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Dichlorido[2-(pyridin-2-yl-κN)benzo[*b*][1,5]-naphthyridine-κN^1]zinc

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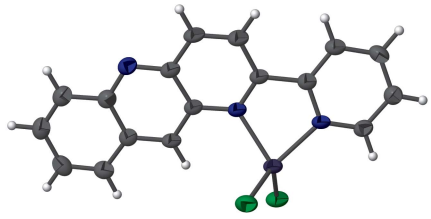
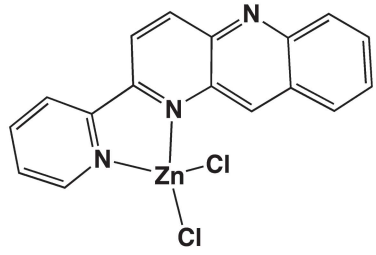
Structural data: full structural data are available from iucrdata.iucr.org

The coordination environment of the Zn^{II} atom in the title complex, $[ZnCl_2(C_{17}H_{11}N_3)]$, is distorted tetrahedral. The NAD$^+$/NADH-analogous ligand is twisted and chelates through one pyridine N atom and one N atom of the benzonaphthyridine ring system. In the crystal, molecules are stacked along the *a* axis and are held together through π–π interactions.

3D view



Chemical scheme



Structure description

Much attention has been paid to transition-metal complexes incorporating the NAD$^+$/NADH-analogous ligand pbn {pbn = 2-(pyridin-2-yl)benzo[*b*][1,5]naphthyridine, $C_{17}H_{11}N_3$} because these compounds can feature remarkable photo-induced multi-electron storage (Fukushima *et al.*, 2010; Ohtsu & Tanaka, 2012*a*) and exhibit photo-driven CO_2 reduction abilities (Ohtsu & Tanaka, 2012*b*; Ohtsu *et al.*, 2015). In this context, the title complex, $[Zn(pbn)Cl_2]$, was prepared. Its molecular structure is shown in Fig. 1. The zinc(II) cation is tetracoordinated by two N atoms of the pbn ligand and two Cl^- ions with Zn—N distances of 2.044 (3) and 2.090 (3) Å and Zn—Cl distances of 2.1944 (7) and 2.2313 (10) Å. The quantitative descriptor for fourfold coordination, τ_4, which can range from τ_4 = 1 for a perfect tetrahedral configuration to τ_4 = 0 for a perfect square-planar configuration (Yang *et al.*, 2007) is τ_4 = 0.85 for the zinc(II) atom by using the equation τ_4 = (360-(α+β))/141, where α = Cl2—Zn1—N3 [120.36 (7)°] and β = Cl1—Zn1—N1 [119.35 (6)°], respectively. Thus, the coordination environment of the zinc(II) atom in $[Zn(pbn)Cl_2]$ is slightly distorted tetrahedral. The pyridine ring and the benzonaphthyridine ring in the pbn ligand are twisted, as revealed by the dihedral angle of 16.36 (7)° between the two least-squares planes.

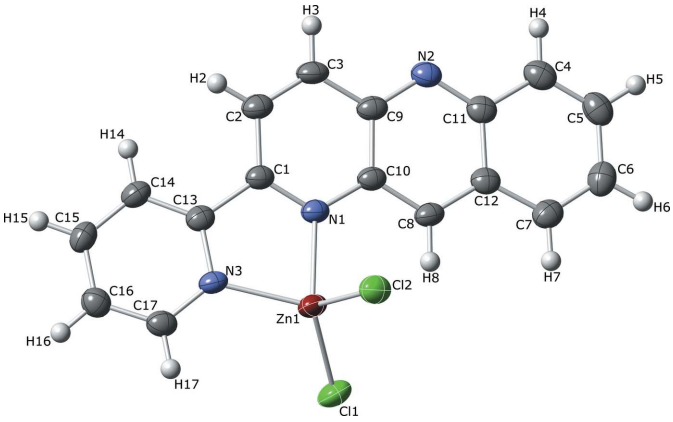


Figure 1
The molecular structure of the title compound, with displacement ellipsoids for non-H atoms drawn at the 50% probability level.

