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Crystal structure and Hirshfeld surface analysis of aqua(1,10-phenanthroline-κ^2N,N')bis[3-(2-sulfanylidene-2,3-dihydro-1,3-benzoxazol-3-yl)propanoato-κO]zinc(II) monohydrate

Zoxida Rasuljon qizi Mamadaliyeva,[a] Tulqinjon Abdusattor ogli Sattarov,[b] Odil Irgashevich Choriyev,[c] Jalil Tulqin ogli Qadirov[c] and Jamshid Mengnorovich Ashurov[c,d]*

[a]Namangan State University, 161 Bobursho Street, Namangan 160107, Uzbekistan, [b]University of Business and Science, 111 Beshkapa Street, Namangan 160107, Uzbekistan, [c]Institute of Bioorganic Chemistry, Academy of Sciences of Uzbekistan, 100125, M. Ulugbek Str 83, Tashkent, Uzbekistan, and [d]Termez University of Economics and Service, 4-b Farovon Street, Termez 190111, Uzbekistan. *Correspondence e-mail: ashurovjamshid1@gmail.com

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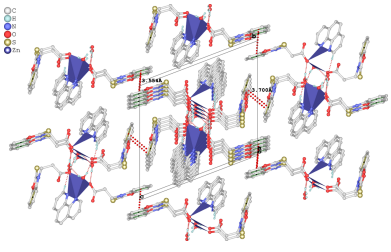
The crystal structure of the title compound, $[Zn(C_{10}H_8NO_3S)_2(C_{12}H_8N_2)(H_2O)]\cdot H_2O$, is reported together with an analysis of its intermolecular interactions. The Zn^{II} ion is five-coordinate, being bonded to two monodentate carboxylate O atoms from two crystallographically independent 3-(2-sulfanylidene-2,3-dihydro-1,3-benzoxazol-3-yl)propanoate ligands, two N atoms of a chelating 1,10-phenanthroline ligand and one water O atom. The coordination geometry is distorted square-pyramidal ($\tau_5 \simeq 0.30$). Although the two carboxylate ligands adopt the same κO coordination mode, they differ in their Zn—O bond lengths and in the conformations of their propanoate chains. In the crystal, O—H···O hydrogen bonds involving the coordinated and solvent water molecules link the complexes into one-dimensional ribbons parallel to [100], reinforced by C—H···O and C—H···S contacts. Additional consolidation is provided by π–π stacking interactions involving the phenanthroline and benzoxazoline-derived aromatic rings. Hirshfeld surface analysis shows that H···H (42.0%), H···O/O···H (19.1%), H···S/S···H (13.7%) and H···C/C···H (11.9%) contacts dominate the intermolecular surface, while C···C contacts (5.8%) are consistent with the observed π–π stacking.

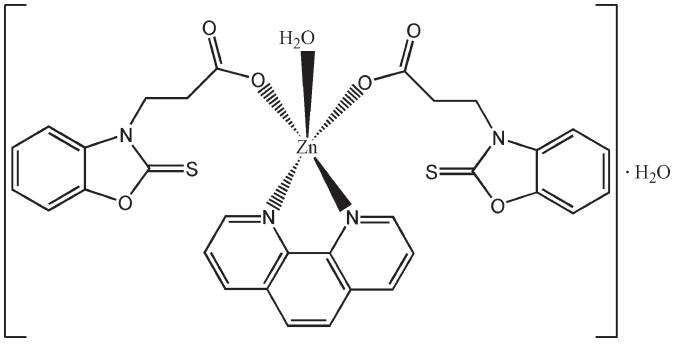
1. Chemical context

Heterocyclic compounds containing N, O and S atoms are of considerable interest because their diverse donor properties make them useful in coordination chemistry and in the design of biologically active compounds (Contreras *et al.*, 2009). Benzoxazolin-2-one and benzoxazolin-2-thione derivatives form an important class of such compounds, and substitution at the ring N atom provides a convenient means of modifying their physicochemical and biological properties. Derivatives of these heterocycles have been reported to exhibit anticancer, analgesic, anti-inflammatory and neuroprotective activities (Prasher *et al.*, 2023). In particular, sulfur-containing benzoxazole derivatives are of interest because replacement of the carbonyl O atom by S increases the polarizability of the heterocycle and may influence both metal-ion interactions and intermolecular contacts. The ability of this sulfur-containing system to interact with Zn centres is illustrated by the inhibition of human carbonic anhydrase II by 2-mercaptobenzoxazole, for which coordination of the S atom to the catalytic Zn ion has been demonstrated crystallographically (Bozdag *et al.*, 2020).



The ligand used in the present study, 3-(2-sulfanylidene-2,3-dihydro-1,3-benzoxazol-3-yl)propanoic acid, combines a carboxylic acid group capable of metal coordination with a benzoxazole-2-thione fragment that can participate in supramolecular interactions. The crystal structure of the free acid and those of its monoethanolammonium and ethylenediammonium salts have previously been reported (Ashurov *et al.*, 2017*a*). In combination with this ligand, 1,10-phenanthroline provides a rigid chelating *N*,*N*′-donor environment and an extended aromatic surface that may contribute to the consolidation of the coordination unit and to π-related intermolecular interactions (Sammes & Yahioglu, 1994).

In this work, we report the synthesis, crystal structure and Hirshfeld surface analysis of the title compound (I). The structural analysis focuses on the coordination environment of the Zn^{II} ion and on the intermolecular interactions responsible for the crystal packing.



2. Structural commentary

The asymmetric unit of the title compound, $[Zn(NBA)_2(phen)(H_2O)]\cdot H_2O$, where NBA denotes the 3-(2-sulfanylidene-2,3-dihydro-1,3-benzoxazol-3-yl)propanoate anion and phen is 1,10-phenanthroline, comprises one neutral Zn^{II} complex molecule and one water molecule of crystallization (Fig. 1). The two crystallographically independent NBA ligands are distinguished by the suffixes *A* and *B*. The phen ligand is represented by atoms N1, N2 and C1–C12, while O1*W* and O2*W* correspond to the coordinated and solvent water molecules, respectively.

The Zn1 atom is five-coordinate, being bonded to one carboxylate O atom from each of the two independent NBA ligands (O2*A* and O2*B*), the two N atoms of the chelating phen ligand (N1 and N2), and the O atom of the coordinated water molecule O1*W*. The Zn–donor bond lengths are Zn1—O2*A* = 1.9682 (15), Zn1—O2*B* = 2.0457 (17), Zn1—N2 = 2.092 (18), Zn1—O1*W* = 2.133 (2) and Zn1—N1 = 2.1729 (19) Å. Thus, both NBA ligands adopt the same monodentate κO coordination mode, although the Zn1—O2*A* bond is shorter than Zn1—O2*B* by *ca* 0.078 Å.

In both NBA ligands, the second carboxylate O atom lies outside the primary coordination sphere. The Zn1···O3*A* and Zn1···O3*B* separations are 3.0871 (19) and 2.6375 (18) Å, respectively. The shorter Zn1···O3*B* separation may be regarded as a secondary contact, but it is substantially longer than the normal Zn1—O2*B* coordination bond and is not included in the primary coordination number. The corresponding carboxylate C—O distances are O2*A*—C10*A* = 1.282 (3) and O3*A*—C10*A* = 1.224 (3) Å for ligand *A*, and O2*B*—C10*B* = 1.285 (3) and O3*B*—C10*B* = 1.231 (3) Å for ligand *B*.

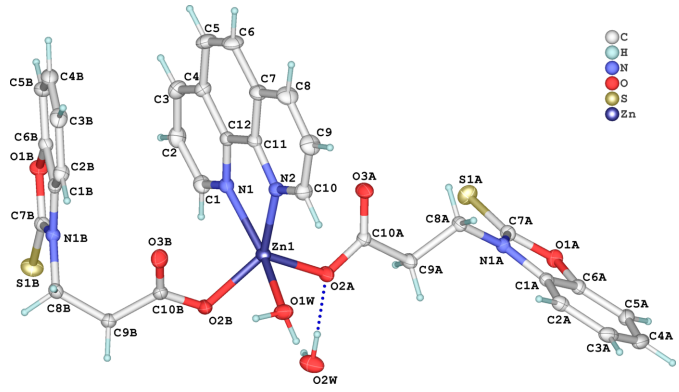


Figure 1
Molecular structure of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are shown as small spheres of arbitrary radii. The dashed line indicates the O—H···O hydrogen bond involving the water molecule of crystallization.

