



Synthesis, crystal structure and Hirshfeld surface analysis of a zinc(II) coordination polymer of 5-phenyl-1,3,4-oxadiazole-2-thiolate

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Received 15 June 2022

Accepted 6 July 2022

Edited by G. Díaz de Delgado, Universidad de Los Andes, Venezuela

Keywords: crystal structure; zinc complex; 5-phenyl-1,3,4-oxadiazole-2-thiol; coordination polymer; Hirshfeld surface analysis.

CCDC reference: 2184492

Supporting information: this article has supporting information at journals.iucr.org/e

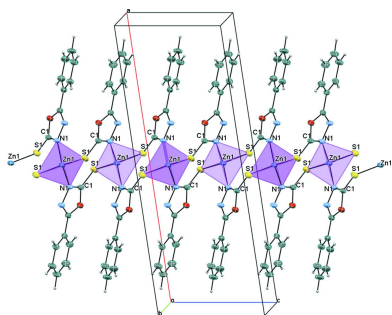
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A new zinc coordination polymer with 5-phenyl-1,3,4-oxadiazole-2-thiolate, namely, *catena*-poly[zinc(II)-bis(μ_2 -5-phenyl-1,3,4-oxadiazole-2-thiolato)- $\kappa^2N^3:S;\kappa^2S:N^3$], [Zn(C₈H₅N₂OS)₂]_n, was synthesized. The single-crystal X-ray diffraction analysis shows that the polymeric structure crystallizes in the centrosymmetric monoclinic *C2/c* space group. The Zn^{II} atom is coordinated to two S and two N atoms from four crystallographically independent (*L*) ligands, forming zigzag chains along the [001] direction. This polymer complex forms an eight-membered [Zn–S–C–N–Zn–S–C–N] chair-like ring with two Zn^{II} atoms and two ligand molecules. On the Hirshfeld surface, the largest contributions come from the short contacts such as van der Waals forces, including H···H, C···H and S···H. Interactions including N···H, O···H and C···C contacts were also observed; however, their contribution to the overall stability of the crystal lattice is minor.

1. Chemical context

Among heterocyclic organic compounds, 1,3,4-oxadiazoles have become an important class of heterocycles because of their broad spectrum of biological activity (De Oliveira *et al.*, 2012; Vaidya *et al.*, 2020). Scientists have identified many properties of 1,3,4-oxadiazole derivatives, such as antimicrobial (Bala *et al.*, 2014; Zachariah *et al.*, 2015; Ahmed *et al.*, 2017; Razzoqova *et al.*, 2019), antituberculosis (Makane *et al.*, 2019; Wang *et al.*, 2022), anticancer (Alam, 2022; Vaidya *et al.*, 2020; Zhang *et al.*, 2005), anti-inflammatory (Abd-Ellah *et al.*, 2017), analgesic (Husain & Ajmal, 2009), herbicidal (Sun *et al.*, 2014; Duan *et al.*, 2011) and antifungal (Zhang *et al.*, 2013; Capoci *et al.*, 2019) activities. Heterocyclic thiones are an important type of compound in coordination chemistry because of their potential multifunctional donor sites, namely either exocyclic sulfur or endocyclic nitrogen (Reddy *et al.*, 2011; Wang *et al.*, 2010). The presence of the 1,3,4-oxadiazole ring affects the physicochemical and pharmacokinetic properties of the entire compound. An exciting feature of these metal complexes is that they can be mononuclear (Singh *et al.*, 2008; Ouilia *et al.*, 2012), binuclear (Xiao *et al.*, 2011; Wang *et al.*, 2007) and/or polymeric (Beghidja *et al.*, 2007).

