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Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.008$ Å
 R factor = 0.054
 wR factor = 0.124
Data-to-parameter ratio = 13.6For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.A new zinc(II) complex with a peptide
ligand: aqua{*N,N*-bis[2-(2-pyridyl)methyl]-
pyridine-2,6-dicarboxamide}dichlorozinc(II)

The title compound, $[\text{ZnCl}_2(\text{C}_{19}\text{H}_{17}\text{N}_5\text{O}_2)(\text{H}_2\text{O})]$, was prepared from the peptide ligand *N,N*-bis[2-(2-pyridyl)methyl]pyridine-2,6-dicarboxamide and zinc chloride. The Zn atom exists in a tetrahedral geometry and is coordinated by a pyridine N atom of the ligand, two chloride ions and one water O atom. The ligand coordinates to the zinc ion in a monodentate fashion.

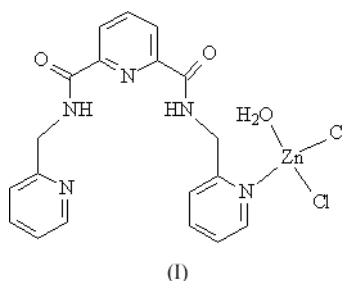
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Comment

Amides play an important role in nature and the amidate function participates in the coordination chemistry of iron-containing biomolecules, such as the antitumor drug bleomycin and nitrile hydratase (Burger, 2000; Tsujimura *et al.*, 1997). The strong donor ability of a deprotonated amide is expected to imbue the metal center, to which it is coordinated, with novel electronic properties. Recently, several designed ligands with pyridine-2-carboxamide units have been synthesized by different groups and their coordination properties with many transition metal ions have been explored (Rowland *et al.*, 2000; Zhu *et al.*, 2002).



The crystal structure of the title complex, (I), a new zinc(II) complex with a peptide ligand, is shown in Fig. 1. It is a discrete mononuclear complex in which the zinc(II) ion exists in a distorted tetrahedral geometry. Selected geometric parameters are given in Table 1. The peptide ligand coordin-

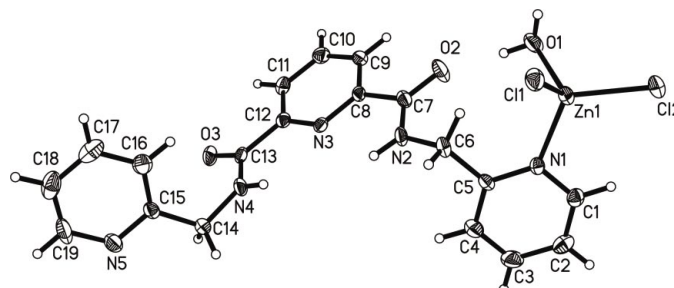


Figure 1

A view of the title compound, (I), shown with 30% probability displacement ellipsoids.

ates to the zinc ion in a monodentate fashion, *via* a pyridine N atom of one arm of the ligand, with a Zn–N bond length of 2.057 (4) Å. The pyridine-2,6-dicarboxamide moiety and the other pyridine arm remain uncoordinated. The other three coordination sites of the zinc ion are occupied by one water molecule and two chloride ions. The Zn–O bond length is 1.994 (3) Å and the Zn–Cl bond lengths are 2.263 (2) and 2.224 (2) Å.

In the complex, a three-dimensional structure is formed through intermolecular hydrogen-bonding interactions (Table 2), and the packing diagram of (I) is shown in Fig. 2.

Experimental

The title compound was prepared by adding an aqueous solution (5 ml) of ZnCl₂ (0.1 mmol) to a methanol solution (10 ml) of *N,N*-bis[2-(2-pyridyl)methyl]pyridine-2,6-dicarboxamide (0.1 mmol). The mixture was stirred for 1 h and then filtered. The filtrate was evaporated slowly at room temperature and colorless block-shaped crystals suitable for X-ray analysis were obtained. Analysis calculated for C₁₉H₁₉Cl₂N₅O₃Zn: C 45.45, H 3.79, N 13.95%; found: C 45.76, H 4.06, N 13.77%.

