# (5-Hydroxy-3-methyl-5-phenyl-4,5-dihydro-1H-pyrazol-1-yl)(pyridin-4-yl)-methanone monohydrate

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In the title compound, $C_{16}H_{15}N_3O_2 \cdot H_2O$, the mean plane of the approximately planar pyrazole ring [maximum deviation = 0.0474 (18) Å] makes dihedral angles of 86.32 (11) and 45.04 (10)° with the phenyl and pyridine rings, respectively. The dihedral angle between the phenyl and pyridine rings is 69.62 (11)°. In the crystal, intermolecular O—H···O and O—H···N hydrogen bonds connect the components into chains along [010]. The crystal structure is further stabilized by $\pi$–$\pi$ stacking interactions with centroid–centroid distances of 3.7730 (12) Å.

## Related literature

For standard values of bond lengths, see: Allen et al. (1987).
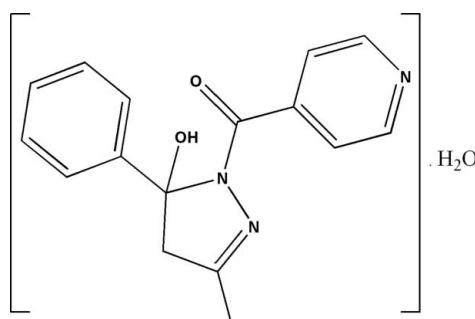


## Experimental

### Crystal data

| | |
|---|---|
| $C_{16}H_{15}N_3O_2 \cdot H_2O$ | $V$ = 1501.77 (16) Å³ |
| $M_r$ = 299.33 | $Z$ = 4 |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation |
| $a$ = 16.9676 (10) Å | $\mu$ = 0.09 mm⁻¹ |
| $b$ = 7.0266 (5) Å | $T$ = 296 K |
| $c$ = 12.6135 (6) Å | 0.32 × 0.24 × 0.18 mm |
| $\beta$ = 93.004 (3)° | |

### Data collection

| | |
|---|---|
| Bruker SMART APEXII CCD area-detector diffractometer | 8525 measured reflections |
| | 3059 independent reflections |
| Absorption correction: multi-scan (SADABS; Bruker, 2005) | 1916 reflections with $I > 2\sigma(I)$ |
| $T_{min}$ = 0.971, $T_{max}$ = 0.983 | $R_{int}$ = 0.038 |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.048 | 200 parameters |
| $wR(F^2)$ = 0.121 | H-atom parameters constrained |
| $S$ = 1.03 | $\Delta\rho_{max}$ = 0.15 e Å⁻³ |
| 3059 reflections | $\Delta\rho_{min}$ = −0.18 e Å⁻³ |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···O1$W^i$ | 0.92 | 1.84 | 2.7490 (19) | 173 |
| O1$W$—H1$W$1···O2$^{ii}$ | 0.92 | 1.89 | 2.8003 (19) | 169 |
| O1$W$—H2$W$1···N3$^{iii}$ | 0.85 | 2.13 | 2.976 (2) | 173 |

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

Data collection: APEX2 (Bruker, 2005); cell refinement: SAINT (Bruker, 2005); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL and PLATON (Spek, 2009); software used to prepare material for publication: SHELXTL and PLATON.

## References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). J. Chem. Soc. Perkin Trans. 2, pp. S1–19.
Bruker (2005). APEX2, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2008). Acta Cryst. A64, 112–122.
Spek, A. L. (2009). Acta Cryst. D65, 148–155.

# (5-Hydroxy-3-methyl-5-phenyl-4,5-dihydro-1*H*-pyrazol-1-yl)(pyridin-4-yl)methanone monohydrate

**Hadi Kargar, Reza Kia, Fatemeh Froozandeh, Moayad Hossaini Sadr and Muhammad Nawaz Tahir**

### S1. Comment

The asymmetric unit of the title compound, Fig. 1, comprises a substituted pyrazole molecule and a solvent water molecule. The bond lengths (Allen *et al.,* 1987) and angles are within the normal ranges. The dihedral angle the mean plane of the pyrazole ring makes with the phenyl and pyridine rings are 86.32 (11) and 45.04 (10)°, respectively. The dihedral angle between the phenyl ring and the pyridine ring is 69.62 (11)Å.

In the crystal structure, intermolecular O—H···O and O—H···N hydrogen bonds connect the components of the structure to form one-dimensional chains along [0 1 0]. The crystal structure is further stabilized by intermolecular $\pi$–$\pi$ stacking interactions [$Cg1···Cg1^{iv}$ = 3.7730 (11)Å, (iv) -*x*, 1 - *y*, -*z*, $Cg1$ is the centroid of the C12-C16/N3 ring].

