

catena-Poly[[[aqua(pyrazine-2-carboxamide- κ^2N^1,O)zinc]- μ -pyrazine-2-carboxamide- $\kappa^3N^1,O:N^4$] dinitrate]

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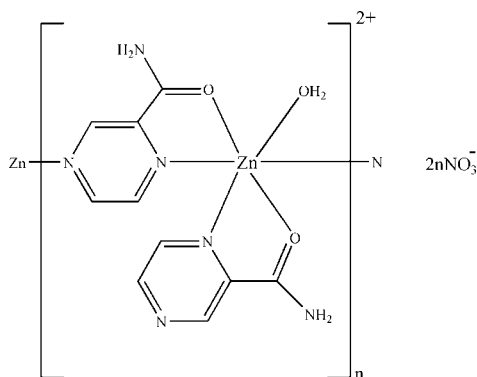
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(C-C) = 0.009$ Å; R factor = 0.076; wR factor = 0.103; data-to-parameter ratio = 12.2.

In the crystal of the title compound, $\{[Zn(C_5H_5N_3O)_2(H_2O)](NO_3)_2\}_n$, the Zn^{II} cation is N,O -chelated by two pyrazine-2-carboxamide (PCA) ligands and is further coordinated by one water molecule and by one pyrazine-N atom from an adjacent PCA ligand in a distorted ZnN_3O_3 octahedral geometry. One of the two independent PCA ligands bridges two Zn^{II} cations, forming a zigzag polymeric chain running along the c axis. In the crystal, the NO_3^- anions link to the chain via $O-H\cdots O$ and $N-H\cdots O$ hydrogen bonding. Weak intermolecular $C-H\cdots O$ interactions also occur.

Related literature

For related structures, see: Shirvan & Haydari Dezfali (2012); Abu-Youssef *et al.* (2006); Azhdari Tehrani *et al.* (2010); Goher & Mautner (2000); Kristiansson (2002); Mir Mohammad Sadegh *et al.* (2010); Munakata *et al.* (1997); Pacigova *et al.* (2008).



Experimental

Crystal data

$[Zn(C_5H_5N_3O)_2(H_2O)](NO_3)_2$
 $M_r = 453.67$
Monoclinic, $P2_1/c$

$a = 10.4889$ (11) Å
 $b = 15.7477$ (16) Å
 $c = 9.9332$ (10) Å

$\beta = 97.664$ (8)°
 $V = 1626.1$ (3) Å³
 $Z = 4$
Mo $K\alpha$ radiation

$\mu = 1.58$ mm⁻¹
 $T = 298$ K
 $0.23 \times 0.12 \times 0.10$ mm

Data collection

Bruker APEXII CCD area detector
diffractometer
Absorption correction: multi-scan
(*SADABS*; Bruker, 2001)
 $T_{min} = 0.070$, $T_{max} = 0.240$

9288 measured reflections
3192 independent reflections
2088 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.123$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.076$
 $wR(F^2) = 0.103$
 $S = 1.06$
3192 reflections
261 parameters

H atoms treated by a mixture of
independent and constrained
refinement
 $\Delta\rho_{max} = 0.46$ e Å⁻³
 $\Delta\rho_{min} = -0.52$ e Å⁻³

Table 1

Selected bond lengths (Å).

Zn1—O1	2.064 (3)	Zn1—N1	2.180 (5)
Zn1—O2	2.073 (3)	Zn1—N4	2.193 (5)
Zn1—O3	2.042 (6)	Zn1—N5 ⁱ	2.179 (5)

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3B $\cdots$ O8 ⁱⁱ	0.76 (7)	2.05 (7)	2.810 (8)	177 (7)
O3—H3C $\cdots$ O4	0.75 (6)	2.06 (7)	2.781 (8)	162 (9)
N3—H3D $\cdots$ O3 ⁱⁱ	0.86	2.50	3.193 (8)	138
N3—H3D $\cdots$ O5 ⁱⁱ	0.86	2.42	3.163 (8)	144
N3—H3E $\cdots$ O7	0.86	2.08	2.937 (8)	172
N6—H6B $\cdots$ O4 ⁱⁱⁱ	0.86	2.07	2.913 (7)	166
N6—H6C $\cdots$ O5 ^{iv}	0.86	2.41	3.231 (8)	161
C1—H1 $\cdots$ O8 ^v	0.93	2.39	3.292 (8)	162
C3—H3 $\cdots$ O7	0.93	2.31	3.227 (8)	169
C6—H6 $\cdots$ O6 ^{vi}	0.93	2.60	3.295 (8)	132
C7—H7 $\cdots$ O5 ^{vi}	0.93	2.49	3.362 (8)	156
C8—H8 $\cdots$ O4 ⁱⁱⁱ	0.93	2.39	3.298 (7)	167

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

We are grateful to the Islamic Azad University, Omidieh Branch for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5508).

