Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

OPEN ACCESS

ISSN 2056-9890

Crystal structure of 1-(5-amino-2*H*-tetrazol-2-yl)-2-methylpropan-2-ol

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Received 5 December 2015; accepted 10 December 2015

Edited by H. Stoeckli-Evans, University of Neuchâtel, Switzerland

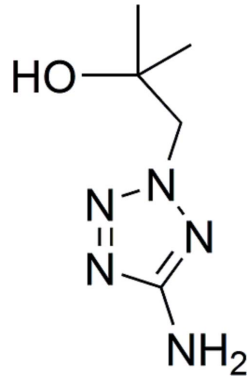
The title compound, $C_5H_{11}N_5O$, crystallized with two independent molecules in the asymmetric unit. The two molecules differ in the orientation of the 2-methylpropan-2-ol unit, with the hydroxy H atoms pointing in opposite directions. In the crystal, molecules are linked *via* O—H···O and N—H···O hydrogen bonds, forming ribbons propagating along [10$\bar{1}$]. The ribbons are linked *via* N—H···N hydrogen bonds, forming a three-dimensional structure.

Keywords: crystal structure; 5-aminotetrazole; 2-methylpropan-2-ol; hydrogen bonding.

CCDC reference: 1441577

1. Related literature

For the crystal structure of 5-aminotetrazole monohydrate, see: Britts & Karle (1967); and for that of 5-aminotetrazole, see: Fujihisa *et al.* (2011). For the crystal structures of alkali salts of 5-aminotetrazole, see: Ernst *et al.* (2007). For the crystal structure of 5-azido-1*H*-tetrazole, a highly explosive compound, see: Stierstorfer *et al.* (2008). For some examples of the use of 5-aminotetrazole in the synthesis of metal–organic frameworks, see: Karaghiosoff *et al.* (2009); Liu *et al.* (2013).



2. Experimental

2.1. Crystal data

$C_5H_{11}N_5O$
M_r = 157.19
Triclinic, $P\bar{1}$
a = 8.2472 (19) Å
b = 9.731 (2) Å
c = 10.087 (2) Å
α = 90.30 (1)°
β = 96.228 (10)°
γ = 96.259 (10)°
V = 799.8 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 296 K
0.12 × 0.10 × 0.08 mm

2.2. Data collection

Bruker SMART 1K CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2006)
T_{min} = 0.90, T_{max} = 0.95
11190 measured reflections
2953 independent reflections
2148 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.122
S = 1.06
2953 reflections
227 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*O*···O2^{i}	0.91 (3)	2.04 (3)	2.946 (2)	171 (2)
N1—H1*A*···O2^{ii}	0.92 (2)	2.53 (2)	3.243 (2)	135 (2)
N1—H1*A*···N9^{ii}	0.92 (2)	2.58 (2)	3.287 (3)	134 (2)
N1—H1*B*···N10^{iii}	0.84 (2)	2.24 (2)	3.082 (2)	173 (2)
O2—H2*O*···N2^{ii}	0.82 (3)	2.14 (3)	2.930 (2)	162 (3)
N6—H6*A*···O1^{iv}	0.93 (2)	2.22 (2)	3.114 (3)	161 (2)
N6—H6*B*···N5^{v}	0.82 (2)	2.41 (2)	3.213 (2)	167 (2)

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

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *Mercury* (Macrae *et al.*, 2008) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL2014* and *PLATON*.

Acknowledgements

This work was supported by a Chonnam National University research grant in 2014.

Supporting information for this paper is available from the IUCr electronic archives (Reference: SU5257).

