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N′-[(1*E*)-4-Hydroxy-3-methoxybenzylidene]-isonicotinohydrazide monohydrate

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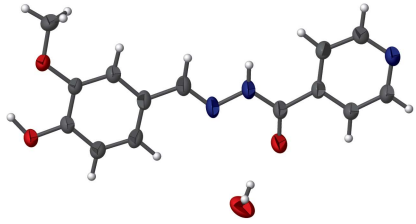
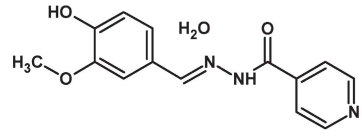
Structural data: full structural data are available from iucrdata.iucr.org

In the title hydrate, $C_{14}H_{13}N_3O_3\cdot H_2O$, the dihedral angle between the pyridine and benzene rings is 2.52 (9)°. Intramolecular O—H···O hydrogen bonds occur. In the crystal, O—H···O, O—H···N, N—H···O and C—H···O hydrogen bonds link the components into a three-dimensional network. π–π interactions are also observed.

3D view



Chemical scheme



Structure description

Hydrazones have been reported to be antitubercular (Vavříková *et al.*, 2011; Koçyiğit Kaymakçıoğlu & Rollas, 2002), anticancer (Bhat *et al.*, 2015), antifungal, antimicrobial, antiviral and antimalarial agents (Maccari *et al.*, 2005; Mallikarjuna *et al.*, 2009; Bekhit *et al.*, 2015). The development of new classes of hydrazones may overcome antimicrobial resistance.

The asymmetric unit of the title compound is shown in Fig. 1. The dihedral angle between the pyridine ring and the benzene rings is 2.52 (9)°. Intramolecular O—H···O hydrogen bonds (Table 1) occur. In the crystal, O—H···O, O—H···N, N—H···O and C—H···O hydrogen bonds (Table 1) link the components into a three-dimensional network. In addition, π–π interactions are observed between the pyridine and benzene rings of neighbouring molecules with centroid–centroid distances of 3.8251 (11) and 3.8984 (11) Å. The crystal packing is illustrated in Fig. 2.

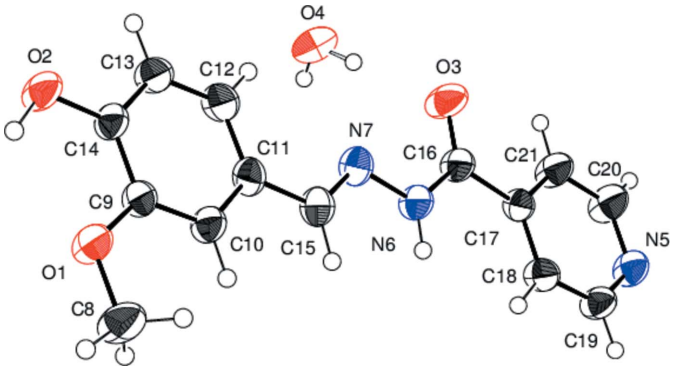


Figure 1
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms are shown as spheres of arbitrary radius.

Synthesis and crystallization

Equimolar quantities of vanillin (50 mmol) and isonicotinic acid hydrazide (50 mmol) were heated to reflux in the presence of absolute ethanol (50 ml) for 6 h; the completion of the reaction was monitored by TLC. After cooling and concentration of reaction mixture, the product was added to ice-cold water. The precipitated product was collected and dried. The crude product was recrystallized from 70 *v*/*v* ethanol solution, affording colourless prismatic crystals (yield 82%).

Spectroscopic data: IR (KBr disk, cm-1) 3356 (OH), 3324 (NH), 2969 (C—H), 1590 (Ar—C═C), 1265 (–OCH3); ^{1}H NMR (400 MHz, DMSO-d_6): 11.85 (*s*, 1H), 9.58 (*s*, 1H), 8.75 (*s*, 2H), 8.32 (*s*, 1H), 7.79 (*d*, 2H), 7.30 (*d*, 1H), 7.10 (*dd*, 1H), 6.83 (*d*, 1H). 3.81 (*s*, 3H); LC–MS *m*/*z*: 272.15 $(M + H)^+$.

