Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-Benzyl-1*H*-benzotriazole

P. Selvarathy Grace,[a] Samuel Robinson Jebas,[b] B. Ravindran Durai Nayagam[a]* and Dieter Schollmeyer[c]

[a]Department of Chemistry, Popes College, Sawyerpuram 628 251, Tamilnadu, India, [b]Department of Physics, Sethupathy Govt. Arts College, Ramanathapuram 623 502, Tamilnadu, India, and [c]Institut für Organische Chemie, Universität Mainz, Duesbergweg 10-14, 55099 Mainz, Germany
Correspondence e-mail: b_ravidurai@yahoo.com

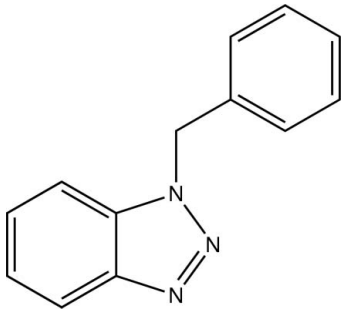
Received 24 February 2012; accepted 13 March 2012

Key indicators: single-crystal X-ray study; T = 193 K; mean σ(C–C) = 0.003 Å; R factor = 0.055; wR factor = 0.138; data-to-parameter ratio = 13.9.

In the title compound, $C_{13}H_{11}N_3$, the benzotriazole ring system is essentially planar, with a maximum deviation of 0.0173 (18) Å, and forms a dihedral angle of 75.08 (8)Å with the phenyl ring. In the crystal, pairs of weak C—H···N hydrogen bonds form inversion dimers. In addition, there are weak C—H···π(arene) interactions and weak π–π stacking interactions, with a centroid–centroid distance of 3.673 (11) Å.

Related literature

For the biological activity of benzotriazole derivatives, see: Katarzyna *et al.* (2005); Sarala *et al.* (2007). For their applications, see: Kopec *et al.* (2008); Krawczyk & Gdaniec (2005); Smith *et al.* (2001); Sha *et al.* (1996). For a related structure, see: Ravindran *et al.* (2009). For standard bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{13}H_{11}N_3$
M_r = 209.25
Monoclinic, $P2_1/c$
a = 11.5734 (10) Å
b = 5.9705 (4) Å
c = 16.1202 (14) Å
β = 106.490 (4)°
V = 1068.07 (15) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 0.64 mm^{-1}
T = 193 K
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (*CORINC*; Dräger & Gattow, 1971; Wiehl & Schollmeyer, 1994)
T_{min} = 0.832, T_{max} = 0.939
2125 measured reflections
2020 independent reflections
1788 reflections with $I > 2\sigma(I)$
R_{int} = 0.108
3 standard reflections every 60 min
intensity decay: 2%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.138
S = 1.12
2020 reflections
145 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

Cg is the centroid of the C4–C9 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···N1^{i}	0.95	2.62	3.513 (3)	158
C14—H14···Cg^{ii}	0.95	2.69	3.583 (2)	157

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *CORINC* (Dräger & Gattow, 1971; Wiehl & Schollmeyer, 1994); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *PLATON* (Spek, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5426).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Dräger, M. & Gattow, G. (1971). *Acta Chem. Scand.* **25**, 761–762.
Enraf–Nonius (1989). *CAD-4 Software*. Enraf–Nonius, Delft, The Netherlands.
Katarzyna, K., Najda, A., Zebrowska, J., Chomicz, L., Piekarczyk, J., Myjak, P. & Bretner, M. (2005). *Bioorg. Med. Chem.* **13**, 3601–3616.
Kopec, E. A., Zwolska, Z. & Kazimierczuk, A. O. Z. (2008). *Acta Pol. Pharm. Drug Res.* **65**, 435–439.
Krawczyk, S. & Gdaniec, M. (2005). *Acta Cryst.* E**61**, o2967–o2969.
Ravindran Durai Nayagam, B., Jebas, S. R., Edward Rajkumar, J. P. & Schollmeyer, D. (2009). *Acta Cryst.* E**65**, o917.
Sarala, G., Swamy, S. N., Prabhuswamy, B., Andalwar, S. M., Prasad, J. S. & Rangappa, K. S. (2007). *Anal. Sci.* **23**, 25–26.
Sha, G., Wang, W. & Ren, T. (1996). *Mocha Xuebao*, **16**, 344–350.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Smith, G., Bottle, S. E., Reid, D. A., Schweinsberg, D. P. & Bott, R. C. (2001). *Acta Cryst.* E**57**, o531–o532.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Wiehl, L. & Schollmeyer, D. (1994). *CORINC*. University of Mainz, Germany.

