# organic compounds

# 6-Amino-3,4-dimethyl-4-phenyl-2H,4H-pyrano[2,3-c]pyrazole-5-carbonitrile

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In the title compound, $C_{15}H_{14}N_4O$, the pyrazole ring is aligned at 88.23 (4)° with respect to the aromatic ring and at 3.75 (4)° with respect to the pyran ring. In the crystal, N—H···N hydrogen bonds link adjacent molecules into a linear chain motif. C—H···N interactions are also observed.

## Related literature

For the synthesis, see: Vasuki & Kumaravel (2008). For the use of related compounds in organic synthesis, see: Liang *et al.* (2009). For related structures, see: Kannan *et al.* (2010).



## Experimental

### Crystal data

| | |
|---|---|
| $C_{15}H_{14}N_4O$ | $c = 11.078$ (5) Å |
| $M_r = 266.3$ | $\alpha = 99.213$ (5)° |
| Triclinic, $P\bar{1}$ | $\beta = 102.740$ (5)° |
| $a = 6.682$ (5) Å | $\gamma = 97.767$ (5)° |
| $b = 9.347$ (5) Å | $V = 655.6$ (7) Å$^3$ |

| | |
|---|---|
| $Z = 2$ | $T = 293$ K |
| Mo $K\alpha$ radiation | $0.22 \times 0.20 \times 0.16$ mm |
| $\mu = 0.09$ mm$^{-1}$ | |

### Data collection

| | |
|---|---|
| Bruker APEXII Kappa CCD detector diffractometer | 4996 independent reflections |
| | 3169 reflections with $I > 2\sigma(I)$ |
| 18424 measured reflections | $R_{int} = 0.036$ |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.057$ | 183 parameters |
| $wR(F^2) = 0.173$ | H-atom parameters constrained |
| $S = 0.99$ | $\Delta\rho_{max} = 0.30$ e Å$^{-3}$ |
| 4996 reflections | $\Delta\rho_{min} = -0.29$ e Å$^{-3}$ |

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

| $D—H\cdots A$ | $D—H$ | $H\cdots A$ | $D\cdots A$ | $D—H\cdots A$ |
|---|---|---|---|---|
| N3—H3A···N1$^i$ | 0.86 | 2.27 | 3.129 (2) | 173 |
| N3—H3B···N4$^{ii}$ | 0.86 | 2.26 | 3.087 (2) | 160 |
| C10—H10···N4$^{iii}$ | 0.93 | 2.53 | 3.455 (3) | 172 |
| C14—H14A···N1$^{iv}$ | 0.96 | 2.59 | 3.522 (3) | 163 |

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); 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).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5120).

## References

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Liang, F., Cheng, X., Liu, J. & Liu, Q. (2009). *Chem. Commun.* pp. 3636–3538.
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Vasuki, G. & Kumaravel, K. (2008). *Tetrahedron Lett.* **49**, 5636–5638.

# supporting information

## 6-Amino-3,4-dimethyl-4-phenyl-2*H*,4*H*-pyrano[2,3-*c*]pyrazole-5-carbonitrile

**Nishith Saurav Topno, Kandhasamy Kumaravel, M. Kannan, Gnanasambandam Vasuki and R. Krishna**

### S1. Comment

The pyrano pyrazole derivatives are widely used as organic intermediates (Liang *et al.*, 2009) and are well known for their biological contribution as ChK1 inhibitors. In view of the growing importance of the pyrano pyrazole derivatives, we have synthesized the title compound by Rapid four-component reactions in water (Vasuki & Kumaravel, 2008) and the single-crystal structure analysis was undertaken.

In the title compound, the attached benzyl ring makes the dihedral angle of 88.23 (4) ° and orient in (+)-*syn*-clinal conforamtion with pyrazole ring, whereas the fused pyrazole ring makes 3.75 (4) ° dihedral angle and orient by an (+)-*syn*-periplanar conformation with respect to the pyran ring (Fig. 1). The methyl group is attached to C6 atom of pyran with an angle of 109.29 (11) °. Two N—H⋯N and C—H⋯N intermolecular hydrogen bond interactions (Fig. 2) are observed for maintaining the crystal packing (Fig. 3), in which the N3—H⋯N4 intermolecular interaction are observed to form $R_2^2$ (12) ring motifs (Fig. 4). The weak N—H⋯$\pi$ intermolecular interaction is also observed for the stabilization of the crystal packing, with a bond distance of 3.382 (3) Å (Fig. 5).

