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Crystal structure and Hirshfeld surface analysis of bis(2-amino-1-methylbenzimidazole-κN^3) bis(salicylato-$\kappa^2 O,O'$)copper(II)

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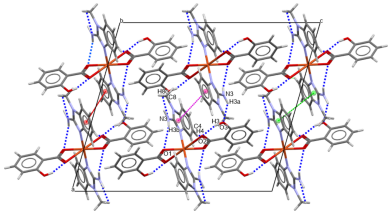
The title complex, $[Cu(C_7H_5O_3)_2(C_8H_9N_3)_2]$, crystallizes in the monoclinic space group $C2/c$. The Cu^{II} cation is located on an inversion center and adopts a distorted octahedral coordination environment defined by two aromatic N atoms from neutral 2-amino-1-methylbenzimidazole ligands and by four O atoms from two bidentate salicylate anions coordinating *via* their carboxylate groups. The tri-periodic supramolecular network features intra- and intermolecular O—H···O, N—H···O and C—H···O hydrogen bonds, along with π–π stacking and C—H···π interactions. Hirshfeld surface analysis indicates that H···H (43.7% contribution), C···H/H···C (35.8%), and O···H/H···O (14.1%) contacts dominate the intermolecular interactions.

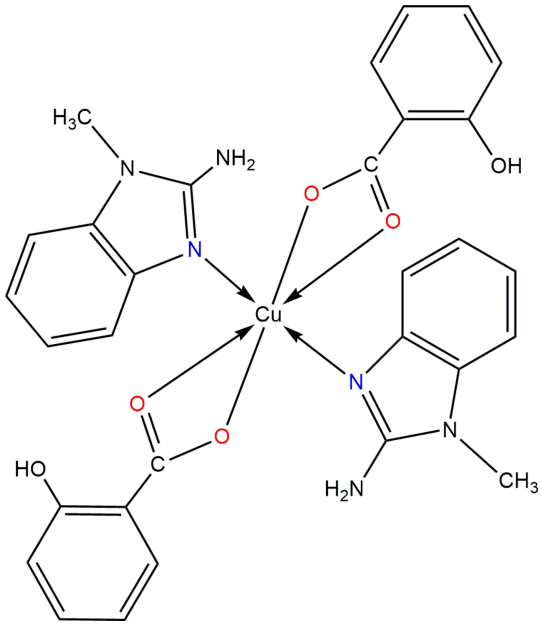
1. Chemical context

Salicylic acid or derivatives thereof form stable complexes with the central metal cation (*e.g.* copper) *via* strong coordination bonds either in a monodentate or bidentate fashion, forming bonds to the oxygen atoms of the carboxyl group and/or the hydroxyl group (Iravani *et al.*, 2013; Hoang *et al.*, 1992). Corresponding complexes exhibit distinctive magnetic and optical properties, influenced by the electronic configuration of the central metal cation and the π-electron system of the ligand, thereby enhancing potential applications in catalysis, optical materials, or biological systems (Costes *et al.*, 2003).

Copper(II) complexes formed by salicylic acid and a co-ligand, such as benzimidazole and its derivatives, have continued to attract attention due to their structural diversity and biological potential. In these mixed N,O-donor ligand systems, salicylic acid can coordinate via its hydroxyl and carboxylate groups, while aromatic amines bind through nitrogen atoms (Lawal *et al.*, 2017). These combinations of ligands provide favorable coordination environments, influencing the crystal packing and stability of the resulting complexes.

In the context given above, we report here on the crystal structure, Hirshfeld and void analysis of a new Cu^{II} complex derived from salicylic acid and benzimidazole, $[Cu(C_7H_5O_3)_2(C_8H_9N_3)_2]$ (Fig. 1).





