



Crystal structure of ethyl *N*-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-4-yl)carbamate

Muhammad Danish,^a Muhammad Nawaz Tahir,^{b*} Uzma Anwar^a and Muhammad Asam Raza^a

^aDepartment of Chemistry, Institute of Natural Sciences, University of Gujrat, Gujrat 50700, Pakistan, and ^bDepartment of Physics, University of Sargodha, Sargodha, Punjab, Pakistan. *Correspondence e-mail: dmntahir_uos@yahoo.com

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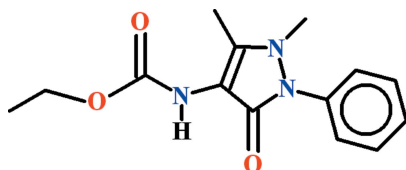
In the title compound, C₁₄H₁₇N₃O₃, the dihedral angle between the benzene ring and the five-membered dihydropyrazole ring is 52.26 (9)°. The ethyl ester group is approximately planar (r.m.s. deviation 0.0568 Å) and subtends an angle 67.73 (8)° to the pyrazole ring. In the crystal, molecules are linked by pairs of N—H···O hydrogen bonds, forming inversion dimers with an R₂²(10) ring motif. Weaker C—H···O contacts link these dimers into a three-dimensional network of molecules stacked along the *a*-axis direction. Offset π–π stacking interactions between the benzene rings [centroid-to-centroid distance = 3.8832 (12) Å] further stabilize the crystal packing.

Keywords: crystal structure; dihydropyrazole; ethyl ester; carbamate; hydrogen bonding; π–π stacking interactions.

CCDC reference: 1056157

1. Related literature

For related structures see: Li *et al.* (2013).



2. Experimental

2.1. Crystal data

C₁₄H₁₇N₃O₃

M_r = 275.30

Monoclinic, *P*2₁/*c*
a = 8.2100 (4) Å
b = 11.4137 (6) Å
c = 15.1594 (8) Å
β = 93.403 (3)°
V = 1418.03 (13) Å³

Z = 4
Mo *K*α radiation
μ = 0.09 mm⁻¹
T = 296 K
0.38 × 0.34 × 0.20 mm

2.2. Data collection

Bruker Kappa APEXII CCD
diffractometer
Absorption correction: multi-scan
(*SADABS*; Bruker, 2005)
*T*_{min} = 0.968, *T*_{max} = 0.983

1712 measured reflections
3098 independent reflections
2368 reflections with *I* > 2σ(*I*)
*R*_{int} = 0.022

2.3. Refinement

R[*F*² > 2σ(*F*²)] = 0.043
wR(*F*²) = 0.127
S = 1.06
3098 reflections

185 parameters
H-atom parameters constrained
Δρ_{max} = 0.19 e Å⁻³
Δρ_{min} = -0.17 e Å⁻³

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

| <i>D</i> —H··· <i>A</i> | <i>D</i> —H | H··· <i>A</i> | <i>D</i> ··· <i>A</i> | <i>D</i> —H··· <i>A</i> |
|------------------------------|-------------|---------------|-----------------------|-------------------------|
| N3—H3A···O1 ⁱ | 0.86 | 1.99 | 2.8223 (17) | 164 |
| C10—H10A···O1 ⁱⁱ | 0.96 | 2.56 | 3.343 (2) | 139 |
| C11—H11B···O2 ⁱⁱⁱ | 0.96 | 2.66 | 3.576 (2) | 161 |

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014/6* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON*.

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: SJ5447).

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supporting information

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Crystal structure of ethyl *N*-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-4-yl)carbamate

Muhammad Danish, Muhammad Nawaz Tahir, Uzma Anwar and Muhammad Asam Raza

S1. Comment

The title compound (I), (Fig. 1) has been synthesized to examine its DNA binding potential and anti-microbial activity. The crystal structures of two closely related compounds, methyl (1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-4-yl)carbamate and methyl (1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-4-yl)methylcarbamate monohydrate have been reported previously (Li *et al.*, 2013).

