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# *N*′-(3-Phenylallylidene)nicotinohydrazide monohydrate

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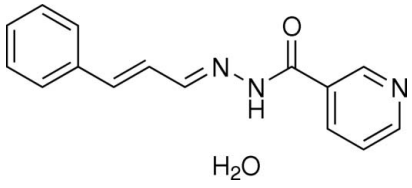
Key indicators: single-crystal X-ray study; $T$ = 110 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.043; $wR$ factor = 0.125; data-to-parameter ratio = 14.2.

In the title compound, $C_{15}H_{13}N_3O\cdot H_2O$, the dihedral angle between the pyridine and phenyl rings is 35.45 (7)°. Intermolecular O—H···O, O—H···N, N—H···O and C—H···O hydrogen bonds are found in the crystal structure. In addition, C—H···$\pi$ interactions involving the pyridine and phenyl rings are also found.

## Related literature

For a related crystal structure and its chemical and biological applications, see: Archana *et al.* (2009).



## Experimental

### *Crystal data*

$C_{15}H_{13}N_3O\cdot H_2O$
$M_r$ = 269.30
Monoclinic, $P2_1/c$
$a$ = 9.8456 (3) Å
$b$ = 9.1288 (3) Å
$c$ = 15.5389 (5) Å
$\beta$ = 95.938 (3)°
$V$ = 1389.12 (8) Å$^3$
$Z$ = 4
Cu $K\alpha$ radiation
$\mu$ = 0.72 mm$^{-1}$
$T$ = 110 K
0.48 × 0.45 × 0.24 mm

### *Data collection*

Oxford Diffraction Xcalibur, Ruby, Gemini diffractometer
Absorption correction: multi-scan (CrysAlisPro; Oxford Diffraction, 2009)
$T_{min}$ = 0.704, $T_{max}$ = 1.000
6007 measured reflections
2742 independent reflections
2346 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.022

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.125
$S$ = 1.05
2742 reflections
193 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.29 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.21 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1$W$—H1$W$···O7$^{i}$ | 0.86 (3) | 2.52 (3) | 3.1550 (14) | 131.9 (19) |
| O1$W$—H1$W$···N9$^{i}$ | 0.86 (3) | 2.16 (3) | 2.9655 (15) | 157 (2) |
| O1$W$—H2$W$···N1$^{ii}$ | 0.88 (3) | 2.05 (3) | 2.9222 (15) | 176 (2) |
| N8—H8···O1$W$ | 0.914 (18) | 1.944 (18) | 2.8486 (15) | 170.3 (17) |
| C2—H2···O7$^{iii}$ | 0.95 | 2.33 | 3.2253 (17) | 157 |
| C4—H4···O1$W$ | 0.95 | 2.54 | 3.2392 (16) | 130 |
| C10—H10···O7$^{i}$ | 0.95 | 2.57 | 3.1507 (17) | 120 |
| C22—H22···$Cg1^{iv}$ | 0.95 | 2.94 | 3.7742 (16) | 148 |
| C5—H5···$Cg2^{v}$ | 0.95 | 2.54 | 3.4342 (15) | 157 |

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (iii) $-x+1, -y+1, -z$; (iv) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (v) $x-1, -y+\frac{1}{2}, z-\frac{1}{2}$. $Cg1$ and $Cg2$ are the centroids of the N1–C6 and C21–C26 rings, respectively.

Data collection: *CrysAlisPro* (Oxford Diffraction, 2009); cell refinement: *CrysAlisPro*; data reduction: *CrysAlisPro*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2355).

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# supporting information

*Acta Cryst.* (2009). E**65**, o2833 [https://doi.org/10.1107/S1600536809043001]

## *N*′-(3-Phenylallylidene)nicotinohydrazide monohydrate

**R. Archana, N. Saradhadevi, A. Manimekalai, A. Thiruvalluvar and R. J. Butcher**

### S1. Comment

As part of our research, we have synthesized the title compound and report its crystal structure here. Archana *et al.* (2009) have reported a related crystal structure, *N*′-(2-methyl-3-phenylallylidene) nicotinohydrazide monohydrate.

