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Crystal structure, Hirshfeld surface analysis and HOMO–LUMO analysis of (*E*)-*N*′-(3-hydroxy-4-methoxybenzylidene)nicotinohydrazide monohydrate

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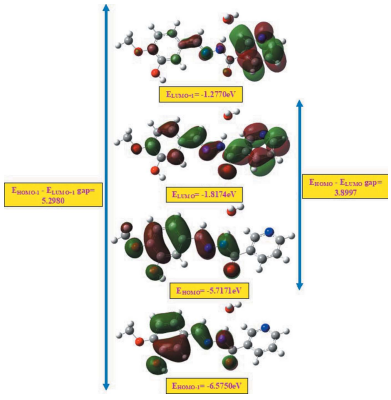
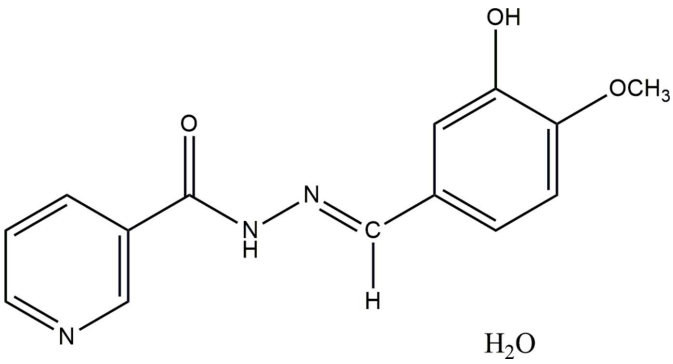
The molecule of the title Schiff base compound, $C_{14}H_{13}N_3O_3\cdot H_2O$, displays a *trans* configuration with respect to the C=N bond. The dihedral angle between the benzene and pyridine rings is 29.63 (7)°. The crystal structure features intermolecular N—H···O, C—H···O, O—H···O and O—H···N hydrogen-bonding interactions, leading to the formation of a supramolecular framework. A Hirshfeld surface analysis indicates that the most important contributions to the crystal packing are from H···H (37.0%), O···H/H···O (23.7%)), C···H/H···C (17.6%) and N···H/H···N (11.9%) interactions. The title compound has also been characterized by frontier molecular orbital analysis.

1. Chemical context

Schiff bases are nitrogen-containing compounds that were first obtained by the condensation reaction of aromatic amines and aldehydes (Schiff, 1864). A wide range of these compounds, with the general formula $RHC{=}NR_1$ (R and R_1 can be alkyl, aryl, cycloalkyl or heterocyclic groups) have been synthesized. Schiff bases are of great importance in the field of coordination chemistry because they are able to form stable complexes with metal ions (Souza *et al.*, 1985). The chemical and biological significance of Schiff bases can be attributed to the presence of a lone electron pair in the sp^2-hybridized orbital of the nitrogen atom of the azomethine group (Singh *et al.*, 1975). These compounds are used in the fields of organic synthesis, chemical catalysis, medicine and pharmacy, as well as other new technologies (Tanaka *et al.*, 2010). Schiff bases are also used as probes for investigating the structure of DNA (Tiwari *et al.*, 2011) and have gained special attention in pharmacophore research and in the development of several bioactive lead molecules (Muralisankar *et al.*, 2016). Schiff bases showing photochromic and thermochromic properties have been used in information storage, electronic display systems, optical switching devices and ophthalmic glasses (Amimoto *et al.*, 2005). As a further contribution to this field of research, we report herein the crystal structure of the title compound, (*E*)-*N*′-(3-hydroxy-4-methoxybenzylidene)nicotinohydrazide monohydrate.





2. Structural commentary

The asymmetric unit of the title compound (Fig. 1) consists of one independent Schiff base molecule displaying a *trans* configuration with respect to the C=N bond and a water molecule. All the bond lengths are within the normal ranges (Allen *et al.*, 1987). The C7=N3 bond length of 1.274 (2) Å is consistent with a double-bond character. The C6—N2 and N2—N3 bond lengths of 1.343 (2) and 1.3866 (16) Å, respectively, are comparable to those observed in related compounds (Sivajeyanthi *et al.*, 2017; Balasubramani *et al.*, 2018). The O1/C6/N2/N3/C7 core is almost planar (r.m.s. deviation = 0.022 Å) and forms dihedral angles of 20.75 (7) and 8.93 (5)°, respectively, with the pyridine and benzene rings.