### S2. Experimental

The title compound was synthesized by adding isoniazide (2 mmol) to a solution of benzoylacetone (2 mmol) in ethanol (20 ml). The mixture was refluxed with stirring for half an hour. The resultant solution was filtered and the white single crystals suitable for *X*-ray structure determination were recrystallized from ethanol by slow evaporation of the solvents at room temperature over several days.

### S3. Refinement

The H atoms of the water and hydroxy groups were located in a difference Fourier map and constraied to refine on the parent atom with $U_{iso}(H)$ = 1.5 $U_{eq}(O)$, see Table 1. The remaining H atoms were positioned geometrically with C—H = 0.93-0.97 Å and included in a riding-model approximation with $U_{iso}(H)$ = 1.2 or 1.5 $U_{eq}(C)$. A rotating group model was used for the methyl group.
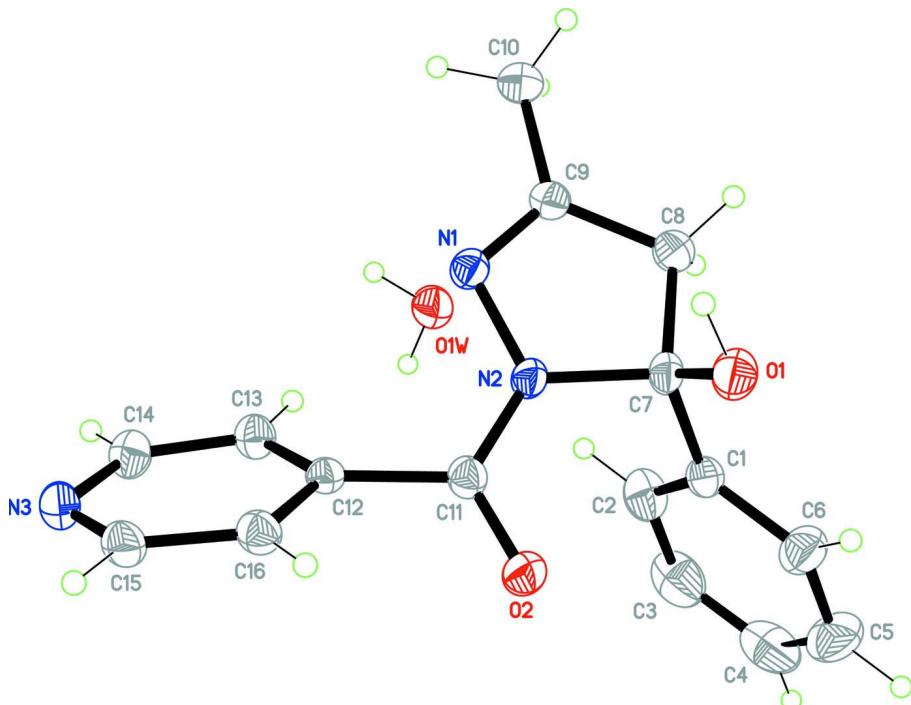
**Figure 1**

The asymmetric unit of the title compound, showing 30% probability displacement ellipsoids and the atomic numbering.
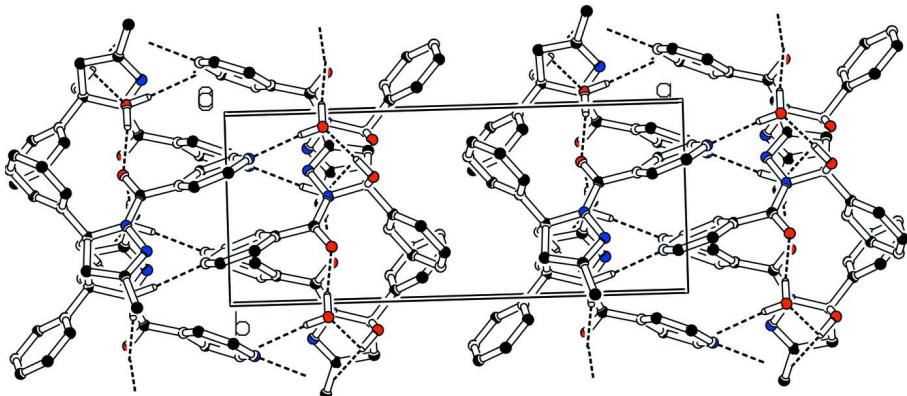


**Figure 2**

The packing of the compound viewed along the *c*-axis showing 1-D extended chains along the *b*-axis through hydrogen bonds. All H atoms removed except those involved in the hydrogen bonds. Hydrogen bonds are shown as dashed lines.

