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Aquabis[3,6-bis(pyridin-2-yl)pyridazine-κ^2N^1,N^6]-copper(II) bis(trifluoromethanesulfonate)

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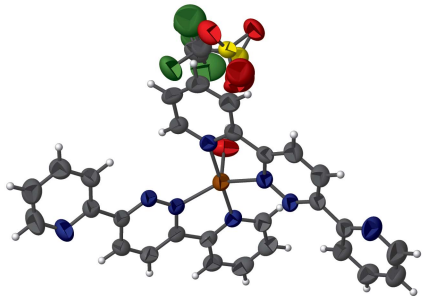
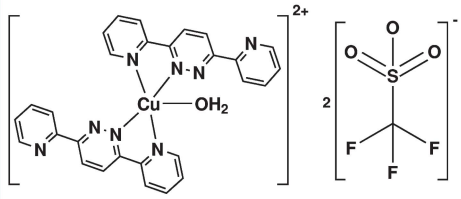
Structural data: full structural data are available from iucrdata.iucr.org

The title salt, $[Cu(C_{14}H_{10}N_4)_2(H_2O)](CF_3SO_3)_2$, contains a Cu^{2+} cation coordinated by two bidentate 3,6-bis(pyridin-2-yl)pyridazine ligands and one water molecule. The charge is balanced by two disordered trifluoromethanesulfonate anions. The asymmetric unit contains half of a cation (point group symmetry 2) and one anion. The coordinating water molecule is engaged in intermolecular O—H···O hydrogen bonds, which connect the cation to the anion. C—H···X (X = N, O, F) interactions stabilize the crystal structure.

3D view



Chemical scheme



Structure description

The coordination chemistry of aromatic diazine and related ligands has gained immense popularity (Xu & Thompson, 2004). 3,6-Bis(pyridin-2-yl)pyridazine is a potential candidate for forming a grid-type architecture because of the multiple binding sites, which can permit coordination of one or two metal atoms depending on the *cis–cis* or *trans–trans* configuration it can adopt (Yuste *et al.*, 2007; Schottel *et al.*, 2006). Understanding the properties and structures of smaller building units with a similar ligand structure will help us to understand the chemistry of larger arrays and synergistic effects in supramolecular frameworks containing the secondary building units (SBU). A large number of transition-metal complexes with a grid-type architecture in two-dimensional arrays, interconnected by the above ligand are known (Constable *et al.*, 2008; Alam *et al.*, 2005; Grove *et al.*, 2001). Furthermore, copper complexes with these ligands can accommodate different oxidation states as bipyridine is an ambivalent ligand (Desbouis *et al.*, 2012). Since the redox potentials of several copper complexes are appropriate for

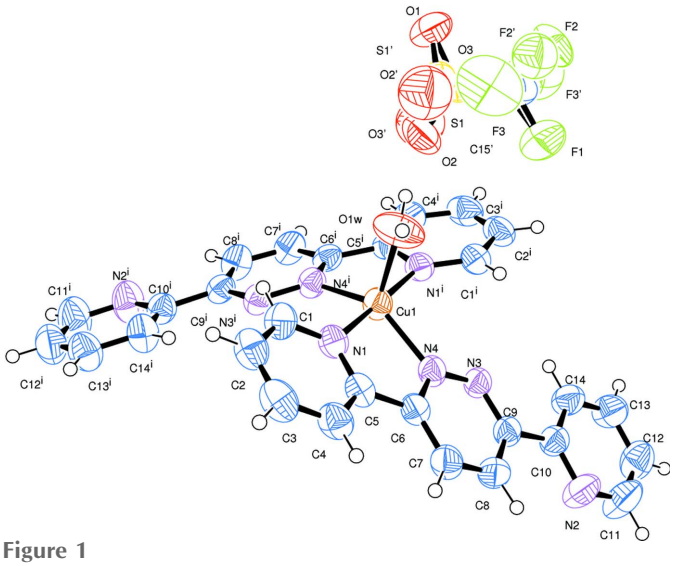


Figure 1
The atom-numbering scheme and 50% probability displacement ellipsoids of the copper complex cation and the anion. The trifluoromethanesulfonate anion shows disorder over two positions with 0.82 and 0.18 site occupancies.

carrying out catalytic redox functions, they are important in technological and biological applications (Farver & Pecht, 1989).

