

catena-Poly[[[aqua(4,4'-dimethyl-2,2'-bipyridine- κ^2N,N')zinc]- μ -3-chlorobenzene-1,2-dicarboxylato- $\kappa^2O^2:O^3$][[(4,4'-dimethyl-2,2'-bipyridine- κ^2N,N')zinc]- μ -3-chlorobenzene-1,2-dicarboxylato- $\kappa^2O^2:O^3$]]

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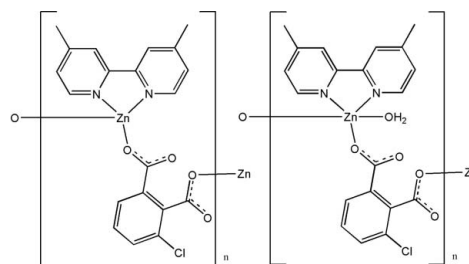
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Key indicators: single-crystal X-ray study; $T = 291$ K; mean $\sigma(C-C) = 0.009$ Å; R factor = 0.056; wR factor = 0.104; data-to-parameter ratio = 12.3.

In the title compound, $\{[Zn(C_8H_3ClO_4)(C_{12}H_{12}N_2)(H_2O)] \cdot [Zn(C_8H_3ClO_4)(C_{12}H_{12}N_2)]\}_n$, one Zn^{2+} ion is five-coordinated by two O atoms from two different 3-chlorobenzene-1,2-dicarboxylate ligands, one O atom from a water molecule and two N atoms from a 4,4'-dimethyl-2,2'-bipyridine ligand, while the second Zn^{2+} ion is four-coordinated by two O atoms from two different 3-chlorobenzene-1,2-dicarboxylate ligands, and two N atoms from a 4,4'-bimethyl-2,2'-bipyridine ligand. The crystal structure exhibits a three-dimensional supramolecular structure composed of alternate $Zn(C_8H_3O_4Cl)(C_{12}H_{12}N_2)$ and $Zn(C_8H_3O_4Cl)(C_{12}H_{12}N_2)(H_2O)$ chains, which are linked together by face-to-face $\pi-\pi$ interactions [shortest centroid-centroid distances of 3.661 (4) and 3.6901 (3) Å], O—H...O and C—H...O hydrogen bonds.

Related literature

For background to the network topologies and applications of coordination polymers, see: Maspoche *et al.* (2007); Ockwig *et al.* (2005); Zang *et al.* (2011). For related O—H...O hydrogen bonds, see: Desiraju *et al.* (2004). For related $\pi-\pi$ interactions, see: Zang *et al.* (2010). For related C—H...O hydrogen bonds, see: Desiraju *et al.* (1996). For related C—H... π interactions, see: Nishio *et al.* (1998).



Experimental

Crystal data

$[Zn(C_8H_3ClO_4)(C_{12}H_{12}N_2)(H_2O)] \cdot [Zn(C_8H_3ClO_4)(C_{12}H_{12}N_2)]$
 $M_r = 914.38$
 Orthorhombic, $Pna2_1$
 $a = 34.050$ (4) Å
 $b = 14.1831$ (10) Å
 $c = 7.8764$ (6) Å
 $V = 3803.8$ (6) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 1.47$ mm⁻¹
 $T = 291$ K
 $0.20 \times 0.18 \times 0.16$ mm

Data collection

Oxford Diffraction Xcalibur Eos Gemini diffractometer
 Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2007)
 $T_{min} = 0.971$, $T_{max} = 1.000$
 10533 measured reflections
 6396 independent reflections
 5076 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.044$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.056$
 $wR(F^2) = 0.104$
 $S = 1.07$
 6396 reflections
 518 parameters
 1 restraint
 H-atom parameters constrained
 $\Delta\rho_{max} = 0.63$ e Å⁻³
 $\Delta\rho_{min} = -0.37$ e Å⁻³
 Absolute structure: Flack (1983), 2200 Friedel pairs
 Flack parameter: 0.093 (14)

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1W—H1WA...O4 ⁱ	0.85	2.10	2.768 (6)	135
O1W—H1WB...O4 ⁱⁱ	0.85	1.79	2.644 (6)	179
O1W—H1WB...O3 ⁱⁱⁱ	0.85	2.43	2.930 (5)	118
C17—H17...O4 ⁱ	0.93	2.36	3.202 (8)	150
C20—H20...O6 ⁱⁱⁱ	0.93	2.28	3.171 (8)	160
C23—H23...O6 ⁱⁱⁱ	0.93	2.40	3.306 (8)	164
C32—H32...O2 ⁱ	0.93	2.57	3.459 (8)	161
C35—H35...O2 ⁱ	0.93	2.45	3.353 (8)	165

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2007); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZQ2156).

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supporting information

Acta Cryst. (2012). E68, m574–m575 [doi:10.1107/S1600536812014006]

catena-Poly[[[aqua(4,4'-dimethyl-2,2'-bipyridine- κ^2N,N')zinc]- μ -3-chlorobenzene-1,2-dicarboxylato- $\kappa^2O^2:O^3$] [(4,4'-dimethyl-2,2'-bipyridine- κ^2N,N')zinc]- μ -3-chlorobenzene-1,2-dicarboxylato- $\kappa^2O^2:O^3$]]

Yu Zhu, Hai-Yang Li and Ming-Li Ma

S1. Comment

In recent years, metallosupramolecular compounds have received much attention due to their variety of architectures and the potential applications as functional materials (MasPOCH *et al.*, 2007; Ockwig *et al.*, 2005). Early reports have shown that carboxylate compounds and nitrogen heterocyclic ligands have been successfully employed in the generation of many novel structures (Zang *et al.*, 2011). To further explore various factors that influence the properties and construction of coordination compounds, we undertake synthetic and structural studies on a novel Zn^{II} complex based on 3-chlorophthalic acid (H₂cp) and 4,4'-dimethyl-2,2'-bipyridine (dmbpy).

