# organic compounds

# 2-(4-Phenyl-1*H*-1,2,3-triazol-1-yl)-*N*-(*p*-tolyl)acetamide

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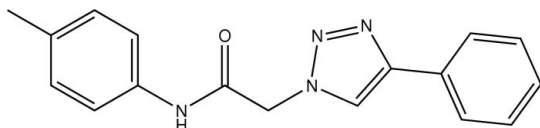
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In the title molecule, $C_{17}H_{16}N_4O$, the triazole ring makes dihedral angles of 29.00 (1) and 77.74 (1)°, respectively, with the phenyl and benzene rings. In the crystal structure, intermolecular N—H···O hydrogen bonds link the molecules into chains extending along the *c* axis.

## Related literature

For related literature, see: Kolb *et al.* (2001); Kolb & Sharpless (2003); Allen *et al.* (1987).



## Experimental

### Crystal data

$C_{17}H_{16}N_4O$
$M_r = 292.34$
Monoclinic, $P2_1/c$
$a = 5.5923$ (7) Å
$b = 30.438$ (4) Å
$c = 9.6112$ (10) Å
$\beta = 115.595$ (6)°

$V = 1475.5$ (3) Å$^3$
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.09$ mm$^{-1}$
$T = 293$ (2) K
$0.39 \times 0.26 \times 0.04$ mm

### Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.967$, $T_{max} = 0.997$

8229 measured reflections
2896 independent reflections
1970 reflections with $I > 2\sigma(I)$
$R_{int} = 0.038$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.136$
$S = 1.00$
2896 reflections

199 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.30$ e Å$^{-3}$
$\Delta\rho_{min} = -0.17$ e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
| --- | --- | --- | --- | --- |
| N4—H4A···O1$^i$ | 0.86 | 2.09 | 2.878 (3) | 152 |

Symmetry code: (i) $x, -y + \frac{3}{2}, z + \frac{1}{2}$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; 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: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

## References

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# supporting information

## 2-(4-Phenyl-1*H*-1,2,3-triazol-1-yl)-*N*-(*p*-tolyl)acetamide

Qing-Zhu Chu, Bao-Ping Qi and Xiao-Ru Zhang

### S1. Comment

The Huisgen 1,3-dipolar cycloaddition of alkynes with azides *via* Cu(I) catalysis is the most well known example of click chemistry (Kolb & Sharpless, 2003; Kolb *et al.*, 2001), which leads to the synthesis of 1,4-disubstituted 1,2,3-triazoles. In this study, a new 1,2,3-triazole derivative was prepared by such "click" reaction and its structure was characterized by X-ray crystallographic analysis.

