

Aquabis(2-iodoacetato- κ O)(1,10-phenanthroline- κ^2 N,N')copper(II)

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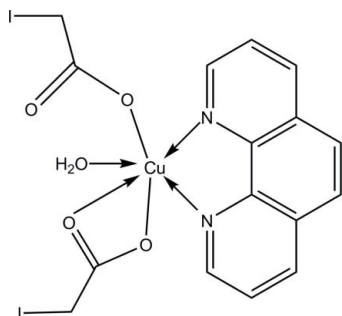
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 Key indicators: single-crystal X-ray study; $T = 273$ K; mean $\sigma(\text{C}-\text{C}) = 0.009$ Å; R factor = 0.038; wR factor = 0.104; data-to-parameter ratio = 13.9.

In the title compound, $[\text{Cu}(\text{C}_2\text{H}_2\text{IO}_2)_2(\text{C}_{12}\text{H}_8\text{N}_2)(\text{H}_2\text{O})]$, the Cu^{II} ion is coordinated by two N atoms [$\text{Cu}-\text{N} = 2.013$ (4) and 2.024 (4) Å] from a 1,10-phenanthroline ligand and three O atoms [$\text{Cu}-\text{O} = 1.940$ (4)– 2.261 (4) Å] from two carboxyl ligands and a water molecule in a distorted square-pyramidal geometry. One iodoacetate O atom [$\text{Cu}-\text{O} = 2.775$ (4) Å] completes the coordination to form a distorted octahedron. Intermolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds link the molecules into centrosymmetric dimers, which are further packed by $\pi-\pi$ interactions between the 1,10-phenanthroline ligands into layers parallel to the ab plane. The crystal packing also exhibits short intermolecular $\text{I}\cdots\text{I}$ contacts of 3.6772 (9) Å and weak $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

The related crystal structure of aquabis(2,4-dichlorophenoxyacetato- O)(1,10-phenanthroline- κ^2 N,N')copper(II) has been reported by Liu *et al.* (2006).



Experimental

Crystal data

$[\text{Cu}(\text{C}_2\text{H}_2\text{IO}_2)_2(\text{C}_{12}\text{H}_8\text{N}_2)(\text{H}_2\text{O})]$	$b = 10.6293$ (12) Å
$M_r = 631.63$	$c = 11.3441$ (13) Å
Triclinic, $P\bar{1}$	$\alpha = 65.803$ (2)°
$a = 9.5156$ (11) Å	$\beta = 65.598$ (2)°

$\gamma = 72.451$ (2)°
 $V = 940.94$ (19) Å³
 $Z = 2$
 Mo $K\alpha$ radiation

$\mu = 4.47$ mm⁻¹
 $T = 273$ (2) K
 $0.26 \times 0.23 \times 0.21$ mm

Data collection

Bruker SMART APEX diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.389$, $T_{\text{max}} = 0.454$
 (expected range = 0.336–0.391)

4948 measured reflections
 3305 independent reflections
 2934 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.016$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.104$
 $S = 1.01$
 3305 reflections
 237 parameters

3 restraints
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 1.53$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.68$ e Å⁻³

Table 1

Selected interatomic distances (Å).

$\text{Cg}1$, $\text{Cg}2$ and $\text{Cg}3$ are the centroids of the $\text{C}4-\text{C}7/\text{C}11/\text{C}12$, $\text{C}6-\text{C}10/\text{N}2$ and $\text{C}1-\text{C}5/\text{N}1$ rings, respectively.

$\text{Cg}1\cdots\text{Cg}3^{\text{i}}$	3.505 (6)	$\text{Cg}2\cdots\text{Cg}1^{\text{ii}}$	3.634 (6)
$\text{Cg}1\cdots\text{Cg}1^{\text{ii}}$	3.584 (6)	$\text{I}2\cdots\text{I}2^{\text{iii}}$	3.6772 (9)
$\text{Cg}2\cdots\text{Cg}3^{\text{i}}$	3.625 (6)		

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O}1-\text{H}1\text{B}\cdots\text{O}3$	0.85	1.84	2.639 (6)	156
$\text{O}1-\text{H}1\text{C}\cdots\text{O}4^{\text{iv}}$	0.85	1.97	2.785 (5)	161
$\text{C}3-\text{H}3\cdots\text{O}1^{\text{ii}}$	0.93	2.44	3.240 (7)	144
$\text{C}11-\text{H}11\cdots\text{O}5^{\text{i}}$	0.93	2.71	3.508 (8)	144
$\text{C}10-\text{H}10\cdots\text{O}3^{\text{iv}}$	0.93	2.68	3.431 (8)	138
$\text{C}14-\text{H}14\text{B}\cdots\text{O}2^{\text{v}}$	0.97	2.59	3.436 (8)	146
$\text{C}14-\text{H}14\text{A}\cdots\text{O}5^{\text{v}}$	0.97	2.64	3.219 (8)	119

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

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2511).

