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# 1-[(1-Benzyl-1*H*-1,2,3-triazol-4-yl)methyl]-1*H*-1,3-benzodiazole

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**Keywords:** crystal structure; triazole; benzodiazole; hydrogen bond.

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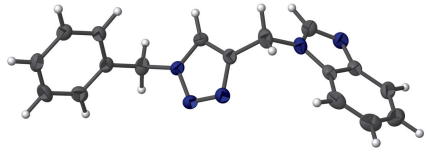
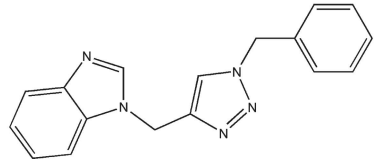
**Structural data**: full structural data are available from iucrdata.iucr.org

The title molecule, $C_{17}H_{15}N_5$, adopts a Z-shaped conformation, with the benzyl and benzodiazole substituents disposed on opposite sides of the plane of the triazole ring. A three-dimensional network is generated in the crystal by a combination of C—H···N hydrogen bonds and C—H···$\pi$(ring) interactions.

**3D view**



**Chemical scheme**



## Structure description

Benzimidazol-2-one derivatives are useful heterocyclic building blocks and are prominent structural elements of compounds presenting a wide variety of pharmacological and biochemical properties (Refaat, 2010; Olesen *et al.*, 1994; Soderlind *et al.*, 1999). As a continuation of our research devoted to the development of 1,2,3-triazole derivatives (Sahbi *et al.*, 2017), we report in this work the synthesis by a 1,3-dipolar cycloaddition reaction of a new 1,2,3-triazole derivative containing the benzimidazole moiety.

The title molecule (Fig. 1) adopts a Z-shaped conformation with the benzyl and benzodiazole substituents disposed on opposite sides of the plane of the triazole ring. The dihedral angle between the phenyl ring of the benzyl group and the triazole ring is 74.26 (4)°, while the dihedral angle between the triazole and benzodiazole units is 72.41 (4)°. Four sets of C—H···N hydrogen bonds (Table 1), two sets being quite weak, as well as a set of C—H···$\pi$(ring) interactions form the molecules into a three-dimensional network in the crystal (Table 1 and Figs. 2 and 3).

## Synthesis and crystallization

In a vial fitted with a screw cap, benzyl azide (100 mg, 0.75 mmol) and alkyled benzimidazol (90 mg, 0.58 mmol) were added to a mixture of copper(II) sulfate pentahydrate

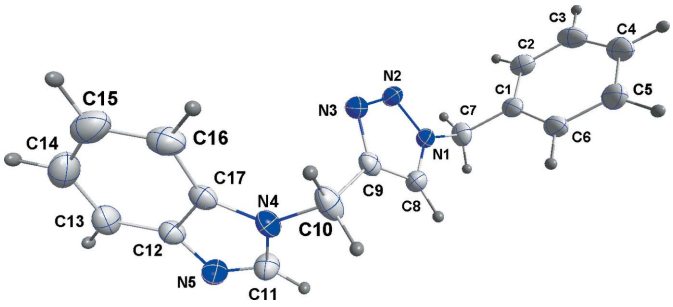



**Figure 1**
The structure of the title molecule with the labeling scheme and 50% probability displacement ellipsoids.

(9.3 mg, 0.037 mmol), sodium ascorbate (22.3 mg, 0.11 mmol), and $\beta$-cyclodextrin (21.33 mg, 0.019 mmol) dissolved in $H_2O$ (1 ml) at room temperature. The reaction mixture was stirred for 15 min at room temperature. The resulting mixture was poured into $CH_2Cl_2$ (3 ml) and $H_2O$ (3 ml), and the organic layer was separated. The aqueous layer was extracted with $CH_2Cl_2$ (3 ml) three times. The product was crystallized by slow evaporation from a hexane–$CH_2Cl_2$ mixture (3:1) (yield 89%).

