

[*N,N'*-Bis(4-chlorobenzyl)propane-1,2-diamine]dichloridozinc(II)

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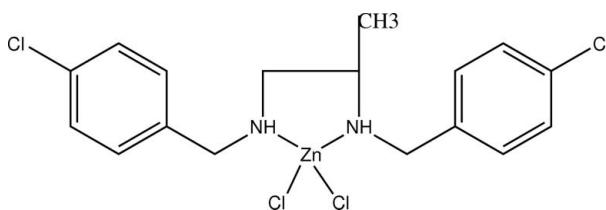
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Key indicators: single-crystal X-ray study; $T = 298\text{ K}$; mean $\sigma(\text{C}-\text{C}) = 0.017\text{ \AA}$; R factor = 0.115; wR factor = 0.217; data-to-parameter ratio = 15.9.

In the title complex, $[\text{ZnCl}_2(\text{C}_{17}\text{H}_{20}\text{Cl}_2\text{N}_2)]$, the Zn^{II} atom is coordinated by two Cl atoms and two N atoms of the *N,N'*-bis(4-chlorobenzyl)propane-1,2-diamine ligand, and displays a tetrahedral coordination geometry. Two $\text{N}-\text{H}\cdots\text{Cl}$ hydrogen bonds link the molecules into a chain of $R_2^2(8)$ rings.

Related literature

For related literature, see: Bernstein *et al.* (1995); Han *et al.* (2006); Liu *et al.* (2007).



Experimental

Crystal data

$[\text{ZnCl}_2(\text{C}_{17}\text{H}_{20}\text{Cl}_2\text{N}_2)]$

$M_r = 459.52$

Orthorhombic, $Pbca$

$a = 14.638 (2)\text{ \AA}$

$b = 10.770 (1)\text{ \AA}$

$c = 26.090 (3)\text{ \AA}$

$V = 4113.2 (9)\text{ \AA}^3$

$Z = 8$

Mo $K\alpha$ radiation

$\mu = 1.72\text{ mm}^{-1}$

$T = 298 (2)\text{ K}$

$0.59 \times 0.18 \times 0.14\text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.431$, $T_{\max} = 0.795$

15270 measured reflections
3458 independent reflections
1720 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.216$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.115$
 $wR(F^2) = 0.217$
 $S = 1.29$
3458 reflections

218 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.61\text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.68\text{ e \AA}^{-3}$

Table 1
Selected geometric parameters (\AA , $^\circ$).

Zn1–N2	2.076 (7)	Zn1–Cl1	2.196 (3)
Zn1–N1	2.098 (8)	Zn1–Cl2	2.249 (3)
N2–Zn1–N1	86.2 (3)	N2–Zn1–Cl2	104.3 (2)
N2–Zn1–Cl1	121.1 (2)	N1–Zn1–Cl2	107.7 (2)
N1–Zn1–Cl1	117.4 (2)	Cl1–Zn1–Cl2	115.9 (1)

Table 2
Hydrogen-bond geometry (\AA , $^\circ$).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
N1–H1 ⁱ –Cl1 ⁱ	0.91	2.68	3.585 (8)	175
N2–H2 ^j –Cl2 ⁱⁱ	0.91	2.47	3.295 (8)	151

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CF2157).

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supplementary materials

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[*N,N'*-Bis(4-chlorobenzyl)propane-1,2-diamine]dichloridozinc(II)

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Comment

We have reported recently the crystal structure of a Zn^{II} complex (Han *et al.*, 2006). As part of our study of Zn^{II} complexes with diamine derivatives, We report here the crystal structure of a new Zn^{II} complex, the title compound, (I).

Complex (I) is a mononuclear compound. The central zinc ion is coordinated by two Cl atoms and two N atoms of the *N,N'*-bis(4-chlorobenzyl)propane-1,2-diamino ligand, forming a distorted tetrahedral coordination geometry (Fig. 1). The Zn—Cl and Zn—N bond lengths are comparable with those of Zn^{II} complexes reported previously (Han *et al.*, 2006; Liu *et al.*, 2007), and the bond angle range around Zn^{II} is 86.2 (3)^o–121.1 (2)^o. The N1/Zn1/N2 and Cl1/Zn1/Cl2 planes are nearly perpendicular, enclosing a dihedral angle of 87.2 (2)^o; the sum of the internal angles is 517^o in the five-membered ring Zn/N1/N2/C15–C16, the two benzene rings are located on opposite sides of the five-membered ring, and they enclose a dihedral angle of 20.2 (5)^o.