References

- Liu, J.-W., Zhu, B., Tian, Y. & Gu, C.-S. (2006). *Acta Cryst.* **E62**, m2030–m2032.
 Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Siemens (1996). *SMART* and *SAINTE*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

supplementary materials

Acta Cryst. (2009). E65, m241 [doi:10.1107/S1600536809002682]

Aquabis(2-iodoacetato- κO)(1,10-phenanthroline- $\kappa^2 N, N'$)copper(II)

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Comment

Metal complexes with carboxylates are among the most investigated complexes in the field of coordination chemistry. Due to their versatile bonding modes with metal ions, they have also been used in the synthesis of mononuclear monomeric and polymeric complexes (Liu *et al.*, 2006). In order to develop some new topological structures, we study the reaction of the copper(II) ion and 2-iodoacetic acid with the presence of 1,10-phenanthroline.

The molecular structure of the title complex is shown in Fig. 1. The Cu atom exhibits a six-coordinated distorted octahedral pyramidal geometry with two carboxyl O atoms from (Cu2—O4 2.000 (4) Å, Cu2—O5 2.775 (4) Å), a water molecule (Cu—O 2.261 (4) Å) and a nitrogen atom (Cu2—N2 2.024 (4) Å) occupying the equatorial planar position. A nitrogen atom N2 (Cu2—N2 2.013 (4) Å) and a carboxyl O atom (Cu2—O2 1.940 (4) Å) occupy the apical positions. The displacement of the metal atom from the basal plane is 0.0640 (2) Å. The crystal packing exhibits short intermolecular I...I contacts (Table 1) and weak C—H...O hydrogen bonds (Table 2).

Experimental

The reaction was carried out by the solvothermal method. 2-iodoacetic acid(0.372 g, 2 mmol) and cupric acetate(0.199 g, 1 mmol) and 1,10-phenanthroline(0.180 g, 1 mmol) were added to the airtight vessel with 20 ml water. The resulting green solution was filtered. The filtrate was placed for several days yielding blue block-shaped crystals.

The yield is 81%. Elemental analysis: calc. for C₁₆H₁₄CuI₂N₂O₅: C 30.42, H 2.23, N 4.43; found: C 30.15, H 2.49, N 4.22. The elemental analyses were performed with PERKIN ELMER MODEL 2400 SERIES II.

Refinement

All the H atoms were found in Fourier map, but placed in idealized positions(C—H 0.93–0.97 Å, O—H 0.85 Å), with the $U_{iso}(H)$ values were set at $1.2U_{eq}(C, O)$ of the parent atoms.

Figures

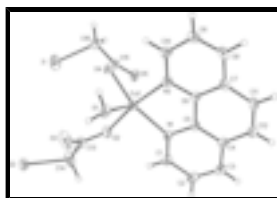


Fig. 1. The molecular structure of the title compound showing the atomic numbering and 30% probability displacement ellipsoids.

Aquabis(2-iodoacetato- κO)(1,10-phenanthroline- $\kappa^2 N, N'$)copper(II)

Crystal data

$[\text{Cu}(\text{C}_2\text{H}_2\text{IO}_2)_2(\text{C}_{12}\text{H}_8\text{N}_2)(\text{H}_2\text{O})]$	$Z = 2$
$M_r = 631.63$	$F_{000} = 598$
Triclinic, $P\bar{1}$	$D_x = 2.229 \text{ Mg m}^{-3}$
$a = 9.5156 (11) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 10.6293 (12) \text{ \AA}$	$\lambda = 0.71073 \text{ \AA}$
$c = 11.3441 (13) \text{ \AA}$	Cell parameters from 3047 reflections
$\alpha = 65.803 (2)^\circ$	$\theta = 2.6\text{--}28.1^\circ$
$\beta = 65.598 (2)^\circ$	$\mu = 4.47 \text{ mm}^{-1}$
$\gamma = 72.451 (2)^\circ$	$T = 273 (2) \text{ K}$
$V = 940.94 (19) \text{ \AA}^3$	Block, blue
	$0.26 \times 0.23 \times 0.21 \text{ mm}$

