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6-Methyl-1,3,5-triazine-2,4-diamine butane-1,4-diol monosolvate

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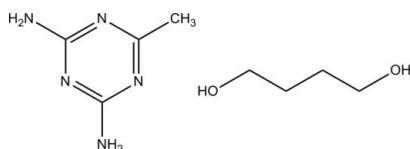
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 Key indicators: single-crystal X-ray study; $T = 123$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.041; wR factor = 0.093; data-to-parameter ratio = 12.3.

The title co-crystal, $\text{C}_4\text{H}_7\text{N}_5 \cdot \text{C}_4\text{H}_{10}\text{O}_2$, crystallizes with one molecule of 6-methyl-1,3,5-triazine-2,4-diamine (DMT) and one molecule of butane-1,4-diol in the asymmetric unit. The DMT molecules form ribbons involving centrosymmetric $R_2^2(8)$ dimer motifs between DMT molecules along the c -axis direction. These ribbons are further hydrogen bonded to each other through butane-1,4-diol, forming sheets parallel to (121).

Related literature

For background to DMT and related structural studies, see: Šebenik *et al.* (1989); Kaczmarek *et al.* (2008); Portalone (2008); Xiao (2008); Fan *et al.* (2009); Qian & Huang (2010); Thanigaimani *et al.* (2010); Perpétuo & Janczak (2007); Portalone & Colapietro (2007); Delori *et al.* (2008). For details of experimental methods used, see: Florence *et al.* (2003). For ring-motif nomenclature, see: Etter (1990).



Experimental

Crystal data

 $\text{C}_4\text{H}_7\text{N}_5 \cdot \text{C}_4\text{H}_{10}\text{O}_2$
 $M_r = 215.27$

 Triclinic, $P\bar{1}$
 $a = 5.8755$ (3) Å

 $b = 9.0515$ (5) Å

 $c = 10.7607$ (5) Å

 $\alpha = 87.911$ (3)°

 $\beta = 74.346$ (3)°

 $\gamma = 83.550$ (3)°

 $V = 547.55$ (5) Å³
 $Z = 2$

 Mo $K\alpha$ radiation

 $\mu = 0.10$ mm⁻¹
 $T = 123$ K

 $0.50 \times 0.05 \times 0.04$ mm

Data collection

Bruker APEXII CCD diffractometer

Absorption correction: multi-scan (SADABS; Bruker, 2007)

 $T_{\min} = 0.637, T_{\max} = 0.745$

 7713 measured reflections
 1911 independent reflections

 1288 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.045$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.093$
 $S = 1.00$

1911 reflections

155 parameters

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\text{max}} = 0.20$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.22$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H \cdots A$ | $D-H$ | $H \cdots A$ | $D \cdots A$ | $D-H \cdots A$ |
|--------------------------|----------|--------------|--------------|----------------|
| $O1-H1 \cdots O2^i$ | 0.84 | 1.92 | 2.764 (2) | 176 |
| $O2-H2 \cdots N1^{ii}$ | 0.84 | 1.94 | 2.777 (2) | 178 |
| $N4-H7N \cdots O1^{iii}$ | 0.92 (3) | 2.52 (2) | 3.173 (2) | 128.5 (7) |
| $N4-H8N \cdots N2^{iv}$ | 0.85 (2) | 2.19 (2) | 3.037 (2) | 178 (2) |
| $N5-H9N \cdots O1^v$ | 0.88 (2) | 2.069 (19) | 2.909 (2) | 160.1 (18) |
| $N5-H10N \cdots N3^v$ | 0.87 (2) | 2.14 (2) | 3.008 (3) | 179 (2) |

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

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: Mercury (Macrae *et al.*, 2008) and ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: enCIFer (Allen *et al.*, 2004) and WinGX (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2459).

