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Bis[(4-chlorophenoxy)acetato-κO](ethylenediamine-$\kappa^2 N,N'$)zinc

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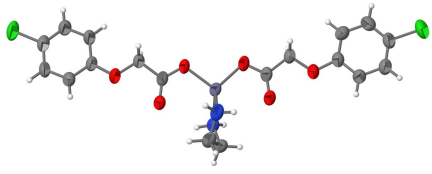
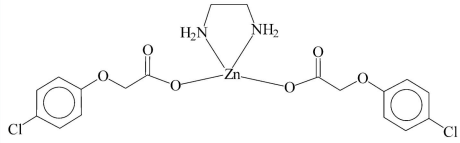
Structural data: full structural data are available from iucrdata.iucr.org

The mononuclear title complex, $[Zn(C_8H_6ClO_3)_2(C_2H_8N_2)]$, was obtained by the reaction of zinc(II) acetate dihydrate with *p*-chlorophenoxyacetic acid (pCPA) and ethylenediamine (EDA) in a water/ethanol mixture. The Zn^{II} cation has a distorted tetrahedral coordination sphere involving two carboxylate O atoms of two monodentate pCPA ligands and two N atoms of one chelating EDA ligand. The pCPA ligands coordinate asymmetrically to the Zn^{II} cation with two different Zn—O distances of 1.967 (3) and 1.978 (3) Å. In the crystal, molecules are linked by N—H···O hydrogen bonds, forming chains propagating parallel to [100]. These chains are linked by C—H···O hydrogen bonds, C—H···π stacking and Cl···Cl interactions, generating a three-dimensional supramolecular network.

3D view



Chemical scheme



Structure description

Phenoxyacetic acid (pCPA) and its derivatives are biologically active compounds which are widely used as herbicides and plant-growth substances. The interaction of metal ions with pCPA results in the formation of complexes in which it demonstrates monodentate (Ashurov *et al.*, 2012; Ma *et al.*, 2013, 2014; Li *et al.*, 2014) and bidentate (Li *et al.*, 2014; Smith *et al.*, 1981; Sun *et al.*, 2007) coordination. pCPA ligands can also show bridging properties (Liwporncharoenvong & Luck, 2005; Li *et al.*, 2013; Jin *et al.*, 2015; An *et al.*, 2002) and form chain structures (Wang *et al.*, 2006, 2008; Li *et al.*, 2013). Ethylenediamine (EDA) ligands can coordinate to metal ions in a monodentate fashion (Xue *et al.*, 2016; Mitzinger *et al.*, 2016; Zhang *et al.*, 2009; Fanizzi *et al.*, 1984; Saidi *et al.*, 2013) and in some complexes behave as bridging ligands (Binnemans *et al.*, 2013; House & Steel, 1999; Bratsos *et al.*, 2011; Doring & Jones, 2013; Kuhn *et al.*, 2008). In many cases, EDA

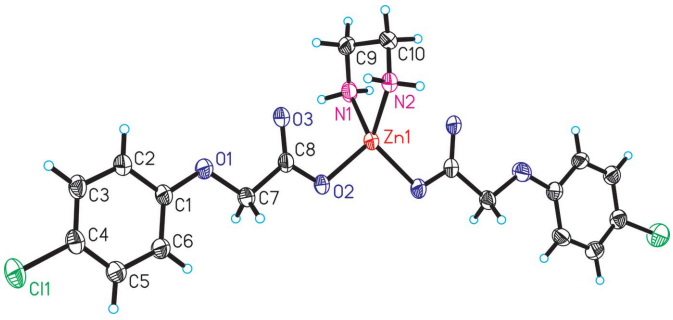


Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level. Unlabelled atoms of the second cCPA ligand are related to the first by a prime character but are not crystallographically equivalent.

demonstrates a chelating property. There are metal complexes in which noncoordinating EDA molecules are situated in the outer sphere (Peipei *et al.*, 2017; Tian *et al.*, 2017; Mirzaei *et al.*, 2014). A search in the Cambridge Structural Database (CSD; Groom *et al.,* 2016) revealed that crystal structures have been reported for complexes of pCPA and EDA with many metal ions. However, no mixed-ligand metal complex including pCPA and EDA is documented in the CSD. Here, the synthesis and structure of the related title compound bis[(4-chlorophenoxy)acetato-κO](ethylenediamine-$\kappa^2 N,N'$)zinc is described.

