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# (*E*)-*N*′-[4-(Dimethylamino)benzylidene]propionohydrazide monohydrate

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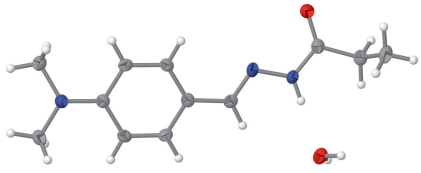
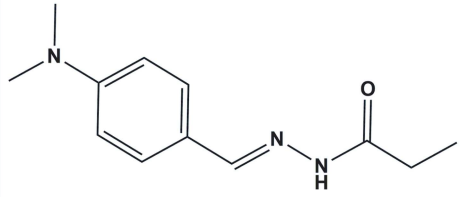
**Structural data**: full structural data are available from iucrdata.iucr.org

In the title hydrated hydrazine compound, $C_{12}H_{17}N_3O\cdot H_2O$, the C=N bond adopts an *E* conformation. In the crystal, water molecules bridge the hydrazine molecules, *via* N—H···O and O—H···O hydrogen bonds, forming sheets parallel to the *bc* plane. There are C—H···$\pi$ interactions present within the sheets, and further C—H···$\pi$ interactions link the sheets to form a three-dimensional structure.

3D view



Chemical scheme




## Structure description

A number of industrial and biologically active compounds can be synthesized using Schiff bases as substrates *via* cycloaddition, ring closure and replacement reactions. In addition, Schiff bases are also known to have biological activities, such as antifungal (Singh & Dash, 1988), antimicrobial (El-Masry *et al.*, 2000) and antitumor (Desai *et al.*, 2001), and they have been used as herbicides. Schiff bases have also been employed as ligands for the complexation of metal ions (Aydogan *et al.*, 2001), since many of these complexes may be useful and serve as models for biologically important species (Dharmaraj *et al.*, 2001). In view of the importance of Schiff base hydrazones, we report herein on the synthesis and crystal structure of the title compound.

In the title compound (Fig. 1), the C9=N2 double bond adopts an *E* conformation. The methyleneformohydrazide unit [atoms O1/N2/N3/C9/C10; maximum deviation = 0.043 (1) Å for atom N2] is inclined to the benzene ring (C3–C8) by 8.94 (9)°. The solvent water molecule is linked to the hydrazine molecule by an N—H···O hydrogen bond (Fig. 1 and Table 1).

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

*Cg*1 is the centroid of the C3–C8 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H8···O2 | 0.86 | 1.98 | 2.8330 (18) | 175 |
| O2—H18···O1$^{i}$ | 0.83 (2) | 2.21 (2) | 2.9272 (18) | 144 (2) |
| O2—H18···N2$^{i}$ | 0.83 (2) | 2.45 (2) | 3.1684 (18) | 145 (2) |
| O2—H19···O1$^{ii}$ | 0.82 (3) | 1.97 (2) | 2.7845 (18) | 172 (2) |
| C1—H14···*Cg*1$^{iii}$ | 0.96 | 2.83 | 3.567 (2) | 135 |
| C2—H16···*Cg*1$^{iv}$ | 0.96 | 2.91 | 3.701 (2) | 140 |

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

In the crystal, water molecules bridge the hydrazine molecules *via* N—H···O and O—H···O hydrogen bonds, forming sheets parallel to the *bc* plane (Table 1 and Fig. 2). There are C—H···$\pi$ interactions present within the sheets, and further

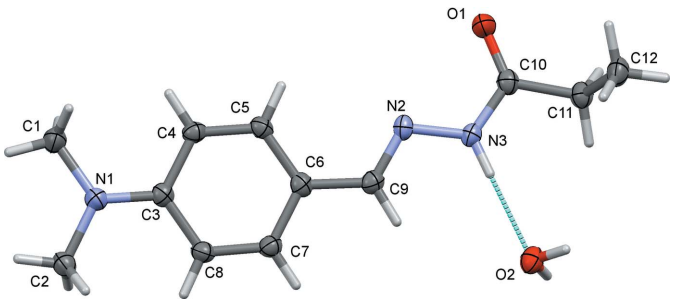



**Figure 1**
A view of the molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level and the N—H···O hydrogen bond is shown as a dashed line (see Table 1).