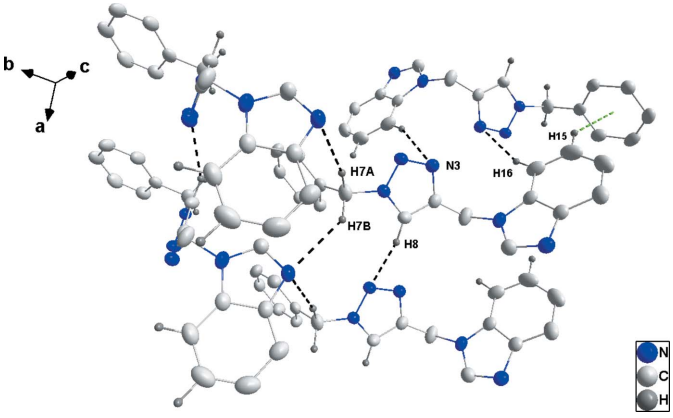



**Figure 2**
Detail of the intermolecular interactions. C—H···N hydrogen bonds and C—H···$\pi$(ring) interactions are shown, respectively, as black and green dashed lines.

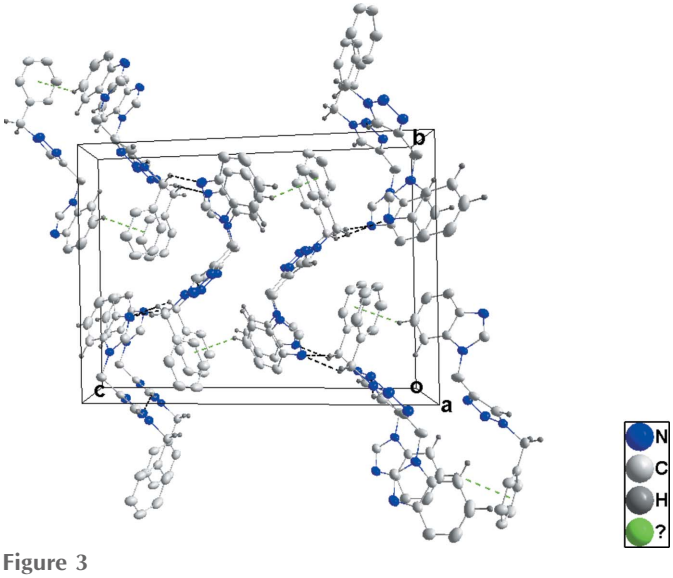



**Figure 3**
Packing viewed along the *a*-axis direction. The intermolecular interactions are depicted as in Fig. 2.

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

*Cg*3 is the centroid of the C1–C6 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C7—H7*A*···N5$^{i}$ | 1.03 (2) | 2.59 (2) | 3.602 (2) | 170 (2) |
| C7—H7*B*···N5$^{ii}$ | 1.01 (2) | 2.66 (2) | 3.508 (2) | 142 (1) |
| C8—H8···N2$^{iii}$ | 0.98 (2) | 2.44 (2) | 3.323 (2) | 151 (2) |
| C16—H16···N3$^{iv}$ | 1.00 (2) | 2.69 (2) | 3.652 (2) | 161 (2) |
| C15—H15···*Cg*3$^{iv}$ | 0.99 (2) | 2.77 (2) | 3.622 (2) | 144 (2) |

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

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{17}H_{15}N_5$ |
| $M_r$ | 289.34 |
| Crystal system, space group | Monoclinic, $P2_1/c$ |
| Temperature (K) | 150 |
| *a*, *b*, *c* (Å) | 5.3483 (1), 14.1861 (4), 19.1408 (5) |
| $\beta$ (°) | 97.451 (1) |
| $V$ (Å$^3$) | 1439.98 (6) |
| $Z$ | 4 |
| Radiation type | Cu $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.67 |
| Crystal size (mm) | 0.13 × 0.03 × 0.02 |
| | |
| Data collection | |
| Diffractometer | Bruker D8 VENTURE PHOTON 100 CMOS |
| Absorption correction | Multi-scan (*SADABS*; Bruker, 2016) |
| $T_{min}$, $T_{max}$ | 0.88, 0.99 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 10936, 2817, 2427 |
| $R_{int}$ | 0.037 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.618 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.040, 0.097, 1.04 |
| No. of reflections | 2817 |
| No. of parameters | 260 |
| H-atom treatment | All H-atom parameters refined |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.22, −0.19 |

Computer programs: *APEX3* (Bruker, 2016), *SAINT* (Bruker, 2016), *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012), *SHELXTL* (Sheldrick, 2008).