The asymmetric unit of the title compound consists of a mononuclear complex of formula $[Zn(C_8H_7ClO_3)_2(C_2H_8N_2)]$, as shown in Fig. 1. The coordination polyhedron of the Zn^{II} cation is a distorted tetrahedron defined by an N_2O_2 coordination set. The distortion is indicated by bond angles O2—Zn1—O2′ [99.47 (11)°], O2—Zn1—N1 [117.37 (11)°], O2—Zn1—N2 [114.42 (12)°], O2′—Zn1—N1 [119.57 (13)°], O2′—Zn1—N2 [122.20 (12)°] and N1—Zn1—N2 [85.14 (13)°]. The dihedral angle between the N1/Zn1/N2 plane and the O2/Zn1/O2′ plane is 87.60 (16)°. The Zn^{II} cation is coordinated by one EDA molecule, which acts as an *N*,*N*′-chelating ligand. The Zn1—N1 and Zn1—N2 distances are 2.041 (4) and 2.052 (3) Å, respectively. The bidentate coordination of the EDA ligand results in the formation of a five-membered chelate ring with an internal angle of 116.0 (15)° for N1—Zn1—N2. The N1—C9—C10—N2 torsion angle within the EDA molecule is −53.0 (4)°. The two pCPA ligands are asymmetrically coordinated to the Zn^{II} cation, with Zn—O distances of 1.967 (3) and 1.978 (3) Å. The dihedral angle between the N1/Zn/N2 plane and the O2/Zn/O2′ plane is 87.61 (7)°. In both pCPA ligands, the oxyacetate group and the aromatic ring are not perfectly coplanar, the torsion angles being −174.2 (3) (C1—O1—C7—C8) and −170.8 (3)° (C1′—O1′—C7′—C8′). The dihedral angles between the acetate and 4-chlorophenoxy least-squares planes in the two independent ligands are 5.985 (3) and 5.513 (3)°.

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1B···O3^{i}	0.89	2.06	2.931 (4)	166
N2—H2B···O3^{ii}	0.89	2.08	2.950 (4)	167
C3—H3···O3^{iii}	0.93	2.59	3.346 (5)	139
C3′—H3′···O3^{iv}	0.93	2.50	3.314 (5)	146

Symmetry codes: (i) $x+1, y, z$; (ii) $x-1, y, z$; (iii) $x+\frac{3}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (iv) $x-\frac{3}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$.

In the crystal, molecules are linked by N—H···O hydrogen bonds (Table 1 and Fig. 2), forming chains propagating parallel to [100] (Figs. 2 and 3). The N—H···O hydrogen-bonding interactions between amine donor groups and carboxylate acceptors groups result in $R_4^2(12)$ ring motifs. The chains are linked by C—H···O hydrogen bonds (Table 1), forming a sheet structure extending parallel to (010) (Fig. 3). The molecules are further linked by C—H···π stacking [3.438 (3) Å] between benzene rings and methylene groups of pCPA, and by Cl1···Cl1^{i,ii} interactions {3.438 (2) [symmetry code: (i) $-x+4, -y+1, -z$] and 3.801(3) Å [symmetry code: (ii) $-x+3, -y+1, -z$]}, generating a three-dimensional supramolecular network.