supporting information

Acta Cryst. (2012). E**68**, o1132 [https://doi.org/10.1107/S1600536812010951]

1-Benzyl-1*H*-benzotriazole

P. Selvarathy Grace, Samuel Robinson Jebas, B. Ravindran Durai Nayagam and Dieter Schollmeyer

S1. Comment

Benzotriazole derivatives show biological activities such as anti-inflammatory, diuretic, antiviral and are antihypertensive agents (Katarzyna *et al.*, 2005; Sarala *et al.*, 2007). They are used as corrosion inhibitors, antifreeze agents, ultraviolet light stabilizer for plastics and as antifoggants in photography (Krawczyk & Gdaniec, 2005; Smith *et al.*, 2001). *N*-Aryloxy derivatives of benzotriazole have anti-mycobacterial activity (Kopec *et al.*, 2008). Benzotriazole possessing three vicinal N atoms, is used as an antifouling and antiwear reagent (Sha *et al.*, 1996). These applications of benzotriazole compounds prompted us to synthesize the title compound and herein we report the crystal structure.

In (I) (Fig 1), the bond lengths (Allen *et al.*, 1987) and bond angles have normal values. The benzotriazole ring system is essentially planar with a maximum deviation of 0.0173 (18) Å for atom N3. The mean plane of the benzotriazole ring system (N1—N3/C4—C9) forms a dihedral angle of 75.08 (8) Å with the mean plane of the phenyl ring (C11—C16).

In the crystal, pairs of weak C—H···N hydrogen bonds form centrosymmetric dimers (Fig. 2). In addition, there are weak π–π stacking interactions between ring N1-N3/C4/C9 and ring C4—C9(1-*x*, 1-y, 1-*z*) with a centroid-centroid distance of 3.673 (11)Å.

S2. Experimental

A mixture of the sodium salt of benzotriazole (0.148 g, 1 mmol) benzyl chloride (0.126 g, 1 mmol) in ethanol and water (5 ml) were heated at 333K with continous stirring for 4 h. The mixture was kept aside for slow evaporation. After two weeks crystals of (I) suitable for X-ray diffraction were formed.

S3. Refinement

H atoms were positioned geometrically [C—H = 0.95 (aromatic) or 0.99 Å (methylene)] and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C).

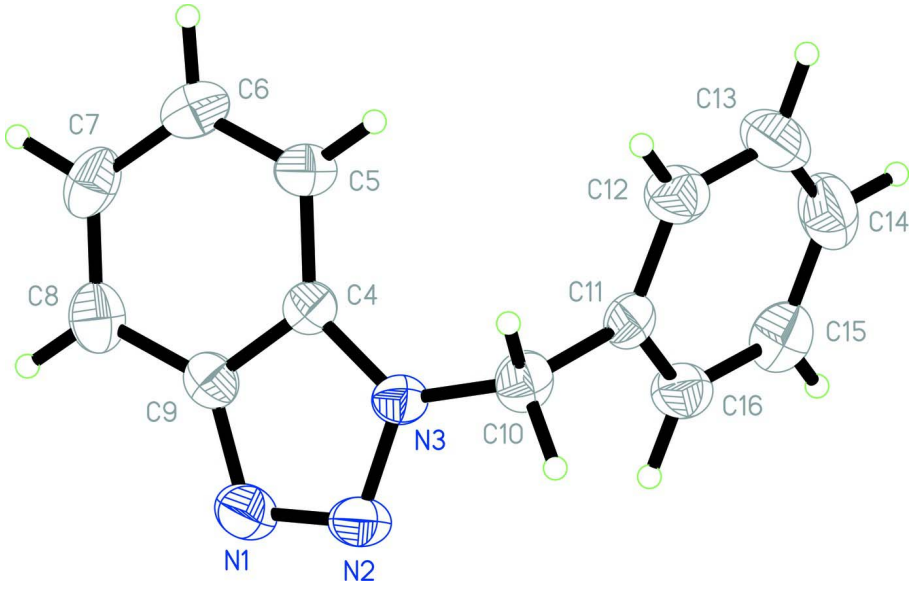


Figure 1

The molecular structure of (I) with displacement ellipsoids are drawn at the 50% probability level.

