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# (Anilino{(*Z*)-2-[(*E*)-5-bromo-3-methoxy-2-oxidobenzylidene]hydrazin-1-ylidene-$\kappa^2O^2,N^2$}methanethiolato-$\kappa S$)(4,4′-dimethyl-2,2′-bipyridine-$\kappa^2N,N'$)zinc *N*,*N*-dimethylformamide monosolvate

**Jinsa Mary Jacob,[a] M. R. Prathapachandra Kurup[a] and Seik Weng Ng[b,c]***

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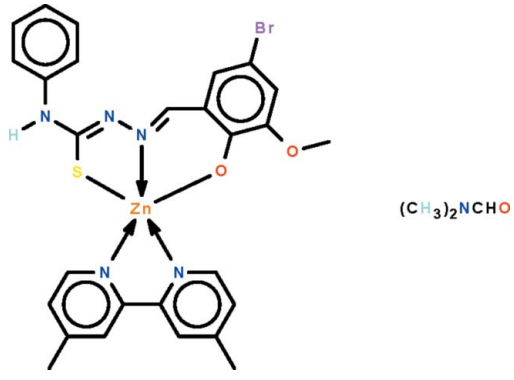
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.012 Å; disorder in main residue; $R$ factor = 0.070; $wR$ factor = 0.211; data-to-parameter ratio = 21.1.

The asymmetric unit of the title compound, [Zn($C_{15}H_{12}BrN_3O_2S$)($C_{12}H_{12}N_2$)]·$C_3H_7NO$, contains two independent molecules with a similar structure. The doubly deprotonated Schiff base ligand *O*,*N*,*S*-chelates to the metal atom, and the three coordinating atoms along with one N atom of the substituted 2,2′-bipyridine ligand constitute the square plane of the distorted square pyramid surrounding the metal atom. The apical site is occupied by the second N atom of the substituted 2,2′-bipyridine. The secondary amine group of the Schiff base dianion forms a hydrogen bond to the O atom of the dimethylformamide solvent. In the crystal, the phenyl ring of one of the two Schiff base anions is disordered over two positions in a 1:1 ratio. The crystal studied is a racemic twin.

## Related literature

For a related zinc structure, see: Seena & Kurup (2008).




## Experimental

### Crystal data

[Zn($C_{15}H_{12}BrN_3O_2S$)($C_{12}H_{12}N_2$)]·$C_3H_7NO$
$M_r$ = 700.95
Monoclinic, $P2_1$
$a$ = 15.2674 (3) Å
$b$ = 12.2422 (3) Å
$c$ = 22.3402 (5) Å
$\beta$ = 131.425 (1)°
$V$ = 3130.90 (12) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 2.17 mm$^{-1}$
$T$ = 293 K
0.40 × 0.30 × 0.25 mm

### Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.478, $T_{max}$ = 0.613
52133 measured reflections
14238 independent reflections
9143 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.051

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.211
$S$ = 1.01
14238 reflections
676 parameters
66 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.22 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.64 e Å$^{-3}$
Absolute structure: Flack (1983), 6722 Friedel pairs
Flack parameter: 0.50 (2)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H3···O5 | 0.88 | 2.07 | 2.95 (1) | 175 |
| N8—H8···O6 | 0.88 | 2.07 | 2.95 (1) | 172 |

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5589).

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# supporting information

*Acta Cryst.* (2012). E**68**, m1089 [https://doi.org/10.1107/S1600536812031777]

## (Anilino{(*Z*)-2-[(*E*)-5-bromo-3-methoxy-2-oxidobenzylidene]hydrazin-1-ylidene-$\kappa^2O^2,N^2$}methanethiolato-$\kappa S$)(4,4′-dimethyl-2,2′-bipyridine-$\kappa^2N,N'$)zinc *N*,*N*-dimethylformamide monosolvate

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### S1. Comment

A large number of first-row transition metal derivatives of Schiff bases that are synthesized by reacting salicylaldehyde-type of aldehydes with 4-phenylthiosemicarbazide has been reported. The zinc homolog has been isolated as a 2,2′-bipyridine adduct (Seena & Kurup, 2008). The metal center shows square-pyramidal coordination as one of the pyridine N atoms occupy the apical site. Substituents in the Schiff base as well as in the 2,2′-bipyridine do not perturb the square pyramidal coordination geometry in $Zn(C_{12}H_{12}N_2)(C_{15}H_{12}BrN_3O_2S)\cdot DMF$ (Scheme I). The compound crystallizes as a DMF solvate (Figs. 1 and 2).

The doubly-deprotonated Schiff base in *O*,*N*,*S*-chelates to the metal atom, and the three coordinating atoms along with the N atom of the substituted bipyridine ligand comprise the square plane of the square pyramid surrounding it. The apical site is occupied by the second N atom of the substituted 2,2′-bipyridine. In one molecule, the Zn is displaced by 0.305 (3) Å in the direction of the apical occupant (Fig. 1) whereas in the other, the displacement is 0.103 (6) Å in the opposite direction (Fig. 2). The secondary amino group of the Schiff-base dianion forms a hydrogen bond to the O atom of the DMF (Table 1).

### S2. Experimental

To a stirred mixture of 2-(5-bromo-2-hydroxy-3-methoxybenzylidene)-*N*-phenylhydrazinecarbothioamide (0.190 g, 0.5 mmol) in a 1:1 mixture of DMF and methanol and 4,4′-dimethyl-2,2′-bipyridine (0.092 g, 0.5 mmol) in methanol, zinc(II) acetate dihydrate (0.109 g, 0.5 mmol) was added. The resulting yellow solution was heated for 3 h. Yellow crystals separated from the solution after several days.

### S3. Refinement

Carbon- and nitrogen bound H-atoms were placed in calculated positions (C–H 0.93 to 0.96 Å, N–H 0.88 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2 to 1.5*U*(C,*N*).

Omitted owing to bad disagreement was (0 1 1).

All aromatic and pyridine rings were refined as rigid hexagons of 1.39 Å sides. One of the phenyl rings of the Schiff-base anion is disordered over two positions in a 1:1 ratio. The temperature factors of the primed atoms were set to those of the unprimed ones but in the reverse order (*i.e.*, those of C11 to those of C15), and the pair of *N*–$C_{phenyl}$ distances were restrained to within 0.01 Å of each other.

The molecules of DMF were each restrained to lie on a plane; their. The anisotropic temperature factors were restrained to be nearly isotropic.

The final difference Fourier map had a peak at 0.91 Å from Br1 and a hole at 0.96 Å from Br2.
The base scale factor was explicitly refined.

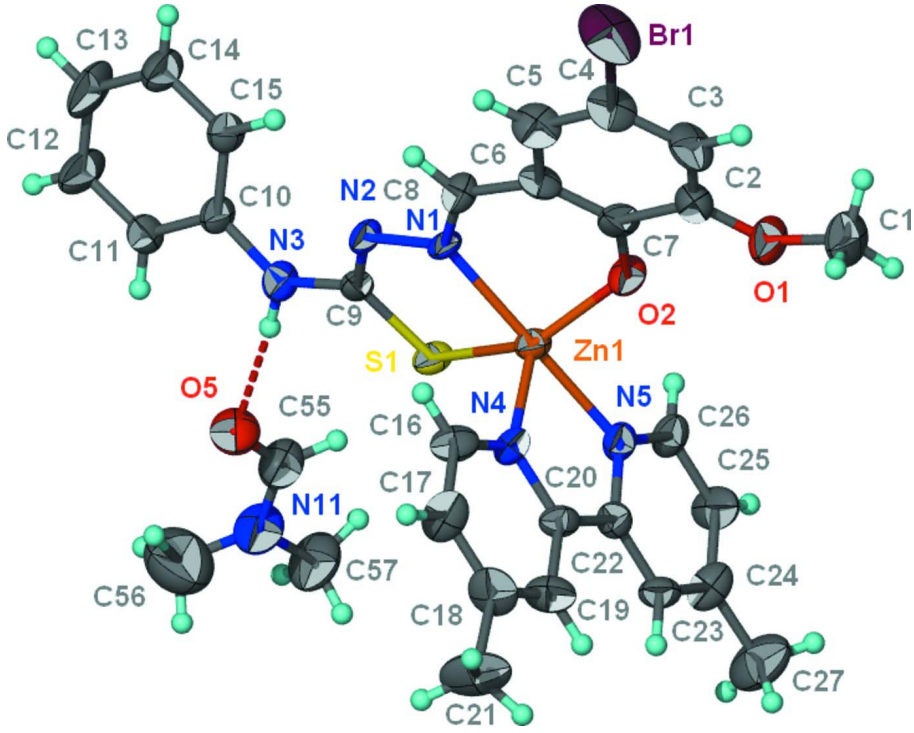


**Figure 1**

Thermal ellipsoid plot (Barbour, 2001) of one $Zn(C_{12}H_{12}N_2)(C_{15}H_{12}BrN_3O_2S)\cdot DMF$ molecule at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius. The disorder in one of the phenyl rings is not shown.