**(5-Hydroxy-3-methyl-5-phenyl-4,5-dihydro-1*H*-pyrazol-1-yl)(pyridin- 4-yl)methanone monohydrate**

*Crystal data*

| | |
|---|---|
| $C_{16}H_{15}N_3O_2 \cdot H_2O$ | $\beta = 93.004 (3)°$ |
| $M_r = 299.33$ | $V = 1501.77 (16)$ Å$^3$ |
| Monoclinic, $P2_1/c$ | $Z = 4$ |
| Hall symbol: -P 2ybc | $F(000) = 632$ |
| $a = 16.9676 (10)$ Å | $D_x = 1.324$ Mg m$^{-3}$ |
| $b = 7.0266 (5)$ Å | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $c = 12.6135 (6)$ Å | Cell parameters from 2540 reflections |

$\theta = 2.5$–$27.5°$

$\mu = 0.09$ mm$^{-1}$

$T = 296$ K

Prism, white

$0.32 \times 0.24 \times 0.18$ mm

*Data collection*

| | |
|---|---|
| Bruker SMART APEXII CCD area-detector diffractometer | 8525 measured reflections |
| Radiation source: fine-focus sealed tube | 3059 independent reflections |
| Graphite monochromator | 1916 reflections with $I > 2\sigma(I)$ |
| $\varphi$ and $\omega$ scans | $R_{int} = 0.038$ |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2005) | $\theta_{max} = 26.5°$, $\theta_{min} = 2.4°$ |
| | $h = -18 \rightarrow 21$ |
| | $k = -7 \rightarrow 8$ |
| $T_{min} = 0.971$, $T_{max} = 0.983$ | $l = -15 \rightarrow 14$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | |
| $R[F^2 > 2\sigma(F^2)] = 0.048$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.121$ | |
| $S = 1.03$ | H-atom parameters constrained |
| 3059 reflections | $w = 1/[\sigma^2(F_o^2) + (0.0554P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 200 parameters | |
| 0 restraints | $(\Delta/\sigma)_{max} < 0.001$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{max} = 0.15$ e Å$^{-3}$ |
| | $\Delta\rho_{min} = -0.18$ 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.

**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 $F^2 > 2\mathrm{sigma}(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.32045 (8) | 0.3424 (2) | −0.01490 (10) | 0.0461 (4) |
| H1 | 0.2849 | 0.2478 | −0.0322 | 0.069* |
| O2 | 0.22503 (8) | 0.70361 (19) | 0.00147 (10) | 0.0455 (4) |
| O1W | 0.21323 (8) | 0.4293 (2) | 0.41563 (10) | 0.0522 (4) |
| H1W1 | 0.2123 | 0.5449 | 0.4498 | 0.078* |
| H2W1 | 0.1656 | 0.3911 | 0.4143 | 0.078* |
| N1 | 0.17899 (8) | 0.3038 (2) | 0.15669 (11) | 0.0339 (4) |
| N2 | 0.22186 (8) | 0.4400 (2) | 0.10150 (11) | 0.0347 (4) |
| N3 | −0.05005 (9) | 0.7733 (2) | 0.10396 (13) | 0.0431 (4) |
| C1 | 0.36077 (10) | 0.5444 (3) | 0.12956 (14) | 0.0370 (5) |
| C2 | 0.35148 (13) | 0.6223 (3) | 0.22873 (16) | 0.0544 (6) |
| H2 | 0.3115 | 0.5788 | 0.2703 | 0.065* |
| C3 | 0.40176 (17) | 0.7653 (4) | 0.2661 (2) | 0.0726 (8) |

