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(*E*)-*N*′-(4-Methoxybenzylidene)pyridine-3-carbohydrazide dihydrate

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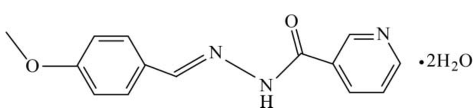
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.046; wR factor = 0.155; data-to-parameter ratio = 16.7.

In the title compound, $C_{14}H_{13}N_3O_2\cdot 2H_2O$, the hydrazone molecule adopts an E conformation with respect to the C═N bond. The dihedral angle between the benzene and pyridine rings is 8.55 (10)°. The methylidene–hydrazide [–C(═O)–N–N═C–] fragment is essentially planar, with a maximum deviation of 0.0375 (13) Å. The mean planes of the benzene and pyridine rings make dihedral angles of 2.71 (14) and 11.25 (13)°, respectively, with mean plane of the methylidene-hydrazide fragment. In the crystal, the benzohydrazide and water molecules are linked by N—H···O, O—H···O and O—H···N hydrogen bonds into a three-dimensional network.

Related literature

For the biological activity of benzohydrazides, see: Hai-Yun (2011); Havanur *et al.* (2010); Parashar *et al.* (2009). For details of the ability of benzohydrazone compounds to inhibit cell growth and DNA synthesis, see: Ambwani *et al.* (2011); Despaigne *et al.* (2010); Havanur *et al.* (2010). For background to the use of benzohydrazides as catalysts, see: Seleem *et al.* (2011); Singh & Raghav (2011). For related structures, see: Ahmad *et al.* (2010); Hu & Liu (2012); Shi & Li (2012).



Experimental

Crystal data

$C_{14}H_{13}N_3O_2\cdot 2H_2O$
M_r = 291.31
Monoclinic, $P2_1/n$
a = 7.6534 (6) Å
b = 16.3503 (11) Å
c = 11.4887 (6) Å
β = 96.889 (2)°
V = 1427.26 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 296 K
0.30 × 0.25 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004) T_{min} = 0.970, T_{max} = 0.980
11391 measured reflections
3449 independent reflections
2050 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.155
S = 0.93
3449 reflections
206 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2N2···O1W	0.86	2.08	2.9013 (17)	161
O1W—H1O1···N3^{i}	0.81 (1)	2.08 (1)	2.8697 (18)	166 (2)
O1W—H2O1···O2W^{ii}	0.83 (1)	1.93 (1)	2.749 (2)	171 (2)
O2W—H1O2···N1^{iii}	0.83 (2)	2.40 (2)	3.209 (2)	166 (3)
O2W—H2O2···O2	0.83 (2)	2.01 (2)	2.8182 (17)	164 (2)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5336).

References

Ahmad, T., Zia-ur-Rehman, M., Siddiqui, H. L., Mahmud, S. & Parvez, M. (2010). *Acta Cryst.* E**66**, o976.
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
Ambwani, J., Dikshit, S. N., Tiwari, V. K., Dubey, A. K. & Rahul, A. (2011). *Asian J. Chem. Environ. Res.* **4**, 33–35.
Bruker (2004). *APEX2*, *SAINT*, *XPREP* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Despaigne, A. A. R., Vieira, L. F., Mendes, I. C., da Costa, F. B., Speziali, N. L. & Beraldo, H. (2010). *J. Braz. Chem. Soc.* **21**, 1247–1257.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Hai-Yun, Z. (2011). *Chin. J. Struct. Chem.* **30**, 724–730.
Havanur, V. C., Badiger, D. S., Ligade, S. G. & Gudasi, K. B. (2010). *Pharma Chem.* **2**, 390–404.
Hu, H.-N. & Liu, S.-Y. (2012). *Acta Cryst.* E**68**, o1613.
Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
Parashar, B., Punjabi, P. B., Gupta, G. D. & Sharma, V. K. (2009). *Int. J. Chem. Tech. Res.* **1**, 1022–1025.
Seleem, H. S., El-Inany, G. A., El-Shetary, B. A., Mousa, M. A. & Hanafy, F. I. (2011). *Chem. Cent. J.* **5**, 1–9.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Shi, Z.-F. & Li, J.-M. (2012). *Acta Cryst.* E**68**, o1726.
Singh, M. & Raghav, N. (2011). *Int. J. Pharm. Pharm. Sci.* **3**, 26–32.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

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(*E*)-*N*′-(4-Methoxybenzylidene)pyridine-3-carbohydrazide dihydrate