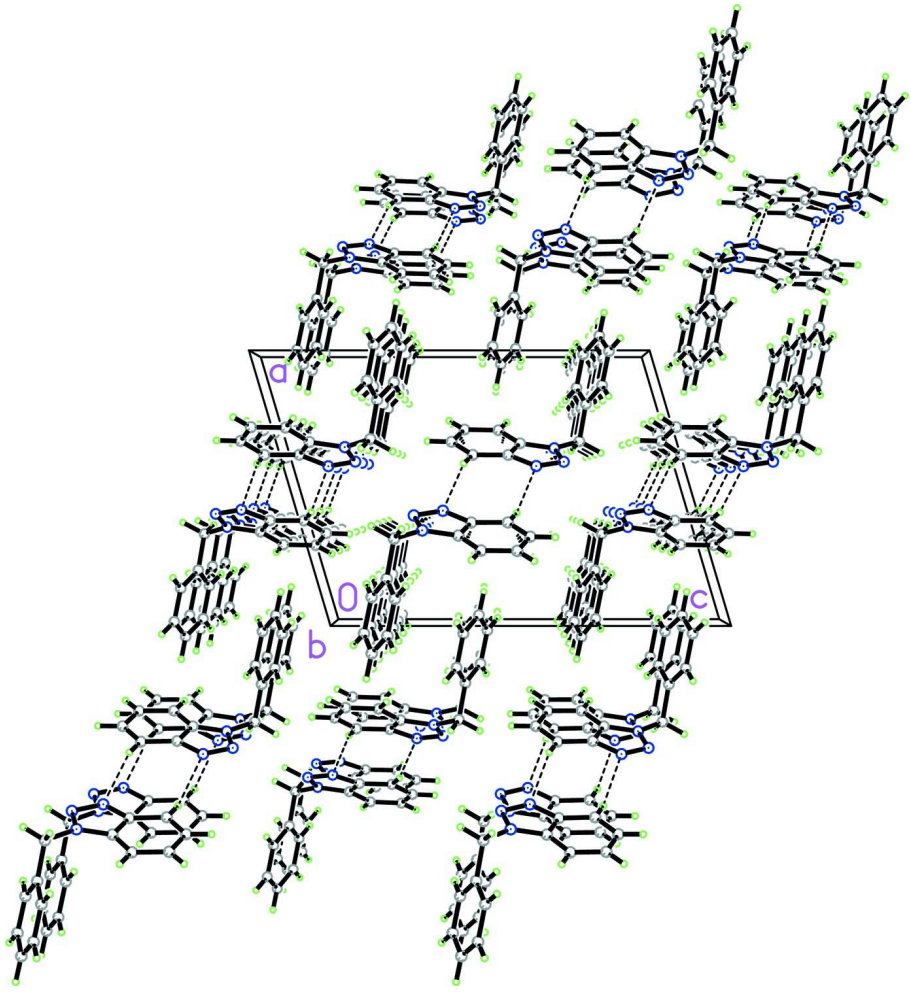


Figure 2

The crystal packing of the title compound, viewed along the *b* axis. Hydrogen bonds are shown as dashed lines.

1-Benzyl-1*H*-benzotriazole

Crystal data

$C_{13}H_{11}N_3$
$M_r = 209.25$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 11.5734\ (10)$ Å
$b = 5.9705\ (4)$ Å
$c = 16.1202\ (14)$ Å
$\beta = 106.490\ (4)°$
$V = 1068.07\ (15)$ Å^3
$Z = 4$
$F(000) = 440$
$D_x = 1.301$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 25 reflections
$\theta = 55–68°$
$\mu = 0.64$ mm^{-1}
$T = 193$ K
Block, colourless
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: rotating anode
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: ψ scan (*CORINC*; Dräger & Gattow, 1971; Wiehl & Schollmeyer, 1994)

