



Received 29 January 2020

Accepted 27 February 2020

Edited by W. T. A. Harrison, University of
Aberdeen, Scotland**Keywords:** crystal structure; molecular salt;
hydrogen bonding.**CCDC reference:** 1986654**Supporting information:** this article has
supporting information at journals.iucr.org/e

Crystal structure and Hirshfeld surface analysis of (C₇H₉N₄O₂)[ZnCl₃(H₂O)]

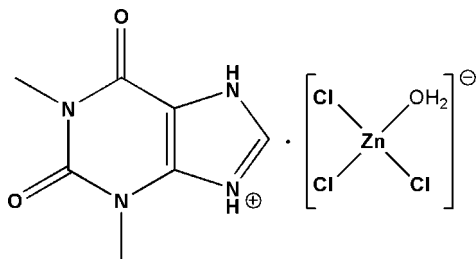
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In the title molecular salt, 1,3-dimethyl-2,6-dioxo-2,3,6,7-tetrahydro-1*H*-purin-9-ium aquatrichloridozincate(II), (C₇H₉N₄O₂)[ZnCl₃(H₂O)], the fused ring system of the cation is close to planar, with the largest deviation from the mean plane being 0.037 (3) Å. In the complex anion, the Zn^{II} cation is coordinated by three chloride ions and one oxygen atom from the water ligand in a distorted tetrahedral geometry. In the crystal, inversion dimers between pairs of cations linked by pairwise N—H···O hydrogen bonds generate R₂²(10) rings. The anions are linked into dimers by pairs of O—H···Cl hydrogen bonds and the respective dimers are linked by O—H···O and N—H···Cl hydrogen bonds. Together, these generate a three-dimensional supramolecular network. Hirshfeld surfaces were generated to gain further insight into the packing.

1. Chemical context

Theophylline, C₇H₈N₄O₂, is an alkaloid derivative of xanthine, containing a fused pyrimidine-imidazole ring system with conjugated double bonds. It has many biological and pharmacological properties (see, for example, Rao *et al.*, 2005; Piosik *et al.*, 2005). Various studies have shown that theophylline can be used as a medicine for the treatment of asthmatic bronchitis and chronic obstructive bronchitis (under several brand names), and as anticancer drugs (Nafisi *et al.* 2003; Rao *et al.* 2005; Piosik *et al.* 2005). Furthermore, theophylline complexes with transition metals can be used in anticancer drugs (David *et al.*, 1999).



As part of our studies in this area, we reacted theophylline with ZnCl₂ under acid conditions to give the molecular salt (C₇H₉N₄O₂)[ZnCl₃(H₂O)] and its crystal structure is described herein.

2. Structural commentary

The asymmetric unit of the title molecular salt (Fig. 1) comprises one theophyllinium (C₇H₉N₄O₂)⁺ cation proto-

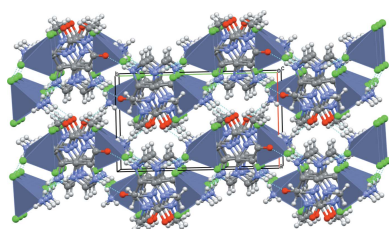


Table 1
Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1\cdots O2^i$	0.86	1.87	2.7067 (18)	163
$N2-H2\cdots Cl2^{ii}$	0.86	2.21	3.0652 (15)	174
$C6-H6C\cdots O2^{iii}$	0.96	2.65	3.431 (3)	139
$O3-H3A\cdots Cl3^{iv}$	0.77	2.43	3.1915 (17)	176
$O3-H3B\cdots O1$	0.82	1.90	2.718 (2)	173

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

nated at N2 and one $[ZnCl_3(H_2O)]^{-1}$ anion. As expected, the $[ZnCl_3(H_2O)]$ tetrahedron contains one short Zn–O bond distance [2.0240 (15) Å] and three longer Zn–Cl bonds distances [in the range 2.2121 (7)–2.2745 (6) Å]. These bond lengths are consistent with the values observed in analogous compounds such as $[H_3N(CH_2)_8NH_3]ZnCl_4$, $[C_6H_5-C_2H_4-NH_3]_2ZnCl_4$, $(Cl_2H_{12}N_2)[ZnCl_4]$ and $(C_{10}H_{22}N_2)[ZnCl_4]$ (El Mrabet *et al.*, 2017), as are the Cl–Zn–Cl [111.45 (3)–116.99 (3)°] and Cl–Zn–O [101.36 (5)–108.19 (5)°] bond angles (Kassou *et al.*, 2016; Campos-Gaxiola *et al.*, 2015; Soudani *et al.*, 2013).

