (3)	122
N7—H7···O3^{iv}	0.86	2.56	3.204 (4)	133
C2—H2···O1	0.93	2.55	2.926 (5)	105
C6—H6···O1^{v}	0.93	2.53	3.389 (4)	154

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

Data collection: *FEBO* (Belletti, 1996); cell refinement: *MolEN* (Fair, 1990); data reduction: *MolEN*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2536).

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supplementary materials

Acta Cryst. (2007). E**63**, o4312-o4313 [**doi:10.1107/S1600536807049446**]

Hydrogen-bonding patterns in 4-[(5-methylisoxazol-3-yl)aminosulfonyl]anilinium chloride

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Comment

Sulfonamides constitute an important class of antimicrobical agents. The drug, 4-amino-*N*-(5-methyl-3-isoxzolyl) benzene sulfonamide [Sulfamethoxazole (SMZ)] prevents the formation of dihydrofolic acid, a compound that bacteria must be able to make in order to survive. The two polymorphs of SMZ (Bettinetti *et al.*, 1982) have already been reported in literature.

An *ORTEPII* (Johnson, 1976) view of the title compound (I), is shown in Fig.1. The asymmetric unit contains one 4-ammonio-*N*-(5-methyl-3-isoxazolyl) benzene sulfonamide cation and a chloride anion. The cation is protonated on the amine nitrogen (N4) atom. The distances around the S atom in the SMZ molecule agree well with the corresponding distances in other sulfonamides. The atoms around the sulfonamide S atom in (I) are arranged in a slightly distorted tetrahedral configuration. The largest deviation is in the angle O1—S1—O2 [120.92 (17)°], but it confirms to the non-tetrahedral nature commonly observed in sulfonamides (Chatterjee *et al.*, 1982; Haridas *et al.*, 1984; Ghosh *et al.*, 1991; Kendi *et al.*, 2000; Takasuka & Nakai, 2001; Özbey *et al.*, 2005). The S1—C1 distance of 1.775 (3)Å (I) is a normal single-bond value and matches well with those observed in other sulfonamides (Singh *et al.*, 1984; Abramenko & Sergienko, 2002). In the present structure the dihedral angle between the isoxazole and ammonio phenyl plane is found to be 58.0 (2)°, whereas in neutral SMZ structures the dihedral angles are 73.15° for form 1 and 79.66° for form 2 (Bettinetti *et al.*, 1982) respectively. The two torsion angles τ_1 (C—C—S—N) and τ_2 (C—S—N—C) defining the conformation of the sulfonamide group are reported to lie in the range 70–120° and 60–90°, respectively (Kálmán *et al.*, 1981). The torsion angles τ_1 is 73.2 (3)° (C6—C1—S1—N7) and τ_2 is −71.2 (3) Å (C1—S1—N7—C8). In the neutral forms, the torsion angles τ_1 are −76.59° (Form 1) and −78.55° (Form 2). The torsion angles τ_2 are −56.14° in form 1 and −61.58° in form 2. The cations and chloride anions are involved in a network of intermolecular hydrogen bonds, resulting in the formation of infinite chains propagating in the−b direction (Fig. 2). The chloride anion participates in N—H···Cl hydrogen-bond formation as a three proton acceptor, interacting with both the ammonio and amide NH groups [N—Cl = 3.093 (3)–3.177 (3) Å]. The amide N—H group also acts as a donor to the oxygen atom of isoxazole moiety, with an N—O distance of 3.204 (4) Å. The sulfonyl O atom (O1) is involved in a weak interaction with C6 of the phenyl ring through C—H···O hydrogen bonds (Fig 3).

Experimental

2 ml of HCl (20%) was added slowly to a solution of 4-amino-*N*-(5-methyl-3-isoxazolyl) benzene sulfonamide in hot ethanol. After a few days, colourless crystals of the title compound (I), were appeared.

Refinement

All H atoms were placed in idealized locations and were refined using a riding model, with C—H = 0.93 Å, N—H = 0.86–0.92 Å and U_{iso}(H) = 1.2Ueq (C,*N*).