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supporting information

Acta Cryst. (2012). E68, o3377 [doi:10.1107/S1600536812044480]

6-Methyl-1,3,5-triazine-2,4-diamine butane-1,4-diol monosolvate

Rajni M. Bhardwaj, Iain Oswald and Alastair J. Florence

S1. Comment

2,4-diamino-6-methyl-1,3,5-triazine (DMT, acetoguanamine, Fig. 1) is used as an intermediate for pharmaceutical and resin synthesis (Šebenik *et al.*, 1989). The crystal structures of the methanol, ethanol, DMF solvates and trifluoroacetate, phthalate, nitrate and chloride salts as well as of various complexes with aliphatic dicarboxylic acids have been reported in the literature (Kaczmarek *et al.*, 2008; Portalone, 2008; Xiao, 2008; Fan *et al.*, 2009; Qian & Huang, 2010; Thanigaimani *et al.*, 2010; Portalone & Colapietro, 2007; Perpétuo & Janczak, 2007; Delori *et al.*, 2008). The sample of DMT butane-1,4-diol solvate was isolated during an experimental physical form screen. The sample was identified as a novel form using multi-sample foil transmission X-ray powder diffraction analysis (Florence *et al.*, 2003). A suitable sample for single-crystal X-ray diffraction analysis was obtained from slow evaporation of saturated butane-1,4-diol solution at room temperature. The title compound crystallizes in space group $P\bar{1}$, with one molecule of DMT and one molecule of butane-1,4-diol in the asymmetric unit. Each DMT molecule forms two hydrogen-bonded dimers *via* an $R_2^2(8)$ motif (Etter, 1990) that extends to form a ribbon structure along the *c*-direction (Fig. 2). The hydrogen bonded DMT ribbons connect to adjacent ribbons through the solvent molecule, butane-1,4-diol, thus forming a second $R_3^2(8)$ ring motif (Fig. 2). These solvent separated ribbon structures extended to form sheets parallel to (121) plane, and are connected through hydrogen bond interactions *via* the hydroxyl groups. Solvent hydroxyl group also donates a hydrogen bond to the solvent in adjacent sheet, creating a three-dimensional layered structure (Fig. 3).

S2. Experimental

A single needle shape crystal was grown from the saturated solution of DMT in butane-1,4-diol by isothermal solvent evaporation at 298 K.

S3. Refinement

The positions of the N-bound H atoms were refined freely. All other H atoms were placed in calculated positions and refined in riding modes with $X-H = 0.98$ or 0.99 or 0.84 Å for the CH_3 , CH_2 and OH groups, respectively. The $U_{iso}(H)$ values were set to 1.5 or 1.2 times U_{eq} of their parent C atoms for the CH_3 and CH_2 groups, respectively. The $U_{iso}(H)$ values were set to 1.5 times U_{eq} of their parent O atoms for the OH groups.

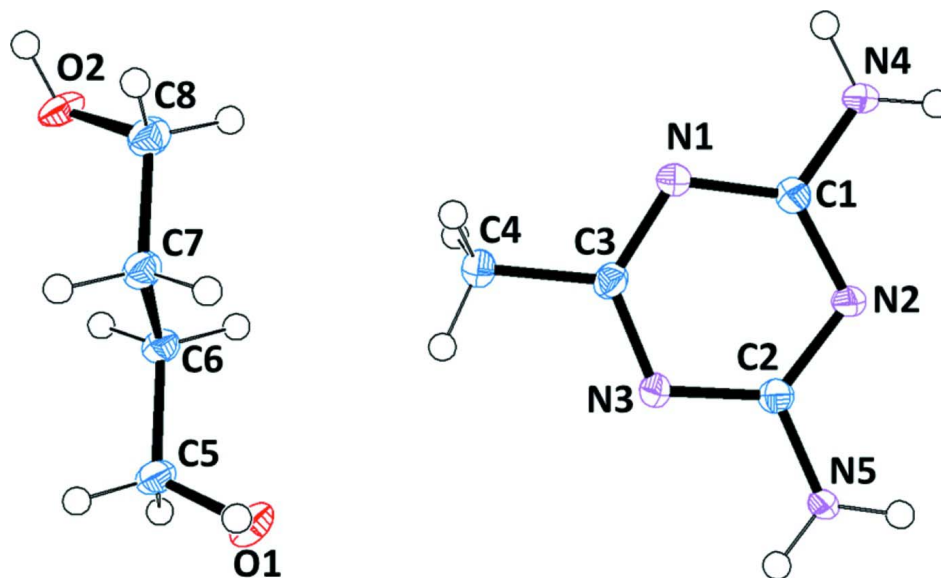


Figure 1

The asymmetric unit of 2,4-diamino-6-methyl-1,3,5-triazine (DMT), butane-1,4-diol solvate. Displacement ellipsoids are drawn at 50% probability level.