3. Supramolecular features

The packing is consolidated by a network of hydrogen bonds (Table 1, Fig. 2). The cations are linked into inversion dimers by pairs of $N1-H1\cdots O2$ hydrogen bonds, which generate $R_2^2(10)$ rings. The anions also form inversion dimers, being

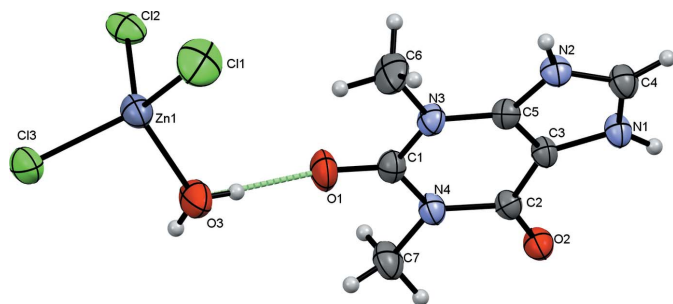


Figure 1
Molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level.

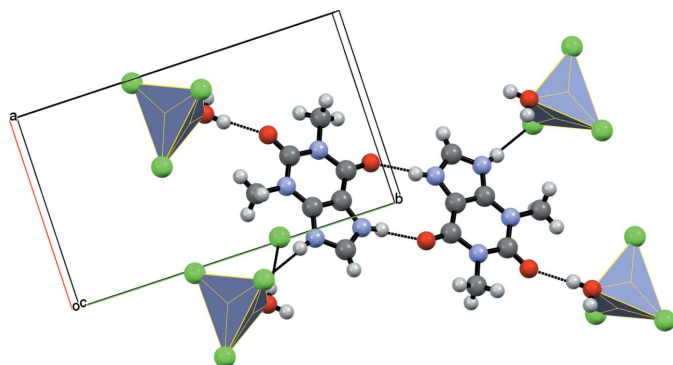


Figure 2
Molecules linked by $O-H\cdots O$ and $O-H\cdots Cl$ strong hydrogen bonds.

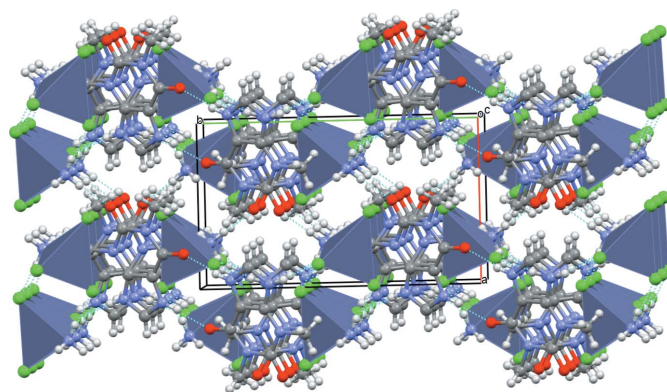


Figure 3
Perspective view of the crystal structure along the c axis showing the layered organization.

linked by pairwise $O3-H3A\cdots Cl3$ hydrogen bonds. The anions are linked to the cations *via* $O3-H3B\cdots O1$ hydrogen bonds from the water molecule to a carbonyl group of the pyrimidine ring. Finally, the cations are linked to the anions *via* $N2-H2\cdots Cl2$ hydrogen bonds. Taken together, these hydrogen bonds generate a three-dimensional supramolecular network (Fig. 3), which also features short $Cl\cdots\pi$ contacts [$Cl\cdots$ centroid distances in the range of 3.533 (2)–3.620 (2) Å].

