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Dichlorido{2-[(5-methyl-1*H*-pyrazol-3-yl-κN^2)-methyl]-1*H*-1,3-benzimidazole-κN^3}zinc

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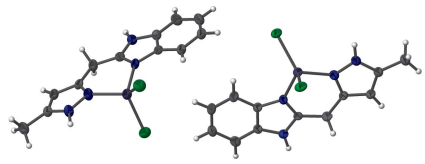
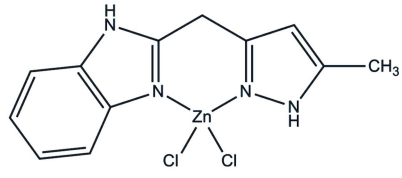
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title complex, $[ZnCl_2(C_{12}H_{12}N_4)]$, contains two independent molecules having similar conformations. The coordination about the Zn^{II} atom is distorted tetrahedral, with the geometrical constraints of the chelating ligand responsible for the observed distortion. Each of the independent molecules forms chains in the crystal through pairs of N—H···Cl hydrogen bonds, using the pyrazole and benzimidazole N—H groups as donors. The first molecule forms chains running parallel to the *b* axis, while the other molecule affords the same kind of one-dimensional supramolecular structure parallel to the *a* axis. The structure was refined as a two-component twin with BASF = 0.0437 (4).

3D view



Chemical scheme



Structure description

Benzimidazole and pyrazole derivatives have shown significant anti-cancer activities when evaluated for their potential antiproliferative activity against human tumour cells (Reddy *et al.*, 2015). The ability of the benzimidazole derivatives to form stable complexes with metal ions gives rise to a variety of metal-ligand coordination modes. Their reactions with metal salts have played an important role in the development of coordination chemistry (Téllez *et al.*, 2008; Qiao *et al.*, 2014). Several research teams investigated the coordination behaviour of benzimidazole derivatives toward transition metal ions (Constable & Steel, 1989). Other studies have explored the biological activity of coordination compounds containing the benzimidazole moiety (Devereux *et al.*, 2007). Benzimidazole-based complexes have relatively high antibacterial and antifungal power (Bouchouit *et al.*, 2016). Their zinc complexes, in addition to their antimicrobial activity, have been used in *in vitro* and *in vivo* anticancer studies and have been shown to have an

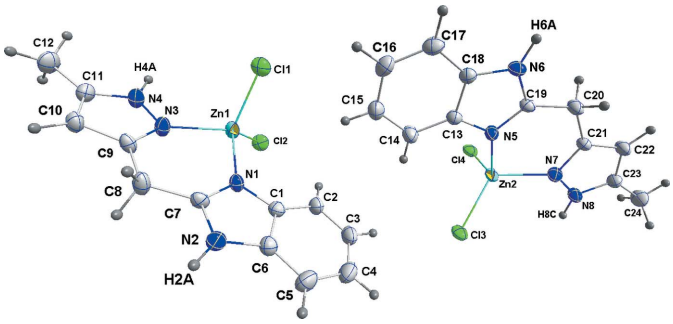


Figure 1
The asymmetric unit of the title compound, showing the labelling scheme and 50% probability displacement ellipsoids.

important role in the chemotherapeutic process (Tabassum *et al.*, 2012) as well as exerting a significant cytotoxic activity (Li *et al.*, 2012).

Continuing our research in this field (Chkirate *et al.*, 2001; Sbai *et al.*, 2002), we synthesized a zinc chloride complex having 2-[(5-methylpyrazol-3-yl)methyl]benzimidazole, obtained by the action of hydrazine on 4-acetonylidene-1,5-benzodiazepin-2-one (Essassi *et al.*, 1987), as the main ligand. The asymmetric unit of the title compound consists of two independent molecules with modest but distinct differences in their conformations (Fig. 1). Each zinc atom adopts a distorted tetrahedral coordination with angles at Zn ranging from 92.17 (18) to 120.88 (15)°, with the smallest angle in each molecule due to the geometrical constraints of the chelating ligand.