2. Structural commentary

The asymmetric unit of the title complex comprises one half of the $[Cu(C_7H_5O_3)_2(C_8H_9N_3)_2]$ molecule, the complete complex being generated by inversion symmetry. The central Cu^{II} cation adopts a distorted octahedral coordination environment defined by two nitrogen atoms [N1, N1^{i}; symmetry code: (i) $-x+\frac{1}{2}, -y+\frac{3}{2}, -z+1$] from two neutral 2-amino-1-methylbenzimidazole (MAB) ligands and four oxygen atoms from two bidentate salicylate ligands, coordinating in a κ^2O,O' fashion (O1, O2; O1^{i}, O2^{i}) through the carboxylate groups. The Cu—N and Cu—O bond lengths fall within expected ranges for the typical Jahn–Teller distortion, with the Cu1—N1, Cu1—O1, and Cu1—O2 distances being 1.9781 (16), 1.9849 (14), and 2.5672 (15) Å, respectively. The salicylate ligand forms a four-membered chelate ring with a bite angle of 56.60 (5)° for O1—Cu1—O2 and a *cis* angle of 123.40 (5)° for O1—Cu1—O2^{i}. Within the salicylate ligand an intramolecular O—H···O hydrogen bond between the phenolic hydroxyl group (O3—H3) and the adjacent carboxylate oxygen atom (O2) helps to consolidate the molecular conformation (Table 1). The N—Cu1—O angles are 88.95 (6) and 91.05 (6)°. These values are consistent with those observed in previously reported Cu^{II} complexes bearing mixed N,O-donor ligands (Puchoňová *et al.*, 2017). The dihedral angle between the benzimidazole ring of the MAB ligand and the aromatic ring of the coordinated salicylate ligand is 82.68 (11)°.

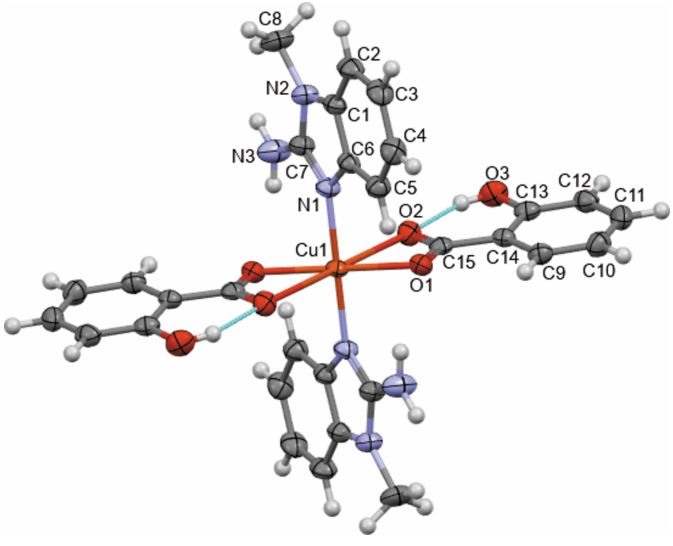


Figure 1
Molecular structure of the title complex. Displacement ellipsoids are drawn at the 50% probability level; non-labeled atoms are generated by symmetry operation $\frac{1}{2}-x, \frac{3}{2}-y, 1-z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O2	0.81 (1)	1.81 (1)	2.538 (2)	150 (1)
N3—H3*a*···O3^{i}	0.88 (1)	2.33 (1)	3.046 (3)	139 (1)
N3—H3*b*···O1	0.88 (1)	2.49 (1)	3.020 (3)	119 (1)
C4—H4···O2^{ii}	0.95 (1)	2.57 (1)	3.373 (2)	143 (1)

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

3. Supramolecular features

The title compound exhibits a tri-periodic supramolecular network defined by a variety of non-covalent interactions. Two key intermolecular N—H···O hydrogen bonds (Table 1) are observed between the amino group of the benzimidazole ligand (N3) and neighboring salicylate oxygen atoms (O3). Additional weaker C—H···O contacts further contribute to the supramolecular cohesion (Table 1). π–π stacking interactions are observed between aromatic rings N1/C6/C1/N2/C7 (centroid *Cg*3) and C1–C6 (*Cg*4) with a centroid-to-centroid distances of 3.8831 (13) Å for *Cg*3···*Cg*4($1-x, 1-y, 1-z$; slippage = 1.769 Å), as shown in Fig. 2. Furthermore, a weak C—H···π interactions is present between the C11—H11

