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## Structure Reports

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(1-{2-[2-(2-Ammonioethylamino)ethyl-amino]ethyliminomethyl}-2-naphtholato-κ<sup>4</sup>O,N,N',N''})chloridocopper(II) chloride

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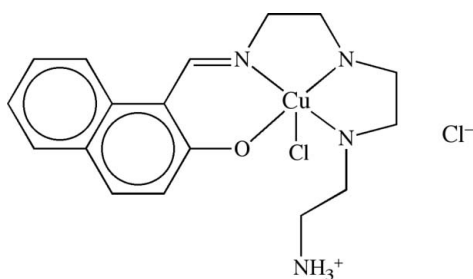
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Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.034;  $wR$  factor = 0.099; data-to-parameter ratio = 14.7.

In the square-pyramidal title complex,  $[\text{CuCl}(\text{C}_{17}\text{H}_{24}\text{N}_4\text{O})]\text{Cl}$ , the  $\text{Cu}^{\text{II}}$  atom is coordinated by three N atoms  $[\text{Cu}-\text{N}$  1.946 (2), 2.010 (2), 2.085 (3) Å], one O atom  $[\text{Cu}-\text{O}$  1.910 (2) Å] and one apical Cl atom  $[\text{Cu}-\text{Cl}$  2.6437 (9) Å]. The three coordinated N and one O atom are almost coplanar, with a maximum deviation of 0.0268 Å. The tetradentate ligand forms two five-membered (N—Cu—N) and one six-membered (N—Cu—O) chelate rings with bite angles of 84.06 (10), 85.30 (10) and 91.70 (9)°, respectively. The two N—Cu—N chelate rings are non-planar.

## Related literature

For the general role of Schiff bases, see: Gamovski *et al.* (1993). For the crystal structures of related complexes, see: Nanda *et al.* (2006).



## Experimental

## Crystal data

$[\text{CuCl}(\text{C}_{17}\text{H}_{24}\text{N}_4\text{O})]\text{Cl}$   
 $M_r = 434.84$

Monoclinic,  $P2_1/c$   
 $a = 12.2687$  (17) Å

$b = 13.0277$  (18) Å  
 $c = 12.7118$  (18) Å  
 $\beta = 111.365$  (2)°  
 $V = 1892.1$  (5) Å<sup>3</sup>  
 $Z = 4$

Mo  $K\alpha$  radiation  
 $\mu = 1.45$  mm<sup>-1</sup>  
 $T = 298$  (2) K  
 $0.48 \times 0.40 \times 0.37$  mm

## Data collection

Bruker SMART CCD area-detector diffractometer  
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)  
 $T_{\text{min}} = 0.543$ ,  $T_{\text{max}} = 0.616$   
 (expected range = 0.515–0.585)

9597 measured reflections  
 3320 independent reflections  
 2646 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.027$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.034$   
 $wR(F^2) = 0.099$   
 $S = 1.00$   
 3320 reflections

226 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.59$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.40$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2 $\cdots$ Cl2 <sup>i</sup>	0.91	2.44	3.225 (3)	144
N3—H3 $\cdots$ Cl1 <sup>ii</sup>	0.91	2.50	3.388 (3)	165
N4—H4A $\cdots$ Cl1 <sup>iii</sup>	0.89	2.31	3.204 (3)	177
N4—H4B $\cdots$ Cl2 <sup>ii</sup>	0.89	2.25	3.079 (4)	156
N4—H4C $\cdots$ O1	0.89	1.83	2.703 (4)	167

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LN2007).

## References

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**supplementary materials**

*Acta Cryst.* (2008). E64, m118 [ doi:10.1107/S1600536807064033 ]

**(1-{2-[2-(2-Ammonioethylamino)ethylamino]ethyliminomethyl}-2-naphtholato- $\kappa^4$ O,N,N',N''}chloridocopper(II) chloride**

**R. Xue and M. Niu**

**Comment**

Schiff base complexes play an important role in coordination chemistry (Gamovski *et al.*, 1993). In a continuation of a study of Schiff base ligands and their copper(II) complexes, we report here the title complex (Fig. 1), in which the ligand donor atoms consist of three nitrogen atoms (one imine and two amine) and one phenolic oxygen atom. Another Cu<sup>II</sup> complex containing the same tetradentate ligand has been reported by Nanda *et al.* (2006). In the crystal structure of (I), intermolecular N—H...Cl hydrogen bonds involving all amine and the ammonium groups link the molecules into two-dimensional networks, which lie parallel to the (100) plane (Table 1, Fig. 2). The ammonium group also forms an intramolecular hydrogen bond with the phenolic O atom.

