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# 2,3,9,10,15,16-Hexaazatetracyclo-[6.6.2.0$^{4,16}$.0$^{11,15}$]hexadecane dihydrate

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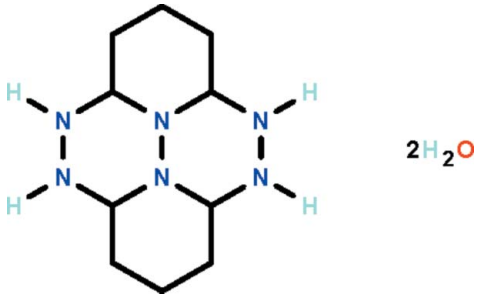
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.043; $wR$ factor = 0.116; data-to-parameter ratio = 14.9.

The four six-membered fused rings in the title compound, $C_{10}H_{20}N_6\cdot 2H_2O$, adopt chair conformations; the H atoms of the four secondary N atoms occupy axial positions. Hydrogen bonds of the types N—H···N, N—H···O and O—H···N link the organic and water molecules into a three-dimensional network.

## Related literature

For background to the reaction of glutaraldehyde and monosubstituted hydrazines, see: Katritzky & Fan (1990).



## Experimental

### Crystal data

$C_{10}H_{20}N_6\cdot 2H_2O$ $M_r$ = 260.35
Monoclinic, $P2_1/c$
$a$ = 9.5154 (10) Å
$b$ = 16.0667 (17) Å
$c$ = 9.1097 (10) Å
$\beta$ = 114.916 (1)°
$V$ = 1263.1 (2) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.10 mm$^{-1}$
$T$ = 100 K
0.20 × 0.20 × 0.05 mm

### Data collection

Bruker SMART APEX diffractometer
14226 measured reflections
2896 independent reflections
2138 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.048

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.116
$S$ = 1.02
2896 reflections
195 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.31 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.23 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1$W$—H11···N3$^{i}$ | 0.93 (3) | 1.99 (3) | 2.922 (2) | 174 (2) |
| O1$W$—H12···N5$^{ii}$ | 0.92 (3) | 2.05 (3) | 2.960 (2) | 178 (2) |
| O2$W$—H21···N2 | 0.88 (3) | 2.05 (3) | 2.925 (2) | 172 (2) |
| O2$W$—H22···N4$^{ii}$ | 0.86 (3) | 2.02 (3) | 2.863 (2) | 167 (2) |
| N1—H1···O1$W$ | 0.88 (2) | 2.08 (2) | 2.964 (2) | 175 (2) |
| N2—H2···O2$W^{iii}$ | 0.91 (2) | 2.18 (2) | 3.071 (2) | 166 (2) |
| N4—H4···N5$^{iv}$ | 0.87 (2) | 2.57 (2) | 3.354 (2) | 150.1 (15) |
| N5—H5···N1$^{iii}$ | 0.96 (2) | 2.25 (2) | 3.163 (2) | 159 (2) |

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5969).

## References

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Katritzky, A. R. & Fan, W.-Q. (1990). *J. Org. Chem.* **55**, 3205–3209.
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Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

# supporting information

*Acta Cryst.* (2012). E**68**, o2545 [https://doi.org/10.1107/S1600536812030735]

## 2,3,9,10,15,16-Hexaazatetracyclo[6.6.2.$0^{4,16}$.$0^{11,15}$]hexadecane dihydrate

**Fiona N.-F. How, Z. A. Rahima, Yee Seng Tan, S. Nadiah Abdul Halim and Seik Weng Ng**

### S1. Comment

Glutaraldehyde, CH═O($CH_2$)$_3$CH═O, condenses with mono-substituted hydrazines to yield *N*-substituted piperidines; for example, it reacts with phenylhydrazine to yield *N*-phenylpiperidin-1-amine (Katritzky & Fan, 1990). The direct reaction of the di-aldehyde with hydrazine itself does not lead to the formation of a polymeric Schiff-base product; the compound is, in fact, 2,3,9,10,15,16-hexaazatetracyclo[6,2,$0^{4,16}$.$0^{11,15}$]hexadecane, which crystallizes as a dihydrate (Scheme I). The four six-membered fused rings adopt chair conformations (Fig. 1). Hydrogen bonds of the type N–H···N, N–H···O and O–H···N link the organic and water molecules into a three dimensional network (Table 1).

