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1-Methyl-5-nitro-3-phenyl-1*H*-indazole

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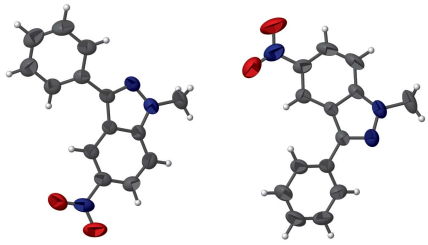
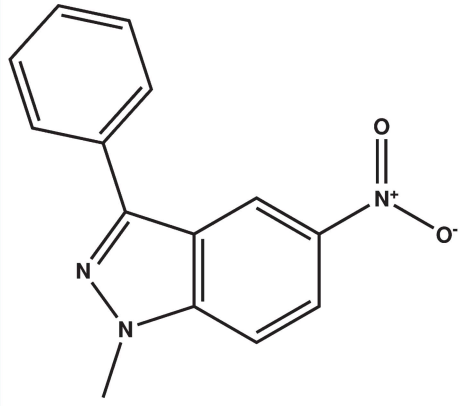
The title compound, $C_{14}H_{11}N_3O_2$, crystallizes with two molecules in the asymmetric unit. The indazole ring system and the nitro group are nearly coplanar, with the largest deviations from the mean plane being 0.070 (4) Å in one molecule and 0.022 (3) Å in the second. The dihedral angle between the mean plane through the phenyl ring and the mean plane of the indazole ring system is of 23.24 (18)° in the first molecule and 26.87 (18)° in the second. In the crystal, molecules are linked by two C—H···O hydrogen bonds, forming linear zigzag tapes running along the *c*-axis direction, and by π–π stacking of molecules along the *b* axis, generating a three-dimensional structure.

3D view



Chemical scheme



Structure description

3-Substituted indazoles obtained from different cross-coupling reactions are common components of drugs and have been found to be of pharmaceutical interest in a variety of therapeutic areas (Cerecetto *et al.*, 2005; Jennings *et al.*, 2007; Sun *et al.*, 1997, Bouissane *et al.*, 2006; Naas *et al.*, 2014). They frequently comprise the core frame of numerous pharmaceutically active compounds, such as Lonidamine [1-(2,4-dichlorobenzyl)-1*H*-indazole-3-carboxylic acid] and Granisetron {1-methyl-*N*-[(1*R*,3*R*,5*S*)-9-methyl-9-azabicyclo[3.3.1]nonan-3-yl]-1*H*-indazole-3-carboxamide}. The present paper is a continuation of our research work devoted to the development of the indazole derivatives with potential pharmacological activities (El Brahmi *et al.*, 2011; El Brahmi *et al.*, 2012).

The asymmetric unit of the title compound is built up from two independent molecules with different orientations, Fig. 1. The two fused five- and six-membered ring systems in each molecule are almost planar, with a maximum deviation of 0.018 (4) Å for C7 in the first molecule (N1,N2,N3,O1,O2,C1–C14) and 0.022 (3) Å for C22 in the second

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

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14B···O2^{i}	0.96	2.51	3.395 (6)	154
C19—H19···O4^{ii}	0.93	2.46	3.288 (6)	148

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

(N4,N5,N6,O3,O4,C15–C28). The dihedral angle between the two phenyl rings is 26.1 (2)°. Moreover, the mean plane of the indazole ring system makes a dihedral angle of 23.24 (18)° with the mean plane through the phenyl ring belonging to the first molecule and 26.87 (18)° in the second molecule. A least-squares overlay of the two molecules (Spek, 2009) is shown in Fig. 2 and reveals that the principal difference between the two is the relative inclinations of the C1–C6 and C19–C25 phenyl rings with respect to the planes of the indazole ring systems.

In the crystal, molecules are linked by C19—H19···O4 and C14—H14B···O2 hydrogen bonds (Table 1), forming linear, zigzag tapes running along the c-axis direction (Fig. 3). In addition, molecules are linked by five π–π stacking interactions between the fused rings, Fig. 4, with centroid–centroid distances in the range 3.852 (2) to 3.917 (2) Å.

