Bis[*N*-benzyl-*N*-(2-phenylethyl)dithiocarbamato-κ²*S*,*S′*](1,10-phenanthroline-κ²*N*,*N′*)zinc(II)

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In the title compound, [Zn(C$_{16}$H$_{16}$NS$_2$)$_2$(C$_{12}$H$_8$N$_2$)], the Zn^{II} atom exists within an N$_2$S$_4$ donor set that defines a distorted octahedral geometry; weak intramolecular C—H···S hydrogen bonds are noted. In the crystal, molecules are linked *via* weak C—H···π interactions, forming *C*(11) chains propagating along [001].

3D view
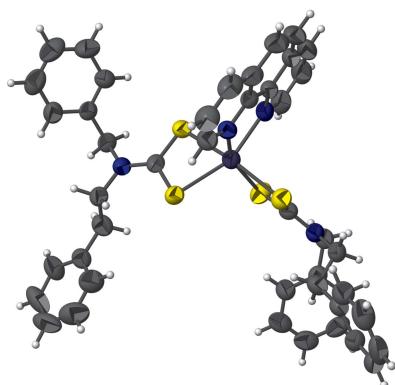
Chemical scheme
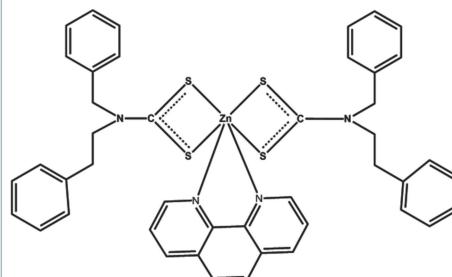
Structure description

Dithiocarbamates are long known to be versatile ligands (Coucouvanis, 1979; Hogarth, 2005) due to their binding capacity to metal atoms, and they can also be used as chemotherapeutics, pesticides and fungicides (Hulanicki, 1967; Ivanov *et al.*, 1999). Dithiocarbamates are the most frequently used bidentate sulfur ligands. In recent years, zinc dithiocarbamates have continued to attract attention on account of their industrial applications (Jones & Jones, 1983). The affinity of zinc towards sulfur-containing ligands leads to many structurally novel complexes (Tiekink, 2003). Metal dithiocarbamate complexes and their nitrogen-donor adducts are useful precursors for the synthesis of metal–sulfide nanoparticles (Srinivasan & Thirumaran, 2012; Yan *et al.*, 1999). In view of the above importance of dithiocarbamate derivatives, we have undertaken the single-crystal X-ray diffraction study of the title compound, and the results are presented herein.

The molecular structure of the title compound is illustrated in Fig. 1. The Zn—S bond lengths are in good agreement with other zinc dithiocarbamate complexes (Kant *et al.*, 2012; Ivanov *et al.*, 2006). The short thiouriede C—N bond lengths indicate that these have significant double-bond character. Similarly, the C—S distances lie between single- and double-bond lengths and prove that these bonds to have partial double-bond character. The zinc metal ion exists within an N$_2$S$_4$ donor set that defines a distorted
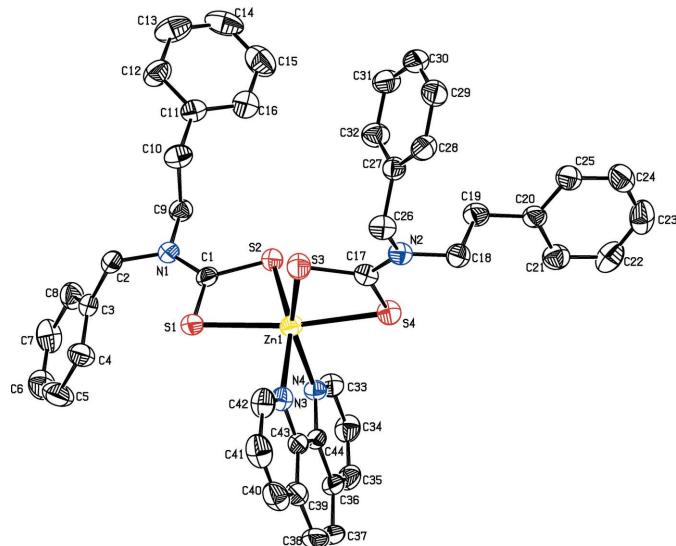
Figure 1
The molecular structure of the title compound, with the atom labelling. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.

octahedral geometry. The distortion is due in part to the acute bond angles subtended at zinc by the chelating ligands.

The molecular structure maybe influenced by weak intramolecular C—H···S hydrogen bonds (Table 1). In the crystal packing, C—H···π interactions link the molecules into $C(11)$ chains propagating along [001]; see Fig. 2 and Table 1. In addition to this, intermolecular π–π interactions are also observed between the centroid of the rings (N4/C33–C36/C44) and (C36–C39/C43–C44) at $(-x, -y, 1 - z)$ with a centroid–centroid distance of 3.766 (2) Å.