There is no precedent for the fused-ring system in the crystallographic literature.

### S2. Experimental

Hydrazine hydrate (0.08 mol, 2.7 ml) was added to glutaraldehyde (0.08 g, 8.1 ml) to give a white solid. and stirred at room temperature to yield a white solid. This was recrystallized from ethanol; several drops of DMSO was added to aid crystallization.

### S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.99 to 1.00 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2 *U*(C).

The amino and water H-atoms were located in a difference Fourier map, and were freely refined.

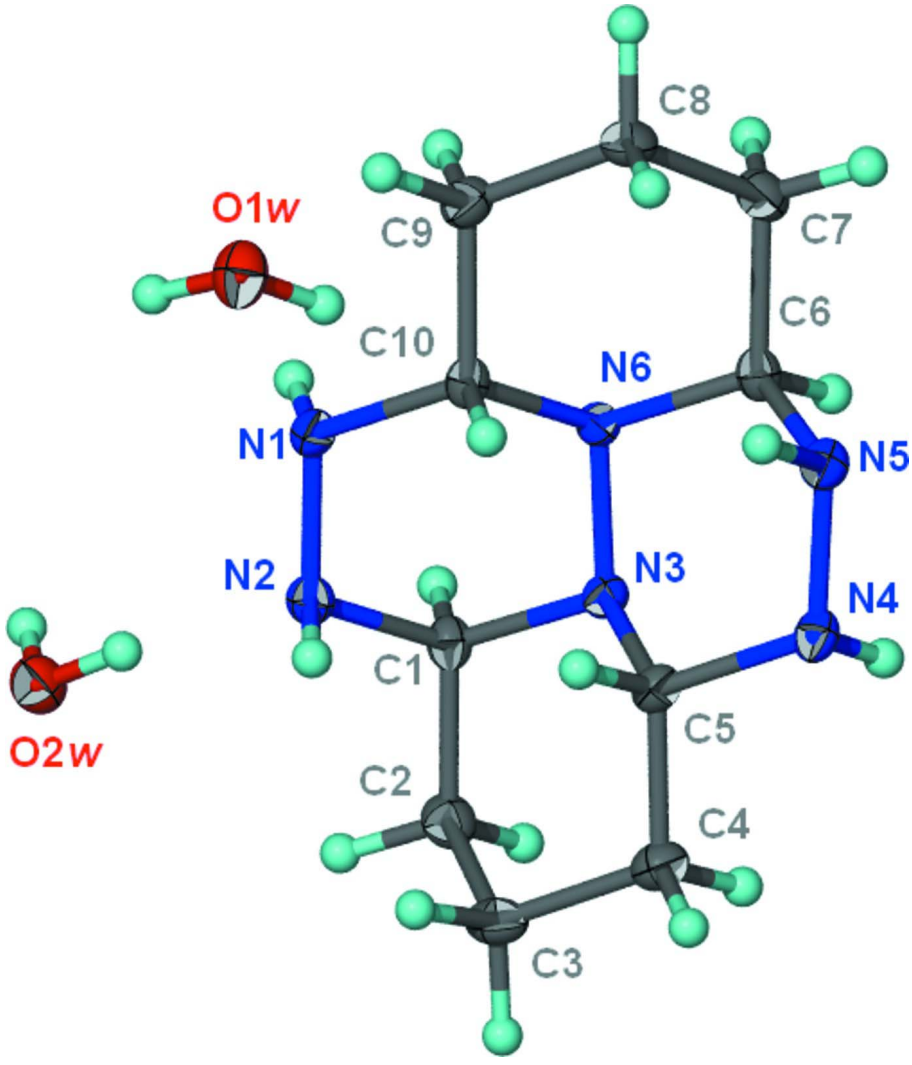


**Figure 1**

Anisotropic displacement ellipsoid plot (Barbour, 2001) of $C_{10}H_{20}N_6{\cdot}2H_2O$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

**2,3,9,10,15,16-Hexaazatetracyclo[6.6.2.0$^{4,16}$.0$^{11,15}$]hexadecane dihydrate**

*Crystal data*

$C_{10}H_{20}N_6{\cdot}2H_2O$
$M_r$ = 260.35
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a$ = 9.5154 (10) Å
$b$ = 16.0667 (17) Å
$c$ = 9.1097 (10) Å
$\beta$ = 114.916 (1)°
$V$ = 1263.1 (2) Å$^3$
$Z$ = 4
$F$(000) = 568
$D_x$ = 1.369 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 2285 reflections
$\theta$ = 2.3–30.0°
$\mu$ = 0.10 mm$^{-1}$
$T$ = 100 K
Prism, colorless
0.20 × 0.20 × 0.05 mm

