



Crystal structure of [bis(2-aminoethyl- κ N)(2-[[4-(trifluoromethyl)benzylidene]amino]ethyl)amine- κ N]dichloridocopper(II)

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Keywords: crystal structure; four-coordinate copper(II) complex; trifluoromethyl group analogue; ligand disorder

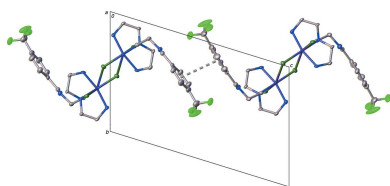
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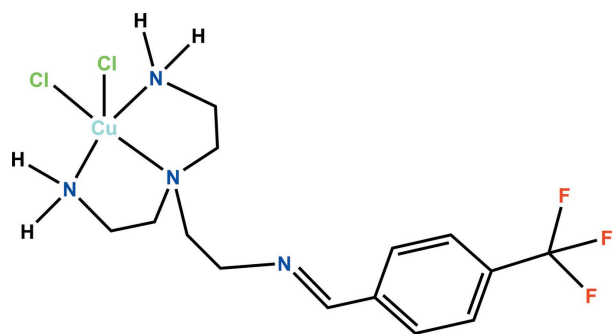
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The Cu^{II} atom in the title compound, [CuCl₂(C₁₄H₂₁F₃N₄)], adopts a coordination geometry that is between distorted square-based pyramidal and very Jahn–Teller-elongated octahedral. It is coordinated by three N atoms from the bis(2-aminoethyl)(2-[[4-(trifluoromethyl)benzylidene]amino]ethyl)amine and two chloride ligands. The two crystallographically unique copper complexes present in the asymmetric unit exhibit noticeable differences in the coordination bond lengths. Considering the Cu^{II} atoms as having square-pyramidal geometry, the basal Cu–Cl bond lengths are typical [2.2701 (12) and 2.2777 (12) Å], while the apical distances are considerably elongated [2.8505 (12) and 2.9415 (12) Å]. For each molecule, a Cu^{II} atom from inversion-related molecules are in nearby proximity to the remaining axial Cu^{II} sites, but the Cu···Cl distances are very long [3.4056 (12) and 3.1645 (12) Å], attributable to van der Waals contacts. Nonetheless, these contacts appear to have some structure-directing properties, leading to association into dimers. These dimers associate *via* stacking of the aromatic rings to form extended zigzag chains.

1. Chemical context

The introduction of a fluorine atom or perfluoroalkyl group into a compound can bring about significant changes in its physical, chemical, and biological properties, making organo-fluorine derivatives suitable for diverse applications in areas of material science, agrochemistry, and medicinal chemistry (Singh & Shreeve, 2000). Modifications include polarity and conformational changes, increased chemical or metabolic stability, and enhanced lipophilicity (Böhm *et al.*, 2004). As many as 30–40% of agrochemicals and 20% of pharmaceuticals on the market are estimated to contain fluorine, including three of the top eight drugs sold in 2007 (Dubinia *et al.*, 2008). Fluorination can also serve as a diagnostic tool, enabling techniques such as ¹⁹F NMR spectroscopy and positron emission tomography, with some organo-fluorine compounds exhibiting interesting NMR spectra (Purser *et al.*, 2008). The simplest perfluoroalkyl group, trifluoromethyl, has become an important structural component for many compounds, mainly because of its polar influence and effect on lipophilicity (Dolbier, 2009). Its electronegativity and relatively small size (only two and one-half times the volume of a methyl group) contribute to this behavior (Welch, 1987). As such, synthesis of simple and complex compounds incorporating fluorinated analogues of the methyl group has become a growing area of interest. In this context, we report the synthesis and crystal structure of the title compound [CuCl₂(C₁₄H₂₁N₄F₃)] (1).





2. Structural commentary

The asymmetric unit of the title compound contains two Cu–ligand complexes (Fig. 1). The coordination geometries of both Cu^{II} ions are between distorted square-based pyramidal and very Jahn–Teller-distorted octahedral. The first complex displays Cu–Cl bond lengths of 2.2701 (12) and 2.8505 (12) Å, while Cu–Cl lengths of 2.2777 (12) and 2.9415 (12) Å are observed in the second (Table 1, Fig. 2). Some studies suggest that copper(II) complexes adopting square-pyramidal geometries with apical Cu–L bonds longer than the basal bonds by up to 0.5 Å may not be due to Jahn–Teller distortion, but the result of a double electron occupancy of the antibonding *a₁* orbital and single occupancy of the *b₁* orbital, leading to increased anti-bonding electron density along the apical Cu–L axis (Rossi & Hoffmann, 1975). Copper(II) complexes with a square plane of ligand donors and one or two axial Cu–L interactions of 2.1–2.8 Å are very common (Murphy & Hathaway, 2003). Taking into consideration the covalent and van der Waals radii of copper (1.4 Å), an axial Cu–Cl bond length of less than 2.8 Å can be viewed as a genuine bond while bond lengths between 2.8–3.2 Å represent a weaker secondary interaction that is predominantly electrostatic in nature. Distances greater than 3.2 Å can be considered as purely van der Waals contacts (Halcrow, 2013). Following these criteria, it would seem that the inter-

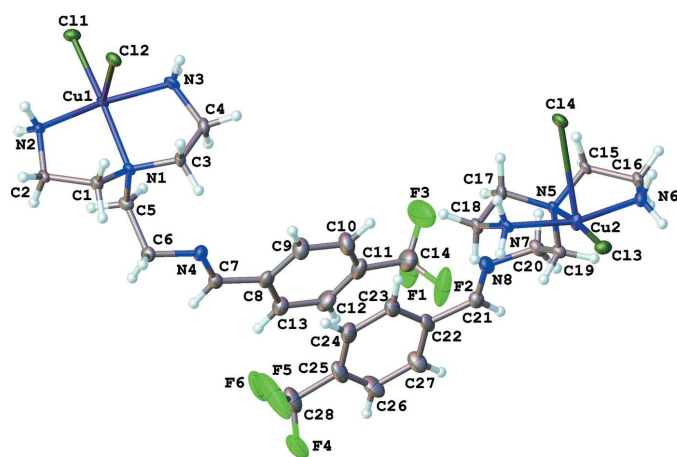


Figure 1
Asymmetric unit of the title compound, showing atomic displacement ellipsoids at the 50% probability level and the atom-numbering scheme.

Table 1
Selected geometric parameters (Å, °).