In (I), the C1—C6 benzene ring and dihydropyrazol-3-one system, O1/N1/N2/N3/C7—C9 are planar with *r.m.s.* deviations of 0.0037 and 0.0398 Å, respectively. The dihedral angle between the two systems is 53.64 (5)°. The ethyl ester group, C12/C13/C14/O2/O3, is also planar (*r.m.s.* deviation 0.0568 Å) and subtends an angle 67.73 (8)° to the pyrazole ring. In the crystal structure classical N3—H3A···O1 hydrogen bonds form inversion dimers (Table 1, Fig. 2) with $R_2^2(10)$ ring motifs. Weaker C10—H10A···O1 and C11—H11B···O2 contacts link these dimers into a three dimensional network of molecules stacked along the *a* axis direction. Offset π ··· π stacking interactions between the benzene rings with $\text{Cg2} \cdots \text{Cg2}^i = 3.8832$ (12) Å further stabilise the crystal packing (Cg2 is the centroid of the C1—C6 benzene ring; $i = 2 - x, -y, 1 - z$).

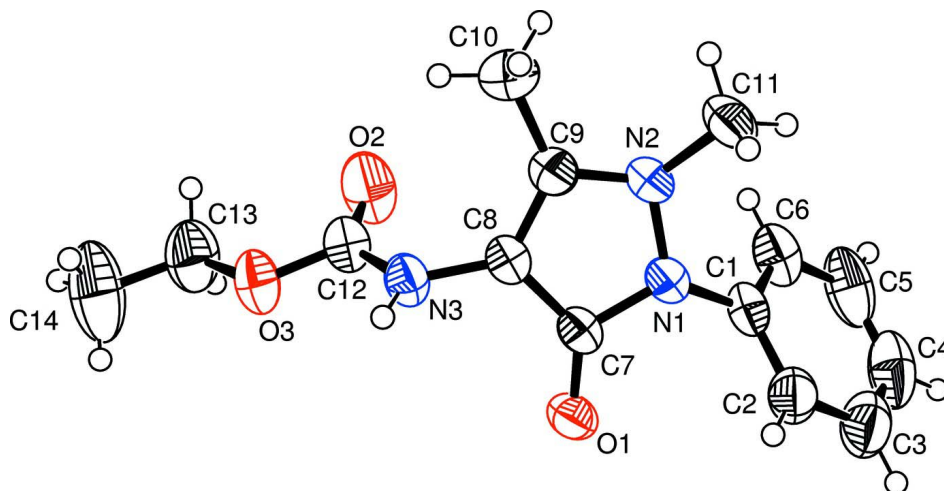
S2. Experimental

4-aminoantipyrene (2 g, 9.84 mmole) was dissolved in 50 ml dimethyl formamide and anhydrous potassium carbonate (0.68 g, 4.92 mmole) was added with continuous stirring over 50 minutes. Ethyl chloroformate (1.3 ml) was added dropwise with stirring over three minutes at 323 K. TLC monitoring showed the reaction to be complete in almost 4 h. The reaction mixture was then cooled to room temperature and transferred to crushed ice leading to the formation of a precipitate. This was separated by filtration and recrystallized from aqueous ethanol to yield (I) as light yellow plates.

Melting point: 477–479 K.

S3. Refinement

The H-atoms were positioned geometrically (N—H = 0.86, C—H = 0.93–0.97 Å) and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$.

**Figure 1**

View of the asymmetric unit of title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small circles of arbitrary radii.