| | | | |
|---|---|---|---|
| H3A | 0.3947 | 0.8188 | 0.3323 | 0.087* |
| C4 | 0.46131 (16) | 0.8286 (4) | 0.2071 (3) | 0.0770 (8) |
| H4 | 0.4951 | 0.9238 | 0.2333 | 0.092* |
| C5 | 0.47118 (14) | 0.7520 (4) | 0.1099 (2) | 0.0726 (8) |
| H5 | 0.5119 | 0.7947 | 0.0694 | 0.087* |
| C6 | 0.42080 (12) | 0.6104 (3) | 0.07061 (17) | 0.0521 (6) |
| H6 | 0.4277 | 0.5596 | 0.0036 | 0.062* |
| C7 | 0.30659 (10) | 0.3854 (3) | 0.09099 (13) | 0.0359 (5) |
| C8 | 0.31075 (11) | 0.2087 (3) | 0.16286 (16) | 0.0449 (5) |
| H8A | 0.3310 | 0.1000 | 0.1255 | 0.054* |
| H8B | 0.3443 | 0.2320 | 0.2262 | 0.054* |
| C9 | 0.22789 (11) | 0.1762 (3) | 0.19037 (13) | 0.0339 (4) |
| C10 | 0.20331 (12) | 0.0106 (3) | 0.25333 (15) | 0.0469 (5) |
| H10A | 0.1476 | 0.0176 | 0.2628 | 0.070* |
| H10B | 0.2314 | 0.0116 | 0.3214 | 0.070* |
| H10C | 0.2150 | −0.1048 | 0.2166 | 0.070* |
| C11 | 0.18790 (11) | 0.5957 (3) | 0.05705 (13) | 0.0334 (4) |
| C12 | 0.10340 (10) | 0.6415 (2) | 0.07655 (13) | 0.0297 (4) |
| C13 | 0.07060 (11) | 0.6357 (3) | 0.17484 (14) | 0.0375 (5) |
| H13 | 0.0990 | 0.5858 | 0.2335 | 0.045* |
| C14 | −0.00432 (12) | 0.7045 (3) | 0.18447 (15) | 0.0430 (5) |
| H14 | −0.0247 | 0.7031 | 0.2515 | 0.052* |
| C15 | −0.01844 (11) | 0.7738 (3) | 0.00927 (15) | 0.0407 (5) |
| H15 | −0.0493 | 0.8176 | −0.0488 | 0.049* |
| C16 | 0.05681 (11) | 0.7135 (3) | −0.00760 (14) | 0.0361 (5) |
| H16 | 0.0764 | 0.7210 | −0.0750 | 0.043* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0399 (8) | 0.0500 (9) | 0.0490 (8) | −0.0025 (7) | 0.0074 (6) | −0.0062 (7) |
| O2 | 0.0370 (8) | 0.0445 (9) | 0.0556 (8) | 0.0018 (7) | 0.0082 (6) | 0.0166 (7) |
| O1W | 0.0428 (8) | 0.0447 (9) | 0.0690 (9) | −0.0001 (7) | 0.0023 (6) | −0.0063 (7) |
| N1 | 0.0297 (9) | 0.0353 (9) | 0.0368 (8) | −0.0024 (8) | 0.0008 (7) | 0.0024 (7) |
| N2 | 0.0240 (8) | 0.0362 (9) | 0.0438 (8) | 0.0016 (7) | 0.0022 (6) | 0.0106 (7) |
| N3 | 0.0319 (9) | 0.0421 (10) | 0.0553 (11) | 0.0033 (8) | 0.0027 (8) | −0.0013 (8) |
| C1 | 0.0274 (10) | 0.0373 (11) | 0.0457 (11) | 0.0028 (9) | −0.0031 (8) | 0.0043 (9) |
| C2 | 0.0458 (13) | 0.0606 (16) | 0.0564 (13) | 0.0085 (12) | −0.0017 (10) | −0.0066 (11) |
| C3 | 0.0676 (18) | 0.0689 (19) | 0.0786 (17) | 0.0129 (16) | −0.0232 (14) | −0.0247 (14) |
| C4 | 0.0537 (17) | 0.0506 (17) | 0.123 (2) | −0.0011 (14) | −0.0303 (16) | −0.0094 (16) |
| C5 | 0.0484 (15) | 0.0663 (19) | 0.102 (2) | −0.0183 (14) | −0.0027 (14) | 0.0144 (16) |
| C6 | 0.0413 (12) | 0.0551 (15) | 0.0598 (13) | −0.0080 (11) | 0.0028 (10) | 0.0046 (11) |
| C7 | 0.0253 (10) | 0.0393 (12) | 0.0434 (11) | 0.0041 (9) | 0.0048 (8) | 0.0036 (9) |
| C8 | 0.0352 (11) | 0.0387 (12) | 0.0605 (12) | 0.0049 (10) | 0.0006 (9) | 0.0118 (10) |
| C9 | 0.0355 (11) | 0.0314 (11) | 0.0345 (9) | 0.0005 (9) | 0.0000 (8) | −0.0005 (8) |
| C10 | 0.0472 (12) | 0.0370 (12) | 0.0567 (12) | 0.0009 (11) | 0.0055 (9) | 0.0069 (10) |
| C11 | 0.0294 (10) | 0.0355 (11) | 0.0349 (10) | 0.0017 (9) | −0.0009 (8) | 0.0008 (9) |
| C12 | 0.0289 (10) | 0.0249 (10) | 0.0351 (10) | −0.0014 (8) | 0.0004 (8) | −0.0009 (8) |

