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ISSN 2414-3146

1-(Cyclohex-1-en-1-yl)-3-[(1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl]-1*H*-benzimidazol-2(3*H*)-one

Mohamed Adardour,[a] Mohamed Loughzail,[a]* Slimane Dahaoui,[b] Abdesselam Baouid[a] and Moha Berraho[c]

[a]Laboratoire de Chimie Moléculaire, Département de Chimie, Faculté des Sciences Semlalia, BP 2390, Université Cadi Ayyad, 40001 Marrakech, Morocco, [b]Cristallographie, Résonance Magnétique et Modélisation (CRM2), Université Henri Poincaré, Nancy 1, Faculté des Sciences, BP 70239, 54506 Vandoeuvre lès Nancy Cedex, France, and [c]Laboratoire de Chimie des Substances Naturelles, Unité Associé au CNRST (URAC16), Faculté des Sciences Semlalia, BP 2390 Bd My Abdellah, Université Cadi Ayyad, 40000 Marrakech, Morocco. *Correspondence e-mail: loughzail@gmail.com

Received 13 June 2017
Accepted 17 June 2017

Edited by J. Simpson, University of Otago, New Zealand

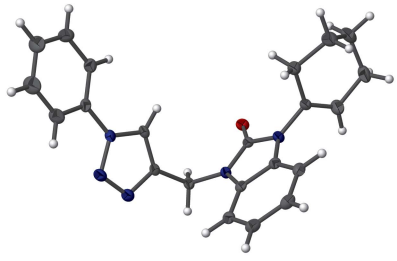
Keywords: crystal structure; benzimidazolone; benzyl azide; triazole; hydrogen bonding.

CCDC reference: 1556697

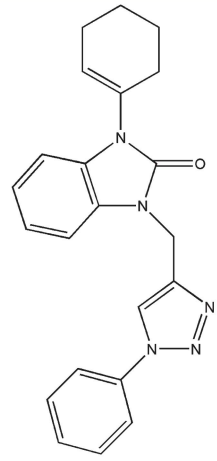
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{22}H_{21}N_5O$, the triazole ring is inclined at 16.88 (12)° to its phenyl substituent and is almost normal to the benzimidazole ring system, making a dihedral angle of 88.40 (8)°. The cyclohexenyl ring adopts a half-chair conformation and its mean plane is inclined to the benzimidazole ring system by 78.75 (12)°. In the crystal, molecules are linked by C—H···O and C—H···N hydrogen bonds, forming a three-dimensional network.

3D view



Chemical scheme



Structure description

Heterocyclic triazole derivatives are important components of materials with both agrochemical (Bowyer & Denning, 2014) and medicinal (Kumar *et al.*, 2013) applications. 1,2,3-Triazoles display a wide range of interesting biological activities, and are used as anti-inflammatory (De Simone *et al.*, 2011), anti-allergic (Buckle *et al.*, 1986) and anti-HIV agents (Giffin *et al.*, 2008; Whiting *et al.*, 2006). They are also effective in the inhibition of histidine biosynthesis (Ventura *et al.*, 1997). The most widely used method for the synthesis of 1,2,3-triazoles is the Huisgen (1963) 1,3-dipolar cycloaddition of alkynes with organic azides. The condensation reaction of 1-cyclohexenyl-3-prop-2-ynyl-1,3-dihydro-benzoimidazol-2-one with azidobenzene in the presence of copper iodide (CuI) under reflux in acetonitrile for one hour gives a single regioisomer of the title compound in good yield.

The molecular structure of the title compound is illustrated in Fig. 1. The triazole ring (N3/N4/N5/C10/C9) is almost normal to the plane of the benzimidazole ring system, making a dihedral angle of 88.36 (8)°. The cyclohexenyl ring (C17/C18–C22), displays a

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O1^{i}	0.93	2.53	3.303 (2)	141
C16—H16···N4^{ii}	0.93	2.62	3.413 (3)	144
C10—H10···O1^{iii}	0.93	2.26	3.174 (2)	167

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

half chair conformation, as indicated by the total puckering amplitude Q_T = 0.494 (3) Å and the spherical polar angle θ_2 = 52.3 (3)° with φ_2 = 144.4 (4)°. This ring makes a dihedral angle of 78.75 (12)° with the benzimidazole ring system.