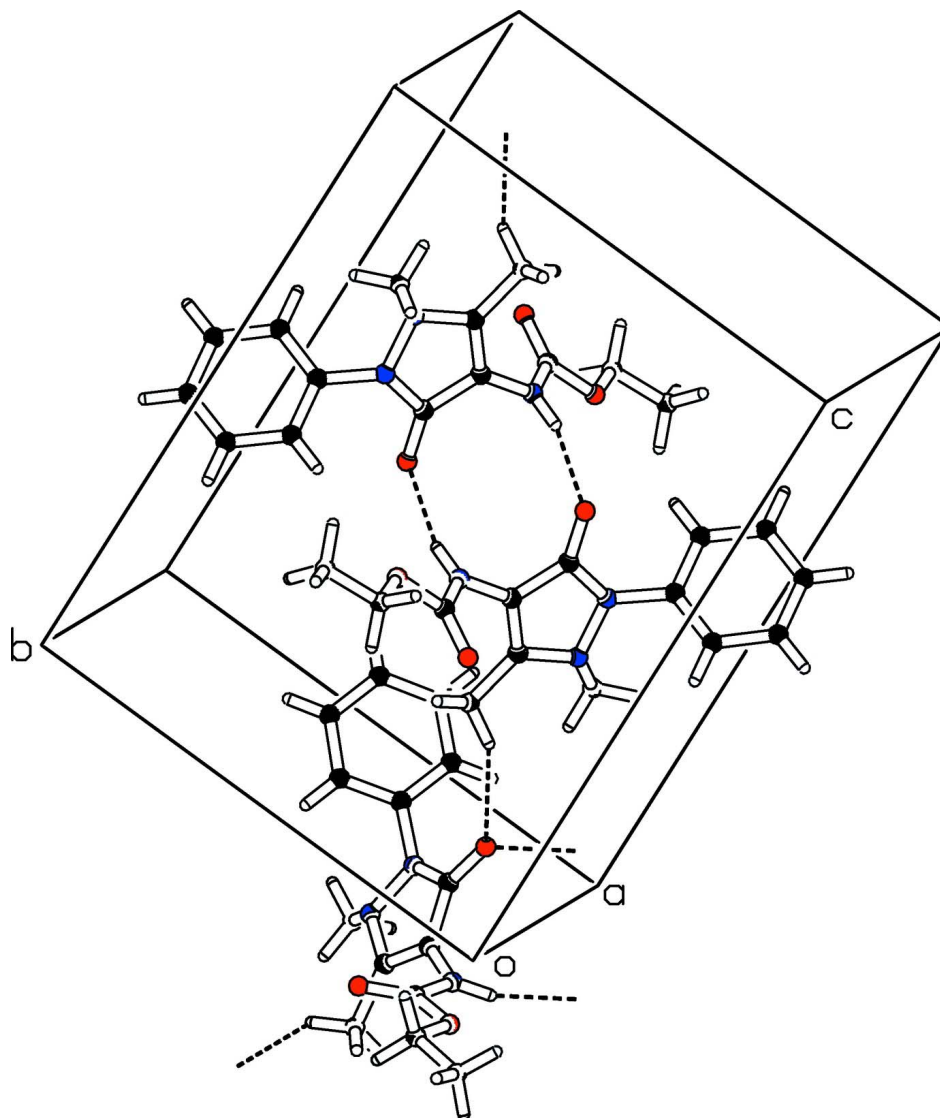


Figure 2

The crystal packing of (I), viewed along the *a* axis, with hydrogen bonds shown as dashed lines.

Ethyl *N*-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-4-yl)carbamate

Crystal data

$C_{14}H_{17}N_3O_3$

$M_r = 275.30$

Monoclinic, $P2_1/c$

$a = 8.2100$ (4) Å

$b = 11.4137$ (6) Å

$c = 15.1594$ (8) Å

$\beta = 93.403$ (3)°

$V = 1418.03$ (13) Å³

$Z = 4$

$F(000) = 584$

$D_x = 1.290$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2368 reflections

$\theta = 2.2$ – 27.0 °

$\mu = 0.09$ mm⁻¹

$T = 296$ K

Plate, light yellow

$0.38 \times 0.34 \times 0.20$ mm

Data collection

Bruker Kappa APEXII CCD
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 Detector resolution: 7.80 pixels mm⁻¹
 ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2005)
 $T_{\min} = 0.968$, $T_{\max} = 0.983$