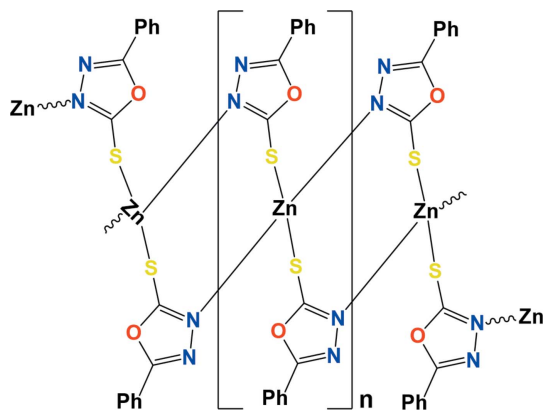
Oxadiazole ligands are ideal objects for creating new coordination compounds with great potential in various fields. Scientists have written extensive literature on the biological properties of oxadiazole-based complex compounds,



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especially on their anticancer effects. In addition to these, in the field of electrical engineering, metal complexes bearing oxadiazole ligands have been used as emitting particles in light-emitting diodes. The introduction of various functionalized oxadiazole ligands makes it easy to control the emission color, thermal stability, and film-forming properties of such complexes (Salassa & Terenzi, 2019).



Herein, we report on the synthesis and crystal structure of a new polymeric complex, $[\text{ZnL}_2]_n$, with $L = 5\text{-phenyl-1,3,4-oxadiazole-2-thiol}$.

2. Structural commentary

The single crystal X-ray structure of 5-phenyl-1,3,4-oxadiazole-2-thiolate Zn^{II} shows a polymeric structure that crystallizes in the centrosymmetric monoclinic space group $C2/c$ (Table 2). As seen in Fig. 1, its asymmetric unit contains half a zinc atom and one ligand anion. The central Zn^{II} atom has a distorted tetrahedral environment comprising two sulfur and two nitrogen atoms. It is coordinated by four crystallographically independent (L) ligands, forming zigzag chains along the $[001]$ direction, which are linked by two sulfur atoms and two nitrogen atoms of four ligands. The Zn1-S1 and Zn1-N1 bond lengths are 2.3370 (5) Å, 2.0184 (14) Å, respectively. In this case, the bond angles of the atom forming the tetrahedral polyhedron are slightly different from the angles of the ideal tetrahedron [$\text{N1-Zn1-N1} = 111.37$ (9)°,

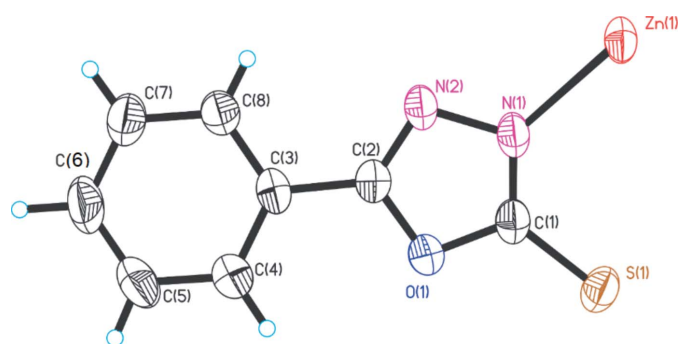


Figure 1
The molecular structure of $[\text{Zn}_{0.5}\text{L}]$ with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are displayed as small spheres of arbitrary radii.

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

$D\text{-H}\cdots A$	$D\text{-H}$	$\text{H}\cdots A$	$D\cdots A$	$D\text{-H}\cdots A$
$\text{C6-H6}\cdots\text{S1}^i$	1.00 (3)	2.86 (3)	3.608 (2)	132 (2)

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

$\text{S1-Zn1-S1} = 100.46$ (3)° and $\text{N1-Zn1-S1} = 108.51$ (4)°]. It is known from the literature (Razzoqova *et al.*, 2019) that the sulfur atom in the 1,3,4-oxadiazole-2-thione molecule is attached to the ring by a double bond. In this polymer complex synthesized based on Zn^{II} ion, the oxadiazole derivative transforms into the thiol tautomeric form and binds to the Zn ion. The N1 atom in the ligand molecule, on the other hand, forms a bond with another Zn^{II} ion due to its high electron-donating property, resulting in an eight-membered $[\text{Zn-S-C-N-Zn-S-C-N}]$ chair-like ring with two Zn^{II} atoms and two ligand molecules (Fig. 2). The dihedral angle between the mean planes of the phenyl (C3-C8) and oxadiazole (C1/O1/C2/N2/N1) rings of the ligand molecule is 13.42 (8)°. The conformation of the oxadiazole-thiol fragment of the ligand is approximately planar (r.m.s. deviation 0.006 Å), with a maximum deviation from the least-squares plane of 0.009 (1) Å for atom O1. The dihedral angle between the planes of the two neighboring independent oxadiazole-thiol (C1/O1/C2/N2/N1/S1) fragments is 64.10 (9)°.

