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Bis[2-(2-pyridylmethylamino)ethanesulfonato-κ^3N,N',O]zinc(II)

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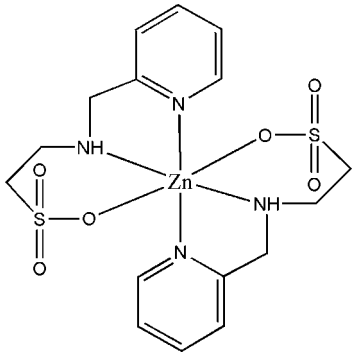
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.003 Å; R factor = 0.023; wR factor = 0.062; data-to-parameter ratio = 17.7.

The title mononuclear complex, $[Zn(C_8H_{11}N_2O_3S)_2]$, is a zinc salt of 2-(2-pyridylmethylamino)ethanesulfonic acid (Hpmt). The Zn^{II} ion is located on an inversion centre and is octahedrally surrounded by four N and two O atoms. The deprotonated pmt^- anion coordinates in a facial arrangement through its two N atoms and one of the sulfonate O atoms. The crystal packing is determined by intermolecular N—H···O and C—H···O hydrogen bonds.

Related literature

For the structures of the Co(II) and Ni(II) analogues, see: Li *et al.* (2008); Liao *et al.* (2007). For the preparation of the Hpmt ligand, see: Li *et al.* (2006).



Experimental

Crystal data

$[Zn(C_8H_{11}N_2O_3S)_2]$
M_r = 495.87
Monoclinic, $P2_1/c$
a = 9.6288 (13) Å
b = 10.0047 (13) Å
c = 11.3624 (15) Å
β = 105.965 (1)°
V = 1052.4 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.41 mm^{-1}
T = 291 K
0.50 × 0.39 × 0.29 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.540, T_{max} = 0.689
6318 measured reflections
2419 independent reflections
2221 reflections with $I > 2\sigma(I)$
R_{int} = 0.012

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.062
S = 1.07
2419 reflections
137 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N2	2.1336 (12)	Zn1—N1	2.2130 (13)
Zn1—O1	2.1465 (11)		
N2—Zn1—O1	92.40 (5)	O1—Zn1—N1^{i}	89.78 (5)
N2^{i}—Zn1—O1	87.60 (4)	N2—Zn1—N1	78.06 (5)
N2—Zn1—N1^{i}	101.93 (5)	O1—Zn1—N1	90.22 (5)

Symmetry code: (i) $-x+1, -y, -z+1$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H1*N*···O2^{ii}	0.855 (18)	2.079 (18)	2.9259 (17)	170.6 (16)
C1—H1···O2^{iii}	0.93	2.47	3.388 (2)	169
C4—H4···O3^{iv}	0.93	2.49	3.324 (2)	150
C6—H6*B*···O1^{i}	0.97	2.56	3.056 (2)	112
C8—H8*B*···O2^{v}	0.97	2.56	3.265 (2)	130

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

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: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2794).

References

Bruker (2004). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Li, J.-X., Jiang, Y.-M. & Li, H.-Y. (2006). *Acta Cryst.* E**62**, m2984–m2986.
Li, J.-X., Jiang, Y.-M. & Lian, B.-R. (2008). *J. Chem. Crystallogr.* **38**, 711–715.
Liao, B.-L., Li, J.-X. & Jiang, Y.-M. (2007). *Acta Cryst.* E**63**, m1974.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2009). E**65**, m706 [doi:10.1107/S1600536809019990]

Bis[2-(2-pyridylmethylamino)ethanesulfonato-κ^3N,N',O]zinc(II)

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S1. Comment

The complex (I) is isostructural with its analogues $[Co(C_8H_{11}N_2O_3S)_2]$ (Li *et al.*, 2006), $[Ni(C_8H_{11}N_2O_3S)_2]$ (Liao *et al.*, 2007) and $[Cu(C_8H_{11}N_2O_3S)_2].2H_2O$ (Li *et al.*, 2008), whose structures have been described in detail. The six-coordinate Zn^{II} ion locates on a centre of symmetry with two deprotonated pmt^- anions coordinate in a tridentate facial arrangement with its three donor atoms (Fig.1). The bond lengths and angles of (I) are in good agreement with its Co(II) and Ni(II) analogues (Table 1).

The N—H donor and S═O acceptor groups of the pmt ions are involved in hydrogen bonding interactions and forms a two-dimensional network in the *bc* plane (Table 2 and Fig. 2).

