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5-Acetamido-1*H*-pyrazole-4-carboxamide monohydrate

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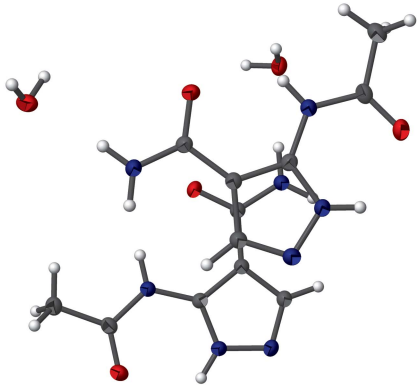
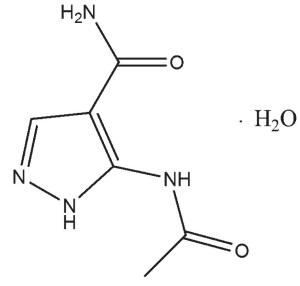
Structural data: full structural data are available from iucrdata.iucr.org

There are two independent molecules of the title carboxamide compound, $C_6H_8N_4O_2\cdot H_2O$, as well as two independent water molecules in the asymmetric unit. The two independent carboxamide molecules differ primarily in the relative orientations of the peripheral methyl and amino groups. Intramolecular N—H···O hydrogen bonds assist in determining the orientations of the acetamido substituents. The three-dimensional crystal packing is directed by a large network of O—H···O, N—H···O, C—H···O and C—H···N hydrogen bonds.

3D view



Chemical scheme



Structure description

Compounds that contain the pyrazole moiety are known to exhibit a wide range of biological properties (Tantawy *et al.*, 2012). As a continuation of our research devoted to the development of carboxamide derivatives of pyrazole (Ramli *et al.*, 2013; Karrouchi *et al.*, 2015), we prepared the title compound and characterized it by X-ray diffraction. There are two independent molecules of the carboxamide compound as well as two independent water molecules in the asymmetric unit (Fig. 1). The former differ primarily in the orientations of the peripheral methyl and amino groups and their conformations are mainly determined by a pair of intramolecular N—H···O hydrogen bonds in each. Intermolecular O—H···O, N—H···O, C—H···O and C—H···N hydrogen bonds which include those with the lattice water form sheets which are tied to one another by hydrogen bonding with the lattice water (Table 1 and Fig. 2).

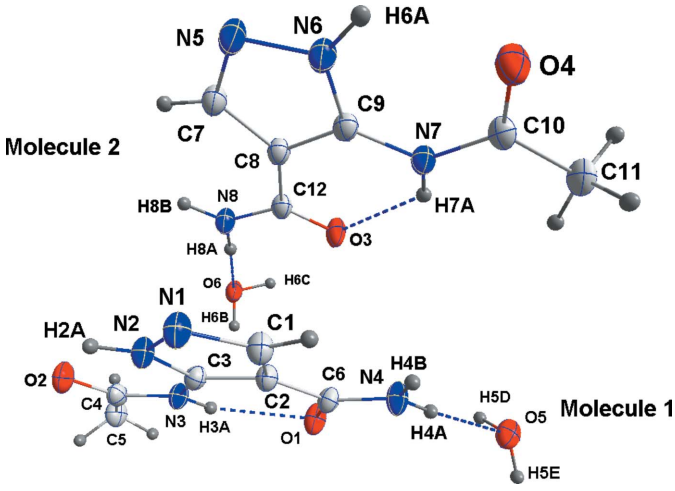


Figure 1
The asymmetric unit of the title compound, showing the atom-labelling scheme and 50% probability displacement ellipsoids.

Synthesis and crystallization

5-Amino-1*H*-pyrazole-4-carboxamide (0.669 g, 3.69 mmol) was stirred in refluxing glacial acetic acid for 1 h. The mixture was cooled to room temperature and the resulting solid was filtered off and dried to obtain the acetylated product (yield; 80%; m.p. = 387–389 K). Crystals suitable for X-ray analysis were obtained by recrystallization from wet ethanol.

Refinement

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

Acknowledgements

The support of NSF–MRI Grant No. 1228232 for the purchase of the diffractometer and Tulane University for support of the Tulane Crystallography Laboratory are gratefully acknowledged.