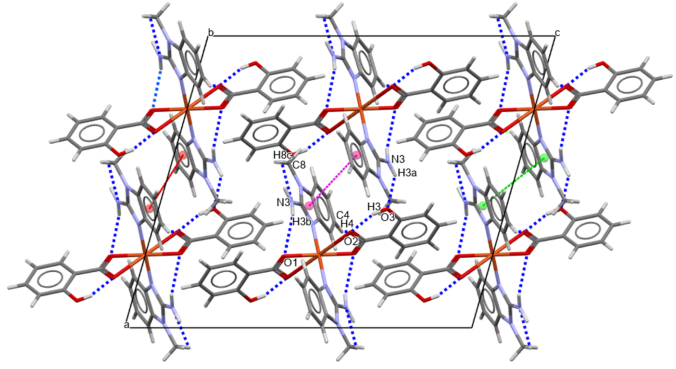


Figure 2
The molecular packing of the title compound along [010]. Intra- and intermolecular hydrogen bonds are shown as dashed lines. π–π stacking interactions are indicated as follows: *Cg*3···*Cg*3 in green, *Cg*3···*Cg*4 in pink, and *Cg*4···*Cg*4 in red.

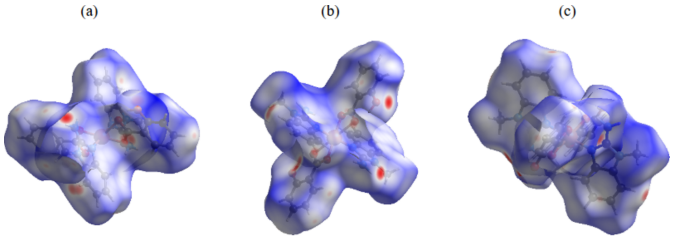


Figure 3
HS plotted over d_{norm} (*a*) along [100], (*b*) along [010] and (*c*) along [001].

group and the π-systems represented by *Cg*4. The H11···*Cg* distance is 2.637 (3), the C11···*Cg* distance is 3.543 (3) and the C11—H11···*Cg* angle is 159.6 (3)°.

4. Hirshfeld surface and void analysis

In order to quantify and visualize intermolecular interactions, a Hirshfeld surface (HS) analysis (Spackman & Jayatilaka, 2009) was performed and the associated two-dimensional fingerprint plots (McKinnon *et al.*, 2007) calculated with *CrystalExplorer*21 (Spackman *et al.*, 2021). The HS mapped with d_{norm} is represented in Fig. 3, where white regions indicate contacts at van der Waals separations, red spots denote shorter contacts (*e.g.* hydrogen bonds) and blue areas longer contacts. The overall two-dimensional fingerprint plot is shown in Fig. 4*a*. H···H contacts make the largest contribution (43.7%, Fig. 4*b*) to the HS. Other significant contacts are H···C/C···H (35.8%, Fig. 4*c*) and H···O/O···H (14.1%, Fig. 4*d*), while H···N/N···H (3%, Fig. 4*e*), C···C (2%, Fig. 4*f*) and C···N/N···C (1.4%, Fig. 4*g*) contacts contribute only to a minor amount.

Void analysis was performed using *CrystalExplorer* with a probe radius of 1.2 Å and a grid spacing of 0.2 Å. The total void volume within the unit cell was calculated to be 327.6 Å^3, which corresponds to 11.7% of the unit-cell volume. The voids are visualized as transparent isosurfaces in the crystal packing diagram (Fig. 5).

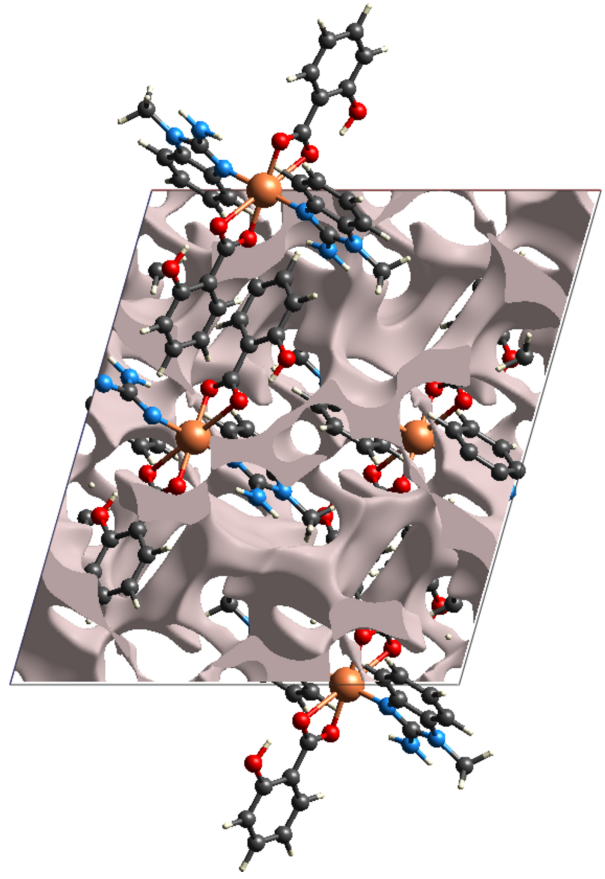


Figure 5
The void surface packing in a view along [010].