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supporting information

Acta Cryst. (2015). E**71**, o1057–o1058 [https://doi.org/10.1107/S2056989015023713]

Crystal structure of 1-(5-amino-2*H*-tetrazol-2-yl)-2-methylpropan-2-ol

Hyun Sik Park, Ji Yeon Ryu and Junseong Lee

S1. Comments

Tetrazole compounds are useful building blocks for the construction of high dimensional metal-organic frameworks, and they have provided various binding modes toward metal centers (Karaghiosoff *et al.*, 2009; Liu *et al.*, 2013). The title compound was easily prepared by the reaction of 5-aminotetrazole and *iso*-butylene oxide, and introduces an hydroxyl group which we hope will be useful as an additional coordination center.

The title compound, Fig. 1, crystallized with two independent molecules(A and B) in the asymmetric unit. The two molecules differ in the orientation of the 2-methylpropan-2-ol unit, with the hydroxyl H atoms pointing in opposite directions (Fig. 2).

In the crystal, molecules are linked *via* O—H···O and N—H···O hydrogen bonds (Table 1) forming ribbons propagating along direction [10$\bar{1}$]. The ribbons are linked via N—H···N hydrogen bonds forming a three-dimensional structure (Table 1 and Fig. 3).

S2. Synthesis and crystallization

The title compound was synthesized by heating 5-aminotetrazole with an excess amount of *iso*-butylene oxide, without solvent, at 333 K. Crystals were obtained on cooling the reaction mixture.

S3. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The OH and NH_2 H atoms were located in difference Fourier maps and freely refined. The C-bound H atoms were positioned geometrically and refined using a riding model: C—H = 0.96-0.97 Å with U_{iso}(H) = 1.5U_{eq}(C-methyl) and 1.2U_{eq}(C) for other H atoms.

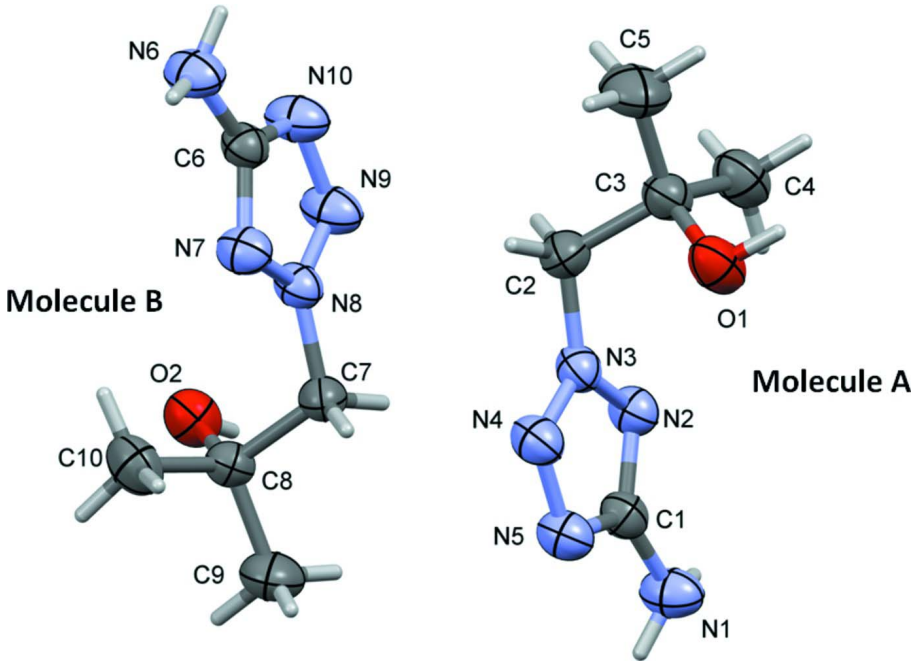

Figure 1

The molecular structure of the two independent molecules (A and B) of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