Synthesis and crystallization

The title compound was prepared according to the literature procedure (Rani & Thirumaran, 2013). Single crystals were obtained by slow evaporation of dichloromethane and ethyl acetate (2:1) solution of the title compound.
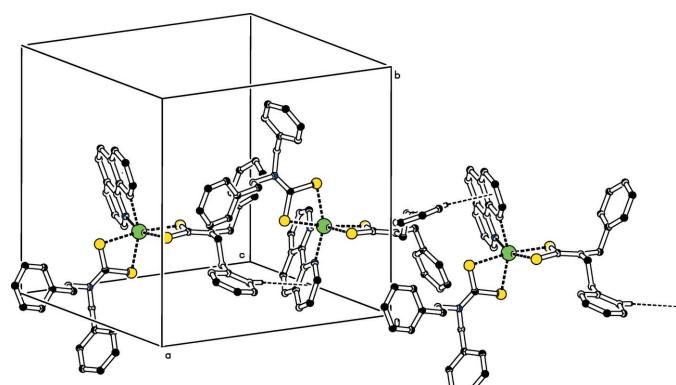

Figure 2
The crystal packing of the title compound. Weak C—H···π interactions are shown as dashed lines (see Table 2). For clarity, H atoms not involved in these interactions have been omitted.

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

Cg is the centroid of the N1/C33–C36/C44 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2B···S1	0.97	2.63	3.046 (4)	106
C9—H9B···S2	0.97	2.59	3.016 (4)	107
C18—H18A···S4	0.97	2.65	3.000 (4)	102
C26—H26B···S3	0.97	2.53	3.060 (4)	115
C12—H12···Cg^{i}	0.93	2.89	3.777 (5)	160

Symmetry code: (i) $x - \frac{3}{2}, -y - \frac{1}{2}, z - \frac{3}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Zn(C_{16}H_{16}NS_2)_2(C_{12}H_8N_2)]$
M_r	818.41
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	298
a, b, c (Å)	16.076 (3), 14.572 (2), 17.151 (2)
β (°)	96.629 (8)
V (Å^3)	3990.9 (10)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.86
Crystal size (mm)	0.24 × 0.22 × 0.20
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (SADABS; Bruker, 1999)
T_{min}, T_{max}	0.84, 0.85
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	18230, 9051, 6001
R_{int}	0.044
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.055, 0.181, 1.04
No. of reflections	9051
No. of parameters	478
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	1.11, −0.39

Computer programs: APEX2, SAINT and XPREP (Bruker, 2004), SHELXS97 (Sheldrick, 2008), SHELXL2014 (Sheldrick, 2015), ORTEP-3 for Windows (Farrugia, 2012) and PLATON (Spek, 2009).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The maximum and minimum residual electron density peaks of 1.11 and 0.39 e Å^{-3}, respectively, are located 0.03 and 0.83 Å from the Zn1 atom.

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full crystallographic data

Bis[*N*-benzyl-*N*-(2-phenylethyl)dithiocarbamato-κ^2S,S'](1,10-phenanthroline-κ^2N,N')zinc(II)

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Bis[*N*-benzyl-*N*-(2-phenylethyl)dithiocarbamato-κ^2S,S'](1,10-phenanthrolineκ^2-*N*,*N'*)zinc(II)

Crystal data

[Zn(C$_{16}$H$_{16}$NS$_2$)$_2$(C$_{12}$H$_8$N$_2$)]	$F(000) = 1704$
$M_r = 818.41$	$D_x = 1.362$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 16.076$ (3) Å	Cell parameters from 12234 reflections
$b = 14.572$ (2) Å	$\theta = 3.3$–26.4°
$c = 17.151$ (2) Å	$\mu = 0.86$ mm^{-1}
$\beta = 96.629$ (8)°	$T = 298$ K
$V = 3990.9$ (10) Å^3	Block, brown
$Z = 4$	$0.24 \times 0.22 \times 0.20$ mm

