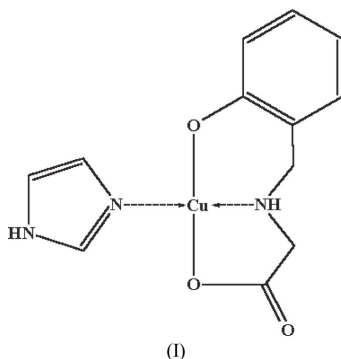


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Key indicators

Single-crystal X-ray study
 $T = 273$ K
Mean $\sigma(\text{C}-\text{C}) = 0.008$ Å
 R factor = 0.044
 wR factor = 0.111
Data-to-parameter ratio = 13.9For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**(1*H*-Imidazole- κ N³)[*N*-(2-oxidobenzyl)-
L-leucinato- κ^3 O,*N*,*O'*']copper(II)**In the title compound, $[\text{Cu}(\text{C}_{13}\text{H}_{17}\text{NO}_3)(\text{C}_3\text{H}_4\text{N}_2)]$, the Cu^{II}
atom is coordinated by two N [$\text{Cu}-\text{N} = 1.965$ (4) and
 1.999 (4) Å] and two O [$\text{Cu}-\text{O} = 1.907$ (3) and
 1.934 (3) Å] atoms in a square-planar geometry. The crystal packing is
stabilized by intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds.Received 13 December 2006
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Comment

Copper(II) complexes of the tridentate Schiff base pyridoxal,
or its analogues, and amino acids provide potential models for
a number of important biological systems (Raso *et al.*, 1999).
We present here the crystal structure of the title Cu^{II} complex,
(I).In (I) (Fig. 1), the Cu atom is coordinated by the imidazole
and tridentate dianionic reduced Schiff base *N*-(2-hydroxy-
benzyl)-L-leucine in a square-planar geometry (Table 1),
which corresponds well to that observed in $[\text{Cu}(\text{salicylidene-}S\text{-alaninato})\text{pyrazole}]\text{pyrazole}$ (Kettmann & Frešová, 1993).
The Cu–amine distance [$\text{Cu}-\text{N}1 = 1.999$ (4) Å] is significantly
longer than known Cu–imine bond lengths [1.890 (3) Å;
Kettmann & Frešová, 1993]. The successful *in situ* reduction of
the imine is evident from the $\text{N}1-\text{C}7$ distance of 1.494 (6) Å
versus $1.27\text{--}1.30$ Å observed in related Cu^{II} complexes with
salicylidene ligands. The $\text{C}6-\text{C}7$ [1.485 (7) Å] and $\text{N}1-\text{C}8$
[1.470 (6) Å] bond lengths, significantly longer than those in
imine complexes, are typical for single bonds and indicate the
absence of conjugation.Intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds (Table 2) form a
three-dimensional hydrogen-bonding network, which stabi-
lizes the crystal structure (Fig. 2).

Experimental

The reduced Schiff base ligand was prepared by a modified literature
method (Koh *et al.*, 1996). The title compound was synthesized as
follows. To the royal blue solution formed from copper(II) acetate

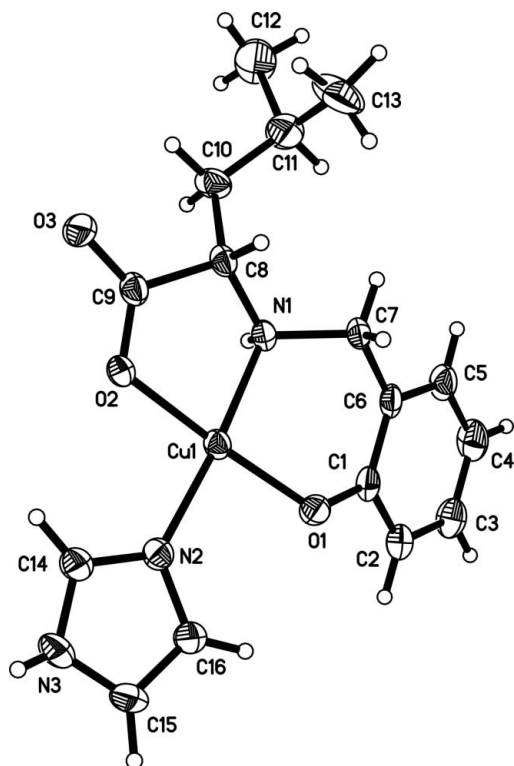


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

monohydrate (200 mg, 1.00 mmol) in ethanol (15 ml) and imidazole (110 mg, 1.00 mmol) in ethanol (10 ml) was added a filtered solution of *N*-(2-hydroxybenzyl)-*L*-leucine (238 mg, 1.00 mmol) in water (20 ml) with KOH (1.0 ml, 1 *M*). The dark-blue solution was stirred for 2 h, then filtered and left for several days. The resulting dark-blue crystals were filtered off, washed with ethanol, and dried under vacuum.

