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3-[5-Methyl-1-(4-methylphenyl)-1*H*-1,2,3-triazol-4-yl]-1-phenyl-1*H*-pyrazole-4-carbaldehyde

Gamal A. El-Hiti,[a]* Bakr F. Abdel-Wahab,[b,c] Alaa Alqahtani,[d] Amany S. Hegazy[e] and Benson M. Kariuki[e]‡

[a]Department of Optometry, College of Applied Medical Sciences, King Saud University, PO Box 10219, Riyadh 11433, Saudi Arabia, [b]Department of Chemistry, College of Science and Humanities, Shaqra University, Duwadimi, Saudi Arabia, [c]Applied Organic Chemistry Department, National Research, Centre, Dokki, Giza, Egypt, [d]Pharmaceutical Chemistry Department, College of Pharmacy, Umm Al-Qura University, Makkah, Saudi Arabia, and [e]School of Chemistry, Cardiff University, Main Building, Park Place, Cardiff CF10 3AT, UK. *Correspondence e-mail: gelhiti@ksu.edu.sa

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‡ Additional correspondence author, e-mail: kariukib@cardiff.ac.uk.

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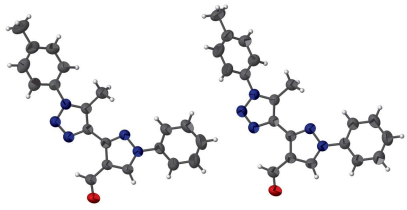
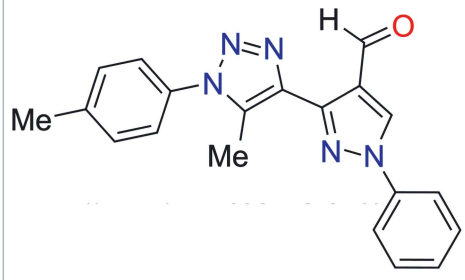
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, $C_{20}H_{17}N_5O$, consists of two independent molecules. The molecules comprise tolyl (*A*), triazolyl (*B*), pyrazolecarbaldehydyl (*C*) and phenyl (*D*) groups. The angles between the planes through neighouring rings *A*/*B*, *B*/*C* and *C*/*D* are 39.1 (1), 6.0 (1) and 12.6 (1)°, respectively, for the first molecule and 46.0 (1), 4.6 (1) and 8.5 (2)°, respectively, for the second. In the crystal, the two independent molecules form dimers linked by four C—H···O hydrogen bonds with each O atom accepting two such links.

3D view



Chemical scheme



Structure description

1,2,3-Triazoles are biologically active heterocycles (Bonandi *et al.*, 2017). Pyrazoles have been used in various pharmacological agents of diverse therapeutic categories (Karrouchi *et al.*, 2018). As part of our ongoing studies in this area (Abdel-Wahab *et al.*, 2015), we now describe the crystal structure of the title compound.

The asymmetric unit consists of two independent molecules **1** (containing C1) and **2** (containing C21). Each molecule comprises tolyl (*A*), triazolyl (*B*), pyrazole-carbaldehydyl (*C*) and phenyl (*D*) groups (Fig. 1). The angles between the planes through neighouring rings *A*/*B*, *B*/*C* and *C*/*D* are 39.1 (1), 6.0 (1) and 12.6 (1)°, respectively, for molecule **1** and 46.0 (1), 4.6 (1) and 8.5 (2)°, respectively, for molecule **2**. In the crystal, the independent molecules are linked by four C—H···O hydrogen bonds (two with O1

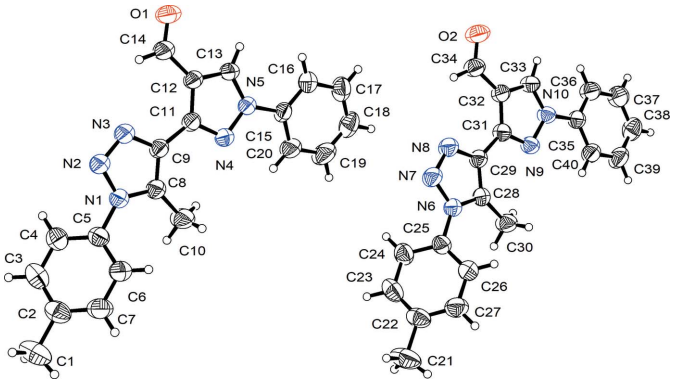


Figure 1
The molecular structure of the title compound showing 50% displacement ellipsoids.

and two with O2 as the acceptors) to form dimers (Table 1, Fig. 2). The dimers are arranged in layers parallel to the (101) plane in the extended structure.

