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(*E*)-*N*′-(2,3,4-Trihydroxybenzylidene)-isonicotinohydrazide dihydrate

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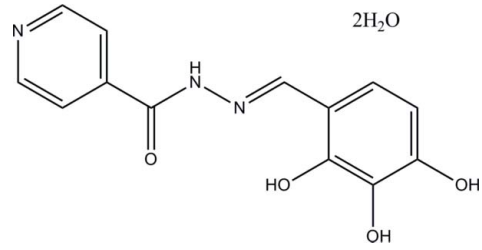
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.001 Å; R factor = 0.038; wR factor = 0.113; data-to-parameter ratio = 21.8.

In the title isoniazid derivative, $C_{13}H_{11}N_3O_4\cdot 2H_2O$, the Schiff base molecule exists in an *E* configuration with respect to the acyclic C=N bond. An intramolecular O—H···N hydrogen bond forms a six-membered ring, producing an $S(6)$ ring motif. The essentially planar pyridine ring [maximum deviation = 0.0119 (8) Å] is inclined at a dihedral angle of 7.30 (4)° with respect to the benzene ring. In the crystal, intermolecular O—H···N, O—H···O, N—H···O and C—H···O hydrogen bonds link the molecules into two-dimensional arrays lying parallel to the $(10\overline{1})$ plane. These arrays are further interconnected into a three-dimensional extended network *via* O—H···O and C—H···O hydrogen bonds. A weak intermolecular π–π interaction [centroid-to-centroid distance = 3.5627 (5) Å] is also observed.

Related literature

For general background to and applications of the title isoniazid derivative, see: Janin (2007); Kahwa *et al.* (1986); Maccari *et al.* (2005); Slayden & Barry (2000). For the preparation of the title compound, see: Lourenço *et al.* (2008). For closely related isoniazid structures, see: Naveenkumar *et al.* (2009, 2010*a*,*b*,*c*); Shi (2005). For hydrogen-bond ring motifs, see: Bernstein *et al.* (1995). For the stability of the temperature controller used for the data collection, see: Cosier & Glazer (1986).



Experimental

Crystal data

$C_{13}H_{11}N_3O_4\cdot 2H_2O$
M_r = 309.28
Monoclinic, $P2_1/c$
a = 6.9504 (5) Å
b = 19.9077 (13) Å
c = 10.0930 (7) Å
β = 106.416 (2)°
V = 1339.60 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 100 K
0.35 × 0.18 × 0.09 mm

Data collection

Bruker APEXII DUO CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.959, T_{max} = 0.989
21520 measured reflections
5656 independent reflections
4668 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.113
S = 1.03
5656 reflections
259 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H1O2···N3	0.883 (18)	1.854 (18)	2.6561 (9)	150.1 (16)
O3—H1O3···N1^{i}	0.869 (19)	1.835 (19)	2.6911 (10)	168.4 (18)
O4—H1O4···O1W	0.895 (18)	1.769 (18)	2.6559 (9)	170.5 (18)
N2—H1N2···O2W^{ii}	0.890 (16)	2.132 (15)	2.9910 (9)	162.1 (14)
O1W—H1W1···O1^{iii}	0.926 (18)	1.880 (18)	2.7834 (9)	164.6 (16)
O1W—H2W1···O2W	0.837 (19)	2.077 (18)	2.8980 (11)	167.0 (18)
O2W—H1W2···O2^{iv}	0.831 (15)	2.161 (15)	2.9570 (11)	160.3 (14)
O2W—H2W2···O4^{v}	0.86 (2)	1.91 (2)	2.7688 (9)	173.3 (19)
C4—H4A···O1^{vi}	0.922 (14)	2.575 (14)	3.2930 (11)	135.1 (11)
C7—H7A···O2W^{ii}	0.988 (14)	2.347 (14)	3.2176 (10)	146.7 (12)

Symmetry codes: (i) $-x+2, y+\frac{1}{2}, -z+\frac{5}{2}$; (ii) $-x+1, -y+1, -z+1$; (iii) $x-1, y, z-1$; (iv) $x, y, z-1$; (v) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (vi) $-x+2, -y+1, -z+3$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2508).

