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3-(2,5-Dimethylfuran-3-yl)-1*H*-pyrazol-5-ol–ethyl 3-(propan-2-ylidene)carbazate (1/1). Corrigendum

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The address of three of the authors in the paper by Shahani *et al.* [*Acta Cryst.* (2010), E**66**, o3020–o3021] is corrected.

In the paper by Shahani *et al.* (2010), the address of the third, fourth and fifth authors is given incorrectly. The correct address is 'Organic Chemistry Division, School of Advanced Sciences, VIT University, Vellore 632 014, India', as given above.

References

Shahani, T., Fun, H.-K., Venkat Ragavan, R., Vijayakumar, V. & Sarveswari, S. (2010). *Acta Cryst.* E**66**, o3020–o3021.

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3-(2,5-Dimethylfuran-3-yl)-1*H*-pyrazol-5-ol–ethyl 3-(propan-2-ylidene)carbazate (1/1)

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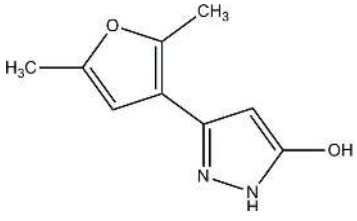
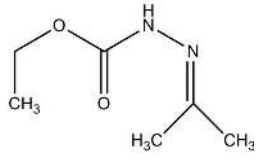
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.033; wR factor = 0.099; data-to-parameter ratio = 14.5.

In the title 1:1 adduct, $C_6H_{12}N_2O_2\cdot C_9H_{10}N_2O_2$, the maximum deviations from the 1*H*-pyrazole-5-ol and furan rings are 0.014 (1) and 0.003 (1) Å, respectively. The dihedral angle formed between the 1*H*-pyrazol-5-ol and 2,5-dimethylfuran rings is 21.07 (5)°. In the crystal, pairs of intermolecular O—H···N hydrogen bonds form inversion dimers of the 3-(2,5-dimethylfuran-3-yl)-1*H*-pyrazol-5-ol species, generating $R_2^2(8)$ ring motifs. Molecules are further linked by intermolecular N—H···O, N—H···N and C—H···O hydrogen bonds to form ribbons along the [010] direction containing bifurcated $R_1^2(5)$ and $R_2^1(7)$ ring motifs. Further stablization of the packing is provided by weak π–π [centroid–centroid distance = 3.5686 (15) Å] and C—H···π interactions.

Related literature

For pyrazole derivatives and their microbial activities, see: Ragavan *et al.* (2009, 2010). For a related structure, see: Shahani *et al.* (2010). For ring conformations, see: Cremer & Pople (1975). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For bond-length data, see: Allen *et al.* (1987). For the stability of the temperature controller used for the data collection, see: Cosier & Glazer (1986).





‡ Thomson Reuters ResearcherID: A-3561-2009.

Experimental

Crystal data

$C_6H_{12}N_2O_2\cdot C_9H_{10}N_2O_2$
M_r = 322.37
Triclinic, $P\overline{1}$
a = 8.6988 (17) Å
b = 9.4830 (19) Å
c = 11.837 (4) Å
α = 107.293 (4)°
β = 100.354 (5)°
γ = 108.346 (3)°
V = 843.7 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 K
0.40 × 0.21 × 0.13 mm

Data collection

Bruker APEXII DUO CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.964, T_{max} = 0.988
13322 measured reflections
3264 independent reflections
2911 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.099
S = 1.11
3264 reflections
225 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*1···O4^{i}	0.883 (18)	2.304 (19)	3.0363 (19)	140.1 (16)
N1—H1*N*1···N4^{i}	0.883 (18)	2.288 (19)	3.043 (2)	143.1 (16)
N3—H1*N*3···O2^{ii}	0.872 (18)	2.076 (19)	2.9293 (19)	166.7 (18)
O2—H1*O*2···N2^{iii}	0.93 (2)	1.73 (2)	2.6602 (17)	176 (2)
C5—H5*A*···O4^{i}	0.93	2.35	3.212 (2)	153
C11—H11*B*···*Cg*2^{iv}	0.97	2.71	3.50 (2)	138

Symmetry codes: (i) $x+1, y, z$; (ii) $x-1, y-1, z$; (iii) $-x+3, -y+2, -z+1$; (iv) $-x+1, -y+1, -z+1$. *Cg*2 is the centroid of the 1*H*-pyrazole ring (N1/N2/C1–C3).