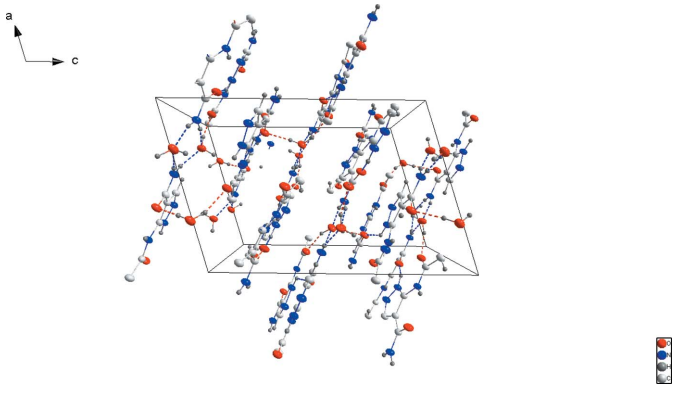


Figure 2
Packing viewed along the *b* axis with O—H···O and N—H···O hydrogen bonds when shown, indicated as red and blue dotted lines, respectively.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O1^{i}	0.90 (2)	2.07 (2)	2.7514 (14)	131.9 (17)
N2—H2*A*···O2	0.90 (2)	2.09 (2)	2.6441 (14)	118.6 (16)
N3—H3*A*···O1	0.883 (19)	2.226 (18)	2.8307 (14)	125.4 (15)
N4—H4*A*···O5	0.897 (19)	2.10 (2)	2.9919 (15)	173.9 (17)
N4—H4*B*···O6^{ii}	0.90 (2)	2.12 (2)	2.9893 (15)	163.2 (17)
C1—H1···O6^{ii}	0.95	2.51	3.3791 (16)	153
N6—H6*A*···O3^{iii}	0.89 (2)	2.01 (2)	2.7112 (14)	135.8 (18)
N6—H6*A*···O4	0.89 (2)	2.14 (2)	2.6558 (15)	116.4 (16)
N7—H7*A*···O3	0.887 (18)	2.204 (18)	2.8325 (14)	127.4 (15)
N8—H8*A*···O6	0.914 (19)	2.13 (2)	3.0338 (15)	169.7 (17)
N8—H8*B*···O5^{iv}	0.907 (18)	2.052 (19)	2.9354 (15)	164.5 (16)
C7—H7···O5^{iv}	0.95	2.63	3.4683 (17)	147
C11—H11*B*···N5^{v}	0.98	2.44	3.3337 (17)	152
O5—H5*D*···O2^{vi}	0.93 (2)	1.87 (2)	2.7658 (14)	161.1 (19)
O5—H5*E*···O1^{vii}	0.87 (2)	1.97 (2)	2.8269 (15)	168 (2)
O6—H6*B*···N1^{vi}	0.85 (2)	2.13 (2)	2.9448 (16)	162.5 (18)
O6—H6*C*···O4^{v}	0.93 (2)	1.83 (2)	2.7406 (14)	165.0 (18)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_6H_8N_4O_2·H_2O$
M_r	186.18
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	150
a, *b*, *c* (Å)	9.7953 (3), 12.4179 (3), 14.4833 (4)
β (°)	107.490 (1)
V (Å^3)	1680.26 (8)
Z	8
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.02
Crystal size (mm)	0.18 × 0.11 × 0.11
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.81, 0.90
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13029, 3358, 2970
R_{int}	0.030
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.036, 0.096, 1.07
No. of reflections	3358
No. of parameters	285
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.20, −0.32

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

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full crystallographic data

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5-Acetamido-1*H*-pyrazole-4-carboxamide monohydrate

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5-Acetamido-1*H*-pyrazole-4-carboxamide monohydrate