The phen ligand acts as a conventional chelating $\kappa^2 N,N'$ donor. The Zn1—N1 and Zn1—N2 bond lengths are 2.1729 (19) and 2.0982 (18) Å, respectively, and the N1—Zn1—N2 bite angle is 78.10 (7)°. Coordination generates a five-membered Zn1/N1/C12/C11/N2 chelate ring, while the fused phenanthroline framework remains essentially planar.

The five-coordinate geometry around Zn1 is strongly distorted. The two largest coordination angles are O1*W*—Zn1—N1 = 161.44 (7)° and O2*B*—Zn1—N2 = 143.68 (7)°. These values give an Addison parameter $\tau_5 = (\beta - \alpha)/60$ of 0.30, indicating that the coordination geometry is substantially closer to the square-pyramidal limit ($\tau_5 = 0$) than to the trigonal-bipyramidal limit ($\tau_5 = 1$). The Zn^{II} centre is therefore best described as having a distorted square-pyramidal five-coordinate environment.

Although the two crystallographically independent NBA ligands have the same κO coordination mode, they differ in both the Zn—O bond lengths and the conformations of their N-substituted propanoate chains. Their benzoxazoline-2-thione ring systems are essentially planar and the C=S bond lengths are very similar [S1*A*—C7*A* = 1.647 (2) and S1*B*—C7*B* = 1.644 (2) Å]. The conformational differences are reflected in the C1*A*—N1*A*—C8*A*—C9*A* and C1B—N1*B*—C8*B*—C9*B* torsion angles of −92.4 (2) and −112.2 (2)°, respectively, and are particularly pronounced in the N1*A*—C8*A*—C9*A*—C10*A* and N1*B*—C8*B*—C9*B*—C10*B* torsion angles of −179.54 (18) and 61.4 (3)°, respectively. Thus, the two NBA ligands retain the same mode of coordination to Zn^{II} but adopt distinctly different conformations in the crystal.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O2W^{i}	0.85 (3)	1.95 (3)	2.749 (3)	155 (3)
O1W—H1WB···O2B^{i}	0.86 (3)	1.94 (3)	2.751 (3)	159 (3)
O2W—H2WA···O2A	0.85	1.96	2.797 (3)	170
O2W—H2WB···O2B^{ii}	0.85	2.46	3.245 (3)	154
C1—H1···O2W^{ii}	0.93	2.39	3.319 (4)	178
C8A—H8AB···S1A^{iii}	0.97	2.87	3.716 (2)	146

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

3. Supramolecular features

The crystal packing is dominated by a cooperative water-mediated O—H···O hydrogen-bonding network (Table 1) involving the coordinated water molecule O1W, the water molecule of crystallization O2W and the carboxylate O atoms O2A and O2B (Fig. 2). The coordinated water molecule acts as a double donor through O1W—H1WA···O2W^{i} [H···A = 1.95 (3) Å, D···A = 2.749 (3) Å and D—H···A = 155 (3)°] and O1W—H1WB···O2B^{i} [1.94 (3), 2.751 (3) Å and 159 (3)°, respectively], where symmetry code (i) is $-x, 1-y, 1-z$. The water molecule of crystallization donates through O2W—H2WA···O2A [H···A = 1.96 Å, D···A = 2.797 (3) Å and D—H···A = 170°] and O2W—H2WB···O2B^{ii} [2.46, 3.245 (3) Å and 154°, respectively; symmetry code: (ii) $1-x$, $1-y$, $1-z$]. These interactions link the complex molecules and water molecules of crystallization into fused cyclic motifs, generating a one-dimensional hydrogen-bonded ribbon parallel to [100] (Figs. 2 and 3). The ribbon is reinforced by the nearly linear C1—H1···O2W^{ii} interaction [H···A = 2.39 Å, D···A = 3.319 (4) Å and D—H···A = 178°] and by the intermolecular C8A—H8AB···S1A^{iii} contact [H···A = 2.87 Å, D···A = 3.716 (2) Å and D—H···A = 146°; symmetry code: (iii) $x-1, y, z$], the latter also propagating along [100].

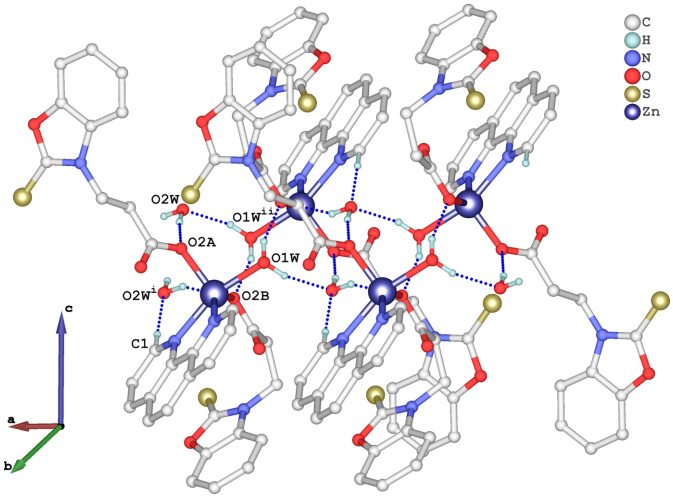


Figure 2
Partial crystal packing showing the intermolecular O—H···O and C—H···O hydrogen bonds (blue dashed lines) involving the coordinated and solvent water molecules. H atoms not involved in these interactions have been omitted for clarity.

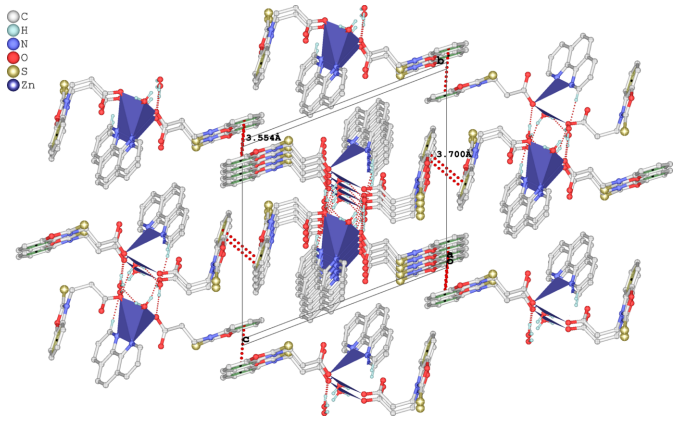


Figure 3
Crystal packing showing the intermolecular hydrogen-bonding network (cyan dashed lines) and π–π stacking interactions (red dotted lines). The centroid–centroid separations for the selected π–π contacts are 3.554 and 3.700 Å. The Zn^{II} coordination polyhedra are shown in blue.