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(*E*)-*N*′-(2,3,4-Trihydroxybenzylidene)isonicotinohydrazide dihydrate

H. S. Naveenkumar, Amirin Sadikun, Pazilah Ibrahim, Jia Hao Goh and Hoong-Kun Fun

S1. Comment

In the search of new compounds, isoniazid derivatives have been found to possess potential tuberculostatic activity (Janin, 2007; Maccari *et al.*, 2005; Slayden & Barry, 2000). Schiff bases have attracted much attention because of their biological activity (Kahwa *et al.*, 1986). As a part of our current work on synthesis of (*E*)-*N*′-substituted isonicotinohydrazide derivatives, in this paper we present the crystal structure of the title compound.

The title isoniazid derivative comprises of a (*E*)-*N*′-(2,3,4-trihydroxybenzylidene)isonicotinohydrazide molecule and two water molecules of crystallization (Fig. 1). The Schiff base molecule exists in an *E* configuration with respect to the acyclic C7═N3 bond [C7═N3 = 1.2921 (10) Å; torsion angle N2—N3—C7—C8 = 178.85 (7)°]. An intramolecular O2—H1O2···N3 hydrogen bond (Table 1) generates a six-membered ring, producing an *S*(6) ring motifs (Bernstein *et al.*, 1995). The pyridine ring with atom sequence C1/C2/N1/C3/C4/C5 is essentially planar, with a maximum deviation of 0.0119 (8) Å at atom C5. There is a slight inclination between the pyridine and benzene rings, as indicated by the dihedral angle formed of 7.30 (4)°. All bond lengths and angles are consistent to those observed in closely related isoniazid structures (Naveenkumar *et al.*, 2009, 2010*a*,*b*,*c*; Shi, 2005).

In the crystal packing, water molecules play an extensive part in forming the hydrogen-bonded structure. Neighbouring molecules are linked into two-dimensional arrays parallel to the (10$\bar{1}$) plane (Fig. 2) by intermolecular O3—H1O3···N1, O4—H1O4···O1W, N2—H1N2···O2W, O1W—H1W1···O1, O2W—H2W2···O4 and C7—H7A···O2W hydrogen bonds (Table 1). These arrays are further interconnected by intermolecular O1W—H2W1···O2W, O2W—H1W2···O2 and C4—H4A···O1 hydrogen bonds (Table 1) into a three-dimensional extended structure (Fig. 3). Weak intermolecular *π*–*π* aromatic stacking interactions involving the pyridine and benzene rings [*Cg*1···*Cg*2 = 3.5627 (5) Å, symmetry code: -x + 2, -y + 1, -z + 2] stabilizing the crystal structure.

S2. Experimental

The isoniazid derivative was prepared following the procedure by Lourenço *et al.*, 2008. The title compound was prepared by the reaction between 2,3,4-trihydroxybenzaldehyde (1.0 eq) with isoniazid (1.0 eq) in ethanol/water. After stirring for 1–3 h at room temperature, the resulting mixture was concentrated under reduced pressure. The residue, purified by washing with cold ethanol and ethyl ether, afforded the pure derivative. The brown-coloured single crystals suitable for X-ray analysis were obtained by recrystallization with ethanol.

S3. Refinement

All H atoms were located from difference Fourier map and allowed to refine freely with N—H = 0.890 (16), O—H = 0.834 (16)–0.926 (18) and C—H = 0.921 (14)–0.988 (13) Å.

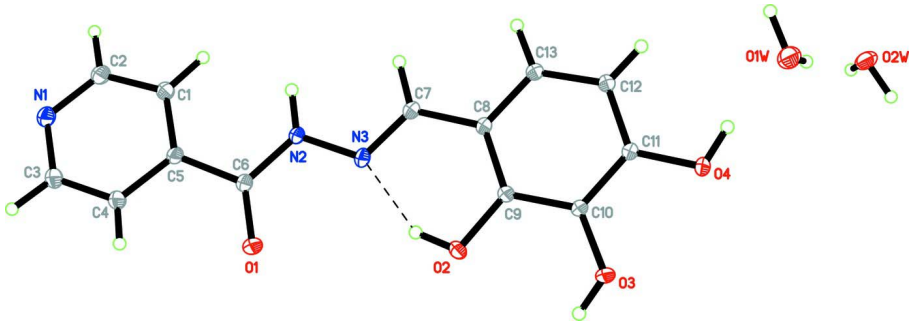

Figure 1

The asymmetric unit of the title isoniazid derivative, showing 50% probability displacement ellipsoids for non-H atoms and the atom-numbering scheme. An intramolecular hydrogen bond is shown as dashed line.