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supporting information

Acta Cryst. (2012). E68, m627–m628 [https://doi.org/10.1107/S1600536812016017]

catena-Poly[[[aqua(pyrazine-2-carboxamide- $\kappa^2 N^1, O$)zinc]- μ -pyrazine-2-carboxamide- $\kappa^3 N^1, O:N^4$] dinitrate]

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S1. Comment

In a recent paper, we reported the synthesis and crystal structure of $[ZnBr_2(pzc)_2]$ (Shirvan & Haydari Dezfuli, 2012), where pzc is the pyrazine-2-carboxamide. Pyrazine-2-carboxamide is a good ligand, and a few complexes with pzc have been prepared, such as that of mercury (Azhdari Tehrani *et al.*, 2010; Mir Mohammad Sadegh *et al.*, 2010) and vanadium (Pacigova *et al.*, 2008), manganese (Abu-Youssef *et al.*, 2006) and copper (Kristiansson, 2002; Munakata *et al.*, 1997; Goher & Mautner, 2000). Here, we report the synthesis and structure of the title compound.

The asymmetric unit of the title compound, (Fig. 1), contains one Zn^{II} cation, two pyrazine-2-carboxamide ligands, one water molecule and two NO_3^- counter-ions. The Zn^{II} atom is six-coordinated in a distorted octahedral configuration by two N and two O atoms from two pyrazine-2-carboxamide ligands and one O atom from one water molecule. The sixth coordination site is occupied by N atom from one bridging pyrazine-2-carboxamide ligand. The Zn—O and Zn—N bond lengths and angles are collected in Table 1.

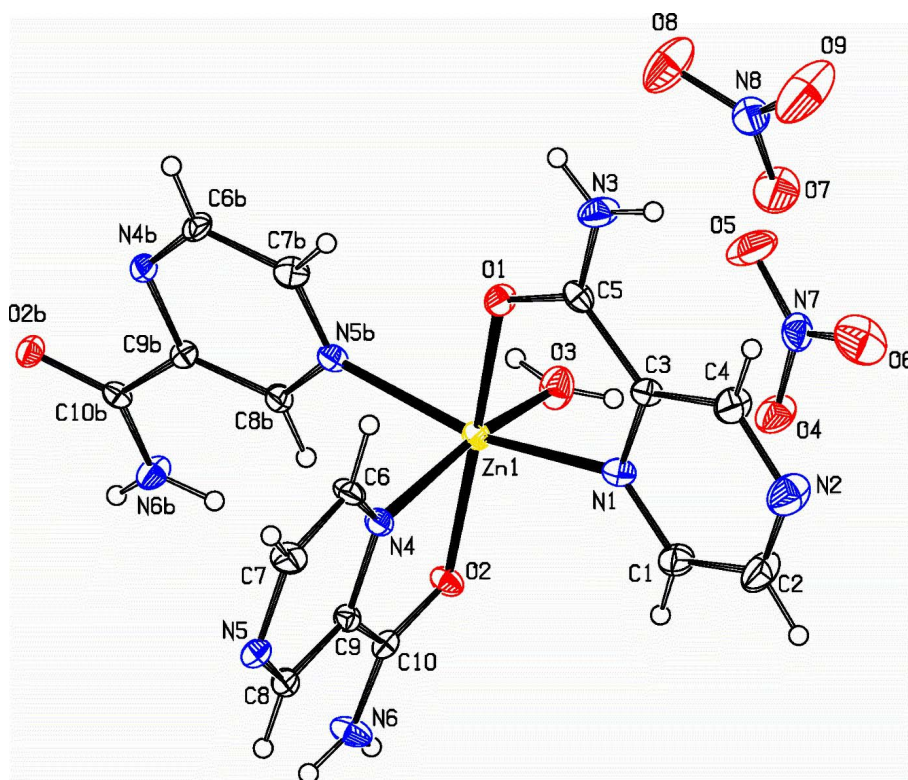
In the crystal structure, intra and intermolecular O—H $\cdots$ O, N—H $\cdots$ O and C—H $\cdots$ O hydrogen bonds (Table 2, Fig. 2) may stabilize the structure.

S2. Experimental

A solution of pyrazine-2-carboxamide (0.25 g, 2.0 mmol) in methanol (10 ml) was added to a solution of $Zn(NO_3)_2 \cdot 4H_2O$ (0.26 g, 1.0 mmol) in methanol (10 ml) and the resulting colorless solution was stirred for 15 min at room temperature. This solution was left to evaporate slowly at room temperature. After one week, colorless block crystals of the title compound were isolated (yield 0.36 g, 79.3%).

S3. Refinement

Water H atoms were located in a difference Fourier map and refined isotropically. Other H atoms were positioned geometrically with C—H = 0.93 and N—H = 0.86 Å, and constrained to ride on their parent atoms with $U_{iso}(H) = 1.2U_{eq}(N,C)$.

**Figure 1**

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (b) $x, 3/2 - y, 1/2 + z$].