The X-ray diffraction study revealed that the title compound crystallizes in the orthorhombic space group *Pna*2₁. The Zn1 atom is five-coordinated by two O atoms from two different 3-chlorobenzene-1,2-dicarboxylato ligands, one O atom from a water molecule and two N atoms from a 4,4'-dimethyl-2,2'-bipyridine ligand, while the Zn2 atom is four-coordinated by two O atoms from two different 3-chlorobenzene-1,2-dicarboxylato ligands, and two N atoms from a 4,4'-bimethyl-2,2'-bipyridine ligand (Fig. 1). Each cp²⁻ ligand acts as a μ_2 -bridge linking two Zn atoms with both carboxylate groups in monodentate fashion resulting into two chains along the *c* axis. These two chains are further connected together by face-to-face π - π interactions (Zang *et al.*, 2010) involving pyridine rings of different chains. The shortest Cg \cdots Cg distances of 3.661 (4) and 3.6901 (3) are observed between Cg2 and Cg4, and Cg1 and Cg3, respectively (Cg1 is the centroid of the N1/C17–C21 ring, Cg2 of N2/C22–C26, Cg3 of N3/C34–C38, and Cg4 of N4/C29–C33). Adjacent zippered structures are linked together to form tetra-chain units by intermolecular O1w—H1wa \cdots O4ⁱⁱⁱ hydrogen bonds (Desiraju *et al.*, 2004) and C17—H17 \cdots O4ⁱⁱⁱ interactions (symmetry code: *iii* = -*x* + 1, -*y* + 1, *z* + 1/2). Each unit is further connected to other units through C20—H20 \cdots O6^{iv}, C23—H23 \cdots O6^{iv} (symmetry code: *iv* = -*x* + 1, -*y* + 1, *z* - 1/2), C32—H32 \cdots O2ⁱⁱⁱ, C35—H35 \cdots O2ⁱⁱⁱ (Desiraju *et al.*, 1996) and C—H \cdots π interactions (the shortest one being C37—H37 \cdots Cg5^v = 2.79 Å; Cg5 centroid of C11–C16; symmetry code: *v* = -*x* + 3/2, *y* - 1/2, *z* - 1/2) (Nishio *et al.*, 1998) to form a three-dimensional supramolecular structure (Fig. 3).

S2. Experimental

The title compound was synthesized hydrothermally in a Teflon-lined stainless steel container by heating a mixture of 3-chlorophthalic acid (H₂cp) (0.0100 g, 0.05 mmol), 4,4'-bimethyl-2,2'-bipyridine (dmbpy) (0.0092 g, 0.05 mmol), Zn(NO₃)₂·6H₂O (0.0149 g, 0.05 mmol) and NaOH (0.0040 g, 0.1 mmol) in 7 ml of distilled water at 120°C for 3 days, and then cooled to room temperature. Colourless block crystals were obtained in 71% yield (based on zinc).

S3. Refinement

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å for aromatic H atoms, C—H = 0.97 Å for methylene H atoms [with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$], and O—H = 0.85 Å for the water H atoms [with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$].

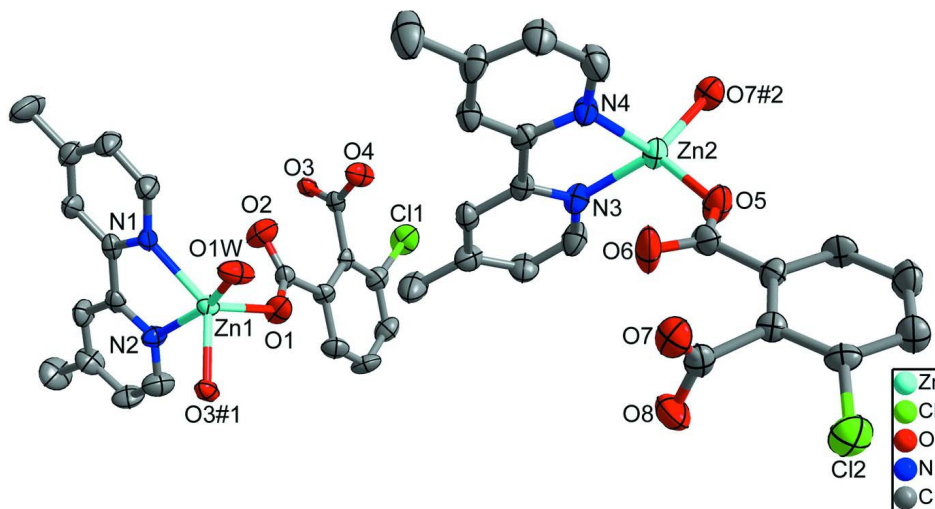


Figure 1

Metal coordination and atom labeling in the title compound (thermal ellipsoids drawn at the 50% probability level). All hydrogen atoms are omitted for clarity. Symmetry code: $x, y, z - 1$.

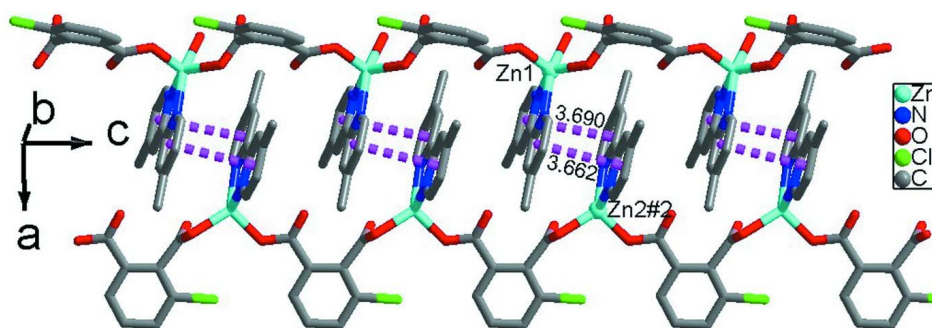
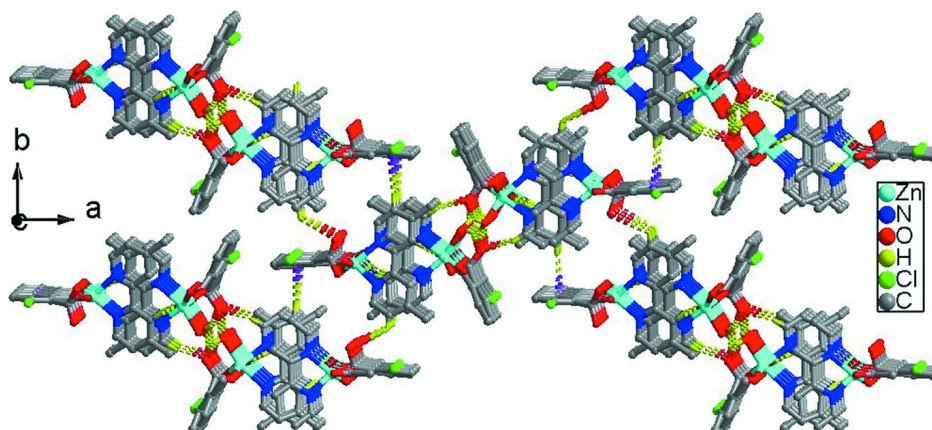


Figure 2

A view of the layered structure of the title compound. Dotted lines represent the π - π interactions (symmetry code: $-x + 1, -y + 1, z + 0.5$.)

