Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

Crystal structure and Hirshfeld surface analysis of [2-(1*H*-benzimidazol-2-yl-κN^3)aniline-κN]dichloridozinc(II) *N*,*N*-dimethylformamide monosolvate

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Received 11 February 2021
Accepted 5 April 2021

Edited by J. Ellena, Universidade de São Paulo, Brazil

Keywords: crystal structure; benzimidazole; aniline; bidentate ligand; heterocyclic; zinc(II) complex.

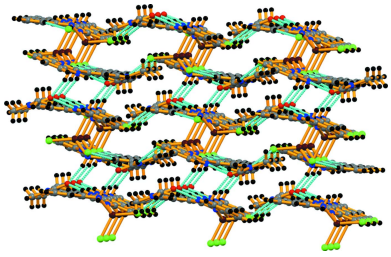
CCDC reference: 2033195

Supporting information: this article has supporting information at journals.iucr.org/e

The title compound, $[ZnCl_2(C_{13}H_{11}N_3)]\cdot C_3H_7NO$, crystallized in the monoclinic crystal system in space group $P2_1/n$. The asymmetric unit contains one neutral complex molecule, which consists of a zinc ion, a bidentate ligand, and two chlorido ligands with dimethylformamide monosolvate. The ligand has two moieties, a benzimidazole and an aniline group. The benzimidazole and aniline planes are not coplanar, subtending a dihedral angle of 18.24 (8)°. The Zn(II) ion shows distorted tetrahedral geometry, being coordinated by an imidazole N atom, the aniline N atom, and two chlorido ligands. The packing features N—H···O, N—H···Cl, C—H···Cl hydrogen bonding.

1. Chemical context

Benzimidazoles as organic ligands have attracted interest with regard to the synthesis of metal–organic frameworks, not only because of their coordination abilities to metal ions, but also their significant potential applications in biological systems (Ahmad & Bharadwaj; 2013; Sharma *et al.*, 2016; Gu *et al.*, 2017). Benzimidazole compounds and their metal complexes have been found to show diverse biological activity (Podunavac-Kuzmanovic & Cvetkovic, 2010), including inhibition against enteroviruses (Xue *et al.*, 2011) and potent antitumor activity (Galarce *et al.*, 2008). The bidentate ligand 2-(1*H*-benzo[*d*]imidazol-2-yl) aniline (*L*) has been used to prepare a series of mononuclear transition-metal complexes with halide anions as the active leaving group in our catalytic research. In this work, a mononuclear zinc complex $ZnLCl_2$ is reported. Zinc complexes bearing various ancillary ligands have been applied in the catalysis of the copolymerization of cyclohexene oxide and CO_2 (Kember *et al.*, 2009).



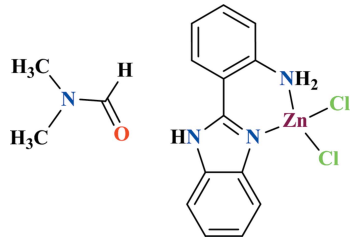


Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.89	2.11	2.923 (2)	152
N1—H1B···Cl2^{ii}	0.89	2.48	3.3592 (17)	170
N3—H3···O1	0.86	1.99	2.807 (2)	157
C2—H2···Cl2^{ii}	0.93	2.93	3.734 (2)	145
C14—H14···Cl1^{iii}	0.93	2.95	3.836 (3)	160

Symmetry codes: (i) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+1, -y+2, -z+1$; (iii) $x+\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$.

2. Structural commentary

The asymmetric unit of the title complex (Fig. 1) contains one neutral complex molecule, which consists of one central zinc ion, one bidentate ligand, and two chlorido ligands with dimethylformamide solvent. The two ligand moieties, benzimidazole and aniline, are not coplanar structure, subtending a dihedral angle of 18.24 (8)°. The C1—N1 and C7—N2 bond lengths are 1.449 (2) and 1.335 (2) Å, respectively. The complex is a four-coordinated system by one imidazole nitrogen atom N2, one aniline nitrogen atom N1, and two chlorido ligands. The distances from the zinc(II) ion to the coordinating atoms are all in the expected ranges. The bond angles around the zinc(II) atom are in the range 88.64 (7) to 118.57 (3)°, of which the smallest angle N1—Zn1—N2 is formed by the two nitrogen atoms from the bidentate ligand.