In the crystal, the molecules are stacked along the *a* axis as shown in Fig. 2. The distance between the centroids of the benzonaphthyridine moieties is 3.7369 (4) Å, which is indicative of intermolecular π–π stacking interactions.

Synthesis and crystallization

The NAD$^+$/NADH-analogous ligand, 2-(pyridin-2-yl)benzo-[*b*][1,5]naphthyridine (pbn), was prepared according to the literature protocol (Koizumi & Tanaka, 2005). To a hot methanolic solution (20 ml) of pbn (51.6 mg, 0.20 mmol) was added dropwise $ZnCl_2$ (27.4 mg, 0.20 mmol) in methanol (10 ml), and the resulting hot solution was filtered. After the solution was left to stand for a few days at room temperature, yellow crystals of the title compound were obtained (yield; 34.9 mg, 44%). Elemental analysis, found: C 51.92, H 3.17, N 10.73%; calculated for $C_{17}H_{11}Cl_2N_3Zn$: C 51.87, H 2.82, N 10.68%.

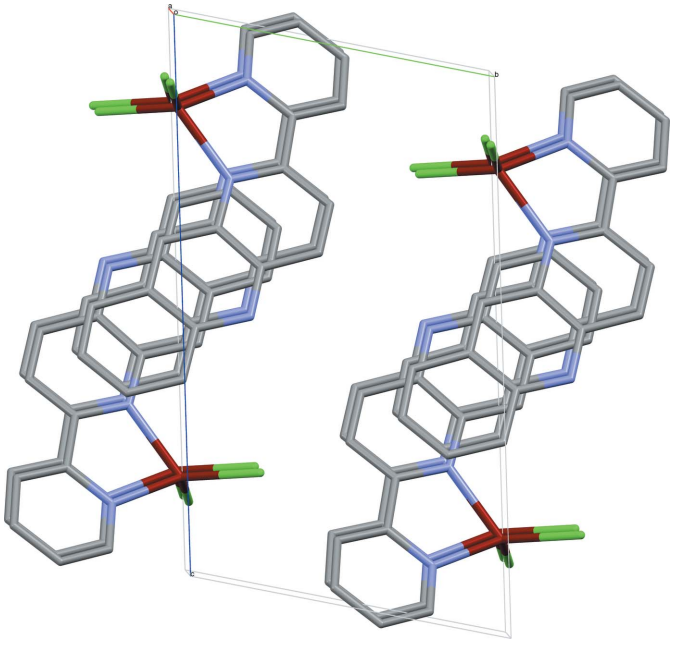


Figure 2
The crystal packing of the title compound, viewed along the *a* axis. H atoms have been omitted for clarity.

Table 1
Experimental details.

Crystal data	
Chemical formula	$[ZnCl_2(C_{17}H_{11}N_3)]$
M_r	393.58
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	173
a, *b*, *c* (Å)	7.90780 (14), 8.27871 (15), 13.4075 (3)
α, β, γ (°)	73.8395 (7), 79.2764 (7), 68.1246 (7)
V (Å^3)	779.00 (3)
Z	2
Radiation type	Cu $K\alpha$
μ (mm^{-1})	5.35
Crystal size (mm)	0.09 × 0.06 × 0.02
Data collection	
Diffractometer	Rigaku R-AXIS RAPID
Absorption correction	Multi-scan (*ABSCOR*; Higashi, 1995)
T_{min}, T_{max}	0.740, 0.899
No. of measured, independent and observed [$F^2 > 2.0\sigma(F^2)$] reflections	9141, 2799, 2338
R_{int}	0.046
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.602
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.039, 0.108, 1.08
No. of reflections	2799
No. of parameters	208
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.59, −0.41

Computer programs: RAPID AUTO (Rigaku, 2001), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *CrystalStructure* (Rigaku, 2010), *Mercury* (Macrae *et al.*, 2008), *CrystalMaker* (Palmer, 2007) and *publCIF* (Westrip, 2010).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

