Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diaquabis[2-(4-bromophenyl)acetato]-bis(N^4,N^4-dimethylpyridin-4-amine)-copper(II)

Yong-Ming Cui, Xi-Bin Dai, Ru-Hua Zha and Qing-Fu Zeng*

Engineering Research Center for Clean Production of Textile Dyeing and Printing, Ministry of Education, Wuhan 430073, People's Republic of China
Correspondence e-mail: qfzeng@wuse.edu.cn

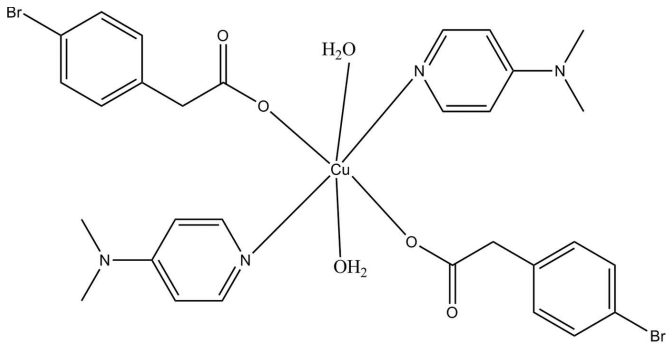
Received 24 August 2009; accepted 28 August 2009

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.035; wR factor = 0.099; data-to-parameter ratio = 14.2.

In the title compound, $[Cu(C_8H_6BrO_2)_2(C_7H_{10}N_2)_2(H_2O)_2]$, the Cu^{II} atom (site symmetry $\overline{1}$) adopts a Jahn–Teller-distorted *trans*-CuN_2O_4 octahedral coordination, with the aqua O atoms in axially extended sites. An intramolecular O—H···O hydrogen bond helps to establish the conformation and an intermolecular O—H···O hydrogen bond is seen in the crystal packing.

Related literature

For background to coordination networks, see: Liu & Zhu (2004); Yang *et al.* (2004); You *et al.* (2004). For reference structural data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[Cu(C_8H_6BrO_2)_2(C_7H_{10}N_2)_2(H_2O)_2]$
M_r = 771.99
Monoclinic, $P2_1/c$
a = 10.4792 (10) Å
b = 6.1059 (6) Å
c = 25.450 (2) Å
β = 100.958 (4)°
V = 1598.7 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 3.23 mm^{-1}
T = 293 K
0.25 × 0.20 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.499, T_{max} = 0.564
8029 measured reflections
2815 independent reflections
2189 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
200 standard reflections
every 3 reflections
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.099
S = 1.01
2815 reflections
198 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.71 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—O2	2.0006 (17)	Cu1—O3	2.5052 (19)
Cu1—N2	2.004 (2)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3B···O2^{i}	0.90	2.03	2.901 (3)	161
O3—H3A···O1	0.92	1.79	2.688 (3)	163

Symmetry code: (i) $x, y-1, z$.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); 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*.

The project was supported by the Scientific Research Foundation for Returned Overseas Chinese Scholars, State Education Ministry, Educational Commission of Hubei Province (D20091703) and the Natural Science Foundation of Hubei Province (2008CDB038).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5065).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1-19.
Enraf–Nonius (1989). *CAD-4 Software*. Enraf–Nonius, Delft, The Netherlands.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
Liu, Z.-D. & Zhu, H.-L. (2004). *Acta Cryst.* E**60**, m1866–m1868.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Yang, H.-L., You, Z.-L. & Zhu, H.-L. (2004). *Acta Cryst.* E**60**, m1213–m1214.
You, Z.-L., Zhu, H.-L. & Liu, W.-S. (2004). *Acta Cryst.* E**60**, m1863–m1865.

supporting information

Acta Cryst. (2009). E**65**, m1163 [doi:10.1107/S1600536809034461]

Diaquabis[2-(4-bromophenyl)acetato]bis(N^4,N^4-dimethylpyridin-4-amine)-copper(II)

Yong-Ming Cui, Xi-Bin Dai, Ru-Hua Zha and Qing-Fu Zeng

S1. Comment

There has been much research interest in the acid and amine metal complexes due to their molecular architectures (Liu *et al.*, 2004; Yang *et al.*, 2004; You *et al.*, 2004). In this work, we report here the crystal structure of the title compound, (I). In (I), all bond lengths are within normal ranges (Allen *et al.*, 1987) (Fig. 1). The Cu^{II} atom is six-coordinated by two N atoms from *N*,*N*-dimethylpyridin-4-amine, two O atoms from 2-(4-bromophenyl)acetic acid and two O atoms from the water molecules, forming a distorted octahedral coordination.