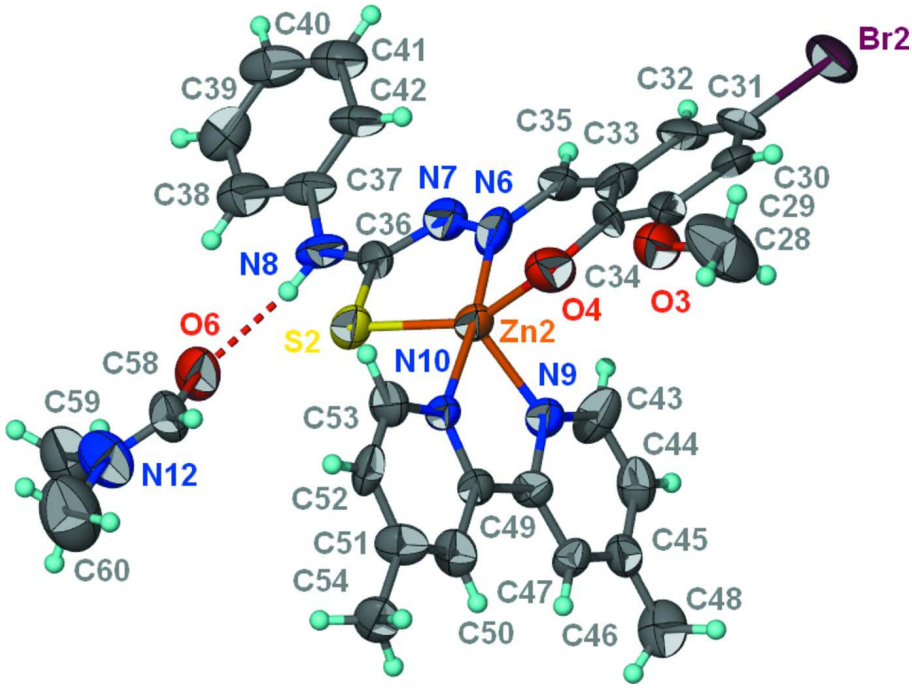


**Figure 2**

Thermal ellipsoid plot (Barbour, 2001) of second $Zn(C_{12}H_{12}N_2)(C_{15}H_{12}BrN_3O_2S)\cdot$DMF molecule at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius. The disorder in one of the phenyl rings is not shown

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*Crystal data*

$[Zn(C_{15}H_{12}BrN_3O_2S)(C_{12}H_{12}N_2)]\cdot C_3H_7NO$
$M_r = 700.95$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 15.2674$ (3) Å
$b = 12.2422$ (3) Å
$c = 22.3402$ (5) Å
$\beta = 131.425$ (1)°
$V = 3130.90$ (12) Å$^3$
$Z = 4$
$F(000) = 1432$
$D_x = 1.487$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9863 reflections
$\theta = 2.5$–$26.3°$
$\mu = 2.17$ mm$^{-1}$
$T = 293$ K
Prism, yellow
0.40 × 0.30 × 0.25 mm

*Data collection*

Bruker APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.478$, $T_{max} = 0.613$
52133 measured reflections
14238 independent reflections
9143 reflections with $I > 2\sigma(I)$
$R_{int} = 0.051$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.2°$
$h = -19\rightarrow19$
$k = -15\rightarrow15$
$l = -29\rightarrow28$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.070$
$wR(F^2) = 0.211$
$S = 1.01$
14238 reflections
676 parameters
66 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0841P)^2 + 9.813P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.22$ e Å$^{-3}$
$\Delta\rho_{min} = -1.64$ e Å$^{-3}$
Absolute structure: Flack (1983), 6722 Friedel pairs
Absolute structure parameter: 0.50 (2)

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Br1 | 1.72718 (11) | −0.00210 (15) | 1.13837 (9) | 0.0914 (5) | |
| Br2 | 1.72867 (13) | 0.40505 (18) | 0.63979 (13) | 0.1416 (9) | |
| Zn1 | 1.12332 (8) | 0.22235 (8) | 0.86185 (6) | 0.0366 (2) | |
| Zn2 | 1.12382 (11) | 0.18373 (10) | 0.36192 (8) | 0.0669 (4) | |
| S1 | 1.02546 (19) | 0.3730 (2) | 0.85966 (14) | 0.0399 (5) | |
| S2 | 1.0257 (3) | 0.0344 (3) | 0.35998 (18) | 0.0745 (9) | |
| O1 | 1.3542 (6) | 0.0420 (9) | 0.8358 (4) | 0.074 (3) | |
| O2 | 1.2468 (5) | 0.1673 (6) | 0.8630 (3) | 0.0452 (15) | |
| O3 | 1.3522 (8) | 0.3694 (10) | 0.3332 (6) | 0.096 (3) | |
| O4 | 1.2447 (8) | 0.2454 (9) | 0.3637 (6) | 0.098 (3) | |
| O5 | 0.8524 (6) | 0.5244 (8) | 0.8923 (4) | 0.066 (2) | |
| O6 | 0.8553 (8) | −0.1344 (9) | 0.3904 (5) | 0.090 (3) | |
| N1 | 1.2588 (5) | 0.2765 (7) | 0.9809 (4) | 0.0347 (16) | |
| N2 | 1.2354 (5) | 0.3571 (6) | 1.0123 (4) | 0.0353 (15) | |
| N3 | 1.1036 (6) | 0.4821 (7) | 0.9878 (4) | 0.0450 (19) | |
| H3 | 1.0279 | 0.4927 | 0.9571 | 0.054* | 0.50 |
| H3′ | 1.0283 | 0.4963 | 0.9555 | 0.054* | 0.50 |
| N4 | 1.0594 (4) | 0.0801 (4) | 0.8728 (3) | 0.0368 (17) | |
| C16 | 1.1041 (4) | 0.0322 (5) | 0.9445 (2) | 0.049 (2) | |
| H16 | 1.1681 | 0.0632 | 0.9927 | 0.058* | |
| C17 | 1.0531 (6) | −0.0620 (5) | 0.9444 (3) | 0.060 (3) | |
| H17 | 1.0830 | −0.0940 | 0.9924 | 0.071* | |
| C18 | 0.9574 (6) | −0.1083 (5) | 0.8724 (4) | 0.061 (3) | |
| C19 | 0.9127 (5) | −0.0604 (5) | 0.8006 (3) | 0.055 (3) | |
| H19 | 0.8486 | −0.0914 | 0.7525 | 0.066* | |
| C20 | 0.9637 (5) | 0.0337 (4) | 0.8008 (2) | 0.0382 (19) | |
| N5 | 0.9842 (4) | 0.1788 (5) | 0.7400 (2) | 0.0400 (17) | |
| C22 | 0.9212 (5) | 0.0881 (4) | 0.7305 (3) | 0.039 (2) | |
| C23 | 0.8202 (5) | 0.0574 (4) | 0.6547 (3) | 0.044 (2) | |
| H23 | 0.7781 | −0.0033 | 0.6483 | 0.053* | |
| C24 | 0.7822 (4) | 0.1174 (5) | 0.5884 (2) | 0.055 (3) | |
| C25 | 0.8451 (5) | 0.2081 (5) | 0.5979 (3) | 0.066 (3) | |

| | | | | | |
|---|---|---|---|---|---|
| H25 | 0.8197 | 0.2482 | 0.5535 | 0.079* | |
| C26 | 0.9461 (5) | 0.2388 (4) | 0.6737 (3) | 0.047 (2) | |
| H26 | 0.9882 | 0.2995 | 0.6801 | 0.057* | |
| N6 | 1.2560 (10) | 0.1274 (9) | 0.4763 (7) | 0.080 (3) | |
| N7 | 1.2368 (9) | 0.0517 (10) | 0.5138 (6) | 0.085 (3) | |
| N8 | 1.1032 (9) | −0.0762 (10) | 0.4868 (6) | 0.073 (3) | |
| H8 | 1.0276 | −0.0868 | 0.4566 | 0.088* | |
| N9 | 1.0634 (5) | 0.3279 (5) | 0.3726 (4) | 0.059 (2) | |
| C43 | 1.1100 (5) | 0.3757 (6) | 0.4448 (3) | 0.085 (4) | |
| H43 | 1.1769 | 0.3467 | 0.4925 | 0.102* | |
| C44 | 1.0566 (6) | 0.4668 (6) | 0.4458 (3) | 0.072 (4) | |
| H44 | 1.0878 | 0.4988 | 0.4941 | 0.086* | |
| C45 | 0.9566 (6) | 0.5102 (5) | 0.3745 (4) | 0.063 (3) | |
| C46 | 0.9099 (5) | 0.4624 (5) | 0.3022 (3) | 0.051 (2) | |
| H46 | 0.8430 | 0.4914 | 0.2545 | 0.061* | |
| C47 | 0.9633 (5) | 0.3712 (5) | 0.3013 (3) | 0.049 (2) | |
| N10 | 0.9844 (4) | 0.2266 (6) | 0.2407 (3) | 0.0542 (19) | |
| C49 | 0.9190 (5) | 0.3154 (5) | 0.2305 (3) | 0.051 (2) | |
| C50 | 0.8194 (6) | 0.3466 (5) | 0.1543 (4) | 0.067 (3) | |
| H50 | 0.7757 | 0.4061 | 0.1475 | 0.080* | |
| C51 | 0.7853 (5) | 0.2890 (6) | 0.0882 (3) | 0.069 (3) | |
| C52 | 0.8507 (6) | 0.2001 (6) | 0.0983 (3) | 0.065 (3) | |
| H52 | 0.8278 | 0.1616 | 0.0541 | 0.078* | |
| C53 | 0.9502 (6) | 0.1689 (5) | 0.1746 (4) | 0.073 (3) | |
| H53 | 0.9940 | 0.1095 | 0.1814 | 0.087* | |
| N11 | 0.6681 (7) | 0.5698 (6) | 0.7784 (5) | 0.072 (3) | |
| N12 | 0.6763 (11) | −0.1722 (9) | 0.2820 (7) | 0.103 (4) | |
| C1 | 1.3953 (11) | −0.0425 (12) | 0.8147 (8) | 0.085 (4) | |
| H1A | 1.3449 | −0.0467 | 0.7576 | 0.127* | |
| H1B | 1.3950 | −0.1113 | 0.8352 | 0.127* | |
| H1C | 1.4733 | −0.0257 | 0.8371 | 0.127* | |
| C2 | 1.4122 (5) | 0.0630 (6) | 0.9134 (3) | 0.050 (2) | |
| C3 | 1.5234 (5) | 0.0242 (5) | 0.9767 (4) | 0.062 (3) | |
| H3A | 1.5613 | −0.0219 | 0.9669 | 0.074* | |
| C4 | 1.5781 (4) | 0.0542 (6) | 1.0544 (3) | 0.055 (3) | |
| C5 | 1.5216 (5) | 0.1230 (6) | 1.0690 (3) | 0.055 (3) | |
| H5 | 1.5582 | 0.1431 | 1.1210 | 0.066* | |
| C6 | 1.4103 (4) | 0.1619 (5) | 1.0057 (3) | 0.040 (2) | |
| C7 | 1.3556 (4) | 0.1319 (5) | 0.9279 (3) | 0.051 (3) | |
| C8 | 1.3598 (8) | 0.2388 (9) | 1.0255 (5) | 0.042 (2) | |
| H8A | 1.4094 | 0.2629 | 1.0782 | 0.051* | |
| C9 | 1.1356 (8) | 0.3981 (7) | 0.9630 (6) | 0.039 (2) | |
| C10 | 1.1736 (15) | 0.5524 (14) | 1.0541 (8) | 0.043 (2) | 0.50 |
| C11 | 1.1131 (11) | 0.622 (2) | 1.0646 (13) | 0.043 (4) | 0.50 |
| H11 | 1.0322 | 0.6178 | 1.0308 | 0.051* | 0.50 |
| C12 | 1.1735 (18) | 0.699 (2) | 1.1259 (17) | 0.083 (7) | 0.50 |
| H12 | 1.1330 | 0.7457 | 1.1329 | 0.100* | 0.50 |
| C13 | 1.2944 (18) | 0.7056 (18) | 1.1765 (13) | 0.080 (6) | 0.50 |