11712 measured reflections
 3098 independent reflections
 2368 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.022$
 $\theta_{\max} = 27.0^\circ$, $\theta_{\min} = 2.2^\circ$
 $h = -10 \rightarrow 10$
 $k = -14 \rightarrow 13$
 $l = -19 \rightarrow 19$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.127$
 $S = 1.06$
 3098 reflections
 185 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
 $w = 1/[\sigma^2(F_o^2) + (0.0592P)^2 + 0.2848P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.19 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.17 \text{ e } \text{\AA}^{-3}$
 Extinction correction: SHELXL,
 $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.027 (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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|--------------|----------------------------------|
| O1 | 0.54493 (13) | 0.33953 (9) | 0.54004 (6) | 0.0503 (3) |
| O2 | 0.13321 (16) | 0.32771 (12) | 0.33957 (11) | 0.0819 (5) |
| O3 | 0.09391 (13) | 0.51504 (10) | 0.38192 (8) | 0.0617 (3) |
| N1 | 0.65770 (15) | 0.23072 (11) | 0.42996 (8) | 0.0458 (3) |
| N2 | 0.62265 (16) | 0.21412 (12) | 0.33892 (8) | 0.0510 (3) |
| N3 | 0.34531 (15) | 0.44615 (11) | 0.38501 (8) | 0.0480 (3) |
| H3A | 0.3728 | 0.5172 | 0.3977 | 0.058* |
| C1 | 0.72550 (18) | 0.13738 (13) | 0.48290 (10) | 0.0472 (4) |
| C2 | 0.8305 (2) | 0.16528 (17) | 0.55395 (11) | 0.0592 (4) |
| H2 | 0.8595 | 0.2428 | 0.5653 | 0.071* |
| C3 | 0.8922 (3) | 0.0764 (2) | 0.60812 (14) | 0.0791 (6) |
| H3 | 0.9628 | 0.0945 | 0.6565 | 0.095* |
| C4 | 0.8508 (3) | -0.0376 (2) | 0.59139 (18) | 0.0851 (7) |
| H4 | 0.8924 | -0.0967 | 0.6285 | 0.102* |

