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3-Phenyl-1*H*-1,2,4-triazol-5-amine–5-phenyl-1*H*-1,2,4-triazol-3-amine (1/1)

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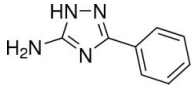
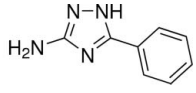
Key indicators: single-crystal X-ray study; T = 223 K; mean σ(C–C) = 0.004 Å; R factor = 0.067; wR factor = 0.168; data-to-parameter ratio = 14.6.

In the title compound, $C_8H_8N_4\cdot C_8H_8N_4$, two tautomers, *viz*. 3-phenyl-1,2,4-triazol-5-amine and 5-phenyl-1,2,4-triazol-3-amine, are crystallized together in equal amounts. The 3-phenyl-1,2,4-triazol-5-amine molecule is essentially planar; the phenyl ring makes a dihedral angle of 2.3 (2)° with the mean plane of the 1,2,4-triazole ring. In the 5-phenyl-1,2,4-triazol-3-amine tautomer, the mean planes of the phenyl and 1,2,4-triazole rings form a dihedral angle of 30.8 (2)°. The π-electron delocalization of the amino group with the 1,2,4-triazole nucleus in the 3-phenyl-1,2,4-triazol-5-amine molecule is more extensive than that in the 5-phenyl-1,2,4-triazol-3-amine tautomer. The molecules are linked into a two-dimensional network parallel to (100) by N—H···N hydrogen bonds.

Related literature

For a summary of structural data for 1,2,4-triazoles, see: Buzykin *et al.* (2006). For the crystal structure of 3-pyridin-2-yl-1,2,4-triazol-5-amine, see: Dolzhenko *et al.* (2009). For the use of 1,2,4-triazol-5-amines as building blocks in the synthesis of fused heterocyclic systems, see: Dolzhenko *et al.* (2006, 2007*a*,*b*); Fischer (2007).

Experimental

Crystal data

$C_8H_8N_4\cdot C_8H_8N_4$
M_r = 320.36
Monoclinic, $P2_1/c$
a = 17.817 (2) Å
b = 5.0398 (6) Å
c = 18.637 (2) Å
β = 113.573 (4)°
V = 1533.9 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 223 (2) K
0.60 × 0.10 × 0.06 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.947, T_{max} = 0.995
10288 measured reflections
3523 independent reflections
2394 reflections with $I > 2\sigma(I)$
R_{int} = 0.063

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.168
S = 0.99
3523 reflections
241 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3*N*···N2^{i}	0.89 (3)	2.08 (3)	2.966 (3)	175 (3)
N4—H4*A*···N1^{ii}	0.92 (3)	2.09 (3)	3.011 (3)	173 (3)
N4—H4*B*···N8^{i}	0.85 (3)	2.25 (3)	3.091 (3)	170 (3)
N6—H6*N*···N5^{iii}	0.87 (4)	2.04 (4)	2.879 (3)	159 (3)
N8—H8*A*···N2	0.81 (3)	2.41 (3)	3.206 (3)	168 (3)
N8—H8*B*···N7^{iv}	0.94 (4)	2.19 (4)	3.115 (3)	169 (3)

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXS97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2720).

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supporting information

Acta Cryst. (2009). E**65**, o126 [doi:10.1107/S1600536808042165]

3-Phenyl-1*H*-1,2,4-triazol-5-amine–5-phenyl-1*H*-1,2,4-triazol-3-amine (1/1)

Anton V. Dolzhenko, Geok Kheng Tan, Lip Lin Koh, Anna V. Dolzhenko and Wai Keung Chui

S1. Comment

1,2,4-Triazol-5-amines have been used as building blocks for the synthesis of fused heterocyclic systems, *e.g.* 1,2,4-triazolo[1,5-*a*]pyrimidines (Fischer, 2007) and 1,2,4-triazolo[1,5-*a*][1,3,5]triazines (Dolzhenko *et al.*, 2006). Herein, we report the structural study of 3(5)-phenyl-1,2,4-triazol-5(3)-amine, which was used as a synthon in our previous works (Dolzhenko *et al.*, 2007*a*,b).