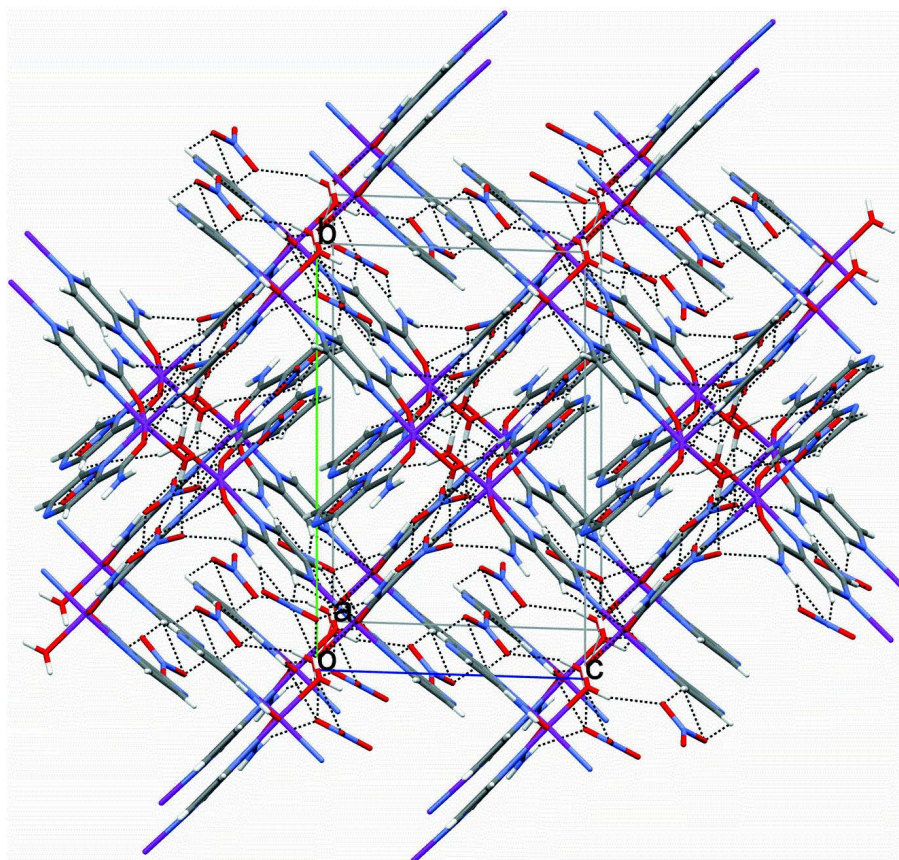


Figure 2

Unit-cell packing diagram for title molecule. Hydrogen bonds are shown as dashed lines.

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Crystal data

$[\text{Zn}(\text{C}_5\text{H}_5\text{N}_3\text{O})_2(\text{H}_2\text{O})](\text{NO}_3)_2$

$M_r = 453.67$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1\text{ybc}$

$a = 10.4889\ (11)\ \text{\AA}$

$b = 15.7477\ (16)\ \text{\AA}$

$c = 9.9332\ (10)\ \text{\AA}$

$\beta = 97.664\ (8)^\circ$

$V = 1626.1\ (3)\ \text{\AA}^3$

$Z = 4$

$F(000) = 920$

$D_x = 1.853\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 9288 reflections

$\theta = 2.4\text{--}26.0^\circ$

$\mu = 1.58\ \text{mm}^{-1}$

$T = 298\ \text{K}$

Block, colorless

$0.23 \times 0.12 \times 0.10\ \text{mm}$

Data collection

Bruker APEXII CCD area detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2001)

$T_{\min} = 0.070$, $T_{\max} = 0.240$

9288 measured reflections

3192 independent reflections

2088 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.123$

$\theta_{\max} = 26.0^\circ$, $\theta_{\min} = 2.4^\circ$

$h = -12 \rightarrow 12$

$k = -19 \rightarrow 19$

$l = -12 \rightarrow 11$

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.076$ $wR(F^2) = 0.103$ $S = 1.06$