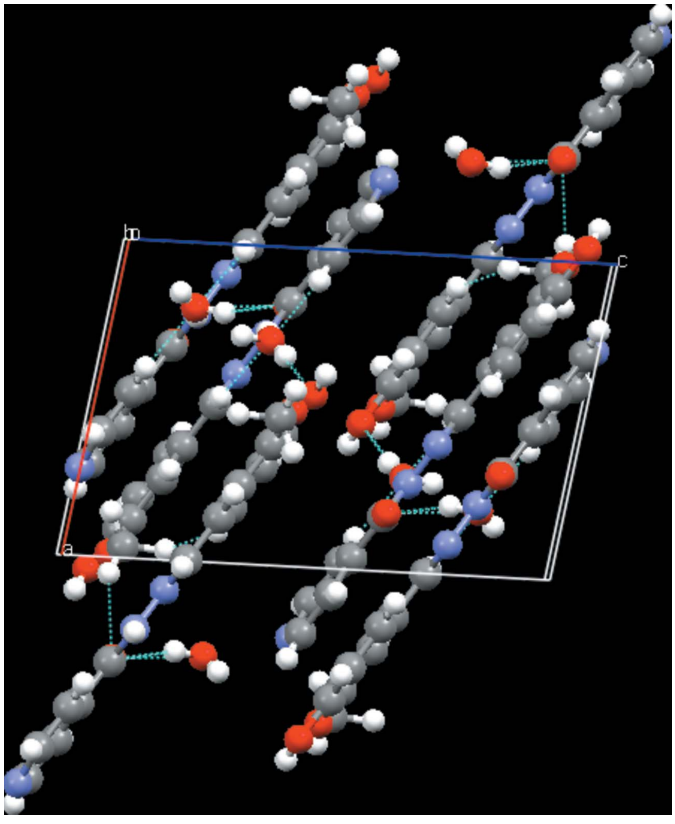


Figure 2
The packing of molecules. Hydrogen bonds are shown as dashed lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1	1.00 (3)	2.24 (3)	2.7081 (18)	107.4 (18)
O2—H2···N5^{i}	1.00 (3)	1.79 (3)	2.699 (2)	150 (2)
O4—H4*A*···O2^{ii}	0.73 (4)	2.28 (4)	2.986 (2)	163 (4)
O4—H4*B*···O3	0.92 (3)	1.93 (3)	2.832 (3)	166 (3)
N6—H6···O4^{iii}	0.89 (2)	2.10 (2)	2.976 (2)	169 (2)
C8—H8*A*···O3^{iv}	0.95 (2)	2.51 (2)	3.390 (3)	154 (2)
C15—H15···O4^{iii}	1.00 (2)	2.58 (2)	3.436 (3)	143.1 (14)
C18—H18···O4^{iii}	0.977 (18)	2.316 (18)	3.272 (3)	165.9 (16)
C20—H20···O1^{v}	0.94 (2)	2.56 (2)	3.189 (2)	124.5 (17)

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

Table 2
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, $P2_1/n$
Temperature (K)	296
a, b, c (Å)	8.3687 (7), 13.0913 (10), 12.6778 (11)
β (°)	99.086 (5)
V (Å^3)	1371.5 (2)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.88
Crystal size (mm)	0.24 × 0.20 × 0.12
Data collection	
Diffractometer	Bruker SMART CCD area-detector
Absorption correction	Multi-scan (*SADABS*; Sheldrick, 2007)
T_{min}, T_{max}	0.770, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7361, 2249, 1805
R_{int}	0.042
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.586
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.114, 1.04
No. of reflections	2249
No. of parameters	251
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.25, −0.25

Computer programs: *SMART* and *SAINT* (Bruker, 2001), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014/7* (Sheldrick, 2015*b*) and *ORTEP-3 for Windows* (Farrugia, 2012).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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References

Bekhit, A. A., Hassan, A. M. M., Abd El Razik, H. A., El-Miligy, M. M. M., El-Agroudy, E. J. & Bekhit, A. E. A. (2015). *Eur. J. Med. Chem.* **94**, 30–44.