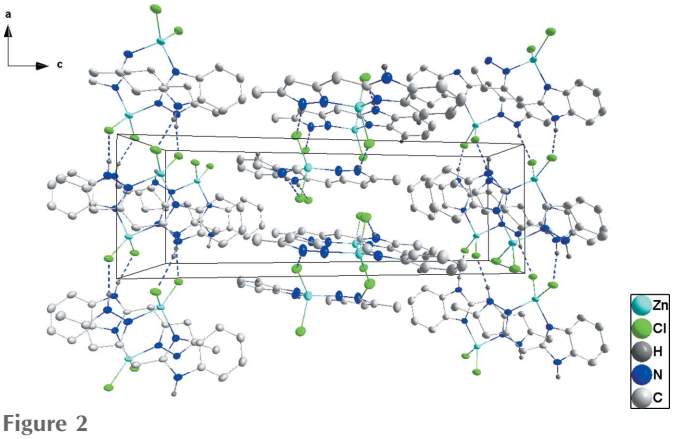


Figure 2
The packing of the title compound, viewed along the *b* axis, with N—H···Cl hydrogen bonds shown as dotted lines.

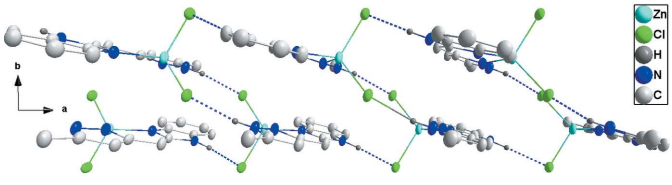


Figure 3
Detail of the N—H···Cl hydrogen-bonded chain containing atom Zn1, viewed along the *c* axis.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···Cl1^{i}	0.91	2.23	3.125 (5)	169
N4—H4*A*···Cl2^{ii}	0.91	2.33	3.161 (5)	152
N6—H6*A*···Cl4^{iii}	0.91	2.24	3.133 (5)	169
N8—H8*C*···Cl3^{iv}	0.91	2.32	3.211 (5)	168

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$[ZnCl_2(C_{12}H_{12}N_4)]$
M_r	348.53
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	150
a, *b*, *c* (Å)	7.7912 (3), 7.8345 (3), 23.3600 (9)
α, β, γ (°)	98.310 (1), 90.397 (2), 90.701 (2)
V (Å^3)	1410.77 (9)
Z	4
Radiation type	Cu *K*α
μ (mm^{-1})	5.83
Crystal size (mm)	0.18 × 0.08 × 0.05
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*TWINABS*; Sheldrick, 2009)
T_{min}, T_{max}	0.46, 0.76
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	19443, 19443, 11989
R_{int}	0.039
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.057, 0.165, 1.07
No. of reflections	19443
No. of parameters	346
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	2.44, −1.49

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008*b*).

In the crystal, the molecule containing Zn1 forms chains running parallel to the *b* axis through a combination of N2—H2*A*···Cl1^{i} and N4—H4*A*···Cl2^{ii} [symmetry codes: (i) $x, 1+y, z$; (ii) $-x, -y, 1-z$] hydrogen bonds. That containing Zn2 similarly forms chains parallel to the *a* axis through a combination of N6—H6*A*···Cl4^{iii} and N8—H8*C*···Cl3^{iv} [symmetry codes: (iii) $1+x, y, z$; (iv) $-x, 1-y, 2-z$] hydrogen bonds (Table 1 and Figs. 2 and 3).

Synthesis and crystallization

6.25×10^{-5} mol of $ZnCl_2$ dissolved in 2.5 ml of ethanol was added to a solution of 6.25×10^{-5} mol of 2-[(5-methylpyrazol-3-yl)methyl]benzimidazole in 2.5 ml of ethanol. The mixture was warmed slightly and then left at room temperature. After 24 h, some white crystals were observed in the mother liquor. The solution was filtered and then evaporated in an oven to give single crystals with a yield of 78%.