Synthesis and crystallization

The title compound was synthesized as previously reported (Abdel-Wahab *et al.*, 2015) from the treatment of 5-methyl-4-(1-(2-phenylhydrazono)ethyl)-1-*p*-tolyl-1*H*-1,2,3-triazole with phosphorus oxychloride in dimethylformamide (DMF) at 0°C and then at 25°C for 12 h. The resulting mixture was neutralized with ammonium hydroxide solution (5%) and the solid obtained was filtered, dried and recrystallized from DMF solution to give colourless blocks (83%), m.p. 195–196°C.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

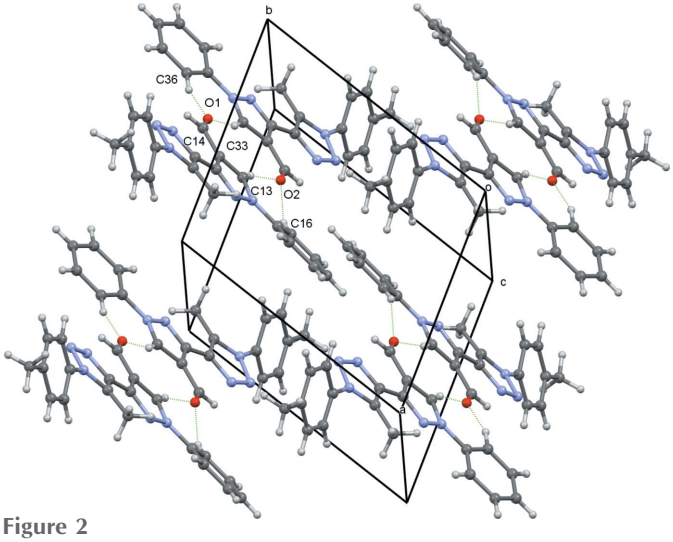


Figure 2
A view of the crystal structure along [001] showing intermolecular contacts as dotted lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13···O2^{i}	0.93	2.54	3.452 (3)	168
C16—H16···O2^{i}	0.93	2.54	3.432 (3)	161
C33—H33···O1^{i}	0.93	2.42	3.329 (3)	165
C36—H36···O1^{i}	0.93	2.41	3.297 (3)	160

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{17}N_5O$
M_r	343.39
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, b, c (Å)	9.7894 (7), 10.9830 (6), 17.2596 (8)
α, β, γ (°)	93.490 (4), 95.702 (5), 107.729 (6)
V (Å^3)	1750.67 (19)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.51 × 0.29 × 0.21
Data collection	
Diffractometer	Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, Atlas
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.988, 0.993
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	16161, 8348, 4289
R_{int}	0.033
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.703
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.065, 0.186, 1.02
No. of reflections	8348
No. of parameters	474
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.21, −0.18

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXS97* (Sheldrick, 2008), *SHELXL2018* (Sheldrick, 2015), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012), *CHEMDRAW Ultra* (Cambridge Soft, 2001).