**Figure 3**

The three-dimensional supramolecular structure of the title compound (hydrogen bonds and C—H \cdots π interactions as dotted lines).

catena-Poly[[[aqua(4,4'-dimethyl-2,2'-bipyridine- κ^2N,N')zinc]- μ -3-chlorobenzene-1,2-dicarboxylato- $\kappa^2O^2:O^3$][[(4,4'-dimethyl-2,2'-bipyridine- κ^2N,N')zinc]- μ -3-chlorobenzene-1,2-dicarboxylato- $\kappa^2O^2:O^3$]]

Crystal data

$[\text{Zn}(\text{C}_8\text{H}_3\text{ClO}_4)(\text{C}_{12}\text{H}_{12}\text{N}_2)(\text{H}_2\text{O})] \cdot [\text{Zn}(\text{C}_8\text{H}_3\text{ClO}_4)$
 $(\text{C}_{12}\text{H}_{12}\text{N}_2)]$

$M_r = 914.38$

Orthorhombic, $Pna2_1$

$a = 34.050$ (4) Å

$b = 14.1831$ (10) Å

$c = 7.8764$ (6) Å

$V = 3803.8$ (6) Å³

$Z = 4$

$F(000) = 1864$

$D_x = 1.597$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.7107$ Å

Cell parameters from 1842 reflections

$\theta = 2.9\text{--}29.3^\circ$

$\mu = 1.47$ mm⁻¹

$T = 291$ K

Prismatic, colourless

$0.20 \times 0.18 \times 0.16$ mm

Data collection

Oxford Diffraction Xcalibur Eos Gemini
 diffractometer

Radiation source: Enhance (Mo) X-ray Source

Graphite monochromator

Detector resolution: 16.2312 pixels mm⁻¹

ω scans

Absorption correction: multi-scan

(*CrysAlis PRO*; Oxford Diffraction, 2007)

$T_{\min} = 0.971$, $T_{\max} = 1.000$

10533 measured reflections

6396 independent reflections

5076 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.044$

$\theta_{\max} = 26.4^\circ$, $\theta_{\min} = 2.9^\circ$

$h = -18 \rightarrow 42$

$k = -17 \rightarrow 17$

$l = -7 \rightarrow 9$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.056$

$wR(F^2) = 0.104$

$S = 1.07$

6396 reflections

518 parameters

1 restraint

Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map

Hydrogen site location: inferred from
 neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0355P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.63$ e Å⁻³

$\Delta\rho_{\min} = -0.37$ e Å⁻³

Absolute structure: Flack (1983), 2200 Friedel pairs

Absolute structure parameter: 0.093 (14)

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.446526 (19)	0.36444 (4)	0.62772 (9)	0.02863 (16)
Zn2	0.73030 (2)	0.67276 (5)	0.37248 (10)	0.03441 (18)
Cl1	0.53270 (7)	0.15962 (15)	-0.2478 (2)	0.0655 (6)
Cl2	0.84880 (6)	0.65033 (13)	1.2682 (2)	0.0487 (5)
O1	0.48307 (15)	0.3004 (3)	0.4755 (5)	0.0462 (13)
O1W	0.47741 (14)	0.4839 (3)	0.7036 (6)	0.0493 (13)
H1WA	0.4918	0.5028	0.6220	0.074*
H1WB	0.4881	0.4524	0.7830	0.074*
O2	0.45488 (16)	0.3521 (3)	0.2380 (6)	0.0524 (14)
O3	0.46114 (11)	0.2980 (3)	-0.1501 (5)	0.0289 (9)
O4	0.51092 (14)	0.3849 (3)	-0.0516 (5)	0.0450 (12)
O5	0.77114 (14)	0.6635 (4)	0.5400 (6)	0.0487 (13)
O6	0.73636 (14)	0.6683 (4)	0.7724 (6)	0.0651 (17)
O7	0.75751 (13)	0.7136 (3)	1.1661 (5)	0.0400 (11)
O8	0.76227 (13)	0.5605 (3)	1.1177 (7)	0.0553 (13)
N1	0.39925 (14)	0.4462 (3)	0.5397 (6)	0.0282 (12)
N2	0.39966 (14)	0.2639 (3)	0.6065 (7)	0.0315 (12)
N3	0.68490 (14)	0.5810 (3)	0.3955 (6)	0.0335 (12)
N4	0.68816 (15)	0.7651 (3)	0.4601 (6)	0.0329 (13)
C1	0.47656 (19)	0.2992 (5)	0.3164 (7)	0.0305 (15)
C1A	0.49032 (19)	0.3121 (4)	-0.0579 (7)	0.0266 (14)
C2	0.5919 (2)	0.9246 (5)	0.6602 (12)	0.072 (3)
H2A	0.5960	0.9384	0.7781	0.107*
H2B	0.5682	0.8888	0.6473	0.107*
H2C	0.5898	0.9824	0.5975	0.107*
C3	0.49776 (19)	0.2223 (4)	0.2198 (7)	0.0264 (14)
C4	0.50368 (18)	0.2278 (4)	0.0461 (7)	0.0263 (14)
C5	0.5226 (2)	0.1537 (4)	-0.0331 (9)	0.0388 (18)
C6	0.5346 (2)	0.0737 (5)	0.0544 (9)	0.0463 (19)
H6	0.5470	0.0246	-0.0028	0.056*
C7	0.5282 (2)	0.0680 (5)	0.2251 (9)	0.0447 (19)
H7	0.5356	0.0143	0.2846	0.054*
C8	0.5105 (2)	0.1420 (4)	0.3089 (8)	0.0404 (18)