Refinement

Crystal and refinement details are given in Table 2. Analysis of 2601 reflections having $I/\sigma(I) > 12$ and chosen from the full data set with *CELL_NOW* (Sheldrick, 2008*a*) showed the crystal to belong to the triclinic system and to be twinned by a 180° rotation about the reciprocal axis [$\bar{1}$10]. The raw data were processed using the multi-component version of *SAINT* under control of the two-component orientation file generated by *CELL_NOW*. The model was refined as a two-component twin with BASF = 0.0437 (4) and twin law −0.00559 1.00489 0.04907/0.99567 0.00642 0.04978/−0.01138 − 0.01717 − 1.00083. The largest difference peak is 0.6 Å from Zn2 while the largest hole is 1.1 Å from Zn2. Other smaller but noticeable difference peaks are < 1 Å from the metal atoms. We attribute these to errors in the absorption correction due to the anisotropic habit of the crystal.

Acknowledgements

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full crystallographic data

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Dichlorido{2-[(5-methyl-1*H*-pyrazol-3-yl-κN^2)methyl]-1*H*-1,3-benzimidazole-κN^3}zinc

Crystal data

$[ZnCl_2(C_{12}H_{12}N_4)]$
M_r = 348.53
Triclinic, $P\overline{1}$
a = 7.7912 (3) Å
b = 7.8345 (3) Å
c = 23.3600 (9) Å
α = 98.310 (1)°
β = 90.397 (2)°
γ = 90.701 (2)°
V = 1410.77 (9) Å^3
Z = 4
$F(000)$ = 704
D_x = 1.641 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9898 reflections
θ = 3.8–72.4°
μ = 5.83 mm^{-1}
T = 150 K
Plate, colourless
0.18 × 0.08 × 0.05 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro-focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*TWINABS*; Sheldrick, 2009)
T_{min} = 0.46, T_{max} = 0.76
19443 measured reflections
19443 independent reflections
11989 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 74.6°, θ_{min} = 3.8°
h = −9→9
k = −9→9
l = −29→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.165
S = 1.07
19443 reflections
346 parameters
0 restraints
0 constraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.041P)^2 + 3.0857P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 2.44 e Å^{-3}
$\Delta\rho_{min}$ = −1.49 e Å^{-3}

Special details

Experimental. =?

Refinement. H-atoms attached to carbon were placed in calculated positions (C—H = 0.95 - 0.99 Å) while those attached to nitrogen were placed in locations derived from a difference map and their parameters adjusted to give N—H = 0.91 Å. All were included as riding contributions with isotropic displacement parameters 1.2 - 1.5 times those of the attached atoms. Refined as a 2-component twin.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.18794 (9)	0.28030 (9)	0.56443 (3)	0.0263 (2)
Cl1	0.43018 (18)	0.14063 (17)	0.58122 (6)	0.0328 (3)
Cl2	−0.04210 (18)	0.13877 (17)	0.59034 (6)	0.0342 (3)
H2A	0.2996	0.9082	0.6062	0.041*
N1	0.1925 (6)	0.5264 (6)	0.60146 (18)	0.0244 (9)
N2	0.2643 (6)	0.8028 (6)	0.6138 (2)	0.0290 (10)
N3	0.2051 (7)	0.3469 (6)	0.4845 (2)	0.0311 (11)
N4	0.2061 (7)	0.2360 (6)	0.43401 (19)	0.0314 (11)
H4A	0.1976	0.1189	0.4300	0.038*
C1	0.1704 (7)	0.5926 (7)	0.6593 (2)	0.0249 (11)
C2	0.1125 (7)	0.5128 (8)	0.7054 (2)	0.0307 (12)
H2	0.0790	0.3945	0.7002	0.037*
C3	0.1061 (8)	0.6138 (9)	0.7587 (3)	0.0365 (14)
H3	0.0666	0.5634	0.7909	0.044*
C4	0.1555 (8)	0.7870 (9)	0.7671 (3)	0.0397 (15)
H4	0.1506	0.8510	0.8048	0.048*
C5	0.2117 (8)	0.8678 (8)	0.7216 (3)	0.0369 (14)
H5	0.2452	0.9860	0.7270	0.044*
C6	0.2166 (7)	0.7667 (7)	0.6677 (2)	0.0272 (11)
C7	0.2479 (7)	0.6574 (6)	0.5757 (2)	0.0233 (11)
C8	0.2897 (8)	0.6581 (7)	0.5139 (2)	0.0320 (13)
H8A	0.4111	0.6957	0.5122	0.038*
H8B	0.2192	0.7483	0.4999	0.038*
C9	0.2672 (7)	0.4968 (7)	0.4713 (2)	0.0249 (11)
C10	0.3060 (7)	0.4792 (7)	0.4129 (2)	0.0286 (12)
H10	0.3513	0.5661	0.3925	0.034*
C11	0.2662 (7)	0.3110 (7)	0.3900 (2)	0.0275 (11)
C12	0.2785 (9)	0.2154 (8)	0.3302 (2)	0.0379 (14)
H12A	0.1651	0.2093	0.3115	0.057*
H12B	0.3192	0.0983	0.3319	0.057*
H12C	0.3592	0.2756	0.3078	0.057*
Zn2	0.25313 (8)	0.28490 (10)	0.93401 (3)	0.0254 (2)
Cl3	0.09426 (16)	0.50253 (18)	0.91272 (6)	0.0309 (3)
Cl4	0.09997 (16)	0.03585 (18)	0.91796 (6)	0.0320 (3)
N5	0.4837 (5)	0.2668 (6)	0.89591 (18)	0.0246 (9)
N6	0.7549 (5)	0.1970 (6)	0.88353 (19)	0.0258 (9)
H6A	0.8604	0.1528	0.8886	0.031*
N7	0.3582 (5)	0.2981 (6)	1.01354 (19)	0.0274 (10)