Synthesis and crystallization

To an aqueous solution (2.5 ml) of $Zn(CH_3COO)_2$ (0.049 g, 0.268 mmol) was added slowly under constant stirring an ethanol solution (5 ml) containing EDA (0.016 g) and pCPA (0.1 g, 0.536 mmol). Colourless crystals were obtained by

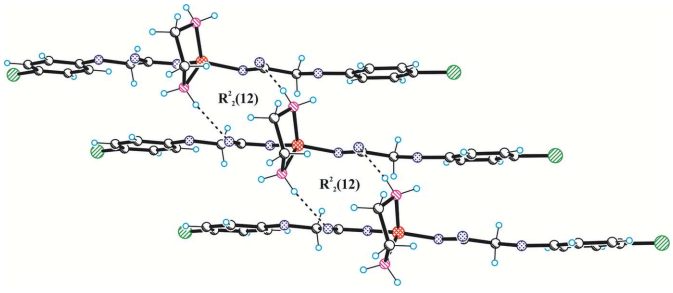


Figure 2
Formation of chains and hydrogen bonds in the title complex. Hydrogen bonds are shown as dashed lines.

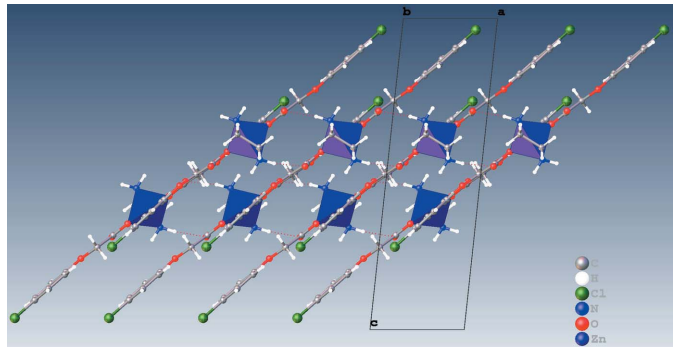


Figure 3
The packing of the molecules in the title complex in a view along [010]. Intermolecular hydrogen bonding is shown as dashed red lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Zn(C_8H_6ClO_3)_2(C_2H_8N_2)]$
M_r	496.63
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	293
a, b, c (Å)	5.6621 (11), 19.366 (13), 18.816 (4)
β (°)	96.09 (2)
V (Å^3)	2051.6 (15)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	4.40
Crystal size (mm)	0.42 × 0.36 × 0.12
Data collection	
Diffractometer	Oxford Diffraction Xcalibur Ruby
Absorption correction	Multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
T_{min}, T_{max}	0.569, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8985, 4125, 2146
R_{int}	0.041
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.627
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.123, 0.84
No. of reflections	4125
No. of parameters	262
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.97, −0.35

Computer programs: *CrysAlis PRO* (Oxford Diffraction, 2009), *olex2.solve* (Bourhis *et al.*, 2015), *SHELXL2014* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

solvent evaporation at room temperature after one week (yield 75%). Elemental analysis calculated for $C_{18}H_{20}Cl_2N_2O_6Zn$: C 43.53, H 4.06, N 5.64%; found: C 43.58, H 4.12, N 5.69%.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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full crystallographic data

IUCrData (2018). **3**, x181250 [https://doi.org/10.1107/S2414314618012506]

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Crystal data

$[Zn(C_8H_6ClO_3)_2(C_2H_8N_2)]$
M_r = 496.63
Monoclinic, $P2_1/n$
a = 5.6621 (11) Å
b = 19.366 (13) Å
c = 18.816 (4) Å
β = 96.09 (2)°
V = 2051.6 (15) Å^3
Z = 4
$F(000)$ = 1016
D_x = 1.608 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 568 reflections
θ = 3.3–75.7°
μ = 4.40 mm^{-1}
T = 293 K
Block, colorless
0.42 × 0.36 × 0.12 mm

