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# 2-[(1*S*,3*S*)-3-Acetyl-2,2-dimethylcyclobutyl]-*N*-(*m*-tolyl)acetamide

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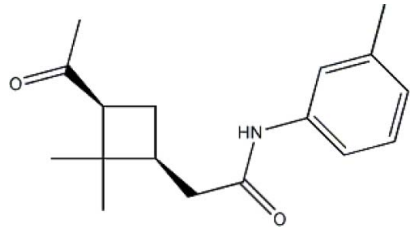
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.073; $wR$ factor = 0.170; data-to-parameter ratio = 17.2.

The title compound, $C_{17}H_{23}NO_2$, contains two chiral centres and was synthesized from 2-(3-acetyl-2,2-dimethylcyclobutyl)acetic acid and *m*-toluidine. The cyclobutane ring is not flat but flexed as though folded from the dimethyl-substituted C atom to the unsubstituted C atom, with a dihedral angle of 25.9°. The crystal structure is stabilized by N—H···O and C—H···O hydrogen-bonding interactions.

## Related literature

For related literature, see: Mitra & Khanra (1977); Yin *et al.* (2007).




## Experimental

### *Crystal data*

$C_{17}H_{23}NO_2$
$M_r$ = 273.36
Orthorhombic, *Pbca*
$a$ = 12.513 (3) Å
$b$ = 9.5190 (19) Å
$c$ = 26.844 (5) Å
$V$ = 3197.4 (11) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.07 mm$^{-1}$
$T$ = 293 (2) K
0.40 × 0.20 × 0.20 mm

### *Data collection*

Enraf–Nonius CAD-4 diffractometer
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.951, $T_{max}$ = 0.975
3150 measured reflections
3120 independent reflections
1385 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.032
3 standard reflections
every 200 reflections
intensity decay: none

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.073
$wR(F^2)$ = 0.170
$S$ = 1.04
3120 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.14 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N—H0$A$···O2$^{i}$ | 0.86 | 2.04 | 2.892 (4) | 169 |
| C12—H12$A$···O2 | 0.93 | 2.49 | 2.931 (5) | 109 |
| C13—H13$A$···O1$^{ii}$ | 0.93 | 2.55 | 3.440 (5) | 161 |

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); 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: AT2522).

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# supporting information

*Acta Cryst.* (2008). E**64**, o291 [https://doi.org/10.1107/S160053680706641X]

## 2-[(1*S*,3*S*)-3-Acetyl-2,2-dimethylcyclobutyl]-*N*-(*m*-tolyl)acetamide

**Yan-Bai Yin, Zhan-Qian Song, Zong-De Wang and Shi-Bin Shang**

### S1. Comment

Terpenes are convenient chiral precursors due to their availability and low cost, and among them, a-pinene (both enantiomers) and verbenone are prominent. For instance, pinene has been used as starting material for the production of some compounds of industrial interest (Mitra & Khanra, 1977). Chiral cyclobutane compound, pinonic acid, can be synthesized from a-pinene. Many derivatives of pinonic acid have interesting biological properties. So we synthesized several derivatives of pinonic acid. In our previous paper we have reported the crystal structure of 2-[(1*S*,3S)-3-acetyl-2,2-dimethylcyclobutyl]-*N*-(2,6-difluorophenyl) acetamide (Yin *et al.*, 2007). Now we synthesized the title compound (I) and report here its crystal structure.

The molecular structure of (I) is shown in Fig. 1. A l l bond lengths and angles are normal. The crystal structure is stabilized by N—H···O and C—H···O hydrogen bonding interactions (Table 1).