3. Supramolecular features

The $[(\text{ZnL}_2)_n]$ unit is given as a monomer of the polymeric chain that extends parallel to the c -axis. Along the polymeric chain, the hydrophilic groups are concentrated within the core of the chain while the phenyl rings project approximately normal to the chain. Neighboring chains across the ab plane are loosely connected *via* a rather weak $\text{C6-H6}\cdots\text{S1}$ hydrogen bond (Table 1, Fig. 3).

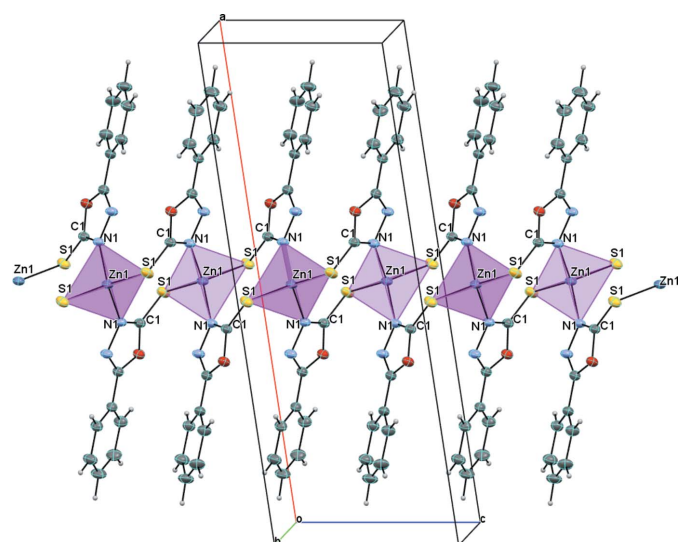


Figure 2
The view of the molecular packing showing the polymeric chain extended along the c -axis.

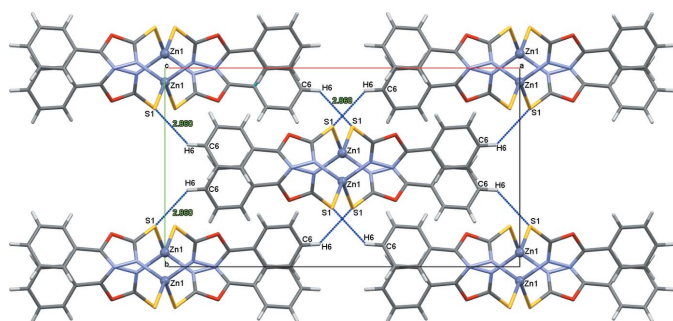


Figure 3
Crystal packing of the polymeric chains in the $[(ZnL_2)_n]$ structure. The projection is along the $[001]$ direction. Hydrogen bonds are shown by cyan lines.

4. Hirshfeld surface analysis

To further investigate the intermolecular interactions present in the title compound, a Hirshfeld surface analysis was performed, and the two-dimensional fingerprint plots were generated with *CrystalExplorer17* (Turner *et al.*, 2017). The Hirshfeld surface mapped over d_{norm} and corresponding colors representing various interactions are shown in Fig. 4. We chose the ZnL_2 molecular fragment as the monomer unit for calculating the Hirshfeld surface of this polymer complex.

The large red areas on the Hirshfeld surface correspond to the $Zn \cdots N$ interactions. The two-dimensional (2D) fingerprint plots (McKinnon *et al.*, 2007) are shown in Fig. 5. On the Hirshfeld surface, the largest contributions (19.2%, 19.5% and 19%) come from short contacts such as van der Waals forces, $H \cdots H$, $C \cdots H$ and $S \cdots H$ contacts. $N \cdots H$ (8.1%), $O \cdots H$ (8%) and $C \cdots C$ (4.7%) contacts are also observed. These interactions play a crucial role in the overall stabilization of the crystal packing.