Due to annular tautomerism in 1,2,4-triazole ring, there is a theoretical possibility of three tautomeric forms, namely 3-phenyl-1,2,4-triazol-5-amine (**I**), 5-phenyl-1,2,4-triazol-3-amine (**II**), and 5-phenyl-4*H*-1,2,4-triazol-3-amine (**III**) (Fig.1).

Usually, tautomerizable 1,2,4-triazoles with nonequivalent substituents at positions 3 and 5 crystallize as a tautomer bearing at position 5 substituent with relatively more pronounced electronodonor properties (Buzykin *et al.*, 2006). Considering significant difference in electronic properties of phenyl and amino group, the crystal would be assembled from the molecules of tautomer **I** analogously to the reported 3-pyridin-2-yl-1,2,4-triazol-5-amine (Dolzhenko *et al.*, 2009). Surprisingly, two tautomeric forms **I** and **II** were found crystallized together in the crystal. To the best of our knowledge, this is the first example of existence in crystal of unequally 3,5-disubstituted tautomerizable 1,2,4-triazole tautomeric form with electronodonor group located at position 3.

The geometry of the tautomer **I** molecule is essentially planar (Fig.2). The amino group is involved in π-electron delocalization with the 1,2,4-triazole nucleus. It is almost planar with small deviation 0.06 (2) Å of the nitrogen atom from the C8/H4A/H4B plane. The length of the C8—N4 bond is 1.337 (3) Å. The π-electron delocalization of the amino group of **II** with the 1,2,4-triazole nucleus is significantly lower. The nitrogen atom (N8) of the amino group adopts a pyramidal configuration with 0.21 (2) Å deviation of the nitrogen atom from the C16/H8A/H8B plane. The C16—N8 bond [1.372 (3) Å] is also longer. The phenyl ring of **I** makes a small dihedral angle of 2.3 (2)° with the mean plane of the 1,2,4-triazole ring. The molecule of tautomer **II** loses this planarity. The mean planes of the phenyl and 1,2,4-triazole rings of **II** form a dihedral angle of 30.8 (2)°.

The molecules are linked into a two-dimensional network parallel to the (100) by N—H···N hydrogen bonds (Table 1 and Fig.3).

S2. Experimental

(5)-Phenyl-1,2,4-triazol-5(3)-amine was prepared according to Dolzhenko *et al.* (2007*a*,b). The crystals suitable for crystallographic analysis were grown by recrystallization from ethanol.

S3. Refinement

N-bound H-atoms were located in a difference map and refined freely. C-bound H atoms were positioned geometrically (C-H = 0.94 Å) and were constrained in a riding motion approximation with U_{iso}(H) = 1.2U_{eq}(C).