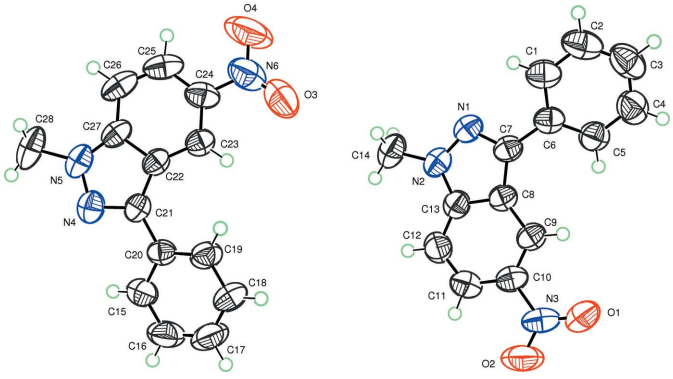


Figure 1
The molecular structure of the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small circles.

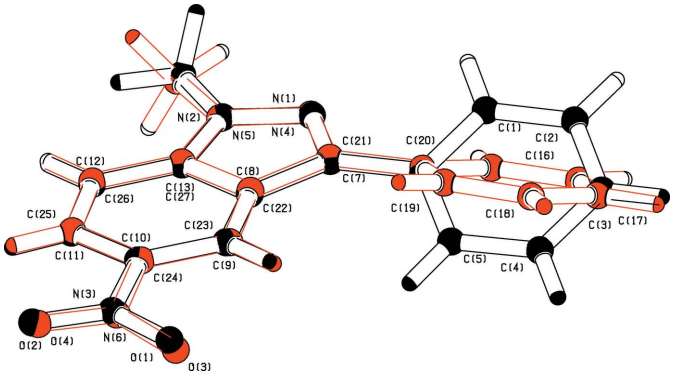


Figure 2
Least-squares fit of the two molecules in the asymmetric unit (one molecule is inverted).

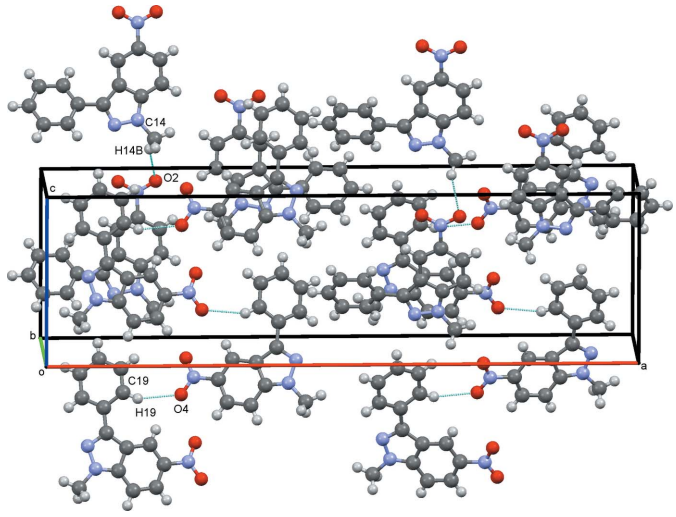


Figure 3
Packing of the title compound viewed along the b-axis direction showing the C—H···O hydrogen bonds.

Synthesis and crystallization

In a 10 ml flask, a solution of phenanthroline (0.048 g, 0.31 mmol) in *N*,*N*-dimethylacetamide (DMA) (5 ml) was degassed by bubbling argon through the solution, and then palladium acetate (0.045 g, 0.14 mmol) was added. The solution was stirred at room temperature for 3 min, then K_2CO_3 (0.39 g, 2.1 mmol), 1-methyl-5-nitro-indazole (0.12 g, 0.7 mmol) and iodobenzene (0.18 g, 0.9 mmol) were successively added. The reaction mixture was heated at reflux under argon for 48 h, and then it was allowed to cool. The mixture was filtered through Celite and the DMA phase was extracted three times with ethyl acetate, dried with magnesium sulfate, and concentrated under reduced pressure. The title compound (m.p. = 396 K; yield = 65%) was purified by flash chromatography on silica gel with a petroleum:ethyl acetate (9:1) solvent system and recrystallized from ethanol to afford colourless crystals of a suitable size for the X-ray diffraction study.