## Refinement

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

## Acknowledgements

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# full crystallographic data

*IUCrData* (2017). **2**, x170944 [https://doi.org/10.1107/S2414314617009440]

## 1-[(1-Benzyl-1*H*-1,2,3-triazol-4-yl)methyl]-1*H*-1,3-benzodiazole

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**1-[(1-Benzyl-1*H*-1,2,3-triazol-4-yl)methyl]-1*H*-1,3-benzodiazole**

*Crystal data*

$C_{17}H_{15}N_5$
$M_r$ = 289.34
Monoclinic, $P2_1/c$
$a$ = 5.3483 (1) Å
$b$ = 14.1861 (4) Å
$c$ = 19.1408 (5) Å
$\beta$ = 97.451 (1)°
$V$ = 1439.98 (6) Å$^3$
$Z$ = 4
$F(000)$ = 608
$D_x$ = 1.335 Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda$ = 1.54178 Å
Cell parameters from 8031 reflections
$\theta$ = 3.9–72.4°
$\mu$ = 0.67 mm$^{-1}$
$T$ = 150 K
Column, colourless
0.13 × 0.03 × 0.02 mm

*Data collection*

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC I$\mu$S micro-focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
$T_{min}$ = 0.88, $T_{max}$ = 0.99
10936 measured reflections
2817 independent reflections
2427 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.037
$\theta_{max}$ = 72.4°, $\theta_{min}$ = 3.9°
$h$ = −6→6
$k$ = −14→16
$l$ = −23→20

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.097
$S$ = 1.04
2817 reflections
260 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0421P)^2 + 0.4698P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.19 e Å$^{-3}$
Extinction correction: *SHELXL2014* (Sheldrick, 2015*b*), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0040 (4)

*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 $F^2 > 2\text{sigma}(F^2)$ 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 | 0.7517 (2) | 0.58381 (8) | 0.31394 (6) | 0.0260 (3) |
| N2 | 0.5371 (2) | 0.57393 (8) | 0.34255 (7) | 0.0304 (3) |
| N3 | 0.5770 (2) | 0.50948 (8) | 0.39222 (6) | 0.0311 (3) |
| N4 | 0.8363 (2) | 0.30988 (8) | 0.42456 (6) | 0.0294 (3) |
| N5 | 0.8012 (2) | 0.17383 (9) | 0.36442 (7) | 0.0333 (3) |
| C1 | 0.8262 (3) | 0.75148 (10) | 0.28669 (7) | 0.0288 (3) |
| C2 | 0.6539 (3) | 0.82402 (11) | 0.26945 (8) | 0.0361 (4) |
| H2 | 0.501 (3) | 0.8069 (11) | 0.2382 (9) | 0.032 (4)* |
| C3 | 0.7079 (3) | 0.91481 (11) | 0.29475 (9) | 0.0400 (4) |
| H3 | 0.583 (4) | 0.9651 (14) | 0.2822 (11) | 0.054 (6)* |
| C4 | 0.9291 (3) | 0.93358 (11) | 0.33753 (9) | 0.0374 (4) |
| H4 | 0.968 (4) | 0.9963 (14) | 0.3562 (10) | 0.049 (5)* |
| C5 | 1.1014 (3) | 0.86152 (11) | 0.35485 (9) | 0.0369 (4) |
| H5 | 1.261 (4) | 0.8760 (14) | 0.3857 (11) | 0.057 (6)* |
| C6 | 1.0509 (3) | 0.77114 (10) | 0.32907 (8) | 0.0325 (3) |
| H6 | 1.180 (4) | 0.7212 (14) | 0.3406 (10) | 0.048 (5)* |
| C7 | 0.7674 (3) | 0.65365 (11) | 0.25806 (8) | 0.0345 (3) |
| H7A | 0.597 (4) | 0.6530 (13) | 0.2267 (10) | 0.046 (5)* |
| H7B | 0.906 (4) | 0.6283 (13) | 0.2324 (10) | 0.047 (5)* |
| C8 | 0.9303 (3) | 0.52577 (10) | 0.34520 (8) | 0.0304 (3) |
| H8 | 1.098 (4) | 0.5242 (14) | 0.3302 (11) | 0.057 (6)* |
| C9 | 0.8188 (3) | 0.47873 (9) | 0.39500 (7) | 0.0275 (3) |
| C10 | 0.9266 (3) | 0.40447 (10) | 0.44536 (9) | 0.0386 (4) |
| H10A | 0.865 (4) | 0.4130 (14) | 0.4933 (11) | 0.052 (5)* |
| H10B | 1.120 (4) | 0.4052 (14) | 0.4484 (11) | 0.055 (6)* |
| C11 | 0.9143 (3) | 0.25572 (10) | 0.37299 (8) | 0.0331 (3) |
| H11 | 1.051 (3) | 0.2804 (12) | 0.3460 (9) | 0.038 (4)* |
| C12 | 0.6362 (3) | 0.17317 (10) | 0.41504 (7) | 0.0283 (3) |
| C13 | 0.4702 (3) | 0.10355 (11) | 0.43167 (9) | 0.0366 (4) |
| H13 | 0.455 (4) | 0.0418 (14) | 0.4059 (10) | 0.048 (5)* |
| C14 | 0.3266 (3) | 0.12212 (13) | 0.48488 (9) | 0.0449 (4) |
| H14 | 0.209 (4) | 0.0736 (15) | 0.4972 (11) | 0.055 (6)* |
| C15 | 0.3451 (3) | 0.20763 (14) | 0.52117 (9) | 0.0468 (4) |
| H15 | 0.243 (4) | 0.2214 (15) | 0.5597 (11) | 0.059 (6)* |
| C16 | 0.5087 (3) | 0.27775 (12) | 0.50617 (8) | 0.0376 (4) |