In the crystal structure of (I), the molecules are linked by two N—H···Cl hydrogen bonds into a chain of $R_2^2(8)$ rings (Bernstein *et al.*, 1995) along the [010] direction (Fig. 2).

Experimental

To a solution containing *N,N'*-bis(4-chlorobenzyl)propane-1,2-diamine (3.20 g, 10 mmol) and ethanol (30 ml), a solution of zinc chloride (1.36 g, 10 mmol) and ethanol (10 ml) was added with stirring for 6 h at room temperature (298–300 K); the solid obtained was filtered off, washed successively with chloroform and ethanol, and dried at room temperature. Colourless crystals of (I) suitable for X-ray structure analysis were obtained by slow evaporation of a DMF-ethanol(1:10) solution containing the product over a period of three weeks (*M.p.* 499–501 K).

Refinement

The overall quality of the data is poor due to the poor crystal quality and weak diffraction, resulting in high *R*-factors.

All H atoms were located in difference Fourier maps and then treated as riding atoms, with C—H distances of 0.93 Å (aryl), 0.96 Å (methyl), 0.97 Å (methylene), and N—H = 0.91 Å, and with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ (methyl) and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$ (aryl, methylene, amine).

supplementary materials

Figures

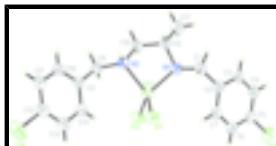


Fig. 1. The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

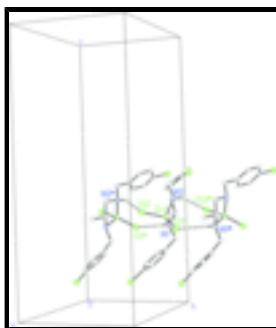


Fig. 2. Part of the crystal structure of (I), showing the formation of a [010] chain of $R_2^2(8)$ rings. For clarity, H atoms have been omitted. Dashed lines indicate hydrogen bonds. [Symmetry codes: (*) $1/2 - x, -1/2 + y, z$; (#) $1/2 - x, 1/2 + y, z$.]

[*N,N'*-Bis(4-chlorobenzyl)propane-1,2-diamine]dichloridozinc(II)