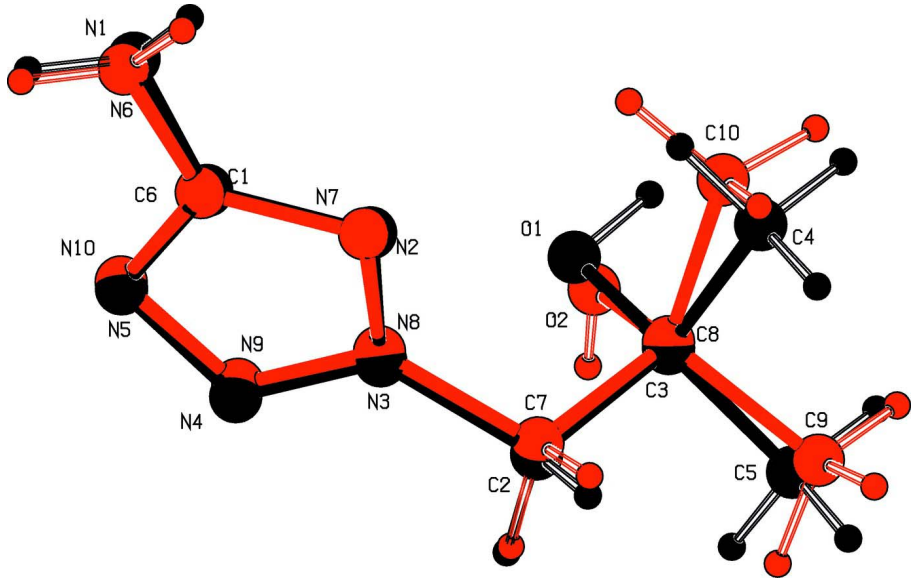

Figure 2

A view of the molecular overlap of molecules A (black) and B (red); calculated using the AutoMolfit routine in PLATON (Spek, 2009).