Cu1–N2	1.986 (3)	Cu2–N7	1.986 (4)
Cu1–N3	1.988 (4)	Cu2–N6	1.989 (4)
Cu1–N1	2.062 (4)	Cu2–N5	2.070 (4)
Cu1–Cl1	2.2701 (12)	Cu2–Cl3	2.2777 (12)
Cu1–Cl2	2.8505 (12)	Cu2–Cl4	2.9415 (12)
Cu1–Cl1 ⁱ	3.4056 (12)	Cu2–Cl3 ⁱⁱ	3.1645 (12)
N2–Cu1–N3	166.47 (15)	N7–Cu2–N6	163.80 (16)
N2–Cu1–N1	84.81 (14)	N7–Cu2–N5	85.50 (15)
N3–Cu1–N1	85.31 (14)	N6–Cu2–N5	85.18 (14)
N2–Cu1–Cl1	95.85 (11)	N7–Cu2–Cl3	95.55 (11)
N3–Cu1–Cl1	95.68 (11)	N6–Cu2–Cl3	95.56 (11)
N1–Cu1–Cl1	168.47 (11)	N5–Cu2–Cl3	171.82 (11)
N2–Cu1–Cl2	88.27 (11)	N7–Cu2–Cl4	81.07 (11)
N3–Cu1–Cl2	83.37 (11)	N6–Cu2–Cl4	86.35 (11)
N1–Cu1–Cl2	94.77 (10)	N5–Cu2–Cl4	93.74 (10)
Cl1–Cu1–Cl2	96.76 (4)	Cl3–Cu2–Cl4	94.44 (4)
N2–Cu1–Cl1 ⁱ	115.18 (11)	N7–Cu2–Cl3 ⁱⁱ	80.52 (11)
N3–Cu1–Cl1 ⁱ	74.19 (11)	N6–Cu2–Cl3 ⁱⁱ	113.16 (12)
N1–Cu1–Cl1 ⁱ	90.95 (10)	N5–Cu2–Cl3 ⁱⁱ	92.88 (10)
Cl1–Cu1–Cl1 ⁱ	78.32 (4)	Cl3–Cu2–Cl3 ⁱⁱ	79.32 (4)
Cl2–Cu1–Cl1 ⁱ	156.30 (3)	Cl4–Cu2–Cl3 ⁱⁱ	159.87 (3)

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

action observed between Cu2···Cl3ⁱⁱ [3.1645 (12) Å; symmetry code: (ii) $-x, -y, -z + 2$] is a weaker secondary interaction with electrostatic characteristics. However, an elongated Cu1···Cl2ⁱ distance of 3.4056 (12) Å is also observed, which can be attributed to a van der Waals contact [Halcrow, 2013; symmetry code: (i) $-x + 1, -y + 1, -z$]. These contacts appear to have some structure-directing properties, producing chlorine-bridged dimers in the crystal structure of (**1**).

3. Supramolecular features

In addition to electrostatic interactions observed in each complex, the aromatic rings engage in offset face-to-face π – π interactions with an observed centroid-to-centroid distance of 3.906 (3) Å and a dihedral angle of 10.6 (3)° (Fig. 3). Inspection of the extended structure shows that the orientation of these phenyl rings (C8–C13 and C22–C27) reduces interactions of the CF₃ groups associated with these rings. Coupled

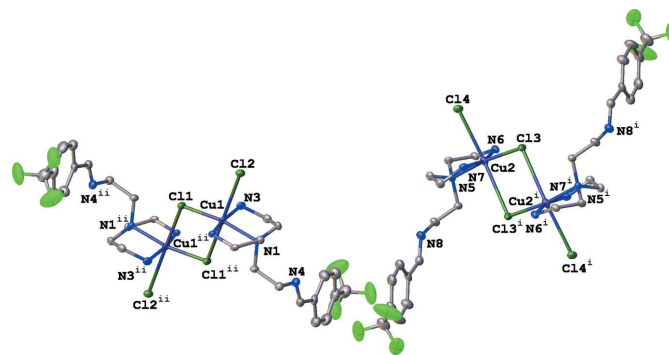
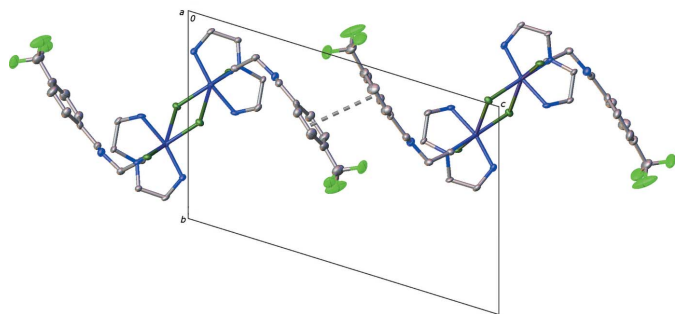


Figure 2
Dimer interactions between [CuCl₂(C₁₄H₂₁N₄F₃)] molecules, shown with 50% probability ellipsoids. H atoms were removed for clarity. Symmetry codes: (i) $-x + 1, -y + 1, -z$; (ii) $-x, -y, -z + 2$.


Figure 3

View along the a axis showing weak intermolecular interactions present in the crystal lattice. Atomic displacement ellipsoids depicted at 50% probability level with π - π interactions shown as dashed gray lines.

with the chlorine-bridged dimer we find that chains of molecules extend through the crystal parallel to the $[221]$ direction (Fig. 3).

Inspection of intermolecular/intramolecular contacts reveals that amine nitrogen atoms N2, N3, N6 and N7 are involved in $N-H\cdots Cl$ hydrogen-bonds (Table 2). However, several of the contacts [$N3\cdots Cl3^i$, $N3\cdots Cl2$, $N7\cdots Cl4$; symmetry code: (i) $-x + 1, -y + 1, -z$] have severely constrained $N-H\cdots Cl$ angles and are merely contacts to chlorine atoms bonded to the same Cu^{II} atom. The remaining hydrogen-bond contacts are intermolecular interactions, and while relatively long, they likely contribute to structure-directed organization.

4. Database survey

There are 318 structures that incorporate the *N*-2-bis(2-aminoethyl)aminoethyl ligand skeleton (Groom & Allen, 2014; CSD Version 5.36). Of those 318 structures, five incorporate one *para*-substituted benzene ring as presented in this article. Of those five, two have bromo-substituted phenyl rings displaying a nickel metal atom with perchlorate counter-ion

Table 2

 Hydrogen-bond geometry ($\text{\AA}, ^\circ$).