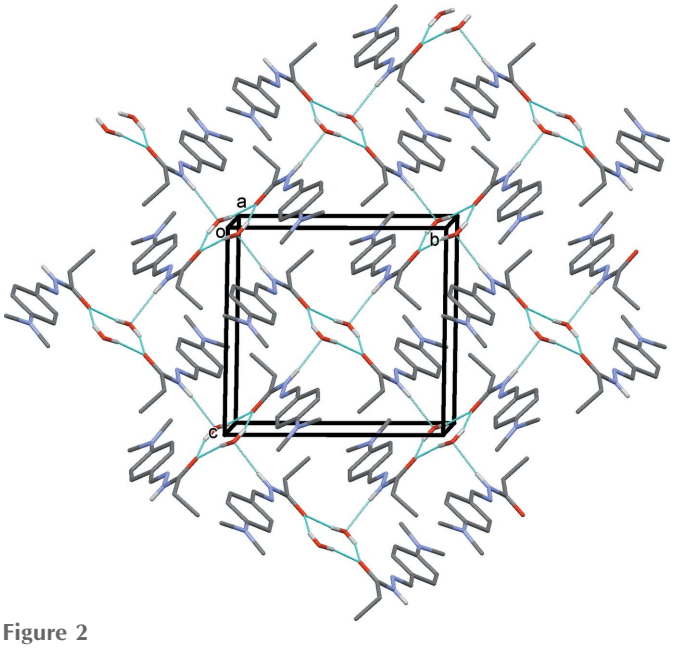



**Figure 2**
A view along the *a* axis of the crystal packing of the title compound. The hydrogen bonds are shown as dashed lines (see Table 1) and, for clarity, H atoms not involved in hydrogen bonding have been omitted.

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{12}H_{17}N_3O{\cdot}H_2O$ |
| $M_r$ | 237.30 |
| Crystal system, space group | Monoclinic, $P2_1/c$ |
| Temperature (K) | 296 |
| *a*, *b*, *c* (Å) | 12.5756 (7), 10.5214 (6), 10.5737 (6) |
| $\beta$ (°) | 112.279 (3) |
| $V$ (Å$^3$) | 1294.60 (13) |
| $Z$ | 4 |
| Radiation type | Cu $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.69 |
| Crystal size (mm) | 0.29 × 0.26 × 0.22 |
| | |
| Data collection | |
| Diffractometer | Bruker X8 Proteum |
| Absorption correction | Multi-scan (*SADABS*; Bruker, 2013) |
| $T_{min}$, $T_{max}$ | 0.826, 0.864 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 10783, 2072, 1799 |
| $R_{int}$ | 0.053 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.581 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.043, 0.141, 1.11 |
| No. of reflections | 2072 |
| No. of parameters | 163 |
| No. of restraints | 3 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.21, −0.24 |

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXS97* and *SHELXL97* (Sheldrich, 2008), *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008).

C—H···$\pi$ interactions link the sheets to form a three-dimensional structure (Table 1 and Fig. 3).