Crystal data

$C_6H_8N_4O_2·H_2O$
M_r = 186.18
Monoclinic, $P2_1/n$
a = 9.7953 (3) Å
b = 12.4179 (3) Å
c = 14.4833 (4) Å
β = 107.490 (1)°
V = 1680.26 (8) Å^3
Z = 8
$F(000)$ = 784
D_x = 1.472 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9957 reflections
θ = 3.2–74.5°
μ = 1.02 mm^{-1}
T = 150 K
Block, colourless
0.18 × 0.11 × 0.11 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro–focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.81, T_{max} = 0.90
13029 measured reflections
3358 independent reflections
2970 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 74.5°, θ_{min} = 4.8°
h = −12→12
k = −14→15
l = −16→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.096
S = 1.07
3358 reflections
285 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.055P)^2 + 0.420P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-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. H-atoms attached to carbon were placed in calculated positions (C—H = 0.95 - 0.98 Å) and included as riding contributions with isotropic displacement parameters 1.2 - 1.5 times those of the attached atoms.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.64084 (10)	0.12975 (7)	0.15757 (7)	0.0275 (2)
O2	1.01723 (10)	0.38984 (7)	0.35365 (7)	0.0275 (2)
N1	0.64268 (12)	0.49783 (9)	0.18328 (9)	0.0243 (2)
N2	0.76322 (12)	0.44563 (9)	0.23727 (8)	0.0216 (2)
H2A	0.839 (2)	0.4803 (16)	0.2766 (16)	0.047 (5)*
N3	0.85744 (12)	0.26580 (9)	0.27281 (8)	0.0216 (2)
H3A	0.8390 (19)	0.1967 (15)	0.2611 (13)	0.036 (5)*
N4	0.43236 (12)	0.20207 (9)	0.06553 (9)	0.0253 (3)
H4A	0.3977 (19)	0.1368 (16)	0.0443 (13)	0.038 (5)*
H4B	0.379 (2)	0.2609 (16)	0.0446 (14)	0.039 (5)*
C1	0.55571 (13)	0.42000 (10)	0.13782 (10)	0.0220 (3)
H1	0.4627	0.4320	0.0945	0.026*
C2	0.61742 (13)	0.31744 (10)	0.16125 (9)	0.0194 (3)
C3	0.75180 (13)	0.33861 (10)	0.22646 (9)	0.0190 (3)
C4	0.98718 (13)	0.29469 (10)	0.33478 (9)	0.0216 (3)
C5	1.08922 (14)	0.20491 (11)	0.37679 (11)	0.0281 (3)
H5A	1.0576	0.1391	0.3390	0.042*
H5B	1.0916	0.1926	0.4441	0.042*
H5C	1.1852	0.2243	0.3747	0.042*
C6	0.56270 (13)	0.20997 (10)	0.12835 (9)	0.0201 (3)
O3	0.40206 (10)	0.25721 (7)	0.29665 (7)	0.0273 (2)
O4	0.00312 (10)	0.51118 (7)	0.11825 (7)	0.0280 (2)
N5	0.33747 (12)	0.61884 (9)	0.33187 (9)	0.0256 (3)
N6	0.23058 (12)	0.56693 (9)	0.26354 (8)	0.0229 (2)
H6A	0.154 (2)	0.6021 (16)	0.2283 (15)	0.048 (5)*
N7	0.17347 (11)	0.39040 (9)	0.19132 (8)	0.0206 (2)
H7A	0.2026 (19)	0.3224 (15)	0.1970 (13)	0.035 (5)*
N8	0.59719 (12)	0.33310 (9)	0.40152 (9)	0.0237 (2)
H8A	0.642 (2)	0.2676 (16)	0.4097 (13)	0.040 (5)*
H8B	0.6437 (19)	0.3930 (15)	0.4305 (13)	0.032 (4)*
C7	0.43460 (14)	0.54373 (10)	0.36760 (10)	0.0229 (3)
H7	0.5221	0.5564	0.4170	0.028*
C8	0.39327 (13)	0.44268 (10)	0.32381 (9)	0.0196 (3)
C9	0.26034 (13)	0.46235 (10)	0.25628 (9)	0.0193 (3)
C10	0.04738 (13)	0.41788 (10)	0.12501 (9)	0.0212 (3)
C11	−0.03388 (14)	0.32910 (11)	0.06167 (10)	0.0258 (3)
H11A	−0.1205	0.3127	0.0796	0.039*
H11B	0.0264	0.2647	0.0703	0.039*