**Experimental**

A solution of triethylenetetramine(1 mmol) in hot methanol (10 ml) was added dropwise to a methanol solution (5 ml) of 2-hydroxy-1-naphthaldehyde (2 mmol, 344.3 mg). The mixture was then stirred at 323 K for 2 h. An aqueous solution (2 ml) of cupric chloride dihydrate (1 mmol, 170.8 mg) was then added dropwise and the mixture stirred for another 5 h. The solution was held at room temperature for about one week, whereupon green prism-shaped crystals suitable for X-ray diffraction analysis were obtained (m.p. > 573 K).

**Refinement**

All H atoms were placed in geometrically idealized positions and refined using a riding model, with C—H = 0.97 Å (methylene) or 0.93 Å (aromatic, methenyl), N—H = 0.91 Å (imine) or 0.89 Å (ammonium) and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  or  $1.5U_{\text{eq}}(\text{N})$ .

**Figures**

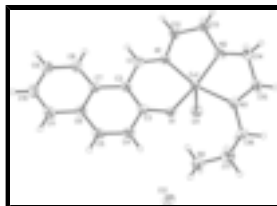


Fig. 1. The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms.

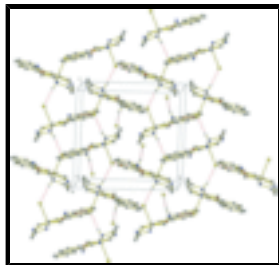


Fig. 2. Crystal packing of the title complex showing the hydrogen bonding interactions as dashed lines.

**(1-{2-[2-(2-Ammonioethylamino)ethylamino]ethyliminomethyl}-2-naphtholato- $\kappa^4$ O,N,N',N''})chloridocopper(II) chloride**

*Crystal data*

[CuCl(C<sub>17</sub>H<sub>24</sub>N<sub>4</sub>O)]Cl

$M_r = 434.84$

Monoclinic,  $P2_1/c$

$a = 12.2687$  (17) Å

$b = 13.0277$  (18) Å

$c = 12.7118$  (18) Å

$\beta = 111.365$  (2)°

$V = 1892.1$  (5) Å<sup>3</sup>

$Z = 4$

$F_{000} = 900$

$D_x = 1.526$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 3813 reflections

$\theta = 2.5$ – $26.7$ °

$\mu = 1.45$  mm<sup>-1</sup>

$T = 298$  (2) K

Block, green

$0.48 \times 0.40 \times 0.37$  mm

*Data collection*

Bruker CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298$ (2) K

phi and  $\omega$  scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.543$ ,  $T_{\max} = 0.616$

9597 measured reflections

3320 independent reflections

2646 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.027$

$\theta_{\text{max}} = 25.0$ °

$\theta_{\text{min}} = 1.8$ °

$h = -14 \rightarrow 14$

$k = -15 \rightarrow 12$

$l = -14 \rightarrow 15$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.034$

$wR(F^2) = 0.099$

$S = 1.00$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0538P)^2 + 1.3872P]$

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

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

3320 reflections  $\Delta\rho_{\max} = 0.59 \text{ e } \text{\AA}^{-3}$   
 226 parameters  $\Delta\rho_{\min} = -0.40 \text{ e } \text{\AA}^{-3}$   
 Primary atom site location: structure-invariant direct methods Extinction correction: none

