Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4,5-Dibromo-*N*-(8-quinolyl)thiophene-2-sulfonamide

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Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.011 Å
R factor = 0.045
wR factor = 0.103
Data-to-parameter ratio = 16.0

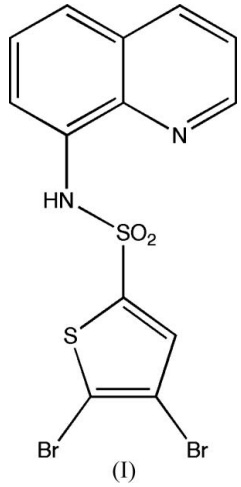
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

There are two independent molecules in the asymmetric unit of the title compound, $C_{13}H_8Br_2N_2O_2S_2$. Intermolecular C—H···O hydrogen bonds are observed, linking each non-planar molecule to a symmetry-equivalent molecule.

Received 17 November 2005
Accepted 13 December 2005
Online 21 December 2005

Comment

Zinc fluorophores have recently been attracting much interest in biological and environmental applications. Following carbonic anhydrase-based biosensors with fluorescent aromatic sulfonamides, a chemosensor, Zinquin, is now extensively used to study the role of intracellular Zn^{2+} in cellular biology (Kimura & Koike, 1998). 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).



(I)

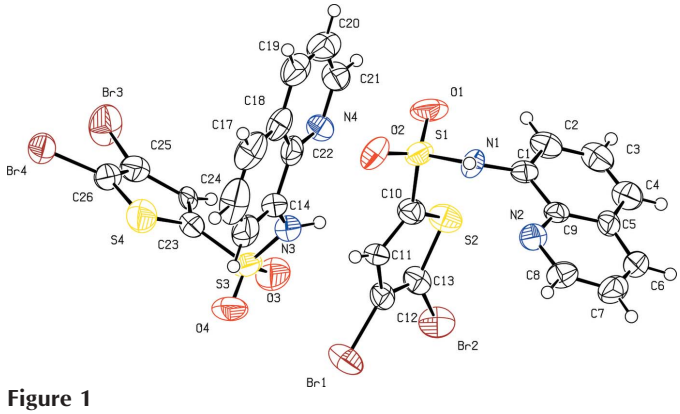


Figure 1
The asymmetric unit of (I), showing the atom labelling and with displacement ellipsoids drawn at the 50% probability level.

The quinoline ring system of each of the two independent molecules in the asymmetric unit (Fig. 1) is nearly planar. The torsion angles C1—N1—S1—C10 and C14—N3—S3—C23 are 59.7 (6) and 60.3 (7)°, respectively. Molecules of the title compound are linked by intermolecular C—H···O hydrogen bonds to form a chain, as shown in Fig. 2 and detailed in Table 1. The contributions of the two inversion twin components refined to 0.23 (1) and 0.77 (1).

Experimental

The title compound, (I), was prepared according to the literature procedure of Xue *et al.* (2000). Suitable crystals were obtained by recrystallization from methanol–dichloromethane (1:1 *v*/*v*).

Crystal data

$C_{13}H_8Br_2N_2O_2S_2$
M_r = 448.15
Orthorhombic, $Pna2_1$
a = 28.318 (2) Å
b = 7.0471 (5) Å
c = 15.094 (1) Å
V = 3012.2 (4) Å^3
Z = 8
D_x = 1.976 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2740 reflections
θ = 2.8–18.0°
μ = 5.66 mm^{-1}
T = 299 (2) K
Rod, pink
0.28 × 0.10 × 0.08 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with Sapphire CCD detector
ω and φ scans
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2004)
T_{min} = 0.344, T_{max} = 0.760
20485 measured reflections
6068 independent reflections
3494 reflections with $I > 2\sigma(I)$
R_{int} = 0.063
θ_{max} = 26.4°
$h = -35 \rightarrow 34$
$k = -5 \rightarrow 8$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.103
S = 0.88
6068 reflections
380 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0499P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.022
$\Delta\rho_{max}$ = 0.69 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}
Absolute structure: Flack (1983)
Flack parameter: 0.23 (1), with 2891 Friedel pairs

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O1^{i}	0.93	2.51	3.215 (9)	133
C20—H20···O3^{ii}	0.93	2.60	3.253 (10)	127

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

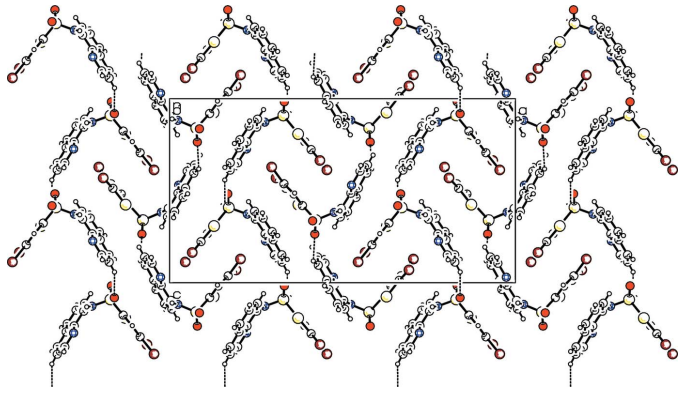


Figure 2
The molecular packing of (I), with hydrogen bonds shown as dashed lines.

H atoms were positioned with idealized geometry using a riding model (C—H = 0.93 Å and N—H = 0.86 Å) and were refined with isotropic displacement parameters (set to 1.2 times U_{eq} of the parent atom).

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2003); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2004); data reduction: *CrysAlis RED*; 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*.

The authors thank Professor Dr Hartmut Fuess, FG Strukturforschung, FB Material- und Geowissenschaften, Technische Universität Darmstadt, Petersenstrasse 23, 64287 Darmstadt, for diffractometer time.

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