### S2. Experimental

The title compound was prepared by the successive addition of acetophenone 2 (0.240 g, 2 mmol), malononitrile (0.132 g, 2 mmol) and piperidine (5 mol%) to a stirred aqueous mixture of hydrazine hydrate 96% 1 (0.107 g, 2 mmol) and ethyl acetoacetate 2 (0.520 g, 2 mmol) at room temperature under an open atmosphere with vigorous stirring for 5–10 min. The precipitated solid was then filtered, followed by washing with water and then with a mixture of ethyl acetate/hexane (20:80). The product obtained was pure by TLC and 1H NMR spectroscopy. Nevertheless, the products were further purified by recrystallization from ethanol. Analysis calculated for 6-amino-3,4-dimethyl-4-phenyl-2*H*,4*H*-pyrano[2,3-*c*]pyrazole-5-carbonitrile showed that it has $C_{15}H_{14}N_4O$.

### S3. Refinement

All hydrogen atoms were placed in calculated positions, with N—H=0.86 and C—H=0.93–0.97 and included in the final cycles of refinement using a riding model with $U(H) = 1.2\ U_{eq}(C)$.
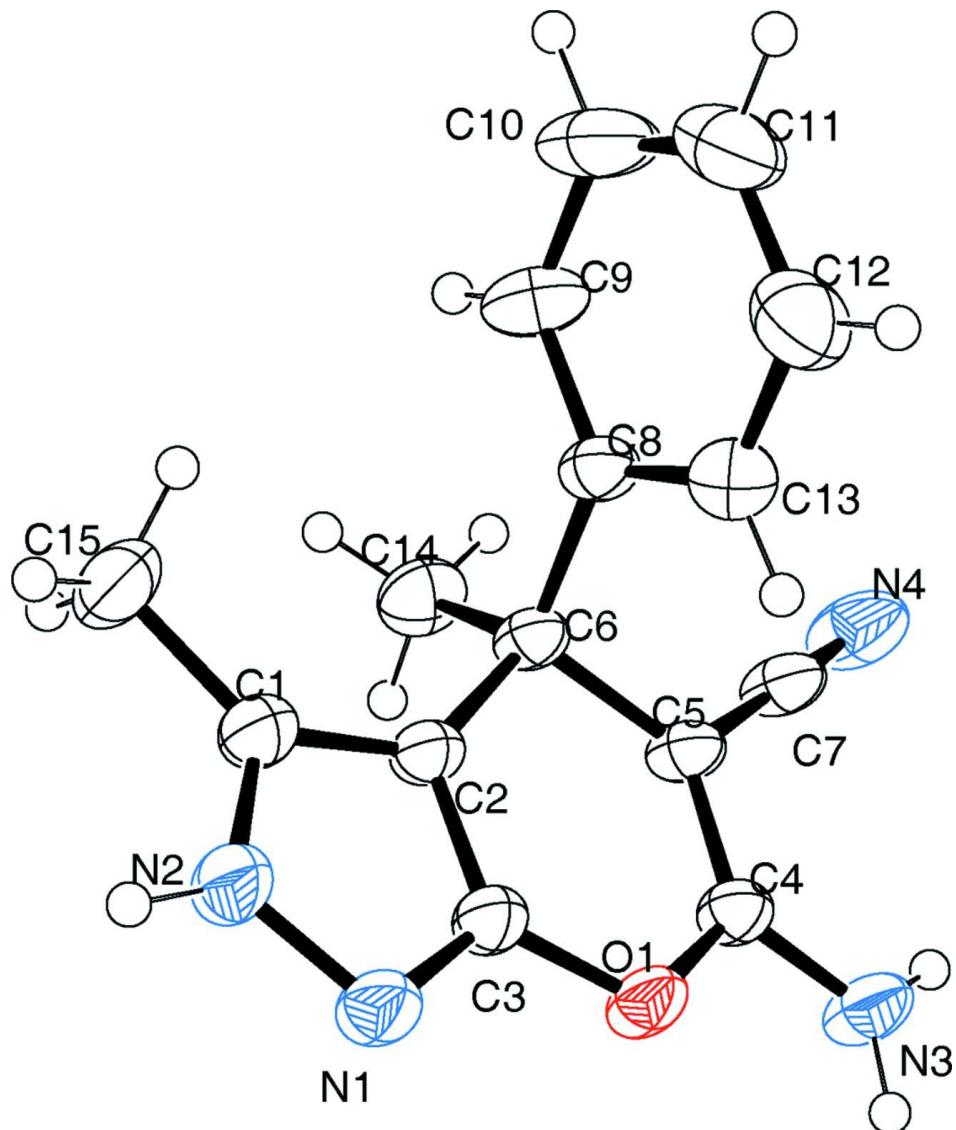
**Figure 1**