S2. Experimental

A mixture of *N*,*N*-dimethylpyridin-4-amine (244 mg, 2 mmol), 2-(4-bromophenyl)acetic acid (428 mg, 2 mmol) and $CuCl_2.2H_2O$ (169 mg, 1 mmol) in methanol (10 ml) was stirred for 3 h. After keeping the filtrate in air for 7 d, green blocks of (I) were formed.

S3. Refinement

All H atoms were positioned geometrically (C—H = 0.93 Å for the aromatic H atoms and C—H = 0.96 Å for the aliphatic H atoms) and were refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) and U_{iso}(H) = 1.2U_{eq}(N).

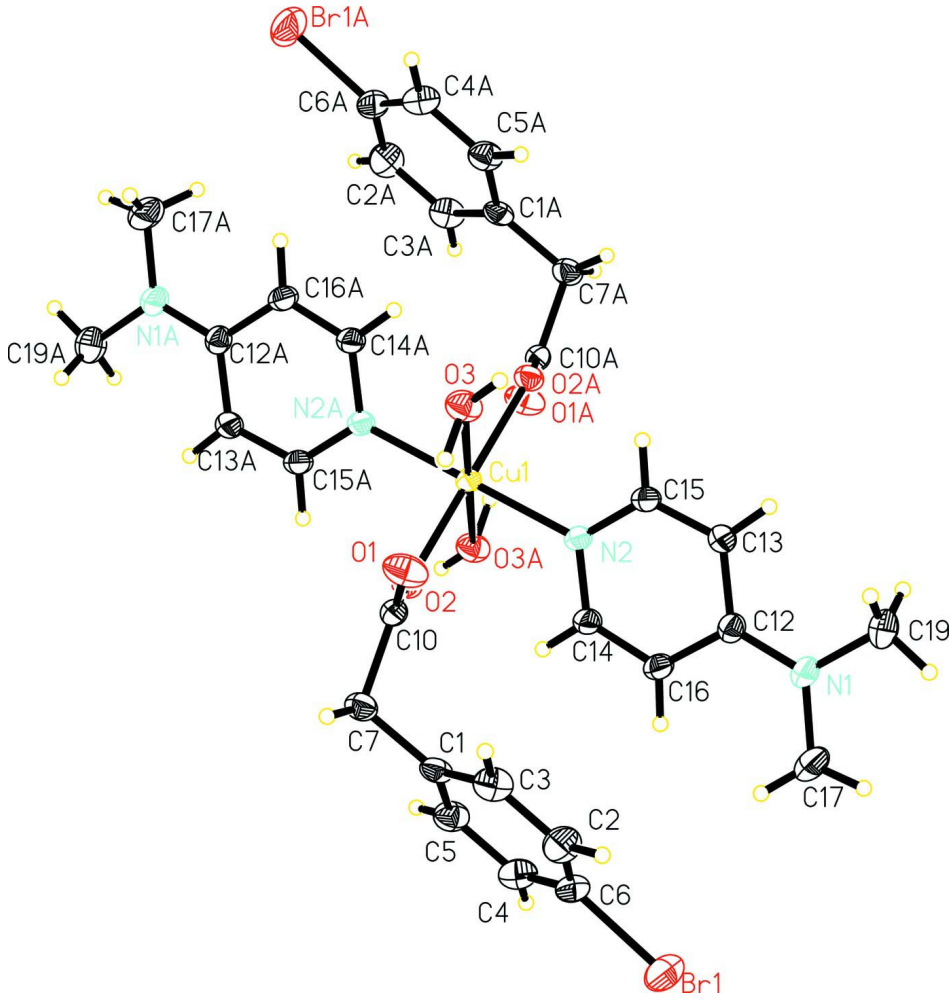


Figure 1

The molecular structure of (I) showing 30% probability displacement ellipsoids. Atoms with the suffix A are generated by the symmetry operation (1–x, 1–y, –z).

