Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Bis(3-aminopyrazine-2-carboxylato-κ^2N^1,O)diaquacobalt(II)

Rafika Bouchene,[a,b] Sofiane Bouacida,[c,b]* Fadila Berrah,[a,b] Ratiba Belhouas[c] and Hocine Merazig[c]

[a]Laboratoire de Chimie Appliquée et Technologie des Matériaux LCATM, Université Oum El Bouaghi, Algeria, [b]Département Sciences de la Matière, Faculté des Sciences Exactes et Sciences de la Nature et de la Vie, Université Oum El Bouaghi, Algeria, and [c]Unité de Recherche de Chimie de l'Environnement et Moléculaire Structurale, CHEMS, Faculté des Sciences Exactes, Université Mentouri Constantine 25000, Algeria
Correspondence e-mail: bouacida_sofiane@yahoo.fr

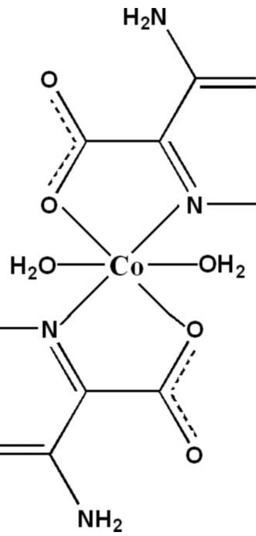
Received 17 January 2013; accepted 22 January 2013

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.001 Å; R factor = 0.034; wR factor = 0.082; data-to-parameter ratio = 43.2.

In the title compound, $[Co(C_5H_4N_3O_2)_2(H_2O)_2]$, the Co^{II} atom is situated on a twofold rotation axis and is *N*,*O*-chelated by two 3-aminopyrazine-2-carboxylate anions and additionally bonded to the O atoms of two water molecules, leading to a slightly distorted octahedral coordination environment. The crystal packing is dominated by intermolecular O—H···O, O—H···N and N—H···O hydrogen bonding involving the water molecules and amino groups as donors and carboxylate O atoms, as well as the non-coordinating heterocyclic N atoms as acceptors, resulting in a three-dimensional network. An intramolecular N—H···O hydrogen bond is also observed.

Related literature

For the role of *N*,*O*-coordination in the crystal structures of metal complexes with pyrazine-2-carboxylate as ligand, see: Alcock *et al.* (1996); Dong *et al.* (2000); Kubota *et al.* (2006); Luo *et al.* (2004). For related pyrazine-2-carboxylate cobalt(II) complexes and their applications, see: Fan *et al.* (2007); Liu *et al.* (2007); McCleverty & Meyer (2004); Shi *et al.* (2011); Sun *et al.* (2004); Tanase *et al.* (2006). For the influence of hydrogen bonding in related systems, see: Bouacida *et al.* (2007, 2009).



Experimental

Crystal data

$[Co(C_5H_4N_3O_2)_2(H_2O)_2]$
M_r = 371.19
Monoclinic, $C2/c$
a = 7.8823 (2) Å
b = 12.7467 (2) Å
c = 13.6851 (3) Å
β = 91.918 (1)°
V = 1374.22 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.29 mm^{-1}
T = 295 K
0.11 × 0.09 × 0.05 mm

Data collection

Bruker APEXII CCD diffractometer
17706 measured reflections
4800 independent reflections
3043 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.082
S = 0.92
4800 reflections
111 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W···N2^i	0.761 (18)	2.070 (18)	2.8254 (12)	172.2 (17)
O1W—H2W···O52^{ii}	0.762 (18)	1.898 (17)	2.6470 (12)	167.1 (16)
N3—H3A···O51^{iii}	0.86	2.33	3.0525 (12)	141
N3—H3B···O52	0.86	2.07	2.7036 (13)	130

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

Data collection: *APEX2* (Bruker, 2011); cell refinement: *SAINT* (Bruker, 2011); data reduction: *SAINT*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg & Berndt, 2001); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

We are grateful to the personal of the LCATM laboratory, Université Oum El Bouaghi, Algeria, for their assistance.

Thanks are due to the MESRS and ATRST (Ministére de l'Enseignement Supérieur et de la Recherche Scientifique et l'Agence thématique de recherche en sciences et technologie - Algérie) *via* the PNR programm for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2721).