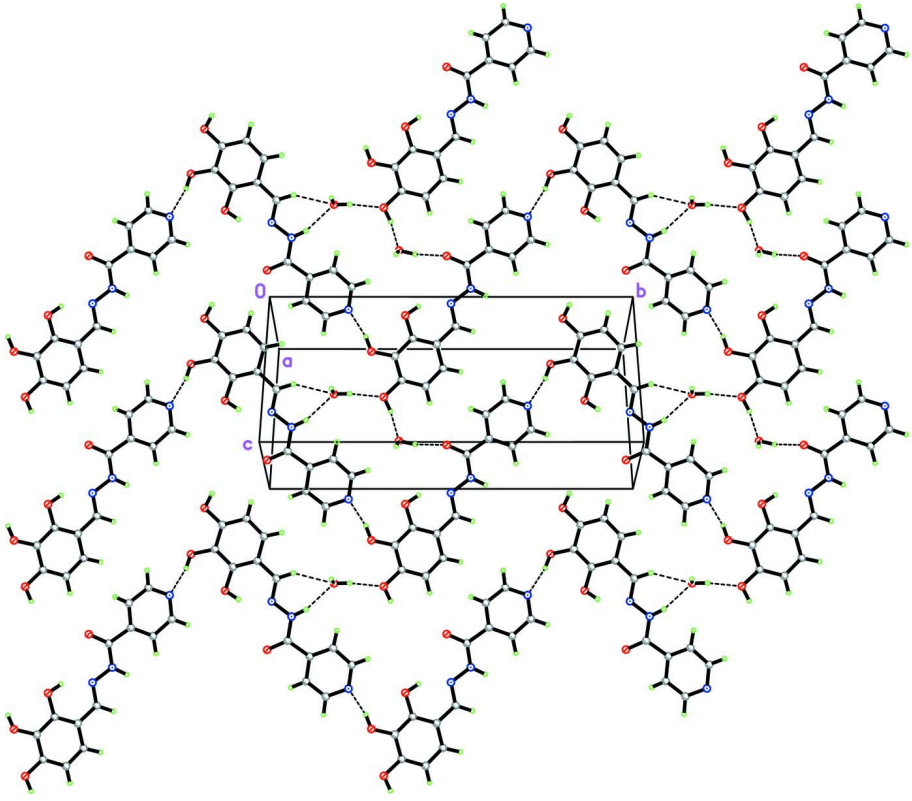

Figure 2

Part of the crystal structure, viewed along the [10$\bar{1}$] direction, showing a hydrogen-bonded 2D array. Intermolecular hydrogen bonds are shown as dashed lines.