In the title compound, (I), all bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The N1–N3/C7/C8 triazole ring makes dihedral angles of 29.00 (1) and 77.74 (1)° with C1–C6 and C11–C16 rings, respectively, and the dihedral angle between the latter two aromatic rings is 88.00 (1)°.
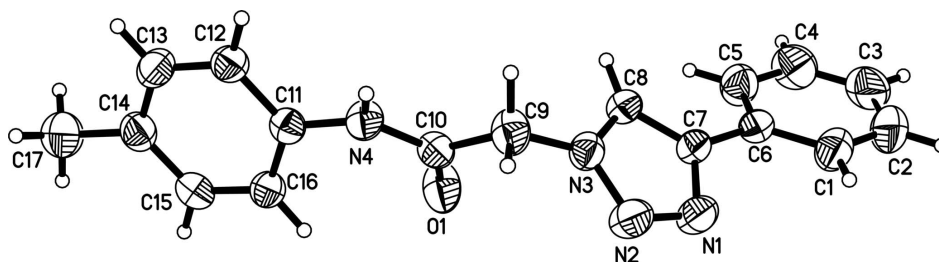
In the crystal, intermolecular N—H···O hydrogen bond (Table 1) link the molecules into chains extended along *c* axis.
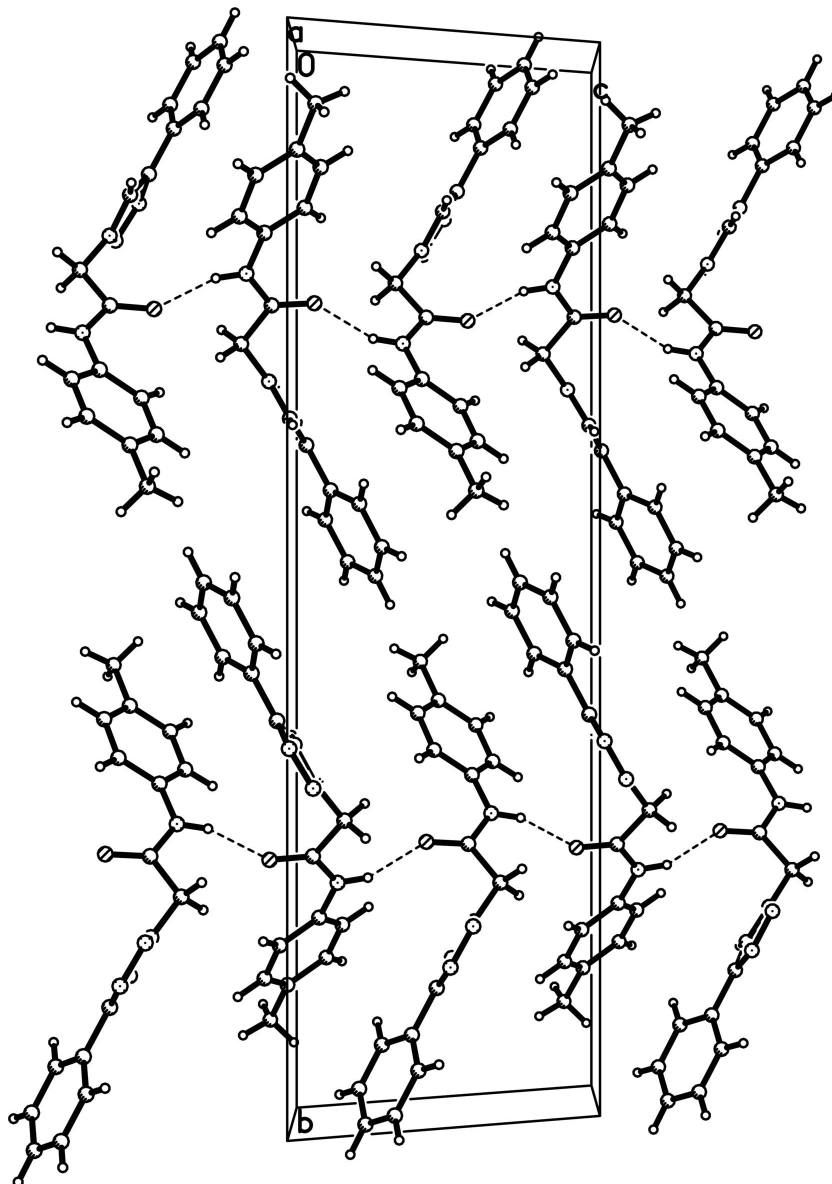
### S2. Experimental

To a solution of 4-methylaniline (2.61 g, 24.36 mmol), triethylamine (3.05 ml, 21.92 mmol) in dry $CH_2Cl_2$ (90 ml), chloroacetyl chloride (1.74 ml, 21.92 mmol) in dry $CH_2Cl_2$ (10 ml) was added dropwisely at 273 K under an inert atmosphere. The mixture was stirred at r.t. for 5 h, followed by dilution with $CH_2Cl_2$ (50 ml). Then washed by water for three times and the organic phase was dried over anhydrous sodium sulfate. After removal of the solvents *in vacuo*, 2-chloro-*N*-(4-methylphenyl)acetamide (3.82 g, 94.76%) was obtain. To a solution of 2-chloro-*N*-(4-methylxyphenyl)-acetamide (1.72 g, 9.37 mmol) in 50 ml DMF/$H_2O$ (1:1, *v/v*), $NaN_3$ (0.79 g, 12.15 mmol), phenylacetylene (3.08 ml, 28.08 mmol), $CuSO_4.5H_2O$ (0.24 g, 0.94 mmol), *L*-Ascorbic acid sodium salt (0.37 g, 1.87 mmol) were added successively. The mixture was stirred at 333 K for 36 h. Then $NH_3.H_2O$ (25 ml) was added, and the solvent was extracted with ethyl acetate, washed with water for three times. The organic phase was dried over anhydrous $Na_2SO_4$. After evaporation, the resulting solid was recrystallized from ethyl acetate, yielding the title compound (I) (2.13 g, 77.9%). Colourless single crystals suitable for X-ray crystallographic analysis were grown by slow evaporation of ethyl acetate.