Data collection

Bruker APEXII diffractometer	3305 independent reflections
Radiation source: fine-focus sealed tube	2934 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.016$
$T = 273(2) \text{ K}$	$\theta_{\text{max}} = 25.1^\circ$
φ and ω scans	$\theta_{\text{min}} = 2.1^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -11 \rightarrow 11$
$T_{\text{min}} = 0.389$, $T_{\text{max}} = 0.454$	$k = -12 \rightarrow 10$
4948 measured reflections	$l = -13 \rightarrow 12$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.038$	H-atom parameters constrained
$wR(F^2) = 0.104$	$w = 1/[\sigma^2(F_o^2) + (0.056P)^2 + 3.6149P]$
$S = 1.01$	where $P = (F_o^2 + 2F_c^2)/3$
3305 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
237 parameters	$\Delta\rho_{\text{max}} = 1.53 \text{ e \AA}^{-3}$
3 restraints	$\Delta\rho_{\text{min}} = -1.68 \text{ e \AA}^{-3}$
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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu2	0.76967 (7)	0.67482 (6)	0.13753 (6)	0.02670 (17)
I1	0.95532 (7)	0.21497 (5)	0.43653 (6)	0.06644 (19)
I2	0.43146 (5)	0.18948 (4)	0.45215 (4)	0.04345 (15)
N1	0.6118 (5)	0.8490 (4)	0.1546 (4)	0.0255 (9)
N2	0.9024 (5)	0.8189 (4)	-0.0095 (4)	0.0280 (9)
O1	0.7777 (4)	0.6019 (4)	-0.0268 (4)	0.0341 (9)
H1C	0.8711	0.5671	-0.0635	0.031 (15)*
H1B	0.7272	0.5340	0.0231	0.06 (2)*
O2	0.6142 (4)	0.5607 (4)	0.2794 (4)	0.0359 (9)
O3	0.6083 (7)	0.4189 (6)	0.1825 (5)	0.0661 (15)
O4	0.9474 (4)	0.5270 (4)	0.1793 (4)	0.0329 (8)
O5	0.8852 (5)	0.6118 (4)	0.3468 (4)	0.0429 (10)
C1	0.4672 (6)	0.8592 (6)	0.2411 (5)	0.0307 (11)
H1A	0.4265	0.7782	0.3029	0.037*
C2	0.3740 (7)	0.9891 (6)	0.2417 (6)	0.0382 (13)
H2	0.2725	0.9934	0.3032	0.046*
C3	0.4311 (7)	1.1090 (6)	0.1529 (6)	0.0382 (13)
H3	0.3693	1.1954	0.1536	0.046*
C4	0.5840 (6)	1.1012 (5)	0.0602 (6)	0.0302 (11)
C5	0.6710 (6)	0.9677 (5)	0.0657 (5)	0.0241 (10)
C6	0.8265 (6)	0.9512 (5)	-0.0244 (5)	0.0249 (10)
C7	0.8936 (6)	1.0689 (6)	-0.1235 (5)	0.0305 (11)
C8	1.0481 (7)	1.0437 (6)	-0.2087 (6)	0.0380 (13)
H8	1.0990	1.1181	-0.2742	0.046*
C9	1.1228 (7)	0.9109 (6)	-0.1952 (6)	0.0392 (13)
H9	1.2240	0.8936	-0.2535	0.047*
C10	1.0475 (6)	0.8002 (6)	-0.0934 (6)	0.0356 (12)
H10	1.1012	0.7096	-0.0841	0.043*
C11	0.8014 (8)	1.2041 (6)	-0.1279 (7)	0.0432 (14)
H11	0.8440	1.2830	-0.1935	0.052*
C12	0.6551 (7)	1.2204 (6)	-0.0396 (6)	0.0381 (13)
H12	0.5997	1.3098	-0.0436	0.046*
C13	0.5693 (6)	0.4601 (6)	0.2801 (6)	0.0336 (12)