Diaquabis[2-(4-bromophenyl)acetato]bis(*N*^{4},*N*^{4}- dimethylpyridin-4-amine)copper(II)

Crystal data

$[Cu(C_8H_6BrO_2)_2(C_7H_{10}N_2)_2(H_2O)_2]$
$M_r = 771.99$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 10.4792\ (10)$ Å
$b = 6.1059\ (6)$ Å
$c = 25.450\ (2)$ Å
$\beta = 100.958\ (4)°$
$V = 1598.7\ (3)$ Å^3
$Z = 2$
$F(000) = 782$
$D_x = 1.604$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 9–12°$
$\mu = 3.23$ mm^{-1}
$T = 293$ K
Block, green
0.25 × 0.20 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.499, T_{max} = 0.564
8029 measured reflections
2815 independent reflections
2189 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 25.0°, θ_{min} = 1.6°
$h = -10 \rightarrow 12$
$k = -7 \rightarrow 7$
$l = -30 \rightarrow 28$
200 standard reflections every 3 reflections
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.099
S = 1.01
2815 reflections
198 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
$w = 1/[\sigma^2(F_o^2) + (0.0539P)^2 + 0.7463P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.71 e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.10163 (4)	0.98365 (8)	0.229572 (18)	0.0870 (2)
C1	0.4910 (3)	0.8264 (4)	0.17361 (10)	0.0366 (6)
C2	0.3209 (3)	0.7210 (6)	0.21980 (12)	0.0567 (9)
H2	0.2854	0.6195	0.2402	0.068*
C3	0.4355 (3)	0.6766 (5)	0.20345 (11)	0.0479 (8)
H3	0.4767	0.5433	0.2126	0.058*
C4	0.3099 (3)	1.0674 (6)	0.17612 (13)	0.0525 (8)
H4	0.2669	1.1991	0.1668	0.063*
C5	0.4259 (3)	1.0225 (5)	0.15993 (13)	0.0462 (8)
H5	0.4608	1.1250	0.1396	0.055*
C6	0.2591 (3)	0.9156 (6)	0.20593 (12)	0.0492 (8)
C7	0.6186 (3)	0.7783 (5)	0.15678 (10)	0.0411 (7)
H7A	0.6807	0.7252	0.1873	0.049*
H7B	0.6529	0.9121	0.1443	0.049*
C10	0.6013 (3)	0.6071 (5)	0.11224 (10)	0.0354 (6)