Offset π–π stacking interactions provide a further contribution to the crystal packing (Fig. 3). For the phen ligand, *Cg*5 and *Cg*6 are the centroids of the N1/C1–C4/C12 and N2/C7–C11 rings, respectively. The translational *Cg*5···*Cg*6^{iv} interaction [symmetry code: (iv) $1+x, y, z$] has a centroid–centroid distance of 3.9453 (15) Å, an interplanar angle of 3.49 (12)° and a slippage of 1.921 Å; the corresponding perpendicular separations are 3.5263 (10) and 3.4460 (11) Å. Ligand A participates in two inversion-related π–π contacts. The *Cg*7···*Cg*7^{v} interaction, where *Cg*7 is the centroid of the C1*A*–C6*A* benzene ring, has a centroid–centroid distance of 3.5541 (15) Å and a slippage of 1.304 Å. A second contact, *Cg*3···*Cg*7^{v}, occurs at 3.7201 (14) Å with a slippage of 1.722 Å, where *Cg*3 is the centroid of the O1*A*/C6*A*/C1*A*/N1*A*/C7*A* heterocyclic ring. Both contacts involve symmetry code (v), $1-x, 2-y, 2-z$. Ligand B displays a different π–π stacking arrangement. The shortest contact is *Cg*4···*Cg*8^{vi} = 3.5381 (13) Å, where *Cg*4 and *Cg*8 are the centroids of the O1*B*/C6*B*/C1*B*/N1*B*/C7*B* and C1*B*–C6*B* rings, respectively. This interaction has an interplanar angle of 2.41 (12)° and a small slippage of 0.855 Å. A second benzene–benzene interaction, *Cg*8···*Cg*8^{vi}, occurs at 3.6998 (14) Å with a slippage of 1.373 Å [symmetry code: (vi) $-x, 1-y, -z$]. Thus, ligand *A* exhibits the shorter benzene–benzene stacking contact, whereas the heterocycle–benzene contact involving ligand *B* shows the more direct overlap. Together with the hydrogen-bonding network, these π–π interactions consolidate the crystal packing.

4. Hirshfeld surface analysis

To quantify the intermolecular contacts contributing to the crystal packing, a Hirshfeld surface analysis (Spackman & Jayatilaka, 2009) was performed using *CrystalExplorer17* (Turner *et al.*, 2017). The percentage contributions of the different contact types are summarized in Fig. 4, while the two-dimensional fingerprint plots and corresponding filtered Hirshfeld surface views are shown in Fig. 5. H···H contacts

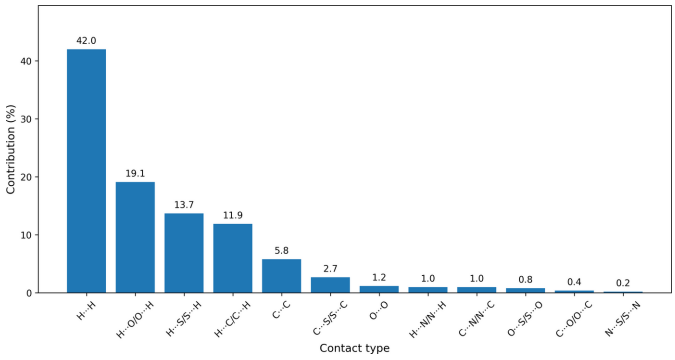


Figure 4
Percentage contributions of the various intermolecular contacts to the Hirshfeld surface.

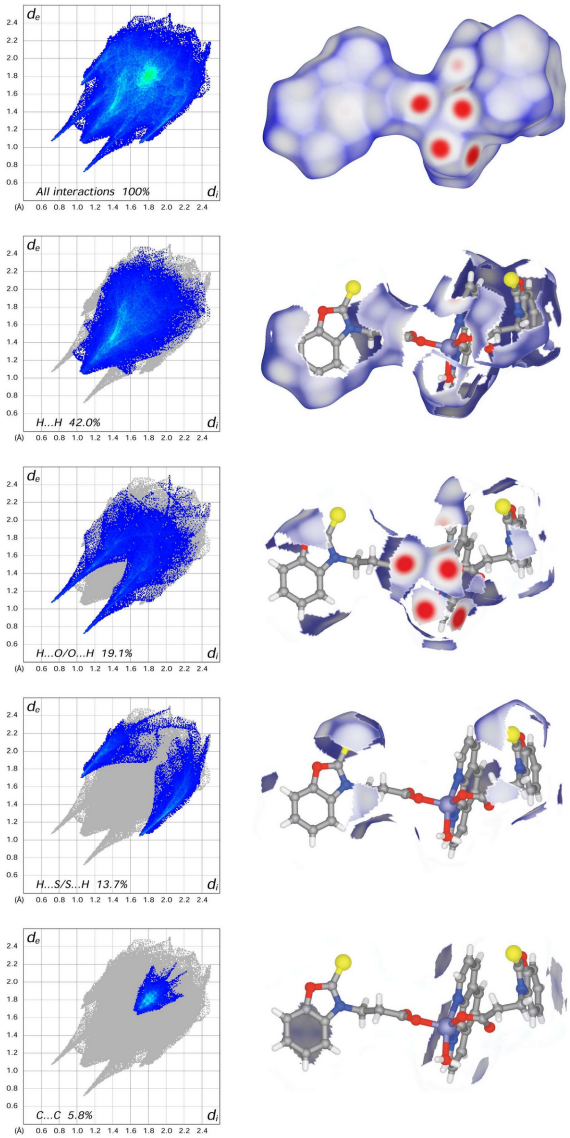


Figure 5
Two-dimensional fingerprint plots (left) and corresponding Hirshfeld surface views (right), showing all intermolecular contacts and the contributions from H···H (42.0%), H···O/O···H (19.1%), H···S/S···H (13.7%), and C···C (5.8%) contacts.

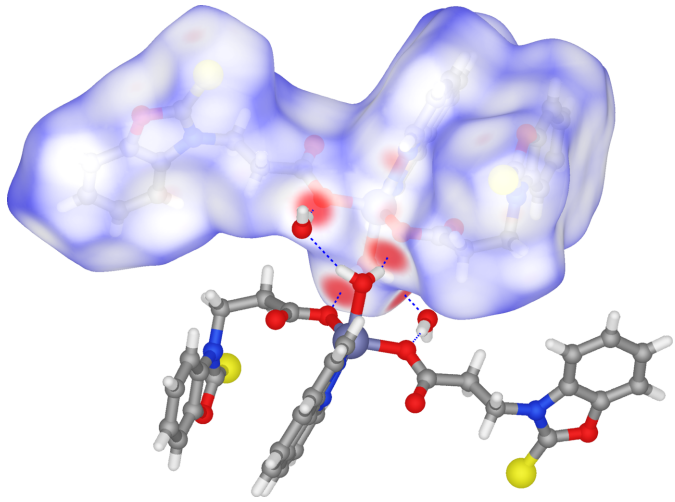


Figure 6
Hirshfeld surface mapped over d_{norm} (−0.6163 to 1.3068 a.u.), showing the intermolecular O—H···O hydrogen-bonding contacts.

make the largest contribution, accounting for 42.0% of the total surface. The next most important contributions are H···O/O···H (19.1%), H···S/S···H (13.7%) and C···C (5.8%) contacts.

The H···O/O···H contacts are associated with the O—H···O and C—H···O interactions described in the supramolecular analysis (Table 1). These short contacts appear as intense red regions on the Hirshfeld surface mapped over d_{norm} (Fig. 6). The appreciable H···S/S···H contribution is likewise consistent with the observed C—H···S interactions. Taken together, the H···O/O···H and H···S/S···H contacts account for 32.8% of the Hirshfeld surface, emphasizing the importance of hydrogen-bonding and related directional contacts in the crystal packing. C···C contacts contribute 5.8% of the surface and are consistent with the π–π stacking interactions identified crystallographically, including the phenanthroline and benzoxazoline-derived aromatic stacks discussed above (Figs. 3 and 7). Smaller contributions arise from C···S/S···C (2.7%), O···O (1.2%), H···N/N···H (1.0%), C···N/N···C (1.0%), O···S/S···O (0.8%), C···O/O···C (0.4%) and N···S/S···N (0.2%) contacts. Overall, the Hirshfeld surface analysis confirms that hydrogen-based contacts dominate the intermolecular association, while the

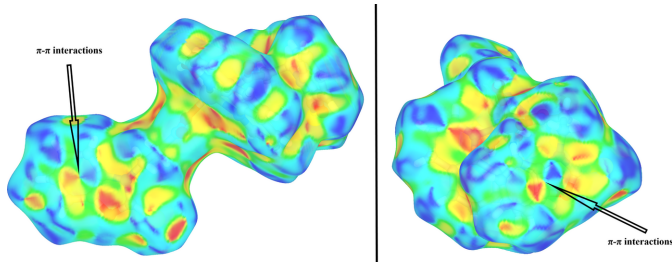


Figure 7
Shape-index surfaces of the two crystallographically independent molecules, *A* (left) and *B* (right), showing the regions involved in π–π stacking interactions.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Zn(C_{10}H_8NO_3S)_2(C_{12}H_8N_2)\cdot(H_2O)]\cdot H_2O$
M_r	726.07
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	291
a, b, c (Å)	6.9071 (3), 14.8406 (7), 16.3048 (7)
α, β, γ (°)	110.602 (4), 94.604 (3), 90.039 (4)
V (Å^3)	1558.65 (13)
Z	2
Radiation type	Cu $K\alpha$
μ (mm^{-1})	2.86
Crystal size (mm)	0.3 × 0.22 × 0.14
Data collection	
Diffractometer	Xcalibur, Ruby
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2014)
T_{min}, T_{max}	0.772, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11088, 6306, 5486
R_{int}	0.026
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.630
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.039, 0.109, 1.04
No. of reflections	6306
No. of parameters	436
No. of restraints	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.34, −0.41

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2025/1* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

measurable C···C contribution provides additional support for the aromatic π–π stacking that consolidates the crystal structure.