Bhat, M. A., Iqbal, M., Al-Dhfyan, A. & Shakeel, F. (2015). *J. Mol. Liq.* **203**, 111–119.

Bruker (2001). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.

Koçyiğit Kaymakçıoğlu, B. & Rollas, S. (2002). *Farmaco*, **57**, 595–599.

Maccari, R., Ottanà, R. & Vigorita, M. G. (2005). *Bioorg. Med. Chem. Lett.* **15**, 2509–2513.

Mallikarjuna, B. P., Sastry, B. S., Suresh Kumar, G. V., Rajendraprasad, Y., Chandrashekar, S. M. & Sathisha, K. (2009). *Eur. J. Med. Chem.* **44**, 4739–4746.

Sheldrick, G. M. (2007). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

Vavříková, E., Polanc, S., Kočevar, M., Košmrlj, J., Horváti, K., Bősze, S., Stolaříková, J., Imramovský, A. & Vinšová, J. (2011). *Eur. J. Med. Chem.* **46**, 5902–5909.

full crystallographic data

IUCrData (2016). **1**, x161300 [doi:10.1107/S2414314616013006]

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Crystal data

$C_{14}H_{13}N_3O_3·H_2O$
M_r = 289.29
Monoclinic, $P2_1/n$
a = 8.3687 (7) Å
b = 13.0913 (10) Å
c = 12.6778 (11) Å
β = 99.086 (5)°
V = 1371.5 (2) Å^3
Z = 4
F(000) = 576
D_x = 1.401 Mg m^{-3}
Melting point: 298 K
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 2249 reflections
θ = 4.9–64.5°
μ = 0.88 mm^{-1}
T = 296 K
Prism, colourless
0.24 × 0.20 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2007)
T_{min} = 0.770, T_{max} = 1.000
7361 measured reflections
2249 independent reflections
1805 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 64.5°, θ_{min} = 4.9°
h = −7→9
k = −14→15
l = −14→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.114
S = 1.04
2249 reflections
251 parameters
0 restraints
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.059P)^2 + 0.2398P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Extinction correction: SHELXL-2014/7 (Sheldrick 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0065 (7)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.01283 (15)	0.81847 (9)	0.90314 (11)	0.0528 (4)
O2	−0.04008 (15)	0.61830 (10)	0.93903 (12)	0.0539 (4)
O3	0.81796 (17)	0.55219 (9)	0.64551 (13)	0.0627 (4)