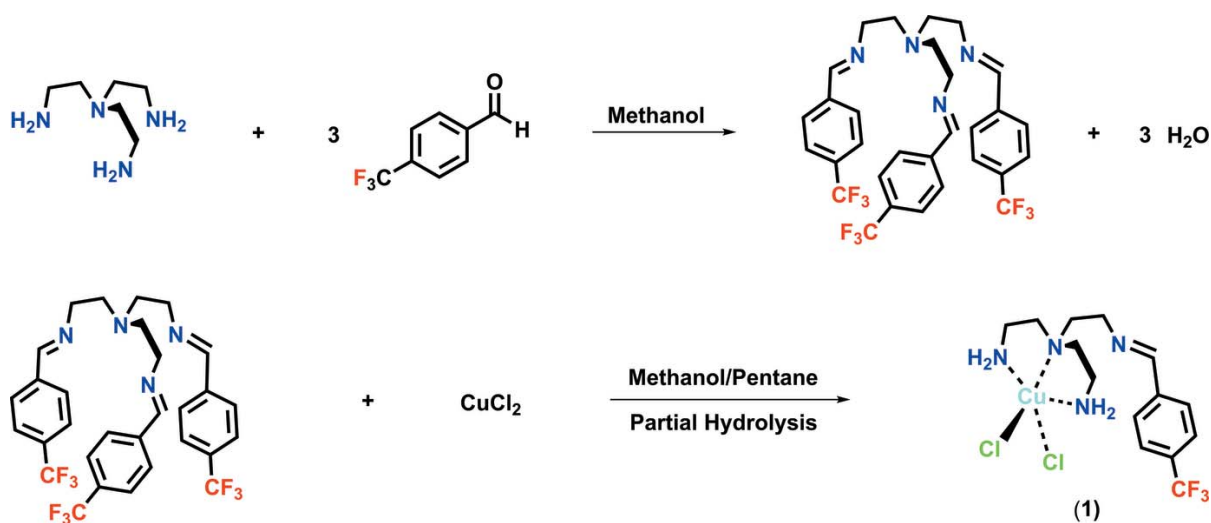
$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N2-H2A\cdots Cl3^{iii}$	0.91	2.84	3.591 (4)	141
$N2-H2B\cdots Cl4^{iv}$	0.91	2.46	3.365 (4)	171
$N3-H3A\cdots Cl1^i$	0.91	2.95	3.444 (4)	115
$N3-H3A\cdots Cl4^v$	0.91	2.60	3.334 (4)	139
$N3-H3B\cdots Cl2$	0.91	2.83	3.281 (4)	112
$N6-H6C\cdots Cl1^v$	0.91	2.96	3.681 (4)	138
$N6-H6D\cdots Cl2^{vi}$	0.91	2.45	3.342 (4)	167
$N7-H7A\cdots Cl2^{iii}$	0.91	2.57	3.348 (4)	143
$N7-H7B\cdots Cl4$	0.91	2.79	3.284 (4)	115

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

and a zinc metal atom with tetrafluoroborate counter-ion, respectively. Two display nitro-substituted phenyl rings with a copper metal atom and perchlorate counter-ions. Of those two, one contains a bidentate ligand with an ammonium derivative group not coordinating to the metal atom. The final structure is a zinc complex incorporating an unsubstituted phenyl ring with a perchlorate counter-ion. Of the 318 structures, none incorporates the trifluoromethyl-substituted phenyl group presented here and none displays the dichloride counterions presented here. A survey of $Cu-Cl$ bond-length elongations of similar structures in the literature produced examples such as 2.6061 (18) and 2.609 (2) \AA (Tucker *et al.*, 1991), 2.843 (1) to 3.140 (1) \AA (Krysiak *et al.*, 2014), 2.665 (3) and 2.731 (2) \AA (Ferrari *et al.*, 1998) and 2.7546 (9) \AA (Odoko *et al.*, 2002).

5. Synthesis and crystallization

Synthesis of tris(2-(4-trifluoromethylbenzylideneamino)ethyl)amine ligand: In a drybox, *tris*(2-(amino)ethyl)amine (2.56 mL, 17.10 mmol) was dissolved in 100 mL methanol in a 250 mL round-bottom flask (Fig. 4). Ligand precursor 4-(trifluoromethyl)benzaldehyde (6.90 mL, 51.29 mmol) was added


Figure 4

Synthetic scheme for $[Cu(C_{14}H_{21}N_4Cl_2F_3)(Cl_2)]$

Table 3
Experimental details.

Crystal data	
Chemical formula	[CuCl ₂ (C ₁₄ H ₂₁ F ₃ N ₄)]
<i>M_r</i>	436.80
Crystal system, space group	Triclinic, <i>P</i> $\bar{1}$
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	9.8506 (6), 11.0603 (7), 17.8574 (12)
α , β , γ (°)	73.110 (3), 75.530 (2), 89.010 (2)
<i>V</i> (Å ³)	1799.4 (2)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	1.54
Crystal size (mm)	0.30 × 0.19 × 0.05
Data collection	
Diffraction	Broker AXS D8 Quest CMOS
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2013)
<i>T_{min}</i> , <i>T_{max}</i>	0.573, 0.746
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	49937, 8937, 7063
<i>R_{int}</i>	0.079
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.073, 0.151, 1.22
No. of reflections	8937
No. of parameters	433
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	1.32, -0.74

Computer programs: *APEX2* and *SAINTE* (Bruker, 2013), *SHELXS97* (Sheldrick, 2008), *SHELXL* (Sheldrick, 2015), *CrystalMaker* (Palmer, 2007) and *OLEX2* (Dolomanov et al., 2009), *pubCIF* (Westrip, 2010), and *PLATON* (Spek, 2009).

to the flask to give a light-yellow colored solution. Reaction was sealed and allowed to mix for 48 h producing a clear yellow solution. Solvent was removed using a rotary evaporator and dried under vacuum for one h to yield a yellow solid (10.40 g, 99%). ¹H NMR (CDCl₃, 500 MHz): δ 2.94 (*t*, *J* = 7.6 Hz, 2H), 3.70 (*t*, *J* = 7.5 Hz, 2H), 7.56 (*br*, 2H), 8.08 (*s*, 1H). ¹³C NMR (CDCl₃, 500 MHz): δ 55.62, 60.32, 122.85 (*q*), 125.73 (*q*), 128.35, 132.44 (*q*), 139.62, 160.42. FT-IR (solid) ν (cm⁻¹): 1321 (*s*), 1169 (*s*), 1118 (*s*), 1062 (*s*), 834 (*s*). Melting Point: 344 K. TOF-ESI-MS: (*m/z*) [*M* + (*H*)]⁺ calculated for C₃₀H₂₈N₄F₉ = 615.2165, found 615.2194 (4.8 p.p.m.).

Synthesis of 2-(4-trifluoromethylbenzylideneamino)ethylamine-bis(2-aminoethyl)amine copper(II) chloride complex: *tris*(2-(4-Trifluoromethylbenzylideneamino)ethyl)amine (1.000 g, 1.63 mmol) was dissolved in 20 mL methanol in a 100 mL round-bottom flask. CuCl₂ (0.219 g, 1.63 mmol) was added to the flask to give a teal-colored solution. The reaction was allowed to mix for six h then 20 mL of pentane was slowly added to the solution to generate a teal-colored precipitate. Solvent was removed from the round-bottom flask by connecting it to a rotary evaporator. The precipitate obtained was washed twice by transferring 15 mL of pentane into the flask and stirring vigorously for thirty minutes. Solvent was removed and precipitate dried under vacuum for one h to yield a teal-colored solid (1.140 g, 93%). FT-IR (solid): ν (cm⁻¹) = 1636 (*m*), 1506 (*s*), 1473 (*s*), 1317 (*s*), 1163 (*s*), 1109 (*br*), 830 (*s*). UV-Vis (MeOH) λ_{\max} = 668 nm. TOF-ESI-MS: (*m/z*) [*M* - 2(Cl)]²⁺ calculated for C₃₀H₂₇N₄F₉Cu = 677.1383,

found 677.1381 (0.2 p.p.m.). Blue single crystal plates suitable for X-ray analysis were obtained by slow diffusion of diethyl ether into a complex solution made in acetonitrile at room temperature. The structure obtained is indicative of hydrolysis occurring on two amine positions of the intended copper(II) complex.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. Hydrogen atoms were placed at calculated positions and constrained to ride on their parent atoms with *U*_{iso}(H) = 1.2*U*_{eq}(C,N) for methylene, aromatic and amide groups with C–H distances set at 0.99 Å (methylene), 0.95 Å (aromatic) and N–H = 0.91 Å.

