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2,4,6-Triisopropyl-*N*-(8-quinolyl)benzenesulfonamide

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Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.007 Å
Disorder in main residue
R factor = 0.062
wR factor = 0.184
Data-to-parameter ratio = 13.1

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

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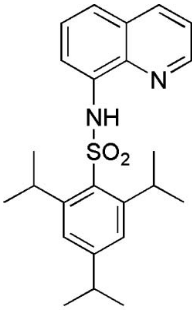
There are two independent molecules in the asymmetric unit of the title compound, $C_{24}H_{30}N_2O_2S$. Intramolecular N—H$\cdots$N hydrogen bonds are observed in each non-planar molecule.

Comment

A large number of quinoline derivatives have been synthesized as the quinoline group has well defined and attractive ionophoric properties towards a variety of important metal ions (Kim *et al.*, 2005). In particular, fluorimetric probes based on the 8-aminoquinolinosulfonamide system have been developed in recent years because of their interesting capacity as metal ion coordinators (Macías *et al.*, 2003). In the context of a project to investigate new fluorophore quinoline derivatives, the crystal structure of the title compound, (I), was determined.



(I)

The quinoline ring system of each of the two independent molecules in the asymmetric unit (Fig. 1) is nearly planar. The dihedral angles between the quinoline residue and the benzene ring, *i.e.* C1—N1—S1—C10 and C25—N3—S2—C35, are 66.5 (3) and −61.2 (4)°, respectively, indicating non-planarity in the molecules. The NH groups form intramolecular hydrogen bonds to the quinoline N atoms [N—H$\cdots$N = 2.30 (4) and 2.13 (5) Å], as shown in the packing diagram (Fig. 2) and detailed in Table 1.

Experimental

Compound (I) was prepared by the overnight reaction of one equivalent of 8-aminoquinoline and a 1.1 equivalent of 2,4,6-triisopropylbenzene-1-sulfonyl chloride in the presence of pyridine, according to the literature procedure of Kimber *et al.* (2000). Single crystals suitable for X-ray data collection were obtained by recrystallization from a methanol–dichloromethane (1:1) solution of (I).

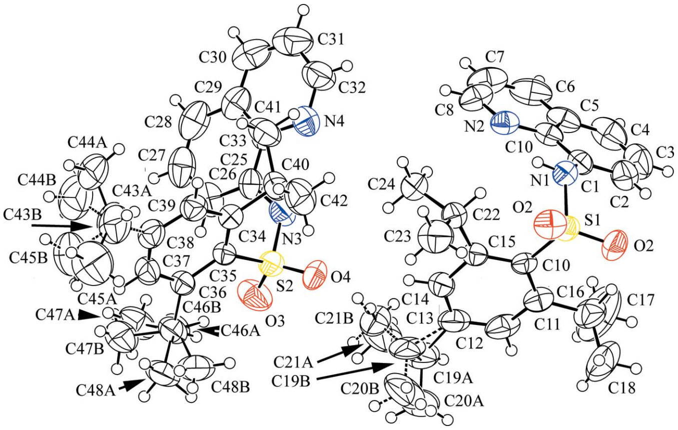


Figure 1

The asymmetric unit of (I), showing the atom labeling and displacement ellipsoids drawn at the 50% probability level. The minor disorder components are shown with dashed bonds.

Crystal data

$C_{24}H_{30}N_2O_2S$
$M_r = 410.56$
Triclinic, $P\overline{1}$
$a = 8.921$ (1) Å
$b = 14.303$ (2) Å
$c = 18.888$ (3) Å
$\alpha = 78.00$ (1)°
$\beta = 77.77$ (1)°
$\gamma = 78.25$ (1)°
$V = 2271.6$ (5) Å^3
$Z = 4$
$D_x = 1.201$ Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 3.2$–20.4°
$\mu = 1.43$ mm^{-1}
$T = 299$ (2) K
Needle, colorless
0.33 × 0.15 × 0.10 mm

Data collection

Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min} = 0.736$, $T_{\max} = 0.867$
8744 measured reflections
8016 independent reflections
4265 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.038$
$\theta_{\max} = 67.9°$
$h = -10 \rightarrow 1$
$k = -17 \rightarrow 17$
$l = -22 \rightarrow 22$
3 standard reflections
frequency: 120 min
intensity decay: 1.0%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.062$
$wR(F^2) = 0.184$
$S = 1.02$
8016 reflections
610 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0873P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.014$
$\Delta\rho_{\max} = 0.33$ e Å^{-3}
$\Delta\rho_{\min} = -0.31$ e Å^{-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$\cdots$N2	0.85 (4)	2.30 (4)	2.699 (5)	109 (3)
N3—H3n$\cdots$N4	0.85 (1)	2.13 (4)	2.626 (5)	116 (3)

Some of the methyl groups, *viz.* C19, C20 and C21 (molecule 1), and C43, C44, C45, C46, C47 and C48 (molecule 2), were found to be disordered and were refined anisotropically using a split model. The corresponding site occupancy factors were refined but later fixed at 0.6:0.4 for molecule 1 and 0.5:0.5 for molecule 2. The H atoms of the NH groups were located in a difference map and refined freely; see Table 1 for parameters. All other H atoms were included in the riding-model approximation with C—H = 0.93 (aromatic), 0.98 (methine) and 0.96 Å (methyl). $U_{\rm iso}$(H) values were set at $1.2U_{\rm eq}$(N,C).

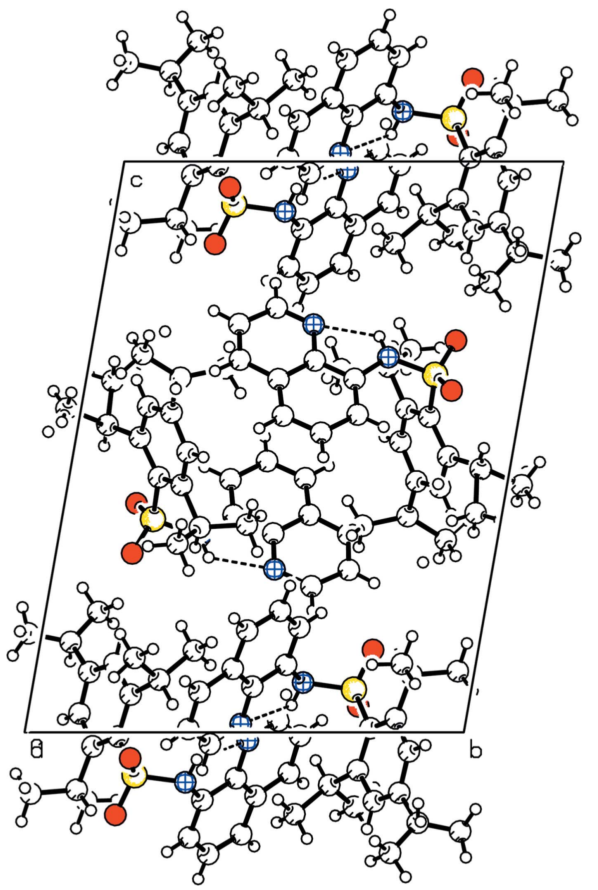


Figure 2

Molecular packing of (I), with hydrogen bonds shown as dashed lines.

Data collection: *CAD-4/PC Software* (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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