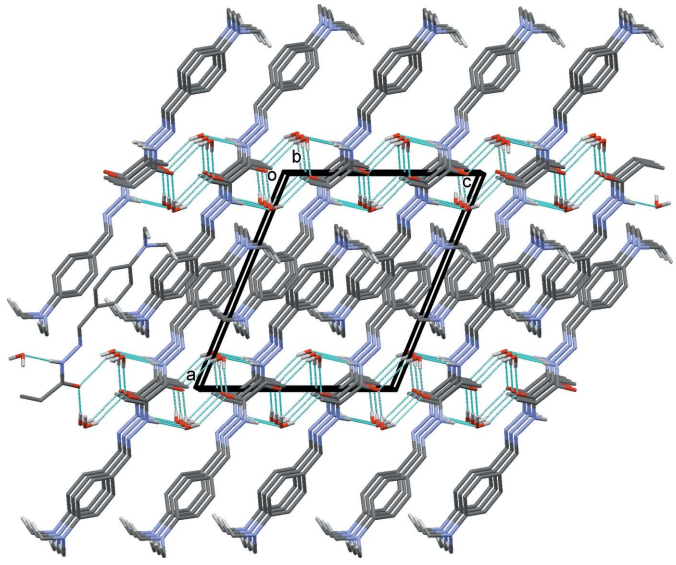



**Figure 3**
A view along the *b* axis of the crystal packing of the title compound. The hydrogen bonds are shown as dashed lines (see Table 1) and, for clarity, H atoms not involved in the various intermolecular interactions have been omitted.

## Synthesis and crystallization

A mixture of 4-(dimethylamino)benzaldehyde (0.01 mol) and hydrazine hydrate (0.01 mol) in 15 ml of propanoic acid was refluxed for *ca* 2 h. On cooling, the solid that separated was filtered off and recrystallized from dimethylformamide (DMF). Colourless block-like crystals were grown from DMF by slow evaporation of the solvent (yield 82%, m.p. 409 K).

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The water H atoms were located in a difference Fourier map and refined, with $U_{iso}(H) = 1.5U_{eq}(O)$.

## Acknowledgements

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# full crystallographic data

*IUCrData* (2016). **1**, x161716 [https://doi.org/10.1107/S2414314616017168]

## (*E*)-*N*′-[4-(Dimethylamino)benzylidene]propionohydrazide monohydrate

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**(*E*)-*N*′-[4-(Dimethylamino)benzylidene]propionohydrazide monohydrate**

*Crystal data*

$C_{12}H_{17}N_3O·H_2O$
$M_r$ = 237.30
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a$ = 12.5756 (7) Å
$b$ = 10.5214 (6) Å
$c$ = 10.5737 (6) Å
$\beta$ = 112.279 (3)°
$V$ = 1294.60 (13) Å$^3$
$Z$ = 4
$F(000)$ = 512
$D_x$ = 1.217 Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda$ = 1.54178 Å
Cell parameters from 2072 reflections
$\theta$ = 3.8–63.7°
$\mu$ = 0.69 mm$^{-1}$
$T$ = 296 K
Block, colourless
0.29 × 0.26 × 0.22 mm

*Data collection*

Bruker X8 Proteum diffractometer
Radiation source: Bruker MicroStar microfocus rotating anode
Helios multilayer optics monochromator
Detector resolution: 18.4 pixels mm$^{-1}$
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (SADABS; Bruker, 2013)
$T_{min}$ = 0.826, $T_{max}$ = 0.864
10783 measured reflections
2072 independent reflections
1799 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.053
$\theta_{max}$ = 63.7°, $\theta_{min}$ = 3.8°
$h$ = −14→14
$k$ = −12→11
$l$ = −11→12

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.141
$S$ = 1.11
2072 reflections
163 parameters
3 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
$w = 1/[\sigma^2(F_o^2) + (0.0887P)^2 + 0.250P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.24 e Å$^{-3}$