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References

- Böhm, H. J., Banner, D., Bendels, S., Kansy, M., Kuhn, B., Müller, K., Obst-Sander, U. & Stahl, M. (2004). *ChemBioChem*, **5**, 637–643.
- Bruker (2013). *APEX2*, *SAINTE*, and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Dolbier, W. R. (2009). *Guide to Fluorine NMR for Organic Chemists*, ch. 5, pp. 137–176. Hoboken: John Wiley and Sons.
- Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
- Dubinina, G. G., Ogikubo, J. & Vivic, D. A. (2008). *Organometallics*, **27**, 6233–6235.
- Ferrari, M. B., Fava, G. G., Loporati, E., Pelosi, G. K., Rossi, R., Tarasconi, P., Albertini, R., Bonati, A., Lunghi, P. & Pinelli, S. (1998). *J. Inorg. Biochem.* **70**, 145–154.
- Groom, C. R. & Allen, F. H. (2014). *Angew. Chem. Int. Ed.* **53**, 662–671.
- Halcrow, M. A. (2013). *Chem. Soc. Rev.* **42**, 1784–1795.
- Krysiak, Y., Fink, L., Bernert, T., Glinemann, J., Kapuscinski, M., Zhao, H., Alig, E. & Schmidt, M. U. (2014). *Z. Anorg. Allg. Chem.* **640**, 3190–3196.
- Murphy, B. & Hathaway, B. (2003). *Coord. Chem. Rev.* **243**, 2370–262.
- Odoko, M., Yamamoto, K. & Okabe, N. (2002). *Acta Cryst.* **C58**, m506–m508.
- Palmer, D. (2007). *CrystalMaker*. CrystalMaker Software, Bicester, England.
- Purser, S., Moore, P. R., Swallow, S. & Gouverneur, V. (2008). *Chem. Soc. Rev.* **37**, 320–330.
- Rossi, A. R. & Hoffmann, R. (1975). *Inorg. Chem.* **14**, 365–374.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Sheldrick, G. M. (2015). *Acta Cryst.* **C71**, 3–8.
- Singh, R. P. & Shreeve, J. M. (2000). *Tetrahedron*, **56**, 7613–7632.
- Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.
- Tucker, D. A., White, P. S., Trojan, K. L., Kirk, M. J. & Hatfield, W. E. (1991). *Inorg. Chem.* **30**, 823–826.
- Welch, J. T. (1987). *Tetrahedron*, **43**, 3123–3197.
- Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supporting information

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Crystal structure of [bis(2-aminoethyl- κ N)(2-{[4-(trifluoromethyl)benzylidene]amino}ethyl)amine- κ N]dichloridocopper(II)

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Computing details

Data collection: *APEX2* (Bruker, 2013); cell refinement: *SAINTE* (Bruker, 2013); data reduction: *SAINTE* (Bruker, 2013); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015); molecular graphics: *CrystalMaker* (Palmer, 2007) and *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009), *publCIF* (Westrip, 2010) and *PLATON* (Spek, 2009).

[Bis(2-aminoethyl- κ N)(2-{[4-(trifluoromethyl)benzylidene]amino}ethyl)amine- κ N]dichloridocopper(II)

Crystal data

[CuCl₂(C₁₄H₂₁F₃N₄)]
 $M_r = 436.80$
 Triclinic, $P\bar{1}$
 $a = 9.8506$ (6) Å
 $b = 11.0603$ (7) Å
 $c = 17.8574$ (12) Å
 $\alpha = 73.110$ (3)°
 $\beta = 75.530$ (2)°
 $\gamma = 89.010$ (2)°
 $V = 1799.4$ (2) Å³

$Z = 4$
 $F(000) = 892$
 $D_x = 1.612$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 9961 reflections
 $\theta = 2.5$ – 28.3 °
 $\mu = 1.54$ mm⁻¹
 $T = 100$ K
 Plate, blue
 $0.30 \times 0.19 \times 0.05$ mm

Data collection

Bruker AXS D8 Quest CMOS
 diffractometer
 Radiation source: I- μ -S microsource X-ray
 tube
 Laterally graded multilayer (Goebel) mirror
 monochromator
 ω and ϕ scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2013)

$T_{\min} = 0.573$, $T_{\max} = 0.746$
 49937 measured reflections
 8937 independent reflections
 7063 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.079$
 $\theta_{\max} = 28.3$ °, $\theta_{\min} = 2.5$ °
 $h = -13 \rightarrow 13$
 $k = -14 \rightarrow 14$
 $l = -23 \rightarrow 23$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.073$
 $wR(F^2) = 0.151$

$S = 1.22$
 8937 reflections
 433 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
 $w = 1/[\sigma^2(F_o^2) + (0.0341P)^2 + 8.3032P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 1.32 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.74 \text{ e } \text{\AA}^{-3}$

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.37014 (6)	0.32211 (5)	0.07300 (3)	0.01576 (13)
Cl1	0.34574 (11)	0.47852 (10)	-0.03695 (7)	0.0181 (2)
Cl2	0.08223 (11)	0.23298 (9)	0.13230 (7)	0.0178 (2)
N1	0.4341 (4)	0.1932 (3)	0.1650 (2)	0.0148 (7)
N2	0.4034 (4)	0.1876 (3)	0.0182 (2)	0.0153 (7)
H2A	0.3259	0.1748	0.0018	0.018*
H2B	0.4768	0.2135	-0.0265	0.018*
N3	0.3162 (4)	0.4228 (3)	0.1506 (2)	0.0180 (8)
H3A	0.3559	0.5029	0.1269	0.022*
H3B	0.2213	0.4275	0.1638	0.022*
N4	0.6465 (4)	0.1886 (4)	0.2797 (2)	0.0220 (8)
C1	0.3888 (5)	0.0696 (4)	0.1598 (3)	0.0165 (8)
H1A	0.2853	0.0565	0.1796	0.020*
H1B	0.4309	0.0006	0.1945	0.020*
C2	0.4347 (4)	0.0663 (4)	0.0728 (3)	0.0157 (8)
H2C	0.5367	0.0540	0.0581	0.019*
H2D	0.3841	-0.0054	0.0666	0.019*
C3	0.3557 (5)	0.2219 (4)	0.2404 (3)	0.0173 (9)
H3C	0.3981	0.1805	0.2855	0.021*
H3D	0.2566	0.1893	0.2555	0.021*
C4	0.3632 (5)	0.3641 (4)	0.2247 (3)	0.0200 (9)
H4A	0.3018	0.3866	0.2712	0.024*
H4B	0.4607	0.3951	0.2175	0.024*
C5	0.5900 (4)	0.2083 (4)	0.1504 (3)	0.0171 (9)
H5A	0.6154	0.2982	0.1425	0.020*
H5B	0.6343	0.1892	0.0993	0.020*
C6	0.6539 (5)	0.1267 (4)	0.2166 (3)	0.0192 (9)
H6A	0.6021	0.0428	0.2407	0.023*
H6B	0.7530	0.1136	0.1927	0.023*
C7	0.7616 (5)	0.2140 (4)	0.2922 (3)	0.0207 (9)
H7	0.8456	0.1851	0.2650	0.025*
C8	0.7687 (5)	0.2881 (4)	0.3484 (3)	0.0229 (10)
C9	0.6476 (6)	0.3277 (5)	0.3926 (3)	0.0317 (12)