3. Supramolecular features

In the crystal of the title compound (Fig. 2), the water molecule interacts with three neighbouring nicotinohydrazide molecules with the O4 water oxygen atom acting as a hydrogen acceptor through N2—H2*N*···O4 and C2—H2···O4 hydrogen bonds (Table 1), and both water H atoms acting as bifurcated donors to form rings of $R_2^1(5)$ graph-set motif. The nicotinohydrazide molecules are further linked by O—H···N and C—H···O hydrogen bonds to form a three-dimensional network.

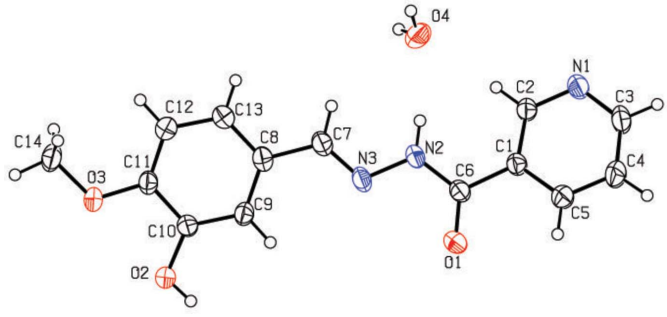


Figure 1
The asymmetric unit of the title compound with displacement ellipsoids drawn at the 50% probability level..

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4*WA*···O2^{i}	0.85	2.28	3.0483 (17)	150
O4—H4*WA*···O3^{i}	0.85	2.49	3.2011 (16)	141
O4—H4*WB*···O1^{ii}	0.85	2.08	2.8429 (19)	150
O4—H4*WB*···N3^{ii}	0.85	2.50	3.1875 (18)	139
N2—H2*N*···O4	0.86	2.06	2.8889 (18)	162
O2—H10···N1^{iii}	0.82	1.96	2.7411 (17)	159
C2—H2···O4	0.93	2.25	3.129 (2)	156
C4—H4···O3^{iv}	0.93	2.45	3.347 (2)	163

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

4. Hirshfeld surface analysis

The three-dimensional d_{norm} surface is a useful tool for analysing and visualizing the intermolecular interactions, as it shows negative or positive values depending on whether an intermolecular contact is shorter or longer, respectively, than the sum of the van der Waals radii (Spackman & Jayatilaka, 2009; McKinnon *et al.*, 2007). The d_{norm} surface of the title compound is shown in Fig. 3. The red points, which represent closer contacts and negative d_{norm} values, correspond to the N—H···O, O—H···O, O—H···N and C—H···O interactions. Two-dimensional fingerprint plots from the Hirshfeld surface analysis (Fig. 4) provide information about the intermolecular contacts and their percentage distributions on the Hirshfeld surface. The percentage of H···H contacts as closest contacts on the Hirshfeld surfaces is a universally applicable measure

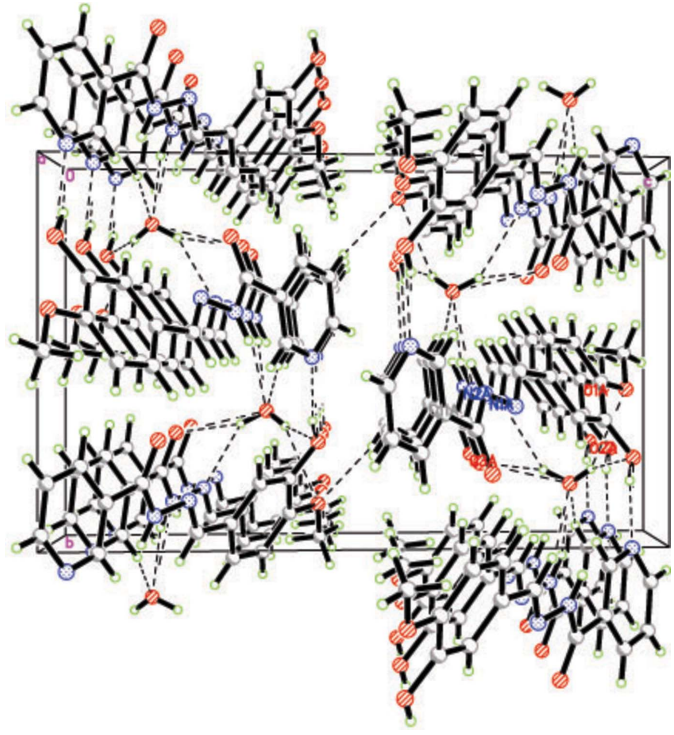


Figure 2
Crystal packing of the title compound, viewed down the *a* axis. Hydrogen bonds are shown as dashed lines.