The molecular structure of the asymmetric unit is shown in Fig. 1. The dihedral angle between the pyridine ring and the phenyl ring is 35.45 (7)°. Intermolecular O—H···O, O—H···N, N—H···O and C—H···O hydrogen bonds are found in the crystal structure. Furthermore, a C22—H22···$\pi$ interaction involving the pyridine (N1—C6) ring and a C5—H5···$\pi$ interaction involving the phenyl (C21—C26) ring are also found.

### S2. Experimental

Sodium hydroxide (0.4 g, 0.01 mol) in a stoppered conical flask was kept in an ice-cold environment. Ethanol (40 ml) was added to dissolve it and the mixture was stirred continuously using a magnetic stirrer. An equimolar quantity of nicotinic hydrazide (1.371 g, 0.01 mol) and cinnamaldehyde (1.32 g, 0.01 mol) was added to this mixture. The stirring was continued for 5 h in ice-cold conditions. The mixture was kept overnight in a refrigerator. The mixture was then allowed to stand for four days under normal conditions. A yellow solid was obtained. This was filtered, washed and recrystallized from ethanol. Yield 2.3 g, 46.80%.

### S3. Refinement

H8 attached to N8, and H1W and H2W attached to O1W were located in a difference Fourier map and refined freely. The remaining H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.95 Å. $U_{iso}$(H) = 1.2$U_{eq}$(C).

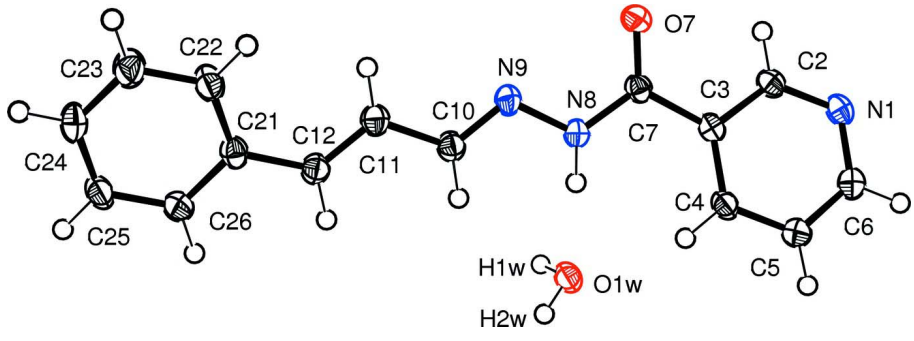


**Figure 1**

The molecular structure of the asymmetric unit, showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radius.

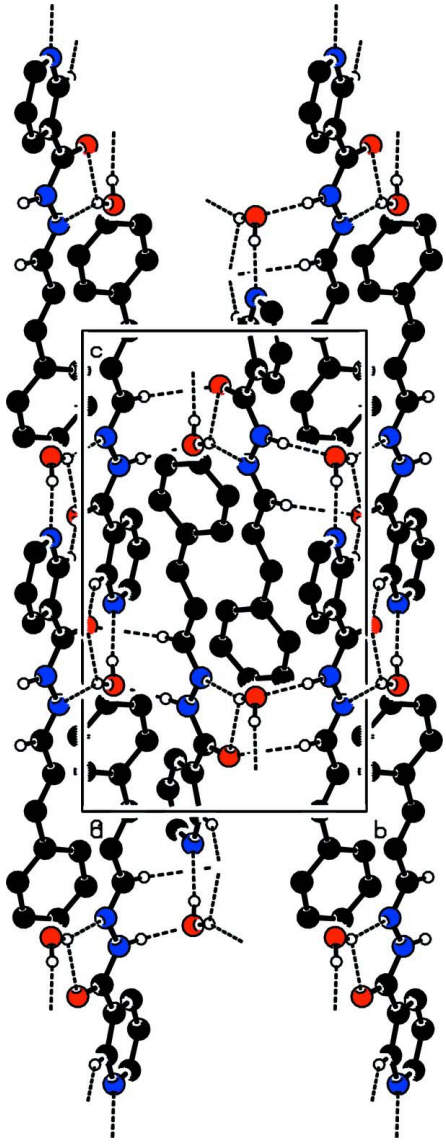


**Figure 2**

The packing of the title compound, viewed down the *a* axis. Dashed lines indicate hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted.