### S2. Experimental

The title compound was synthesized from *m*-toluidine and 2-(3-acetyl-2,2-dimethylcyclobutyl) acetyl chloride at room temperature. The acetyl chloride was obtained using 2-(3-acetyl-2,2-dimethylcyclobutyl)acetic acid (pinonic acid), thionyl chloride as raw materials and dichloromethane as solvent. Pinonic acid (27 mmol) and thionyl chloride (32 mmol) were dissolved in dichloromethane (50 ml). The resulting mixture was refluxed for 8 h. After refluxing the solvent was distilled away under vacuum and the remainder was 2-(3-acetyl-2,2-dimethylcyclobutyl)acetyl chloride. The acetyl chloride reacted with *m*-toluidine (27 mmol) for 24 h using dichloromethane as solvent. After the reaction was complete the solvent was distilled away and the crude title compound was gained. The pure compound was obtained by crystallizing from a mixture of ethanol (40 ml) and water (40 ml). Crystals of the title compound suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

### S3. Refinement

All H atoms were placed geometrically, with the C—H distances in the range 0.93–0.98 Å and N—H = 0.86 Å, and included in the refinement in riding motion approximation with $U_{iso}$(H) = 1.2 or 1.5$U_{eq}$(H) of the carrier atom.

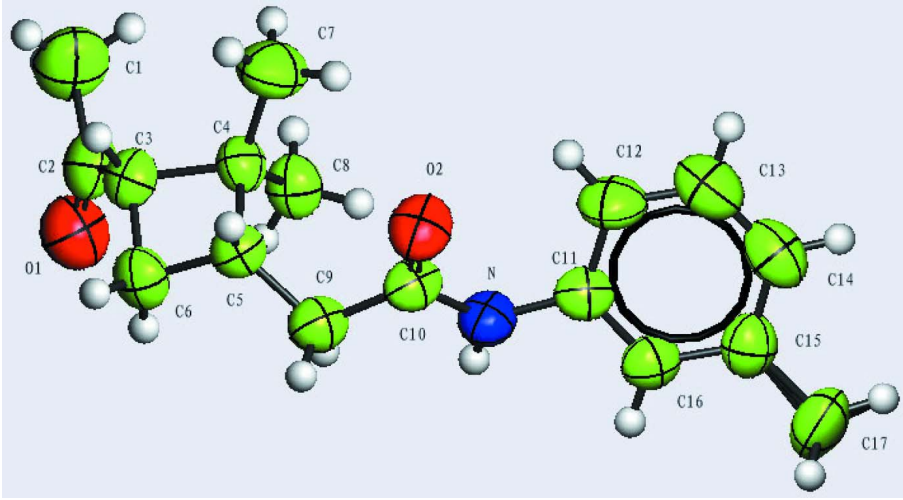


**Figure 1**

A view of the molecular structure of (I), showing displacement ellipsoids at the 50% probability level.

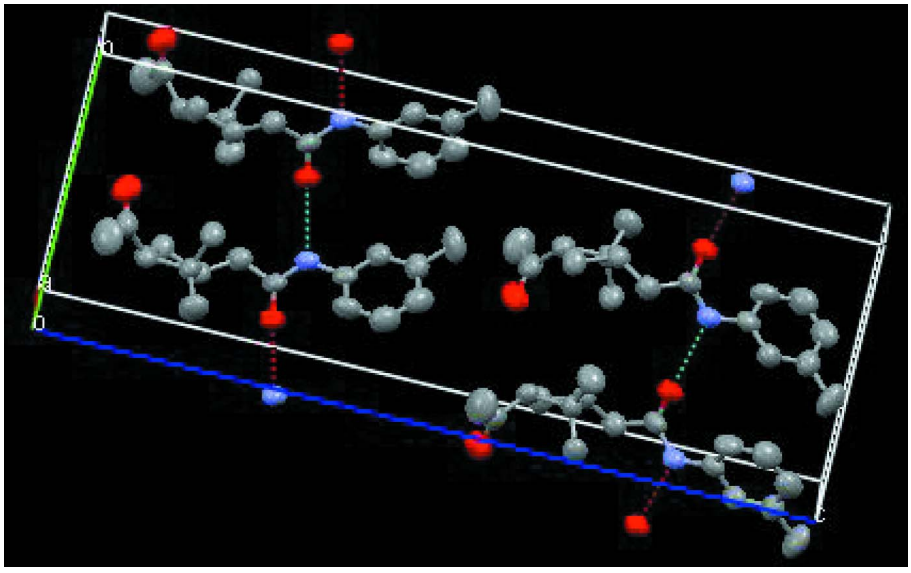

**Figure 2**

A view of the packing and N—H···O hydrogen bondings (dash lines) of the title compound.