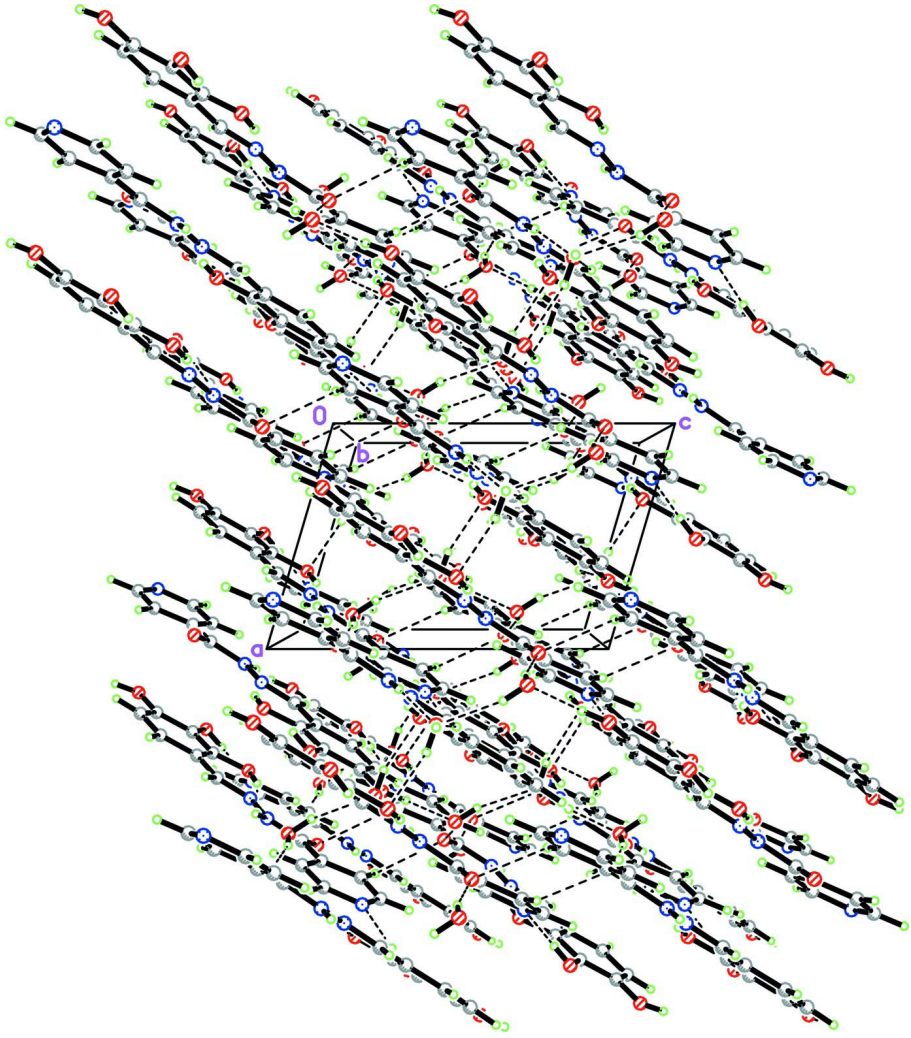

Figure 3

The crystal structure of the title derivative, viewed along the *b* axis, showing the 2D arrays being linked into a 3D extended network. Intermolecular hydrogen bonds are shown as dashed lines.

(*E*)-*N*′-(2,3,4-Trihydroxybenzylidene)isonicotinohydrazide dihydrate

Crystal data

$C_{13}H_{11}N_3O_4·2H_2O$
M_r = 309.28
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 6.9504 (5) Å
b = 19.9077 (13) Å
c = 10.0930 (7) Å
β = 106.416 (2)°
V = 1339.60 (16) Å^3
Z = 4
$F(000)$ = 648
D_x = 1.534 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7532 reflections
θ = 2.9–34.5°
μ = 0.12 mm^{-1}
T = 100 K
Plate, brown
0.35 × 0.18 × 0.09 mm

Data collection

Bruker APEXII DUO CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.959, T_{max} = 0.989
21520 measured reflections
5656 independent reflections
4668 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 34.5°, θ_{min} = 2.3°
h = −11→11
k = −31→31
l = −16→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.113
S = 1.03
5656 reflections
259 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
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0651P)^2 + 0.2238P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1)K.

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2$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}
O1	1.01608 (10)	0.51301 (3)	1.29712 (6)	0.01639 (12)
O2	0.67646 (10)	0.62875 (3)	0.99244 (6)	0.01723 (13)
O3	0.48628 (10)	0.72385 (3)	0.80029 (6)	0.01782 (13)
O4	0.29346 (10)	0.68845 (3)	0.54245 (6)	0.01504 (12)
N1	1.23127 (11)	0.28684 (4)	1.50037 (7)	0.01687 (14)
N2	0.86827 (10)	0.44582 (3)	1.11516 (6)	0.01251 (12)
N3	0.78423 (10)	0.50085 (3)	1.03671 (7)	0.01281 (12)
C1	1.05976 (13)	0.33042 (4)	1.27584 (8)	0.01494 (14)
C2	1.14706 (13)	0.27828 (4)	1.36485 (8)	0.01646 (15)
C3	1.22531 (14)	0.34874 (4)	1.55190 (8)	0.01760 (15)
C4	1.14150 (13)	0.40355 (4)	1.47177 (8)	0.01499 (14)
C5	1.05899 (11)	0.39475 (4)	1.32999 (7)	0.01165 (13)
C6	0.97938 (12)	0.45639 (4)	1.24693 (7)	0.01180 (13)
C7	0.68132 (12)	0.48824 (4)	0.91109 (8)	0.01247 (13)