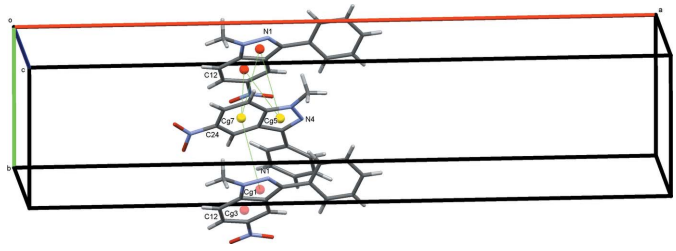


Figure 4
π–π stacking interactions viewed along c. *Cg*1, *Cg*3, *Cg*5 and *Cg*7 are the centroids of the N1/N2/C7/C8/C13, C8–C13, N4/N5/C21/C22/C27 and C22–C27 rings, respectively, with centroids shown as colored spheres and *Cg*···*Cg* contacts drawn as green dotted lines.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The structure was refined as a two-component inversion twin with equal domain ratios.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{11}N_3O_2$
M_r	253.26
Crystal system, space group	Orthorhombic, $Pca2_1$
Temperature (K)	296
a, b, c (Å)	33.4769 (17), 7.4977 (3), 9.7916 (4)
V (Å^3)	2457.69 (19)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.10
Crystal size (mm)	0.33 × 0.28 × 0.19
Data collection	
Diffractometer	Bruker X8 *APEX*
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.638, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13395, 5245, 3328
R_{int}	0.040
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.641
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.049, 0.130, 1.01
No. of reflections	5245
No. of parameters	344
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.16, −0.15
Absolute structure	Refined as an inversion twin.
Absolute structure parameter	2 (2)

Computer programs: *APEX2* and *SAINT-Plus* (Bruker, 2009), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

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full crystallographic data

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Crystal data

$C_{14}H_{11}N_3O_2$
M_r = 253.26
Orthorhombic, $Pca2_1$
a = 33.4769 (17) Å
b = 7.4977 (3) Å
c = 9.7916 (4) Å
V = 2457.69 (19) Å^3
Z = 8
$F(000)$ = 1056
D_x = 1.369 Mg m^{-3}
Melting point: 396 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5245 reflections
θ = 2.4–27.1°
μ = 0.10 mm^{-1}
T = 296 K
Block, colourless
0.33 × 0.28 × 0.19 mm

Data collection

Bruker X8 APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2009)
T_{min} = 0.638, T_{max} = 0.746
13395 measured reflections
5245 independent reflections
3328 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 27.1°, θ_{min} = 2.4°
h = −30→42
k = −9→9
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.130
S = 1.01
5245 reflections
344 parameters
1 restraint
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0579P)^2 + 0.091P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Absolute structure: Refined as an inversion twin.
Absolute structure parameter: 2 (2)