The molecular structure of (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level.
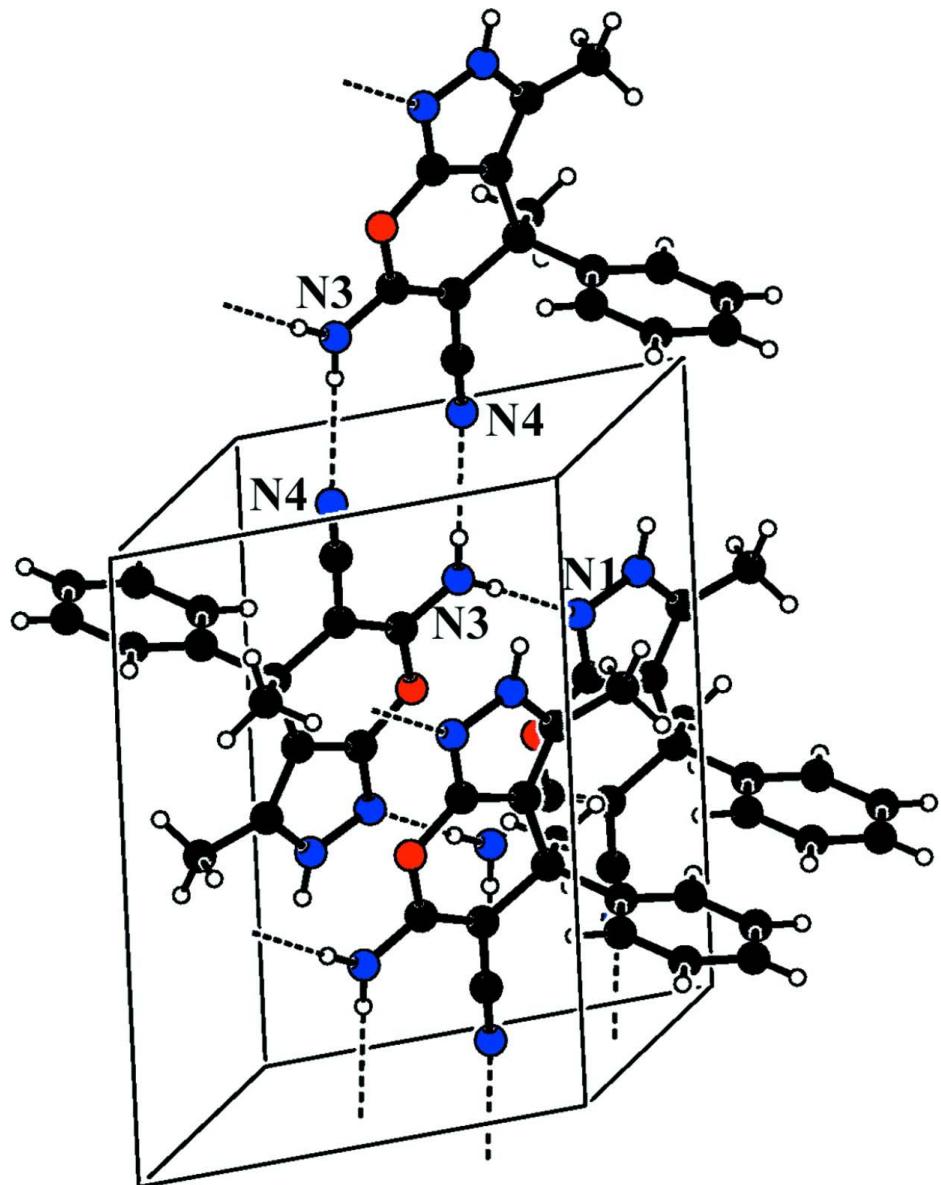
**Figure 2**
The crystal packing of (I), showing intermolecular hydrogen bonding interactions as dashed lines.
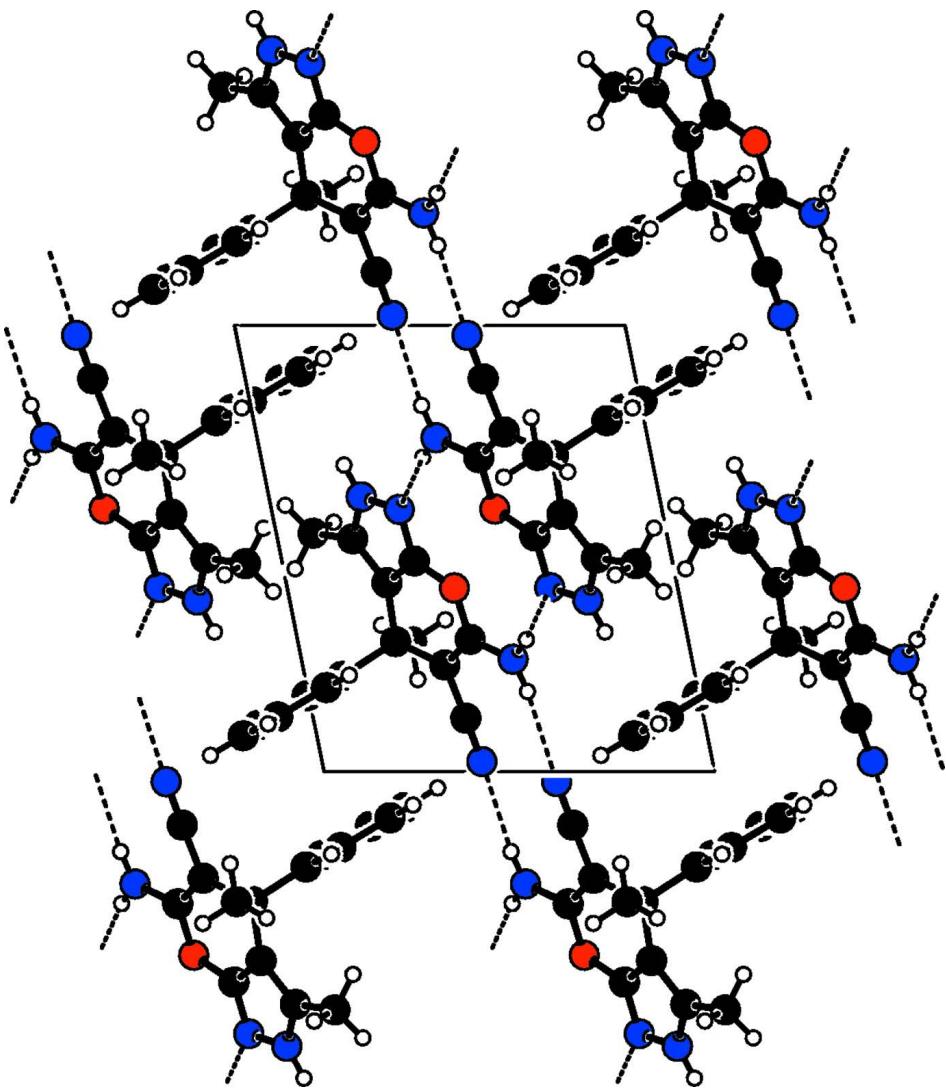
**Figure 3**