*Data collection*

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
14226 measured reflections
2896 independent reflections
2138 reflections with $I > 2\sigma(I)$
$R_{int} = 0.048$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.5°$
$h = -12 \rightarrow 12$
$k = -20 \rightarrow 20$
$l = -11 \rightarrow 11$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.116$
$S = 1.02$
2896 reflections
195 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0493P)^2 + 0.6276P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.31$ e Å$^{-3}$
$\Delta\rho_{min} = -0.23$ e Å$^{-3}$

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1W | 0.34037 (14) | 0.59785 (8) | 0.67888 (15) | 0.0195 (3) |
| O2W | 0.75367 (14) | 0.67859 (7) | 0.93500 (16) | 0.0182 (3) |
| N1 | 0.47258 (15) | 0.70228 (8) | 0.49990 (16) | 0.0129 (3) |
| N2 | 0.63553 (16) | 0.68083 (8) | 0.58207 (16) | 0.0134 (3) |
| N3 | 0.60274 (15) | 0.57645 (8) | 0.36983 (15) | 0.0115 (3) |
| N4 | 0.61057 (16) | 0.59177 (9) | 0.11065 (16) | 0.0138 (3) |
| N5 | 0.44386 (15) | 0.60328 (8) | 0.03409 (16) | 0.0136 (3) |
| N6 | 0.43683 (15) | 0.59445 (8) | 0.30232 (15) | 0.0111 (3) |
| C1 | 0.66679 (19) | 0.59553 (9) | 0.54388 (18) | 0.0132 (3) |
| H1A | 0.6175 | 0.5564 | 0.5937 | 0.016* |
| C2 | 0.84013 (19) | 0.57828 (10) | 0.6218 (2) | 0.0170 (4) |
| H2A | 0.8576 | 0.5176 | 0.6203 | 0.020* |
| H2B | 0.8837 | 0.5965 | 0.7362 | 0.020* |
| C3 | 0.92503 (19) | 0.62308 (10) | 0.5346 (2) | 0.0177 (4) |
| H3A | 0.9182 | 0.6840 | 0.5462 | 0.021* |
| H3B | 1.0358 | 0.6071 | 0.5839 | 0.021* |
| C4 | 0.85215 (18) | 0.59957 (10) | 0.3555 (2) | 0.0166 (3) |
| H4A | 0.9039 | 0.6307 | 0.2984 | 0.020* |
| H4B | 0.8673 | 0.5394 | 0.3439 | 0.020* |
| C5 | 0.68021 (18) | 0.61943 (9) | 0.27960 (18) | 0.0128 (3) |
| H5A | 0.6657 | 0.6809 | 0.2837 | 0.015* |
| C6 | 0.36997 (18) | 0.56712 (10) | 0.13338 (19) | 0.0130 (3) |
| H6 | 0.3851 | 0.5055 | 0.1344 | 0.016* |
| C7 | 0.19610 (19) | 0.58261 (10) | 0.0546 (2) | 0.0168 (4) |
| H7A | 0.1451 | 0.5442 | 0.1021 | 0.020* |

