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1-Isopropyl-4-tosylpiperazin-1-ium trifluoroacetate

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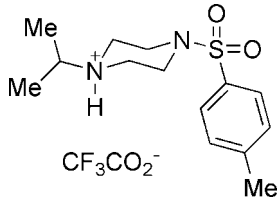
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.004 Å; disorder in solvent or counterion; R factor = 0.054; wR factor = 0.124; data-to-parameter ratio = 11.9.

In the title compound, $C_{14}H_{23}N_2O_2S^+\cdot C_2F_3O_2^-$, the piperazine ring adopts a chair conformation. The crystal packing is stabilized by C—H···O and N—H···O hydrogen bonds between the cation and anion. The F atoms are disordered over two positions; the site occupancy factors are 0.55 (2) and 0.45 (2).

Related literature

For related literature on benzenesulfonamides, see: Yu *et al.* (2007); Xing *et al.* (2006, 2005).



Experimental

Crystal data

$C_{14}H_{23}N_2O_2S^+\cdot C_2F_3O_2^-$
M_r = 396.42
Monoclinic, $P2_1/n$
a = 11.659 (2) Å
b = 8.4274 (17) Å
c = 19.404 (4) Å
β = 105.87 (3)°
V = 1833.8 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 113 (2) K
0.10 × 0.08 × 0.02 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.977, T_{max} = 0.995
10902 measured reflections
3226 independent reflections
2517 reflections with $I > 2\sigma(I)$
R_{int} = 0.072

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.124
S = 1.03
3226 reflections
270 parameters
43 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O4^{i}	0.902 (11)	1.828 (12)	2.724 (3)	172 (3)
C9—H9A···O2^{ii}	0.97	2.52	3.405 (4)	151
C10—H10A···O4^{ii}	0.97	2.45	3.357 (4)	155
C2—H2···O3^{iii}	0.93	2.58	3.225 (4)	127

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *CrystalStructure* (Rigaku/MSC, 2005).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2629).

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supplementary materials

Acta Cryst. (2008). E**64**, o22 [**doi:10.1107/S1600536807061570**]

1-Isopropyl-4-tosylpiperazin-1-ium trifluoroacetate

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Comment

In the title compound (Fig. 1) both N atoms have a pyramidal arrangement, but the pyramid of the amide is somewhat shallower than that of the protonated N. The protonated piperazin ring adopts a chair conformation.

The crystal packing is stabilized by C—H···O and N—H···O hydrogen bonds (Table 1) between the cation and anion. Weak intermolecular C—H···O hydrogen bonds involving an S=O group as acceptor play an important role in the moleclular packing.

Experimental

A solution of 4-methylbenzenesulfonyl chloride (3.28 g, 17 mmol) in CH_2Cl_2 was added dropwise to a mixture of 1-isopropylpiperazine (2.23 g, 82%, 0.14 mmol) and sodium biscarbonate (3.36 g, 40 mmol) in CH_2Cl_2 (30 ml) at room temperature with stirring. After stirring for 4 h followed by filtration, the organic filtrate was rotoevaporated under vacuum. The resulting solid, in a yield of 53.8%, was purified by recrystallization from methanol. Crystals in the form of colourless blocks were grown by evaporation of a trifluoroacetic solution.

Refinement

The N-bound H atoms were refined freely with the restraint of 0.90 (1) Å, while the other H atoms were positioned geometrically (C—H = 0.93, 0.96 and 0.97 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C). The three F atoms are disordered over two site occupancy of 0.55 (2): 0.45 (2). The C—F distances were restrained to 1.36 (1) Å and their displacement parameters were restrained to be isotropic by means of the instruction ISOR (tolerance 0.01) in *SHELXL*.

Figures

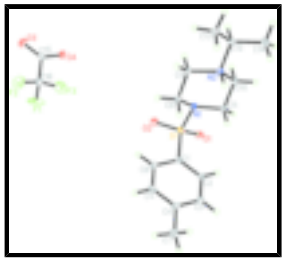


Fig. 1. The molecular structure of (I) with the atom-numbering scheme and 30% probability displacement ellipsoids. Only one component of the disordered CF_3 group is shown.

