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Diaquabis[5-(2-pyridylmethyl)tetrazolato-κ^2N^1,N^5]zinc(II)

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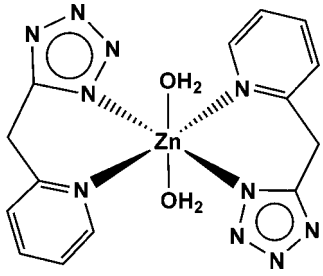
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.022; wR factor = 0.053; data-to-parameter ratio = 11.2.

In the title mononuclear complex, $[Zn(C_7H_6N_5)_2(H_2O)_2]$, the Zn^{II} atom, located on an inversion centre, is in a distorted octahedral coordination geometry formed by four N atoms from two chelating 5-(2-pyridylmethyl)tetrazolate ligands and two O donors from two water molecules. Intermolecular O—H···N hydrogen bonds between the coordinated water molecule and the tetrazolyl group of the 5-(2-pyridylmethyl)tetrazolate ligand lead to the formation of a three-dimensional network.

Related literature

For metal-organic frameworks with tetrazolate ligands and their applications in magnetism, fluorescence and gas storage, see: Yang *et al.* (2011); Feng *et al.* (2010); Zhao *et al.* (2008); Panda *et al.* (2011). For metal complexes with *in situ*-generated 5-(2-pyridylmethyl)-tetrazolate ligands, see: Xu *et al.* (2009); Wang (2008).



Experimental

Crystal data

$[Zn(C_7H_6N_5)_2(H_2O)_2]$ M_r = 421.74
Monoclinic, $P2_1/c$
a = 6.6695 (4) Å
b = 13.8949 (8) Å
c = 10.8718 (5) Å
β = 127.055 (2)°
V = 804.05 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.57 mm^{-1}
T = 173 K
0.20 × 0.10 × 0.08 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.745, T_{max} = 0.885
3929 measured reflections
1388 independent reflections
1335 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.053
S = 1.05
1388 reflections
124 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···N4^{i}	0.85	2.00	2.8395 (19)	171
O1—H1B···N2^{ii}	0.85	2.16	2.9386 (18)	152

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

Data collection: *APEX2* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2001); 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) and *DIAMOND* (Brandenburg & Berndt, 1999); 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: BT5553).

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supporting information

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Diaquabis[5-(2-pyridylmethyl)tetrazolato-κ^2N^1,N^5]zinc(II)

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S1. Comment

Design and construction of metal-organic frameworks (MOFs) with *in situ* generated tetrazolate ligands are of great interest due to their intriguing structures and topology (Zhao *et al.*, 2008), promising applications in magnetism (Yang *et al.* 2011), luminscence (Feng *et al.* 2010), and gas storage (Panda *et al.* 2011) as well as the effectiveness, simplicity, and environmental friendliness of the *in situ* synthetic route. Up to date, lots of tetrazolyl-based MOFs have been reported with special interest on the tuning of the organic nitrile and metal ions (Xu *et al.* 2009; Wang *et al.*, 2008). Herein, as our continuing investigations on the coordination chemistry of the tetrazolyl ligand, we report the crystal structure of a diaquazinc(II) complex with an *in situ* generated 5-(2-pyridylmethyl)-tetrazolate ligand.

The molecular structure of the title mononuclear complex is show Figure 1. The Zn^{II} ion in the mononuclear structure of I, locating on an inversion center, exhibits a slightly distorted octahedral geometry involoving four N donors from two in situ generated 5-(pyridin-2-ylmethyl)tetrazolate ligands, and two O atoms from a pair of coordinated water molecules. The flexible 5-(pyridin-2-ylmethyl)tetrazolate anion acts as a bidentate chelating ligand to coordinate with Zn^{II} through pyridyl and tetrazolyl N donors.

In the crystal structure, intermolecular O—H···N hydrogen bonds between the coordinated water molecules and the tetrazolyl group of 5-(2-pyridylmethyl)- tetrazolate ligand (Table 2) lead to the formation of a three-dimensional network (Figure 2).

