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Chlorido(2-{(2-hydroxyethyl)[tris(hydroxymethyl)methyl]amino}ethanolato- $\kappa^5 N, O, O', O'', O'''$)-copper(II)

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Keywords: crystal structure; coordination compound; bis-tris; supramolecular structure; very strong hydrogen bonds.

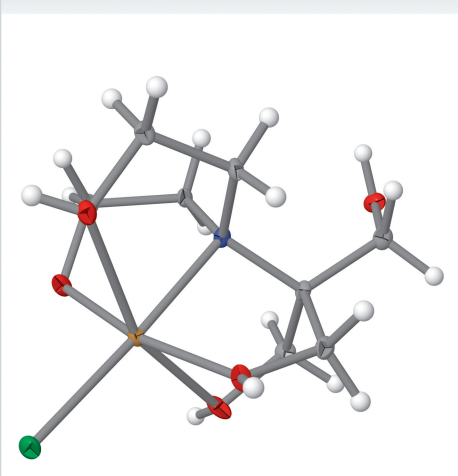
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Structural data: full structural data are available from iucrdata.iucr.org

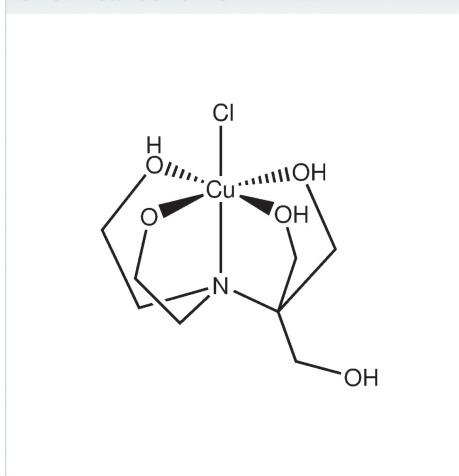
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The title complex, [Cu(C₈H₁₈NO₅)Cl] or [Cu(H₄bis-tris)Cl], was obtained starting from the previously reported [Cu(H₅bis-tris)Cl]Cl compound. The deprotonation of the aminopolyol ligand H₅bis-tris {[bis(2-hydroxyethyl)amino]tris(hydroxymethyl)methane, C₈H₁₉NO₅} promotes the formation of a very strong O—H...O intermolecular hydrogen bond, characterized by an H...O separation of 1.553 (19) Å and an O—H...O angle of 178 (4)°. The remaining hydroxy groups are also engaged in hydrogen bonds, forming R₂²(8), R₄⁴(16), R₄⁴(20) and R₄⁴(22) ring motifs, which stabilize the triperiodic supramolecular network.

3D view



Chemical scheme



Structure description

Aminopolyol [bis(2-hydroxyethyl)amino]tris(hydroxymethyl)methane, generally abbreviated H₅bis-tris, is able to coordinate first-row late transition metals and lanthanides (Nicholson *et al.*, 2001). This molecule behaves systematically as a chelating pentadentate ligand, through the tertiary N atom and four of the five alcohol arms. The metal coordination sphere is then completed with an ancillary ligand, frequently an aqua or a chlorido ligand. Furthermore, depending on the reaction conditions, H₅bis-tris can be deprotonated, affording chelating anions. While anions (H_{5-n}bis-tris)ⁿ⁻ with *n* = 2 to 4 have been determined by X-ray structure analysis in several compounds (*e.g.* Stamatatos *et al.*, 2009), it seems that to date the anionic ligand with *n* = 1, (H₄bis-tris)⁻, has been observed only once: Kirillova *et al.* (2017) reported a crystal structure comprising [Cu(H₅bis-tris)(inic)]⁺ and [Cu(H₄bis-tris)(inic)] entities, where inic stands for the isonicotinate anion. We now report the structure of the second complex where (H₄bis-