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C14	0.4522 (9)	0.3957 (7)	0.4171 (7)	0.0550 (19)
H14A	0.3507	0.4539	0.4228	0.066*
H14B	0.4825	0.3950	0.4891	0.066*
C15	0.9541 (6)	0.5230 (5)	0.2913 (5)	0.0293 (11)
C16	1.0576 (7)	0.3988 (6)	0.3569 (6)	0.0354 (12)
H16A	1.0700	0.4144	0.4303	0.043*
H16B	1.1602	0.3872	0.2894	0.043*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu2	0.0264 (3)	0.0205 (3)	0.0253 (3)	-0.0018 (2)	-0.0022 (3)	-0.0080 (2)
I1	0.0913 (4)	0.0355 (3)	0.0650 (3)	-0.0196 (2)	-0.0323 (3)	0.0035 (2)
I2	0.0464 (3)	0.0329 (2)	0.0460 (3)	-0.01190 (17)	-0.00496 (18)	-0.01484 (18)
N1	0.028 (2)	0.025 (2)	0.022 (2)	-0.0010 (17)	-0.0070 (17)	-0.0096 (17)
N2	0.029 (2)	0.026 (2)	0.026 (2)	-0.0039 (18)	-0.0058 (18)	-0.0100 (18)
O1	0.036 (2)	0.032 (2)	0.0267 (19)	0.0013 (18)	-0.0049 (16)	-0.0137 (17)
O2	0.040 (2)	0.031 (2)	0.031 (2)	-0.0118 (17)	0.0021 (17)	-0.0139 (16)
O3	0.093 (4)	0.070 (3)	0.038 (3)	-0.050 (3)	0.012 (2)	-0.030 (2)
O4	0.034 (2)	0.0286 (19)	0.0270 (19)	0.0040 (16)	-0.0075 (16)	-0.0095 (16)
O5	0.049 (2)	0.034 (2)	0.044 (2)	-0.0013 (19)	-0.0081 (19)	-0.0224 (19)
C1	0.028 (3)	0.035 (3)	0.024 (3)	-0.003 (2)	-0.003 (2)	-0.012 (2)
C2	0.031 (3)	0.046 (3)	0.032 (3)	0.003 (3)	-0.007 (2)	-0.018 (3)
C3	0.036 (3)	0.037 (3)	0.043 (3)	0.009 (2)	-0.019 (3)	-0.019 (3)
C4	0.034 (3)	0.027 (3)	0.037 (3)	-0.001 (2)	-0.019 (2)	-0.013 (2)
C5	0.031 (3)	0.022 (2)	0.025 (2)	-0.002 (2)	-0.014 (2)	-0.009 (2)
C6	0.025 (3)	0.025 (3)	0.025 (2)	0.000 (2)	-0.010 (2)	-0.010 (2)
C7	0.035 (3)	0.029 (3)	0.030 (3)	-0.011 (2)	-0.013 (2)	-0.006 (2)
C8	0.040 (3)	0.042 (3)	0.032 (3)	-0.020 (3)	-0.010 (2)	-0.005 (2)
C9	0.031 (3)	0.049 (4)	0.032 (3)	-0.010 (3)	-0.001 (2)	-0.016 (3)
C10	0.032 (3)	0.038 (3)	0.031 (3)	-0.002 (2)	-0.002 (2)	-0.017 (2)
C11	0.055 (4)	0.024 (3)	0.051 (4)	-0.013 (3)	-0.025 (3)	-0.001 (3)
C12	0.042 (3)	0.025 (3)	0.050 (4)	-0.002 (2)	-0.022 (3)	-0.010 (3)
C13	0.033 (3)	0.030 (3)	0.031 (3)	-0.010 (2)	-0.001 (2)	-0.010 (2)
C14	0.071 (5)	0.048 (4)	0.039 (4)	-0.034 (4)	0.013 (3)	-0.022 (3)
C15	0.029 (3)	0.024 (3)	0.028 (3)	-0.007 (2)	-0.002 (2)	-0.007 (2)
C16	0.040 (3)	0.034 (3)	0.033 (3)	-0.003 (2)	-0.015 (3)	-0.010 (2)

Geometric parameters (\AA , $^\circ$)

Cu2—O2	1.940 (4)	C3—C4	1.402 (8)
Cu2—O4	2.000 (4)	C3—H3	0.9300
Cu2—O5	2.775 (4)	C4—C5	1.402 (7)
Cu2—N2	2.013 (4)	C4—C12	1.433 (8)
Cu2—N1	2.024 (4)	C5—C6	1.416 (7)
Cu2—O1	2.261 (4)	C6—C7	1.404 (7)
I1—C16	2.134 (6)	C7—C8	1.403 (8)
I2—I2 ⁱ	3.6772 (9)	C7—C11	1.434 (8)