Acknowledgements

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full crystallographic data

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Crystal data

$[ZnCl_2(C_{17}H_{11}N_3)]$
M_r = 393.58
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 7.90780 (14) Å
b = 8.27871 (15) Å
c = 13.4075 (3) Å
α = 73.8395 (7)°
β = 79.2764 (7)°
γ = 68.1246 (7)°
V = 779.00 (3) Å^3
Z = 2
$F(000)$ = 396.00
D_x = 1.678 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54187 Å
Cell parameters from 6125 reflections
θ = 3.4–68.1°
μ = 5.35 mm^{-1}
T = 173 K
Block, yellow
0.09 × 0.06 × 0.02 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Detector resolution: 10.000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.740, T_{max} = 0.899
9141 measured reflections
2799 independent reflections
2338 reflections with $F^2 > 2.0\sigma(F^2)$
R_{int} = 0.046
θ_{max} = 68.3°
h = −9→9
k = −9→9
l = −16→16

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.108
S = 1.08
2799 reflections
208 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.065P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

Special details

Geometry. ENTER SPECIAL DETAILS OF THE MOLECULAR GEOMETRY
Refinement. Refinement was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F^2. R-factor (gt) are based on F. The threshold expression of $F^2 > 2.0$ sigma(F^2) is used only for calculating R-factor (gt).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.41698 (5)	0.98623 (4)	0.82997 (3)	0.03376 (16)
Cl1	0.18049 (10)	1.23090 (9)	0.79219 (6)	0.0427 (2)
Cl2	0.66287 (9)	1.01287 (9)	0.87332 (5)	0.0407 (2)
N1	0.5368 (3)	0.8306 (3)	0.71983 (16)	0.0297 (5)
N2	0.8589 (3)	0.7866 (3)	0.48422 (17)	0.0339 (6)
N3	0.3436 (3)	0.7661 (3)	0.90061 (16)	0.0296 (5)
C1	0.5507 (4)	0.6619 (4)	0.7581 (2)	0.0295 (6)
C2	0.6749 (4)	0.5228 (4)	0.7104 (2)	0.0355 (7)
C3	0.7792 (4)	0.5637 (4)	0.6216 (2)	0.0353 (7)
C4	0.9435 (4)	1.0064 (5)	0.3483 (2)	0.0387 (7)
C5	0.9299 (4)	1.1799 (5)	0.3057 (3)	0.0411 (7)
C6	0.8138 (4)	1.3189 (4)	0.3550 (3)	0.0414 (7)
C7	0.7110 (4)	1.2813 (4)	0.4452 (3)	0.0380 (7)
C8	0.6182 (4)	1.0558 (4)	0.5861 (2)	0.0319 (6)
C9	0.7600 (4)	0.7458 (4)	0.5748 (2)	0.0316 (6)
C10	0.6373 (4)	0.8776 (4)	0.6281 (2)	0.0293 (6)
C11	0.8396 (4)	0.9589 (4)	0.4439 (2)	0.0333 (6)
C12	0.7194 (4)	1.1003 (4)	0.4934 (2)	0.0315 (6)
C13	0.4260 (4)	0.6276 (4)	0.8532 (2)	0.0312 (6)
C14	0.3886 (4)	0.4706 (4)	0.8888 (2)	0.0342 (7)
C15	0.2615 (4)	0.4546 (4)	0.9738 (3)	0.0366 (7)
C16	0.1745 (4)	0.5958 (4)	1.0209 (2)	0.0373 (7)
C17	0.2187 (4)	0.7500 (4)	0.9823 (2)	0.0345 (7)
H2	0.6843	0.4018	0.7408	0.0426*
H3	0.8650	0.4713	0.5907	0.0424*
H4	1.0231	0.9157	0.3141	0.0465*
H5	0.9994	1.2086	0.2417	0.0493*
H6	0.8081	1.4389	0.3246	0.0496*
H7	0.6325	1.3755	0.4771	0.0455*
H8	0.5371	1.1459	0.6204	0.0383*
H14	0.4495	0.3741	0.8554	0.0411*
H15	0.2345	0.3468	0.9993	0.0439*
H16	0.0858	0.5877	1.0788	0.0447*
H17	0.1588	0.8478	1.0148	0.0414*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0323 (3)	0.0270 (3)	0.0444 (3)	−0.00862 (17)	0.00031 (17)	−0.01653 (17)
Cl1	0.0410 (4)	0.0304 (4)	0.0549 (5)	−0.0030 (3)	−0.0077 (4)	−0.0175 (4)
Cl2	0.0381 (4)	0.0379 (5)	0.0531 (5)	−0.0139 (4)	−0.0040 (3)	−0.0200 (4)
N1	0.0269 (11)	0.0267 (12)	0.0378 (12)	−0.0069 (10)	−0.0034 (9)	−0.0140 (10)
N2	0.0269 (12)	0.0359 (14)	0.0384 (12)	−0.0062 (10)	−0.0027 (10)	−0.0141 (10)
N3	0.0305 (12)	0.0244 (12)	0.0370 (12)	−0.0080 (10)	−0.0033 (10)	−0.0135 (9)
C1	0.0268 (13)	0.0276 (14)	0.0363 (14)	−0.0063 (11)	−0.0048 (11)	−0.0134 (11)