5. Database survey

A survey of the Cambridge Structural Database (CSD, version 5.43, update of November 2021; Groom *et al.*, 2016) revealed that crystal structures had been reported for complexes of 1,3,4-oxadiazole derivatives and a number of metal ions, including zinc, copper, nickel, manganese, cadmium, cobalt and silver. No polymer complexes containing $[M-S-C-N-M-S-C-N]$ eight-membered cyclization have been reported. The

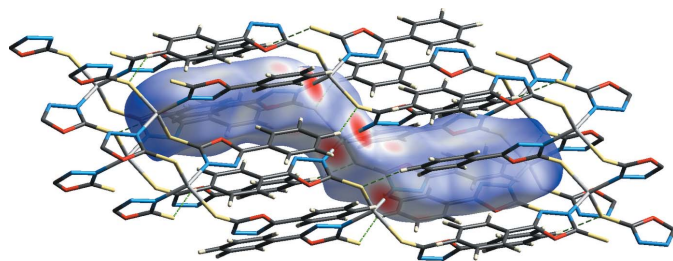


Figure 4
Hirshfeld surfaces mapped over d_{norm} calculated for the monomer part of the polymer molecule.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Zn(C_8H_5N_2OS)_2]$
M_r	419.79
Crystal system, space group	Monoclinic, $C2/c$
Temperature (K)	293
a, b, c (Å)	20.4223 (3), 11.3260 (2), 7.4019 (1)
β (°)	98.310 (1)
V (Å ³)	1694.11 (5)
Z	4
Radiation type	Cu $K\alpha$
μ (mm ⁻¹)	4.48
Crystal size (mm)	0.60 × 0.14 × 0.08
Data collection	
Diffractometer	XtaLAB Synergy, single source at home/near, HyPix3000
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Rigaku OD, 2020)
T_{min}, T_{max}	0.099, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7033, 1634, 1536
R_{int}	0.028
$(\sin \theta/\lambda)_{max}$ (Å ⁻¹)	0.615
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.026, 0.073, 1.09
No. of reflections	1634
No. of parameters	134
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å ⁻³)	0.26, -0.33

Computer programs: *CrysAlis PRO* (Rigaku OD, 2020), *SHELXT2014/5* (Sheldrick, 2015a), *SHELXL2016/6* (Sheldrick, 2015b) and *OLEX2* (Dolomanov *et al.*, 2009).

structures of complexes of Pt, Sn and Au based on 5-phenyl-1,3,4-oxadiazole-2-thiole with additional ligands have been deposited in the CSD (FATNIZ, Al-Jibori *et al.*, 2012; HAXTAC, Ma *et al.*, 2005; and YIVVEG, Chaves *et al.*, 2014). However, no complexes containing only the zinc ion and 5-phenyl-1,3,4-oxadiazole-2-thiolate have been documented in the CSD.

6. Synthesis and crystallization

$ZnCl_2$ (0.136 g, 0.001 mol) and 5-phenyl-1,3,4-oxadiazole-2-thiol (ligand) (0.354 g, 0.002 mol) were dissolved separately in ethanol (10 mL). To a solution of the ligand, an aqueous

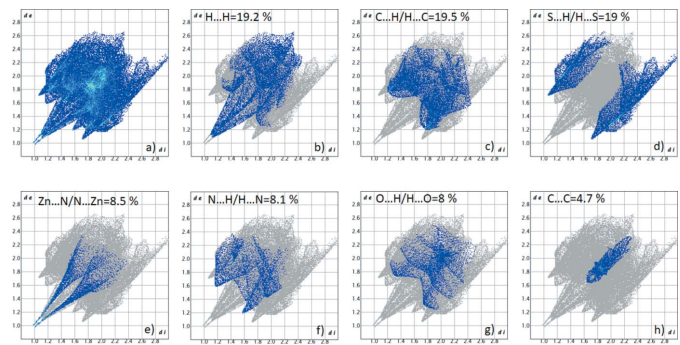


Figure 5
Contributions of the various contacts to the fingerprint plot built using the Hirshfeld surface of the title compound.

solution of KOH (0.112 g, 0.002 mol) was added. The obtained solutions were mixed together and stirred at 323 K for 20 min. A white precipitate was obtained. The precipitate was filtered and allowed to dry. The solid residue was dissolved in DMF to crystallize for the single crystal X-ray diffraction studies. X-ray quality single crystals were produced after 10 days by slow evaporation of the solution.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All the hydrogen atoms were located in difference-Fourier maps and refined isotropically.