H11C	−0.0607	0.3520	−0.0062	0.039*
C12	0.46470 (13)	0.33801 (10)	0.33990 (9)	0.0197 (3)
O5	0.29513 (11)	−0.00815 (8)	−0.01083 (8)	0.0294 (2)
H5D	0.340 (2)	−0.0463 (17)	0.0455 (17)	0.051 (6)*
H5E	0.322 (2)	−0.0375 (18)	−0.0572 (17)	0.057 (6)*
O6	0.75030 (11)	0.11930 (8)	0.45538 (8)	0.0289 (2)
H6B	0.790 (2)	0.0974 (16)	0.4142 (15)	0.042 (5)*
H6C	0.667 (2)	0.0781 (16)	0.4413 (14)	0.047 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0272 (5)	0.0164 (4)	0.0306 (5)	0.0028 (4)	−0.0038 (4)	−0.0002 (4)
O2	0.0243 (5)	0.0243 (5)	0.0283 (5)	−0.0054 (4)	−0.0005 (4)	−0.0008 (4)
N1	0.0216 (5)	0.0179 (5)	0.0291 (6)	0.0007 (4)	0.0010 (5)	0.0015 (4)
N2	0.0195 (5)	0.0167 (5)	0.0249 (6)	−0.0016 (4)	0.0008 (5)	0.0001 (4)
N3	0.0197 (5)	0.0179 (5)	0.0231 (5)	−0.0001 (4)	0.0003 (4)	0.0001 (4)
N4	0.0222 (6)	0.0166 (5)	0.0304 (6)	−0.0009 (4)	−0.0024 (5)	−0.0015 (5)
C1	0.0199 (6)	0.0180 (6)	0.0251 (6)	0.0003 (5)	0.0022 (5)	0.0007 (5)
C2	0.0183 (6)	0.0178 (6)	0.0203 (6)	−0.0004 (4)	0.0029 (5)	0.0004 (5)
C3	0.0203 (6)	0.0171 (6)	0.0186 (6)	−0.0009 (4)	0.0043 (5)	0.0001 (5)
C4	0.0184 (6)	0.0256 (6)	0.0193 (6)	−0.0018 (5)	0.0034 (5)	0.0009 (5)
C5	0.0210 (6)	0.0288 (7)	0.0297 (7)	0.0022 (5)	0.0004 (5)	0.0023 (6)
C6	0.0216 (6)	0.0169 (6)	0.0192 (6)	0.0001 (5)	0.0022 (5)	−0.0001 (5)
O3	0.0228 (5)	0.0164 (4)	0.0361 (5)	−0.0024 (3)	−0.0012 (4)	−0.0038 (4)
O4	0.0237 (5)	0.0220 (5)	0.0320 (5)	0.0042 (4)	−0.0012 (4)	0.0015 (4)
N5	0.0239 (5)	0.0179 (5)	0.0292 (6)	−0.0014 (4)	−0.0009 (5)	−0.0032 (4)
N6	0.0207 (5)	0.0161 (5)	0.0269 (6)	0.0015 (4)	−0.0004 (5)	−0.0005 (4)
N7	0.0189 (5)	0.0165 (5)	0.0231 (5)	0.0006 (4)	0.0011 (4)	−0.0002 (4)
N8	0.0200 (5)	0.0172 (5)	0.0289 (6)	0.0007 (4)	−0.0003 (5)	−0.0009 (5)
C7	0.0209 (6)	0.0188 (6)	0.0252 (6)	−0.0012 (5)	0.0011 (5)	−0.0010 (5)
C8	0.0181 (6)	0.0166 (6)	0.0218 (6)	−0.0003 (4)	0.0026 (5)	0.0004 (5)
C9	0.0188 (6)	0.0164 (6)	0.0215 (6)	−0.0004 (4)	0.0041 (5)	0.0006 (5)
C10	0.0184 (6)	0.0219 (6)	0.0216 (6)	0.0000 (5)	0.0034 (5)	0.0025 (5)
C11	0.0241 (6)	0.0232 (6)	0.0256 (7)	−0.0025 (5)	0.0006 (5)	0.0015 (5)
C12	0.0191 (6)	0.0169 (6)	0.0216 (6)	−0.0013 (4)	0.0037 (5)	0.0008 (5)
O5	0.0303 (5)	0.0244 (5)	0.0280 (5)	0.0074 (4)	0.0005 (4)	0.0002 (4)
O6	0.0222 (5)	0.0249 (5)	0.0358 (6)	−0.0022 (4)	0.0030 (4)	−0.0093 (4)