S2. Experimental

A mixture containing 2-(pyridin-2-yl)acetonitrile (26 mg, 0.2 mmol), $Zn(NO_3)_2$ (29.7 mg, 0.1 mmol), 1,3,5-benzenetricarboxylic acid (21.0 mg, 0.1 mmol), NaN_3 (13.0 mg, 0.2 mmol), and doubly deionized water (10.0 ml) was sealed in a Teflon-lined reactor (23.0 ml) and heated at 125 °C for 72 h. After the mixture was cooled to room temperature at a rate of 5.5°C/h, pale-yellow block-shaped crystals suitable for X-ray diffraction analysis were obtained. Yield: 56% based on Zn^{II} salt. Anal. Calcd.for $C_{14}H_{16}N_{10}O_2Zn$: C, 39.87; H, 3.82; N, 33.21%. Found: C, 39.85; H, 3.82; N, 33.24%.

S3. Refinement

H atoms were located in a difference map but refined using a riding model with O-H = 0.85Å, $C_{aromatic}$-H = 0.95Å, $C_{methylene}$-H = 0.99Å and with U(H) set to 1.2 U of the parent atom.

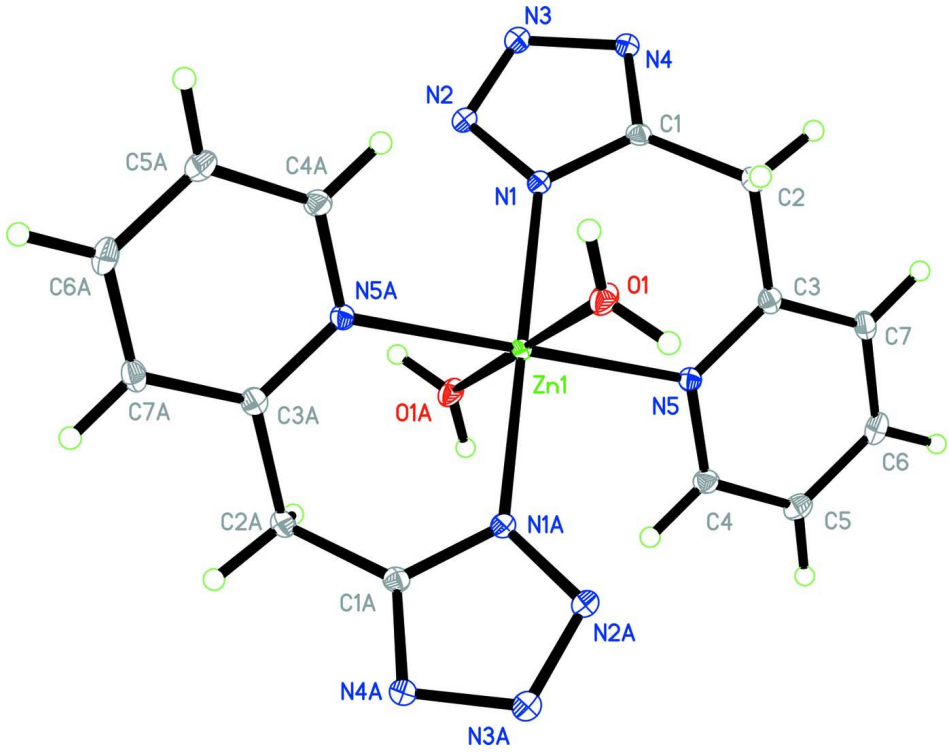

Figure 1

The molecular structure of the title complex with the atomic numbering scheme. Displacement ellipsoids were drawn at the 30% probability level [Symmetry code: (A) $1 - x$, $2 - y$, $- z$].