*Special details*

**Geometry**. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

**Refinement**. Refinement on $F^2$ for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs 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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.01204 (10) | 0.62894 (12) | 0.61531 (12) | 0.0317 (4) |
| N1 | 0.66806 (12) | 0.86484 (13) | 0.57578 (14) | 0.0262 (4) |
| N2 | 0.20753 (11) | 0.76812 (13) | 0.69793 (13) | 0.0223 (4) |
| N3 | 0.12447 (11) | 0.78061 (13) | 0.75446 (13) | 0.0223 (4) |
| C1 | 0.67145 (15) | 0.78096 (18) | 0.46817 (17) | 0.0300 (5) |
| C2 | 0.74862 (15) | 0.97087 (16) | 0.61820 (18) | 0.0276 (5) |
| C3 | 0.57562 (14) | 0.86170 (15) | 0.61455 (15) | 0.0214 (5) |
| C4 | 0.49094 (14) | 0.76498 (15) | 0.56646 (15) | 0.0218 (5) |
| C5 | 0.39942 (13) | 0.75970 (15) | 0.60754 (15) | 0.0213 (5) |
| C6 | 0.38583 (14) | 0.85007 (15) | 0.69790 (15) | 0.0215 (5) |
| C7 | 0.46896 (14) | 0.94588 (15) | 0.74484 (16) | 0.0229 (5) |
| C8 | 0.56171 (14) | 0.95285 (15) | 0.70483 (16) | 0.0232 (5) |
| C9 | 0.29009 (14) | 0.84864 (15) | 0.74319 (15) | 0.0222 (5) |
| C10 | 0.03017 (14) | 0.70707 (15) | 0.70870 (16) | 0.0235 (5) |
| C11 | −0.05031 (14) | 0.72381 (16) | 0.78285 (17) | 0.0261 (5) |
| C12 | −0.03320 (16) | 0.61625 (18) | 0.88521 (18) | 0.0314 (6) |
| O2 | 0.16326 (10) | 0.94926 (11) | 0.97640 (12) | 0.0275 (4) |
| H1 | 0.67440 | 0.69420 | 0.49750 | 0.0450* |
| H2 | 0.04330 | 0.62020 | 0.95350 | 0.0470* |
| H3 | 0.80850 | 0.95850 | 0.58410 | 0.0410* |
| H4 | 0.49740 | 0.70410 | 0.50610 | 0.0260* |
| H5 | 0.34550 | 0.69500 | 0.57480 | 0.0260* |
| H6 | 0.61510 | 1.01800 | 0.73770 | 0.0280* |
| H7 | 0.46170 | 1.00680 | 0.80480 | 0.0270* |
| H8 | 0.13350 | 0.83510 | 0.81830 | 0.0270* |
| H9 | −0.03550 | 0.80470 | 0.83030 | 0.0310* |
| H10 | −0.12920 | 0.72380 | 0.71760 | 0.0310* |
| H11 | −0.04420 | 0.53610 | 0.83860 | 0.0470* |
| H12 | −0.08790 | 0.62460 | 0.92800 | 0.0470* |
| H13 | 0.28860 | 0.90830 | 0.80740 | 0.0270* |
| H14 | 0.60380 | 0.79370 | 0.38730 | 0.0450* |
| H15 | 0.73840 | 0.79950 | 0.44860 | 0.0450* |
| H16 | 0.70880 | 1.04870 | 0.58230 | 0.0410* |
| H17 | 0.78160 | 0.97520 | 0.71620 | 0.0410* |
| H18 | 0.1452 (18) | 0.9041 (17) | 1.0300 (19) | 0.0410* |