N8	0.2700 (6)	0.3138 (7)	1.06422 (19)	0.0302 (10)
H8C	0.1605	0.3533	1.0666	0.036*
C13	0.5233 (6)	0.2698 (7)	0.8382 (2)	0.0244 (11)
C14	0.4239 (7)	0.3104 (8)	0.7924 (2)	0.0310 (12)
H14	0.3073	0.3425	0.7975	0.037*
C15	0.5018 (8)	0.3020 (8)	0.7394 (2)	0.0338 (13)
H15	0.4366	0.3280	0.7073	0.041*
C16	0.6741 (8)	0.2564 (8)	0.7312 (2)	0.0351 (13)
H16	0.7229	0.2528	0.6939	0.042*
C17	0.7748 (7)	0.2165 (8)	0.7765 (3)	0.0330 (13)
H17	0.8915	0.1846	0.7713	0.040*
C18	0.6949 (7)	0.2258 (7)	0.8302 (2)	0.0250 (11)
C19	0.6252 (6)	0.2239 (7)	0.9216 (2)	0.0226 (10)
C20	0.6553 (7)	0.2051 (8)	0.9832 (2)	0.0301 (12)
H20A	0.7539	0.2810	0.9972	0.036*
H20B	0.6918	0.0850	0.9843	0.036*
C21	0.5134 (6)	0.2424 (7)	1.0263 (2)	0.0247 (11)
C22	0.5243 (7)	0.2259 (7)	1.0847 (2)	0.0283 (12)
H22	0.6212	0.1901	1.1046	0.034*
C23	0.3677 (7)	0.2715 (7)	1.1077 (2)	0.0267 (11)
C24	0.3001 (8)	0.2795 (9)	1.1675 (2)	0.0367 (14)
H24A	0.1955	0.2085	1.1667	0.055*
H24B	0.2738	0.3993	1.1829	0.055*
H24C	0.3866	0.2360	1.1922	0.055*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0354 (4)	0.0185 (3)	0.0261 (4)	−0.0062 (3)	0.0028 (3)	0.0071 (3)
Cl1	0.0330 (7)	0.0248 (6)	0.0424 (8)	−0.0043 (6)	0.0037 (5)	0.0113 (6)
Cl2	0.0360 (7)	0.0253 (6)	0.0423 (8)	−0.0086 (6)	0.0061 (6)	0.0087 (6)
N1	0.030 (2)	0.022 (2)	0.022 (2)	−0.0043 (19)	−0.0008 (17)	0.0083 (18)
N2	0.036 (3)	0.021 (2)	0.029 (2)	−0.003 (2)	0.0015 (19)	0.0030 (19)
N3	0.047 (3)	0.022 (2)	0.025 (2)	−0.009 (2)	0.001 (2)	0.0046 (19)
N4	0.049 (3)	0.020 (2)	0.024 (2)	−0.008 (2)	0.000 (2)	0.0020 (18)
C1	0.024 (3)	0.027 (3)	0.025 (3)	0.003 (2)	−0.0003 (19)	0.007 (2)
C2	0.035 (3)	0.033 (3)	0.026 (3)	0.003 (3)	0.004 (2)	0.011 (2)
C3	0.039 (3)	0.046 (4)	0.027 (3)	0.009 (3)	0.006 (2)	0.014 (3)
C4	0.043 (3)	0.048 (4)	0.027 (3)	0.007 (3)	0.002 (2)	0.000 (3)
C5	0.043 (3)	0.032 (3)	0.034 (3)	−0.004 (3)	0.001 (3)	−0.003 (3)
C6	0.027 (3)	0.028 (3)	0.027 (3)	−0.003 (2)	0.001 (2)	0.006 (2)
C7	0.026 (3)	0.017 (2)	0.027 (3)	−0.004 (2)	−0.001 (2)	0.003 (2)
C8	0.048 (3)	0.024 (3)	0.025 (3)	−0.007 (3)	0.001 (2)	0.007 (2)
C9	0.030 (3)	0.021 (2)	0.025 (3)	−0.003 (2)	−0.004 (2)	0.009 (2)
C10	0.034 (3)	0.026 (3)	0.027 (3)	−0.003 (2)	0.003 (2)	0.011 (2)
C11	0.030 (3)	0.029 (3)	0.024 (3)	−0.002 (2)	0.000 (2)	0.006 (2)
C12	0.047 (4)	0.037 (3)	0.028 (3)	−0.003 (3)	0.002 (2)	−0.001 (3)
Zn2	0.0158 (3)	0.0359 (4)	0.0246 (4)	0.0054 (3)	−0.0021 (2)	0.0044 (3)