## *N*′-(3-Phenylallylidene)nicotinohydrazide monohydrate

*Crystal data*

$C_{15}H_{13}N_3O{\cdot}H_2O$
$M_r = 269.30$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 9.8456\ (3)$ Å
$b = 9.1288\ (3)$ Å
$c = 15.5389\ (5)$ Å
$\beta = 95.938\ (3)°$
$V = 1389.12\ (8)$ Å$^3$
$Z = 4$
$F(000) = 568$
$D_x = 1.288$ Mg m$^{-3}$
Melting point: 463 K
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 3706 reflections
$\theta = 4.5–74.0°$
$\mu = 0.72$ mm$^{-1}$
$T = 110$ K
Plate, colourless
0.48 × 0.45 × 0.24 mm

*Data collection*

Oxford Diffraction Xcalibur, Ruby, Gemini diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 10.5081 pixels $mm^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
$T_{min}$ = 0.704, $T_{max}$ = 1.000
6007 measured reflections
2742 independent reflections
2346 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.022
$\theta_{max}$ = 74.6°, $\theta_{min}$ = 4.5°
$h = -12 \rightarrow 12$
$k = -10 \rightarrow 9$
$l = -13 \rightarrow 18$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.125
$S$ = 1.05
2742 reflections
193 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
$w = 1/[\sigma^2(F_o^2) + (0.0821P)^2 + 0.2609P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.29 e $Å^{-3}$
$\Delta\rho_{min}$ = −0.21 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 e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**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 $F^2 > 2\sigma(F^2)$ 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.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O7 | 0.47479 (10) | 0.51591 (11) | 0.11459 (6) | 0.0278 (3) |
| N1 | 0.16249 (12) | 0.38852 (13) | −0.06770 (7) | 0.0251 (3) |
| N8 | 0.40129 (11) | 0.37087 (13) | 0.21906 (7) | 0.0229 (3) |
| N9 | 0.50761 (11) | 0.41751 (13) | 0.27801 (7) | 0.0239 (3) |
| C2 | 0.26809 (14) | 0.41542 (15) | −0.00816 (8) | 0.0234 (4) |
| C3 | 0.26600 (13) | 0.38761 (14) | 0.08017 (8) | 0.0213 (3) |
| C4 | 0.14754 (14) | 0.32800 (15) | 0.10770 (8) | 0.0245 (4) |
| C5 | 0.03714 (14) | 0.30162 (16) | 0.04673 (9) | 0.0266 (4) |
| C6 | 0.04847 (14) | 0.33422 (15) | −0.03908 (9) | 0.0249 (4) |
| C7 | 0.39013 (13) | 0.43067 (15) | 0.13894 (8) | 0.0214 (3) |
| C10 | 0.51203 (13) | 0.35650 (15) | 0.35280 (9) | 0.0244 (4) |
| C11 | 0.61459 (14) | 0.39886 (15) | 0.42168 (9) | 0.0253 (4) |
| C12 | 0.61879 (13) | 0.33520 (16) | 0.49986 (8) | 0.0252 (4) |
| C21 | 0.71252 (14) | 0.36867 (15) | 0.57704 (8) | 0.0241 (4) |
| C22 | 0.79857 (16) | 0.49073 (16) | 0.58318 (9) | 0.0308 (4) |
| C23 | 0.89016 (17) | 0.51244 (18) | 0.65604 (10) | 0.0366 (5) |

