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4-Fluoro-*N*-(quinolin-8-yl)benzenesulfonamide

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Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.003 Å
R factor = 0.035
wR factor = 0.096
Data-to-parameter ratio = 10.7

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

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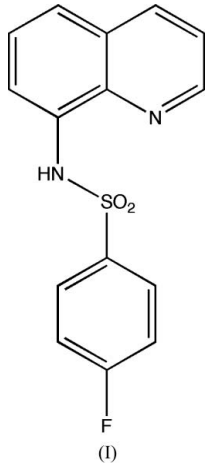
In the crystal structure of the title compound, $C_{15}H_{11}FN_2O_2S$, the torsion angle about the N—S bond between the quinoline ring system and the benzene ring is −59.0 (2)°. The sulfonamide H atom forms one intramolecular hydrogen bond to the quinoline N atom [N—H···N = 2.25 (2) Å] and an intermolecular hydrogen bond to a sulfonyl O atom [N—H···O =2.53 (2) Å]. The C atom adjacent to the quinoline N atom forms one intermolecular contact to the F atom [H···F = 2.48 (2) Å].

Comment

We have focused on 8-aminoquinolinosulfonamide derivatives (da Silva *et al.*, 2005*a*,*b*,*c*,*d*), which have been developed in recent years because of their interesting capacity as metal chelators (Pearce *et al.*, 2001). We report here the structure of the title compound, (I), as part of our search for fluorescent agents that could be use to detect and measure the available zinc(II) within cells. The nearly planar quinoline ring system of (I) forms a C1—N1—S1—C10 torsion angle with the benzene ring of −59.0 (2)°. The NH group has one intramolecular hydrogen bond to the quinoline N atom and another to a sulfonyl O atom (Table 1). An intermolecular hydrogen bond of type C—H···F is also observed. The molecular packing of the title compound is stabilized by these hydrogen bonds, as shown in Fig. 2 and detailed in Table 1.



(I)

Experimental

Compound (I) was prepared according to a literature procedure (Xue *et al.*, 2000). Single crystals of (I) suitable for X-ray data collection were obtained by recrystallization from methanol–dichloromethane (1:1). (m.p. 412–413 K, yield 79%).

Crystal data

$C_{15}H_{11}FN_2O_2S$
M_r = 302.32
Monoclinic, $P2_1/c$
a = 11.984 (1) Å
b = 12.408 (1) Å
c = 9.2792 (7) Å
β = 102.74 (1)°
V = 1345.82 (19) Å^3
Z = 4
D_x = 1.492 Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 5.2–19.0°
μ = 2.31 mm^{-1}
T = 299 (2) K
Prism, colorless
0.28 × 0.28 × 0.23 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
4785 measured reflections
2396 independent reflections
2064 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 66.9°
$h = -14 \rightarrow 14$
$k = -14 \rightarrow 0$
$l = -11 \rightarrow 11$
3 standard reflections
frequency: 120 min
intensity decay: 1.0%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.096
S = 1.03
2396 reflections
224 parameters
Only H-atom coordinates refined
$w = 1/[\sigma^2(F_o^2) + (0.0471P)^2 + 0.2885P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0050 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*···N2	0.89 (2)	2.25 (2)	2.682 (2)	109 (2)
N1—H1*N*···O2^{i}	0.89 (2)	2.53 (2)	3.330 (2)	150 (2)
C8—H8···F1^{ii}	1.01 (2)	2.48 (3)	3.413 (3)	154 (2)

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

The H atoms were located in a difference map and refined with isotropic displacement parameters (set to 1.2 times U_{eq} of the parent atom).

Data collection: *CAD-4/PC Software* (Enraf–Nonius, 1996); cell refinement: *CAD-4/PC Software*; data reduction: *REDU4* (Stoe & Cie, 1987); 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: *SHELXL97*.

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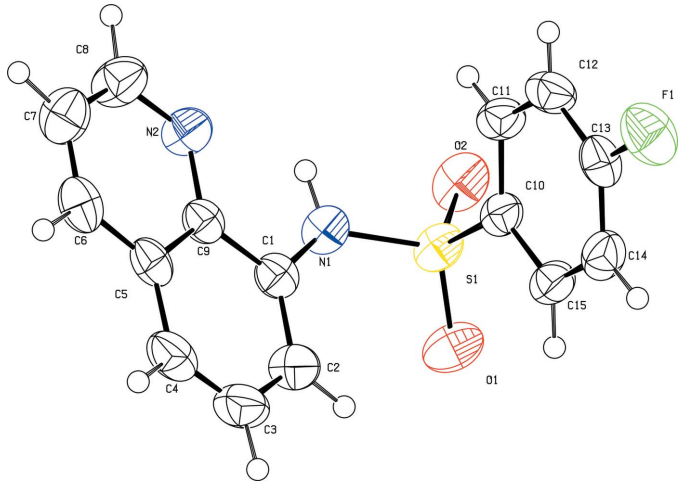

Figure 1
The molecular structure of (I), showing the atom labeling and displacement ellipsoids drawn at the 50% probability level.

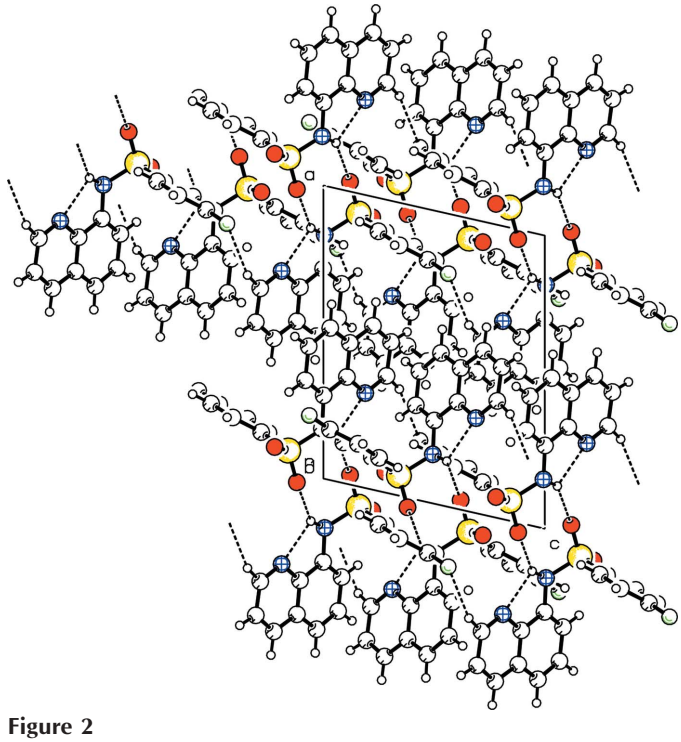

Figure 2
The molecular packing of (I), with hydrogen bonds shown as dashed lines.

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