| | | | | | |
|---|---|---|---|---|---|
| H13 | 1.3348 | 0.7569 | 1.2175 | 0.096* | 0.50 |
| C14 | 1.3550 (10) | 0.6357 (15) | 1.1659 (9) | 0.060 (4) | 0.50 |
| H14 | 1.4359 | 0.6402 | 1.1998 | 0.072* | 0.50 |
| C15 | 1.2946 (15) | 0.5591 (11) | 1.1047 (10) | 0.043 (4) | 0.50 |
| H15 | 1.3351 | 0.5123 | 1.0976 | 0.052* | 0.50 |
| C10′ | 1.1748 (15) | 0.5472 (15) | 1.0570 (8) | 0.043 (2) | 0.50 |
| C11′ | 1.1224 (10) | 0.635 (2) | 1.0620 (11) | 0.043 (4) | 0.50 |
| H11′ | 1.0431 | 0.6488 | 1.0207 | 0.052* | 0.50 |
| C12′ | 1.1883 (17) | 0.7029 (19) | 1.1285 (14) | 0.060 (4) | 0.50 |
| H12′ | 1.1532 | 0.7618 | 1.1318 | 0.072* | 0.50 |
| C13′ | 1.3067 (17) | 0.6826 (18) | 1.1902 (10) | 0.080 (6) | 0.50 |
| H13′ | 1.3508 | 0.7279 | 1.2347 | 0.096* | 0.50 |
| C14′ | 1.3592 (11) | 0.5946 (16) | 1.1853 (8) | 0.083 (7) | 0.50 |
| H14′ | 1.4384 | 0.5810 | 1.2265 | 0.100* | 0.50 |
| C15′ | 1.2933 (16) | 0.5269 (10) | 1.1187 (10) | 0.043 (4) | 0.50 |
| H15′ | 1.3284 | 0.4680 | 1.1154 | 0.051* | 0.50 |
| C21 | 0.8951 (12) | −0.2053 (11) | 0.8731 (8) | 0.089 (4) | |
| H21A | 0.8491 | −0.1801 | 0.8855 | 0.134* | |
| H21B | 0.9519 | −0.2571 | 0.9127 | 0.134* | |
| H21C | 0.8450 | −0.2395 | 0.8215 | 0.134* | |
| C27 | 0.6743 (14) | 0.0869 (17) | 0.5059 (7) | 0.101 (5) | |
| H27A | 0.6592 | 0.0103 | 0.5042 | 0.152* | |
| H27B | 0.6850 | 0.1026 | 0.4690 | 0.152* | |
| H27C | 0.6093 | 0.1282 | 0.4916 | 0.152* | |
| C28 | 1.3964 (16) | 0.454 (2) | 0.3172 (13) | 0.170 (11) | |
| H28A | 1.3466 | 0.4635 | 0.2605 | 0.255* | |
| H28B | 1.4737 | 0.4350 | 0.3390 | 0.255* | |
| H28C | 1.3992 | 0.5202 | 0.3412 | 0.255* | |
| C29 | 1.4093 (6) | 0.3422 (7) | 0.4112 (4) | 0.092 (5) | |
| C30 | 1.5205 (6) | 0.3817 (6) | 0.4740 (6) | 0.096 (5) | |
| H30 | 1.5574 | 0.4282 | 0.4637 | 0.115* | |
| C31 | 1.5764 (5) | 0.3518 (8) | 0.5520 (5) | 0.095 (5) | |
| C32 | 1.5212 (7) | 0.2824 (8) | 0.5673 (4) | 0.094 (5) | |
| H32 | 1.5587 | 0.2624 | 0.6195 | 0.112* | |
| C33 | 1.4100 (7) | 0.2428 (7) | 0.5046 (5) | 0.080 (4) | |
| C34 | 1.3541 (5) | 0.2728 (7) | 0.4266 (4) | 0.071 (3) | |
| C35 | 1.3670 (10) | 0.1683 (13) | 0.5301 (8) | 0.086 (4) | |
| H35 | 1.4152 | 0.1478 | 0.5834 | 0.103* | |
| C36 | 1.1316 (9) | 0.0013 (10) | 0.4594 (6) | 0.059 (3) | |
| C37 | 1.1745 (6) | −0.1450 (7) | 0.5566 (4) | 0.064 (3) | |
| C38 | 1.1170 (5) | −0.2253 (8) | 0.5633 (5) | 0.081 (4) | |
| H38 | 1.0359 | −0.2292 | 0.5258 | 0.098* | |
| C39 | 1.1807 (9) | −0.2998 (7) | 0.6258 (6) | 0.091 (4) | |
| H39 | 1.1423 | −0.3536 | 0.6302 | 0.110* | |
| C40 | 1.3020 (9) | −0.2940 (7) | 0.6817 (5) | 0.095 (5) | |
| H40 | 1.3446 | −0.3438 | 0.7236 | 0.114* | |
| C41 | 1.3595 (5) | −0.2136 (8) | 0.6751 (4) | 0.086 (4) | |
| H41 | 1.4406 | −0.2097 | 0.7125 | 0.103* | |