Crystal data

$[ZnCl_2(C_{17}H_{20}Cl_2N_2)]$	$D_x = 1.484 \text{ Mg m}^{-3}$
$M_r = 459.52$	Melting point: 497 K
Orthorhombic, $Pbca$	Mo $K\alpha$ radiation
Hall symbol: -P 2ac 2ab	$\lambda = 0.71073 \text{ \AA}$
$a = 14.638 (2) \text{ \AA}$	Cell parameters from 1955 reflections
$b = 10.770 (1) \text{ \AA}$	$\theta = 2.5\text{--}20.8^\circ$
$c = 26.090 (3) \text{ \AA}$	$\mu = 1.72 \text{ mm}^{-1}$
$V = 4113.2 (9) \text{ \AA}^3$	$T = 298 (2) \text{ K}$
$Z = 8$	Prism, colourless
$F_{000} = 1872$	$0.59 \times 0.18 \times 0.14 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer	3458 independent reflections
Radiation source: fine-focus sealed tube	1720 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.216$
$T = 298(2) \text{ K}$	$\theta_{\text{max}} = 25.0^\circ$
ϕ and ω scans	$\theta_{\text{min}} = 2.5^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -10 \rightarrow 17$
$T_{\text{min}} = 0.431, T_{\text{max}} = 0.795$	$k = -12 \rightarrow 11$
15270 measured reflections	$l = -31 \rightarrow 31$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.115$	H-atom parameters constrained
$wR(F^2) = 0.217$	$w = 1/[\sigma^2(F_o^2) + (0.0488P)^2 + 0.5373P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.29$	$(\Delta/\sigma)_{\max} = 0.001$
3458 reflections	$\Delta\rho_{\max} = 0.61 \text{ e \AA}^{-3}$
218 parameters	$\Delta\rho_{\min} = -0.68 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.28774 (7)	0.94334 (11)	0.82844 (4)	0.0514 (4)
Cl1	0.3749 (2)	1.0772 (2)	0.78794 (10)	0.0687 (8)
Cl2	0.3531 (2)	0.7603 (2)	0.84790 (12)	0.0775 (9)
Cl3	0.2262 (3)	0.5655 (4)	0.58833 (11)	0.1036 (12)
Cl4	0.5868 (3)	1.2971 (4)	0.98538 (16)	0.1283 (15)
N1	0.1588 (6)	0.9061 (7)	0.7969 (3)	0.054 (2)
H1	0.1537	0.8223	0.7938	0.065*
N2	0.2181 (5)	0.9931 (7)	0.8947 (2)	0.051 (2)
H2	0.2073	1.0762	0.8930	0.061*
C1	0.1418 (7)	0.9612 (10)	0.7448 (3)	0.064 (3)
H1A	0.1792	1.0347	0.7405	0.077*
H1B	0.0783	0.9855	0.7419	0.077*
C2	0.1646 (9)	0.8677 (11)	0.7035 (4)	0.063 (3)
C3	0.0958 (9)	0.8106 (11)	0.6772 (4)	0.074 (3)
H3	0.0356	0.8340	0.6831	0.089*
C4	0.1148 (9)	0.7179 (12)	0.6418 (4)	0.076 (4)
H4	0.0668	0.6809	0.6240	0.092*
C5	0.2029 (9)	0.6795 (12)	0.6323 (4)	0.070 (3)

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C6	0.2716 (9)	0.7410 (13)	0.6581 (4)	0.077 (3)
H6	0.3323	0.7205	0.6516	0.092*
C7	0.2518 (10)	0.8318 (13)	0.6931 (4)	0.074 (3)
H7	0.2996	0.8703	0.7103	0.089*
C8	0.2633 (8)	0.9668 (11)	0.9458 (3)	0.061 (3)
H8A	0.2190	0.9788	0.9729	0.073*
H8B	0.2827	0.8807	0.9466	0.073*
C9	0.3446 (7)	1.0486 (11)	0.9558 (4)	0.058 (3)
C10	0.3392 (8)	1.1473 (11)	0.9888 (4)	0.064 (3)
H10	0.2839	1.1632	1.0050	0.077*
C11	0.4120 (9)	1.2236 (11)	0.9989 (4)	0.072 (3)
H11	0.4065	1.2894	1.0217	0.086*
C12	0.4930 (9)	1.2006 (12)	0.9745 (4)	0.075 (3)
C13	0.5032 (9)	1.1033 (12)	0.9416 (4)	0.077 (4)
H13	0.5592	1.0891	0.9257	0.092*
C14	0.4298 (9)	1.0259 (11)	0.9320 (4)	0.070 (3)
H14	0.4365	0.9589	0.9098	0.084*
C15	0.0914 (7)	0.9464 (9)	0.8355 (3)	0.053 (2)
H15	0.0793	1.0350	0.8304	0.063*
C16	0.1287 (7)	0.9288 (9)	0.8889 (3)	0.055 (3)
H16A	0.0857	0.9617	0.9137	0.066*
H16B	0.1364	0.8409	0.8958	0.066*
C17	0.0017 (8)	0.8766 (11)	0.8300 (4)	0.083 (4)
H17A	-0.0237	0.8924	0.7967	0.125*
H17B	-0.0403	0.9042	0.8559	0.125*
H17C	0.0124	0.7892	0.8339	0.125*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0501 (7)	0.0421 (7)	0.0619 (7)	-0.0004 (6)	0.0054 (6)	0.0067 (6)
Cl1	0.070 (2)	0.0510 (16)	0.0855 (18)	-0.0078 (14)	0.0194 (15)	0.0113 (14)
Cl2	0.068 (2)	0.0388 (15)	0.126 (2)	0.0107 (14)	0.0061 (17)	0.0128 (15)
Cl3	0.133 (4)	0.110 (3)	0.0682 (17)	-0.005 (3)	0.0009 (19)	-0.0178 (18)
Cl4	0.085 (3)	0.132 (3)	0.168 (4)	-0.039 (3)	-0.030 (3)	-0.002 (3)
N1	0.054 (6)	0.050 (5)	0.059 (5)	-0.010 (4)	0.000 (4)	0.006 (4)
N2	0.053 (6)	0.048 (5)	0.052 (4)	-0.006 (4)	0.011 (4)	0.011 (4)
C1	0.063 (8)	0.066 (7)	0.063 (6)	-0.010 (6)	-0.006 (6)	0.008 (6)
C2	0.066 (9)	0.076 (8)	0.046 (6)	-0.005 (7)	0.002 (6)	0.009 (6)
C3	0.065 (8)	0.099 (9)	0.057 (7)	-0.015 (7)	-0.005 (6)	-0.006 (7)
C4	0.075 (10)	0.097 (10)	0.057 (7)	-0.020 (8)	-0.011 (6)	-0.004 (7)
C5	0.075 (9)	0.082 (9)	0.052 (6)	-0.009 (8)	0.000 (7)	-0.003 (6)
C6	0.069 (9)	0.097 (10)	0.064 (7)	-0.007 (7)	0.003 (7)	-0.005 (7)
C7	0.070 (9)	0.095 (10)	0.058 (6)	-0.007 (8)	-0.005 (6)	-0.007 (6)
C8	0.062 (8)	0.073 (8)	0.047 (6)	-0.002 (6)	0.007 (5)	0.014 (5)
C9	0.056 (8)	0.066 (8)	0.053 (6)	0.005 (7)	-0.006 (5)	0.010 (6)
C10	0.059 (9)	0.075 (8)	0.058 (7)	0.011 (7)	-0.002 (6)	0.008 (6)
C11	0.068 (9)	0.079 (9)	0.068 (7)	-0.003 (7)	-0.013 (7)	0.004 (6)