Figures

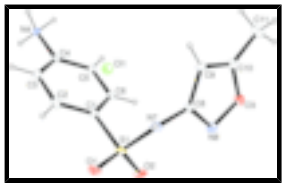

Fig. 1. An *ORTEP* view of the asymmetric unit of (I) showing 50% probability displacement ellipsoids.

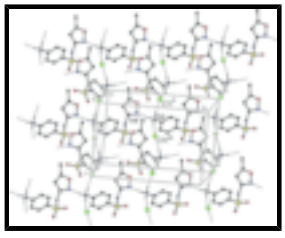

Fig. 2. Hydrogen bonding patterns in compound (I). Symmetry codes: (i) *x* − 1/2,*y* + 1/2,*z*; (ii) *x* − 1,-*y* + 1,*z* − 1/2; (iii) *x* − 1,*y*,*z*.

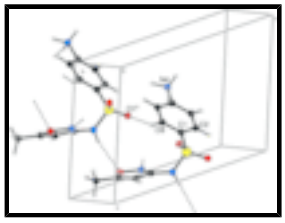

Fig. 3. A view of C—H···O interaction in compound (I). Symmetry codes: (v) *x* − 1/2,-*y* + 1/2,*z* − 1/2.

4-[(5-methylisoxazol-3-yl)aminosulfonyl]anilinium chloride

Crystal data

$C_{10}H_{12}N_3O_3S^+\cdot Cl^-$	F_{000} = 600
M_r = 289.75	D_x = 1.461 Mg m^{-3}
Monoclinic, *Cc*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: C -2yc	Cell parameters from 25 reflections
a = 8.677 (2) Å	θ = 3.0–30.0º
b = 15.615 (3) Å	μ = 0.45 mm^{-1}
c = 10.435 (2) Å	*T* = 293 K
β = 111.29 (2)º	Prism, colourless
V = 1317.4 (5) Å^3	0.15 × 0.14 × 0.13 mm
Z = 4	

Data collection

Philips PW 1100 diffractometer	R_{int} = 0.0000
Radiation source: fine-focus sealed tube	θ_{max} = 30.0º
Monochromator: graphite	θ_{min} = 3.4º
T = 293 K	*h* = −12→11
ω scans	*k* = 0→21
Absorption correction: none	*l* = 0→14
2021 measured reflections	1 standard reflections

2021 independent reflections
1318 reflections with $I > 2\sigma(I)$
every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.071$
$S = 0.90$
2021 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0282P)^2]$, where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ e Å^{-3}
Extinction correction: ?
Absolute structure: Flack (1983), 89 Friedel pairs
Flack parameter: −0.05 (7)

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All e.s.d.'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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.33023 (10)	0.30198 (5)	1.02704 (8)	0.0452 (3)
O1	0.4305 (3)	0.32910 (17)	1.1625 (2)	0.0622 (10)
O2	0.2677 (3)	0.21625 (14)	1.0016 (3)	0.0592 (10)
O3	0.3264 (3)	0.21386 (15)	0.6159 (3)	0.0564 (10)
N4	−0.2378 (3)	0.54615 (16)	0.8049 (3)	0.0418 (10)
N7	0.4442 (3)	0.31761 (16)	0.9346 (3)	0.0436 (9)
N8	0.3621 (4)	0.21322 (17)	0.7594 (3)	0.0525 (11)
C1	0.1613 (4)	0.3740 (2)	0.9626 (3)	0.0384 (10)
C2	0.1549 (5)	0.4471 (2)	1.0364 (4)	0.0501 (11)
C3	0.0266 (5)	0.5039 (2)	0.9840 (4)	0.0514 (14)
C4	−0.0967 (4)	0.48678 (19)	0.8594 (3)	0.0370 (10)
C5	−0.0929 (4)	0.4144 (2)	0.7853 (3)	0.0438 (11)
C6	0.0384 (4)	0.3578 (2)	0.8374 (3)	0.0443 (11)
C8	0.3984 (4)	0.29307 (19)	0.7974 (3)	0.0351 (10)