| | | | | |
|---|---|---|---|---|
| H16 | 0.528 (4) | 0.3390 (15) | 0.5321 (11) | 0.056 (6)* |
| C17 | 0.6542 (3) | 0.25882 (9) | 0.45272 (7) | 0.0278 (3) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0261 (6) | 0.0254 (6) | 0.0274 (6) | −0.0019 (4) | 0.0063 (4) | −0.0013 (4) |
| N2 | 0.0259 (6) | 0.0307 (6) | 0.0360 (7) | 0.0012 (5) | 0.0090 (5) | 0.0032 (5) |
| N3 | 0.0319 (6) | 0.0283 (6) | 0.0345 (7) | 0.0020 (5) | 0.0092 (5) | 0.0011 (5) |
| N4 | 0.0360 (6) | 0.0219 (6) | 0.0292 (6) | 0.0004 (5) | 0.0004 (5) | −0.0015 (4) |
| N5 | 0.0378 (7) | 0.0295 (6) | 0.0333 (6) | 0.0010 (5) | 0.0074 (5) | −0.0056 (5) |
| C1 | 0.0330 (7) | 0.0290 (7) | 0.0265 (7) | −0.0003 (5) | 0.0117 (6) | 0.0042 (5) |
| C2 | 0.0345 (8) | 0.0410 (9) | 0.0333 (8) | 0.0050 (6) | 0.0058 (6) | 0.0061 (6) |
| C3 | 0.0470 (9) | 0.0324 (8) | 0.0425 (9) | 0.0138 (7) | 0.0135 (7) | 0.0087 (6) |
| C4 | 0.0452 (9) | 0.0246 (7) | 0.0457 (9) | −0.0017 (6) | 0.0184 (7) | 0.0031 (6) |
| C5 | 0.0325 (8) | 0.0312 (8) | 0.0478 (9) | −0.0034 (6) | 0.0084 (7) | 0.0005 (6) |
| C6 | 0.0316 (7) | 0.0262 (7) | 0.0410 (8) | 0.0031 (6) | 0.0093 (6) | 0.0035 (6) |
| C7 | 0.0451 (9) | 0.0329 (8) | 0.0263 (7) | −0.0041 (6) | 0.0076 (6) | 0.0037 (6) |
| C8 | 0.0244 (7) | 0.0274 (7) | 0.0399 (8) | −0.0006 (5) | 0.0059 (6) | −0.0018 (6) |
| C9 | 0.0302 (7) | 0.0213 (6) | 0.0297 (7) | −0.0014 (5) | −0.0007 (5) | −0.0048 (5) |
| C10 | 0.0479 (9) | 0.0240 (8) | 0.0398 (9) | −0.0024 (6) | −0.0100 (7) | −0.0016 (6) |
| C11 | 0.0364 (8) | 0.0325 (8) | 0.0312 (7) | −0.0023 (6) | 0.0072 (6) | −0.0024 (6) |
| C12 | 0.0315 (7) | 0.0268 (7) | 0.0257 (7) | 0.0033 (5) | 0.0006 (5) | 0.0003 (5) |
| C13 | 0.0379 (8) | 0.0321 (8) | 0.0383 (8) | −0.0032 (6) | −0.0015 (6) | 0.0058 (6) |
| C14 | 0.0390 (9) | 0.0533 (11) | 0.0420 (9) | −0.0044 (7) | 0.0041 (7) | 0.0176 (8) |
| C15 | 0.0433 (9) | 0.0660 (12) | 0.0328 (8) | 0.0120 (8) | 0.0115 (7) | 0.0107 (8) |
| C16 | 0.0440 (9) | 0.0419 (9) | 0.0267 (7) | 0.0128 (7) | 0.0037 (6) | −0.0018 (6) |
| C17 | 0.0318 (7) | 0.0263 (7) | 0.0240 (7) | 0.0061 (5) | −0.0009 (5) | 0.0022 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N1—C8 | 1.3416 (18) | C5—H5 | 1.00 (2) |
| N1—N2 | 1.3420 (16) | C6—H6 | 0.992 (19) |
| N1—C7 | 1.4684 (18) | C7—H7A | 1.025 (19) |
| N2—N3 | 1.3163 (17) | C7—H7B | 1.01 (2) |
| N3—C9 | 1.3592 (18) | C8—C9 | 1.363 (2) |
| N4—C11 | 1.3585 (19) | C8—H8 | 0.98 (2) |
| N4—C17 | 1.3784 (18) | C9—C10 | 1.492 (2) |
| N4—C10 | 1.4638 (18) | C10—H10A | 1.02 (2) |
| N5—C11 | 1.3102 (19) | C10—H10B | 1.03 (2) |
| N5—C12 | 1.3927 (18) | C11—H11 | 1.011 (18) |
| C1—C6 | 1.388 (2) | C12—C13 | 1.392 (2) |
| C1—C2 | 1.392 (2) | C12—C17 | 1.4100 (19) |
| C1—C7 | 1.510 (2) | C13—C14 | 1.378 (2) |
| C2—C3 | 1.393 (2) | C13—H13 | 1.00 (2) |
| C2—H2 | 0.977 (18) | C14—C15 | 1.395 (3) |
| C3—C4 | 1.374 (3) | C14—H14 | 0.98 (2) |
| C3—H3 | 0.98 (2) | C15—C16 | 1.379 (3) |