S2. Experimental

The ligand Hpmt was prepared according to the method of Li *et al.*, 2006. To the solution of Hpmt (2.0 mmol, 0.43 g) in water (25 ml), solid $ZnCl_2$ (1 mmol, 0.14 g) was added. The resulting mixture was stirred at 333 K for 5 h, then cooled to room temperature. After filtration, the filtrate was left to stand at room temperature for slow evaporation. Colourless block-shaped crystals suitable for X-ray diffraction were obtained in a yield of 42%. Analysis, found: C 38.66, H 4.37, N 11.32, S 12.95%; $C_{16}H_{22}N_4O_6S_2Zn$ requires: C 38.72, H 4.44, N 11.29, S 12.90%. IR (KBr, ν, cm^{-1}): 771.3 [γ(C=C—H)], 746.5(γCH_2); 1190.3, 1151.4, 1038.8(ν SO_3^-); 1607.2, 1572.3(ν C=C + ν C=N); 3198.2(ν N—H).

S3. Refinement

H atoms bonded to C were positioned geometrically with C—H distance of 0.93–0.97 Å, and treated as riding atoms, with U_{iso}(H) =1.2U_{eq}(C). The N—H hydrogen atom was located in a difference Fourier map and refined isotropically.

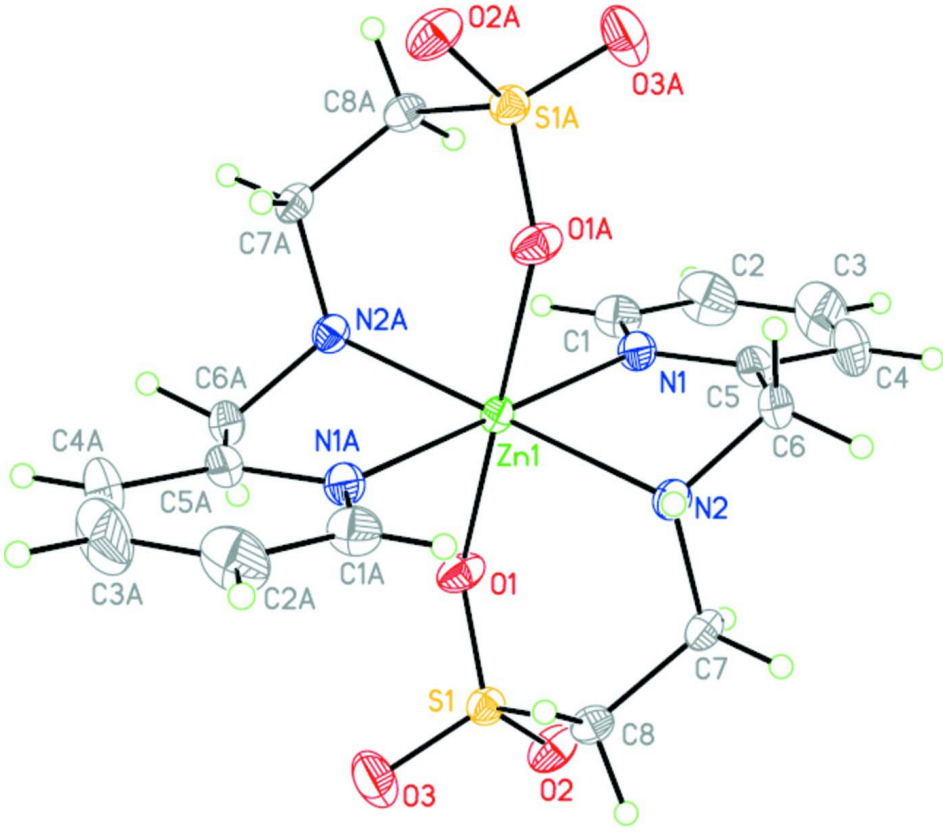

Figure 1

Molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level. Atoms with the suffix A are at the symmetry position (-*x*, -*y*, -*z*).