| C13 | 0.0348 (11) | 0.0420 (12) | 0.0355 (10) | 0.0022 (10) | −0.0015 (8) | 0.0012 (9) |
| C14 | 0.0381 (12) | 0.0480 (13) | 0.0431 (11) | −0.0005 (10) | 0.0053 (9) | −0.0035 (9) |
| C15 | 0.0343 (11) | 0.0386 (12) | 0.0480 (12) | 0.0020 (10) | −0.0095 (9) | 0.0048 (9) |
| C16 | 0.0363 (11) | 0.0358 (11) | 0.0360 (10) | 0.0017 (9) | −0.0013 (8) | 0.0013 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C7 | 1.401 (2) | C5—C6 | 1.386 (3) |
| O1—H1 | 0.9166 | C5—H5 | 0.9300 |
| O2—C11 | 1.229 (2) | C6—H6 | 0.9300 |
| O1W—H1W1 | 0.9200 | C7—C8 | 1.536 (3) |
| O1W—H2W1 | 0.8517 | C8—C9 | 1.483 (3) |
| N1—C9 | 1.279 (2) | C8—H8A | 0.9700 |
| N1—N2 | 1.408 (2) | C8—H8B | 0.9700 |
| N2—C11 | 1.345 (2) | C9—C10 | 1.481 (3) |
| N2—C7 | 1.501 (2) | C10—H10A | 0.9600 |
| N3—C15 | 1.334 (2) | C10—H10B | 0.9600 |
| N3—C14 | 1.336 (2) | C10—H10C | 0.9600 |
| C1—C6 | 1.373 (3) | C11—C12 | 1.502 (2) |
| C1—C2 | 1.382 (3) | C12—C16 | 1.386 (2) |
| C1—C7 | 1.511 (3) | C12—C13 | 1.386 (2) |
| C2—C3 | 1.384 (3) | C13—C14 | 1.371 (3) |
| C2—H2 | 0.9300 | C13—H13 | 0.9300 |
| C3—C4 | 1.360 (4) | C14—H14 | 0.9300 |
| C3—H3A | 0.9300 | C15—C16 | 1.372 (3) |
| C4—C5 | 1.358 (4) | C15—H15 | 0.9300 |
| C4—H4 | 0.9300 | C16—H16 | 0.9300 |
| | | | |
| C7—O1—H1 | 104.0 | C9—C8—H8A | 110.9 |
| H1W1—O1W—H2W1 | 104.4 | C7—C8—H8A | 110.9 |
| C9—N1—N2 | 107.33 (14) | C9—C8—H8B | 110.9 |
| C11—N2—N1 | 122.54 (15) | C7—C8—H8B | 110.9 |
| C11—N2—C7 | 124.25 (15) | H8A—C8—H8B | 108.9 |
| N1—N2—C7 | 113.06 (13) | N1—C9—C10 | 122.21 (17) |
| C15—N3—C14 | 115.90 (17) | N1—C9—C8 | 114.87 (16) |
| C6—C1—C2 | 118.6 (2) | C10—C9—C8 | 122.91 (17) |
| C6—C1—C7 | 122.12 (17) | C9—C10—H10A | 109.5 |
| C2—C1—C7 | 119.22 (17) | C9—C10—H10B | 109.5 |
| C1—C2—C3 | 119.9 (2) | H10A—C10—H10B | 109.5 |
| C1—C2—H2 | 120.1 | C9—C10—H10C | 109.5 |
| C3—C2—H2 | 120.1 | H10A—C10—H10C | 109.5 |
| C4—C3—C2 | 120.9 (2) | H10B—C10—H10C | 109.5 |
| C4—C3—H3A | 119.5 | O2—C11—N2 | 121.24 (17) |
| C2—C3—H3A | 119.5 | O2—C11—C12 | 118.90 (16) |
| C5—C4—C3 | 119.6 (2) | N2—C11—C12 | 119.85 (16) |
| C5—C4—H4 | 120.2 | C16—C12—C13 | 117.15 (17) |
| C3—C4—H4 | 120.2 | C16—C12—C11 | 117.65 (15) |
| C4—C5—C6 | 120.3 (2) | C13—C12—C11 | 124.86 (16) |