In the crystal, pairs of C16—H16···N4 and C10—H10···O1 hydrogen bonds (Table 1) each form inversion dimers, enclosing $R_2^2(10)$ and $R_2^2(14)$ rings, respectively. These combine with an additional C4—H4···O2 hydrogen bond to link the molecules into a three-dimensional network, as shown in Fig. 2.

Synthesis and crystallization

To a solution of 1-cyclohexenyl-3-prop-2-ynyl-1,3-dihydro-benzoimidazol-2-one (3.96 mmole) dissolved in acetonitrile was added azidobenzene (4.69 mmol), in the presence of CuI. The mixture was refluxed for 1 h; the reaction was monitored by thin layer chromatography. The mixture was filtered and the solvent removed under vacuum. The solid was purified by column chromatography on silica gel using hexane/ethyl acetate as eluent. The solid product was recrystallized from ethanol solution.

^{1}H NMR (300 MHz, $CDCl_3$), δ (p.p.m.): 1.78, 1.90, 2.33, 2.43 (4 *m*, 8H, CH_2–cyclohexenyl), 5.31 (*s*, 2H, N—CH2), 5.98 (*m*, 1H, C═CH; *H*–cyclohexenyl), 7.06–7,74 (*m*, 9H, H—Ar), 8.09 (*s*, 1H, H-triazolic). ^{13}C NMR (75 MHz, $CDCl_3$), δ (p.p.m.): 21.66, 22.60, 24.73, 26.85 (4 C, CH_2–cyclohexenyl), 36.35 (N—CH_2), 127.36 (CH═C, *C*–cyclohexenyl), 121.21 (N—CH=C, C-triazolic), 108.68, 120.56, 121.58, 128.89, 129.74 (C, CH=C, C—Ar), 121.67, 129.53, 132.21, 136.92, 144.00 (6C, ═C–), 152,92 (1C, C═O).

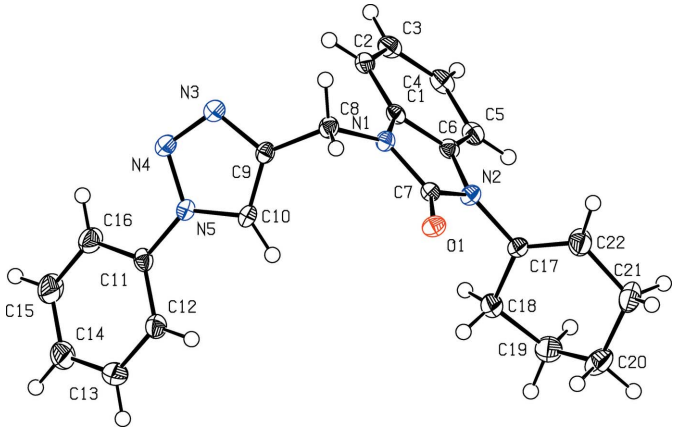


Figure 1
The molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 30% probability level.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{21}N_5O$
M_r	371.43
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	293
a, b, c (Å)	8.5878 (8), 9.0603 (8), 12.8566 (12)
α, β, γ (°)	85.076 (7), 82.558 (7), 70.917 (8)
V (Å^3)	936.40 (16)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.48 × 0.20 × 0.15
Data collection	
Diffractometer	Bruker X8 APEX Diffractometer
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.811, 1.0
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5162, 3592, 2866
R_{int}	0.029
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.054, 0.143, 1.03
No. of reflections	3592
No. of parameters	253
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.67, −0.30

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS2014* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009).