5. Database survey

A search of the Cambridge Structural Database (CSD, Version 6.01, November 2025, including the February 2026 updates; Groom *et al.*, 2016) for the benzoxazole-derived fragment of the ligand used here yielded 215 hits. The most relevant are the free acid YEDCOC and its monoethanolammonium and ethylenediammonium salts, YEDCUI and YEDDAP (Ashurov *et al.*, 2017*a*), the related Zn^{II} complex $[Zn(L)_2(H_2O)_4]$ (UNODOR; Ashurov *et al.*, 2011) and its isostructural Co^{II}/Cu^{II} analogues (Ashurov *et al.*, 2014), the (2-oxo-1,3-benzoxazol-3(2*H*)-yl)acetate derivatives NUZSIM (Wang *et al.*, 2016) with polymorphs NUZSIM01/NUZSIM02 (Ashurov *et al.*, 2017*b*) and the solvate, salts and hydrate ULIBUO, ULICAV, ULICAV01 and ULICOJ (Ashurov *et al.*, 2015*b*), and related triethanolamine mixed-ligand carboxylate complexes of Zn^{II}, Cd^{II} and Cu^{II} (Ashurov *et al.*, 2015*a*, 2016*a*,*b*). No entry corresponding to a Zn^{II} complex of this thione-containing propanoate ligand together with 1,10-phenanthroline was found.

A further search for the $[Zn(phen)(\kappa O\text{-}RCOO)_2(H_2O)]$ fragment – a chelating phen ligand, two monodentate carboxylates and one aqua ligand, as found here – retrieved 61 hits, confirming that this five-coordinate geometry is well established for Zn^{II}, even though it has not previously been combined with the present thione-containing ligand. To compare parameters rather than connectivity alone, the Zn—donor bond lengths of the title compound may be set against four representative examples: ADUROH (Luo *et al.*, 2007), QAHNUK (Liu *et al.*, 2011), ETUXAT (Nie *et al.*, 2011) and BUBYOO (Huang *et al.*, 2014), the last of which, like the title compound, crystallizes with an additional water molecule of crystallization. The Zn1—O(carboxylate) bond lengths in the title compound [1.9682 (15) and 2.0457 (17) Å] compare closely with those in the four analogues [1.988 (3)/2.055 (2), 1.968 (2)/2.000 (2), 2.015 (2)/2.032 (2) and 1.997 (2)/2.064 (2) Å, respectively, in the order above]. Similarly, the Zn1—O(aqua) distance of the title compound [2.133 (2) Å] lies close to the corresponding values [2.030 (3), 2.128 (2), 2.110 (3) and 2.107 (2) Å], and the two Zn1—N(phen) distances [2.098 (2) and 2.173 (2) Å] are comparable with those in the same four structures [2.087 (4)/2.194 (3), 2.103 (2)/2.184 (2), 2.126 (3)/2.131 (2) and 2.095 (2)/2.163 (2) Å]. In every case, including the title compound, the two symmetry-independent Zn—O(carboxylate) bonds are slightly inequivalent [Δ = 0.078 Å in the title compound, *versus* 0.067, 0.032, 0.017 and 0.067 Å in the four analogues, respectively], showing that this small asymmetry is a general feature of bis(monodentate-carboxylato) coordination at Zn^{II} rather than a peculiarity of the title compound.

6. Synthesis and crystallization

Zinc chloride dihydrate, 3-(2-sulfanylidene-2,3-dihydro-1,3-benzoxazol-3-yl)propanoic acid (HNBA) and 1,10-phenanthroline were mixed in a 1:2:1 molar ratio. An aqueous solution of $ZnCl_2\cdot 2H_2O$ (0.10 mmol, 17.2 mg) in 5 mL of distilled water was stirred while an ethanolic solution containing the two organic ligands was added dropwise over approximately 15 min. The ligand solution was prepared by dissolving HNBA (0.20 mmol, 44.7 mg) in 6 mL of warm ethanol, followed by the addition of 1,10-phenanthroline (0.10 mmol, 18.0 mg), dissolved in 4 mL of ethanol. The resulting clear, colourless solution was stirred for a further 30 min at room temperature and then filtered through a fine-porosity glass frit. The filtrate was left to evaporate slowly at room temperature. Colourless single crystals suitable for X-ray diffraction were obtained, collected by filtration, washed with a small amount of cold ethanol–water (1:1, *v*/*v*), and air-dried. The isolated yield was approximately 65% based on Zn. Analysis calculated for $C_{32}H_{28}N_4O_8S_2Zn$: C 52.93, H 3.89, N 7.72, S 8.83%. Found: C 52.88, H 3.81, N 7.66, S 8.78%.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms bonded to C atoms were placed in geometrically calculated positions and refined using a riding model, with C—H distances of 0.93 Å for aromatic H atoms and 0.97 Å for methylene H atoms. The H atoms of the

coordinated water molecule O1*W* (H1*WA* and H1*WB*) were located from difference-Fourier maps and refined with restrained O—H distances, giving O1*W*—H1*WA* = 0.85 (3) and O1*W*—H1*WB* = 0.86 (3) Å. The H atoms of the water molecule of crystallization O2*W* (H2*WA* and H2*WB*) were retained at fixed positions with O—H = 0.85 Å. Two least-squares restraints were used in the final refinement.

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References

Agilent (2014). *CrysAlis PRO*. Agilent Technologies Ltd, Yarnton, Oxfordshire, England.
Ashurov, J. M. (2016*b*). *Acta Cryst.* E**72**, 526–529.
Ashurov, J. M., Ibragimov, A. B. & Ibragimov, B. T. (2015*a*). *Polyhedron* **102**, 441–446.
Ashurov, J. M., Ibragimov, B. T. & Mukhamedov, N. S. (2014). *Russ. J. Coord. Chem.* **40**, 246–250.
Ashurov, J. M., Izotova, L. Yu., Ibragimov, B. T. & Mukhamedov, N. S. (2017*b*). *Russ. J. Phys. Chem.* **91**, 106–110.
Ashurov, J., Karimova, G., Mukhamedov, N., Parpiev, N. A. & Ibragimov, B. (2011). *Acta Cryst.* E**67**, m432.
Ashurov, J. M., Mukhamedov, N. S., Tashkhodzhaev, B. & Ibragimov, B. T. (2015*b*). *J. Struct. Chem.* **56**, 1148–1153.
Ashurov, J. M., Obidova, N. J., Abdireymov, H. B. & Ibragimov, B. T. (2016*a*). *Acta Cryst.* E**72**, 420–423.
Ashurov, Zh. M., Tashkhodjaev, B., Izotova, L. Yu., Olimova, M. I. & Ibragimov, B. T. (2017*a*). *J. Struct. Chem.* **58**, 544–549.
Bozdag, M., Supuran, C. T., Esposito, D., Angeli, A., Carta, F., Monti, S. M., De Simone, G. & Alterio, V. (2020). *Chem. Commun.* **56**, 8297–8300.
Contreras, R., Flores-Parra, A., Mijangos, E., Téllez, F., López-Sandoval, H. & Barba-Behrens, N. (2009). *Coord. Chem. Rev.* **253**, 1979–1999.
Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.
Huang, M.-L., Weng, W.-T. & Chen, Q. (2014). *Wuji Huaxue Xuebao (Chin. J. Inorg. Chem.)* **30**, 2032–2038.
Liu, J.-Z., Zhang, Z., Shi, Z.-W. & Gao, P. (2011). *Acta Cryst.* E**67**, m30.
Luo, B.-C., Li, C.-H., Peng, Y.-L. & Kuang, Y.-F. (2007). *Jiegou Huaxue (Chin. J. Struct. Chem.)* **26**, 649–653.
Nie, J.-J., Xu, X. & Xu, D.-J. (2011). *Acta Cryst.* E**67**, m855–m856.
Prasher, P., Mall, T. & Sharma, M. (2023). *Arch. Pharm.* **356**, e2300245.
Sammes, P. G. & Yahioglu, G. (1994). *Chem. Soc. Rev.* **23**, 327–334.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Spackman, M. A. & Jayatilaka, D. (2009). *CrystEngComm* **11**, 19–32.
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.
Wang, A., Ashurov, J., Ibragimov, A., Wang, R., Mouhib, H., Mukhamedov, N. & Englert, U. (2016). *Acta Cryst.* B**72**, 142–150.