| | | | |
|---|---|---|---|
| C4—C5—H5 | 119.9 | C14—C13—C12 | 119.10 (17) |
| C6—C5—H5 | 119.9 | C14—C13—H13 | 120.4 |
| C1—C6—C5 | 120.7 (2) | C12—C13—H13 | 120.4 |
| C1—C6—H6 | 119.7 | N3—C14—C13 | 124.36 (18) |
| C5—C6—H6 | 119.7 | N3—C14—H14 | 117.8 |
| O1—C7—N2 | 110.42 (13) | C13—C14—H14 | 117.8 |
| O1—C7—C1 | 109.67 (14) | N3—C15—C16 | 123.97 (17) |
| N2—C7—C1 | 110.60 (15) | N3—C15—H15 | 118.0 |
| O1—C7—C8 | 112.56 (16) | C16—C15—H15 | 118.0 |
| N2—C7—C8 | 99.74 (14) | C15—C16—C12 | 119.47 (17) |
| C1—C7—C8 | 113.51 (15) | C15—C16—H16 | 120.3 |
| C9—C8—C7 | 104.34 (15) | C12—C16—H16 | 120.3 |
| | | | |
| C9—N1—N2—C11 | −179.02 (16) | N2—C7—C8—C9 | 7.23 (18) |
| C9—N1—N2—C7 | 5.31 (18) | C1—C7—C8—C9 | 124.87 (16) |
| C6—C1—C2—C3 | 0.6 (3) | N2—N1—C9—C10 | 179.31 (16) |
| C7—C1—C2—C3 | 178.63 (19) | N2—N1—C9—C8 | 0.2 (2) |
| C1—C2—C3—C4 | −1.1 (4) | C7—C8—C9—N1 | −5.2 (2) |
| C2—C3—C4—C5 | 0.7 (4) | C7—C8—C9—C10 | 175.69 (17) |
| C3—C4—C5—C6 | 0.2 (4) | N1—N2—C11—O2 | −173.53 (15) |
| C2—C1—C6—C5 | 0.2 (3) | C7—N2—C11—O2 | 1.7 (3) |
| C7—C1—C6—C5 | −177.7 (2) | N1—N2—C11—C12 | 7.4 (2) |
| C4—C5—C6—C1 | −0.6 (4) | C7—N2—C11—C12 | −177.38 (15) |
| C11—N2—C7—O1 | −64.9 (2) | O2—C11—C12—C16 | 39.6 (2) |
| N1—N2—C7—O1 | 110.71 (15) | N2—C11—C12—C16 | −141.39 (18) |
| C11—N2—C7—C1 | 56.7 (2) | O2—C11—C12—C13 | −133.48 (19) |
| N1—N2—C7—C1 | −127.72 (15) | N2—C11—C12—C13 | 45.6 (3) |
| C11—N2—C7—C8 | 176.49 (17) | C16—C12—C13—C14 | −1.5 (3) |
| N1—N2—C7—C8 | −7.92 (18) | C11—C12—C13—C14 | 171.52 (18) |
| C6—C1—C7—O1 | −8.6 (2) | C15—N3—C14—C13 | −0.4 (3) |
| C2—C1—C7—O1 | 173.52 (17) | C12—C13—C14—N3 | 2.0 (3) |
| C6—C1—C7—N2 | −130.57 (19) | C14—N3—C15—C16 | −1.7 (3) |
| C2—C1—C7—N2 | 51.5 (2) | N3—C15—C16—C12 | 2.1 (3) |
| C6—C1—C7—C8 | 118.3 (2) | C13—C12—C16—C15 | −0.4 (3) |
| C2—C1—C7—C8 | −59.6 (2) | C11—C12—C16—C15 | −173.97 (17) |
| O1—C7—C8—C9 | −109.82 (17) | | |

*Hydrogen-bond geometry (Å, º)*

| D—H⋯A | D—H | H⋯A | D⋯A | D—H⋯A |
|---|---|---|---|---|
| O1—H1⋯O1Wⁱ | 0.92 | 1.84 | 2.7490 (19) | 173 |
| O1W—H1W1⋯O2ⁱⁱ | 0.92 | 1.89 | 2.8003 (19) | 169 |
| O1W—H2W1⋯N3ⁱⁱⁱ | 0.85 | 2.13 | 2.976 (2) | 173 |

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