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Diaquabis(4-chlorobenzoato-κO)bis-(*N*,*N*′-diethylnicotinamide-κ*N*)zinc(II)

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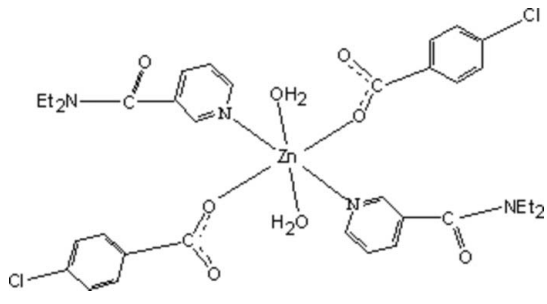
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.063; wR factor = 0.169; data-to-parameter ratio = 24.0.

The title compound, $[Zn(C_7H_4ClO_2)_2(C_{10}H_{14}N_2O)_2(H_2O)_2]$, is a monomeric complex, where the Zn^{II} ion resides on a centre of symmetry in an octahedral coordination environment comprising two pyridyl N, two carboxylate O and two water O atoms. There is an intramolecular hydrogen bond linking each water molecule with one carboxylate group.

Related literature

For related literature, see: Adiwidjaja *et al.* (1978); Bigoli *et al.* (1972, 1973); Catterick *et al.* (1974); Györyová *et al.* (1995); Hökelek & Necefoğlu (1996, 1997); Hökelek *et al.* (1995); Shnulin *et al.* (1981); Szunyogová *et al.* (2007).



Experimental

Crystal data

$[Zn(C_7H_4ClO_2)_2(C_{10}H_{14}N_2O)_2(H_2O)_2]$
M_r = 768.99
Triclinic, $P\overline{1}$
a = 7.3570 (2) Å
b = 8.6887 (10) Å
c = 15.9114 (10) Å
α = 85.047 (5)°
β = 78.476 (5)°
γ = 67.321 (4)°
V = 919.49 (13) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.87 mm^{-1}
T = 296 (2) K
0.35 × 0.20 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID-S diffractometer
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.812, T_{max} = 0.917
27286 measured reflections
5615 independent reflections
3800 reflections with $I > 2\sigma(I)$
R_{int} = 0.073

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.169
S = 1.02
5615 reflections
234 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.85 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn—O2	2.097 (2)	Zn—N1	2.168 (2)
Zn—O1*W*	2.143 (2)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*B*···O3^{i}	0.91 (5)	1.75 (5)	2.654 (4)	168 (5)

Symmetry code: (i) $-x, -y, -z$.

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2071).

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supplementary materials

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Diaquabis(4-chlorobenzoato-κ*O*)bis-(*N*,*N*'-diethylnicotinamide-κ*N*)zinc(II)

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Comment

Zn(II)plays a key role in many biological processes and its interactions are a subject of considerable interest. The metal takes part in more than 300 metalloenzymes and many of its complexes have antimicrobial effect against bacteria, fungi and viruses (Szunyogová *et al.*; 2007). They are interesting both from a chemical point of view as due to their biological activity (Györyová *et al.*, 1995). In particular, *N*,*N*'-Diethylnicotinamide (DENA) is an important respiratory stimulant (Bigoli *et al.*, 1972). The structures of some complexes obtained from the reactions of transition metal(II) ions with DENA have been determined previously; (Bigoli *et al.*, 1972; Hökelek *et al.*, 1995; Hökelek & Necefoğlu, 1996, Hökelek & Necefoğlu, 1997).

On the other hand, the structure-function-coordination relationships of the arylcarboxylate ion in Zn(II) complexes of benzoic acid derivatives change depending on the nature and position of the substituted groups in the phenyl ring, the nature of the additional ligand molecule or solvent, and the pH and temperature of synthesis (Shnulin *et al.*, 1981; Adiwidjaja *et al.*, 1978). When pyridine and its derivatives are coordinated instead of water molecules, the structure is completely different (Catterick *et al.*, 1974).

We report here the structure of the title compound, (I), a monomeric zinc complex combining both the chlorobenzoate and diethylnicotinamide ligands.