3192 reflections

261 parameters

0 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sitesH atoms treated by a mixture of independent
and constrained refinement $w = 1/[\sigma^2(F_o^2) + (0.0237P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.006$ $\Delta\rho_{\max} = 0.46 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.52 \text{ e } \text{\AA}^{-3}$ *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 ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.7871 (6)	0.4587 (4)	0.1320 (7)	0.0329 (15)
H1	0.8748	0.4701	0.1417	0.039*
C2	0.7334 (6)	0.4048 (5)	0.0291 (7)	0.0445 (17)
H2	0.7859	0.3819	−0.0300	0.053*
C3	0.5393 (6)	0.4184 (4)	0.1012 (7)	0.0387 (16)
H3	0.4526	0.4043	0.0946	0.046*
C4	0.5906 (5)	0.4738 (3)	0.2038 (6)	0.0210 (12)
C5	0.5169 (5)	0.5161 (3)	0.3017 (6)	0.0237 (13)
C6	0.6418 (5)	0.7234 (4)	0.1580 (7)	0.0248 (14)
H6	0.5624	0.7048	0.1782	0.030*
C7	0.6463 (5)	0.7868 (4)	0.0610 (7)	0.0292 (15)
H7	0.5699	0.8084	0.0154	0.035*
C8	0.8651 (5)	0.7831 (3)	0.0990 (6)	0.0240 (14)
H8	0.9445	0.8033	0.0814	0.029*
C9	0.8615 (5)	0.7189 (3)	0.1932 (6)	0.0189 (12)
C10	0.9758 (5)	0.6759 (3)	0.2712 (6)	0.0207 (13)
N1	0.7158 (4)	0.4940 (3)	0.2159 (5)	0.0246 (12)
N2	0.6089 (5)	0.3848 (4)	0.0128 (6)	0.0483 (16)
N3	0.3939 (5)	0.5002 (3)	0.3014 (6)	0.0366 (14)
H3D	0.3515	0.5264	0.3571	0.044*
H3E	0.3558	0.4637	0.2454	0.044*
N4	0.7479 (4)	0.6893 (3)	0.2219 (5)	0.0228 (12)
N5	0.7584 (4)	0.8170 (3)	0.0325 (5)	0.0225 (11)
N6	1.0915 (4)	0.7048 (3)	0.2613 (5)	0.0317 (13)

H6C	1.1576	0.6814	0.3071	0.038*
H6B	1.1012	0.7472	0.2090	0.038*
N7	0.7146 (5)	0.3192 (3)	0.4190 (7)	0.0350 (13)
N8	0.1273 (5)	0.4024 (4)	0.1241 (6)	0.0361 (13)
O1	0.5749 (3)	0.5684 (2)	0.3812 (4)	0.0300 (11)
O2	0.9561 (3)	0.6152 (2)	0.3448 (4)	0.0252 (9)
O3	0.8371 (5)	0.5012 (4)	0.5193 (6)	0.0397 (13)
H3C	0.850 (7)	0.456 (4)	0.503 (8)	0.04 (3)*
H3B	0.853 (6)	0.510 (4)	0.595 (7)	0.03 (2)*
O4	0.8335 (4)	0.3362 (3)	0.4190 (5)	0.0437 (12)
O5	0.6640 (5)	0.3426 (4)	0.5181 (7)	0.080 (2)
O6	0.6571 (5)	0.2815 (4)	0.3235 (6)	0.0633 (16)
O7	0.2393 (5)	0.3816 (3)	0.1188 (7)	0.0622 (15)
O8	0.1027 (5)	0.4586 (4)	0.2039 (6)	0.0669 (17)
O9	0.0400 (5)	0.3687 (4)	0.0522 (8)	0.098 (3)
Zn1	0.76855 (6)	0.58798 (4)	0.37477 (7)	0.02037 (17)

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.021 (3)	0.037 (3)	0.042 (4)	0.001 (3)	0.007 (3)	−0.005 (3)
C2	0.044 (4)	0.049 (4)	0.041 (4)	0.003 (4)	0.008 (3)	−0.020 (4)
C3	0.030 (3)	0.048 (4)	0.038 (4)	−0.012 (3)	0.004 (3)	−0.020 (4)
C4	0.020 (3)	0.028 (3)	0.015 (3)	−0.003 (2)	0.000 (2)	−0.001 (3)
C5	0.023 (3)	0.023 (3)	0.025 (4)	−0.003 (2)	−0.001 (3)	0.005 (3)
C6	0.018 (3)	0.025 (3)	0.033 (4)	−0.004 (2)	0.007 (3)	0.006 (3)
C7	0.013 (3)	0.035 (4)	0.039 (4)	0.001 (2)	0.001 (3)	0.003 (3)
C8	0.021 (3)	0.019 (3)	0.033 (4)	0.001 (2)	0.007 (3)	−0.001 (3)
C9	0.017 (3)	0.020 (3)	0.018 (3)	−0.002 (2)	0.001 (2)	−0.001 (2)
C10	0.022 (3)	0.021 (3)	0.020 (3)	0.003 (2)	0.004 (2)	−0.004 (3)
N1	0.021 (2)	0.030 (3)	0.023 (3)	−0.001 (2)	0.003 (2)	0.003 (2)
N2	0.038 (3)	0.060 (4)	0.046 (4)	−0.004 (3)	0.003 (3)	−0.021 (3)
N3	0.023 (3)	0.052 (3)	0.035 (4)	−0.004 (2)	0.009 (2)	−0.011 (3)
N4	0.020 (2)	0.020 (3)	0.029 (3)	0.000 (2)	0.006 (2)	0.003 (2)
N5	0.022 (2)	0.024 (2)	0.021 (3)	0.005 (2)	0.004 (2)	−0.002 (2)
N6	0.015 (2)	0.039 (3)	0.041 (4)	0.001 (2)	0.003 (2)	0.017 (3)
N7	0.027 (3)	0.025 (3)	0.053 (4)	0.002 (2)	0.004 (3)	−0.004 (3)
N8	0.030 (3)	0.035 (3)	0.042 (4)	0.003 (3)	0.002 (3)	0.001 (3)
O1	0.022 (2)	0.034 (3)	0.035 (3)	−0.0099 (18)	0.0051 (19)	−0.017 (2)
O2	0.020 (2)	0.025 (2)	0.031 (3)	0.0002 (16)	0.0029 (18)	0.0098 (18)
O3	0.053 (3)	0.034 (3)	0.030 (4)	0.009 (3)	0.000 (3)	0.005 (3)
O4	0.024 (2)	0.052 (3)	0.056 (4)	0.001 (2)	0.007 (2)	−0.017 (3)
O5	0.063 (4)	0.087 (4)	0.103 (5)	−0.015 (3)	0.057 (4)	−0.041 (4)
O6	0.045 (3)	0.077 (4)	0.063 (4)	−0.022 (3)	−0.009 (3)	−0.006 (3)
O7	0.028 (3)	0.065 (3)	0.094 (4)	−0.006 (3)	0.010 (3)	−0.022 (3)
O8	0.052 (3)	0.088 (4)	0.056 (4)	0.018 (3)	−0.009 (3)	−0.039 (3)
O9	0.026 (3)	0.135 (6)	0.127 (6)	0.003 (3)	−0.007 (3)	−0.092 (5)
Zn1	0.0182 (3)	0.0208 (3)	0.0216 (3)	−0.0026 (3)	0.0009 (2)	−0.0004 (4)

