



# Crystal structure of (4-hydroxypiperidin-1-yl)(4-methylphenyl)methanone

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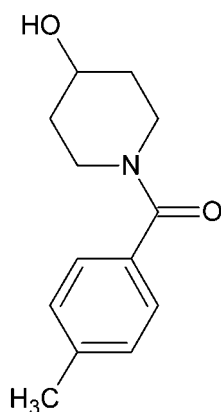
In the title compound, C<sub>13</sub>H<sub>17</sub>NO<sub>2</sub>, the dihedral angle between the planes of the piperidine and benzene rings is 51.7 (2)°. The bond-angle sum around the N atom [359.8 (3)°] indicates *sp*<sup>2</sup> hybridization of the atom. In the crystal, O—H...O hydrogen bonds link the molecules, forming chains along [001].

**Keywords:** crystal structure; piperidine derivative; hydrogen bonding.

**CCDC reference:** 1428660

## 1. Related literature

For the biological activity of piperidine derivatives, see: Pissamitski *et al.* (2007); Katritzky *et al.* (1995); Dimmock *et al.* (2001); Watson *et al.* (2000); Thomas *et al.* (1998); Sambath *et al.* (2004). For related structures, see: Revathi *et al.* (2015); Prathebha *et al.* (2015). For the synthesis, see: Revathi *et al.* (2015).



## 2. Experimental

### 2.1. Crystal data

|   |                                      |
|---|--------------------------------------|
| C <sub>13</sub> H <sub>17</sub> NO <sub>2</sub> | <i>V</i> = 1216.3 (4) Å <sup>3</sup> |
| <i>M<sub>r</sub></i> = 219.28                   | <i>Z</i> = 4                         |
| Orthorhombic, <i>Pca</i> 2 <sub>1</sub>         | Mo <i>K</i> α radiation              |
| <i>a</i> = 23.933 (5) Å                         | <i>μ</i> = 0.08 mm <sup>-1</sup>     |
| <i>b</i> = 6.3317 (12) Å                        | <i>T</i> = 293 K                     |
| <i>c</i> = 8.0269 (14) Å                        | 0.24 × 0.22 × 0.22 mm                |

### 2.2. Data collection

|   |   |
|---|---|
| Bruker Kappa APEXII CCD diffractometer                            | 10595 measured reflections                      |
| Absorption correction: multi-scan ( <i>SADABS</i> ; Bruker, 2004) | 3454 independent reflections                    |
| <i>T<sub>min</sub></i> = 0.981, <i>T<sub>max</sub></i> = 0.985    | 1668 reflections with <i>I</i> > 2σ( <i>I</i> ) |
|   | <i>R<sub>int</sub></i> = 0.039                  |

### 2.3. Refinement

|   |   |
|---|---|
| <i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )] = 0.066 | 1 restraint                                 |
| <i>wR</i> ( <i>F</i> <sup>2</sup> ) = 0.208                             | H-atom parameters constrained               |
| <i>S</i> = 1.04   | Δρ <sub>max</sub> = 0.28 e Å <sup>-3</sup>  |
| 3454 reflections  | Δρ <sub>min</sub> = -0.22 e Å <sup>-3</sup> |
| 145 parameters  |   |

**Table 1**

Hydrogen-bond geometry (Å, °).

| <i>D</i> —H... <i>A</i>  | <i>D</i> —H | H... <i>A</i> | <i>D</i> ... <i>A</i> | <i>D</i> —H... <i>A</i> |
|--------------------------|-------------|---------------|-----------------------|-------------------------|
| O2—H2A...O1 <sup>i</sup> | 0.82        | 1.97          | 2.741 (4)             | 156                     |

Symmetry code: (i) *x*, *y*, *z* - 1.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *SHELXL97*.

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Supporting information for this paper is available from the IUCr electronic archives (Reference: ZS2344).

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## supporting information

*Acta Cryst.* (2015). E71, o817–o818 [https://doi.org/10.1107/S2056989015018307]

## Crystal structure of (4-hydroxypiperidin-1-yl)(4-methylphenyl)methanone

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### S1. Comment

The piperidine ring is one of the most recognizable structural entities among heterocyclic molecules (Katritzky, 1995). A piperidine series of gamma-secretase inhibitors have been evaluated for treatment of Alzheimer's disease (AD) (Pissamitski *et al.*, 2007). Some piperidines were found to possess high profile biological activities, including cytotoxic and anticancer properties (Dimmock *et al.*, 2001). The piperidine ring is a feature of oral anaesthetics and narcotic analgesics (Watson *et al.*, 2000); Thomas *et al.*, 1998). Piperidine derivatives are used clinically to prevent post-operative vomiting, to speed up gastric emptying before anaesthesia, to facilitate radiological investigations and to correct a variety of disturbances of gastrointestinal functions (Sambath *et al.*, 2004).