C12	0.063 (9)	0.082 (9)	0.079 (8)	-0.003 (7)	-0.017 (7)	0.008 (7)
C13	0.061 (9)	0.091 (10)	0.078 (8)	0.003 (7)	-0.003 (7)	0.009 (7)
C14	0.068 (10)	0.078 (9)	0.064 (7)	0.001 (7)	-0.004 (7)	-0.002 (6)
C15	0.055 (6)	0.044 (5)	0.060 (6)	-0.008 (6)	-0.003 (5)	0.000 (5)
C16	0.049 (7)	0.056 (6)	0.059 (6)	-0.009 (5)	0.006 (5)	0.003 (5)
C17	0.070 (9)	0.077 (8)	0.103 (9)	-0.014 (7)	0.008 (7)	0.003 (7)

Geometric parameters (\AA , $^\circ$)

Zn1—N2	2.076 (7)	C6—H6	0.930
Zn1—N1	2.098 (8)	C7—H7	0.930
Zn1—Cl1	2.196 (3)	C8—C9	1.503 (14)
Zn1—Cl2	2.249 (3)	C8—H8A	0.970
Cl3—C5	1.714 (13)	C8—H8B	0.970
Cl4—C12	1.746 (13)	C9—C10	1.371 (14)
N1—C15	1.476 (12)	C9—C14	1.414 (14)
N1—C1	1.502 (11)	C10—C11	1.371 (14)
N1—H1	0.910	C10—H10	0.930
N2—C16	1.488 (12)	C11—C12	1.367 (16)
N2—C8	1.515 (11)	C11—H11	0.930
N2—H2	0.910	C12—C13	1.363 (14)
C1—C2	1.511 (14)	C13—C14	1.383 (15)
C1—H1A	0.970	C13—H13	0.930
C1—H1B	0.970	C14—H14	0.930
C2—C7	1.362 (16)	C15—C16	1.509 (11)
C2—C3	1.365 (15)	C15—C17	1.520 (13)
C3—C4	1.389 (15)	C15—H15	0.980
C3—H3	0.930	C16—H16A	0.970
C4—C5	1.377 (16)	C16—H16B	0.970
C4—H4	0.930	C17—H17A	0.960
C5—C6	1.380 (15)	C17—H17B	0.960
C6—C7	1.369 (16)	C17—H17C	0.960
N2—Zn1—N1	86.2 (3)	C9—C8—N2	112.9 (8)
N2—Zn1—Cl1	121.1 (2)	C9—C8—H8A	109.0
N1—Zn1—Cl1	117.4 (2)	N2—C8—H8A	109.0
N2—Zn1—Cl2	104.3 (2)	C9—C8—H8B	109.0
N1—Zn1—Cl2	107.7 (2)	N2—C8—H8B	109.0
Cl1—Zn1—Cl2	115.9 (1)	H8A—C8—H8B	107.8
C15—N1—C1	113.1 (8)	C10—C9—C14	117.4 (11)
C15—N1—Zn1	106.1 (5)	C10—C9—C8	121.2 (10)
C1—N1—Zn1	115.3 (6)	C14—C9—C8	121.4 (11)
C15—N1—H1	107.3	C9—C10—C11	122.7 (11)
C1—N1—H1	107.3	C9—C10—H10	118.6
Zn1—N1—H1	107.3	C11—C10—H10	118.6
C16—N2—C8	112.7 (7)	C12—C11—C10	118.4 (11)
C16—N2—Zn1	103.2 (5)	C12—C11—H11	120.8
C8—N2—Zn1	118.0 (6)	C10—C11—H11	120.8
C16—N2—H2	107.5	C13—C12—C11	121.9 (12)
C8—N2—H2	107.5	C13—C12—Cl4	118.2 (11)

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Zn1—N2—H2	107.5	C11—C12—Cl4	119.9 (11)
N1—C1—C2	110.2 (8)	C12—C13—C14	119.5 (12)
N1—C1—H1A	109.6	C12—C13—H13	120.3