supporting information

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Crystal structure and Hirshfeld surface analysis of aqua(1,10-phenanthroline-κ^2N,N')bis[3-(2-sulfanylidene-2,3-dihydro-1,3-benzoxazol-3-yl)propanoato-κO]zinc(II) monohydrate

Zoxida Rasuljon qizi Mamadaliyeva, Tulqinjon Abdusattor ogli Sattarov, Odil Irgashevich Choriyev, Jalil Tulqin ogli Qadirov and Jamshid Mengnorovich Ashurov

Computing details

Aqua(1,10-phenanthroline-κ^2N,N')bis[3-(2-sulfanylidene-2,3-dihydro-1,3-benzoxazol-3-yl)propanoato-κO]zinc(II) monohydrate

Crystal data

$[Zn(C_{10}H_8NO_3S)_2(C_{12}H_8N_2)(H_2O)]\cdot H_2O$
$M_r = 726.07$
Triclinic, $P\overline{1}$
$a = 6.9071$ (3) Å
$b = 14.8406$ (7) Å
$c = 16.3048$ (7) Å
$\alpha = 110.602$ (4)°
$\beta = 94.604$ (3)°
$\gamma = 90.039$ (4)°
$V = 1558.65$ (13) Å^3
$Z = 2$
$F(000) = 748$
$D_x = 1.547$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 6283 reflections
$\theta = 5.0$–$75.8°$
$\mu = 2.86$ mm^{-1}
$T = 291$ K
Block, colourless
0.3 × 0.22 × 0.14 mm

Data collection

Xcalibur, Ruby diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 10.2576 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Agilent, 2014)
$T_{min} = 0.772$, $T_{max} = 1.000$
11088 measured reflections
6306 independent reflections
5486 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 76.3°$, $\theta_{min} = 3.2°$
$h = -8\rightarrow8$
$k = -18\rightarrow17$
$l = -16\rightarrow20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.109$
$S = 1.04$
6306 reflections
436 parameters
2 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0594P)^2 + 0.2152P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.41$ e Å^{-3}

Extinction correction: SHELXL-2025/1 (Sheldrick 2015b), $Fc^{*}=kFc[1+0.001xFc^{2}\lambda^{3}/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00062 (16)

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	0.06762 (4)	0.65940 (2)	0.47043 (2)	0.04569 (11)
S1A	0.95185 (9)	0.88039 (6)	0.77354 (4)	0.06117 (17)
S1B	0.45542 (10)	0.36073 (5)	0.12867 (5)	0.06746 (19)
O1A	0.8755 (2)	0.88855 (12)	0.93312 (10)	0.0491 (4)
O1B	0.3695 (2)	0.51840 (12)	0.09501 (11)	0.0511 (4)
O1W	−0.1818 (3)	0.62099 (14)	0.52147 (13)	0.0633 (5)
H1WA	−0.268 (4)	0.591 (2)	0.4804 (16)	0.085 (11)*
H1WB	−0.143 (5)	0.589 (2)	0.5539 (19)	0.084 (11)*
O2A	0.2398 (2)	0.68238 (11)	0.57848 (10)	0.0523 (4)
O2B	0.1181 (3)	0.51751 (12)	0.40405 (10)	0.0657 (5)
O3A	0.2952 (3)	0.83758 (12)	0.60212 (12)	0.0635 (5)
O3B	−0.0825 (3)	0.55723 (13)	0.31048 (11)	0.0605 (4)
N1	0.2497 (3)	0.70306 (13)	0.38743 (11)	0.0448 (4)
N1A	0.6125 (2)	0.87668 (12)	0.84374 (11)	0.0394 (4)
N1B	0.1228 (2)	0.45948 (12)	0.14092 (11)	0.0404 (4)
N2	−0.0759 (3)	0.77999 (12)	0.46006 (11)	0.0444 (4)
C1	0.4102 (4)	0.66383 (18)	0.35236 (16)	0.0570 (6)
H1	0.460365	0.612170	0.365960	0.068*
C1A	0.5493 (3)	0.87933 (14)	0.92400 (13)	0.0399 (4)
C1B	0.0551 (3)	0.53864 (14)	0.12113 (12)	0.0408 (4)
C2	0.5066 (4)	0.6969 (2)	0.29597 (18)	0.0663 (7)
H2	0.619772	0.668386	0.273219	0.080*
C2A	0.3672 (4)	0.87639 (16)	0.95211 (16)	0.0512 (5)
H2A	0.254143	0.870642	0.915339	0.061*
C2B	−0.1256 (4)	0.57964 (18)	0.12254 (15)	0.0523 (5)
H2B	−0.231964	0.556153	0.141242	0.063*
C3	0.4323 (4)	0.7717 (2)	0.27473 (18)	0.0658 (7)
H3	0.494006	0.793949	0.236581	0.079*
C3A	0.3636 (4)	0.88257 (17)	1.03909 (18)	0.0616 (7)
H3A	0.244233	0.880536	1.061111	0.074*
C3B	−0.1386 (4)	0.65749 (19)	0.09452 (17)	0.0626 (7)
H3B	−0.256988	0.687391	0.094711	0.075*
C4	0.2628 (4)	0.81509 (17)	0.31037 (15)	0.0529 (5)
C4A	0.5315 (5)	0.89164 (18)	1.09390 (17)	0.0641 (7)
H4A	0.521670	0.895669	1.151636	0.077*

