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# Ethyl 2-(6-amino-5-cyano-3,4-dimethyl-2*H*,4*H*-pyrano[2,3-c]pyrazol-4-yl)acetate

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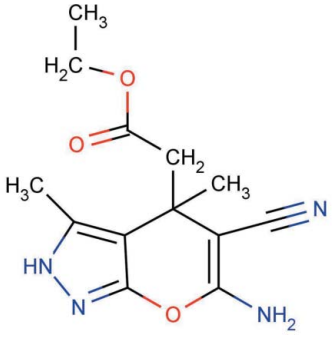
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.041; $wR$ factor = 0.117; data-to-parameter ratio = 12.9.

In he title compound, $C_{13}H_{16}N_4O_3$, the pyrazole ring is planar (r.m.s. deviation = 0.054 Å). The pyran ring is not planar; the mean plane makes a dihedral angle of 1.9 (1)° with the pyrazole ring. In the crystal structure, intermolecular N—H···N and N—H···O interactions lead to a linear chain motif.

## Related literature

For biological applications of pyrazole and pyranopyrazole derivatives, see: Wamhoff *et al.* (1993).; Velaparthi *et al.* (2008); Magedov *et al.* (2007); Rovnyak *et al.* (1982). For the synthesis, see: Vasuki & Kumaravel (2008).




## Experimental

### Crystal data

$C_{13}H_{16}N_4O_3$
$M_r$ = 276.30
Triclinic, $P\overline{1}$
$a$ = 6.961 (5) Å
$b$ = 7.373 (5) Å
$c$ = 14.535 (5) Å
$\alpha$ = 86.405 (5)°
$\beta$ = 85.183 (5)°
$\gamma$ = 65.726 (5)°
$V$ = 677.3 (7) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.10 mm$^{-1}$
$T$ = 293 K
0.25 × 0.20 × 0.20 mm

### Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker 2004)
$T_{min}$ = 0.976, $T_{max}$ = 0.981
12811 measured reflections
2385 independent reflections
2130 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.020

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.117
$S$ = 1.02
2378 reflections
184 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.26 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2···O2$^{i}$ | 0.86 | 2.55 | 3.274 (2) | 142 |
| N2—H2···N1$^{ii}$ | 0.86 | 2.37 | 2.956 (2) | 126 |
| N3—H3*A*···N4$^{iii}$ | 0.86 | 2.19 | 3.012 (2) | 160 |
| N3—H3*B*···O3$^{iv}$ | 0.86 | 2.40 | 3.192 (2) | 154 |

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

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 for Windows* (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: NG2761).

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# supporting information

*Acta Cryst.* (2010). E**66**, o1242 [https://doi.org/10.1107/S1600536810015540]

## Ethyl 2-(6-amino-5-cyano-3,4-dimethyl-2*H*,4*H*-pyrano[2,3-*c*]pyrazol-4-yl)acetate

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

### S1. Comment

Pyrazole, Pyranopyrazoles and its derivates possess antimicrobial (Velaparthi *et al.*,2008),anticancer (Magedov *et al.*,2007) and anti-inflammatory (Rovnyak *et al.*,1982) properties,which made them to be used as a medicines and as biodegradable agrochemiclas (Wamhoff *et al.*, 1993).Wide variety of biological importances of these molecules made the quest for their crystal study and accordingly we have synthesized the title compound by multi-component reaction which compiles with the principles of green chemistry and reported the crystal structure of the title compound.

The compound was crystallized by slow evaporation technique using ethanol as solvent at room temperature. The title compound, (I) was centrosymmetric and it has triclinic crystal system with the space group of P-1. The pyrazole groups are essentially planar, with a mean deviation of 0.0542 Å from the least square plane defined by the five atoms (N1 to C1). The pyran ring deviates significantly from the plane and it has dihedral angle of 1.93 (0.06)° with pyrazole ring. The ethyl acetate group has dihedral angle of 49.99 (0.07)° with pyran ring to which it is attached (Fig. 1). The intermolecular hydrogen bond was formed between N2···N1, N3···N4, N2—H···O2 and N3—H···O3 with distance of 2.956 (2), 3.012 (2), 3.274 (2) and 3.192 (2) Å respectively (Table.1). These intermolecular interactions help in theformation three-dimensional network and crystal packing (Fig. 2) of (I).