Data collection

Bruker Kappa APEXII CCD diffractometer	9051 independent reflections
Radiation source: Sealed tube	6001 reflections with $I > 2\sigma(I)$
ω and φ scan	$R_{int} = 0.044$
Absorption correction: multi-scan (SADABS; Bruker, 1999)	$\theta_{max} = 27.5°$, $\theta_{min} = 3.0°$
$T_{min} = 0.84$, $T_{max} = 0.85$	$h = -20 \rightarrow 18$
18230 measured reflections	$k = -18 \rightarrow 13$
	$l = -12 \rightarrow 22$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.055$	$w = 1/[\sigma^2(F_o^2) + (0.0923P)^2 + 1.0518P]$
$wR(F^2) = 0.181$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.001$
9051 reflections	$\Delta\rho_{max} = 1.11$ e Å^{-3}
478 parameters	$\Delta\rho_{min} = -0.39$ e Å^{-3}
0 restraints	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.44340 (2)	0.78266 (2)	0.11581 (2)	0.05327 (14)
S1	0.60074 (5)	0.76988 (6)	0.15144 (5)	0.0606 (2)
S2	0.47447 (5)	0.77993 (6)	0.26228 (5)	0.0595 (2)
S3	0.42542 (6)	0.95155 (6)	0.09034 (6)	0.0682 (3)
S4	0.28729 (6)	0.81866 (6)	0.08990 (5)	0.0601 (2)
N1	0.63881 (16)	0.77183 (19)	0.30803 (16)	0.0554 (6)
N2	0.26299 (18)	0.99571 (19)	0.05570 (16)	0.0577 (7)
N3	0.45893 (16)	0.7483 (2)	−0.00687 (16)	0.0556 (6)
N4	0.41053 (16)	0.63575 (16)	0.10380 (14)	0.0491 (6)
C1	0.57767 (19)	0.7727 (2)	0.2472 (2)	0.0520 (7)
C2	0.7285 (2)	0.7759 (2)	0.2971 (2)	0.0591 (8)
H2A	0.7580	0.8101	0.3403	0.071*
H2B	0.7345	0.8092	0.2491	0.071*
C3	0.76887 (18)	0.6826 (2)	0.29289 (19)	0.0534 (7)
C4	0.7812 (2)	0.6460 (3)	0.2216 (2)	0.0738 (10)
H4	0.7627	0.6777	0.1759	0.089*
C5	0.8207 (3)	0.5627 (4)	0.2169 (3)	0.0990 (15)
H5	0.8286	0.5388	0.1680	0.119*
C6	0.8485 (3)	0.5147 (3)	0.2834 (3)	0.0891 (13)
H6	0.8757	0.4587	0.2798	0.107*
C7	0.8362 (3)	0.5492 (3)	0.3547 (3)	0.0843 (12)
H7	0.8542	0.5163	0.3999	0.101*
C8	0.7970 (2)	0.6334 (3)	0.3603 (2)	0.0717 (10)
H8	0.7895	0.6570	0.4094	0.086*
C9	0.6197 (2)	0.7765 (2)	0.3904 (2)	0.0579 (8)
H9A	0.6610	0.7417	0.4239	0.070*
H9B	0.5651	0.7498	0.3943	0.070*
C10	0.6205 (3)	0.8758 (3)	0.4175 (2)	0.0709 (10)
H10A	0.5821	0.9108	0.3812	0.085*
H10B	0.6762	0.9007	0.4158	0.085*
C11	0.5962 (2)	0.8882 (2)	0.5000 (2)	0.0620 (8)
C12	0.6528 (3)	0.9198 (3)	0.5598 (2)	0.0834 (12)
H12	0.7085	0.9280	0.5516	0.100*
C13	0.6276 (4)	0.9396 (4)	0.6319 (3)	0.1032 (17)
H13	0.6661	0.9629	0.6716	0.124*
C14	0.5475 (5)	0.9255 (3)	0.6458 (3)	0.1020 (17)
H14	0.5310	0.9391	0.6947	0.122*
C15	0.4910 (4)	0.8914 (4)	0.5876 (4)	0.1061 (17)
H15	0.4361	0.8805	0.5972	0.127*
C16	0.5147 (3)	0.8730 (3)	0.5151 (3)	0.0905 (13)
H16	0.4756	0.8502	0.4757	0.109*
C17	0.3196 (2)	0.9295 (2)	0.07673 (19)	0.0549 (7)
C18	0.1722 (2)	0.9789 (3)	0.0535 (2)	0.0612 (8)
H18A	0.1588	0.9197	0.0294	0.073*
H18B	0.1419	1.0255	0.0213	0.073*