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full crystallographic data

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Crystal data

$C_{20}H_{17}N_5O$
M_r = 343.39
Triclinic, $P\overline{1}$
a = 9.7894 (7) Å
b = 10.9830 (6) Å
c = 17.2596 (8) Å
α = 93.490 (4)°
β = 95.702 (5)°
γ = 107.729 (6)°
V = 1750.67 (19) Å^3
Z = 4
$F(000)$ = 720
D_x = 1.303 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3321 reflections
θ = 3.9–26.0°
μ = 0.09 mm^{-1}
T = 296 K
Block, colourless
0.51 × 0.29 × 0.21 mm

Data collection

Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, Atlas diffractometer
ω scans
Absorption correction: gaussian (CrysAlisPro; Rigaku OD, 2015)
T_{min} = 0.988, T_{max} = 0.993
16161 measured reflections
8348 independent reflections
4289 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 30.0°, θ_{min} = 1.2°
h = −11→12
k = −14→14
l = −22→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.186
S = 1.02
8348 reflections
474 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0654P)^2 + 0.3491P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Extinction correction: SHELXL2018 (Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0073 (12)

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. All hydrogen atoms were placed in calculated positions and refined using a riding model. Bond distances for sp^2 C—H hydrogen atoms were set to 0.93 Å and their U_{iso} set to 1.2 times U_{eq}(C). Bond distances for methyl C—H hydrogen atoms were set to 0.96 Å and their U_{iso} set to 1.5 times U_{eq}(C) with the group free to rotate about the C—C bond.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.0712 (4)	−0.3249 (3)	1.28244 (17)	0.1113 (12)
H1A	0.052641	−0.415552	1.284534	0.167*
H1B	−0.016407	−0.304173	1.286566	0.167*
H1C	0.142888	−0.279085	1.324964	0.167*
C2	0.1253 (3)	−0.2870 (2)	1.20609 (15)	0.0772 (8)
C3	0.2465 (3)	−0.3124 (2)	1.18414 (15)	0.0784 (8)
H3	0.292625	−0.356492	1.216383	0.094*
C4	0.3012 (3)	−0.2741 (2)	1.11560 (14)	0.0683 (7)
H4	0.383419	−0.291762	1.102293	0.082*
C5	0.2333 (3)	−0.2101 (2)	1.06756 (13)	0.0606 (6)
C6	0.1083 (3)	−0.1885 (2)	1.08590 (16)	0.0775 (8)
H6	0.059060	−0.149184	1.051878	0.093*
C7	0.0567 (3)	−0.2258 (3)	1.15538 (17)	0.0846 (8)
H7	−0.026400	−0.209094	1.168172	0.101*
C8	0.2966 (3)	−0.0657 (2)	0.95852 (13)	0.0593 (6)
C9	0.3572 (2)	−0.08357 (19)	0.89240 (13)	0.0551 (5)
C10	0.2546 (4)	0.0452 (2)	0.98959 (17)	0.0928 (10)
H10A	0.263488	0.049410	1.045658	0.139*
H10B	0.156385	0.034654	0.969319	0.139*
H10C	0.316988	0.123090	0.973863	0.139*
C11	0.3917 (2)	−0.00234 (19)	0.82856 (13)	0.0541 (5)
C12	0.4634 (2)	−0.01785 (19)	0.76307 (13)	0.0564 (6)
C13	0.4665 (2)	0.0866 (2)	0.72310 (13)	0.0569 (6)
H13	0.506839	0.105062	0.676932	0.068*
C14	0.5234 (3)	−0.1176 (2)	0.74118 (16)	0.0792 (8)
H14	0.514676	−0.183787	0.773318	0.095*
C15	0.3862 (2)	0.2794 (2)	0.74615 (14)	0.0571 (6)
C16	0.4153 (3)	0.3263 (2)	0.67588 (15)	0.0695 (7)
H16	0.444824	0.279264	0.638028	0.083*
C17	0.4001 (3)	0.4442 (3)	0.66179 (18)	0.0809 (8)
H17	0.418989	0.476358	0.613998	0.097*
C18	0.3579 (3)	0.5140 (3)	0.7172 (2)	0.0882 (9)
H18	0.346166	0.592598	0.707025	0.106*
C19	0.3328 (4)	0.4676 (3)	0.7881 (2)	0.1017 (10)
H19	0.306254	0.516093	0.826522	0.122*