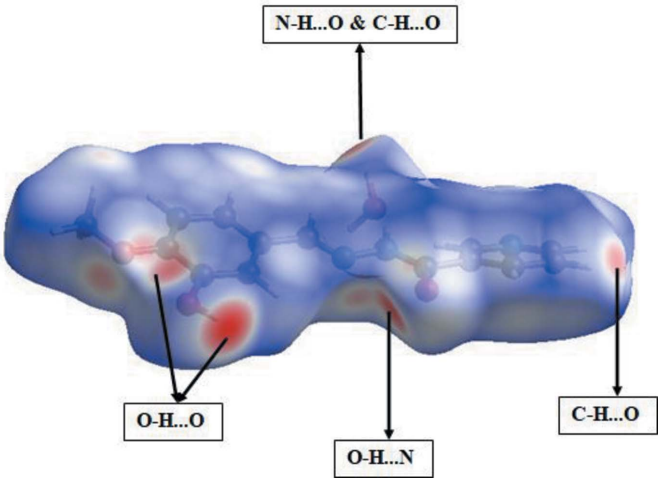


Figure 3
Hirshfeld surfaces of the title compound mapped over d_{norm}.

of the crystal lattice energy and can be used as a reference for the importance of other types of contacts. In the title compound, the percentage contributions of the various intermolecular contacts to the total Hirshfeld surface are as follows: H···H (37.0%), C···H/H···C (17.6%), N···H/H···N (11.9%), C···N/N···C (3.7%), O···H/H···O (23.7%), C···C (4.5%), N···N (0.3%) and O···C/C···O (1.2%).

5. Frontier molecular orbitals

The HOMO (highest occupied molecular orbital) acts as an electron donor and LUMO (lowest occupied molecular orbital) acts as an electron acceptor. If the HOMO–LUMO energy gap is small, then the molecule is highly polarizable and has high chemical reactivity. The energy levels for the title compound were computed by DFT-B3LYP/6-311G++(d,p) method (Sivajeyanthi *et al.*, 2017). The energy levels, energy gaps, chemical hardness, chemical potential, electronegativity and electrophilicity index are given in Table 2. As shown in Fig. 5, the frontier molecular orbital LUMO is located over the whole of the molecule. The energy gap of the molecule clearly shows the charge-transfer interaction involving donor and acceptor groups. If the HOMO–LUMO energy gap is small, then the molecule is defined as soft, *i.e.* it is highly polarizable and has high chemical reactivity, whereas if the energy gap is large the molecule can be defined as hard. Therefore from Table 2 we conclude that the title molecule belongs to the really hard materials.

Table 2
Calculated frontier molecular orbital energies (eV).

FMO	Energy
E_{HOMO}	−5.7171
E_{LUMO}	−1.8174
E_{HOMO-1}	−6.5750
E_{LUMO+1}	−1.2770
(E_{HOMO} − E_{LUMO}) gap	3.8997
(E_{HOMO-1} − E_{LUMO+1}) gap	5.2980
Chemical hardness	1.9498
Chemical potential	3.7672
Electronegativity	−3.7672
Electrophilicity index	3.6393

