

# *N*-(5,7-Dibromo-8-quinolyl)-4-fluorobenzene-sulfonamide

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## Key indicators

Single-crystal X-ray study  
*T* = 299 K  
Mean  $\sigma$ (C–C) = 0.009 Å  
*R* factor = 0.055  
*wR* factor = 0.182  
Data-to-parameter ratio = 13.2

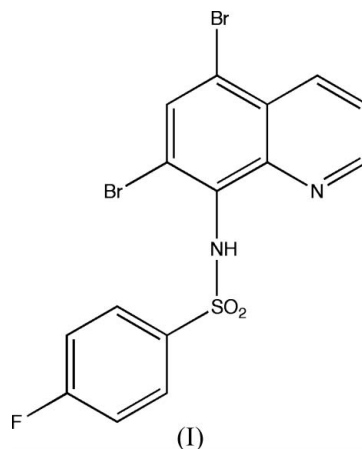
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

Molecules of the non-planar title compound, C<sub>15</sub>H<sub>9</sub>Br<sub>2</sub>FN<sub>2</sub>O<sub>2</sub>S, are linked by intermolecular N–H···O and C–H···N hydrogen bonds to form a chain.

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## Comment

Quinoline sulfonamide derivatives have recently been described as useful reagents for the detection of zinc(II) in histochemical staining procedures (Frederickson *et al.*, 1987; Savage *et al.*, 1989; Kimber *et al.*, 2000). Moreover, Hendrickson *et al.* (1997) have investigated the synthesis of zinc(II)- and copper(II)-specific fluorescence agents that can be used to detect and measure the available metals within cells. Our interest in such metal chelators as potential agents for neuroprotection in Alzheimer's disease (Zheng *et al.*, 2005) led to the X-ray study of the title compound, (I) (Fig. 1).



The nearly planar quinoline ring system of (I) forms a C1–N1–S1–C10 dihedral angle with the benzene ring of  $-71.3(3)^\circ$ , indicating non-planarity in the molecule.

Intermolecular N–H···O and C–H···N hydrogen bonds lead to the formation of a chain, as shown in Fig. 2; details are given in Table 1.

## Experimental

To an ice-cooled solution of 5,7-dibromo-8-aminoquinoline (50 mg, 0.1736 mmol) in anhydrous pyridine (5 ml) was added *p*-fluorobenzenesulfonyl chloride (37.15 mg, 0.1909 mmol). The mixture was stirred at 273 K for 90 min and then overnight at room temperature. The reaction mixture was quenched with iced water (20 ml) and the precipitated product filtered off. Recrystallization from ethanol yielded 61 mg (75%) of (I). Single crystals of (I) suitable for X-ray diffraction study were obtained by recrystallization from a methanol–dichloromethane (1:1) solution of (I).

## Crystal data

$C_{15}H_9Br_2FN_2O_2S$   
 $M_r = 460.12$   
 Monoclinic,  $P2_1/c$   
 $a = 18.636$  (1) Å  
 $b = 4.9871$  (7) Å  
 $c = 17.914$  (1) Å  
 $\beta = 110.628$  (7)°  
 $V = 1558.2$  (3) Å<sup>3</sup>  
 $Z = 4$

$D_x = 1.961$  Mg m<sup>-3</sup>  
 Cu  $K\alpha$  radiation  
 Cell parameters from 25 reflections  
 $\theta = 10.1$ – $19.5^\circ$   
 $\mu = 8.06$  mm<sup>-1</sup>  
 $T = 299$  (2) K  
 Prism, colorless  
 $0.15 \times 0.15 \times 0.10$  mm

## Data collection

Nonius CAD-4 diffractometer  
 $\omega/2\theta$  scans  
 Absorption correction:  $\psi$  scan  
 (North *et al.*, 1968)  
 $T_{min} = 0.360$ ,  $T_{max} = 0.447$   
 2893 measured reflections  
 2760 independent reflections  
 2096 reflections with  $I > 2\sigma(I)$

$R_{int} = 0.052$   
 $\theta_{max} = 66.9^\circ$   
 $h = -21 \rightarrow 22$   
 $k = 0 \rightarrow 5$   
 $l = -21 \rightarrow 1$   
 3 standard reflections  
 frequency: 120 min  
 intensity decay: 10.0%

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.055$   
 $wR(F^2) = 0.182$   
 $S = 1.03$   
 2760 reflections  
 209 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1263P)^2 + 0.7796P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} = 0.001$   
 $\Delta\rho_{max} = 1.20$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -1.44$  e Å<sup>-3</sup>  
 Extinction correction: *SHELXL97*  
 (Sheldrick, 1997)  
 Extinction coefficient: 0.0014 (3)

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1N\cdots O2^i$	0.86	2.37	3.000 (7)	130
$C11-H11\cdots N2^{ii}$	0.93	2.51	3.421 (9)	165

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

H atoms were included in the riding-model approximation, with  $N-H = 0.86$  Å and  $C-H = 0.93$  Å, and with  $U_{iso}(H) = 1.2U_{eq}(N,C)$ . The residual electron-density peaks were located in the region of the Br atoms. The highest peak and deepest hole are 1.43 and 0.75 Å<sup>-3</sup>, respectively, from atom Br1.

Data collection: *CAD-4-PC Software* (Nonius, 1996); cell refinement: *CAD-4-PC Software*; data reduction: *REDU4* (Stoe & Cie, 1988); 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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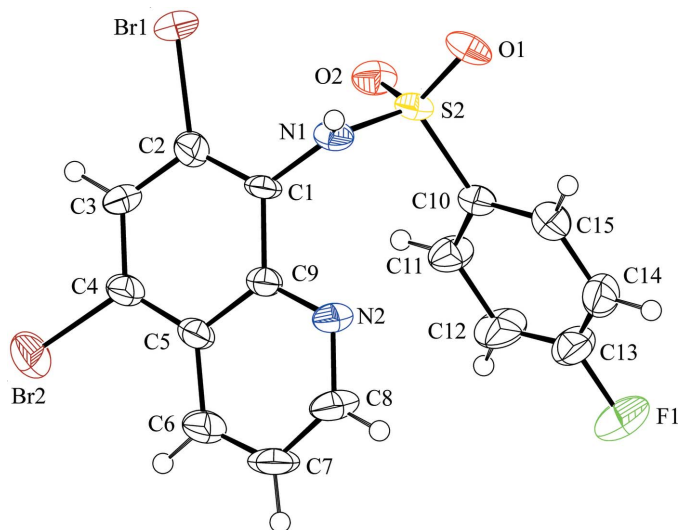


Figure 1

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

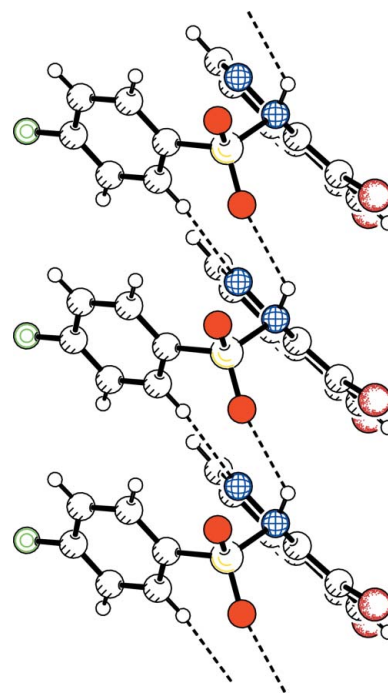


Figure 2

The chain in (I), mediated by hydrogen bonds (dashed lines).

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