### S3. Refinement

All H atoms were located in difference Fourier maps, placed in idealized positions (C—H 0.93–0.97 Å, N—H 0.86 Å) and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2–1.5U_{eq}$ of the parent atom.

**Figure 1**

The molecular structure of (I) showing 50% probability displacement ellipsoids and the atom numbering scheme.



**Figure 2**

A packing diagram of (I), viewed down the *a* axis. Dashed lines denote N—H⋯O hydrogen bonds.

**2-(4-Phenyl-1*H*-1,2,3-triazol-1-yl)-*N*-(*p*-tolyl)acetamide**

*Crystal data*

| | |
|---|---|
| $C_{17}H_{16}N_4O$ | $F(000) = 616$ |
| $M_r = 292.34$ | $D_x = 1.316$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 5.5923$ (7) Å | Cell parameters from 1236 reflections |
| $b = 30.438$ (4) Å | $\theta = 2.4–21.9°$ |
| $c = 9.6112$ (10) Å | $\mu = 0.09$ mm$^{-1}$ |
| $\beta = 115.595$ (6)° | $T = 293$ K |
| $V = 1475.5$ (3) Å$^3$ | Plate, colourless |
| $Z = 4$ | $0.39 \times 0.26 \times 0.04$ mm |

*Data collection*

| | |
|---|---|
| Siemens SMART 1000 CCD area-detector diffractometer | 8229 measured reflections |
| | 2896 independent reflections |
| Radiation source: fine-focus sealed tube | 1970 reflections with $I > 2\sigma(I)$ |
| Graphite monochromator | $R_{int} = 0.039$ |
| Detector resolution: 8.33 pixels mm$^{-1}$ | $\theta_{max} = 26.1°$, $\theta_{min} = 2.4°$ |
| $\omega$ scans | $h = -6\rightarrow6$ |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | $k = -37\rightarrow33$ |
| | $l = -9\rightarrow11$ |
| $T_{min} = 0.967$, $T_{max} = 0.997$ | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | |
| $R[F^2 > 2\sigma(F^2)] = 0.056$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.136$ | |
| $S = 1.01$ | H-atom parameters constrained |
| 2896 reflections | $w = 1/[\sigma^2(F_o^2) + (0.0529P)^2 + 0.5144P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 199 parameters | |
| 0 restraints | $(\Delta/\sigma)_{max} < 0.001$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{max} = 0.30$ e Å$^{-3}$ |
| | $\Delta\rho_{min} = -0.17$ e Å$^{-3}$ |

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N4 | 0.5557 (4) | 0.72043 (6) | 0.6455 (2) | 0.0390 (5) |
| H4A | 0.6141 | 0.7249 | 0.7431 | 0.047* |
| N3 | 0.9051 (4) | 0.81474 (6) | 0.5865 (2) | 0.0386 (5) |
| O1 | 0.5915 (4) | 0.74454 (5) | 0.43200 (19) | 0.0558 (5) |