C2	0.0332 (15)	0.0286 (15)	0.0444 (16)	−0.0053 (12)	−0.0044 (12)	−0.0144 (12)
C3	0.0295 (14)	0.0298 (15)	0.0470 (16)	−0.0026 (12)	−0.0034 (12)	−0.0199 (13)
C4	0.0303 (15)	0.0482 (19)	0.0376 (15)	−0.0103 (13)	−0.0051 (12)	−0.0126 (14)
C5	0.0336 (16)	0.053 (2)	0.0352 (15)	−0.0153 (14)	−0.0045 (12)	−0.0067 (14)
C6	0.0390 (17)	0.0384 (17)	0.0460 (17)	−0.0156 (14)	−0.0125 (13)	0.0004 (14)
C7	0.0316 (15)	0.0359 (17)	0.0470 (17)	−0.0092 (13)	−0.0080 (13)	−0.0107 (13)
C8	0.0289 (14)	0.0264 (15)	0.0420 (15)	−0.0055 (12)	−0.0055 (12)	−0.0142 (12)
C9	0.0257 (14)	0.0333 (16)	0.0382 (14)	−0.0056 (12)	−0.0064 (11)	−0.0154 (12)
C10	0.0239 (13)	0.0305 (15)	0.0360 (14)	−0.0065 (11)	−0.0046 (11)	−0.0142 (11)
C11	0.0261 (14)	0.0385 (16)	0.0364 (14)	−0.0093 (12)	−0.0064 (11)	−0.0105 (12)
C12	0.0246 (14)	0.0357 (16)	0.0353 (14)	−0.0082 (12)	−0.0068 (11)	−0.0103 (12)
C13	0.0261 (14)	0.0314 (15)	0.0375 (14)	−0.0080 (12)	−0.0066 (11)	−0.0104 (12)
C14	0.0337 (15)	0.0287 (15)	0.0414 (15)	−0.0069 (12)	−0.0066 (12)	−0.0127 (12)
C15	0.0376 (16)	0.0311 (16)	0.0451 (16)	−0.0158 (13)	−0.0084 (13)	−0.0062 (13)
C16	0.0343 (15)	0.0421 (18)	0.0379 (15)	−0.0145 (13)	−0.0029 (12)	−0.0111 (13)
C17	0.0285 (14)	0.0373 (16)	0.0408 (15)	−0.0089 (13)	−0.0032 (12)	−0.0168 (13)

Geometric parameters (Å, º)