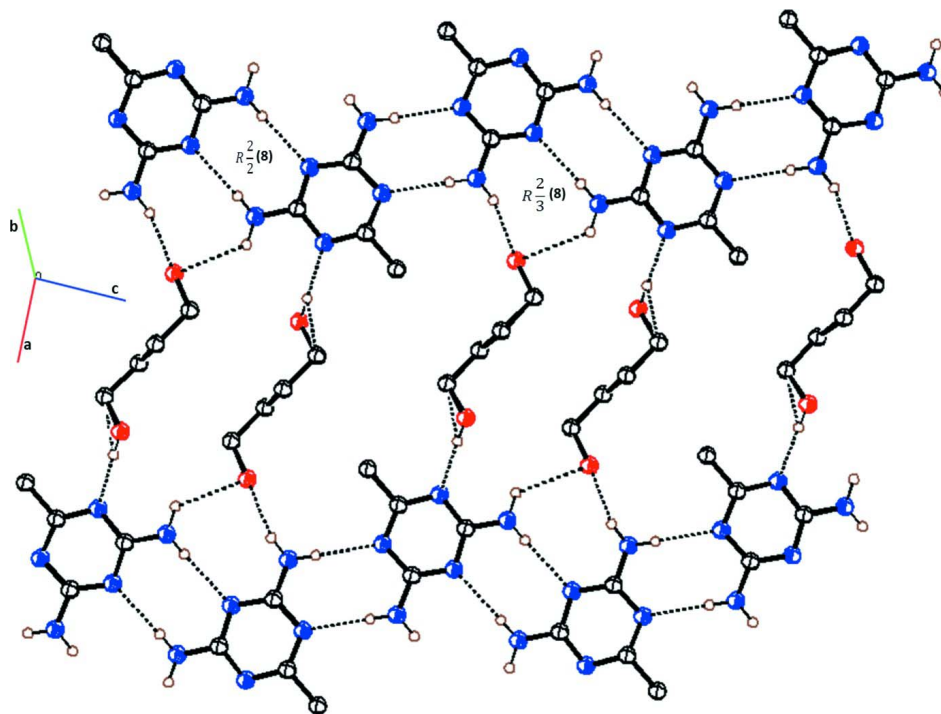
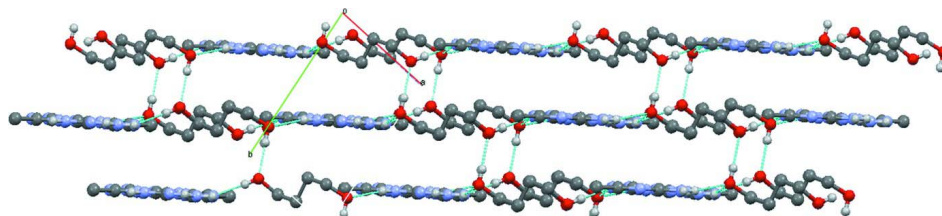


Figure 2

DMT molecules form ribbons through $R_2^2(8)$ dimer, ribbons are connected *via* H-bonding (shown in cyan dotted line) interactions mediated by butane-1,4-diol, thus give rise to sheet structure. C, N and H atoms are shown in black, blue and tan colour respectively. Other H atoms are omitted for clarity.

**Figure 3**

3-D Layered structure formed by sheets connected through H-bonding (cyan dotted line) mediated by butane-1,4-diol. C, N and H atoms are shown in grey, blue and white colour respectively. Other H atoms are omitted for clarity.

6-Methyl-1,3,5-triazine-2,4-diamine butane-1,4-diol monosolvate

Crystal data

$C_4H_7N_5 \cdot C_4H_{10}O_2$

$M_r = 215.27$

Triclinic, $P1$

Hall symbol: $-P 1$

$a = 5.8755 (3) \text{ \AA}$

$b = 9.0515 (5) \text{ \AA}$

$c = 10.7607 (5) \text{ \AA}$

$\alpha = 87.911 (3)^\circ$

$\beta = 74.346 (3)^\circ$

$\gamma = 83.550 (3)^\circ$

$V = 547.55 (5) \text{ \AA}^3$

$Z = 2$

$F(000) = 232$

$D_x = 1.306 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 1602 reflections