Cl3	0.0224 (6)	0.0360 (7)	0.0354 (7)	0.0079 (6)	−0.0015 (5)	0.0082 (6)
Cl4	0.0221 (6)	0.0331 (7)	0.0407 (8)	0.0054 (6)	−0.0050 (5)	0.0048 (6)
N5	0.019 (2)	0.034 (2)	0.020 (2)	0.002 (2)	−0.0022 (16)	0.0029 (18)
N6	0.017 (2)	0.033 (2)	0.028 (2)	0.0031 (19)	0.0013 (16)	0.0050 (19)
N7	0.019 (2)	0.039 (3)	0.024 (2)	0.005 (2)	−0.0006 (16)	0.002 (2)
N8	0.022 (2)	0.043 (3)	0.025 (2)	0.008 (2)	0.0021 (17)	0.004 (2)
C13	0.020 (2)	0.029 (3)	0.024 (3)	0.001 (2)	−0.0021 (19)	0.004 (2)
C14	0.026 (3)	0.041 (3)	0.026 (3)	0.003 (3)	−0.005 (2)	0.007 (2)
C15	0.036 (3)	0.042 (3)	0.024 (3)	0.003 (3)	−0.005 (2)	0.007 (2)
C16	0.039 (3)	0.042 (3)	0.024 (3)	0.003 (3)	0.004 (2)	0.006 (2)
C17	0.025 (3)	0.042 (3)	0.033 (3)	0.002 (3)	0.006 (2)	0.005 (3)
C18	0.023 (3)	0.028 (3)	0.023 (3)	0.001 (2)	0.0006 (19)	0.002 (2)
C19	0.016 (2)	0.026 (3)	0.025 (3)	0.003 (2)	−0.0004 (18)	0.003 (2)
C20	0.020 (2)	0.044 (3)	0.027 (3)	0.007 (3)	−0.001 (2)	0.005 (2)
C21	0.020 (2)	0.029 (3)	0.024 (3)	0.003 (2)	−0.0034 (19)	0.003 (2)
C22	0.023 (3)	0.036 (3)	0.027 (3)	0.006 (2)	−0.002 (2)	0.006 (2)
C23	0.025 (3)	0.031 (3)	0.024 (3)	0.002 (2)	−0.002 (2)	0.002 (2)
C24	0.035 (3)	0.049 (4)	0.027 (3)	0.008 (3)	0.004 (2)	0.006 (3)