Funding information

This work was supported by Uzbekistan Ministry of Innovation Development.

References

- Abd-Allah, H. S., Abdel-Aziz, M., Shoman, M. E., Beshr, E. A. M., Kaoud, T. S. & Ahmed, A. F. F. (2017). *Bioorg. Chem.* **74**, 15–29.
- Ahmed, M. N., Yasin, K. A., Hameed, S., Ayub, K., Haq, I., Tahir, M. N. & Mahmood, T. (2017). *J. Mol. Struct.* **1129**, 50–59.
- Alam, M. M. (2022). *Biointerface Res. Appl. Chem.* **12**, 5727–5744.
- Al-Jibori, S. A., Khaleel, T. F., Ahmed, S. A. O., Al-Hayaly, L. J., Merzweiler, K., Wagner, C. & Hogarth, G. (2012). *Polyhedron*, **41**, 20–24.
- Bala, S., Kamboj, S., Kajal, A., Saini, V. & Prasad, D. N. (2014). *BioMed Res. Int.* 172791.
- Beghidja, C., Rogez, G. & Welter, R. (2007). *New J. Chem.* **31**, 1403–1406.
- Capoci, I. R. G., Sakita, K. M., Faria, D. R., Rodrigues-Vendramini, F. A. V., Arita, G. S., de Oliveira, A. G. & Svidzinski, T. I. E. (2019). *Front. Microbiol.* **10**, 1–11.
- Chaves, J. D. S., Neumann, F., Francisco, T. M., Corrêa, C. C., Lopes, M. T. P., Silva, H., Fontes, A. P. S. & de Almeida, M. V. (2014). *Inorg. Chim. Acta*, **414**, 85–90.
- Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
- Duan, W.-G., Li, X.-R., Mo, Q.-J., Huang, J.-X., Cen, B., Xu, X.-T. & Lei, F.-H. (2011). *Holzforchung*, **65**, 191–197.
- Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* **B72**, 171–179.
- Husain, A. & Ajmal, M. (2009). *Acta Pharm.* **59**, 223–233.
- Ma, C.-L., Tian, G.-R. & Zhang, R.-F. (2005). *Polyhedron*, **24**, 1773–1780.
- Makane, V. B., Krishna, V. S., Krishna, E. V., Shukla, M., Mahizhaveni, B., Misra, S., Chopra, S., Sriram, D., Azger Dusthacker, V. N. & Rode, H. B. (2019). *Future Med. Chem.* **11**, 499–510.
- McKinnon, J. J., Jayatilaka, D. & Spackman, M. A. (2007). *Chem. Commun.* pp. 3814–3816.
- Oliveira, C. S. de, Lira, B. F., Barbosa-Filho, J. M., Lorenzo, J. G. F. & de Athayde-Filho, P. F. (2012). *Molecules*, **17**, 10192–10231.
- Ouilia, S., Beghidja, C., Beghidja, A. & Michaud, F. (2012). *Acta Cryst.* **E68**, m943.
- Razzoqova, S. R., Kadirova, S., Ashurov, J. M., Rakhmonova, D. S., Ziyayev, A. & Parpiev, N. A. (2019). *IUCrData*, **4**, x191532.
- Reddy, M. A., Malleshm, G., Thomas, A., Srinivas, K., Rao, V. J., Bhanuprakash, K., Giribabu, L., Grover, R., Kumar, A., Kamalasanan, M. N. & Srivastava, R. (2011). *Synth. Met.* **161**, 869–880.
- Rigaku OD (2020). *CrysAlis PRO*. Rigaku Oxford Diffraction, Yarnton, England.
- Salassa, G. & Terenzi, A. (2019). *Int. J. Mol. Sci.* **20**, 3483.
- Sheldrick, G. M. (2015a). *Acta Cryst.* **A71**, 3–8.
- Sheldrick, G. M. (2015b). *Acta Cryst.* **C71**, 3–8.
- Singh, M., Butcher, R. J. & Singh, N. K. (2008). *Polyhedron*, **27**, 3151–3159.
- Sun, G.-X., Yang, M.-Y., Sun, Z.-H., Wu, H.-K., Liu, X.-H. & Wei, Y.-Y. (2014). *Phosphorus Sulfur Silicon*, **189**, 1895–1900.
- Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Spackman, P. R., Jayatilaka, D. & Spackman, M. A. (2017). *CrystalExplorer17*. University of Western Australia. <http://Hirshfeldsurface.net>
- Vaidya, A., Pathak, D. & Shah, K. (2020). *Chem. Biol. Drug Des.* **97**, 572–591.
- Wang, A., Xu, S., Chai, Y., Xia, G., Wang, B., Lv, K., Wang, D., Qin, X., Jiang, B., Wu, W., Liu, M. & Lu, Y. (2022). *Bioorg. Med. Chem.* **53**, 116529.
- Wang, Y.-T., Tang, G.-M. & Qiang, Z.-W. (2007). *Polyhedron*, **26**, 4542–4550.
- Wang, Y. T., Wan, W. Z., Tang, G. M., Qiang, Z. W. & Li, T. D. J. (2010). *J. Coord. Chem.* **63**, 206–213.
- Xiao, J., Ma, J.-P., Huang, R.-Q. & Dong, Y.-B. (2011). *Acta Cryst.* **C67**, m90–m92.
- Zachariah, S. M., Ramkumar, M., George, N. & Ashif, M. S. (2015). *Res. J. Pharm. Biol. Chem. Sci.* **6**, 205–219.
- Zhang, H.-Z., Kasibhatla, S., Kueimmerle, J., Kemnitzer, W., Ollis-Mason, K., Qiu, L., Crogan-Grundy, C., Tseng, B., Drewe, J. & Cai, S. X. (2005). *J. Med. Chem.* **48**, 5215–5223.
- Zhang, M.-Z., Mulholland, N., Beattie, D., Irwin, D., Gu, Y.-C., Chen, Q., Yang, G. F. & Clough, J. (2013). *Eur. J. Med. Chem.* **63**, 22–32.