| | | | |
|---|---|---|---|
| C7 | 0.9236 (4) | 0.87351 (7) | 0.4663 (3) | 0.0372 (5) |
| N1 | 1.1547 (4) | 0.85049 (7) | 0.5105 (2) | 0.0481 (5) |
| N2 | 1.1417 (4) | 0.81467 (7) | 0.5828 (2) | 0.0495 (6) |
| C11 | 0.3715 (4) | 0.68575 (7) | 0.5825 (2) | 0.0348 (5) |
| C8 | 0.7636 (5) | 0.85028 (7) | 0.5150 (3) | 0.0385 (6) |
| H8A | 0.5935 | 0.8576 | 0.5014 | 0.046* |
| C16 | 0.3509 (5) | 0.66145 (7) | 0.4563 (3) | 0.0383 (6) |
| H16A | 0.4596 | 0.6679 | 0.4081 | 0.046* |
| C12 | 0.2094 (5) | 0.67507 (8) | 0.6535 (3) | 0.0412 (6) |
| H12A | 0.2224 | 0.6909 | 0.7393 | 0.049* |
| C10 | 0.6489 (5) | 0.74713 (7) | 0.5694 (3) | 0.0373 (6) |
| C15 | 0.1688 (5) | 0.62767 (7) | 0.4016 (3) | 0.0422 (6) |
| H15A | 0.1568 | 0.6117 | 0.3164 | 0.051* |
| C6 | 0.8802 (5) | 0.91601 (8) | 0.3866 (3) | 0.0409 (6) |
| C14 | 0.0036 (5) | 0.61689 (8) | 0.4702 (3) | 0.0445 (6) |
| C13 | 0.0295 (5) | 0.64126 (8) | 0.5975 (3) | 0.0465 (6) |
| H13A | −0.0775 | 0.6346 | 0.6465 | 0.056* |
| C9 | 0.8423 (5) | 0.78126 (8) | 0.6729 (3) | 0.0474 (6) |
| H9A | 0.7666 | 0.7952 | 0.7355 | 0.057* |
| H9B | 1.0047 | 0.7667 | 0.7420 | 0.057* |
| C5 | 0.6276 (5) | 0.92969 (9) | 0.2884 (3) | 0.0533 (7) |
| H5A | 0.4834 | 0.9117 | 0.2715 | 0.064* |
| C1 | 1.0916 (6) | 0.94323 (9) | 0.4090 (3) | 0.0557 (7) |
| H1B | 1.2632 | 0.9345 | 0.4743 | 0.067* |
| C4 | 0.5868 (6) | 0.96997 (10) | 0.2147 (4) | 0.0668 (8) |
| H4B | 0.4158 | 0.9788 | 0.1487 | 0.080* |
| C3 | 0.7971 (7) | 0.99692 (10) | 0.2385 (4) | 0.0690 (9) |
| H3A | 0.7693 | 1.0241 | 0.1900 | 0.083* |
| C2 | 1.0483 (7) | 0.98348 (9) | 0.3341 (4) | 0.0694 (9) |
| H2B | 1.1918 | 1.0015 | 0.3492 | 0.083* |
| C17 | −0.1951 (6) | 0.58006 (9) | 0.4079 (4) | 0.0701 (9) |
| H17A | −0.1834 | 0.5672 | 0.3198 | 0.105* |
| H17B | −0.3706 | 0.5914 | 0.3780 | 0.105* |
| H17C | −0.1578 | 0.5581 | 0.4862 | 0.105* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N4 | 0.0487 (12) | 0.0423 (11) | 0.0276 (10) | −0.0047 (9) | 0.0180 (9) | −0.0002 (9) |
| N3 | 0.0409 (12) | 0.0390 (11) | 0.0379 (11) | −0.0043 (9) | 0.0190 (9) | 0.0001 (9) |
| O1 | 0.0874 (14) | 0.0507 (11) | 0.0314 (10) | −0.0180 (10) | 0.0277 (10) | −0.0014 (8) |
| C7 | 0.0375 (13) | 0.0394 (13) | 0.0394 (13) | −0.0022 (10) | 0.0210 (11) | −0.0007 (10) |
| N1 | 0.0435 (13) | 0.0523 (13) | 0.0560 (14) | 0.0042 (10) | 0.0285 (11) | 0.0084 (11) |
| N2 | 0.0462 (13) | 0.0533 (13) | 0.0556 (14) | 0.0078 (10) | 0.0283 (11) | 0.0093 (11) |
| C11 | 0.0370 (13) | 0.0343 (12) | 0.0314 (12) | 0.0033 (10) | 0.0131 (10) | 0.0036 (10) |
| C8 | 0.0334 (13) | 0.0410 (13) | 0.0440 (14) | −0.0011 (11) | 0.0194 (11) | −0.0024 (11) |
| C16 | 0.0424 (14) | 0.0383 (13) | 0.0363 (13) | 0.0012 (11) | 0.0191 (11) | 0.0034 (10) |
| C12 | 0.0489 (15) | 0.0392 (13) | 0.0403 (14) | 0.0035 (11) | 0.0238 (12) | 0.0031 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C10 | 0.0469 (14) | 0.0344 (13) | 0.0319 (13) | 0.0023 (10) | 0.0184 (11) | 0.0016 (10) |
| C15 | 0.0456 (15) | 0.0372 (13) | 0.0407 (14) | 0.0042 (11) | 0.0157 (12) | −0.0029 (11) |
| C6 | 0.0460 (14) | 0.0402 (13) | 0.0451 (14) | −0.0018 (11) | 0.0279 (12) | −0.0018 (11) |
| C14 | 0.0394 (14) | 0.0376 (13) | 0.0536 (16) | 0.0006 (11) | 0.0175 (12) | 0.0011 (12) |
| C13 | 0.0439 (15) | 0.0489 (15) | 0.0532 (16) | 0.0009 (12) | 0.0270 (13) | 0.0072 (13) |
| C9 | 0.0616 (17) | 0.0450 (15) | 0.0367 (14) | −0.0083 (12) | 0.0221 (13) | 0.0006 (12) |
| C5 | 0.0494 (16) | 0.0478 (16) | 0.0624 (18) | 0.0007 (12) | 0.0239 (14) | 0.0063 (13) |
| C1 | 0.0520 (17) | 0.0538 (17) | 0.0674 (19) | −0.0052 (13) | 0.0315 (15) | 0.0039 (14) |
| C4 | 0.069 (2) | 0.0564 (18) | 0.073 (2) | 0.0146 (16) | 0.0296 (18) | 0.0155 (16) |
| C3 | 0.096 (3) | 0.0428 (16) | 0.085 (2) | 0.0112 (17) | 0.056 (2) | 0.0156 (16) |
| C2 | 0.078 (2) | 0.0487 (17) | 0.097 (2) | −0.0096 (16) | 0.052 (2) | 0.0070 (17) |
| C17 | 0.065 (2) | 0.0576 (18) | 0.095 (2) | −0.0155 (15) | 0.0414 (19) | −0.0156 (17) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N4—C10 | 1.341 (3) | C15—H15A | 0.9300 |
| N4—C11 | 1.415 (3) | C6—C5 | 1.381 (3) |
| N4—H4A | 0.8600 | C6—C1 | 1.382 (3) |
| N3—N2 | 1.339 (3) | C14—C13 | 1.384 (3) |
| N3—C8 | 1.341 (3) | C14—C17 | 1.508 (3) |
| N3—C9 | 1.450 (3) | C13—H13A | 0.9300 |
| O1—C10 | 1.219 (3) | C9—H9A | 0.9700 |
| C7—N1 | 1.367 (3) | C9—H9B | 0.9700 |
| C7—C8 | 1.372 (3) | C5—C4 | 1.385 (4) |
| C7—C6 | 1.469 (3) | C5—H5A | 0.9300 |
| N1—N2 | 1.312 (3) | C1—C2 | 1.388 (4) |
| C11—C16 | 1.383 (3) | C1—H1B | 0.9300 |
| C11—C12 | 1.388 (3) | C4—C3 | 1.370 (4) |
| C8—H8A | 0.9300 | C4—H4B | 0.9300 |
| C16—C15 | 1.381 (3) | C3—C2 | 1.368 (4) |
| C16—H16A | 0.9300 | C3—H3A | 0.9300 |
| C12—C13 | 1.376 (3) | C2—H2B | 0.9300 |
| C12—H12A | 0.9300 | C17—H17A | 0.9600 |
| C10—C9 | 1.520 (3) | C17—H17B | 0.9600 |
| C15—C14 | 1.386 (3) | C17—H17C | 0.9600 |
| | | | |
| C10—N4—C11 | 126.96 (19) | C13—C14—C17 | 121.8 (2) |
| C10—N4—H4A | 116.5 | C15—C14—C17 | 121.0 (2) |
| C11—N4—H4A | 116.5 | C12—C13—C14 | 121.8 (2) |
| N2—N3—C8 | 111.02 (18) | C12—C13—H13A | 119.1 |
| N2—N3—C9 | 120.0 (2) | C14—C13—H13A | 119.1 |
| C8—N3—C9 | 128.7 (2) | N3—C9—C10 | 112.66 (19) |
| N1—C7—C8 | 107.4 (2) | N3—C9—H9A | 109.1 |
| N1—C7—C6 | 122.3 (2) | C10—C9—H9A | 109.1 |
| C8—C7—C6 | 130.3 (2) | N3—C9—H9B | 109.1 |
| N2—N1—C7 | 109.24 (18) | C10—C9—H9B | 109.1 |
| N1—N2—N3 | 107.11 (19) | H9A—C9—H9B | 107.8 |
| C16—C11—C12 | 118.8 (2) | C6—C5—C4 | 120.7 (3) |