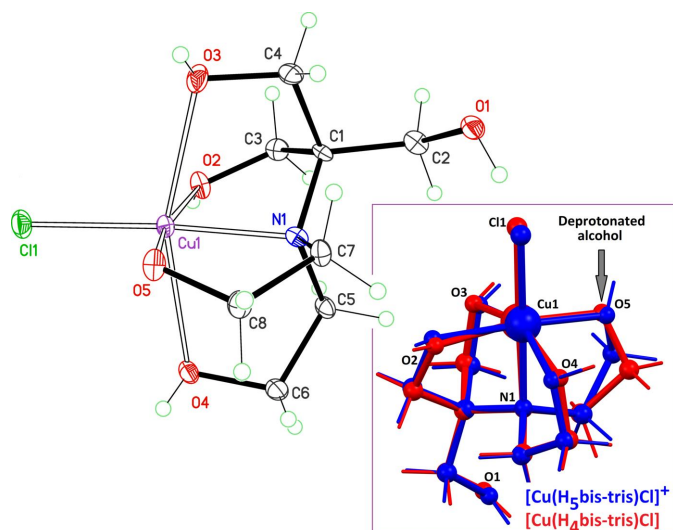


Figure 1
Molecular structure of the title compound, with displacement ellipsoids for non-H atoms at the 60% probability level. The inset is an overlay calculated with Mercury (Macrae *et al.*, 2020), comparing the shape of $[\text{Cu}(\text{H}_5\text{bis-tris})\text{Cl}]^+$ (blue) and the title complex $[\text{Cu}(\text{H}_4\text{bis-tris})\text{Cl}]$ (red). The crystal structure of $[\text{Cu}(\text{H}_5\text{bis-tris})\text{Cl}]\text{Cl}$ has been published (Inomata *et al.*, 2004; CCDC refcode FIPRAY); however, the authors did not deposit a CIF file at that time. A CSD communication for this compound was thus used for the fit (FIPRAY01; Fortis-Valera *et al.*, 2018).

tris^- acts as a ligand, namely $[\text{Cu}(\text{H}_4\text{bis-tris})\text{Cl}]$, which was obtained serendipitously from $[\text{Cu}(\text{H}_5\text{bis-tris})\text{Cl}]^+\text{Cl}$ (Inomata *et al.*, 2004).

The new Cu^{II} molecular complex displays the expected distorted octahedral shape (Fig. 1). Since all H atoms could be located from electron-difference maps, the deprotonated

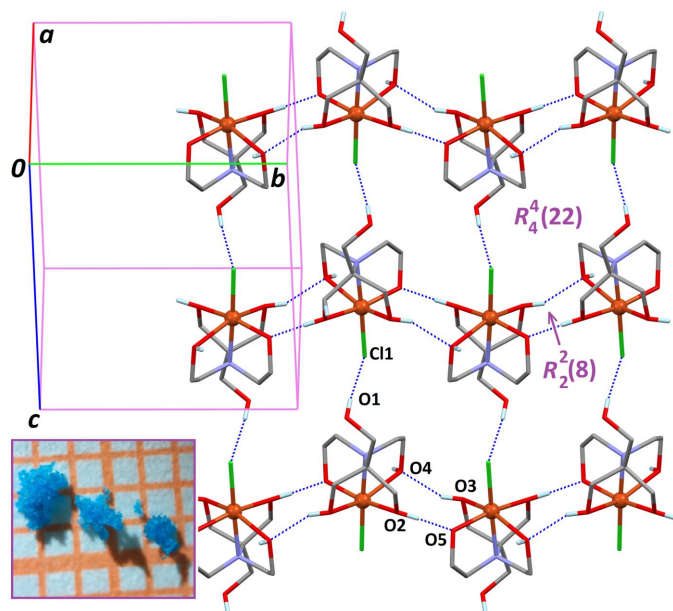


Figure 2
The supramolecular framework based on intermolecular $\text{O}-\text{H}\cdots(\text{O}, \text{Cl})$ hydrogen bonds (dashed blue lines) corresponding to entries 1–3 in Table 1. The inset shows single crystals suitable for X-ray diffraction.