Geometric parameters (Å, °)

Zn1—O1	2.064 (3)	N4—C9	1.345 (7)
Zn1—O2	2.073 (3)	N4—C6	1.320 (7)
Zn1—O3	2.042 (6)	N5—C8	1.333 (7)
Zn1—N1	2.180 (5)	N5—C7	1.333 (7)
Zn1—N4	2.193 (5)	N6—C10	1.312 (7)
Zn1—N5 ⁱ	2.179 (5)	N3—H3E	0.8600
O1—C5	1.243 (6)	N3—H3D	0.8600
O2—C10	1.237 (6)	N6—H6B	0.8600
O3—H3B	0.76 (7)	N6—H6C	0.8600
O3—H3C	0.75 (6)	C1—C2	1.389 (10)
O4—N7	1.276 (7)	C3—C4	1.394 (9)
O5—N7	1.235 (9)	C4—C5	1.479 (8)
O6—N7	1.210 (9)	C6—C7	1.393 (9)
O7—N8	1.227 (8)	C8—C9	1.382 (7)
O8—N8	1.238 (9)	C9—C10	1.500 (8)
O9—N8	1.207 (9)	C1—H1	0.9300
N1—C4	1.341 (7)	C2—H2	0.9300
N1—C1	1.315 (8)	C3—H3	0.9300
N2—C2	1.332 (8)	C6—H6	0.9300
N2—C3	1.325 (9)	C7—H7	0.9300
N3—C5	1.314 (7)	C8—H8	0.9300
Zn1...H3D ⁱⁱ	3.5800	N4...C10	2.385 (7)
O1...O3	3.092 (6)	N4...N5 ⁱ	3.074 (7)
O1...N1	2.627 (6)	N5...N4 ^{viii}	3.074 (7)
O1...N4	3.192 (6)	N5...O3 ^{viii}	2.987 (8)
O1...C4	2.330 (7)	N5...O1 ^{viii}	2.907 (6)
O1...O5 ⁱⁱ	3.148 (7)	N5...N4	2.766 (7)
O1...N5 ⁱ	2.907 (6)	N5...O2 ^{viii}	3.154 (6)
O1...C7 ⁱ	2.932 (7)	N6...O6 ^{ix}	3.117 (7)
O2...C9	2.350 (6)	N6...O4 ^{ix}	2.913 (7)
O2...O3	2.892 (7)	N6...O4 ⁱⁱⁱ	3.233 (7)
O2...N4	2.629 (6)	N6...O5 ⁱⁱⁱ	3.231 (8)
O2...C8 ⁱ	3.240 (7)	N7...C4	3.383 (8)
O2...O3 ⁱⁱⁱ	3.018 (7)	N7...O3	3.243 (8)
O2...O4 ⁱⁱⁱ	3.095 (6)	N8...C8 ^v	3.323 (8)
O2...N5 ⁱ	3.154 (6)	N8...C9 ^v	3.406 (8)
O3...N1	3.113 (8)	N2...H6 ^{vii}	2.8100
O3...O5	3.087 (8)	N3...H3B ⁱⁱ	2.92 (6)
O3...N5 ⁱ	2.987 (8)	N3...H3	2.6900
O3...O2 ⁱⁱⁱ	3.018 (7)	N5...H3B ^{viii}	2.94 (6)
O3...O1	3.092 (6)	N6...H8	2.6900
O3...O2	2.892 (7)	N7...H6C ⁱⁱⁱ	2.8700
O3...O4	2.781 (8)	N7...H3C	2.65 (7)
O3...O8 ⁱⁱ	2.810 (8)	N7...H6B ^{iv}	2.7000
O3...N7	3.243 (8)	N8...H1 ^{vi}	2.8800