The crystal packing of Compound (I) viewed down the *XO*-axis, showing intermolecular hydrogen bonding interactions as dashed lines.
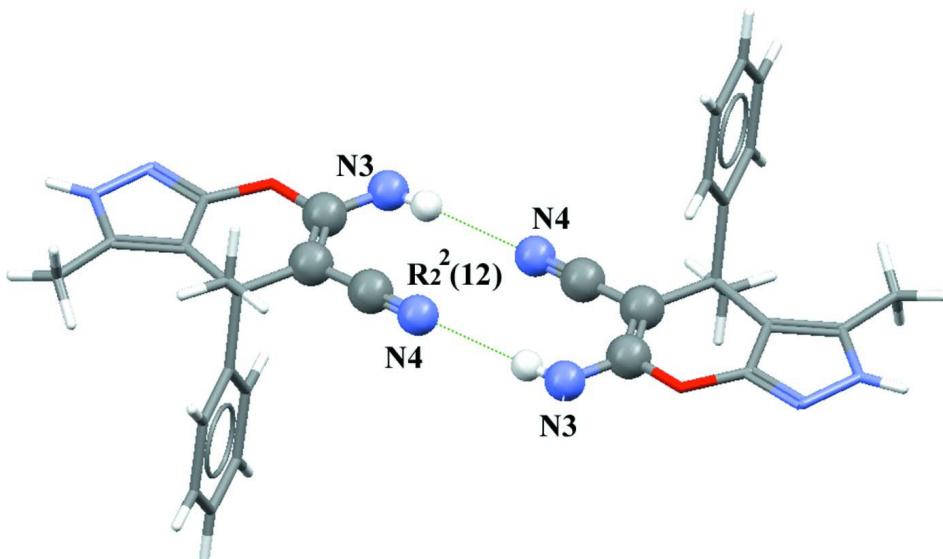
**Figure 4**