The title compound crystallizes in a monoclinic *C*-centered lattice with four molecules per unit cell. The asymmetric unit contains half of a cation and one anion (Fig. 1). In the anion, except for one of the O atoms (O1) and one of the F atoms (F1), all the atoms are disordered over two positions with major and minor site occupancies of 0.82 and 0.18, respectively. The copper atom is coordinated by nitrogen atoms of the pyridazine and pyridine rings. Hence, the metal coordination, with four Cu—N bonds and one Cu—O(water) bond, adopts a pyramidal geometry with the N atoms forming the base and the O atom at the top of the pyramid. The Cu—N distances are 1.984 (3) and 2.013 (3) Å, while the Cu—O1*W* distance amounts to 2.128 (6) Å. The ligands are inclined at an angle of 49.58 (2)° to each other.

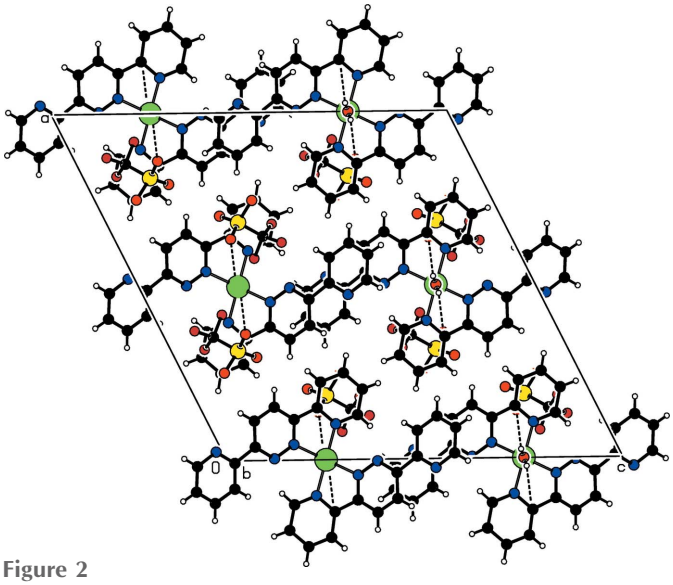


Figure 2
Packing diagram of the title compound viewed down the *b* axis. Hydrogen bonds are shown as dashed lines. The minor component of the disordered trifluoromethanesulfonate anion has been omitted for clarity.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···N3^{i}	0.93	2.63	3.104 (5)	112
C2—H2···O3^{ii}	0.93	2.55	3.376 (6)	149
C11—H11···F1^{iii}	0.93	2.55	3.334 (7)	142
C12—H12···O2^{iv}	0.93	2.59	3.443 (8)	152
O1*W*—H1*W*···O2^{i}	0.83 (1)	1.91 (3)	2.710 (6)	161 (7)
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Symmetry codes: (i) $-x+2, y, -z+\frac{3}{2}$; (ii) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (iii) $-x+2, -y, -z+2$; (iv) $x, -y, z+\frac{1}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Cu(C_{14}H_{10}N_4)_2H_2O](CF_3O_3S)_2$
M_r	848.21
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	293
a, *b*, *c* (Å)	20.7092 (13), 8.7911 (8), 21.1274 (14)
β (°)	116.292 (9)
V (Å^3)	3448.5 (5)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.85
Crystal size (mm)	0.22 × 0.14 × 0.12
Data collection	
Diffractometer	Bruker SMART APEX CCD area-detector
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	3562, 3038, 1662
R_{int}	0.036
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.594
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.043, 0.136, 1.03
No. of reflections	3038
No. of parameters	273
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.41, −0.28

Computer programs: *SMART* and *SAINT* (Bruker, 2001), *SHELX2014* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *PLATON* (Spek, 2009).