C20	0.3465 (3)	0.3496 (2)	0.80313 (17)	0.0830 (8)
H20	0.328967	0.318124	0.851216	0.100*
C21	−0.2941 (4)	0.5864 (3)	0.98610 (19)	0.1168 (13)
H21A	−0.241402	0.636997	1.033160	0.175*
H21B	−0.306369	0.497299	0.991423	0.175*
H21C	−0.387077	0.598747	0.977108	0.175*
C22	−0.2114 (4)	0.6273 (2)	0.91809 (16)	0.0783 (8)
C23	−0.0752 (4)	0.6162 (2)	0.91614 (16)	0.0821 (8)
H23	−0.035778	0.580842	0.956870	0.098*
C24	0.0042 (3)	0.6561 (2)	0.85547 (15)	0.0720 (7)
H24	0.096526	0.648968	0.855653	0.086*
C25	−0.0551 (3)	0.7065 (2)	0.79484 (14)	0.0618 (6)
C26	−0.1919 (3)	0.7160 (2)	0.79411 (16)	0.0765 (7)
H26	−0.232868	0.748106	0.752328	0.092*
C27	−0.2682 (3)	0.6769 (3)	0.85651 (17)	0.0845 (8)
H27	−0.360245	0.684591	0.856511	0.101*
C28	0.0488 (2)	0.8566 (2)	0.69514 (13)	0.0569 (6)
C29	0.1348 (2)	0.8423 (2)	0.63965 (13)	0.0569 (6)
C30	−0.0065 (3)	0.9633 (2)	0.71839 (16)	0.0752 (7)
H30A	−0.097793	0.952025	0.687926	0.113*
H30B	0.061226	1.043504	0.709403	0.113*
H30C	−0.018804	0.963322	0.772884	0.113*
C31	0.1888 (2)	0.92652 (19)	0.57980 (13)	0.0561 (5)
C32	0.2710 (2)	0.9107 (2)	0.51911 (13)	0.0576 (6)
C33	0.2840 (3)	1.0170 (2)	0.47884 (13)	0.0600 (6)
H33	0.331495	1.035272	0.434849	0.072*
C34	0.3304 (3)	0.8080 (2)	0.50072 (15)	0.0704 (7)
H34	0.321107	0.744151	0.534681	0.084*
C35	0.2025 (3)	1.2106 (2)	0.49593 (13)	0.0576 (6)
C36	0.2778 (3)	1.2760 (2)	0.44062 (16)	0.0752 (7)
H36	0.337994	1.241736	0.414163	0.090*
C37	0.2636 (3)	1.3934 (3)	0.42448 (18)	0.0846 (8)
H37	0.312940	1.437398	0.386147	0.102*
C38	0.1782 (3)	1.4455 (3)	0.46404 (18)	0.0845 (8)
H38	0.169949	1.525055	0.453187	0.101*
C39	0.1041 (3)	1.3800 (3)	0.52007 (19)	0.0872 (8)
H39	0.046390	1.415715	0.547634	0.105*
C40	0.1150 (3)	1.2619 (2)	0.53551 (16)	0.0723 (7)
H40	0.063151	1.216867	0.572699	0.087*
N1	0.2891 (2)	−0.17216 (16)	0.99594 (11)	0.0587 (5)
N2	0.3447 (2)	−0.25196 (18)	0.95537 (12)	0.0697 (6)
N3	0.3860 (2)	−0.19775 (18)	0.89270 (12)	0.0686 (6)
N4	0.3537 (2)	0.10420 (16)	0.82772 (11)	0.0574 (5)
N5	0.4016 (2)	0.15758 (16)	0.76206 (10)	0.0547 (5)
N6	0.0278 (2)	0.74817 (17)	0.73213 (11)	0.0614 (5)
N7	0.0988 (2)	0.67146 (19)	0.70172 (13)	0.0741 (6)
N8	0.1638 (2)	0.72915 (18)	0.64519 (12)	0.0719 (6)
N9	0.1551 (2)	1.03480 (17)	0.57660 (11)	0.0605 (5)