A view of $R_2^2$ (12) ring motifs formed by N—H···N interaction between two molecules. The ring forming atoms are shown in ball and stick model and the Hydrogen bond are shown in green dashed lines.
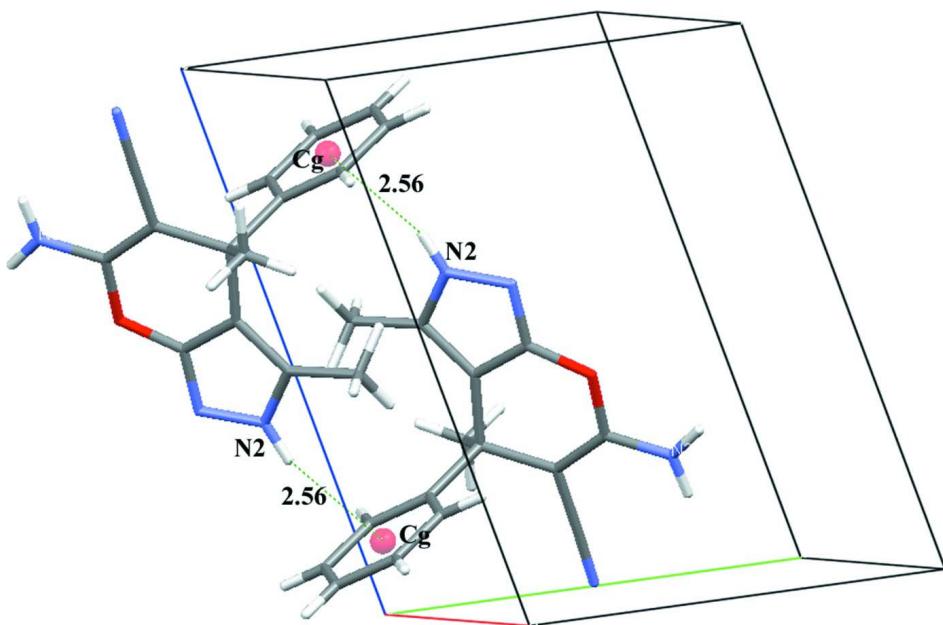


**Figure 5**

The molecular interaction showing the weak N—H···pi interaction in Compound (I). *Cg* is a centroid of $C_8$—$C_{13}$ ring.

**6-Amino-3,4-dimethyl-4-phenyl-2*H*,4*H*-pyrano[2,3-*c*]pyrazole- 5-carbonitrile**

*Crystal data*

| | |
|---|---|
| $C_{15}H_{14}N_4O$ | $b = 9.347$ (5) Å |
| $M_r = 266.3$ | $c = 11.078$ (5) Å |
| Triclinic, $P\overline{1}$ | $\alpha = 99.213$ (5)° |
| Hall symbol: -P 1 | $\beta = 102.740$ (5)° |
| $a = 6.682$ (5) Å | $\gamma = 97.767$ (5)° |

$V = 655.6$ (7) Å$^3$

$Z = 2$

$F(000) = 280$

$D_x = 1.349$ Mg m$^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å

Cell parameters from 4350 reflections

$\theta = 1.9–33.3°$

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

$T = 293$ K

Prism, colourless

$0.22 \times 0.20 \times 0.16$ mm

*Data collection*

Bruker APEXII Kappa CCD-detector diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 0 pixels mm$^{-1}$

$\omega$ and $\varphi$ scans

18424 measured reflections

4996 independent reflections

3169 reflections with $I > 2\sigma(I)$

$R_{int} = 0.036$

$\theta_{max} = 33.3°$, $\theta_{min} = 1.9°$

$h = -10 \rightarrow 9$

$k = -14 \rightarrow 14$

$l = -17 \rightarrow 16$

*Refinement*

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.057$

$wR(F^2) = 0.173$

$S = 0.99$

4996 reflections

183 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-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0847P)^2 + 0.1309P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.014$

$\Delta\rho_{max} = 0.30$ e Å$^{-3}$

$\Delta\rho_{min} = -0.29$ e Å$^{-3}$

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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 ($Å^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.22065 (13) | 0.57205 (11) | 0.58851 (9) | 0.0380 (2) |
| C2 | 0.52515 (18) | 0.74174 (14) | 0.57658 (11) | 0.0306 (3) |
| N1 | 0.23543 (18) | 0.67259 (14) | 0.41251 (11) | 0.0406 (3) |
| C6 | 0.64969 (18) | 0.74989 (14) | 0.70869 (12) | 0.0304 (2) |
| C5 | 0.52503 (19) | 0.63581 (14) | 0.76101 (12) | 0.0315 (3) |
| C7 | 0.6205 (2) | 0.60943 (15) | 0.88018 (13) | 0.0377 (3) |
| C4 | 0.32984 (19) | 0.55767 (14) | 0.70373 (12) | 0.0315 (3) |
| C3 | 0.32497 (19) | 0.66098 (15) | 0.52808 (12) | 0.0320 (3) |
| C8 | 0.6664 (2) | 0.90474 (14) | 0.78630 (12) | 0.0332 (3) |
| N3 | 0.21879 (18) | 0.45814 (14) | 0.74817 (12) | 0.0439 (3) |
| H3A | 0.0968 | 0.4142 | 0.7044 | 0.053* |
| H3B | 0.2692 | 0.4379 | 0.8206 | 0.053* |