**2-[(1*S*,3*S*)-3-Acetyl-2,2-dimethylcyclobutyl]-*N*-(*m*- tolyl)acetamide**

*Crystal data*

$C_{17}H_{23}NO_2$
$M_r = 273.36$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 12.513\ (3)$ Å
$b = 9.5190\ (19)$ Å
$c = 26.844\ (5)$ Å
$V = 3197.4\ (11)$ Å$^3$
$Z = 8$
$F(000) = 1184$
$D_x = 1.136$ Mg m$^{-3}$
Melting point: 367 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 8–13°$
$\mu = 0.07$ mm$^{-1}$
$T = 293$ K
Quadrate, colourless
0.40 × 0.20 × 0.20 mm

*Data collection*

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.951, $T_{max}$ = 0.975
3150 measured reflections
3120 independent reflections
1385 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.032
$\theta_{max}$ = 26.0°, $\theta_{min}$ = 1.5°
$h$ = 0→15
$k$ = 0→11
$l$ = 0→32
3 standard reflections every 200 reflections
intensity decay: none

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.073
$wR(F^2)$ = 0.170
$S$ = 1.04
3120 reflections
181 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
$w = 1/[\sigma^2(F_o^2) + (0.05P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.14 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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N | 0.7095 (2) | 0.0658 (3) | 0.68825 (10) | 0.0721 (8) |
| H0A | 0.7277 | −0.0171 | 0.6977 | 0.087* |
| O1 | 0.6178 (2) | −0.0407 (3) | 0.92753 (10) | 0.1064 (9) |
| C1 | 0.4701 (3) | 0.1175 (5) | 0.93668 (16) | 0.1272 (16) |
| H1A | 0.4414 | 0.0449 | 0.9576 | 0.191* |
| H1B | 0.4227 | 0.1333 | 0.9091 | 0.191* |
| H1C | 0.4774 | 0.2026 | 0.9556 | 0.191* |
| O2 | 0.7021 (2) | 0.2940 (2) | 0.71316 (9) | 0.0883 (8) |
| C2 | 0.5782 (3) | 0.0728 (4) | 0.91735 (14) | 0.0830 (11) |
| C3 | 0.6333 (3) | 0.1758 (3) | 0.88408 (12) | 0.0684 (9) |
| H3A | 0.6270 | 0.2708 | 0.8978 | 0.082* |
| C4 | 0.5977 (3) | 0.1749 (3) | 0.82785 (11) | 0.0643 (9) |
| C5 | 0.7192 (2) | 0.1983 (3) | 0.81526 (11) | 0.0642 (8) |
| H5A | 0.7331 | 0.2993 | 0.8128 | 0.077* |
| C6 | 0.7475 (3) | 0.1488 (4) | 0.86728 (11) | 0.0777 (10) |