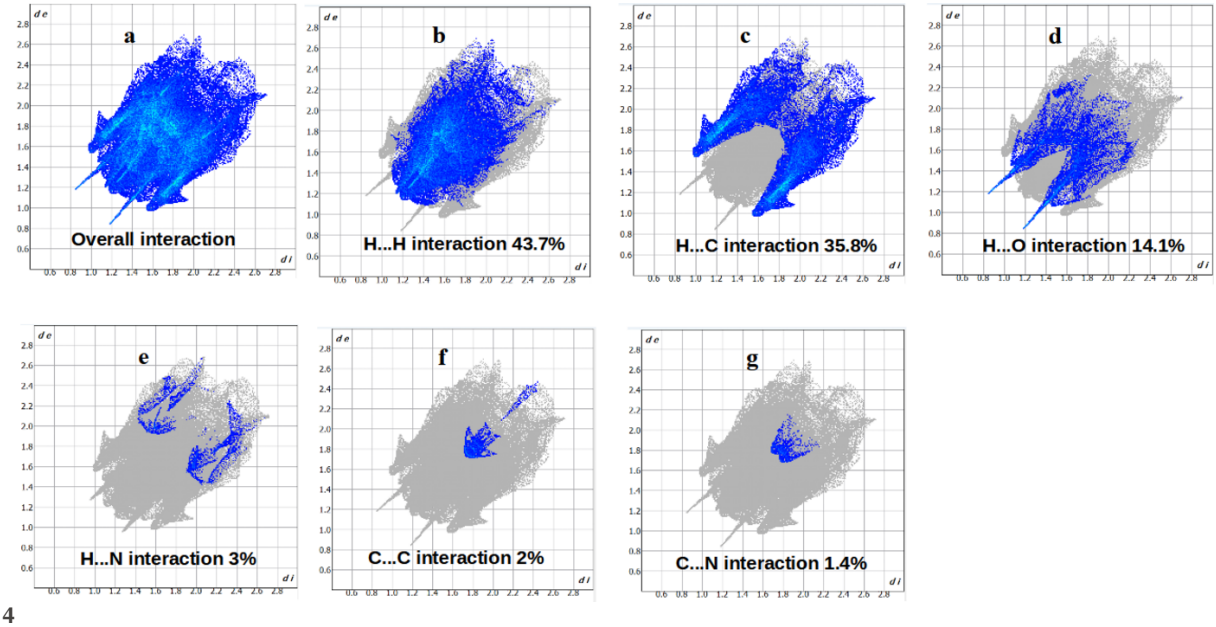


Figure 4
Two-dimensional fingerprint plots for (*a*) all interactions and (*b*)–(*g*) individual interatomic contacts.

5. Database survey

A search of the Cambridge Structural Database (CSD, version 5.46, updated November 2024; Groom *et al.*, 2016) for similar coordination environments (bidentate carboxylate group and an aromatic monodentate N-donor ligand) yielded several complexes including the first-row transition metal complex: *catena*-[bis(μ-carbonato)tetrakis(2,4′-bipyridine)bis(aqua)-dicopper(II) dihydrate] (RITBEE01; Mulrooney *et al.*, 2018), which features a bidentate binding and bridging carbonate anion and monodentately binding 2,2′-bipyridine entities, resulting in the formation of a polymeric chain.

6. Synthesis and crystallization

An aqueous solution of copper(II) sulfate pentahydrate (0.05 *M*, 10 ml) was prepared by dissolving the salt in distilled water. An ethanolic solution of salicylic acid (0.1 *M*, 10 ml) was added, and the resulting mixture stirred magnetically at room temperature for 4 h. No noticeable color change was observed during this step. Subsequently, an ethanolic solution of 2-amino-1-methylbenzimidazole (0.1 *M*, 10 ml) was added, and stirring was continued for additional 4 h, resulting in a green-colored solution. The reaction mixture was then filtered and left to stand at room temperature for 2–3 weeks to allow the growth of green crystals suitable for X-ray diffraction analysis.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Hydrogen atoms were positioned geometrically (aromatic C—H = 0.95 Å, N—H = 0.89 Å, O—H = 0.84 Å and methyl C—H = 0.98 Å) and refined using a riding model with U_{iso}(H) = 1.2U_{eq}(aromatic C, N) or 1.5U_{eq}(methyl C, O).