### S2. Experimental

The titled compound was prepared bythe successive addition of 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, 4 mmol) at room temperature under an openatmosphere with vigorous stirring for 5–10 min. The precipitated solid wasfiltered, washed with water and then with a mixture of ethyl acetate/hexane(20:80) (Vasuki & Kumaravel, 2008). The product obtained was pure by TLCand $^1$H NMR spectroscopy. However, the products were further purifiedby recrystallization from ethanol. Analysis calculated for ethyl2-(6-amino-5-cyano-3,4-dimethyl-2,4-dihydropyrano[2,3-c]pyrazol-4-yl) acetate showed that it has $C_{13}$, $H_{16}$,$N_4$, $O_3$.

### S3. Refinement

The non-hydrogen atoms where refined anisotropically whereas hydrogen atoms were refined isotropically. The H atoms were geometrically placed (N—H = 0.86 Å, and C—H=0.93-0.97 Å) and refined as riding with $U_{iso}$(H) = 1.2-1.5 $U_{eq}$ (parent atom).

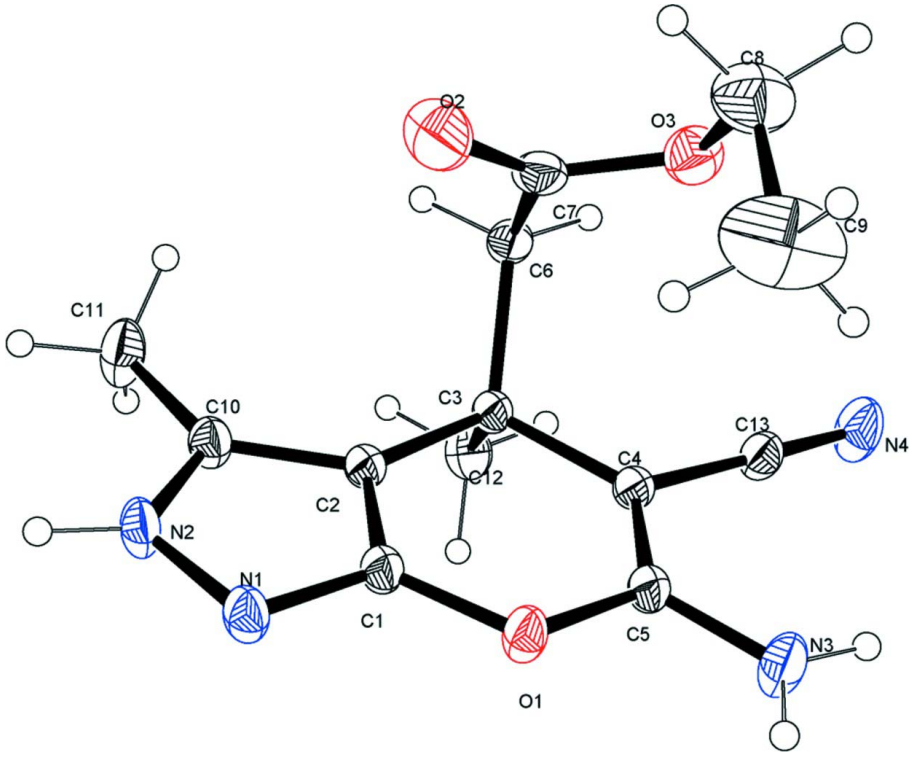


**Figure 1**

The molecular structure of (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level.