Zn1—Cl1	2.1944 (7)	C8—C10	1.385 (4)
Zn1—Cl2	2.2313 (10)	C8—C12	1.385 (4)
Zn1—N1	2.090 (3)	C9—C10	1.425 (4)
Zn1—N3	2.044 (3)	C11—C12	1.444 (4)
N1—C1	1.317 (4)	C13—C14	1.376 (5)
N1—C10	1.376 (4)	C14—C15	1.384 (4)
N2—C9	1.347 (4)	C15—C16	1.375 (5)
N2—C11	1.337 (4)	C16—C17	1.385 (5)
N3—C13	1.356 (4)	C2—H2	0.950
N3—C17	1.344 (4)	C3—H3	0.950
C1—C2	1.426 (4)	C4—H4	0.950
C1—C13	1.489 (4)	C5—H5	0.950
C2—C3	1.353 (4)	C6—H6	0.950
C3—C9	1.424 (4)	C7—H7	0.950
C4—C5	1.361 (5)	C8—H8	0.950
C4—C11	1.428 (4)	C14—H14	0.950
C5—C6	1.419 (5)	C15—H15	0.950
C6—C7	1.354 (4)	C16—H16	0.950
C7—C12	1.438 (5)	C17—H17	0.950
Zn1···C8	3.354 (3)	Cl2···H14^{vi}	2.8000
N1···C3	2.795 (4)	Cl2···H15^{v}	2.8859
N2···C8	2.832 (4)	Cl2···H17^{iii}	2.9212
N3···C15	2.764 (5)	N2···H3^{viii}	2.6908
C1···C8	3.590 (4)	N2···H8^{i}	3.4609
C1···C9	2.767 (4)	N3···H5^{i}	3.5104
C2···C10	2.758 (4)	N3···H15^{v}	3.5289
C2···C14	3.028 (4)	C1···H16^{v}	3.5650
C4···C7	2.808 (5)	C2···H4^{viii}	3.5916

C5···C12	2.806 (4)	C2···H7^{i}	3.5369
C6···C11	2.829 (5)	C2···H16^{v}	3.4158
C9···C12	2.748 (4)	C3···H4^{viii}	3.5936
C10···C11	2.743 (4)	C3···H6^{iv}	3.4625
C13···C16	2.735 (4)	C3···H7^{ix}	3.3748
C14···C17	2.721 (5)	C3···H7^{i}	3.5525
Cl1···C4^{i}	3.543 (4)	C4···H3^{viii}	3.5778
Cl1···C16^{ii}	3.550 (3)	C7···H3^{vi}	3.4319
Cl2···C17^{iii}	3.554 (4)	C7···H7^{vii}	3.3738
N2···C6^{iv}	3.384 (5)	C8···H4^{iv}	3.4607
N2···C7^{iv}	3.501 (4)	C9···H3^{viii}	3.5701
N3···C14^{v}	3.514 (4)	C9···H5^{iv}	3.5510
N3···C15^{v}	3.453 (4)	C9···H6^{iv}	3.5360
C1···C6^{i}	3.433 (5)	C9···H8^{i}	3.5466
C1···C7^{i}	3.550 (5)	C10···H5^{iv}	3.3836
C4···Cl1^{i}	3.543 (4)	C11···H3^{viii}	3.5598
C4···C8^{iv}	3.550 (5)	C12···H4^{iv}	3.5206
C4···C12^{iv}	3.421 (5)	C13···H5^{i}	3.4659
C5···C9^{iv}	3.478 (5)	C13···H6^{i}	3.5412
C5···C10^{iv}	3.522 (5)	C14···H5^{i}	3.5878
C5···C13^{i}	3.464 (4)	C14···H6^{i}	3.2800
C6···N2^{iv}	3.384 (5)	C15···H16^{x}	3.1201
C6···C1^{i}	3.433 (5)	C16···H2^{v}	3.5826
C6···C9^{iv}	3.477 (5)	C16···H15^{x}	3.1414
C6···C13^{i}	3.498 (5)	C16···H16^{x}	3.5802
C7···N2^{iv}	3.501 (4)	C17···H14^{v}	3.3974
C7···C1^{i}	3.550 (5)	C17···H17^{ii}	3.5522
C8···C4^{iv}	3.550 (5)	H2···Cl2^{ix}	3.2656
C9···C5^{iv}	3.478 (5)	H2···C16^{v}	3.5826
C9···C6^{iv}	3.477 (5)	H2···H4^{viii}	2.9524
C10···C5^{iv}	3.522 (5)	H2···H8^{ix}	3.5908
C10···C12^{i}	3.435 (5)	H2···H16^{v}	3.3215
C11···C11^{iv}	3.528 (5)	H2···H17^{v}	3.5191
C11···C12^{iv}	3.564 (5)	H3···N2^{viii}	2.6908
C12···C4^{iv}	3.421 (5)	H3···C4^{viii}	3.5778
C12···C10^{i}	3.435 (5)	H3···C7^{ix}	3.4319
C12···C11^{iv}	3.564 (5)	H3···C9^{viii}	3.5701
C13···C5^{i}	3.464 (4)	H3···C11^{viii}	3.5598
C13···C6^{i}	3.498 (5)	H3···H3^{viii}	2.9792
C13···C15^{v}	3.458 (5)	H3···H4^{viii}	2.9517
C13···C16^{v}	3.484 (4)	H3···H6^{iv}	3.3951
C14···N3^{v}	3.514 (4)	H3···H7^{ix}	3.0208
C14···C17^{v}	3.461 (4)	H4···Cl1^{i}	3.0609
C15···N3^{v}	3.453 (4)	H4···Cl2^{iv}	3.2821
C15···C13^{v}	3.458 (5)	H4···C2^{viii}	3.5916
C16···Cl1^{ii}	3.550 (3)	H4···C3^{viii}	3.5936
C16···C13^{v}	3.484 (4)	H4···C8^{iv}	3.4607
C17···Cl2^{iii}	3.554 (4)	H4···C12^{iv}	3.5206