C19	0.1441 (2)	0.9805 (3)	0.1350 (2)	0.0713 (10)
H19A	0.1762	0.9356	0.1676	0.086*
H19B	0.1561	1.0405	0.1581	0.086*
C20	0.0524 (2)	0.9604 (3)	0.13529 (19)	0.0609 (8)
C21	0.0215 (3)	0.8714 (3)	0.1240 (2)	0.0761 (11)
H21	0.0574	0.8239	0.1140	0.091*
C22	−0.0627 (3)	0.8534 (4)	0.1278 (3)	0.0906 (14)
H22	−0.0831	0.7941	0.1193	0.109*
C23	−0.1160 (3)	0.9227 (5)	0.1439 (2)	0.0968 (16)
H23	−0.1720	0.9100	0.1480	0.116*
C24	−0.0866 (3)	1.0097 (4)	0.1540 (2)	0.0877 (14)
H24	−0.1229	1.0568	0.1640	0.105*
C25	−0.0040 (2)	1.0288 (3)	0.1495 (2)	0.0709 (10)
H25	0.0147	1.0889	0.1561	0.085*
C26	0.2877 (2)	1.0887 (2)	0.0327 (2)	0.0646 (9)
H26A	0.2597	1.1024	−0.0191	0.078*
H26B	0.3476	1.0893	0.0295	0.078*
C27	0.2670 (2)	1.1634 (2)	0.0890 (2)	0.0592 (8)
C28	0.2173 (2)	1.2358 (3)	0.0622 (3)	0.0720 (10)
H28	0.1962	1.2395	0.0094	0.086*
C29	0.1986 (3)	1.3047 (3)	0.1149 (3)	0.0844 (12)
H29	0.1658	1.3546	0.0968	0.101*
C30	0.2283 (3)	1.2984 (3)	0.1924 (3)	0.0787 (11)
H30	0.2147	1.3434	0.2273	0.094*
C31	0.2776 (3)	1.2270 (3)	0.2188 (3)	0.0806 (12)
H31	0.2984	1.2237	0.2716	0.097*
C32	0.2970 (3)	1.1591 (3)	0.1679 (2)	0.0747 (10)
H32	0.3305	1.1101	0.1867	0.090*
C33	0.3880 (2)	0.5807 (2)	0.1593 (2)	0.0621 (8)
H33	0.3874	0.6039	0.2098	0.075*
C34	0.3651 (2)	0.4894 (3)	0.1449 (3)	0.0725 (10)
H34	0.3509	0.4524	0.1855	0.087*
C35	0.3637 (2)	0.4550 (3)	0.0712 (3)	0.0726 (10)
H35	0.3477	0.3944	0.0611	0.087*
C36	0.3863 (2)	0.5104 (2)	0.0104 (2)	0.0625 (9)
C37	0.3880 (2)	0.4803 (3)	−0.0691 (3)	0.0794 (12)
H37	0.3716	0.4207	−0.0830	0.095*
C38	0.4129 (3)	0.5371 (3)	−0.1234 (3)	0.0816 (12)
H38	0.4130	0.5157	−0.1745	0.098*
C39	0.4390 (2)	0.6287 (3)	−0.1058 (2)	0.0690 (10)
C40	0.4692 (3)	0.6887 (4)	−0.1596 (2)	0.0883 (14)
H40	0.4731	0.6696	−0.2107	0.106*
C41	0.4930 (3)	0.7753 (4)	−0.1366 (3)	0.0898 (15)
H41	0.5135	0.8155	−0.1720	0.108*
C42	0.4863 (2)	0.8031 (3)	−0.0601 (2)	0.0728 (10)
H42	0.5016	0.8628	−0.0456	0.087*
C43	0.43604 (18)	0.6620 (2)	−0.02923 (18)	0.0525 (7)
C44	0.40974 (17)	0.6017 (2)	0.02984 (18)	0.0486 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0580 (2)	0.0468 (2)	0.0536 (2)	−0.00002 (15)	0.00018 (17)	−0.00421 (16)
S1	0.0571 (5)	0.0653 (5)	0.0581 (5)	0.0045 (4)	0.0014 (4)	−0.0148 (4)
S2	0.0494 (4)	0.0664 (5)	0.0614 (5)	0.0048 (4)	0.0010 (4)	−0.0096 (4)
S3	0.0610 (5)	0.0534 (5)	0.0898 (7)	−0.0001 (4)	0.0067 (5)	0.0041 (5)
S4	0.0629 (5)	0.0519 (5)	0.0657 (5)	0.0007 (4)	0.0082 (4)	0.0078 (4)
N1	0.0489 (14)	0.0607 (17)	0.0551 (15)	0.0023 (12)	−0.0001 (12)	−0.0111 (12)
N2	0.0642 (16)	0.0549 (15)	0.0533 (15)	0.0067 (13)	0.0033 (12)	0.0009 (12)
N3	0.0543 (14)	0.0599 (16)	0.0518 (15)	−0.0003 (13)	0.0029 (12)	0.0055 (13)