H8	0.5071	0.1388	0.4258	0.049*
C9	0.7673 (2)	0.6666 (5)	0.7003 (9)	0.0356 (17)
C10	0.77225 (18)	0.6434 (4)	1.0906 (7)	0.0325 (15)
C11	0.80563 (19)	0.6689 (4)	0.7983 (7)	0.0292 (15)
C12	0.80732 (19)	0.6604 (4)	0.9751 (7)	0.0251 (14)
C13	0.8441 (2)	0.6620 (4)	1.0484 (8)	0.0308 (15)
C14	0.8786 (2)	0.6732 (4)	0.9570 (9)	0.0384 (17)
H14	0.9028	0.6751	1.0115	0.046*
C15	0.8759 (2)	0.6812 (5)	0.7839 (10)	0.0473 (19)
H15	0.8986	0.6874	0.7192	0.057*
C16	0.8403 (2)	0.6802 (4)	0.7065 (7)	0.0354 (16)
H16	0.8390	0.6873	0.5892	0.043*
C17	0.4015 (2)	0.5397 (4)	0.5072 (9)	0.0426 (17)
H17	0.4248	0.5717	0.5298	0.051*
C18	0.3702 (2)	0.5882 (4)	0.4417 (9)	0.0448 (18)
H18	0.3724	0.6526	0.4209	0.054*
C19	0.3356 (2)	0.5428 (4)	0.4066 (8)	0.0404 (17)
C20	0.33365 (19)	0.4466 (4)	0.4388 (8)	0.0378 (16)
H20	0.3105	0.4136	0.4181	0.045*
C21	0.36621 (18)	0.4002 (4)	0.5020 (7)	0.0281 (14)
C22	0.36610 (18)	0.2978 (4)	0.5409 (7)	0.0285 (14)
C23	0.33407 (19)	0.2400 (4)	0.5094 (8)	0.0371 (16)
H23	0.3112	0.2650	0.4631	0.045*
C24	0.3363 (2)	0.1447 (4)	0.5475 (9)	0.0441 (18)
C25	0.3715 (2)	0.1119 (4)	0.6178 (11)	0.0478 (18)
H25	0.3743	0.0485	0.6453	0.057*
C26	0.4011 (2)	0.1728 (4)	0.6454 (9)	0.0471 (18)
H26	0.4240	0.1497	0.6947	0.057*
C27	0.3001 (2)	0.5942 (5)	0.3372 (12)	0.074 (3)
H27A	0.2881	0.6302	0.4263	0.111*
H27B	0.2816	0.5492	0.2937	0.111*
H27C	0.3082	0.6357	0.2475	0.111*
C28	0.3008 (2)	0.0812 (5)	0.5202 (10)	0.064 (2)
H28A	0.2998	0.0345	0.6084	0.096*
H28B	0.3029	0.0506	0.4119	0.096*
H28C	0.2772	0.1184	0.5233	0.096*
C29	0.6922 (2)	0.8562 (5)	0.4932 (10)	0.0499 (19)
H29	0.7161	0.8853	0.4702	0.060*
C30	0.6618 (2)	0.9098 (4)	0.5612 (9)	0.049 (2)
H30	0.6656	0.9734	0.5847	0.059*
C31	0.62615 (19)	0.8681 (4)	0.5935 (9)	0.0410 (18)
C32	0.62257 (19)	0.7715 (4)	0.5612 (8)	0.0356 (16)
H32	0.5989	0.7408	0.5827	0.043*
C33	0.65364 (19)	0.7224 (4)	0.4983 (7)	0.0290 (14)
C34	0.65222 (19)	0.6193 (4)	0.4647 (7)	0.0296 (15)
C35	0.61938 (19)	0.5652 (4)	0.5012 (7)	0.0351 (16)
H35	0.5973	0.5938	0.5480	0.042*
C36	0.6189 (2)	0.4691 (4)	0.4691 (8)	0.0384 (17)