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supporting information

Acta Cryst. (2013). E**69**, m129–m130 [doi:10.1107/S1600536813002183]

Bis(3-aminopyrazine-2-carboxylato-$\kappa^2 N^1$,*O*)diaquacobalt(II)

Rafika Bouchene, Sofiane Bouacida, Fadila Berrah, Ratiba Belhouas and Hocine Merazig

S1. Comment

During our recent research in the field of *N,O*-donor stabilized metal complexes we have prepared the title compound. As ligand we have chosen pyrazine-2-carboxylate that already has been extensively studied (Alcock *et al.*, 1996; Dong *et al.*, 2000; Kubota *et al.*, 2006; Luo *et al.*, 2004; Shi *et al.*, 2011; Fan *et al.*, 2007; Liu *et al.*, 2007). Some of its cobalt(II) complexes have also been reported for multitude applications (Tanase *et al.*, 2006; Sun *et al.*, 2004; McCleverty & Meyer, 2004).

In continuation of our investigations on the influence of hydrogen bonds on the structural features (Bouacida *et al.*, 2007,2009), we report here the crystal growth and crystal structure of the title compound, $[Co(C_5H_4N_3O_2)_2(H_2O)_2]$ (I).

The asymmetric unit of (I) consists of one-half of the complex molecule, with the other half being generated by a twofold rotation axis running through the Co^{II} atom (Wyckoff site 4 *e*). The latter is octahedrally coordinated by two 3-aminopyrazine-2-carboxylate anions acting in a bidentate manner and by two water molecules. The molecular geometry and the atom-numbering scheme of (I) are shown in Fig. 1.

Bond lengths and angles observed in the different entities show normal features and are consistent with those reported previously for related systems (Shi *et al.*, 2011). Fig. 2 shows a packing diagram of the structure. Parallel to the *c* axis channels with a square cross-section are formed. The crystal packing can be described by stacking of alternating layers parallel to (110). The layers are linked together by O1W—H···N, O1W—H···O and N—H···O interactions involving the water molecules and amino functions as donors and carboxylate O atoms as well as the non-coordinating heterocyclic N atoms as acceptors (Fig. 3, Table 1). These interactions lead to the formation of a three-dimensional network.

S2. Experimental

The title compound was obtained from a mixture of cobalt(II) chloride hexahydrate (0.05 g, 0.2 mmol), 3-amino-pyrazine-2-carboxylic acid (0.03 g, 0.2 mmol) and acidified water (25 ml, HCl 37%). The solution was evaporated at room temperature for two weeks. Yellow single crystals were obtained and were carefully isolated under a polarizing microscope for analysis by X-ray diffraction.

S3. Refinement

The H atoms were localized in Fourier maps but were eventually introduced in calculated positions and treated as riding on their parent atoms (C or N) with C—H = 0.93 Å and N—H = 0.86 Å with $U_{iso}(H) = 1.2U_{eq}$(C or N). The water H atoms H1W and H2W were also located in a difference Fourier map. Their positions were refined freely, but their temperature factors were refined isotropically with $U_{iso}(H) = 1.5U_{eq}(OW)$.

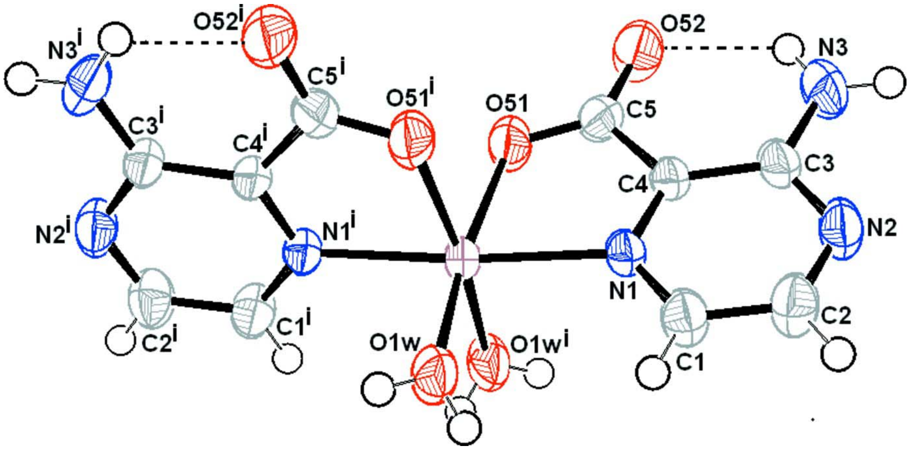

Figure 1

A view of the coordination environment of the Co^{II} atom of (I) with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radius. [Symmetry code: (i)-*x*, *y*, -*z* + 3/2.]