| | | | | |
|---|---|---|---|---|
| C42 | 1.2958 (6) | −0.1391 (7) | 0.6126 (5) | 0.075 (3) |
| H42 | 1.3342 | −0.0854 | 0.6081 | 0.090* |
| C48 | 0.8976 (13) | 0.6037 (14) | 0.3730 (8) | 0.086 (4) |
| H48A | 0.9371 | 0.6693 | 0.3788 | 0.130* |
| H48B | 0.8981 | 0.5985 | 0.4161 | 0.130* |
| H48C | 0.8184 | 0.6056 | 0.3231 | 0.130* |
| C54 | 0.6715 (11) | 0.3223 (13) | 0.0054 (6) | 0.077 (4) |
| H54A | 0.6260 | 0.2582 | −0.0236 | 0.116* |
| H54B | 0.6894 | 0.3593 | −0.0232 | 0.116* |
| H54C | 0.6278 | 0.3701 | 0.0113 | 0.116* |
| C55 | 0.7803 (10) | 0.5459 (7) | 0.8201 (7) | 0.068 (3) |
| H55 | 0.8067 | 0.5452 | 0.7926 | 0.082* |
| C56 | 0.6333 (15) | 0.5697 (15) | 0.8199 (11) | 0.143 (6) |
| H56A | 0.6947 | 0.5413 | 0.8724 | 0.214* |
| H56B | 0.5651 | 0.5248 | 0.7931 | 0.214* |
| H56C | 0.6152 | 0.6430 | 0.8238 | 0.214* |
| C57 | 0.5914 (11) | 0.5943 (11) | 0.6963 (6) | 0.086 (4) |
| H57A | 0.6356 | 0.6161 | 0.6818 | 0.129* |
| H57B | 0.5403 | 0.6527 | 0.6850 | 0.129* |
| H57C | 0.5458 | 0.5308 | 0.6662 | 0.129* |
| C58 | 0.7778 (10) | −0.1278 (9) | 0.3182 (8) | 0.080 (3) |
| H58 | 0.7912 | −0.0906 | 0.2886 | 0.096* |
| C59 | 0.6513 (12) | −0.2339 (13) | 0.3288 (9) | 0.112 (5) |
| H59A | 0.7138 | −0.2215 | 0.3849 | 0.168* |
| H59B | 0.6453 | −0.3106 | 0.3178 | 0.168* |
| H59C | 0.5793 | −0.2083 | 0.3131 | 0.168* |
| C60 | 0.5787 (17) | −0.1630 (16) | 0.1896 (12) | 0.161 (8) |
| H60A | 0.5966 | −0.1041 | 0.1708 | 0.241* |
| H60B | 0.5051 | −0.1492 | 0.1755 | 0.241* |
| H60C | 0.5741 | −0.2301 | 0.1654 | 0.241* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Br1 | 0.0544 (7) | 0.1203 (13) | 0.0898 (9) | 0.0469 (8) | 0.0437 (7) | 0.0423 (9) |
| Br2 | 0.0536 (8) | 0.1371 (17) | 0.1670 (18) | −0.0138 (9) | 0.0445 (11) | −0.0857 (15) |
| Zn1 | 0.0284 (4) | 0.0361 (5) | 0.0374 (5) | −0.0018 (5) | 0.0184 (4) | −0.0056 (5) |
| Zn2 | 0.0540 (7) | 0.0451 (7) | 0.0582 (8) | 0.0078 (6) | 0.0185 (6) | 0.0086 (7) |
| S1 | 0.0290 (10) | 0.0372 (13) | 0.0389 (12) | −0.0004 (10) | 0.0163 (10) | −0.0066 (11) |
| S2 | 0.0691 (19) | 0.0521 (18) | 0.0518 (17) | 0.0037 (16) | 0.0185 (15) | 0.0069 (15) |
| O1 | 0.045 (4) | 0.105 (7) | 0.063 (4) | 0.007 (4) | 0.033 (4) | −0.032 (5) |
| O2 | 0.029 (3) | 0.059 (4) | 0.028 (3) | 0.010 (3) | 0.011 (3) | −0.003 (3) |
| O3 | 0.073 (6) | 0.074 (6) | 0.112 (7) | −0.001 (5) | 0.049 (6) | 0.013 (6) |
| O4 | 0.072 (6) | 0.077 (7) | 0.112 (8) | 0.009 (5) | 0.048 (6) | 0.027 (6) |
| O5 | 0.043 (3) | 0.085 (5) | 0.054 (4) | 0.012 (3) | 0.025 (3) | 0.005 (4) |
| O6 | 0.086 (5) | 0.081 (5) | 0.052 (4) | −0.009 (4) | 0.024 (4) | −0.009 (4) |
| N1 | 0.020 (3) | 0.044 (4) | 0.026 (3) | −0.004 (3) | 0.009 (3) | −0.012 (3) |
| N2 | 0.031 (3) | 0.034 (4) | 0.033 (3) | 0.002 (3) | 0.017 (3) | −0.011 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N3 | 0.032 (4) | 0.052 (5) | 0.044 (4) | 0.011 (4) | 0.023 (4) | −0.008 (4) |
| N4 | 0.041 (4) | 0.030 (4) | 0.030 (4) | 0.000 (3) | 0.020 (4) | −0.003 (3) |
| C16 | 0.033 (4) | 0.045 (6) | 0.047 (5) | 0.002 (4) | 0.018 (4) | 0.005 (5) |
| C17 | 0.081 (8) | 0.039 (6) | 0.053 (6) | 0.002 (6) | 0.042 (7) | 0.007 (5) |
| C18 | 0.087 (8) | 0.036 (6) | 0.079 (7) | −0.005 (6) | 0.063 (7) | 0.013 (6) |
| C19 | 0.045 (5) | 0.051 (6) | 0.059 (6) | −0.006 (5) | 0.030 (5) | 0.007 (5) |
| C20 | 0.034 (4) | 0.026 (4) | 0.050 (5) | −0.003 (4) | 0.026 (4) | −0.004 (4) |
| N5 | 0.050 (4) | 0.035 (4) | 0.040 (4) | −0.003 (4) | 0.032 (4) | −0.005 (4) |
| C22 | 0.038 (4) | 0.042 (5) | 0.040 (5) | 0.001 (4) | 0.026 (4) | −0.001 (4) |
| C23 | 0.039 (5) | 0.042 (5) | 0.048 (5) | −0.013 (4) | 0.028 (5) | −0.006 (5) |
| C24 | 0.062 (6) | 0.040 (5) | 0.041 (5) | 0.008 (5) | 0.025 (5) | 0.002 (5) |
| C25 | 0.063 (6) | 0.095 (10) | 0.027 (5) | −0.020 (6) | 0.024 (5) | 0.008 (6) |
| C26 | 0.067 (6) | 0.033 (5) | 0.048 (5) | −0.008 (5) | 0.041 (5) | −0.007 (5) |
| N6 | 0.089 (7) | 0.041 (6) | 0.079 (7) | −0.003 (5) | 0.043 (6) | −0.009 (5) |
| N7 | 0.066 (6) | 0.066 (8) | 0.077 (7) | 0.006 (6) | 0.028 (6) | −0.007 (6) |
| N8 | 0.064 (6) | 0.071 (7) | 0.055 (6) | 0.032 (5) | 0.027 (5) | 0.013 (5) |
| N9 | 0.056 (5) | 0.048 (6) | 0.048 (5) | 0.002 (4) | 0.024 (5) | 0.003 (5) |
| C43 | 0.129 (11) | 0.053 (8) | 0.046 (7) | 0.009 (8) | 0.047 (8) | 0.008 (6) |
| C44 | 0.084 (9) | 0.070 (9) | 0.052 (7) | −0.023 (7) | 0.041 (7) | −0.014 (7) |
| C45 | 0.053 (6) | 0.054 (7) | 0.059 (6) | −0.009 (5) | 0.028 (5) | 0.005 (6) |
| C46 | 0.062 (6) | 0.041 (6) | 0.042 (5) | 0.005 (5) | 0.031 (5) | 0.009 (5) |
| C47 | 0.049 (5) | 0.054 (6) | 0.034 (5) | 0.006 (5) | 0.023 (5) | 0.006 (5) |
| N10 | 0.044 (4) | 0.040 (4) | 0.050 (5) | 0.004 (4) | 0.019 (4) | 0.000 (5) |
| C49 | 0.048 (5) | 0.043 (6) | 0.047 (6) | 0.002 (5) | 0.025 (5) | 0.005 (5) |
| C50 | 0.066 (7) | 0.072 (8) | 0.035 (6) | −0.006 (6) | 0.022 (6) | 0.001 (6) |
| C51 | 0.065 (7) | 0.091 (10) | 0.045 (6) | 0.018 (7) | 0.034 (6) | 0.013 (7) |
| C52 | 0.089 (8) | 0.035 (6) | 0.054 (6) | −0.014 (5) | 0.041 (6) | −0.005 (5) |
| C53 | 0.062 (7) | 0.067 (8) | 0.063 (7) | −0.008 (6) | 0.030 (6) | −0.021 (7) |
| N11 | 0.043 (4) | 0.090 (6) | 0.050 (5) | 0.020 (4) | 0.018 (4) | 0.002 (4) |
| N12 | 0.086 (7) | 0.133 (8) | 0.073 (6) | −0.014 (6) | 0.045 (5) | −0.015 (6) |
| C1 | 0.076 (8) | 0.088 (9) | 0.102 (9) | 0.009 (7) | 0.064 (8) | −0.035 (8) |
| C2 | 0.050 (5) | 0.057 (7) | 0.053 (6) | −0.004 (5) | 0.038 (5) | −0.005 (5) |
| C3 | 0.044 (5) | 0.080 (8) | 0.067 (7) | 0.022 (5) | 0.039 (5) | 0.012 (6) |
| C4 | 0.045 (5) | 0.042 (5) | 0.075 (7) | 0.024 (4) | 0.038 (6) | 0.014 (5) |
| C5 | 0.040 (5) | 0.058 (7) | 0.049 (6) | 0.020 (5) | 0.022 (5) | 0.020 (5) |
| C6 | 0.024 (4) | 0.042 (5) | 0.048 (5) | 0.011 (4) | 0.021 (4) | 0.009 (4) |
| C7 | 0.054 (6) | 0.033 (5) | 0.077 (7) | −0.018 (4) | 0.048 (6) | −0.025 (5) |
| C8 | 0.045 (5) | 0.042 (6) | 0.034 (4) | 0.002 (4) | 0.024 (4) | −0.003 (4) |
| C9 | 0.043 (5) | 0.033 (5) | 0.053 (5) | −0.014 (4) | 0.036 (5) | −0.019 (4) |
| C10 | 0.038 (4) | 0.041 (5) | 0.048 (5) | 0.001 (4) | 0.028 (4) | −0.014 (4) |
| C11 | 0.055 (9) | 0.027 (6) | 0.060 (9) | −0.003 (6) | 0.044 (8) | −0.006 (6) |
| C12 | 0.051 (10) | 0.091 (14) | 0.089 (14) | −0.009 (8) | 0.039 (10) | −0.058 (11) |
| C13 | 0.087 (10) | 0.061 (12) | 0.072 (10) | 0.005 (9) | 0.044 (9) | −0.035 (10) |
| C14 | 0.052 (9) | 0.061 (10) | 0.058 (10) | −0.004 (7) | 0.033 (9) | −0.021 (8) |
| C15 | 0.046 (8) | 0.037 (8) | 0.050 (8) | 0.003 (6) | 0.032 (8) | −0.004 (7) |
| C10′ | 0.038 (4) | 0.041 (5) | 0.048 (5) | 0.001 (4) | 0.028 (4) | −0.014 (4) |
| C11′ | 0.046 (8) | 0.037 (8) | 0.050 (8) | 0.003 (6) | 0.032 (8) | −0.004 (7) |
| C12′ | 0.052 (9) | 0.061 (10) | 0.058 (10) | −0.004 (7) | 0.033 (9) | −0.021 (8) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C13′ | 0.087 (10) | 0.061 (12) | 0.072 (10) | 0.005 (9) | 0.044 (9) | −0.035 (10) |
| C14′ | 0.051 (10) | 0.091 (14) | 0.089 (14) | −0.009 (8) | 0.039 (10) | −0.058 (11) |
| C15′ | 0.055 (9) | 0.027 (6) | 0.060 (9) | −0.003 (6) | 0.044 (8) | −0.006 (6) |
| C21 | 0.091 (9) | 0.054 (7) | 0.096 (10) | −0.030 (7) | 0.050 (8) | 0.015 (7) |
| C27 | 0.104 (11) | 0.110 (14) | 0.048 (8) | −0.024 (11) | 0.033 (8) | −0.005 (9) |
| C28 | 0.101 (14) | 0.23 (3) | 0.19 (2) | −0.026 (17) | 0.101 (16) | 0.03 (2) |
| C29 | 0.043 (6) | 0.047 (7) | 0.148 (13) | 0.001 (6) | 0.046 (8) | 0.001 (9) |
| C30 | 0.059 (7) | 0.045 (7) | 0.132 (13) | 0.021 (6) | 0.041 (8) | 0.003 (8) |
| C31 | 0.027 (5) | 0.103 (12) | 0.098 (10) | 0.010 (7) | 0.017 (6) | −0.043 (9) |
| C32 | 0.044 (7) | 0.089 (11) | 0.090 (10) | 0.024 (7) | 0.020 (7) | −0.013 (9) |
| C33 | 0.066 (7) | 0.042 (7) | 0.081 (9) | 0.017 (6) | 0.027 (7) | 0.010 (6) |
| C34 | 0.028 (5) | 0.053 (7) | 0.066 (7) | −0.009 (5) | 0.003 (5) | −0.017 (6) |
| C35 | 0.041 (6) | 0.063 (8) | 0.071 (8) | 0.013 (6) | 0.002 (6) | −0.001 (7) |
| C36 | 0.045 (5) | 0.052 (7) | 0.047 (6) | −0.002 (5) | 0.017 (5) | −0.016 (5) |
| C37 | 0.059 (6) | 0.083 (9) | 0.038 (5) | 0.029 (6) | 0.027 (5) | −0.003 (6) |
| C38 | 0.082 (8) | 0.082 (10) | 0.071 (8) | 0.018 (7) | 0.047 (7) | 0.008 (7) |
| C39 | 0.120 (12) | 0.073 (10) | 0.095 (10) | 0.007 (8) | 0.077 (10) | 0.002 (8) |
| C40 | 0.095 (10) | 0.119 (14) | 0.054 (7) | 0.048 (10) | 0.043 (8) | 0.017 (8) |
| C41 | 0.069 (7) | 0.101 (11) | 0.074 (8) | 0.025 (7) | 0.041 (7) | 0.006 (7) |
| C42 | 0.052 (6) | 0.091 (9) | 0.061 (6) | 0.034 (6) | 0.029 (5) | 0.016 (7) |
| C48 | 0.106 (10) | 0.095 (11) | 0.080 (9) | −0.015 (9) | 0.070 (9) | −0.021 (8) |
| C54 | 0.067 (8) | 0.074 (10) | 0.040 (6) | 0.004 (7) | 0.014 (6) | 0.005 (6) |
| C55 | 0.064 (6) | 0.072 (6) | 0.057 (5) | 0.006 (5) | 0.035 (5) | −0.008 (5) |
| C56 | 0.114 (9) | 0.177 (11) | 0.142 (10) | 0.006 (7) | 0.087 (8) | 0.006 (8) |
| C57 | 0.072 (6) | 0.103 (7) | 0.050 (5) | 0.017 (5) | 0.026 (5) | 0.001 (5) |
| C58 | 0.066 (6) | 0.075 (7) | 0.064 (6) | −0.020 (5) | 0.028 (5) | −0.006 (5) |
| C59 | 0.099 (7) | 0.119 (8) | 0.105 (8) | −0.025 (6) | 0.061 (6) | −0.007 (6) |
| C60 | 0.154 (11) | 0.165 (12) | 0.130 (10) | −0.038 (8) | 0.079 (8) | 0.015 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Br1—C4 | 1.877 (4) | C1—H1B | 0.9600 |
| Br2—C31 | 1.908 (5) | C1—H1C | 0.9600 |
| Zn1—O2 | 1.987 (6) | C2—C3 | 1.3900 |
| Zn1—N4 | 2.088 (4) | C2—C7 | 1.3900 |
| Zn1—N1 | 2.124 (6) | C3—C4 | 1.3900 |
| Zn1—N5 | 2.134 (4) | C3—H3A | 0.9300 |
| Zn1—S1 | 2.353 (2) | C4—C5 | 1.3900 |
| Zn2—O4 | 1.970 (9) | C5—C6 | 1.3900 |
| Zn2—N6 | 2.063 (11) | C5—H5 | 0.9300 |
| Zn2—N9 | 2.077 (5) | C6—C7 | 1.3900 |
| Zn2—N10 | 2.124 (4) | C6—C8 | 1.459 (10) |
| Zn2—S2 | 2.346 (4) | C8—H8A | 0.9300 |
| S1—C9 | 1.765 (10) | C10—C11 | 1.3900 |
| S2—C36 | 1.720 (11) | C10—C15 | 1.3900 |
| O1—C2 | 1.351 (8) | C11—C12 | 1.3900 |
| O1—C1 | 1.441 (12) | C11—H11 | 0.9300 |
| O2—C7 | 1.364 (7) | C12—C13 | 1.3900 |