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Cu(C_7H_5O_3)_2(C_8H_9N_3)_2]$
M_r	632.14
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	150
a, *b*, *c* (Å)	16.7892 (5), 9.0355 (2), 19.2315 (6)
β (°)	106.011 (3)
V (Å^3)	2804.23 (14)
Z	4
Radiation type	Cu *K*α
μ (mm^{-1})	1.58
Crystal size (mm)	0.54 × 0.18 × 0.06
Data collection	
Diffractometer	XtaLAB Synergy, Single source at home/near, HyPix3000
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2023)
T_{min}, T_{max}	0.710, 1.000
No. of measured, independent and observed [$I \geq 2u(I)$] reflections	13358, 2710, 2351
R_{int}	0.046
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.616
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.038, 0.108, 1.02
No. of reflections	2710
No. of parameters	197
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.36, −0.44

Computer programs: *CrysAlis PRO* (Rigaku OD, 2023), *OLEX2.solve* (Bourhis *et al.*, 2015), *SHELXL* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

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Crystal structure and Hirshfeld surface analysis of bis(2-amino-1-methylbenzimidazole-κN^3)bis(salicylato-$\kappa^2 O,O'$)copper(II)

Salmon Mukhammadiev, Feruza Fayzullayeva, Zukhra Kadirova, Akmaljon Tojiboev, Jamshid Ashurov and Shahlo Daminova

Computing details

Bis(2-hydroxybenzoato-$\kappa^2 O^1,O^{1'}$)bis(1-methyl-1*H*-1,3-benzodiazol-2-amine-κN^3)copper(II)

Crystal data

$[Cu(C_7H_5O_3)_2(C_8H_9N_3)_2]$
$M_r = 632.14$
Monoclinic, $C2/c$
$a = 16.7892$ (5) Å
$b = 9.0355$ (2) Å
$c = 19.2315$ (6) Å
$\beta = 106.011$ (3)°
$V = 2804.23$ (14) Å^3
$Z = 4$
$F(000) = 1308.0$
$D_x = 1.497$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 6926 reflections
$\theta = 4.8$–$71.0°$
$\mu = 1.58$ mm^{-1}
$T = 150$ K
Block, dark green
0.54 × 0.18 × 0.06 mm