supporting information

Acta Cryst. (2022). E78, 794-797 [https://doi.org/10.1107/S2056989022006922]

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Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2020); cell refinement: *CrysAlis PRO* (Rigaku OD, 2020); data reduction: *CrysAlis PRO* (Rigaku OD, 2020); program(s) used to solve structure: *SHELXT2014/5* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2016/6* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

catena-Poly[zinc(II)-bis(μ_2 -5-phenyl-1,3,4-oxadiazole-2-thiolato)- $\kappa^2N^3:S;\kappa^2S:N^3$]

Crystal data

[Zn(C₈H₅N₂OS)₂]
 $M_r = 419.79$
 Monoclinic, *C2/c*
 $a = 20.4223$ (3) Å
 $b = 11.3260$ (2) Å
 $c = 7.4019$ (1) Å
 $\beta = 98.310$ (1)°
 $V = 1694.11$ (5) Å³
 $Z = 4$

$F(000) = 848$
 $D_x = 1.646$ Mg m⁻³
 Cu *K* α radiation, $\lambda = 1.54184$ Å
 Cell parameters from 5128 reflections
 $\theta = 4.4\text{--}71.1^\circ$
 $\mu = 4.48$ mm⁻¹
 $T = 293$ K
 Block, colourless
 $0.60 \times 0.14 \times 0.08$ mm

Data collection

XtaLAB Synergy, single source at home/near,
 HyPix3000
 diffractometer
 Radiation source: micro-focus sealed X-ray
 tube, PhotonJet (Cu) X-ray Source
 Mirror monochromator
 Detector resolution: 10.0000 pixels mm⁻¹
 ω scans
 Absorption correction: multi-scan
 (CrysAlisPro; Rigaku OD, 2020)

$T_{\min} = 0.099$, $T_{\max} = 1.000$
 7033 measured reflections
 1634 independent reflections
 1536 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.028$
 $\theta_{\max} = 71.5^\circ$, $\theta_{\min} = 4.4^\circ$
 $h = -25 \rightarrow 23$
 $k = -13 \rightarrow 13$
 $l = -9 \rightarrow 8$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.026$
 $wR(F^2) = 0.073$
 $S = 1.09$
 1634 reflections