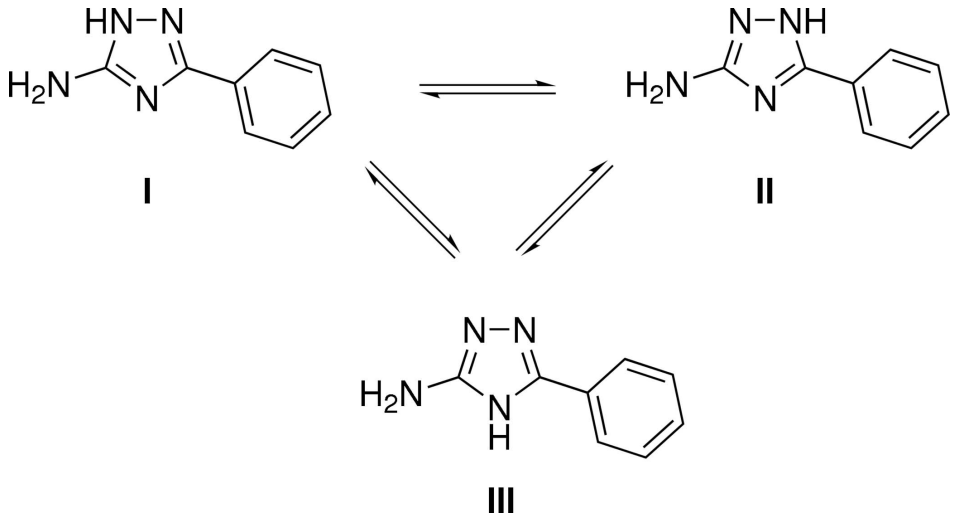

Figure 1

Possible tautomers of 3(5)-phenyl-1,2,4-triazol-5(3)-amine.

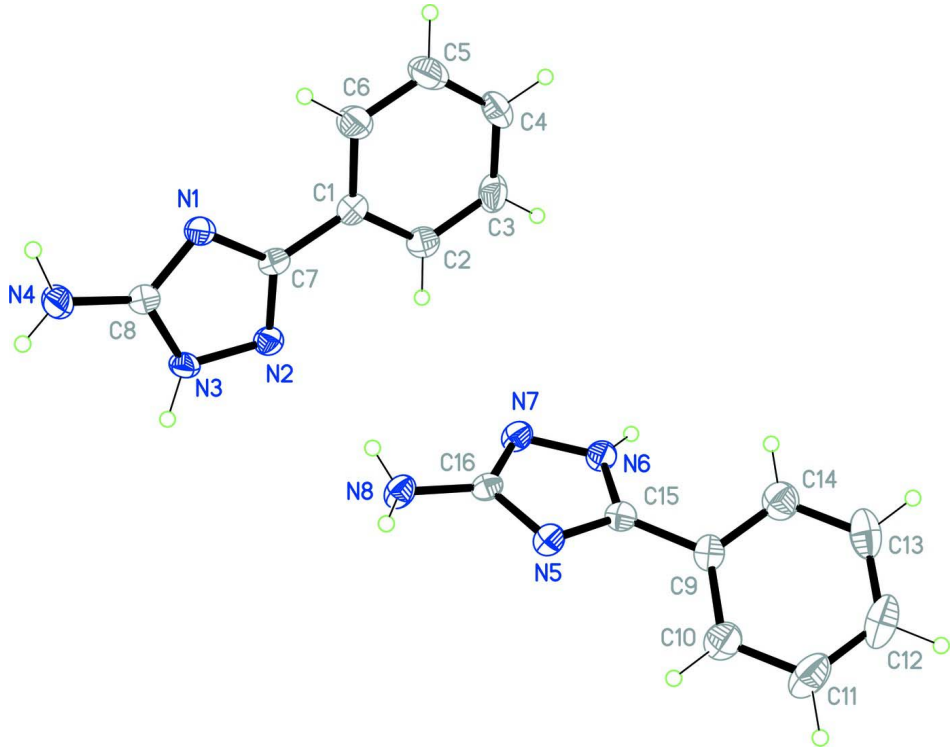

Figure 2

The molecular structure of 3(5)-phenyl-1,2,4-triazol-5(3)-amine with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