Fig. 1 shows an ellipsoid plot of (I). The Zn cation is located on a symmetry centre in a slightly distorted octahedral environment. The metal is coordinated by two O atoms from two equivalent carboxylate groups and two O atoms from two water molecules to form a distorted square-planar base (Table 1). Two pyridine N atoms from diethylnicotinamide (DENA) ligands (Table 1), complete the Jahn-Teller distorted octahedral coordination at a longer distance (Zn—N: 2.168 (2) Å), in good agreement with values reported for other octahedrally coordinated Zn^{II} complexes [*viz*., $Zn(DENA)_2(NCS)_2{\cdot}2H_2O$, Zn—N: 2.171 (4) Å; Bigoli *et al.*,1973]. The carboxylate group is approximately coplanar with the attached benzene ring, the dihedral angle between both planes being 2.8 (3)°. The pyridine and benzene rings are planar, the maximum deviation from the least-squares planes being −0.0072 (10) Å for atom C10 and 0.0006 (1) Å for atom C2. There is an intramolecular hydrogen bond between O1w and the carboxyl O3 (Table 2).

Experimental

In the synthesis of the complex, sodium *p*-chlorobenzoate was preapared firstly, for what 0.02 mole *p*-chlorobenzoic acid was reacted with aqueous solution (50 ml) of 0,02 mole sodium bicarbonate. In order to remove completely the carbon dioxide formed in the reaction, the solution was stirred with heating at 363 K for 1 h and allowed to cool at room temperature. In another beaker, an aqueous solution (25 ml) of diethylnicotinamide (0.02 mole) was added to an aqueous solution (25 ml) of zinc nitrate (0,01 mole) and the previously prepared solution of sodium *p*-chlorobenzoate was added. This final mixed solution was kept unperturbed for 3–5 days, to allow for crystallization. The crystals formed were filtered off, washed with cold water and dried at room temperature. Analysis found: C 52.49, H 5.00, N 7.26%; calculated for $C_{34}H_{40}Cl_2N_4O_8Zn$: C 53.10, H 5.24, N 7.29%.

Refinement

Water H atoms were located in difference maps and refined with isotropic displacement factors. Other H atoms were placed in geometrically idealized positions and refined constrained to ride on their parent atoms with distances in the range 0.93–0.97 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$, or $1.5U_{eq}(C)$ for methyl atoms.

Figures

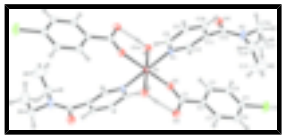


Fig. 1. The molecular sructure and atomic labelling scheme of the title compound. Hydrogen bonds are indicated by open dashed lines. Displacement ellipsoids are drawn at the 30% probability level·Unlabelled atoms are related to labelled atoms by −*x*, −*y*, −*z*.

Diaquabis(4-chlorobenzoato-κ*O*)bis-(*N*,*N*'- diethylnicotinamide-κ*N*)zinc(II)

Crystal data

$[Zn(C_7H_4ClO_2)_2(C_{10}H_{14}N_2O)_2(H_2O)_2]$	$Z = 1$
$M_r = 768.99$	$F_{000} = 400$
Triclinic, $P\overline{1}$	$D_x = 1.389$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71069$ Å
$a = 7.3570$ (2) Å	Cell parameters from 25 reflections
$b = 8.6887$ (10) Å	$\theta = 2.5$–30.5º
$c = 15.9114$ (10) Å	$\mu = 0.87$ mm^{-1}
$\alpha = 85.047$ (5)º	$T = 296$ (2) K
$\beta = 78.476$ (5)º	Prism, yellow
$\gamma = 67.321$ (4)º	0.35 × 0.20 × 0.10 mm
$V = 919.49$ (13) Å^3	

Data collection

Rigaku R-AXIS RAPID-S diffractometer	5615 independent reflections
Radiation source: sealed X-ray tube	3800 reflections with $I > 2\sigma(I)$
Monochromator: Graphite Monochromator	$R_{int} = 0.073$
Detector resolution: 10.000 pixels mm^{-1}	$\theta_{max} = 30.5$º
$T = 296(2)$ K	$\theta_{min} = 2.5$º
ω scans	$h = -10 \rightarrow 10$
Absorption correction: multi-scan (Blessing, 1995)	$k = -12 \rightarrow 12$
$T_{min} = 0.812$, $T_{max} = 0.917$	$l = -22 \rightarrow 22$
27286 measured reflections	

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.063$

$wR(F^2) = 0.169$

$S = 1.02$

5615 reflections

234 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0647P)^2 + 0.5887P]$ where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 0.85$ e Å^{-3}