The coordinating water molecule is engaged in intermolecular O—H···O hydrogen bonds, which connects the cation with two anions. Further, the crystal structure is stabilized by C—H···*X* (*X* = N, O, F) intermolecular interactions (Fig. 2, Table 1).

Synthesis and crystallization

Two moles of 3,6-bis(pyridin-2-yl)pyridazine (bppz) and one mole of $Cu(CF_3SO_3)_2$ were dissolved in dry benzene (10 ml)

separately and stirred for 2 h at 323 K. The bppz solution was then added dropwise to the $Cu(CF_3SO_3)_2$ solution and stirred well. The colour of the solution slowly turned to a light blue and a precipitate of the same colour was formed. It was filtered off and washed with benzene. Good quality needle-shaped crystals were obtained from methanol by the solvent evaporation method.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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full crystallographic data

IUCrData (2017). **2**, x171142 [https://doi.org/10.1107/S2414314617011427]

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Aquabis[3,6-bis(pyridin-2-yl)pyridazine-κ^2N^1,N^6]copper(II) bis(trifluoromethanesulfonate)

Crystal data

$[Cu(C_{14}H_{10}N_4)_2H_2O](CF_3O_3S)_2$
M_r = 848.21
Monoclinic, $C2/c$
a = 20.7092 (13) Å
b = 8.7911 (8) Å
c = 21.1274 (14) Å
β = 116.292 (9)°
V = 3448.5 (5) Å^3
Z = 4
$F(000)$ = 1716
D_x = 1.634 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2463 reflections
θ = 2.4–24.5°
μ = 0.85 mm^{-1}
T = 293 K
Needle, light blue
0.22 × 0.14 × 0.12 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
ω scans
3562 measured reflections
3038 independent reflections
1662 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 25.0°, θ_{min} = 2.2°
h = 0→24
k = −1→10
l = −25→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.136
S = 1.03
3038 reflections
273 parameters
1 restraint
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0652P)^2 + 1.9713P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 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. All the H atoms, except water hydrogen atoms, were constrained and refined in the riding atom approximation with C—H = 0.93 Å and U_{iso}(H) = 1.2 U_{eq}(parent carbon atom). The water hydrogen atoms were located from difference Fourier map and refined isotropically with the O—H distance restrained to 0.84 (1) Å. All the atoms in the anion, except O1 and F1, are disordered over two positions with major and minor site occupancies of 0.82 and 0.18, respectively. The minor occupied atoms were isotropically refined.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.8715 (2)	0.0852 (5)	0.6131 (2)	0.0585 (12)	
H1	0.9039	0.1137	0.5957	0.070*	
C2	0.7985 (3)	0.0927 (5)	0.5689 (2)	0.0644 (13)	
H2	0.7820	0.1242	0.5223	0.077*	
C3	0.7508 (3)	0.0527 (6)	0.5951 (3)	0.0699 (14)	
H3	0.7015	0.0564	0.5662	0.084*	
C4	0.7765 (2)	0.0071 (5)	0.6644 (2)	0.0622 (13)	
H4	0.7449	−0.0179	0.6832	0.075*	
C5	0.8502 (2)	−0.0009 (5)	0.7056 (2)	0.0509 (11)	
C6	0.8834 (2)	−0.0565 (5)	0.7791 (2)	0.0482 (10)	
C7	0.8475 (2)	−0.1223 (5)	0.8134 (2)	0.0614 (12)	
H7	0.7977	−0.1334	0.7909	0.074*	
C8	0.8861 (2)	−0.1704 (6)	0.8804 (2)	0.0627 (12)	
H8	0.8632	−0.2133	0.9054	0.075*	
C9	0.9612 (2)	−0.1545 (5)	0.9117 (2)	0.0492 (10)	
C10	1.0075 (2)	−0.2088 (5)	0.9842 (2)	0.0539 (11)	