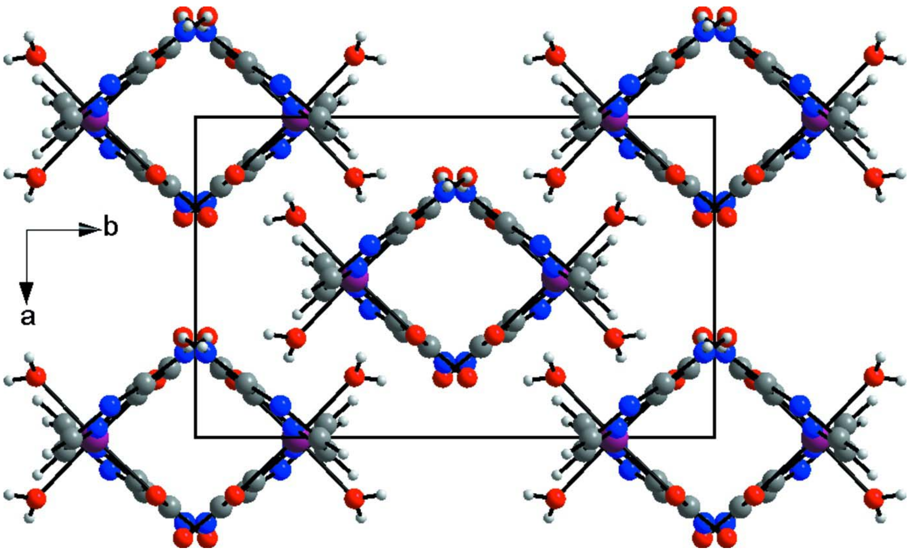

Figure 2

The packing of the structure of (I) viewed along the *c* axis

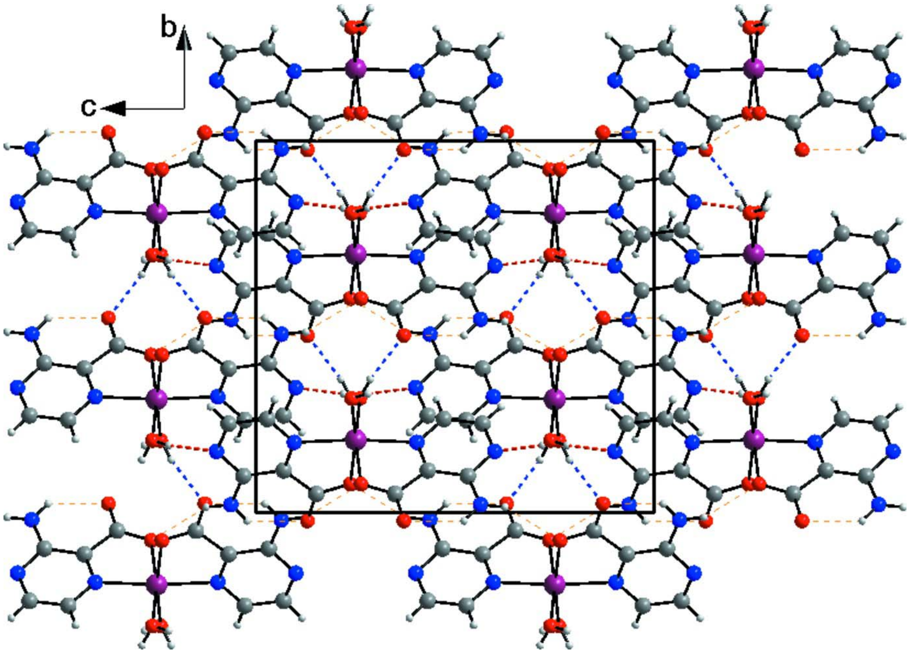

Figure 3

Hydrogen bonding interactions (dashed lines) in the structure of (I)

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Crystal data

$[Co(C_5H_4N_3O_2)_2(H_2O)_2]$
$M_r = 371.19$
Monoclinic, $C2/c$
$a = 7.8823$ (2) Å
$b = 12.7467$ (2) Å
$c = 13.6851$ (3) Å
$\beta = 91.918$ (1)°
$V = 1374.22$ (5) Å^3
$Z = 4$

$F(000) = 756$
$D_x = 1.794$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6448 reflections
$\theta = 3.0$–38.7°
$\mu = 1.29$ mm^{-1}
$T = 295$ K
Block, yellow
0.11 × 0.09 × 0.05 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
17706 measured reflections
4800 independent reflections