C17···C14^{v}	3.461 (4)	H4···H2^{viii}	2.9524
Zn1···H8	2.9018	H4···H3^{viii}	2.9517
Zn1···H17	3.1467	H4···H8^{iv}	3.5627
Cl1···H8	3.2804	H5···Cl2^{iv}	3.0437
Cl2···H8	3.4733	H5···N3^{i}	3.5104
N1···H2	3.2434	H5···C9^{iv}	3.5510
N1···H8	2.5801	H5···C10^{iv}	3.3836
N2···H3	2.5905	H5···C13^{i}	3.4659
N2···H4	2.5706	H5···C14^{i}	3.5878
N3···H14	3.2371	H5···H15^{xi}	3.5494
N3···H16	3.2419	H5···H16^{xi}	3.5093
C1···H3	3.2683	H6···Cl1^{vii}	2.7717
C1···H14	2.7054	H6···C3^{iv}	3.4625
C2···H14	2.7354	H6···C9^{iv}	3.5360
C4···H6	3.2714	H6···C13^{i}	3.5412
C5···H7	3.2644	H6···C14^{i}	3.2800
C6···H4	3.2782	H6···H3^{iv}	3.3951
C7···H5	3.2533	H6···H14^{i}	3.1252
C7···H8	2.6727	H7···C2^{i}	3.5369
C8···H7	2.6759	H7···C3^{vi}	3.3748
C9···H2	3.2665	H7···C3^{i}	3.5525
C9···H8	3.2900	H7···C7^{vii}	3.3738
C10···H3	3.3015	H7···H3^{vi}	3.0208
C11···H5	3.2816	H7···H7^{vii}	2.4550
C11···H7	3.3392	H8···N2^{i}	3.4609
C11···H8	3.3004	H8···C9^{i}	3.5466
C12···H4	3.3234	H8···H2^{vi}	3.5908
C12···H6	3.2881	H8···H4^{iv}	3.5627
C13···H2	2.7408	H14···Zn1^{ix}	3.4282
C13···H15	3.2430	H14···Cl1^{ix}	3.1240
C13···H17	3.1793	H14···Cl2^{ix}	2.8000
C14···H2	2.7638	H14···C17^{v}	3.3974
C14···H16	3.2462	H14···H6^{i}	3.1252
C15···H17	3.2283	H14···H17^{v}	3.4623
C16···H14	3.2430	H15···Cl1^{ix}	3.3230
C17···H15	3.2383	H15···Cl2^{v}	2.8859
H2···H3	2.3072	H15···N3^{v}	3.5289
H2···H14	2.2180	H15···C16^{x}	3.1414
H4···H5	2.2965	H15···H5^{xii}	3.5494
H5···H6	2.3581	H15···H16^{x}	2.7302
H6···H7	2.2969	H16···Cl1^{ii}	2.7231
H7···H8	2.5235	H16···C1^{v}	3.5650
H14···H15	2.3422	H16···C2^{v}	3.4158
H15···H16	2.3379	H16···C15^{x}	3.1201
H16···H17	2.3279	H16···C16^{x}	3.5802
Zn1···H14^{vi}	3.4282	H16···H2^{v}	3.3215
Cl1···H4^{i}	3.0609	H16···H5^{xii}	3.5093
Cl1···H6^{vii}	2.7717	H16···H15^{x}	2.7302

