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Azido{1-[2-(propylamino)ethyliminomethyl]naphthalen-2-olato}copper(II)

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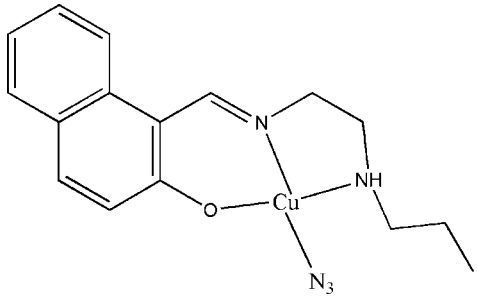
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.013 Å; disorder in main residue; R factor = 0.069; wR factor = 0.214; data-to-parameter ratio = 17.2.

The title compound, $[Cu(C_{16}H_{19}N_2O)(N_3)]$, was synthesized by the reaction of equimolar quantities of 2-hydroxy-1-naphthaldehyde, *N*-propylethane-1,2-diamine, sodium azide and copper(II) acetate in a methanol solution. The Cu^{II} ion in the compound is four-coordinated by one imine N, one amine N, and one phenolate O atoms of the Schiff base ligand 1-[2-(propylamino)ethyliminomethyl]naphthalen-2-ol and by one terminal N atom of an azide anion, forming a square-planar coordination. The propyl group and attached NH are disordered over two positions; the site occupancy factors are *ca* 0.6 and 0.4.

Related literature

For related literature, see: Allen *et al.* (1987); Arnold *et al.* (2003); Collinson & Fenton (1996); García-Raso *et al.* (2003); Hossain *et al.* (1996); Musie *et al.* (2003); Raptopoulou *et al.* (1998); Ray *et al.* (2003); Tarafder *et al.* (2002); Wei & Wang (2006); Zhu *et al.* (2006); Butcher *et al.* (2003); Hebbachi & Benali-Cherif (2005).



Experimental

Crystal data

$[Cu(C_{16}H_{19}N_2O)(N_3)]$
M_r = 360.90
Monoclinic, $C2/c$
a = 12.465 (4) Å
b = 24.772 (8) Å
c = 11.047 (4) Å
β = 103.007 (4)°
V = 3323.7 (19) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.33 mm^{-1}
T = 298 (2) K
0.20 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.778, T_{max} = 0.796
13362 measured reflections
3452 independent reflections
1816 reflections with $I > 2\sigma(I)$
R_{int} = 0.069

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.214
S = 1.01
3452 reflections
201 parameters
12 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.808 (4)	Cu1—N3	1.900 (5)
Cu1—N1	1.843 (5)	Cu1—N2	1.928 (6)
O1—Cu1—N1	93.8 (2)	O1—Cu1—N2	177.3 (2)
O1—Cu1—N3	88.3 (2)	N1—Cu1—N2	87.2 (2)
N1—Cu1—N3	177.8 (2)	N3—Cu1—N2	90.7 (2)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2′—H2′A···N3^{i}	0.91	2.35	3.233 (8)	165
N2—H2A···N3^{i}	0.91	2.35	3.233 (8)	162

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); 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: GD2027).

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supplementary materials

Acta Cryst. (2007). E**63**, m3197-m3198 [**doi:10.1107/S1600536807062514**]

Azido{1-[2-(propylamino)ethyliminomethyl]naphthalen-2-olato}copper(II)

C.-G. Zhu, Y.-J. Wei and F.-W. Wang

Comment

During the last few years, there has been a great effort to identify the biological role of copper (Collinson & Fenton, 1996; Hossain *et al.*, 1996; Tarafder *et al.*, 2002). It appears that the biological role of copper is primarily in redox reactions and as a biological catalyst, although much remains to be understood (Musie *et al.*, 2003; García-Raso *et al.*, 2003). The peculiarity of copper lies in its ability to form complexes with coordination number four, five, and six (Ray *et al.*, 2003; Arnold *et al.*, 2003; Raptopoulou *et al.*, 1998). Recently, we have reported several Schiff base copper(II) complexes with azide ligand (Zhu *et al.*, 2006; Wei & Wang, 2006). Here the structure of the title complex (I), Fig. 1, is reported.