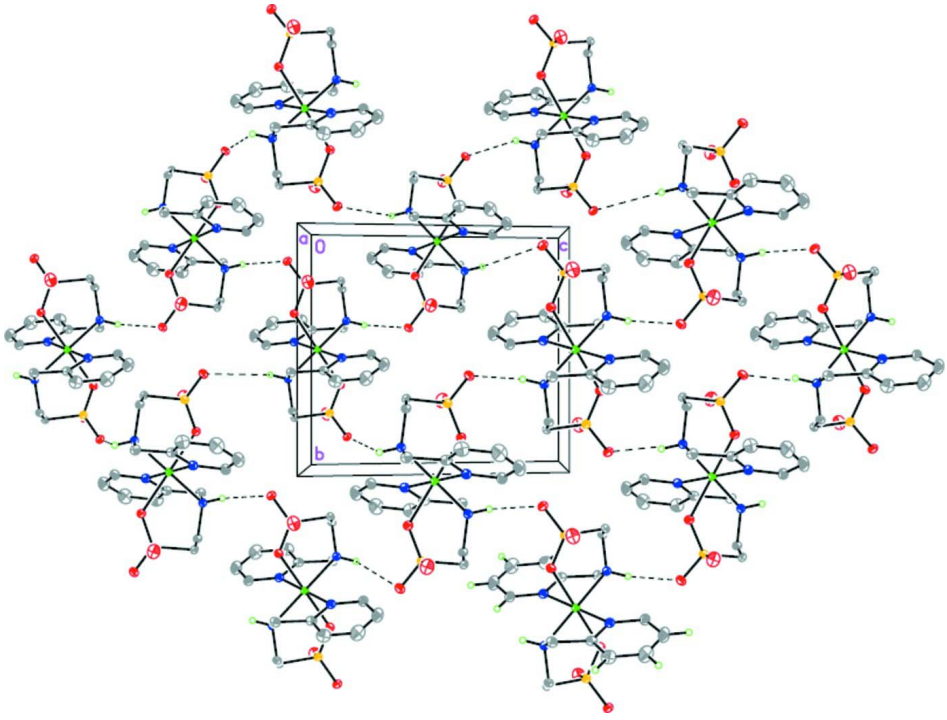

Figure 2

The hydrogen bonding interactions in (I) (dashed lines) projected in *bc* plane. H atoms on C atoms have been omitted.

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$M_r = 495.87$
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Hall symbol: -P 2ybc
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$b = 10.0047\ (13)$ Å
$c = 11.3624\ (15)$ Å
$\beta = 105.965\ (1)°$
$V = 1052.4\ (2)$ Å^3
$Z = 2$
$F(000) = 512$
$D_x = 1.565$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4168 reflections
$\theta = 2.8–28.2°$
$\mu = 1.41$ mm^{-1}
$T = 291$ K
Block, colourless
0.50 × 0.39 × 0.29 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.540$, $T_{max} = 0.689$
6318 measured reflections
2419 independent reflections
2221 reflections with $I > 2\sigma(I)$
$R_{int} = 0.012$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.8°$
$h = -11\rightarrow12$
$k = -9\rightarrow12$
$l = -14\rightarrow14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.062$
$S = 1.07$
2419 reflections
137 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0322P)^2 + 0.3355P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.38$ e Å^{-3}

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.5000	0.0000	0.5000	0.02437 (8)
S1	0.63235 (4)	0.29294 (4)	0.45567 (3)	0.02858 (10)
O1	0.57188 (13)	0.16226 (11)	0.40792 (10)	0.0375 (3)
O2	0.55332 (14)	0.40018 (12)	0.37950 (10)	0.0428 (3)
O3	0.78676 (14)	0.30037 (16)	0.47547 (13)	0.0573 (4)
N1	0.27433 (14)	0.03618 (13)	0.39160 (12)	0.0309 (3)
N2	0.42452 (13)	0.13247 (12)	0.61609 (11)	0.0274 (3)
C1	0.2143 (2)	0.02195 (18)	0.27020 (16)	0.0412 (4)
H1	0.2677	−0.0185	0.2232	0.049*
C2	0.0760 (2)	0.0655 (3)	0.2137 (2)	0.0633 (6)
H2	0.0370	0.0549	0.1297	0.076*
C3	−0.0031 (2)	0.1249 (3)	0.2834 (2)	0.0746 (7)
H3	−0.0961	0.1558	0.2468	0.090*
C4	0.05670 (19)	0.1385 (2)	0.4085 (2)	0.0584 (5)
H4	0.0044	0.1775	0.4571	0.070*
C5	0.19633 (16)	0.09248 (16)	0.45981 (15)	0.0350 (3)
C6	0.26892 (17)	0.10136 (17)	0.59524 (15)	0.0360 (3)
H6A	0.2233	0.1707	0.6313	0.043*
H6B	0.2584	0.0171	0.6342	0.043*
C7	0.44409 (17)	0.27835 (15)	0.59923 (13)	0.0303 (3)
H7A	0.4184	0.3273	0.6639	0.036*
H7B	0.3796	0.3066	0.5217	0.036*