| | | | | |
|---|---|---|---|---|
| H19 | 0.1159 (16) | 1.0074 (15) | 0.955 (2) | 0.0410* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0339 (7) | 0.0360 (7) | 0.0292 (7) | −0.0111 (5) | 0.0165 (5) | −0.0072 (5) |
| N1 | 0.0251 (7) | 0.0296 (8) | 0.0265 (8) | −0.0065 (6) | 0.0126 (6) | −0.0058 (6) |
| N2 | 0.0233 (7) | 0.0256 (7) | 0.0212 (7) | 0.0004 (5) | 0.0120 (6) | 0.0020 (5) |
| N3 | 0.0242 (7) | 0.0253 (7) | 0.0206 (7) | −0.0012 (5) | 0.0120 (6) | −0.0019 (5) |
| C1 | 0.0277 (9) | 0.0365 (10) | 0.0292 (9) | −0.0041 (7) | 0.0145 (7) | −0.0067 (7) |
| C2 | 0.0262 (9) | 0.0271 (9) | 0.0309 (9) | −0.0042 (7) | 0.0125 (7) | 0.0007 (7) |
| C3 | 0.0223 (8) | 0.0228 (8) | 0.0177 (8) | −0.0001 (6) | 0.0061 (6) | 0.0033 (6) |
| C4 | 0.0259 (9) | 0.0204 (8) | 0.0178 (8) | −0.0005 (6) | 0.0068 (6) | −0.0007 (6) |
| C5 | 0.0218 (8) | 0.0211 (8) | 0.0192 (8) | −0.0027 (6) | 0.0056 (6) | 0.0018 (6) |
| C6 | 0.0231 (8) | 0.0221 (8) | 0.0184 (8) | 0.0007 (6) | 0.0069 (6) | 0.0049 (6) |
| C7 | 0.0281 (9) | 0.0209 (8) | 0.0202 (8) | −0.0009 (6) | 0.0098 (6) | −0.0012 (6) |
| C8 | 0.0252 (8) | 0.0208 (8) | 0.0226 (8) | −0.0042 (6) | 0.0078 (6) | −0.0011 (6) |
| C9 | 0.0264 (9) | 0.0217 (8) | 0.0183 (8) | 0.0012 (6) | 0.0081 (6) | 0.0020 (6) |
| C10 | 0.0254 (9) | 0.0235 (8) | 0.0227 (8) | 0.0012 (6) | 0.0104 (7) | 0.0045 (6) |
| C11 | 0.0228 (9) | 0.0281 (9) | 0.0284 (9) | 0.0024 (7) | 0.0109 (7) | 0.0015 (7) |
| C12 | 0.0354 (10) | 0.0341 (10) | 0.0323 (10) | 0.0016 (8) | 0.0216 (8) | 0.0028 (7) |
| O2 | 0.0310 (7) | 0.0269 (7) | 0.0278 (7) | 0.0054 (5) | 0.0148 (5) | 0.0026 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C10 | 1.238 (2) | C11—C12 | 1.524 (2) |
| O2—H18 | 0.83 (2) | C1—H1 | 0.9600 |
| O2—H19 | 0.823 (18) | C1—H15 | 0.9600 |
| N1—C1 | 1.453 (2) | C1—H14 | 0.9600 |
| N1—C3 | 1.372 (2) | C2—H16 | 0.9600 |
| N1—C2 | 1.459 (2) | C2—H17 | 0.9600 |
| N2—N3 | 1.393 (2) | C2—H3 | 0.9600 |
| N2—C9 | 1.284 (2) | C4—H4 | 0.9300 |
| N3—C10 | 1.343 (2) | C5—H5 | 0.9300 |
| N3—H8 | 0.8600 | C7—H7 | 0.9300 |
| C3—C4 | 1.420 (2) | C8—H6 | 0.9300 |
| C3—C8 | 1.410 (2) | C9—H13 | 0.9300 |
| C4—C5 | 1.377 (3) | C11—H10 | 0.9700 |
| C5—C6 | 1.404 (2) | C11—H9 | 0.9700 |
| C6—C7 | 1.401 (2) | C12—H12 | 0.9600 |
| C6—C9 | 1.455 (3) | C12—H2 | 0.9600 |
| C7—C8 | 1.385 (3) | C12—H11 | 0.9600 |
| C10—C11 | 1.507 (3) | | |
| | | | |
| H18—O2—H19 | 105 (2) | N1—C1—H15 | 109.00 |
| C1—N1—C2 | 118.82 (15) | N1—C2—H3 | 109.00 |
| C1—N1—C3 | 119.94 (14) | N1—C2—H16 | 109.00 |
| C2—N1—C3 | 119.67 (14) | H3—C2—H16 | 109.00 |