O4	0.7956 (2)	0.43537 (13)	0.83061 (19)	0.0730 (5)
N5	1.22351 (17)	0.77082 (12)	0.50647 (12)	0.0476 (4)
N6	0.72171 (17)	0.70837 (12)	0.67777 (13)	0.0439 (4)
N7	0.59405 (17)	0.66654 (11)	0.72119 (12)	0.0469 (4)
C8	0.0359 (3)	0.92178 (15)	0.8789 (2)	0.0645 (7)
C9	0.12124 (18)	0.74987 (12)	0.87380 (13)	0.0378 (4)
C10	0.25461 (19)	0.77494 (14)	0.82747 (14)	0.0404 (4)
C11	0.35901 (19)	0.69995 (13)	0.80039 (14)	0.0413 (4)
C12	0.3261 (2)	0.59800 (14)	0.82145 (16)	0.0478 (5)
C13	0.1922 (2)	0.57302 (13)	0.86640 (16)	0.0468 (5)
C14	0.0886 (2)	0.64756 (13)	0.89347 (14)	0.0400 (4)
C15	0.4981 (2)	0.73119 (15)	0.75230 (15)	0.0452 (5)
C16	0.8276 (2)	0.64568 (13)	0.64171 (14)	0.0411 (4)
C17	0.96296 (18)	0.69426 (12)	0.59529 (13)	0.0361 (4)
C18	0.9779 (2)	0.79793 (13)	0.57671 (15)	0.0423 (4)
C19	1.1081 (2)	0.83129 (14)	0.53230 (15)	0.0446 (5)
C20	1.2073 (2)	0.67153 (15)	0.52461 (19)	0.0570 (6)
C21	1.0808 (2)	0.63071 (14)	0.56764 (17)	0.0499 (5)
H2	−0.106 (3)	0.678 (2)	0.955 (2)	0.107 (9)*
H6	0.731 (3)	0.7757 (18)	0.6774 (16)	0.058 (6)*
H10	0.283 (2)	0.8450 (16)	0.8173 (16)	0.058 (6)*
H13	0.168 (2)	0.5017 (16)	0.8816 (16)	0.064 (6)*
H18	0.900 (2)	0.8477 (15)	0.5953 (15)	0.055 (5)*
H12	0.402 (3)	0.5455 (15)	0.8037 (16)	0.063 (6)*
H19	1.118 (2)	0.9016 (16)	0.5182 (16)	0.058 (6)*
H15	0.519 (2)	0.8058 (17)	0.7452 (15)	0.057 (6)*
H21	1.075 (3)	0.5576 (17)	0.5790 (17)	0.068 (6)*
H20	1.289 (3)	0.6279 (17)	0.5081 (17)	0.070 (7)*
H8A	−0.051 (3)	0.9615 (18)	0.8970 (19)	0.080 (7)*
H8B	0.143 (3)	0.9463 (18)	0.918 (2)	0.089 (8)*
H8C	0.031 (3)	0.930 (2)	0.792 (2)	0.102 (9)*
H4B	0.785 (4)	0.475 (2)	0.770 (2)	0.103 (10)*
H4A	0.841 (4)	0.472 (3)	0.867 (3)	0.132 (15)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0479 (7)	0.0351 (7)	0.0847 (10)	0.0084 (5)	0.0386 (7)	0.0072 (6)
O2	0.0455 (8)	0.0385 (7)	0.0868 (11)	0.0000 (5)	0.0386 (7)	0.0034 (6)
O3	0.0569 (8)	0.0407 (7)	0.1011 (12)	−0.0071 (6)	0.0452 (8)	−0.0036 (7)
O4	0.0819 (12)	0.0538 (9)	0.0861 (13)	−0.0240 (8)	0.0218 (10)	0.0032 (9)
N5	0.0380 (8)	0.0474 (8)	0.0618 (10)	−0.0014 (6)	0.0216 (7)	0.0035 (7)

