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# Poly[[$\mu$-chlorido-$\mu$-[2-(2,4-difluorophenyl)-1,3-bis(1,2,4-triazol-1-yl)propan-2-ol-$\kappa^2N^4:N^{4'}$]-zinc] chloride dihydrate]

**Gang-Hong Pan, Jin-Niu Tang, Shi-Hua Xu, Zhong-Jing Huang* and Bo-Fa Mo**

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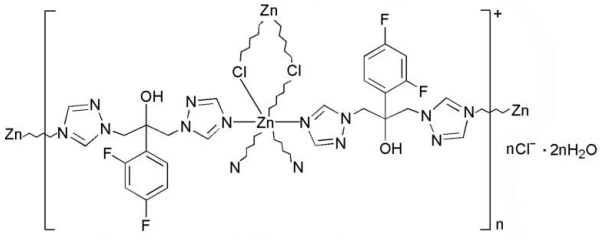
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.015 Å; $R$ factor = 0.080; $wR$ factor = 0.306; data-to-parameter ratio = 12.3.

The title compound, $\{[ZnCl(C_{13}H_{12}F_2N_6O)_2]Cl\cdot 2H_2O\}_n$, is a two-dimensional coordination polymer. The $Zn^{II}$ atom is six-coordinated by four N atoms from four 2-(2,4-difluorophenyl)-1,3-bis(1,2,4-triazol-1-yl)propan-2-ol (HFlu) ligands and by two Cl atoms in a distorted octahedral geometry. Two Cl atoms bridge two $Zn^{II}$ atoms, forming a centrosymmetric dinuclear unit. The HFlu ligands connect the dinuclear units into a $4^4$ net parallel to (001) when the dinuclear unit is considered as a node. O—H···O and O—H···Cl hydrogen bonds link the cationic layer, free chloride anions and lattice water molecules. Intralayer $\pi$–$\pi$ interactions between the triazole rings are observed [centroid–centroid distance = 3.716 (6) Å].

## Related literature

For background to this class of compounds, see: Han *et al.* (2006*a*,*b*). For related structures, see: Gao *et al.* (2001); Zhang *et al.* (2007).




## Experimental

### Crystal data

$[ZnCl(C_{13}H_{12}F_2N_6O)_2]Cl\cdot 2H_2O$ $M_r$ = 784.89
Triclinic, $P\overline{1}$
$a$ = 10.2310 (6) Å
$b$ = 11.8118 (6) Å
$c$ = 14.3588 (9) Å
$\alpha$ = 91.191 (7)°
$\beta$ = 107.481 (5)°
$\gamma$ = 106.074 (6)°
$V$ = 1580.11 (18) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 1.03 mm$^{-1}$
$T$ = 296 K
0.25 × 0.25 × 0.21 mm

### Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min}$ = 0.784, $T_{max}$ = 0.813
8374 measured reflections
5465 independent reflections
3137 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.064

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.080
$wR(F^2)$ = 0.306
$S$ = 1.07
5465 reflections
444 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.92 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.09 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···Cl2$^{i}$ | 0.82 | 2.29 | 3.103 (7) | 172 |
| O2—H2···O4$^{i}$ | 0.82 | 1.87 | 2.653 (9) | 160 |
| O3—H3*A*···Cl2$^{ii}$ | 0.85 | 2.32 | 3.163 (11) | 170 |
| O3—H3*B*···Cl1$^{iii}$ | 0.85 | 2.38 | 3.221 (10) | 170 |
| O4—H4*A*···O2$^{iv}$ | 0.85 | 2.24 | 2.784 (9) | 122 |
| O4—H4*B*···Cl2 | 0.85 | 2.29 | 3.101 (8) | 160 |

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

This work was supported by the Innovation Project of Guangxi University for Nationalities.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2637).

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# supporting information

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# Poly[[$\mu$-chlorido-$\mu$-[2-(2,4-difluorophenyl)-1,3-bis(1,2,4-triazol-1-yl)propan-2-ol-$\kappa^2N^4:N^{4'}$]-zinc] chloride dihydrate]

**Gang-Hong Pan, Jin-Niu Tang, Shi-Hua Xu, Zhong-Jing Huang and Bo-Fa Mo**

## S1. Comment

Fluconazole 2-(2,4-difluorophenyl)-1,3-bis(1,2,4-triazol-1-yl) propan-2-ol, which is a 1,2,4-triazole derivative, is not only a widely used antifungal medicine but also a good flexible ligand to construct metal-organic polymers with optical properties and medical applications (Han *et al.*, 2006*a*,*b*). Fluconazole can coordinate to metal ions in different configurations. We here report a new coordination polymer based on fluconazole.

The asymmetric unit of the title compound contains one $Zn^{II}$ ion, two 2-(2,4-difluorophenyl)-1,3-bis(1,2,4-triazol-1-yl)propan-2-ol (HFlu) ligands, one coordinated $Cl^{-1}$ anion, one free $Cl^{-1}$ anion and two free water molecules. As shown in Fig. 1, the $Zn^{II}$ ion is six-coordinated by four N atoms from four HFlu ligands and two bridging $Cl^{-1}$ anions. The Zn—N bond lengths range from 2.127 (8) to 2.197 (7) Å, and the Zn—Cl bond distances are 2.418 (3) and 2.732 (3) Å. The Zn—N bond lengths are in the normal range as observed in other Zn(II) complexes (Zhang *et al.*, 2007). However, the Zn—Cl bond distances are longer than those as observed in other Zn(II) complexe (Gao *et al.*, 2001). Two $Zn^{II}$ ions are connected by two HFlu ligands, forming a $Zn_2(HFlu)_2$ macrocycle, in which the Zn···Zn distance is 11.297 (2)Å. The other two HFlu ligands link the macrocycle along the *a* axis with a Zn···Zn distance of 10.231 (2) Å to form a grid unit with dimensions of 11.30 × 10.23 $Å^2$ (Fig. 2a). These grid units are further connected by two $Cl^{-1}$ anions with a Zn···Zn distance of 3.879 (1) Å into a two-dimensional structure (Fig. 2b), in which another type of grid with dimensions of 10.231 (2) × 3.879 (1) $Å^2$ is formed.