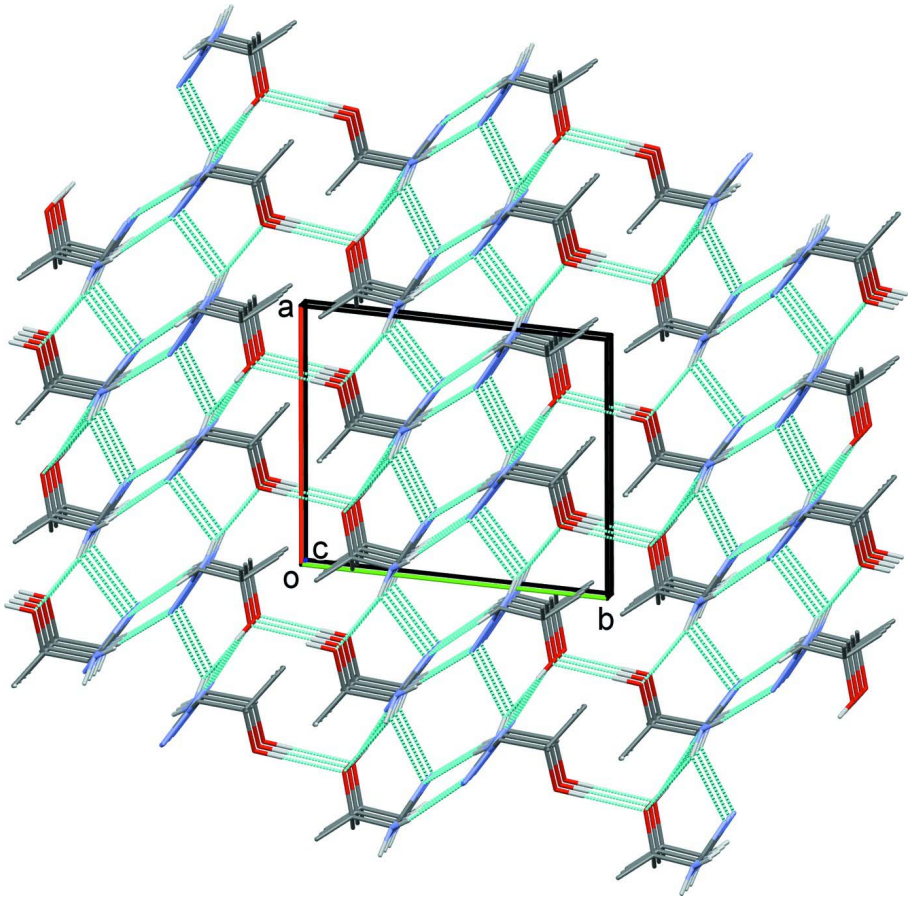

Figure 3

A view along the *c* axis of the crystal packing of the title compound. The hydrogen bonds are shown as dashed lines (see Table 1). H atoms not involved in hydrogen bonding have been omitted for clarity.

1-(5-Amino-2*H*-tetrazol-2-yl)-2-methylpropan-2-ol

Crystal data

$C_5H_{11}N_5O$
$M_r = 157.19$
Triclinic, $P\overline{1}$
$a = 8.2472$ (19) Å
$b = 9.731$ (2) Å
$c = 10.087$ (2) Å
$\alpha = 90.30$ (1)°
$\beta = 96.228$ (10)°
$\gamma = 96.259$ (10)°
$V = 799.8$ (3) Å^3
$Z = 4$
$F(000) = 336$
$D_x = 1.305$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4382 reflections
$\theta = 2.0$–29.9°
$\mu = 0.10$ mm^{-1}
$T = 296$ K
Block, colourless
0.12 × 0.10 × 0.08 mm

Data collection

Bruker SMART 1K CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
profile data from ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2006)
$T_{min} = 0.90$, $T_{max} = 0.95$
11190 measured reflections
2953 independent reflections

2148 reflections with $I > 2\sigma(I)$
$R_{int} = 0.047$
$\theta_{max} = 25.5°$, $\theta_{min} = 2.5°$

$h = -9 \rightarrow 9$
$k = -11 \rightarrow 11$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.122$
$S = 1.06$
2953 reflections
227 parameters
0 restraints

Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0588P)^2 + 0.018P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.28249 (16)	0.86314 (15)	0.81161 (14)	0.0536 (4)
H1O	0.270 (3)	0.952 (3)	0.789 (3)	0.101 (9)*
N1	0.4219 (2)	0.6570 (2)	1.28100 (17)	0.0530 (5)
H1A	0.527 (3)	0.690 (2)	1.315 (2)	0.063 (7)*
H1B	0.378 (2)	0.592 (2)	1.3251 (19)	0.048 (6)*
N2	0.48661 (17)	0.69286 (15)	1.05833 (15)	0.0405 (4)
N3	0.40258 (18)	0.64638 (14)	0.94250 (14)	0.0383 (4)
N4	0.26829 (19)	0.56520 (15)	0.95690 (15)	0.0463 (4)
N5	0.25930 (18)	0.55592 (16)	1.08764 (15)	0.0458 (4)
C1	0.3924 (2)	0.63485 (18)	1.14668 (18)	0.0376 (4)
C2	0.4501 (2)	0.68157 (18)	0.80986 (18)	0.0456 (5)
H2A	0.3810	0.6223	0.7440	0.055*
H2B	0.5624	0.6622	0.8062	0.055*
C3	0.4370 (2)	0.83230 (18)	0.77215 (18)	0.0432 (5)
C4	0.5765 (2)	0.9290 (2)	0.8434 (2)	0.0572 (6)
H4A	0.5651	1.0223	0.8165	0.086*
H4B	0.6794	0.9034	0.8208	0.086*
H4C	0.5732	0.9226	0.9380	0.086*
C5	0.4359 (3)	0.8413 (2)	0.6213 (2)	0.0730 (7)
H5A	0.3447	0.7815	0.5786	0.110*
H5B	0.5363	0.8133	0.5957	0.110*
H5C	0.4260	0.9348	0.5945	0.110*
O2	0.24050 (17)	0.15721 (15)	0.77069 (15)	0.0509 (4)
H2O	0.301 (4)	0.198 (3)	0.831 (3)	0.131 (13)*
N6	0.0533 (3)	0.3192 (2)	0.24056 (16)	0.0523 (5)
H6A	−0.054 (3)	0.283 (2)	0.214 (2)	0.065 (7)*
H6B	0.093 (2)	0.377 (2)	0.191 (2)	0.057 (7)*