Complex (I) is a mononuclear copper(II) compound. The Cu^{II} ion is four-coordinated by one imine N, one amine N, and one phenolate O atoms of a Schiff base ligand, and by one terminal N atom of an azide anion, forming a square planar coordination. All the bond lengths are in normal ranges (Allen *et al.*, 1987). The bond lengths (Table 1) related to the Cu^{II} ion are comparable to the values of the complexes we reported previously corresponding, and also comparable to the values of other Schiff base copper(II) complexes (Hebbachi & Benali-Cherif, 2005; Butcher *et al.*, 2003). The bond angles around the central metal ion show somewhat deviations from ideal square planar geometry, ranging from 87.2 (2) to 93.8 (2) °. The two *trans* bond angles are 177.3 (2) and 177.8 (2) °, respectively.

Experimental

2-Hydroxy-1-naphthaldehyde (1.0 mmol, 172.3 mg), *N*-propylethane-1,2-diamine (1.0 mmol, 102.2 mg), sodium azide (1.0 mmol, 65.0 mg), and copper acetate (1.0 mmol, 199.1 mg) were dissolved in a methanol solution (150 ml). The mixture was refluxed at 340 K for about 1 h to give a clear blue solution. After keeping the cooled resulting solution in dark for 12 days, blue block-shaped crystals were formed.

Refinement

All the H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, N—H distances of 0.91 Å, and with U_{iso}(H) = 1.2U_{eq}(C/N) and 1.5U_{eq}(C16 and C16'). The propyl group is disordered and it was modelled using two sets of atom sites, refined isotropically with occupancies of 0.37 (3) and 0.63 (3), respectively.

Figures

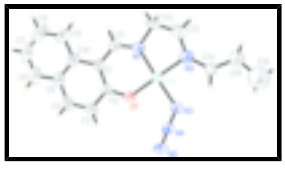


Fig. 1. The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Only the major orientation of the disordered propyl group is shown.

Azido{1-[2-(propylamino)ethyliminomethyl]naphthalen-2-olato}copper(II)

Crystal data

$[Cu(C_{16}H_{19}N_2O)(N_3)]$	F_{000} = 1496
M_r = 360.90	D_x = 1.442 Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 12.465 (4) Å	Cell parameters from 1297 reflections
b = 24.772 (8) Å	θ = 2.4–24.5º
c = 11.047 (4) Å	μ = 1.33 mm^{-1}
β = 103.007 (4)º	T = 298 (2) K
V = 3323.7 (19) Å^3	Block, blue
Z = 8	0.20 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer	3452 independent reflections
Radiation source: fine-focus sealed tube	1816 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.069
T = 298(2) K	θ_{max} = 26.5º
ω scan	θ_{min} = 1.6º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −15→15
T_{min} = 0.778, T_{max} = 0.796	k = −31→31
13362 measured reflections	l = −13→13

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.069	H-atom parameters constrained
$wR(F^2)$ = 0.214	$w = 1/[\sigma^2(F_o^2) + (0.0886P)^2 + 3.7952P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.01	$(\Delta/\sigma)_{max} < 0.001$
3452 reflections	$\Delta\rho_{max}$ = 0.53 e Å^{-3}
201 parameters	$\Delta\rho_{min}$ = −0.30 e Å^{-3}
12 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cu1	0.12391 (5)	0.23867 (3)	0.35451 (7)	0.0733 (4)	
O1	0.1921 (3)	0.19640 (17)	0.2615 (4)	0.0785 (11)	
N1	0.0746 (4)	0.1811 (2)	0.4326 (4)	0.0701 (13)	
N3	0.1703 (5)	0.2997 (2)	0.2755 (6)	0.0891 (16)	
N4	0.2368 (4)	0.2975 (2)	0.2131 (5)	0.0789 (14)	
N5	0.2984 (5)	0.2977 (3)	0.1539 (6)	0.120 (2)	
C1	0.1459 (5)	0.1089 (3)	0.3270 (6)	0.0715 (16)	
C2	0.1936 (5)	0.1440 (3)	0.2545 (6)	0.0739 (16)	
C3	0.2508 (6)	0.1221 (3)	0.1681 (7)	0.098 (2)	
H3	0.2832	0.1450	0.1200	0.117*	
C4	0.2585 (7)	0.0675 (4)	0.1554 (8)	0.114 (3)	
H4	0.2952	0.0540	0.0973	0.137*	
C5	0.2128 (7)	0.0310 (3)	0.2272 (8)	0.101 (2)	
C6	0.2267 (8)	−0.0239 (4)	0.2101 (11)	0.136 (3)	
H6	0.2666	−0.0364	0.1540	0.163*	
C7	0.1800 (12)	−0.0588 (4)	0.2783 (14)	0.158 (5)	
H7	0.1882	−0.0957	0.2675	0.190*	
C8	0.1220 (11)	−0.0419 (5)	0.3614 (12)	0.156 (5)	
H8	0.0907	−0.0669	0.4060	0.187*	
C9	0.1097 (7)	0.0133 (4)	0.3796 (8)	0.118 (3)	
H9	0.0705	0.0250	0.4371	0.142*	
C10	0.1555 (6)	0.0514 (3)	0.3125 (7)	0.0852 (19)	
C11	0.0889 (5)	0.1310 (3)	0.4126 (6)	0.0762 (17)	
H11	0.0585	0.1065	0.4593	0.091*	
C12	0.0082 (6)	0.1975 (4)	0.5219 (7)	0.105 (2)	
H12A	−0.0692	0.1909	0.4866	0.126*	
H12B	0.0297	0.1765	0.5977	0.126*	
C13	0.0263 (8)	0.2541 (4)	0.5491 (9)	0.128 (3)	
H13A	−0.0377	0.2688	0.5738	0.154*	
H13B	0.0889	0.2581	0.6188	0.154*	
N2	0.0461 (5)	0.2847 (2)	0.4465 (5)	0.0914 (16)*	0.37 (3)
H2A	−0.0223	0.2847	0.3955	0.110*	0.37 (3)
C14	0.0697 (19)	0.3422 (4)	0.455 (3)	0.081 (7)*	0.37 (3)