134 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods
 Hydrogen site location: difference Fourier map
 All H-atom parameters refined

$$w = 1/[\sigma^2(F_o^2) + (0.0425P)^2 + 0.6399P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$

$$\Delta\rho_{\max} = 0.26 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.33 \text{ e } \text{\AA}^{-3}$$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.500000	0.42861 (3)	0.750000	0.03700 (13)
S1	0.52858 (2)	0.70338 (4)	0.49120 (6)	0.04489 (15)
O1	0.64980 (6)	0.66497 (11)	0.66937 (16)	0.0378 (3)
N1	0.57974 (7)	0.52907 (14)	0.7241 (2)	0.0381 (3)
N2	0.64167 (7)	0.49941 (14)	0.8226 (2)	0.0402 (3)
C2	0.68103 (8)	0.58151 (15)	0.7854 (2)	0.0360 (4)
C3	0.75171 (8)	0.59280 (16)	0.8505 (2)	0.0370 (4)
C1	0.58617 (8)	0.62555 (15)	0.6334 (2)	0.0362 (4)
C8	0.78515 (9)	0.49670 (18)	0.9351 (3)	0.0442 (4)
C4	0.78562 (10)	0.69688 (18)	0.8287 (3)	0.0472 (4)
C7	0.85194 (10)	0.5044 (2)	0.9992 (3)	0.0572 (5)
C5	0.85239 (11)	0.7043 (2)	0.8940 (3)	0.0578 (5)
C6	0.88524 (10)	0.6091 (2)	0.9798 (3)	0.0613 (6)
H8	0.7634 (11)	0.4299 (18)	0.946 (3)	0.042 (6)*
H5	0.8723 (13)	0.772 (3)	0.874 (3)	0.068 (7)*
H4	0.7642 (12)	0.761 (2)	0.771 (3)	0.059 (7)*
H7	0.8758 (14)	0.443 (2)	1.056 (4)	0.074 (8)*
H6	0.9339 (15)	0.614 (3)	1.020 (4)	0.088 (9)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.02217 (18)	0.0460 (2)	0.0416 (2)	0.000	0.00048 (13)	0.000
S1	0.0363 (3)	0.0440 (3)	0.0508 (3)	0.00848 (17)	-0.00577 (19)	-0.00479 (18)
O1	0.0309 (6)	0.0384 (6)	0.0423 (6)	-0.0034 (5)	-0.0009 (5)	0.0004 (5)
N1	0.0228 (7)	0.0461 (8)	0.0440 (8)	-0.0019 (6)	0.0001 (6)	0.0003 (6)
N2	0.0243 (7)	0.0483 (8)	0.0462 (8)	-0.0030 (6)	-0.0012 (6)	0.0056 (6)
C2	0.0291 (8)	0.0410 (9)	0.0368 (8)	-0.0004 (6)	0.0010 (7)	-0.0010 (6)
C3	0.0276 (8)	0.0468 (9)	0.0359 (8)	-0.0050 (7)	0.0019 (6)	-0.0033 (7)
C1	0.0273 (8)	0.0418 (9)	0.0386 (8)	0.0008 (7)	0.0013 (6)	-0.0070 (7)
C8	0.0357 (9)	0.0498 (11)	0.0459 (9)	-0.0059 (8)	0.0012 (7)	0.0053 (8)
C4	0.0380 (10)	0.0446 (10)	0.0578 (11)	-0.0048 (8)	0.0027 (8)	0.0008 (9)
C7	0.0363 (10)	0.0697 (14)	0.0620 (12)	0.0004 (10)	-0.0044 (9)	0.0124 (11)
C5	0.0393 (11)	0.0591 (13)	0.0741 (14)	-0.0179 (9)	0.0052 (10)	-0.0027 (11)
C6	0.0288 (10)	0.0797 (15)	0.0722 (14)	-0.0108 (10)	-0.0035 (9)	0.0046 (12)

Geometric parameters (Å, °)