| | | | | |
|---|---|---|---|---|
| C24 | 0.89795 (15) | 0.41399 (17) | 0.72450 (9) | 0.0319 (4) |
| C25 | 0.80997 (15) | 0.29477 (17) | 0.72029 (9) | 0.0306 (4) |
| C26 | 0.71789 (14) | 0.27272 (17) | 0.64743 (9) | 0.0273 (4) |
| O1W | 0.26480 (10) | 0.11005 (11) | 0.26235 (6) | 0.0266 (3) |
| H2 | 0.34889 | 0.45566 | −0.02707 | 0.0281* |
| H4 | 0.14252 | 0.30588 | 0.16702 | 0.0294* |
| H5 | −0.04511 | 0.26171 | 0.06373 | 0.0320* |
| H6 | −0.02844 | 0.31734 | −0.08004 | 0.0299* |
| H8 | 0.3493 (18) | 0.294 (2) | 0.2342 (11) | 0.035 (5)* |
| H10 | 0.44733 | 0.28292 | 0.36291 | 0.0293* |
| H11 | 0.67948 | 0.47225 | 0.41157 | 0.0304* |
| H12 | 0.55372 | 0.26002 | 0.50588 | 0.0302* |
| H22 | 0.79430 | 0.55943 | 0.53706 | 0.0369* |
| H23 | 0.94833 | 0.59572 | 0.65915 | 0.0440* |
| H24 | 0.96260 | 0.42804 | 0.77357 | 0.0383* |
| H25 | 0.81272 | 0.22804 | 0.76735 | 0.0366* |
| H26 | 0.65768 | 0.19119 | 0.64543 | 0.0328* |
| H1W | 0.335 (3) | 0.054 (3) | 0.2663 (14) | 0.057 (6)* |
| H2W | 0.232 (3) | 0.106 (3) | 0.3128 (16) | 0.070 (7)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O7 | 0.0289 (5) | 0.0327 (5) | 0.0219 (5) | −0.0068 (4) | 0.0028 (4) | 0.0027 (4) |
| N1 | 0.0305 (6) | 0.0268 (6) | 0.0179 (5) | 0.0013 (5) | 0.0022 (4) | −0.0001 (4) |
| N8 | 0.0222 (5) | 0.0268 (6) | 0.0192 (6) | −0.0023 (4) | −0.0006 (4) | 0.0013 (4) |
| N9 | 0.0247 (5) | 0.0273 (6) | 0.0191 (5) | −0.0010 (4) | −0.0004 (4) | −0.0012 (4) |
| C2 | 0.0267 (6) | 0.0245 (7) | 0.0194 (6) | 0.0002 (5) | 0.0046 (5) | 0.0002 (5) |
| C3 | 0.0246 (6) | 0.0204 (6) | 0.0189 (6) | 0.0021 (5) | 0.0023 (5) | 0.0008 (5) |
| C4 | 0.0263 (7) | 0.0281 (7) | 0.0194 (6) | 0.0018 (5) | 0.0032 (5) | 0.0042 (5) |
| C5 | 0.0245 (6) | 0.0295 (7) | 0.0259 (7) | −0.0008 (5) | 0.0029 (5) | 0.0033 (5) |
| C6 | 0.0263 (6) | 0.0242 (7) | 0.0235 (7) | 0.0020 (5) | −0.0007 (5) | −0.0009 (5) |
| C7 | 0.0231 (6) | 0.0233 (6) | 0.0182 (6) | 0.0019 (5) | 0.0036 (5) | −0.0004 (5) |
| C10 | 0.0249 (6) | 0.0262 (7) | 0.0219 (7) | 0.0004 (5) | 0.0014 (5) | 0.0000 (5) |
| C11 | 0.0267 (7) | 0.0260 (7) | 0.0230 (7) | −0.0003 (5) | 0.0013 (5) | −0.0019 (5) |
| C12 | 0.0241 (6) | 0.0274 (7) | 0.0236 (7) | −0.0002 (5) | 0.0008 (5) | −0.0009 (5) |
| C21 | 0.0251 (6) | 0.0268 (7) | 0.0203 (6) | 0.0040 (5) | 0.0023 (5) | −0.0016 (5) |
| C22 | 0.0424 (8) | 0.0250 (7) | 0.0233 (7) | −0.0025 (6) | −0.0042 (6) | 0.0028 (5) |
| C23 | 0.0461 (9) | 0.0304 (8) | 0.0310 (8) | −0.0089 (7) | −0.0074 (7) | −0.0004 (6) |
| C24 | 0.0352 (8) | 0.0385 (8) | 0.0202 (7) | 0.0001 (6) | −0.0053 (6) | −0.0034 (6) |
| C25 | 0.0338 (7) | 0.0383 (8) | 0.0194 (6) | 0.0016 (6) | 0.0021 (5) | 0.0044 (5) |
| C26 | 0.0263 (6) | 0.0332 (7) | 0.0229 (7) | −0.0011 (5) | 0.0044 (5) | 0.0011 (5) |
| O1W | 0.0283 (5) | 0.0294 (5) | 0.0220 (5) | 0.0024 (4) | 0.0023 (4) | 0.0048 (4) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O7—C7 | 1.2283 (16) | C21—C26 | 1.3980 (19) |
| O1W—H1W | 0.86 (3) | C22—C23 | 1.387 (2) |