| | | | | |
|---|---|---|---|---|
| H7B | 0.1556 | 0.5703 | −0.0626 | 0.020* |
| C8 | 0.15525 (19) | 0.67222 (10) | 0.0773 (2) | 0.0170 (4) |
| H8A | 0.1920 | 0.7104 | 0.0157 | 0.020* |
| H8B | 0.0414 | 0.6781 | 0.0353 | 0.020* |
| C9 | 0.23099 (19) | 0.69524 (10) | 0.25679 (19) | 0.0156 (3) |
| H9A | 0.2083 | 0.7542 | 0.2700 | 0.019* |
| H9B | 0.1867 | 0.6604 | 0.3165 | 0.019* |
| C10 | 0.40528 (18) | 0.68252 (9) | 0.32748 (18) | 0.0125 (3) |
| H10A | 0.4508 | 0.7199 | 0.2711 | 0.015* |
| H1 | 0.427 (2) | 0.6716 (12) | 0.548 (2) | 0.018 (5)* |
| H2 | 0.687 (2) | 0.7182 (13) | 0.547 (2) | 0.023 (5)* |
| H4 | 0.629 (2) | 0.5389 (14) | 0.108 (2) | 0.027 (5)* |
| H5 | 0.427 (2) | 0.6621 (13) | 0.024 (2) | 0.024 (5)* |
| H11 | 0.364 (3) | 0.5434 (17) | 0.661 (3) | 0.053 (7)* |
| H12 | 0.371 (3) | 0.5987 (15) | 0.789 (3) | 0.051 (7)* |
| H21 | 0.711 (3) | 0.6761 (14) | 0.829 (3) | 0.039 (7)* |
| H22 | 0.704 (3) | 0.6475 (15) | 0.974 (3) | 0.045 (7)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1W | 0.0256 (7) | 0.0162 (6) | 0.0178 (6) | 0.0021 (5) | 0.0100 (5) | 0.0008 (5) |
| O2W | 0.0192 (7) | 0.0204 (6) | 0.0158 (6) | −0.0034 (5) | 0.0083 (5) | −0.0005 (5) |
| N1 | 0.0130 (7) | 0.0144 (7) | 0.0120 (6) | 0.0006 (5) | 0.0060 (6) | −0.0009 (5) |
| N2 | 0.0135 (7) | 0.0115 (6) | 0.0147 (7) | −0.0002 (5) | 0.0054 (6) | −0.0009 (5) |
| N3 | 0.0114 (7) | 0.0122 (6) | 0.0118 (6) | 0.0001 (5) | 0.0057 (5) | 0.0003 (5) |
| N4 | 0.0162 (7) | 0.0121 (7) | 0.0137 (7) | 0.0023 (5) | 0.0070 (6) | −0.0006 (5) |
| N5 | 0.0149 (7) | 0.0134 (7) | 0.0128 (7) | 0.0014 (5) | 0.0060 (6) | 0.0006 (5) |
| N6 | 0.0106 (6) | 0.0101 (6) | 0.0117 (6) | 0.0007 (5) | 0.0040 (5) | −0.0005 (5) |
| C1 | 0.0166 (8) | 0.0111 (7) | 0.0119 (7) | −0.0001 (6) | 0.0060 (6) | −0.0002 (6) |
| C2 | 0.0162 (8) | 0.0156 (8) | 0.0163 (8) | 0.0016 (6) | 0.0041 (7) | −0.0002 (6) |
| C3 | 0.0121 (8) | 0.0171 (8) | 0.0220 (9) | 0.0017 (6) | 0.0055 (7) | 0.0011 (6) |
| C4 | 0.0142 (8) | 0.0171 (8) | 0.0199 (8) | 0.0012 (6) | 0.0084 (7) | 0.0005 (6) |
| C5 | 0.0137 (8) | 0.0121 (7) | 0.0145 (8) | 0.0007 (6) | 0.0076 (6) | 0.0004 (6) |
| C6 | 0.0159 (8) | 0.0112 (7) | 0.0122 (7) | −0.0010 (6) | 0.0061 (6) | −0.0006 (6) |
| C7 | 0.0147 (8) | 0.0191 (8) | 0.0147 (8) | −0.0030 (6) | 0.0044 (7) | −0.0020 (6) |
| C8 | 0.0120 (8) | 0.0194 (8) | 0.0177 (8) | 0.0020 (6) | 0.0043 (7) | −0.0005 (6) |
| C9 | 0.0153 (8) | 0.0161 (8) | 0.0160 (8) | 0.0023 (6) | 0.0073 (7) | 0.0003 (6) |
| C10 | 0.0149 (8) | 0.0108 (7) | 0.0127 (8) | 0.0005 (6) | 0.0066 (6) | −0.0003 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1W—H11 | 0.93 (3) | C2—H2A | 0.9900 |
| O1W—H12 | 0.92 (3) | C2—H2B | 0.9900 |
| O2W—H21 | 0.88 (3) | C3—C4 | 1.528 (2) |
| O2W—H22 | 0.86 (3) | C3—H3A | 0.9900 |
| N1—N2 | 1.4509 (19) | C3—H3B | 0.9900 |
| N1—C10 | 1.460 (2) | C4—C5 | 1.518 (2) |