Free water molecules and free $Cl^{-1}$ anions are accommodated in the residual empties to shrink the void space and stabilize the structure. Moreover, there are intermolecular O—H···O and O—H···Cl hydrogen bonds involving the cationic layer, free $Cl^{-1}$ anions and water molecules (Table 1, Fig. 3). These interactions further stabilize the structural framework.

## S2. Experimental

A mixture of fluconazole (153 mg, 0.5 mmol), $ZnCl_2$ (136 mg, 1.0 mmol), 15 ml $H_2O$, and 3 ml ethanol was placed in a Parr Teflon-lined stainless steel vessel (30 ml), and then the vessel was sealed and heated at 423 K for 3 days. After the mixture was slowly cooled to room temperature, colorless block-shaped crystals of the title compound was obtained. Analysis, calculated for $C_{26}H_{28}Cl_2F_4N_{12}O_4Zn$: C 39.79, H 3.60, N 21.42%; found: C 39.66, H 3.52, N 21.28%.

## S3. Refinement

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 (aromatic), 0.97(methylene) and O—H = 0.82 Å and with $U_{iso}$(H) = 1.2(1.5 for hydroxyl)$U_{eq}$(C,O). H atoms of the water molecules were located in a difference Fourier map and refined as riding, with O—H = 0.85 Å and $U_{iso}$(H) = 1.2$U_{eq}$(O). The maximum remaining electron density was found 1.00 Å from Zn1 and the minimum density 0.83 Å from Zn1.

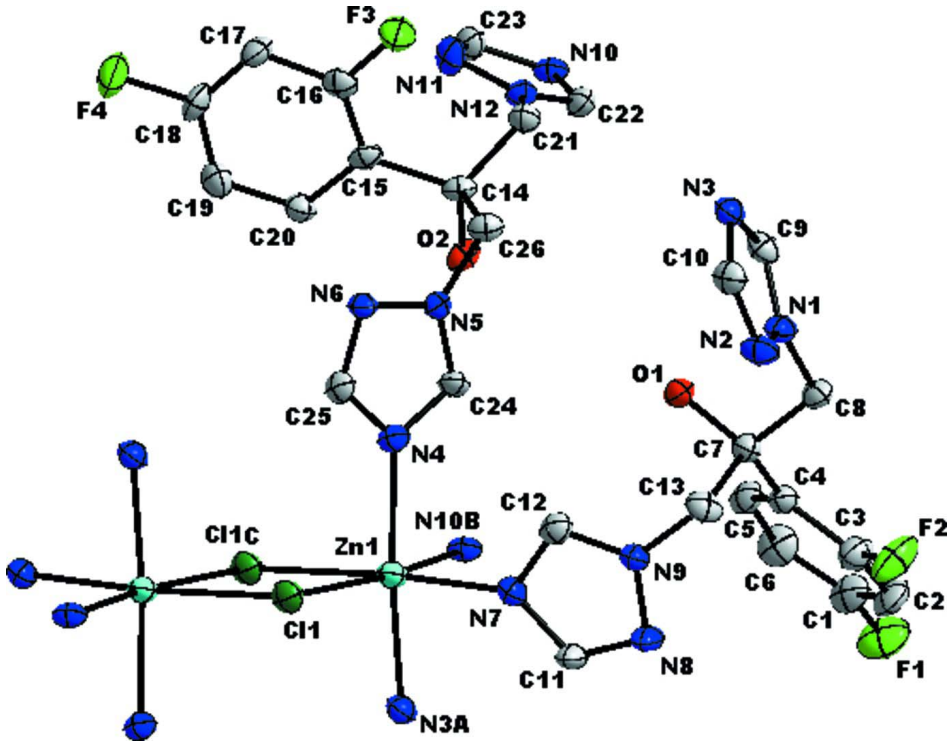


**Figure 1**

The coordination environment around the $Zn^{II}$ atom in the title compound (uncoordinated Cl atom, water molecules and H atoms have been omitted for clarity). Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (A) 1+x, y, z; (B) 2-x, -y, 1-z; (C) 3-x, 1-y, 1-z.]