$\theta = 2.3\text{--}24.6^\circ$

$\mu = 0.10 \text{ mm}^{-1}$

$T = 123 \text{ K}$

Needle, colourless

$0.50 \times 0.05 \times 0.04 \text{ mm}$

Data collection

Bruker APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2007)

$T_{\min} = 0.637$, $T_{\max} = 0.745$

7713 measured reflections

1911 independent reflections

1288 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.045$

$\theta_{\max} = 25.0^\circ$, $\theta_{\min} = 2.0^\circ$

$h = -6 \rightarrow 6$

$k = -10 \rightarrow 10$

$l = -12 \rightarrow 12$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.041$

$wR(F^2) = 0.093$

$S = 1.00$

1911 reflections

155 parameters

0 restraints

0 constraints

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

$w = 1/[\sigma^2(F_o^2) + (0.0401P)^2 + 0.1476P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.20 \text{ e \AA}^{-3}$

$\Delta\rho_{\min} = -0.22 \text{ e \AA}^{-3}$

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|------------|---------------|--------------|----------------------------------|
| C1 | 0.5923 (3) | 0.3881 (2) | 0.16893 (18) | 0.0160 (5) |
| C2 | 0.2419 (3) | 0.4825 (2) | 0.30267 (18) | 0.0163 (5) |
| C3 | 0.5020 (3) | 0.3277 (2) | 0.38201 (19) | 0.0174 (5) |
| C4 | 0.5670 (4) | 0.2448 (2) | 0.49230 (19) | 0.0243 (5) |
| H4A | 0.4317 | 0.2559 | 0.5692 | 0.036* |
| H4B | 0.7035 | 0.2850 | 0.5095 | 0.036* |
| H4C | 0.6083 | 0.1393 | 0.4705 | 0.036* |
| C5 | 0.3181 (3) | 0.1867 (2) | 0.9133 (2) | 0.0207 (5) |
| H5A | 0.2639 | 0.1078 | 0.9771 | 0.025* |
| H5B | 0.3114 | 0.2788 | 0.9615 | 0.025* |
| C6 | 0.5730 (3) | 0.1418 (2) | 0.83897 (19) | 0.0182 (5) |
| H6A | 0.6744 | 0.1373 | 0.8993 | 0.022* |
| H6B | 0.6254 | 0.2195 | 0.7737 | 0.022* |
| C7 | 0.6115 (3) | -0.0072 (2) | 0.77120 (19) | 0.0191 (5) |
| H7A | 0.5611 | -0.0855 | 0.8363 | 0.023* |
| H7B | 0.5099 | -0.0033 | 0.7110 | 0.023* |
| C8 | 0.8673 (3) | -0.0489 (2) | 0.69683 (19) | 0.0220 (5) |
| H8A | 0.8820 | -0.1465 | 0.6551 | 0.026* |
| H8B | 0.9165 | 0.0260 | 0.6282 | 0.026* |
| N1 | 0.6600 (3) | 0.31119 (18) | 0.26599 (15) | 0.0175 (4) |
| N2 | 0.3851 (3) | 0.47401 (18) | 0.18167 (15) | 0.0162 (4) |
| N3 | 0.2928 (3) | 0.41094 (18) | 0.40710 (15) | 0.0174 (4) |
| N4 | 0.7434 (3) | 0.3769 (2) | 0.05127 (17) | 0.0221 (4) |
| N5 | 0.0347 (3) | 0.5670 (2) | 0.32441 (19) | 0.0201 (4) |
| O1 | 0.1589 (2) | 0.21134 (16) | 0.83288 (14) | 0.0238 (4) |
| H1 | 0.1221 | 0.1293 | 0.8146 | 0.036* |
| O2 | 1.0196 (2) | -0.05639 (16) | 0.78135 (13) | 0.0229 (4) |
| H2 | 1.1154 | -0.1339 | 0.7660 | 0.034* |
| H7N | 0.883 (4) | 0.316 (3) | 0.040 (2) | 0.037 (7)* |
| H8N | 0.704 (4) | 0.418 (2) | -0.013 (2) | 0.028 (7)* |
| H9N | -0.008 (3) | 0.618 (2) | 0.262 (2) | 0.019 (6)* |
| H10N | -0.059 (4) | 0.572 (2) | 0.402 (2) | 0.026 (6)* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|----|-------------|-------------|-------------|-------------|--------------|-------------|
| C1 | 0.0178 (11) | 0.0139 (11) | 0.0162 (11) | -0.0025 (9) | -0.0042 (9) | 0.0004 (9) |
| C2 | 0.0158 (11) | 0.0155 (11) | 0.0169 (11) | -0.0015 (9) | -0.0036 (9) | 0.0005 (9) |
| C3 | 0.0192 (12) | 0.0152 (11) | 0.0180 (11) | 0.0017 (9) | -0.0069 (9) | -0.0010 (9) |
| C4 | 0.0269 (12) | 0.0266 (13) | 0.0167 (11) | 0.0075 (10) | -0.0055 (10) | 0.0007 (9) |
| C5 | 0.0165 (11) | 0.0232 (13) | 0.0221 (11) | 0.0028 (9) | -0.0062 (9) | -0.0016 (9) |
| C6 | 0.0144 (11) | 0.0194 (12) | 0.0210 (11) | -0.0004 (9) | -0.0055 (9) | -0.0001 (9) |
| C7 | 0.0166 (11) | 0.0200 (12) | 0.0212 (11) | -0.0005 (9) | -0.0067 (9) | 0.0007 (9) |
| C8 | 0.0202 (12) | 0.0240 (13) | 0.0230 (11) | 0.0021 (9) | -0.0088 (10) | -0.0032 (9) |
| N1 | 0.0176 (9) | 0.0180 (10) | 0.0151 (9) | 0.0024 (7) | -0.0031 (8) | -0.0012 (7) |