3043 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.041$
$\theta_{\max} = 42.1°$, $\theta_{\min} = 3.0°$
$h = -14 \rightarrow 10$
$k = -24 \rightarrow 22$
$l = -25 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.082$
$S = 0.92$
4800 reflections
111 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0413P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.48$ e Å^{-3}
$\Delta\rho_{min} = -0.38$ 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Co1	0	0.195326 (13)	0.75	0.02207 (5)
O1W	0.19025 (11)	0.30652 (6)	0.76033 (6)	0.03609 (17)
H1W	0.250 (2)	0.3194 (11)	0.7195 (13)	0.054*
H2W	0.1779 (19)	0.3585 (14)	0.7867 (12)	0.054*
O51	−0.18087 (10)	0.07591 (6)	0.76347 (5)	0.03603 (17)
O52	−0.31276 (13)	−0.02336 (7)	0.87118 (6)	0.0538 (2)
N1	−0.03120 (10)	0.18853 (6)	0.90389 (5)	0.02230 (13)
N2	−0.09937 (11)	0.16410 (8)	1.09943 (6)	0.03211 (17)
C1	0.04090 (12)	0.25148 (8)	0.97172 (6)	0.02822 (18)
H1	0.1164	0.3035	0.9535	0.034*
N3	−0.26554 (13)	0.02032 (8)	1.06349 (7)	0.0453 (2)
H3A	−0.2827	0.0138	1.1249	0.054*
H3B	−0.3112	−0.0232	1.0224	0.054*
C2	0.00267 (13)	0.23880 (9)	1.06893 (7)	0.0327 (2)
H2	0.0508	0.2847	1.1148	0.039*
C3	−0.16811 (12)	0.09790 (7)	1.03189 (7)	0.02792 (18)
C4	−0.13532 (11)	0.11308 (7)	0.93095 (6)	0.02309 (15)
C5	−0.21616 (13)	0.04957 (8)	0.84893 (7)	0.03098 (19)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.02920 (9)	0.02103 (9)	0.01636 (7)	0	0.00654 (5)	0
O1W	0.0437 (4)	0.0371 (4)	0.0284 (3)	−0.0159 (3)	0.0152 (3)	−0.0072 (3)
O51	0.0514 (4)	0.0342 (4)	0.0230 (3)	−0.0146 (3)	0.0090 (3)	−0.0052 (3)
O52	0.0808 (6)	0.0417 (5)	0.0405 (4)	−0.0356 (4)	0.0263 (4)	−0.0128 (4)
N1	0.0249 (3)	0.0230 (3)	0.0193 (3)	0.0009 (3)	0.0057 (2)	0.0015 (2)
N2	0.0378 (4)	0.0383 (4)	0.0207 (3)	0.0010 (4)	0.0071 (3)	0.0019 (3)
C1	0.0285 (4)	0.0338 (5)	0.0225 (4)	−0.0058 (4)	0.0025 (3)	0.0005 (3)
N3	0.0686 (7)	0.0378 (5)	0.0307 (4)	−0.0167 (5)	0.0196 (4)	0.0032 (4)
C3	0.0343 (4)	0.0259 (4)	0.0242 (4)	0.0031 (3)	0.0112 (3)	0.0041 (3)

C5	0.0410 (5)	0.0242 (4)	0.0284 (4)	−0.0072 (4)	0.0117 (4)	−0.0050 (3)
C4	0.0285 (4)	0.0202 (4)	0.0210 (3)	0.0010 (3)	0.0083 (3)	0.0014 (3)
C2	0.0348 (5)	0.0411 (6)	0.0221 (4)	−0.0031 (4)	0.0007 (3)	−0.0024 (4)

Geometric parameters (Å, º)