Refinement

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

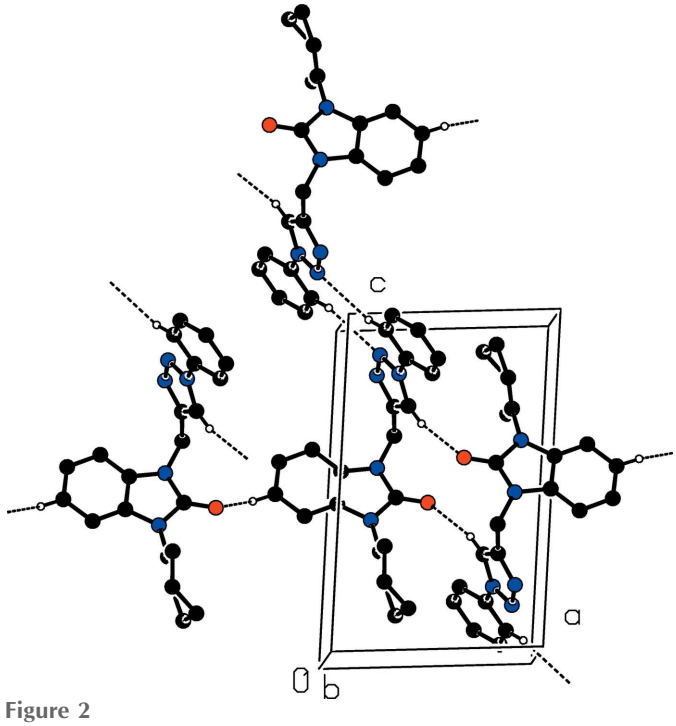


Figure 2
A partial view of the crystal packing of the title compound, viewed along the *b*-axis direction.

Acknowledgements

The authors thank the Laboratoire de Cristallographie, Résonance Magnétique et Modélization (CRM2), Université Henri Poincaré, Nancy 1, Faculté des Sciences, BP 70239, 54506 Vandoeuvre lès Nancy CEDEX, France, for the data collection.

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full crystallographic data

IUCrData (2017). **2**, x170907 [https://doi.org/10.1107/S2414314617009075]

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1-(Cyclohex-1-en-1-yl)-3-[(1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl]-1*H*-benzimidazol-2(3*H*)-one

Crystal data

$C_{22}H_{21}N_5O$
M_r = 371.43
Triclinic, $P\overline{1}$
a = 8.5878 (8) Å
b = 9.0603 (8) Å
c = 12.8566 (12) Å
α = 85.076 (7)°
β = 82.558 (7)°
γ = 70.917 (8)°
V = 936.40 (16) Å^3
Z = 2
$F(000)$ = 392
D_x = 1.317 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3592 reflections
θ = 3.1–26.4°
μ = 0.09 mm^{-1}
T = 293 K
Block, colourless
0.48 × 0.20 × 0.15 mm