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S1. Comment

Hydrazones have attracted much attention for their excellent biological properties, such as antimicrobial, anti-convulsant, analgestic, anti-inflammatory, antiplatelet, antitubercular, anticancer, antitumor (Hai-Yun, 2011), antiviral and vasodilator activities (Parashar *et al.*, 2009). Hydrazones possessing azomethine –NHN═CH– groups constitute an important class of compounds for new drug development (Hai-Yun, 2011). Moreover, hydrazones derived from 2-acetylpyridine are known to inhibit the proliferation of tumour cells to a greater extent compared to standard anticancer agents (Havanur *et al.*, 2010). In addition, metal complexes with hydrazones exhibit antimicrobial, DNA-binding and cytotoxic activities. It has also been shown that these metal complexes can be potent inhibitors of cell growth and DNA synthesis (Despaigne *et al.*, 2010; Havanur *et al.*, 2010; Ambwani *et al.*, 2011). Metal complexes with hydrazones also have potential applications as catalysts, luminescent probes and molecular sensors (Seleem *et al.*, 2011; Singh & Raghav, 2011). We report herein the crystal structure of the title compound, a new hydrazone.

The title compound (Fig. 1), $C_{14}H_{13}N_3O_2.2H_2O$, comprises one benzohydrazide molecule and two water molecules. The hydrazone molecule adopts an E conformation with respect to the C═N bond with the torsion angle of -177.41 (16)° (C8—N1—N2—C9). Phenyl and pyridine rings (C2—C7 and N3/C10—C14, respectively) are each planner with a dihedral angle 8.55 (10)° between their mean-planes. The methylidenehydrazide fragment O2/C9/N2/N1/C8 in the title compound is essentially planar with maximum deviation being -0.0375 (13) Å for the N1 atom. The mean-planes of the benzene and pyridine rings make dihedral angles of 2.71 (14)° and 11.25 (13)°, respectively, with mean–plane of the methylidenehydrazide fragment. The C8═N1 and C9═O2 bond lengths are 1.270 (2) and 1.2199 (18) Å, respectively, which is very close to the values found in related structures (Hu & Liu, 2012; Shi & Li, 2012; Ahmad *et al.*, 2010). The methoxy group is co–planar with the benzene ring to which it is bound with the C1—O1—C2—C3 torsion angle = -0.26 (27)°.

In the crystal packing (Fig. 2), the molecules of benzohydrazide and water are linked by N2—H2N2···O1W, O1W—H2O1···O2W, O2W—H2O2···O2, O1W—H1O1···N3 and O2W—H1O2···N1 hydrogen bonds (Table 1) into a three–dimensional network.

S2. Experimental

Anisaldehyde (1.2 ml, 0.01 mol) and benzoic acid hydrazide (1.37 g, 0.01 mol) were added to ethanol(10 ml) of and stirred for an hour in the presence of hydrochloric acid to form a white precipitate. The precipitate was washed with sodium bicarbonate solution and filtered and again washed with petroleum ether (40–60%)and dried in air. The compound was recrystallized from absolute ethanol.

S3. Refinement

H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H = 0.93 Å, CH_3 = 0.96 Å, N—H = 0.86 Å and O—H = 0.81–0.83 Å with $U_{iso}(H) = 1.5U_{eq}(CH_3)$ and $1.2U_{eq}(CH, NH)$.

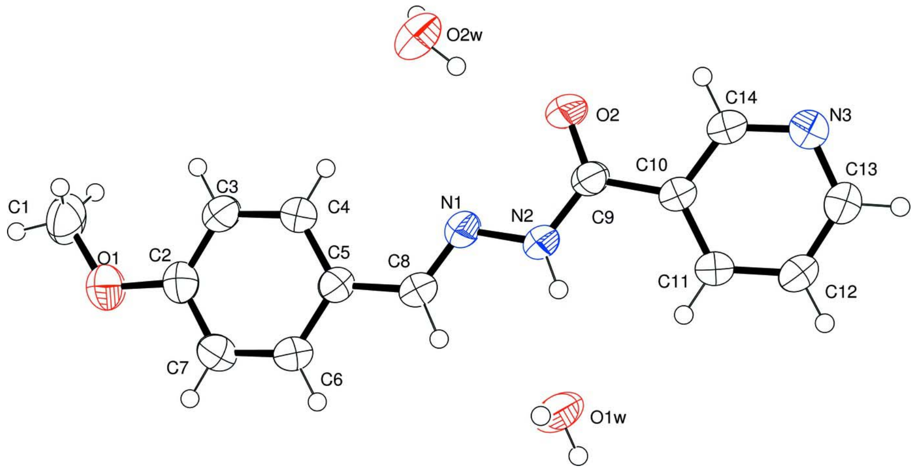

Figure 1

The molecular structure of the title molecule, with the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