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

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5696).

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supporting information

Acta Cryst. (2010). E**66**, o3020–o3021 [https://doi.org/10.1107/S1600536810043886]

3-(2,5-Dimethylfuran-3-yl)-1*H*-pyrazol-5-ol–ethyl 3-(propan-2-ylidene)carbazate (1/1)

Tara Shahani, Hoong-Kun Fun, R. Venkat Ragavan, V. Vijayakumar and S. Sarveswari

S1. Comment

Antibacterial and antifungal activities of the azoles are most widely studied and some of them are in clinical practice as anti-microbial agents. However, the azole-resistant strain had led to the development of new antimicrobial compounds. In particular, pyrazole derivatives are extensively studied and used as antimicrobial agents. Pyrazole is an important class of heterocyclic compounds and many pyrazole derivatives are reported to have the broad spectrum of biological properties such as anti-inflammatory, antifungal, herbicidal, anti-tumour, cytotoxic, molecular modelling and antiviral activities. Pyrazole derivatives also act as antiangiogenic agents, A3 adenosine receptor antagonists, neuropeptide YY5 receptor antagonists, kinase inhibitor for treatment of type 2 diabetes, hyperlipidemia, obesity, and thrombopiotinmimetics. Recently urea derivatives of pyrazoles have been reported as potent inhibitors of p38 kinase. Since the high electronegativity of halogens (particularly chlorine and fluorine) in the aromatic part of the drug molecules play an important role in enhancing their biological activity, we are interested to have 4-fluoro or 4-chloro substitution in the aryls of 1,5-diaryl pyrazoles. As part of our on-going research aiming the synthesis of new antimicrobial compounds, we have reported the synthesis of novel pyrazole derivatives and their microbial activities (Ragavan *et al.*, 2009; 2010). The structure of the title compound is presented here.

The asymmetric unit of the title compound, (Fig. 1), consists of one 3-(2,5-dimethylfuran-3-yl)-1*H*-pyrazol-5-ol and one ethyl2- (propan-2-ylidene)hydrazine carboxylate. The maximum deviations in 1*H*- pyrazole-5-ol (N1/N2/C1–C3/O2) and furan (C4–C7/O1) rings are 0.014 (1) and 0.003 (1) Å at atoms C2 and C7, respectively. The dihedral angles formed between the 1*H*-pyrazole-5-ol ring and 2,5-dimethylfuran ring (C4–C9/O1) is 21.07 (5)°. The bond lengths (Allen *et al.*,1987) and angles are within normal ranges and comparable to those closely related structures (Shahani *et al.*, 2010).

In the crystal packing (Fig. 2), pairs of intermolecular N2—H1O2···O2 hydrogen bonds form dimers with neighbouring molecules, generating $R^2_2(8)$ ring motif. Furthermore N1—H1N1···O4, N1—H1N1···N4, N3—H1N3···O2, O2—H1O2···N2 and C5—H5A···O4 hydrogen bonds (Table 1) link the molecules into ribbons along [010] direction with bifurcated $R_1^2(5)$ and $R_2^1(7)$ ring motifs. The crystal structure is stablilized by weak π–π and C—H···π interactions [Cg1···Cg1 = 3.5686 (15) Å, symmetry code, 2-*X*, 1-Y, –*Z*], Cg1 is the centroids of the 1*H*-pyrazole ring (N1/N2/C1—C3) and Cg2 is the centroids of the 1*H*-pyrazole ring (N1/N2/C1–C3).

S2. Experimental

The compound has been synthesized using the method available in the literature (Ragavan *et al.*,2009) and recrystallized using the ethanol-chloroform 1:1 mixture to yield colourless blocks of (I). Yield: 78%. M.p. 225.5–227.5 °C.

S3. Refinement

The hydrogen atoms bound to C atoms were positioned geometrically [C–H = 0.96–0.97 Å] with U_{iso}(H) =1.2 or 1.5U_{iso}(C). A rotating group model was applied to the methyl groups. The hydrogen atoms attached to the N and O atoms were located from the difference map and refined freely, [N–H = 0.872 (18)–0.883 (18) Å, O–H = 0.93 Å].