C37	0.6532 (2)	0.4317 (4)	0.3981 (10)	0.0473 (19)
H37	0.6547	0.3676	0.3745	0.057*
C38	0.6845 (2)	0.4887 (4)	0.3632 (10)	0.0460 (17)
H38	0.7067	0.4617	0.3144	0.055*
C39	0.5834 (2)	0.4107 (5)	0.5081 (10)	0.059 (2)
H39A	0.5900	0.3642	0.5920	0.088*
H39B	0.5746	0.3799	0.4066	0.088*
H39C	0.5629	0.4506	0.5509	0.088*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0277 (4)	0.0328 (3)	0.0254 (3)	0.0020 (3)	0.0000 (4)	0.0016 (3)
Zn2	0.0264 (4)	0.0442 (4)	0.0327 (4)	0.0009 (3)	0.0010 (4)	-0.0032 (4)
Cl1	0.0765 (16)	0.0915 (15)	0.0283 (10)	0.0279 (13)	0.0089 (10)	-0.0091 (10)
Cl2	0.0505 (13)	0.0658 (12)	0.0297 (9)	0.0041 (10)	-0.0054 (8)	-0.0054 (8)
O1	0.053 (3)	0.070 (3)	0.016 (2)	0.021 (3)	0.002 (2)	-0.005 (2)
O1W	0.060 (4)	0.040 (3)	0.048 (3)	-0.014 (2)	-0.011 (2)	0.015 (2)
O2	0.071 (4)	0.056 (3)	0.031 (3)	0.027 (3)	-0.005 (3)	-0.011 (2)
O3	0.029 (2)	0.038 (2)	0.020 (2)	-0.0047 (18)	-0.0028 (19)	0.0053 (19)
O4	0.048 (3)	0.044 (3)	0.043 (3)	-0.015 (2)	-0.017 (2)	0.007 (2)
O5	0.034 (3)	0.081 (4)	0.030 (3)	0.004 (3)	-0.003 (2)	-0.001 (2)
O6	0.025 (3)	0.127 (5)	0.043 (3)	-0.006 (3)	0.003 (3)	0.007 (3)
O7	0.041 (3)	0.048 (3)	0.032 (3)	0.008 (2)	0.004 (2)	-0.010 (2)
O8	0.048 (3)	0.041 (3)	0.077 (3)	-0.002 (2)	0.018 (3)	0.015 (3)
N1	0.024 (3)	0.027 (3)	0.033 (3)	0.001 (2)	0.008 (2)	0.000 (2)
N2	0.032 (3)	0.029 (3)	0.033 (3)	-0.001 (2)	-0.006 (3)	0.001 (2)
N3	0.031 (3)	0.033 (3)	0.037 (3)	0.003 (2)	0.000 (3)	-0.011 (3)
N4	0.024 (3)	0.030 (3)	0.045 (3)	0.001 (2)	0.000 (2)	-0.007 (2)
C1	0.025 (4)	0.039 (4)	0.028 (3)	-0.001 (3)	0.002 (3)	0.000 (3)
C1A	0.028 (4)	0.033 (3)	0.019 (3)	-0.002 (3)	0.002 (3)	-0.004 (3)
C2	0.050 (5)	0.046 (4)	0.120 (8)	-0.003 (4)	0.028 (5)	-0.024 (5)
C3	0.029 (4)	0.032 (3)	0.019 (3)	-0.002 (3)	-0.005 (3)	-0.003 (3)
C4	0.017 (3)	0.032 (3)	0.029 (3)	-0.003 (3)	-0.004 (3)	-0.004 (3)
C5	0.038 (5)	0.037 (4)	0.041 (4)	-0.001 (3)	-0.007 (3)	-0.004 (3)
C6	0.048 (5)	0.037 (4)	0.054 (5)	0.011 (4)	-0.003 (4)	-0.007 (3)
C7	0.057 (5)	0.039 (4)	0.038 (4)	0.013 (4)	-0.015 (4)	0.007 (3)
C8	0.049 (5)	0.044 (4)	0.027 (4)	0.000 (4)	-0.007 (3)	0.004 (3)
C9	0.035 (4)	0.040 (4)	0.033 (4)	0.005 (3)	0.008 (3)	0.002 (3)
C10	0.030 (4)	0.045 (4)	0.022 (4)	-0.003 (3)	-0.004 (3)	-0.003 (3)
C11	0.027 (4)	0.029 (3)	0.031 (3)	0.003 (3)	-0.002 (3)	-0.004 (3)
C12	0.029 (4)	0.023 (3)	0.023 (3)	0.000 (3)	0.000 (3)	-0.006 (2)
C13	0.039 (4)	0.025 (3)	0.028 (3)	0.005 (3)	0.000 (3)	-0.002 (3)
C14	0.034 (4)	0.048 (4)	0.033 (4)	-0.003 (3)	0.001 (3)	-0.005 (3)
C15	0.028 (4)	0.059 (5)	0.055 (5)	0.002 (4)	0.007 (4)	0.000 (4)
C16	0.043 (5)	0.049 (4)	0.014 (3)	-0.002 (3)	-0.001 (3)	-0.002 (3)
C17	0.033 (4)	0.030 (3)	0.064 (5)	0.003 (3)	0.009 (4)	0.004 (3)
C18	0.042 (5)	0.026 (3)	0.066 (5)	0.008 (3)	0.007 (4)	0.001 (3)

C19	0.036 (4)	0.042 (4)	0.043 (4)	0.012 (3)	0.000 (3)	0.000 (3)
C20	0.027 (4)	0.042 (4)	0.044 (4)	0.002 (3)	-0.002 (3)	0.008 (3)
C21	0.022 (3)	0.038 (3)	0.024 (3)	-0.003 (3)	0.002 (3)	-0.005 (3)
C22	0.028 (4)	0.041 (3)	0.017 (3)	0.000 (3)	0.002 (3)	-0.002 (3)
C23	0.026 (4)	0.038 (4)	0.047 (4)	-0.005 (3)	-0.001 (3)	-0.005 (3)
C24	0.051 (5)	0.035 (4)	0.047 (4)	-0.015 (4)	-0.001 (4)	-0.005 (3)
C25	0.064 (5)	0.025 (3)	0.055 (4)	0.002 (3)	-0.006 (5)	0.001 (4)
C26	0.054 (5)	0.039 (3)	0.048 (4)	-0.003 (3)	-0.014 (4)	0.005 (4)
C27	0.053 (5)	0.057 (5)	0.112 (8)	0.018 (4)	-0.018 (6)	0.022 (5)
C28	0.059 (6)	0.048 (4)	0.086 (6)	-0.023 (4)	-0.006 (5)	-0.005 (4)
C29	0.040 (5)	0.046 (4)	0.064 (5)	-0.011 (4)	0.011 (4)	-0.004 (4)
C30	0.043 (4)	0.028 (3)	0.076 (5)	-0.005 (3)	0.003 (4)	-0.011 (3)
C31	0.034 (4)	0.040 (3)	0.050 (5)	0.008 (3)	0.006 (3)	-0.015 (3)
C32	0.028 (4)	0.038 (4)	0.041 (4)	-0.005 (3)	0.001 (3)	-0.004 (3)
C33	0.030 (4)	0.031 (3)	0.026 (3)	0.000 (3)	-0.006 (3)	-0.002 (3)
C34	0.027 (4)	0.034 (3)	0.027 (3)	0.000 (3)	-0.002 (3)	-0.004 (3)
C35	0.025 (4)	0.043 (4)	0.038 (4)	-0.004 (3)	0.000 (3)	0.000 (3)
C36	0.039 (4)	0.031 (3)	0.045 (4)	-0.004 (3)	-0.011 (3)	-0.001 (3)
C37	0.047 (5)	0.029 (3)	0.066 (5)	-0.001 (3)	0.002 (4)	-0.002 (4)
C38	0.034 (4)	0.043 (4)	0.061 (5)	0.007 (3)	-0.001 (4)	-0.012 (4)
C39	0.044 (5)	0.034 (4)	0.098 (6)	0.000 (4)	-0.001 (5)	0.007 (4)

Geometric parameters (Å, °)