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. Refined as a 2-component inversion twin.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.45757 (13)	0.7758 (5)	0.8046 (5)	0.0631 (11)
H1	0.4420	0.7154	0.7410	0.076*
C2	0.49860 (16)	0.7540 (6)	0.8036 (6)	0.0797 (14)
H2	0.5105	0.6813	0.7382	0.096*
C3	0.52212 (14)	0.8402 (7)	0.8998 (6)	0.0784 (14)
H3	0.5497	0.8247	0.8998	0.094*
C4	0.50432 (14)	0.9486 (6)	0.9949 (5)	0.0708 (13)
H4	0.5200	1.0059	1.0599	0.085*
C5	0.46349 (12)	0.9737 (5)	0.9955 (4)	0.0579 (10)
H5	0.4519	1.0488	1.0600	0.069*
C6	0.43943 (12)	0.8867 (5)	0.8996 (4)	0.0488 (9)
C7	0.39618 (12)	0.9148 (5)	0.8928 (4)	0.0477 (9)
C8	0.36860 (11)	0.9732 (4)	0.9954 (4)	0.0461 (9)
C9	0.37031 (13)	1.0185 (4)	1.1343 (4)	0.0494 (9)
H9	0.3942	1.0138	1.1827	0.059*
C10	0.33550 (14)	1.0697 (5)	1.1956 (4)	0.0544 (10)
C11	0.29892 (13)	1.0770 (6)	1.1283 (5)	0.0622 (11)
H11	0.2762	1.1139	1.1751	0.075*
C12	0.29627 (13)	1.0300 (5)	0.9938 (5)	0.0615 (11)
H12	0.2720	1.0332	0.9473	0.074*
C13	0.33147 (11)	0.9771 (5)	0.9290 (4)	0.0496 (9)
C14	0.30967 (14)	0.9067 (6)	0.6881 (4)	0.0697 (13)
H14A	0.2835	0.9377	0.7204	0.105*
H14B	0.3172	0.9860	0.6155	0.105*
H14C	0.3095	0.7862	0.6548	0.105*
C15	0.06659 (14)	0.6121 (5)	0.7116 (5)	0.0586 (11)
H15	0.0443	0.6102	0.6551	0.070*
C16	0.06358 (16)	0.6833 (7)	0.8421 (6)	0.0804 (14)
H16	0.0393	0.7283	0.8727	0.096*
C17	0.09621 (17)	0.6875 (7)	0.9256 (5)	0.0807 (14)
H17	0.0941	0.7362	1.0127	0.097*
C18	0.13218 (16)	0.6199 (6)	0.8814 (4)	0.0709 (13)
H18	0.1544	0.6233	0.9384	0.085*
C19	0.13518 (14)	0.5474 (6)	0.7527 (4)	0.0582 (11)
H19	0.1594	0.5001	0.7240	0.070*
C20	0.10261 (12)	0.5436 (5)	0.6649 (4)	0.0456 (9)
C21	0.10652 (11)	0.4730 (4)	0.5262 (4)	0.0443 (9)
C22	0.14088 (11)	0.4648 (4)	0.4399 (4)	0.0439 (8)
C23	0.18067 (12)	0.5160 (5)	0.4490 (4)	0.0492 (9)
H23	0.1909	0.5688	0.5275	0.059*
C24	0.20434 (13)	0.4850 (5)	0.3366 (5)	0.0598 (11)
C25	0.19033 (17)	0.4081 (6)	0.2148 (5)	0.0700 (13)
H25	0.2077	0.3899	0.1420	0.084*
C26	0.15079 (16)	0.3597 (5)	0.2040 (4)	0.0665 (13)
H26	0.1408	0.3085	0.1245	0.080*