| | | | |
|---|---|---|---|
| O3—C29 | 1.379 (12) | C12—H12 | 0.9300 |
| O3—C28 | 1.40 (2) | C13—C14 | 1.3900 |
| O4—C34 | 1.330 (11) | C13—H13 | 0.9300 |
| O5—C55 | 1.239 (13) | C14—C15 | 1.3900 |
| O6—C58 | 1.218 (14) | C14—H14 | 0.9300 |
| N1—C8 | 1.246 (11) | C15—H15 | 0.9300 |
| N1—N2 | 1.388 (9) | C10′—C11′ | 1.3900 |
| N2—C9 | 1.251 (11) | C10′—C15′ | 1.3900 |
| N3—C9 | 1.401 (11) | C11′—C12′ | 1.3900 |
| N3—C10′ | 1.409 (10) | C11′—H11′ | 0.9300 |
| N3—C10 | 1.407 (10) | C12′—C13′ | 1.3900 |
| N3—H3 | 0.8800 | C12′—H12′ | 0.9300 |
| N3—H3′ | 0.8800 | C13′—C14′ | 1.3900 |
| N4—C16 | 1.3900 | C13′—H13′ | 0.9300 |
| N4—C20 | 1.3900 | C14′—C15′ | 1.3900 |
| C16—C17 | 1.3900 | C14′—H14′ | 0.9300 |
| C16—H16 | 0.9300 | C15′—H15′ | 0.9300 |
| C17—C18 | 1.3900 | C21—H21A | 0.9600 |
| C17—H17 | 0.9300 | C21—H21B | 0.9600 |
| C18—C19 | 1.3900 | C21—H21C | 0.9600 |
| C18—C21 | 1.527 (11) | C27—H27A | 0.9600 |
| C19—C20 | 1.3900 | C27—H27B | 0.9600 |
| C19—H19 | 0.9300 | C27—H27C | 0.9600 |
| C20—C22 | 1.408 (5) | C28—H28A | 0.9600 |
| N5—C22 | 1.3900 | C28—H28B | 0.9600 |
| N5—C26 | 1.3900 | C28—H28C | 0.9600 |
| C22—C23 | 1.3900 | C29—C30 | 1.3900 |
| C23—C24 | 1.3900 | C29—C34 | 1.3900 |
| C23—H23 | 0.9300 | C30—C31 | 1.3900 |
| C24—C25 | 1.3900 | C30—H30 | 0.9300 |
| C24—C27 | 1.493 (14) | C31—C32 | 1.3900 |
| C25—C26 | 1.3900 | C32—C33 | 1.3900 |
| C25—H25 | 0.9300 | C32—H32 | 0.9300 |
| C26—H26 | 0.9300 | C33—C34 | 1.3900 |
| N6—C35 | 1.368 (16) | C33—C35 | 1.443 (17) |
| N6—N7 | 1.403 (15) | C35—H35 | 0.9300 |
| N7—C36 | 1.362 (15) | C37—C38 | 1.3900 |
| N8—C36 | 1.347 (16) | C37—C42 | 1.3900 |
| N8—C37 | 1.443 (11) | C38—C39 | 1.3900 |
| N8—H8 | 0.8800 | C38—H38 | 0.9300 |
| N9—C43 | 1.3900 | C39—C40 | 1.3900 |
| N9—C47 | 1.3900 | C39—H39 | 0.9300 |
| C43—C44 | 1.3900 | C40—C41 | 1.3900 |
| C43—H43 | 0.9300 | C40—H40 | 0.9300 |
| C44—C45 | 1.3900 | C41—C42 | 1.3900 |
| C44—H44 | 0.9300 | C41—H41 | 0.9300 |
| C45—C46 | 1.3900 | C42—H42 | 0.9300 |
| C45—C48 | 1.444 (15) | C48—H48A | 0.9600 |