N7	0.00343 (18)	0.29922 (16)	0.46818 (14)	0.0436 (4)
N8	0.09725 (18)	0.34753 (14)	0.57877 (14)	0.0382 (4)
N9	0.23381 (19)	0.42091 (16)	0.55631 (15)	0.0505 (4)
N10	0.23478 (19)	0.42088 (17)	0.42439 (15)	0.0516 (5)
C6	0.0940 (2)	0.34662 (18)	0.37369 (17)	0.0377 (4)
C7	0.0495 (2)	0.32626 (18)	0.71339 (17)	0.0416 (5)
H7A	−0.0649	0.3416	0.7126	0.050*
H7B	0.1138	0.3952	0.7729	0.050*
C8	0.0714 (2)	0.18313 (18)	0.76967 (17)	0.0386 (4)
C9	0.0260 (3)	0.1839 (2)	0.9121 (2)	0.0652 (7)
H9A	0.0504	0.0992	0.9542	0.098*
H9B	−0.0891	0.1923	0.9108	0.098*
H9C	0.0881	0.2607	0.9610	0.098*
C10	−0.0294 (3)	0.0686 (2)	0.6850 (2)	0.0573 (6)
H10A	0.0133	0.0630	0.6005	0.086*
H10B	−0.1416	0.0880	0.6710	0.086*
H10C	−0.0237	−0.0178	0.7298	0.086*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0434 (8)	0.0474 (9)	0.0716 (10)	0.0081 (7)	0.0097 (7)	0.0127 (7)
N1	0.0503 (12)	0.0632 (12)	0.0421 (11)	−0.0055 (10)	0.0018 (9)	0.0068 (9)
N2	0.0397 (9)	0.0411 (9)	0.0389 (9)	0.0004 (7)	0.0010 (7)	0.0029 (7)
N3	0.0432 (9)	0.0329 (8)	0.0379 (9)	0.0030 (7)	0.0023 (7)	0.0032 (7)
N4	0.0500 (10)	0.0425 (9)	0.0436 (10)	−0.0031 (8)	0.0008 (7)	0.0055 (7)
N5	0.0436 (10)	0.0482 (10)	0.0436 (10)	−0.0011 (8)	0.0021 (7)	0.0076 (7)
C1	0.0356 (10)	0.0374 (10)	0.0395 (11)	0.0052 (8)	0.0015 (8)	0.0049 (8)
C2	0.0558 (12)	0.0436 (11)	0.0389 (11)	0.0073 (9)	0.0095 (9)	0.0002 (9)
C3	0.0446 (11)	0.0401 (11)	0.0454 (11)	0.0035 (9)	0.0083 (9)	0.0069 (9)
C4	0.0513 (13)	0.0492 (13)	0.0705 (15)	−0.0013 (10)	0.0098 (11)	0.0077 (11)
C5	0.0948 (19)	0.0761 (17)	0.0485 (13)	0.0069 (14)	0.0111 (13)	0.0190 (12)
O2	0.0433 (8)	0.0501 (9)	0.0586 (10)	0.0054 (7)	0.0015 (7)	0.0067 (7)
N6	0.0598 (12)	0.0577 (12)	0.0362 (10)	−0.0039 (10)	0.0007 (9)	0.0061 (8)
N7	0.0432 (9)	0.0492 (10)	0.0355 (9)	−0.0032 (7)	−0.0013 (7)	0.0030 (7)
N8	0.0410 (9)	0.0374 (9)	0.0347 (9)	0.0003 (7)	0.0010 (7)	0.0052 (7)
N9	0.0506 (10)	0.0563 (11)	0.0403 (10)	−0.0081 (8)	−0.0015 (8)	0.0093 (8)
N10	0.0489 (10)	0.0637 (11)	0.0390 (9)	−0.0062 (8)	0.0027 (8)	0.0102 (8)
C6	0.0413 (11)	0.0361 (10)	0.0357 (10)	0.0051 (8)	0.0030 (8)	0.0059 (8)
C7	0.0529 (12)	0.0379 (11)	0.0348 (10)	0.0059 (9)	0.0078 (9)	0.0018 (8)
C8	0.0396 (11)	0.0383 (11)	0.0380 (10)	0.0031 (8)	0.0056 (8)	0.0049 (8)
C9	0.0835 (17)	0.0633 (15)	0.0513 (13)	0.0076 (12)	0.0191 (12)	0.0159 (11)
C10	0.0582 (14)	0.0447 (12)	0.0648 (14)	−0.0055 (10)	−0.0005 (11)	0.0037 (10)