Geometric parameters (Å, º)

O1—C6	1.2500 (15)	N5—C7	1.3218 (17)
O2—C4	1.2284 (16)	N5—N6	1.3668 (15)
N1—C1	1.3252 (17)	N6—C9	1.3420 (16)
N1—N2	1.3677 (15)	N6—H6A	0.89 (2)
N2—C3	1.3389 (16)	N7—C10	1.3606 (17)
N2—H2A	0.90 (2)	N7—C9	1.3878 (16)
N3—C4	1.3652 (17)	N7—H7A	0.887 (18)

N3—C3	1.3863 (16)	N8—C12	1.3373 (17)
N3—H3A	0.883 (19)	N8—H8A	0.914 (19)
N4—C6	1.3301 (17)	N8—H8B	0.907 (18)
N4—H4A	0.897 (19)	C7—C8	1.4094 (17)
N4—H4B	0.90 (2)	C7—H7	0.9500
C1—C2	1.4069 (17)	C8—C9	1.3950 (18)
C1—H1	0.9500	C8—C12	1.4612 (17)
C2—C3	1.3952 (17)	C10—C11	1.5005 (18)
C2—C6	1.4635 (17)	C11—H11A	0.9800
C4—C5	1.4989 (18)	C11—H11B	0.9800
C5—H5A	0.9800	C11—H11C	0.9800
C5—H5B	0.9800	O5—H5D	0.93 (2)
C5—H5C	0.9800	O5—H5E	0.87 (2)
O3—C12	1.2429 (15)	O6—H6B	0.85 (2)
O4—C10	1.2307 (16)	O6—H6C	0.93 (2)

C1—N1—N2	104.71 (10)	C9—N6—N5	112.09 (11)
C3—N2—N1	112.09 (11)	C9—N6—H6A	126.8 (13)
C3—N2—H2A	125.0 (13)	N5—N6—H6A	121.1 (13)
N1—N2—H2A	122.8 (13)	C10—N7—C9	123.96 (11)
C4—N3—C3	123.98 (11)	C10—N7—H7A	120.2 (12)
C4—N3—H3A	118.6 (12)	C9—N7—H7A	115.8 (12)
C3—N3—H3A	117.4 (12)	C12—N8—H8A	117.2 (12)
C6—N4—H4A	119.2 (12)	C12—N8—H8B	121.5 (11)
C6—N4—H4B	121.0 (12)	H8A—N8—H8B	121.1 (16)
H4A—N4—H4B	119.8 (16)	N5—C7—C8	112.11 (11)
N1—C1—C2	112.02 (11)	N5—C7—H7	123.9
N1—C1—H1	124.0	C8—C7—H7	123.9
C2—C1—H1	124.0	C9—C8—C7	103.94 (11)
C3—C2—C1	104.02 (11)	C9—C8—C12	124.67 (11)
C3—C2—C6	124.82 (11)	C7—C8—C12	131.39 (12)
C1—C2—C6	131.16 (12)	N6—C9—N7	124.94 (11)
N2—C3—N3	124.53 (11)	N6—C9—C8	107.06 (11)
N2—C3—C2	107.15 (11)	N7—C9—C8	127.99 (11)
N3—C3—C2	128.32 (11)	O4—C10—N7	121.03 (12)
O2—C4—N3	120.83 (12)	O4—C10—C11	122.25 (12)
O2—C4—C5	122.63 (12)	N7—C10—C11	116.72 (11)
N3—C4—C5	116.54 (11)	C10—C11—H11A	109.5
C4—C5—H5A	109.5	C10—C11—H11B	109.5
C4—C5—H5B	109.5	H11A—C11—H11B	109.5
H5A—C5—H5B	109.5	C10—C11—H11C	109.5
C4—C5—H5C	109.5	H11A—C11—H11C	109.5
H5A—C5—H5C	109.5	H11B—C11—H11C	109.5
H5B—C5—H5C	109.5	O3—C12—N8	122.18 (12)
O1—C6—N4	122.48 (12)	O3—C12—C8	119.84 (11)
O1—C6—C2	119.30 (11)	N8—C12—C8	117.98 (11)
N4—C6—C2	118.18 (11)	H5D—O5—H5E	106.9 (19)
C7—N5—N6	104.79 (10)	H6B—O6—H6C	102.9 (17)