C8	0.59850 (16)	0.31189 (15)	0.60131 (13)	0.0292 (3)
H8A	0.6637	0.2542	0.6599	0.035*
H8B	0.6190	0.4034	0.6287	0.035*
H1N	0.4634 (18)	0.1133 (17)	0.6913 (16)	0.032 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.02484 (13)	0.02218 (13)	0.02641 (12)	0.00349 (8)	0.00760 (9)	−0.00102 (8)
S1	0.03239 (19)	0.02599 (19)	0.02848 (17)	0.00050 (14)	0.01027 (14)	0.00143 (13)
O1	0.0591 (7)	0.0267 (6)	0.0308 (5)	−0.0037 (5)	0.0194 (5)	−0.0023 (4)
O2	0.0672 (8)	0.0301 (6)	0.0319 (5)	0.0094 (5)	0.0148 (5)	0.0068 (5)
O3	0.0353 (7)	0.0786 (11)	0.0625 (8)	−0.0049 (6)	0.0208 (6)	−0.0068 (7)
N1	0.0272 (6)	0.0305 (6)	0.0330 (6)	0.0024 (5)	0.0051 (5)	0.0010 (5)
N2	0.0307 (6)	0.0268 (6)	0.0253 (6)	0.0022 (5)	0.0087 (5)	0.0003 (5)
C1	0.0404 (9)	0.0424 (10)	0.0366 (8)	−0.0027 (7)	0.0035 (7)	0.0020 (7)
C2	0.0453 (11)	0.0799 (16)	0.0501 (11)	−0.0037 (11)	−0.0114 (9)	0.0067 (11)
C3	0.0310 (10)	0.097 (2)	0.0817 (16)	0.0137 (11)	−0.0080 (10)	0.0102 (15)
C4	0.0270 (8)	0.0691 (14)	0.0786 (14)	0.0112 (9)	0.0137 (9)	0.0001 (11)
C5	0.0259 (7)	0.0329 (8)	0.0474 (9)	0.0013 (6)	0.0118 (6)	0.0005 (7)
C6	0.0327 (8)	0.0387 (9)	0.0430 (8)	0.0013 (7)	0.0210 (7)	−0.0030 (7)
C7	0.0367 (8)	0.0245 (7)	0.0313 (7)	0.0042 (6)	0.0120 (6)	−0.0028 (6)
C8	0.0348 (7)	0.0268 (7)	0.0241 (6)	−0.0009 (6)	0.0048 (5)	−0.0029 (5)

Geometric parameters (Å, º)

Zn1—N2	2.1336 (12)	C1—H1	0.9300
Zn1—N2^{i}	2.1336 (12)	C2—C3	1.376 (4)
Zn1—O1	2.1465 (11)	C2—H2	0.9300
Zn1—O1^{i}	2.1465 (11)	C3—C4	1.386 (3)
Zn1—N1^{i}	2.2130 (13)	C3—H3	0.9300
Zn1—N1	2.2130 (13)	C4—C5	1.388 (2)
S1—O3	1.4431 (13)	C4—H4	0.9300
S1—O2	1.4549 (12)	C5—C6	1.508 (2)
S1—O1	1.4727 (11)	C6—H6A	0.9700
S1—C8	1.7825 (15)	C6—H6B	0.9700
N1—C5	1.342 (2)	C7—C8	1.518 (2)
N1—C1	1.349 (2)	C7—H7A	0.9700
N2—C6	1.4841 (19)	C7—H7B	0.9700
N2—C7	1.4908 (19)	C8—H8A	0.9700
N2—H1N	0.856 (17)	C8—H8B	0.9700
C1—C2	1.380 (3)		
N2—Zn1—N2^{i}	180.0	N1—C1—H1	119.0
N2—Zn1—O1	92.40 (5)	C2—C1—H1	119.0
N2^{i}—Zn1—O1	87.60 (4)	C3—C2—C1	118.96 (19)
N2—Zn1—O1^{i}	87.60 (5)	C3—C2—H2	120.5
N2^{i}—Zn1—O1^{i}	92.40 (5)	C1—C2—H2	120.5