N10	0.2162 (2)	1.08935 (16)	0.51417 (11)	0.0580 (5)
O1	0.5843 (3)	−0.12112 (19)	0.68400 (12)	0.1063 (8)
O2	0.3917 (2)	0.80038 (17)	0.44354 (12)	0.0902 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.144 (3)	0.101 (2)	0.074 (2)	0.008 (2)	0.040 (2)	0.0128 (16)
C2	0.096 (2)	0.0605 (15)	0.0641 (16)	0.0059 (14)	0.0200 (15)	0.0026 (12)
C3	0.087 (2)	0.0705 (16)	0.0652 (16)	0.0068 (14)	0.0003 (15)	0.0151 (12)
C4	0.0671 (17)	0.0643 (14)	0.0689 (16)	0.0136 (12)	0.0065 (13)	0.0098 (11)
C5	0.0720 (17)	0.0538 (12)	0.0563 (14)	0.0173 (11)	0.0165 (12)	0.0064 (10)
C6	0.093 (2)	0.0785 (17)	0.0757 (18)	0.0398 (15)	0.0318 (16)	0.0174 (13)
C7	0.101 (2)	0.0785 (17)	0.085 (2)	0.0324 (15)	0.0422 (17)	0.0120 (14)
C8	0.0672 (16)	0.0532 (12)	0.0622 (14)	0.0229 (10)	0.0153 (12)	0.0071 (10)
C9	0.0568 (14)	0.0509 (12)	0.0619 (14)	0.0207 (10)	0.0136 (11)	0.0068 (9)
C10	0.145 (3)	0.0704 (17)	0.087 (2)	0.0547 (17)	0.054 (2)	0.0168 (14)
C11	0.0531 (14)	0.0516 (12)	0.0608 (13)	0.0194 (10)	0.0116 (11)	0.0068 (9)
C12	0.0634 (15)	0.0528 (12)	0.0596 (13)	0.0245 (10)	0.0176 (11)	0.0067 (10)
C13	0.0648 (15)	0.0580 (13)	0.0537 (13)	0.0249 (10)	0.0173 (11)	0.0052 (10)
C14	0.111 (2)	0.0722 (16)	0.0775 (18)	0.0512 (15)	0.0417 (17)	0.0198 (13)
C15	0.0570 (14)	0.0526 (12)	0.0675 (15)	0.0245 (10)	0.0098 (11)	0.0094 (10)
C16	0.0777 (18)	0.0673 (15)	0.0711 (16)	0.0314 (12)	0.0118 (13)	0.0155 (12)
C17	0.080 (2)	0.0735 (17)	0.095 (2)	0.0288 (14)	0.0089 (16)	0.0280 (14)
C18	0.085 (2)	0.0627 (16)	0.126 (3)	0.0344 (14)	0.0134 (19)	0.0214 (16)
C19	0.125 (3)	0.084 (2)	0.125 (3)	0.0628 (19)	0.049 (2)	0.0189 (18)
C20	0.110 (2)	0.0732 (17)	0.0891 (19)	0.0511 (15)	0.0407 (17)	0.0199 (14)
C21	0.173 (4)	0.088 (2)	0.101 (2)	0.036 (2)	0.078 (3)	0.0295 (17)
C22	0.107 (2)	0.0591 (15)	0.0721 (17)	0.0218 (14)	0.0352 (16)	0.0124 (12)
C23	0.111 (3)	0.0705 (16)	0.0643 (16)	0.0251 (15)	0.0124 (16)	0.0208 (12)
C24	0.0776 (18)	0.0693 (15)	0.0713 (16)	0.0234 (13)	0.0105 (14)	0.0207 (12)
C25	0.0690 (17)	0.0595 (13)	0.0603 (14)	0.0218 (11)	0.0141 (12)	0.0132 (10)
C26	0.0767 (19)	0.0902 (18)	0.0752 (17)	0.0375 (14)	0.0216 (15)	0.0259 (14)
C27	0.086 (2)	0.0864 (18)	0.093 (2)	0.0335 (15)	0.0396 (17)	0.0244 (15)
C28	0.0613 (15)	0.0559 (13)	0.0580 (13)	0.0228 (10)	0.0110 (11)	0.0115 (10)
C29	0.0617 (15)	0.0528 (12)	0.0617 (14)	0.0232 (10)	0.0134 (11)	0.0098 (10)
C30	0.096 (2)	0.0646 (15)	0.0789 (17)	0.0362 (13)	0.0351 (15)	0.0152 (12)
C31	0.0607 (14)	0.0505 (12)	0.0582 (13)	0.0176 (10)	0.0120 (11)	0.0061 (9)
C32	0.0596 (15)	0.0556 (12)	0.0606 (14)	0.0200 (10)	0.0143 (11)	0.0064 (10)
C33	0.0641 (15)	0.0590 (13)	0.0598 (14)	0.0196 (11)	0.0207 (12)	0.0057 (10)
C34	0.0821 (19)	0.0619 (14)	0.0759 (17)	0.0289 (12)	0.0279 (15)	0.0102 (12)
C35	0.0623 (15)	0.0531 (12)	0.0598 (14)	0.0205 (10)	0.0099 (11)	0.0076 (10)
C36	0.091 (2)	0.0647 (15)	0.0822 (18)	0.0324 (13)	0.0331 (15)	0.0203 (12)
C37	0.097 (2)	0.0700 (17)	0.095 (2)	0.0297 (15)	0.0285 (17)	0.0278 (14)
C38	0.090 (2)	0.0625 (16)	0.108 (2)	0.0327 (14)	0.0123 (18)	0.0197 (15)
C39	0.089 (2)	0.0835 (19)	0.110 (2)	0.0512 (16)	0.0255 (18)	0.0232 (16)
C40	0.0728 (18)	0.0739 (16)	0.0822 (18)	0.0340 (13)	0.0226 (14)	0.0204 (13)
N1	0.0696 (13)	0.0540 (10)	0.0591 (11)	0.0256 (9)	0.0167 (10)	0.0091 (8)