| | | | |
|---|---|---|---|
| N2 | 0.38757 (19) | 0.76374 (15) | 0.38430 (11) | 0.0432 (3) |
| H2 | 0.3736 | 0.7912 | 0.3129 | 0.052* |
| N4 | 0.7004 (2) | 0.59058 (17) | 0.97741 (14) | 0.0571 (4) |
| C1 | 0.5621 (2) | 0.80702 (16) | 0.47848 (13) | 0.0376 (3) |
| C14 | 0.8640 (2) | 0.70915 (18) | 0.70847 (16) | 0.0438 (3) |
| H14A | 0.8467 | 0.6116 | 0.6599 | 0.066* |
| H14B | 0.9397 | 0.7124 | 0.7936 | 0.066* |
| H14C | 0.9401 | 0.7779 | 0.6718 | 0.066* |
| C13 | 0.4882 (2) | 0.95084 (17) | 0.81184 (15) | 0.0442 (3) |
| H13 | 0.3617 | 0.8859 | 0.7841 | 0.053* |
| C9 | 0.8513 (3) | 1.00406 (18) | 0.82993 (17) | 0.0517 (4) |
| H9 | 0.9738 | 0.9768 | 0.8150 | 0.062* |
| C10 | 0.8558 (3) | 1.1452 (2) | 0.89631 (18) | 0.0639 (5) |
| H10 | 0.9817 | 1.2109 | 0.9251 | 0.077* |
| C15 | 0.7477 (3) | 0.9053 (2) | 0.46603 (16) | 0.0536 (4) |
| H15A | 0.8448 | 0.8469 | 0.4411 | 0.080* |
| H15B | 0.8130 | 0.9701 | 0.5456 | 0.080* |
| H15C | 0.7051 | 0.9625 | 0.4033 | 0.080* |
| C12 | 0.4943 (3) | 1.0905 (2) | 0.87732 (17) | 0.0568 (4) |
| H12 | 0.3727 | 1.1186 | 0.8930 | 0.068* |
| C11 | 0.6797 (4) | 1.18818 (19) | 0.91953 (16) | 0.0595 (5) |
| H11 | 0.6843 | 1.2826 | 0.9635 | 0.071* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0256 (4) | 0.0500 (6) | 0.0318 (5) | −0.0082 (4) | −0.0019 (3) | 0.0142 (4) |
| C2 | 0.0260 (5) | 0.0314 (6) | 0.0302 (6) | −0.0015 (4) | 0.0032 (4) | 0.0049 (4) |
| N1 | 0.0346 (6) | 0.0480 (7) | 0.0319 (6) | −0.0072 (5) | −0.0007 (4) | 0.0116 (5) |
| C6 | 0.0233 (5) | 0.0309 (6) | 0.0322 (6) | −0.0011 (4) | 0.0012 (4) | 0.0056 (4) |
| C5 | 0.0272 (5) | 0.0296 (6) | 0.0320 (6) | −0.0019 (4) | −0.0014 (4) | 0.0073 (5) |
| C7 | 0.0308 (6) | 0.0350 (7) | 0.0397 (7) | −0.0061 (5) | −0.0026 (5) | 0.0109 (5) |
| C4 | 0.0266 (5) | 0.0338 (6) | 0.0303 (6) | 0.0004 (4) | 0.0013 (4) | 0.0072 (5) |
| C3 | 0.0273 (5) | 0.0362 (6) | 0.0290 (6) | −0.0015 (4) | 0.0029 (4) | 0.0073 (5) |
| C8 | 0.0330 (6) | 0.0318 (6) | 0.0286 (6) | −0.0033 (5) | −0.0005 (5) | 0.0066 (5) |
| N3 | 0.0331 (6) | 0.0509 (7) | 0.0396 (6) | −0.0111 (5) | −0.0038 (5) | 0.0191 (5) |
| N2 | 0.0415 (6) | 0.0517 (7) | 0.0308 (6) | −0.0082 (5) | 0.0030 (5) | 0.0144 (5) |
| N4 | 0.0472 (7) | 0.0635 (9) | 0.0477 (8) | −0.0143 (6) | −0.0114 (6) | 0.0260 (7) |
| C1 | 0.0327 (6) | 0.0407 (7) | 0.0352 (7) | −0.0031 (5) | 0.0057 (5) | 0.0075 (5) |
| C14 | 0.0271 (6) | 0.0477 (8) | 0.0529 (9) | 0.0045 (5) | 0.0052 (6) | 0.0076 (7) |
| C13 | 0.0464 (8) | 0.0385 (8) | 0.0450 (8) | 0.0025 (6) | 0.0122 (6) | 0.0034 (6) |
| C9 | 0.0384 (7) | 0.0422 (8) | 0.0600 (10) | −0.0085 (6) | −0.0025 (7) | 0.0016 (7) |