H9	0.5578	0.2990	0.3917	0.038*
C10	0.6578 (6)	0.4083 (6)	0.4375 (4)	0.0380 (13)
H10	0.5750	0.4342	0.4679	0.046*
C11	0.7877 (7)	0.4513 (5)	0.4381 (3)	0.0339 (12)
C12	0.9094 (6)	0.4099 (6)	0.3972 (4)	0.0365 (13)
H12	0.9987	0.4374	0.3993	0.044*
C13	0.8989 (6)	0.3276 (5)	0.3529 (3)	0.0296 (11)
H13	0.9818	0.2978	0.3254	0.036*
C14	0.7966 (7)	0.5463 (6)	0.4827 (4)	0.0439 (15)
F1	0.9161 (5)	0.6165 (4)	0.4552 (2)	0.0643 (13)
F2	0.7837 (6)	0.4938 (4)	0.5606 (2)	0.0708 (14)
F3	0.6983 (6)	0.6312 (5)	0.4752 (4)	0.093 (2)
Cu2	-0.05556 (6)	0.17013 (5)	0.92597 (3)	0.01768 (14)
Cl3	-0.18291 (11)	0.01387 (10)	1.03343 (7)	0.0185 (2)
Cl4	-0.30093 (11)	0.26904 (10)	0.86714 (7)	0.0194 (2)
N5	0.0850 (4)	0.3019 (3)	0.8338 (2)	0.0139 (7)
N6	-0.0796 (4)	0.3026 (4)	0.9827 (2)	0.0175 (7)
H6C	-0.1725	0.3161	0.9980	0.021*
H6D	-0.0480	0.2753	1.0281	0.021*
N7	-0.0460 (4)	0.0769 (3)	0.8452 (2)	0.0172 (8)
H7A	-0.0292	-0.0054	0.8669	0.021*
H7B	-0.1297	0.0788	0.8320	0.021*
N8	0.4024 (4)	0.3011 (4)	0.7164 (2)	0.0242 (9)
C15	0.0291 (5)	0.4249 (4)	0.8417 (3)	0.0162 (8)
H15A	-0.0582	0.4383	0.8232	0.019*
H15B	0.0986	0.4951	0.8073	0.019*
C16	-0.0011 (5)	0.4240 (4)	0.9293 (3)	0.0170 (9)
H16A	0.0882	0.4326	0.9437	0.020*
H16B	-0.0576	0.4963	0.9372	0.020*
C17	0.0714 (5)	0.2776 (4)	0.7581 (3)	0.0176 (9)
H17A	0.1522	0.3193	0.7125	0.021*
H17B	-0.0158	0.3123	0.7447	0.021*
C18	0.0672 (5)	0.1352 (4)	0.7717 (3)	0.0190 (9)
H18A	0.0483	0.1155	0.7244	0.023*
H18B	0.1585	0.1018	0.7788	0.023*
C19	0.2302 (4)	0.2903 (4)	0.8443 (3)	0.0165 (8)
H19A	0.2529	0.2006	0.8532	0.020*
H19B	0.2315	0.3122	0.8941	0.020*
C20	0.3469 (5)	0.3718 (4)	0.7746 (3)	0.0214 (10)
H20A	0.3091	0.4512	0.7471	0.026*
H20B	0.4233	0.3941	0.7960	0.026*
C21	0.5325 (5)	0.2848 (4)	0.7024 (3)	0.0221 (10)
H21	0.5900	0.3247	0.7249	0.027*
C22	0.5967 (5)	0.2040 (5)	0.6508 (3)	0.0240 (10)
C23	0.5150 (6)	0.1411 (5)	0.6187 (3)	0.0288 (11)
H23	0.4183	0.1565	0.6248	0.035*
C24	0.5744 (6)	0.0561 (5)	0.5779 (3)	0.0330 (12)
H24	0.5180	0.0109	0.5577	0.040*