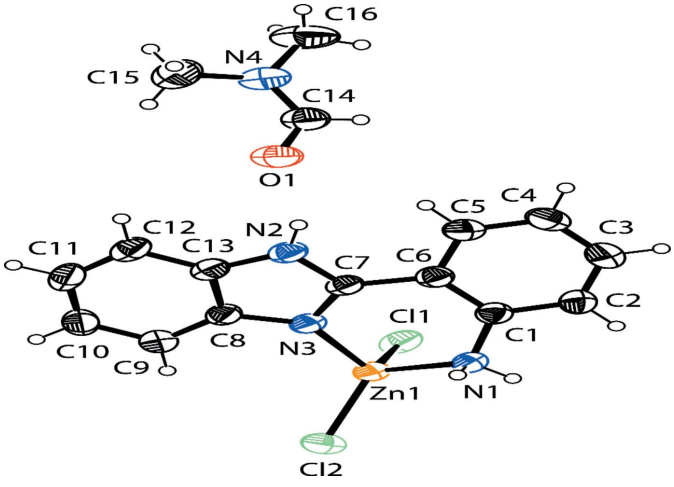


Figure 1
A view of the title complex with the atom labeling and displacement ellipsoids drawn at the 40% level.

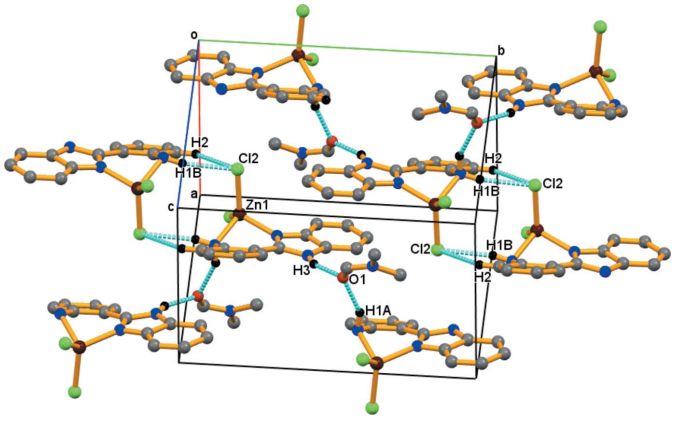


Figure 2
A packing view approximately along [10$\bar{1}$] of the title complex. Hydrogen atoms are omitted for clarity.

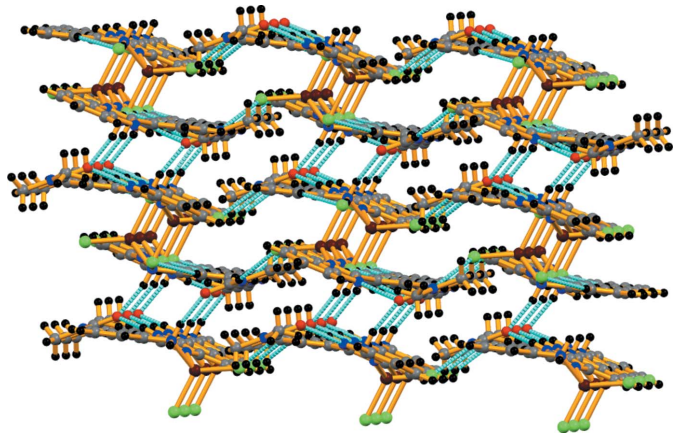


Figure 3
Supramolecular view along the b axis of the crystal structure of the title complex formed through C—H···π, hydrogen-bonding, and other weak interactions.

3. Supramolecular features

In the crystal, molecules are linked by N—H···Cl hydrogen bonds (Table 1, Fig. 2), forming sheets propagating along the b-axis direction (Fig. 3).

4. Hirshfeld Surface analysis

A Hirshfeld surface analysis (Spackman & Jayatilaka, 2009) was undertaken and the associated two-dimensional fingerprint plots (McKinnon, *et al.*, 2007) generated using *Crystal Explorer* (Turner *et al.*, 2017) to investigate the intermolecular interactions and surface morphology of the crystal structure.