Table 1
Hydrogen-bond geometry (\AA , $^\circ$).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O1}-\text{H1}\cdots\text{Cl1}^{\text{i}}$	0.83 (2)	2.24 (2)	3.068 (2)	174 (4)
$\text{O2}-\text{H2}\cdots\text{O5}^{\text{ii}}$	0.86 (2)	1.55 (2)	2.408 (3)	178 (4)
$\text{O3}-\text{H3}\cdots\text{O4}^{\text{iii}}$	0.82 (2)	2.00 (2)	2.758 (3)	154 (4)
$\text{O4}-\text{H4}\cdots\text{O1}^{\text{iv}}$	0.82 (2)	1.85 (2)	2.663 (3)	171 (4)

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

alcohol group was clearly identified as being O5. Moreover, the anion formula for $(\text{H}_4\text{bis-tris})^-$ is consistent with the charge balance in the complex. The tetragonal distortion resulting from the Jahn–Teller effect for Cu^{II} increases bond lengths $\text{Cu1}-\text{O3}$ and $\text{Cu1}-\text{O4}$ [2.361 (3) and 2.436 (2) \AA] in comparison with bond lengths in the equatorial plane $\text{N1}/\text{O2}/\text{O5}/\text{Cl1}$ [1.943 (2) to 2.2812 (10) \AA]. The shape of the neutral molecule $[\text{Cu}(\text{H}_4\text{bis-tris})\text{Cl}]$ is actually close to that observed for the cation $[\text{Cu}(\text{H}_5\text{bis-tris})\text{Cl}]^+$: a molecular overlay gives a root-mean-square (r.m.s.) deviation of 0.28 \AA and a maximum deviation of 0.91 \AA (Fig. 1, inset).

The space group and the network of hydrogen bonds are however modified upon deprotonation of $\text{H}_5\text{bis-tris}$. In the new complex, all hydroxy groups are donors for hydrogen bonding, and the deprotonated hydroxy group, O5, is an acceptor (Table 1). The latter is engaged in the strongest interaction, $\text{O2}-\text{H2}\cdots\text{O5}$, with a very short $\text{H2}\cdots\text{O5}$ distance of 1.553 (19) \AA and with an angle $\text{O2}-\text{H2}\cdots\text{O5} = 178 (4)^\circ$. Indeed, only few shorter intermolecular $\text{H}\cdots\text{O}$ separations

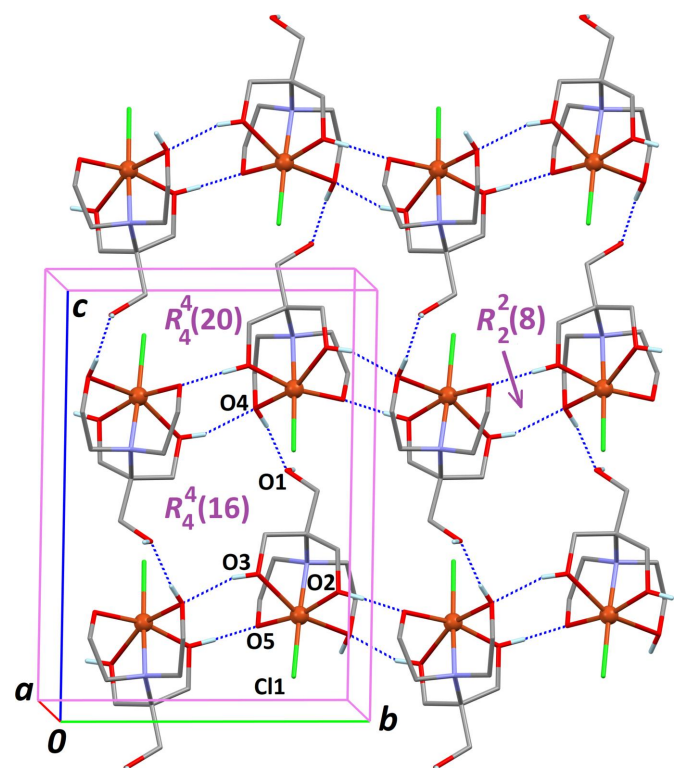


Figure 3
The supramolecular framework based on intermolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds (dashed blue lines) corresponding to entries 2–4 in Table 1.

can be retrieved from the Cambridge Structural Database (CSD v. 5.45, updated March 2024; Groom *et al.*, 2016) for $\text{CH}_2\text{—CH}_2\text{—O}\cdots\text{H—O}$ fragments (see, for example: Yilmaz *et al.*, 2002). Together with contact $\text{O3—H3}\cdots\text{O4}$, $R_2^2(8)$ ring motifs are formed in the crystal structure. Combined with another hydrogen bond involving the non-coordinating alcohol group, $\text{O1—H1}\cdots\text{Cl1}$, a diperiodic framework is formed parallel to (101), based on $R_2^2(8)$ and $R_4^4(22)$ supra-molecular motifs (Fig. 2). The last hydrogen bond, $\text{O4—H4}\cdots\text{O1}$, expands the supramolecular network through the formation of centrosymmetric $R_4^4(16)$ and $R_4^4(20)$ rings (Fig. 3), affording a stable triperiodic crystal structure.