N2	0.0860 (15)	0.0680 (12)	0.0720 (13)	0.0403 (11)	0.0296 (12)	0.0191 (10)
N3	0.0815 (15)	0.0659 (12)	0.0729 (13)	0.0362 (10)	0.0286 (11)	0.0185 (10)
N4	0.0600 (12)	0.0587 (11)	0.0600 (11)	0.0240 (9)	0.0172 (9)	0.0110 (8)
N5	0.0581 (12)	0.0540 (10)	0.0580 (11)	0.0236 (8)	0.0138 (9)	0.0095 (8)
N6	0.0687 (13)	0.0632 (11)	0.0628 (12)	0.0307 (9)	0.0189 (10)	0.0167 (9)
N7	0.0845 (16)	0.0707 (13)	0.0863 (15)	0.0420 (11)	0.0322 (13)	0.0260 (11)
N8	0.0841 (16)	0.0666 (12)	0.0811 (14)	0.0371 (11)	0.0322 (12)	0.0239 (10)
N9	0.0693 (13)	0.0582 (11)	0.0593 (12)	0.0232 (9)	0.0190 (10)	0.0122 (8)
N10	0.0654 (13)	0.0536 (10)	0.0590 (11)	0.0200 (9)	0.0191 (10)	0.0101 (8)
O1	0.160 (2)	0.1014 (14)	0.0995 (15)	0.0799 (14)	0.0765 (15)	0.0327 (11)
O2	0.1142 (16)	0.0829 (12)	0.0947 (14)	0.0493 (11)	0.0510 (13)	0.0147 (10)

Geometric parameters (Å, º)