O3...N3 ⁱⁱ	3.193 (8)	N8...H3E	2.7100
O4...O3	2.781 (8)	C1...O9 ^x	3.199 (9)
O4...C8 ^{iv}	3.298 (7)	C1...O8 ^x	3.292 (8)
O4...N6 ⁱⁱⁱ	3.233 (7)	C2...O9 ^x	3.244 (8)
O4...O2 ⁱⁱⁱ	3.095 (6)	C3...O6	3.213 (9)
O4...N6 ^{iv}	2.913 (7)	C3...O7	3.227 (8)
O5...C7 ^v	3.362 (8)	C3...C4 ^{vii}	3.580 (9)
O5...N6 ⁱⁱⁱ	3.231 (8)	C3...C3 ^{vii}	3.299 (9)
O5...N3 ⁱⁱ	3.163 (8)	C4...C3 ^{vii}	3.580 (9)
O5...O1 ⁱⁱ	3.148 (7)	C4...O6	3.294 (8)
O5...O3	3.087 (8)	C4...N7	3.383 (8)
O6...N6 ^{iv}	3.117 (7)	C6...N2 ^{vii}	3.392 (8)
O6...C4	3.294 (8)	C6...O6 ^{xi}	3.295 (8)
O6...C3	3.213 (9)	C7...O5 ^{xi}	3.362 (8)
O6...C6 ^v	3.295 (8)	C8...N8 ^{xi}	3.323 (8)
O7...C3	3.227 (8)	C8...O9 ^{vii}	3.059 (8)
O7...N3	2.937 (8)	C8...O8 ^{xi}	3.378 (8)
O8...C8 ^v	3.378 (8)	C8...O4 ^{ix}	3.298 (7)
O8...C1 ^{vi}	3.292 (8)	C9...N8 ^{xi}	3.406 (8)
O8...N3	3.148 (8)	C9...O9 ^{vii}	3.096 (9)
O8...O3 ⁱⁱ	2.810 (8)	C10...O9 ^{vii}	3.271 (10)
O9...C9 ^{vii}	3.096 (9)	C3...H3E	2.6500
O9...C2 ^{vi}	3.244 (8)	C8...H6B	2.6300
O9...C8 ^{vii}	3.059 (8)	H1...O8 ^x	2.3900
O9...C1 ^{vi}	3.199 (9)	H1...O9 ^x	2.6000
O9...C10 ^{vii}	3.271 (10)	H1...N8 ^x	2.8800
O1...H7 ⁱ	2.3600	H2...O9 ^x	2.6900
O2...H3C ⁱⁱⁱ	2.62 (7)	H3...N3	2.6900
O2...H3B ⁱⁱⁱ	2.82 (6)	H3...H3E	2.1300
O2...H8 ⁱ	2.6900	H3...O7	2.3100
O3...H3D ⁱⁱ	2.5000	H3B...O2 ⁱⁱⁱ	2.82 (6)
O4...H3C	2.06 (7)	H3B...H3D ⁱⁱ	2.3300
O4...H6C ⁱⁱⁱ	2.7200	H3B...O8 ⁱⁱ	2.05 (7)
O4...H6B ^{iv}	2.0700	H3B...N3 ⁱⁱ	2.92 (6)
O4...H8 ^{iv}	2.3900	H3C...O5	2.66 (7)
O5...H3C	2.66 (7)	H3C...O4	2.06 (7)
O5...H6C ⁱⁱⁱ	2.4100	H3C...N7	2.65 (7)
O5...H7 ^v	2.4900	H3C...O2 ⁱⁱⁱ	2.62 (7)
O5...H3D ⁱⁱ	2.4200	H3D...Zn1 ⁱⁱ	3.5800
O6...H6 ^v	2.6000	H3D...H3B ⁱⁱ	2.3300
O6...H6B ^{iv}	2.6500	H3D...O3 ⁱⁱ	2.5000
O7...H3	2.3100	H3D...O5 ⁱⁱ	2.4200
O7...H3E	2.0800	H3E...O7	2.0800
O8...H3E	2.6300	H3E...O8	2.6300
O8...H1 ^{vi}	2.3900	H3E...N8	2.7100
O8...H3B ⁱⁱ	2.05 (7)	H3E...C3	2.6500
O9...H2 ^{vi}	2.6900	H3E...H3	2.1300
O9...H1 ^{vi}	2.6000	H6...N2 ^{vii}	2.8100