C4B	0.0199 (4)	0.69217 (19)	0.06617 (17)	0.0629 (7)
H4B	0.004782	0.744855	0.048179	0.075*
C5	0.1755 (5)	0.8952 (2)	0.29361 (19)	0.0687 (7)
H5	0.230319	0.919649	0.255192	0.082*
C5A	0.7135 (4)	0.89488 (17)	1.06535 (15)	0.0564 (6)
H5A	0.826852	0.901560	1.102091	0.068*
C5B	0.1996 (4)	0.65080 (17)	0.06383 (16)	0.0562 (6)
H5B	0.305907	0.673314	0.044289	0.067*
C6	0.0172 (5)	0.9358 (2)	0.33178 (19)	0.0674 (7)
H6	−0.034647	0.988298	0.320036	0.081*
C6A	0.7157 (3)	0.88755 (15)	0.97876 (14)	0.0446 (4)
C6B	0.2099 (3)	0.57408 (15)	0.09244 (14)	0.0441 (4)
C7	−0.0736 (4)	0.89968 (17)	0.39044 (17)	0.0541 (5)
C7A	0.8072 (3)	0.88153 (15)	0.84943 (14)	0.0432 (4)
C7B	0.3108 (3)	0.44668 (16)	0.12318 (14)	0.0463 (5)
C8	−0.2364 (4)	0.9408 (2)	0.4337 (2)	0.0691 (7)
H8	−0.291333	0.994427	0.425374	0.083*
C8A	0.4879 (3)	0.87262 (15)	0.76538 (13)	0.0426 (4)
H8AA	0.551563	0.907883	0.734519	0.051*
H8AB	0.366806	0.903599	0.783206	0.051*
C8B	0.0067 (3)	0.39299 (15)	0.16722 (14)	0.0470 (5)
H8BA	0.026357	0.327505	0.128808	0.056*
H8BB	−0.129891	0.406184	0.159830	0.056*
C9	−0.3137 (4)	0.9012 (2)	0.4883 (2)	0.0700 (7)
H9	−0.421087	0.928295	0.517837	0.084*
C9A	0.4445 (3)	0.77031 (15)	0.70392 (14)	0.0489 (5)
H9AA	0.379984	0.735210	0.734669	0.059*
H9AB	0.565726	0.739188	0.686507	0.059*
C9B	0.0584 (4)	0.40123 (16)	0.26168 (14)	0.0535 (6)
H9BA	−0.018119	0.353486	0.274145	0.064*
H9BB	0.194228	0.386427	0.268395	0.064*
C10	−0.2311 (4)	0.82006 (19)	0.49962 (17)	0.0567 (6)
H10	−0.286786	0.793191	0.536139	0.068*
C10A	0.3166 (3)	0.76591 (15)	0.62222 (13)	0.0427 (4)
C10B	0.0249 (4)	0.49929 (16)	0.32831 (14)	0.0503 (5)
C11	0.0041 (3)	0.81968 (14)	0.40680 (13)	0.0429 (4)
C12	0.1766 (3)	0.77751 (14)	0.36722 (13)	0.0421 (4)
O2W	0.4199 (3)	0.52157 (16)	0.59806 (17)	0.0789 (6)
H2WA	0.378693	0.573354	0.592736	0.118*
H2WB	0.535657	0.518267	0.583319	0.118*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0585 (2)	0.03806 (16)	0.04177 (17)	−0.00106 (12)	−0.00615 (12)	0.01790 (12)
S1A	0.0439 (3)	0.0827 (4)	0.0627 (4)	−0.0012 (3)	0.0104 (3)	0.0316 (3)
S1B	0.0560 (4)	0.0598 (4)	0.0937 (5)	0.0164 (3)	0.0080 (3)	0.0354 (3)
O1A	0.0407 (8)	0.0570 (9)	0.0473 (8)	0.0028 (7)	−0.0037 (6)	0.0174 (7)

O1B	0.0435 (8)	0.0511 (9)	0.0630 (10)	0.0006 (7)	0.0058 (7)	0.0252 (7)
O1W	0.0723 (12)	0.0603 (11)	0.0643 (11)	−0.0140 (9)	−0.0059 (9)	0.0332 (9)
O2A	0.0672 (10)	0.0419 (8)	0.0450 (8)	−0.0058 (7)	−0.0153 (7)	0.0160 (6)
O2B	0.1151 (16)	0.0402 (8)	0.0407 (8)	−0.0109 (9)	−0.0088 (9)	0.0163 (7)
O3A	0.0870 (13)	0.0469 (9)	0.0585 (10)	−0.0056 (8)	−0.0189 (9)	0.0262 (8)
O3B	0.0701 (11)	0.0571 (10)	0.0522 (9)	0.0103 (8)	0.0114 (8)	0.0153 (8)
N1	0.0525 (10)	0.0400 (9)	0.0419 (9)	0.0061 (8)	−0.0011 (7)	0.0155 (7)
N1A	0.0375 (8)	0.0395 (8)	0.0386 (8)	−0.0007 (7)	0.0001 (6)	0.0113 (7)
N1B	0.0430 (9)	0.0391 (8)	0.0390 (8)	−0.0001 (7)	0.0035 (7)	0.0137 (7)
N2	0.0507 (10)	0.0397 (9)	0.0436 (9)	0.0018 (7)	0.0007 (7)	0.0163 (7)
C1	0.0594 (14)	0.0517 (13)	0.0561 (13)	0.0126 (11)	−0.0004 (11)	0.0156 (11)
C1A	0.0443 (11)	0.0313 (9)	0.0432 (10)	0.0027 (8)	0.0043 (8)	0.0116 (7)
C1B	0.0476 (11)	0.0382 (10)	0.0341 (9)	0.0032 (8)	0.0011 (8)	0.0102 (7)
C2	0.0620 (16)	0.0728 (17)	0.0582 (15)	0.0139 (13)	0.0134 (12)	0.0140 (13)
C2A	0.0502 (12)	0.0420 (11)	0.0612 (13)	0.0005 (9)	0.0118 (10)	0.0166 (10)
C2B	0.0499 (12)	0.0578 (13)	0.0478 (12)	0.0107 (10)	0.0067 (9)	0.0163 (10)
C3	0.0719 (17)	0.0726 (17)	0.0575 (15)	0.0019 (14)	0.0181 (13)	0.0259 (13)
C3A	0.0730 (17)	0.0454 (12)	0.0734 (16)	0.0061 (11)	0.0307 (14)	0.0243 (11)
C3B	0.0699 (17)	0.0588 (14)	0.0575 (14)	0.0258 (13)	0.0041 (12)	0.0186 (11)
C4	0.0629 (14)	0.0521 (13)	0.0473 (12)	0.0000 (11)	0.0058 (10)	0.0219 (10)
C4A	0.100 (2)	0.0467 (13)	0.0529 (13)	0.0105 (13)	0.0224 (14)	0.0238 (11)
C4B	0.089 (2)	0.0474 (12)	0.0538 (14)	0.0122 (13)	0.0014 (13)	0.0205 (11)
C5	0.089 (2)	0.0644 (16)	0.0696 (17)	0.0039 (14)	0.0143 (15)	0.0429 (14)
C5A	0.0795 (17)	0.0446 (12)	0.0459 (12)	0.0100 (11)	0.0001 (11)	0.0181 (9)
C5B	0.0720 (16)	0.0450 (12)	0.0542 (13)	−0.0040 (11)	0.0050 (11)	0.0206 (10)
C6	0.0830 (19)	0.0566 (15)	0.0789 (18)	0.0114 (13)	0.0064 (15)	0.0442 (14)
C6A	0.0503 (12)	0.0382 (10)	0.0438 (11)	0.0027 (8)	0.0020 (9)	0.0131 (8)
C6B	0.0488 (12)	0.0396 (10)	0.0412 (10)	0.0007 (9)	0.0003 (8)	0.0115 (8)
C7	0.0622 (14)	0.0451 (11)	0.0577 (13)	0.0073 (10)	0.0002 (11)	0.0227 (10)
C7A	0.0379 (10)	0.0429 (10)	0.0461 (11)	−0.0007 (8)	−0.0018 (8)	0.0137 (8)
C7B	0.0466 (11)	0.0430 (11)	0.0477 (11)	−0.0013 (9)	0.0004 (9)	0.0151 (9)
C8	0.0709 (17)	0.0552 (15)	0.086 (2)	0.0230 (13)	0.0087 (14)	0.0306 (14)
C8A	0.0422 (11)	0.0401 (10)	0.0435 (10)	0.0009 (8)	−0.0053 (8)	0.0142 (8)
C8B	0.0536 (12)	0.0399 (10)	0.0437 (11)	−0.0082 (9)	0.0029 (9)	0.0101 (8)
C9	0.0642 (16)	0.0640 (16)	0.0813 (19)	0.0228 (13)	0.0178 (14)	0.0226 (14)
C9A	0.0571 (13)	0.0404 (11)	0.0466 (11)	−0.0030 (9)	−0.0104 (9)	0.0153 (9)
C9B	0.0758 (16)	0.0413 (11)	0.0443 (11)	−0.0052 (11)	0.0046 (10)	0.0162 (9)
C10	0.0585 (14)	0.0563 (14)	0.0569 (13)	0.0062 (11)	0.0110 (11)	0.0206 (11)
C10A	0.0474 (11)	0.0418 (10)	0.0380 (10)	0.0009 (8)	−0.0005 (8)	0.0137 (8)
C10B	0.0712 (15)	0.0421 (11)	0.0394 (11)	−0.0094 (10)	0.0085 (10)	0.0157 (9)
C11	0.0517 (12)	0.0355 (9)	0.0415 (10)	0.0013 (8)	−0.0019 (8)	0.0149 (8)
C12	0.0492 (11)	0.0375 (10)	0.0391 (10)	−0.0006 (8)	−0.0021 (8)	0.0143 (8)
O2W	0.0720 (13)	0.0618 (12)	0.1090 (17)	−0.0081 (10)	−0.0172 (12)	0.0429 (12)