Data collection

Bruker X8 APEX Diffractometer
Radiation source: fine-focus sealed X-ray tube
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2009)
T_{min} = 0.811, T_{max} = 1.0
5162 measured reflections
3592 independent reflections
2866 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 26.4°, θ_{min} = 3.1°
h = −10→8
k = −11→11
l = −10→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.143
S = 1.03
3592 reflections
253 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0628P)^2 + 0.6025P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 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. All H atoms attached to C atoms were fixed geometrically and treated as riding with C—H = 0.99 Å (methylene), 0.98 Å (methyl), 1.0Å (methine) with $U_{iso}(H) = 1.2U_{eq}$(CH and CH_2). The coordinates of H atoms attached to N atoms were freely refined with $U_{iso}(H) = 1.2U_{eq}(N)$ and the H attached to hydroxyl O atoms were fixed geometrically and treated as riding with O—H = 0.84Å and $U_{iso}(H) = 1.5U_{eq}(O)$.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C12	0.3923 (3)	−0.3191 (2)	0.80138 (16)	0.0229 (5)
H12	0.4612	−0.2984	0.7440	0.028*
C16	0.1680 (3)	−0.2279 (3)	0.93894 (17)	0.0280 (5)
H16	0.0878	−0.1458	0.9733	0.034*
C21	0.3016 (3)	0.1477 (3)	0.10909 (17)	0.0319 (5)
H21A	0.3956	0.1775	0.0756	0.038*
H21B	0.2138	0.1851	0.0635	0.038*
C18	0.2255 (3)	−0.0204 (2)	0.30745 (17)	0.0315 (5)
H18A	0.1314	−0.0343	0.3528	0.038*
H18B	0.3255	−0.0812	0.3385	0.038*
C19	0.2295 (3)	−0.0802 (3)	0.19899 (19)	0.0332 (5)
H19A	0.2611	−0.1934	0.2033	0.040*
H19B	0.1199	−0.0393	0.1754	0.040*
C14	0.3050 (3)	−0.5029 (3)	0.92148 (19)	0.0363 (6)
H14	0.3161	−0.6057	0.9442	0.044*
C15	0.1856 (3)	−0.3810 (3)	0.97239 (19)	0.0361 (6)
H15	0.1166	−0.4022	1.0295	0.043*
C20	0.3520 (3)	−0.0292 (3)	0.12117 (18)	0.0321 (5)
H20A	0.3574	−0.0717	0.0536	0.039*
H20B	0.4613	−0.0699	0.1451	0.039*
C13	0.4079 (3)	−0.4719 (3)	0.83683 (19)	0.0324 (5)
H13	0.4887	−0.5542	0.8031	0.039*
C22	0.2430 (3)	0.2252 (3)	0.21187 (17)	0.0300 (5)
H22	0.2268	0.3316	0.2137	0.036*
O1	0.43046 (16)	0.19506 (16)	0.44443 (11)	0.0200 (3)
N1	0.1877 (2)	0.29311 (18)	0.55563 (12)	0.0159 (3)
N2	0.1672 (2)	0.22461 (19)	0.39825 (13)	0.0170 (4)
N5	0.2507 (2)	−0.03975 (19)	0.81699 (12)	0.0168 (4)
N4	0.1623 (2)	0.0792 (2)	0.87935 (13)	0.0226 (4)
C1	0.0200 (2)	0.3188 (2)	0.54935 (15)	0.0163 (4)
C2	−0.1186 (2)	0.3784 (2)	0.61908 (16)	0.0191 (4)
H2	−0.1105	0.4075	0.6853	0.023*
C6	0.0074 (2)	0.2742 (2)	0.45008 (15)	0.0165 (4)
N3	0.1596 (2)	0.2099 (2)	0.82603 (13)	0.0231 (4)
C10	0.3051 (2)	0.0162 (2)	0.72346 (15)	0.0179 (4)
H10	0.3686	−0.0407	0.6671	0.021*
C7	0.2799 (2)	0.2326 (2)	0.46372 (15)	0.0164 (4)
C8	0.2612 (2)	0.3012 (2)	0.64997 (15)	0.0180 (4)
H8A	0.2064	0.4025	0.6797	0.022*
H8B	0.3774	0.2906	0.6317	0.022*