Data collection

XtaLAB Synergy, Single source at home/near, HyPix3000 diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2023)
$T_{min} = 0.710$, $T_{max} = 1.000$
13358 measured reflections
2710 independent reflections
2351 reflections with $I \geq 2u(I)$
$R_{int} = 0.046$
$\theta_{max} = 71.7°$, $\theta_{min} = 4.8°$
$h = -20 \rightarrow 17$
$k = -11 \rightarrow 10$
$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.108$
$S = 1.02$
2710 reflections
197 parameters
0 restraints
25 constraints
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0592P)^2 + 2.8103P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = -0.001$
$\Delta\rho_{max} = 0.36$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.25	0.75	0.5	0.02441 (15)
O1	0.24551 (8)	0.80636 (16)	0.59860 (8)	0.0287 (3)
O2	0.17132 (9)	0.60031 (16)	0.57333 (8)	0.0331 (4)
O3	0.09241 (9)	0.50418 (17)	0.65918 (9)	0.0385 (4)
H3	0.10951 (9)	0.50901 (17)	0.62385 (9)	0.0577 (6)*
N1	0.35479 (10)	0.64351 (19)	0.54380 (9)	0.0284 (4)
N2	0.48415 (10)	0.5937 (2)	0.60893 (10)	0.0321 (4)
N3	0.43028 (12)	0.8317 (2)	0.62124 (12)	0.0469 (6)
H3a	0.47667 (12)	0.8575 (2)	0.65315 (12)	0.0563 (7)*
H3b	0.38887 (12)	0.8948 (2)	0.60864 (12)	0.0563 (7)*
C1	0.45469 (12)	0.4673 (2)	0.57009 (12)	0.0292 (5)
C2	0.49118 (14)	0.3304 (3)	0.56638 (13)	0.0367 (5)
H2	0.54675 (14)	0.3105 (3)	0.59311 (13)	0.0441 (6)*
C3	0.44333 (16)	0.2248 (3)	0.52229 (14)	0.0401 (6)
H3c	0.46642 (16)	0.1301 (3)	0.51867 (14)	0.0481 (7)*
C4	0.36121 (16)	0.2540 (2)	0.48257 (14)	0.0386 (5)
H4	0.32941 (16)	0.1784 (2)	0.45334 (14)	0.0463 (7)*
C5	0.32582 (14)	0.3926 (2)	0.48553 (12)	0.0334 (5)
H5	0.27066 (14)	0.4134 (2)	0.45803 (12)	0.0401 (6)*
C6	0.37341 (12)	0.4982 (2)	0.52959 (11)	0.0276 (4)
C7	0.42262 (12)	0.6952 (2)	0.59162 (12)	0.0308 (5)
C8	0.56419 (14)	0.6094 (3)	0.66364 (14)	0.0458 (6)
H8a	0.5682 (5)	0.5360 (14)	0.7020 (5)	0.0686 (9)*
H8b	0.60917 (14)	0.594 (2)	0.6410 (3)	0.0686 (9)*
H8c	0.5687 (5)	0.7091 (8)	0.6844 (8)	0.0686 (9)*
C9	0.22167 (13)	0.8228 (2)	0.73737 (12)	0.0310 (5)
H9	0.25920 (13)	0.8908 (2)	0.72568 (12)	0.0373 (5)*
C10	0.20417 (14)	0.8346 (3)	0.80299 (12)	0.0380 (5)
H10	0.22939 (14)	0.9099 (3)	0.83627 (12)	0.0456 (6)*
C11	0.14918 (15)	0.7351 (3)	0.82013 (13)	0.0387 (6)
H11	0.13671 (15)	0.7428 (3)	0.86527 (13)	0.0464 (7)*
C12	0.11264 (13)	0.6251 (3)	0.77193 (12)	0.0362 (5)
H12	0.07531 (13)	0.5577 (3)	0.78424 (12)	0.0434 (6)*
C13	0.13000 (12)	0.6125 (2)	0.70566 (12)	0.0298 (5)
C14	0.18537 (12)	0.7131 (2)	0.68769 (11)	0.0259 (4)
C15	0.20180 (12)	0.7050 (2)	0.61594 (11)	0.0270 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0213 (2)	0.0226 (2)	0.0293 (2)	0.00500 (15)	0.00676 (17)	0.00076 (16)
O1	0.0257 (7)	0.0291 (7)	0.0324 (8)	0.0017 (6)	0.0101 (6)	0.0006 (6)
O2	0.0384 (8)	0.0271 (8)	0.0333 (8)	0.0027 (6)	0.0088 (6)	−0.0039 (6)
O3	0.0366 (8)	0.0323 (8)	0.0444 (9)	−0.0093 (7)	0.0078 (7)	−0.0011 (7)
N1	0.0253 (8)	0.0253 (9)	0.0344 (9)	0.0051 (7)	0.0077 (7)	−0.0008 (7)