Geometric parameters (Å, º)

Zn1—O1W	2.133 (2)	C3A—H3A	0.9300
Zn1—O2A	1.9682 (15)	C3A—C4A	1.382 (4)

Zn1—O2B	2.0457 (17)	C3B—H3B	0.9300
Zn1—N1	2.1729 (19)	C3B—C4B	1.388 (4)
Zn1—N2	2.0982 (18)	C4—C5	1.434 (4)
S1A—C7A	1.647 (2)	C4—C12	1.406 (3)
S1B—C7B	1.644 (2)	C4A—H4A	0.9300
O1A—C6A	1.382 (3)	C4A—C5A	1.381 (4)
O1A—C7A	1.375 (3)	C4B—H4B	0.9300
O1B—C6B	1.385 (3)	C4B—C5B	1.382 (4)
O1B—C7B	1.372 (3)	C5—H5	0.9300
O1W—H1WA	0.854 (10)	C5—C6	1.339 (4)
O1W—H1WB	0.853 (10)	C5A—H5A	0.9300
O2A—C10A	1.282 (3)	C5A—C6A	1.379 (3)
O2B—C10B	1.285 (3)	C5B—H5B	0.9300
O3A—C10A	1.224 (3)	C5B—C6B	1.374 (3)
O3B—C10B	1.231 (3)	C6—H6	0.9300
N1—C1	1.328 (3)	C6—C7	1.433 (4)
N1—C12	1.347 (3)	C7—C8	1.400 (4)
N1A—C1A	1.400 (3)	C7—C11	1.403 (3)
N1A—C7A	1.341 (3)	C8—H8	0.9300
N1A—C8A	1.465 (2)	C8—C9	1.365 (4)
N1B—C1B	1.395 (3)	C8A—H8AA	0.9700
N1B—C7B	1.351 (3)	C8A—H8AB	0.9700
N1B—C8B	1.468 (3)	C8A—C9A	1.510 (3)
N2—C10	1.327 (3)	C8B—H8BA	0.9700
N2—C11	1.358 (3)	C8B—H8BB	0.9700
C1—H1	0.9300	C8B—C9B	1.515 (3)
C1—C2	1.395 (4)	C9—H9	0.9300
C1A—C2A	1.379 (3)	C9—C10	1.397 (4)
C1A—C6A	1.376 (3)	C9A—H9AA	0.9700
C1B—C2B	1.387 (3)	C9A—H9AB	0.9700
C1B—C6B	1.375 (3)	C9A—C10A	1.520 (3)
C2—H2	0.9300	C9B—H9BA	0.9700
C2—C3	1.362 (4)	C9B—H9BB	0.9700
C2A—H2A	0.9300	C9B—C10B	1.510 (3)
C2A—C3A	1.391 (4)	C10—H10	0.9300
C2B—H2B	0.9300	C11—C12	1.438 (3)
C2B—C3B	1.384 (4)	O2W—H2WA	0.8499
C3—H3	0.9300	O2W—H2WB	0.8500
C3—C4	1.404 (4)		

O1W—Zn1—N1	161.44 (7)	C6A—C5A—C4A	115.5 (2)
O2A—Zn1—O1W	94.89 (7)	C6A—C5A—H5A	122.2
O2A—Zn1—O2B	100.29 (7)	C4B—C5B—H5B	122.4
O2A—Zn1—N1	102.93 (7)	C6B—C5B—C4B	115.2 (2)
O2A—Zn1—N2	115.84 (7)	C6B—C5B—H5B	122.4
O2B—Zn1—O1W	91.01 (8)	C5—C6—H6	119.5
O2B—Zn1—N1	90.88 (7)	C5—C6—C7	121.0 (2)
O2B—Zn1—N2	143.68 (7)	C7—C6—H6	119.5

N2—Zn1—O1W	89.57 (8)	C1A—C6A—O1A	109.13 (18)
N2—Zn1—N1	78.10 (7)	C1A—C6A—C5A	123.0 (2)
C7A—O1A—C6A	107.32 (16)	C5A—C6A—O1A	127.9 (2)
C7B—O1B—C6B	107.20 (17)	C1B—C6B—O1B	108.95 (18)
Zn1—O1W—H1WA	112 (2)	C5B—C6B—O1B	127.2 (2)
Zn1—O1W—H1WB	107 (2)	C5B—C6B—C1B	123.8 (2)
H1WA—O1W—H1WB	113 (3)	C8—C7—C6	123.3 (2)
C10A—O2A—Zn1	121.33 (14)	C8—C7—C11	117.6 (2)
C10B—O2B—Zn1	104.12 (15)	C11—C7—C6	119.1 (2)
C1—N1—Zn1	129.16 (16)	O1A—C7A—S1A	122.84 (15)
C1—N1—C12	118.5 (2)	N1A—C7A—S1A	128.85 (16)
C12—N1—Zn1	112.20 (14)	N1A—C7A—O1A	108.30 (18)
C1A—N1A—C8A	126.06 (17)	O1B—C7B—S1B	122.14 (17)
C7A—N1A—C1A	109.79 (17)	N1B—C7B—S1B	129.23 (17)
C7A—N1A—C8A	124.12 (18)	N1B—C7B—O1B	108.60 (18)
C1B—N1B—C8B	126.43 (18)	C7—C8—H8	120.3
C7B—N1B—C1B	109.11 (17)	C9—C8—C7	119.3 (2)
C7B—N1B—C8B	124.12 (18)	C9—C8—H8	120.3
C10—N2—Zn1	127.26 (16)	N1A—C8A—H8AA	109.2
C10—N2—C11	118.4 (2)	N1A—C8A—H8AB	109.2
C11—N2—Zn1	114.32 (14)	N1A—C8A—C9A	111.89 (17)
N1—C1—H1	118.6	H8AA—C8A—H8AB	107.9
N1—C1—C2	122.7 (2)	C9A—C8A—H8AA	109.2
C2—C1—H1	118.6	C9A—C8A—H8AB	109.2
C2A—C1A—N1A	132.7 (2)	N1B—C8B—H8BA	109.1
C6A—C1A—N1A	105.45 (18)	N1B—C8B—H8BB	109.1
C6A—C1A—C2A	121.8 (2)	N1B—C8B—C9B	112.67 (18)
C2B—C1B—N1B	133.0 (2)	H8BA—C8B—H8BB	107.8
C6B—C1B—N1B	106.08 (18)	C9B—C8B—H8BA	109.1
C6B—C1B—C2B	120.8 (2)	C9B—C8B—H8BB	109.1
C1—C2—H2	120.5	C8—C9—H9	120.1
C3—C2—C1	119.0 (2)	C8—C9—C10	119.8 (3)
C3—C2—H2	120.5	C10—C9—H9	120.1
C1A—C2A—H2A	122.2	C8A—C9A—H9AA	109.2
C1A—C2A—C3A	115.6 (2)	C8A—C9A—H9AB	109.2
C3A—C2A—H2A	122.2	C8A—C9A—C10A	112.01 (18)
C1B—C2B—H2B	121.9	H9AA—C9A—H9AB	107.9
C3B—C2B—C1B	116.2 (2)	C10A—C9A—H9AA	109.2
C3B—C2B—H2B	121.9	C10A—C9A—H9AB	109.2
C2—C3—H3	120.0	C8B—C9B—H9BA	108.8
C2—C3—C4	120.1 (2)	C8B—C9B—H9BB	108.8
C4—C3—H3	120.0	H9BA—C9B—H9BB	107.6
C2A—C3A—H3A	118.9	C10B—C9B—C8B	114.0 (2)
C4A—C3A—C2A	122.2 (2)	C10B—C9B—H9BA	108.8
C4A—C3A—H3A	118.9	C10B—C9B—H9BB	108.8
C2B—C3B—H3B	119.1	N2—C10—C9	122.2 (2)
C2B—C3B—C4B	121.8 (2)	N2—C10—H10	118.9
C4B—C3B—H3B	119.1	C9—C10—H10	118.9