| | | | |
|---|---|---|---|
| N1—H1 | 0.88 (2) | C4—H4A | 0.9900 |
| N2—C1 | 1.4748 (19) | C4—H4B | 0.9900 |
| N2—H2 | 0.91 (2) | C5—H5A | 1.0000 |
| N3—N6 | 1.4615 (17) | C6—C7 | 1.521 (2) |
| N3—C1 | 1.4715 (19) | C6—H6 | 1.0000 |
| N3—C5 | 1.4853 (19) | C7—C8 | 1.528 (2) |
| N4—N5 | 1.4508 (19) | C7—H7A | 0.9900 |
| N4—C5 | 1.465 (2) | C7—H7B | 0.9900 |
| N4—H4 | 0.87 (2) | C8—C9 | 1.528 (2) |
| N5—C6 | 1.479 (2) | C8—H8A | 0.9900 |
| N5—H5 | 0.96 (2) | C8—H8B | 0.9900 |
| N6—C6 | 1.4633 (19) | C9—C10 | 1.519 (2) |
| N6—C10 | 1.4843 (19) | C9—H9A | 0.9900 |
| C1—C2 | 1.521 (2) | C9—H9B | 0.9900 |
| C1—H1A | 1.0000 | C10—H10A | 1.0000 |
| C2—C3 | 1.530 (2) | | |

| | | | |
|---|---|---|---|
| H11—O1W—H12 | 103 (2) | C3—C4—H4A | 109.5 |
| H21—O2W—H22 | 110 (2) | C5—C4—H4B | 109.5 |
| N2—N1—C10 | 113.12 (12) | C3—C4—H4B | 109.5 |
| N2—N1—H1 | 104.6 (12) | H4A—C4—H4B | 108.1 |
| C10—N1—H1 | 109.1 (13) | N4—C5—N3 | 109.28 (12) |
| N1—N2—C1 | 112.14 (12) | N4—C5—C4 | 109.79 (13) |
| N1—N2—H2 | 106.1 (12) | N3—C5—C4 | 109.95 (13) |
| C1—N2—H2 | 109.9 (13) | N4—C5—H5A | 109.3 |
| N6—N3—C1 | 107.21 (11) | N3—C5—H5A | 109.3 |
| N6—N3—C5 | 112.03 (11) | C4—C5—H5A | 109.3 |
| C1—N3—C5 | 115.01 (12) | N6—C6—N5 | 114.67 (12) |
| N5—N4—C5 | 112.67 (12) | N6—C6—C7 | 110.60 (13) |
| N5—N4—H4 | 107.5 (13) | N5—C6—C7 | 110.49 (13) |
| C5—N4—H4 | 108.6 (13) | N6—C6—H6 | 106.9 |
| N4—N5—C6 | 111.18 (12) | N5—C6—H6 | 106.9 |
| N4—N5—H5 | 106.0 (12) | C7—C6—H6 | 106.9 |
| C6—N5—H5 | 110.3 (12) | C6—C7—C8 | 112.24 (13) |
| N3—N6—C6 | 107.29 (11) | C6—C7—H7A | 109.2 |
| N3—N6—C10 | 112.12 (11) | C8—C7—H7A | 109.2 |
| C6—N6—C10 | 114.95 (12) | C6—C7—H7B | 109.2 |
| N3—C1—N2 | 114.49 (12) | C8—C7—H7B | 109.2 |
| N3—C1—C2 | 109.88 (13) | H7A—C7—H7B | 107.9 |
| N2—C1—C2 | 110.24 (13) | C9—C8—C7 | 109.92 (13) |
| N3—C1—H1A | 107.3 | C9—C8—H8A | 109.7 |
| N2—C1—H1A | 107.3 | C7—C8—H8A | 109.7 |
| C2—C1—H1A | 107.3 | C9—C8—H8B | 109.7 |
| C1—C2—C3 | 112.22 (13) | C7—C8—H8B | 109.7 |
| C1—C2—H2A | 109.2 | H8A—C8—H8B | 108.2 |
| C3—C2—H2A | 109.2 | C10—C9—C8 | 111.07 (13) |
| C1—C2—H2B | 109.2 | C10—C9—H9A | 109.4 |
| C3—C2—H2B | 109.2 | C8—C9—H9A | 109.4 |