| | | | | |
|------|--------------|---------------|--------------|-------------|
| C5 | 0.7481 (3) | -0.06516 (17) | 0.52008 (19) | 0.0841 (7) |
| H5 | 0.7216 | -0.1431 | 0.5085 | 0.101* |
| C6 | 0.6830 (2) | 0.02230 (15) | 0.46480 (14) | 0.0639 (5) |
| H6 | 0.6122 | 0.0038 | 0.4166 | 0.077* |
| C7 | 0.55368 (17) | 0.31534 (12) | 0.46080 (9) | 0.0406 (3) |
| C8 | 0.46691 (17) | 0.35940 (13) | 0.38352 (9) | 0.0430 (3) |
| C9 | 0.51590 (19) | 0.30017 (14) | 0.31216 (10) | 0.0487 (4) |
| C10 | 0.4694 (3) | 0.3221 (2) | 0.21696 (12) | 0.0755 (6) |
| H10A | 0.4626 | 0.2489 | 0.1858 | 0.113* |
| H10B | 0.5502 | 0.3709 | 0.1921 | 0.113* |
| H10C | 0.3654 | 0.3607 | 0.2117 | 0.113* |
| C11 | 0.7583 (2) | 0.17664 (16) | 0.28711 (12) | 0.0621 (5) |
| H11A | 0.7971 | 0.1016 | 0.3078 | 0.093* |
| H11B | 0.8452 | 0.2329 | 0.2937 | 0.093* |
| H11C | 0.7217 | 0.1709 | 0.2259 | 0.093* |
| C12 | 0.1866 (2) | 0.42031 (14) | 0.36699 (11) | 0.0528 (4) |
| C13 | -0.0815 (2) | 0.4956 (2) | 0.37242 (17) | 0.0818 (6) |
| H13A | -0.1108 | 0.4609 | 0.3152 | 0.098* |
| H13B | -0.1145 | 0.4424 | 0.4179 | 0.098* |
| C14 | -0.1628 (3) | 0.6069 (3) | 0.3803 (2) | 0.1237 (11) |
| H14A | -0.2786 | 0.5946 | 0.3798 | 0.186* |
| H14B | -0.1381 | 0.6563 | 0.3316 | 0.186* |
| H14C | -0.1259 | 0.6438 | 0.4348 | 0.186* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|-------------|-------------|-------------|
| O1 | 0.0619 (7) | 0.0475 (6) | 0.0425 (6) | 0.0067 (5) | 0.0099 (5) | -0.0044 (4) |
| O2 | 0.0552 (7) | 0.0589 (9) | 0.1307 (13) | -0.0026 (6) | -0.0010 (8) | -0.0187 (8) |
| O3 | 0.0453 (6) | 0.0558 (7) | 0.0849 (8) | 0.0115 (5) | 0.0113 (6) | 0.0010 (6) |
| N1 | 0.0493 (7) | 0.0440 (7) | 0.0445 (7) | 0.0090 (6) | 0.0050 (5) | -0.0052 (5) |
| N2 | 0.0517 (7) | 0.0558 (8) | 0.0458 (7) | 0.0106 (6) | 0.0067 (6) | -0.0112 (6) |
| N3 | 0.0459 (7) | 0.0395 (7) | 0.0586 (8) | 0.0054 (5) | 0.0037 (6) | -0.0030 (5) |
| C1 | 0.0421 (7) | 0.0439 (8) | 0.0568 (9) | 0.0089 (6) | 0.0134 (6) | 0.0019 (7) |
| C2 | 0.0558 (9) | 0.0613 (11) | 0.0607 (10) | 0.0102 (8) | 0.0043 (8) | 0.0035 (8) |
| C3 | 0.0691 (12) | 0.0960 (17) | 0.0724 (12) | 0.0247 (12) | 0.0054 (10) | 0.0187 (11) |
| C4 | 0.0744 (14) | 0.0786 (15) | 0.1049 (17) | 0.0307 (12) | 0.0268 (13) | 0.0369 (13) |
| C5 | 0.0725 (13) | 0.0453 (11) | 0.138 (2) | 0.0119 (10) | 0.0371 (14) | 0.0176 (12) |
| C6 | 0.0542 (10) | 0.0488 (10) | 0.0901 (13) | 0.0032 (8) | 0.0156 (9) | -0.0036 (9) |
| C7 | 0.0411 (7) | 0.0350 (7) | 0.0464 (8) | -0.0002 (6) | 0.0086 (6) | -0.0038 (6) |
| C8 | 0.0423 (7) | 0.0396 (8) | 0.0476 (8) | 0.0030 (6) | 0.0067 (6) | -0.0019 (6) |
| C9 | 0.0472 (8) | 0.0521 (9) | 0.0470 (8) | 0.0031 (7) | 0.0029 (6) | -0.0056 (6) |
| C10 | 0.0805 (13) | 0.0979 (16) | 0.0474 (10) | 0.0178 (11) | -0.0019 (9) | -0.0074 (9) |
| C11 | 0.0611 (10) | 0.0664 (11) | 0.0605 (10) | 0.0110 (9) | 0.0174 (8) | -0.0146 (8) |
| C12 | 0.0487 (8) | 0.0479 (9) | 0.0622 (10) | 0.0056 (7) | 0.0067 (7) | 0.0021 (7) |
| C13 | 0.0470 (10) | 0.0869 (15) | 0.1121 (17) | 0.0083 (10) | 0.0091 (10) | 0.0007 (13) |
| C14 | 0.0581 (13) | 0.105 (2) | 0.211 (3) | 0.0252 (14) | 0.0337 (17) | 0.016 (2) |