| | | | |
|---|---|---|---|
| C4—C5 | 1.387 (2) | C15—H15 | 0.99 (2) |
| C4—H4 | 0.97 (2) | C16—C17 | 1.389 (2) |
| C5—C6 | 1.388 (2) | C16—H16 | 1.00 (2) |
| | | | |
| C8—N1—N2 | 110.57 (11) | N1—C8—C9 | 105.16 (12) |
| C8—N1—C7 | 129.36 (12) | N1—C8—H8 | 120.7 (12) |
| N2—N1—C7 | 120.03 (12) | C9—C8—H8 | 134.1 (12) |
| N3—N2—N1 | 107.45 (11) | N3—C9—C8 | 108.42 (12) |
| N2—N3—C9 | 108.41 (11) | N3—C9—C10 | 122.53 (14) |
| C11—N4—C17 | 106.63 (12) | C8—C9—C10 | 129.04 (14) |
| C11—N4—C10 | 126.47 (13) | N4—C10—C9 | 112.66 (12) |
| C17—N4—C10 | 126.90 (13) | N4—C10—H10A | 102.7 (11) |
| C11—N5—C12 | 104.06 (12) | C9—C10—H10A | 110.8 (11) |
| C6—C1—C2 | 119.09 (14) | N4—C10—H10B | 108.6 (11) |
| C6—C1—C7 | 121.34 (13) | C9—C10—H10B | 109.3 (11) |
| C2—C1—C7 | 119.56 (14) | H10A—C10—H10B | 112.7 (16) |
| C1—C2—C3 | 120.01 (15) | N5—C11—N4 | 114.34 (13) |
| C1—C2—H2 | 115.8 (10) | N5—C11—H11 | 126.6 (10) |
| C3—C2—H2 | 124.1 (10) | N4—C11—H11 | 119.1 (10) |
| C4—C3—C2 | 120.65 (14) | C13—C12—N5 | 130.10 (13) |
| C4—C3—H3 | 120.6 (12) | C13—C12—C17 | 119.86 (14) |
| C2—C3—H3 | 118.8 (12) | N5—C12—C17 | 110.04 (12) |
| C3—C4—C5 | 119.56 (15) | C14—C13—C12 | 117.79 (15) |
| C3—C4—H4 | 121.5 (12) | C14—C13—H13 | 120.8 (11) |
| C5—C4—H4 | 119.0 (12) | C12—C13—H13 | 121.4 (11) |
| C4—C5—C6 | 120.22 (15) | C13—C14—C15 | 121.59 (16) |
| C4—C5—H5 | 118.9 (12) | C13—C14—H14 | 118.7 (12) |
| C6—C5—H5 | 120.9 (12) | C15—C14—H14 | 119.7 (12) |
| C5—C6—C1 | 120.47 (14) | C16—C15—C14 | 121.96 (15) |
| C5—C6—H6 | 118.9 (11) | C16—C15—H15 | 116.0 (13) |
| C1—C6—H6 | 120.7 (11) | C14—C15—H15 | 122.1 (13) |
| N1—C7—C1 | 112.61 (12) | C15—C16—C17 | 116.42 (15) |
| N1—C7—H7A | 106.8 (11) | C15—C16—H16 | 123.4 (12) |
| C1—C7—H7A | 110.3 (11) | C17—C16—H16 | 120.2 (12) |
| N1—C7—H7B | 103.3 (11) | N4—C17—C16 | 132.69 (14) |
| C1—C7—H7B | 112.0 (11) | N4—C17—C12 | 104.93 (12) |
| H7A—C7—H7B | 111.5 (15) | C16—C17—C12 | 122.38 (14) |
| | | | |
| C8—N1—N2—N3 | −0.05 (15) | N3—C9—C10—N4 | 74.92 (19) |
| C7—N1—N2—N3 | −178.06 (12) | C8—C9—C10—N4 | −104.13 (18) |
| N1—N2—N3—C9 | 0.14 (15) | C12—N5—C11—N4 | −0.66 (17) |
| C6—C1—C2—C3 | −0.1 (2) | C17—N4—C11—N5 | −0.01 (18) |
| C7—C1—C2—C3 | −179.06 (13) | C10—N4—C11—N5 | −179.34 (13) |
| C1—C2—C3—C4 | −0.8 (2) | C11—N5—C12—C13 | −178.60 (15) |
| C2—C3—C4—C5 | 0.8 (2) | C11—N5—C12—C17 | 1.07 (16) |
| C3—C4—C5—C6 | 0.1 (2) | N5—C12—C13—C14 | −179.81 (15) |
| C4—C5—C6—C1 | −1.0 (2) | C17—C12—C13—C14 | 0.5 (2) |
| C2—C1—C6—C5 | 1.1 (2) | C12—C13—C14—C15 | 0.1 (2) |