Synthesis and crystallization

Single crystals of the title complex were unexpectedly obtained in an attempt to substitute the chlorido ligand in $[\text{Cu}(\text{H}_5\text{bis-tris})\text{Cl}]^+$ by a heterocyclic compound. Complex $[\text{Cu}(\text{H}_5\text{bis-tris})\text{Cl}]^+\text{Cl}^-$ (1 mmol, 0.343 g) and fluconazole (1 mmol, 0.307 g) were dissolved in ethanol (70% *v/v* solution, 15 ml). The mixture was heated to 323 K under stirring for 20 min, and filtered to eliminate a blue precipitate. The resulting solution was evaporated over 3 days, affording a blue product. The crude product was recrystallized in methanol, giving sky-blue crystals used for the diffraction study (see Fig. 2, inset).

Refinement

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

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Table 2

Experimental details.

Crystal data	
Chemical formula	$[\text{Cu}(\text{C}_8\text{H}_{18}\text{NO}_5)\text{Cl}]$
M_r	307.22
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	109
a, b, c (Å)	7.2605 (9), 10.4221 (14), 14.668 (2)
β (°)	94.366 (12)
V (Å ³)	1106.7 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	2.22
Crystal size (mm)	0.17 × 0.06 × 0.04
Data collection	
Diffractometer	Xcalibur, Atlas, Gemini
Absorption correction	Analytical (<i>CrysAlis PRO</i> ; Rigaku OD, 2022)
T_{\min}, T_{\max}	0.848, 0.917
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5523, 2582, 2002
R_{int}	0.046
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.694
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.048, 0.130, 1.05
No. of reflections	2582
No. of parameters	157
No. of restraints	4
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	1.18, -1.17

Computer programs: *CrysAlis PRO* (Rigaku OD, 2022), *SHELXT2018/2* (Sheldrick, 2015a), *SHELXL2018/3* (Sheldrick, 2015b), *XP* in *SHELXTL-Plus* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2020) and *pubCIF* (Westrip, 2010).

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full crystallographic data

IUCrData (2024). **9**, x240439 [https://doi.org/10.1107/S2414314624004395]

Chlorido(2-[(2-hydroxyethyl)[tris(hydroxymethyl)methyl]amino]ethanolato- $\kappa^5 N, O, O', O'', O'''$)copper(II)

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Chlorido(2-[(2-hydroxyethyl)[tris(hydroxymethyl)methyl]amino]ethanolato- $\kappa^5 N, O, O', O'', O'''$)copper(II)

Crystal data

[Cu(C₈H₁₈NO₅)Cl]

$M_r = 307.22$

Monoclinic, $P2_1/n$

$a = 7.2605$ (9) Å

$b = 10.4221$ (14) Å

$c = 14.668$ (2) Å

$\beta = 94.366$ (12)°

$V = 1106.7$ (3) Å³

$Z = 4$

$F(000) = 636$

$D_x = 1.844$ Mg m⁻³

Melting point: 435 K

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

Cell parameters from 1395 reflections

$\theta = 3.4$ – 29.6 °

$\mu = 2.22$ mm⁻¹

$T = 109$ K

Prism, blue

$0.17 \times 0.06 \times 0.04$ mm

Data collection

Xcalibur, Atlas, Gemini
diffractometer

Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator

Detector resolution: 10.4685 pixels mm⁻¹
 ω scans

Absorption correction: analytical
(CrysAlisPro; Rigaku OD, 2022)

$T_{\min} = 0.848$, $T_{\max} = 0.917$

5523 measured reflections

2582 independent reflections

2002 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.046$

$\theta_{\max} = 29.6$ °, $\theta_{\min} = 3.4$ °

$h = -9 \rightarrow 10$

$k = -14 \rightarrow 13$

$l = -18 \rightarrow 18$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.048$

$wR(F^2) = 0.130$

$S = 1.05$

2582 reflections

157 parameters

4 restraints

0 constraints

Primary atom site location: dual

Secondary atom site location: difference Fourier
map

Hydrogen site location: mixed

H atoms treated by a mixture of independent
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0646P)^2]$

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

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

$\Delta\rho_{\max} = 1.18$ e Å⁻³

$\Delta\rho_{\min} = -1.17$ e Å⁻³

Special details

Refinement. Methylene H atoms were refined using a riding model (C—H: 0.99 Å); hydroxy H atoms (H1, H2, H3, H4) were located from electron-difference maps and were refined freely, with the O—H bond lengths restrained to 0.85 (2) Å.

