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N-(5,7-Dibromo-8-quinolyl)-3,5-difluorobenzenesulfonamide

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Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.007 Å
R factor = 0.044
wR factor = 0.122
Data-to-parameter ratio = 12.8

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

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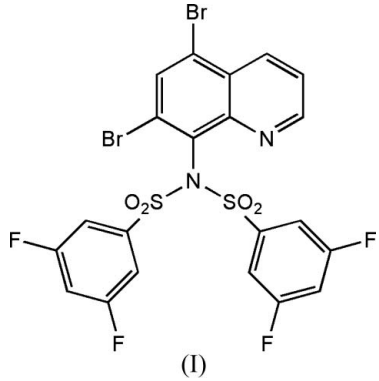
In the title compound, $C_{21}H_{10}Br_2F_4N_2O_4S$, the quinoline ring system, carrying two Br atoms, is essentially planar. The torsion angles about the N—S bonds connecting the quinoline ring to the aromatic rings are 84.0 (3) and 120.8 (3)°. Intermolecular C—H···O hydrogen bonds link molecules into a three-dimensional array.

Comment

The importance of zinc-specific fluorescent probes is particularly apparent in understanding the zinc chemistry of the brain (Fahrni & O'Halloran, 1999). As more roles for non-enzymatic zinc pools become apparent, so has the need for well characterized cell-permeable chemical probes for zinc biology. Various fluorescence-based zinc probes have recently been developed. Zinc chelators based on a quinoline core, such as 6-methoxy-(8-*p*-toluenesulfomido)quinoline (TSQ), are currently the most widely used zinc-activated fluorophores (Frederickson *et al.*, 1987). As part of our ongoing search for fluorophores based on quinolinesulfonamide as potential fluorophores for neurodegenerative diseases (da Silva *et al.*, 2005*a*,*b*,*c*,*d*), we report here the title structure, (I).



(I)

The effectively planar quinoline ring system (Fig. 1) carrying the two Br atoms [maximum deviation from the least-squares plane is 0.049 (2) Å for Br2] forms C1—N1—S1—C10 and C1—N1—S2—C16 torsion angles with the aromatic rings of 84.0 (3) and 120.8 (3)°, respectively, indicating non-planarity in the molecule.

Intermolecular C—H···O hydrogen bonds (Table 1) build a three-dimensional network, as shown in the packing diagram (Fig. 2).

Experimental

Compound (I) was prepared according to the literature procedure of da Silva *et al.* (2005*e*). Single crystals of (I) suitable for X-ray data

collection were obtained by recrystallization from a solution of the compound in a dichloromethane–methanol (1:1) mixture (m.p. 443 K).

Crystal data

$C_{21}H_{10}Br_2F_4N_2O_4S_2$
M_r = 654.25
Monoclinic, $P2_1/n$
a = 9.758 (1) Å
b = 24.091 (2) Å
c = 9.851 (1) Å
β = 99.56 (1)°
V = 2283.6 (4) Å^3
Z = 4
D_x = 1.903 Mg m^{-3}
Cu $K\alpha$ radiation
μ = 6.83 mm^{-1}
T = 299 (2) K
Prism, light pink
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.188, T_{max} = 0.456
(expected range = 0.208–0.505)
4450 measured reflections
4057 independent reflections
3269 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 66.9°
3 standard reflections
frequency: 120 min
intensity decay: 1.0%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.122
S = 1.04
4057 reflections
316 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0603P)^2 + 3.291P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.93 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C19—H19···O1^{i}	0.93	2.40	3.264 (5)	155
C7—H7···O2^{ii}	0.93	2.48	3.333 (6)	152

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

All H atoms were included in the riding-model approximation, with C—H = 0.93 Å, and with U_{iso}(H) = 1.2U_{eq}(C).

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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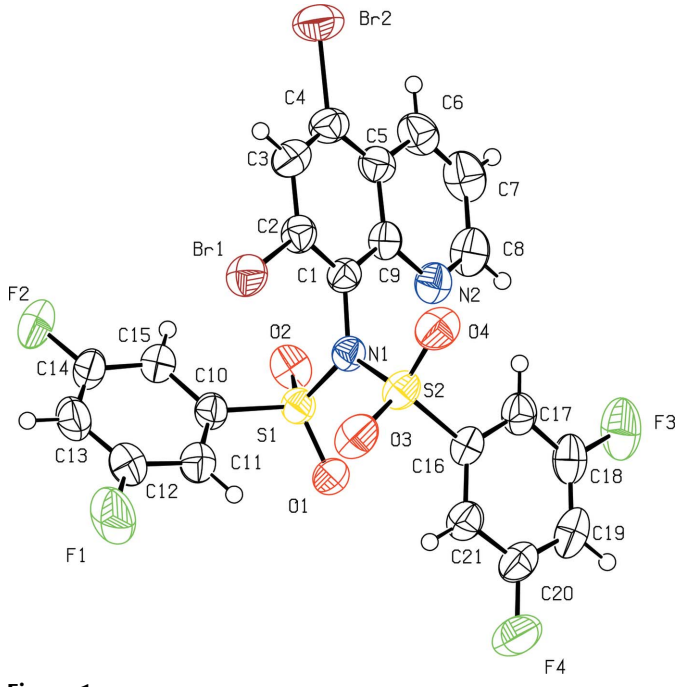

Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

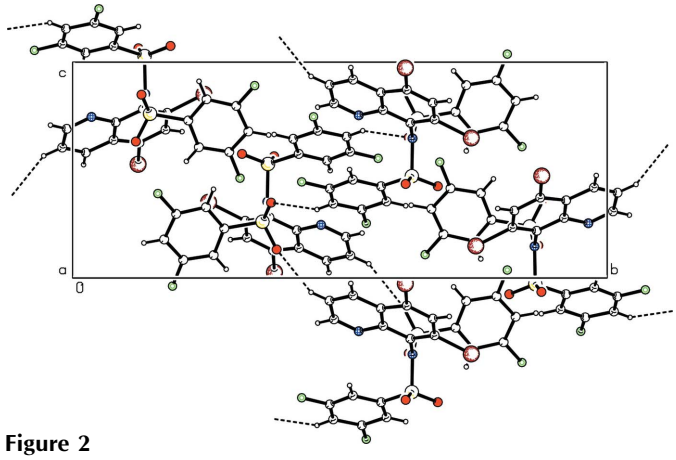

Figure 2
The molecular packing in (I), with hydrogen bonds shown as dashed lines.

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