Geometric parameters (Å, º)

Zn1—N1	1.996 (4)	Zn2—N5	2.007 (4)
Zn1—N3	2.014 (4)	Zn2—N7	2.014 (4)
Zn1—Cl2	2.2291 (14)	Zn2—Cl3	2.2304 (15)
Zn1—Cl1	2.2533 (16)	Zn2—Cl4	2.2577 (16)
N1—C7	1.332 (6)	N5—C19	1.322 (7)
N1—C1	1.388 (7)	N5—C13	1.389 (6)
N2—C7	1.345 (7)	N6—C19	1.350 (6)
N2—C6	1.381 (7)	N6—C18	1.377 (7)
N2—H2A	0.9088	N6—H6A	0.9100
N3—C9	1.342 (7)	N7—C21	1.337 (7)
N3—N4	1.361 (6)	N7—N8	1.364 (6)
N4—C11	1.340 (7)	N8—C23	1.347 (7)
N4—H4A	0.9100	N8—H8C	0.9100
C1—C6	1.392 (8)	C13—C14	1.392 (7)
C1—C2	1.396 (7)	C13—C18	1.392 (7)
C2—C3	1.377 (8)	C14—C15	1.377 (8)
C2—H2	0.9500	C14—H14	0.9500
C3—C4	1.392 (10)	C15—C16	1.400 (9)
C3—H3	0.9500	C15—H15	0.9500
C4—C5	1.384 (9)	C16—C17	1.387 (9)
C4—H4	0.9500	C16—H16	0.9500
C5—C6	1.390 (8)	C17—C18	1.397 (7)
C5—H5	0.9500	C17—H17	0.9500
C7—C8	1.483 (7)	C19—C20	1.484 (7)
C8—C9	1.499 (8)	C20—C21	1.504 (7)
C8—H8A	0.9900	C20—H20A	0.9900
C8—H8B	0.9900	C20—H20B	0.9900

C9—C10	1.387 (7)	C21—C22	1.390 (7)
C10—C11	1.379 (8)	C22—C23	1.368 (7)
C10—H10	0.9500	C22—H22	0.9500
C11—C12	1.493 (7)	C23—C24	1.489 (7)
C12—H12A	0.9800	C24—H24A	0.9800
C12—H12B	0.9800	C24—H24B	0.9800
C12—H12C	0.9800	C24—H24C	0.9800