Data collection

Oxford Diffraction 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 (CrysAlis PRO; Oxford Diffraction, 2009)
T_{min} = 0.569, T_{max} = 1.000
8985 measured reflections
4125 independent reflections
2146 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 75.3°, θ_{min} = 3.3°
h = −6→7
k = −14→24
l = −23→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.123
S = 0.84
4125 reflections
262 parameters
0 restraints
Primary atom site location: iterative
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0653P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.97 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.48309 (8)	0.70588 (3)	0.38879 (3)	0.05115 (17)
Cl1	1.7835 (2)	0.54592 (7)	0.03685 (7)	0.0914 (4)
Cl1′	−0.8303 (3)	0.54629 (7)	0.73405 (8)	0.1022 (5)
O2	0.6929 (4)	0.64544 (13)	0.33966 (14)	0.0542 (7)
O2′	0.2828 (4)	0.63502 (13)	0.42866 (14)	0.0569 (7)
O3	0.8426 (5)	0.74137 (14)	0.29750 (16)	0.0583 (7)
O3′	0.1265 (5)	0.72723 (13)	0.47574 (16)	0.0602 (8)
O1	1.1489 (5)	0.67189 (13)	0.22793 (16)	0.0692 (9)
O1′	−0.1830 (5)	0.65479 (15)	0.53761 (19)	0.0882 (11)
N1	0.6398 (5)	0.78062 (16)	0.45419 (19)	0.0613 (9)
H1A	0.5691	0.7834	0.4941	0.074*
H1B	0.7926	0.7708	0.4658	0.074*
N2	0.3406 (5)	0.78667 (15)	0.32804 (18)	0.0588 (9)
H2A	0.4137	0.7911	0.2887	0.071*
H2B	0.1867	0.7794	0.3152	0.071*
C8	0.8322 (6)	0.6779 (2)	0.3031 (2)	0.0492 (9)
C1	1.2919 (7)	0.6383 (2)	0.1844 (2)	0.0540 (10)
C8′	0.1401 (6)	0.6639 (2)	0.4674 (2)	0.0504 (10)
C7	0.9894 (6)	0.63128 (19)	0.2646 (2)	0.0518 (10)
H7A	1.0791	0.6011	0.2987	0.062*
H7B	0.8926	0.6027	0.2307	0.062*
C7′	−0.0217 (6)	0.6143 (2)	0.5016 (2)	0.0548 (10)
H7′A	−0.1083	0.5857	0.4654	0.066*
H7′B	0.0709	0.5845	0.5353	0.066*
C6	1.3034 (7)	0.5669 (2)	0.1764 (2)	0.0618 (12)
H6	1.2102	0.5381	0.2013	0.074*
C2	1.4358 (7)	0.6799 (2)	0.1478 (2)	0.0615 (11)
H2	1.4320	0.7275	0.1545	0.074*
C3	1.5848 (7)	0.6527 (2)	0.1017 (2)	0.0602 (11)
H3	1.6782	0.6812	0.0763	0.072*
C2′	−0.4549 (7)	0.6694 (2)	0.6210 (2)	0.0643 (12)
H2′	−0.4363	0.7167	0.6151	0.077*
C3′	−0.6059 (7)	0.6452 (2)	0.6682 (2)	0.0627 (12)
H3′	−0.6882	0.6757	0.6948	0.075*
C4′	−0.6321 (7)	0.5753 (2)	0.6751 (2)	0.0616 (11)
C1′	−0.3307 (7)	0.6237 (2)	0.5824 (2)	0.0608 (11)
C6′	−0.3578 (8)	0.5530 (2)	0.5898 (2)	0.0659 (12)
H6′	−0.2745	0.5223	0.5637	0.079*
C5′	−0.5131 (8)	0.5287 (2)	0.6373 (2)	0.0661 (12)
H5′	−0.5353	0.4816	0.6431	0.079*
C4	1.5910 (7)	0.5819 (2)	0.0942 (2)	0.0613 (11)
C9	0.6155 (7)	0.8462 (2)	0.4149 (3)	0.0699 (13)
H9A	0.7391	0.8500	0.3832	0.084*
H9B	0.6325	0.8845	0.4483	0.084*
C5	1.4556 (8)	0.5395 (2)	0.1306 (2)	0.0671 (13)