Zn1—O1	1.952 (4)	C12—C13	1.378 (9)
Zn1—O1W	2.082 (4)	C13—C14	1.387 (9)
Zn1—O3 ⁱ	2.049 (4)	C14—H14	0.9300
Zn1—N1	2.102 (5)	C14—C15	1.371 (8)
Zn1—N2	2.146 (4)	C15—H15	0.9300
Zn2—O5	1.921 (5)	C15—C16	1.357 (9)
Zn2—O7 ⁱⁱ	1.958 (4)	C16—H16	0.9300
Zn2—N3	2.029 (5)	C17—H17	0.9300
Zn2—N4	2.062 (5)	C17—C18	1.370 (9)
C11—C5	1.729 (7)	C18—H18	0.9300
C12—C13	1.747 (6)	C18—C19	1.372 (9)
O1—C1	1.273 (7)	C19—C20	1.389 (8)
O1W—H1WA	0.8512	C19—C27	1.513 (9)
O1W—H1WB	0.8501	C20—H20	0.9300
O2—C1	1.220 (8)	C20—C21	1.382 (8)
O3—Zn1 ⁱⁱ	2.049 (4)	C21—C22	1.484 (8)
O3—C1A	1.246 (7)	C22—C23	1.387 (8)
O4—C1A	1.249 (7)	C23—H23	0.9300
O5—C9	1.270 (7)	C23—C24	1.386 (9)
O6—C9	1.196 (8)	C24—C25	1.400 (9)
O7—Zn2 ⁱ	1.958 (4)	C24—C28	1.523 (9)
O7—C10	1.264 (7)	C25—H25	0.9300
O8—C10	1.242 (7)	C25—C26	1.347 (8)
N1—C17	1.352 (8)	C26—H26	0.9300

N1—C21	1.334 (7)	C27—H27A	0.9600
N2—C22	1.343 (7)	C27—H27B	0.9600
N2—C26	1.329 (7)	C27—H27C	0.9600
N3—C34	1.353 (7)	C28—H28A	0.9600
N3—C38	1.334 (7)	C28—H28B	0.9600
N4—C29	1.325 (8)	C28—H28C	0.9600
N4—C33	1.357 (8)	C29—H29	0.9300
C1—C3	1.514 (8)	C29—C30	1.391 (9)
C1A—C4	1.520 (8)	C30—H30	0.9300
C2—H2A	0.9600	C30—C31	1.374 (9)
C2—H2B	0.9600	C31—C32	1.400 (8)
C2—H2C	0.9600	C32—H32	0.9300
C2—C31	1.507 (8)	C32—C33	1.360 (8)
C3—C4	1.385 (7)	C33—C34	1.487 (8)
C3—C8	1.407 (8)	C34—C35	1.386 (8)
C4—C5	1.381 (9)	C35—H35	0.9300
C5—C6	1.389 (9)	C35—C36	1.386 (8)
C6—H6	0.9300	C36—C37	1.399 (9)
C6—C7	1.365 (9)	C36—C39	1.498 (9)
C7—H7	0.9300	C37—H37	0.9300
C7—C8	1.377 (9)	C37—C38	1.364 (9)
C8—H8	0.9300	C38—H38	0.9300
C9—C11	1.518 (9)	C39—H39A	0.9600
C10—C12	1.521 (9)	C39—H39B	0.9600
C11—C12	1.399 (7)	C39—H39C	0.9600
C11—C16	1.394 (9)		
O1—Zn1—O1W	103.5 (2)	C16—C15—C14	120.3 (7)
O1—Zn1—O3 ⁱ	98.96 (17)	C16—C15—H15	119.9
O1—Zn1—N1	122.84 (18)	C11—C16—H16	119.2
O1—Zn1—N2	96.7 (2)	C15—C16—C11	121.7 (6)
O1W—Zn1—N1	91.85 (18)	C15—C16—H16	119.2
O1W—Zn1—N2	159.80 (19)	N1—C17—H17	119.4
O3 ⁱ —Zn1—O1W	90.36 (16)	N1—C17—C18	121.3 (6)
O3 ⁱ —Zn1—N1	136.19 (17)	C18—C17—H17	119.4
O3 ⁱ —Zn1—N2	86.66 (17)	C17—C18—H18	119.7
N1—Zn1—N2	76.79 (18)	C17—C18—C19	120.6 (6)
O5—Zn2—O7 ⁱⁱ	104.35 (19)	C19—C18—H18	119.7
O5—Zn2—N3	116.5 (2)	C18—C19—C20	117.7 (6)
O5—Zn2—N4	108.5 (2)	C18—C19—C27	122.1 (6)
O7 ⁱⁱ —Zn2—N3	128.6 (2)	C20—C19—C27	120.1 (6)
O7 ⁱⁱ —Zn2—N4	114.78 (19)	C19—C20—H20	120.1
N3—Zn2—N4	81.22 (19)	C21—C20—C19	119.7 (6)
C1—O1—Zn1	120.0 (4)	C21—C20—H20	120.1
Zn1—O1W—H1WA	109.3	N1—C21—C20	121.6 (6)
Zn1—O1W—H1WB	89.9	N1—C21—C22	115.8 (5)
H1WA—O1W—H1WB	118.4	C20—C21—C22	122.6 (6)
C1A—O3—Zn1 ⁱⁱ	128.1 (4)	N2—C22—C21	115.3 (5)