C1—C2	1.504 (3)	C21—H21C	0.9600
C1—H1A	0.9600	C22—C27	1.368 (4)
C1—H1B	0.9600	C22—C23	1.379 (4)
C1—H1C	0.9600	C23—C24	1.380 (3)
C2—C7	1.378 (4)	C23—H23	0.9300
C2—C3	1.380 (4)	C24—C25	1.373 (3)
C3—C4	1.383 (3)	C24—H24	0.9300
C3—H3	0.9300	C25—C26	1.374 (3)
C4—C5	1.367 (3)	C25—N6	1.431 (3)
C4—H4	0.9300	C26—C27	1.387 (3)
C5—C6	1.378 (3)	C26—H26	0.9300
C5—N1	1.435 (3)	C27—H27	0.9300
C6—C7	1.384 (3)	C28—N6	1.356 (3)
C6—H6	0.9300	C28—C29	1.369 (3)
C7—H7	0.9300	C28—C30	1.483 (3)
C8—N1	1.356 (3)	C29—N8	1.363 (3)
C8—C9	1.368 (3)	C29—C31	1.459 (3)
C8—C10	1.486 (3)	C30—H30A	0.9600
C9—N3	1.367 (3)	C30—H30B	0.9600
C9—C11	1.461 (3)	C30—H30C	0.9600
C10—H10A	0.9600	C31—N9	1.330 (3)
C10—H10B	0.9600	C31—C32	1.416 (3)
C10—H10C	0.9600	C32—C33	1.374 (3)
C11—N4	1.332 (3)	C32—C34	1.450 (3)
C11—C12	1.416 (3)	C33—N10	1.337 (3)
C12—C13	1.369 (3)	C33—H33	0.9300
C12—C14	1.440 (3)	C34—O2	1.216 (3)
C13—N5	1.336 (3)	C34—H34	0.9300
C13—H13	0.9300	C35—C36	1.368 (3)
C14—O1	1.207 (3)	C35—C40	1.372 (3)
C14—H14	0.9300	C35—N10	1.429 (3)
C15—C16	1.368 (3)	C36—C37	1.380 (3)
C15—C20	1.371 (3)	C36—H36	0.9300
C15—N5	1.430 (3)	C37—C38	1.360 (4)

C16—C17	1.381 (3)	C37—H37	0.9300
C16—H16	0.9300	C38—C39	1.373 (4)
C17—C18	1.363 (4)	C38—H38	0.9300
C17—H17	0.9300	C39—C40	1.373 (3)
C18—C19	1.370 (4)	C39—H39	0.9300
C18—H18	0.9300	C40—H40	0.9300
C19—C20	1.380 (4)	N1—N2	1.359 (3)
C19—H19	0.9300	N2—N3	1.306 (2)
C20—H20	0.9300	N4—N5	1.366 (2)
C21—C22	1.505 (3)	N6—N7	1.358 (3)
C21—H21A	0.9600	N7—N8	1.308 (3)
C21—H21B	0.9600	N9—N10	1.366 (2)

C2—C1—H1A	109.5	C22—C23—C24	121.9 (3)
C2—C1—H1B	109.5	C22—C23—H23	119.1
H1A—C1—H1B	109.5	C24—C23—H23	119.1
C2—C1—H1C	109.5	C25—C24—C23	119.0 (3)
H1A—C1—H1C	109.5	C25—C24—H24	120.5
H1B—C1—H1C	109.5	C23—C24—H24	120.5
C7—C2—C3	117.4 (2)	C24—C25—C26	120.6 (2)
C7—C2—C1	121.7 (3)	C24—C25—N6	118.8 (2)
C3—C2—C1	121.0 (3)	C26—C25—N6	120.6 (2)
C2—C3—C4	121.9 (3)	C25—C26—C27	119.1 (3)
C2—C3—H3	119.0	C25—C26—H26	120.4
C4—C3—H3	119.0	C27—C26—H26	120.4
C5—C4—C3	119.4 (3)	C22—C27—C26	121.6 (3)
C5—C4—H4	120.3	C22—C27—H27	119.2
C3—C4—H4	120.3	C26—C27—H27	119.2
C4—C5—C6	120.1 (2)	N6—C28—C29	103.65 (18)
C4—C5—N1	119.3 (2)	N6—C28—C30	124.0 (2)
C6—C5—N1	120.5 (2)	C29—C28—C30	132.2 (2)
C5—C6—C7	119.4 (3)	N8—C29—C28	109.49 (18)
C5—C6—H6	120.3	N8—C29—C31	121.5 (2)
C7—C6—H6	120.3	C28—C29—C31	129.0 (2)
C2—C7—C6	121.6 (3)	C28—C30—H30A	109.5
C2—C7—H7	119.2	C28—C30—H30B	109.5
C6—C7—H7	119.2	H30A—C30—H30B	109.5
N1—C8—C9	104.48 (18)	C28—C30—H30C	109.5
N1—C8—C10	124.7 (2)	H30A—C30—H30C	109.5
C9—C8—C10	130.7 (2)	H30B—C30—H30C	109.5
N3—C9—C8	108.58 (19)	N9—C31—C32	111.11 (18)
N3—C9—C11	121.1 (2)	N9—C31—C29	118.7 (2)
C8—C9—C11	130.3 (2)	C32—C31—C29	130.2 (2)
C8—C10—H10A	109.5	C33—C32—C31	104.39 (19)
C8—C10—H10B	109.5	C33—C32—C34	125.8 (2)
H10A—C10—H10B	109.5	C31—C32—C34	129.8 (2)
C8—C10—H10C	109.5	N10—C33—C32	107.81 (19)
H10A—C10—H10C	109.5	N10—C33—H33	126.1