H5	1.4649	0.4919	0.1249	0.081*
C10	0.3740 (7)	0.8491 (2)	0.3721 (2)	0.0690 (13)
H10A	0.2509	0.8519	0.4041	0.083*
H10B	0.3632	0.8897	0.3418	0.083*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0394 (2)	0.0495 (3)	0.0668 (4)	0.0015 (3)	0.0163 (2)	−0.0043 (3)
Cl1	0.0874 (9)	0.1086 (10)	0.0866 (9)	0.0091 (7)	0.0490 (7)	−0.0154 (8)
Cl1′	0.1095 (11)	0.1037 (10)	0.1036 (11)	−0.0081 (9)	0.0589 (9)	0.0235 (9)
O2	0.0457 (15)	0.0576 (15)	0.0637 (18)	0.0021 (12)	0.0256 (13)	−0.0020 (14)
O2′	0.0452 (14)	0.0623 (16)	0.0669 (19)	−0.0009 (13)	0.0236 (13)	−0.0063 (15)
O3	0.0477 (16)	0.0576 (16)	0.073 (2)	0.0030 (14)	0.0237 (14)	0.0016 (16)
O3′	0.0441 (15)	0.0581 (16)	0.082 (2)	−0.0018 (12)	0.0249 (14)	−0.0045 (15)
O1	0.0669 (19)	0.0579 (16)	0.091 (2)	−0.0050 (14)	0.0453 (17)	−0.0115 (16)
O1′	0.080 (2)	0.0644 (18)	0.133 (3)	0.0086 (16)	0.068 (2)	0.016 (2)
N1	0.0416 (18)	0.071 (2)	0.073 (3)	−0.0009 (16)	0.0118 (16)	−0.013 (2)
N2	0.0435 (17)	0.059 (2)	0.076 (2)	0.0024 (16)	0.0179 (16)	0.0044 (19)
C8	0.039 (2)	0.058 (2)	0.052 (3)	−0.0022 (18)	0.0112 (18)	−0.008 (2)
C1	0.050 (2)	0.059 (2)	0.056 (3)	0.0027 (19)	0.0201 (19)	−0.006 (2)
C8′	0.037 (2)	0.061 (2)	0.054 (3)	0.0005 (18)	0.0092 (18)	0.000 (2)
C7	0.052 (2)	0.054 (2)	0.052 (2)	0.0012 (19)	0.0202 (19)	−0.003 (2)
C7′	0.049 (2)	0.062 (2)	0.056 (3)	0.0040 (19)	0.0186 (19)	−0.001 (2)
C6	0.065 (3)	0.057 (2)	0.068 (3)	−0.006 (2)	0.031 (2)	−0.009 (2)
C2	0.053 (2)	0.060 (2)	0.075 (3)	0.003 (2)	0.022 (2)	0.004 (2)
C3	0.054 (2)	0.074 (3)	0.056 (3)	0.003 (2)	0.024 (2)	0.007 (2)
C2′	0.061 (3)	0.050 (2)	0.086 (3)	−0.006 (2)	0.028 (2)	−0.005 (2)
C3′	0.059 (3)	0.067 (3)	0.066 (3)	−0.002 (2)	0.021 (2)	−0.008 (2)
C4′	0.058 (3)	0.071 (3)	0.059 (3)	−0.003 (2)	0.019 (2)	0.007 (2)
C1′	0.054 (2)	0.062 (2)	0.071 (3)	−0.002 (2)	0.024 (2)	0.002 (2)
C6′	0.066 (3)	0.057 (2)	0.078 (3)	0.011 (2)	0.020 (2)	0.000 (2)
C5′	0.067 (3)	0.060 (2)	0.072 (3)	−0.005 (2)	0.013 (2)	0.011 (2)
C4	0.056 (2)	0.078 (3)	0.052 (3)	0.005 (2)	0.016 (2)	−0.006 (2)
C9	0.055 (3)	0.052 (2)	0.106 (4)	−0.009 (2)	0.027 (3)	−0.020 (3)
C5	0.071 (3)	0.062 (3)	0.073 (3)	−0.002 (2)	0.030 (2)	−0.009 (2)
C10	0.058 (3)	0.051 (2)	0.101 (4)	0.010 (2)	0.028 (3)	0.005 (2)

Geometric parameters (Å, º)