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

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
Cu1	0.22842 (5)	0.75373 (4)	0.75931 (3)	0.00775 (16)
Cl1	0.31899 (12)	0.76196 (8)	0.61387 (6)	0.0145 (2)
O1	0.2269 (3)	0.8024 (2)	1.09572 (16)	0.0130 (5)
H1	0.116 (3)	0.790 (4)	1.103 (3)	0.019*
O2	0.3908 (3)	0.6168 (2)	0.80600 (16)	0.0096 (5)
H2	0.407 (5)	0.539 (2)	0.790 (3)	0.014*
O3	0.4592 (3)	0.8730 (2)	0.84389 (17)	0.0143 (5)
H3	0.462 (5)	0.9507 (19)	0.836 (3)	0.022*
O4	−0.0338 (3)	0.6104 (2)	0.72784 (16)	0.0104 (5)
H4	−0.113 (4)	0.641 (4)	0.692 (2)	0.016*
O5	0.0620 (3)	0.8995 (2)	0.74310 (16)	0.0111 (5)
N1	0.1319 (4)	0.7390 (2)	0.8869 (2)	0.0075 (6)
C1	0.3128 (5)	0.7294 (3)	0.9443 (2)	0.0080 (7)
C2	0.2964 (5)	0.6976 (3)	1.0446 (2)	0.0121 (7)
H2A	0.213089	0.622927	1.048817	0.015*
H2B	0.419525	0.672641	1.072706	0.015*
C3	0.4235 (4)	0.6194 (3)	0.9021 (2)	0.0109 (7)
H3A	0.557130	0.631837	0.918562	0.013*
H3B	0.386836	0.536144	0.927768	0.013*
C4	0.4244 (4)	0.8542 (3)	0.9372 (2)	0.0104 (7)
H4A	0.353726	0.927666	0.959330	0.012*
H4B	0.542532	0.847779	0.975361	0.012*
C5	0.0232 (4)	0.6181 (3)	0.8917 (2)	0.0096 (7)
H5A	−0.039617	0.617991	0.949336	0.012*
H5B	0.109414	0.544400	0.893907	0.012*
C6	−0.1206 (4)	0.5993 (3)	0.8123 (2)	0.0118 (7)
H6A	−0.178021	0.513531	0.816363	0.014*
H6B	−0.218735	0.664857	0.814672	0.014*
C7	0.0172 (4)	0.8544 (3)	0.9019 (2)	0.0094 (7)
H7A	0.095096	0.922177	0.932473	0.011*
H7B	−0.081487	0.832157	0.942142	0.011*
C8	−0.0692 (4)	0.9044 (3)	0.8101 (2)	0.0114 (7)
H8A	−0.177933	0.851406	0.789966	0.014*
H8B	−0.111298	0.993927	0.817219	0.014*

Atomic displacement parameters (Å²)

	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³
Cu1	0.0099 (3)	0.0069 (2)	0.0065 (2)	0.00093 (15)	0.00096 (17)	0.00036 (15)
Cl1	0.0135 (4)	0.0219 (5)	0.0084 (4)	0.0024 (3)	0.0025 (3)	0.0011 (3)
O1	0.0108 (11)	0.0173 (13)	0.0108 (13)	−0.0005 (11)	0.0007 (9)	−0.0040 (11)