C8	0.58229 (11)	0.54102 (3)	0.81860 (7)	0.01120 (13)
C9	0.58328 (11)	0.60855 (4)	0.85957 (7)	0.01149 (13)
C10	0.48749 (12)	0.65802 (4)	0.76616 (7)	0.01176 (13)
C11	0.38589 (11)	0.63908 (4)	0.63033 (7)	0.01128 (13)
C12	0.38052 (12)	0.57192 (4)	0.58943 (7)	0.01307 (13)
C13	0.47908 (12)	0.52365 (4)	0.68254 (7)	0.01302 (13)
O1W	0.13931 (13)	0.64535 (3)	0.28519 (7)	0.02289 (15)
O2W	0.30816 (11)	0.67273 (3)	0.05904 (7)	0.01959 (13)
H1O2	0.732 (3)	0.5922 (9)	1.0365 (17)	0.041 (4)*
H1O3	0.582 (3)	0.7387 (9)	0.8694 (18)	0.045 (5)*
H1O4	0.247 (3)	0.6695 (9)	0.4591 (19)	0.045 (5)*
H1N2	0.836 (2)	0.4055 (8)	1.0773 (15)	0.034 (4)*
H1A	1.001 (2)	0.3205 (7)	1.1767 (14)	0.023 (3)*
H2A	1.146 (2)	0.2338 (7)	1.3281 (14)	0.023 (3)*
H3A	1.282 (2)	0.3542 (6)	1.6527 (14)	0.021 (3)*
H4A	1.135 (2)	0.4445 (7)	1.5129 (14)	0.028 (3)*
H7A	0.665 (2)	0.4412 (7)	0.8788 (15)	0.029 (3)*
H12A	0.306 (2)	0.5605 (7)	0.4985 (13)	0.020 (3)*
H13A	0.479 (2)	0.4751 (7)	0.6573 (14)	0.021 (3)*
H1W1	0.102 (3)	0.6006 (9)	0.2736 (17)	0.043 (4)*
H2W1	0.206 (3)	0.6521 (8)	0.2292 (17)	0.038 (4)*
H1W2	0.425 (2)	0.6675 (7)	0.0549 (15)	0.030 (4)*
H2W2	0.309 (3)	0.7161 (10)	0.0608 (19)	0.049 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0222 (3)	0.0097 (2)	0.0151 (2)	−0.0004 (2)	0.0018 (2)	−0.00091 (18)
O2	0.0237 (3)	0.0122 (2)	0.0108 (2)	0.0021 (2)	−0.0033 (2)	−0.00140 (18)
O3	0.0247 (3)	0.0080 (2)	0.0154 (2)	0.0006 (2)	−0.0029 (2)	−0.00218 (18)
O4	0.0206 (3)	0.0099 (2)	0.0112 (2)	0.00154 (19)	−0.0010 (2)	0.00164 (17)
N1	0.0185 (3)	0.0132 (3)	0.0162 (3)	0.0008 (2)	0.0005 (2)	0.0031 (2)
N2	0.0154 (3)	0.0084 (2)	0.0115 (2)	0.0012 (2)	0.0002 (2)	0.00147 (19)
N3	0.0139 (3)	0.0104 (2)	0.0126 (3)	0.0018 (2)	0.0014 (2)	0.00298 (19)
C1	0.0188 (4)	0.0110 (3)	0.0133 (3)	0.0015 (2)	0.0017 (3)	0.0002 (2)
C2	0.0195 (4)	0.0109 (3)	0.0169 (3)	0.0021 (3)	0.0018 (3)	0.0012 (2)
C3	0.0218 (4)	0.0148 (3)	0.0129 (3)	0.0008 (3)	−0.0006 (3)	0.0023 (2)
C4	0.0179 (4)	0.0121 (3)	0.0125 (3)	0.0008 (2)	0.0003 (2)	0.0006 (2)
C5	0.0121 (3)	0.0097 (3)	0.0121 (3)	0.0005 (2)	0.0017 (2)	0.0012 (2)
C6	0.0127 (3)	0.0103 (3)	0.0115 (3)	0.0006 (2)	0.0021 (2)	0.0009 (2)
C7	0.0146 (3)	0.0095 (3)	0.0126 (3)	0.0010 (2)	0.0026 (2)	0.0011 (2)
C8	0.0128 (3)	0.0088 (3)	0.0110 (3)	0.0007 (2)	0.0018 (2)	0.0008 (2)
C9	0.0129 (3)	0.0097 (3)	0.0101 (3)	0.0001 (2)	0.0004 (2)	−0.0001 (2)
C10	0.0137 (3)	0.0084 (3)	0.0116 (3)	−0.0001 (2)	0.0010 (2)	0.0001 (2)
C11	0.0129 (3)	0.0093 (3)	0.0106 (3)	0.0002 (2)	0.0015 (2)	0.0010 (2)
C12	0.0163 (3)	0.0102 (3)	0.0110 (3)	0.0005 (2)	0.0011 (2)	−0.0003 (2)
C13	0.0165 (3)	0.0093 (3)	0.0117 (3)	0.0006 (2)	0.0015 (2)	−0.0004 (2)
O1W	0.0385 (4)	0.0160 (3)	0.0140 (3)	−0.0034 (3)	0.0071 (3)	−0.0002 (2)