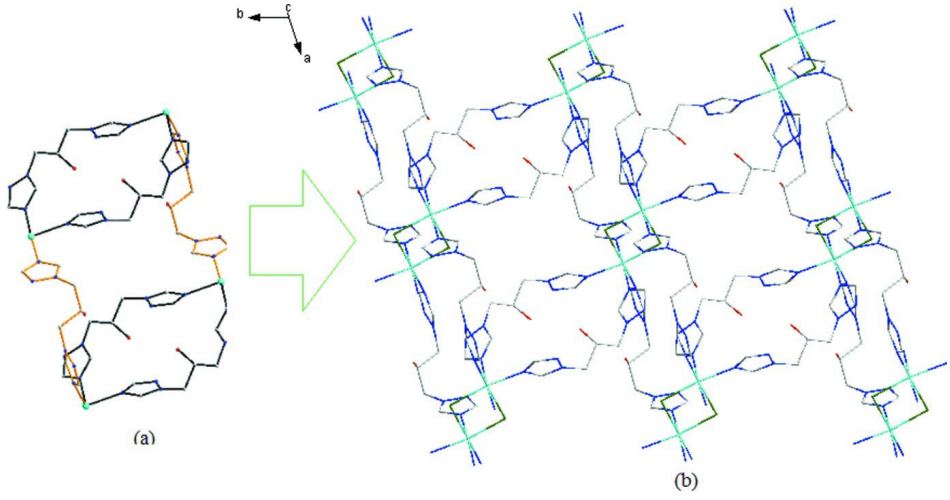


**Figure 2**

(a) A view of the grid unit in the title compound. (b) A view of the two-dimensional framework. H atoms and difluorophenyl groups of HFlu are omitted for clarity.

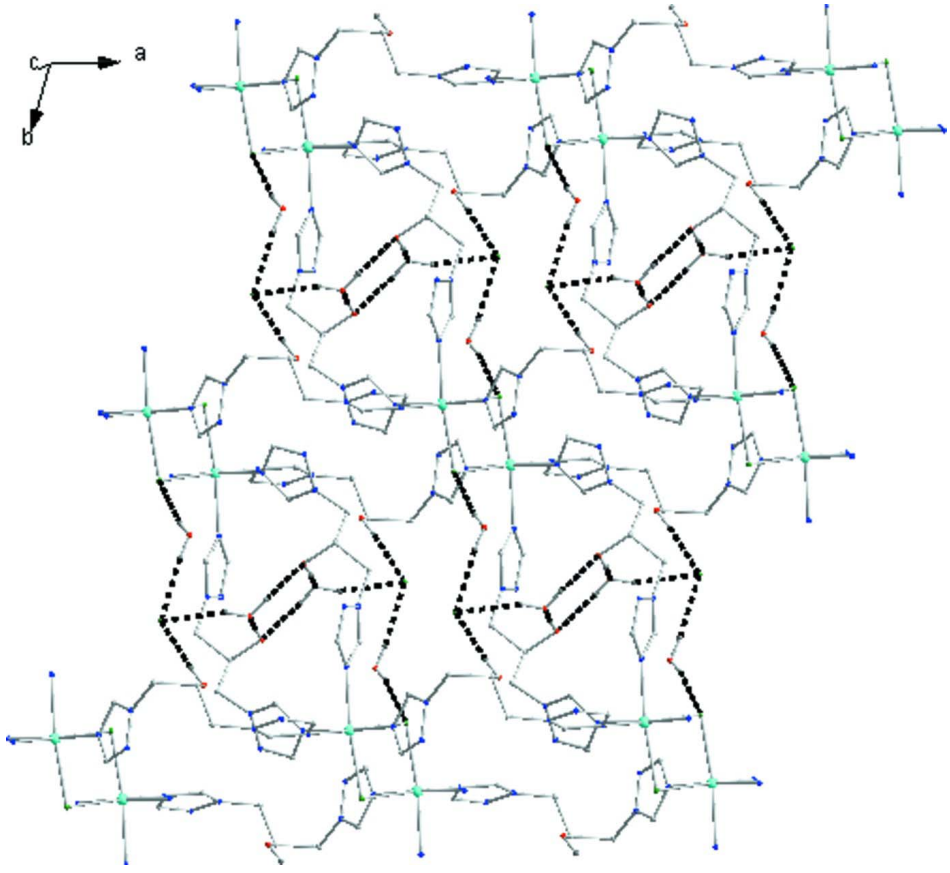


**Figure 3**

A view of hydrogen bonding interactions (dashed lines) in the title compound. H atoms and difluorophenyl groups of HFlu are omitted for clarity.

**Poly[[$\mu$-chlorido-$\mu$-[2-(2,4-difluorophenyl)-1,3-bis(1,2,4-triazol-1-yl)propan-2-ol-$\kappa^2N^4:N^{4'}$]-zinc] chloride dihydrate]**

*Crystal data*

$[ZnCl(C_{13}H_{12}F_2N_6O)_2]Cl\cdot 2H_2O$
$M_r = 784.89$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 10.2310\ (6)$ Å
$b = 11.8118\ (6)$ Å
$c = 14.3588\ (9)$ Å
$\alpha = 91.191\ (7)°$
$\beta = 107.481\ (5)°$
$\gamma = 106.074\ (6)°$
$V = 1580.11\ (18)$ Å$^3$
$Z = 2$
$F(000) = 800$
$D_x = 1.650$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 859 reflections
$\theta = 2.2–22.1°$
$\mu = 1.03$ mm$^{-1}$
$T = 296$ K
Block, colorless
0.25 × 0.25 × 0.21 mm

*Data collection*

Bruker SMART 1000 CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.784$, $T_{max} = 0.813$

8374 measured reflections
5465 independent reflections
3137 reflections with $I > 2\sigma(I)$
$R_{int} = 0.064$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.5°$
$h = -12 \rightarrow 12$
$k = -14 \rightarrow 12$
$l = -14 \rightarrow 17$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.080$
$wR(F^2) = 0.306$
$S = 1.07$
5465 reflections
444 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
$w = 1/[\sigma^2(F_o^2) + (0.1513P)^2 + 4.0805P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.92$ e Å$^{-3}$
$\Delta\rho_{min} = -1.09$ 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.