N4	0.0557 (14)	0.0428 (13)	0.0490 (14)	−0.0008 (11)	0.0073 (11)	−0.0019 (11)
C1	0.0513 (16)	0.0419 (16)	0.0604 (19)	−0.0001 (12)	−0.0037 (14)	−0.0103 (13)
C2	0.0492 (16)	0.059 (2)	0.066 (2)	−0.0035 (14)	−0.0030 (15)	−0.0088 (16)
C3	0.0407 (14)	0.0590 (19)	0.0592 (18)	−0.0035 (13)	0.0008 (13)	−0.0049 (15)
C4	0.080 (2)	0.079 (3)	0.062 (2)	0.018 (2)	0.0058 (18)	−0.0100 (19)
C5	0.107 (3)	0.093 (3)	0.097 (3)	0.033 (3)	0.011 (3)	−0.028 (3)
C6	0.078 (3)	0.058 (2)	0.131 (4)	0.011 (2)	0.008 (3)	0.004 (3)
C7	0.070 (2)	0.086 (3)	0.097 (3)	0.010 (2)	0.011 (2)	0.034 (3)
C8	0.060 (2)	0.089 (3)	0.065 (2)	0.0057 (19)	0.0032 (17)	0.003 (2)
C9	0.0608 (18)	0.0516 (18)	0.0596 (19)	0.0034 (14)	−0.0007 (15)	−0.0028 (15)
C10	0.089 (3)	0.059 (2)	0.064 (2)	−0.0055 (19)	0.0059 (19)	−0.0022 (17)
C11	0.074 (2)	0.0536 (18)	0.0574 (19)	−0.0016 (16)	0.0024 (16)	−0.0027 (15)
C12	0.086 (3)	0.099 (3)	0.062 (2)	−0.015 (2)	−0.005 (2)	−0.008 (2)
C13	0.153 (5)	0.100 (4)	0.053 (2)	−0.022 (3)	−0.003 (3)	−0.005 (2)
C14	0.165 (5)	0.077 (3)	0.072 (3)	0.016 (3)	0.050 (3)	0.000 (2)
C15	0.103 (4)	0.104 (4)	0.120 (4)	0.006 (3)	0.051 (4)	0.001 (3)
C16	0.078 (3)	0.098 (3)	0.096 (3)	−0.004 (2)	0.011 (2)	−0.016 (3)
C17	0.0644 (18)	0.0510 (17)	0.0501 (17)	0.0059 (15)	0.0098 (14)	0.0010 (14)
C18	0.0623 (19)	0.065 (2)	0.0545 (19)	0.0067 (16)	−0.0006 (15)	0.0010 (16)
C19	0.074 (2)	0.085 (3)	0.054 (2)	0.005 (2)	0.0047 (17)	−0.0108 (18)
C20	0.0639 (19)	0.068 (2)	0.0490 (17)	0.0059 (17)	0.0014 (14)	−0.0074 (16)
C21	0.083 (3)	0.073 (3)	0.071 (2)	0.005 (2)	0.002 (2)	−0.003 (2)
C22	0.091 (3)	0.101 (3)	0.075 (3)	−0.026 (3)	−0.009 (2)	0.010 (2)
C23	0.066 (2)	0.167 (6)	0.055 (2)	0.001 (3)	−0.0039 (19)	0.016 (3)
C24	0.074 (3)	0.123 (4)	0.063 (2)	0.030 (3)	−0.004 (2)	−0.005 (3)
C25	0.073 (2)	0.074 (2)	0.064 (2)	0.0131 (19)	−0.0002 (18)	−0.0025 (19)
C26	0.081 (2)	0.0561 (19)	0.0562 (19)	0.0052 (17)	0.0066 (17)	0.0082 (16)
C27	0.0578 (18)	0.0548 (19)	0.064 (2)	−0.0002 (15)	0.0053 (15)	−0.0006 (16)
C28	0.073 (2)	0.060 (2)	0.080 (3)	0.0028 (18)	−0.0090 (19)	−0.0021 (19)
C29	0.074 (2)	0.057 (2)	0.121 (4)	0.0095 (19)	0.008 (3)	−0.010 (2)
C30	0.075 (2)	0.070 (3)	0.092 (3)	−0.012 (2)	0.018 (2)	−0.023 (2)
C31	0.088 (3)	0.082 (3)	0.073 (3)	−0.010 (2)	0.012 (2)	−0.020 (2)
C32	0.086 (3)	0.072 (2)	0.064 (2)	0.010 (2)	0.0000 (19)	−0.0037 (19)
C33	0.071 (2)	0.0561 (19)	0.0590 (19)	0.0010 (16)	0.0060 (16)	0.0014 (16)
C34	0.072 (2)	0.055 (2)	0.091 (3)	−0.0109 (17)	0.010 (2)	0.010 (2)
C35	0.062 (2)	0.0501 (19)	0.104 (3)	−0.0102 (16)	0.000 (2)	−0.010 (2)
C36	0.0527 (17)	0.0552 (19)	0.077 (2)	0.0012 (15)	−0.0032 (16)	−0.0199 (18)