C9	0.3927 (4)	0.3457 (2)	0.6865 (4)	0.0451 (11)
C10	0.3460 (4)	0.2944 (2)	0.5764 (4)	0.0459 (12)
C11	0.3117 (5)	0.3066 (3)	0.4289 (4)	0.0645 (16)
Cl1	0.56666 (11)	0.50480 (6)	0.99302 (10)	0.0488 (3)
H2	0.23760	0.45760	1.12130	0.0600*
H3	0.02290	0.55350	1.03210	0.0620*
H4A	−0.19790	0.60040	0.80070	0.067 (12)*
H4B	−0.30140	0.53420	0.70750	0.054 (10)*
H4C	−0.29630	0.54180	0.85610	0.045 (10)*
H5	−0.17730	0.40360	0.70150	0.0520*
H6	0.04350	0.30910	0.78780	0.0530*
H7	0.53820	0.34250	0.97280	0.0520*
H9	0.41650	0.40390	0.68910	0.0540*
H11A	0.22950	0.35040	0.39360	0.0970*
H11B	0.27180	0.25390	0.38090	0.0970*
H11C	0.41150	0.32340	0.41590	0.0970*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0562 (5)	0.0374 (4)	0.0361 (4)	−0.0009 (4)	0.0098 (4)	0.0115 (4)
O1	0.0727 (19)	0.0673 (17)	0.0342 (14)	0.0047 (14)	0.0045 (13)	0.0126 (12)
O2	0.0734 (19)	0.0353 (13)	0.0663 (18)	−0.0031 (12)	0.0223 (16)	0.0181 (12)
O3	0.0714 (19)	0.0473 (15)	0.0525 (16)	−0.0147 (13)	0.0248 (15)	−0.0153 (12)
N4	0.0492 (17)	0.0319 (15)	0.0492 (18)	−0.0021 (13)	0.0236 (15)	−0.0003 (13)
N7	0.0384 (15)	0.0434 (15)	0.0400 (16)	−0.0101 (12)	0.0036 (12)	0.0025 (13)
N8	0.070 (2)	0.0338 (15)	0.054 (2)	−0.0064 (14)	0.0228 (17)	−0.0027 (13)
C1	0.0472 (19)	0.0312 (16)	0.0365 (17)	−0.0034 (14)	0.0150 (15)	0.0033 (14)
C2	0.054 (2)	0.047 (2)	0.0397 (19)	−0.0065 (18)	0.0054 (17)	−0.0115 (17)
C3	0.061 (3)	0.0392 (19)	0.052 (2)	−0.0047 (19)	0.018 (2)	−0.0172 (18)
C4	0.0479 (19)	0.0289 (16)	0.0368 (17)	−0.0075 (14)	0.0185 (15)	−0.0002 (13)
C5	0.051 (2)	0.0370 (18)	0.0382 (18)	−0.0006 (16)	0.0101 (16)	−0.0074 (15)
C6	0.058 (2)	0.0350 (18)	0.0340 (19)	0.0021 (17)	0.0098 (17)	−0.0061 (15)
C8	0.0299 (16)	0.0297 (16)	0.0416 (18)	−0.0035 (14)	0.0082 (14)	−0.0004 (14)
C9	0.052 (2)	0.0323 (18)	0.051 (2)	−0.0081 (15)	0.0187 (18)	0.0008 (16)
C10	0.042 (2)	0.044 (2)	0.056 (2)	−0.0075 (17)	0.023 (2)	−0.0054 (17)
C11	0.072 (3)	0.076 (3)	0.049 (2)	−0.018 (2)	0.026 (2)	−0.006 (2)
Cl1	0.0622 (5)	0.0392 (5)	0.0495 (5)	−0.0109 (4)	0.0257 (4)	−0.0048 (4)

Geometric parameters (Å, °)

S1—O1	1.429 (2)	C2—C3	1.372 (6)
S1—O2	1.433 (2)	C3—C4	1.377 (5)
S1—N7	1.631 (3)	C4—C5	1.377 (4)
S1—C1	1.775 (3)	C5—C6	1.387 (5)
O3—N8	1.415 (4)	C8—C9	1.406 (5)
O3—C10	1.353 (4)	C9—C10	1.337 (5)
N4—C4	1.475 (4)	C10—C11	1.470 (6)
N7—C8	1.393 (4)	C2—H2	0.9301