Co1—O1W	2.0648 (8)	N1—C1	1.3390 (11)
Co1—O1W^{i}	2.0648 (8)	N2—C2	1.3230 (14)
Co1—O51	2.0979 (7)	N2—C3	1.3515 (13)
Co1—O51^{i}	2.0979 (7)	C1—C2	1.3834 (13)
Co1—N1^{i}	2.1303 (7)	C1—H1	0.93
Co1—N1	2.1303 (7)	N3—C3	1.3329 (13)
O1W—H1W	0.760 (18)	N3—H3A	0.86
O1W—H2W	0.763 (18)	N3—H3B	0.86
O51—C5	1.2568 (12)	C3—C4	1.4270 (12)
O52—C5	1.2460 (12)	C5—C4	1.5078 (13)
N1—C4	1.3252 (11)	C2—H2	0.93
O1W—Co1—O1W^{i}	93.31 (5)	C1—N1—Co1	126.91 (6)
O1W—Co1—O51	170.46 (3)	C2—N2—C3	117.88 (8)
O1W^{i}—Co1—O51	90.57 (4)	N1—C1—C2	119.71 (9)
O1W—Co1—O51^{i}	90.57 (4)	N1—C1—H1	120.1
O1W^{i}—Co1—O51^{i}	170.46 (3)	C2—C1—H1	120.1
O51—Co1—O51^{i}	86.97 (5)	C3—N3—H3A	120
O1W—Co1—N1^{i}	89.31 (3)	C3—N3—H3B	120
O1W^{i}—Co1—N1^{i}	93.89 (3)	H3A—N3—H3B	120
O51—Co1—N1^{i}	99.13 (3)	N3—C3—N2	117.61 (8)
O51^{i}—Co1—N1^{i}	77.43 (3)	N3—C3—C4	122.66 (9)
O1W—Co1—N1	93.89 (3)	N2—C3—C4	119.73 (8)
O1W^{i}—Co1—N1	89.31 (3)	O52—C5—O51	125.65 (9)
O51—Co1—N1	77.43 (3)	O52—C5—C4	117.72 (8)
O51^{i}—Co1—N1	99.13 (3)	O51—C5—C4	116.63 (8)
N1^{i}—Co1—N1	175.34 (4)	N1—C4—C3	120.19 (8)
Co1—O1W—H1W	124.2 (12)	N1—C4—C5	115.59 (7)
Co1—O1W—H2W	121.7 (11)	C3—C4—C5	124.20 (8)
H1W—O1W—H2W	104.7 (15)	N2—C2—C1	122.81 (9)
C5—O51—Co1	116.60 (6)	N2—C2—H2	118.6
C4—N1—C1	119.58 (7)	C1—C2—H2	118.6
C4—N1—Co1	113.50 (6)		
O1W^{i}—Co1—O51—C5	−93.84 (8)	Co1—O51—C5—O52	−175.74 (10)
O51^{i}—Co1—O51—C5	95.39 (8)	Co1—O51—C5—C4	4.97 (12)
N1^{i}—Co1—O51—C5	172.13 (8)	C1—N1—C4—C3	−1.05 (13)
N1—Co1—O51—C5	−4.67 (7)	Co1—N1—C4—C3	179.46 (6)
O1W—Co1—N1—C4	−172.54 (6)	C1—N1—C4—C5	177.36 (8)
O1W^{i}—Co1—N1—C4	94.19 (6)	Co1—N1—C4—C5	−2.13 (10)
O51—Co1—N1—C4	3.45 (6)	N3—C3—C4—N1	−176.88 (9)
O51^{i}—Co1—N1—C4	−81.34 (6)	N2—C3—C4—N1	3.34 (13)

O1W—Co1—N1—C1	8.01 (8)	N3—C3—C4—C5	4.85 (15)
O1W^{i}—Co1—N1—C1	−85.25 (8)	N2—C3—C4—C5	−174.93 (9)
O51—Co1—N1—C1	−175.99 (8)	O52—C5—C4—N1	178.82 (10)
O51^{i}—Co1—N1—C1	99.22 (8)	O51—C5—C4—N1	−1.84 (13)
C4—N1—C1—C2	−1.63 (14)	O52—C5—C4—C3	−2.84 (15)
Co1—N1—C1—C2	177.78 (7)	O51—C5—C4—C3	176.50 (9)
C2—N2—C3—N3	177.46 (9)	C3—N2—C2—C1	0.07 (16)
C2—N2—C3—C4	−2.76 (14)	N1—C1—C2—N2	2.23 (16)

Symmetry code: (i) −*x*, *y*, −*z*+3/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*···N2^{ii}	0.761 (18)	2.070 (18)	2.8254 (12)	172.2 (17)
O1*W*—H2*W*···O52^{iii}	0.762 (18)	1.898 (17)	2.6470 (12)	167.1 (16)
N3—H3*A*···O51^{iv}	0.86	2.33	3.0525 (12)	141
N3—H3*B*···O52	0.86	2.07	2.7036 (13)	130
C1—H1···O52^{iii}	0.93	2.55	3.4010 (13)	153

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