C11	0.2720 (2)	−0.1982 (2)	0.85310 (15)	0.0190 (4)
C9	0.2458 (2)	0.1753 (2)	0.73019 (15)	0.0163 (4)
C5	−0.1435 (3)	0.2862 (2)	0.41806 (16)	0.0207 (4)
H5	−0.1512	0.2551	0.3524	0.025*
C17	0.2133 (2)	0.1475 (2)	0.30030 (15)	0.0169 (4)
C3	−0.2715 (2)	0.3932 (2)	0.58592 (17)	0.0224 (4)
H3	−0.3676	0.4351	0.6306	0.027*
C4	−0.2841 (3)	0.3470 (2)	0.48808 (17)	0.0225 (5)
H4	−0.3879	0.3567	0.4690	0.027*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C12	0.0240 (11)	0.0246 (11)	0.0192 (10)	−0.0076 (9)	−0.0007 (8)	0.0013 (8)
C16	0.0344 (13)	0.0270 (11)	0.0227 (11)	−0.0129 (10)	0.0054 (9)	−0.0021 (9)
C21	0.0428 (14)	0.0381 (13)	0.0183 (11)	−0.0185 (11)	−0.0018 (10)	−0.0001 (9)
C18	0.0492 (15)	0.0207 (11)	0.0211 (11)	−0.0067 (10)	−0.0038 (10)	0.0003 (9)
C19	0.0457 (15)	0.0244 (11)	0.0303 (13)	−0.0120 (10)	−0.0033 (11)	−0.0033 (9)
C14	0.0582 (17)	0.0238 (12)	0.0281 (12)	−0.0177 (11)	0.0003 (11)	0.0037 (9)
C15	0.0497 (16)	0.0322 (13)	0.0276 (12)	−0.0204 (12)	0.0085 (11)	0.0020 (10)
C20	0.0310 (12)	0.0407 (14)	0.0251 (12)	−0.0096 (11)	−0.0021 (9)	−0.0127 (10)
C13	0.0435 (14)	0.0206 (11)	0.0286 (12)	−0.0060 (10)	0.0007 (10)	−0.0018 (9)
C22	0.0463 (14)	0.0250 (11)	0.0227 (11)	−0.0168 (10)	−0.0048 (10)	0.0002 (9)
O1	0.0151 (7)	0.0224 (7)	0.0216 (7)	−0.0051 (6)	0.0006 (5)	−0.0039 (6)
N1	0.0161 (8)	0.0175 (8)	0.0148 (8)	−0.0058 (6)	−0.0022 (6)	−0.0011 (6)
N2	0.0167 (8)	0.0190 (8)	0.0159 (8)	−0.0059 (7)	−0.0015 (6)	−0.0031 (6)
N5	0.0183 (8)	0.0190 (8)	0.0135 (8)	−0.0065 (7)	−0.0017 (6)	−0.0011 (6)
N4	0.0283 (10)	0.0211 (9)	0.0167 (9)	−0.0065 (7)	0.0022 (7)	−0.0033 (7)
C1	0.0181 (10)	0.0128 (9)	0.0181 (10)	−0.0059 (7)	−0.0021 (7)	0.0026 (7)
C2	0.0217 (10)	0.0166 (10)	0.0176 (10)	−0.0057 (8)	0.0002 (8)	0.0016 (8)
C6	0.0175 (10)	0.0141 (9)	0.0181 (10)	−0.0060 (8)	−0.0007 (7)	0.0012 (7)
N3	0.0284 (10)	0.0205 (9)	0.0184 (9)	−0.0057 (7)	−0.0001 (7)	−0.0018 (7)
C10	0.0193 (10)	0.0223 (10)	0.0123 (9)	−0.0075 (8)	0.0001 (7)	−0.0019 (7)
C7	0.0189 (10)	0.0139 (9)	0.0157 (9)	−0.0048 (8)	−0.0011 (7)	0.0000 (7)
C8	0.0214 (10)	0.0187 (10)	0.0157 (10)	−0.0078 (8)	−0.0041 (8)	−0.0014 (7)
C11	0.0230 (10)	0.0198 (10)	0.0166 (10)	−0.0093 (8)	−0.0062 (8)	0.0015 (8)
C9	0.0159 (9)	0.0203 (10)	0.0139 (9)	−0.0067 (8)	−0.0033 (7)	−0.0015 (7)
C5	0.0236 (11)	0.0179 (10)	0.0226 (10)	−0.0080 (8)	−0.0076 (8)	0.0009 (8)
C17	0.0161 (9)	0.0179 (10)	0.0167 (9)	−0.0050 (8)	−0.0016 (7)	−0.0028 (7)
C3	0.0174 (10)	0.0199 (10)	0.0265 (11)	−0.0042 (8)	0.0025 (8)	0.0025 (8)
C4	0.0168 (10)	0.0207 (10)	0.0300 (11)	−0.0067 (8)	−0.0040 (8)	0.0051 (8)

Geometric parameters (Å, º)

C12—C11	1.384 (3)	N1—C7	1.382 (2)
C12—C13	1.388 (3)	N1—C1	1.394 (2)
C12—H12	0.9300	N1—C8	1.455 (2)
C16—C15	1.382 (3)	N2—C7	1.385 (2)

C16—C11	1.392 (3)	N2—C6	1.393 (2)
C16—H16	0.9300	N2—C17	1.439 (2)
C21—C22	1.500 (3)	N5—C10	1.351 (2)
C21—C20	1.517 (3)	N5—N4	1.355 (2)
C21—H21A	0.9700	N5—C11	1.431 (2)
C21—H21B	0.9700	N4—N3	1.312 (2)
C18—C17	1.486 (3)	C1—C2	1.378 (3)
C18—C19	1.531 (3)	C1—C6	1.399 (3)
C18—H18A	0.9700	C2—C3	1.394 (3)
C18—H18B	0.9700	C2—H2	0.9300
C19—C20	1.512 (3)	C6—C5	1.378 (3)
C19—H19A	0.9700	N3—C9	1.358 (3)
C19—H19B	0.9700	C10—C9	1.370 (3)
C14—C13	1.380 (3)	C10—H10	0.9300
C14—C15	1.381 (4)	C8—C9	1.498 (3)
C14—H14	0.9300	C8—H8A	0.9700
C15—H15	0.9300	C8—H8B	0.9700
C20—H20A	0.9700	C5—C4	1.393 (3)
C20—H20B	0.9700	C5—H5	0.9300
C13—H13	0.9300	C3—C4	1.387 (3)
C22—C17	1.326 (3)	C3—H3	0.9300
C22—H22	0.9300	C4—H4	0.9300
O1—C7	1.222 (2)		