N8—C8	1.312 (4)	C3—H3	0.9298
N4—H4B	0.9824	C5—H5	0.9297
N4—H4C	0.8629	C6—H6	0.9299
N4—H4A	0.9222	C9—H9	0.9302
N7—H7	0.8597	C11—H11A	0.9599
C1—C2	1.389 (5)	C11—H11B	0.9602
C1—C6	1.377 (4)	C11—H11C	0.9604
Cl1···N4^{i}	3.093 (3)	C5···Cl1^{ix}	3.616 (3)
Cl1···N7	3.094 (3)	C6···C11^{xi}	3.569 (6)
Cl1···C5^{ii}	3.616 (3)	C6···C8	3.450 (5)
Cl1···C11^{iii}	3.597 (5)	C6···O1^{vi}	3.389 (4)
Cl1···N4^{ii}	3.177 (3)	C8···C6	3.450 (5)
Cl1···H4C^{i}	2.2412	C11···O1^{xii}	3.316 (5)
Cl1···H7	2.5476	C11···C6^{xiii}	3.569 (6)
Cl1···H11C^{iii}	2.9783	C11···Cl1^{xiv}	3.597 (5)
Cl1···H9^{iii}	3.1389	C6···H11B^{xi}	3.0598
Cl1···H5^{ii}	2.8644	C8···H6	3.0548
Cl1···H4B^{ii}	2.1977	H2···O1	2.5475
S1···H6^{iv}	3.1907	H3···H4A	2.5842
O1···C11^{v}	3.316 (5)	H4A···O2^{x}	2.8655
O1···C6^{iv}	3.389 (4)	H4A···O3^{x}	2.6828
O2···N8	2.926 (4)	H4A···N8^{x}	1.9296
O3···N7^{vi}	3.204 (4)	H4A···H3	2.5842
O1···H11C^{v}	2.7099	H4B···H5	2.3176
O1···H2	2.5475	H4B···Cl1^{ix}	2.1977
O1···H6^{iv}	2.5292	H4C···Cl1^{viii}	2.2412
O2···H5^{iv}	2.7126	H5···Cl1^{ix}	2.8644
O2···H4A^{vii}	2.8655	H5···H4B	2.3176
O2···H6	2.7771	H5···O2^{vi}	2.7126
O3···H4A^{vii}	2.6828	H6···O2	2.7771
O3···H7^{vi}	2.5585	H6···C8	3.0548
N4···Cl1^{viii}	3.093 (3)	H6···S1^{vi}	3.1907
N4···Cl1^{ix}	3.177 (3)	H6···O1^{vi}	2.5292
N4···N8^{x}	2.843 (4)	H7···O3^{iv}	2.5586
N7···O3^{iv}	3.204 (4)	H7···Cl1	2.5476
N7···Cl1	3.094 (3)	H9···Cl1^{xiv}	3.1389
N8···N4^{vii}	2.843 (4)	H11B···C6^{xiii}	3.0598
N8···O2	2.926 (4)	H11C···O1^{xii}	2.7099
N8···H4A^{vii}	1.9296	H11C···Cl1^{xiv}	2.9783
O1—S1—O2	120.92 (17)	C4—C5—C6	119.1 (3)
O1—S1—N7	104.98 (16)	C1—C6—C5	119.8 (3)
O1—S1—C1	108.03 (15)	N7—C8—C9	126.6 (3)