C2—C1—H1A	109.6	C14—C13—H13	120.3
N1—C1—H1B	109.6	C13—C14—C9	120.1 (11)
C2—C1—H1B	109.6	C13—C14—H14	120.0
H1A—C1—H1B	108.1	C9—C14—H14	120.0
C7—C2—C3	117.5 (11)	N1—C15—C16	110.6 (8)
C7—C2—C1	122.6 (11)	N1—C15—C17	111.6 (8)
C3—C2—C1	119.8 (12)	C16—C15—C17	109.8 (8)
C2—C3—C4	120.8 (11)	N1—C15—H15	108.3
C2—C3—H3	119.6	C16—C15—H15	108.3
C4—C3—H3	119.6	C17—C15—H15	108.3
C5—C4—C3	121.5 (11)	N2—C16—C15	110.6 (7)
C5—C4—H4	119.2	N2—C16—H16A	109.5
C3—C4—H4	119.2	C15—C16—H16A	109.5
C4—C5—C6	116.8 (11)	N2—C16—H16B	109.5
C4—C5—Cl3	121.5 (10)	C15—C16—H16B	109.5
C6—C5—Cl3	121.6 (11)	H16A—C16—H16B	108.1
C7—C6—C5	120.9 (12)	C15—C17—H17A	109.5
C7—C6—H6	119.6	C15—C17—H17B	109.5
C5—C6—H6	119.6	H17A—C17—H17B	109.5
C2—C7—C6	122.4 (12)	C15—C17—H17C	109.5
C2—C7—H7	118.8	H17A—C17—H17C	109.5
C6—C7—H7	118.8	H17B—C17—H17C	109.5
N2—Zn1—N1—C15	5.5 (6)	C1—C2—C7—C6	175.4 (10)
Cl1—Zn1—N1—C15	−117.7 (5)	C5—C6—C7—C2	−1.3 (19)
Cl2—Zn1—N1—C15	109.3 (5)	C16—N2—C8—C9	−169.7 (9)
N2—Zn1—N1—C1	131.5 (7)	Zn1—N2—C8—C9	70.2 (10)
Cl1—Zn1—N1—C1	8.3 (7)	N2—C8—C9—C10	103.3 (11)
Cl2—Zn1—N1—C1	−124.7 (6)	N2—C8—C9—C14	−77.4 (13)
N1—Zn1—N2—C16	21.4 (6)	C14—C9—C10—C11	0.6 (15)
Cl1—Zn1—N2—C16	141.3 (5)	C8—C9—C10—C11	179.9 (9)
Cl2—Zn1—N2—C16	−85.9 (6)	C9—C10—C11—C12	0.6 (16)
N1—Zn1—N2—C8	146.4 (7)	C10—C11—C12—C13	−1.2 (17)
Cl1—Zn1—N2—C8	−93.7 (7)	C10—C11—C12—C14	178.9 (8)
Cl2—Zn1—N2—C8	39.1 (7)	C11—C12—C13—C14	0.6 (17)
C15—N1—C1—C2	−143.6 (9)	C14—C12—C13—C14	−179.5 (8)
Zn1—N1—C1—C2	94.1 (9)	C12—C13—C14—C9	0.7 (16)
N1—C1—C2—C7	−69.9 (13)	C10—C9—C14—C13	−1.2 (15)
N1—C1—C2—C3	106.2 (11)	C8—C9—C14—C13	179.4 (9)
C7—C2—C3—C4	1.0 (16)	C1—N1—C15—C16	−159.4 (8)
C1—C2—C3—C4	−175.2 (10)	Zn1—N1—C15—C16	−32.1 (8)
C2—C3—C4—C5	0.6 (18)	C1—N1—C15—C17	78.1 (10)
C3—C4—C5—C6	−2.6 (18)	Zn1—N1—C15—C17	−154.6 (7)
C3—C4—C5—Cl3	−179.8 (9)	C8—N2—C16—C15	−173.8 (8)
C4—C5—C6—C7	2.9 (18)	Zn1—N2—C16—C15	−45.5 (9)
Cl3—C5—C6—C7	−179.9 (9)	N1—C15—C16—N2	54.7 (10)
C3—C2—C7—C6	−0.7 (17)	C17—C15—C16—N2	178.2 (8)