Cl1···H14^{vi}	3.1240	H16···H16^{x}	3.5584
Cl1···H15^{vi}	3.3230	H17···Cl1^{ii}	3.4786
Cl1···H16^{ii}	2.7231	H17···Cl2^{iii}	2.9212
Cl1···H17^{ii}	3.4786	H17···C17^{ii}	3.5522
Cl2···H2^{vi}	3.2656	H17···H2^{v}	3.5191
Cl2···H4^{iv}	3.2821	H17···H14^{v}	3.4623
Cl2···H5^{iv}	3.0437	H17···H17^{ii}	2.8125

Cl1—Zn1—Cl2	117.48 (4)	C7—C12—C8	122.6 (3)
Cl1—Zn1—N1	119.35 (6)	C7—C12—C11	118.8 (3)
Cl1—Zn1—N3	112.79 (7)	C8—C12—C11	118.5 (3)
Cl2—Zn1—N1	100.96 (7)	N3—C13—C1	115.2 (3)
Cl2—Zn1—N3	120.36 (7)	N3—C13—C14	121.5 (3)
N1—Zn1—N3	79.60 (9)	C1—C13—C14	123.2 (3)
Zn1—N1—C1	112.42 (17)	C13—C14—C15	119.4 (3)
Zn1—N1—C10	125.4 (2)	C14—C15—C16	119.5 (3)
C1—N1—C10	119.8 (3)	C15—C16—C17	118.7 (3)
C9—N2—C11	117.8 (3)	N3—C17—C16	122.2 (3)
Zn1—N3—C13	113.79 (17)	C1—C2—H2	120.136
Zn1—N3—C17	127.4 (2)	C3—C2—H2	120.142
C13—N3—C17	118.7 (3)	C2—C3—H3	120.126
N1—C1—C2	122.0 (3)	C9—C3—H3	120.130
N1—C1—C13	115.4 (3)	C5—C4—H4	119.588
C2—C1—C13	122.6 (3)	C11—C4—H4	119.590
C1—C2—C3	119.7 (3)	C4—C5—H5	119.377
C2—C3—C9	119.7 (3)	C6—C5—H5	119.371
C5—C4—C11	120.8 (3)	C5—C6—H6	119.860
C4—C5—C6	121.3 (3)	C7—C6—H6	119.865
C5—C6—C7	120.3 (3)	C6—C7—H7	119.612
C6—C7—C12	120.8 (3)	C12—C7—H7	119.611
C10—C8—C12	118.8 (3)	C10—C8—H8	120.577
N2—C9—C3	119.6 (3)	C12—C8—H8	120.580
N2—C9—C10	122.8 (3)	C13—C14—H14	120.314
C3—C9—C10	117.6 (3)	C15—C14—H14	120.313
N1—C10—C8	119.8 (3)	C14—C15—H15	120.273
N1—C10—C9	121.0 (3)	C16—C15—H15	120.274
C8—C10—C9	119.2 (3)	C15—C16—H16	120.642
N2—C11—C4	119.1 (3)	C17—C16—H16	120.644
N2—C11—C12	122.9 (3)	N3—C17—H17	118.876
C4—C11—C12	118.0 (3)	C16—C17—H17	118.876