Zn1—O2	1.967 (2)	C7′—H7′A	0.9700
Zn1—O2′	1.978 (3)	C7′—H7′B	0.9700
Zn1—N1	2.041 (3)	C6—H6	0.9300
Zn1—N2	2.052 (3)	C6—C5	1.386 (5)
Cl1—C4	1.757 (4)	C2—H2	0.9300
Cl1′—C4′	1.752 (4)	C2—C3	1.377 (5)
O2—C8	1.267 (4)	C3—H3	0.9300
O2′—C8′	1.274 (4)	C3—C4	1.379 (6)

O3—C8	1.235 (4)	C2′—H2′	0.9300
O3′—C8′	1.240 (4)	C2′—C3′	1.378 (5)
O1—C1	1.375 (4)	C2′—C1′	1.384 (5)
O1—C7	1.430 (4)	C3′—H3′	0.9300
O1′—C7′	1.428 (4)	C3′—C4′	1.369 (5)
O1′—C1′	1.386 (4)	C4′—C5′	1.370 (6)
N1—H1A	0.8900	C1′—C6′	1.385 (6)
N1—H1B	0.8900	C6′—H6′	0.9300
N1—C9	1.469 (5)	C6′—C5′	1.401 (6)
N2—H2A	0.8900	C5′—H5′	0.9300
N2—H2B	0.8900	C4—C5	1.359 (6)
N2—C10	1.466 (5)	C9—H9A	0.9700
C8—C7	1.506 (5)	C9—H9B	0.9700
C1—C6	1.392 (5)	C9—C10	1.513 (6)
C1—C2	1.381 (5)	C5—H5	0.9300
C8′—C7′	1.516 (5)	C10—H10A	0.9700
C7—H7A	0.9700	C10—H10B	0.9700
C7—H7B	0.9700		

O2—Zn1—O2′	99.47 (11)	C5—C6—C1	119.2 (4)
O2—Zn1—N1	117.37 (12)	C5—C6—H6	120.4
O2—Zn1—N2	114.42 (12)	C1—C2—H2	119.2
O2′—Zn1—N1	119.57 (13)	C3—C2—C1	121.6 (4)
O2′—Zn1—N2	122.20 (12)	C3—C2—H2	119.2
N1—Zn1—N2	85.14 (14)	C2—C3—H3	121.0
C8—O2—Zn1	113.7 (2)	C2—C3—C4	117.9 (4)
C8′—O2′—Zn1	109.7 (2)	C4—C3—H3	121.0
C1—O1—C7	118.0 (3)	C3′—C2′—H2′	119.8
C1′—O1′—C7′	120.5 (3)	C3′—C2′—C1′	120.4 (4)
Zn1—N1—H1A	110.2	C1′—C2′—H2′	119.8
Zn1—N1—H1B	110.2	C2′—C3′—H3′	120.7
H1A—N1—H1B	108.5	C4′—C3′—C2′	118.5 (4)
C9—N1—Zn1	107.4 (3)	C4′—C3′—H3′	120.7
C9—N1—H1A	110.2	C3′—C4′—Cl1′	117.4 (3)
C9—N1—H1B	110.2	C3′—C4′—C5′	122.5 (4)
Zn1—N2—H2A	110.3	C5′—C4′—Cl1′	120.0 (3)
Zn1—N2—H2B	110.3	C2′—C1′—O1′	114.5 (4)
H2A—N2—H2B	108.6	C2′—C1′—C6′	120.7 (4)
C10—N2—Zn1	107.1 (3)	C6′—C1′—O1′	124.8 (4)
C10—N2—H2A	110.3	C1′—C6′—H6′	120.7
C10—N2—H2B	110.3	C1′—C6′—C5′	118.7 (4)
O2—C8—C7	113.4 (3)	C5′—C6′—H6′	120.7
O3—C8—O2	125.3 (4)	C4′—C5′—C6′	119.2 (4)
O3—C8—C7	121.3 (3)	C4′—C5′—H5′	120.4
O1—C1—C6	124.9 (4)	C6′—C5′—H5′	120.4
O1—C1—C2	115.9 (4)	C3—C4—Cl1	118.8 (3)
C2—C1—C6	119.2 (4)	C5—C4—Cl1	119.3 (4)
O2′—C8′—C7′	114.4 (3)	C5—C4—C3	121.9 (4)