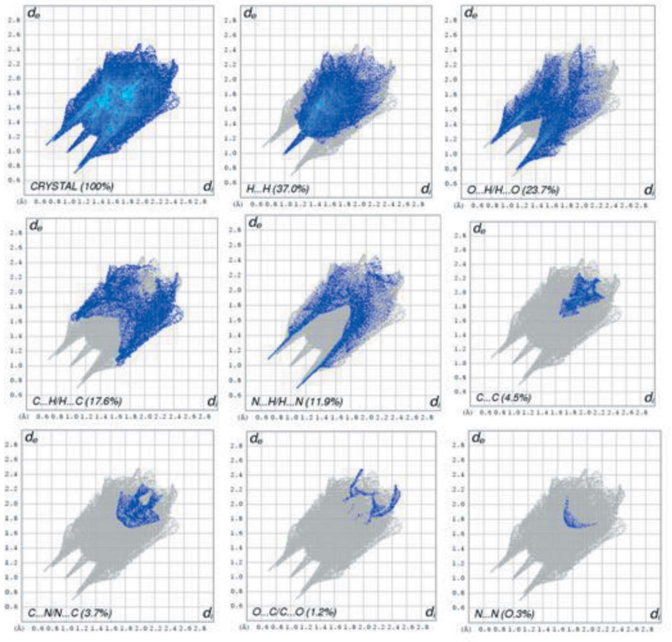


Figure 4
Two-dimensional fingerprint plots for the title compound and relative contributions of the atom pairs to the Hirshfeld surface.

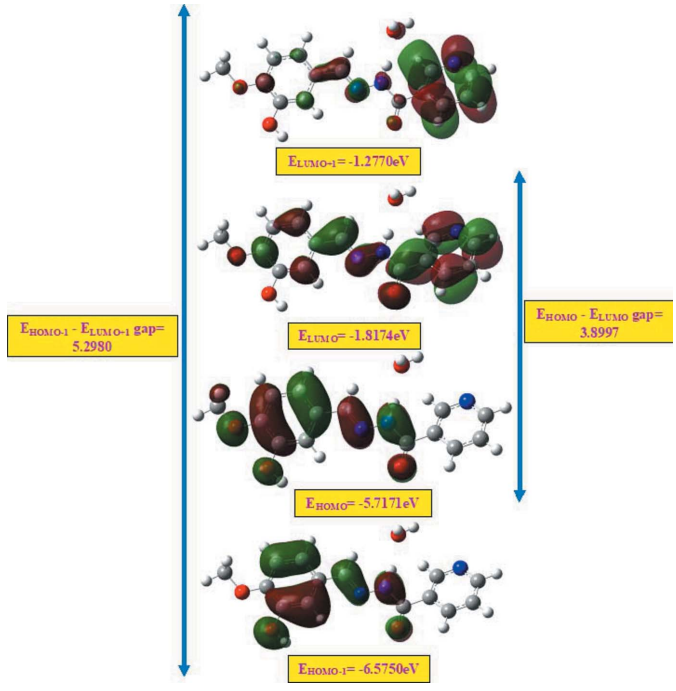


Figure 5
Molecular orbital energy levels of the title compound.

6. Database survey

A search of the Cambridge Structural Database (Version 5.40, update November 2018; Groom *et al.*, 2016) for uncoordinated *N*′-(benzylidene)nicotinohydrazide derivatives O-substituted at the 3,4 positions of the benzene ring yielded three hits, namely *N*′-(1,3-benzodioxol-5-ylmethylene)nicotinohydrazide monohydrate (refcode BUDNIY; Bao *et al.*, 2009), *N*′-(3,4-dimethoxybenzylidene)nicotinohydrazide monohydrate (XODZOH; Novina *et al.*, 2014) and the isomer *N*′-(4-hydroxy-3-methoxybenzylidene)nicotinohydrazide monohydrate (SEZREV; Shi *et al.*, 2007). The conformation of the last molecule differs from the title compound mainly in the relative orientation of the pyridine ring with respect to the carbonyl group, as indicated by the value of 158.03 (15)° for the O1—C6—C1—C2 torsion angle in the title compound and of 10.2 (3)° for the corresponding angle in SEZREV. Moreover, in SEZREV the water molecule acts as acceptor of three H atoms from the same nicotinohydrazide molecule and as donor in two O—H···O hydrogen bonds.

7. Synthesis and crystallization

The title compound was synthesized by the reaction of a 1:1 molar ratio mixture of a hot ethanolic solution (20 ml) of nicotinohydrazide (0.137 mg) and a hot ethanolic solution of 3-hydroxy-4-methoxy benzaldehyde (0.152 mg). After refluxing for 8 h, the solution was then cooled and kept at room temperature to precipitate. Colourless block-shaped crystals suitable for X-ray analysis were obtained by slow evaporation of a 10 ml dimethyl sulfoxide/water (1:1 *v*/*v*) solution.

8. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. H atoms were positioned geometrically (O—H = 0.82 Å, N–H = 0.86 Å, C—H = 0.93–0.96 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C,N) or 1.5U_{eq}(O, C-methyl)

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{13}N_3O_3{\cdot}H_2O$
M_r	289.29
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	295
a, b, c (Å)	7.1153 (4), 11.0075 (6), 18.2771 (10)
β (°)	105.766 (5)
V (Å^3)	1377.64 (14)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.10
Crystal size (mm)	0.30 × 0.25 × 0.18
Data collection	
Diffractometer	Agilent Xcalibur Eos
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2012)
T_{min}, T_{max}	0.969, 0.981
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8396, 2549, 2027
R_{int}	0.027
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.606
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.036, 0.101, 1.04
No. of reflections	2549
No. of parameters	192
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.16, −0.13

Computer programs: *CrysAlis PRO* (Agilent, 2012), *SHELXS97* (Sheldrick, 2008), *SHELXL2017* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2006).

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supporting information

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Crystal structure, Hirshfeld surface analysis and HOMO–LUMO analysis of (*E*)-*N*′-(3-hydroxy-4-methoxybenzylidene)nicotinohydrazide monohydrate

Palaniyappan Sivajeyanthi, Bellarmin Edison, Kasthuri Balasubramani, Ganesan Premkumar and Toka Swu

Computing details

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO* (Agilent, 2012); data reduction: *CrysAlis PRO* (Agilent, 2012); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2017* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL2017* (Sheldrick, 2015).

(*E*)-*N*′-(3-Hydroxy-4-methoxybenzylidene)nicotinohydrazide monohydrate

Crystal data

$C_{14}H_{13}N_3O_3·H_2O$
M_r = 289.29
Monoclinic, $P2_1/c$
a = 7.1153 (4) Å
b = 11.0075 (6) Å
c = 18.2771 (10) Å
β = 105.766 (5)°
V = 1377.64 (14) Å^3
Z = 4
$F(000)$ = 608
D_x = 1.395 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3729 reflections
θ = 3.9–29.2°
μ = 0.10 mm^{-1}
T = 295 K
Block, colourless
0.30 × 0.25 × 0.18 mm

Data collection

Agilent Xcalibur Eos diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 15.9821 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2012)
T_{min} = 0.969, T_{max} = 0.981
8396 measured reflections
2549 independent reflections
2027 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 25.5°, θ_{min} = 3.9°
h = −8→8
k = −13→12
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.101
S = 1.04
2549 reflections
192 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0462P)^2 + 0.2987P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.13$ e Å^{-3}

Extinction correction: SHELXL2017 (Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.030 (3)

Special details

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 $F^2 > 2\text{sigma}(F^2)$ 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}
O3	−0.03769 (14)	0.40424 (10)	0.06695 (6)	0.0455 (3)
O2	0.20750 (15)	0.23383 (10)	0.06507 (7)	0.0537 (3)
H10	0.287088	0.178188	0.073527	0.081*
O1	1.15498 (17)	0.21431 (11)	0.30304 (8)	0.0604 (4)
N3	0.85559 (17)	0.37007 (12)	0.26300 (7)	0.0418 (3)
N2	1.03456 (17)	0.40123 (12)	0.31206 (7)	0.0410 (3)
H2N	1.053128	0.472235	0.332397	0.049*
N1	1.61018 (19)	0.51282 (12)	0.42610 (8)	0.0452 (4)
C8	0.5291 (2)	0.43898 (15)	0.20366 (8)	0.0371 (4)
C9	0.4682 (2)	0.33704 (14)	0.15750 (8)	0.0384 (4)
H9	0.555924	0.274429	0.157443	0.046*
C10	0.2791 (2)	0.32888 (14)	0.11216 (8)	0.0372 (4)
C11	0.1465 (2)	0.42290 (14)	0.11294 (8)	0.0355 (4)
C12	0.2059 (2)	0.52410 (15)	0.15746 (9)	0.0409 (4)
H12	0.118419	0.586791	0.157676	0.049*
C13	0.3972 (2)	0.53171 (15)	0.20196 (9)	0.0423 (4)
H13	0.437730	0.600772	0.231319	0.051*
C14	−0.1795 (2)	0.49637 (17)	0.06553 (10)	0.0492 (4)
H14A	−0.192906	0.508196	0.115902	0.074*
H14B	−0.302791	0.472017	0.032256	0.074*
H14C	−0.138193	0.570937	0.047468	0.074*
C7	0.7260 (2)	0.45278 (15)	0.25379 (8)	0.0411 (4)
H7	0.758441	0.525352	0.280265	0.049*
C6	1.1785 (2)	0.31829 (14)	0.32729 (9)	0.0390 (4)
C2	1.4323 (2)	0.47808 (14)	0.38578 (8)	0.0387 (4)
H2	1.343594	0.537888	0.362746	0.046*
C1	1.3728 (2)	0.35815 (13)	0.37638 (8)	0.0354 (4)
C5	1.5059 (2)	0.27035 (15)	0.41019 (10)	0.0502 (4)
H5	1.472088	0.188603	0.404400	0.060*
C4	1.6891 (2)	0.30435 (17)	0.45260 (11)	0.0599 (5)
H4	1.780614	0.246398	0.476287	0.072*