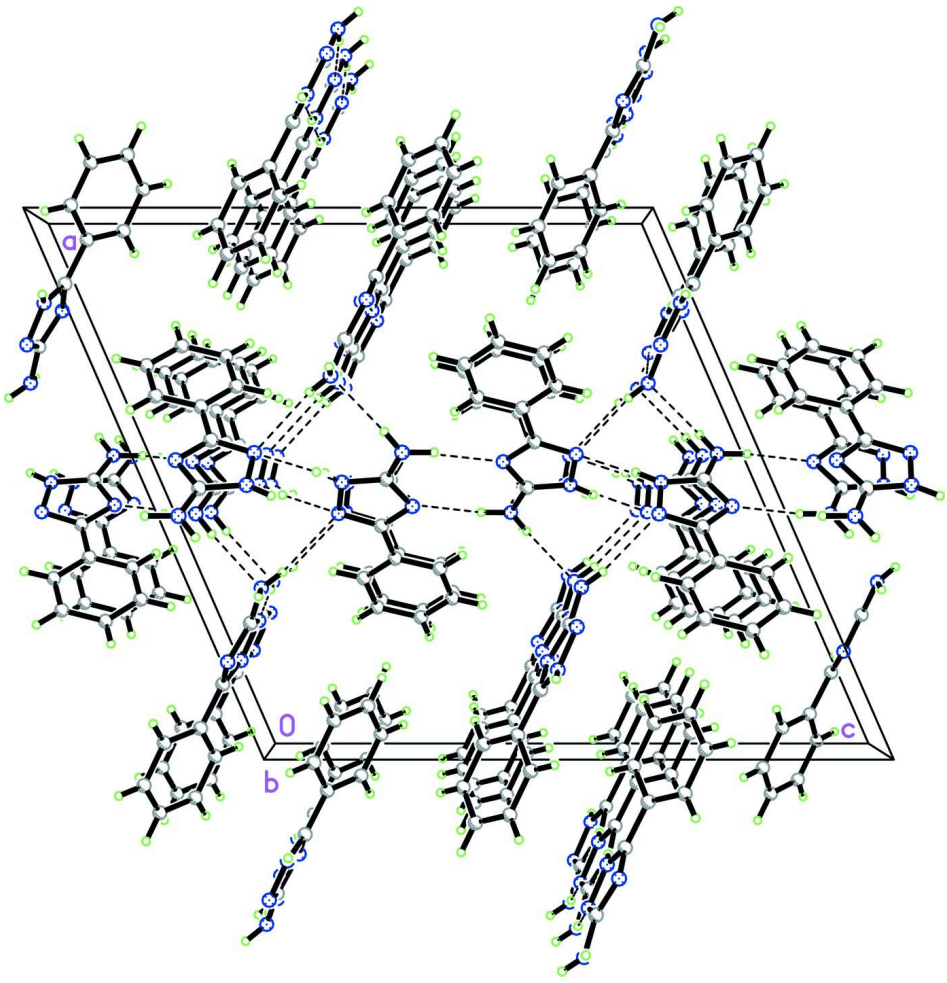

Figure 3

Molecular packing in the crystal, viewed along the *b* axis. Hydrogen bonds are shown as dashed lines.

3-Phenyl-1*H*-1,2,4-triazol-5-amine–5-phenyl-1*H*-1,2,4-triazol- 3-amine (1/1)

Crystal data

$C_8H_8N_4{\cdot}C_8H_8N_4$
$M_r = 320.36$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 17.817\ (2)$ Å
$b = 5.0398\ (6)$ Å
$c = 18.637\ (2)$ Å
$\beta = 113.573\ (4)°$
$V = 1533.9\ (3)$ Å^3
$Z = 4$

$F(000) = 672$
$D_x = 1.387$ Mg m^{-3}
Melting point: 460 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1028 reflections
$\theta = 2.4–22.6°$
$\mu = 0.09$ mm^{-1}
$T = 223$ K
Rod, colourless
0.60 × 0.10 × 0.06 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator

φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
$T_{min} = 0.947$, $T_{max} = 0.995$