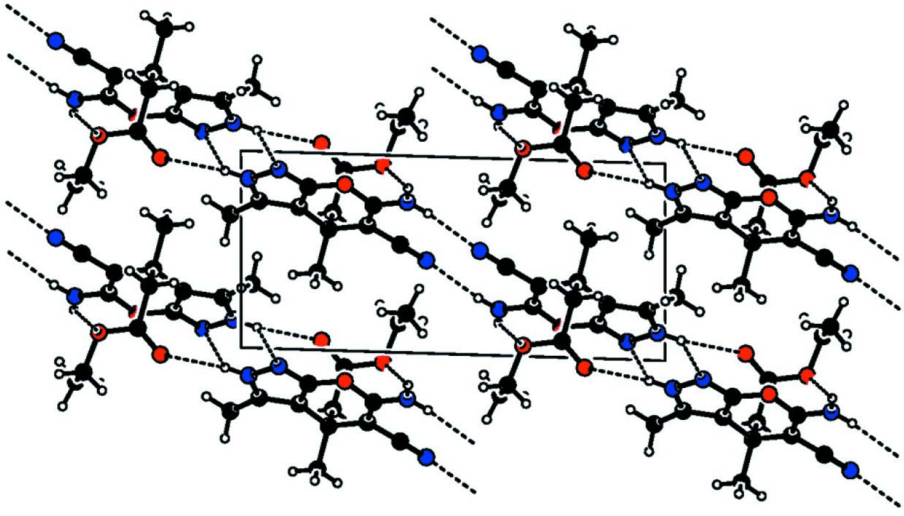

**Figure 2**

The crystal packing of (I), showing intermolecular hydrogen bonding interactions as dashed lines.

**Ethyl 2-(6-amino-5-cyano-3,4-dimethyl-2*H*,4*H*- pyrano[2,3-*c*]pyrazol-4-yl)acetate**

*Crystal data*

$C_{13}H_{16}N_4O_3$
$M_r = 276.30$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.961$ (5) Å
$b = 7.373$ (5) Å
$c = 14.535$ (5) Å
$\alpha = 86.405$ (5)°
$\beta = 85.183$ (5)°
$\gamma = 65.726$ (5)°
$V = 677.3$ (7) Å$^3$
$Z = 2$
$F(000) = 292$
$D_x = 1.355$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 7682 reflections
$\theta = 2.8$–$32.8°$
$\mu = 0.10$ mm$^{-1}$
$T = 293$ K
Block, colourless
0.25 × 0.20 × 0.20 mm

*Data collection*

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0 pixels mm$^{-1}$
$\omega$ and $\varphi$ scan
Absorption correction: multi-scan (*SADABS*; Bruker 2004)
$T_{min} = 0.976$, $T_{max} = 0.981$
12811 measured reflections
2385 independent reflections
2130 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.8°$
$h = -8 \rightarrow 8$
$k = -8 \rightarrow 8$
$l = -17 \rightarrow 17$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.117$
$S = 1.02$
2378 reflections
184 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
$w = 1/[\sigma^2(F_o^2) + (0.0655P)^2 + 0.2561P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.30$ e Å$^{-3}$
$\Delta\rho_{min} = -0.26$ 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 $F^2 > \sigma(F^2)$ 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.
Some "bad" relections were omitted in the refinement.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.4375 (2) | 0.8266 (2) | 0.84125 (10) | 0.0288 (3) |
| C2 | 0.3125 (2) | 0.7231 (2) | 0.86328 (9) | 0.0271 (3) |