**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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Zn1 | 1.32995 (12) | 0.41377 (10) | 0.39336 (8) | 0.0404 (4) |
| Cl1 | 1.4508 (3) | 0.6199 (2) | 0.45651 (17) | 0.0448 (6) |
| Cl2 | 0.4395 (3) | 0.9322 (2) | 0.6822 (2) | 0.0584 (8) |
| F1 | 0.7971 (10) | −0.0762 (7) | −0.0678 (5) | 0.086 (2) |
| F2 | 0.6122 (9) | 0.2436 (7) | −0.0664 (4) | 0.083 (2) |
| F3 | 0.8098 (7) | 0.2576 (6) | 0.7540 (4) | 0.0657 (18) |
| F4 | 1.2544 (8) | 0.3386 (7) | 0.9953 (4) | 0.079 (2) |
| N1 | 0.5148 (8) | 0.3554 (8) | 0.1793 (5) | 0.043 (2) |
| N2 | 0.5348 (9) | 0.4724 (7) | 0.1718 (6) | 0.048 (2) |
| N3 | 0.4536 (8) | 0.4152 (7) | 0.2976 (5) | 0.041 (2) |
| N4 | 1.1903 (9) | 0.4025 (7) | 0.4804 (5) | 0.041 (2) |
| N5 | 1.0061 (8) | 0.3403 (6) | 0.5307 (5) | 0.0335 (18) |
| N6 | 1.0891 (8) | 0.4430 (6) | 0.5911 (5) | 0.0345 (18) |
| N7 | 1.1616 (8) | 0.4340 (7) | 0.2632 (5) | 0.041 (2) |
| N8 | 1.0182 (9) | 0.4016 (9) | 0.1051 (6) | 0.054 (2) |
| N9 | 0.9478 (8) | 0.4220 (7) | 0.1671 (5) | 0.0388 (19) |
| N10 | 0.7509 (8) | −0.2201 (7) | 0.6379 (5) | 0.0393 (19) |
| N11 | 0.8367 (9) | −0.0419 (7) | 0.7239 (6) | 0.048 (2) |
| N12 | 0.7677 (8) | −0.0339 (7) | 0.6293 (5) | 0.0381 (19) |
| O1 | 0.7534 (7) | 0.2765 (6) | 0.2468 (4) | 0.0446 (17) |
| H1 | 0.6956 | 0.2212 | 0.2602 | 0.067* |

| | | | | |
|---|---|---|---|---|
| O2 | 0.9802 (7) | 0.1089 (6) | 0.5651 (4) | 0.0417 (16) |
| H2 | 0.9323 | 0.0797 | 0.5087 | 0.063* |
| O3 | 0.5759 (12) | 0.8041 (10) | 0.3197 (8) | 0.106 (4) |
| H3A | 0.5660 | 0.8728 | 0.3247 | 0.127* |
| H3B | 0.5394 | 0.7628 | 0.3585 | 0.127* |
| O4 | 0.1267 (8) | 0.9438 (6) | 0.6285 (5) | 0.055 (2) |
| H4A | 0.0960 | 0.9921 | 0.6543 | 0.065* |
| H4B | 0.2165 | 0.9582 | 0.6394 | 0.065* |
| C1 | 0.7769 (15) | 0.0150 (10) | −0.0176 (9) | 0.061 (3) |
| C2 | 0.7008 (14) | 0.0812 (11) | −0.0685 (8) | 0.061 (3) |
| H2A | 0.6611 | 0.0669 | −0.1366 | 0.073* |
| C3 | 0.6831 (12) | 0.1716 (11) | −0.0163 (8) | 0.055 (3) |
| C4 | 0.7305 (10) | 0.1914 (8) | 0.0866 (6) | 0.037 (2) |
| C5 | 0.8047 (12) | 0.1152 (9) | 0.1326 (7) | 0.048 (3) |
| H5 | 0.8379 | 0.1228 | 0.2009 | 0.058* |
| C6 | 0.8309 (14) | 0.0295 (9) | 0.0817 (8) | 0.059 (3) |
| H6 | 0.8848 | −0.0178 | 0.1146 | 0.071* |
| C7 | 0.7064 (10) | 0.2849 (8) | 0.1446 (6) | 0.038 (2) |
| C8 | 0.5481 (11) | 0.2778 (9) | 0.1112 (7) | 0.044 (2) |
| H8A | 0.5219 | 0.3018 | 0.0456 | 0.053* |
| H8B | 0.4911 | 0.1963 | 0.1083 | 0.053* |
| C9 | 0.4661 (10) | 0.3227 (9) | 0.2527 (7) | 0.043 (2) |
| H9 | 0.4441 | 0.2460 | 0.2701 | 0.051* |
| C10 | 0.4963 (11) | 0.5041 (9) | 0.2440 (7) | 0.045 (2) |
| H10 | 0.4978 | 0.5816 | 0.2584 | 0.054* |
| C11 | 1.1463 (11) | 0.4096 (10) | 0.1657 (7) | 0.050 (3) |
| H11 | 1.2202 | 0.3997 | 0.1446 | 0.060* |
| C12 | 1.0311 (11) | 0.4394 (8) | 0.2601 (7) | 0.042 (2) |
| H12 | 1.0035 | 0.4532 | 0.3144 | 0.051* |
| C13 | 0.7955 (10) | 0.4106 (9) | 0.1330 (7) | 0.045 (3) |
| H13A | 0.7669 | 0.4244 | 0.0644 | 0.054* |
| H13B | 0.7766 | 0.4699 | 0.1706 | 0.054* |
| C14 | 0.9018 (10) | 0.1666 (8) | 0.6051 (6) | 0.035 (2) |
| C15 | 0.9956 (10) | 0.2149 (8) | 0.7112 (6) | 0.036 (2) |
| C16 | 0.9466 (11) | 0.2552 (8) | 0.7784 (7) | 0.043 (2) |
| C17 | 1.0282 (12) | 0.2959 (9) | 0.8753 (6) | 0.047 (3) |
| H17 | 0.9900 | 0.3211 | 0.9202 | 0.056* |
| C18 | 1.1686 (12) | 0.2967 (10) | 0.9008 (6) | 0.050 (3) |
| C19 | 1.2280 (12) | 0.2644 (9) | 0.8356 (7) | 0.052 (3) |
| H19 | 1.3248 | 0.2691 | 0.8550 | 0.062* |
| C20 | 1.1427 (10) | 0.2248 (8) | 0.7411 (7) | 0.040 (2) |
| H20 | 1.1826 | 0.2039 | 0.6955 | 0.048* |
| C21 | 0.7561 (10) | 0.0805 (8) | 0.5970 (7) | 0.043 (2) |
| H21A | 0.7120 | 0.1149 | 0.6367 | 0.052* |
| H21B | 0.6944 | 0.0683 | 0.5292 | 0.052* |
| C22 | 0.7170 (11) | −0.1387 (9) | 0.5789 (7) | 0.045 (3) |
| H22 | 0.6653 | −0.1546 | 0.5122 | 0.054* |
| C23 | 0.8252 (11) | −0.1510 (9) | 0.7257 (7) | 0.046 (3) |