I2—C14	2.117 (6)	C8—C9	1.352 (8)
N1—C1	1.322 (6)	C8—H8	0.9300
N1—C5	1.357 (6)	C9—C10	1.394 (8)
N2—C10	1.325 (7)	C9—H9	0.9300
N2—C6	1.349 (6)	C10—H10	0.9300
O1—H1C	0.8500	C11—C12	1.348 (9)
O1—H1B	0.8500	C11—H11	0.9300
O2—C13	1.262 (7)	C12—H12	0.9300
O3—C13	1.230 (7)	C13—C14	1.511 (8)
O4—C15	1.282 (6)	C14—H14A	0.9700
O5—C15	1.221 (6)	C14—H14B	0.9700
C1—C2	1.399 (8)	C15—C16	1.510 (7)
C1—H1A	0.9300	C16—H16A	0.9700
C2—C3	1.359 (9)	C16—H16B	0.9700
C2—H2	0.9300		
Cg1...Cg3 ⁱⁱ	3.505 (6)	Cg2...Cg4 ⁱⁱⁱ	3.634 (6)
Cg1...Cg4 ⁱⁱⁱ	3.584 (6)	I2...I2 ⁱ	3.6772 (9)
Cg2...Cg3 ⁱⁱ	3.625 (6)		
O2—Cu2—O4	92.78 (16)	C7—C6—C5	120.1 (4)
O2—Cu2—N2	170.83 (17)	C8—C7—C6	116.6 (5)
O4—Cu2—N2	96.04 (17)	C8—C7—C11	125.3 (5)
O2—Cu2—N1	89.71 (17)	C6—C7—C11	118.1 (5)
O4—Cu2—N1	153.55 (16)	C9—C8—C7	119.8 (5)
N2—Cu2—N1	81.29 (17)	C9—C8—H8	120.1
O2—Cu2—O1	93.26 (15)	C7—C8—H8	120.1
O4—Cu2—O1	92.60 (14)	C8—C9—C10	119.7 (5)
N2—Cu2—O1	88.81 (16)	C8—C9—H9	120.2
N1—Cu2—O1	113.56 (15)	C10—C9—H9	120.2
C1—N1—C5	118.9 (4)	N2—C10—C9	122.7 (5)
C1—N1—Cu2	128.7 (4)	N2—C10—H10	118.7
C5—N1—Cu2	112.3 (3)	C9—C10—H10	118.7
C10—N2—C6	117.8 (5)	C12—C11—C7	122.0 (5)
C10—N2—Cu2	129.0 (4)	C12—C11—H11	119.0
C6—N2—Cu2	113.1 (3)	C7—C11—H11	119.0
Cu2—O1—H1C	109.3	C11—C12—C4	120.6 (5)
Cu2—O1—H1B	99.7	C11—C12—H12	119.7
H1C—O1—H1B	106.6	C4—C12—H12	119.7
C13—O2—Cu2	130.1 (3)	O3—C13—O2	126.2 (5)
C15—O4—Cu2	108.2 (3)	O3—C13—C14	122.0 (5)
N1—C1—C2	121.5 (5)	O2—C13—C14	111.7 (5)
N1—C1—H1A	119.2	C13—C14—I2	113.9 (4)
C2—C1—H1A	119.2	C13—C14—H14A	108.8
C3—C2—C1	120.4 (5)	I2—C14—H14A	108.8
C3—C2—H2	119.8	C13—C14—H14B	108.8
C1—C2—H2	119.8	I2—C14—H14B	108.8
C2—C3—C4	119.3 (5)	H14A—C14—H14B	107.7
C2—C3—H3	120.4	O5—C15—O4	125.0 (5)
C4—C3—H3	120.4	O5—C15—C16	118.5 (5)

supplementary materials

C5—C4—C3	117.3 (5)	O4—C15—C16	116.5 (4)
C5—C4—C12	118.6 (5)	C15—C16—I1	109.7 (4)
C3—C4—C12	124.1 (5)	C15—C16—H16A	109.7
N1—C5—C4	122.6 (5)	I1—C16—H16A	109.7
N1—C5—C6	116.8 (4)	C15—C16—H16B	109.7
C4—C5—C6	120.6 (5)	I1—C16—H16B	109.7
N2—C6—C7	123.4 (5)	H16A—C16—H16B	108.2
N2—C6—C5	116.5 (4)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1B \cdots O3	0.85	1.84	2.639 (6)	156
O1—H1C \cdots O4 ^{iv}	0.85	1.97	2.785 (5)	161
C3—H3 \cdots O1 ⁱⁱⁱ	0.93	2.44	3.240 (7)	144
C11—H11 \cdots O5 ⁱⁱ	0.93	2.71	3.508 (8)	144
C10—H10 \cdots O3 ^{iv}	0.93	2.68	3.431 (8)	138
C14—H14B \cdots O2 ^v	0.97	2.59	3.436 (8)	146
C14—H14A \cdots O5 ^v	0.97	2.64	3.219 (8)	119

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

Fig. 1