C1—N1—N2—C3	−0.37 (14)	C7—N5—N6—C9	−0.37 (15)
N2—N1—C1—C2	0.03 (15)	N6—N5—C7—C8	−0.04 (15)
N1—C1—C2—C3	0.29 (15)	N5—C7—C8—C9	0.41 (15)
N1—C1—C2—C6	−179.28 (13)	N5—C7—C8—C12	−179.72 (13)
N1—N2—C3—N3	−179.73 (11)	N5—N6—C9—N7	−178.19 (12)
N1—N2—C3—C2	0.56 (15)	N5—N6—C9—C8	0.63 (15)
C4—N3—C3—N2	−0.6 (2)	C10—N7—C9—N6	1.4 (2)
C4—N3—C3—C2	179.02 (12)	C10—N7—C9—C8	−177.21 (13)
C1—C2—C3—N2	−0.50 (14)	C7—C8—C9—N6	−0.60 (14)
C6—C2—C3—N2	179.11 (12)	C12—C8—C9—N6	179.51 (12)
C1—C2—C3—N3	179.81 (12)	C7—C8—C9—N7	178.17 (12)
C6—C2—C3—N3	−0.6 (2)	C12—C8—C9—N7	−1.7 (2)
C3—N3—C4—O2	0.5 (2)	C9—N7—C10—O4	0.81 (19)
C3—N3—C4—C5	−178.89 (12)	C9—N7—C10—C11	−178.96 (12)
C3—C2—C6—O1	−1.9 (2)	C9—C8—C12—O3	−5.3 (2)
C1—C2—C6—O1	177.57 (13)	C7—C8—C12—O3	174.86 (13)
C3—C2—C6—N4	−179.75 (12)	C9—C8—C12—N8	174.62 (12)
C1—C2—C6—N4	−0.3 (2)	C7—C8—C12—N8	−5.2 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O1^{i}	0.90 (2)	2.07 (2)	2.7514 (14)	131.9 (17)
N2—H2*A*···O2	0.90 (2)	2.09 (2)	2.6441 (14)	118.6 (16)
N3—H3*A*···O1	0.883 (19)	2.226 (18)	2.8307 (14)	125.4 (15)
N4—H4*A*···O5	0.897 (19)	2.10 (2)	2.9919 (15)	173.9 (17)
N4—H4*B*···O6^{ii}	0.90 (2)	2.12 (2)	2.9893 (15)	163.2 (17)
C1—H1···O6^{ii}	0.95	2.51	3.3791 (16)	153
N6—H6*A*···O3^{iii}	0.89 (2)	2.01 (2)	2.7112 (14)	135.8 (18)
N6—H6*A*···O4	0.89 (2)	2.14 (2)	2.6558 (15)	116.4 (16)
N7—H7*A*···O3	0.887 (18)	2.204 (18)	2.8325 (14)	127.4 (15)
N8—H8*A*···O6	0.914 (19)	2.13 (2)	3.0338 (15)	169.7 (17)
N8—H8*B*···O5^{iv}	0.907 (18)	2.052 (19)	2.9354 (15)	164.5 (16)
C7—H7···O5^{iv}	0.95	2.63	3.4683 (17)	147
C11—H11*B*···N5^{v}	0.98	2.44	3.3337 (17)	152
O5—H5*D*···O2^{vi}	0.93 (2)	1.87 (2)	2.7658 (14)	161.1 (19)
O5—H5*E*···O1^{vii}	0.87 (2)	1.97 (2)	2.8269 (15)	168 (2)
O6—H6*B*···N1^{vi}	0.85 (2)	2.13 (2)	2.9448 (16)	162.5 (18)
O6—H6*C*···O4^{v}	0.93 (2)	1.83 (2)	2.7406 (14)	165.0 (18)

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