C11	1.0151 (3)	−0.3321 (8)	1.0818 (3)	0.0950 (19)	
H11	0.9925	−0.3833	1.1049	0.114*	
C12	1.0885 (3)	−0.3126 (7)	1.1172 (3)	0.0819 (16)	
H12	1.1146	−0.3505	1.1627	0.098*	
C13	1.1217 (3)	−0.2369 (6)	1.0843 (3)	0.0729 (14)	
H13	1.1712	−0.2208	1.1068	0.088*	
C14	1.0811 (2)	−0.1837 (6)	1.0166 (2)	0.0653 (13)	
H14	1.1029	−0.1315	0.9929	0.078*	
N1	0.89698 (18)	0.0381 (4)	0.68029 (17)	0.0502 (8)	
N2	0.9741 (2)	−0.2823 (6)	1.0161 (2)	0.0796 (13)	
N3	0.99497 (17)	−0.0912 (4)	0.87806 (16)	0.0492 (9)	
N4	0.95559 (17)	−0.0410 (4)	0.81159 (16)	0.0492 (8)	
Cu1	1.0000	0.03557 (9)	0.7500	0.0529 (3)	
O1W	1.0000	0.2776 (6)	0.7500	0.0893 (16)	
C15	1.1403 (6)	0.6066 (12)	0.8757 (5)	0.092 (3)	0.82
S1	1.18594 (9)	0.50258 (19)	0.83360 (9)	0.0587 (4)	0.82
O2	1.1340 (4)	0.3927 (7)	0.7914 (3)	0.0942 (18)	0.82
O3	1.2477 (2)	0.4436 (6)	0.8942 (2)	0.0850 (13)	0.82
F2	1.1834 (4)	0.7126 (7)	0.9176 (3)	0.124 (2)	0.82
F3	1.0797 (3)	0.6670 (7)	0.8270 (4)	0.153 (2)	0.82
O1	1.2036 (2)	0.6180 (4)	0.79347 (19)	0.0887 (11)	
F1	1.1262 (2)	0.5086 (5)	0.9157 (2)	0.1269 (15)	
C15′	1.169 (2)	0.560 (5)	0.877 (2)	0.075 (12)*	0.18
S1′	1.1532 (6)	0.5444 (11)	0.7986 (5)	0.072 (2)*	0.18
O2′	1.0868 (19)	0.578 (4)	0.7664 (17)	0.155 (11)*	0.18
O3′	1.169 (2)	0.381 (6)	0.799 (2)	0.139 (17)*	0.18
F2′	1.1434 (16)	0.715 (4)	0.8872 (16)	0.107 (9)*	0.18
F3′	1.237 (2)	0.560 (4)	0.9289 (19)	0.183 (11)*	0.18
H1W	0.964 (2)	0.332 (6)	0.741 (4)	0.13 (3)*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.055 (3)	0.063 (3)	0.052 (3)	0.009 (2)	0.019 (2)	0.004 (2)
C2	0.059 (3)	0.063 (3)	0.054 (3)	0.014 (2)	0.009 (2)	0.002 (2)
C3	0.048 (3)	0.073 (3)	0.069 (3)	0.011 (3)	0.008 (2)	−0.006 (3)
C4	0.044 (2)	0.074 (4)	0.062 (3)	−0.001 (2)	0.017 (2)	−0.007 (2)
C5	0.045 (2)	0.053 (3)	0.049 (2)	0.002 (2)	0.016 (2)	−0.0096 (19)
C6	0.041 (2)	0.055 (3)	0.049 (2)	0.000 (2)	0.0199 (19)	−0.009 (2)
C7	0.041 (2)	0.085 (4)	0.057 (3)	−0.008 (2)	0.021 (2)	−0.011 (2)
C8	0.052 (3)	0.080 (3)	0.059 (3)	−0.015 (3)	0.027 (2)	−0.006 (3)
C9	0.045 (2)	0.058 (3)	0.047 (2)	−0.002 (2)	0.023 (2)	−0.006 (2)
C10	0.052 (3)	0.061 (3)	0.051 (3)	−0.002 (2)	0.025 (2)	−0.001 (2)
C11	0.087 (4)	0.134 (6)	0.077 (4)	0.002 (4)	0.048 (3)	0.032 (4)
C12	0.082 (4)	0.101 (4)	0.059 (3)	0.010 (3)	0.027 (3)	0.016 (3)
C13	0.060 (3)	0.083 (4)	0.069 (3)	−0.003 (3)	0.022 (3)	0.010 (3)
C14	0.056 (3)	0.079 (3)	0.058 (3)	−0.009 (3)	0.023 (2)	0.007 (3)
N1	0.0452 (19)	0.054 (2)	0.0465 (19)	0.0034 (17)	0.0153 (17)	−0.0025 (18)
N2	0.066 (3)	0.110 (4)	0.069 (3)	−0.008 (3)	0.036 (2)	0.020 (2)
N3	0.0422 (19)	0.062 (2)	0.0424 (19)	−0.0037 (17)	0.0178 (17)	−0.0025 (17)
N4	0.0427 (19)	0.060 (2)	0.0421 (18)	−0.0029 (18)	0.0161 (16)	−0.0047 (17)
Cu1	0.0402 (4)	0.0692 (6)	0.0453 (4)	0.000	0.0154 (3)	0.000
O1W	0.060 (4)	0.056 (3)	0.132 (5)	0.000	0.025 (4)	0.000
C15	0.106 (8)	0.063 (6)	0.138 (8)	−0.008 (6)	0.082 (7)	−0.012 (5)
S1	0.0556 (9)	0.0612 (10)	0.0614 (9)	−0.0086 (8)	0.0277 (9)	−0.0031 (8)
O2	0.089 (4)	0.094 (4)	0.095 (4)	−0.035 (4)	0.036 (4)	−0.039 (3)
O3	0.061 (3)	0.098 (3)	0.091 (3)	0.023 (3)	0.029 (2)	0.039 (3)
F2	0.163 (6)	0.098 (4)	0.121 (4)	−0.050 (4)	0.072 (4)	−0.059 (3)
F3	0.085 (3)	0.141 (5)	0.214 (6)	0.045 (3)	0.049 (4)	−0.005 (4)
O1	0.089 (3)	0.096 (3)	0.090 (3)	−0.010 (2)	0.047 (2)	0.024 (2)
F1	0.153 (4)	0.133 (3)	0.138 (3)	−0.039 (3)	0.104 (3)	−0.010 (2)