C3	1.7334 (2)	0.42511 (17)	0.45907 (10)	0.0533 (5)
H3	1.857046	0.447633	0.488254	0.064*
O4	1.07802 (17)	0.65762 (11)	0.34578 (7)	0.0594 (4)
H4WA	1.034030	0.696974	0.377588	0.089*
H4WB	1.043530	0.692674	0.302788	0.089*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.0286 (5)	0.0448 (7)	0.0558 (7)	0.0044 (5)	−0.0009 (5)	−0.0023 (5)
O2	0.0385 (6)	0.0378 (6)	0.0712 (8)	0.0062 (5)	−0.0085 (5)	−0.0115 (6)
O1	0.0513 (7)	0.0382 (7)	0.0744 (9)	−0.0022 (5)	−0.0127 (6)	−0.0079 (6)
N3	0.0309 (6)	0.0455 (8)	0.0416 (7)	−0.0061 (6)	−0.0029 (5)	0.0026 (6)
N2	0.0311 (6)	0.0390 (7)	0.0448 (7)	−0.0032 (6)	−0.0037 (5)	−0.0026 (6)
N1	0.0361 (7)	0.0419 (8)	0.0509 (8)	−0.0062 (6)	0.0006 (6)	0.0030 (6)
C8	0.0317 (7)	0.0424 (9)	0.0351 (8)	−0.0033 (7)	0.0054 (6)	0.0051 (7)
C9	0.0306 (7)	0.0373 (8)	0.0437 (8)	0.0036 (6)	0.0039 (6)	0.0062 (7)
C10	0.0343 (8)	0.0327 (8)	0.0408 (8)	−0.0019 (6)	0.0038 (6)	0.0024 (7)
C11	0.0281 (7)	0.0388 (9)	0.0369 (8)	−0.0003 (6)	0.0039 (6)	0.0052 (7)
C12	0.0369 (8)	0.0403 (9)	0.0435 (8)	0.0051 (7)	0.0073 (6)	−0.0004 (7)
C13	0.0399 (8)	0.0422 (9)	0.0412 (8)	−0.0020 (7)	0.0049 (7)	−0.0052 (7)
C14	0.0325 (8)	0.0598 (11)	0.0520 (10)	0.0118 (8)	0.0056 (7)	0.0013 (8)
C7	0.0348 (8)	0.0446 (9)	0.0397 (8)	−0.0055 (7)	0.0030 (6)	0.0012 (7)
C6	0.0370 (8)	0.0345 (9)	0.0398 (8)	−0.0047 (7)	0.0007 (6)	0.0025 (7)
C2	0.0320 (8)	0.0364 (8)	0.0432 (8)	−0.0003 (6)	0.0023 (6)	0.0041 (7)
C1	0.0321 (7)	0.0359 (8)	0.0345 (7)	−0.0008 (6)	0.0026 (6)	0.0024 (6)
C5	0.0457 (9)	0.0361 (9)	0.0580 (10)	−0.0003 (7)	−0.0041 (8)	0.0050 (8)
C4	0.0432 (10)	0.0477 (11)	0.0728 (13)	0.0060 (8)	−0.0114 (9)	0.0120 (9)
C3	0.0328 (8)	0.0540 (11)	0.0611 (11)	−0.0043 (8)	−0.0075 (7)	0.0063 (9)
O4	0.0627 (8)	0.0475 (7)	0.0583 (7)	0.0186 (6)	−0.0002 (6)	−0.0017 (6)