O1—Zn1—O1^{i}	180.0	C2—C3—C4	119.55 (18)
N2—Zn1—N1^{i}	101.93 (5)	C2—C3—H3	120.2
N2^{i}—Zn1—N1^{i}	78.06 (5)	C4—C3—H3	120.2
O1—Zn1—N1^{i}	89.78 (5)	C3—C4—C5	118.7 (2)
O1^{i}—Zn1—N1^{i}	90.22 (5)	C3—C4—H4	120.7
N2—Zn1—N1	78.06 (5)	C5—C4—H4	120.7
N2^{i}—Zn1—N1	101.94 (5)	N1—C5—C4	121.82 (16)
O1—Zn1—N1	90.22 (5)	N1—C5—C6	115.98 (13)
O1^{i}—Zn1—N1	89.78 (5)	C4—C5—C6	122.19 (16)
N1^{i}—Zn1—N1	180.0	N2—C6—C5	109.85 (12)
O3—S1—O2	113.74 (9)	N2—C6—H6A	109.7
O3—S1—O1	112.90 (8)	C5—C6—H6A	109.7
O2—S1—O1	110.27 (7)	N2—C6—H6B	109.7
O3—S1—C8	107.06 (8)	C5—C6—H6B	109.7
O2—S1—C8	105.93 (7)	H6A—C6—H6B	108.2
O1—S1—C8	106.36 (7)	N2—C7—C8	111.86 (12)
S1—O1—Zn1	129.76 (6)	N2—C7—H7A	109.2
C5—N1—C1	118.96 (14)	C8—C7—H7A	109.2
C5—N1—Zn1	111.53 (10)	N2—C7—H7B	109.2
C1—N1—Zn1	129.14 (12)	C8—C7—H7B	109.2
C6—N2—C7	110.03 (12)	H7A—C7—H7B	107.9
C6—N2—Zn1	105.77 (9)	C7—C8—S1	112.98 (10)
C7—N2—Zn1	116.88 (9)	C7—C8—H8A	109.0
C6—N2—H1N	104.9 (12)	S1—C8—H8A	109.0
C7—N2—H1N	108.2 (12)	C7—C8—H8B	109.0
Zn1—N2—H1N	110.4 (11)	S1—C8—H8B	109.0
N1—C1—C2	122.03 (19)	H8A—C8—H8B	107.8

O3—S1—O1—Zn1	103.94 (10)	N1—Zn1—N2—C7	−90.09 (10)
O2—S1—O1—Zn1	−127.61 (9)	C5—N1—C1—C2	1.1 (3)
C8—S1—O1—Zn1	−13.19 (11)	Zn1—N1—C1—C2	−171.19 (16)
N2—Zn1—O1—S1	33.74 (10)	N1—C1—C2—C3	−0.2 (3)
N2^{i}—Zn1—O1—S1	−146.26 (10)	C1—C2—C3—C4	−0.7 (4)
N1^{i}—Zn1—O1—S1	−68.19 (10)	C2—C3—C4—C5	0.7 (4)
N1—Zn1—O1—S1	111.81 (10)	C1—N1—C5—C4	−1.1 (3)
N2—Zn1—N1—C5	−14.41 (11)	Zn1—N1—C5—C4	172.45 (15)
N2^{i}—Zn1—N1—C5	165.59 (11)	C1—N1—C5—C6	178.25 (15)
O1—Zn1—N1—C5	−106.82 (11)	Zn1—N1—C5—C6	−8.16 (17)
O1^{i}—Zn1—N1—C5	73.18 (11)	C3—C4—C5—N1	0.3 (3)
N2—Zn1—N1—C1	158.35 (15)	C3—C4—C5—C6	−179.1 (2)
N2^{i}—Zn1—N1—C1	−21.65 (15)	C7—N2—C6—C5	80.21 (15)
O1—Zn1—N1—C1	65.94 (14)	Zn1—N2—C6—C5	−46.87 (14)
O1^{i}—Zn1—N1—C1	−114.06 (14)	N1—C5—C6—N2	37.7 (2)
O1—Zn1—N2—C6	122.46 (10)	C4—C5—C6—N2	−142.93 (17)
O1^{i}—Zn1—N2—C6	−57.54 (10)	C6—N2—C7—C8	−171.67 (11)
N1^{i}—Zn1—N2—C6	−147.26 (9)	Zn1—N2—C7—C8	−51.08 (14)
N1—Zn1—N2—C6	32.74 (9)	N2—C7—C8—S1	85.42 (13)
O1—Zn1—N2—C7	−0.37 (10)	O3—S1—C8—C7	−168.32 (11)

O1^{i}—Zn1—N2—C7	179.63 (10)	O2—S1—C8—C7	69.97 (12)
N1^{i}—Zn1—N2—C7	89.91 (10)	O1—S1—C8—C7	−47.37 (12)

Symmetry code: (i) −*x*+1, −*y*, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H1*N*···O2^{ii}	0.855 (18)	2.079 (18)	2.9259 (17)	170.6 (16)
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C6—H6*B*···O1^{i}	0.97	2.56	3.056 (2)	112
C8—H8*B*···O2^{v}	0.97	2.56	3.265 (2)	130

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) *x*, −*y*+1/2, *z*+1/2; (iii) −*x*+1, *y*−1/2, −*z*+1/2; (iv) *x*−1, *y*, *z*; (v) −*x*+1, −*y*+1, −*z*+1.