O3′—C8′—O2′	123.9 (4)	N1—C9—H9A	109.8
O3′—C8′—C7′	121.6 (3)	N1—C9—H9B	109.8
O1—C7—C8	109.8 (3)	N1—C9—C10	109.3 (3)
O1—C7—H7A	109.7	H9A—C9—H9B	108.3
O1—C7—H7B	109.7	C10—C9—H9A	109.8
C8—C7—H7A	109.7	C10—C9—H9B	109.8
C8—C7—H7B	109.7	C6—C5—H5	119.9
H7A—C7—H7B	108.2	C4—C5—C6	120.1 (4)
O1′—C7′—C8′	107.4 (3)	C4—C5—H5	119.9
O1′—C7′—H7′A	110.2	N2—C10—C9	109.1 (3)
O1′—C7′—H7′B	110.2	N2—C10—H10A	109.9
C8′—C7′—H7′A	110.2	N2—C10—H10B	109.9
C8′—C7′—H7′B	110.2	C9—C10—H10A	109.9
H7′A—C7′—H7′B	108.5	C9—C10—H10B	109.9
C1—C6—H6	120.4	H10A—C10—H10B	108.3
Zn1—O2—C8—O3	0.4 (6)	C7—O1—C1—C6	−3.9 (6)
Zn1—O2—C8—C7	−179.0 (2)	C7—O1—C1—C2	177.4 (4)
Zn1—O2′—C8′—O3′	2.5 (5)	C7′—O1′—C1′—C2′	171.9 (4)
Zn1—O2′—C8′—C7′	−179.4 (3)	C7′—O1′—C1′—C6′	−8.1 (7)
Zn1—N1—C9—C10	38.5 (4)	C6—C1—C2—C3	2.2 (7)
Zn1—N2—C10—C9	39.2 (4)	C2—C1—C6—C5	−1.3 (7)
Cl1—C4—C5—C6	179.7 (3)	C2—C3—C4—Cl1	−178.9 (3)
Cl1′—C4′—C5′—C6′	179.2 (4)	C2—C3—C4—C5	0.1 (7)
O2—C8—C7—O1	−176.9 (3)	C3—C4—C5—C6	0.7 (7)
O2′—C8′—C7′—O1′	−174.9 (3)	C2′—C3′—C4′—Cl1′	−178.6 (3)
O3—C8—C7—O1	3.7 (6)	C2′—C3′—C4′—C5′	0.4 (7)
O3′—C8′—C7′—O1′	3.1 (6)	C2′—C1′—C6′—C5′	−0.2 (7)
O1—C1—C6—C5	−180.0 (4)	C3′—C2′—C1′—O1′	−179.2 (4)
O1—C1—C2—C3	−179.0 (4)	C3′—C2′—C1′—C6′	0.8 (7)
O1′—C1′—C6′—C5′	179.8 (4)	C3′—C4′—C5′—C6′	0.2 (7)
N1—C9—C10—N2	−53.0 (4)	C1′—O1′—C7′—C8′	−170.8 (4)
C1—O1—C7—C8	−174.2 (3)	C1′—C2′—C3′—C4′	−0.9 (7)
C1—C6—C5—C4	−0.1 (7)	C1′—C6′—C5′—C4′	−0.3 (7)
C1—C2—C3—C4	−1.6 (7)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*B*···O3′^{i}	0.89	2.06	2.931 (4)	166
N2—H2*B*···O3^{ii}	0.89	2.08	2.950 (4)	167
C3—H3···O3′^{iii}	0.93	2.59	3.346 (5)	139
C3′—H3′···O3^{iv}	0.93	2.50	3.314 (5)	146

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) *x*−1, *y*, *z*; (iii) *x*+3/2, −*y*+3/2, *z*−1/2; (iv) *x*−3/2, −*y*+3/2, *z*+1/2.