| | | | | |
|---|---|---|---|---|
| C3 | 0.2551 (2) | 0.6151 (2) | 0.79351 (9) | 0.0271 (3) |
| C4 | 0.3682 (2) | 0.6404 (2) | 0.70213 (9) | 0.0282 (3) |
| C5 | 0.4908 (2) | 0.7439 (2) | 0.68793 (10) | 0.0306 (3) |
| C6 | 0.0126 (2) | 0.7009 (2) | 0.78369 (10) | 0.0329 (3) |
| H6A | −0.0164 | 0.6276 | 0.7375 | 0.040* |
| H6B | −0.0563 | 0.6818 | 0.8420 | 0.040* |
| C7 | −0.0780 (2) | 0.9167 (2) | 0.75667 (11) | 0.0378 (4) |
| C8 | −0.1525 (3) | 1.1488 (3) | 0.62848 (17) | 0.0654 (6) |
| H8A | −0.2528 | 1.2402 | 0.6724 | 0.078* |
| H8B | −0.2217 | 1.1636 | 0.5715 | 0.078* |
| C9 | 0.0317 (5) | 1.1990 (4) | 0.6104 (3) | 0.1088 (12) |
| H9A | 0.0887 | 1.2023 | 0.6679 | 0.163* |
| H9B | −0.0109 | 1.3271 | 0.5794 | 0.163* |
| H9C | 0.1375 | 1.1003 | 0.5722 | 0.163* |
| C10 | 0.2672 (2) | 0.7477 (2) | 0.95731 (10) | 0.0320 (3) |
| C11 | 0.1408 (3) | 0.6754 (3) | 1.02539 (11) | 0.0487 (5) |
| H11A | 0.2177 | 0.5356 | 1.0380 | 0.073* |
| H11B | 0.0091 | 0.6978 | 1.0006 | 0.073* |
| H11C | 0.1140 | 0.7461 | 1.0816 | 0.073* |
| C12 | 0.3282 (3) | 0.3931 (2) | 0.82003 (11) | 0.0385 (4) |
| H12A | 0.4780 | 0.3351 | 0.8261 | 0.058* |
| H12B | 0.2951 | 0.3270 | 0.7729 | 0.058* |
| H12C | 0.2574 | 0.3782 | 0.8777 | 0.058* |
| C13 | 0.3419 (2) | 0.5481 (2) | 0.62484 (10) | 0.0354 (4) |
| N1 | 0.4738 (2) | 0.9108 (2) | 0.91081 (8) | 0.0351 (3) |
| N2 | 0.3649 (2) | 0.8596 (2) | 0.98199 (8) | 0.0357 (3) |
| H2 | 0.3589 | 0.8954 | 1.0377 | 0.043* |
| N3 | 0.5923 (2) | 0.7662 (2) | 0.60839 (9) | 0.0474 (4) |
| H3A | 0.5831 | 0.7114 | 0.5594 | 0.057* |
| H3B | 0.6667 | 0.8352 | 0.6064 | 0.057* |
| N4 | 0.3189 (3) | 0.4715 (3) | 0.56322 (10) | 0.0555 (4) |
| O1 | 0.52556 (17) | 0.84545 (17) | 0.75515 (7) | 0.0367 (3) |
| O2 | −0.1338 (2) | 1.0482 (2) | 0.81014 (10) | 0.0659 (4) |
| O3 | −0.08990 (18) | 0.94621 (17) | 0.66504 (8) | 0.0450 (3) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0306 (7) | 0.0354 (7) | 0.0243 (7) | −0.0169 (6) | −0.0013 (5) | −0.0047 (6) |
| C2 | 0.0271 (7) | 0.0322 (7) | 0.0246 (7) | −0.0142 (6) | −0.0018 (5) | −0.0038 (5) |
| C3 | 0.0277 (7) | 0.0322 (7) | 0.0250 (7) | −0.0153 (6) | −0.0012 (5) | −0.0050 (5) |
| C4 | 0.0269 (7) | 0.0353 (7) | 0.0253 (7) | −0.0148 (6) | −0.0007 (5) | −0.0071 (6) |
| C5 | 0.0307 (7) | 0.0399 (8) | 0.0245 (7) | −0.0172 (6) | −0.0006 (6) | −0.0069 (6) |
| C6 | 0.0291 (7) | 0.0450 (8) | 0.0312 (8) | −0.0213 (6) | 0.0005 (6) | −0.0068 (6) |
| C7 | 0.0250 (7) | 0.0454 (9) | 0.0434 (9) | −0.0128 (6) | −0.0036 (6) | −0.0124 (7) |
| C8 | 0.0592 (12) | 0.0478 (11) | 0.0810 (15) | −0.0144 (9) | −0.0116 (11) | 0.0124 (10) |
| C9 | 0.096 (2) | 0.0740 (17) | 0.171 (3) | −0.0526 (16) | −0.029 (2) | 0.0415 (19) |
| C10 | 0.0376 (8) | 0.0365 (8) | 0.0267 (7) | −0.0196 (6) | −0.0016 (6) | −0.0048 (6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C11 | 0.0692 (12) | 0.0637 (11) | 0.0298 (8) | −0.0450 (10) | 0.0083 (8) | −0.0090 (8) |
| C12 | 0.0481 (9) | 0.0344 (8) | 0.0364 (8) | −0.0197 (7) | −0.0038 (7) | −0.0028 (6) |
| C13 | 0.0362 (8) | 0.0488 (9) | 0.0289 (8) | −0.0255 (7) | 0.0042 (6) | −0.0088 (7) |
| N1 | 0.0430 (7) | 0.0457 (7) | 0.0273 (6) | −0.0284 (6) | −0.0011 (5) | −0.0067 (5) |
| N2 | 0.0487 (8) | 0.0459 (7) | 0.0224 (6) | −0.0286 (6) | −0.0015 (5) | −0.0069 (5) |
| N3 | 0.0591 (9) | 0.0738 (10) | 0.0300 (7) | −0.0484 (8) | 0.0114 (6) | −0.0162 (7) |
| N4 | 0.0675 (10) | 0.0859 (12) | 0.0357 (8) | −0.0534 (9) | 0.0097 (7) | −0.0243 (8) |
| O1 | 0.0446 (6) | 0.0537 (7) | 0.0266 (6) | −0.0350 (5) | 0.0047 (4) | −0.0106 (5) |
| O2 | 0.0652 (9) | 0.0518 (8) | 0.0677 (9) | −0.0048 (7) | −0.0160 (7) | −0.0270 (7) |
| O3 | 0.0440 (7) | 0.0432 (6) | 0.0457 (7) | −0.0163 (5) | −0.0008 (5) | −0.0005 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—N1 | 1.3125 (19) | C8—H8A | 0.9700 |
| C1—O1 | 1.3714 (18) | C8—H8B | 0.9700 |
| C1—C2 | 1.383 (2) | C9—H9A | 0.9600 |
| C2—C10 | 1.383 (2) | C9—H9B | 0.9600 |
| C2—C3 | 1.5006 (19) | C9—H9C | 0.9600 |
| C3—C4 | 1.527 (2) | C10—N2 | 1.346 (2) |
| C3—C12 | 1.535 (2) | C10—C11 | 1.487 (2) |
| C3—C6 | 1.556 (2) | C11—H11A | 0.9600 |
| C4—C5 | 1.356 (2) | C11—H11B | 0.9600 |
| C4—C13 | 1.411 (2) | C11—H11C | 0.9600 |
| C5—N3 | 1.341 (2) | C12—H12A | 0.9600 |
| C5—O1 | 1.3616 (17) | C12—H12B | 0.9600 |
| C6—C7 | 1.490 (2) | C12—H12C | 0.9600 |
| C6—H6A | 0.9700 | C13—N4 | 1.144 (2) |
| C6—H6B | 0.9700 | N1—N2 | 1.3572 (18) |
| C7—O2 | 1.195 (2) | N2—H2 | 0.8600 |
| C7—O3 | 1.340 (2) | N3—H3A | 0.8600 |
| C8—O3 | 1.452 (2) | N3—H3B | 0.8600 |
| C8—C9 | 1.474 (4) | | |