| | | | |
|---|---|---|---|
| C46—C47 | 1.3900 | C48—H48B | 0.9600 |
| C46—H46 | 0.9300 | C48—H48C | 0.9600 |
| C47—C49 | 1.418 (6) | C54—H54A | 0.9600 |
| N10—C49 | 1.3900 | C54—H54B | 0.9600 |
| N10—C53 | 1.3900 | C54—H54C | 0.9600 |
| C49—C50 | 1.3900 | C55—H55 | 0.9300 |
| C50—C51 | 1.3900 | C56—H56A | 0.9600 |
| C50—H50 | 0.9300 | C56—H56B | 0.9600 |
| C51—C52 | 1.3900 | C56—H56C | 0.9600 |
| C51—C54 | 1.534 (12) | C57—H57A | 0.9600 |
| C52—C53 | 1.3900 | C57—H57B | 0.9600 |
| C52—H52 | 0.9300 | C57—H57C | 0.9600 |
| C53—H53 | 0.9300 | C58—H58 | 0.9300 |
| N11—C55 | 1.333 (14) | C59—H59A | 0.9600 |
| N11—C56 | 1.339 (17) | C59—H59B | 0.9600 |
| N11—C57 | 1.407 (14) | C59—H59C | 0.9600 |
| N12—C58 | 1.301 (16) | C60—H60A | 0.9600 |
| N12—C59 | 1.528 (18) | C60—H60B | 0.9600 |
| N12—C60 | 1.56 (2) | C60—H60C | 0.9600 |
| C1—H1A | 0.9600 | | |

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| O2—Zn1—N4 | 103.2 (3) | O2—C7—C2 | 116.8 (5) |
| O2—Zn1—N1 | 87.7 (2) | C6—C7—C2 | 120.0 |
| N4—Zn1—N1 | 104.9 (3) | N1—C8—C6 | 128.3 (8) |
| O2—Zn1—N5 | 93.9 (2) | N1—C8—H8A | 115.9 |
| N4—Zn1—N5 | 78.0 (2) | C6—C8—H8A | 115.9 |
| N1—Zn1—N5 | 176.3 (3) | N2—C9—N3 | 119.1 (8) |
| O2—Zn1—S1 | 148.2 (2) | N2—C9—S1 | 129.3 (6) |
| N4—Zn1—S1 | 108.48 (15) | N3—C9—S1 | 111.4 (7) |
| N1—Zn1—S1 | 82.0 (2) | C11—C10—C15 | 120.0 |
| N5—Zn1—S1 | 94.97 (17) | C11—C10—N3 | 115.3 (14) |
| O4—Zn2—N6 | 88.1 (4) | C15—C10—N3 | 124.6 (14) |
| O4—Zn2—N9 | 98.8 (4) | C12—C11—C10 | 120.0 |
| N6—Zn2—N9 | 106.6 (3) | C12—C11—H11 | 120.0 |
| O4—Zn2—N10 | 93.8 (3) | C10—C11—H11 | 120.0 |
| N6—Zn2—N10 | 174.8 (4) | C13—C12—C11 | 120.0 |
| N9—Zn2—N10 | 77.9 (2) | C13—C12—H12 | 120.0 |
| O4—Zn2—S2 | 151.3 (4) | C11—C12—H12 | 120.0 |
| N6—Zn2—S2 | 81.5 (3) | C12—C13—C14 | 120.0 |
| N9—Zn2—S2 | 109.7 (2) | C12—C13—H13 | 120.0 |
| N10—Zn2—S2 | 94.6 (2) | C14—C13—H13 | 120.0 |
| C9—S1—Zn1 | 93.8 (3) | C15—C14—C13 | 120.0 |
| C36—S2—Zn2 | 96.7 (4) | C15—C14—H14 | 120.0 |
| C2—O1—C1 | 120.0 (9) | C13—C14—H14 | 120.0 |
| C7—O2—Zn1 | 126.8 (4) | C14—C15—C10 | 120.0 |
| C29—O3—C28 | 119.4 (13) | C14—C15—H15 | 120.0 |
| C34—O4—Zn2 | 128.5 (8) | C10—C15—H15 | 120.0 |
| C8—N1—N2 | 117.1 (7) | C11′—C10′—C15′ | 120.0 |

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| C8—N1—Zn1 | 123.4 (6) | C11′—C10′—N3 | 117.3 (15) |
| N2—N1—Zn1 | 119.5 (5) | C15′—C10′—N3 | 122.7 (15) |
| C9—N2—N1 | 114.2 (6) | C12′—C11′—C10′ | 120.0 |
| C9—N3—C10′ | 129.2 (11) | C12′—C11′—H11′ | 120.0 |
| C9—N3—C10 | 130.1 (11) | C10′—C11′—H11′ | 120.0 |
| C10′—N3—C10 | 3.4 (16) | C11′—C12′—C13′ | 120.0 |
| C9—N3—H3 | 115.0 | C11′—C12′—H12′ | 120.0 |
| C10′—N3—H3 | 115.8 | C13′—C12′—H12′ | 120.0 |
| C10—N3—H3 | 115.0 | C14′—C13′—C12′ | 120.0 |
| C9—N3—H3′ | 115.4 | C14′—C13′—H13′ | 120.0 |
| C10′—N3—H3′ | 115.4 | C12′—C13′—H13′ | 120.0 |
| C10—N3—H3′ | 114.4 | C15′—C14′—C13′ | 120.0 |
| C16—N4—C20 | 120.0 | C15′—C14′—H14′ | 120.0 |
| C16—N4—Zn1 | 125.1 (3) | C13′—C14′—H14′ | 120.0 |
| C20—N4—Zn1 | 114.9 (3) | C14′—C15′—C10′ | 120.0 |
| C17—C16—N4 | 120.0 | C14′—C15′—H15′ | 120.0 |
| C17—C16—H16 | 120.0 | C10′—C15′—H15′ | 120.0 |
| N4—C16—H16 | 120.0 | C18—C21—H21A | 109.5 |
| C16—C17—C18 | 120.0 | C18—C21—H21B | 109.5 |
| C16—C17—H17 | 120.0 | H21A—C21—H21B | 109.5 |
| C18—C17—H17 | 120.0 | C18—C21—H21C | 109.5 |
| C17—C18—C19 | 120.0 | H21A—C21—H21C | 109.5 |
| C17—C18—C21 | 119.4 (7) | H21B—C21—H21C | 109.5 |
| C19—C18—C21 | 120.4 (7) | C24—C27—H27A | 109.5 |
| C20—C19—C18 | 120.0 | C24—C27—H27B | 109.5 |
| C20—C19—H19 | 120.0 | H27A—C27—H27B | 109.5 |
| C18—C19—H19 | 120.0 | C24—C27—H27C | 109.5 |
| C19—C20—N4 | 120.0 | H27A—C27—H27C | 109.5 |
| C19—C20—C22 | 123.1 (4) | H27B—C27—H27C | 109.5 |
| N4—C20—C22 | 116.9 (4) | O3—C28—H28A | 109.5 |
| C22—N5—C26 | 120.0 | O3—C28—H28B | 109.5 |
| C22—N5—Zn1 | 113.5 (3) | H28A—C28—H28B | 109.5 |
| C26—N5—Zn1 | 126.1 (3) | O3—C28—H28C | 109.5 |
| C23—C22—N5 | 120.0 | H28A—C28—H28C | 109.5 |
| C23—C22—C20 | 123.5 (4) | H28B—C28—H28C | 109.5 |
| N5—C22—C20 | 116.5 (4) | O3—C29—C30 | 121.3 (7) |
| C22—C23—C24 | 120.0 | O3—C29—C34 | 118.7 (7) |
| C22—C23—H23 | 120.0 | C30—C29—C34 | 120.0 |
| C24—C23—H23 | 120.0 | C29—C30—C31 | 120.0 |
| C25—C24—C23 | 120.0 | C29—C30—H30 | 120.0 |
| C25—C24—C27 | 118.4 (8) | C31—C30—H30 | 120.0 |
| C23—C24—C27 | 121.6 (8) | C32—C31—C30 | 120.0 |
| C24—C25—C26 | 120.0 | C32—C31—Br2 | 118.7 (6) |
| C24—C25—H25 | 120.0 | C30—C31—Br2 | 121.3 (6) |
| C26—C25—H25 | 120.0 | C31—C32—C33 | 120.0 |
| C25—C26—N5 | 120.0 | C31—C32—H32 | 120.0 |
| C25—C26—H26 | 120.0 | C33—C32—H32 | 120.0 |
| N5—C26—H26 | 120.0 | C34—C33—C32 | 120.0 |