$\Delta\rho_{min} = -0.44$ e Å^{-3}

Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.029 (4)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn	0.0000	0.0000	0.0000	0.04307 (17)
Cl1	0.73554 (19)	0.1583 (2)	−0.46678 (7)	0.0998 (4)
O1W	0.2219 (3)	0.0161 (3)	0.06412 (16)	0.0526 (5)
H1A	0.206 (6)	0.113 (5)	0.074 (2)	0.057 (11)*
H1B	0.184 (8)	−0.030 (7)	0.115 (3)	0.112 (19)*
O2	0.1110 (3)	0.1211 (3)	−0.10540 (13)	0.0477 (5)
O3	−0.0778 (3)	0.1279 (3)	−0.20065 (15)	0.0588 (6)
O4	0.8388 (4)	−0.3286 (3)	−0.12444 (17)	0.0645 (6)
N1	0.2253 (4)	−0.2349 (3)	−0.05050 (16)	0.0448 (5)
N2	0.8313 (5)	−0.4147 (5)	−0.2505 (2)	0.0748 (9)
C1	0.0786 (4)	0.1282 (4)	−0.18056 (19)	0.0430 (6)
C2	0.2437 (4)	0.1359 (4)	−0.25251 (19)	0.0437 (6)
C3	0.4176 (5)	0.1423 (4)	−0.2350 (2)	0.0494 (7)
H3	0.4325	0.1415	−0.1783	0.059*
C4	0.5694 (5)	0.1500 (5)	−0.3001 (2)	0.0570 (8)
H4	0.6856	0.1547	−0.2878	0.068*
C5	0.5441 (5)	0.1503 (5)	−0.3838 (2)	0.0616 (9)
C6	0.3747 (5)	0.1419 (5)	−0.4034 (2)	0.0617 (9)
H6	0.3610	0.1416	−0.4602	0.074*
C7	0.2248 (5)	0.1338 (4)	−0.3374 (2)	0.0526 (7)
H7	0.1100	0.1270	−0.3500	0.063*
C8	0.1959 (4)	−0.3783 (4)	−0.0406 (2)	0.0477 (7)
H8	0.0743	−0.3778	−0.0096	0.057*
C9	0.3380 (5)	−0.5276 (4)	−0.0745 (2)	0.0549 (8)
H9	0.3129	−0.6253	−0.0661	0.066*
C10	0.5181 (5)	−0.5280 (4)	−0.1210 (2)	0.0530 (8)
H10	0.6159	−0.6261	−0.1452	0.064*