H10B—C10—H10C	109.5	C32—C33—H33	126.1
N4—C11—C12	110.92 (18)	O2—C34—C32	123.9 (2)
N4—C11—C9	119.4 (2)	O2—C34—H34	118.1
C12—C11—C9	129.7 (2)	C32—C34—H34	118.1
C13—C12—C11	104.52 (18)	C36—C35—C40	120.2 (2)
C13—C12—C14	125.7 (2)	C36—C35—N10	120.5 (2)
C11—C12—C14	129.7 (2)	C40—C35—N10	119.3 (2)
N5—C13—C12	108.00 (19)	C35—C36—C37	119.3 (2)
N5—C13—H13	126.0	C35—C36—H36	120.3
C12—C13—H13	126.0	C37—C36—H36	120.3
O1—C14—C12	124.5 (2)	C38—C37—C36	120.7 (3)
O1—C14—H14	117.7	C38—C37—H37	119.6
C12—C14—H14	117.7	C36—C37—H37	119.6
C16—C15—C20	120.8 (2)	C37—C38—C39	119.7 (3)
C16—C15—N5	120.2 (2)	C37—C38—H38	120.2
C20—C15—N5	119.0 (2)	C39—C38—H38	120.2
C15—C16—C17	119.3 (3)	C38—C39—C40	120.2 (3)
C15—C16—H16	120.4	C38—C39—H39	119.9
C17—C16—H16	120.4	C40—C39—H39	119.9
C18—C17—C16	120.6 (3)	C35—C40—C39	119.8 (2)
C18—C17—H17	119.7	C35—C40—H40	120.1
C16—C17—H17	119.7	C39—C40—H40	120.1
C17—C18—C19	119.6 (3)	C8—N1—N2	110.73 (17)
C17—C18—H18	120.2	C8—N1—C5	130.73 (19)
C19—C18—H18	120.2	N2—N1—C5	118.54 (17)
C18—C19—C20	120.6 (3)	N3—N2—N1	107.00 (17)
C18—C19—H19	119.7	N2—N3—C9	109.21 (18)
C20—C19—H19	119.7	C11—N4—N5	104.88 (17)
C15—C20—C19	119.1 (3)	C13—N5—N4	111.67 (17)
C15—C20—H20	120.4	C13—N5—C15	128.83 (18)
C19—C20—H20	120.4	N4—N5—C15	119.37 (17)
C22—C21—H21A	109.5	C28—N6—N7	111.17 (18)
C22—C21—H21B	109.5	C28—N6—C25	130.08 (19)
H21A—C21—H21B	109.5	N7—N6—C25	118.74 (18)
C22—C21—H21C	109.5	N8—N7—N6	107.05 (18)
H21A—C21—H21C	109.5	N7—N8—C29	108.63 (19)
H21B—C21—H21C	109.5	C31—N9—N10	104.86 (18)
C27—C22—C23	117.8 (2)	C33—N10—N9	111.82 (18)
C27—C22—C21	121.4 (3)	C33—N10—C35	129.31 (19)
C23—C22—C21	120.7 (3)	N9—N10—C35	118.86 (18)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13···O2^{i}	0.93	2.54	3.452 (3)	168
C16—H16···O2^{i}	0.93	2.54	3.432 (3)	161

C33—H33···O1^{i}	0.93	2.42	3.329 (3)	165
C36—H36···O1^{i}	0.93	2.41	3.297 (3)	160

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.