| | | | |
|---|---|---|---|
| C16—C11—N4 | 123.0 (2) | C6—C5—H5A | 119.7 |
| C12—C11—N4 | 118.3 (2) | C4—C5—H5A | 119.7 |
| N3—C8—C7 | 105.3 (2) | C6—C1—C2 | 120.2 (3) |
| N3—C8—H8A | 127.4 | C6—C1—H1B | 119.9 |
| C7—C8—H8A | 127.4 | C2—C1—H1B | 119.9 |
| C15—C16—C11 | 120.0 (2) | C3—C4—C5 | 120.3 (3) |
| C15—C16—H16A | 120.0 | C3—C4—H4B | 119.8 |
| C11—C16—H16A | 120.0 | C5—C4—H4B | 119.8 |
| C13—C12—C11 | 120.3 (2) | C2—C3—C4 | 119.5 (3) |
| C13—C12—H12A | 119.8 | C2—C3—H3A | 120.3 |
| C11—C12—H12A | 119.8 | C4—C3—H3A | 120.3 |
| O1—C10—N4 | 124.7 (2) | C3—C2—C1 | 120.7 (3) |
| O1—C10—C9 | 122.2 (2) | C3—C2—H2B | 119.6 |
| N4—C10—C9 | 113.05 (19) | C1—C2—H2B | 119.6 |
| C16—C15—C14 | 121.9 (2) | C14—C17—H17A | 109.5 |
| C16—C15—H15A | 119.0 | C14—C17—H17B | 109.5 |
| C14—C15—H15A | 119.0 | H17A—C17—H17B | 109.5 |
| C5—C6—C1 | 118.6 (2) | C14—C17—H17C | 109.5 |
| C5—C6—C7 | 120.8 (2) | H17A—C17—H17C | 109.5 |
| C1—C6—C7 | 120.6 (2) | H17B—C17—H17C | 109.5 |
| C13—C14—C15 | 117.2 (2) | | |