*Special details*

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.70712 (3)	0.22917 (3)	0.92710 (3)	0.03282 (14)
Cl1	0.59641 (8)	0.15391 (7)	0.72264 (7)	0.0511 (2)
Cl2	0.26659 (9)	0.14202 (8)	0.07523 (10)	0.0662 (3)
N1	0.8689 (2)	0.22822 (18)	0.9363 (2)	0.0327 (6)
N2	0.7491 (2)	0.09353 (18)	1.0070 (2)	0.0342 (6)
H2	0.7261	0.0426	0.9545	0.041*
N3	0.5626 (2)	0.22573 (19)	0.9765 (2)	0.0377 (6)
H3	0.5809	0.2667	1.0385	0.045*
N4	0.4596 (3)	0.4130 (2)	0.8025 (3)	0.0599 (8)
H4A	0.4462	0.4803	0.7985	0.090*
H4B	0.4206	0.3844	0.7358	0.090*
H4C	0.5359	0.4017	0.8212	0.090*
O1	0.69138 (17)	0.37176 (15)	0.88974 (19)	0.0406 (5)
C1	0.9272 (3)	0.3033 (2)	0.9185 (2)	0.0328 (7)
H1	1.0057	0.2918	0.9308	0.039*
C2	0.8815 (2)	0.4046 (2)	0.8810 (2)	0.0304 (6)
C3	0.7695 (3)	0.4344 (2)	0.8753 (2)	0.0328 (7)
C4	0.7349 (3)	0.5390 (2)	0.8524 (3)	0.0400 (7)
H4	0.6622	0.5597	0.8519	0.048*
C5	0.8061 (3)	0.6090 (2)	0.8313 (3)	0.0418 (8)
H5	0.7816	0.6769	0.8181	0.050*
C6	0.9163 (3)	0.5815 (2)	0.8290 (3)	0.0372 (7)
C7	0.9567 (3)	0.4795 (2)	0.8561 (2)	0.0332 (7)
C8	1.0697 (3)	0.4563 (2)	0.8560 (3)	0.0438 (8)
H8	1.0987	0.3900	0.8728	0.053*
C9	1.1367 (3)	0.5298 (3)	0.8319 (3)	0.0502 (9)
H9	1.2108	0.5127	0.8333	0.060*
C10	1.0955 (3)	0.6301 (3)	0.8050 (3)	0.0499 (9)

## supplementary materials

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H10	1.1418	0.6794	0.7887	0.060*
C11	0.9881 (3)	0.6547 (3)	0.8030 (3)	0.0471 (8)
H11	0.9605	0.7213	0.7842	0.057*
C12	0.9279 (3)	0.1298 (2)	0.9797 (3)	0.0411 (8)
H12A	1.0116	0.1403	1.0163	0.049*
H12B	0.9145	0.0815	0.9182	0.049*
C13	0.8775 (3)	0.0893 (2)	1.0628 (3)	0.0395 (7)
H13A	0.9029	0.0192	1.0836	0.047*
H13B	0.9029	0.1310	1.1307	0.047*
C14	0.6823 (3)	0.0837 (3)	1.0821 (3)	0.0460 (8)
H14A	0.7172	0.1258	1.1490	0.055*
H14B	0.6820	0.0129	1.1055	0.055*
C15	0.5603 (3)	0.1189 (2)	1.0168 (3)	0.0470 (8)
H15A	0.5244	0.0738	0.9527	0.056*
H15B	0.5140	0.1163	1.0644	0.056*
C16	0.4418 (3)	0.2538 (3)	0.9023 (4)	0.0547 (10)
H16A	0.3873	0.2243	0.9333	0.066*
H16B	0.4255	0.2236	0.8284	0.066*
C17	0.4203 (4)	0.3678 (3)	0.8885 (4)	0.0680 (12)
H17A	0.3373	0.3808	0.8678	0.082*
H17B	0.4609	0.4012	0.9604	0.082*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cu1	0.0285 (2)	0.0288 (2)	0.0378 (2)	0.00173 (14)	0.00819 (16)	0.00456 (15)
Cl1	0.0517 (5)	0.0531 (5)	0.0416 (5)	-0.0067 (4)	0.0088 (4)	-0.0052 (4)
Cl2	0.0524 (6)	0.0529 (6)	0.0853 (7)	0.0006 (4)	0.0156 (5)	-0.0208 (5)
N1	0.0287 (13)	0.0297 (13)	0.0362 (14)	0.0036 (10)	0.0075 (11)	0.0021 (11)
N2	0.0332 (14)	0.0299 (13)	0.0334 (14)	-0.0002 (10)	0.0048 (11)	0.0015 (11)
N3	0.0373 (14)	0.0330 (14)	0.0456 (16)	-0.0008 (11)	0.0183 (12)	0.0041 (11)
N4	0.0419 (17)	0.0528 (19)	0.077 (2)	0.0075 (14)	0.0127 (16)	0.0175 (17)
O1	0.0283 (11)	0.0320 (12)	0.0581 (14)	0.0030 (9)	0.0117 (10)	0.0069 (10)
C1	0.0287 (15)	0.0347 (16)	0.0330 (16)	0.0019 (12)	0.0087 (13)	-0.0028 (13)
C2	0.0323 (15)	0.0295 (15)	0.0249 (15)	-0.0011 (12)	0.0050 (12)	-0.0033 (12)
C3	0.0349 (16)	0.0288 (15)	0.0304 (16)	-0.0018 (13)	0.0066 (13)	-0.0024 (12)
C4	0.0362 (17)	0.0326 (17)	0.047 (2)	0.0045 (13)	0.0108 (15)	0.0005 (14)
C5	0.048 (2)	0.0275 (16)	0.0448 (19)	0.0033 (14)	0.0114 (16)	0.0015 (14)
C6	0.0415 (18)	0.0325 (16)	0.0332 (17)	-0.0052 (13)	0.0083 (14)	-0.0007 (13)
C7	0.0345 (16)	0.0344 (16)	0.0258 (15)	-0.0035 (13)	0.0051 (13)	-0.0055 (12)
C8	0.0436 (19)	0.0414 (19)	0.047 (2)	-0.0032 (15)	0.0172 (16)	0.0012 (15)
C9	0.042 (2)	0.057 (2)	0.054 (2)	-0.0056 (16)	0.0204 (17)	0.0024 (17)
C10	0.053 (2)	0.051 (2)	0.047 (2)	-0.0159 (17)	0.0193 (18)	0.0033 (16)
C11	0.058 (2)	0.0377 (18)	0.0417 (19)	-0.0077 (16)	0.0135 (17)	0.0023 (15)
C12	0.0310 (17)	0.0336 (17)	0.054 (2)	0.0074 (13)	0.0098 (15)	0.0043 (14)
C13	0.0352 (17)	0.0320 (17)	0.0422 (18)	0.0044 (13)	0.0032 (14)	0.0063 (13)
C14	0.048 (2)	0.0414 (19)	0.049 (2)	0.0008 (15)	0.0181 (17)	0.0124 (16)
C15	0.047 (2)	0.0382 (18)	0.060 (2)	-0.0022 (15)	0.0240 (18)	0.0106 (16)