C12	0.1011 (3)	0.4106 (5)	0.06736 (10)	0.0354 (6)
C13	0.1512 (3)	0.2454 (5)	0.03830 (11)	0.0410 (7)
H13	0.1083	0.1117	0.0324	0.049*
C14	0.2815 (3)	0.6273 (4)	0.05081 (11)	0.0373 (6)
H14	0.3254	0.7605	0.0548	0.045*
C15	0.2618 (3)	0.2798 (5)	0.01872 (11)	0.0392 (7)
H15	0.2918	0.1658	0.0001	0.047*
C16	0.1726 (3)	0.6080 (5)	0.07202 (11)	0.0393 (7)
H16	0.1447	0.7264	0.0899	0.047*
C17	−0.0511 (4)	0.5523 (6)	0.12039 (17)	0.0694 (11)
H17A	0.0206	0.6143	0.1450	0.104*
H17B	−0.1126	0.4918	0.1399	0.104*
H17C	−0.0924	0.6644	0.0966	0.104*
C19	−0.0777 (3)	0.1795 (6)	0.08259 (15)	0.0640 (10)
H19A	−0.1167	0.1622	0.0455	0.096*
H19B	−0.1445	0.1841	0.1037	0.096*
H19C	−0.0207	0.0583	0.0939	0.096*
Cu1	0.5000	0.5000	0.0000	0.03234 (15)
N1	−0.0042 (2)	0.3814 (4)	0.08968 (10)	0.0462 (6)
N2	0.3302 (2)	0.4658 (3)	0.02439 (9)	0.0331 (5)
O1	0.6222 (2)	0.4143 (4)	0.12444 (8)	0.0570 (6)
O2	0.56545 (17)	0.6809 (3)	0.06509 (7)	0.0372 (4)
O3	0.58520 (19)	0.1416 (3)	0.03998 (7)	0.0469 (5)
H3B	0.5591	0.0050	0.0463	0.056*
H3A	0.6011	0.2105	0.0727	0.056*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0564 (3)	0.1343 (5)	0.0770 (3)	−0.0039 (2)	0.0294 (2)	−0.0350 (3)
C1	0.0497 (17)	0.0354 (15)	0.0256 (13)	−0.0051 (13)	0.0092 (12)	−0.0073 (11)
C2	0.069 (2)	0.065 (2)	0.0416 (17)	−0.0128 (19)	0.0260 (16)	0.0034 (15)
C3	0.065 (2)	0.0413 (17)	0.0386 (15)	0.0014 (16)	0.0123 (15)	0.0054 (13)
C4	0.061 (2)	0.0482 (18)	0.0505 (18)	0.0102 (17)	0.0149 (16)	−0.0055 (15)
C5	0.060 (2)	0.0394 (18)	0.0421 (16)	−0.0025 (15)	0.0167 (15)	−0.0010 (13)
C6	0.0488 (18)	0.064 (2)	0.0388 (16)	−0.0027 (17)	0.0171 (14)	−0.0152 (15)
C7	0.0470 (17)	0.0440 (17)	0.0323 (14)	−0.0046 (14)	0.0080 (12)	−0.0083 (12)
C10	0.0345 (15)	0.0392 (17)	0.0358 (15)	−0.0073 (13)	0.0155 (12)	−0.0071 (12)
C12	0.0330 (14)	0.0396 (15)	0.0348 (14)	−0.0011 (13)	0.0093 (12)	0.0013 (12)
C13	0.0413 (16)	0.0349 (15)	0.0505 (16)	−0.0085 (13)	0.0177 (13)	−0.0096 (13)
C14	0.0407 (15)	0.0298 (15)	0.0447 (16)	−0.0029 (12)	0.0164 (13)	−0.0063 (12)
C15	0.0437 (16)	0.0334 (15)	0.0452 (16)	−0.0045 (13)	0.0199 (13)	−0.0103 (12)
C16	0.0405 (16)	0.0337 (16)	0.0477 (16)	0.0018 (13)	0.0188 (13)	−0.0063 (13)
C17	0.062 (2)	0.073 (2)	0.087 (3)	−0.0086 (19)	0.048 (2)	−0.017 (2)
C19	0.054 (2)	0.067 (2)	0.079 (2)	−0.0204 (18)	0.0334 (18)	−0.0083 (19)
Cu1	0.0321 (3)	0.0372 (3)	0.0304 (3)	−0.0056 (2)	0.01259 (19)	−0.00735 (18)
N1	0.0408 (14)	0.0468 (15)	0.0572 (15)	−0.0077 (12)	0.0249 (12)	−0.0071 (12)
N2	0.0355 (12)	0.0318 (13)	0.0351 (12)	−0.0014 (10)	0.0143 (10)	−0.0048 (9)

O1	0.0861 (18)	0.0371 (12)	0.0473 (12)	−0.0003 (12)	0.0116 (11)	−0.0025 (10)
O2	0.0436 (11)	0.0381 (11)	0.0317 (10)	−0.0060 (9)	0.0114 (8)	−0.0075 (8)
O3	0.0602 (13)	0.0386 (11)	0.0438 (11)	−0.0036 (10)	0.0146 (9)	−0.0017 (9)

Geometric parameters (Å, º)