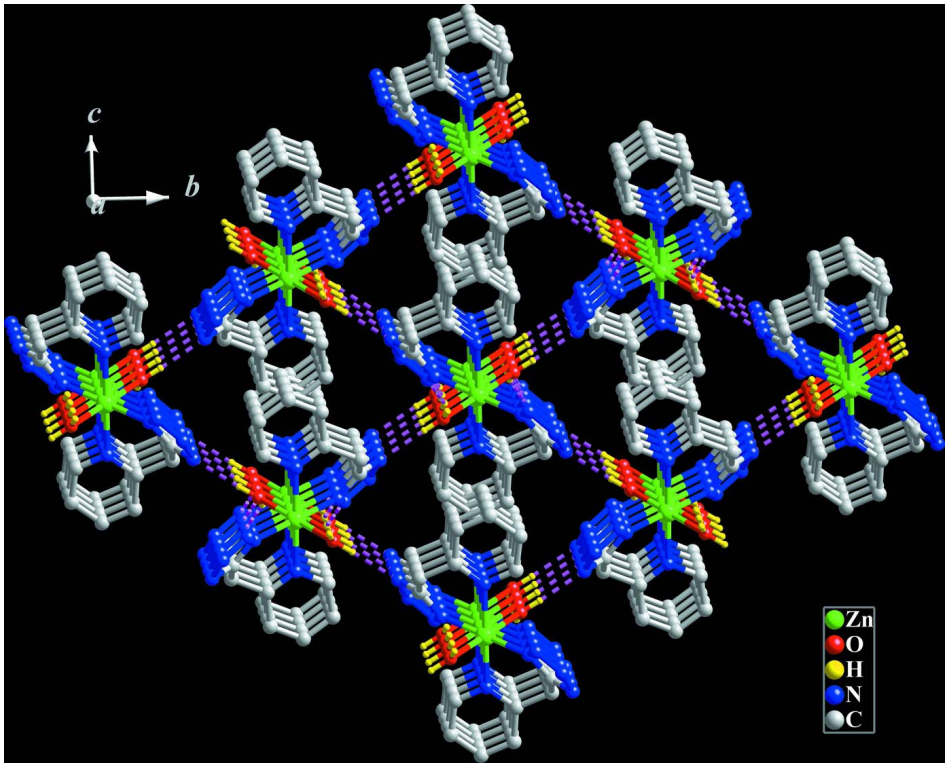

Figure 2

Three-dimensional network of the title complex assembled from hydrogen-bonding interactions.

Diaquabis[5-(2-pyridylmethyl)tetrazolato-κ^2N^1,N^5]zinc(II)

Crystal data

$[Zn(C_7H_6N_5)_2(H_2O)_2]$
$M_r = 421.74$
Monoclinic, $P2_1/c$
$a = 6.6695$ (4) Å
$b = 13.8949$ (8) Å
$c = 10.8718$ (5) Å
$\beta = 127.055$ (2)°
$V = 804.05$ (8) Å^3
$Z = 2$
$F(000) = 432$
$D_x = 1.742$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3869 reflections
$\theta = 2.8$–$28.4°$
$\mu = 1.57$ mm^{-1}
$T = 173$ K
Block, pale yellow
0.20 × 0.10 × 0.08 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.745$, $T_{max} = 0.885$
3929 measured reflections
1388 independent reflections
1335 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.8°$
$h = -7 \rightarrow 7$
$k = -16 \rightarrow 11$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.022$
$wR(F^2) = 0.053$
$S = 1.05$
1388 reflections
124 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
$w = 1/[\sigma^2(F_o^2) + (0.0146P)^2 + 0.7405P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.62$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ 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}
Zn1	0.5000	1.0000	0.0000	0.01318 (11)
O1	0.6481 (2)	0.90283 (9)	−0.08811 (14)	0.0196 (3)
H1A	0.5809	0.8510	−0.1382	0.024*
H1B	0.7995	0.9131	−0.0532	0.024*
N1	0.4006 (3)	0.88555 (10)	0.07937 (16)	0.0144 (3)
N2	0.1830 (3)	0.86762 (11)	0.05983 (17)	0.0164 (3)
N3	0.2217 (3)	0.79864 (11)	0.15370 (17)	0.0185 (3)
N4	0.4661 (3)	0.77039 (11)	0.23846 (16)	0.0161 (3)
N5	0.8595 (3)	0.99858 (9)	0.22729 (17)	0.0135 (3)
C1	0.5681 (3)	0.82608 (12)	0.18945 (19)	0.0140 (4)
C2	0.8406 (3)	0.82446 (13)	0.2548 (2)	0.0166 (4)
H2A	0.8553	0.8047	0.1730	0.020*
H2B	0.9289	0.7759	0.3381	0.020*
C3	0.9670 (3)	0.92064 (13)	0.3181 (2)	0.0146 (4)
C4	0.9710 (3)	1.08445 (13)	0.2853 (2)	0.0159 (4)
H4	0.8952	1.1398	0.2218	0.019*
C5	1.1913 (3)	1.09628 (14)	0.4334 (2)	0.0189 (4)
H5	1.2641	1.1582	0.4704	0.023*
C6	1.3018 (3)	1.01590 (14)	0.5256 (2)	0.0196 (4)
H6	1.4524	1.0216	0.6276	0.023*
C7	1.1908 (3)	0.92742 (14)	0.4676 (2)	0.0175 (4)
H7	1.2659	0.8712	0.5289	0.021*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.01153 (16)	0.01131 (17)	0.01161 (16)	−0.00133 (10)	0.00427 (13)	0.00173 (10)
O1	0.0142 (6)	0.0174 (7)	0.0229 (6)	−0.0019 (5)	0.0089 (5)	−0.0076 (6)
N1	0.0128 (7)	0.0135 (7)	0.0140 (7)	−0.0012 (6)	0.0066 (6)	0.0001 (6)
N2	0.0138 (7)	0.0160 (8)	0.0174 (7)	−0.0018 (6)	0.0083 (6)	−0.0003 (7)
N3	0.0160 (7)	0.0183 (8)	0.0189 (7)	−0.0012 (6)	0.0093 (6)	0.0004 (7)
N4	0.0150 (7)	0.0145 (7)	0.0169 (7)	−0.0003 (6)	0.0086 (6)	0.0018 (6)
N5	0.0127 (7)	0.0136 (8)	0.0141 (7)	0.0005 (5)	0.0080 (6)	0.0011 (5)
C1	0.0160 (8)	0.0104 (8)	0.0143 (8)	−0.0005 (7)	0.0085 (7)	−0.0020 (7)
C2	0.0153 (8)	0.0139 (9)	0.0189 (9)	0.0028 (7)	0.0094 (7)	0.0029 (8)
C3	0.0141 (8)	0.0176 (9)	0.0164 (8)	0.0020 (7)	0.0115 (7)	0.0019 (8)
C4	0.0166 (8)	0.0159 (9)	0.0146 (8)	−0.0015 (7)	0.0092 (7)	0.0008 (8)
C5	0.0180 (9)	0.0212 (10)	0.0169 (9)	−0.0049 (8)	0.0102 (8)	−0.0038 (8)
C6	0.0127 (8)	0.0298 (10)	0.0151 (9)	0.0001 (8)	0.0078 (7)	−0.0005 (8)
C7	0.0145 (8)	0.0214 (10)	0.0172 (9)	0.0051 (7)	0.0100 (7)	0.0058 (8)