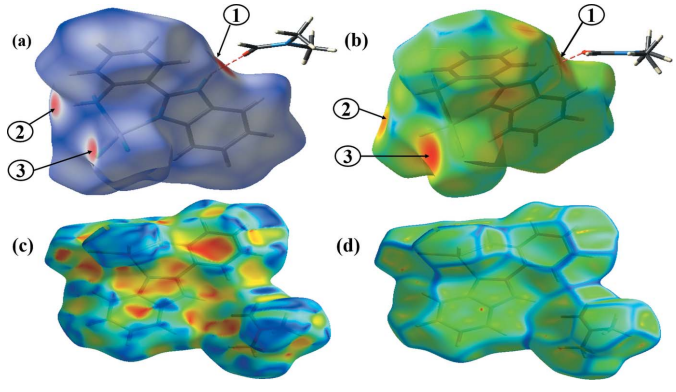


Figure 4
The Hirshfeld surface of the title complex mapped over (*a*) d_{norm}, (*b*) d_e, (*c*) shape-index, and (*d*) curvedness. Red spots 1,2, and 3 in (*a*) and (*b*) correspond to N—H···O, N—H···Cl, and C—H···Cl hydrogen bonds.

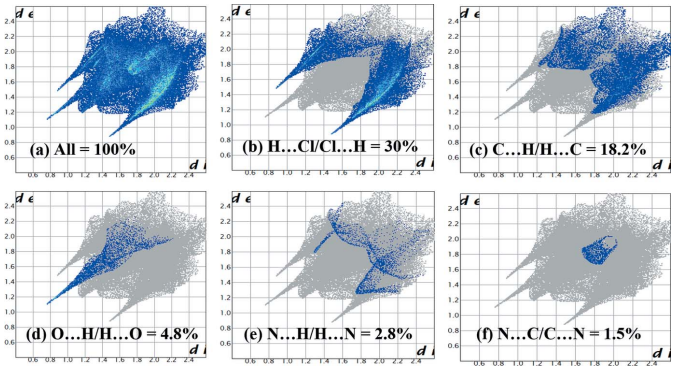


Figure 5
(*a*) A full two-dimensional fingerprint plot of the title complex, and delineated into (*b*) H···Cl/Cl···H (30%), (*c*) C···H/H···C (18.2%), and (*d*) O···H/H···O (4.8%) contacts, which are the major interactions present in the crystal structure.

The Hirshfeld surface mapped over d_{norm} in the color range (−0.464 to 1.340 a.u.) from red (shorter than the sum of the van der Waals radii) and white to blue (longer distance than the sum of the van der Waals radii). The bright red spot on the d_{norm} surface (Fig. 4*a*) indicates the N—H···O hydrogen bonding. C—H···Cl contacts are evident as distinct circular depressions (red spots) and other visible spots on the d_{norm} surface (Fig. 4*a*) are due to H···H contacts. The surfaces of the title complex were also mapped over d_e (0.834 to 2.650 Å), shape-index (−1.0000 to 1.0000 Å), and curvedness (−4.0000 to 0.4000 Å) in the given ranges. The flat green region on the d_e surface represents similar contact distances (Fig. 4*b*). The pattern of red and blue regions in the shape-index surface is characteristic of ring carbon atoms of the molecule inside the surface. The shape of the blue outline on the curved surface shown in Fig. 4*d* is evidence of the flat region toward the bottom of both sides of the molecules.

Five types of major interactions in the crystal structure (H···Cl = 30%, C···H = 18.2%, O···H = 4.8%, N···H = 2.8%, N···C = 1.5%) are shown in the two-dimensional fingerprint plots (Fig. 5). The interaction order (H···Cl)> (C···H)> (O···H)> (N···H)> (N···C) of d_{norm} on the 2D fingerprint plot represents the nature of packing in the title crystal structure (Muslim *et al.*, 2020). The pattern of intermolecular interactions (H···Cl/Cl···H, C···H/H···C, O···H/H···O, N···H/H···O, and N···C/C···N) governs the overall packing and quantifies the contribution of the non-covalent interaction (C—H···Cl) to the extended supramolecular network (Seth *et al.*, 2011; Seth, 2013; Manna *et al.*, 2012; Mitra *et al.*, 2014).