Geometric parameters (Å, º)

C1—N1	1.343 (5)	C12—H12	0.9300
C1—C2	1.381 (6)	C13—C14	1.381 (6)
C1—H1	0.9300	C13—H13	0.9300
C2—C3	1.375 (6)	C14—H14	0.9300
C2—H2	0.9300	N1—Cu1	1.984 (3)
C3—C4	1.377 (7)	N3—N4	1.348 (4)
C3—H3	0.9300	N4—Cu1	2.013 (3)
C4—C5	1.384 (6)	Cu1—N1^{i}	1.984 (3)
C4—H4	0.9300	Cu1—N4^{i}	2.013 (3)
C5—N1	1.342 (5)	Cu1—O1W	2.128 (6)
C5—C6	1.475 (6)	O1W—H1W	0.834 (10)
C6—N4	1.347 (5)	C15—F2	1.323 (10)
C6—C7	1.376 (6)	C15—F1	1.327 (9)
C7—C8	1.349 (6)	C15—F3	1.330 (12)

C7—H7	0.9300	C15—S1	1.808 (10)
C8—C9	1.402 (6)	S1—O2	1.426 (6)
C8—H8	0.9300	S1—O3	1.447 (4)
C9—N3	1.321 (5)	S1—O1	1.469 (4)
C9—C10	1.480 (6)	O1—S1′	1.273 (9)
C10—N2	1.327 (5)	F1—C15′	1.52 (4)
C10—C14	1.385 (6)	C15′—F3′	1.34 (4)
C11—N2	1.340 (6)	C15′—F2′	1.51 (5)
C11—C12	1.375 (7)	C15′—S1′	1.54 (4)
C11—H11	0.9300	S1′—O2′	1.27 (3)
C12—C13	1.351 (7)	S1′—O3′	1.47 (5)