C11—C12—C13	118.7 (2)	C7—N2—C17	123.90 (16)
C11—C12—H12	120.7	C6—N2—C17	125.19 (16)
C13—C12—H12	120.7	C10—N5—N4	110.57 (16)
C15—C16—C11	119.1 (2)	C10—N5—C11	129.19 (17)
C15—C16—H16	120.5	N4—N5—C11	120.23 (16)
C11—C16—H16	120.5	N3—N4—N5	107.21 (16)
C22—C21—C20	112.85 (19)	C2—C1—N1	131.87 (18)
C22—C21—H21A	109.0	C2—C1—C6	121.32 (18)
C20—C21—H21A	109.0	N1—C1—C6	106.80 (17)
C22—C21—H21B	109.0	C1—C2—C3	117.01 (18)
C20—C21—H21B	109.0	C1—C2—H2	121.5
H21A—C21—H21B	107.8	C3—C2—H2	121.5
C17—C18—C19	111.21 (18)	C5—C6—N2	131.24 (18)
C17—C18—H18A	109.4	C5—C6—C1	121.64 (19)
C19—C18—H18A	109.4	N2—C6—C1	107.10 (16)
C17—C18—H18B	109.4	N4—N3—C9	108.87 (16)
C19—C18—H18B	109.4	N5—C10—C9	104.52 (17)
H18A—C18—H18B	108.0	N5—C10—H10	127.7
C20—C19—C18	110.10 (19)	C9—C10—H10	127.7
C20—C19—H19A	109.6	O1—C7—N1	126.60 (18)
C18—C19—H19A	109.6	O1—C7—N2	127.29 (18)
C20—C19—H19B	109.6	N1—C7—N2	106.11 (16)
C18—C19—H19B	109.6	N1—C8—C9	111.45 (15)
H19A—C19—H19B	108.2	N1—C8—H8A	109.3

C13—C14—C15	119.9 (2)	C9—C8—H8A	109.3
C13—C14—H14	120.0	N1—C8—H8B	109.3
C15—C14—H14	120.0	C9—C8—H8B	109.3
C14—C15—C16	120.4 (2)	H8A—C8—H8B	108.0
C14—C15—H15	119.8	C12—C11—C16	121.16 (19)
C16—C15—H15	119.8	C12—C11—N5	119.89 (18)
C19—C20—C21	110.9 (2)	C16—C11—N5	118.93 (19)
C19—C20—H20A	109.5	N3—C9—C10	108.83 (17)
C21—C20—H20A	109.5	N3—C9—C8	121.42 (17)
C19—C20—H20B	109.5	C10—C9—C8	129.73 (18)
C21—C20—H20B	109.5	C6—C5—C4	117.29 (19)
H20A—C20—H20B	108.0	C6—C5—H5	121.4
C14—C13—C12	120.8 (2)	C4—C5—H5	121.4
C14—C13—H13	119.6	C22—C17—N2	120.40 (18)
C12—C13—H13	119.6	C22—C17—C18	124.28 (19)
C17—C22—C21	122.4 (2)	N2—C17—C18	115.31 (17)
C17—C22—H22	118.8	C4—C3—C2	121.76 (19)
C21—C22—H22	118.8	C4—C3—H3	119.1
C7—N1—C1	110.11 (15)	C2—C3—H3	119.1
C7—N1—C8	123.32 (16)	C3—C4—C5	120.95 (19)
C1—N1—C8	125.74 (16)	C3—C4—H4	119.5
C7—N2—C6	109.84 (16)	C5—C4—H4	119.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O1^{i}	0.93	2.53	3.303 (2)	141
C16—H16···N4^{ii}	0.93	2.62	3.413 (3)	144
C10—H10···O1^{iii}	0.93	2.26	3.174 (2)	167

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