10288 measured reflections
3523 independent reflections
2394 reflections with $I > 2\sigma(I)$
$R_{int} = 0.063$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.2°$
$h = -17 \rightarrow 23$
$k = -6 \rightarrow 6$
$l = -24 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.067$
$wR(F^2) = 0.168$
$S = 0.99$
3523 reflections
241 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
$w = 1/[\sigma^2(F_o^2) + (0.0813P)^2 + 0.5041P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.43$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ 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. 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}
N1	0.45958 (12)	0.2679 (4)	0.41243 (11)	0.0227 (5)
N2	0.44655 (12)	0.1498 (4)	0.29112 (11)	0.0228 (5)
N3	0.50228 (12)	0.3557 (4)	0.31965 (12)	0.0232 (5)
H3N	0.5206 (17)	0.441 (6)	0.2883 (17)	0.034 (8)*
N4	0.55437 (15)	0.6210 (5)	0.43462 (14)	0.0306 (5)
H4A	0.5543 (18)	0.650 (6)	0.483 (2)	0.047 (9)*
H4B	0.5900 (18)	0.694 (6)	0.4217 (17)	0.038 (8)*
C1	0.36387 (14)	−0.0976 (5)	0.34673 (13)	0.0221 (5)
C2	0.32601 (15)	−0.2542 (5)	0.28099 (14)	0.0275 (6)
H2	0.3384	−0.2297	0.2369	0.033*
C3	0.26999 (16)	−0.4464 (5)	0.27973 (16)	0.0326 (6)
H3	0.2450	−0.5525	0.2349	0.039*
C4	0.25056 (16)	−0.4837 (5)	0.34337 (16)	0.0317 (6)
H4	0.2119	−0.6128	0.3420	0.038*
C5	0.28814 (18)	−0.3303 (6)	0.40898 (17)	0.0405 (7)
H5	0.2754	−0.3557	0.4528	0.049*
C6	0.34456 (17)	−0.1385 (6)	0.41101 (16)	0.0352 (7)
H6	0.3700	−0.0352	0.4563	0.042*
C7	0.42378 (14)	0.1068 (5)	0.34941 (13)	0.0205 (5)
C8	0.50768 (14)	0.4241 (5)	0.39146 (13)	0.0223 (5)