Geometric parameters (Å, º)

Zn1—N1^{i}	2.0983 (14)	N5—C3	1.345 (2)
Zn1—N1	2.0984 (14)	C1—C2	1.501 (2)
Zn1—N5	2.1714 (15)	C2—C3	1.507 (2)
Zn1—N5^{i}	2.1714 (15)	C2—H2A	0.9900
Zn1—O1	2.2039 (12)	C2—H2B	0.9900
Zn1—O1^{i}	2.2039 (12)	C3—C7	1.399 (2)
O1—H1A	0.8501	C4—C5	1.388 (2)
O1—H1B	0.8500	C4—H4	0.9500
N1—C1	1.324 (2)	C5—C6	1.380 (3)
N1—N2	1.3572 (19)	C5—H5	0.9500
N2—N3	1.307 (2)	C6—C7	1.376 (3)
N3—N4	1.360 (2)	C6—H6	0.9500
N4—C1	1.335 (2)	C7—H7	0.9500
N5—C4	1.345 (2)		
N1^{i}—Zn1—N1	180.00 (7)	C3—N5—Zn1	125.26 (11)
N1^{i}—Zn1—N5	93.96 (5)	N1—C1—N4	111.52 (15)
N1—Zn1—N5	86.04 (5)	N1—C1—C2	123.99 (15)
N1^{i}—Zn1—N5^{i}	86.04 (5)	N4—C1—C2	124.45 (15)
N1—Zn1—N5^{i}	93.96 (5)	C1—C2—C3	112.78 (14)
N5—Zn1—N5^{i}	180.0	C1—C2—H2A	109.0
N1^{i}—Zn1—O1	87.13 (5)	C3—C2—H2A	109.0
N1—Zn1—O1	92.87 (5)	C1—C2—H2B	109.0
N5—Zn1—O1	90.71 (5)	C3—C2—H2B	109.0
N5^{i}—Zn1—O1	89.29 (5)	H2A—C2—H2B	107.8
N1^{i}—Zn1—O1^{i}	92.87 (5)	N5—C3—C7	121.50 (16)
N1—Zn1—O1^{i}	87.13 (5)	N5—C3—C2	118.36 (15)
N5—Zn1—O1^{i}	89.29 (5)	C7—C3—C2	120.14 (16)