1-Isopropyl-4-tosylpiperazin-1-ium trifluoroacetate

Crystal data

$C_{14}H_{23}N_2O_2S^+·C_2F_3O_2^-$	F_{000} = 832
M_r = 396.42	D_x = 1.436 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 3880 reflections
a = 11.659 (2) Å	θ = 2.2–27.9º
b = 8.4274 (17) Å	μ = 0.23 mm^{-1}
c = 19.404 (4) Å	T = 113 (2) K
β = 105.87 (3)º	Block, colorless
V = 1833.8 (6) Å^3	0.10 × 0.08 × 0.02 mm
Z = 4	

Data collection

Rigaku Saturn diffractometer	3226 independent reflections
Radiation source: rotating anode	2517 reflections with $I > 2\sigma(I)$
Monochromator: confocal	R_{int} = 0.072
T = 113(2) K	θ_{max} = 25.0º
ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (CrystalClear; Rigaku/MSC, 2005)	h = −13→9
T_{min} = 0.977, T_{max} = 0.995	k = −9→10
10902 measured reflections	l = −23→23

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.054	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.124	$w = 1/[\sigma^2(F_o^2) + (0.0512P)^2 + 0.9104P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max}$ = 0.003
3226 reflections	$\Delta\rho_{max}$ = 0.40 e Å^{-3}
270 parameters	$\Delta\rho_{min}$ = −0.28 e Å^{-3}
43 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\text{sigma}(F^2)$ 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}	Occ. (<1)
S1	0.63629 (6)	−0.19035 (8)	0.09809 (4)	0.0214 (2)	
F1	0.0952 (9)	0.0965 (13)	0.2419 (6)	0.078 (3)	0.55 (2)
F2	0.1367 (11)	0.3388 (12)	0.2544 (5)	0.077 (3)	0.55 (2)
F3	0.2151 (6)	0.1905 (18)	0.1909 (5)	0.070 (3)	0.55 (2)
F1'	0.0745 (9)	0.175 (2)	0.2595 (5)	0.083 (4)	0.45 (2)
F2'	0.1771 (11)	0.3557 (10)	0.2275 (9)	0.077 (4)	0.45 (2)
F3'	0.1949 (11)	0.1212 (15)	0.2000 (6)	0.066 (4)	0.45 (2)
O1	0.63011 (18)	−0.3355 (2)	0.05863 (10)	0.0265 (5)	
O2	0.53262 (17)	−0.1320 (2)	0.11580 (10)	0.0275 (5)	
O3	−0.0548 (2)	0.3661 (3)	0.14312 (12)	0.0410 (6)	
O4	0.00768 (17)	0.1625 (2)	0.08810 (10)	0.0277 (5)	
N1	0.6753 (2)	−0.0517 (3)	0.04892 (11)	0.0197 (5)	
N2	0.7924 (2)	0.1936 (3)	−0.01082 (12)	0.0183 (5)	
C1	0.7539 (2)	−0.2013 (3)	0.17719 (14)	0.0195 (6)	
C2	0.8553 (3)	−0.2897 (3)	0.17916 (14)	0.0211 (6)	
H2	0.8588	−0.3517	0.1402	0.025*	
C3	0.9508 (3)	−0.2842 (4)	0.23978 (15)	0.0254 (7)	
H3	1.0186	−0.3440	0.2415	0.030*	
C4	0.9472 (3)	−0.1907 (3)	0.29824 (14)	0.0248 (7)	
C5	0.8443 (3)	−0.1060 (4)	0.29589 (15)	0.0281 (7)	
H5	0.8406	−0.0447	0.3351	0.034*	
C6	0.7468 (3)	−0.1113 (3)	0.23611 (15)	0.0258 (7)	
H6	0.6776	−0.0556	0.2353	0.031*	
C7	1.0535 (3)	−0.1813 (4)	0.36274 (16)	0.0373 (8)	
H7A	1.0736	−0.2858	0.3820	0.056*	
H7B	1.0348	−0.1150	0.3984	0.056*	
H7C	1.1199	−0.1371	0.3490	0.056*	
C8	0.6947 (3)	0.1074 (3)	0.08214 (14)	0.0222 (6)	
H8A	0.7690	0.1081	0.1200	0.027*	
H8B	0.6305	0.1321	0.1033	0.027*	
C9	0.6995 (3)	0.2314 (3)	0.02688 (14)	0.0215 (7)	
H9A	0.6221	0.2383	−0.0080	0.026*	
H9B	0.7169	0.3339	0.0501	0.026*	