| | | | |
|---|---|---|---|
| O1W—H2W | 0.88 (3) | C23—C24 | 1.389 (2) |
| N1—C2 | 1.3410 (17) | C24—C25 | 1.388 (2) |
| N1—C6 | 1.3443 (18) | C25—C26 | 1.390 (2) |
| N8—N9 | 1.3848 (15) | C2—H2 | 0.9500 |
| N8—C7 | 1.3534 (17) | C4—H4 | 0.9500 |
| N9—C10 | 1.2854 (18) | C5—H5 | 0.9500 |
| N8—H8 | 0.914 (18) | C6—H6 | 0.9500 |
| C2—C3 | 1.3981 (18) | C10—H10 | 0.9500 |
| C3—C4 | 1.3938 (19) | C11—H11 | 0.9500 |
| C3—C7 | 1.5004 (18) | C12—H12 | 0.9500 |
| C4—C5 | 1.3871 (19) | C22—H22 | 0.9500 |
| C5—C6 | 1.382 (2) | C23—H23 | 0.9500 |
| C10—C11 | 1.4461 (19) | C24—H24 | 0.9500 |
| C11—C12 | 1.3435 (19) | C25—H25 | 0.9500 |
| C12—C21 | 1.4678 (18) | C26—H26 | 0.9500 |
| C21—C22 | 1.397 (2) | | |

| | | | |
|---|---|---|---|
| O1W···N1$^{i}$ | 2.9222 (15) | C22···H11 | 2.8000 |
| O1W···O7$^{ii}$ | 3.1550 (14) | C23···H5$^{ix}$ | 2.9900 |
| O1W···N9$^{ii}$ | 2.9655 (15) | C24···H5$^{ix}$ | 3.0700 |
| O1W···C4 | 3.2392 (16) | C25···H5$^{ix}$ | 2.9900 |
| O1W···N8 | 2.8486 (15) | C26···H5$^{ix}$ | 2.8000 |
| O7···C10$^{iii}$ | 3.1507 (17) | H1W···N9$^{ii}$ | 2.16 (3) |
| O7···N9 | 2.6814 (14) | H1W···H8 | 2.26 (3) |
| O7···C2$^{iv}$ | 3.2253 (17) | H1W···O7$^{ii}$ | 2.52 (3) |
| O7···O1W$^{iii}$ | 3.1550 (14) | H1W···C10$^{ii}$ | 3.09 (3) |
| O1W···H10 | 2.7500 | H2···O7 | 2.4700 |
| O1W···H8 | 1.944 (18) | H2···O7$^{iv}$ | 2.3300 |
| O1W···H4 | 2.5400 | H2W···N1$^{i}$ | 2.05 (3) |
| O7···H2 | 2.4700 | H2W···C2$^{i}$ | 2.78 (2) |
| O7···H10$^{iii}$ | 2.5700 | H2W···H8 | 2.46 (3) |
| O7···H12$^{iii}$ | 2.9100 | H4···O1W | 2.5400 |
| O7···H2$^{iv}$ | 2.3300 | H4···N8 | 2.6600 |
| O7···H26$^{v}$ | 2.6200 | H4···H8 | 2.1900 |
| O7···H1W$^{iii}$ | 2.52 (3) | H5···C21$^{x}$ | 2.6900 |
| N1···O1W$^{v}$ | 2.9222 (15) | H5···C22$^{x}$ | 2.8000 |
| N8···O1W | 2.8486 (15) | H5···C23$^{x}$ | 2.9900 |
| N9···O1W$^{iii}$ | 2.9655 (15) | H5···C24$^{x}$ | 3.0700 |
| N9···O7 | 2.6814 (14) | H5···C25$^{x}$ | 2.9900 |
| N1···H2W$^{v}$ | 2.05 (3) | H5···C26$^{x}$ | 2.8000 |
| N8···H26$^{v}$ | 2.9300 | H6···H24$^{viii}$ | 2.4800 |
| N8···H4 | 2.6600 | H6···H23$^{ii}$ | 2.5400 |
| N9···H1W$^{iii}$ | 2.16 (3) | H8···H1W | 2.26 (3) |
| N9···H26$^{v}$ | 2.8400 | H8···O1W | 1.944 (18) |
| C2···O7$^{iv}$ | 3.2253 (17) | H8···C4 | 2.664 (17) |
| C4···O1W | 3.2392 (16) | H8···H10 | 2.1300 |
| C4···C24$^{vi}$ | 3.576 (2) | H8···H2W | 2.46 (3) |
| C5···C6$^{vii}$ | 3.429 (2) | H8···H4 | 2.1900 |

