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Bis[*N*-(5,7-dibromoquinolin-8-yl)-3,5-bis(trifluoromethyl)benzenesulfonamidato-κ^2N,N']zinc(II)

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.006 Å
R factor = 0.042
wR factor = 0.100
Data-to-parameter ratio = 14.2

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

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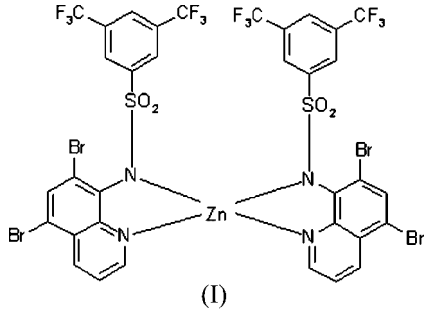
In the title compound, $[Zn(C_{17}H_7Br_2F_6N_2O_2S)_2]$, the zinc(II) ion has a distorted tetrahedral geometry formed by the N atoms of the quinoline and the sulfonamide groups. One intermolecular C—H···O hydrogen bond to a sulfonyl O atom is observed.

Comment

The metal-binding site of β-amyloid (Aβ) is a promising target for pharmacological interventions that may benefit Alzheimer's patients. There is increasing evidence that interactions between (Aβ) and metal ions such as copper and zinc may play an important role in neurogenerative disorder (Miller *et al.*, 2005; Cardoso *et al.*, 2005). Thus, the search for metal-specific fluorescent compounds is of increasing importance in understanding the neurobiological role of metals in the brain. As part of our efforts in search for metal chelators as potential probes for neuroprotection in neurogenerative diseases (da Silva *et al.*, 2006*a*,*b*,*c*,*d*,*e*), the structure of the title compound, (I), has been determined.



(I)

The zinc(II) ion has a distorted tetrahedral geometry formed by two quinoline N and two sulfonamide N atoms (Table 1). The bond angles N1—Zn1—N2 and N3—Zn1—N4 are quite small relative to the ideal tetrahedral angle, whereas the N1—Zn1—N4 and N2—Zn1—N3 are much wider. The other bond angles at the Zn atom, N1—Zn1—N3 and N2—Zn1—N4, are very close to the tetrahedral value. One intermolecular C—H···O hydrogen bond to a sulfonyl O links molecules into a three-dimensional network (Fig. 2 and Table 2).

Experimental

The ligand was prepared as described previously (da Silva *et al.*, 2005). The title compound was prepared according to a literature procedure (Macías *et al.*, 2003). Single crystals of (I) suitable for X-ray data collection appeared after two days of slow evaporation of a methanol solution.

Crystal data

$[Zn(C_{17}H_7Br_2F_6N_2O_2S)_2]$
M_r = 1219.62
Triclinic, $P\overline{1}$
a = 11.7057 (6) Å
b = 12.4768 (6) Å
c = 14.0759 (7) Å
α = 90.091 (4)°
β = 100.293 (4)°
γ = 100.519 (4)°
V = 1987.46 (17) Å^3
Z = 2
D_x = 2.038 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 4.85 mm^{-1}
T = 100 (2) K
Prism, colourless
0.55 × 0.30 × 0.25 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector
ω and φ scans
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2004)
T_{min} = 0.176, T_{max} = 0.377
13514 measured reflections
7836 independent reflections
6792 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 26.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.100
S = 1.06
7836 reflections
550 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0338P)^2 + 9.6563P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.70 e Å^{-3}
$\Delta\rho_{min}$ = −1.14 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N1	2.014 (3)	Zn1—N3	2.096 (3)
Zn1—N4	2.031 (3)	Zn1—N2	2.108 (3)
N1—Zn1—N4	140.30 (13)	N1—Zn1—N2	80.92 (14)
N1—Zn1—N3	109.20 (13)	N4—Zn1—N2	108.37 (14)
N4—Zn1—N3	80.85 (13)	N3—Zn1—N2	152.12 (14)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C23—H23···O4^{i}	0.95	2.30	3.127 (5)	145

Symmetry code: (i) $-x, -y+2, -z$.