| | | | | | | |
|----|-------------|-------------|-------------|------------|-------------|-------------|
| N2 | 0.0151 (9) | 0.0164 (9) | 0.0148 (9) | 0.0024 (7) | -0.0016 (7) | 0.0008 (7) |
| N3 | 0.0184 (9) | 0.0175 (10) | 0.0145 (9) | 0.0025 (7) | -0.0033 (7) | 0.0023 (7) |
| N4 | 0.0184 (11) | 0.0272 (11) | 0.0152 (10) | 0.0082 (9) | 0.0004 (9) | 0.0015 (8) |
| N5 | 0.0172 (10) | 0.0258 (11) | 0.0120 (10) | 0.0071 (8) | 0.0005 (9) | 0.0047 (8) |
| O1 | 0.0201 (8) | 0.0202 (8) | 0.0340 (9) | 0.0013 (7) | -0.0139 (7) | 0.0009 (7) |
| O2 | 0.0171 (8) | 0.0223 (9) | 0.0299 (9) | 0.0073 (6) | -0.0102 (7) | -0.0055 (7) |

Geometric parameters (Å, °)

| | | | |
|------------|-------------|------------|-------------|
| C1—N4 | 1.336 (2) | C6—C7 | 1.522 (3) |
| C1—N2 | 1.345 (2) | C6—H6A | 0.9900 |
| C1—N1 | 1.357 (2) | C6—H6B | 0.9900 |
| C2—N5 | 1.331 (3) | C7—C8 | 1.512 (3) |
| C2—N2 | 1.346 (2) | C7—H7A | 0.9900 |
| C2—N3 | 1.362 (2) | C7—H7B | 0.9900 |
| C3—N3 | 1.334 (2) | C8—O2 | 1.434 (2) |
| C3—N1 | 1.342 (2) | C8—H8A | 0.9900 |
| C3—C4 | 1.494 (3) | C8—H8B | 0.9900 |
| C4—H4A | 0.9800 | N4—H7N | 0.92 (2) |
| C4—H4B | 0.9800 | N4—H8N | 0.85 (2) |
| C4—H4C | 0.9800 | N5—H9N | 0.87 (2) |
| C5—O1 | 1.431 (2) | N5—H10N | 0.87 (2) |
| C5—C6 | 1.512 (3) | O1—H1 | 0.8400 |
| C5—H5A | 0.9900 | O2—H2 | 0.8400 |
| C5—H5B | 0.9900 | | |
| N4—C1—N2 | 117.48 (18) | C7—C6—H6B | 108.7 |
| N4—C1—N1 | 117.24 (18) | H6A—C6—H6B | 107.6 |
| N2—C1—N1 | 125.28 (18) | C8—C7—C6 | 113.03 (17) |
| N5—C2—N2 | 118.72 (19) | C8—C7—H7A | 109.0 |
| N5—C2—N3 | 116.41 (18) | C6—C7—H7A | 109.0 |
| N2—C2—N3 | 124.86 (18) | C8—C7—H7B | 109.0 |
| N3—C3—N1 | 125.76 (18) | C6—C7—H7B | 109.0 |
| N3—C3—C4 | 117.45 (18) | H7A—C7—H7B | 107.8 |
| N1—C3—C4 | 116.79 (17) | O2—C8—C7 | 110.49 (16) |
| C3—C4—H4A | 109.5 | O2—C8—H8A | 109.6 |