N6	0.0354 (8)	0.0421 (9)	0.0599 (10)	−0.0036 (6)	0.0250 (7)	−0.0039 (7)
N7	0.0346 (8)	0.0539 (9)	0.0576 (10)	−0.0046 (7)	0.0237 (7)	−0.0048 (7)
C8	0.0622 (14)	0.0354 (10)	0.105 (2)	0.0109 (9)	0.0420 (14)	0.0106 (11)
C9	0.0327 (8)	0.0353 (9)	0.0485 (10)	0.0047 (7)	0.0156 (7)	0.0002 (7)
C10	0.0348 (9)	0.0390 (9)	0.0504 (11)	0.0001 (7)	0.0160 (7)	0.0013 (8)
C11	0.0335 (9)	0.0479 (10)	0.0457 (10)	0.0003 (7)	0.0161 (7)	−0.0029 (8)
C12	0.0411 (10)	0.0431 (10)	0.0642 (12)	0.0057 (8)	0.0240 (9)	−0.0066 (9)
C13	0.0429 (10)	0.0358 (9)	0.0667 (13)	0.0015 (7)	0.0235 (9)	−0.0030 (9)
C14	0.0351 (9)	0.0388 (9)	0.0498 (10)	−0.0018 (7)	0.0183 (7)	0.0005 (7)
C15	0.0377 (10)	0.0501 (11)	0.0516 (11)	0.0004 (8)	0.0185 (8)	−0.0023 (8)
C16	0.0327 (9)	0.0404 (9)	0.0535 (11)	−0.0031 (7)	0.0170 (7)	−0.0030 (8)
C17	0.0283 (8)	0.0389 (8)	0.0429 (10)	−0.0011 (6)	0.0116 (7)	−0.0035 (7)
C18	0.0356 (9)	0.0384 (9)	0.0557 (11)	0.0010 (7)	0.0155 (8)	−0.0042 (8)
C19	0.0394 (10)	0.0378 (10)	0.0596 (12)	−0.0038 (7)	0.0170 (8)	0.0012 (8)
C20	0.0459 (11)	0.0466 (11)	0.0870 (16)	0.0072 (9)	0.0371 (10)	0.0075 (10)
C21	0.0434 (10)	0.0378 (10)	0.0744 (14)	0.0033 (8)	0.0280 (9)	0.0049 (9)

Geometric parameters (Å, º)

O1—C9	1.3691 (19)	C10—C11	1.393 (2)
O1—C8	1.407 (2)	C10—H10	0.96 (2)
O2—C14	1.355 (2)	C11—C12	1.397 (3)
O2—H2	0.99 (3)	C11—C15	1.455 (2)
O3—C16	1.228 (2)	C12—C13	1.374 (3)
O4—H4B	0.92 (3)	C12—H12	0.99 (2)
O4—H4A	0.73 (3)	C13—C14	1.384 (2)
N5—C19	1.329 (2)	C13—H13	0.98 (2)
N5—C20	1.331 (2)	C15—H15	1.00 (2)
N6—C16	1.340 (2)	C16—C17	1.498 (2)
N6—N7	1.389 (2)	C17—C21	1.377 (2)
N6—H6	0.88 (2)	C17—C18	1.386 (2)
N7—C15	1.272 (2)	C18—C19	1.375 (3)
C8—H8A	0.95 (3)	C18—H18	0.97 (2)
C8—H8B	1.01 (3)	C19—H19	0.94 (2)
C8—H8C	1.10 (3)	C20—C21	1.373 (3)
C9—C10	1.380 (2)	C20—H20	0.94 (2)
C9—C14	1.397 (2)	C21—H21	0.97 (2)
C9—O1—C8	116.83 (14)	C12—C13—H13	120.9 (12)
C14—O2—H2	111.8 (16)	C14—C13—H13	117.9 (13)
H4B—O4—H4A	97 (3)	O2—C14—C13	118.52 (15)
C19—N5—C20	116.19 (16)	O2—C14—C9	122.53 (15)
C16—N6—N7	119.02 (15)	C13—C14—C9	118.95 (16)
C16—N6—H6	123.2 (15)	N7—C15—C11	121.94 (18)
N7—N6—H6	117.8 (15)	N7—C15—H15	119.6 (12)
C15—N7—N6	115.06 (15)	C11—C15—H15	118.4 (12)
O1—C8—H8A	109.6 (15)	O3—C16—N6	123.10 (16)
O1—C8—H8B	109.9 (14)	O3—C16—C17	119.78 (15)