Geometric parameters (Å, º)

O3—C11	1.3664 (17)	C12—C13	1.386 (2)
O3—C14	1.4257 (19)	C12—H12	0.9300
O2—C10	1.3627 (18)	C13—H13	0.9300
O2—H10	0.8198	C14—H14A	0.9600
O1—C6	1.2223 (19)	C14—H14B	0.9600
N3—C7	1.274 (2)	C14—H14C	0.9600
N3—N2	1.3866 (16)	C7—H7	0.9300
N2—C6	1.343 (2)	C6—C1	1.4950 (19)
N2—H2N	0.8602	C2—C1	1.383 (2)
N1—C3	1.333 (2)	C2—H2	0.9300
N1—C2	1.3355 (19)	C1—C5	1.376 (2)
C8—C13	1.381 (2)	C5—C4	1.376 (2)
C8—C9	1.400 (2)	C5—H5	0.9300
C8—C7	1.459 (2)	C4—C3	1.364 (3)
C9—C10	1.378 (2)	C4—H4	0.9300

C9—H9	0.9300	C3—H3	0.9300
C10—C11	1.404 (2)	O4—H4WA	0.8500
C11—C12	1.377 (2)	O4—H4WB	0.8495
C11—O3—C14	117.37 (12)	H14A—C14—H14B	109.5
C10—O2—H10	109.5	O3—C14—H14C	109.5
C7—N3—N2	114.41 (13)	H14A—C14—H14C	109.5
C6—N2—N3	118.71 (13)	H14B—C14—H14C	109.5
C6—N2—H2N	120.6	N3—C7—C8	123.07 (15)
N3—N2—H2N	120.7	N3—C7—H7	118.5
C3—N1—C2	116.76 (14)	C8—C7—H7	118.5
C13—C8—C9	118.80 (13)	O1—C6—N2	122.66 (13)
C13—C8—C7	117.90 (14)	O1—C6—C1	120.37 (14)
C9—C8—C7	123.31 (14)	N2—C6—C1	116.97 (13)
C10—C9—C8	120.43 (14)	N1—C2—C1	123.65 (14)
C10—C9—H9	119.8	N1—C2—H2	118.2
C8—C9—H9	119.8	C1—C2—H2	118.2
O2—C10—C9	124.50 (13)	C5—C1—C2	117.67 (13)
O2—C10—C11	115.81 (12)	C5—C1—C6	118.33 (14)
C9—C10—C11	119.69 (14)	C2—C1—C6	123.84 (13)
O3—C11—C12	125.07 (13)	C4—C5—C1	119.55 (15)
O3—C11—C10	114.71 (13)	C4—C5—H5	120.2
C12—C11—C10	120.22 (13)	C1—C5—H5	120.2
C11—C12—C13	119.40 (14)	C3—C4—C5	118.38 (15)
C11—C12—H12	120.3	C3—C4—H4	120.8
C13—C12—H12	120.3	C5—C4—H4	120.8
C8—C13—C12	121.44 (15)	N1—C3—C4	123.96 (15)
C8—C13—H13	119.3	N1—C3—H3	118.0
C12—C13—H13	119.3	C4—C3—H3	118.0
O3—C14—H14A	109.5	H4WA—O4—H4WB	109.5
O3—C14—H14B	109.5		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4*WA*···O2^{i}	0.85	2.28	3.0483 (17)	150
O4—H4*WA*···O3^{i}	0.85	2.49	3.2011 (16)	141
O4—H4*WB*···O1^{ii}	0.85	2.08	2.8429 (19)	150
O4—H4*WB*···N3^{ii}	0.85	2.50	3.1875 (18)	139
N2—H2*N*···O4	0.86	2.06	2.8889 (18)	162
O2—H10···N1^{iii}	0.82	1.96	2.7411 (17)	159
C2—H2···O4	0.93	2.25	3.129 (2)	156
C4—H4···O3^{iv}	0.93	2.45	3.347 (2)	163

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