N1...C5	2.382 (7)	H6...O6 ^{xi}	2.6000
N1...O1	2.627 (6)	H6B...O6 ^{ix}	2.6500
N1...N2	2.772 (8)	H6B...O4 ^{ix}	2.0700
N1...N4	3.094 (7)	H6B...N7 ^{ix}	2.7000
N1...O3	3.113 (8)	H6B...H8	2.1300
N2...N1	2.772 (8)	H6B...C8	2.6300
N2...C6 ^{vii}	3.392 (8)	H6C...O5 ⁱⁱⁱ	2.4100
N3...O5 ⁱⁱ	3.163 (8)	H6C...O4 ⁱⁱⁱ	2.7200
N3...O7	2.937 (8)	H6C...N7 ⁱⁱⁱ	2.8700
N3...O3 ⁱⁱ	3.193 (8)	H7...O5 ^{xi}	2.4900
N3...O8	3.148 (8)	H7...O1 ^{viii}	2.3600
N4...N1	3.094 (7)	H8...O4 ^{ix}	2.3900
N4...O1	3.192 (6)	H8...O2 ^{viii}	2.6900
N4...O2	2.629 (6)	H8...N6	2.6900
N4...N5	2.766 (7)	H8...H6B	2.1300
O1—Zn1—O2	172.71 (15)	O4—N7—O5	117.5 (6)
O1—Zn1—O3	97.70 (18)	O4—N7—O6	119.2 (6)
O1—Zn1—N1	76.42 (15)	O5—N7—O6	123.3 (6)
O1—Zn1—N4	97.09 (15)	O8—N8—O9	119.1 (6)
O1—Zn1—N5 ⁱ	86.43 (15)	O7—N8—O8	120.0 (6)
O2—Zn1—O3	89.28 (18)	O7—N8—O9	120.8 (6)
O2—Zn1—N1	100.98 (15)	N1—C1—C2	121.0 (6)
O2—Zn1—N4	76.01 (15)	N2—C2—C1	121.9 (6)
O2—Zn1—N5 ⁱ	95.71 (15)	N2—C3—C4	122.8 (6)
O3—Zn1—N1	94.9 (2)	C3—C4—C5	125.3 (5)
O3—Zn1—N4	165.13 (19)	N1—C4—C5	115.2 (5)
O3—Zn1—N5 ⁱ	90.0 (2)	N1—C4—C3	119.5 (5)
N1—Zn1—N4	90.03 (18)	O1—C5—C4	117.5 (5)
N1—Zn1—N5 ⁱ	162.62 (16)	O1—C5—N3	121.7 (5)
N4—Zn1—N5 ⁱ	89.34 (18)	N3—C5—C4	120.8 (5)
Zn1—O1—C5	118.7 (3)	N4—C6—C7	121.4 (5)
Zn1—O2—C10	118.8 (3)	N5—C7—C6	121.0 (5)
H3B—O3—H3C	112 (8)	N5—C8—C9	122.1 (5)
Zn1—O3—H3C	123 (6)	C8—C9—C10	126.0 (5)
Zn1—O3—H3B	126 (5)	N4—C9—C10	113.8 (5)
C1—N1—C4	118.4 (5)	N4—C9—C8	120.2 (5)
Zn1—N1—C4	112.1 (4)	O2—C10—C9	118.0 (5)
Zn1—N1—C1	129.4 (4)	N6—C10—C9	119.2 (5)
C2—N2—C3	116.3 (6)	O2—C10—N6	122.8 (5)
Zn1—N4—C6	128.9 (4)	C2—C1—H1	120.00
Zn1—N4—C9	113.0 (3)	N1—C1—H1	119.00
C6—N4—C9	118.1 (5)	N2—C2—H2	119.00
Zn1 ^{viii} —N5—C8	120.9 (4)	C1—C2—H2	119.00
C7—N5—C8	117.3 (5)	N2—C3—H3	119.00
Zn1 ^{viii} —N5—C7	121.8 (4)	C4—C3—H3	119.00
C5—N3—H3E	120.00	C7—C6—H6	119.00
H3D—N3—H3E	120.00	N4—C6—H6	119.00