Geometric parameters (Å, °)

| | | | |
|------------|-------------|---------------|-------------|
| O1—C7 | 1.2387 (17) | C4—H4 | 0.9300 |
| O2—C12 | 1.208 (2) | C5—C6 | 1.390 (3) |
| O3—C12 | 1.3489 (19) | C5—H5 | 0.9300 |
| O3—C13 | 1.456 (2) | C6—H6 | 0.9300 |
| N1—C7 | 1.3886 (18) | C7—C8 | 1.426 (2) |
| N1—N2 | 1.4057 (17) | C8—C9 | 1.357 (2) |
| N1—C1 | 1.4269 (19) | C9—C10 | 1.492 (2) |
| N2—C9 | 1.362 (2) | C10—H10A | 0.9600 |
| N2—C11 | 1.4645 (19) | C10—H10B | 0.9600 |
| N3—C12 | 1.348 (2) | C10—H10C | 0.9600 |
| N3—C8 | 1.4072 (18) | C11—H11A | 0.9600 |
| N3—H3A | 0.8600 | C11—H11B | 0.9600 |
| C1—C2 | 1.376 (2) | C11—H11C | 0.9600 |
| C1—C6 | 1.383 (2) | C13—C14 | 1.443 (3) |
| C2—C3 | 1.382 (3) | C13—H13A | 0.9700 |
| C2—H2 | 0.9300 | C13—H13B | 0.9700 |
| C3—C4 | 1.365 (3) | C14—H14A | 0.9600 |
| C3—H3 | 0.9300 | C14—H14B | 0.9600 |
| C4—C5 | 1.367 (4) | C14—H14C | 0.9600 |
| | | | |
| C12—O3—C13 | 115.20 (15) | C9—C8—C7 | 108.79 (13) |
| C7—N1—N2 | 109.28 (11) | N3—C8—C7 | 123.72 (12) |
| C7—N1—C1 | 123.86 (12) | C8—C9—N2 | 109.74 (13) |
| N2—N1—C1 | 120.12 (12) | C8—C9—C10 | 128.08 (15) |
| C9—N2—N1 | 106.61 (11) | N2—C9—C10 | 122.17 (14) |
| C9—N2—C11 | 123.19 (14) | C9—C10—H10A | 109.5 |
| N1—N2—C11 | 116.61 (13) | C9—C10—H10B | 109.5 |
| C12—N3—C8 | 121.39 (13) | H10A—C10—H10B | 109.5 |
| C12—N3—H3A | 119.3 | C9—C10—H10C | 109.5 |
| C8—N3—H3A | 119.3 | H10A—C10—H10C | 109.5 |
| C2—C1—C6 | 120.94 (16) | H10B—C10—H10C | 109.5 |
| C2—C1—N1 | 118.21 (15) | N2—C11—H11A | 109.5 |
| C6—C1—N1 | 120.81 (15) | N2—C11—H11B | 109.5 |
| C1—C2—C3 | 119.05 (19) | H11A—C11—H11B | 109.5 |
| C1—C2—H2 | 120.5 | N2—C11—H11C | 109.5 |
| C3—C2—H2 | 120.5 | H11A—C11—H11C | 109.5 |
| C4—C3—C2 | 120.7 (2) | H11B—C11—H11C | 109.5 |
| C4—C3—H3 | 119.6 | O2—C12—N3 | 125.98 (15) |
| C2—C3—H3 | 119.6 | O2—C12—O3 | 124.21 (15) |
| C3—C4—C5 | 120.1 (2) | N3—C12—O3 | 109.79 (14) |
| C3—C4—H4 | 120.0 | C14—C13—O3 | 108.53 (19) |
| C5—C4—H4 | 120.0 | C14—C13—H13A | 110.0 |
| C4—C5—C6 | 120.6 (2) | O3—C13—H13A | 110.0 |
| C4—C5—H5 | 119.7 | C14—C13—H13B | 110.0 |
| C6—C5—H5 | 119.7 | O3—C13—H13B | 110.0 |
| C1—C6—C5 | 118.6 (2) | H13A—C13—H13B | 108.4 |