O2W	0.0281 (4)	0.0104 (2)	0.0201 (3)	−0.0019 (2)	0.0065 (2)	−0.0011 (2)

Geometric parameters (Å, º)

O1—C6	1.2326 (9)	C3—H3A	0.988 (13)
O2—C9	1.3743 (9)	C4—C5	1.3941 (10)
O2—H1O2	0.883 (18)	C4—H4A	0.921 (14)
O3—C10	1.3557 (9)	C5—C6	1.5009 (10)
O3—H1O3	0.868 (18)	C7—C8	1.4442 (10)
O4—C11	1.3577 (9)	C7—H7A	0.987 (15)
O4—H1O4	0.895 (18)	C8—C13	1.4011 (10)
N1—C2	1.3380 (10)	C8—C9	1.4060 (10)
N1—C3	1.3428 (11)	C9—C10	1.3954 (10)
N2—C6	1.3524 (9)	C10—C11	1.4047 (10)
N2—N3	1.3809 (9)	C11—C12	1.3965 (10)
N2—H1N2	0.890 (16)	C12—C13	1.3827 (10)
N3—C7	1.2921 (10)	C12—H12A	0.946 (13)
C1—C5	1.3929 (10)	C13—H13A	1.000 (13)
C1—C2	1.3945 (11)	O1W—H1W1	0.926 (18)
C1—H1A	0.988 (13)	O1W—H2W1	0.838 (18)
C2—H2A	0.960 (14)	O2W—H1W2	0.834 (16)
C3—C4	1.3847 (11)	O2W—H2W2	0.863 (19)
C9—O2—H1O2	105.5 (11)	N2—C6—C5	116.10 (6)
C10—O3—H1O3	118.3 (12)	N3—C7—C8	121.57 (7)
C11—O4—H1O4	106.7 (12)	N3—C7—H7A	119.2 (8)
C2—N1—C3	117.41 (7)	C8—C7—H7A	119.2 (8)
C6—N2—N3	118.17 (6)	C13—C8—C9	118.86 (6)
C6—N2—H1N2	124.5 (10)	C13—C8—C7	118.20 (6)
N3—N2—H1N2	117.1 (10)	C9—C8—C7	122.94 (6)
C7—N3—N2	115.84 (6)	O2—C9—C10	117.13 (6)
C5—C1—C2	118.73 (7)	O2—C9—C8	121.91 (6)
C5—C1—H1A	122.3 (8)	C10—C9—C8	120.96 (6)
C2—C1—H1A	118.9 (8)	O3—C10—C9	123.14 (6)
N1—C2—C1	123.29 (7)	O3—C10—C11	118.03 (6)
N1—C2—H2A	117.8 (8)	C9—C10—C11	118.83 (6)
C1—C2—H2A	118.9 (8)	O4—C11—C12	122.13 (6)
N1—C3—C4	123.43 (7)	O4—C11—C10	117.24 (6)
N1—C3—H3A	117.0 (8)	C12—C11—C10	120.63 (6)
C4—C3—H3A	119.6 (8)	C13—C12—C11	119.85 (7)
C3—C4—C5	118.92 (7)	C13—C12—H12A	121.6 (8)
C3—C4—H4A	119.9 (9)	C11—C12—H12A	118.6 (8)
C5—C4—H4A	121.1 (9)	C12—C13—C8	120.85 (7)
C1—C5—C4	118.18 (7)	C12—C13—H13A	122.3 (8)
C1—C5—C6	125.05 (7)	C8—C13—H13A	116.8 (8)
C4—C5—C6	116.76 (6)	H1W1—O1W—H2W1	105.0 (15)
O1—C6—N2	122.73 (7)	H1W2—O2W—H2W2	97.2 (15)
O1—C6—C5	121.16 (7)		