| | | | | |
|---|---|---|---|---|
| H23 | 0.8644 | −0.1822 | 0.7827 | 0.056* |
| C24 | 1.0684 (10) | 0.3188 (8) | 0.4666 (6) | 0.038 (2) |
| H24 | 1.0314 | 0.2539 | 0.4187 | 0.046* |
| C25 | 1.1980 (11) | 0.4760 (8) | 0.5568 (6) | 0.038 (2) |
| H25 | 1.2742 | 0.5445 | 0.5829 | 0.045* |
| C26 | 0.8744 (10) | 0.2674 (8) | 0.5427 (7) | 0.038 (2) |
| H26A | 0.8054 | 0.2338 | 0.4787 | 0.046* |
| H26B | 0.8341 | 0.3160 | 0.5745 | 0.046* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Zn1 | 0.0408 (7) | 0.0385 (7) | 0.0419 (7) | 0.0027 (5) | 0.0216 (5) | −0.0007 (5) |
| Cl1 | 0.0473 (14) | 0.0335 (13) | 0.0487 (13) | 0.0027 (11) | 0.0168 (11) | 0.0009 (10) |
| Cl2 | 0.0528 (16) | 0.0554 (17) | 0.0658 (17) | 0.0127 (14) | 0.0199 (13) | 0.0137 (13) |
| F1 | 0.126 (7) | 0.067 (5) | 0.085 (5) | 0.039 (5) | 0.054 (5) | −0.006 (4) |
| F2 | 0.127 (7) | 0.099 (6) | 0.043 (4) | 0.071 (5) | 0.020 (4) | 0.013 (3) |
| F3 | 0.048 (4) | 0.095 (5) | 0.059 (4) | 0.027 (4) | 0.019 (3) | −0.005 (3) |
| F4 | 0.073 (5) | 0.105 (6) | 0.040 (3) | 0.023 (4) | −0.002 (3) | −0.014 (3) |
| N1 | 0.037 (4) | 0.057 (6) | 0.040 (4) | 0.018 (4) | 0.017 (3) | 0.006 (4) |
| N2 | 0.052 (5) | 0.038 (5) | 0.060 (5) | 0.008 (4) | 0.030 (4) | 0.008 (4) |
| N3 | 0.031 (4) | 0.048 (5) | 0.045 (4) | 0.010 (4) | 0.014 (3) | 0.009 (4) |
| N4 | 0.044 (5) | 0.045 (5) | 0.037 (4) | 0.012 (4) | 0.019 (3) | 0.009 (4) |
| N5 | 0.035 (4) | 0.034 (4) | 0.031 (4) | 0.007 (3) | 0.012 (3) | 0.002 (3) |
| N6 | 0.035 (4) | 0.037 (4) | 0.036 (4) | 0.009 (4) | 0.019 (3) | 0.003 (3) |
| N7 | 0.033 (4) | 0.053 (5) | 0.039 (4) | 0.012 (4) | 0.013 (3) | 0.005 (4) |
| N8 | 0.039 (5) | 0.091 (7) | 0.038 (4) | 0.022 (5) | 0.021 (4) | 0.004 (4) |
| N9 | 0.031 (4) | 0.051 (5) | 0.037 (4) | 0.010 (4) | 0.015 (3) | 0.007 (4) |
| N10 | 0.042 (5) | 0.039 (5) | 0.042 (4) | 0.009 (4) | 0.023 (4) | 0.011 (4) |
| N11 | 0.058 (5) | 0.025 (4) | 0.045 (4) | −0.005 (4) | 0.008 (4) | −0.001 (3) |
| N12 | 0.043 (5) | 0.036 (5) | 0.033 (4) | 0.005 (4) | 0.014 (3) | 0.009 (3) |
| O1 | 0.048 (4) | 0.046 (4) | 0.036 (3) | 0.002 (3) | 0.018 (3) | −0.002 (3) |
| O2 | 0.054 (4) | 0.043 (4) | 0.034 (3) | 0.023 (3) | 0.015 (3) | 0.005 (3) |
| O3 | 0.112 (9) | 0.096 (8) | 0.138 (9) | 0.039 (7) | 0.071 (7) | 0.047 (7) |
| O4 | 0.060 (5) | 0.052 (5) | 0.051 (4) | 0.025 (4) | 0.010 (3) | −0.002 (3) |
| C1 | 0.083 (9) | 0.036 (6) | 0.061 (7) | 0.006 (6) | 0.031 (6) | −0.010 (5) |
| C2 | 0.080 (9) | 0.064 (8) | 0.036 (6) | 0.018 (7) | 0.020 (5) | −0.011 (5) |
| C3 | 0.057 (7) | 0.067 (8) | 0.045 (6) | 0.023 (6) | 0.017 (5) | 0.011 (5) |
| C4 | 0.038 (5) | 0.040 (5) | 0.035 (5) | 0.011 (4) | 0.015 (4) | 0.007 (4) |
| C5 | 0.061 (7) | 0.040 (6) | 0.040 (5) | 0.007 (5) | 0.020 (5) | −0.005 (4) |
| C6 | 0.076 (8) | 0.035 (6) | 0.067 (7) | 0.019 (6) | 0.024 (6) | 0.002 (5) |
| C7 | 0.035 (5) | 0.039 (5) | 0.038 (5) | 0.009 (4) | 0.013 (4) | 0.002 (4) |
| C8 | 0.046 (6) | 0.047 (6) | 0.039 (5) | 0.007 (5) | 0.020 (4) | −0.009 (4) |