C25	0.7162 (6)	0.0377 (5)	0.5668 (3)	0.0327 (12)
C26	0.7993 (6)	0.1014 (6)	0.5960 (4)	0.0394 (14)
H26	0.8970	0.0888	0.5872	0.047*
C27	0.7394 (6)	0.1846 (5)	0.6383 (4)	0.0327 (12)
H27	0.7963	0.2285	0.6589	0.039*
C28	0.7789 (7)	-0.0583 (6)	0.5239 (4)	0.0425 (15)
F4	0.8768 (6)	-0.1210 (4)	0.5533 (3)	0.0730 (14)
F5	0.8382 (6)	-0.0061 (4)	0.4467 (3)	0.0854 (18)
F6	0.6850 (5)	-0.1463 (6)	0.5298 (5)	0.113 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0205 (3)	0.0126 (2)	0.0166 (3)	0.0093 (2)	-0.0060 (2)	-0.0075 (2)
Cl1	0.0154 (5)	0.0155 (5)	0.0217 (5)	0.0018 (4)	-0.0058 (4)	-0.0018 (4)
Cl2	0.0161 (5)	0.0132 (4)	0.0255 (6)	0.0022 (4)	-0.0049 (4)	-0.0085 (4)
N1	0.0167 (18)	0.0127 (16)	0.0169 (18)	0.0045 (14)	-0.0048 (14)	-0.0070 (14)
N2	0.0155 (17)	0.0170 (17)	0.0157 (18)	0.0062 (14)	-0.0055 (14)	-0.0076 (14)
N3	0.0206 (19)	0.0086 (16)	0.026 (2)	0.0037 (14)	-0.0063 (16)	-0.0061 (15)
N4	0.025 (2)	0.025 (2)	0.019 (2)	0.0040 (16)	-0.0080 (16)	-0.0085 (16)
C1	0.020 (2)	0.0135 (19)	0.017 (2)	0.0017 (16)	-0.0043 (17)	-0.0063 (16)
C2	0.015 (2)	0.017 (2)	0.020 (2)	0.0068 (16)	-0.0071 (17)	-0.0125 (17)
C3	0.021 (2)	0.018 (2)	0.013 (2)	0.0043 (17)	-0.0015 (16)	-0.0077 (17)
C4	0.020 (2)	0.024 (2)	0.020 (2)	0.0028 (18)	-0.0043 (18)	-0.0136 (19)
C5	0.014 (2)	0.015 (2)	0.022 (2)	0.0019 (16)	-0.0045 (17)	-0.0069 (17)
C6	0.020 (2)	0.018 (2)	0.022 (2)	0.0014 (17)	-0.0075 (18)	-0.0094 (18)
C7	0.024 (2)	0.020 (2)	0.018 (2)	0.0044 (18)	-0.0048 (18)	-0.0066 (18)
C8	0.032 (3)	0.021 (2)	0.014 (2)	-0.0002 (19)	-0.0067 (19)	-0.0018 (18)
C9	0.031 (3)	0.037 (3)	0.029 (3)	-0.001 (2)	-0.005 (2)	-0.016 (2)
C10	0.042 (3)	0.043 (3)	0.036 (3)	0.007 (3)	-0.007 (3)	-0.024 (3)
C11	0.055 (4)	0.028 (3)	0.025 (3)	0.003 (2)	-0.018 (3)	-0.011 (2)
C12	0.041 (3)	0.041 (3)	0.035 (3)	0.001 (3)	-0.020 (3)	-0.014 (3)
C13	0.033 (3)	0.034 (3)	0.026 (3)	0.005 (2)	-0.010 (2)	-0.013 (2)
C14	0.053 (4)	0.046 (4)	0.046 (4)	0.010 (3)	-0.024 (3)	-0.025 (3)
F1	0.108 (4)	0.045 (2)	0.045 (2)	-0.023 (2)	-0.017 (2)	-0.0216 (19)
F2	0.121 (4)	0.062 (3)	0.031 (2)	-0.032 (3)	-0.012 (2)	-0.0215 (19)
F3	0.114 (4)	0.085 (4)	0.142 (5)	0.048 (3)	-0.082 (4)	-0.086 (4)
Cu2	0.0214 (3)	0.0159 (3)	0.0160 (3)	-0.0060 (2)	-0.0010 (2)	-0.0079 (2)
Cl3	0.0143 (5)	0.0183 (5)	0.0204 (5)	0.0000 (4)	-0.0045 (4)	-0.0019 (4)
Cl4	0.0191 (5)	0.0137 (5)	0.0277 (6)	0.0046 (4)	-0.0064 (4)	-0.0094 (4)
N5	0.0182 (18)	0.0102 (16)	0.0143 (18)	0.0026 (13)	-0.0037 (14)	-0.0056 (14)
N6	0.0166 (18)	0.0214 (19)	0.0157 (18)	-0.0010 (14)	-0.0026 (14)	-0.0086 (15)
N7	0.0180 (18)	0.0117 (17)	0.025 (2)	0.0040 (14)	-0.0063 (15)	-0.0089 (15)
N8	0.023 (2)	0.026 (2)	0.022 (2)	0.0042 (16)	-0.0009 (16)	-0.0093 (17)
C15	0.019 (2)	0.0127 (19)	0.020 (2)	0.0063 (16)	-0.0040 (17)	-0.0097 (17)
C16	0.016 (2)	0.019 (2)	0.020 (2)	0.0005 (16)	-0.0025 (17)	-0.0126 (18)
C17	0.023 (2)	0.018 (2)	0.015 (2)	0.0040 (17)	-0.0042 (17)	-0.0103 (17)
C18	0.023 (2)	0.017 (2)	0.020 (2)	0.0055 (17)	-0.0045 (18)	-0.0114 (18)

C19	0.016 (2)	0.0143 (19)	0.020 (2)	0.0024 (16)	-0.0044 (17)	-0.0062 (17)
C20	0.020 (2)	0.018 (2)	0.025 (2)	0.0025 (17)	0.0001 (18)	-0.0085 (19)
C21	0.026 (2)	0.020 (2)	0.019 (2)	0.0013 (18)	-0.0044 (19)	-0.0053 (18)
C22	0.028 (3)	0.024 (2)	0.015 (2)	0.0053 (19)	0.0034 (18)	-0.0053 (19)
C23	0.032 (3)	0.033 (3)	0.021 (2)	0.008 (2)	-0.004 (2)	-0.011 (2)
C24	0.039 (3)	0.039 (3)	0.021 (3)	0.006 (2)	-0.005 (2)	-0.012 (2)
C25	0.036 (3)	0.030 (3)	0.026 (3)	0.005 (2)	0.005 (2)	-0.011 (2)
C26	0.025 (3)	0.041 (3)	0.049 (4)	0.008 (2)	0.003 (2)	-0.020 (3)
C27	0.026 (3)	0.033 (3)	0.039 (3)	0.001 (2)	-0.001 (2)	-0.016 (2)
C28	0.043 (3)	0.043 (3)	0.040 (3)	0.006 (3)	0.004 (3)	-0.024 (3)
F4	0.109 (4)	0.060 (3)	0.058 (3)	0.053 (3)	-0.021 (3)	-0.031 (2)
F5	0.145 (5)	0.065 (3)	0.033 (2)	0.053 (3)	0.002 (3)	-0.019 (2)
F6	0.062 (3)	0.106 (4)	0.195 (7)	-0.007 (3)	0.016 (4)	-0.124 (5)

Geometric parameters (Å, °)

Cu1—N2	1.986 (3)	Cu2—N7	1.986 (4)
Cu1—N3	1.988 (4)	Cu2—N6	1.989 (4)
Cu1—N1	2.062 (4)	Cu2—N5	2.070 (4)
Cu1—Cl1	2.2701 (12)	Cu2—Cl3	2.2777 (12)
Cu1—Cl2	2.8505 (12)	Cu2—Cl4	2.9415 (12)
Cu1—Cl1 ⁱ	3.4056 (12)	Cu2—Cl3 ⁱⁱ	3.1645 (12)
N1—C1	1.480 (5)	N5—C19	1.486 (5)
N1—C3	1.493 (5)	N5—C15	1.491 (5)
N1—C5	1.496 (5)	N5—C17	1.491 (5)
N2—C2	1.491 (5)	N6—C16	1.494 (6)
N2—H2A	0.9100	N6—H6C	0.9100
N2—H2B	0.9100	N6—H6D	0.9100
N3—C4	1.478 (6)	N7—C18	1.478 (6)
N3—H3A	0.9100	N7—H7A	0.9100
N3—H3B	0.9100	N7—H7B	0.9100
N4—C7	1.260 (6)	N8—C21	1.263 (6)
N4—C6	1.466 (6)	N8—C20	1.470 (6)
C1—C2	1.518 (6)	C15—C16	1.515 (6)
C1—H1A	0.9900	C15—H15A	0.9900
C1—H1B	0.9900	C15—H15B	0.9900
C2—H2C	0.9900	C16—H16A	0.9900
C2—H2D	0.9900	C16—H16B	0.9900
C3—C4	1.516 (6)	C17—C18	1.522 (6)
C3—H3C	0.9900	C17—H17A	0.9900
C3—H3D	0.9900	C17—H17B	0.9900
C4—H4A	0.9900	C18—H18A	0.9900
C4—H4B	0.9900	C18—H18B	0.9900
C5—C6	1.529 (6)	C19—C20	1.534 (6)
C5—H5A	0.9900	C19—H19A	0.9900
C5—H5B	0.9900	C19—H19B	0.9900
C6—H6A	0.9900	C20—H20A	0.9900
C6—H6B	0.9900	C20—H20B	0.9900