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.40, May 2019; Groom *et al.*, 2016) for organic-inorganic compounds containing theophyllinium in the cation revealed three similar structures: theophyllinium trichloro-theophyllineplatinum(II), bis(theophyllinium) tetrachloroplatinum(II) (Griffith *et al.*, 1979) and bis(theophyllinium) tetrabromopalladium(II) (Salas *et al.*, 1989). In each of the three complexes, the metal cation is surrounded by four ligands in a planar geometry. The crystal structures of these

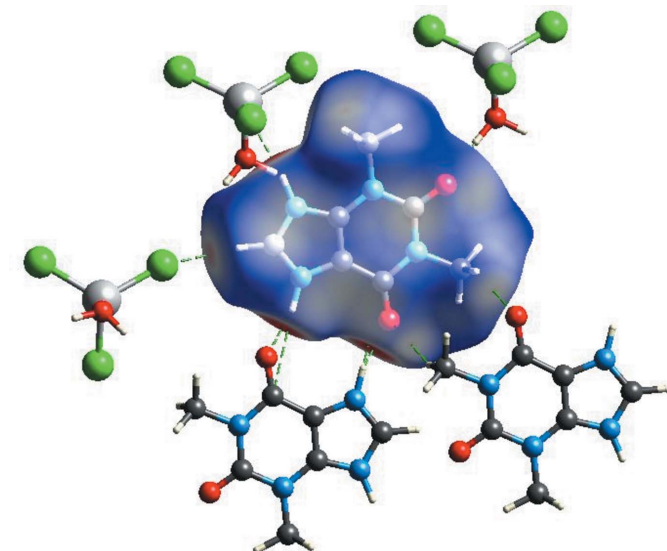


Figure 4
Hirshfeld d_{norm} surface of the $(C_7H_9N_4O_2)^+$ cation in the title compound.

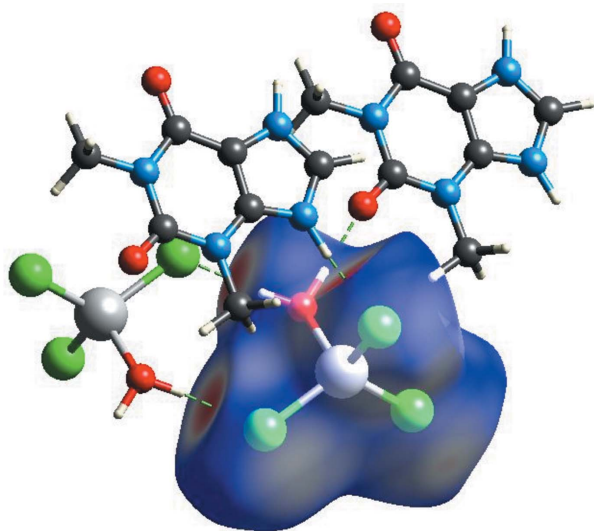


Figure 5
Hirshfeld d_{norm} surface of the $[\text{ZnCl}_3(\text{H}_2\text{O})]^-$ anion in the title compound.

compounds are different from that of the title compound; however, the organic–inorganic moieties are linked through hydrogen bonds in all of these structures.

5. Hirshfeld surface analysis

In order to gain further insight into the intermolecular interactions in the title compound, we used the program *Crystal Explorer* (Spackman & Jayatilaka, 2009), to consider separately the $(\text{C}_7\text{H}_9\text{N}_4\text{O}_2)^+$ organic cation and the $[\text{ZnCl}_3(\text{H}_2\text{O})]^-$ inorganic anion.

The Hirshfeld d_{norm} surface of the cation is depicted in Fig. 4. The most significant interactions are $\text{H}\cdots\text{H}$ (29.6%) contacts and the second largest percentage (25.8%) can be attributed to $\text{H}\cdots\text{O}$ interactions, which are responsible for the appearance of deep-red spots and correlate with the $\text{O}-\text{H}\cdots\text{O}$ and $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds. $\text{H}\cdots\text{Cl}$ (21.9%), $\text{C}\cdots\text{Cl}$ (8.1%), $\text{N}\cdots\text{Cl}$ (5.5%) and $\text{C}\cdots\text{H}$ (3.6%) interactions are also observed, with other contact types making a negligible contribution.