C6—N2—N3—C7	179.26 (7)	C13—C8—C9—O2	178.05 (7)
C3—N1—C2—C1	1.77 (14)	C7—C8—C9—O2	−1.23 (12)
C5—C1—C2—N1	−0.22 (14)	C13—C8—C9—C10	−1.49 (12)
C2—N1—C3—C4	−1.57 (14)	C7—C8—C9—C10	179.23 (7)
N1—C3—C4—C5	−0.19 (14)	O2—C9—C10—O3	1.24 (12)
C2—C1—C5—C4	−1.57 (12)	C8—C9—C10—O3	−179.21 (8)
C2—C1—C5—C6	177.13 (8)	O2—C9—C10—C11	−178.29 (7)
C3—C4—C5—C1	1.76 (12)	C8—C9—C10—C11	1.26 (12)
C3—C4—C5—C6	−177.05 (8)	O3—C10—C11—O4	0.08 (11)
N3—N2—C6—O1	−3.53 (12)	C9—C10—C11—O4	179.64 (7)
N3—N2—C6—C5	177.10 (7)	O3—C10—C11—C12	−179.47 (8)
C1—C5—C6—O1	−166.63 (8)	C9—C10—C11—C12	0.09 (12)
C4—C5—C6—O1	12.09 (12)	O4—C11—C12—C13	179.27 (7)
C1—C5—C6—N2	12.74 (12)	C10—C11—C12—C13	−1.20 (12)
C4—C5—C6—N2	−168.54 (7)	C11—C12—C13—C8	0.97 (12)
N2—N3—C7—C8	178.85 (7)	C9—C8—C13—C12	0.35 (12)
N3—C7—C8—C13	177.91 (8)	C7—C8—C13—C12	179.67 (7)
N3—C7—C8—C9	−2.81 (13)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H1*O*2···N3	0.883 (18)	1.854 (18)	2.6561 (9)	150.1 (16)
O3—H1*O*3···N1^{i}	0.869 (19)	1.835 (19)	2.6911 (10)	168.4 (18)
O4—H1*O*4···O1*W*	0.895 (18)	1.769 (18)	2.6559 (9)	170.5 (18)
N2—H1*N*2···O2*W*^{ii}	0.890 (16)	2.132 (15)	2.9910 (9)	162.1 (14)
O1*W*—H1*W*1···O1^{iii}	0.926 (18)	1.880 (18)	2.7834 (9)	164.6 (16)
O1*W*—H2*W*1···O2*W*	0.837 (19)	2.077 (18)	2.8980 (11)	167.0 (18)
O2*W*—H1*W*2···O2^{iv}	0.831 (15)	2.161 (15)	2.9570 (11)	160.3 (14)
O2*W*—H2*W*2···O4^{v}	0.86 (2)	1.91 (2)	2.7688 (9)	173.3 (19)
C4—H4*A*···O1^{vi}	0.922 (14)	2.575 (14)	3.2930 (11)	135.1 (11)
C7—H7*A*···O2*W*^{ii}	0.988 (14)	2.347 (14)	3.2176 (10)	146.7 (12)

Symmetry codes: (i) −*x*+2, *y*+1/2, −*z*+5/2; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*−1, *y*, *z*−1; (iv) *x*, *y*, *z*−1; (v) *x*, −*y*+3/2, *z*−1/2; (vi) −*x*+2, −*y*+1, −*z*+3.