5. Database survey

A search of the Cambridge Structural Database (CSD, version 5.39; Groom *et al.*, 2016) gave thirteen hits for the [2-(1*H*-benzimidazol-2-yl]aniline)zinc(II) moiety. Two compounds whose structures are very similar to that of the title compound are [2-(1*H*-benzimidazol-2-yl)aniline]dichloridozinc(II) (AWOLEE; Eltayeb *et al.*, 2011*a*) in which the dimethylformamide solvent is absent and dichloro-[2-(1-methyl-1*H*-benzimidazol-2-yl)aniline]zinc(II) (ILELIW; Zhou *et al.*, 2016) in which the NH group is replaced by an N—CH_3 group. Zinc compounds with different ligands include (2-{[2-(1*H*-benzimidazol-2-yl-κN^3)phenyl]iminomethyl-κN}-5-methylphenolato-κO)chloridozinc(II) (AYINEC; Eltayeb *et al.*, 2011*b*) in which the zinc atom is surrounded by two imine nitrogen, one phenolic oxygen and one chlorine atoms. Other complexes include bis{N-[2-(1-butyl-5-nitro-1*H*-benzimidazol-2-yl)phenyl]-4- methylbenzenesulfonamidato}zinc(II) with an unknown solvate (BUXDIJ; Burlov *et al.*, 2016) and bis{4-methyl-*N*-[2-(5-nitro-1-propyl-1*H*-benzimidazole-2-yl)phenyl]benzenesulfonamidato}zinc(II) chloroform solvate (BUXDOP; Burlov *et al.*, 2016), bis{μ-[2-(5-amino-1-propyl-1*H*-benzimidazole-2-yl)phenyl](4-methylbenzene-1-sulfonyl)amido}bis(pivalato)dizinc acetonitrile ethanol solvate dihydrate (EDOVUR; Nikolaevskii *et al.*, 2014), bis(μ_2-3-{[2-(1*H*-benzimidazole-2-yl)phenyl]carbonoimidoyl}benzene-1,2-diolato)dizinc(II) ethanol solvate (GABVUD; Wang *et al.*, 2016), (acetato-*O*,*O*′)-[2-({[2-(1*H*-benzimidazole-2-yl)phenyl]imino}methyl)-5-(diethylamino)phenolato]zinc(II) isopropanol solvate (IKOYUE; Liao *et al.*, 2016).

Table 2
Experimental details.

Crystal data	
Chemical formula	$[ZnCl_2(C_{13}H_{11}N_3)]\cdot C_3H_7NO$
M_r	418.61
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	296
a, *b*, *c* (Å)	10.9394 (9), 13.3041 (7), 13.1665 (11)
β (°)	106.140 (7)
V (Å^3)	1840.7 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.64
Crystal size (mm)	0.60 × 0.50 × 0.39
Data collection	
Diffractometer	Stoe IPDS 2
Absorption correction	Integration (*X-RED32*; Stoe & Cie, 2002)
T_{min}, T_{max}	0.460, 0.567
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	19616, 5643, 3891
R_{int}	0.036
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.717
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.037, 0.097, 1.04
No. of reflections	5643
No. of parameters	219
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.34, −0.62

Computer programs: *X-AREA* (Stoe & Cie, 2002), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012), and *XP* in *SHELXTL* (Sheldrick, 2008).

6. Synthesis and crystallization

A mixture of 2-(2-aminophenylbenzimidazole) (0.05 g, 0.14 mmol) and $ZnCl_2\cdot 4H_2O$ (0.125 g, 0.4 mmol) was dissolved in 5 ml of dimethylformamide (DMF) and then sealed in a

Teflon-lined autoclave and heated under autogenous pressure to 453 K for 2 d and then allow to cool to room temperature at the rate of 1 K per minute. The resulting solution was filtered and kept for slow evaporation. After one week, block-shaped colorless crystals suitable for single-crystal X-ray diffraction data collection were obtained.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Hydrogen atoms were positioned geometrically (N—H = 0.86–0.89, C—H = 0.93–0.96 Å) included with U_{iso}(H) = 1.2U_{eq}(N, C) or 1.5U_{eq}(C-methyl).