| | | | |
|---|---|---|---|
| N1—C1—O1 | 118.81 (13) | H8A—C8—H8B | 108.0 |
| N1—C1—C2 | 115.28 (13) | C8—C9—H9A | 109.5 |
| O1—C1—C2 | 125.90 (13) | C8—C9—H9B | 109.5 |
| C1—C2—C10 | 103.21 (13) | H9A—C9—H9B | 109.5 |
| C1—C2—C3 | 123.21 (13) | C8—C9—H9C | 109.5 |
| C10—C2—C3 | 133.58 (13) | H9A—C9—H9C | 109.5 |
| C2—C3—C4 | 105.90 (12) | H9B—C9—H9C | 109.5 |
| C2—C3—C12 | 111.39 (12) | N2—C10—C2 | 106.01 (13) |
| C4—C3—C12 | 109.91 (12) | N2—C10—C11 | 122.04 (14) |
| C2—C3—C6 | 112.12 (11) | C2—C10—C11 | 131.95 (14) |
| C4—C3—C6 | 110.22 (12) | C10—C11—H11A | 109.5 |
| C12—C3—C6 | 107.33 (12) | C10—C11—H11B | 109.5 |
| C5—C4—C13 | 116.78 (13) | H11A—C11—H11B | 109.5 |
| C5—C4—C3 | 126.29 (13) | C10—C11—H11C | 109.5 |
| C13—C4—C3 | 116.93 (13) | H11A—C11—H11C | 109.5 |