C27	0.12625 (13)	0.3904 (5)	0.3168 (4)	0.0494 (10)
C28	0.05914 (16)	0.2949 (6)	0.2328 (5)	0.0824 (15)
H28A	0.0331	0.2863	0.2733	0.124*
H28B	0.0582	0.3758	0.1569	0.124*
H28C	0.0674	0.1793	0.2017	0.124*
N1	0.37717 (10)	0.8847 (4)	0.7771 (3)	0.0524 (8)
N2	0.33801 (11)	0.9220 (4)	0.7986 (3)	0.0552 (8)
N3	0.33657 (14)	1.1181 (5)	1.3406 (4)	0.0670 (11)
N4	0.07439 (10)	0.4110 (4)	0.4608 (4)	0.0560 (9)
N5	0.08741 (11)	0.3607 (4)	0.3338 (4)	0.0592 (9)
N6	0.24577 (14)	0.5381 (7)	0.3419 (5)	0.0853 (13)
O1	0.36862 (12)	1.1219 (5)	1.4003 (4)	0.0835 (10)
O2	0.30487 (11)	1.1535 (6)	1.3978 (4)	0.0990 (12)
O3	0.25797 (11)	0.6241 (6)	0.4405 (5)	0.1101 (14)
O4	0.26727 (13)	0.4964 (8)	0.2468 (5)	0.146 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.072 (3)	0.055 (2)	0.062 (3)	0.009 (2)	0.010 (2)	−0.001 (2)
C2	0.077 (3)	0.078 (3)	0.084 (4)	0.024 (3)	0.022 (3)	0.000 (3)
C3	0.057 (3)	0.092 (4)	0.086 (4)	0.017 (3)	0.004 (3)	0.026 (3)
C4	0.062 (3)	0.087 (3)	0.063 (3)	0.004 (2)	−0.005 (3)	0.017 (3)
C5	0.060 (3)	0.065 (2)	0.049 (2)	0.007 (2)	−0.001 (2)	0.008 (2)
C6	0.058 (2)	0.047 (2)	0.041 (2)	0.0032 (17)	0.006 (2)	0.0099 (17)
C7	0.057 (2)	0.044 (2)	0.042 (2)	−0.0001 (17)	0.0033 (19)	0.0009 (16)
C8	0.054 (2)	0.0426 (18)	0.041 (2)	−0.0012 (16)	0.003 (2)	0.0037 (17)
C9	0.059 (2)	0.047 (2)	0.042 (2)	−0.0006 (18)	0.0006 (19)	0.0036 (17)
C10	0.067 (3)	0.054 (2)	0.042 (2)	0.0024 (19)	0.008 (2)	0.0028 (17)
C11	0.056 (3)	0.069 (3)	0.061 (3)	0.001 (2)	0.012 (2)	0.001 (2)
C12	0.053 (2)	0.068 (2)	0.064 (3)	−0.003 (2)	−0.003 (2)	0.002 (2)
C13	0.054 (2)	0.049 (2)	0.046 (2)	−0.0069 (17)	−0.001 (2)	0.0020 (18)
C14	0.080 (3)	0.077 (3)	0.052 (3)	−0.010 (2)	−0.017 (2)	−0.002 (2)
C15	0.056 (3)	0.057 (2)	0.063 (3)	0.000 (2)	0.011 (2)	−0.001 (2)
C16	0.072 (3)	0.087 (3)	0.082 (4)	0.006 (3)	0.030 (3)	−0.018 (3)
C17	0.105 (4)	0.090 (3)	0.047 (3)	−0.009 (3)	0.015 (3)	−0.016 (3)
C18	0.085 (4)	0.090 (3)	0.038 (2)	−0.001 (3)	0.000 (2)	−0.005 (2)
C19	0.063 (3)	0.071 (3)	0.041 (2)	0.010 (2)	0.001 (2)	0.0004 (19)
C20	0.052 (2)	0.0429 (19)	0.042 (2)	−0.0002 (16)	0.006 (2)	0.0039 (16)
C21	0.052 (2)	0.0399 (18)	0.041 (2)	0.0009 (16)	−0.0065 (18)	0.0026 (15)
C22	0.054 (2)	0.0421 (18)	0.035 (2)	0.0053 (16)	−0.0066 (19)	0.0015 (15)
C23	0.057 (2)	0.049 (2)	0.042 (2)	0.0047 (16)	−0.0013 (19)	0.0030 (16)
C24	0.061 (3)	0.066 (2)	0.052 (3)	0.011 (2)	0.014 (2)	0.011 (2)
C25	0.096 (4)	0.070 (3)	0.043 (3)	0.021 (3)	0.018 (3)	0.002 (2)
C26	0.106 (4)	0.057 (2)	0.036 (2)	0.012 (2)	−0.006 (2)	−0.0059 (18)
C27	0.070 (3)	0.0414 (19)	0.036 (2)	0.0057 (18)	−0.006 (2)	−0.0012 (16)
C28	0.108 (4)	0.074 (3)	0.065 (3)	−0.016 (3)	−0.044 (3)	−0.003 (2)
N1	0.062 (2)	0.0530 (18)	0.0421 (19)	−0.0014 (15)	−0.0003 (18)	−0.0007 (15)