Crystal data

[ZnCl ₂ (C ₁₉ H ₁₇ N ₅ O ₂)(H ₂ O)]	$D_x = 1.580 \text{ Mg m}^{-3}$
$M_r = 501.66$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 770 reflections
$a = 9.210 (5) \text{ \AA}$	$\theta = 2.6\text{--}24.2^\circ$
$b = 18.394 (10) \text{ \AA}$	$\mu = 1.45 \text{ mm}^{-1}$
$c = 13.215 (7) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 109.657 (8)^\circ$	Block, colorless
$V = 2108.5 (19) \text{ \AA}^3$	$0.22 \times 0.20 \times 0.14 \text{ mm}$
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	3693 independent reflections
φ and ω scans	2504 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.066$
$T_{\text{min}} = 0.576$, $T_{\text{max}} = 0.816$	$\theta_{\text{max}} = 25.0^\circ$
10650 measured reflections	$h = -10 \rightarrow 10$
	$k = -21 \rightarrow 12$
	$l = -14 \rightarrow 15$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.054$	$w = 1/[\sigma^2(F_o^2) + (0.0563P)^2]$
$wR(F^2) = 0.125$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{\text{max}} = 0.004$
3693 reflections	$\Delta\rho_{\text{max}} = 0.63 \text{ e \AA}^{-3}$
271 parameters	$\Delta\rho_{\text{min}} = -0.41 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Zn1–O1	1.994 (3)	O2–C7	1.229 (5)
Zn1–N1	2.057 (4)	O3–C13	1.224 (5)
Zn1–Cl2	2.2239 (18)	N2–C7	1.327 (6)
Zn1–Cl1	2.2629 (17)	N4–C13	1.346 (6)
O1–Zn1–N1	102.31 (14)	O1–Zn1–Cl1	109.04 (12)
O1–Zn1–Cl2	106.17 (11)	N1–Zn1–Cl1	111.76 (10)
N1–Zn1–Cl2	112.60 (11)	Cl2–Zn1–Cl1	114.06 (5)

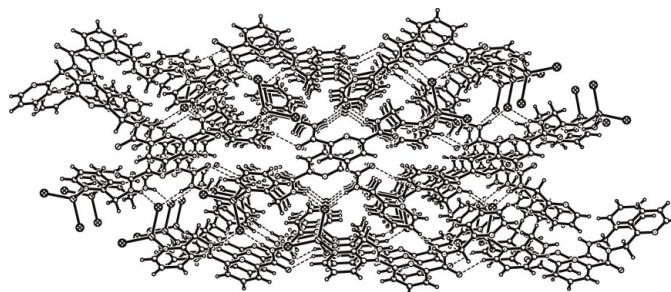


Figure 2

A crystal packing diagram of the title compound, (I), viewed down the a axis. Hydrogen bonds are shown as dashed lines.

Table 2

Hydrogen-bonding geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1–H1A \cdots O2	0.82	1.88	2.695 (5)	171
O1–H1B \cdots N5 ⁱ	0.85	1.89	2.723 (6)	167
N2–H2A \cdots N3	0.86	2.32	2.707 (5)	108
N2–H2A \cdots Cl1 ⁱⁱ	0.86	2.59	3.356 (4)	149
N4–H4A \cdots N3	0.86	2.35	2.720 (6)	106
N4–H4A \cdots Cl1 ⁱⁱ	0.86	2.62	3.364 (4)	145
Cl1–H1 \cdots O3 ⁱⁱⁱ	0.93	2.36	3.140 (6)	142

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

The water H atoms, located in a difference map, were not refined [$U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$]. The N–H, aromatic and CH₂ H atoms were placed in calculated positions (N–H = 0.86 Å and C–H = 0.93–0.97 Å) and allowed to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N or C})$.

Data collection: SMART (Bruker, 1998); cell refinement: SMART; data reduction: SAINT (Bruker, 1998); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1998); software used to prepare material for publication: SHELXTL.

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