C37	0.068 (2)	0.077 (3)	0.089 (3)	0.006 (2)	−0.008 (2)	−0.044 (2)
C38	0.079 (3)	0.100 (3)	0.063 (2)	0.015 (2)	−0.004 (2)	−0.037 (2)
C39	0.0568 (19)	0.098 (3)	0.0502 (19)	0.0176 (19)	−0.0021 (15)	−0.0117 (19)
C40	0.077 (3)	0.139 (4)	0.049 (2)	0.025 (3)	0.0095 (19)	−0.001 (3)
C41	0.078 (3)	0.129 (5)	0.065 (3)	0.008 (3)	0.019 (2)	0.029 (3)
C42	0.065 (2)	0.082 (3)	0.072 (2)	−0.0064 (19)	0.0103 (18)	0.020 (2)
C43	0.0453 (15)	0.0644 (19)	0.0468 (16)	0.0036 (14)	0.0005 (12)	−0.0076 (15)
C44	0.0427 (14)	0.0475 (16)	0.0536 (17)	0.0002 (12)	−0.0029 (12)	−0.0077 (13)

Geometric parameters (Å, º)

Zn1—N3	2.205 (3)	C18—C19	1.519 (5)
Zn1—N4	2.209 (2)	C18—H18A	0.9700
Zn1—S2	2.5043 (10)	C18—H18B	0.9700
Zn1—S3	2.5103 (11)	C19—C20	1.504 (5)
Zn1—S1	2.5394 (10)	C19—H19A	0.9700
Zn1—S4	2.5522 (10)	C19—H19B	0.9700
S1—C1	1.725 (3)	C20—C25	1.387 (5)
S2—C1	1.712 (3)	C20—C21	1.395 (6)
S3—C17	1.721 (4)	C21—C22	1.386 (6)
S4—C17	1.719 (3)	C21—H21	0.9300
N1—C1	1.349 (4)	C22—C23	1.373 (7)
N1—C2	1.476 (4)	C22—H22	0.9300
N1—C9	1.482 (4)	C23—C24	1.358 (7)
N2—C17	1.347 (4)	C23—H23	0.9300
N2—C18	1.475 (4)	C24—C25	1.366 (6)
N2—C26	1.478 (4)	C24—H24	0.9300
N3—C42	1.326 (4)	C25—H25	0.9300
N3—C43	1.353 (4)	C26—C27	1.518 (5)
N4—C33	1.327 (4)	C26—H26A	0.9700
N4—C44	1.361 (4)	C26—H26B	0.9700
C2—C3	1.512 (5)	C27—C28	1.371 (5)
C2—H2A	0.9700	C27—C32	1.383 (5)
C2—H2B	0.9700	C28—C29	1.407 (6)
C3—C4	1.369 (5)	C28—H28	0.9300
C3—C8	1.391 (5)	C29—C30	1.363 (6)
C4—C5	1.377 (6)	C29—H29	0.9300
C4—H4	0.9300	C30—C31	1.354 (6)
C5—C6	1.369 (7)	C30—H30	0.9300
C5—H5	0.9300	C31—C32	1.380 (5)
C6—C7	1.357 (6)	C31—H31	0.9300
C6—H6	0.9300	C32—H32	0.9300
C7—C8	1.387 (6)	C33—C34	1.394 (5)
C7—H7	0.9300	C33—H33	0.9300
C8—H8	0.9300	C34—C35	1.359 (6)
C9—C10	1.519 (5)	C34—H34	0.9300
C9—H9A	0.9700	C35—C36	1.399 (5)
C9—H9B	0.9700	C35—H35	0.9300

C10—C11	1.520 (5)	C36—C44	1.413 (4)
C10—H10A	0.9700	C36—C37	1.435 (5)
C10—H10B	0.9700	C37—C38	1.342 (6)
C11—C12	1.371 (5)	C37—H37	0.9300
C11—C16	1.382 (6)	C38—C39	1.421 (6)
C12—C13	1.375 (6)	C38—H38	0.9300
C12—H12	0.9300	C39—C40	1.398 (6)
C13—C14	1.352 (8)	C39—C43	1.407 (4)
C13—H13	0.9300	C40—C41	1.363 (7)
C14—C15	1.364 (8)	C40—H40	0.9300
C14—H14	0.9300	C41—C42	1.389 (6)
C15—C16	1.368 (7)	C41—H41	0.9300
C15—H15	0.9300	C42—H42	0.9300
C16—H16	0.9300	C43—C44	1.441 (5)
N3—Zn1—N4	75.10 (10)	N2—C18—C19	111.9 (3)
N3—Zn1—S2	157.24 (8)	N2—C18—H18A	109.2
N4—Zn1—S2	95.51 (7)	C19—C18—H18A	109.2
N3—Zn1—S3	94.60 (8)	N2—C18—H18B	109.2
N4—Zn1—S3	155.83 (7)	C19—C18—H18B	109.2
S2—Zn1—S3	101.29 (3)	H18A—C18—H18B	107.9
N3—Zn1—S1	89.63 (7)	C20—C19—C18	113.4 (3)
N4—Zn1—S1	99.92 (7)	C20—C19—H19A	108.9
S2—Zn1—S1	71.32 (3)	C18—C19—H19A	108.9
S3—Zn1—S1	101.84 (3)	C20—C19—H19B	108.9
N3—Zn1—S4	95.62 (7)	C18—C19—H19B	108.9
N4—Zn1—S4	87.89 (7)	H19A—C19—H19B	107.7
S2—Zn1—S4	104.85 (3)	C25—C20—C21	117.5 (4)
S3—Zn1—S4	71.16 (3)	C25—C20—C19	121.5 (4)
S1—Zn1—S4	171.52 (3)	C21—C20—C19	121.0 (3)
C1—S1—Zn1	84.82 (11)	C22—C21—C20	120.2 (4)
C1—S2—Zn1	86.19 (12)	C22—C21—H21	119.9
C17—S3—Zn1	86.12 (11)	C20—C21—H21	119.9
C17—S4—Zn1	84.84 (12)	C23—C22—C21	120.4 (5)
C1—N1—C2	122.4 (3)	C23—C22—H22	119.8
C1—N1—C9	121.7 (3)	C21—C22—H22	119.8
C2—N1—C9	115.6 (3)	C24—C23—C22	119.7 (4)
C17—N2—C18	121.6 (3)	C24—C23—H23	120.1
C17—N2—C26	122.3 (3)	C22—C23—H23	120.1
C18—N2—C26	116.2 (3)	C23—C24—C25	120.6 (4)
C42—N3—C43	117.7 (3)	C23—C24—H24	119.7
C42—N3—Zn1	127.1 (3)	C25—C24—H24	119.7
C43—N3—Zn1	115.1 (2)	C24—C25—C20	121.5 (4)
C33—N4—C44	118.3 (3)	C24—C25—H25	119.2
C33—N4—Zn1	126.9 (2)	C20—C25—H25	119.2
C44—N4—Zn1	114.61 (19)	N2—C26—C27	113.7 (3)
N1—C1—S2	121.0 (3)	N2—C26—H26A	108.8
N1—C1—S1	121.3 (2)	C27—C26—H26A	108.8