N2	0.063 (2)	0.0578 (19)	0.045 (2)	0.0003 (16)	−0.0072 (18)	−0.0026 (16)
N3	0.086 (3)	0.068 (2)	0.047 (2)	0.008 (2)	0.021 (2)	0.0023 (17)
N4	0.060 (2)	0.0533 (18)	0.055 (2)	−0.0053 (15)	−0.0106 (18)	0.0037 (16)
N5	0.073 (2)	0.0562 (19)	0.049 (2)	−0.0065 (16)	−0.0162 (19)	−0.0033 (16)
N6	0.064 (3)	0.122 (4)	0.070 (3)	0.014 (3)	0.010 (3)	0.023 (3)
O1	0.091 (3)	0.110 (3)	0.0498 (19)	0.006 (2)	−0.004 (2)	−0.0117 (18)
O2	0.095 (3)	0.143 (3)	0.059 (2)	0.021 (2)	0.029 (2)	−0.001 (2)
O3	0.064 (2)	0.154 (4)	0.113 (4)	−0.018 (2)	0.008 (2)	−0.001 (3)
O4	0.085 (3)	0.253 (6)	0.099 (3)	0.024 (3)	0.044 (3)	0.004 (4)

Geometric parameters (Å, º)

C1—C2	1.383 (6)	C16—C17	1.365 (7)
C1—C6	1.388 (5)	C16—H16	0.9300
C1—H1	0.9300	C17—C18	1.376 (7)
C2—C3	1.388 (8)	C17—H17	0.9300
C2—H2	0.9300	C18—C19	1.377 (6)
C3—C4	1.372 (7)	C18—H18	0.9300
C3—H3	0.9300	C19—C20	1.389 (6)
C4—C5	1.380 (6)	C19—H19	0.9300
C4—H4	0.9300	C20—C21	1.463 (5)
C5—C6	1.399 (6)	C21—N4	1.336 (5)
C5—H5	0.9300	C21—C22	1.429 (5)
C6—C7	1.465 (5)	C22—C23	1.389 (5)
C7—N1	1.319 (5)	C22—C27	1.416 (5)
C7—C8	1.433 (5)	C23—C24	1.376 (6)
C8—C13	1.403 (5)	C23—H23	0.9300
C8—C9	1.403 (6)	C24—C25	1.404 (7)
C9—C10	1.366 (6)	C24—N6	1.444 (6)
C9—H9	0.9300	C25—C26	1.377 (6)
C10—C11	1.391 (6)	C25—H25	0.9300
C10—N3	1.466 (5)	C26—C27	1.396 (6)
C11—C12	1.367 (7)	C26—H26	0.9300
C11—H11	0.9300	C27—N5	1.330 (5)
C12—C13	1.396 (6)	C28—N5	1.455 (5)
C12—H12	0.9300	C28—H28A	0.9600
C13—N2	1.359 (5)	C28—H28B	0.9600
C14—N2	1.444 (5)	C28—H28C	0.9600
C14—H14A	0.9600	N1—N2	1.357 (4)
C14—H14B	0.9600	N3—O1	1.222 (5)
C14—H14C	0.9600	N3—O2	1.229 (4)
C15—C16	1.388 (7)	N4—N5	1.371 (5)
C15—C20	1.388 (6)	N6—O4	1.218 (6)
C15—H15	0.9300	N6—O3	1.231 (6)
C2—C1—C6	120.7 (4)	C16—C17—H17	119.9
C2—C1—H1	119.7	C18—C17—H17	119.9
C6—C1—H1	119.7	C17—C18—C19	119.8 (5)