Geometric parameters (Å, º)

O1—C3	1.437 (2)	O2—C8	1.443 (2)
O1—H1O	0.91 (3)	O2—H2O	0.82 (3)

N1—C1	1.362 (2)	N6—C6	1.366 (2)
N1—H1A	0.92 (2)	N6—H6A	0.93 (2)
N1—H1B	0.844 (19)	N6—H6B	0.82 (2)
N2—C1	1.333 (2)	N7—C6	1.328 (2)
N2—N3	1.342 (2)	N7—N8	1.339 (2)
N3—N4	1.310 (2)	N8—N9	1.308 (2)
N3—C2	1.466 (2)	N8—C7	1.464 (2)
N4—N5	1.332 (2)	N9—N10	1.332 (2)
N5—C1	1.349 (2)	N10—C6	1.347 (2)
C2—C3	1.529 (3)	C7—C8	1.528 (2)
C2—H2A	0.9700	C7—H7A	0.9700
C2—H2B	0.9700	C7—H7B	0.9700
C3—C4	1.518 (3)	C8—C10	1.515 (3)
C3—C5	1.524 (3)	C8—C9	1.524 (2)
C4—H4A	0.9600	C9—H9A	0.9600
C4—H4B	0.9600	C9—H9B	0.9600
C4—H4C	0.9600	C9—H9C	0.9600
C5—H5A	0.9600	C10—H10A	0.9600
C5—H5B	0.9600	C10—H10B	0.9600
C5—H5C	0.9600	C10—H10C	0.9600

C3—O1—H1O	107.4 (15)	C8—O2—H2O	113 (2)
C1—N1—H1A	117.3 (13)	C6—N6—H6A	116.9 (13)
C1—N1—H1B	113.0 (14)	C6—N6—H6B	114.9 (15)
H1A—N1—H1B	114.2 (18)	H6A—N6—H6B	115.5 (19)
C1—N2—N3	101.66 (14)	C6—N7—N8	101.56 (14)
N4—N3—N2	113.70 (14)	N9—N8—N7	114.12 (14)
N4—N3—C2	121.24 (15)	N9—N8—C7	122.32 (15)
N2—N3—C2	125.06 (14)	N7—N8—C7	123.51 (14)
N3—N4—N5	106.41 (14)	N8—N9—N10	105.90 (15)
N4—N5—C1	105.97 (13)	N9—N10—C6	106.18 (14)
N2—C1—N5	112.25 (16)	N7—C6—N10	112.23 (16)
N2—C1—N1	124.33 (17)	N7—C6—N6	124.23 (18)
N5—C1—N1	123.35 (16)	N10—C6—N6	123.49 (16)
N3—C2—C3	114.27 (14)	N8—C7—C8	114.86 (14)
N3—C2—H2A	108.7	N8—C7—H7A	108.6
C3—C2—H2A	108.7	C8—C7—H7A	108.6
N3—C2—H2B	108.7	N8—C7—H7B	108.6
C3—C2—H2B	108.7	C8—C7—H7B	108.6
H2A—C2—H2B	107.6	H7A—C7—H7B	107.5
O1—C3—C4	110.33 (16)	O2—C8—C10	106.22 (15)
O1—C3—C5	110.39 (16)	O2—C8—C9	109.55 (15)
C4—C3—C5	111.14 (16)	C10—C8—C9	112.03 (15)
O1—C3—C2	105.38 (14)	O2—C8—C7	109.61 (13)
C4—C3—C2	111.81 (16)	C10—C8—C7	112.28 (15)
C5—C3—C2	107.60 (16)	C9—C8—C7	107.14 (15)
C3—C4—H4A	109.5	C8—C9—H9A	109.5
C3—C4—H4B	109.5	C8—C9—H9B	109.5