Hydrogen-bond geometry (Å, °)

$D\text{---H}\cdots A$	$D\text{---H}$	$H\cdots A$	$D\cdots A$	$D\text{---H}\cdots A$
N1—H1···Cl1 ⁱ	0.91	2.68	3.585 (8)	175
N2—H2···Cl2 ⁱⁱ	0.91	2.47	3.295 (8)	151

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

supplementary materials

Fig. 1

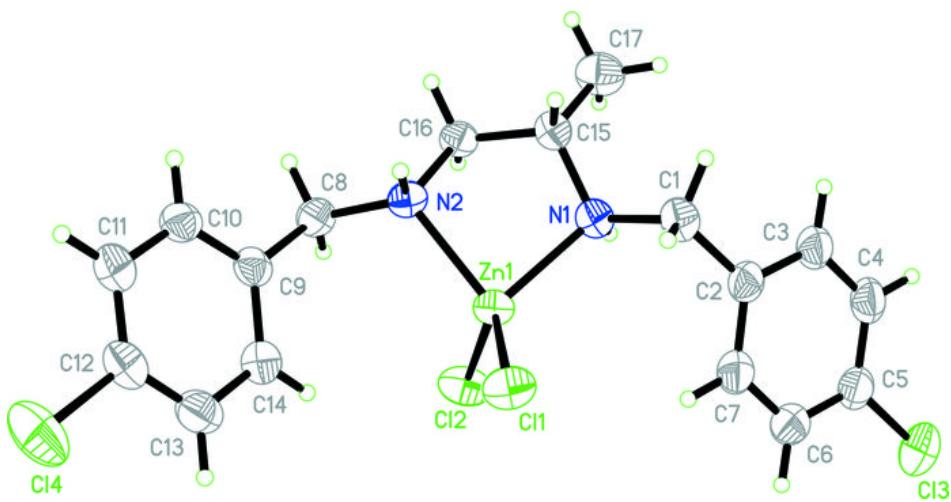


Fig. 2