S2—C1—S1	117.67 (19)	N2—C26—H26B	108.8
N1—C2—C3	113.6 (3)	C27—C26—H26B	108.8
N1—C2—H2A	108.8	H26A—C26—H26B	107.7
C3—C2—H2A	108.8	C28—C27—C32	119.1 (4)
N1—C2—H2B	108.8	C28—C27—C26	120.0 (3)
C3—C2—H2B	108.8	C32—C27—C26	120.8 (3)
H2A—C2—H2B	107.7	C27—C28—C29	119.5 (4)
C4—C3—C8	118.3 (3)	C27—C28—H28	120.2
C4—C3—C2	120.1 (3)	C29—C28—H28	120.2
C8—C3—C2	121.6 (3)	C30—C29—C28	120.2 (4)
C3—C4—C5	120.8 (4)	C30—C29—H29	119.9
C3—C4—H4	119.6	C28—C29—H29	119.9
C5—C4—H4	119.6	C31—C30—C29	120.2 (4)
C6—C5—C4	120.6 (4)	C31—C30—H30	119.9
C6—C5—H5	119.7	C29—C30—H30	119.9
C4—C5—H5	119.7	C30—C31—C32	120.4 (4)
C7—C6—C5	119.6 (4)	C30—C31—H31	119.8
C7—C6—H6	120.2	C32—C31—H31	119.8
C5—C6—H6	120.2	C31—C32—C27	120.5 (4)
C6—C7—C8	120.4 (4)	C31—C32—H32	119.7
C6—C7—H7	119.8	C27—C32—H32	119.7
C8—C7—H7	119.8	N4—C33—C34	122.5 (3)
C7—C8—C3	120.3 (4)	N4—C33—H33	118.7
C7—C8—H8	119.8	C34—C33—H33	118.7
C3—C8—H8	119.8	C35—C34—C33	119.5 (4)
N1—C9—C10	109.9 (3)	C35—C34—H34	120.2
N1—C9—H9A	109.7	C33—C34—H34	120.2
C10—C9—H9A	109.7	C34—C35—C36	120.2 (3)
N1—C9—H9B	109.7	C34—C35—H35	119.9
C10—C9—H9B	109.7	C36—C35—H35	119.9
H9A—C9—H9B	108.2	C35—C36—C44	116.9 (3)
C9—C10—C11	113.8 (3)	C35—C36—C37	124.5 (4)
C9—C10—H10A	108.8	C44—C36—C37	118.6 (4)
C11—C10—H10A	108.8	C38—C37—C36	120.7 (4)
C9—C10—H10B	108.8	C38—C37—H37	119.6
C11—C10—H10B	108.8	C36—C37—H37	119.6
H10A—C10—H10B	107.7	C37—C38—C39	122.4 (4)
C12—C11—C16	118.3 (4)	C37—C38—H38	118.8
C12—C11—C10	121.1 (4)	C39—C38—H38	118.8
C16—C11—C10	120.5 (4)	C40—C39—C43	116.8 (4)
C11—C12—C13	120.3 (5)	C40—C39—C38	124.4 (4)
C11—C12—H12	119.8	C43—C39—C38	118.8 (4)
C13—C12—H12	119.8	C41—C40—C39	119.8 (4)
C14—C13—C12	120.8 (5)	C41—C40—H40	120.1
C14—C13—H13	119.6	C39—C40—H40	120.1
C12—C13—H13	119.6	C40—C41—C42	119.5 (4)
C13—C14—C15	119.6 (4)	C40—C41—H41	120.2
C13—C14—H14	120.2	C42—C41—H41	120.2