H4A—C4—H4B	109.5	H9A—C9—H9B	109.5
C3—C4—H4C	109.5	C8—C9—H9C	109.5
H4A—C4—H4C	109.5	H9A—C9—H9C	109.5
H4B—C4—H4C	109.5	H9B—C9—H9C	109.5
C3—C5—H5A	109.5	C8—C10—H10A	109.5
C3—C5—H5B	109.5	C8—C10—H10B	109.5
H5A—C5—H5B	109.5	H10A—C10—H10B	109.5
C3—C5—H5C	109.5	C8—C10—H10C	109.5
H5A—C5—H5C	109.5	H10A—C10—H10C	109.5
H5B—C5—H5C	109.5	H10B—C10—H10C	109.5
C1—N2—N3—N4	−0.60 (19)	C6—N7—N8—N9	1.0 (2)
C1—N2—N3—C2	178.59 (15)	C6—N7—N8—C7	178.36 (15)
N2—N3—N4—N5	0.2 (2)	N7—N8—N9—N10	−1.1 (2)
C2—N3—N4—N5	−178.98 (14)	C7—N8—N9—N10	−178.47 (14)
N3—N4—N5—C1	0.23 (19)	N8—N9—N10—C6	0.6 (2)
N3—N2—C1—N5	0.74 (19)	N8—N7—C6—N10	−0.5 (2)
N3—N2—C1—N1	−176.40 (17)	N8—N7—C6—N6	177.00 (17)
N4—N5—C1—N2	−0.6 (2)	N9—N10—C6—N7	−0.1 (2)
N4—N5—C1—N1	176.53 (17)	N9—N10—C6—N6	−177.61 (17)
N4—N3—C2—C3	110.47 (19)	N9—N8—C7—C8	−104.44 (19)
N2—N3—C2—C3	−68.7 (2)	N7—N8—C7—C8	78.4 (2)
N3—C2—C3—O1	−44.3 (2)	N8—C7—C8—O2	57.7 (2)
N3—C2—C3—C4	75.5 (2)	N8—C7—C8—C10	−60.1 (2)
N3—C2—C3—C5	−162.14 (16)	N8—C7—C8—C9	176.52 (15)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···O2^{i}	0.91 (3)	2.04 (3)	2.946 (2)	171 (2)
N1—H1*A*···O2^{ii}	0.92 (2)	2.53 (2)	3.243 (2)	135 (2)
N1—H1*A*···N9^{ii}	0.92 (2)	2.58 (2)	3.287 (3)	134 (2)
N1—H1*B*···N10^{iii}	0.84 (2)	2.24 (2)	3.082 (2)	173 (2)
O2—H2*O*···N2^{ii}	0.82 (3)	2.14 (3)	2.930 (2)	162 (3)
N6—H6*A*···O1^{iv}	0.93 (2)	2.22 (2)	3.114 (3)	161 (2)
N6—H6*B*···N5^{v}	0.82 (2)	2.41 (2)	3.213 (2)	167 (2)

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