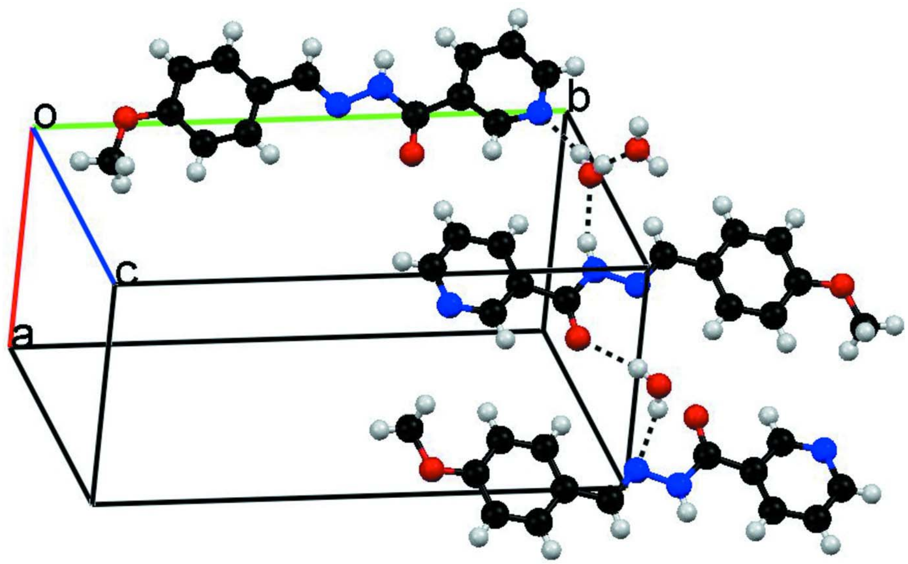

Figure 2

Crystal packing of the title compound viewed along the *a* axis. Hydrogen bonds are shown as dashed lines.

(*E*)-*N*′-(4-Methoxybenzylidene)pyridine-3-carbohydrazide dihydrate

Crystal data

$C_{14}H_{13}N_3O_2\cdot 2H_2O$	$F(000) = 616$
$M_r = 291.31$	$D_x = 1.356$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 2772 reflections
$a = 7.6534$ (6) Å	$\theta = 5.0$–$49.6°$
$b = 16.3503$ (11) Å	$\mu = 0.10$ mm^{-1}
$c = 11.4887$ (6) Å	$T = 296$ K
$\beta = 96.889$ (2)°	Block, colorless
$V = 1427.26$ (17) Å^3	0.30 × 0.25 × 0.20 mm
$Z = 4$	

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.970, T_{max} = 0.980
11391 measured reflections
3449 independent reflections
2050 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 28.2°, θ_{min} = 3.0°
$h = -6 \rightarrow 10$
$k = -21 \rightarrow 21$
$l = -13 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.155$
$S = 0.93$
3449 reflections
206 parameters
6 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
$w = 1/[\sigma^2(F_o^2) + (0.0961P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.009 (2)

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}
O1W	−0.21558 (17)	0.92875 (9)	0.70457 (12)	0.0661 (4)
O1	0.21045 (18)	1.39338 (7)	0.86316 (12)	0.0652 (4)
O2W	0.4378 (2)	1.01711 (9)	1.14079 (13)	0.0670 (4)
N1	0.15479 (18)	1.00258 (8)	0.89482 (11)	0.0459 (4)
N2	0.09417 (18)	0.92297 (7)	0.87676 (11)	0.0449 (4)
H2N2	0.0061	0.9121	0.8253	0.054*
N3	0.1583 (2)	0.63790 (8)	0.97900 (12)	0.0530 (4)
O2	0.29733 (18)	0.87747 (7)	1.01980 (11)	0.0688 (5)
C1	0.3384 (3)	1.42723 (12)	0.9485 (2)	0.0717 (6)
H1A	0.3071	1.4158	1.0253	0.108*
H1B	0.3438	1.4853	0.9375	0.108*
H1C	0.4512	1.4035	0.9408	0.108*
C2	0.1867 (2)	1.31049 (10)	0.86152 (14)	0.0470 (4)
C3	0.2804 (2)	1.25610 (10)	0.93809 (15)	0.0477 (4)
H3	0.3671	1.2753	0.9952	0.057*