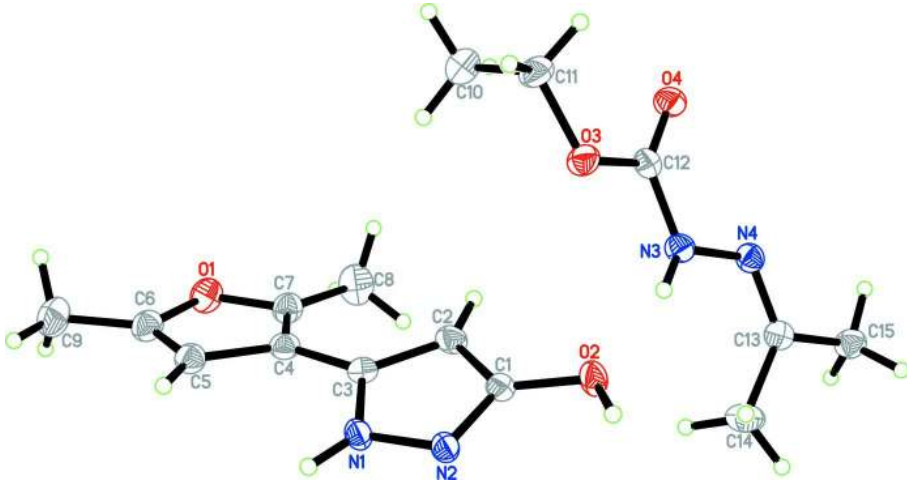

Figure 1

The molecular structure of the title compound, showing 50% probability displacement ellipsoids.

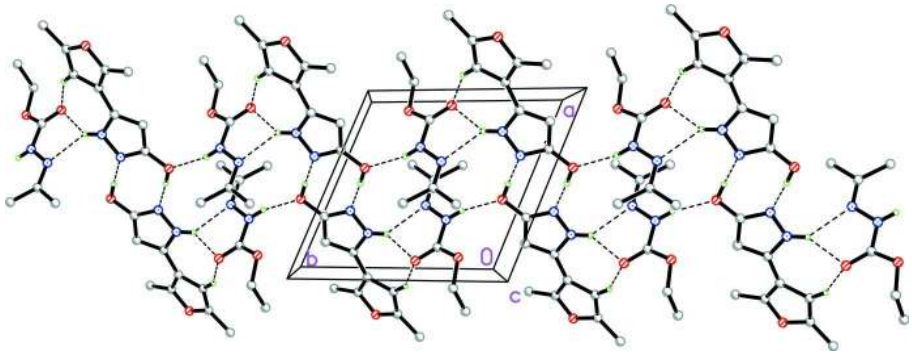

Figure 2

The crystal packing of the title compound, viewed along *c* axis, showing ribbons along the [010] direction..

3-(2,5-Dimethylfuran-3-yl)-1*H*-pyrazol-5-ol–ethyl 3-(propan-2-ylidene)carbazate (1/1)

Crystal data

$C_6H_{12}N_2O_2{\cdot}C_9H_{10}N_2O_2$
M_r = 322.37
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 8.6988 (17) Å
b = 9.4830 (19) Å
c = 11.837 (4) Å
α = 107.293 (4)°
β = 100.354 (5)°
γ = 108.346 (3)°
V = 843.7 (3) Å^3
Z = 2
F(000) = 344
D_x = 1.269 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7782 reflections
θ = 2.6–31.7°
μ = 0.09 mm^{-1}
T = 100 K
Block, colourless
0.40 × 0.21 × 0.13 mm

Data collection

Bruker APEXII DUO CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.964, T_{max} = 0.988
13322 measured reflections
3264 independent reflections
2911 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 26.0°, θ_{min} = 1.9°
h = −10→10
k = −11→11
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.099
S = 1.11
3264 reflections
225 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
$w = 1/[\sigma^2(F_o^2) + (0.045P)^2 + 0.2939P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cyrosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

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	0.72298 (12)	0.49965 (12)	−0.03577 (8)	0.0272 (2)
O2	1.41202 (12)	1.13027 (10)	0.43430 (9)	0.0232 (2)
N1	1.21447 (13)	0.71967 (13)	0.29969 (10)	0.0197 (2)
N2	1.34466 (13)	0.85605 (12)	0.38574 (9)	0.0190 (2)
C1	1.31074 (15)	0.97528 (15)	0.36573 (11)	0.0185 (3)
C2	1.16205 (16)	0.91874 (15)	0.26795 (12)	0.0211 (3)
H2A	1.1136	0.9791	0.2366	0.025*
C3	1.10286 (15)	0.75316 (15)	0.22806 (11)	0.0185 (3)
C4	0.95185 (16)	0.62751 (15)	0.13126 (11)	0.0201 (3)
C5	0.87164 (16)	0.46384 (15)	0.11997 (12)	0.0222 (3)
H5A	0.9076	0.4169	0.1725	0.027*
C6	0.73478 (17)	0.39202 (16)	0.01874 (12)	0.0252 (3)
C7	0.85745 (16)	0.64286 (16)	0.03429 (12)	0.0240 (3)
C8	0.8742 (2)	0.77483 (18)	−0.01199 (14)	0.0344 (3)