The title compound, C<sub>13</sub>H<sub>17</sub>NO<sub>2</sub>, has been synthesized and the structure (Fig. 1) is reported herein. In this compound, The C—C distances in the piperidine ring and the benzene ring are in the range 1.497 (6)–1.515 (5) Å and 1.357 (6)–1.386 (5) Å, respectively and are comparable with literature values. The C—N distances in the piperidine ring are 1.455 (5) Å and 1.462 (5) Å and are in good agreement with values in a similar reported structure (Revathi *et al.*, 2015). The C7—O1 distance is 1.238 (5) Å, indicating double bond character and is comparable with the value reported previously (Prathebha *et al.*, 2015). The dihedral angle between piperidine and benzene rings is 51.7 (2)°. The bond angle sum around the N1 atom are 359.8 (3)° indicating an *sp*<sup>2</sup> hybridization of the atoms. The C8—N1—C7—O1 torsion angle [-9.0 (6)°] indicates that the keto group is in a *syn-periplanar* (*-sp*) orientation with respect to the piperidine ring which adopts a chair conformation, with puckering parameters of  $q_2 = 0.016$  (4) Å,  $\varphi_2 = 168.41^\circ$   $q_3 = -0.560$  (4) Å,  $QT = 0.561$  (4) Å and  $\theta_2 = 178.38$  (4)°.

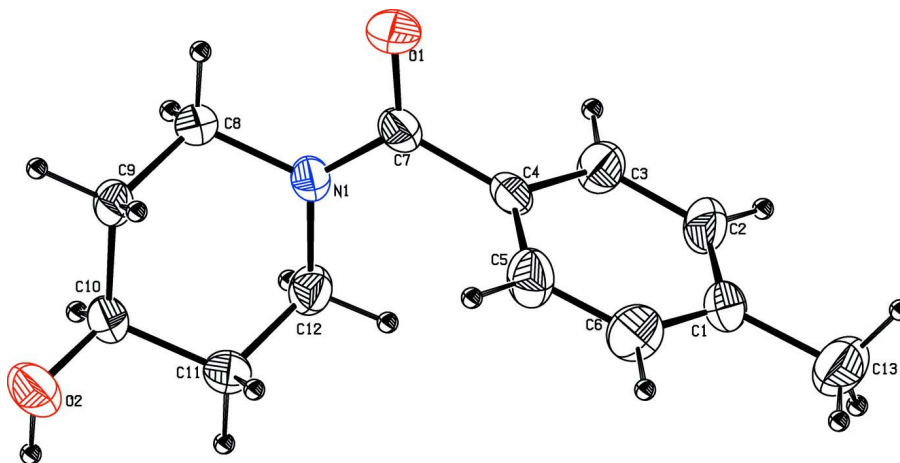
The crystal packing is stabilized by a single intermolecular O2—H···O1<sup>i</sup> hydrogen bond (Table 1), forming one-dimensional chains which extend along [001] (Fig. 2). Present also in the structure is a short intramolecular C8—H···O1 interaction [2.740 (5) Å].

### S2. Experimental

The title compound was synthesized using a published procedure (Revathi *et al.*, 2015). In a 250 ml round-bottomed flask, 120 mL of ethyl methyl ketone was added to 4-hydroxypiperidine (0.02 mol) and stirred at room temperature. After 5 min, triethylamine (0.04 mol) was added and the mixture was stirred for 15 min. 4-Methyl benzoyl chloride (0.04 mol) was then added and the reaction mixture was stirred at room temperature for *ca.* 2 h. A white precipitate of triethylammonium chloride was formed, which was removed by filtration and the filtrate was evaporated to give the crude product. This was recrystallized twice from ethyl methyl ketone giving colourless block-like crystals of the title compound (yield: 82%).