N5^{i}—Zn1—O1^{i}	90.71 (5)	N5—C4—C5	123.28 (17)
O1—Zn1—O1^{i}	180.00 (6)	N5—C4—H4	118.4
Zn1—O1—H1A	126.6	C5—C4—H4	118.4
Zn1—O1—H1B	115.2	C6—C5—C4	118.38 (17)
H1A—O1—H1B	117.0	C6—C5—H5	120.8
C1—N1—N2	105.52 (13)	C4—C5—H5	120.8
C1—N1—Zn1	122.75 (11)	C7—C6—C5	119.06 (17)
N2—N1—Zn1	130.38 (11)	C7—C6—H6	120.5
N3—N2—N1	108.81 (13)	C5—C6—H6	120.5
N2—N3—N4	109.47 (13)	C6—C7—C3	119.69 (17)
C1—N4—N3	104.66 (14)	C6—C7—H7	120.2
C4—N5—C3	118.08 (15)	C3—C7—H7	120.2
C4—N5—Zn1	116.42 (11)		

N1^{i}—Zn1—N1—C1	−100 (10)	O1^{i}—Zn1—N5—C3	116.31 (13)
N5—Zn1—N1—C1	−26.79 (13)	N2—N1—C1—N4	1.07 (19)
N5^{i}—Zn1—N1—C1	153.21 (13)	Zn1—N1—C1—N4	169.09 (11)
O1—Zn1—N1—C1	63.72 (13)	N2—N1—C1—C2	−176.72 (15)
O1^{i}—Zn1—N1—C1	−116.28 (13)	Zn1—N1—C1—C2	−8.7 (2)
N1^{i}—Zn1—N1—N2	65 (10)	N3—N4—C1—N1	−0.63 (19)
N5—Zn1—N1—N2	137.97 (14)	N3—N4—C1—C2	177.15 (15)
N5^{i}—Zn1—N1—N2	−42.03 (14)	N1—C1—C2—C3	56.5 (2)
O1—Zn1—N1—N2	−131.52 (14)	N4—C1—C2—C3	−121.02 (18)
O1^{i}—Zn1—N1—N2	48.48 (14)	C4—N5—C3—C7	−1.2 (2)
C1—N1—N2—N3	−1.10 (18)	Zn1—N5—C3—C7	−175.34 (12)
Zn1—N1—N2—N3	−167.85 (11)	C4—N5—C3—C2	178.95 (15)
N1—N2—N3—N4	0.75 (18)	Zn1—N5—C3—C2	4.8 (2)
N2—N3—N4—C1	−0.09 (18)	C1—C2—C3—N5	−51.8 (2)
N1^{i}—Zn1—N5—C4	34.93 (13)	C1—C2—C3—C7	128.33 (16)
N1—Zn1—N5—C4	−145.07 (13)	C3—N5—C4—C5	0.3 (2)
N5^{i}—Zn1—N5—C4	85.1 (7)	Zn1—N5—C4—C5	174.98 (13)
O1—Zn1—N5—C4	122.11 (12)	N5—C4—C5—C6	0.2 (3)
O1^{i}—Zn1—N5—C4	−57.89 (12)	C4—C5—C6—C7	0.2 (3)
N1^{i}—Zn1—N5—C3	−150.86 (13)	C5—C6—C7—C3	−1.0 (3)
N1—Zn1—N5—C3	29.14 (13)	N5—C3—C7—C6	1.6 (2)
N5^{i}—Zn1—N5—C3	−100.7 (7)	C2—C3—C7—C6	−178.58 (16)
O1—Zn1—N5—C3	−63.69 (13)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···N4^{ii}	0.85	2.00	2.8395 (19)	171
O1—H1*B*···N2^{iii}	0.85	2.16	2.9386 (18)	152

Symmetry codes: (ii) *x*, −*y*+3/2, *z*−1/2; (iii) *x*+1, *y*, *z*.