H8A	0.9922	0.8414	0.0089	0.052*
H8B	0.8166	0.8382	0.0257	0.052*
H8C	0.8246	0.7301	−0.1005	0.052*
C9	0.59939 (19)	0.22804 (18)	−0.04258 (14)	0.0342 (3)
H9A	0.6186	0.1632	0.0027	0.051*
H9B	0.6011	0.1810	−0.1260	0.051*
H9C	0.4909	0.2338	−0.0441	0.051*
O3	0.08857 (11)	0.22838 (11)	0.42456 (9)	0.0236 (2)
O4	0.06433 (11)	0.42612 (11)	0.36063 (9)	0.0244 (2)
N3	0.29597 (14)	0.35988 (13)	0.36500 (10)	0.0209 (2)
N4	0.37772 (13)	0.48909 (12)	0.33504 (10)	0.0201 (2)
C10	−0.21443 (18)	0.07821 (18)	0.31978 (15)	0.0346 (3)
H10A	−0.3233	0.0471	0.3338	0.052*
H10B	−0.1904	−0.0153	0.2871	0.052*
H10C	−0.2154	0.1302	0.2615	0.052*
C11	−0.07996 (17)	0.19197 (17)	0.44018 (13)	0.0267 (3)
H11A	−0.0984	0.2905	0.4695	0.032*
H11B	−0.0878	0.1443	0.5021	0.032*
C12	0.14196 (16)	0.34622 (14)	0.38212 (11)	0.0194 (3)
C13	0.52197 (16)	0.50193 (15)	0.31731 (11)	0.0212 (3)
C14	0.60676 (18)	0.38865 (18)	0.32513 (14)	0.0300 (3)
H14A	0.6155	0.3777	0.4039	0.045*
H14B	0.7183	0.4299	0.3169	0.045*
H14C	0.5408	0.2856	0.2596	0.045*
C15	0.61073 (17)	0.64131 (16)	0.28562 (13)	0.0249 (3)
H15A	0.5436	0.7044	0.2843	0.037*
H15B	0.6259	0.6025	0.2054	0.037*
H15C	0.7196	0.7063	0.3468	0.037*
H1N1	1.211 (2)	0.626 (2)	0.3012 (15)	0.033 (4)*
H1N3	0.347 (2)	0.304 (2)	0.3897 (15)	0.031 (4)*
H1O2	1.496 (3)	1.138 (2)	0.500 (2)	0.057 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0228 (5)	0.0284 (5)	0.0227 (5)	0.0062 (4)	0.0009 (4)	0.0068 (4)
O2	0.0222 (5)	0.0154 (4)	0.0274 (5)	0.0068 (4)	−0.0018 (4)	0.0078 (4)
N1	0.0200 (5)	0.0146 (5)	0.0221 (5)	0.0065 (4)	0.0026 (4)	0.0061 (4)
N2	0.0178 (5)	0.0157 (5)	0.0215 (5)	0.0065 (4)	0.0028 (4)	0.0061 (4)
C1	0.0190 (6)	0.0173 (6)	0.0212 (6)	0.0085 (5)	0.0067 (5)	0.0080 (5)
C2	0.0209 (6)	0.0212 (6)	0.0231 (6)	0.0115 (5)	0.0041 (5)	0.0090 (5)
C3	0.0174 (6)	0.0216 (6)	0.0187 (6)	0.0095 (5)	0.0070 (5)	0.0079 (5)
C4	0.0190 (6)	0.0218 (6)	0.0194 (6)	0.0090 (5)	0.0073 (5)	0.0059 (5)
C5	0.0215 (6)	0.0224 (6)	0.0217 (6)	0.0084 (5)	0.0074 (5)	0.0069 (5)
C6	0.0233 (7)	0.0258 (7)	0.0243 (7)	0.0080 (5)	0.0089 (5)	0.0073 (5)
C7	0.0211 (6)	0.0246 (7)	0.0221 (6)	0.0075 (5)	0.0043 (5)	0.0060 (5)
C8	0.0364 (8)	0.0329 (8)	0.0294 (7)	0.0115 (7)	−0.0003 (6)	0.0139 (6)
C9	0.0279 (7)	0.0295 (8)	0.0323 (8)	0.0019 (6)	0.0049 (6)	0.0067 (6)