O2—S1—N7	107.48 (15)	N8—C8—C9	112.0 (3)
O2—S1—C1	108.47 (16)	N7—C8—N8	121.3 (3)
N7—S1—C1	106.01 (15)	C8—C9—C10	105.4 (3)
N8—O3—C10	109.0 (3)	O3—C10—C11	116.1 (3)
S1—N7—C8	124.0 (2)	C9—C10—C11	134.8 (3)
O3—N8—C8	104.4 (2)	O3—C10—C9	109.1 (3)
H4B—N4—H4C	112.95	C1—C2—H2	120.04
C4—N4—H4C	107.71	C3—C2—H2	119.96
C4—N4—H4A	108.80	C2—C3—H3	120.35
C4—N4—H4B	110.81	C4—C3—H3	120.27
H4A—N4—H4B	101.82	C4—C5—H5	120.39
H4A—N4—H4C	114.65	C6—C5—H5	120.49
S1—N7—H7	118.05	C1—C6—H6	120.09
C8—N7—H7	117.99	C5—C6—H6	120.07
S1—C1—C2	120.3 (3)	C8—C9—H9	127.31
S1—C1—C6	119.4 (2)	C10—C9—H9	127.24
C2—C1—C6	120.3 (3)	C10—C11—H11A	109.50
C1—C2—C3	120.0 (4)	C10—C11—H11B	109.43
C2—C3—C4	119.4 (3)	C10—C11—H11C	109.46
N4—C4—C3	119.6 (3)	H11A—C11—H11B	109.48
N4—C4—C5	119.0 (3)	H11A—C11—H11C	109.49
C3—C4—C5	121.4 (3)	H11B—C11—H11C	109.46
O1—S1—N7—C8	174.6 (3)	O3—N8—C8—C9	−1.6 (4)
O2—S1—N7—C8	44.7 (3)	S1—C1—C6—C5	−179.1 (3)
C1—S1—N7—C8	−71.2 (3)	S1—C1—C2—C3	178.0 (3)
O1—S1—C1—C2	6.7 (3)	C6—C1—C2—C3	−0.6 (6)
O1—S1—C1—C6	−174.7 (3)	C2—C1—C6—C5	−0.5 (5)
O2—S1—C1—C2	139.4 (3)	C1—C2—C3—C4	1.3 (6)
O2—S1—C1—C6	−42.0 (3)	C2—C3—C4—N4	177.9 (3)
N7—S1—C1—C2	−105.4 (3)	C2—C3—C4—C5	−0.9 (6)
N7—S1—C1—C6	73.2 (3)	C3—C4—C5—C6	−0.2 (5)
N8—O3—C10—C11	−179.3 (3)	N4—C4—C5—C6	−179.0 (3)
C10—O3—N8—C8	0.9 (4)	C4—C5—C6—C1	0.9 (5)
N8—O3—C10—C9	0.1 (4)	N8—C8—C9—C10	1.8 (5)
S1—N7—C8—N8	−57.2 (4)	N7—C8—C9—C10	178.6 (4)
S1—N7—C8—C9	126.2 (3)	C8—C9—C10—O3	−1.1 (4)
O3—N8—C8—N7	−178.7 (3)	C8—C9—C10—C11	178.3 (4)

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) *x*+1, −*y*+1, *z*+1/2; (iii) *x*, −*y*+1, *z*+1/2; (iv) *x*+1/2, −*y*+1/2, *z*+1/2; (v) *x*, *y*, *z*+1; (vi) *x*−1/2, −*y*+1/2, *z*−1/2; (vii) *x*+1/2, *y*−1/2, *z*; (viii) *x*−1, *y*, *z*; (ix) *x*−1, −*y*+1, *z*−1/2; (x) *x*−1/2, *y*+1/2, *z*; (xi) *x*−1/2, −*y*+1/2, *z*+1/2; (xii) *x*, *y*, *z*−1; (xiii) *x*+1/2, −*y*+1/2, *z*−1/2; (xiv) *x*, −*y*+1, *z*−1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4A···N8^{x}	0.92	1.93	2.843 (4)	170
N4—H4B···Cl1^{ix}	0.98	2.20	3.177 (3)	175
N4—H4C···Cl1^{viii}	0.86	2.24	3.093 (3)	169
N7—H7···Cl1	0.86	2.55	3.094 (3)	122

N7—H7···O3^{iv}	0.86	2.56	3.204 (4)	133
C2—H2···O1	0.93	2.55	2.926 (5)	105
C6—H6···O1^{vi}	0.93	2.53	3.389 (4)	154

Symmetry codes: (x) *x*−1/2, *y*+1/2, *z*; (ix) *x*−1, −*y*+1, *z*−1/2; (viii) *x*−1, *y*, *z*; (iv) *x*+1/2, −*y*+1/2, *z*+1/2; (vi) *x*−1/2, −*y*+1/2, *z*−1/2.