| | | | |
|---|---|---|---|
| C6···C22$^{ii}$ | 3.575 (2) | H10···O7$^{ii}$ | 2.5700 |
| C6···C6$^{vii}$ | 3.4332 (19) | H10···O1W | 2.7500 |
| C6···C23$^{ii}$ | 3.539 (2) | H10···H8 | 2.1300 |
| C6···C5$^{vii}$ | 3.429 (2) | H10···H12 | 2.3700 |
| C10···C22$^{vi}$ | 3.594 (2) | H11···H22 | 2.2900 |
| C10···O7$^{ii}$ | 3.1507 (17) | H11···C22 | 2.8000 |
| C10···C21$^{vi}$ | 3.5874 (19) | H12···H10 | 2.3700 |
| C21···C10$^{vi}$ | 3.5874 (19) | H12···H26 | 2.3800 |
| C22···C10$^{vi}$ | 3.594 (2) | H12···O7$^{ii}$ | 2.9100 |
| C22···C6$^{iii}$ | 3.575 (2) | H22···C11 | 2.8000 |
| C23···C6$^{iii}$ | 3.539 (2) | H22···H11 | 2.2900 |
| C24···C4$^{vi}$ | 3.576 (2) | H22···C6$^{iii}$ | 2.9500 |
| C2···H2W$^{v}$ | 2.78 (2) | H23···C6$^{iii}$ | 2.8700 |
| C4···H8 | 2.664 (17) | H23···H6$^{iii}$ | 2.5400 |
| C6···H23$^{ii}$ | 2.8700 | H24···C6$^{xi}$ | 3.0700 |
| C6···H22$^{ii}$ | 2.9500 | H24···H6$^{xi}$ | 2.4800 |
| C6···H24$^{viii}$ | 3.0700 | H26···H12 | 2.3800 |
| C7···H26$^{v}$ | 2.8500 | H26···O7$^{i}$ | 2.6200 |
| C10···H1W$^{iii}$ | 3.09 (3) | H26···N8$^{i}$ | 2.9300 |
| C11···H22 | 2.8000 | H26···N9$^{i}$ | 2.8400 |
| C21···H5$^{ix}$ | 2.6900 | H26···C7$^{i}$ | 2.8500 |
| C22···H5$^{ix}$ | 2.8000 | | |