O3	0.0212 (5)	0.0240 (5)	0.0319 (5)	0.0101 (4)	0.0109 (4)	0.0159 (4)
O4	0.0234 (5)	0.0235 (5)	0.0314 (5)	0.0129 (4)	0.0088 (4)	0.0133 (4)
N3	0.0214 (5)	0.0195 (5)	0.0282 (6)	0.0108 (5)	0.0090 (4)	0.0139 (5)
N4	0.0217 (5)	0.0185 (5)	0.0218 (5)	0.0084 (4)	0.0064 (4)	0.0093 (4)
C10	0.0259 (7)	0.0307 (8)	0.0430 (9)	0.0076 (6)	0.0118 (6)	0.0112 (7)
C11	0.0232 (7)	0.0288 (7)	0.0340 (7)	0.0104 (6)	0.0152 (6)	0.0156 (6)
C12	0.0218 (6)	0.0168 (6)	0.0187 (6)	0.0079 (5)	0.0045 (5)	0.0063 (5)
C13	0.0221 (6)	0.0226 (6)	0.0196 (6)	0.0100 (5)	0.0061 (5)	0.0079 (5)
C14	0.0310 (7)	0.0334 (8)	0.0411 (8)	0.0207 (6)	0.0195 (6)	0.0215 (7)
C15	0.0234 (7)	0.0261 (7)	0.0293 (7)	0.0108 (5)	0.0100 (5)	0.0138 (6)

Geometric parameters (Å, º)

O1—C7	1.3719 (16)	C9—H9C	0.9600
O1—C6	1.3792 (17)	O3—C12	1.3445 (15)
O2—C1	1.3468 (15)	O3—C11	1.4558 (15)
O2—H1O2	0.93 (2)	O4—C12	1.2124 (15)
N1—C3	1.3493 (16)	N3—C12	1.3625 (17)
N1—N2	1.3685 (14)	N3—N4	1.3905 (15)
N1—H1N1	0.883 (18)	N3—H1N3	0.872 (18)
N2—C1	1.3288 (16)	N4—C13	1.2834 (17)
C1—C2	1.3988 (18)	C10—C11	1.502 (2)
C2—C3	1.3844 (18)	C10—H10A	0.9600
C2—H2A	0.9300	C10—H10B	0.9600
C3—C4	1.4561 (18)	C10—H10C	0.9600
C4—C7	1.3597 (19)	C11—H11A	0.9700
C4—C5	1.4405 (18)	C11—H11B	0.9700
C5—C6	1.3448 (19)	C13—C14	1.4967 (19)
C5—H5A	0.9300	C13—C15	1.4967 (18)
C6—C9	1.4835 (19)	C14—H14A	0.9600
C7—C8	1.486 (2)	C14—H14B	0.9600
C8—H8A	0.9600	C14—H14C	0.9600
C8—H8B	0.9600	C15—H15A	0.9600
C8—H8C	0.9600	C15—H15B	0.9600
C9—H9A	0.9600	C15—H15C	0.9600
C9—H9B	0.9600		

C7—O1—C6	107.17 (10)	H9A—C9—H9C	109.5
C1—O2—H1O2	110.5 (13)	H9B—C9—H9C	109.5
C3—N1—N2	111.95 (10)	C12—O3—C11	115.88 (10)
C3—N1—H1N1	129.8 (11)	C12—N3—N4	116.20 (11)
N2—N1—H1N1	118.1 (11)	C12—N3—H1N3	119.0 (11)
C1—N2—N1	104.49 (10)	N4—N3—H1N3	123.2 (11)
N2—C1—O2	121.83 (11)	C13—N4—N3	116.67 (11)
N2—C1—C2	111.95 (11)	C11—C10—H10A	109.5
O2—C1—C2	126.22 (11)	C11—C10—H10B	109.5
C3—C2—C1	104.84 (11)	H10A—C10—H10B	109.5
C3—C2—H2A	127.6	C11—C10—H10C	109.5