C5—N3—H3D	120.00	N5—C7—H7	120.00
C10—N6—H6B	120.00	C6—C7—H7	119.00
C10—N6—H6C	120.00	C9—C8—H8	119.00
H6B—N6—H6C	120.00	N5—C8—H8	119.00
O3—Zn1—O1—C5	−92.4 (4)	Zn1—O2—C10—N6	170.5 (4)
N1—Zn1—O1—C5	0.9 (4)	Zn1—O2—C10—C9	−8.1 (6)
N4—Zn1—O1—C5	89.2 (4)	Zn1—N1—C4—C5	−2.1 (6)
N5 ⁱ —Zn1—O1—C5	178.1 (4)	C1—N1—C4—C3	−1.8 (8)
O3—Zn1—O2—C10	−171.7 (4)	C4—N1—C1—C2	3.0 (9)
N1—Zn1—O2—C10	93.4 (4)	Zn1—N1—C4—C3	176.1 (4)
N4—Zn1—O2—C10	6.2 (4)	Zn1—N1—C1—C2	−174.5 (5)
N5 ⁱ —Zn1—O2—C10	−81.7 (4)	C1—N1—C4—C5	−180.0 (5)
O1—Zn1—N1—C1	178.4 (6)	C2—N2—C3—C4	1.9 (10)
O2—Zn1—N1—C1	5.4 (6)	C3—N2—C2—C1	−0.8 (10)
O3—Zn1—N1—C1	−84.9 (5)	Zn1—N4—C9—C8	−179.9 (4)
N4—Zn1—N1—C1	81.1 (5)	Zn1—N4—C6—C7	−178.8 (5)
O1—Zn1—N1—C4	0.8 (4)	C6—N4—C9—C10	−180.0 (5)
O2—Zn1—N1—C4	−172.3 (4)	Zn1—N4—C9—C10	0.3 (6)
O3—Zn1—N1—C4	97.5 (4)	C6—N4—C9—C8	−0.1 (8)
N4—Zn1—N1—C4	−96.5 (4)	C9—N4—C6—C7	1.6 (9)
O1—Zn1—N4—C6	−0.4 (5)	C8—N5—C7—C6	1.0 (9)
O2—Zn1—N4—C6	177.3 (6)	Zn1 ^{viii} —N5—C7—C6	177.2 (5)
N1—Zn1—N4—C6	76.0 (5)	Zn1 ^{viii} —N5—C8—C9	−175.8 (4)
N5 ⁱ —Zn1—N4—C6	−86.7 (5)	C7—N5—C8—C9	0.4 (8)
O1—Zn1—N4—C9	179.3 (4)	N1—C1—C2—N2	−1.7 (11)
O2—Zn1—N4—C9	−3.0 (4)	N2—C3—C4—C5	177.3 (6)
N1—Zn1—N4—C9	−104.3 (4)	N2—C3—C4—N1	−0.7 (9)
N5 ⁱ —Zn1—N4—C9	93.0 (4)	N1—C4—C5—N3	−178.8 (5)
O1 ^{viii} —Zn1 ^{viii} —N5—C7	14.9 (5)	N1—C4—C5—O1	3.0 (7)
O2 ^{viii} —Zn1 ^{viii} —N5—C7	−158.1 (5)	C3—C4—C5—N3	3.2 (9)
O3 ^{viii} —Zn1 ^{viii} —N5—C7	112.6 (5)	C3—C4—C5—O1	−175.1 (5)
N4 ^{viii} —Zn1 ^{viii} —N5—C7	−82.2 (5)	N4—C6—C7—N5	−2.1 (10)
O1 ^{viii} —Zn1 ^{viii} —N5—C8	−169.1 (4)	N5—C8—C9—N4	−0.9 (8)
O2 ^{viii} —Zn1 ^{viii} —N5—C8	17.9 (4)	N5—C8—C9—C10	178.9 (5)
O3 ^{viii} —Zn1 ^{viii} —N5—C8	−71.4 (4)	N4—C9—C10—O2	5.0 (7)
N4 ^{viii} —Zn1 ^{viii} —N5—C8	93.8 (4)	C8—C9—C10—N6	6.5 (8)
Zn1—O1—C5—N3	179.4 (4)	N4—C9—C10—N6	−173.6 (5)
Zn1—O1—C5—C4	−2.3 (6)	C8—C9—C10—O2	−174.9 (5)

Symmetry codes: (i) $x, -y+3/2, z+1/2$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x+2, -y+1, -z+1$; (iv) $-x+2, y-1/2, -z+1/2$; (v) $-x+1, y-1/2, -z+1/2$; (vi) $x-1, y, z$; (vii) $-x+1, -y+1, -z$; (viii) $x, -y+3/2, z-1/2$; (ix) $-x+2, y+1/2, -z+1/2$; (x) $x+1, y, z$; (xi) $-x+1, y+1/2, -z+1/2$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D\cdots H\cdots A$	$D\cdots H$	$H\cdots A$	$D\cdots A$	$D\cdots H\cdots A$
O3—H3B $\cdots$ O8 ⁱⁱ	0.76 (7)	2.05 (7)	2.810 (8)	177 (7)
O3—H3C $\cdots$ O4	0.75 (6)	2.06 (7)	2.781 (8)	162 (9)
N3—H3D $\cdots$ O3 ⁱⁱ	0.86	2.50	3.193 (8)	138

N3—H3 <i>D</i> ...O5 ⁱⁱ	0.86	2.42	3.163 (8)	144
N3—H3 <i>E</i> ...O7	0.86	2.08	2.937 (8)	172
N6—H6 <i>B</i> ...O4 ^{ix}	0.86	2.07	2.913 (7)	166
N6—H6 <i>C</i> ...O5 ⁱⁱⁱ	0.86	2.41	3.231 (8)	161
C1—H1...O8 ^x	0.93	2.39	3.292 (8)	162
C3—H3...O7	0.93	2.31	3.227 (8)	169
C6—H6...O6 ^{xi}	0.93	2.60	3.295 (8)	132
C7—H7...O5 ^{xi}	0.93	2.49	3.362 (8)	156
C8—H8...O4 ^{ix}	0.93	2.39	3.298 (7)	167

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