All H atoms were included in the riding model approximation with C—H = 0.95 Å and with U_{iso}(H) = 1.2 U_{eq}(C). The residual electron-density features are located in the region of Br2. The highest peak and the deepest hole are 0.89 and 0.77 Å from Br2, respectively.

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*.

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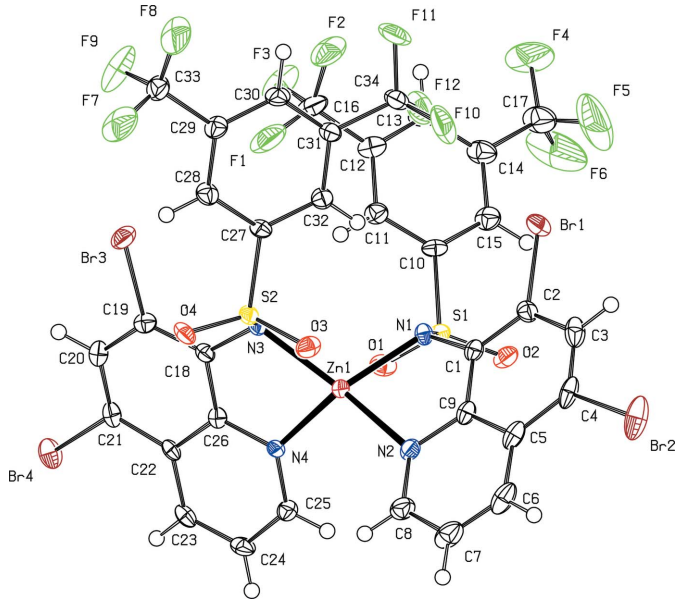

Figure 1
Molecular structure of (I), showing the atom labelling and displacement ellipsoids drawn at the 50% probability level.

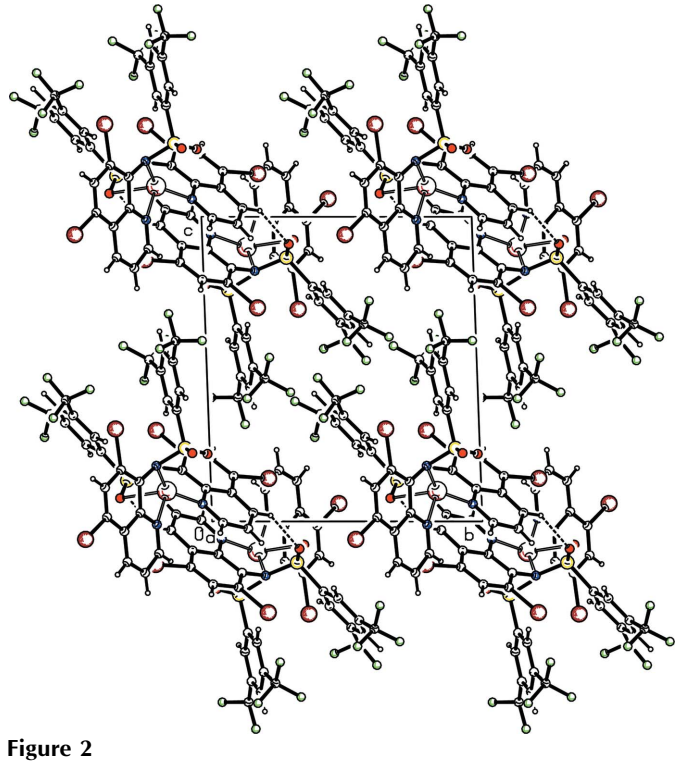

Figure 2
The molecular packing of (I), with hydrogen bonds shown as dashed lines.

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