O2	0.0163 (11)	0.0046 (11)	0.0080 (12)	0.0047 (10)	0.0018 (9)	-0.0025 (10)
O3	0.0218 (12)	0.0108 (11)	0.0110 (13)	-0.0061 (11)	0.0049 (10)	0.0006 (11)
O4	0.0128 (11)	0.0111 (12)	0.0073 (12)	-0.0009 (10)	-0.0007 (9)	0.0000 (10)
O5	0.0154 (11)	0.0085 (11)	0.0100 (12)	0.0031 (10)	0.0037 (9)	0.0011 (10)
N1	0.0095 (13)	0.0039 (13)	0.0088 (14)	0.0006 (10)	-0.0011 (11)	-0.0011 (11)
C1	0.0085 (15)	0.0082 (15)	0.0070 (16)	-0.0009 (13)	-0.0022 (12)	-0.0015 (13)
C2	0.0128 (16)	0.0119 (16)	0.0114 (18)	0.0007 (14)	-0.0012 (13)	-0.0009 (15)
C3	0.0114 (15)	0.0090 (16)	0.0121 (18)	0.0007 (14)	-0.0011 (12)	0.0020 (14)
C4	0.0120 (15)	0.0078 (16)	0.0112 (18)	-0.0019 (14)	0.0001 (12)	-0.0028 (13)
C5	0.0119 (15)	0.0090 (15)	0.0075 (16)	-0.0004 (14)	-0.0013 (12)	0.0018 (14)
C6	0.0137 (15)	0.0113 (16)	0.0101 (17)	-0.0055 (14)	-0.0015 (12)	0.0021 (14)
C7	0.0102 (15)	0.0105 (16)	0.0076 (17)	0.0038 (13)	0.0010 (12)	0.0011 (13)
C8	0.0124 (15)	0.0115 (16)	0.0102 (17)	0.0004 (14)	0.0012 (12)	0.0014 (14)

Geometric parameters (Å, °)

Cu1—O2	1.943 (2)	C1—C4	1.540 (4)
Cu1—O5	1.944 (2)	C1—C3	1.556 (5)
Cu1—N1	2.054 (3)	C2—H2A	0.9900
Cu1—Cl1	2.2812 (10)	C2—H2B	0.9900
Cu1—O3	2.361 (3)	C3—H3A	0.9900
Cu1—O4	2.436 (2)	C3—H3B	0.9900
O1—C2	1.438 (4)	C4—H4A	0.9900
O1—H1	0.833 (19)	C4—H4B	0.9900
O2—C3	1.412 (4)	C5—C6	1.516 (4)
O2—H2	0.856 (19)	C5—H5A	0.9900
O3—C4	1.425 (4)	C5—H5B	0.9900
O3—H3	0.818 (19)	C6—H6A	0.9900
O4—C6	1.437 (4)	C6—H6B	0.9900
O4—H4	0.819 (18)	C7—C8	1.534 (5)
O5—C8	1.420 (4)	C7—H7A	0.9900
N1—C7	1.489 (4)	C7—H7B	0.9900
N1—C5	1.491 (4)	C8—H8A	0.9900
N1—C1	1.509 (4)	C8—H8B	0.9900
C1—C2	1.522 (5)		
O2—Cu1—O5	166.42 (10)	C1—C2—H2A	108.9
O2—Cu1—N1	82.17 (10)	O1—C2—H2B	108.9
O5—Cu1—N1	85.29 (10)	C1—C2—H2B	108.9
O2—Cu1—Cl1	98.45 (7)	H2A—C2—H2B	107.7
O5—Cu1—Cl1	94.41 (7)	O2—C3—C1	111.0 (3)
N1—Cu1—Cl1	176.13 (8)	O2—C3—H3A	109.4
O2—Cu1—O3	79.29 (9)	C1—C3—H3A	109.4
O5—Cu1—O3	93.57 (9)	O2—C3—H3B	109.4
N1—Cu1—O3	80.70 (10)	C1—C3—H3B	109.4
Cl1—Cu1—O3	103.18 (7)	H3A—C3—H3B	108.0
O2—Cu1—O4	93.48 (9)	O3—C4—C1	108.3 (3)
O5—Cu1—O4	89.25 (9)	O3—C4—H4A	110.0