Zn1—S1 ⁱ	2.3370 (5)	C3—C8	1.385 (3)
Zn1—S1 ⁱⁱ	2.3370 (5)	C3—C4	1.388 (3)
Zn1—N1	2.0184 (14)	C8—C7	1.381 (3)
Zn1—N1 ⁱⁱⁱ	2.0184 (14)	C8—H8	0.89 (2)
S1—C1	1.7059 (17)	C4—C5	1.382 (3)
O1—C2	1.371 (2)	C4—H4	0.92 (3)
O1—C1	1.3635 (19)	C7—C6	1.384 (3)
N1—N2	1.4062 (18)	C7—H7	0.92 (3)
N1—C1	1.299 (2)	C5—C6	1.376 (4)
N2—C2	1.285 (2)	C5—H5	0.89 (3)
C2—C3	1.460 (2)	C6—H6	1.00 (3)
S1 ⁱ —Zn1—S1 ⁱⁱ	100.46 (3)	O1—C1—S1	120.26 (13)
N1—Zn1—S1 ⁱⁱ	108.51 (4)	N1—C1—S1	129.90 (13)
N1—Zn1—S1 ⁱ	113.82 (4)	N1—C1—O1	109.83 (14)
N1 ⁱⁱⁱ —Zn1—S1 ⁱ	108.50 (4)	C3—C8—H8	119.3 (14)
N1 ⁱⁱⁱ —Zn1—S1 ⁱⁱ	113.82 (5)	C7—C8—C3	120.24 (19)
N1—Zn1—N1 ⁱⁱⁱ	111.37 (9)	C7—C8—H8	120.5 (14)
C1—S1—Zn1 ⁱ	102.39 (6)	C3—C4—H4	120.8 (16)
C1—O1—C2	103.92 (13)	C5—C4—C3	119.6 (2)
N2—N1—Zn1	119.57 (11)	C5—C4—H4	119.6 (16)
C1—N1—Zn1	131.80 (12)	C8—C7—C6	119.6 (2)
C1—N1—N2	108.57 (13)	C8—C7—H7	122.8 (17)
C2—N2—N1	105.05 (14)	C6—C7—H7	117.6 (17)
O1—C2—C3	119.65 (15)	C4—C5—H5	116.4 (17)
N2—C2—O1	112.61 (14)	C6—C5—C4	120.3 (2)
N2—C2—C3	127.75 (16)	C6—C5—H5	123.3 (17)
C8—C3—C2	118.67 (16)	C7—C6—H6	119.8 (18)
C8—C3—C4	119.85 (17)	C5—C6—C7	120.33 (19)
C4—C3—C2	121.48 (17)	C5—C6—H6	119.8 (18)
Zn1 ⁱ —S1—C1—O1	116.48 (12)	C2—O1—C1—S1	-179.75 (12)
Zn1 ⁱ —S1—C1—N1	-65.24 (17)	C2—O1—C1—N1	1.66 (18)
Zn1—N1—N2—C2	-176.89 (12)	C2—C3—C8—C7	-179.66 (19)
Zn1—N1—C1—S1	-2.7 (3)	C2—C3—C4—C5	179.34 (19)
Zn1—N1—C1—O1	175.68 (11)	C3—C8—C7—C6	0.5 (3)
O1—C2—C3—C8	-166.60 (16)	C3—C4—C5—C6	0.2 (3)
O1—C2—C3—C4	13.2 (3)	C1—O1—C2—N2	-1.25 (19)
N1—N2—C2—O1	0.4 (2)	C1—O1—C2—C3	178.37 (15)
N1—N2—C2—C3	-179.19 (17)	C1—N1—N2—C2	0.68 (19)
N2—N1—C1—S1	-179.91 (13)	C8—C3—C4—C5	-0.9 (3)
N2—N1—C1—O1	-1.49 (19)	C8—C7—C6—C5	-1.2 (4)
N2—C2—C3—C8	13.0 (3)	C4—C3—C8—C7	0.6 (3)
N2—C2—C3—C4	-167.27 (19)	C4—C5—C6—C7	0.9 (4)

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x, -y+1, z+1/2$; (iii) $-x+1, y, -z+3/2$.

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C6—H6 \cdots S1 ^{iv}	1.00 (3)	2.86 (3)	3.608 (2)	132 (2)

Symmetry code: (iv) $x+1/2, -y+3/2, z+1/2$.