N1—C1—C2	121.9 (4)	C5—N1—Cu1	115.5 (3)
N1—C1—H1	119.0	C1—N1—Cu1	125.3 (3)
C2—C1—H1	119.0	C10—N2—C11	116.8 (4)
C3—C2—C1	118.8 (4)	C9—N3—N4	118.6 (3)
C3—C2—H2	120.6	C6—N4—N3	121.4 (3)
C1—C2—H2	120.6	C6—N4—Cu1	115.2 (3)
C2—C3—C4	119.7 (4)	N3—N4—Cu1	123.0 (2)
C2—C3—H3	120.2	N1^{i}—Cu1—N1	178.7 (2)
C4—C3—H3	120.2	N1^{i}—Cu1—N4^{i}	80.48 (13)
C3—C4—C5	118.8 (4)	N1—Cu1—N4^{i}	99.95 (13)
C3—C4—H4	120.6	N1^{i}—Cu1—N4	99.94 (13)
C5—C4—H4	120.6	N1—Cu1—N4	80.48 (13)
N1—C5—C4	121.8 (4)	N4^{i}—Cu1—N4	140.9 (2)
N1—C5—C6	114.9 (4)	N1^{i}—Cu1—O1W	89.37 (10)
C4—C5—C6	123.3 (4)	N1—Cu1—O1W	89.37 (11)
N4—C6—C7	120.7 (4)	N4^{i}—Cu1—O1W	109.53 (10)
N4—C6—C5	113.5 (3)	N4—Cu1—O1W	109.53 (10)
C7—C6—C5	125.8 (4)	Cu1—O1W—H1W	125 (5)
C8—C7—C6	118.6 (4)	F2—C15—F1	107.7 (8)
C8—C7—H7	120.7	F2—C15—F3	111.3 (10)
C6—C7—H7	120.7	F1—C15—F3	110.8 (8)
C7—C8—C9	118.7 (4)	F2—C15—S1	109.9 (7)
C7—C8—H8	120.6	F1—C15—S1	107.2 (7)
C9—C8—H8	120.6	F3—C15—S1	109.9 (7)
N3—C9—C8	122.0 (4)	O2—S1—O3	115.9 (4)
N3—C9—C10	116.0 (3)	O2—S1—O1	114.8 (3)
C8—C9—C10	122.0 (4)	O3—S1—O1	114.2 (2)
N2—C10—C14	122.3 (4)	O2—S1—C15	103.7 (4)
N2—C10—C9	116.0 (4)	O3—S1—C15	101.3 (4)
C14—C10—C9	121.7 (4)	O1—S1—C15	104.6 (4)
N2—C11—C12	124.4 (5)	F3′—C15′—F2′	101 (3)
N2—C11—H11	117.8	F3′—C15′—F1	102 (3)
C12—C11—H11	117.8	F2′—C15′—F1	82 (3)
C13—C12—C11	118.2 (5)	F3′—C15′—S1′	122 (3)
C13—C12—H12	120.9	F2′—C15′—S1′	108 (3)
C11—C12—H12	120.9	F1—C15′—S1′	131 (3)

C12—C13—C14	119.0 (5)	O2′—S1′—O1	124.7 (18)
C12—C13—H13	120.5	O2′—S1′—O3′	115 (2)
C14—C13—H13	120.5	O1—S1′—O3′	107.6 (16)
C13—C14—C10	119.3 (4)	O2′—S1′—C15′	103 (2)
C13—C14—H14	120.3	O1—S1′—C15′	104.6 (17)
C10—C14—H14	120.3	O3′—S1′—C15′	99 (2)
C5—N1—C1	119.0 (4)		