| C9 | 0.035 (5) | 0.043 (6) | 0.053 (6) | 0.014 (5) | 0.014 (4) | 0.005 (5) |
| C10 | 0.050 (6) | 0.031 (5) | 0.053 (6) | 0.007 (5) | 0.020 (5) | −0.002 (4) |
| C11 | 0.037 (6) | 0.083 (8) | 0.036 (5) | 0.020 (6) | 0.020 (4) | 0.010 (5) |
| C12 | 0.051 (6) | 0.036 (5) | 0.040 (5) | 0.009 (5) | 0.017 (4) | 0.001 (4) |
| C13 | 0.041 (6) | 0.049 (6) | 0.056 (6) | 0.023 (5) | 0.020 (5) | 0.015 (5) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C14 | 0.042 (5) | 0.036 (5) | 0.037 (5) | 0.015 (4) | 0.023 (4) | 0.008 (4) |
| C15 | 0.048 (6) | 0.031 (5) | 0.034 (5) | 0.010 (4) | 0.021 (4) | 0.011 (4) |
| C16 | 0.047 (6) | 0.032 (5) | 0.050 (6) | 0.006 (5) | 0.022 (5) | 0.008 (4) |
| C17 | 0.057 (7) | 0.057 (7) | 0.030 (5) | 0.019 (5) | 0.018 (4) | 0.001 (4) |
| C18 | 0.063 (7) | 0.058 (7) | 0.023 (5) | 0.019 (6) | 0.005 (5) | 0.006 (4) |
| C19 | 0.044 (6) | 0.049 (6) | 0.051 (6) | 0.003 (5) | 0.009 (5) | −0.001 (5) |
| C20 | 0.035 (5) | 0.044 (6) | 0.044 (5) | 0.011 (5) | 0.018 (4) | 0.004 (4) |
| C21 | 0.039 (5) | 0.047 (6) | 0.040 (5) | 0.006 (5) | 0.014 (4) | 0.010 (4) |
| C22 | 0.048 (6) | 0.046 (6) | 0.034 (5) | 0.001 (5) | 0.016 (4) | −0.004 (4) |
| C23 | 0.053 (6) | 0.038 (6) | 0.040 (5) | 0.001 (5) | 0.014 (5) | 0.001 (4) |
| C24 | 0.041 (5) | 0.037 (5) | 0.037 (5) | 0.002 (4) | 0.021 (4) | 0.006 (4) |
| C25 | 0.046 (6) | 0.025 (5) | 0.039 (5) | 0.005 (4) | 0.015 (4) | −0.002 (4) |
| C26 | 0.045 (6) | 0.035 (5) | 0.042 (5) | 0.016 (5) | 0.020 (4) | 0.010 (4) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Zn1—N3$^{i}$ | 2.127 (8) | O4—H4B | 0.8500 |
| Zn1—N4 | 2.144 (8) | C1—C2 | 1.331 (16) |
| Zn1—N10$^{ii}$ | 2.192 (8) | C1—C6 | 1.353 (15) |
| Zn1—N7 | 2.197 (7) | C2—C3 | 1.374 (15) |
| Zn1—Cl1 | 2.418 (3) | C2—H2A | 0.9300 |
| Zn1—Cl1$^{iii}$ | 2.732 (3) | C3—C4 | 1.402 (13) |
| F1—C1 | 1.380 (13) | C4—C5 | 1.387 (13) |
| F2—C3 | 1.349 (12) | C4—C7 | 1.487 (13) |
| F3—C16 | 1.345 (12) | C5—C6 | 1.367 (15) |
| F4—C18 | 1.368 (11) | C5—H5 | 0.9300 |
| N1—C9 | 1.317 (12) | C6—H6 | 0.9300 |
| N1—N2 | 1.351 (11) | C7—C8 | 1.521 (13) |
| N1—C8 | 1.500 (12) | C7—C13 | 1.554 (13) |
| N2—C10 | 1.297 (13) | C8—H8A | 0.9700 |
| N3—C9 | 1.312 (13) | C8—H8B | 0.9700 |
| N3—C10 | 1.366 (12) | C9—H9 | 0.9300 |
| N4—C24 | 1.317 (12) | C10—H10 | 0.9300 |
| N4—C25 | 1.354 (12) | C11—H11 | 0.9300 |
| N5—C24 | 1.323 (12) | C12—H12 | 0.9300 |
| N5—N6 | 1.375 (10) | C13—H13A | 0.9700 |
| N5—C26 | 1.446 (12) | C13—H13B | 0.9700 |
| N6—C25 | 1.317 (12) | C14—C21 | 1.524 (13) |
| N7—C12 | 1.342 (13) | C14—C15 | 1.533 (12) |
| N7—C11 | 1.376 (12) | C14—C26 | 1.542 (11) |
| N8—C11 | 1.314 (12) | C15—C16 | 1.346 (14) |
| N8—N9 | 1.356 (11) | C15—C20 | 1.406 (13) |
| N9—C12 | 1.327 (11) | C16—C17 | 1.384 (13) |
| N9—C13 | 1.452 (12) | C17—C18 | 1.369 (15) |
| N10—C22 | 1.343 (12) | C17—H17 | 0.9300 |
| N10—C23 | 1.367 (12) | C18—C19 | 1.359 (16) |
| N11—C23 | 1.262 (12) | C19—C20 | 1.363 (13) |
| N11—N12 | 1.350 (10) | C19—H19 | 0.9300 |