| | | | | |
|---|---|---|---|---|
| H6A | 0.7682 | 0.0507 | 0.8688 | 0.093* |
| H6B | 0.7999 | 0.2077 | 0.8838 | 0.093* |
| C7 | 0.5230 (3) | 0.2938 (4) | 0.81276 (14) | 0.1015 (13) |
| H7A | 0.4510 | 0.2698 | 0.8216 | 0.152* |
| H7B | 0.5274 | 0.3081 | 0.7774 | 0.152* |
| H7C | 0.5435 | 0.3784 | 0.8297 | 0.152* |
| C8 | 0.5565 (3) | 0.0333 (3) | 0.81108 (12) | 0.0782 (10) |
| H8A | 0.4824 | 0.0246 | 0.8197 | 0.117* |
| H8B | 0.5966 | −0.0397 | 0.8272 | 0.117* |
| H8C | 0.5645 | 0.0249 | 0.7756 | 0.117* |
| C9 | 0.7689 (3) | 0.1250 (3) | 0.77045 (12) | 0.0771 (10) |
| H9A | 0.8452 | 0.1427 | 0.7705 | 0.092* |
| H9B | 0.7584 | 0.0245 | 0.7738 | 0.092* |
| C10 | 0.7236 (3) | 0.1716 (3) | 0.72154 (12) | 0.0662 (9) |
| C11 | 0.6677 (3) | 0.0789 (3) | 0.63926 (13) | 0.0650 (9) |
| C12 | 0.5888 (3) | 0.1753 (3) | 0.62739 (16) | 0.0855 (11) |
| H12A | 0.5602 | 0.2353 | 0.6513 | 0.103* |
| C13 | 0.5545 (3) | 0.1783 (4) | 0.57870 (19) | 0.1012 (13) |
| H13A | 0.5033 | 0.2443 | 0.5698 | 0.121* |
| C14 | 0.5914 (3) | 0.0904 (4) | 0.54333 (16) | 0.0931 (12) |
| H14A | 0.5657 | 0.0978 | 0.5109 | 0.112* |
| C15 | 0.6686 (3) | −0.0127 (4) | 0.55487 (14) | 0.0801 (10) |
| C16 | 0.7049 (3) | −0.0140 (3) | 0.60417 (13) | 0.0723 (9) |
| H16A | 0.7559 | −0.0800 | 0.6135 | 0.087* |
| C17 | 0.7134 (3) | −0.1128 (5) | 0.51691 (14) | 0.1146 (14) |
| H17A | 0.6788 | −0.0977 | 0.4854 | 0.172* |
| H17B | 0.7011 | −0.2077 | 0.5276 | 0.172* |
| H17C | 0.7888 | −0.0971 | 0.5134 | 0.172* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N | 0.088 (2) | 0.0515 (15) | 0.077 (2) | 0.0067 (14) | 0.0022 (16) | 0.0046 (15) |
| O1 | 0.115 (2) | 0.099 (2) | 0.105 (2) | −0.0141 (18) | −0.0003 (17) | 0.0199 (17) |
| C1 | 0.085 (3) | 0.175 (4) | 0.122 (4) | −0.020 (3) | 0.026 (3) | −0.006 (3) |
| O2 | 0.124 (2) | 0.0526 (14) | 0.0881 (17) | −0.0010 (13) | 0.0038 (15) | 0.0082 (12) |
| C2 | 0.102 (3) | 0.079 (2) | 0.068 (2) | −0.015 (2) | −0.003 (2) | −0.007 (2) |
| C3 | 0.078 (2) | 0.0583 (18) | 0.069 (2) | −0.0117 (18) | 0.0023 (18) | −0.0043 (17) |
| C4 | 0.074 (2) | 0.0616 (19) | 0.057 (2) | −0.0020 (17) | −0.0052 (17) | 0.0061 (16) |
| C5 | 0.063 (2) | 0.0605 (19) | 0.070 (2) | −0.0078 (16) | 0.0058 (17) | 0.0026 (17) |
| C6 | 0.067 (2) | 0.092 (2) | 0.074 (2) | −0.0174 (18) | −0.0040 (19) | 0.006 (2) |
| C7 | 0.097 (3) | 0.098 (3) | 0.110 (3) | 0.025 (2) | 0.002 (2) | 0.015 (2) |
| C8 | 0.077 (2) | 0.081 (2) | 0.077 (2) | −0.0201 (19) | −0.0042 (19) | 0.0009 (19) |
| C9 | 0.080 (2) | 0.072 (2) | 0.079 (2) | 0.0042 (18) | 0.008 (2) | 0.0053 (19) |
| C10 | 0.078 (2) | 0.0522 (19) | 0.069 (2) | 0.0044 (18) | 0.0147 (18) | 0.0129 (19) |
| C11 | 0.067 (2) | 0.0499 (18) | 0.079 (2) | −0.0047 (16) | 0.0074 (19) | 0.0102 (19) |
| C12 | 0.084 (3) | 0.059 (2) | 0.113 (3) | 0.013 (2) | 0.001 (2) | −0.003 (2) |
| C13 | 0.090 (3) | 0.096 (3) | 0.117 (4) | 0.002 (3) | −0.022 (3) | 0.011 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C14 | 0.088 (3) | 0.090 (3) | 0.101 (3) | −0.015 (2) | −0.025 (2) | 0.014 (3) |
| C15 | 0.085 (3) | 0.085 (3) | 0.071 (3) | −0.012 (2) | 0.003 (2) | 0.000 (2) |
| C16 | 0.074 (2) | 0.068 (2) | 0.075 (2) | 0.0018 (19) | 0.012 (2) | 0.006 (2) |
| C17 | 0.109 (3) | 0.153 (4) | 0.081 (3) | 0.001 (3) | 0.017 (2) | −0.036 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N—C10 | 1.357 (4) | C7—H7B | 0.9600 |
| N—C11 | 1.421 (4) | C7—H7C | 0.9600 |
| N—H0A | 0.8600 | C8—H8A | 0.9600 |
| O1—C2 | 1.219 (4) | C8—H8B | 0.9600 |
| C1—C2 | 1.510 (5) | C8—H8C | 0.9600 |
| C1—H1A | 0.9600 | C9—C10 | 1.497 (4) |
| C1—H1B | 0.9600 | C9—H9A | 0.9700 |
| C1—H1C | 0.9600 | C9—H9B | 0.9700 |
| O2—C10 | 1.217 (3) | C11—C16 | 1.374 (4) |
| C2—C3 | 1.495 (4) | C11—C12 | 1.384 (4) |
| C3—C6 | 1.521 (4) | C12—C13 | 1.376 (5) |
| C3—C4 | 1.574 (4) | C12—H12A | 0.9300 |
| C3—H3A | 0.9800 | C13—C14 | 1.347 (5) |
| C4—C8 | 1.512 (4) | C13—H13A | 0.9300 |
| C4—C7 | 1.522 (4) | C14—C15 | 1.411 (5) |
| C4—C5 | 1.573 (4) | C14—H14A | 0.9300 |
| C5—C6 | 1.516 (4) | C15—C16 | 1.399 (4) |
| C5—C9 | 1.523 (4) | C15—C17 | 1.504 (5) |
| C5—H5A | 0.9800 | C16—H16A | 0.9300 |
| C6—H6A | 0.9700 | C17—H17A | 0.9600 |
| C6—H6B | 0.9700 | C17—H17B | 0.9600 |
| C7—H7A | 0.9600 | C17—H17C | 0.9600 |
| | | | |
| C10—N—C11 | 126.3 (3) | H7B—C7—H7C | 109.5 |
| C10—N—H0A | 116.9 | C4—C8—H8A | 109.5 |
| C11—N—H0A | 116.9 | C4—C8—H8B | 109.5 |
| C2—C1—H1A | 109.5 | H8A—C8—H8B | 109.5 |
| C2—C1—H1B | 109.5 | C4—C8—H8C | 109.5 |
| H1A—C1—H1B | 109.5 | H8A—C8—H8C | 109.5 |
| C2—C1—H1C | 109.5 | H8B—C8—H8C | 109.5 |
| H1A—C1—H1C | 109.5 | C10—C9—C5 | 113.7 (3) |
| H1B—C1—H1C | 109.5 | C10—C9—H9A | 108.8 |
| O1—C2—C3 | 121.8 (4) | C5—C9—H9A | 108.8 |
| O1—C2—C1 | 122.5 (4) | C10—C9—H9B | 108.8 |
| C3—C2—C1 | 115.7 (4) | C5—C9—H9B | 108.8 |
| C2—C3—C6 | 120.0 (3) | H9A—C9—H9B | 107.7 |
| C2—C3—C4 | 116.1 (3) | O2—C10—N | 124.0 (3) |
| C6—C3—C4 | 88.9 (2) | O2—C10—C9 | 121.9 (3) |
| C2—C3—H3A | 110.1 | N—C10—C9 | 114.0 (3) |
| C6—C3—H3A | 110.1 | C16—C11—C12 | 120.7 (4) |
| C4—C3—H3A | 110.1 | C16—C11—N | 116.9 (3) |