C7—C8	1.482 (6)	C21—C22	1.488 (6)
C7—H7	0.9500	C21—H21	0.9500
C8—C13	1.390 (7)	C22—C27	1.390 (7)
C8—C9	1.397 (7)	C22—C23	1.394 (8)
C9—C10	1.381 (8)	C23—C24	1.386 (7)
C9—H9	0.9500	C23—H23	0.9500
C10—C11	1.377 (9)	C24—C25	1.381 (8)
C10—H10	0.9500	C24—H24	0.9500
C11—C12	1.385 (9)	C25—C26	1.373 (9)
C11—C14	1.506 (8)	C25—C28	1.519 (7)
C12—C13	1.387 (8)	C26—C27	1.389 (8)
C12—H12	0.9500	C26—H26	0.9500
C13—H13	0.9500	C27—H27	0.9500
C14—F2	1.317 (8)	C28—F4	1.306 (8)
C14—F1	1.323 (8)	C28—F5	1.312 (7)
C14—F3	1.341 (8)	C28—F6	1.318 (8)
N2—Cu1—N3	166.47 (15)	N7—Cu2—N6	163.80 (16)
N2—Cu1—N1	84.81 (14)	N7—Cu2—N5	85.50 (15)
N3—Cu1—N1	85.31 (14)	N6—Cu2—N5	85.18 (14)
N2—Cu1—Cl1	95.85 (11)	N7—Cu2—Cl3	95.55 (11)
N3—Cu1—Cl1	95.68 (11)	N6—Cu2—Cl3	95.56 (11)
N1—Cu1—Cl1	168.47 (11)	N5—Cu2—Cl3	171.82 (11)
N2—Cu1—Cl2	88.27 (11)	N7—Cu2—Cl4	81.07 (11)
N3—Cu1—Cl2	83.37 (11)	N6—Cu2—Cl4	86.35 (11)
N1—Cu1—Cl2	94.77 (10)	N5—Cu2—Cl4	93.74 (10)
Cl1—Cu1—Cl2	96.76 (4)	Cl3—Cu2—Cl4	94.44 (4)
N2—Cu1—Cl1 ⁱ	115.18 (11)	N7—Cu2—Cl3 ⁱⁱ	80.52 (11)
N3—Cu1—Cl1 ⁱ	74.19 (11)	N6—Cu2—Cl3 ⁱⁱ	113.16 (12)
N1—Cu1—Cl1 ⁱ	90.95 (10)	N5—Cu2—Cl3 ⁱⁱ	92.88 (10)
Cl1—Cu1—Cl1 ⁱ	78.32 (4)	Cl3—Cu2—Cl3 ⁱⁱ	79.32 (4)
Cl2—Cu1—Cl1 ⁱ	156.30 (3)	Cl4—Cu2—Cl3 ⁱⁱ	159.87 (3)
C1—N1—C3	113.3 (3)	C19—N5—C15	111.4 (3)
C1—N1—C5	112.1 (3)	C19—N5—C17	113.2 (3)
C3—N1—C5	112.9 (3)	C15—N5—C17	112.4 (3)
C1—N1—Cu1	103.3 (3)	C19—N5—Cu2	111.7 (3)
C3—N1—Cu1	104.8 (2)	C15—N5—Cu2	102.9 (3)
C5—N1—Cu1	109.8 (3)	C17—N5—Cu2	104.7 (3)
C2—N2—Cu1	111.7 (3)	C16—N6—Cu2	111.2 (3)
C2—N2—H2A	109.3	C16—N6—H6C	109.4
Cu1—N2—H2A	109.3	Cu2—N6—H6C	109.4
C2—N2—H2B	109.3	C16—N6—H6D	109.4
Cu1—N2—H2B	109.3	Cu2—N6—H6D	109.4
H2A—N2—H2B	107.9	H6C—N6—H6D	108.0
C4—N3—Cu1	110.5 (3)	C18—N7—Cu2	110.0 (3)
C4—N3—H3A	109.5	C18—N7—H7A	109.7
Cu1—N3—H3A	109.5	Cu2—N7—H7A	109.7
C4—N3—H3B	109.5	C18—N7—H7B	109.7

Cu1—N3—H3B	109.5	Cu2—N7—H7B	109.7
H3A—N3—H3B	108.1	H7A—N7—H7B	108.2
C7—N4—C6	116.6 (4)	C21—N8—C20	116.4 (4)
N1—C1—C2	109.9 (4)	N5—C15—C16	109.5 (4)
N1—C1—H1A	109.7	N5—C15—H15A	109.8
C2—C1—H1A	109.7	C16—C15—H15A	109.8
N1—C1—H1B	109.7	N5—C15—H15B	109.8
C2—C1—H1B	109.7	C16—C15—H15B	109.8
H1A—C1—H1B	108.2	H15A—C15—H15B	108.2
N2—C2—C1	109.4 (3)	N6—C16—C15	109.5 (3)
N2—C2—H2C	109.8	N6—C16—H16A	109.8
C1—C2—H2C	109.8	C15—C16—H16A	109.8
N2—C2—H2D	109.8	N6—C16—H16B	109.8
C1—C2—H2D	109.8	C15—C16—H16B	109.8
H2C—C2—H2D	108.2	H16A—C16—H16B	108.2
N1—C3—C4	108.3 (4)	N5—C17—C18	108.2 (4)
N1—C3—H3C	110.0	N5—C17—H17A	110.0
C4—C3—H3C	110.0	C18—C17—H17A	110.0
N1—C3—H3D	110.0	N5—C17—H17B	110.0
C4—C3—H3D	110.0	C18—C17—H17B	110.0
H3C—C3—H3D	108.4	H17A—C17—H17B	108.4
N3—C4—C3	108.1 (4)	N7—C18—C17	107.7 (3)
N3—C4—H4A	110.1	N7—C18—H18A	110.2
C3—C4—H4A	110.1	C17—C18—H18A	110.2
N3—C4—H4B	110.1	N7—C18—H18B	110.2
C3—C4—H4B	110.1	C17—C18—H18B	110.2
H4A—C4—H4B	108.4	H18A—C18—H18B	108.5
N1—C5—C6	116.6 (4)	N5—C19—C20	116.6 (4)
N1—C5—H5A	108.1	N5—C19—H19A	108.2
C6—C5—H5A	108.1	C20—C19—H19A	108.2
N1—C5—H5B	108.1	N5—C19—H19B	108.2
C6—C5—H5B	108.1	C20—C19—H19B	108.2
H5A—C5—H5B	107.3	H19A—C19—H19B	107.3
N4—C6—C5	110.1 (4)	N8—C20—C19	109.5 (4)
N4—C6—H6A	109.6	N8—C20—H20A	109.8
C5—C6—H6A	109.6	C19—C20—H20A	109.8
N4—C6—H6B	109.6	N8—C20—H20B	109.8
C5—C6—H6B	109.6	C19—C20—H20B	109.8
H6A—C6—H6B	108.1	H20A—C20—H20B	108.2
N4—C7—C8	121.4 (4)	N8—C21—C22	120.6 (5)
N4—C7—H7	119.3	N8—C21—H21	119.7
C8—C7—H7	119.3	C22—C21—H21	119.7
C13—C8—C9	118.8 (5)	C27—C22—C23	119.1 (5)
C13—C8—C7	119.6 (4)	C27—C22—C21	119.5 (5)
C9—C8—C7	121.5 (5)	C23—C22—C21	121.3 (4)
C10—C9—C8	120.3 (5)	C24—C23—C22	120.2 (5)
C10—C9—H9	119.9	C24—C23—H23	119.9
C8—C9—H9	119.9	C22—C23—H23	119.9