Fig. 1

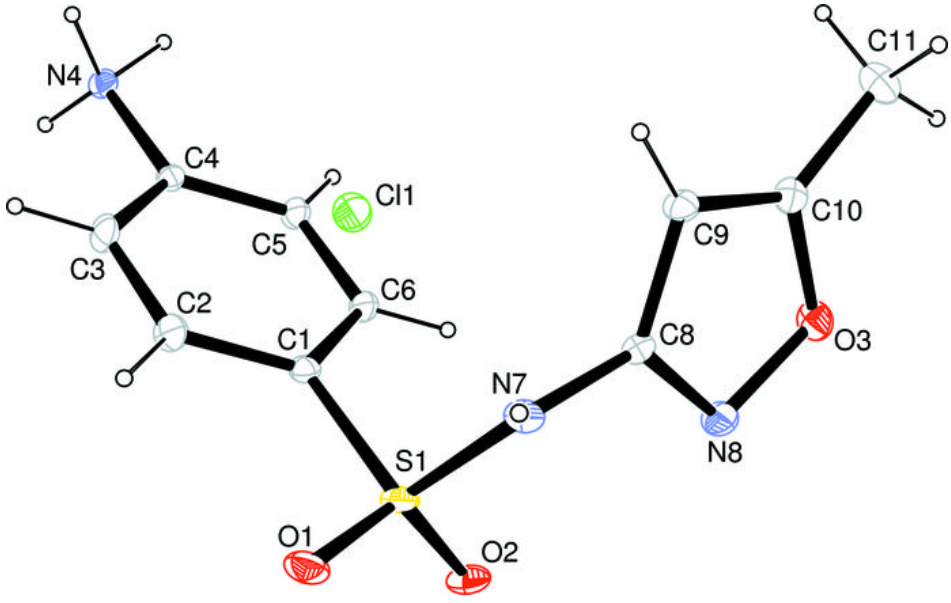

Fig. 2

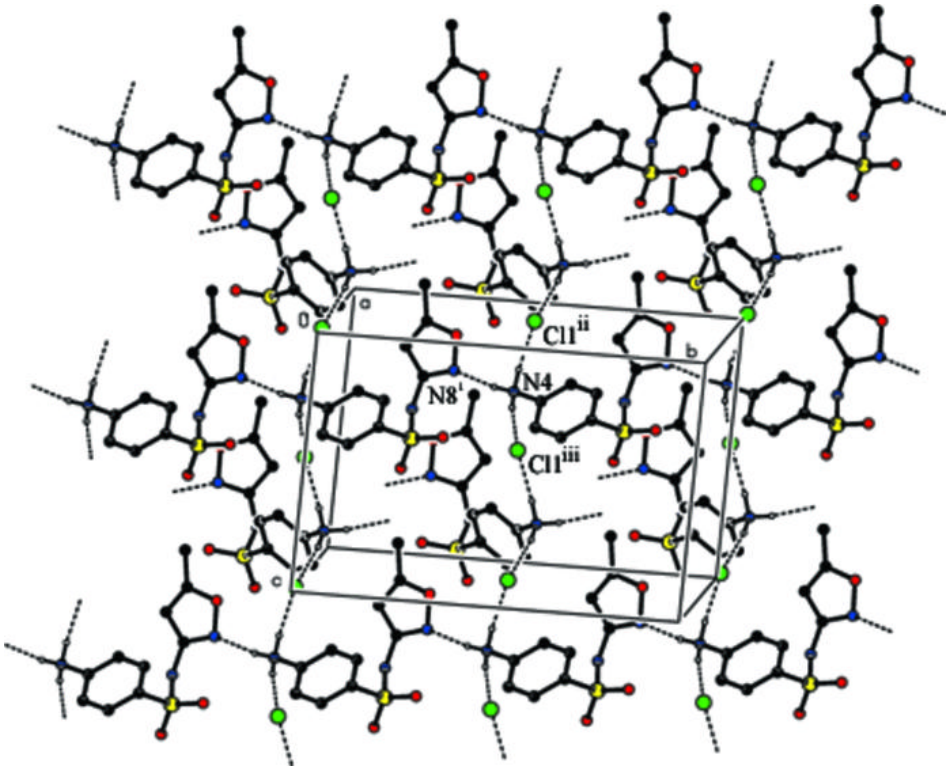

Fig. 3