C10	0.7722 (2)	0.0296 (3)	−0.04174 (14)	0.0201 (6)
H10A	0.8350	0.0033	−0.0639	0.024*
H10B	0.6967	0.0261	−0.0785	0.024*
C11	0.7712 (3)	−0.0907 (3)	0.01589 (14)	0.0213 (6)
H11A	0.7585	−0.1962	−0.0049	0.026*
H11B	0.8474	−0.0898	0.0520	0.026*
C12	0.7963 (3)	0.3177 (3)	−0.06701 (14)	0.0221 (6)
H12	0.7191	0.3189	−0.1033	0.026*
C13	0.8190 (3)	0.4804 (3)	−0.03294 (16)	0.0271 (7)
H13A	0.8896	0.4772	0.0066	0.041*
H13B	0.7522	0.5112	−0.0161	0.041*
H13C	0.8296	0.5558	−0.0677	0.041*
C14	0.8927 (3)	0.2765 (4)	−0.10319 (17)	0.0337 (8)
H14A	0.8996	0.3606	−0.1352	0.051*
H14B	0.8720	0.1797	−0.1298	0.051*
H14C	0.9675	0.2631	−0.0675	0.051*
C15	0.0119 (3)	0.2552 (3)	0.13959 (15)	0.0241 (7)
C16	0.1144 (3)	0.2243 (4)	0.20678 (16)	0.0313 (8)
H2A	0.8653 (14)	0.193 (4)	0.0208 (13)	0.031 (9)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0190 (4)	0.0236 (4)	0.0199 (4)	−0.0031 (3)	0.0026 (3)	0.0009 (3)
F1	0.079 (5)	0.074 (5)	0.064 (4)	−0.015 (3)	−0.010 (3)	0.047 (4)
F2	0.086 (5)	0.073 (5)	0.046 (4)	0.026 (4)	−0.027 (3)	−0.032 (3)
F3	0.028 (3)	0.129 (7)	0.050 (3)	0.014 (4)	0.005 (2)	0.008 (5)
F1'	0.077 (5)	0.139 (9)	0.036 (4)	0.013 (6)	0.019 (3)	0.036 (5)
F2'	0.063 (5)	0.046 (4)	0.085 (7)	−0.023 (3)	−0.040 (4)	−0.008 (4)
F3'	0.062 (6)	0.063 (6)	0.052 (5)	0.044 (4)	−0.021 (4)	−0.016 (4)
O1	0.0317 (13)	0.0237 (11)	0.0212 (10)	−0.0075 (9)	0.0025 (9)	−0.0013 (8)
O2	0.0180 (12)	0.0362 (13)	0.0290 (11)	0.0000 (9)	0.0075 (9)	0.0045 (9)
O3	0.0448 (15)	0.0332 (13)	0.0382 (13)	0.0159 (11)	0.0001 (11)	−0.0083 (11)
O4	0.0216 (12)	0.0312 (12)	0.0270 (11)	0.0039 (9)	0.0012 (9)	−0.0056 (9)
N1	0.0213 (14)	0.0194 (13)	0.0194 (12)	0.0001 (10)	0.0074 (10)	0.0004 (10)
N2	0.0172 (13)	0.0179 (12)	0.0191 (12)	0.0001 (10)	0.0037 (10)	−0.0019 (10)
C1	0.0223 (16)	0.0160 (14)	0.0187 (14)	−0.0008 (11)	0.0031 (12)	0.0019 (11)
C2	0.0250 (17)	0.0199 (15)	0.0186 (14)	−0.0006 (12)	0.0064 (12)	0.0019 (12)
C3	0.0217 (17)	0.0302 (17)	0.0258 (15)	0.0025 (13)	0.0091 (13)	0.0056 (13)
C4	0.0262 (18)	0.0242 (16)	0.0214 (15)	−0.0057 (13)	0.0021 (13)	0.0049 (12)
C5	0.037 (2)	0.0244 (17)	0.0201 (15)	0.0035 (13)	0.0032 (14)	0.0000 (12)
C6	0.0265 (18)	0.0259 (17)	0.0254 (15)	0.0063 (13)	0.0081 (13)	−0.0006 (13)
C7	0.031 (2)	0.046 (2)	0.0276 (17)	−0.0068 (15)	−0.0032 (14)	0.0033 (15)
C8	0.0233 (17)	0.0218 (15)	0.0235 (15)	0.0015 (12)	0.0098 (13)	−0.0025 (12)
C9	0.0202 (17)	0.0208 (15)	0.0249 (15)	0.0036 (12)	0.0085 (12)	−0.0041 (12)
C10	0.0204 (16)	0.0182 (15)	0.0215 (14)	0.0006 (11)	0.0054 (12)	−0.0039 (12)
C11	0.0231 (16)	0.0179 (15)	0.0220 (14)	0.0020 (11)	0.0046 (12)	−0.0017 (12)
C12	0.0234 (16)	0.0193 (15)	0.0221 (15)	0.0009 (12)	0.0038 (12)	0.0056 (12)