Crystal data

[Cu(C ₁₃ H ₁₇ NO ₃)(C ₃ H ₄ N ₂) <i>M_r</i> = 366.90 Orthorhombic, <i>P</i> 2 ₁ 2 ₁ 2 ₁ <i>a</i> = 7.1094 (9) Å <i>b</i> = 12.0945 (15) Å <i>c</i> = 19.731 (3) Å <i>V</i> = 1696.6 (4) Å ³	<i>Z</i> = 4 <i>D_x</i> = 1.436 Mg m ⁻³ Mo <i>K</i> α radiation <i>μ</i> = 1.31 mm ⁻¹ <i>T</i> = 273 (2) K Block, dark blue 0.30 × 0.10 × 0.10 mm
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Data collection

Bruker SMART CCD area-detector diffractometer <i>ω</i> scans Absorption correction: multi-scan (<i>SADABS</i> ; Sheldrick, 1996) <i>T_{min}</i> = 0.696, <i>T_{max}</i> = 0.881	8853 measured reflections 2970 independent reflections 2507 reflections with <i>I</i> > 2σ(<i>I</i>) <i>R_{int}</i> = 0.042 <i>θ_{max}</i> = 25.0°
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Refinement

Refinement on <i>F</i> ² <i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)] = 0.044 <i>wR</i> (<i>F</i> ²) = 0.111 <i>S</i> = 1.08 2970 reflections 214 parameters H atoms treated by a mixture of independent and constrained refinement	<i>w</i> = 1/[σ ² (<i>F_o</i> ²) + (0.0561 <i>P</i>) ²] where <i>P</i> = (<i>F_o</i> ² + 2 <i>F_c</i> ²)/3 (Δ/σ) _{max} < 0.001 Δρ _{max} = 0.77 e Å ⁻³ Δρ _{min} = -0.44 e Å ⁻³ Absolute structure: Flack (1983), 1227 Friedel pairs Flack parameter: 0.01 (2)
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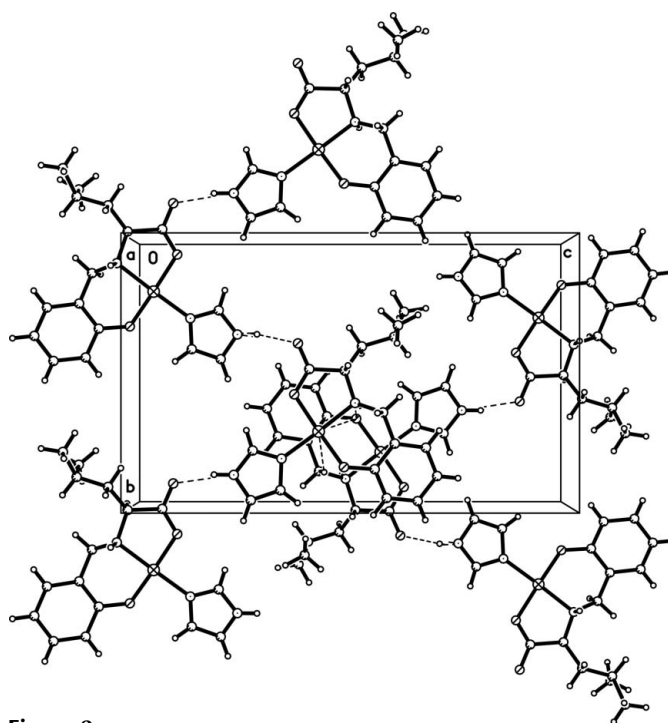


Figure 2
The crystal packing viewed down the *a* axis. Hydrogen bonds are shown as dashed lines.

Table 1

Selected geometric parameters (Å, °).

Cu1—O1	1.907 (3)	Cu1—N2	1.965 (4)
Cu1—O2	1.934 (3)	Cu1—N1	1.999 (4)
O1—Cu1—O2	175.65 (15)	O1—Cu1—N1	94.01 (14)
O1—Cu1—N2	89.24 (15)	O2—Cu1—N1	84.26 (15)
O2—Cu1—N2	92.90 (14)	N2—Cu1—N1	173.22 (19)

Table 2

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>
N3—H3A...O3 ⁱ	0.86	1.85	2.693 (5)	167
N1—H1...O1 ⁱⁱ	0.78 (5)	2.17 (6)	2.932 (6)	164 (5)

Symmetry codes: (i) $-x + 2, y + \frac{1}{2}, -z + \frac{5}{2}$; (ii) $x + \frac{1}{2}, -y + \frac{1}{2}, -z + 2$.

Atom H1 was located in a difference map and refined isotropically. Other H atoms were placed in geometrically idealized positions (C—H = 0.93–0.98 and N—H = 0.86 Å) and refined as riding, with *U_{iso}*(H) = 1.2 or 1.5 times *U_{eq}*(parent atom).

Data collection: *APEX2* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

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