| C10 | 0.0682 (12) | 0.0430 (9) | 0.0577 (11) | −0.0165 (8) | −0.0087 (9) | −0.0007 (8) |
| C15 | 0.0450 (8) | 0.0609 (10) | 0.0498 (9) | −0.0142 (7) | 0.0090 (7) | 0.0193 (8) |
| C12 | 0.0746 (12) | 0.0457 (9) | 0.0514 (10) | 0.0136 (8) | 0.0213 (9) | 0.0032 (7) |
| C11 | 0.0922 (14) | 0.0371 (8) | 0.0405 (8) | 0.0039 (9) | 0.0083 (9) | −0.0001 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C4 | 1.3602 (16) | N2—C1 | 1.3465 (19) |
| O1—C3 | 1.3611 (16) | N2—H2 | 0.8600 |
| C2—C1 | 1.3799 (19) | C1—C15 | 1.486 (2) |
| C2—C3 | 1.3885 (18) | C14—H14A | 0.9600 |
| C2—C6 | 1.5001 (18) | C14—H14B | 0.9600 |
| N1—C3 | 1.3164 (17) | C14—H14C | 0.9600 |
| N1—N2 | 1.3595 (17) | C13—C12 | 1.379 (2) |
| C6—C5 | 1.5289 (18) | C13—H13 | 0.9300 |
| C6—C14 | 1.531 (2) | C9—C10 | 1.397 (3) |
| C6—C8 | 1.5369 (19) | C9—H9 | 0.9300 |
| C5—C4 | 1.3661 (18) | C10—C11 | 1.357 (3) |
| C5—C7 | 1.4091 (19) | C10—H10 | 0.9300 |
| C7—N4 | 1.1440 (19) | C15—H15A | 0.9600 |
| C4—N3 | 1.3340 (17) | C15—H15B | 0.9600 |
| C8—C9 | 1.380 (2) | C15—H15C | 0.9600 |
| C8—C13 | 1.390 (2) | C12—C11 | 1.374 (3) |
| N3—H3A | 0.8600 | C12—H12 | 0.9300 |
| N3—H3B | 0.8600 | C11—H11 | 0.9300 |
| | | | |
| C4—O1—C3 | 115.59 (10) | N2—C1—C2 | 106.17 (12) |
| C1—C2—C3 | 103.33 (11) | N2—C1—C15 | 122.22 (14) |
| C1—C2—C6 | 133.30 (11) | C2—C1—C15 | 131.61 (13) |
| C3—C2—C6 | 123.33 (11) | C6—C14—H14A | 109.5 |
| C3—N1—N2 | 101.74 (11) | C6—C14—H14B | 109.5 |
| C2—C6—C5 | 105.36 (10) | H14A—C14—H14B | 109.5 |
| C2—C6—C14 | 110.78 (11) | C6—C14—H14C | 109.5 |
| C5—C6—C14 | 109.28 (12) | H14A—C14—H14C | 109.5 |
| C2—C6—C8 | 109.09 (10) | H14B—C14—H14C | 109.5 |
| C5—C6—C8 | 109.98 (11) | C12—C13—C8 | 121.64 (15) |
| C14—C6—C8 | 112.12 (10) | C12—C13—H13 | 119.2 |
| C4—C5—C7 | 116.92 (12) | C8—C13—H13 | 119.2 |
| C4—C5—C6 | 126.31 (11) | C8—C9—C10 | 120.50 (17) |
| C7—C5—C6 | 116.77 (11) | C8—C9—H9 | 119.8 |
| N4—C7—C5 | 178.69 (15) | C10—C9—H9 | 119.8 |
| N3—C4—O1 | 110.00 (11) | C11—C10—C9 | 121.11 (17) |
| N3—C4—C5 | 127.07 (12) | C11—C10—H10 | 119.4 |
| O1—C4—C5 | 122.93 (12) | C9—C10—H10 | 119.4 |
| N1—C3—O1 | 119.33 (11) | C1—C15—H15A | 109.5 |
| N1—C3—C2 | 114.94 (12) | C1—C15—H15B | 109.5 |
| O1—C3—C2 | 125.71 (12) | H15A—C15—H15B | 109.5 |
| C9—C8—C13 | 117.40 (14) | C1—C15—H15C | 109.5 |
| C9—C8—C6 | 123.01 (13) | H15A—C15—H15C | 109.5 |
| C13—C8—C6 | 119.57 (11) | H15B—C15—H15C | 109.5 |
| C4—N3—H3A | 120.0 | C11—C12—C13 | 120.16 (18) |
| C4—N3—H3B | 120.0 | C11—C12—H12 | 119.9 |
| H3A—N3—H3B | 120.0 | C13—C12—H12 | 119.9 |