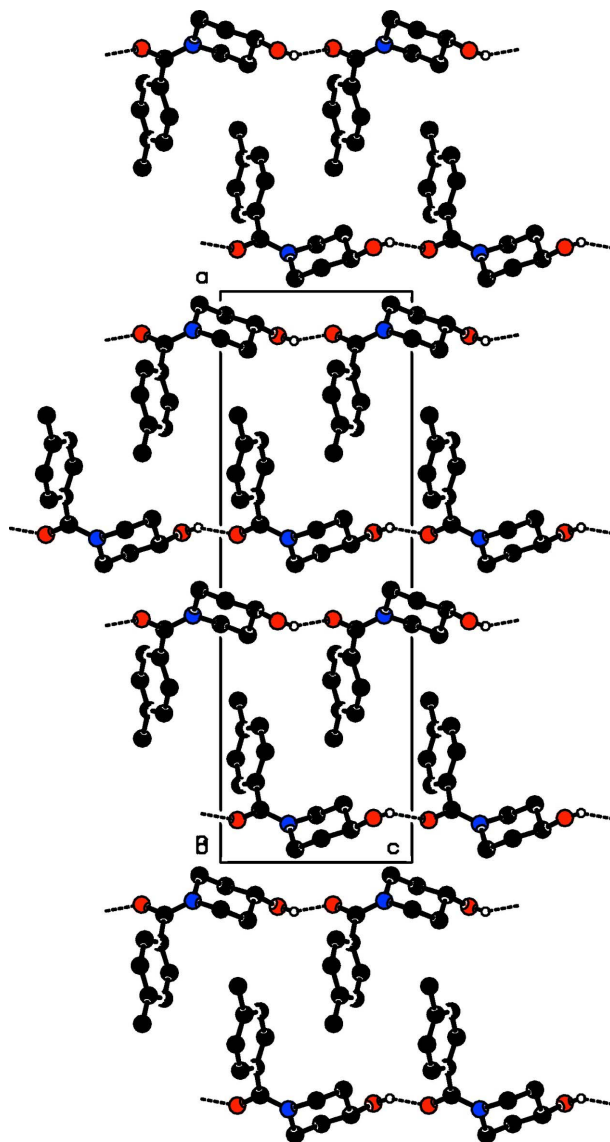
### S3. Refinement

H atoms were positioned geometrically and treated as riding on their parent atoms and refined with C—H distances of 0.93–0.98 Å and an O—H distance of 0.82 Å, with  $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{C-methyl and O})$ ,  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C, O})$  for other H atoms. One reflection (2 0 0) was considered to be affected by the beamstop and was omitted. The value of the absolute structure factor (Flack, 1983), although not of particular relevance but meaningless in this structure, was determined as 0(3) for 1610 Friedel pairs.



**Figure 1**

The molecular structure and atom numbering scheme for the title compound, with displacement ellipsoids drawn at the 30% probability level.



**Figure 2**

The crystal packing in the unit cell viewed along  $b$ . The dashed lines indicate hydrogen bonds.

**(4-Hydroxypiperidin-1-yl)(4-methylphenyl)methanone**

*Crystal data*

$C_{13}H_{17}NO_2$

$M_r = 219.28$

Orthorhombic,  $Pca2_1$

Hall symbol:  $P\ 2c\ -2ac$

$a = 23.933\ (5)\ \text{\AA}$

$b = 6.3317\ (12)\ \text{\AA}$

$c = 8.0269\ (14)\ \text{\AA}$

$V = 1216.3\ (4)\ \text{\AA}^3$

$Z = 4$

$F(000) = 472$

$D_x = 1.197\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$

$\theta = 1.7\text{--}29.8^\circ$

$\mu = 0.08\ \text{mm}^{-1}$

$T = 293\ \text{K}$

Block, colourless

$0.24 \times 0.22 \times 0.22\ \text{mm}$

*Data collection*

|  |  |
|--|--|
| Bruker Kappa APEXII CCD diffractometer                   | 10595 measured reflections   |
| Radiation source: fine-focus sealed tube                 | 3454 independent reflections   |
| Graphite monochromator                                   | 1668 reflections with $I > 2\sigma(I)$                                 |
| $\omega$ and $\varphi$ scans                             | $R_{\text{int}} = 0.039$   |
| Absorption correction: multi-scan (SADABS; Bruker, 2004) | $\theta_{\text{max}} = 29.8^\circ$ , $\theta_{\text{min}} = 3.1^\circ$ |
| $T_{\text{min}} = 0.981$ , $T_{\text{max}} = 0.985$      | $h = -33 \rightarrow 30$   |
|  | $k = -8 \rightarrow 8$   |
|  | $l = -10 \rightarrow 11$   |

*Refinement*

|  |  |
|--|--|
| Refinement on $F^2$  | Secondary atom site location: difference Fourier map         |
| Least-squares matrix: full                                     | Hydrogen site location: inferred from neighbouring sites     |
| $R[F^2 > 2\sigma(F^2)] = 0.066$                                | H-atom parameters constrained                                |
| $wR(F^2) = 0.208$  | $w = 1/[\sigma^2(F_o^2) + (0.121P)^2 + 0.297P]$              |
| $S = 1.04$   | where $P = (F_o^2 + 2F_c^2)/3$                               |
| 3454 reflections   | $(\Delta/\sigma)_{\text{max}} < 0.001$                       |
| 145 parameters   | $\Delta\rho_{\text{max}} = 0.28 \text{ e } \text{\AA}^{-3}$  |
| 1 restraint  | $\Delta\rho_{\text{min}} = -0.22 \text{ e } \text{\AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods |  |