C16	0.0349 (19)	0.059 (2)	0.070 (3)	0.0065 (16)	0.0185 (18)	0.0179 (19)
C17	0.061 (3)	0.067 (3)	0.083 (3)	0.026 (2)	0.035 (2)	0.021 (2)

*Geometric parameters (Å, °)*

Cu1—O1	1.910 (2)	C5—H5	0.9300
Cu1—N1	1.946 (2)	C6—C7	1.415 (4)
Cu1—N2	2.010 (2)	C6—C11	1.417 (4)
Cu1—N3	2.085 (3)	C7—C8	1.420 (4)
Cu1—C11	2.6437 (9)	C8—C9	1.367 (5)
N1—C1	1.280 (4)	C8—H8	0.9300
N1—C12	1.477 (4)	C9—C10	1.398 (5)
N2—C14	1.472 (4)	C9—H9	0.9300
N2—C13	1.475 (4)	C10—C11	1.347 (5)
N2—H2	0.9100	C10—H10	0.9300
N3—C16	1.484 (4)	C11—H11	0.9300
N3—C15	1.487 (4)	C12—C13	1.502 (5)
N3—H3	0.9100	C12—H12A	0.9700
N4—C17	1.470 (5)	C12—H12B	0.9700
N4—H4A	0.8900	C13—H13A	0.9700
N4—H4B	0.8900	C13—H13B	0.9700
N4—H4C	0.8900	C14—C15	1.495 (5)
O1—C3	1.321 (3)	C14—H14A	0.9700
C1—C2	1.445 (4)	C14—H14B	0.9700
C1—H1	0.9300	C15—H15A	0.9700
C2—C3	1.404 (4)	C15—H15B	0.9700
C2—C7	1.455 (4)	C16—C17	1.507 (5)
C3—C4	1.426 (4)	C16—H16A	0.9700
C4—C5	1.355 (4)	C16—H16B	0.9700
C4—H4	0.9300	C17—H17A	0.9700
C5—C6	1.410 (4)	C17—H17B	0.9700
O1—Cu1—N1	91.70 (9)	C6—C7—C2	119.3 (3)
O1—Cu1—N2	164.83 (10)	C8—C7—C2	123.6 (3)
N1—Cu1—N2	84.06 (10)	C9—C8—C7	121.2 (3)
O1—Cu1—N3	94.34 (9)	C9—C8—H8	119.4
N1—Cu1—N3	160.46 (11)	C7—C8—H8	119.4
N2—Cu1—N3	85.30 (10)	C8—C9—C10	121.0 (3)
O1—Cu1—C11	98.46 (7)	C8—C9—H9	119.5
N1—Cu1—C11	101.77 (8)	C10—C9—H9	119.5
N2—Cu1—C11	96.66 (7)	C11—C10—C9	119.5 (3)
N3—Cu1—C11	95.70 (8)	C11—C10—H10	120.3
C1—N1—C12	120.0 (3)	C9—C10—H10	120.3
C1—N1—Cu1	127.5 (2)	C10—C11—C6	121.4 (3)
C12—N1—Cu1	112.23 (19)	C10—C11—H11	119.3
C14—N2—C13	115.7 (2)	C6—C11—H11	119.3
C14—N2—Cu1	107.68 (18)	N1—C12—C13	107.3 (2)
C13—N2—Cu1	107.95 (18)	N1—C12—H12A	110.3
C14—N2—H2	108.4	C13—C12—H12A	110.3
C13—N2—H2	108.4	N1—C12—H12B	110.3