H14A	0.0946	0.3517	0.3801	0.097*	0.37 (3)
H14B	0.1324	0.3470	0.5238	0.097*	0.37 (3)
C15	−0.012 (2)	0.3832 (10)	0.469 (4)	0.127 (11)*	0.37 (3)
H15A	−0.0178	0.3832	0.5548	0.153*	0.37 (3)
H15B	−0.0826	0.3727	0.4183	0.153*	0.37 (3)
C16	0.012 (4)	0.4387 (13)	0.435 (6)	0.27 (2)*	0.37 (3)
H16A	−0.0458	0.4622	0.4464	0.399*	0.37 (3)
H16B	0.0173	0.4395	0.3496	0.399*	0.37 (3)
H16C	0.0808	0.4503	0.4869	0.399*	0.37 (3)
N2'	0.0461 (5)	0.2847 (2)	0.4465 (5)	0.0914 (16)*	0.63 (3)
H2'A	−0.0210	0.2911	0.3959	0.110*	0.63 (3)
C14'	0.0896 (14)	0.3366 (5)	0.492 (2)	0.138 (8)*	0.63 (3)
H14C	0.1101	0.3559	0.4239	0.166*	0.63 (3)
H14D	0.1562	0.3310	0.5554	0.166*	0.63 (3)
C15'	0.0149 (12)	0.3708 (5)	0.5433 (19)	0.107 (6)*	0.63 (3)
H15C	0.0287	0.3647	0.6322	0.129*	0.63 (3)
H15D	−0.0603	0.3598	0.5076	0.129*	0.63 (3)
C16'	0.0258 (16)	0.4291 (6)	0.520 (2)	0.158 (8)*	0.63 (3)
H16D	−0.0282	0.4487	0.5523	0.236*	0.63 (3)
H16E	0.0146	0.4354	0.4326	0.236*	0.63 (3)
H16F	0.0982	0.4410	0.5612	0.236*	0.63 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0607 (5)	0.0843 (6)	0.0809 (6)	−0.0013 (3)	0.0286 (4)	0.0000 (4)
O1	0.086 (3)	0.072 (3)	0.092 (3)	−0.001 (2)	0.050 (2)	0.001 (2)
N1	0.061 (3)	0.090 (4)	0.063 (3)	−0.012 (3)	0.023 (2)	0.002 (3)
N3	0.092 (4)	0.071 (3)	0.115 (4)	0.001 (3)	0.048 (3)	0.008 (3)
N4	0.071 (3)	0.067 (3)	0.105 (4)	−0.007 (3)	0.034 (3)	0.009 (3)
N5	0.119 (5)	0.110 (5)	0.157 (6)	−0.005 (4)	0.085 (5)	0.026 (4)
C1	0.058 (3)	0.072 (4)	0.079 (4)	−0.011 (3)	0.004 (3)	0.006 (3)
C2	0.067 (4)	0.073 (4)	0.087 (4)	0.001 (3)	0.028 (3)	0.001 (3)
C3	0.099 (5)	0.100 (6)	0.105 (5)	−0.003 (4)	0.046 (4)	−0.007 (4)
C4	0.108 (6)	0.098 (6)	0.142 (7)	0.014 (5)	0.042 (5)	−0.034 (6)
C5	0.098 (5)	0.071 (5)	0.124 (7)	0.002 (4)	0.007 (5)	−0.004 (5)
C6	0.146 (8)	0.085 (7)	0.163 (9)	0.020 (6)	0.005 (7)	−0.004 (6)
C7	0.176 (12)	0.079 (7)	0.189 (13)	0.019 (7)	−0.025 (9)	0.005 (8)
C8	0.189 (13)	0.085 (8)	0.178 (12)	−0.026 (7)	0.006 (9)	0.038 (7)
C9	0.122 (7)	0.106 (7)	0.118 (6)	−0.017 (5)	0.011 (5)	0.029 (5)
C10	0.080 (4)	0.077 (5)	0.090 (5)	−0.008 (4)	0.002 (4)	0.011 (4)
C11	0.069 (4)	0.090 (5)	0.071 (4)	−0.019 (3)	0.017 (3)	0.013 (4)
C12	0.102 (5)	0.144 (7)	0.087 (5)	−0.032 (5)	0.061 (4)	−0.015 (5)
C13	0.160 (7)	0.133 (6)	0.109 (5)	0.024 (5)	0.068 (5)	0.002 (5)