C13	0.0293 (18)	0.0233 (16)	0.0295 (16)	0.0040 (13)	0.0096 (13)	0.0055 (13)
C14	0.042 (2)	0.0283 (18)	0.0380 (18)	−0.0016 (14)	0.0228 (16)	0.0014 (14)
C15	0.0239 (18)	0.0234 (16)	0.0246 (15)	−0.0028 (12)	0.0058 (13)	0.0007 (13)
C16	0.032 (2)	0.0311 (19)	0.0285 (17)	−0.0004 (14)	0.0039 (15)	−0.0037 (14)

Geometric parameters (Å, °)

S1—O2	1.431 (2)	C5—C6	1.385 (4)
S1—O1	1.435 (2)	C5—H5	0.9300
S1—N1	1.649 (2)	C6—H6	0.9300
S1—C1	1.758 (3)	C7—H7A	0.9600
F1—C16	1.326 (6)	C7—H7B	0.9600
F2—C16	1.311 (6)	C7—H7C	0.9600
F3—C16	1.323 (7)	C8—C9	1.509 (4)
F1'—C16	1.302 (7)	C8—H8A	0.9700
F2'—C16	1.327 (7)	C8—H8B	0.9700
F3'—C16	1.312 (7)	C9—H9A	0.9700
O3—C15	1.230 (4)	C9—H9B	0.9700
O4—C15	1.259 (3)	C10—C11	1.512 (4)
N1—C11	1.470 (4)	C10—H10A	0.9700
N1—C8	1.478 (3)	C10—H10B	0.9700
N2—C9	1.498 (3)	C11—H11A	0.9700
N2—C10	1.499 (3)	C11—H11B	0.9700
N2—C12	1.521 (3)	C12—C13	1.514 (4)
N2—H2A	0.902 (11)	C12—C14	1.519 (4)
C1—C2	1.389 (4)	C12—H12	0.9800
C1—C6	1.393 (4)	C13—H13A	0.9600
C2—C3	1.382 (4)	C13—H13B	0.9600
C2—H2	0.9300	C13—H13C	0.9600
C3—C4	1.391 (4)	C14—H14A	0.9600
C3—H3	0.9300	C14—H14B	0.9600
C4—C5	1.386 (4)	C14—H14C	0.9600
C4—C7	1.503 (4)	C15—C16	1.531 (4)
O2—S1—O1	119.92 (12)	C11—C10—H10A	109.5
O2—S1—N1	106.25 (12)	N2—C10—H10B	109.5
O1—S1—N1	106.09 (11)	C11—C10—H10B	109.5
O2—S1—C1	108.45 (13)	H10A—C10—H10B	108.1
O1—S1—C1	109.53 (12)	N1—C11—C10	109.5 (2)
N1—S1—C1	105.65 (12)	N1—C11—H11A	109.8
C11—N1—C8	110.4 (2)	C10—C11—H11A	109.8
C11—N1—S1	117.15 (18)	N1—C11—H11B	109.8
C8—N1—S1	115.10 (17)	C10—C11—H11B	109.8
C9—N2—C10	109.7 (2)	H11A—C11—H11B	108.2
C9—N2—C12	111.8 (2)	C13—C12—C14	110.2 (2)
C10—N2—C12	112.3 (2)	C13—C12—N2	110.2 (2)
C9—N2—H2A	109.9 (19)	C14—C12—N2	110.2 (2)
C10—N2—H2A	107 (2)	C13—C12—H12	108.7
C12—N2—H2A	106 (2)	C14—C12—H12	108.7
C2—C1—C6	120.7 (3)	N2—C12—H12	108.7