| | | | |
|---|---|---|---|
| C1—N2—N1 | 113.80 (12) | C10—C11—C12 | 119.19 (17) |
| C1—N2—H2 | 123.1 | C10—C11—H11 | 120.4 |
| N1—N2—H2 | 123.1 | C12—C11—H11 | 120.4 |
| | | | |
| C1—C2—C6—C5 | −173.79 (14) | C6—C2—C3—N1 | 176.69 (12) |
| C3—C2—C6—C5 | 8.91 (17) | C1—C2—C3—O1 | 177.46 (13) |
| C1—C2—C6—C14 | −55.7 (2) | C6—C2—C3—O1 | −4.6 (2) |
| C3—C2—C6—C14 | 126.98 (14) | C2—C6—C8—C9 | −111.80 (15) |
| C1—C2—C6—C8 | 68.17 (18) | C5—C6—C8—C9 | 133.10 (14) |
| C3—C2—C6—C8 | −109.13 (14) | C14—C6—C8—C9 | 11.29 (19) |
| C2—C6—C5—C4 | −7.33 (18) | C2—C6—C8—C13 | 66.30 (15) |
| C14—C6—C5—C4 | −126.40 (15) | C5—C6—C8—C13 | −48.80 (16) |
| C8—C6—C5—C4 | 110.12 (15) | C14—C6—C8—C13 | −170.61 (13) |
| C2—C6—C5—C7 | 173.06 (12) | C3—N1—N2—C1 | −0.42 (17) |
| C14—C6—C5—C7 | 53.99 (16) | N1—N2—C1—C2 | −0.34 (18) |
| C8—C6—C5—C7 | −69.50 (15) | N1—N2—C1—C15 | 179.23 (15) |
| C4—C5—C7—N4 | −158 (8) | C3—C2—C1—N2 | 0.91 (15) |
| C6—C5—C7—N4 | 21 (8) | C6—C2—C1—N2 | −176.77 (14) |
| C3—O1—C4—N3 | −174.36 (12) | C3—C2—C1—C15 | −178.61 (17) |
| C3—O1—C4—C5 | 5.24 (19) | C6—C2—C1—C15 | 3.7 (3) |
| C7—C5—C4—N3 | −0.2 (2) | C9—C8—C13—C12 | 0.5 (2) |
| C6—C5—C4—N3 | −179.80 (13) | C6—C8—C13—C12 | −177.74 (14) |
| C7—C5—C4—O1 | −179.72 (12) | C13—C8—C9—C10 | −0.4 (2) |
| C6—C5—C4—O1 | 0.7 (2) | C6—C8—C9—C10 | 177.75 (15) |
| N2—N1—C3—O1 | −177.77 (12) | C8—C9—C10—C11 | 0.0 (3) |
| N2—N1—C3—C2 | 1.06 (17) | C8—C13—C12—C11 | −0.2 (3) |
| C4—O1—C3—N1 | 175.29 (12) | C9—C10—C11—C12 | 0.3 (3) |
| C4—O1—C3—C2 | −3.4 (2) | C13—C12—C11—C10 | −0.2 (3) |
| C1—C2—C3—N1 | −1.29 (17) | | |

*Hydrogen-bond geometry (Å, º)*

| D—H···A | D—H | H···A | D···A | D—H···A |
|---|---|---|---|---|
| N3—H3A···N1ⁱ | 0.86 | 2.27 | 3.129 (2) | 173 |
| N3—H3B···N4ⁱⁱ | 0.86 | 2.26 | 3.087 (2) | 160 |
| C10—H10···N4ⁱⁱⁱ | 0.93 | 2.53 | 3.455 (3) | 172 |
| C14—H14A···N1ⁱᵛ | 0.96 | 2.59 | 3.522 (3) | 163 |

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