N5	0.18197 (12)	0.2602 (4)	0.01779 (11)	0.0225 (5)
N6	0.17613 (13)	−0.1706 (4)	0.02735 (12)	0.0241 (5)
H6N	0.165 (2)	−0.339 (7)	0.0188 (19)	0.057 (10)*
N7	0.25003 (12)	−0.1005 (4)	0.08543 (11)	0.0247 (5)
N8	0.31434 (13)	0.3193 (5)	0.12197 (13)	0.0257 (5)
H8A	0.3424 (19)	0.261 (6)	0.1652 (19)	0.042 (9)*
H8B	0.302 (2)	0.500 (7)	0.1168 (19)	0.055 (10)*
C9	0.05728 (14)	0.0322 (5)	−0.07822 (14)	0.0237 (5)
C10	0.03648 (17)	0.2181 (5)	−0.13815 (16)	0.0341 (7)
H10	0.0741	0.3502	−0.1371	0.041*
C11	−0.04013 (18)	0.2079 (6)	−0.19945 (17)	0.0444 (8)
H11	−0.0542	0.3339	−0.2399	0.053*
C12	−0.09593 (17)	0.0147 (6)	−0.20168 (17)	0.0423 (8)
H12	−0.1477	0.0092	−0.2435	0.051*
C13	−0.07527 (17)	−0.1708 (6)	−0.14209 (18)	0.0417 (8)
H13	−0.1131	−0.3025	−0.1432	0.050*
C14	0.00090 (17)	−0.1621 (6)	−0.08100 (16)	0.0345 (6)
H14A	0.0148	−0.2891	−0.0408	0.041*
C15	0.13744 (15)	0.0420 (5)	−0.01207 (13)	0.0219 (5)
C16	0.24976 (14)	0.1614 (5)	0.07732 (13)	0.0198 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0273 (11)	0.0216 (10)	0.0205 (10)	−0.0031 (9)	0.0108 (9)	−0.0002 (8)
N2	0.0274 (11)	0.0216 (10)	0.0200 (10)	−0.0022 (9)	0.0099 (8)	−0.0016 (8)
N3	0.0306 (11)	0.0236 (11)	0.0193 (10)	−0.0060 (9)	0.0143 (9)	−0.0013 (9)
N4	0.0378 (13)	0.0325 (13)	0.0266 (12)	−0.0140 (11)	0.0182 (10)	−0.0090 (10)
C1	0.0229 (12)	0.0212 (12)	0.0217 (12)	0.0036 (10)	0.0082 (10)	−0.0010 (10)
C2	0.0293 (13)	0.0302 (14)	0.0244 (13)	−0.0007 (11)	0.0122 (11)	−0.0013 (11)
C3	0.0286 (14)	0.0343 (15)	0.0310 (14)	−0.0080 (12)	0.0079 (11)	−0.0104 (12)
C4	0.0268 (14)	0.0275 (14)	0.0419 (15)	−0.0067 (11)	0.0150 (12)	0.0017 (12)
C5	0.0476 (18)	0.0449 (17)	0.0391 (16)	−0.0131 (15)	0.0279 (14)	−0.0024 (14)
C6	0.0448 (16)	0.0356 (15)	0.0298 (14)	−0.0133 (13)	0.0197 (13)	−0.0075 (12)
C7	0.0249 (12)	0.0190 (12)	0.0176 (11)	0.0031 (10)	0.0085 (9)	0.0007 (9)
C8	0.0237 (12)	0.0228 (13)	0.0208 (12)	0.0009 (10)	0.0093 (10)	0.0011 (10)
N5	0.0246 (10)	0.0196 (10)	0.0214 (10)	0.0019 (8)	0.0072 (8)	−0.0015 (8)
N6	0.0264 (11)	0.0176 (11)	0.0250 (11)	0.0004 (9)	0.0067 (9)	0.0018 (9)
N7	0.0276 (11)	0.0219 (11)	0.0211 (10)	0.0015 (9)	0.0061 (9)	0.0004 (8)
N8	0.0267 (12)	0.0222 (12)	0.0223 (11)	0.0028 (9)	0.0037 (9)	−0.0001 (9)
C9	0.0223 (12)	0.0203 (12)	0.0277 (13)	0.0023 (10)	0.0091 (10)	−0.0052 (10)
C10	0.0383 (15)	0.0234 (13)	0.0338 (14)	0.0007 (12)	0.0073 (12)	0.0002 (11)
C11	0.0453 (18)	0.0347 (17)	0.0357 (16)	0.0085 (14)	−0.0022 (14)	0.0022 (13)
C12	0.0278 (15)	0.0420 (18)	0.0431 (17)	0.0073 (13)	−0.0008 (13)	−0.0139 (14)
C13	0.0285 (15)	0.0431 (17)	0.0506 (18)	−0.0101 (13)	0.0126 (13)	−0.0157 (15)
C14	0.0357 (15)	0.0313 (15)	0.0349 (15)	−0.0016 (12)	0.0123 (12)	−0.0024 (12)
C15	0.0261 (12)	0.0193 (12)	0.0218 (12)	0.0001 (10)	0.0113 (10)	−0.0022 (10)
C16	0.0241 (12)	0.0196 (12)	0.0166 (11)	0.0031 (10)	0.0092 (9)	−0.0009 (9)

Geometric parameters (Å, º)