C11	0.5511 (4)	−0.3795 (4)	−0.13123 (19)	0.0449 (6)
C12	0.4022 (4)	−0.2380 (4)	−0.09404 (19)	0.0454 (6)
H12	0.4256	−0.1394	−0.0994	0.055*
C13	0.7496 (5)	−0.3702 (4)	−0.1696 (2)	0.0513 (7)
C14	0.7386 (8)	−0.4727 (7)	−0.3088 (3)	0.0960 (15)
H14A	0.8306	−0.5810	−0.3312	0.115*
H14B	0.6181	−0.4854	−0.2770	0.115*
C15	0.6889 (14)	−0.3581 (12)	−0.3789 (6)	0.203 (5)
H15A	0.6076	−0.2485	−0.3569	0.208*
H15B	0.6163	−0.3932	−0.4120	0.208*
H15C	0.8096	−0.3560	−0.4146	0.208*
C16	1.0387 (7)	−0.4206 (6)	−0.2822 (3)	0.0845 (13)
H16A	1.1175	−0.4644	−0.2373	0.101*
H16B	1.1008	−0.4953	−0.3307	0.101*
C17	1.0383 (9)	−0.2539 (7)	−0.3086 (4)	0.113 (2)
H17A	0.9436	−0.2030	−0.3461	0.170*
H17B	1.1696	−0.2639	−0.3380	0.170*
H17C	1.0015	−0.1860	−0.2587	0.170*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn	0.0364 (2)	0.0470 (3)	0.0430 (3)	−0.0135 (2)	−0.00279 (18)	−0.0062 (2)
Cl1	0.0809 (7)	0.1576 (13)	0.0650 (6)	−0.0628 (8)	0.0159 (5)	−0.0051 (7)
O1W	0.0482 (12)	0.0575 (15)	0.0573 (14)	−0.0236 (11)	−0.0112 (10)	−0.0056 (12)
O2	0.0464 (11)	0.0523 (12)	0.0432 (11)	−0.0187 (10)	−0.0041 (9)	−0.0039 (9)
O3	0.0438 (11)	0.0772 (16)	0.0568 (13)	−0.0241 (11)	−0.0124 (10)	0.0062 (12)
O4	0.0546 (13)	0.0773 (17)	0.0705 (16)	−0.0328 (13)	−0.0093 (12)	−0.0138 (13)
N1	0.0382 (12)	0.0461 (14)	0.0473 (13)	−0.0146 (10)	−0.0026 (10)	−0.0045 (11)
N2	0.0625 (18)	0.108 (3)	0.0594 (18)	−0.0429 (19)	0.0088 (14)	−0.0224 (18)
C1	0.0395 (13)	0.0392 (14)	0.0456 (15)	−0.0103 (11)	−0.0066 (11)	−0.0011 (12)
C2	0.0420 (14)	0.0414 (15)	0.0452 (15)	−0.0136 (12)	−0.0064 (11)	−0.0020 (12)
C3	0.0481 (16)	0.0536 (18)	0.0484 (16)	−0.0216 (14)	−0.0068 (13)	−0.0033 (13)
C4	0.0489 (17)	0.067 (2)	0.059 (2)	−0.0275 (16)	−0.0064 (14)	−0.0006 (16)
C5	0.0564 (19)	0.076 (2)	0.0484 (18)	−0.0264 (18)	0.0024 (14)	−0.0033 (16)
C6	0.059 (2)	0.078 (2)	0.0448 (17)	−0.0238 (18)	−0.0065 (14)	−0.0005 (16)
C7	0.0481 (16)	0.063 (2)	0.0480 (17)	−0.0212 (15)	−0.0105 (13)	−0.0009 (14)
C8	0.0421 (15)	0.0508 (17)	0.0502 (16)	−0.0177 (13)	−0.0059 (12)	−0.0055 (13)
C9	0.0503 (17)	0.0479 (17)	0.067 (2)	−0.0197 (14)	−0.0063 (15)	−0.0078 (15)
C10	0.0450 (16)	0.0480 (17)	0.063 (2)	−0.0124 (13)	−0.0068 (14)	−0.0152 (15)
C11	0.0373 (13)	0.0492 (16)	0.0455 (15)	−0.0124 (12)	−0.0066 (11)	−0.0072 (13)
C12	0.0398 (14)	0.0452 (15)	0.0496 (16)	−0.0151 (12)	−0.0040 (12)	−0.0055 (12)
C13	0.0420 (15)	0.0560 (18)	0.0543 (18)	−0.0179 (14)	−0.0020 (13)	−0.0113 (14)
C14	0.093 (3)	0.130 (4)	0.069 (3)	−0.050 (3)	−0.002 (2)	−0.011 (3)
C15	0.155 (9)	0.185 (12)	0.152 (9)	−0.102 (9)	−0.100 (8)	0.100 (9)
C16	0.067 (2)	0.085 (3)	0.093 (3)	−0.030 (2)	0.017 (2)	−0.024 (2)
C17	0.120 (5)	0.090 (4)	0.117 (4)	−0.047 (3)	0.025 (4)	−0.006 (3)

Geometric parameters (Å, °)