Acknowledgements

The Department of Applied Chemistry, ZHCET, Faculty of Engineering and Technology, Aligarh Muslim University, UP, India, is gratefully acknowledged for providing laboratory facilities. Author contributions are as follows. Conceptualization, AM, MA and MM; methodology, MA, AM and MSHF; investigation, ND, AA and MA; writing (original draft), MM and MSHF; writing (review and editing of the manuscript), MdA, MM and AA; visualization, MM, AA and MSHF; funding acquisition, AM; resources, ND and MA; supervision, AM and MA.

Funding information

MA and MSHF acknowledge the startup grant received from UGC, India.

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supporting information

Acta Cryst. (2021). E**77**, 491-494 [https://doi.org/10.1107/S2056989021003649]

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Computing details

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA* (Stoe & Cie, 2002); data reduction: *X-AREA* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015b); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *XP* in *SHELXTL* (Sheldrick, 2008).

[2-(1*H*-Benzimidazol-2-yl-κN^3)aniline-κN]dichloridozinc(II) *N*,*N*-dimethylformamide monosolvate

Crystal data

$[ZnCl_2(C_{13}H_{11}N_3)]\cdot C_3H_7NO$
$M_r = 418.61$
Monoclinic, $P2_1/n$
$a = 10.9394$ (9) Å
$b = 13.3041$ (7) Å
$c = 13.1665$ (11) Å
$\beta = 106.140$ (7)°
$V = 1840.7$ (2) Å^3
$Z = 4$
$F(000) = 856$
$D_x = 1.511$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 22582 reflections
$\theta = 1.5$–31.0°
$\mu = 1.64$ mm^{-1}
$T = 296$ K
Prism, yellow
0.60 × 0.50 × 0.39 mm

Data collection

STOE IPDS 2 diffractometer
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus
Plane graphite monochromator
Detector resolution: 6.67 pixels mm^{-1}
rotation method scans
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)
$T_{min} = 0.460$, $T_{max} = 0.567$
19616 measured reflections
5643 independent reflections
3891 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 30.7°$, $\theta_{min} = 2.2°$
$h = -15\rightarrow15$
$k = -17\rightarrow18$
$l = -18\rightarrow18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.097$
$S = 1.04$
5643 reflections
219 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0502P)^2 + 0.0362P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.62$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.40345 (2)	0.83177 (2)	0.52883 (2)	0.04912 (8)
Cl2	0.61440 (5)	0.84302 (4)	0.60104 (5)	0.06630 (16)
Cl1	0.27561 (6)	0.87107 (5)	0.62724 (5)	0.07198 (17)
O1	0.41861 (16)	0.45845 (14)	0.17389 (14)	0.0726 (5)
N1	0.35146 (16)	0.90600 (12)	0.38489 (13)	0.0502 (4)
H1A	0.267634	0.900599	0.357590	0.060*
H1B	0.369650	0.970981	0.395980	0.060*
N3	0.37815 (15)	0.58840 (12)	0.32936 (13)	0.0504 (4)
H3	0.388210	0.563774	0.271825	0.060*
N2	0.36342 (15)	0.70047 (12)	0.44985 (13)	0.0476 (3)
N4	0.5564 (2)	0.35468 (17)	0.12569 (17)	0.0691 (5)
C7	0.38739 (18)	0.68676 (14)	0.35677 (15)	0.0455 (4)
C1	0.41353 (18)	0.86859 (16)	0.30855 (15)	0.0480 (4)
C13	0.34988 (17)	0.53440 (15)	0.40928 (16)	0.0486 (4)
C8	0.33936 (18)	0.60573 (14)	0.48466 (16)	0.0479 (4)
C6	0.42738 (18)	0.76471 (15)	0.29345 (15)	0.0482 (4)
C12	0.3365 (2)	0.43147 (16)	0.42430 (19)	0.0590 (5)
H12	0.345224	0.384308	0.374641	0.071*
C2	0.4613 (2)	0.93761 (18)	0.25020 (18)	0.0582 (5)
H2	0.452680	1.005994	0.261168	0.070*
C9	0.3122 (2)	0.57631 (17)	0.57798 (18)	0.0588 (5)
H9	0.304769	0.623164	0.628334	0.071*
C10	0.2969 (2)	0.47426 (18)	0.5923 (2)	0.0652 (6)
H10	0.277820	0.452174	0.653141	0.078*
C11	0.3097 (2)	0.40357 (18)	0.5165 (2)	0.0658 (6)
H11	0.299785	0.335685	0.529071	0.079*
C5	0.4888 (2)	0.73555 (19)	0.21791 (18)	0.0610 (5)
H5	0.499020	0.667438	0.206631	0.073*
C14	0.5136 (2)	0.4429 (2)	0.1430 (2)	0.0673 (6)
H14	0.558734	0.498851	0.131104	0.081*
C3	0.5212 (2)	0.9066 (2)	0.1763 (2)	0.0674 (6)
H3A	0.552587	0.953741	0.137785	0.081*
C4	0.5345 (2)	0.8051 (2)	0.1598 (2)	0.0694 (6)
H4	0.574124	0.783670	0.109566	0.083*
C15	0.4900 (4)	0.2641 (2)	0.1419 (3)	0.0947 (9)
H15A	0.458046	0.272789	0.202229	0.142*
H15B	0.547714	0.208200	0.153689	0.142*
H15C	0.420336	0.251482	0.080351	0.142*
C16	0.6699 (3)	0.3452 (3)	0.0881 (3)	0.1086 (13)