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|---|---|---|---|
| H1W—O1W—H2W | 106 (2) | C21—C26—C25 | 121.01 (14) |
| C2—N1—C6 | 116.98 (11) | N1—C2—H2 | 118.00 |
| N9—N8—C7 | 117.93 (11) | C3—C2—H2 | 118.00 |
| N8—N9—C10 | 114.67 (11) | C5—C4—H4 | 121.00 |
| C7—N8—H8 | 123.5 (11) | C3—C4—H4 | 121.00 |
| N9—N8—H8 | 118.1 (11) | C4—C5—H5 | 120.00 |
| N1—C2—C3 | 123.71 (12) | C6—C5—H5 | 120.00 |
| C2—C3—C7 | 117.14 (11) | C5—C6—H6 | 118.00 |
| C4—C3—C7 | 124.77 (11) | N1—C6—H6 | 118.00 |
| C2—C3—C4 | 118.03 (12) | N9—C10—H10 | 120.00 |
| C3—C4—C5 | 118.66 (12) | C11—C10—H10 | 120.00 |
| C4—C5—C6 | 119.07 (13) | C12—C11—H11 | 120.00 |
| N1—C6—C5 | 123.52 (13) | C10—C11—H11 | 120.00 |
| N8—C7—C3 | 115.96 (11) | C11—C12—H12 | 116.00 |
| O7—C7—C3 | 120.96 (11) | C21—C12—H12 | 116.00 |
| O7—C7—N8 | 123.08 (12) | C23—C22—H22 | 120.00 |
| N9—C10—C11 | 120.60 (12) | C21—C22—H22 | 120.00 |
| C10—C11—C12 | 120.49 (13) | C22—C23—H23 | 120.00 |
| C11—C12—C21 | 127.36 (13) | C24—C23—H23 | 120.00 |
| C12—C21—C22 | 123.19 (12) | C25—C24—H24 | 120.00 |
| C12—C21—C26 | 118.59 (12) | C23—C24—H24 | 120.00 |
| C22—C21—C26 | 118.21 (12) | C24—C25—H25 | 120.00 |
| C21—C22—C23 | 120.55 (13) | C26—C25—H25 | 120.00 |
| C22—C23—C24 | 120.84 (15) | C21—C26—H26 | 119.00 |
| C23—C24—C25 | 119.11 (14) | C25—C26—H26 | 119.00 |

| | | | |
|---|---|---|---|
| C24—C25—C26 | 120.21 (13) | | |
| | | | |
| C6—N1—C2—C3 | 1.2 (2) | C3—C4—C5—C6 | 0.4 (2) |
| C2—N1—C6—C5 | −2.0 (2) | C4—C5—C6—N1 | 1.2 (2) |
| C7—N8—N9—C10 | 179.89 (12) | N9—C10—C11—C12 | 179.83 (13) |
| N9—N8—C7—O7 | 5.25 (19) | C10—C11—C12—C21 | −177.76 (13) |
| N9—N8—C7—C3 | −174.34 (11) | C11—C12—C21—C22 | 10.7 (2) |
| N8—N9—C10—C11 | −177.62 (12) | C11—C12—C21—C26 | −168.23 (14) |
| N1—C2—C3—C4 | 0.3 (2) | C12—C21—C22—C23 | −176.56 (14) |
| N1—C2—C3—C7 | −177.10 (12) | C26—C21—C22—C23 | 2.4 (2) |
| C2—C3—C4—C5 | −1.10 (19) | C12—C21—C26—C25 | 176.51 (13) |
| C7—C3—C4—C5 | 176.05 (13) | C22—C21—C26—C25 | −2.5 (2) |
| C2—C3—C7—O7 | 16.54 (19) | C21—C22—C23—C24 | −0.3 (2) |
| C2—C3—C7—N8 | −163.87 (12) | C22—C23—C24—C25 | −1.7 (2) |
| C4—C3—C7—O7 | −160.64 (13) | C23—C24—C25—C26 | 1.6 (2) |
| C4—C3—C7—N8 | 18.96 (19) | C24—C25—C26—C21 | 0.5 (2) |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*W*—H1*W*···O7$^{ii}$ | 0.86 (3) | 2.52 (3) | 3.1550 (14) | 131.9 (19) |
| O1*W*—H1*W*···N9$^{ii}$ | 0.86 (3) | 2.16 (3) | 2.9655 (15) | 157 (2) |
| O1*W*—H2*W*···N1$^{i}$ | 0.88 (3) | 2.05 (3) | 2.9222 (15) | 176 (2) |
| N8—H8···O1*W* | 0.914 (18) | 1.944 (18) | 2.8486 (15) | 170.3 (17) |
| C2—H2···O7$^{iv}$ | 0.95 | 2.33 | 3.2253 (17) | 157 |
| C4—H4···O1*W* | 0.95 | 2.54 | 3.2392 (16) | 130 |
| C10—H10···O7$^{ii}$ | 0.95 | 2.57 | 3.1507 (17) | 120 |
| C22—H22···*Cg*1$^{iii}$ | 0.95 | 2.94 | 3.7742 (16) | 148 |
| C5—H5···*Cg*2$^{x}$ | 0.95 | 2.54 | 3.4342 (15) | 157 |

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