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| C35—N6—N7 | 110.1 (11) | C34—C33—C35 | 126.8 (8) |
| C35—N6—Zn2 | 126.4 (10) | C32—C33—C35 | 113.2 (8) |
| N7—N6—Zn2 | 122.7 (8) | O4—C34—C33 | 123.9 (7) |
| C36—N7—N6 | 110.8 (10) | O4—C34—C29 | 115.9 (7) |
| C36—N8—C37 | 131.6 (10) | C33—C34—C29 | 120.0 |
| C36—N8—H8 | 114.2 | N6—C35—C33 | 120.5 (12) |
| C37—N8—H8 | 114.2 | N6—C35—H35 | 119.7 |
| C43—N9—C47 | 120.0 | C33—C35—H35 | 119.7 |
| C43—N9—Zn2 | 124.5 (3) | N8—C36—N7 | 117.3 (11) |
| C47—N9—Zn2 | 115.3 (3) | N8—C36—S2 | 116.2 (8) |
| C44—C43—N9 | 120.0 | N7—C36—S2 | 126.3 (10) |
| C44—C43—H43 | 120.0 | C38—C37—C42 | 120.0 |
| N9—C43—H43 | 120.0 | C38—C37—N8 | 116.8 (7) |
| C45—C44—C43 | 120.0 | C42—C37—N8 | 123.0 (7) |
| C45—C44—H44 | 120.0 | C39—C38—C37 | 120.0 |
| C43—C44—H44 | 120.0 | C39—C38—H38 | 120.0 |
| C44—C45—C46 | 120.0 | C37—C38—H38 | 120.0 |
| C44—C45—C48 | 121.7 (7) | C38—C39—C40 | 120.0 |
| C46—C45—C48 | 118.3 (7) | C38—C39—H39 | 120.0 |
| C47—C46—C45 | 120.0 | C40—C39—H39 | 120.0 |
| C47—C46—H46 | 120.0 | C41—C40—C39 | 120.0 |
| C45—C46—H46 | 120.0 | C41—C40—H40 | 120.0 |
| C46—C47—N9 | 120.0 | C39—C40—H40 | 120.0 |
| C46—C47—C49 | 123.5 (5) | C40—C41—C42 | 120.0 |
| N9—C47—C49 | 116.5 (5) | C40—C41—H41 | 120.0 |
| C49—N10—C53 | 120.0 | C42—C41—H41 | 120.0 |
| C49—N10—Zn2 | 114.0 (3) | C41—C42—C37 | 120.0 |
| C53—N10—Zn2 | 125.7 (3) | C41—C42—H42 | 120.0 |
| N10—C49—C50 | 120.0 | C37—C42—H42 | 120.0 |
| N10—C49—C47 | 115.7 (5) | C45—C48—H48A | 109.5 |
| C50—C49—C47 | 124.2 (5) | C45—C48—H48B | 109.5 |
| C49—C50—C51 | 120.0 | H48A—C48—H48B | 109.5 |
| C49—C50—H50 | 120.0 | C45—C48—H48C | 109.5 |
| C51—C50—H50 | 120.0 | H48A—C48—H48C | 109.5 |
| C50—C51—C52 | 120.0 | H48B—C48—H48C | 109.5 |
| C50—C51—C54 | 118.4 (7) | C51—C54—H54A | 109.5 |
| C52—C51—C54 | 121.5 (7) | C51—C54—H54B | 109.5 |
| C53—C52—C51 | 120.0 | H54A—C54—H54B | 109.5 |
| C53—C52—H52 | 120.0 | C51—C54—H54C | 109.5 |
| C51—C52—H52 | 120.0 | H54A—C54—H54C | 109.5 |
| C52—C53—N10 | 120.0 | H54B—C54—H54C | 109.5 |
| C52—C53—H53 | 120.0 | O5—C55—N11 | 125.5 (10) |
| N10—C53—H53 | 120.0 | O5—C55—H55 | 117.3 |
| C55—N11—C56 | 115.6 (11) | N11—C55—H55 | 117.3 |
| C55—N11—C57 | 122.3 (10) | N11—C56—H56A | 109.5 |
| C56—N11—C57 | 122.1 (11) | N11—C56—H56B | 109.5 |
| C58—N12—C59 | 121.0 (12) | H56A—C56—H56B | 109.5 |
| C58—N12—C60 | 119.7 (13) | N11—C56—H56C | 109.5 |

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| C59—N12—C60 | 119.3 (12) | H56A—C56—H56C | 109.5 |
| O1—C1—H1A | 109.5 | H56B—C56—H56C | 109.5 |
| O1—C1—H1B | 109.5 | N11—C57—H57A | 109.5 |
| H1A—C1—H1B | 109.5 | N11—C57—H57B | 109.5 |
| O1—C1—H1C | 109.5 | H57A—C57—H57B | 109.5 |
| H1A—C1—H1C | 109.5 | N11—C57—H57C | 109.5 |
| H1B—C1—H1C | 109.5 | H57A—C57—H57C | 109.5 |
| O1—C2—C3 | 124.2 (5) | H57B—C57—H57C | 109.5 |
| O1—C2—C7 | 115.8 (5) | O6—C58—N12 | 120.6 (13) |
| C3—C2—C7 | 120.0 | O6—C58—H58 | 119.7 |
| C2—C3—C4 | 120.0 | N12—C58—H58 | 119.7 |
| C2—C3—H3A | 120.0 | N12—C59—H59A | 109.5 |
| C4—C3—H3A | 120.0 | N12—C59—H59B | 109.5 |
| C5—C4—C3 | 120.0 | H59A—C59—H59B | 109.5 |
| C5—C4—Br1 | 121.3 (3) | N12—C59—H59C | 109.5 |
| C3—C4—Br1 | 118.7 (3) | H59A—C59—H59C | 109.5 |
| C4—C5—C6 | 120.0 | H59B—C59—H59C | 109.5 |
| C4—C5—H5 | 120.0 | N12—C60—H60A | 109.5 |
| C6—C5—H5 | 120.0 | N12—C60—H60B | 109.5 |
| C5—C6—C7 | 120.0 | H60A—C60—H60B | 109.5 |
| C5—C6—C8 | 116.6 (5) | N12—C60—H60C | 109.5 |
| C7—C6—C8 | 123.3 (5) | H60A—C60—H60C | 109.5 |
| O2—C7—C6 | 123.2 (4) | H60B—C60—H60C | 109.5 |

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| O2—Zn1—S1—C9 | −80.2 (4) | C46—C47—C49—N10 | 179.3 (4) |
| N4—Zn1—S1—C9 | 95.2 (3) | N9—C47—C49—N10 | −3.0 (7) |
| N1—Zn1—S1—C9 | −7.9 (3) | C46—C47—C49—C50 | 1.7 (8) |
| N5—Zn1—S1—C9 | 174.3 (3) | N9—C47—C49—C50 | 179.4 (4) |
| O4—Zn2—S2—C36 | 77.1 (8) | N10—C49—C50—C51 | 0.0 |
| N6—Zn2—S2—C36 | 7.2 (5) | C47—C49—C50—C51 | 177.6 (7) |
| N9—Zn2—S2—C36 | −97.5 (4) | C49—C50—C51—C52 | 0.0 |
| N10—Zn2—S2—C36 | −176.2 (4) | C49—C50—C51—C54 | 176.8 (9) |
| N4—Zn1—O2—C7 | −75.8 (7) | C50—C51—C52—C53 | 0.0 |
| N1—Zn1—O2—C7 | 29.0 (7) | C54—C51—C52—C53 | −176.7 (9) |
| N5—Zn1—O2—C7 | −154.4 (7) | C51—C52—C53—N10 | 0.0 |
| S1—Zn1—O2—C7 | 99.7 (7) | C49—N10—C53—C52 | 0.0 |
| N6—Zn2—O4—C34 | −23.1 (10) | Zn2—N10—C53—C52 | 174.1 (5) |
| N9—Zn2—O4—C34 | 83.4 (10) | C1—O1—C2—C3 | 13.5 (13) |
| N10—Zn2—O4—C34 | 161.8 (10) | C1—O1—C2—C7 | −169.2 (8) |
| S2—Zn2—O4—C34 | −91.4 (12) | O1—C2—C3—C4 | 177.1 (8) |
| O2—Zn1—N1—C8 | −21.4 (8) | C7—C2—C3—C4 | 0.0 |
| N4—Zn1—N1—C8 | 81.7 (8) | C2—C3—C4—C5 | 0.0 |
| S1—Zn1—N1—C8 | −171.2 (8) | C2—C3—C4—Br1 | 178.8 (5) |
| O2—Zn1—N1—N2 | 159.4 (6) | C3—C4—C5—C6 | 0.0 |
| N4—Zn1—N1—N2 | −97.6 (6) | Br1—C4—C5—C6 | −178.8 (5) |
| S1—Zn1—N1—N2 | 9.5 (6) | C4—C5—C6—C7 | 0.0 |
| C8—N1—N2—C9 | 174.4 (9) | C4—C5—C6—C8 | −176.4 (7) |
| Zn1—N1—N2—C9 | −6.2 (9) | Zn1—O2—C7—C6 | −22.1 (9) |