| | | | |
|---|---|---|---|
| N12—C22 | 1.306 (12) | C20—H20 | 0.9300 |
| N12—C21 | 1.462 (11) | C21—H21A | 0.9700 |
| O1—C7 | 1.415 (10) | C21—H21B | 0.9700 |
| O1—H1 | 0.8200 | C22—H22 | 0.9300 |
| O2—C14 | 1.415 (11) | C23—H23 | 0.9300 |
| O2—H2 | 0.8200 | C24—H24 | 0.9300 |
| O3—H3A | 0.8499 | C25—H25 | 0.9300 |
| O3—H3B | 0.8500 | C26—H26A | 0.9700 |
| O4—H4A | 0.8500 | C26—H26B | 0.9700 |

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|---|---|---|---|
| N3$^{i}$—Zn1—N4 | 175.2 (3) | N1—C8—C7 | 111.8 (8) |
| N3$^{i}$—Zn1—N10$^{ii}$ | 88.7 (3) | N1—C8—H8A | 109.3 |
| N4—Zn1—N10$^{ii}$ | 88.0 (3) | C7—C8—H8A | 109.3 |
| N3$^{i}$—Zn1—N7 | 86.0 (3) | N1—C8—H8B | 109.3 |
| N4—Zn1—N7 | 90.5 (3) | C7—C8—H8B | 109.3 |
| N10$^{ii}$—Zn1—N7 | 91.2 (3) | H8A—C8—H8B | 107.9 |
| N3$^{i}$—Zn1—Cl1 | 93.0 (2) | N3—C9—N1 | 109.5 (9) |
| N4—Zn1—Cl1 | 90.9 (2) | N3—C9—H9 | 125.3 |
| N10$^{ii}$—Zn1—Cl1 | 168.89 (19) | N1—C9—H9 | 125.3 |
| N7—Zn1—Cl1 | 99.8 (2) | N2—C10—N3 | 115.1 (9) |
| N3$^{i}$—Zn1—Cl1$^{iii}$ | 89.1 (2) | N2—C10—H10 | 122.5 |
| N4—Zn1—Cl1$^{iii}$ | 94.2 (2) | N3—C10—H10 | 122.5 |
| N10$^{ii}$—Zn1—Cl1$^{iii}$ | 86.6 (2) | N8—C11—N7 | 114.2 (10) |
| N7—Zn1—Cl1$^{iii}$ | 174.7 (2) | N8—C11—H11 | 122.9 |
| Cl1—Zn1—Cl1$^{iii}$ | 82.44 (8) | N7—C11—H11 | 122.9 |
| Zn1—Cl1—Zn1$^{iii}$ | 97.56 (8) | N9—C12—N7 | 108.9 (9) |
| C9—N1—N2 | 111.4 (9) | N9—C12—H12 | 125.6 |
| C9—N1—C8 | 126.6 (9) | N7—C12—H12 | 125.6 |
| N2—N1—C8 | 122.0 (8) | N9—C13—C7 | 110.6 (7) |
| C10—N2—N1 | 101.5 (8) | N9—C13—H13A | 109.5 |
| C9—N3—C10 | 102.6 (8) | C7—C13—H13A | 109.5 |
| C9—N3—Zn1$^{iv}$ | 127.0 (7) | N9—C13—H13B | 109.5 |
| C10—N3—Zn1$^{iv}$ | 127.3 (7) | C7—C13—H13B | 109.5 |
| C24—N4—C25 | 103.4 (8) | H13A—C13—H13B | 108.1 |
| C24—N4—Zn1 | 125.4 (7) | O2—C14—C21 | 109.9 (8) |
| C25—N4—Zn1 | 131.1 (7) | O2—C14—C15 | 106.4 (7) |
| C24—N5—N6 | 110.1 (7) | C21—C14—C15 | 113.6 (7) |
| C24—N5—C26 | 127.4 (8) | O2—C14—C26 | 107.9 (7) |
| N6—N5—C26 | 122.4 (8) | C21—C14—C26 | 107.4 (7) |
| C25—N6—N5 | 101.7 (7) | C15—C14—C26 | 111.5 (8) |
| C12—N7—C11 | 102.9 (8) | C16—C15—C20 | 116.5 (9) |
| C12—N7—Zn1 | 126.3 (6) | C16—C15—C14 | 123.5 (9) |
| C11—N7—Zn1 | 128.3 (7) | C20—C15—C14 | 119.9 (9) |
| C11—N8—N9 | 102.4 (8) | C15—C16—F3 | 120.6 (9) |
| C12—N9—N8 | 111.5 (8) | C15—C16—C17 | 124.4 (10) |
| C12—N9—C13 | 126.0 (9) | F3—C16—C17 | 115.0 (10) |
| N8—N9—C13 | 122.1 (7) | C18—C17—C16 | 115.8 (10) |
| C22—N10—C23 | 101.2 (8) | C18—C17—H17 | 122.1 |