C11—C10—C9	120.1 (5)	C25—C24—C23	119.5 (5)
C11—C10—H10	120.0	C25—C24—H24	120.2
C9—C10—H10	120.0	C23—C24—H24	120.2
C10—C11—C12	120.7 (5)	C26—C25—C24	121.1 (5)
C10—C11—C14	119.3 (6)	C26—C25—C28	120.0 (5)
C12—C11—C14	120.0 (6)	C24—C25—C28	118.8 (5)
C11—C12—C13	119.0 (5)	C25—C26—C27	119.4 (5)
C11—C12—H12	120.5	C25—C26—H26	120.3
C13—C12—H12	120.5	C27—C26—H26	120.3
C12—C13—C8	121.0 (5)	C26—C27—C22	120.5 (5)
C12—C13—H13	119.5	C26—C27—H27	119.7
C8—C13—H13	119.5	C22—C27—H27	119.7
F2—C14—F1	105.8 (5)	F4—C28—F5	105.2 (5)
F2—C14—F3	107.4 (6)	F4—C28—F6	104.6 (6)
F1—C14—F3	103.8 (6)	F5—C28—F6	107.6 (6)
F2—C14—C11	113.2 (5)	F4—C28—C25	113.6 (6)
F1—C14—C11	113.8 (6)	F5—C28—C25	112.7 (5)
F3—C14—C11	112.1 (5)	F6—C28—C25	112.5 (5)
C3—N1—C1—C2	161.1 (3)	C19—N5—C15—C16	-71.4 (4)
C5—N1—C1—C2	-69.8 (4)	C17—N5—C15—C16	160.5 (4)
Cu1—N1—C1—C2	48.3 (4)	Cu2—N5—C15—C16	48.4 (4)
Cu1—N2—C2—C1	17.1 (4)	Cu2—N6—C16—C15	19.9 (4)
N1—C1—C2—N2	-44.7 (5)	N5—C15—C16—N6	-46.7 (5)
C1—N1—C3—C4	-156.5 (4)	C19—N5—C17—C18	77.8 (4)
C5—N1—C3—C4	74.8 (4)	C15—N5—C17—C18	-155.0 (4)
Cu1—N1—C3—C4	-44.7 (4)	Cu2—N5—C17—C18	-44.0 (4)
Cu1—N3—C4—C3	-33.0 (4)	Cu2—N7—C18—C17	-35.9 (4)
N1—C3—C4—N3	52.3 (5)	N5—C17—C18—N7	54.0 (5)
C1—N1—C5—C6	-70.5 (5)	C15—N5—C19—C20	-72.8 (5)
C3—N1—C5—C6	58.9 (5)	C17—N5—C19—C20	55.0 (5)
Cu1—N1—C5—C6	175.4 (3)	Cu2—N5—C19—C20	172.7 (3)
C7—N4—C6—C5	-120.4 (4)	C21—N8—C20—C19	-122.6 (5)
N1—C5—C6—N4	-84.7 (5)	N5—C19—C20—N8	-89.7 (4)
C6—N4—C7—C8	173.7 (4)	C20—N8—C21—C22	173.9 (4)
N4—C7—C8—C13	-172.1 (5)	N8—C21—C22—C27	-178.1 (5)
N4—C7—C8—C9	3.0 (7)	N8—C21—C22—C23	-1.9 (7)
C13—C8—C9—C10	2.4 (8)	C27—C22—C23—C24	2.8 (8)
C7—C8—C9—C10	-172.7 (5)	C21—C22—C23—C24	-173.4 (5)
C8—C9—C10—C11	0.7 (9)	C22—C23—C24—C25	-2.3 (8)
C9—C10—C11—C12	-3.1 (9)	C23—C24—C25—C26	0.4 (9)
C9—C10—C11—C14	175.8 (6)	C23—C24—C25—C28	178.4 (5)
C10—C11—C12—C13	2.3 (9)	C24—C25—C26—C27	0.9 (9)
C14—C11—C12—C13	-176.6 (5)	C28—C25—C26—C27	-177.0 (6)
C11—C12—C13—C8	0.9 (8)	C25—C26—C27—C22	-0.4 (9)
C9—C8—C13—C12	-3.2 (8)	C23—C22—C27—C26	-1.5 (8)
C7—C8—C13—C12	172.0 (5)	C21—C22—C27—C26	174.8 (5)
C10—C11—C14—F2	84.1 (7)	C26—C25—C28—F4	34.7 (8)

C12—C11—C14—F2	-97.1 (7)	C24—C25—C28—F4	-143.3 (6)
C10—C11—C14—F1	-155.1 (6)	C26—C25—C28—F5	-84.8 (8)
C12—C11—C14—F1	23.8 (8)	C24—C25—C28—F5	97.2 (7)
C10—C11—C14—F3	-37.6 (9)	C26—C25—C28—F6	153.2 (7)
C12—C11—C14—F3	141.2 (6)	C24—C25—C28—F6	-24.8 (9)

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2A \cdots Cl3 ⁱⁱⁱ	0.91	2.84	3.591 (4)	141
N2—H2B \cdots Cl4 ^{iv}	0.91	2.46	3.365 (4)	171
N3—H3A \cdots Cl1 ⁱ	0.91	2.95	3.444 (4)	115
N3—H3A \cdots Cl4 ^v	0.91	2.60	3.334 (4)	139
N3—H3B \cdots Cl2	0.91	2.83	3.281 (4)	112
N6—H6C \cdots Cl1 ^v	0.91	2.96	3.681 (4)	138
N6—H6D \cdots Cl2 ^{vi}	0.91	2.45	3.342 (4)	167
N7—H7A \cdots Cl2 ⁱⁱⁱ	0.91	2.57	3.348 (4)	143
N7—H7B \cdots Cl4	0.91	2.79	3.284 (4)	115

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