Cl1—Zn1—N1—C1	−126.99 (12)	N1—C1—C13—C14	163.5 (3)
Cl1—Zn1—N1—C10	70.47 (18)	C2—C1—C13—N3	167.5 (3)
Cl1—Zn1—N3—C13	126.73 (12)	C2—C1—C13—C14	−15.5 (5)
Cl1—Zn1—N3—C17	−49.2 (2)	C13—C1—C2—C3	177.3 (3)
Cl2—Zn1—N1—C1	102.62 (14)	C1—C2—C3—C9	−2.0 (5)
Cl2—Zn1—N1—C10	−59.92 (16)	C2—C3—C9—N2	−177.4 (3)
Cl2—Zn1—N3—C13	−87.57 (15)	C2—C3—C9—C10	3.8 (5)

Cl2—Zn1—N3—C17	96.51 (17)	C5—C4—C11—N2	−178.9 (3)
N1—Zn1—N3—C13	9.13 (14)	C5—C4—C11—C12	0.3 (5)
N1—Zn1—N3—C17	−166.8 (2)	C11—C4—C5—C6	0.6 (5)
N3—Zn1—N1—C1	−16.58 (15)	C4—C5—C6—C7	−1.2 (5)
N3—Zn1—N1—C10	−179.12 (18)	C5—C6—C7—C12	0.8 (5)
Zn1—N1—C1—C2	−160.27 (19)	C6—C7—C12—C8	179.3 (3)
Zn1—N1—C1—C13	20.7 (3)	C6—C7—C12—C11	0.1 (5)
Zn1—N1—C10—C8	−20.7 (4)	C10—C8—C12—C7	−178.7 (3)
Zn1—N1—C10—C9	159.93 (17)	C10—C8—C12—C11	0.5 (5)
C1—N1—C10—C8	177.9 (3)	C12—C8—C10—N1	−179.4 (3)
C1—N1—C10—C9	−1.4 (4)	C12—C8—C10—C9	−0.1 (5)
C10—N1—C1—C2	3.4 (5)	N2—C9—C10—N1	179.1 (3)
C10—N1—C1—C13	−175.7 (3)	N2—C9—C10—C8	−0.2 (5)
C9—N2—C11—C4	179.6 (3)	C3—C9—C10—N1	−2.1 (5)
C9—N2—C11—C12	0.4 (5)	C3—C9—C10—C8	178.5 (3)
C11—N2—C9—C3	−178.7 (3)	N2—C11—C12—C7	178.5 (3)
C11—N2—C9—C10	0.1 (5)	N2—C11—C12—C8	−0.7 (5)
Zn1—N3—C13—C1	−1.2 (3)	C4—C11—C12—C7	−0.7 (5)
Zn1—N3—C13—C14	−178.26 (17)	C4—C11—C12—C8	−179.9 (3)
Zn1—N3—C17—C16	177.10 (16)	N3—C13—C14—C15	1.2 (4)
C13—N3—C17—C16	1.4 (4)	C1—C13—C14—C15	−175.6 (3)
C17—N3—C13—C1	175.1 (2)	C13—C14—C15—C16	0.1 (5)
C17—N3—C13—C14	−2.0 (4)	C14—C15—C16—C17	−0.7 (5)
N1—C1—C2—C3	−1.7 (5)	C15—C16—C17—N3	−0.0 (5)
N1—C1—C13—N3	−13.5 (4)		

Symmetry codes: (i) $-x+1, -y+2, -z+1$; (ii) $-x, -y+2, -z+2$; (iii) $-x+1, -y+2, -z+2$; (iv) $-x+2, -y+2, -z+1$; (v) $-x+1, -y+1, -z+2$; (vi) $x, y+1, z$; (vii) $-x+1, -y+3, -z+1$; (viii) $-x+2, -y+1, -z+1$; (ix) $x, y-1, z$; (x) $-x, -y+1, -z+2$; (xi) $x+1, y+1, z-1$; (xii) $x-1, y-1, z+1$.