The Hirshfeld surface of the $[\text{ZnCl}_3(\text{H}_2\text{O})]^-$ anion is depicted in Fig. 5 and shows red spots that correspond to the strong $\text{N}-\text{H}\cdots\text{Cl}$ and $\text{O}-\text{H}\cdots\text{Cl}$ hydrogen bonds: $\text{Cl}\cdots\text{H}$ contacts are the most abundant contributor to the surface at 54.7%. Other significant contributions include $\text{Cl}\cdots\text{C}$ (10.3%), $\text{H}\cdots\text{H}$ (9.6%), $\text{Cl}\cdots\text{N}$ (7.3%), $\text{H}\cdots\text{O}$ (5.6%) and $\text{H}\cdots\text{Cl}$ (4.7%). It is notable that the $\text{Cl}\cdots\text{Cl}$ contact percentage is 0%, *i.e.* the chloride anions avoid each other in the crystal.

6. Synthesis and crystallization

$\text{ZnCl}_2\cdot 6\text{H}_2\text{O}$ (0.244 g, 1 mmol) was dissolved in 5 ml of water. Then, theophylline $[\text{C}_7\text{H}_8\text{N}_4\text{O}_2]$ (0.180 g, 1 mmol) was dissolved in 3 ml of ethanol/water (1:1 v:v) with a few drops of conc. HCl (37%). The two solutions were mixed and after two

Table 2
Experimental details.

Crystal data	
Chemical formula	$(\text{C}_7\text{H}_9\text{N}_4\text{O}_2)[\text{ZnCl}_3(\text{H}_2\text{O})]$
M_r	370.92
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	8.0932 (14), 13.744 (3), 12.429 (2)
β (°)	92.290 (6)
V (Å ³)	1381.4 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	2.36
Crystal size (mm)	0.32 × 0.25 × 0.11
Data collection	
Diffractometer	Bruker D8 VENTURE Super DUO
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
$T_{\text{min}}, T_{\text{max}}$	0.587, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	29522, 3046, 2753
R_{int}	0.035
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.025, 0.070, 1.04
No. of reflections	3046
No. of parameters	166
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.42, -0.26

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT2014/5* (Sheldrick, 2015a), *SHELXL2018/3* (Sheldrick 2015b), *Mercury* (Macrae *et al.*, 2020) and *publCIF* (Westrip, 2010).

weeks, colourless crystals of the title molecular salt were obtained.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The H atoms were all located in a difference map, but those attached to C and N atoms were repositioned geometrically ($\text{C}-\text{H} = 0.93\text{--}0.96$, $\text{N}-\text{H} = 0.86$ Å). The water H atoms were located in a difference map and refined as riding atoms in their as-found relative positions. The constraint $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$ or $1.5U_{\text{eq}}(\text{C-methyl})$ was applied in all cases.

Acknowledgements

The authors thank the Faculty of Science, Mohammed V University in Rabat, Morocco for the X-ray data collection.

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supporting information

Acta Cryst. (2020). E76, 506-509 [https://doi.org/10.1107/S2056989020002753]

Crystal structure and Hirshfeld surface analysis of $(\text{C}_7\text{H}_9\text{N}_4\text{O}_2)[\text{ZnCl}_3(\text{H}_2\text{O})]$

Hicham El Hamdani, Mohamed El Amane, Mohamed Saadi and Lahcen El Ammari

Computing details

Data collection: *APEX3* (Bruker, 2016); cell refinement: *SAINT* (Bruker, 2016); data reduction: *SAINT* (Bruker, 2016); program(s) used to solve structure: *SHELXT2014/5* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick 2015b); molecular graphics: *Mercury* (Macrae *et al.*, 2020); software used to prepare material for publication: *publCIF* (Westrip, 2010).