| | | | |
|---|---|---|---|
| C8—C4—C7 | 112.0 (3) | C12—C11—N | 122.3 (3) |
| C8—C4—C3 | 112.7 (3) | C13—C12—C11 | 117.0 (4) |
| C7—C4—C3 | 115.2 (3) | C13—C12—H12A | 121.5 |
| C8—C4—C5 | 113.0 (3) | C11—C12—H12A | 121.5 |
| C7—C4—C5 | 115.5 (3) | C14—C13—C12 | 123.4 (4) |
| C3—C4—C5 | 86.1 (2) | C14—C13—H13A | 118.3 |
| C6—C5—C9 | 119.3 (3) | C12—C13—H13A | 118.3 |
| C6—C5—C4 | 89.1 (2) | C13—C14—C15 | 120.8 (4) |
| C9—C5—C4 | 120.0 (3) | C13—C14—H14A | 119.6 |
| C6—C5—H5A | 108.9 | C15—C14—H14A | 119.6 |
| C9—C5—H5A | 108.9 | C16—C15—C14 | 115.9 (3) |
| C4—C5—H5A | 108.9 | C16—C15—C17 | 120.9 (4) |
| C3—C6—C5 | 90.0 (2) | C14—C15—C17 | 123.2 (4) |
| C3—C6—H6A | 113.6 | C11—C16—C15 | 122.2 (3) |
| C5—C6—H6A | 113.6 | C11—C16—H16A | 118.9 |
| C3—C6—H6B | 113.6 | C15—C16—H16A | 118.9 |
| C5—C6—H6B | 113.6 | C15—C17—H17A | 109.5 |
| H6A—C6—H6B | 110.9 | C15—C17—H17B | 109.5 |
| C4—C7—H7A | 109.5 | H17A—C17—H17B | 109.5 |
| C4—C7—H7B | 109.5 | C15—C17—H17C | 109.5 |
| H7A—C7—H7B | 109.5 | H17A—C17—H17C | 109.5 |
| C4—C7—H7C | 109.5 | H17B—C17—H17C | 109.5 |
| H7A—C7—H7C | 109.5 | | |