C4	0.2445 (2)	1.17334 (10)	0.92929 (14)	0.0460 (4)
H4	0.3080	1.1372	0.9806	0.055*
C5	0.1152 (2)	1.14332 (9)	0.84510 (13)	0.0413 (4)
C8	0.0684 (2)	1.05745 (10)	0.83445 (14)	0.0450 (4)
H8	−0.0278	1.0421	0.7818	0.054*
C9	0.1777 (2)	0.86340 (9)	0.94232 (13)	0.0422 (4)
C10	0.1187 (2)	0.77765 (9)	0.91597 (13)	0.0384 (4)
C14	0.1898 (2)	0.71787 (10)	0.99233 (13)	0.0467 (4)
H14	0.2650	0.7345	1.0577	0.056*
C13	0.0525 (2)	0.61574 (10)	0.88326 (15)	0.0520 (5)
H13	0.0303	0.5603	0.8708	0.062*
C6	0.0240 (2)	1.19971 (10)	0.76869 (14)	0.0482 (4)
H6	−0.0629	1.1809	0.7114	0.058*
C7	0.0592 (2)	1.28169 (10)	0.77585 (15)	0.0509 (4)
H7	−0.0022	1.3178	0.7234	0.061*
C12	−0.0253 (2)	0.67021 (10)	0.80237 (15)	0.0519 (5)
H12	−0.0988	0.6519	0.7373	0.062*
C11	0.0072 (2)	0.75257 (9)	0.81904 (14)	0.0456 (4)
H11	−0.0452	0.7907	0.7658	0.055*
H1O1	−0.266 (2)	0.9158 (11)	0.6408 (10)	0.068*
H2O1	−0.291 (2)	0.9418 (13)	0.7474 (13)	0.068*
H2O2	0.389 (3)	0.9826 (11)	1.0949 (17)	0.077 (7)*
H1O2	0.544 (2)	1.021 (2)	1.134 (3)	0.149 (15)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1W	0.0546 (9)	0.0784 (9)	0.0607 (9)	−0.0029 (7)	−0.0121 (7)	−0.0218 (7)
O1	0.0764 (10)	0.0408 (7)	0.0760 (9)	−0.0070 (6)	−0.0009 (8)	0.0042 (6)
O2W	0.0648 (10)	0.0722 (9)	0.0623 (9)	−0.0155 (8)	0.0000 (8)	−0.0202 (7)
N1	0.0494 (8)	0.0396 (7)	0.0464 (8)	−0.0076 (6)	−0.0043 (7)	−0.0017 (6)
N2	0.0468 (8)	0.0403 (7)	0.0440 (8)	−0.0064 (6)	−0.0088 (6)	−0.0030 (6)
N3	0.0636 (10)	0.0439 (8)	0.0487 (8)	−0.0001 (7)	−0.0054 (7)	0.0017 (6)
O2	0.0731 (9)	0.0519 (7)	0.0702 (9)	−0.0125 (6)	−0.0370 (8)	0.0024 (6)
C1	0.0695 (14)	0.0482 (10)	0.0957 (16)	−0.0127 (9)	0.0025 (12)	−0.0117 (10)
C2	0.0523 (10)	0.0401 (9)	0.0497 (9)	−0.0011 (7)	0.0111 (8)	−0.0009 (7)
C3	0.0489 (10)	0.0472 (9)	0.0450 (9)	−0.0052 (7)	−0.0023 (8)	−0.0042 (7)
C4	0.0500 (10)	0.0418 (9)	0.0439 (9)	0.0017 (7)	−0.0030 (8)	0.0007 (7)
C5	0.0427 (9)	0.0420 (8)	0.0386 (8)	−0.0005 (7)	0.0022 (7)	−0.0033 (6)
C8	0.0447 (9)	0.0457 (9)	0.0420 (9)	−0.0029 (7)	−0.0049 (7)	−0.0037 (7)
C9	0.0428 (9)	0.0436 (9)	0.0383 (8)	−0.0055 (7)	−0.0026 (7)	−0.0010 (6)
C10	0.0380 (8)	0.0421 (8)	0.0343 (8)	−0.0016 (7)	0.0009 (7)	−0.0026 (6)
C14	0.0518 (10)	0.0479 (9)	0.0375 (9)	−0.0021 (8)	−0.0068 (8)	−0.0020 (7)
C13	0.0578 (11)	0.0413 (9)	0.0546 (10)	−0.0017 (8)	−0.0021 (9)	−0.0064 (7)
C6	0.0478 (10)	0.0500 (10)	0.0441 (9)	0.0022 (8)	−0.0062 (8)	−0.0028 (7)
C7	0.0554 (11)	0.0477 (9)	0.0480 (9)	0.0074 (8)	−0.0003 (8)	0.0046 (7)
C12	0.0555 (11)	0.0484 (9)	0.0478 (9)	−0.0034 (8)	−0.0100 (8)	−0.0096 (8)
C11	0.0486 (10)	0.0442 (9)	0.0412 (9)	0.0013 (7)	−0.0068 (8)	0.0003 (7)