C9—O5—Zn2	127.2 (5)	N2—C22—C23	121.8 (5)
C10—O7—Zn2 ⁱ	110.2 (4)	C23—C22—C21	122.9 (6)
C17—N1—Zn1	124.0 (4)	C22—C23—H23	120.2
C21—N1—Zn1	116.7 (4)	C24—C23—C22	119.7 (6)
C21—N1—C17	119.1 (6)	C24—C23—H23	120.2
C22—N2—Zn1	115.1 (4)	C23—C24—C25	117.1 (6)
C26—N2—Zn1	126.8 (4)	C23—C24—C28	120.2 (7)
C26—N2—C22	118.0 (5)	C25—C24—C28	122.6 (6)
C34—N3—Zn2	113.9 (4)	C24—C25—H25	120.2
C38—N3—Zn2	128.4 (4)	C26—C25—C24	119.6 (6)
C38—N3—C34	117.5 (5)	C26—C25—H25	120.2
C29—N4—Zn2	127.8 (5)	N2—C26—C25	123.9 (6)
C29—N4—C33	118.8 (6)	N2—C26—H26	118.1
C33—N4—Zn2	113.2 (4)	C25—C26—H26	118.1
O1—C1—C3	114.9 (6)	C19—C27—H27A	109.5
O2—C1—O1	126.6 (6)	C19—C27—H27B	109.5
O2—C1—C3	118.5 (5)	C19—C27—H27C	109.5
O3—C1A—O4	127.1 (6)	H27A—C27—H27B	109.5
O3—C1A—C4	115.2 (5)	H27A—C27—H27C	109.5
O4—C1A—C4	117.4 (5)	H27B—C27—H27C	109.5
H2A—C2—H2B	109.5	C24—C28—H28A	109.5
H2A—C2—H2C	109.5	C24—C28—H28B	109.5
H2B—C2—H2C	109.5	C24—C28—H28C	109.5
C31—C2—H2A	109.5	H28A—C28—H28B	109.5
C31—C2—H2B	109.5	H28A—C28—H28C	109.5
C31—C2—H2C	109.5	H28B—C28—H28C	109.5
C4—C3—C1	121.7 (6)	N4—C29—H29	118.9
C4—C3—C8	119.5 (6)	N4—C29—C30	122.1 (6)
C8—C3—C1	118.7 (5)	C30—C29—H29	118.9
C3—C4—C1A	122.2 (6)	C29—C30—H30	120.2
C5—C4—C1A	119.7 (5)	C31—C30—C29	119.6 (6)
C5—C4—C3	118.1 (6)	C31—C30—H30	120.2
C4—C5—C11	119.9 (5)	C30—C31—C2	121.3 (6)
C4—C5—C6	122.3 (6)	C30—C31—C32	117.7 (6)
C6—C5—C11	117.8 (5)	C32—C31—C2	121.1 (6)
C5—C6—H6	120.3	C31—C32—H32	120.0
C7—C6—C5	119.3 (7)	C33—C32—C31	120.0 (6)
C7—C6—H6	120.3	C33—C32—H32	120.0
C6—C7—H7	120.1	N4—C33—C32	121.7 (5)
C6—C7—C8	119.8 (6)	N4—C33—C34	115.4 (5)
C8—C7—H7	120.1	C32—C33—C34	122.9 (6)
C3—C8—H8	119.6	N3—C34—C33	116.1 (5)
C7—C8—C3	120.9 (6)	N3—C34—C35	121.7 (5)
C7—C8—H8	119.6	C35—C34—C33	122.2 (6)
O5—C9—C11	114.7 (6)	C34—C35—H35	119.5
O6—C9—O5	124.3 (7)	C36—C35—C34	121.0 (6)
O6—C9—C11	121.0 (6)	C36—C35—H35	119.5
O7—C10—C12	117.9 (5)	C35—C36—C37	115.9 (6)

O8—C10—O7	123.8 (6)	C35—C36—C39	121.0 (6)
O8—C10—C12	117.9 (6)	C37—C36—C39	123.1 (6)
C12—C11—C9	122.7 (6)	C36—C37—H37	119.8
C16—C11—C9	117.9 (6)	C38—C37—C36	120.5 (6)
C16—C11—C12	119.4 (6)	C38—C37—H37	119.8
C11—C12—C10	125.2 (6)	N3—C38—C37	123.4 (6)
C13—C12—C10	117.7 (5)	N3—C38—H38	118.3
C13—C12—C11	117.0 (6)	C37—C38—H38	118.3
C12—C13—C12	119.9 (5)	C36—C39—H39A	109.5
C12—C13—C14	123.6 (6)	C36—C39—H39B	109.5
C14—C13—C12	116.6 (5)	C36—C39—H39C	109.5
C13—C14—H14	121.0	H39A—C39—H39B	109.5
C15—C14—C13	118.0 (8)	H39A—C39—H39C	109.5
C15—C14—H14	121.0	H39B—C39—H39C	109.5
C14—C15—H15	119.9		
Zn1—O1—C1—O2	18.8 (10)	N3—C34—C35—C36	0.5 (9)
Zn1—O1—C1—C3	-159.9 (4)	N4—Zn2—O5—C9	34.9 (7)
Zn1 ⁱⁱ —O3—C1A—O4	22.0 (9)	N4—Zn2—N3—C34	-4.7 (4)
Zn1 ⁱⁱ —O3—C1A—C4	-152.6 (4)	N4—Zn2—N3—C38	-179.3 (6)
Zn1—N1—C17—C18	176.6 (5)	N4—C29—C30—C31	-1.0 (11)
Zn1—N1—C21—C20	-178.3 (5)	N4—C33—C34—N3	-1.9 (8)
Zn1—N1—C21—C22	4.9 (6)	N4—C33—C34—C35	178.3 (6)
Zn1—N2—C22—C21	-3.0 (6)	C1—C3—C4—C1A	1.6 (10)
Zn1—N2—C22—C23	175.9 (4)	C1—C3—C4—C5	-178.7 (6)
Zn1—N2—C26—C25	-175.1 (6)	C1—C3—C8—C7	176.6 (6)
Zn2—O5—C9—O6	6.5 (12)	C1A—C4—C5—C11	2.7 (9)
Zn2—O5—C9—C11	-173.1 (4)	C1A—C4—C5—C6	-178.4 (6)
Zn2 ⁱ —O7—C10—O8	17.5 (8)	C2—C31—C32—C33	178.9 (7)
Zn2 ⁱ —O7—C10—C12	-155.3 (4)	C3—C4—C5—C11	-177.0 (5)
Zn2—N3—C34—C33	5.0 (6)	C3—C4—C5—C6	1.9 (10)
Zn2—N3—C34—C35	-175.2 (4)	C4—C3—C8—C7	-1.3 (10)
Zn2—N3—C38—C37	173.7 (6)	C4—C5—C6—C7	-0.9 (12)
Zn2—N4—C29—C30	-176.3 (5)	C5—C6—C7—C8	-1.3 (12)
Zn2—N4—C33—C32	178.6 (5)	C6—C7—C8—C3	2.3 (11)
Zn2—N4—C33—C34	-2.0 (6)	C8—C3—C4—C1A	179.5 (6)
C11—C5—C6—C7	178.0 (6)	C8—C3—C4—C5	-0.8 (10)
C12—C13—C14—C15	179.1 (5)	C9—C11—C12—C10	3.1 (9)
O1—Zn1—N1—C17	-90.0 (5)	C9—C11—C12—C13	178.9 (5)
O1—Zn1—N1—C21	84.6 (4)	C9—C11—C16—C15	-178.7 (6)
O1—Zn1—N2—C22	-118.1 (4)	C10—C12—C13—C12	-3.1 (7)
O1—Zn1—N2—C26	59.4 (6)	C10—C12—C13—C14	177.4 (6)
O1—C1—C3—C4	-160.0 (6)	C11—C12—C13—C12	-179.2 (4)
O1—C1—C3—C8	22.1 (9)	C11—C12—C13—C14	1.3 (9)
O1W—Zn1—O1—C1	-108.3 (5)	C12—C11—C16—C15	1.5 (10)
O1W—Zn1—N1—C17	17.3 (5)	C12—C13—C14—C15	-1.4 (10)
O1W—Zn1—N1—C21	-168.0 (4)	C13—C14—C15—C16	1.4 (11)
O1W—Zn1—N2—C22	61.4 (8)	C14—C15—C16—C11	-1.5 (11)