C1—C2—C3	120.2 (5)	C17—C18—H18	120.1
C1—C2—H2	119.9	C19—C18—H18	120.1
C3—C2—H2	119.9	C18—C19—C20	121.2 (4)
C4—C3—C2	119.4 (4)	C18—C19—H19	119.4
C4—C3—H3	120.3	C20—C19—H19	119.4
C2—C3—H3	120.3	C15—C20—C19	118.0 (4)
C3—C4—C5	121.0 (5)	C15—C20—C21	121.2 (4)
C3—C4—H4	119.5	C19—C20—C21	120.8 (4)
C5—C4—H4	119.5	N4—C21—C22	110.5 (3)
C4—C5—C6	120.2 (4)	N4—C21—C20	120.0 (4)
C4—C5—H5	119.9	C22—C21—C20	129.5 (4)
C6—C5—H5	119.9	C23—C22—C27	119.6 (4)
C1—C6—C5	118.5 (4)	C23—C22—C21	136.3 (3)
C1—C6—C7	119.2 (4)	C27—C22—C21	104.0 (3)
C5—C6—C7	122.2 (3)	C24—C23—C22	117.1 (4)
N1—C7—C8	110.1 (3)	C24—C23—H23	121.5
N1—C7—C6	119.4 (3)	C22—C23—H23	121.5
C8—C7—C6	130.5 (4)	C23—C24—C25	123.8 (4)
C13—C8—C9	118.7 (4)	C23—C24—N6	118.5 (4)
C13—C8—C7	104.6 (3)	C25—C24—N6	117.7 (4)
C9—C8—C7	136.6 (4)	C26—C25—C24	119.7 (4)
C10—C9—C8	117.3 (4)	C26—C25—H25	120.2
C10—C9—H9	121.3	C24—C25—H25	120.2
C8—C9—H9	121.3	C25—C26—C27	117.5 (4)
C9—C10—C11	123.6 (4)	C25—C26—H26	121.3
C9—C10—N3	118.3 (4)	C27—C26—H26	121.3
C11—C10—N3	118.0 (4)	N5—C27—C26	130.3 (4)
C12—C11—C10	120.2 (4)	N5—C27—C22	107.3 (3)
C12—C11—H11	119.9	C26—C27—C22	122.4 (4)
C10—C11—H11	119.9	N5—C28—H28A	109.5
C11—C12—C13	117.2 (4)	N5—C28—H28B	109.5
C11—C12—H12	121.4	H28A—C28—H28B	109.5
C13—C12—H12	121.4	N5—C28—H28C	109.5
N2—C13—C12	130.5 (4)	H28A—C28—H28C	109.5
N2—C13—C8	106.6 (4)	H28B—C28—H28C	109.5
C12—C13—C8	122.9 (4)	C7—N1—N2	107.3 (3)
N2—C14—H14A	109.5	N1—N2—C13	111.4 (3)
N2—C14—H14B	109.5	N1—N2—C14	120.1 (3)
H14A—C14—H14B	109.5	C13—N2—C14	128.5 (4)
N2—C14—H14C	109.5	O1—N3—O2	122.4 (4)
H14A—C14—H14C	109.5	O1—N3—C10	119.4 (4)
H14B—C14—H14C	109.5	O2—N3—C10	118.3 (5)
C16—C15—C20	120.6 (5)	C21—N4—N5	106.0 (3)
C16—C15—H15	119.7	C27—N5—N4	112.2 (3)
C20—C15—H15	119.7	C27—N5—C28	127.5 (4)
C17—C16—C15	120.2 (5)	N4—N5—C28	120.2 (4)
C17—C16—H16	119.9	O4—N6—O3	122.6 (5)
C15—C16—H16	119.9	O4—N6—C24	118.0 (6)

C16—C17—C18	120.2 (4)	O3—N6—C24	119.4 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14*B*···O2^{i}	0.96	2.51	3.395 (6)	154
C19—H19···O4^{ii}	0.93	2.46	3.288 (6)	148

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