N1—Cu1—O4	79.10 (10)	C1—C4—H4A	110.0
Cl1—Cu1—O4	97.04 (6)	O3—C4—H4B	110.0
O3—Cu1—O4	159.29 (9)	C1—C4—H4B	110.0
C2—O1—H1	110 (3)	H4A—C4—H4B	108.4
C3—O2—Cu1	112.91 (19)	N1—C5—C6	114.1 (3)
C3—O2—H2	106 (3)	N1—C5—H5A	108.7
Cu1—O2—H2	134 (3)	C6—C5—H5A	108.7
C4—O3—Cu1	105.16 (18)	N1—C5—H5B	108.7
C4—O3—H3	106 (3)	C6—C5—H5B	108.7
Cu1—O3—H3	118 (3)	H5A—C5—H5B	107.6
C6—O4—Cu1	105.88 (18)	O4—C6—C5	109.3 (3)
C6—O4—H4	105 (3)	O4—C6—H6A	109.8
Cu1—O4—H4	113 (3)	C5—C6—H6A	109.8
C8—O5—Cu1	112.74 (19)	O4—C6—H6B	109.8
C7—N1—C5	111.8 (3)	C5—C6—H6B	109.8
C7—N1—C1	116.3 (3)	H6A—C6—H6B	108.3
C5—N1—C1	111.1 (2)	N1—C7—C8	109.9 (3)
C7—N1—Cu1	107.9 (2)	N1—C7—H7A	109.7
C5—N1—Cu1	109.0 (2)	C8—C7—H7A	109.7
C1—N1—Cu1	99.8 (2)	N1—C7—H7B	109.7
N1—C1—C2	115.2 (3)	C8—C7—H7B	109.7
N1—C1—C4	110.3 (3)	H7A—C7—H7B	108.2
C2—C1—C4	109.3 (3)	O5—C8—C7	110.1 (3)
N1—C1—C3	106.3 (3)	O5—C8—H8A	109.6
C2—C1—C3	107.7 (3)	C7—C8—H8A	109.6
C4—C1—C3	107.8 (3)	O5—C8—H8B	109.6
O1—C2—C1	113.2 (3)	C7—C8—H8B	109.6
O1—C2—H2A	108.9	H8A—C8—H8B	108.1
C7—N1—C1—C2	72.7 (4)	C4—C1—C3—O2	-82.8 (3)
C5—N1—C1—C2	-56.7 (4)	Cu1—O3—C4—C1	22.4 (3)
Cu1—N1—C1—C2	-171.5 (2)	N1—C1—C4—O3	-60.1 (3)
C7—N1—C1—C4	-51.5 (4)	C2—C1—C4—O3	172.3 (3)
C5—N1—C1—C4	179.1 (3)	C3—C1—C4—O3	55.5 (3)
Cu1—N1—C1—C4	64.2 (3)	C7—N1—C5—C6	69.7 (4)
C7—N1—C1—C3	-168.1 (3)	C1—N1—C5—C6	-158.5 (3)
C5—N1—C1—C3	62.5 (3)	Cu1—N1—C5—C6	-49.5 (3)
Cu1—N1—C1—C3	-52.3 (3)	Cu1—O4—C6—C5	-28.5 (3)
N1—C1—C2—O1	-72.4 (3)	N1—C5—C6—O4	53.5 (4)
C4—C1—C2—O1	52.4 (4)	C5—N1—C7—C8	-91.3 (3)
C3—C1—C2—O1	169.2 (2)	C1—N1—C7—C8	139.7 (3)
Cu1—O2—C3—C1	2.2 (3)	Cu1—N1—C7—C8	28.6 (3)
N1—C1—C3—O2	35.5 (3)	Cu1—O5—C8—C7	34.4 (3)
C2—C1—C3—O2	159.4 (3)	N1—C7—C8—O5	-41.6 (4)

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>
O1—H1···Cl1 ⁱ	0.83 (2)	2.24 (2)	3.068 (2)	174 (4)
O2—H2···O5 ⁱⁱ	0.86 (2)	1.55 (2)	2.408 (3)	178 (4)
O3—H3···O4 ⁱⁱⁱ	0.82 (2)	2.00 (2)	2.758 (3)	154 (4)
O4—H4···O1 ^{iv}	0.82 (2)	1.85 (2)	2.663 (3)	171 (4)
C4—H4B···Cl1 ^v	0.99	2.97	3.906 (3)	157
C5—H5A···Cl1 ⁱ	0.99	2.97	3.887 (4)	155
C7—H7B···Cl1 ⁱ	0.99	2.85	3.727 (3)	148
C8—H8B···O1 ^{vi}	0.99	2.65	3.577 (4)	157

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