| | | | |
|---|---|---|---|
| N3—N2—C9 | 114.20 (13) | H3—C2—H17 | 109.00 |
| N2—N3—C10 | 119.64 (13) | N1—C2—H17 | 109.00 |
| N2—N3—H8 | 120.00 | H16—C2—H17 | 109.00 |
| C10—N3—H8 | 120.00 | C5—C4—H4 | 119.00 |
| C4—C3—C8 | 117.45 (16) | C3—C4—H4 | 119.00 |
| N1—C3—C8 | 121.51 (15) | C4—C5—H5 | 119.00 |
| N1—C3—C4 | 121.03 (14) | C6—C5—H5 | 119.00 |
| C3—C4—C5 | 121.26 (15) | C6—C7—H7 | 119.00 |
| C4—C5—C6 | 121.30 (15) | C8—C7—H7 | 119.00 |
| C7—C6—C9 | 119.37 (14) | C7—C8—H6 | 120.00 |
| C5—C6—C9 | 123.14 (15) | C3—C8—H6 | 120.00 |
| C5—C6—C7 | 117.49 (16) | C6—C9—H13 | 119.00 |
| C6—C7—C8 | 122.11 (15) | N2—C9—H13 | 119.00 |
| C3—C8—C7 | 120.38 (15) | C10—C11—H9 | 110.00 |
| N2—C9—C6 | 122.51 (14) | C12—C11—H9 | 110.00 |
| O1—C10—N3 | 122.71 (17) | C12—C11—H10 | 110.00 |
| N3—C10—C11 | 114.87 (14) | C10—C11—H10 | 110.00 |
| O1—C10—C11 | 122.39 (16) | H9—C11—H10 | 108.00 |
| C10—C11—C12 | 109.93 (15) | C11—C12—H11 | 109.00 |
| N1—C1—H1 | 109.00 | C11—C12—H12 | 109.00 |
| N1—C1—H14 | 109.00 | C11—C12—H2 | 109.00 |
| H1—C1—H14 | 109.00 | H2—C12—H12 | 110.00 |
| H1—C1—H15 | 109.00 | H11—C12—H12 | 109.00 |
| H14—C1—H15 | 109.00 | H2—C12—H11 | 109.00 |

| | | | |
|---|---|---|---|
| C1—N1—C3—C4 | 9.6 (2) | C4—C3—C8—C7 | 0.6 (2) |
| C1—N1—C3—C8 | −171.26 (15) | C3—C4—C5—C6 | 0.4 (2) |
| C2—N1—C3—C4 | 175.19 (14) | C4—C5—C6—C7 | 0.0 (2) |
| C2—N1—C3—C8 | −5.7 (2) | C4—C5—C6—C9 | 179.55 (15) |
| C9—N2—N3—C10 | 175.73 (14) | C5—C6—C7—C8 | 0.0 (2) |
| N3—N2—C9—C6 | 179.26 (13) | C9—C6—C7—C8 | −179.60 (15) |
| N2—N3—C10—O1 | −1.4 (2) | C5—C6—C9—N2 | −3.8 (2) |
| N2—N3—C10—C11 | 176.70 (13) | C7—C6—C9—N2 | 175.81 (15) |
| N1—C3—C4—C5 | 178.48 (15) | C6—C7—C8—C3 | −0.3 (2) |
| C8—C3—C4—C5 | −0.7 (2) | O1—C10—C11—C12 | 77.2 (2) |
| N1—C3—C8—C7 | −178.52 (15) | N3—C10—C11—C12 | −100.88 (17) |

*Hydrogen-bond geometry (Å, º)*

*Cg*1 is the centroid of the C3–C8 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H8···O2 | 0.86 | 1.98 | 2.8330 (18) | 175 |
| O2—H18···O1$^{i}$ | 0.83 (2) | 2.21 (2) | 2.9272 (18) | 144 (2) |
| O2—H18···N2$^{i}$ | 0.83 (2) | 2.45 (2) | 3.1684 (18) | 145 (2) |
| O2—H19···O1$^{ii}$ | 0.82 (3) | 1.97 (2) | 2.7845 (18) | 172 (2) |

| | | | | |
|---|---|---|---|---|
| C1—H14···*Cg*1$^{iii}$ | 0.96 | 2.83 | 3.567 (2) | 135 |
| C2—H16···*Cg*1$^{iv}$ | 0.96 | 2.91 | 3.701 (2) | 140 |

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