C2—C1—S1	120.4 (2)	C12—C13—H13A	109.5
C6—C1—S1	118.7 (2)	C12—C13—H13B	109.5
C3—C2—C1	119.2 (3)	H13A—C13—H13B	109.5
C3—C2—H2	120.4	C12—C13—H13C	109.5
C1—C2—H2	120.4	H13A—C13—H13C	109.5
C2—C3—C4	121.0 (3)	H13B—C13—H13C	109.5
C2—C3—H3	119.5	C12—C14—H14A	109.5
C4—C3—H3	119.5	C12—C14—H14B	109.5
C5—C4—C3	118.9 (3)	H14A—C14—H14B	109.5
C5—C4—C7	120.6 (3)	C12—C14—H14C	109.5
C3—C4—C7	120.5 (3)	H14A—C14—H14C	109.5
C6—C5—C4	121.0 (3)	H14B—C14—H14C	109.5
C6—C5—H5	119.5	O3—C15—O4	128.9 (3)
C4—C5—H5	119.5	O3—C15—C16	116.1 (3)
C5—C6—C1	119.1 (3)	O4—C15—C16	115.0 (3)
C5—C6—H6	120.5	F1'—C16—F2	74.1 (6)
C1—C6—H6	120.5	F1'—C16—F3'	106.7 (6)
C4—C7—H7A	109.5	F2—C16—F3'	123.3 (6)
C4—C7—H7B	109.5	F1'—C16—F3	130.1 (6)
H7A—C7—H7B	109.5	F2—C16—F3	107.7 (6)
C4—C7—H7C	109.5	F3'—C16—F3	29.5 (5)
H7A—C7—H7C	109.5	F1'—C16—F1	35.9 (5)
H7B—C7—H7C	109.5	F2—C16—F1	105.3 (5)
N1—C8—C9	110.5 (2)	F3'—C16—F1	75.0 (6)
N1—C8—H8A	109.6	F3—C16—F1	103.4 (5)
C9—C8—H8A	109.6	F1'—C16—F2'	108.3 (6)
N1—C8—H8B	109.6	F2—C16—F2'	35.5 (5)
C9—C8—H8B	109.6	F3'—C16—F2'	103.5 (7)
H8A—C8—H8B	108.1	F3—C16—F2'	78.5 (6)
N2—C9—C8	111.8 (2)	F1—C16—F2'	132.7 (6)
N2—C9—H9A	109.3	F1'—C16—C15	111.1 (5)
C8—C9—H9A	109.3	F2—C16—C15	115.6 (4)
N2—C9—H9B	109.3	F3'—C16—C15	116.1 (5)
C8—C9—H9B	109.3	F3—C16—C15	112.0 (5)
H9A—C9—H9B	107.9	F1—C16—C15	112.0 (4)
N2—C10—C11	110.8 (2)	F2'—C16—C15	110.6 (5)
N2—C10—H10A	109.5		
O2—S1—N1—C11	−172.47 (19)	C10—N2—C9—C8	54.2 (3)
O1—S1—N1—C11	−43.8 (2)	C12—N2—C9—C8	179.4 (2)
C1—S1—N1—C11	72.4 (2)	N1—C8—C9—N2	−55.7 (3)
O2—S1—N1—C8	55.2 (2)	C9—N2—C10—C11	−56.1 (3)
O1—S1—N1—C8	−176.13 (19)	C12—N2—C10—C11	178.9 (2)
C1—S1—N1—C8	−59.9 (2)	C8—N1—C11—C10	−60.6 (3)
O2—S1—C1—C2	163.9 (2)	S1—N1—C11—C10	164.97 (18)
O1—S1—C1—C2	31.4 (3)	N2—C10—C11—N1	59.7 (3)
N1—S1—C1—C2	−82.5 (2)	C9—N2—C12—C13	57.2 (3)
O2—S1—C1—C6	−20.4 (3)	C10—N2—C12—C13	−179.0 (2)
O1—S1—C1—C6	−152.9 (2)	C9—N2—C12—C14	179.1 (2)
N1—S1—C1—C6	93.2 (2)	C10—N2—C12—C14	−57.1 (3)