N1—C1—C2—C3	1.0 (7)	C5—C6—N4—N3	−177.4 (3)
C1—C2—C3—C4	0.3 (7)	C7—C6—N4—Cu1	173.3 (3)
C2—C3—C4—C5	−1.6 (7)	C5—C6—N4—Cu1	−5.2 (4)
C3—C4—C5—N1	1.7 (7)	C9—N3—N4—C6	−1.1 (6)
C3—C4—C5—C6	−176.4 (4)	C9—N3—N4—Cu1	−172.8 (3)
N1—C5—C6—N4	7.8 (5)	F2—C15—S1—O2	179.3 (8)
C4—C5—C6—N4	−173.9 (4)	F1—C15—S1—O2	62.5 (8)
N1—C5—C6—C7	−170.5 (4)	F3—C15—S1—O2	−58.0 (7)
C4—C5—C6—C7	7.7 (7)	F2—C15—S1—O3	58.8 (9)
N4—C6—C7—C8	0.3 (7)	F1—C15—S1—O3	−57.9 (7)
C5—C6—C7—C8	178.5 (4)	F3—C15—S1—O3	−178.4 (6)
C6—C7—C8—C9	−1.4 (7)	F2—C15—S1—O1	−60.1 (9)
C7—C8—C9—N3	1.4 (7)	F1—C15—S1—O1	−176.9 (6)
C7—C8—C9—C10	−178.1 (4)	F3—C15—S1—O1	62.6 (7)
N3—C9—C10—N2	−175.2 (4)	O2—S1—O1—S1′	44.7 (8)
C8—C9—C10—N2	4.3 (6)	O3—S1—O1—S1′	−178.1 (8)
N3—C9—C10—C14	4.9 (6)	C15—S1—O1—S1′	−68.2 (8)
C8—C9—C10—C14	−175.6 (4)	F2—C15—F1—C15′	−95 (4)
N2—C11—C12—C13	0.7 (10)	F3—C15—F1—C15′	143 (4)
C11—C12—C13—C14	−0.6 (8)	S1—C15—F1—C15′	23 (4)
C12—C13—C14—C10	0.2 (8)	C15—F1—C15′—F3′	124 (6)
N2—C10—C14—C13	0.2 (7)	C15—F1—C15′—F2′	25 (3)
C9—C10—C14—C13	−180.0 (4)	C15—F1—C15′—S1′	−83 (4)
C4—C5—N1—C1	−0.4 (6)	S1—O1—S1′—O2′	166 (3)
C6—C5—N1—C1	177.9 (4)	S1—O1—S1′—O3′	−54.9 (19)
C4—C5—N1—Cu1	174.9 (3)	S1—O1—S1′—C15′	49.2 (18)
C6—C5—N1—Cu1	−6.8 (5)	F3′—C15′—S1′—O2′	−168 (4)
C2—C1—N1—C5	−1.0 (6)	F2′—C15′—S1′—O2′	−52 (3)
C2—C1—N1—Cu1	−175.8 (3)	F1—C15′—S1′—O2′	44 (4)
C14—C10—N2—C11	−0.1 (8)	F3′—C15′—S1′—O1	−37 (4)
C9—C10—N2—C11	−179.9 (5)	F2′—C15′—S1′—O1	79 (3)
C12—C11—N2—C10	−0.4 (9)	F1—C15′—S1′—O1	175 (3)
C8—C9—N3—N4	−0.1 (6)	F3′—C15′—S1′—O3′	74 (4)
C10—C9—N3—N4	179.4 (4)	F2′—C15′—S1′—O3′	−170 (3)
C7—C6—N4—N3	1.1 (6)	F1—C15′—S1′—O3′	−74 (4)

Symmetry code: (i) $-x+2, y, -z+3/2$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···N3^{i}	0.93	2.63	3.104 (5)	112
C2—H2···O3^{ii}	0.93	2.55	3.376 (6)	149
C11—H11···F1^{iii}	0.93	2.55	3.334 (7)	142
C12—H12···O2^{iv}	0.93	2.59	3.443 (8)	152
O1*W*—H1*W*···O2^{i}	0.83 (1)	1.91 (3)	2.710 (6)	161 (7)
C1—H1···N3^{i}	0.93	2.63	3.104 (5)	112
C2—H2···O3^{ii}	0.93	2.55	3.376 (6)	149
C11—H11···F1^{iii}	0.93	2.55	3.334 (7)	142
C12—H12···O2^{iv}	0.93	2.59	3.443 (8)	152
O1*W*—H1*W*···O2^{i}	0.83 (1)	1.91 (3)	2.710 (6)	161 (7)

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