1,3-Dimethyl-2,6-dioxo-2,3,6,7-tetrahydro-1*H*-purin-9-ium aquatrichloridozincate(II)

Crystal data

$(\text{C}_7\text{H}_9\text{N}_4\text{O}_2)[\text{ZnCl}_3(\text{H}_2\text{O})]$

$M_r = 370.92$

Monoclinic, $P2_1/c$

$a = 8.0932$ (14) Å

$b = 13.744$ (3) Å

$c = 12.429$ (2) Å

$\beta = 92.290$ (6)°

$V = 1381.4$ (4) Å³

$Z = 4$

$F(000) = 744$

$D_x = 1.783$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 3046 reflections

$\theta = 2.2$ – 27.1 °

$\mu = 2.36$ mm⁻¹

$T = 296$ K

Plate, colorless

$0.32 \times 0.25 \times 0.11$ mm

Data collection

Bruker D8 VENTURE Super DUO
diffractometer

Radiation source: INCOATEC I μ S micro-focus
source

HELIOS mirror optics monochromator

Detector resolution: 10.4167 pixels mm⁻¹

φ and ω scans

Absorption correction: multi-scan
(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.587$, $T_{\max} = 0.746$

29522 measured reflections

3046 independent reflections

2753 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.035$

$\theta_{\max} = 27.1$ °, $\theta_{\min} = 2.2$ °

$h = -10 \rightarrow 10$

$k = -17 \rightarrow 17$

$l = -15 \rightarrow 15$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.025$

$wR(F^2) = 0.070$

$S = 1.04$

3046 reflections

166 parameters

0 restraints

Primary atom site location: dual

Hydrogen site location: mixed

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0361P)^2 + 0.7104P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.42$ e Å⁻³

$\Delta\rho_{\min} = -0.26$ e Å⁻³

Extinction correction: *SHELXL2018/3*

(Sheldrick 2015b),

$F_c^* = kF_c[1 + 0.001 \times F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0116 (9)

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.3890 (2)	0.73981 (12)	0.43314 (14)	0.0328 (4)
C2	0.23025 (19)	0.88256 (11)	0.49620 (13)	0.0270 (3)
C3	0.09587 (19)	0.84313 (11)	0.43243 (13)	0.0275 (3)
C4	−0.1427 (2)	0.81114 (13)	0.35170 (15)	0.0347 (4)
H4	−0.252141	0.816209	0.326593	0.042*
C5	0.10920 (19)	0.75700 (12)	0.37968 (13)	0.0279 (3)
C6	0.2625 (3)	0.61496 (16)	0.3140 (2)	0.0534 (6)
H6A	0.175032	0.571204	0.331328	0.080*
H6B	0.367334	0.584272	0.329585	0.080*
H6C	0.253138	0.631212	0.238896	0.080*
C7	0.5201 (2)	0.85870 (15)	0.55359 (17)	0.0427 (4)
H7A	0.593033	0.889908	0.505244	0.064*
H7B	0.575456	0.804184	0.587203	0.064*
H7C	0.489054	0.904175	0.607817	0.064*
N1	−0.06417 (17)	0.87524 (10)	0.41341 (12)	0.0314 (3)
H1	−0.105499	0.928117	0.437743	0.038*
N2	−0.04038 (17)	0.73720 (10)	0.33052 (12)	0.0317 (3)
H2	−0.064969	0.686459	0.292687	0.038*
N3	0.25046 (17)	0.70379 (10)	0.37848 (12)	0.0316 (3)
N4	0.37091 (16)	0.82468 (10)	0.49296 (12)	0.0307 (3)
O1	0.52249 (16)	0.69911 (11)	0.42937 (12)	0.0463 (3)
O2	0.22824 (15)	0.95718 (8)	0.54976 (10)	0.0348 (3)
O3	0.7194 (2)	0.54071 (11)	0.46116 (13)	0.0567 (4)
H3A	0.791444	0.560052	0.496924	0.085*
H3B	0.653875	0.586278	0.454444	0.085*
Cl1	0.53785 (8)	0.37606 (5)	0.28558 (6)	0.06943 (19)
Cl2	0.84322 (7)	0.55879 (3)	0.20036 (4)	0.04325 (13)
Cl3	0.98173 (7)	0.36721 (4)	0.39782 (4)	0.05047 (15)
Zn1	0.76669 (3)	0.45595 (2)	0.33282 (2)	0.03798 (10)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0309 (8)	0.0313 (8)	0.0364 (9)	0.0047 (7)	0.0020 (7)	0.0003 (7)
C2	0.0268 (7)	0.0248 (7)	0.0293 (7)	0.0002 (6)	0.0002 (6)	0.0013 (6)
C3	0.0244 (7)	0.0245 (7)	0.0333 (8)	0.0023 (6)	−0.0005 (6)	−0.0009 (6)
C4	0.0276 (8)	0.0346 (9)	0.0414 (9)	−0.0006 (7)	−0.0030 (7)	−0.0028 (7)
C5	0.0289 (8)	0.0250 (7)	0.0299 (8)	−0.0004 (6)	0.0014 (6)	0.0003 (6)
C6	0.0538 (13)	0.0432 (11)	0.0627 (13)	0.0120 (9)	−0.0033 (10)	−0.0252 (10)