N2	0.0231 (8)	0.0331 (10)	0.0371 (10)	0.0025 (7)	0.0033 (7)	0.0011 (8)
N3	0.0320 (10)	0.0344 (11)	0.0650 (14)	0.0041 (8)	−0.0020 (9)	−0.0167 (10)
C1	0.0251 (10)	0.0291 (11)	0.0348 (11)	0.0050 (8)	0.0108 (8)	0.0060 (9)
C2	0.0328 (11)	0.0354 (12)	0.0432 (13)	0.0124 (9)	0.0124 (10)	0.0083 (10)
C3	0.0488 (14)	0.0290 (12)	0.0448 (13)	0.0147 (10)	0.0169 (11)	0.0021 (10)
C4	0.0480 (14)	0.0267 (12)	0.0409 (13)	0.0040 (9)	0.0121 (11)	−0.0047 (9)
C5	0.0329 (11)	0.0305 (11)	0.0355 (12)	0.0043 (9)	0.0073 (9)	−0.0015 (9)
C6	0.0281 (10)	0.0248 (10)	0.0314 (11)	0.0054 (8)	0.0107 (8)	0.0030 (8)
C7	0.0250 (10)	0.0296 (11)	0.0373 (12)	0.0029 (8)	0.0075 (8)	−0.0013 (9)
C8	0.0262 (11)	0.0501 (15)	0.0516 (15)	0.0027 (10)	−0.0052 (10)	0.0012 (12)
C9	0.0267 (10)	0.0312 (11)	0.0339 (11)	−0.0019 (8)	0.0062 (8)	0.0003 (9)
C10	0.0397 (12)	0.0388 (13)	0.0322 (12)	0.0003 (10)	0.0042 (10)	−0.0056 (10)
C11	0.0381 (12)	0.0495 (15)	0.0300 (12)	0.0081 (10)	0.0119 (10)	0.0049 (10)
C12	0.0290 (10)	0.0412 (13)	0.0394 (12)	0.0017 (9)	0.0111 (9)	0.0119 (10)
C13	0.0242 (9)	0.0261 (10)	0.0364 (11)	0.0023 (8)	0.0038 (8)	0.0041 (9)
C14	0.0212 (9)	0.0251 (10)	0.0309 (11)	0.0030 (7)	0.0063 (8)	0.0022 (8)
C15	0.0223 (9)	0.0251 (10)	0.0315 (11)	0.0074 (8)	0.0039 (8)	0.0026 (8)

Geometric parameters (Å, º)

Cu1—O1	1.9849 (14)	C3—H3c	0.9500
Cu1—O1^{i}	1.9849 (14)	C3—C4	1.405 (3)
Cu1—O2	2.5672 (15)	C4—H4	0.9500
Cu1—N1	1.9781 (16)	C4—C5	1.394 (3)
Cu1—N1^{i}	1.9781 (16)	C5—H5	0.9500
O1—C15	1.274 (3)	C5—C6	1.376 (3)
O2—C15	1.264 (3)	C8—H8a	0.9800
O3—H3	0.8084	C8—H8b	0.9800
O3—C13	1.358 (3)	C8—H8c	0.9800
N1—C6	1.394 (3)	C9—H9	0.9500
N1—C7	1.335 (3)	C9—C10	1.376 (3)
N2—C1	1.380 (3)	C9—C14	1.395 (3)
N2—C7	1.352 (3)	C10—H10	0.9500
N2—C8	1.467 (3)	C10—C11	1.392 (3)
N3—H3a	0.8800	C11—H11	0.9500
N3—H3b	0.8800	C11—C12	1.381 (3)
N3—C7	1.350 (3)	C12—H12	0.9500
C1—C2	1.391 (3)	C12—C13	1.388 (3)
C1—C6	1.400 (3)	C13—C14	1.410 (3)
C2—H2	0.9500	C14—C15	1.482 (3)
C2—C3	1.377 (4)		

O1—Cu1—O2^{i}	123.40 (5)	C1—C6—N1	108.42 (18)
O1—Cu1—O2	56.60 (5)	C5—C6—N1	130.57 (19)
O1^{i}—Cu1—O1	180.0	C5—C6—C1	121.01 (19)
N1^{i}—Cu1—O1^{i}	88.95 (6)	N2—C7—N1	112.40 (19)
N1^{i}—Cu1—O1	91.05 (6)	N3—C7—N1	125.03 (19)
N1—Cu1—O1^{i}	91.05 (6)	N3—C7—N2	122.56 (19)