| C3—C4—H4B | 109.5 | C7—C8—H8A | 109.6 |
| H4A—C4—H4B | 109.5 | O2—C8—H8B | 109.6 |
| C3—C4—H4C | 109.5 | C7—C8—H8B | 109.6 |
| H4A—C4—H4C | 109.5 | H8A—C8—H8B | 108.1 |
| H4B—C4—H4C | 109.5 | C3—N1—C1 | 114.53 (16) |
| O1—C5—C6 | 113.42 (16) | C1—N2—C2 | 114.71 (17) |
| O1—C5—H5A | 108.9 | C3—N3—C2 | 114.85 (17) |
| C6—C5—H5A | 108.9 | C1—N4—H7N | 118.7 (14) |
| O1—C5—H5B | 108.9 | C1—N4—H8N | 120.1 (15) |
| C6—C5—H5B | 108.9 | H7N—N4—H8N | 121 (2) |
| H5A—C5—H5B | 107.7 | C2—N5—H9N | 121.4 (13) |
| C5—C6—C7 | 114.11 (17) | C2—N5—H10N | 119.2 (14) |

| | | | |
|-------------|--------------|-------------|--------------|
| C5—C6—H6A | 108.7 | H9N—N5—H10N | 119.4 (19) |
| C7—C6—H6A | 108.7 | C5—O1—H1 | 109.5 |
| C5—C6—H6B | 108.7 | C8—O2—H2 | 109.5 |
| O1—C5—C6—C7 | -64.5 (2) | N1—C1—N2—C2 | 1.1 (3) |
| C5—C6—C7—C8 | 179.55 (17) | N5—C2—N2—C1 | 178.99 (18) |
| C6—C7—C8—O2 | 59.0 (2) | N3—C2—N2—C1 | -0.6 (3) |
| N3—C3—N1—C1 | -0.1 (3) | N1—C3—N3—C2 | 0.5 (3) |
| C4—C3—N1—C1 | 179.68 (18) | C4—C3—N3—C2 | -179.23 (18) |
| N4—C1—N1—C3 | 179.49 (18) | N5—C2—N3—C3 | -179.76 (18) |
| N2—C1—N1—C3 | -0.8 (3) | N2—C2—N3—C3 | -0.1 (3) |
| N4—C1—N2—C2 | -179.17 (19) | | |

Hydrogen-bond geometry (Å, °)

| <i>D</i> —H \cdots <i>A</i> | <i>D</i> —H | H \cdots <i>A</i> | <i>D</i> \cdots <i>A</i> | <i>D</i> —H \cdots <i>A</i> |
|-----------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| O1—H1 \cdots O2 ⁱ | 0.84 | 1.92 | 2.764 (2) | 176 |
| O2—H2 \cdots N1 ⁱⁱ | 0.84 | 1.94 | 2.777 (2) | 178 |
| N4—H7N \cdots O1 ⁱⁱⁱ | 0.92 (3) | 2.52 (2) | 3.173 (2) | 128.5 (7) |
| N4—H8N \cdots N2 ^{iv} | 0.85 (2) | 2.19 (2) | 3.037 (2) | 178 (2) |
| N5—H9N \cdots O1 ^v | 0.88 (2) | 2.069 (19) | 2.909 (2) | 160.1 (18) |
| N5—H10N \cdots N3 ^v | 0.87 (2) | 2.14 (2) | 3.008 (3) | 179 (2) |

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