H8A—C8—H8B	111 (2)	N6—C16—C17	117.12 (15)
O1—C8—H8C	109.3 (14)	C21—C17—C18	117.44 (16)
H8A—C8—H8C	106 (2)	C21—C17—C16	117.37 (15)
H8B—C8—H8C	111 (2)	C18—C17—C16	125.18 (15)
O1—C9—C10	125.07 (15)	C19—C18—C17	118.63 (16)
O1—C9—C14	115.08 (14)	C19—C18—H18	119.2 (12)
C10—C9—C14	119.85 (15)	C17—C18—H18	122.1 (12)
C9—C10—C11	121.21 (16)	N5—C19—C18	124.45 (17)
C9—C10—H10	120.9 (13)	N5—C19—H19	116.3 (13)
C11—C10—H10	117.7 (13)	C18—C19—H19	119.3 (13)
C10—C11—C12	118.41 (16)	N5—C20—C21	123.69 (18)
C10—C11—C15	118.65 (16)	N5—C20—H20	117.2 (14)
C12—C11—C15	122.94 (16)	C21—C20—H20	119.1 (14)
C13—C12—C11	120.34 (16)	C20—C21—C17	119.60 (17)
C13—C12—H12	121.8 (12)	C20—C21—H21	120.1 (14)
C11—C12—H12	117.8 (12)	C17—C21—H21	120.3 (14)
C12—C13—C14	121.23 (17)		

C16—N6—N7—C15	−179.18 (16)	C10—C11—C15—N7	−176.74 (17)
C8—O1—C9—C10	3.4 (3)	C12—C11—C15—N7	3.8 (3)
C8—O1—C9—C14	−176.32 (19)	N7—N6—C16—O3	−0.3 (3)
O1—C9—C10—C11	179.83 (16)	N7—N6—C16—C17	179.83 (14)
C14—C9—C10—C11	−0.5 (3)	O3—C16—C17—C21	−6.0 (3)
C9—C10—C11—C12	−0.2 (3)	N6—C16—C17—C21	173.86 (17)
C9—C10—C11—C15	−179.66 (16)	O3—C16—C17—C18	173.15 (18)
C10—C11—C12—C13	0.9 (3)	N6—C16—C17—C18	−7.0 (3)
C15—C11—C12—C13	−179.58 (18)	C21—C17—C18—C19	−0.1 (3)
C11—C12—C13—C14	−1.1 (3)	C16—C17—C18—C19	−179.19 (17)
C12—C13—C14—O2	−179.03 (18)	C20—N5—C19—C18	0.9 (3)
C12—C13—C14—C9	0.4 (3)	C17—C18—C19—N5	−0.8 (3)
O1—C9—C14—O2	−0.5 (3)	C19—N5—C20—C21	−0.2 (3)
C10—C9—C14—O2	179.79 (17)	N5—C20—C21—C17	−0.6 (4)
O1—C9—C14—C13	−179.92 (16)	C18—C17—C21—C20	0.7 (3)
C10—C9—C14—C13	0.4 (3)	C16—C17—C21—C20	179.90 (19)
N6—N7—C15—C11	−179.50 (16)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1	1.00 (3)	2.24 (3)	2.7081 (18)	107.4 (18)
O2—H2···N5^{i}	1.00 (3)	1.79 (3)	2.699 (2)	150 (2)
O4—H4*A*···O2^{ii}	0.73 (4)	2.28 (4)	2.986 (2)	163 (4)
O4—H4*B*···O3	0.92 (3)	1.93 (3)	2.832 (3)	166 (3)
N6—H6···O4^{iii}	0.89 (2)	2.10 (2)	2.976 (2)	169 (2)
C8—H8*A*···O3^{iv}	0.95 (2)	2.51 (2)	3.390 (3)	154 (2)
C15—H15···O4^{iii}	1.00 (2)	2.58 (2)	3.436 (3)	143.1 (14)

C18—H18···O4^{iii}	0.977 (18)	2.316 (18)	3.272 (3)	165.9 (16)
C20—H20···O1^{v}	0.94 (2)	2.56 (2)	3.189 (2)	124.5 (17)

Symmetry codes: (i) $x-3/2, -y+3/2, z+1/2$; (ii) $x+1, y, z$; (iii) $-x+3/2, y+1/2, -z+3/2$; (iv) $-x+1/2, y+1/2, -z+3/2$; (v) $x+3/2, -y+3/2, z-1/2$.