N1—Zn1—N3	92.17 (18)	N5—Zn2—N7	92.34 (17)
N1—Zn1—Cl2	111.84 (13)	N5—Zn2—Cl3	114.47 (14)
N3—Zn1—Cl2	120.88 (15)	N7—Zn2—Cl3	119.46 (14)
N1—Zn1—Cl1	112.63 (14)	N5—Zn2—Cl4	112.76 (14)
N3—Zn1—Cl1	107.46 (15)	N7—Zn2—Cl4	106.71 (15)
Cl2—Zn1—Cl1	110.69 (6)	Cl3—Zn2—Cl4	110.02 (6)
C7—N1—C1	106.2 (4)	C19—N5—C13	106.9 (4)
C7—N1—Zn1	124.3 (3)	C19—N5—Zn2	123.7 (3)
C1—N1—Zn1	128.6 (3)	C13—N5—Zn2	128.8 (3)
C7—N2—C6	108.4 (4)	C19—N6—C18	108.3 (4)
C7—N2—H2A	127.0	C19—N6—H6A	128.6
C6—N2—H2A	124.6	C18—N6—H6A	122.5
C9—N3—N4	105.3 (4)	C21—N7—N8	105.1 (4)
C9—N3—Zn1	126.2 (4)	C21—N7—Zn2	126.4 (4)
N4—N3—Zn1	125.9 (3)	N8—N7—Zn2	125.6 (3)
C11—N4—N3	112.0 (4)	C23—N8—N7	111.5 (4)
C11—N4—H4A	119.3	C23—N8—H8C	127.1
N3—N4—H4A	126.6	N7—N8—H8C	121.4
N1—C1—C6	108.9 (4)	N5—C13—C14	131.1 (5)
N1—C1—C2	130.4 (5)	N5—C13—C18	108.2 (4)
C6—C1—C2	120.7 (5)	C14—C13—C18	120.8 (5)
C3—C2—C1	116.8 (6)	C15—C14—C13	117.2 (5)
C3—C2—H2	121.6	C15—C14—H14	121.4
C1—C2—H2	121.6	C13—C14—H14	121.4
C2—C3—C4	122.3 (5)	C14—C15—C16	122.1 (5)
C2—C3—H3	118.8	C14—C15—H15	118.9
C4—C3—H3	118.8	C16—C15—H15	118.9
C5—C4—C3	121.3 (6)	C17—C16—C15	121.2 (5)
C5—C4—H4	119.3	C17—C16—H16	119.4
C3—C4—H4	119.3	C15—C16—H16	119.4
C4—C5—C6	116.5 (6)	C16—C17—C18	116.3 (5)
C4—C5—H5	121.8	C16—C17—H17	121.9
C6—C5—H5	121.8	C18—C17—H17	121.9
N2—C6—C5	132.3 (5)	N6—C18—C13	105.8 (4)
N2—C6—C1	105.3 (5)	N6—C18—C17	131.8 (5)
C5—C6—C1	122.4 (5)	C13—C18—C17	122.4 (5)
N1—C7—N2	111.1 (5)	N5—C19—N6	110.8 (4)
N1—C7—C8	128.6 (5)	N5—C19—C20	129.4 (4)
N2—C7—C8	120.3 (5)	N6—C19—C20	119.7 (4)
C7—C8—C9	120.1 (5)	C19—C20—C21	119.9 (4)

C7—C8—H8A	107.3	C19—C20—H20A	107.3
C9—C8—H8A	107.3	C21—C20—H20A	107.3
C7—C8—H8B	107.3	C19—C20—H20B	107.3
C9—C8—H8B	107.3	C21—C20—H20B	107.3
H8A—C8—H8B	106.9	H20A—C20—H20B	106.9
N3—C9—C10	109.9 (5)	N7—C21—C22	110.4 (4)
N3—C9—C8	124.3 (5)	N7—C21—C20	124.2 (5)
C10—C9—C8	125.7 (5)	C22—C21—C20	125.4 (5)
C11—C10—C9	106.6 (5)	C23—C22—C21	106.3 (5)
C11—C10—H10	126.7	C23—C22—H22	126.9
C9—C10—H10	126.7	C21—C22—H22	126.9
N4—C11—C10	106.1 (5)	N8—C23—C22	106.7 (5)
N4—C11—C12	121.9 (5)	N8—C23—C24	121.5 (5)
C10—C11—C12	131.9 (5)	C22—C23—C24	131.8 (5)
C11—C12—H12A	109.5	C23—C24—H24A	109.5
C11—C12—H12B	109.5	C23—C24—H24B	109.5
H12A—C12—H12B	109.5	H24A—C24—H24B	109.5
C11—C12—H12C	109.5	C23—C24—H24C	109.5
H12A—C12—H12C	109.5	H24A—C24—H24C	109.5
H12B—C12—H12C	109.5	H24B—C24—H24C	109.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···Cl1^{i}	0.91	2.23	3.125 (5)	169
N4—H4*A*···Cl2^{ii}	0.91	2.33	3.161 (5)	152
N6—H6*A*···Cl4^{iii}	0.91	2.24	3.133 (5)	169
N8—H8*C*···Cl3^{iv}	0.91	2.32	3.211 (5)	168

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