| | | | |
|---|---|---|---|
| C7—C1—C6—C5 | 179.97 (13) | C13—C14—C15—C16 | −0.4 (3) |
| C8—N1—C7—C1 | −94.48 (17) | C14—C15—C16—C17 | 0.2 (2) |
| N2—N1—C7—C1 | 83.11 (16) | C11—N4—C17—C16 | −179.96 (15) |
| C6—C1—C7—N1 | 62.58 (18) | C10—N4—C17—C16 | −0.6 (2) |
| C2—C1—C7—N1 | −118.51 (15) | C11—N4—C17—C12 | 0.66 (15) |
| N2—N1—C8—C9 | −0.06 (15) | C10—N4—C17—C12 | 179.99 (13) |
| C7—N1—C8—C9 | 177.71 (13) | C15—C16—C17—N4 | −178.83 (15) |
| N2—N3—C9—C8 | −0.18 (16) | C15—C16—C17—C12 | 0.5 (2) |
| N2—N3—C9—C10 | −179.41 (12) | C13—C12—C17—N4 | 178.63 (13) |
| N1—C8—C9—N3 | 0.14 (16) | N5—C12—C17—N4 | −1.09 (15) |
| N1—C8—C9—C10 | 179.30 (13) | C13—C12—C17—C16 | −0.8 (2) |
| C11—N4—C10—C9 | 76.8 (2) | N5—C12—C17—C16 | 179.45 (13) |
| C17—N4—C10—C9 | −102.42 (17) | | |

*Hydrogen-bond geometry (Å, º)*

Cg3 is the centroid of the C1–C6 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C7—H7*A*···N5$^{i}$ | 1.025 (19) | 2.59 (2) | 3.602 (2) | 170.2 (15) |
| C7—H7*B*···N5$^{ii}$ | 1.01 (2) | 2.66 (2) | 3.5076 (19) | 142.4 (14) |
| C8—H8···N2$^{iii}$ | 0.98 (2) | 2.44 (2) | 3.3228 (18) | 151.1 (17) |
| C16—H16···N3$^{iv}$ | 1.00 (2) | 2.69 (2) | 3.652 (2) | 161.2 (16) |
| C15—H15···*Cg*3$^{iv}$ | 0.99 (2) | 2.77 (2) | 3.6216 (18) | 143.9 (16) |

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