C3—C4—C5	124.4 (2)	O2A—C10A—C9A	114.07 (18)
C3—C4—C12	117.0 (2)	O3A—C10A—O2A	125.2 (2)
C12—C4—C5	118.7 (2)	O3A—C10A—C9A	120.73 (19)
C3A—C4A—H4A	119.1	O2B—C10B—C9B	114.9 (2)
C5A—C4A—C3A	121.9 (2)	O3B—C10B—O2B	123.0 (2)
C5A—C4A—H4A	119.1	O3B—C10B—C9B	122.1 (2)
C3B—C4B—H4B	119.0	N2—C11—C7	122.6 (2)
C5B—C4B—C3B	122.0 (2)	N2—C11—C12	117.59 (18)
C5B—C4B—H4B	119.0	C7—C11—C12	119.8 (2)
C4—C5—H5	119.1	N1—C12—C4	122.7 (2)
C6—C5—C4	121.8 (2)	N1—C12—C11	117.61 (19)
C6—C5—H5	119.1	C4—C12—C11	119.7 (2)
C4A—C5A—H5A	122.2	H2WA—O2W—H2WB	104.5

Zn1—O2A—C10A—O3A	−1.1 (3)	C4B—C5B—C6B—C1B	0.5 (3)
Zn1—O2A—C10A—C9A	179.76 (15)	C5—C4—C12—N1	−179.3 (2)
Zn1—O2B—C10B—O3B	−6.5 (3)	C5—C4—C12—C11	0.1 (3)
Zn1—O2B—C10B—C9B	172.80 (16)	C5—C6—C7—C8	178.4 (3)
Zn1—N1—C1—C2	176.36 (19)	C5—C6—C7—C11	−0.9 (4)
Zn1—N1—C12—C4	−176.40 (17)	C6—C7—C8—C9	179.8 (3)
Zn1—N1—C12—C11	4.1 (2)	C6—C7—C11—N2	−178.6 (2)
Zn1—N2—C10—C9	179.4 (2)	C6—C7—C11—C12	2.2 (4)
Zn1—N2—C11—C7	178.84 (17)	C6A—O1A—C7A—S1A	179.91 (16)
Zn1—N2—C11—C12	−1.9 (2)	C6A—O1A—C7A—N1A	0.2 (2)
N1—C1—C2—C3	−0.9 (4)	C6A—C1A—C2A—C3A	0.2 (3)
N1A—C1A—C2A—C3A	−178.9 (2)	C6B—O1B—C7B—S1B	175.81 (16)
N1A—C1A—C6A—O1A	−0.8 (2)	C6B—O1B—C7B—N1B	−2.3 (2)
N1A—C1A—C6A—C5A	178.3 (2)	C6B—C1B—C2B—C3B	−0.6 (3)
N1A—C8A—C9A—C10A	−179.54 (18)	C7—C8—C9—C10	−0.6 (5)
N1B—C1B—C2B—C3B	−177.5 (2)	C7—C11—C12—N1	177.62 (19)
N1B—C1B—C6B—O1B	−0.4 (2)	C7—C11—C12—C4	−1.8 (3)
N1B—C1B—C6B—C5B	177.8 (2)	C7A—O1A—C6A—C1A	0.4 (2)
N1B—C8B—C9B—C10B	61.4 (3)	C7A—O1A—C6A—C5A	−178.6 (2)
N2—C11—C12—N1	−1.6 (3)	C7A—N1A—C1A—C2A	−179.9 (2)
N2—C11—C12—C4	178.91 (19)	C7A—N1A—C1A—C6A	0.9 (2)
C1—N1—C12—C4	0.2 (3)	C7A—N1A—C8A—C9A	89.8 (2)
C1—N1—C12—C11	−179.2 (2)	C7B—O1B—C6B—C1B	1.7 (2)
C1—C2—C3—C4	0.9 (4)	C7B—O1B—C6B—C5B	−176.5 (2)
C1A—N1A—C7A—S1A	179.61 (17)	C7B—N1B—C1B—C2B	176.1 (2)
C1A—N1A—C7A—O1A	−0.7 (2)	C7B—N1B—C1B—C6B	−1.1 (2)
C1A—N1A—C8A—C9A	−92.4 (2)	C7B—N1B—C8B—C9B	75.1 (3)
C1A—C2A—C3A—C4A	0.4 (3)	C8—C7—C11—N2	2.1 (4)
C1B—N1B—C7B—S1B	−175.82 (17)	C8—C7—C11—C12	−177.1 (2)
C1B—N1B—C7B—O1B	2.1 (2)	C8—C9—C10—N2	1.2 (5)
C1B—N1B—C8B—C9B	−112.2 (2)	C8A—N1A—C1A—C2A	2.1 (3)
C1B—C2B—C3B—C4B	0.4 (4)	C8A—N1A—C1A—C6A	−177.11 (18)
C2—C3—C4—C5	178.7 (3)	C8A—N1A—C7A—S1A	−2.3 (3)
C2—C3—C4—C12	−0.3 (4)	C8A—N1A—C7A—O1A	177.39 (17)

C2A—C1A—C6A—O1A	179.91 (19)	C8A—C9A—C10A—O2A	−164.8 (2)
C2A—C1A—C6A—C5A	−1.0 (3)	C8A—C9A—C10A—O3A	16.0 (3)
C2A—C3A—C4A—C5A	−0.2 (4)	C8B—N1B—C1B—C2B	2.6 (3)
C2B—C1B—C6B—O1B	−178.00 (19)	C8B—N1B—C1B—C6B	−174.67 (18)
C2B—C1B—C6B—C5B	0.2 (3)	C8B—N1B—C7B—S1B	−2.1 (3)
C2B—C3B—C4B—C5B	0.3 (4)	C8B—N1B—C7B—O1B	175.90 (17)
C3—C4—C5—C6	−177.7 (3)	C8B—C9B—C10B—O2B	−160.3 (2)
C3—C4—C12—N1	−0.3 (3)	C8B—C9B—C10B—O3B	19.1 (3)
C3—C4—C12—C11	179.2 (2)	C10—N2—C11—C7	−1.6 (3)
C3A—C4A—C5A—C6A	−0.6 (4)	C10—N2—C11—C12	177.6 (2)
C3B—C4B—C5B—C6B	−0.7 (4)	C11—N2—C10—C9	−0.1 (4)
C4—C5—C6—C7	−0.9 (5)	C11—C7—C8—C9	−0.9 (4)
C4A—C5A—C6A—O1A	−179.9 (2)	C12—N1—C1—C2	0.4 (4)
C4A—C5A—C6A—C1A	1.2 (3)	C12—C4—C5—C6	1.2 (4)
C4B—C5B—C6B—O1B	178.3 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O2*W*^{i}	0.85 (3)	1.95 (3)	2.749 (3)	155 (3)
O1*W*—H1*WB*···O2*B*^{i}	0.86 (3)	1.94 (3)	2.751 (3)	159 (3)
O2*W*—H2*WA*···O2*A*	0.85	1.96	2.797 (3)	170
O2*W*—H2*WB*···O2*B*^{ii}	0.85	2.46	3.245 (3)	154
C1—H1···O2*W*^{ii}	0.93	2.39	3.319 (4)	178
C8*A*—H8*AB*···S1*A*^{iii}	0.97	2.87	3.716 (2)	146

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