T_{min} = 0.832, T_{max} = 0.939
2125 measured reflections
2020 independent reflections
1788 reflections with $I > 2\sigma(I)$
R_{int} = 0.108
θ_{max} = 70.0°, θ_{min} = 4.0°
h = 0→14
k = 0→7
l = −19→18
3 standard reflections every 60 min
intensity decay: 2%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.138
S = 1.12
2020 reflections
145 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0628P)^2 + 0.3976P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.30 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. 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 $F^2 > 2$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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
N1	0.42315 (15)	0.1763 (3)	0.37392 (11)	0.0331 (4)
N2	0.40768 (14)	0.2958 (3)	0.30376 (10)	0.0312 (4)
N3	0.35886 (13)	0.4957 (3)	0.31508 (10)	0.0255 (4)
C4	0.34149 (14)	0.5049 (3)	0.39488 (11)	0.0232 (4)
C5	0.29338 (17)	0.6694 (3)	0.43720 (12)	0.0291 (4)
H5	0.2638	0.8079	0.4105	0.035*
C6	0.29158 (18)	0.6177 (4)	0.52002 (13)	0.0345 (5)
H6	0.2588	0.7231	0.5513	0.041*
C7	0.33691 (17)	0.4130 (4)	0.55981 (12)	0.0332 (5)
H7	0.3349	0.3858	0.6174	0.040*
C8	0.38387 (17)	0.2517 (4)	0.51801 (13)	0.0324 (5)
H8	0.4147	0.1145	0.5453	0.039*
C9	0.38385 (15)	0.3007 (3)	0.43252 (12)	0.0256 (4)
C10	0.33293 (16)	0.6650 (3)	0.24689 (12)	0.0300 (4)
H10A	0.3745	0.6244	0.2031	0.036*
H10B	0.3648	0.8114	0.2721	0.036*
C11	0.19948 (16)	0.6862 (3)	0.20336 (11)	0.0254 (4)
C12	0.13833 (19)	0.8816 (3)	0.21182 (13)	0.0343 (5)
H12	0.1804	1.0015	0.2461	0.041*

C13	0.0167 (2)	0.9019 (4)	0.17048 (15)	0.0425 (5)
H13	−0.0246	1.0354	0.1769	0.051*
C14	−0.04510 (19)	0.7302 (4)	0.12006 (15)	0.0434 (6)
H14	−0.1285	0.7459	0.0912	0.052*
C15	0.01477 (19)	0.5340 (4)	0.11147 (13)	0.0376 (5)
H15	−0.0276	0.4148	0.0769	0.045*
C16	0.13627 (17)	0.5127 (3)	0.15333 (12)	0.0310 (4)
H16	0.1769	0.3778	0.1478	0.037*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0330 (9)	0.0294 (9)	0.0363 (9)	0.0057 (7)	0.0088 (7)	−0.0014 (7)
N2	0.0301 (8)	0.0319 (9)	0.0331 (9)	0.0056 (7)	0.0113 (7)	−0.0050 (7)
N3	0.0241 (7)	0.0282 (8)	0.0260 (8)	0.0022 (6)	0.0099 (6)	−0.0012 (6)
C4	0.0192 (8)	0.0264 (9)	0.0247 (9)	−0.0029 (7)	0.0072 (6)	−0.0010 (7)
C5	0.0314 (9)	0.0262 (10)	0.0323 (10)	0.0010 (8)	0.0133 (8)	−0.0016 (8)
C6	0.0370 (10)	0.0374 (11)	0.0331 (10)	−0.0026 (9)	0.0164 (8)	−0.0062 (9)
C7	0.0329 (10)	0.0446 (12)	0.0232 (9)	−0.0092 (9)	0.0097 (7)	0.0026 (8)
C8	0.0303 (9)	0.0327 (11)	0.0322 (10)	−0.0045 (8)	0.0059 (8)	0.0069 (8)
C9	0.0213 (8)	0.0250 (9)	0.0294 (9)	−0.0012 (7)	0.0055 (7)	0.0002 (7)
C10	0.0289 (9)	0.0354 (11)	0.0288 (9)	−0.0016 (8)	0.0130 (8)	0.0051 (8)
C11	0.0285 (9)	0.0303 (10)	0.0212 (8)	0.0005 (7)	0.0129 (7)	0.0064 (7)
C12	0.0410 (11)	0.0291 (10)	0.0356 (11)	0.0025 (9)	0.0155 (9)	0.0016 (9)
C13	0.0417 (12)	0.0384 (12)	0.0501 (13)	0.0146 (10)	0.0174 (10)	0.0082 (10)
C14	0.0303 (10)	0.0581 (15)	0.0403 (12)	0.0073 (10)	0.0074 (9)	0.0125 (11)
C15	0.0372 (11)	0.0433 (12)	0.0319 (10)	−0.0057 (9)	0.0090 (8)	−0.0009 (9)
C16	0.0345 (10)	0.0298 (10)	0.0315 (10)	0.0027 (8)	0.0137 (8)	0.0010 (8)

Geometric parameters (Å, º)