C15—C14—H14	120.2	N3—C42—C41	122.9 (4)
C14—C15—C16	120.3 (5)	N3—C42—H42	118.6
C14—C15—H15	119.8	C41—C42—H42	118.6
C16—C15—H15	119.8	N3—C43—C39	123.2 (3)
C15—C16—C11	120.6 (5)	N3—C43—C44	117.4 (3)
C15—C16—H16	119.7	C39—C43—C44	119.4 (3)
C11—C16—H16	119.7	N4—C44—C36	122.5 (3)
N2—C17—S4	120.2 (3)	N4—C44—C43	117.5 (3)
N2—C17—S3	121.9 (3)	C36—C44—C43	120.0 (3)
S4—C17—S3	117.83 (19)		
C2—N1—C1—S2	−173.1 (2)	C21—C20—C25—C24	1.4 (5)
C9—N1—C1—S2	0.4 (4)	C19—C20—C25—C24	−176.4 (4)
C2—N1—C1—S1	5.0 (4)	C17—N2—C26—C27	−114.4 (4)
C9—N1—C1—S1	178.5 (2)	C18—N2—C26—C27	66.2 (4)
Zn1—S2—C1—N1	177.3 (3)	N2—C26—C27—C28	−122.9 (4)
Zn1—S2—C1—S1	−0.82 (16)	N2—C26—C27—C32	56.6 (5)
Zn1—S1—C1—N1	−177.3 (3)	C32—C27—C28—C29	0.6 (6)
Zn1—S1—C1—S2	0.81 (16)	C26—C27—C28—C29	−180.0 (4)
C1—N1—C2—C3	−92.6 (4)	C27—C28—C29—C30	−1.2 (6)
C9—N1—C2—C3	93.6 (3)	C28—C29—C30—C31	1.5 (7)
N1—C2—C3—C4	100.2 (4)	C29—C30—C31—C32	−1.1 (7)
N1—C2—C3—C8	−82.0 (4)	C30—C31—C32—C27	0.5 (6)
C8—C3—C4—C5	−0.2 (6)	C28—C27—C32—C31	−0.2 (6)
C2—C3—C4—C5	177.6 (4)	C26—C27—C32—C31	−179.7 (4)
C3—C4—C5—C6	0.0 (7)	C44—N4—C33—C34	1.1 (5)
C4—C5—C6—C7	0.7 (8)	Zn1—N4—C33—C34	177.3 (3)
C5—C6—C7—C8	−1.1 (7)	N4—C33—C34—C35	−1.5 (6)
C6—C7—C8—C3	0.9 (6)	C33—C34—C35—C36	0.9 (6)
C4—C3—C8—C7	−0.2 (5)	C34—C35—C36—C44	−0.1 (5)
C2—C3—C8—C7	−178.0 (3)	C34—C35—C36—C37	179.1 (4)
C1—N1—C9—C10	−92.1 (4)	C35—C36—C37—C38	−177.9 (4)
C2—N1—C9—C10	81.8 (4)	C44—C36—C37—C38	1.3 (5)
N1—C9—C10—C11	176.4 (3)	C36—C37—C38—C39	0.3 (6)
C9—C10—C11—C12	114.3 (4)	C37—C38—C39—C40	176.8 (4)
C9—C10—C11—C16	−69.7 (5)	C37—C38—C39—C43	−2.2 (6)
C16—C11—C12—C13	−2.8 (7)	C43—C39—C40—C41	−0.9 (6)
C10—C11—C12—C13	173.3 (4)	C38—C39—C40—C41	−179.8 (4)
C11—C12—C13—C14	2.0 (8)	C39—C40—C41—C42	−0.4 (7)
C12—C13—C14—C15	0.0 (8)	C43—N3—C42—C41	−0.7 (5)
C13—C14—C15—C16	−1.3 (9)	Zn1—N3—C42—C41	−179.2 (3)
C14—C15—C16—C11	0.5 (8)	C40—C41—C42—N3	1.3 (7)
C12—C11—C16—C15	1.5 (7)	C42—N3—C43—C39	−0.8 (5)
C10—C11—C16—C15	−174.6 (4)	Zn1—N3—C43—C39	177.9 (2)
C18—N2—C17—S4	8.2 (4)	C42—N3—C43—C44	177.5 (3)
C26—N2—C17—S4	−171.1 (2)	Zn1—N3—C43—C44	−3.8 (3)
C18—N2—C17—S3	−172.5 (2)	C40—C39—C43—N3	1.5 (5)
C26—N2—C17—S3	8.3 (4)	C38—C39—C43—N3	−179.5 (3)

Zn1—S4—C17—N2	177.3 (3)	C40—C39—C43—C44	−176.7 (3)
Zn1—S4—C17—S3	−2.12 (17)	C38—C39—C43—C44	2.3 (5)
Zn1—S3—C17—N2	−177.2 (3)	C33—N4—C44—C36	−0.3 (4)
Zn1—S3—C17—S4	2.15 (17)	Zn1—N4—C44—C36	−176.9 (2)
C17—N2—C18—C19	77.9 (4)	C33—N4—C44—C43	−178.8 (3)
C26—N2—C18—C19	−102.8 (4)	Zn1—N4—C44—C43	4.6 (3)
N2—C18—C19—C20	−178.0 (3)	C35—C36—C44—N4	−0.2 (5)
C18—C19—C20—C25	−107.5 (4)	C37—C36—C44—N4	−179.5 (3)
C18—C19—C20—C21	74.8 (5)	C35—C36—C44—C43	178.2 (3)
C25—C20—C21—C22	−0.5 (6)	C37—C36—C44—C43	−1.1 (5)
C19—C20—C21—C22	177.3 (4)	N3—C43—C44—N4	−0.5 (4)
C20—C21—C22—C23	−1.2 (6)	C39—C43—C44—N4	177.8 (3)
C21—C22—C23—C24	2.0 (7)	N3—C43—C44—C36	−179.1 (3)
C22—C23—C24—C25	−1.1 (7)	C39—C43—C44—C36	−0.8 (4)
C23—C24—C25—C20	−0.6 (6)		

Hydrogen-bond geometry (Å, °)

Cg is the centroid of the N1/C33–C36/C44 ring.

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C2—H2B⋯S1	0.97	2.63	3.046 (4)	106
C9—H9B⋯S2	0.97	2.59	3.016 (4)	107
C18—H18A⋯S4	0.97	2.65	3.000 (4)	102
C26—H26B⋯S3	0.97	2.53	3.060 (4)	115
C12—H12⋯Cgⁱ	0.93	2.89	3.777 (5)	160

Symmetry code: (i) x−3/2, −y−1/2, z−3/2.