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2,2-Dichloro-*N*-{[1-(fluoromethyl)-2-hydroxy-2-[4-(methylsulfonyl)phenyl]ethyl}acetamide

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.006 Å
Disorder in main residue
R factor = 0.053
wR factor = 0.155
Data-to-parameter ratio = 14.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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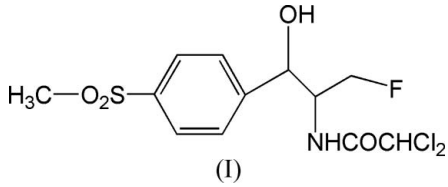
The crystal structure of the title compound, $C_{12}H_{14}Cl_2FNO_4S$, shows that, although there are no intra- or intermolecular π–π stacking interactions, there are O—H···O, C—H···F and C—H···O hydrogen bonds.

Comment

The title compound, (I), is a synthetic broad-spectrum antibiotic that has been developed for veterinary medicine (Hillaert & Van den Bossche, 2004). In this paper, we present the X-ray crystallographic analysis of (I). A perspective view is shown in Fig.1 and selected geometric parameters which describe the molecular conformation are listed in Table 1.



(I)

As shown in Fig. 2, the molecules are linked by intermolecular O—H···O, C—H···O and C—H···F hydrogen bonds (Table 2). There is no π–π stacking in the crystal structure. The disordered F-atom position was described as two components, F1 and F1′, with site-occupancy factors refined to 0.516 (5) and 0.484 (5), respectively.

Experimental

The title compound was synthesized according to Clark *et al.* (1995). Crystals appropriate for data collection were obtained by slow evaporation of an ethanol solution at room temperature.

Crystal data

$C_{12}H_{13}Cl_2FNO_4S$
M_r = 357.19
Monoclinic, $P2_1$
a = 11.2407 (18) Å
b = 5.0994 (8) Å
c = 13.412 (2) Å
β = 103.499 (3)°
V = 747.6 (2) Å^3
Z = 2
D_x = 1.587 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1667 reflections
θ = 2.7–24.1°
μ = 0.60 mm^{-1}
T = 292 (2) K
Block, colorless
0.30 × 0.20 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.841, T_{max} = 0.921
4249 measured reflections
2839 independent reflections
2427 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 26.0°
$h = -13 \rightarrow 11$
$k = -6 \rightarrow 6$
$l = -16 \rightarrow 15$

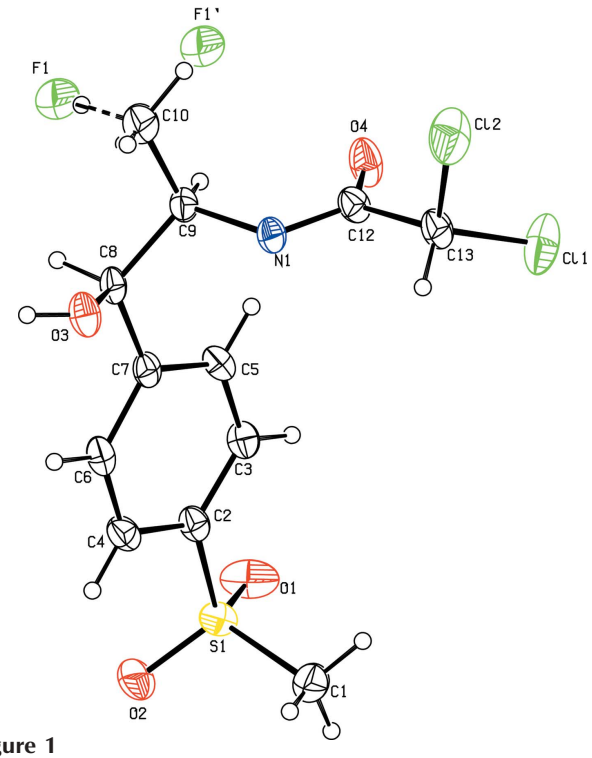


Figure 1
View of the molecule of (I), showing the atom-labelling scheme, with displacement ellipsoids drawn at the 50% probability level. Both disordered F atoms are shown and H atoms are represented by circles of arbitrary size.

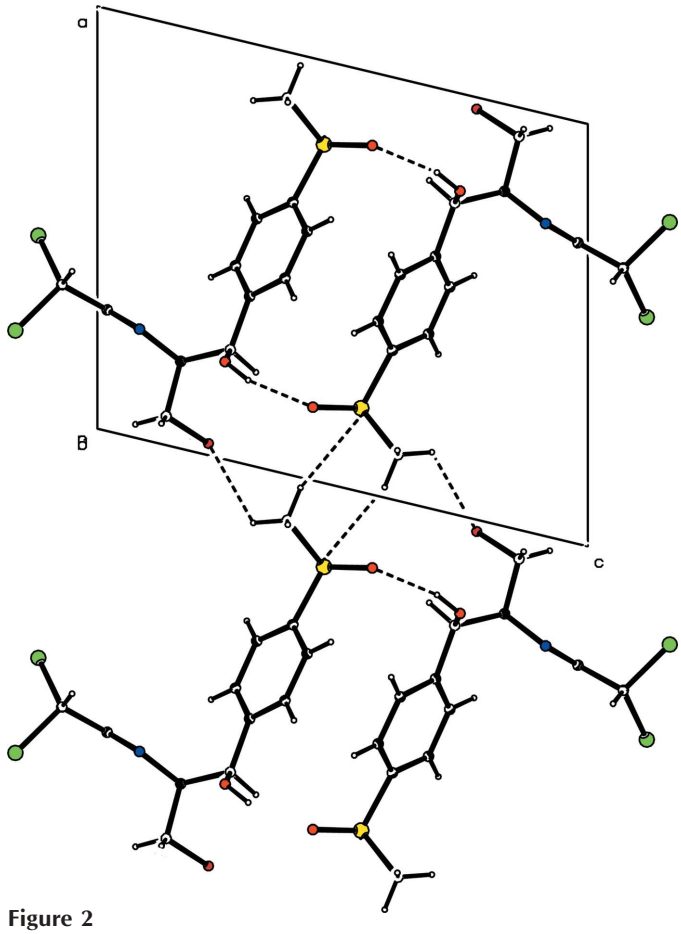


Figure 2
The intermolecular hydrogen bonding (dashed lines) in the crystal structure of (I).

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0885P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.053$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.155$	$\Delta\rho_{max} = 0.38$ e Å^{-3}
$S = 1.07$	$\Delta\rho_{min} = -0.29$ e Å^{-3}
2839 reflections	Absolute structure: Flack (1983), 1200 Friedel pairs
196 parameters	Flack parameter: −0.07 (12)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

C10—F1'	1.404 (8)	C10—F1	1.445 (8)
C8—O3—H3*A*	109.5	C1—S1—C2	106.3 (2)
C6—C7—C8—O3	37.0 (5)	C13—C12—N1—C9	170.5 (3)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*A*···O2^{i}	0.82	2.02	2.815 (4)	164
C1—H1*A*···O1^{ii}	0.96	2.57	3.418 (6)	148
C1—H1*B*···O1^{iii}	0.96	2.39	3.260 (8)	151
C1—H1*C*···F1^{iv}	0.96	2.51	3.077 (9)	118
C9—H9···O3^{v}	0.98	2.32	3.239 (5)	156

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

H atoms were placed at calculated positions and treated as riding atoms (C—H = 0.93–0.98 Å), with U_{iso}(H) values set equal to 1.2 (CH) or 1.5 (CH and CH_3) times U_{eq} of the parent atom.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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