N1—N2	1.306 (2)	C10—C11	1.509 (2)
N1—C9	1.376 (2)	C10—H10A	0.9900
N2—N3	1.354 (2)	C10—H10B	0.9900
N3—C4	1.358 (2)	C11—C16	1.387 (3)
N3—C10	1.460 (2)	C11—C12	1.391 (3)
C4—C9	1.388 (3)	C12—C13	1.382 (3)
C4—C5	1.399 (3)	C12—H12	0.9500
C5—C6	1.376 (3)	C13—C14	1.376 (3)
C5—H5	0.9500	C13—H13	0.9500
C6—C7	1.411 (3)	C14—C15	1.388 (3)
C6—H6	0.9500	C14—H14	0.9500
C7—C8	1.373 (3)	C15—C16	1.382 (3)
C7—H7	0.9500	C15—H15	0.9500
C8—C9	1.409 (3)	C16—H16	0.9500
C8—H8	0.9500		
N2—N1—C9	108.00 (16)	N3—C10—H10A	109.2

N1—N2—N3	108.93 (15)	C11—C10—H10A	109.2
N2—N3—C4	110.05 (15)	N3—C10—H10B	109.2
N2—N3—C10	120.85 (15)	C11—C10—H10B	109.2
C4—N3—C10	129.11 (15)	H10A—C10—H10B	107.9
N3—C4—C9	104.45 (16)	C16—C11—C12	118.97 (18)
N3—C4—C5	132.60 (17)	C16—C11—C10	120.57 (17)
C9—C4—C5	122.94 (17)	C12—C11—C10	120.46 (18)
C6—C5—C4	115.70 (18)	C13—C12—C11	120.2 (2)
C6—C5—H5	122.2	C13—C12—H12	119.9
C4—C5—H5	122.2	C11—C12—H12	119.9
C5—C6—C7	121.96 (19)	C14—C13—C12	120.5 (2)
C5—C6—H6	119.0	C14—C13—H13	119.8
C7—C6—H6	119.0	C12—C13—H13	119.8
C8—C7—C6	122.18 (18)	C13—C14—C15	119.8 (2)
C8—C7—H7	118.9	C13—C14—H14	120.1
C6—C7—H7	118.9	C15—C14—H14	120.1
C7—C8—C9	116.38 (18)	C16—C15—C14	119.8 (2)
C7—C8—H8	121.8	C16—C15—H15	120.1
C9—C8—H8	121.8	C14—C15—H15	120.1
N1—C9—C4	108.56 (16)	C15—C16—C11	120.71 (19)
N1—C9—C8	130.63 (18)	C15—C16—H16	119.6
C4—C9—C8	120.80 (18)	C11—C16—H16	119.6
N3—C10—C11	111.88 (15)		

C9—N1—N2—N3	−0.1 (2)	N3—C4—C9—C8	177.98 (16)
N1—N2—N3—C4	−0.4 (2)	C5—C4—C9—C8	−2.1 (3)
N1—N2—N3—C10	179.31 (15)	C7—C8—C9—N1	−179.62 (19)
N2—N3—C4—C9	0.78 (18)	C7—C8—C9—C4	1.9 (3)
C10—N3—C4—C9	−178.94 (17)	N2—N3—C10—C11	106.88 (18)
N2—N3—C4—C5	−179.12 (18)	C4—N3—C10—C11	−73.4 (2)
C10—N3—C4—C5	1.2 (3)	N3—C10—C11—C16	−67.4 (2)
N3—C4—C5—C6	−179.41 (18)	N3—C10—C11—C12	113.53 (19)
C9—C4—C5—C6	0.7 (3)	C16—C11—C12—C13	−0.3 (3)
C4—C5—C6—C7	0.8 (3)	C10—C11—C12—C13	178.74 (17)
C5—C6—C7—C8	−1.0 (3)	C11—C12—C13—C14	−0.5 (3)
C6—C7—C8—C9	−0.4 (3)	C12—C13—C14—C15	0.8 (3)
N2—N1—C9—C4	0.6 (2)	C13—C14—C15—C16	−0.3 (3)
N2—N1—C9—C8	−178.05 (18)	C14—C15—C16—C11	−0.5 (3)
N3—C4—C9—N1	−0.84 (19)	C12—C11—C16—C15	0.9 (3)
C5—C4—C9—N1	179.07 (17)	C10—C11—C16—C15	−178.22 (17)

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the C4–C9 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···N1^{i}	0.95	2.62	3.513 (3)	158

C14—H14···*Cg*^{ii}	0.95	2.69	3.583 (2)	157

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