Geometric parameters (Å, °)

Cu1—O1	1.808 (4)	C11—H11	0.9300
Cu1—N1	1.843 (5)	C12—C13	1.441 (11)

Cu1—N3	1.900 (5)	C12—H12A	0.9700
Cu1—N2	1.928 (6)	C12—H12B	0.9700
O1—C2	1.301 (7)	C13—N2	1.430 (9)
N1—C11	1.278 (8)	C13—H13A	0.9700
N1—C12	1.480 (7)	C13—H13B	0.9700
N3—N4	1.193 (7)	N2—C14	1.454 (9)
N4—N5	1.116 (7)	N2—H2A	0.9100
C1—C2	1.402 (8)	C14—C15	1.468 (10)
C1—C11	1.414 (9)	C14—H14A	0.9700
C1—C10	1.442 (9)	C14—H14B	0.9700
C2—C3	1.421 (9)	C15—C16	1.471 (10)
C3—C4	1.365 (10)	C15—H15A	0.9700
C3—H3	0.9300	C15—H15B	0.9700
C4—C5	1.405 (11)	C16—H16A	0.9600
C4—H4	0.9300	C16—H16B	0.9600
C5—C6	1.390 (11)	C16—H16C	0.9600
C5—C10	1.398 (10)	C14'—C15'	1.465 (9)
C6—C7	1.360 (15)	C14'—H14C	0.9700
C6—H6	0.9300	C14'—H14D	0.9700
C7—C8	1.357 (15)	C15'—C16'	1.478 (9)
C7—H7	0.9300	C15'—H15C	0.9700
C8—C9	1.397 (14)	C15'—H15D	0.9700
C8—H8	0.9300	C16'—H16D	0.9600
C9—C10	1.398 (10)	C16'—H16E	0.9600
C9—H9	0.9300	C16'—H16F	0.9600
O1—Cu1—N1	93.8 (2)	C13—C12—H12B	109.9
O1—Cu1—N3	88.3 (2)	N1—C12—H12B	109.9
N1—Cu1—N3	177.8 (2)	H12A—C12—H12B	108.3
O1—Cu1—N2	177.3 (2)	N2—C13—C12	113.4 (7)
N1—Cu1—N2	87.2 (2)	N2—C13—H13A	108.9
N3—Cu1—N2	90.7 (2)	C12—C13—H13A	108.9
C2—O1—Cu1	128.8 (4)	N2—C13—H13B	108.9
C11—N1—C12	120.2 (5)	C12—C13—H13B	108.9
C11—N1—Cu1	126.6 (4)	H13A—C13—H13B	107.7
C12—N1—Cu1	113.2 (5)	C13—N2—C14	122.7 (12)
N4—N3—Cu1	123.4 (5)	C13—N2—Cu1	107.6 (5)
N5—N4—N3	176.9 (7)	C14—N2—Cu1	119.5 (9)
C2—C1—C11	118.9 (6)	C13—N2—H2A	100.7
C2—C1—C10	119.5 (6)	C14—N2—H2A	100.7
C11—C1—C10	121.6 (6)	Cu1—N2—H2A	100.7
O1—C2—C1	124.9 (6)	N2—C14—C15	123.3 (17)
O1—C2—C3	115.9 (6)	N2—C14—H14A	106.5
C1—C2—C3	119.2 (6)	C15—C14—H14A	106.5
C4—C3—C2	120.3 (7)	N2—C14—H14B	106.5
C4—C3—H3	119.8	C15—C14—H14B	106.5
C2—C3—H3	119.8	H14A—C14—H14B	106.5
C3—C4—C5	122.2 (7)	C14—C15—C16	116 (3)
C3—C4—H4	118.9	C14—C15—H15A	108.3
C5—C4—H4	118.9	C16—C15—H15A	108.3