Geometric parameters (Å, º)

O1W—H1O1	0.814 (9)	C3—H3	0.9300
O1W—H2O1	0.828 (9)	C4—C5	1.388 (2)
O1—C2	1.3672 (19)	C4—H4	0.9300
O1—C1	1.413 (2)	C5—C6	1.400 (2)
O2W—H2O2	0.830 (15)	C5—C8	1.450 (2)
O2W—H1O2	0.828 (17)	C8—H8	0.9300
N1—C8	1.270 (2)	C9—C10	1.493 (2)
N1—N2	1.3890 (17)	C10—C11	1.382 (2)
N2—C9	1.3451 (19)	C10—C14	1.381 (2)
N2—H2N2	0.8600	C14—H14	0.9300
N3—C14	1.335 (2)	C13—C12	1.370 (2)
N3—C13	1.335 (2)	C13—H13	0.9300
O2—C9	1.2199 (18)	C6—C7	1.368 (2)
C1—H1A	0.9600	C6—H6	0.9300
C1—H1B	0.9600	C7—H7	0.9300
C1—H1C	0.9600	C12—C11	1.379 (2)
C2—C7	1.383 (2)	C12—H12	0.9300
C2—C3	1.388 (2)	C11—H11	0.9300
C3—C4	1.382 (2)		
H1O1—O1W—H2O1	108.4 (17)	N1—C8—H8	119.0
C2—O1—C1	118.54 (14)	C5—C8—H8	119.0
H2O2—O2W—H1O2	111 (2)	O2—C9—N2	122.46 (14)
C8—N1—N2	115.97 (13)	O2—C9—C10	120.50 (14)
C9—N2—N1	117.85 (12)	N2—C9—C10	117.04 (13)
C9—N2—H2N2	121.1	C11—C10—C14	117.41 (14)
N1—N2—H2N2	121.1	C11—C10—C9	125.79 (14)
C14—N3—C13	116.33 (13)	C14—C10—C9	116.70 (13)
O1—C1—H1A	109.5	N3—C14—C10	124.64 (14)
O1—C1—H1B	109.5	N3—C14—H14	117.7
H1A—C1—H1B	109.5	C10—C14—H14	117.7
O1—C1—H1C	109.5	N3—C13—C12	123.60 (15)
H1A—C1—H1C	109.5	N3—C13—H13	118.2
H1B—C1—H1C	109.5	C12—C13—H13	118.2
O1—C2—C7	115.38 (14)	C7—C6—C5	121.87 (14)
O1—C2—C3	124.65 (14)	C7—C6—H6	119.1
C7—C2—C3	119.97 (14)	C5—C6—H6	119.1
C4—C3—C2	119.85 (14)	C6—C7—C2	119.58 (15)
C4—C3—H3	120.1	C6—C7—H7	120.2
C2—C3—H3	120.1	C2—C7—H7	120.2
C3—C4—C5	121.08 (14)	C13—C12—C11	118.95 (14)
C3—C4—H4	119.5	C13—C12—H12	120.5
C5—C4—H4	119.5	C11—C12—H12	120.5
C4—C5—C6	117.64 (14)	C12—C11—C10	119.05 (14)
C4—C5—C8	123.31 (14)	C12—C11—H11	120.5
C6—C5—C8	119.04 (13)	C10—C11—H11	120.5

N1—C8—C5	122.07 (14)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*N*2···O1*W*	0.86	2.08	2.9013 (17)	161
O1*W*—H1*O*1···N3^{i}	0.81 (1)	2.08 (1)	2.8697 (18)	166 (2)
O1*W*—H2*O*1···O2*W*^{ii}	0.83 (1)	1.93 (1)	2.749 (2)	171 (2)
O2*W*—H1*O*2···N1^{iii}	0.83 (2)	2.40 (2)	3.209 (2)	166 (3)
O2*W*—H2*O*2···O2	0.83 (2)	2.01 (2)	2.8182 (17)	164 (2)

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