Zn—O2^{i}	2.097 (2)	C6—C7	1.381 (5)
Zn—O2	2.097 (2)	C6—H6	0.9300
Zn—O1W^{i}	2.143 (2)	C7—H7	0.9300
Zn—O1W	2.143 (2)	C8—C9	1.384 (4)
Zn—N1	2.168 (2)	C8—H8	0.9300
Zn—N1^{i}	2.168 (2)	C9—C10	1.381 (5)
Cl1—C5	1.746 (4)	C9—H9	0.9300
O1W—H1A	0.83 (4)	C10—C11	1.393 (4)
O1W—H1B	0.91 (4)	C10—H10	0.9300
O2—C1	1.257 (3)	C11—C12	1.375 (4)
O3—C1	1.255 (4)	C11—C13	1.496 (4)
O4—C13	1.222 (4)	C12—H12	0.9300
N1—C8	1.336 (4)	C14—C15	1.435 (11)
N1—C12	1.338 (4)	C14—H14A	0.9700
N2—C13	1.328 (4)	C14—H14B	0.9700
N2—C14	1.478 (6)	C15—H15A	0.9600
N2—C16	1.489 (5)	C15—H15B	0.9600
C1—C2	1.511 (4)	C15—H15C	0.9600
C2—C3	1.385 (4)	C16—C17	1.473 (7)
C2—C7	1.387 (4)	C16—H16A	0.9700
C3—C4	1.381 (4)	C16—H16B	0.9700
C3—H3	0.9300	C17—H17A	0.9600
C4—C5	1.382 (5)	C17—H17B	0.9600
C4—H4	0.9300	C17—H17C	0.9600
C5—C6	1.373 (5)		
O2^{i}—Zn—O2	180.0	C6—C7—H7	119.7
O2^{i}—Zn—O1W^{i}	87.86 (9)	C2—C7—H7	119.7
O2—Zn—O1W^{i}	92.14 (9)	N1—C8—C9	123.0 (3)
O2^{i}—Zn—O1W	92.14 (9)	N1—C8—H8	118.5
O2—Zn—O1W	87.86 (9)	C9—C8—H8	118.5
O1W^{i}—Zn—O1W	180.00 (11)	C10—C9—C8	118.5 (3)
O2^{i}—Zn—N1	91.50 (9)	C10—C9—H9	120.8
O2—Zn—N1	88.50 (9)	C8—C9—H9	120.8
O1W^{i}—Zn—N1	93.59 (10)	C9—C10—C11	119.1 (3)
O1W—Zn—N1	86.41 (10)	C9—C10—H10	120.5
O2^{i}—Zn—N1^{i}	88.50 (9)	C11—C10—H10	120.5
O2—Zn—N1^{i}	91.50 (9)	C12—C11—C10	118.3 (3)
O1W^{i}—Zn—N1^{i}	86.41 (10)	C12—C11—C13	117.8 (3)
O1W—Zn—N1^{i}	93.59 (10)	C10—C11—C13	123.4 (3)
N1—Zn—N1^{i}	180.00 (13)	N1—C12—C11	123.3 (3)
Zn—O1W—H1A	114 (3)	N1—C12—H12	118.4
Zn—O1W—H1B	96 (3)	C11—C12—H12	118.4
H1A—O1W—H1B	108 (4)	O4—C13—N2	120.8 (3)