H16A	0.700566	0.410905	0.077503	0.163*
H16B	0.648854	0.308946	0.022441	0.163*
H16C	0.734825	0.309531	0.139603	0.163*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.05561 (14)	0.04018 (13)	0.05557 (14)	−0.00002 (10)	0.02208 (10)	−0.00610 (10)
Cl2	0.0557 (3)	0.0485 (3)	0.0914 (4)	0.0007 (2)	0.0149 (3)	−0.0107 (3)
Cl1	0.0790 (4)	0.0697 (4)	0.0814 (4)	0.0010 (3)	0.0458 (3)	−0.0117 (3)
O1	0.0641 (9)	0.0727 (11)	0.0876 (11)	−0.0039 (8)	0.0320 (9)	−0.0269 (9)
N1	0.0536 (9)	0.0383 (8)	0.0625 (10)	0.0024 (7)	0.0226 (8)	−0.0004 (7)
N3	0.0548 (9)	0.0409 (9)	0.0557 (9)	−0.0016 (7)	0.0155 (7)	−0.0098 (7)
N2	0.0513 (8)	0.0383 (8)	0.0561 (9)	0.0002 (7)	0.0198 (7)	−0.0054 (7)
N4	0.0641 (11)	0.0695 (13)	0.0731 (12)	0.0084 (10)	0.0178 (10)	−0.0187 (10)
C7	0.0450 (9)	0.0381 (10)	0.0536 (10)	0.0006 (7)	0.0138 (8)	−0.0064 (8)
C1	0.0458 (9)	0.0458 (10)	0.0531 (10)	0.0001 (8)	0.0152 (8)	−0.0010 (8)
C13	0.0411 (9)	0.0405 (10)	0.0621 (11)	0.0009 (7)	0.0108 (8)	−0.0044 (8)
C8	0.0442 (9)	0.0393 (9)	0.0612 (11)	−0.0011 (7)	0.0162 (8)	−0.0023 (8)
C6	0.0462 (9)	0.0459 (10)	0.0533 (10)	−0.0012 (8)	0.0152 (8)	−0.0047 (8)
C12	0.0551 (11)	0.0406 (11)	0.0781 (14)	−0.0027 (9)	0.0131 (10)	−0.0075 (10)
C2	0.0593 (12)	0.0504 (12)	0.0690 (13)	−0.0024 (9)	0.0245 (10)	0.0031 (10)
C9	0.0626 (12)	0.0531 (12)	0.0657 (12)	0.0021 (10)	0.0259 (10)	0.0019 (10)
C10	0.0634 (13)	0.0587 (14)	0.0778 (15)	−0.0017 (11)	0.0269 (11)	0.0136 (11)
C11	0.0586 (12)	0.0436 (11)	0.0936 (17)	−0.0033 (10)	0.0185 (12)	0.0092 (11)
C5	0.0686 (13)	0.0557 (13)	0.0651 (12)	0.0001 (10)	0.0295 (11)	−0.0092 (10)
C14	0.0619 (13)	0.0669 (15)	0.0772 (14)	−0.0053 (11)	0.0262 (11)	−0.0206 (12)
C3	0.0711 (14)	0.0680 (15)	0.0716 (14)	−0.0072 (12)	0.0340 (12)	0.0047 (12)
C4	0.0759 (15)	0.0767 (16)	0.0670 (14)	−0.0022 (13)	0.0388 (12)	−0.0059 (12)
C15	0.122 (3)	0.0664 (18)	0.098 (2)	0.0083 (18)	0.0341 (19)	−0.0014 (16)
C16	0.0760 (19)	0.124 (3)	0.134 (3)	0.0120 (18)	0.0440 (19)	−0.051 (2)