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| O2—Zn1—N4—C16 | 88.1 (4) | Zn1—O2—C7—C2 | 158.2 (5) |
| N1—Zn1—N4—C16 | −3.1 (4) | C5—C6—C7—O2 | −179.7 (7) |
| N5—Zn1—N4—C16 | 179.3 (4) | C8—C6—C7—O2 | −3.5 (9) |
| S1—Zn1—N4—C16 | −89.4 (3) | C5—C6—C7—C2 | 0.0 |
| O2—Zn1—N4—C20 | −92.8 (3) | C8—C6—C7—C2 | 176.2 (7) |
| N1—Zn1—N4—C20 | 176.0 (3) | O1—C2—C7—O2 | 2.3 (8) |
| N5—Zn1—N4—C20 | −1.6 (3) | C3—C2—C7—O2 | 179.7 (7) |
| S1—Zn1—N4—C20 | 89.7 (3) | O1—C2—C7—C6 | −177.4 (8) |
| C20—N4—C16—C17 | 0.0 | C3—C2—C7—C6 | 0.0 |
| Zn1—N4—C16—C17 | 179.1 (4) | N2—N1—C8—C6 | −173.8 (8) |
| N4—C16—C17—C18 | 0.0 | Zn1—N1—C8—C6 | 6.9 (14) |
| C16—C17—C18—C19 | 0.0 | C5—C6—C8—N1 | −172.7 (9) |
| C16—C17—C18—C21 | −174.2 (9) | C7—C6—C8—N1 | 11.0 (13) |
| C17—C18—C19—C20 | 0.0 | N1—N2—C9—N3 | −178.5 (7) |
| C21—C18—C19—C20 | 174.1 (9) | N1—N2—C9—S1 | −3.7 (12) |
| C18—C19—C20—N4 | 0.0 | C10′—N3—C9—N2 | 15.3 (17) |
| C18—C19—C20—C22 | −178.4 (6) | C10—N3—C9—N2 | 19.6 (17) |
| C16—N4—C20—C19 | 0.0 | C10′—N3—C9—S1 | −160.3 (12) |
| Zn1—N4—C20—C19 | −179.2 (4) | C10—N3—C9—S1 | −156.0 (12) |
| C16—N4—C20—C22 | 178.5 (6) | Zn1—S1—C9—N2 | 9.6 (9) |
| Zn1—N4—C20—C22 | −0.7 (5) | Zn1—S1—C9—N3 | −175.2 (6) |
| O2—Zn1—N5—C22 | 106.4 (3) | C9—N3—C10—C11 | −175.4 (13) |
| N4—Zn1—N5—C22 | 3.7 (3) | C15—C10—C11—C12 | 0.0 |
| S1—Zn1—N5—C22 | −104.2 (3) | N3—C10—C11—C12 | −176.7 (17) |
| O2—Zn1—N5—C26 | −81.3 (4) | C10—C11—C12—C13 | 0.0 |
| N4—Zn1—N5—C26 | 176.0 (4) | C11—C12—C13—C14 | 0.0 |
| S1—Zn1—N5—C26 | 68.2 (3) | C12—C13—C14—C15 | 0.0 |
| C26—N5—C22—C23 | 0.0 | C13—C14—C15—C10 | 0.0 |
| Zn1—N5—C22—C23 | 172.8 (4) | C11—C10—C15—C14 | 0.0 |
| C26—N5—C22—C20 | −178.2 (5) | N3—C10—C15—C14 | 176.3 (19) |
| Zn1—N5—C22—C20 | −5.3 (5) | C9—N3—C10′—C11′ | 171.4 (12) |
| C19—C20—C22—C23 | 4.4 (6) | C15′—C10′—C11′—C12′ | 0.0 |
| N4—C20—C22—C23 | −174.0 (4) | N3—C10′—C11′—C12′ | −179.5 (17) |
| C19—C20—C22—N5 | −177.5 (3) | C10′—C11′—C12′—C13′ | 0.0 |
| N4—C20—C22—N5 | 4.1 (6) | C11′—C12′—C13′—C14′ | 0.0 |
| N5—C22—C23—C24 | 0.0 | C12′—C13′—C14′—C15′ | 0.0 |
| C20—C22—C23—C24 | 178.0 (6) | C13′—C14′—C15′—C10′ | 0.0 |
| C22—C23—C24—C25 | 0.0 | C11′—C10′—C15′—C14′ | 0.0 |
| C22—C23—C24—C27 | 179.9 (10) | N3—C10′—C15′—C14′ | 179.4 (18) |
| C23—C24—C25—C26 | 0.0 | C28—O3—C29—C30 | −12.1 (17) |
| C27—C24—C25—C26 | −179.9 (10) | C28—O3—C29—C34 | 168.7 (14) |
| C24—C25—C26—N5 | 0.0 | O3—C29—C30—C31 | −179.2 (9) |
| C22—N5—C26—C25 | 0.0 | C34—C29—C30—C31 | 0.0 |
| Zn1—N5—C26—C25 | −171.9 (4) | C29—C30—C31—C32 | 0.0 |
| O4—Zn2—N6—C35 | 23.3 (12) | C29—C30—C31—Br2 | −179.6 (6) |
| N9—Zn2—N6—C35 | −75.4 (11) | C30—C31—C32—C33 | 0.0 |
| S2—Zn2—N6—C35 | 176.5 (11) | Br2—C31—C32—C33 | 179.6 (6) |
| O4—Zn2—N6—N7 | −167.5 (10) | C31—C32—C33—C34 | 0.0 |

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| N9—Zn2—N6—N7 | 93.9 (9) | C31—C32—C33—C35 | 177.5 (9) |
| S2—Zn2—N6—N7 | −14.3 (9) | Zn2—O4—C34—C33 | 12.8 (14) |
| C35—N6—N7—C36 | −173.2 (11) | Zn2—O4—C34—C29 | −162.2 (7) |
| Zn2—N6—N7—C36 | 16.0 (13) | C32—C33—C34—O4 | −174.8 (10) |
| O4—Zn2—N9—C43 | −88.2 (5) | C35—C33—C34—O4 | 8.0 (12) |
| N6—Zn2—N9—C43 | 2.5 (5) | C32—C33—C34—C29 | 0.0 |
| N10—Zn2—N9—C43 | 179.8 (4) | C35—C33—C34—C29 | −177.1 (10) |
| S2—Zn2—N9—C43 | 89.2 (4) | O3—C29—C34—O4 | −5.5 (10) |
| O4—Zn2—N9—C47 | 97.4 (5) | C30—C29—C34—O4 | 175.2 (9) |
| N6—Zn2—N9—C47 | −171.9 (4) | O3—C29—C34—C33 | 179.2 (9) |
| N10—Zn2—N9—C47 | 5.4 (4) | C30—C29—C34—C33 | 0.0 |
| S2—Zn2—N9—C47 | −85.2 (4) | N7—N6—C35—C33 | 176.1 (10) |
| C47—N9—C43—C44 | 0.0 | Zn2—N6—C35—C33 | −13.5 (18) |
| Zn2—N9—C43—C44 | −174.1 (5) | C34—C33—C35—N6 | −6.9 (16) |
| N9—C43—C44—C45 | 0.0 | C32—C33—C35—N6 | 175.8 (10) |
| C43—C44—C45—C46 | 0.0 | C37—N8—C36—N7 | −24.5 (17) |
| C43—C44—C45—C48 | 179.1 (9) | C37—N8—C36—S2 | 160.5 (9) |
| C44—C45—C46—C47 | 0.0 | N6—N7—C36—N8 | 178.0 (9) |
| C48—C45—C46—C47 | −179.1 (8) | N6—N7—C36—S2 | −7.6 (15) |
| C45—C46—C47—N9 | 0.0 | Zn2—S2—C36—N8 | 172.4 (8) |
| C45—C46—C47—C49 | 177.6 (7) | Zn2—S2—C36—N7 | −2.1 (11) |
| C43—N9—C47—C46 | 0.0 | C36—N8—C37—C38 | −173.7 (10) |
| Zn2—N9—C47—C46 | 174.6 (4) | C36—N8—C37—C42 | 1.4 (15) |
| C43—N9—C47—C49 | −177.8 (6) | C42—C37—C38—C39 | 0.0 |
| Zn2—N9—C47—C49 | −3.2 (6) | N8—C37—C38—C39 | 175.2 (7) |
| O4—Zn2—N10—C49 | −105.2 (5) | C37—C38—C39—C40 | 0.0 |
| N9—Zn2—N10—C49 | −6.9 (4) | C38—C39—C40—C41 | 0.0 |
| S2—Zn2—N10—C49 | 102.3 (3) | C39—C40—C41—C42 | 0.0 |
| O4—Zn2—N10—C53 | 80.4 (5) | C40—C41—C42—C37 | 0.0 |
| N9—Zn2—N10—C53 | 178.7 (4) | C38—C37—C42—C41 | 0.0 |
| S2—Zn2—N10—C53 | −72.2 (4) | N8—C37—C42—C41 | −174.9 (8) |
| C53—N10—C49—C50 | 0.0 | C56—N11—C55—O5 | −0.1 (4) |
| Zn2—N10—C49—C50 | −174.8 (4) | C57—N11—C55—O5 | 179.4 (4) |
| C53—N10—C49—C47 | −177.8 (6) | C59—N12—C58—O6 | 0.0 (3) |
| Zn2—N10—C49—C47 | 7.5 (6) | C60—N12—C58—O6 | −179.8 (3) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H3···O5 | 0.88 | 2.07 | 2.95 (1) | 175 |
| N8—H8···O6 | 0.88 | 2.07 | 2.95 (1) | 172 |