| | | | |
|---|---|---|---|
| C8—C7—N1—N2 | 0.1 (3) | N1—C7—C6—C1 | −27.7 (3) |
| C6—C7—N1—N2 | 178.1 (2) | C8—C7—C6—C1 | 149.7 (3) |
| C7—N1—N2—N3 | −0.5 (3) | C16—C15—C14—C13 | −0.5 (4) |
| C8—N3—N2—N1 | 0.7 (3) | C16—C15—C14—C17 | 179.6 (2) |
| C9—N3—N2—N1 | −173.9 (2) | C11—C12—C13—C14 | 0.0 (4) |
| C10—N4—C11—C16 | 30.6 (3) | C15—C14—C13—C12 | 0.6 (4) |
| C10—N4—C11—C12 | −151.1 (2) | C17—C14—C13—C12 | −179.5 (2) |
| N2—N3—C8—C7 | −0.7 (3) | N2—N3—C9—C10 | −106.1 (2) |
| C9—N3—C8—C7 | 173.4 (2) | C8—N3—C9—C10 | 80.4 (3) |
| N1—C7—C8—N3 | 0.3 (3) | O1—C10—C9—N3 | 11.7 (3) |
| C6—C7—C8—N3 | −177.4 (2) | N4—C10—C9—N3 | −169.56 (19) |
| C12—C11—C16—C15 | 0.9 (3) | C1—C6—C5—C4 | −0.5 (4) |
| N4—C11—C16—C15 | 179.2 (2) | C7—C6—C5—C4 | 179.3 (2) |
| C16—C11—C12—C13 | −0.8 (3) | C5—C6—C1—C2 | 0.3 (4) |
| N4—C11—C12—C13 | −179.2 (2) | C7—C6—C1—C2 | −179.5 (2) |
| C11—N4—C10—O1 | −1.9 (4) | C6—C5—C4—C3 | −0.1 (4) |
| C11—N4—C10—C9 | 179.3 (2) | C5—C4—C3—C2 | 0.9 (5) |
| C11—C16—C15—C14 | −0.2 (4) | C4—C3—C2—C1 | −1.0 (5) |
| N1—C7—C6—C5 | 152.5 (2) | C6—C1—C2—C3 | 0.5 (4) |
| C8—C7—C6—C5 | −30.1 (4) | | |

*Hydrogen-bond geometry (Å, º)*

| D—H···A | D—H | H···A | D···A | D—H···A |
|---|---|---|---|---|
| | | | | |

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|---|---|---|---|---|
| N4—H4*A*⋯O1[i] | 0.86 | 2.09 | 2.878 (3) | 152 |

Symmetry code: (i) $x$, $-y+3/2$, $z+1/2$.