C7	0.0269 (8)	0.0451 (10)	0.0551 (12)	0.0004 (7)	-0.0089 (8)	-0.0086 (9)
N1	0.0257 (7)	0.0273 (7)	0.0411 (8)	0.0027 (5)	-0.0018 (6)	-0.0044 (6)
N2	0.0307 (7)	0.0281 (7)	0.0359 (7)	-0.0026 (5)	-0.0021 (6)	-0.0055 (6)
N3	0.0316 (7)	0.0269 (7)	0.0364 (7)	0.0046 (5)	0.0013 (6)	-0.0055 (6)
N4	0.0246 (6)	0.0305 (7)	0.0366 (7)	0.0018 (5)	-0.0027 (5)	-0.0025 (6)
O1	0.0334 (7)	0.0440 (8)	0.0612 (9)	0.0146 (6)	-0.0020 (6)	-0.0063 (6)
O2	0.0335 (6)	0.0302 (6)	0.0401 (7)	0.0031 (5)	-0.0052 (5)	-0.0086 (5)
O3	0.0556 (9)	0.0577 (9)	0.0556 (9)	0.0250 (7)	-0.0129 (7)	-0.0217 (7)
Cl1	0.0508 (3)	0.0742 (4)	0.0829 (4)	-0.0221 (3)	-0.0032 (3)	-0.0209 (3)
Cl2	0.0543 (3)	0.0337 (2)	0.0405 (2)	-0.00102 (19)	-0.0130 (2)	-0.00533 (17)
Cl3	0.0538 (3)	0.0503 (3)	0.0467 (3)	0.0195 (2)	-0.0059 (2)	0.0006 (2)
Zn1	0.03676 (14)	0.03346 (14)	0.04306 (15)	0.00315 (8)	-0.00657 (9)	-0.00676 (8)

Geometric parameters (Å, °)