Br1—C6	1.906 (3)	C14—N2	1.347 (3)
C1—C3	1.386 (4)	C14—C16	1.357 (4)
C1—C5	1.389 (4)	C14—H14	0.9300
C1—C7	1.508 (4)	C15—N2	1.336 (3)
C2—C6	1.367 (5)	C15—H15	0.9300
C2—C3	1.371 (4)	C16—H16	0.9300
C2—H2	0.9300	C17—N1	1.445 (4)
C3—H3	0.9300	C17—H17A	0.9600
C4—C6	1.368 (5)	C17—H17B	0.9600
C4—C5	1.384 (5)	C17—H17C	0.9600
C4—H4	0.9300	C19—N1	1.447 (4)
C5—H5	0.9300	C19—H19A	0.9600
C7—C10	1.527 (4)	C19—H19B	0.9600
C7—H7A	0.9700	C19—H19C	0.9600
C7—H7B	0.9700	Cu1—O2^{i}	2.0006 (17)
C10—O1	1.226 (4)	Cu1—O2	2.0006 (17)
C10—O2	1.270 (3)	Cu1—N2	2.004 (2)
C12—N1	1.345 (3)	Cu1—N2^{i}	2.004 (2)
C12—C13	1.410 (4)	Cu1—O3	2.5052 (19)
C12—C16	1.412 (4)	Cu1—O3^{i}	2.5052 (19)
C13—C15	1.362 (4)	O3—H3B	0.9018
C13—H13	0.9300	O3—H3A	0.9200
C3—C1—C5	117.9 (3)	C14—C16—C12	120.9 (3)
C3—C1—C7	121.0 (3)	C14—C16—H16	119.6
C5—C1—C7	121.1 (3)	C12—C16—H16	119.6
C6—C2—C3	119.5 (3)	N1—C17—H17A	109.5
C6—C2—H2	120.2	N1—C17—H17B	109.5
C3—C2—H2	120.2	H17A—C17—H17B	109.5
C2—C3—C1	121.3 (3)	N1—C17—H17C	109.5
C2—C3—H3	119.4	H17A—C17—H17C	109.5
C1—C3—H3	119.4	H17B—C17—H17C	109.5
C6—C4—C5	119.2 (3)	N1—C19—H19A	109.5
C6—C4—H4	120.4	N1—C19—H19B	109.5
C5—C4—H4	120.4	H19A—C19—H19B	109.5
C4—C5—C1	120.9 (3)	N1—C19—H19C	109.5
C4—C5—H5	119.5	H19A—C19—H19C	109.5
C1—C5—H5	119.5	H19B—C19—H19C	109.5
C2—C6—C4	121.1 (3)	O2^{i}—Cu1—O2	180.00 (6)
C2—C6—Br1	120.3 (3)	O2^{i}—Cu1—N2	90.81 (8)
C4—C6—Br1	118.6 (3)	O2—Cu1—N2	89.19 (8)
C1—C7—C10	111.0 (2)	O2^{i}—Cu1—N2^{i}	89.19 (8)

C1—C7—H7A	109.4	O2—Cu1—N2^{i}	90.81 (8)
C10—C7—H7A	109.4	N2—Cu1—N2^{i}	180.00 (11)
C1—C7—H7B	109.4	O2—Cu1—O3	96.11 (7)
C10—C7—H7B	109.4	O2—Cu1—O3^{i}	83.89 (7)
H7A—C7—H7B	108.0	O3—Cu1—N2	92.98 (7)
O1—C10—O2	125.9 (2)	O3—Cu1—O2^{i}	83.89 (7)
O1—C10—C7	118.6 (2)	O3—Cu1—O3^{i}	180.00 (7)
O2—C10—C7	115.5 (2)	O3—Cu1—N2^{i}	87.02 (7)
N1—C12—C13	122.9 (3)	N2—Cu1—O3^{i}	87.02 (7)
N1—C12—C16	122.8 (3)	O2^{i}—Cu1—O3^{i}	96.11 (7)
C13—C12—C16	114.2 (2)	O3^{i}—Cu1—N2^{i}	92.98 (7)
C15—C13—C12	120.6 (3)	C12—N1—C17	121.5 (3)
C15—C13—H13	119.7	C12—N1—C19	121.4 (3)
C12—C13—H13	119.7	C17—N1—C19	117.1 (3)
N2—C14—C16	124.2 (3)	C15—N2—C14	115.4 (2)
N2—C14—H14	117.9	C15—N2—Cu1	123.04 (18)
C16—C14—H14	117.9	C14—N2—Cu1	121.40 (18)
N2—C15—C13	124.6 (2)	C10—O2—Cu1	125.44 (18)
N2—C15—H15	117.7	H3B—O3—H3A	105.6
C13—C15—H15	117.7		

Symmetry code: (i) $-x+1, -y+1, -z$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*B*···O2^{ii}	0.90	2.03	2.901 (3)	161
O3—H3*A*···O1	0.92	1.79	2.688 (3)	163

Symmetry code: (ii) $x, y-1, z$.