C1—O2—Zn	126.4 (2)	O4—C13—C11	119.0 (3)
C8—N1—C12	117.8 (3)	N2—C13—C11	120.1 (3)
C8—N1—Zn	123.0 (2)	C15—C14—N2	111.6 (6)
C12—N1—Zn	119.1 (2)	C15—C14—H14A	108.9
C13—N2—C14	124.9 (3)	N2—C14—H14A	108.9
C13—N2—C16	117.6 (3)	C15—C14—H14B	108.9
C14—N2—C16	117.4 (3)	N2—C14—H14B	108.9
O3—C1—O2	125.6 (3)	H14A—C14—H14B	107.7
O3—C1—C2	117.6 (3)	C14—C15—H15A	109.5
O2—C1—C2	116.8 (3)	C14—C15—H15B	109.5
C3—C2—C7	118.8 (3)	H15A—C15—H15B	109.5
C3—C2—C1	120.7 (3)	C14—C15—H15C	109.5
C7—C2—C1	120.4 (3)	H15A—C15—H15C	109.5
C4—C3—C2	121.4 (3)	H15B—C15—H15C	109.5
C4—C3—H3	119.3	C17—C16—N2	111.3 (4)
C2—C3—H3	119.3	C17—C16—H16A	109.4
C3—C4—C5	118.2 (3)	N2—C16—H16A	109.4
C3—C4—H4	120.9	C17—C16—H16B	109.4
C5—C4—H4	120.9	N2—C16—H16B	109.4
C6—C5—C4	121.9 (3)	H16A—C16—H16B	108.0
C6—C5—Cl1	119.4 (3)	C16—C17—H17A	109.5
C4—C5—Cl1	118.7 (3)	C16—C17—H17B	109.5
C5—C6—C7	119.0 (3)	H17A—C17—H17B	109.5
C5—C6—H6	120.5	C16—C17—H17C	109.5
C7—C6—H6	120.5	H17A—C17—H17C	109.5
C6—C7—C2	120.7 (3)	H17B—C17—H17C	109.5
O1W^{i}—Zn—O2—C1	−16.0 (2)	C3—C2—C7—C6	−1.4 (5)
O1W—Zn—O2—C1	164.0 (2)	C1—C2—C7—C6	179.6 (3)
N1—Zn—O2—C1	77.5 (2)	C12—N1—C8—C9	−1.2 (5)
N1^{i}—Zn—O2—C1	−102.5 (2)	Zn—N1—C8—C9	178.5 (2)
O2^{i}—Zn—N1—C8	32.6 (2)	N1—C8—C9—C10	−0.4 (5)
O2—Zn—N1—C8	−147.4 (2)	C8—C9—C10—C11	0.8 (5)
O1W—Zn—N1—C8	124.6 (2)	C9—C10—C11—C12	0.2 (5)
O2^{i}—Zn—N1—C12	−147.8 (2)	C9—C10—C11—C13	171.2 (3)
O2—Zn—N1—C12	32.2 (2)	C8—N1—C12—C11	2.3 (4)
O1W^{i}—Zn—N1—C12	124.3 (2)	Zn—N1—C12—C11	−177.4 (2)
O1W—Zn—N1—C12	−55.7 (2)	C10—C11—C12—N1	−1.8 (5)
Zn—O2—C1—O3	30.9 (4)	C13—C11—C12—N1	−173.4 (3)
Zn—O2—C1—C2	−148.4 (2)	C14—N2—C13—O4	177.6 (4)
O3—C1—C2—C3	177.8 (3)	C16—N2—C13—O4	3.2 (6)
O2—C1—C2—C3	−2.9 (4)	C14—N2—C13—C11	1.0 (6)
O3—C1—C2—C7	−3.2 (4)	C16—N2—C13—C11	−173.4 (4)
O2—C1—C2—C7	176.1 (3)	C12—C11—C13—O4	57.2 (4)
C7—C2—C3—C4	1.3 (5)	C10—C11—C13—O4	−113.9 (4)
C1—C2—C3—C4	−179.8 (3)	C12—C11—C13—N2	−126.1 (4)
C2—C3—C4—C5	−0.3 (5)	C10—C11—C13—N2	62.8 (5)
C3—C4—C5—C6	−0.6 (6)	C13—N2—C14—C15	114.2 (7)
C3—C4—C5—Cl1	−179.5 (3)	C16—N2—C14—C15	−70.5 (8)

C4—C5—C6—C7	0.4 (6)	C13—N2—C16—C17	−82.4 (6)
Cl1—C5—C6—C7	179.3 (3)	C14—N2—C16—C17	102.7 (5)
C5—C6—C7—C2	0.6 (6)		

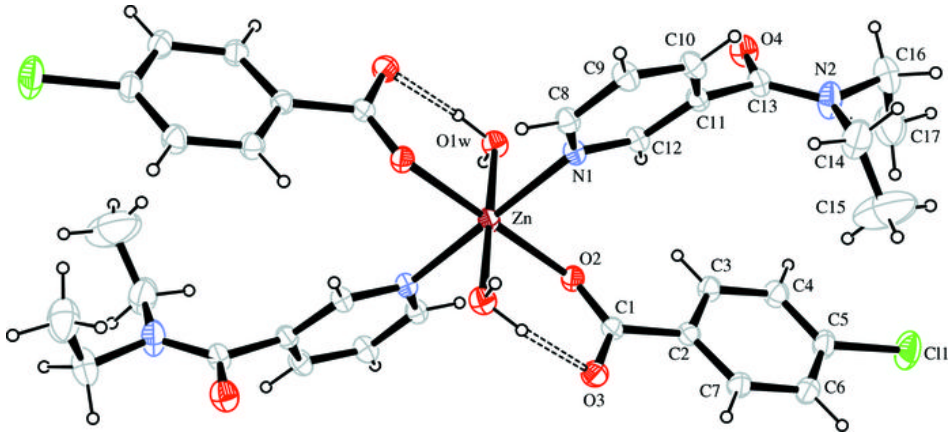
Symmetry codes: (i) −*x*, −*y*, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1B···O3^{i}	0.91 (5)	1.75 (5)	2.654 (4)	168 (5)

Symmetry codes: (i) −*x*, −*y*, −*z*.

Fig. 1


C10
O4
C16
C9
N2
C8
C13
C11
C17
O1w
C12
C14
N1
Zn
C15
O2
C3
C4
C1
C5
C2
Cl1
C7
C6
O3