O1W—Zn1—N2—C26	-121.2 (6)	C16—C11—C12—C10	-177.1 (6)
O2—C1—C3—C4	21.2 (10)	C16—C11—C12—C13	-1.3 (8)
O2—C1—C3—C8	-156.7 (6)	C17—N1—C21—C20	-3.4 (9)
O3 ⁱ —Zn1—O1—C1	159.2 (5)	C17—N1—C21—C22	179.8 (5)
O3 ⁱ —Zn1—N1—C17	109.8 (5)	C17—C18—C19—C20	-0.3 (10)
O3 ⁱ —Zn1—N1—C21	-75.6 (5)	C17—C18—C19—C27	178.9 (7)
O3 ⁱ —Zn1—N2—C22	143.3 (4)	C18—C19—C20—C21	-0.9 (9)
O3 ⁱ —Zn1—N2—C26	-39.3 (6)	C19—C20—C21—N1	2.8 (9)
O3—C1A—C4—C3	-106.9 (7)	C19—C20—C21—C22	179.4 (5)
O3—C1A—C4—C5	73.4 (7)	C20—C21—C22—N2	-178.0 (6)
O4—C1A—C4—C3	77.9 (8)	C20—C21—C22—C23	3.2 (9)
O4—C1A—C4—C5	-101.8 (7)	C21—N1—C17—C18	2.1 (9)
O5—Zn2—N3—C34	101.7 (4)	C21—C22—C23—C24	179.3 (6)
O5—Zn2—N3—C38	-72.9 (6)	C22—N2—C26—C25	2.3 (11)
O5—Zn2—N4—C29	63.2 (6)	C22—C23—C24—C25	0.4 (9)
O5—Zn2—N4—C33	-111.5 (4)	C22—C23—C24—C28	177.5 (6)
O5—C9—C11—C12	-171.7 (6)	C23—C24—C25—C26	0.1 (11)
O5—C9—C11—C16	8.5 (9)	C24—C25—C26—N2	-1.4 (12)
O6—C9—C11—C12	8.7 (10)	C26—N2—C22—C21	179.3 (6)
O6—C9—C11—C16	-171.1 (7)	C26—N2—C22—C23	-1.8 (9)
O7 ⁱⁱ —Zn2—O5—C9	157.7 (6)	C27—C19—C20—C21	179.9 (7)
O7 ⁱⁱ —Zn2—N3—C34	-119.5 (4)	C28—C24—C25—C26	-177.0 (7)
O7 ⁱⁱ —Zn2—N3—C38	65.9 (7)	C29—N4—C33—C32	3.5 (9)
O7 ⁱⁱ —Zn2—N4—C29	-53.1 (6)	C29—N4—C33—C34	-177.2 (6)
O7 ⁱⁱ —Zn2—N4—C33	132.3 (4)	C29—C30—C31—C2	-177.3 (7)
O7—C10—C12—C11	-99.1 (7)	C29—C30—C31—C32	2.2 (10)
O7—C10—C12—C13	85.1 (7)	C30—C31—C32—C33	-0.7 (10)
O8—C10—C12—C11	87.7 (8)	C31—C32—C33—N4	-2.2 (9)
O8—C10—C12—C13	-88.1 (7)	C31—C32—C33—C34	178.6 (5)
N1—Zn1—O1—C1	-7.1 (6)	C32—C33—C34—N3	177.4 (6)
N1—Zn1—N2—C22	4.2 (4)	C32—C33—C34—C35	-2.4 (9)
N1—Zn1—N2—C26	-178.4 (6)	C33—N4—C29—C30	-1.9 (10)
N1—C17—C18—C19	-0.3 (10)	C33—C34—C35—C36	-179.8 (5)
N1—C21—C22—N2	-1.2 (7)	C34—N3—C38—C37	-0.7 (11)
N1—C21—C22—C23	180.0 (6)	C34—C35—C36—C37	-0.2 (9)
N2—Zn1—O1—C1	71.5 (5)	C34—C35—C36—C39	-179.9 (6)
N2—Zn1—N1—C17	-179.5 (5)	C35—C36—C37—C38	-0.5 (10)
N2—Zn1—N1—C21	-4.9 (4)	C36—C37—C38—N3	1.0 (12)
N2—C22—C23—C24	0.5 (9)	C38—N3—C34—C33	-179.8 (6)
N3—Zn2—O5—C9	-54.4 (7)	C38—N3—C34—C35	0.0 (9)
N3—Zn2—N4—C29	178.3 (6)	C39—C36—C37—C38	179.2 (7)
N3—Zn2—N4—C33	3.6 (4)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1WA \cdots O4 ⁱⁱⁱ	0.85	2.10	2.768 (6)	135

O1 <i>W</i> —H1 <i>WB</i> ···O4 ⁱ	0.85	1.79	2.644 (6)	179
O1 <i>W</i> —H1 <i>WB</i> ···O3 ⁱ	0.85	2.43	2.930 (5)	118
C17—H17···O4 ⁱⁱⁱ	0.93	2.36	3.202 (8)	150
C20—H20···O6 ^{iv}	0.93	2.28	3.171 (8)	160
C23—H23···O6 ^{iv}	0.93	2.40	3.306 (8)	164
C32—H32···O2 ⁱⁱⁱ	0.93	2.57	3.459 (8)	161
C35—H35···O2 ⁱⁱⁱ	0.93	2.45	3.353 (8)	165

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