N1—C8	1.332 (3)	N5—C15	1.340 (3)
N1—C7	1.359 (3)	N5—C16	1.366 (3)
N2—C7	1.321 (3)	N6—C15	1.326 (3)
N2—N3	1.387 (3)	N6—N7	1.375 (3)
N3—C8	1.348 (3)	N6—H6N	0.87 (4)
N3—H3N	0.89 (3)	N7—C16	1.328 (3)
N4—C8	1.337 (3)	N8—C16	1.372 (3)
N4—H4A	0.92 (3)	N8—H8A	0.81 (3)
N4—H4B	0.85 (3)	N8—H8B	0.94 (4)
C1—C2	1.385 (3)	C9—C14	1.389 (4)
C1—C6	1.388 (3)	C9—C10	1.390 (4)
C1—C7	1.470 (3)	C9—C15	1.468 (3)
C2—C3	1.385 (4)	C10—C11	1.387 (4)
C2—H2	0.94	C10—H10	0.94
C3—C4	1.375 (4)	C11—C12	1.380 (4)
C3—H3	0.94	C11—H11	0.94
C4—C5	1.373 (4)	C12—C13	1.384 (4)
C4—H4	0.94	C12—H12	0.94
C5—C6	1.384 (4)	C13—C14	1.380 (4)
C5—H5	0.94	C13—H13	0.94
C6—H6	0.94	C14—H14A	0.94
C8—N1—C7	103.55 (19)	C15—N5—C16	102.86 (19)
C7—N2—N3	102.47 (18)	C15—N6—N7	110.6 (2)
C8—N3—N2	109.15 (19)	C15—N6—H6N	131 (2)
C8—N3—H3N	129.2 (18)	N7—N6—H6N	118 (2)
N2—N3—H3N	120.4 (18)	C16—N7—N6	101.93 (18)
C8—N4—H4A	118 (2)	C16—N8—H8A	115 (2)
C8—N4—H4B	121 (2)	C16—N8—H8B	113 (2)
H4A—N4—H4B	120 (3)	H8A—N8—H8B	119 (3)
C2—C1—C6	118.5 (2)	C14—C9—C10	119.3 (2)
C2—C1—C7	121.3 (2)	C14—C9—C15	120.1 (2)
C6—C1—C7	120.2 (2)	C10—C9—C15	120.7 (2)
C3—C2—C1	120.4 (2)	C11—C10—C9	119.7 (3)
C3—C2—H2	119.8	C11—C10—H10	120.2
C1—C2—H2	119.8	C9—C10—H10	120.2
C4—C3—C2	120.6 (2)	C12—C11—C10	120.7 (3)
C4—C3—H3	119.7	C12—C11—H11	119.6
C2—C3—H3	119.7	C10—C11—H11	119.6
C5—C4—C3	119.3 (2)	C11—C12—C13	119.7 (3)
C5—C4—H4	120.3	C11—C12—H12	120.2
C3—C4—H4	120.3	C13—C12—H12	120.2
C4—C5—C6	120.5 (3)	C14—C13—C12	119.9 (3)
C4—C5—H5	119.7	C14—C13—H13	120.0
C6—C5—H5	119.7	C12—C13—H13	120.0
C5—C6—C1	120.5 (3)	C13—C14—C9	120.7 (3)

C5—C6—H6	119.7	C13—C14—H14A	119.6
C1—C6—H6	119.7	C9—C14—H14A	119.6
N2—C7—N1	114.8 (2)	N6—C15—N5	110.0 (2)
N2—C7—C1	123.0 (2)	N6—C15—C9	123.7 (2)
N1—C7—C1	122.1 (2)	N5—C15—C9	126.3 (2)
N1—C8—N4	125.5 (2)	N7—C16—N5	114.6 (2)
N1—C8—N3	110.0 (2)	N7—C16—N8	122.9 (2)
N4—C8—N3	124.6 (2)	N5—C16—N8	122.4 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*N*···N2^{i}	0.89 (3)	2.08 (3)	2.966 (3)	175 (3)
N4—H4*A*···N1^{ii}	0.92 (3)	2.09 (3)	3.011 (3)	173 (3)
N4—H4*B*···N8^{i}	0.85 (3)	2.25 (3)	3.091 (3)	170 (3)
N6—H6*N*···N5^{iii}	0.87 (4)	2.04 (4)	2.879 (3)	159 (3)
N8—H8*A*···N2	0.81 (3)	2.41 (3)	3.206 (3)	168 (3)
N8—H8*B*···N7^{iv}	0.94 (4)	2.19 (4)	3.115 (3)	169 (3)

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