| | | | |
|---|---|---|---|
| H2A—C2—H2B | 107.9 | C10—C9—H9B | 109.4 |
| C4—C3—C2 | 109.67 (14) | C8—C9—H9B | 109.4 |
| C4—C3—H3A | 109.7 | H9A—C9—H9B | 108.0 |
| C2—C3—H3A | 109.7 | N1—C10—N6 | 110.36 (12) |
| C4—C3—H3B | 109.7 | N1—C10—C9 | 109.43 (13) |
| C2—C3—H3B | 109.7 | N6—C10—C9 | 108.58 (12) |
| H3A—C3—H3B | 108.2 | N1—C10—H10A | 109.5 |
| C5—C4—C3 | 110.60 (13) | N6—C10—H10A | 109.5 |
| C5—C4—H4A | 109.5 | C9—C10—H10A | 109.5 |

| | | | |
|---|---|---|---|
| C10—N1—N2—C1 | −48.61 (17) | C1—N3—C5—C4 | 56.60 (16) |
| C5—N4—N5—C6 | −50.99 (16) | C3—C4—C5—N4 | −176.52 (13) |
| C1—N3—N6—C6 | −174.01 (11) | C3—C4—C5—N3 | −56.27 (17) |
| C5—N3—N6—C6 | 58.93 (14) | N3—N6—C6—N5 | −55.08 (16) |
| C1—N3—N6—C10 | 58.87 (15) | C10—N6—C6—N5 | 70.36 (17) |
| C5—N3—N6—C10 | −68.19 (15) | N3—N6—C6—C7 | 179.18 (12) |
| N6—N3—C1—N2 | −55.16 (16) | C10—N6—C6—C7 | −55.38 (17) |
| C5—N3—C1—N2 | 70.13 (17) | N4—N5—C6—N6 | 52.05 (17) |
| N6—N3—C1—C2 | −179.84 (12) | N4—N5—C6—C7 | 177.85 (12) |
| C5—N3—C1—C2 | −54.55 (16) | N6—C6—C7—C8 | 51.81 (18) |
| N1—N2—C1—N3 | 51.03 (17) | N5—C6—C7—C8 | −76.24 (17) |
| N1—N2—C1—C2 | 175.52 (12) | C6—C7—C8—C9 | −53.06 (18) |
| N3—C1—C2—C3 | 53.32 (17) | C7—C8—C9—C10 | 56.33 (18) |
| N2—C1—C2—C3 | −73.78 (17) | N2—N1—C10—N6 | 52.49 (17) |
| C1—C2—C3—C4 | −55.36 (17) | N2—N1—C10—C9 | 171.91 (12) |
| C2—C3—C4—C5 | 56.48 (17) | N3—N6—C10—N1 | −59.00 (16) |
| N5—N4—C5—N3 | 55.05 (16) | C6—N6—C10—N1 | 178.11 (12) |
| N5—N4—C5—C4 | 175.72 (12) | N3—N6—C10—C9 | −178.95 (11) |
| N6—N3—C5—N4 | −60.10 (15) | C6—N6—C10—C9 | 58.17 (16) |
| C1—N3—C5—N4 | 177.16 (12) | C8—C9—C10—N1 | −178.00 (13) |
| N6—N3—C5—C4 | 179.34 (12) | C8—C9—C10—N6 | −57.48 (17) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*W*—H11···N3$^{i}$ | 0.93 (3) | 1.99 (3) | 2.922 (2) | 174 (2) |
| O1*W*—H12···N5$^{ii}$ | 0.92 (3) | 2.05 (3) | 2.960 (2) | 178 (2) |
| O2*W*—H21···N2 | 0.88 (3) | 2.05 (3) | 2.925 (2) | 172 (2) |
| O2*W*—H22···N4$^{ii}$ | 0.86 (3) | 2.02 (3) | 2.863 (2) | 167 (2) |
| N1—H1···O1*W* | 0.88 (2) | 2.08 (2) | 2.964 (2) | 175 (2) |
| N2—H2···O2*W*$^{iii}$ | 0.91 (2) | 2.18 (2) | 3.071 (2) | 166 (2) |
| N4—H4···N5$^{iv}$ | 0.87 (2) | 2.57 (2) | 3.354 (2) | 150.1 (15) |
| N5—H5···N1$^{iii}$ | 0.96 (2) | 2.25 (2) | 3.163 (2) | 159 (2) |

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