| | | | |
|---|---|---|---|
| C22—N10—Zn1$^{ii}$ | 128.2 (7) | C16—C17—H17 | 122.1 |
| C23—N10—Zn1$^{ii}$ | 129.6 (6) | C19—C18—C17 | 123.1 (9) |
| C23—N11—N12 | 103.6 (7) | C19—C18—F4 | 118.8 (10) |
| C22—N12—N11 | 110.1 (7) | C17—C18—F4 | 118.0 (10) |
| C22—N12—C21 | 129.4 (8) | C18—C19—C20 | 118.6 (10) |
| N11—N12—C21 | 120.5 (8) | C18—C19—H19 | 120.7 |
| C7—O1—H1 | 109.5 | C20—C19—H19 | 120.7 |
| C14—O2—H2 | 109.5 | C19—C20—C15 | 121.3 (10) |
| H3A—O3—H3B | 108.7 | C19—C20—H20 | 119.4 |
| H4A—O4—H4B | 119.4 | C15—C20—H20 | 119.4 |
| C2—C1—C6 | 123.2 (12) | N12—C21—C14 | 112.1 (8) |
| C2—C1—F1 | 118.7 (10) | N12—C21—H21A | 109.2 |
| C6—C1—F1 | 118.0 (11) | C14—C21—H21A | 109.2 |
| C1—C2—C3 | 117.2 (10) | N12—C21—H21B | 109.2 |
| C1—C2—H2A | 121.4 | C14—C21—H21B | 109.2 |
| C3—C2—H2A | 121.4 | H21A—C21—H21B | 107.9 |
| F2—C3—C2 | 118.5 (9) | N12—C22—N10 | 109.7 (8) |
| F2—C3—C4 | 117.7 (10) | N12—C22—H22 | 125.1 |
| C2—C3—C4 | 123.8 (9) | N10—C22—H22 | 125.1 |
| C5—C4—C3 | 114.2 (10) | N11—C23—N10 | 115.4 (8) |
| C5—C4—C7 | 121.1 (8) | N11—C23—H23 | 122.3 |
| C3—C4—C7 | 124.7 (8) | N10—C23—H23 | 122.3 |
| C6—C5—C4 | 122.7 (9) | N4—C24—N5 | 110.2 (9) |
| C6—C5—H5 | 118.6 | N4—C24—H24 | 124.9 |
| C4—C5—H5 | 118.6 | N5—C24—H24 | 124.9 |
| C1—C6—C5 | 118.6 (10) | N6—C25—N4 | 114.7 (8) |
| C1—C6—H6 | 120.7 | N6—C25—H25 | 122.6 |
| C5—C6—H6 | 120.7 | N4—C25—H25 | 122.6 |
| O1—C7—C4 | 112.2 (7) | N5—C26—C14 | 110.9 (7) |
| O1—C7—C8 | 109.6 (8) | N5—C26—H26A | 109.5 |
| C4—C7—C8 | 110.1 (8) | C14—C26—H26A | 109.5 |
| O1—C7—C13 | 104.5 (7) | N5—C26—H26B | 109.5 |
| C4—C7—C13 | 111.2 (8) | C14—C26—H26B | 109.5 |
| C8—C7—C13 | 109.0 (7) | H26A—C26—H26B | 108.1 |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···Cl2$^{v}$ | 0.82 | 2.29 | 3.103 (7) | 172 |
| O2—H2···O4$^{v}$ | 0.82 | 1.87 | 2.653 (9) | 160 |
| O3—H3*A*···Cl2$^{vi}$ | 0.85 | 2.32 | 3.163 (11) | 170 |
| O3—H3*B*···Cl1$^{iv}$ | 0.85 | 2.38 | 3.221 (10) | 170 |
| O4—H4*A*···O2$^{vii}$ | 0.85 | 2.24 | 2.784 (9) | 122 |
| O4—H4*B*···Cl2 | 0.85 | 2.29 | 3.101 (8) | 160 |

Symmetry codes: (iv) $x-1, y, z$; (v) $-x+1, -y+1, -z+1$; (vi) $-x+1, -y+2, -z+1$; (vii) $x-1, y+1, z$.