## supplementary materials

Cu1—N2—H2	108.4	C13—C12—H12B	110.3
C16—N3—C15	108.0 (2)	H12A—C12—H12B	108.5
C16—N3—Cu1	124.5 (2)	N2—C13—C12	106.9 (2)
C15—N3—Cu1	104.42 (18)	N2—C13—H13A	110.4
C16—N3—H3	106.3	C12—C13—H13A	110.4
C15—N3—H3	106.3	N2—C13—H13B	110.4
Cu1—N3—H3	106.3	C12—C13—H13B	110.4
C17—N4—H4A	109.5	H13A—C13—H13B	108.6
C17—N4—H4B	109.5	N2—C14—C15	107.1 (3)
H4A—N4—H4B	109.5	N2—C14—H14A	110.3
C17—N4—H4C	109.5	C15—C14—H14A	110.3
H4A—N4—H4C	109.5	N2—C14—H14B	110.3
H4B—N4—H4C	109.5	C15—C14—H14B	110.3
C3—O1—Cu1	128.49 (18)	H14A—C14—H14B	108.6
N1—C1—C2	125.5 (3)	N3—C15—C14	109.7 (3)
N1—C1—H1	117.2	N3—C15—H15A	109.7
C2—C1—H1	117.2	C14—C15—H15A	109.7
C3—C2—C1	121.6 (3)	N3—C15—H15B	109.7
C3—C2—C7	119.3 (3)	C14—C15—H15B	109.7
C1—C2—C7	118.9 (3)	H15A—C15—H15B	108.2
O1—C3—C2	124.6 (3)	N3—C16—C17	114.1 (3)
O1—C3—C4	116.2 (3)	N3—C16—H16A	108.7
C2—C3—C4	119.2 (3)	C17—C16—H16A	108.7
C5—C4—C3	121.2 (3)	N3—C16—H16B	108.7
C5—C4—H4	119.4	C17—C16—H16B	108.7
C3—C4—H4	119.4	H16A—C16—H16B	107.6
C4—C5—C6	121.7 (3)	N4—C17—C16	113.0 (3)
C4—C5—H5	119.1	N4—C17—H17A	109.0
C6—C5—H5	119.1	C16—C17—H17A	109.0
C5—C6—C7	119.1 (3)	N4—C17—H17B	109.0
C5—C6—C11	121.1 (3)	C16—C17—H17B	109.0
C7—C6—C11	119.8 (3)	H17A—C17—H17B	107.8
C6—C7—C8	117.0 (3)		

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2 $\cdots$ C12 <sup>i</sup>	0.91	2.44	3.225 (3)	144
N3—H3 $\cdots$ C11 <sup>ii</sup>	0.91	2.50	3.388 (3)	165
N4—H4A $\cdots$ C11 <sup>iii</sup>	0.89	2.31	3.204 (3)	177
N4—H4B $\cdots$ C12 <sup>ii</sup>	0.89	2.25	3.079 (4)	156
N4—H4C $\cdots$ O1	0.89	1.83	2.703 (4)	167

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



Fig. 2