Geometric parameters (Å, º)

Zn1—N2	2.0177 (16)	C6—C5	1.401 (3)
Zn1—N1	2.0715 (17)	C12—C11	1.376 (3)
Zn1—Cl1	2.2171 (6)	C12—H12	0.9300
Zn1—Cl2	2.2432 (7)	C2—C3	1.379 (3)
O1—C14	1.234 (3)	C2—H2	0.9300
N1—C1	1.449 (2)	C9—C10	1.387 (3)
N1—H1A	0.8900	C9—H9	0.9300
N1—H1B	0.8900	C10—C11	1.406 (4)
N3—C7	1.354 (2)	C10—H10	0.9300
N3—C13	1.378 (3)	C11—H11	0.9300
N3—H3	0.8600	C5—C4	1.380 (3)
N2—C7	1.335 (2)	C5—H5	0.9300
N2—C8	1.391 (2)	C14—H14	0.9300
N4—C14	1.307 (3)	C3—C4	1.382 (4)

N4—C15	1.453 (4)	C3—H3A	0.9300
N4—C16	1.465 (3)	C4—H4	0.9300
C7—C6	1.471 (3)	C15—H15A	0.9600
C1—C2	1.389 (3)	C15—H15B	0.9600
C1—C6	1.410 (3)	C15—H15C	0.9600
C13—C12	1.397 (3)	C16—H16A	0.9600
C13—C8	1.401 (3)	C16—H16B	0.9600
C8—C9	1.398 (3)	C16—H16C	0.9600

N2—Zn1—N1	88.64 (7)	C13—C12—H12	121.8
N2—Zn1—Cl1	115.06 (5)	C3—C2—C1	121.2 (2)
N1—Zn1—Cl1	111.40 (5)	C3—C2—H2	119.4
N2—Zn1—Cl2	109.06 (5)	C1—C2—H2	119.4
N1—Zn1—Cl2	110.14 (5)	C10—C9—C8	117.2 (2)
Cl1—Zn1—Cl2	118.57 (3)	C10—C9—H9	121.4
C1—N1—Zn1	114.12 (12)	C8—C9—H9	121.4
C1—N1—H1A	108.7	C9—C10—C11	121.2 (2)
Zn1—N1—H1A	108.7	C9—C10—H10	119.4
C1—N1—H1B	108.7	C11—C10—H10	119.4
Zn1—N1—H1B	108.7	C12—C11—C10	122.2 (2)
H1A—N1—H1B	107.6	C12—C11—H11	118.9
C7—N3—C13	108.43 (16)	C10—C11—H11	118.9
C7—N3—H3	125.8	C4—C5—C6	121.8 (2)
C13—N3—H3	125.8	C4—C5—H5	119.1
C7—N2—C8	106.38 (16)	C6—C5—H5	119.1
C7—N2—Zn1	121.43 (13)	O1—C14—N4	125.6 (3)
C8—N2—Zn1	130.43 (13)	O1—C14—H14	117.2
C14—N4—C15	120.1 (2)	N4—C14—H14	117.2
C14—N4—C16	121.0 (3)	C2—C3—C4	119.7 (2)
C15—N4—C16	118.9 (3)	C2—C3—H3A	120.2
N2—C7—N3	110.96 (17)	C4—C3—H3A	120.2
N2—C7—C6	126.08 (17)	C5—C4—C3	119.8 (2)
N3—C7—C6	122.84 (17)	C5—C4—H4	120.1
C2—C1—C6	119.87 (18)	C3—C4—H4	120.1
C2—C1—N1	118.52 (18)	N4—C15—H15A	109.5
C6—C1—N1	121.60 (17)	N4—C15—H15B	109.5
N3—C13—C12	132.33 (19)	H15A—C15—H15B	109.5
N3—C13—C8	105.54 (17)	N4—C15—H15C	109.5
C12—C13—C8	122.1 (2)	H15A—C15—H15C	109.5
N2—C8—C9	130.48 (18)	H15B—C15—H15C	109.5
N2—C8—C13	108.66 (17)	N4—C16—H16A	109.5
C9—C8—C13	120.83 (19)	N4—C16—H16B	109.5
C5—C6—C1	117.58 (19)	H16A—C16—H16B	109.5
C5—C6—C7	118.94 (18)	N4—C16—H16C	109.5
C1—C6—C7	123.39 (17)	H16A—C16—H16C	109.5
C11—C12—C13	116.5 (2)	H16B—C16—H16C	109.5
C11—C12—H12	121.8		