| | | | |
|---|---|---|---|
| N3—C5—C4 | 126.98 (14) | H11B—C11—H11C | 109.5 |
| N3—C5—O1 | 109.58 (13) | C3—C12—H12A | 109.5 |
| C4—C5—O1 | 123.44 (13) | C3—C12—H12B | 109.5 |
| C7—C6—C3 | 112.62 (12) | H12A—C12—H12B | 109.5 |
| C7—C6—H6A | 109.1 | C3—C12—H12C | 109.5 |
| C3—C6—H6A | 109.1 | H12A—C12—H12C | 109.5 |
| C7—C6—H6B | 109.1 | H12B—C12—H12C | 109.5 |
| C3—C6—H6B | 109.1 | N4—C13—C4 | 178.79 (17) |
| H6A—C6—H6B | 107.8 | C1—N1—N2 | 101.70 (12) |
| O2—C7—O3 | 123.82 (17) | C10—N2—N1 | 113.80 (12) |
| O2—C7—C6 | 124.23 (16) | C10—N2—H2 | 123.1 |
| O3—C7—C6 | 111.94 (13) | N1—N2—H2 | 123.1 |
| O3—C8—C9 | 111.08 (18) | C5—N3—H3A | 120.0 |
| O3—C8—H8A | 109.4 | C5—N3—H3B | 120.0 |
| C9—C8—H8A | 109.4 | H3A—N3—H3B | 120.0 |
| O3—C8—H8B | 109.4 | C5—O1—C1 | 115.14 (12) |
| C9—C8—H8B | 109.4 | C7—O3—C8 | 117.56 (15) |

| | | | |
|---|---|---|---|
| N1—C1—C2—C10 | 0.13 (17) | C12—C3—C6—C7 | −179.24 (12) |
| O1—C1—C2—C10 | 179.38 (13) | C3—C6—C7—O2 | −85.9 (2) |
| N1—C1—C2—C3 | −179.36 (12) | C3—C6—C7—O3 | 94.18 (15) |
| O1—C1—C2—C3 | −0.1 (2) | C1—C2—C10—N2 | 0.13 (16) |
| C1—C2—C3—C4 | 2.14 (18) | C3—C2—C10—N2 | 179.54 (14) |
| C10—C2—C3—C4 | −177.17 (15) | C1—C2—C10—C11 | −179.84 (17) |
| C1—C2—C3—C12 | 121.60 (15) | C3—C2—C10—C11 | −0.4 (3) |
| C10—C2—C3—C12 | −57.7 (2) | C5—C4—C13—N4 | 169 (9) |
| C1—C2—C3—C6 | −118.10 (15) | C3—C4—C13—N4 | −11 (9) |
| C10—C2—C3—C6 | 62.6 (2) | O1—C1—N1—N2 | −179.63 (12) |
| C2—C3—C4—C5 | −1.37 (19) | C2—C1—N1—N2 | −0.32 (17) |
| C12—C3—C4—C5 | −121.80 (16) | C2—C10—N2—N1 | −0.35 (17) |
| C6—C3—C4—C5 | 120.10 (16) | C11—C10—N2—N1 | 179.63 (15) |
| C2—C3—C4—C13 | 178.97 (12) | C1—N1—N2—C10 | 0.41 (17) |
| C12—C3—C4—C13 | 58.54 (17) | N3—C5—O1—C1 | −177.10 (12) |
| C6—C3—C4—C13 | −59.56 (17) | C4—C5—O1—C1 | 3.8 (2) |
| C13—C4—C5—N3 | −0.9 (2) | N1—C1—O1—C5 | 176.23 (12) |
| C3—C4—C5—N3 | 179.41 (14) | C2—C1—O1—C5 | −3.0 (2) |
| C13—C4—C5—O1 | 178.03 (13) | O2—C7—O3—C8 | 7.0 (2) |
| C3—C4—C5—O1 | −1.6 (2) | C6—C7—O3—C8 | −173.07 (14) |
| C2—C3—C6—C7 | 58.13 (16) | C9—C8—O3—C7 | 87.2 (3) |
| C4—C3—C6—C7 | −59.57 (16) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2···O2$^{i}$ | 0.86 | 2.55 | 3.274 (2) | 142 |
| N2—H2···N1$^{ii}$ | 0.86 | 2.37 | 2.956 (2) | 126 |

| | | | | |
|---|---|---|---|---|
| N3—H3*A*···N4$^{iii}$ | 0.86 | 2.19 | 3.012 (2) | 160 |
| N3—H3*B*···O3$^{iv}$ | 0.86 | 2.40 | 3.192 (2) | 154 |

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