N1—Cu1—O1	88.95 (6)	H8a—C8—N2	109.5
N1^{i}—Cu1—N1	180.0	H8b—C8—N2	109.5
C15—O1—Cu1	104.01 (13)	H8b—C8—H8a	109.5
C13—O3—H3	107.8	H8c—C8—N2	109.5
C6—N1—Cu1	126.57 (14)	H8c—C8—H8a	109.5
C7—N1—Cu1	127.78 (14)	H8c—C8—H8b	109.5
C7—N1—C6	105.64 (16)	C10—C9—H9	119.36 (13)
C7—N2—C1	107.01 (17)	C14—C9—H9	119.36 (13)
C8—N2—C1	126.06 (19)	C14—C9—C10	121.3 (2)
C8—N2—C7	126.7 (2)	H10—C10—C9	120.31 (13)
H3b—N3—H3a	120.0	C11—C10—C9	119.4 (2)
C7—N3—H3a	120.0	C11—C10—H10	120.31 (14)
C7—N3—H3b	120.0	H11—C11—C10	119.79 (14)
C2—C1—N2	131.8 (2)	C12—C11—C10	120.4 (2)
C6—C1—N2	106.52 (18)	C12—C11—H11	119.79 (14)
C6—C1—C2	121.6 (2)	H12—C12—C11	119.72 (14)
H2—C2—C1	121.41 (13)	C13—C12—C11	120.6 (2)
C3—C2—C1	117.2 (2)	C13—C12—H12	119.72 (13)
C3—C2—H2	121.41 (13)	C12—C13—O3	119.12 (19)
H3c—C3—C2	119.23 (13)	C14—C13—O3	121.4 (2)
C4—C3—C2	121.5 (2)	C14—C13—C12	119.4 (2)
C4—C3—H3c	119.23 (13)	C13—C14—C9	118.9 (2)
H4—C4—C3	119.61 (13)	C15—C14—C9	120.95 (19)
C5—C4—C3	120.8 (2)	C15—C14—C13	120.10 (19)
C5—C4—H4	119.61 (14)	O2—C15—O1	121.9 (2)
H5—C5—C4	121.09 (14)	C14—C15—O1	118.49 (18)
C6—C5—C4	117.8 (2)	C14—C15—O2	119.64 (19)
C6—C5—H5	121.09 (12)		

Cu1—O1—C15—O2	−0.95 (13)	N3—C7—N2—C1	178.8 (2)
Cu1—O1—C15—C14	−179.75 (10)	N3—C7—N2—C8	4.1 (3)
Cu1—N1—C6—C1	178.22 (18)	C1—C2—C3—C4	0.1 (3)
Cu1—N1—C6—C5	−2.4 (2)	C1—C6—N1—C7	−0.6 (2)
Cu1—N1—C7—N2	−178.35 (19)	C1—C6—C5—C4	0.0 (2)
Cu1—N1—C7—N3	2.8 (2)	C2—C1—N2—C7	179.4 (3)
O1—C15—C14—C9	−4.6 (2)	C2—C1—N2—C8	−5.8 (3)
O1—C15—C14—C13	173.06 (17)	C2—C1—C6—C5	1.4 (3)
O2—C15—C14—C9	176.60 (18)	C2—C3—C4—C5	1.2 (3)
O2—C15—C14—C13	−5.8 (2)	C3—C2—C1—C6	−1.4 (3)
O3—C13—C12—C11	−179.33 (19)	C3—C4—C5—C6	−1.2 (3)
O3—C13—C14—C9	179.50 (19)	C5—C6—N1—C7	178.7 (3)
O3—C13—C14—C15	1.8 (2)	C6—C1—N2—C7	−0.2 (2)
N1—C6—C1—N2	0.55 (18)	C6—C1—N2—C8	174.49 (18)
N1—C6—C1—C2	−179.18 (18)	C9—C10—C11—C12	0.2 (3)
N1—C6—C5—C4	−179.3 (3)	C9—C14—C13—C12	0.3 (2)
N1—C7—N2—C1	−0.2 (2)	C10—C9—C14—C13	−0.2 (2)
N1—C7—N2—C8	−174.86 (19)	C10—C9—C14—C15	177.42 (19)
N2—C1—C2—C3	178.9 (3)	C10—C11—C12—C13	−0.2 (3)

N2—C1—C6—C5	−178.89 (17)	C11—C10—C9—C14	0.0 (3)
N2—C7—N1—C6	0.5 (2)	C11—C12—C13—C14	−0.1 (3)
N3—C7—N1—C6	−178.4 (3)	C12—C13—C14—C15	−177.40 (18)

Symmetry code: (i) −*x*+1/2, −*y*+3/2, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O2	0.81 (1)	1.81 (1)	2.538 (2)	150 (1)
N3—H3*a*···O3^{ii}	0.88 (1)	2.33 (1)	3.046 (3)	139 (1)
N3—H3*b*···O1	0.88 (1)	2.49 (1)	3.020 (3)	119 (1)
C4—H4···O2^{iii}	0.95 (1)	2.57 (1)	3.373 (2)	143 (1)
C8—H8*c*···N3	0.98 (1)	2.56 (1)	2.957 (3)	104 (1)

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