C8—N2—C7—N3	0.9 (2)	N1—C1—C6—C7	−3.5 (3)
Zn1—N2—C7—N3	167.25 (13)	N2—C7—C6—C5	158.9 (2)
C8—N2—C7—C6	−175.14 (18)	N3—C7—C6—C5	−16.7 (3)
Zn1—N2—C7—C6	−8.8 (3)	N2—C7—C6—C1	−17.5 (3)
C13—N3—C7—N2	−1.5 (2)	N3—C7—C6—C1	166.93 (18)
C13—N3—C7—C6	174.63 (18)	N3—C13—C12—C11	178.7 (2)
Zn1—N1—C1—C2	−135.94 (17)	C8—C13—C12—C11	1.3 (3)
Zn1—N1—C1—C6	43.4 (2)	C6—C1—C2—C3	0.7 (3)
C7—N3—C13—C12	−176.2 (2)	N1—C1—C2—C3	−179.9 (2)
C7—N3—C13—C8	1.5 (2)	N2—C8—C9—C10	−177.7 (2)
C7—N2—C8—C9	178.2 (2)	C13—C8—C9—C10	0.2 (3)
Zn1—N2—C8—C9	13.6 (3)	C8—C9—C10—C11	0.7 (3)
C7—N2—C8—C13	0.1 (2)	C13—C12—C11—C10	−0.3 (3)
Zn1—N2—C8—C13	−164.58 (13)	C9—C10—C11—C12	−0.7 (4)
N3—C13—C8—N2	−1.0 (2)	C1—C6—C5—C4	0.0 (3)
C12—C13—C8—N2	177.06 (18)	C7—C6—C5—C4	−176.6 (2)
N3—C13—C8—C9	−179.33 (19)	C15—N4—C14—O1	0.5 (4)
C12—C13—C8—C9	−1.3 (3)	C16—N4—C14—O1	179.4 (3)
C2—C1—C6—C5	−0.7 (3)	C1—C2—C3—C4	−0.1 (4)
N1—C1—C6—C5	−179.96 (19)	C6—C5—C4—C3	0.7 (4)
C2—C1—C6—C7	175.8 (2)	C2—C3—C4—C5	−0.6 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O1^{i}	0.89	2.11	2.923 (2)	152
N1—H1*B*···Cl2^{ii}	0.89	2.48	3.3592 (17)	170
N3—H3···O1	0.86	1.99	2.807 (2)	157
C2—H2···Cl2^{ii}	0.93	2.93	3.734 (2)	145
C14—H14···Cl1^{iii}	0.93	2.95	3.836 (3)	160

Symmetry codes: (i) −*x*+1/2, *y*+1/2, −*z*+1/2; (ii) −*x*+1, −*y*+2, −*z*+1; (iii) *x*+1/2, −*y*+3/2, *z*−1/2.