| | | | |
|---|---|---|---|
| O1—C2—C3—C6 | −7.8 (5) | C4—C5—C6—C3 | −18.5 (2) |
| C1—C2—C3—C6 | 173.1 (3) | C6—C5—C9—C10 | 172.5 (3) |
| O1—C2—C3—C4 | 97.1 (4) | C4—C5—C9—C10 | 64.8 (4) |
| C1—C2—C3—C4 | −82.0 (4) | C11—N—C10—O2 | −0.5 (5) |
| C2—C3—C4—C8 | −27.7 (4) | C11—N—C10—C9 | 179.7 (3) |
| C6—C3—C4—C8 | 95.5 (3) | C5—C9—C10—O2 | 40.0 (5) |
| C2—C3—C4—C7 | 102.6 (4) | C5—C9—C10—N | −140.2 (3) |
| C6—C3—C4—C7 | −134.3 (3) | C10—N—C11—C16 | 149.2 (3) |
| C2—C3—C4—C5 | −141.0 (3) | C10—N—C11—C12 | −34.2 (5) |
| C6—C3—C4—C5 | −17.8 (2) | C16—C11—C12—C13 | −3.5 (5) |
| C8—C4—C5—C6 | −95.2 (3) | N—C11—C12—C13 | −180.0 (3) |
| C7—C4—C5—C6 | 134.0 (3) | C11—C12—C13—C14 | 2.1 (6) |
| C3—C4—C5—C6 | 17.9 (2) | C12—C13—C14—C15 | 0.5 (6) |
| C8—C4—C5—C9 | 28.6 (4) | C13—C14—C15—C16 | −1.6 (5) |
| C7—C4—C5—C9 | −102.2 (3) | C13—C14—C15—C17 | −179.5 (4) |
| C3—C4—C5—C9 | 141.7 (3) | C12—C11—C16—C15 | 2.5 (5) |
| C2—C3—C6—C5 | 138.2 (3) | N—C11—C16—C15 | 179.1 (3) |
| C4—C3—C6—C5 | 18.5 (2) | C14—C15—C16—C11 | 0.2 (5) |
| C9—C5—C6—C3 | −142.9 (3) | C17—C15—C16—C11 | 178.1 (3) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N—H0*A*···O2$^{i}$ | 0.86 | 2.04 | 2.892 (4) | 169 |

| | | | | |
|---|---|---|---|---|
| C12—H12*A*···O2 | 0.93 | 2.49 | 2.931 (5) | 109 |
| C13—H13*A*···O1$^{ii}$ | 0.93 | 2.55 | 3.440 (5) | 161 |

Symmetry codes: (i) *x*+1, −*y*−3/2, *z*−1/2; (ii) *x*+3/2, −*y*+1/2, −*z*+1.