C1—O1	1.219 (2)	C6—H6B	0.9600
C1—N3	1.379 (2)	C6—H6C	0.9600
C1—N4	1.394 (2)	C7—N4	1.474 (2)
C2—O2	1.223 (2)	C7—H7A	0.9600
C2—N4	1.391 (2)	C7—H7B	0.9600
C2—C3	1.427 (2)	C7—H7C	0.9600
C3—C5	1.360 (2)	N1—H1	0.8600
C3—N1	1.380 (2)	N2—H2	0.8600
C4—N1	1.315 (2)	O3—H3A	0.7665
C4—N2	1.343 (2)	O3—H3B	0.8227
C4—H4	0.9300	Zn1—O3	2.0240 (15)
C5—N3	1.358 (2)	Zn1—Cl1	2.2121 (7)
C5—N2	1.362 (2)	Zn1—Cl2	2.2745 (6)
C6—N3	1.466 (2)	Zn1—Cl3	2.2487 (6)
C6—H6A	0.9600		
O1—C1—N3	121.36 (16)	N4—C7—H7C	109.5
O1—C1—N4	121.10 (16)	H7A—C7—H7C	109.5
N3—C1—N4	117.55 (14)	H7B—C7—H7C	109.5
O2—C2—N4	121.61 (15)	C4—N1—C3	108.30 (14)
O2—C2—C3	126.47 (15)	C4—N1—H1	125.8
N4—C2—C3	111.92 (14)	C3—N1—H1	125.8
C5—C3—N1	106.73 (14)	C4—N2—C5	107.74 (14)
C5—C3—C2	121.68 (15)	C4—N2—H2	126.1
N1—C3—C2	131.54 (15)	C5—N2—H2	126.1
N1—C4—N2	109.50 (15)	C5—N3—C1	117.99 (14)
N1—C4—H4	125.2	C5—N3—C6	121.95 (15)
N2—C4—H4	125.2	C1—N3—C6	119.84 (15)
N3—C5—C3	123.88 (15)	C2—N4—C1	126.70 (14)
N3—C5—N2	128.42 (15)	C2—N4—C7	117.30 (14)
C3—C5—N2	107.71 (14)	C1—N4—C7	115.90 (14)
N3—C6—H6A	109.5	Zn1—O3—H3A	119.6
N3—C6—H6B	109.5	Zn1—O3—H3B	120.0

H6A—C6—H6B	109.5	H3A—O3—H3B	105.5
N3—C6—H6C	109.5	O3—Zn1—Cl3	101.36 (5)
H6A—C6—H6C	109.5	O3—Zn1—Cl2	106.16 (6)
H6B—C6—H6C	109.5	O3—Zn1—Cl1	108.19 (5)
N4—C7—H7A	109.5	Cl1—Zn1—Cl2	111.45 (3)
N4—C7—H7B	109.5	Cl3—Zn1—Cl2	111.58 (2)
H7A—C7—H7B	109.5	Cl1—Zn1—Cl3	116.99 (3)
O2—C2—C3—C5	-176.95 (16)	N2—C5—N3—C1	178.75 (17)
N4—C2—C3—C5	2.2 (2)	C3—C5—N3—C6	-175.40 (18)
O2—C2—C3—N1	0.2 (3)	N2—C5—N3—C6	4.0 (3)
N4—C2—C3—N1	179.38 (17)	O1—C1—N3—C5	-175.01 (17)
N1—C3—C5—N3	179.06 (15)	N4—C1—N3—C5	5.0 (2)
C2—C3—C5—N3	-3.2 (3)	O1—C1—N3—C6	-0.2 (3)
N1—C3—C5—N2	-0.48 (18)	N4—C1—N3—C6	179.78 (18)
C2—C3—C5—N2	177.31 (15)	O2—C2—N4—C1	-178.35 (16)
N2—C4—N1—C3	0.8 (2)	C3—C2—N4—C1	2.4 (2)
C5—C3—N1—C4	-0.18 (19)	O2—C2—N4—C7	-2.2 (2)
C2—C3—N1—C4	-177.67 (18)	C3—C2—N4—C7	178.56 (15)
N1—C4—N2—C5	-1.1 (2)	O1—C1—N4—C2	173.82 (17)
N3—C5—N2—C4	-178.56 (16)	N3—C1—N4—C2	-6.1 (3)
C3—C5—N2—C4	0.95 (19)	O1—C1—N4—C7	-2.3 (3)
C3—C5—N3—C1	-0.7 (2)	N3—C1—N4—C7	177.68 (16)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N1—H1...O2 ⁱ	0.86	1.87	2.7067 (18)	163
N2—H2...Cl2 ⁱⁱ	0.86	2.21	3.0652 (15)	174
C6—H6C...O2 ⁱⁱⁱ	0.96	2.65	3.431 (3)	139
O3—H3A...Cl3 ^{iv}	0.77	2.43	3.1915 (17)	176
O3—H3B...O1	0.82	1.90	2.718 (2)	173

Symmetry codes: (i) $-x, -y+2, -z+1$; (ii) $x-1, y, z$; (iii) $x, -y+3/2, z-1/2$; (iv) $-x+2, -y+1, -z+1$.