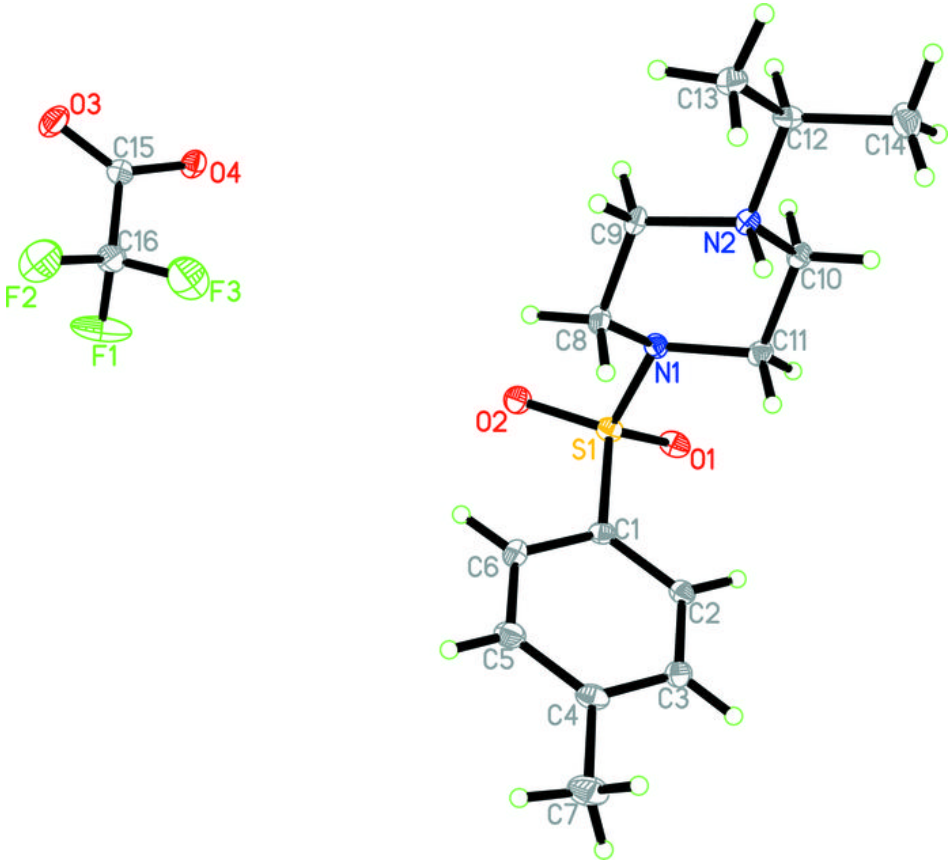
C6—C1—C2—C3	−1.7 (4)	O3—C15—C16—F1'	67.0 (11)
S1—C1—C2—C3	173.9 (2)	O4—C15—C16—F1'	−112.9 (10)
C1—C2—C3—C4	−0.6 (4)	O3—C15—C16—F2	−14.9 (9)
C2—C3—C4—C5	2.0 (4)	O4—C15—C16—F2	165.2 (9)
C2—C3—C4—C7	−177.8 (3)	O3—C15—C16—F3'	−170.9 (9)
C3—C4—C5—C6	−1.1 (4)	O4—C15—C16—F3'	9.3 (10)
C7—C4—C5—C6	178.7 (3)	O3—C15—C16—F3	−138.8 (8)
C4—C5—C6—C1	−1.1 (4)	O4—C15—C16—F3	41.4 (8)
C2—C1—C6—C5	2.5 (4)	O3—C15—C16—F1	105.7 (9)
S1—C1—C6—C5	−173.2 (2)	O4—C15—C16—F1	−74.2 (9)
C11—N1—C8—C9	58.7 (3)	O3—C15—C16—F2'	−53.3 (11)
S1—N1—C8—C9	−165.91 (18)	O4—C15—C16—F2'	126.8 (10)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···O4^{i}	0.902 (11)	1.828 (12)	2.724 (3)	172 (3)
C9—H9A···O2^{ii}	0.97	2.52	3.405 (4)	151
C10—H10A···O4^{ii}	0.97	2.45	3.357 (4)	155
C2—H2···O3^{iii}	0.93	2.58	3.225 (4)	127

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

Fig. 1


O3
C15
O4
C16
F2
F3
F1
C13
C12
C14
C9
N2
C10
C8
C11
N1
O2
S1
O1
C1
C6
C2
C5
C3
C4
C7