| | | | |
|--------------|--------------|----------------|--------------|
| C1—C6—H6 | 120.7 | C13—C14—H14A | 109.5 |
| C5—C6—H6 | 120.7 | C13—C14—H14B | 109.5 |
| O1—C7—N1 | 123.62 (13) | H14A—C14—H14B | 109.5 |
| O1—C7—C8 | 131.54 (13) | C13—C14—H14C | 109.5 |
| N1—C7—C8 | 104.82 (12) | H14A—C14—H14C | 109.5 |
| C9—C8—N3 | 127.41 (14) | H14B—C14—H14C | 109.5 |
| | | | |
| C7—N1—N2—C9 | 9.01 (16) | C12—N3—C8—C9 | 67.6 (2) |
| C1—N1—N2—C9 | 161.31 (13) | C12—N3—C8—C7 | -108.89 (18) |
| C7—N1—N2—C11 | 151.05 (14) | O1—C7—C8—C9 | -177.01 (16) |
| C1—N1—N2—C11 | -56.66 (19) | N1—C7—C8—C9 | 1.68 (16) |
| C7—N1—C1—C2 | -64.2 (2) | O1—C7—C8—N3 | 0.0 (3) |
| N2—N1—C1—C2 | 147.71 (14) | N1—C7—C8—N3 | 178.73 (13) |
| C7—N1—C1—C6 | 113.91 (17) | N3—C8—C9—N2 | -172.97 (14) |
| N2—N1—C1—C6 | -34.2 (2) | C7—C8—C9—N2 | 3.95 (18) |
| C6—C1—C2—C3 | -0.7 (2) | N3—C8—C9—C10 | 8.5 (3) |
| N1—C1—C2—C3 | 177.40 (15) | C7—C8—C9—C10 | -174.57 (18) |
| C1—C2—C3—C4 | 0.4 (3) | N1—N2—C9—C8 | -7.90 (17) |
| C2—C3—C4—C5 | 0.5 (3) | C11—N2—C9—C8 | -146.82 (15) |
| C3—C4—C5—C6 | -1.0 (3) | N1—N2—C9—C10 | 170.73 (16) |
| C2—C1—C6—C5 | 0.2 (2) | C11—N2—C9—C10 | 31.8 (3) |
| N1—C1—C6—C5 | -177.87 (15) | C8—N3—C12—O2 | -8.1 (3) |
| C4—C5—C6—C1 | 0.7 (3) | C8—N3—C12—O3 | 173.51 (13) |
| N2—N1—C7—O1 | 172.30 (14) | C13—O3—C12—O2 | 6.8 (3) |
| C1—N1—C7—O1 | 21.3 (2) | C13—O3—C12—N3 | -174.78 (15) |
| N2—N1—C7—C8 | -6.52 (16) | C12—O3—C13—C14 | -173.5 (2) |
| C1—N1—C7—C8 | -157.55 (14) | | |

Hydrogen-bond geometry (Å, °)

| <i>D</i> —H \cdots <i>A</i> | <i>D</i> —H | H \cdots <i>A</i> | <i>D</i> \cdots <i>A</i> | <i>D</i> —H \cdots <i>A</i> |
|-------------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| N3—H3A \cdots O1 ⁱ | 0.86 | 1.99 | 2.8223 (17) | 164 |
| C10—H10A \cdots O1 ⁱⁱ | 0.96 | 2.56 | 3.343 (2) | 139 |
| C11—H11B \cdots O2 ⁱⁱⁱ | 0.96 | 2.66 | 3.576 (2) | 161 |

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