C1—C2—H2A	127.6	H10A—C10—H10C	109.5
N1—C3—C2	106.77 (11)	H10B—C10—H10C	109.5
N1—C3—C4	122.08 (11)	O3—C11—C10	110.77 (11)
C2—C3—C4	131.15 (12)	O3—C11—H11A	109.5
C7—C4—C5	106.49 (11)	C10—C11—H11A	109.5
C7—C4—C3	126.43 (12)	O3—C11—H11B	109.5
C5—C4—C3	127.08 (12)	C10—C11—H11B	109.5
C6—C5—C4	106.74 (12)	H11A—C11—H11B	108.1
C6—C5—H5A	126.6	O4—C12—O3	125.45 (12)
C4—C5—H5A	126.6	O4—C12—N3	125.31 (12)
C5—C6—O1	109.97 (12)	O3—C12—N3	109.22 (10)
C5—C6—C9	134.00 (13)	N4—C13—C14	125.22 (12)
O1—C6—C9	116.02 (12)	N4—C13—C15	116.82 (12)
C4—C7—O1	109.62 (12)	C14—C13—C15	117.96 (11)
C4—C7—C8	134.17 (13)	C13—C14—H14A	109.5
O1—C7—C8	116.15 (11)	C13—C14—H14B	109.5
C7—C8—H8A	109.5	H14A—C14—H14B	109.5
C7—C8—H8B	109.5	C13—C14—H14C	109.5
H8A—C8—H8B	109.5	H14A—C14—H14C	109.5
C7—C8—H8C	109.5	H14B—C14—H14C	109.5
H8A—C8—H8C	109.5	C13—C15—H15A	109.5
H8B—C8—H8C	109.5	C13—C15—H15B	109.5
C6—C9—H9A	109.5	H15A—C15—H15B	109.5
C6—C9—H9B	109.5	C13—C15—H15C	109.5
H9A—C9—H9B	109.5	H15A—C15—H15C	109.5
C6—C9—H9C	109.5	H15B—C15—H15C	109.5

C3—N1—N2—C1	0.09 (13)	C7—O1—C6—C5	0.06 (14)
N1—N2—C1—O2	179.58 (11)	C7—O1—C6—C9	179.60 (11)
N1—N2—C1—C2	−0.44 (14)	C5—C4—C7—O1	0.55 (14)
N2—C1—C2—C3	0.62 (14)	C3—C4—C7—O1	−178.68 (11)
O2—C1—C2—C3	−179.40 (11)	C5—C4—C7—C8	−176.26 (16)
N2—N1—C3—C2	0.30 (14)	C3—C4—C7—C8	4.5 (2)
N2—N1—C3—C4	−178.86 (10)	C6—O1—C7—C4	−0.39 (14)
C1—C2—C3—N1	−0.53 (13)	C6—O1—C7—C8	177.06 (12)
C1—C2—C3—C4	178.51 (12)	C12—N3—N4—C13	−179.21 (11)
N1—C3—C4—C7	−161.23 (13)	C12—O3—C11—C10	84.10 (14)
C2—C3—C4—C7	19.8 (2)	C11—O3—C12—O4	2.70 (18)
N1—C3—C4—C5	19.70 (19)	C11—O3—C12—N3	−176.27 (10)
C2—C3—C4—C5	−159.23 (13)	N4—N3—C12—O4	8.26 (18)
C7—C4—C5—C6	−0.50 (14)	N4—N3—C12—O3	−172.77 (10)
C3—C4—C5—C6	178.72 (12)	N3—N4—C13—C14	0.65 (19)
C4—C5—C6—O1	0.27 (14)	N3—N4—C13—C15	−179.72 (11)
C4—C5—C6—C9	−179.15 (15)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*1···O4^{i}	0.883 (18)	2.304 (19)	3.0363 (19)	140.1 (16)
N1—H1*N*1···N4^{i}	0.883 (18)	2.288 (19)	3.043 (2)	143.1 (16)
N3—H1*N*3···O2^{ii}	0.872 (18)	2.076 (19)	2.9293 (19)	166.7 (18)
O2—H1*O*2···N2^{iii}	0.93 (2)	1.73 (2)	2.6602 (17)	176 (2)
C5—H5*A*···O4^{i}	0.93	2.35	3.212 (2)	153
C11—H11*B*···*Cg*2^{iv}	0.97	2.71	3.50 (2)	138

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) *x*−1, *y*−1, *z*; (iii) −*x*+3, −*y*+2, −*z*+1; (iv) −*x*+1, −*y*+1, −*z*+1.