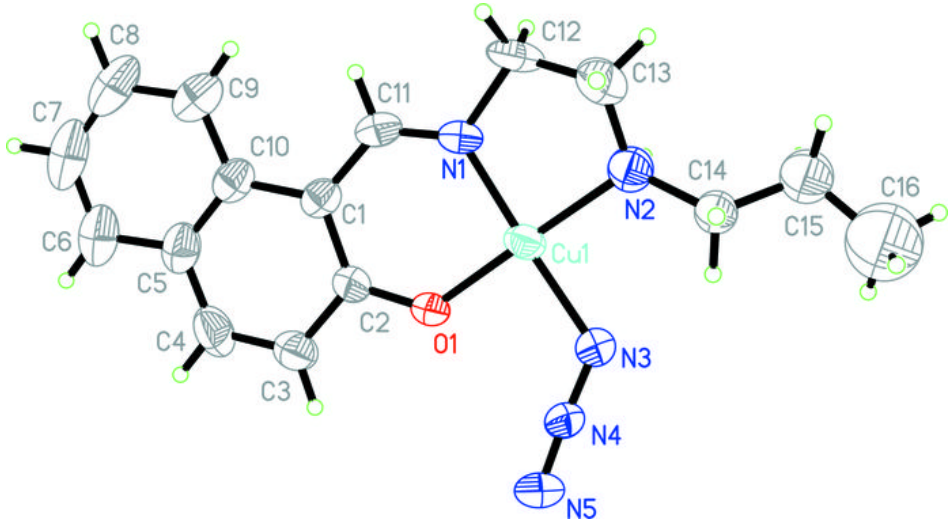
C6—C5—C10	122.9 (9)	C14—C15—H15B	108.3
C6—C5—C4	118.3 (10)	C16—C15—H15B	108.3
C10—C5—C4	118.8 (7)	H15A—C15—H15B	107.4
C7—C6—C5	117.7 (11)	C15—C16—H16A	109.5
C7—C6—H6	121.1	C15—C16—H16B	109.5
C5—C6—H6	121.1	H16A—C16—H16B	109.5
C8—C7—C6	122.6 (11)	C15—C16—H16C	109.5
C8—C7—H7	118.7	H16A—C16—H16C	109.5
C6—C7—H7	118.7	H16B—C16—H16C	109.5
C7—C8—C9	119.5 (11)	C15'—C14'—H14C	108.4
C7—C8—H8	120.3	C15'—C14'—H14D	108.4
C9—C8—H8	120.3	H14C—C14'—H14D	107.5
C8—C9—C10	120.9 (10)	C14'—C15'—C16'	114.0 (12)
C8—C9—H9	119.6	C14'—C15'—H15C	108.8
C10—C9—H9	119.6	C16'—C15'—H15C	108.8
C9—C10—C5	116.5 (8)	C14'—C15'—H15D	108.8
C9—C10—C1	123.6 (8)	C16'—C15'—H15D	108.8
C5—C10—C1	120.0 (6)	H15C—C15'—H15D	107.6
N1—C11—C1	127.0 (5)	C15'—C16'—H16D	109.5
N1—C11—H11	116.5	C15'—C16'—H16E	109.5
C1—C11—H11	116.5	H16D—C16'—H16E	109.5
C13—C12—N1	108.8 (6)	C15'—C16'—H16F	109.5
C13—C12—H12A	109.9	H16D—C16'—H16F	109.5
N1—C12—H12A	109.9	H16E—C16'—H16F	109.5

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2'—H2'A···N3^{i}	0.91	2.35	3.233 (8)	165
N2—H2A···N3^{i}	0.91	2.35	3.233 (8)	162

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

Fig. 1


C8
C9
C7
C10
C11
C12
C13
N1
N2
C14
C16
C15
C1
C6
C5
Cu1
C2
O1
N3
C4
C3
N4
N5