*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 ( $\text{\AA}^2$ )*

|      | <i>x</i>     | <i>y</i>   | <i>z</i>   | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|--------------|------------|------------|----------------------------------|
| O2   | 0.42250 (13) | 0.9019 (5) | 0.2011 (4) | 0.0766 (9)                       |
| H2A  | 0.4137       | 0.8390     | 0.1158     | 0.115*                           |
| N1   | 0.43269 (12) | 0.5768 (5) | 0.6446 (4) | 0.0502 (8)                       |
| O1   | 0.42609 (13) | 0.6719 (6) | 0.9120 (3) | 0.0885 (11)                      |
| C10  | 0.44267 (16) | 0.7574 (6) | 0.3187 (5) | 0.0533 (9)                       |
| H10  | 0.4759       | 0.6870     | 0.2737     | 0.064*                           |
| C4   | 0.35949 (13) | 0.4254 (6) | 0.8163 (4) | 0.0482 (8)                       |
| C1   | 0.26666 (15) | 0.1641 (8) | 0.8753 (5) | 0.0628 (11)                      |
| C12  | 0.41754 (16) | 0.4528 (6) | 0.4989 (5) | 0.0545 (9)                       |
| H12A | 0.3877       | 0.3558     | 0.5279     | 0.065*                           |
| H12B | 0.4495       | 0.3701     | 0.4632     | 0.065*                           |
| C7   | 0.40802 (15) | 0.5691 (6) | 0.7925 (4) | 0.0505 (9)                       |
| C11  | 0.39864 (16) | 0.5930 (6) | 0.3578 (4) | 0.0524 (9)                       |
| H11A | 0.3640       | 0.6627     | 0.3883     | 0.063*                           |
| H11B | 0.3916       | 0.5077     | 0.2596     | 0.063*                           |
| C6   | 0.26126 (15) | 0.3547 (9) | 0.7954 (6) | 0.0758 (13)                      |

|      |              |             |            |             |
|------|--------------|-------------|------------|-------------|
| H6   | 0.2261       | 0.3976      | 0.7599     | 0.091*      |
| C5   | 0.30623 (16) | 0.4839 (7)  | 0.7665 (6) | 0.0669 (11) |
| H5   | 0.3009       | 0.6125      | 0.7128     | 0.080*      |
| C2   | 0.31909 (18) | 0.1055 (7)  | 0.9206 (6) | 0.0742 (13) |
| H2   | 0.3245       | -0.0261     | 0.9694     | 0.089*      |
| C8   | 0.47699 (16) | 0.7294 (7)  | 0.6096 (5) | 0.0598 (10) |
| H8A  | 0.5107       | 0.6557      | 0.5758     | 0.072*      |
| H8B  | 0.4853       | 0.8099      | 0.7094     | 0.072*      |
| C3   | 0.36470 (16) | 0.2363 (7)  | 0.8960 (6) | 0.0679 (12) |
| H3   | 0.3996       | 0.1943      | 0.9346     | 0.082*      |
| C9   | 0.45847 (17) | 0.8752 (5)  | 0.4737 (5) | 0.0527 (9)  |
| H9A  | 0.4884       | 0.9732      | 0.4482     | 0.063*      |
| H9B  | 0.4266       | 0.9566      | 0.5121     | 0.063*      |
| C13  | 0.2170 (2)   | 0.0223 (10) | 0.9085 (8) | 0.0951 (16) |
| H13A | 0.1836       | 0.0885      | 0.8674     | 0.143*      |
| H13B | 0.2135       | -0.0011     | 1.0262     | 0.143*      |
| H13C | 0.2223       | -0.1105     | 0.8530     | 0.143*      |

*Atomic displacement parameters (Å<sup>2</sup>)*

|     | $U^{11}$    | $U^{22}$    | $U^{33}$    | $U^{12}$     | $U^{13}$     | $U^{23}$     |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| O2  | 0.097 (2)   | 0.0792 (19) | 0.0541 (17) | 0.0001 (17)  | -0.0073 (14) | 0.0175 (16)  |
| N1  | 0.0614 (17) | 0.0478 (18) | 0.0413 (15) | -0.0129 (14) | 0.0013 (12)  | 0.0037 (14)  |
| O1  | 0.105 (2)   | 0.117 (3)   | 0.0441 (16) | -0.045 (2)   | -0.0064 (15) | -0.0106 (18) |
| C10 | 0.0621 (19) | 0.056 (2)   | 0.0418 (18) | -0.0096 (18) | 0.0032 (15)  | 0.0054 (18)  |
| C4  | 0.056 (2)   | 0.056 (2)   | 0.0323 (15) | 0.0001 (16)  | -0.0009 (13) | 0.0075 (17)  |
| C1  | 0.062 (2)   | 0.079 (3)   | 0.0472 (19) | -0.016 (2)   | 0.0102 (17)  | 0.005 (2)    |
| C12 | 0.061 (2)   | 0.046 (2)   | 0.056 (2)   | -0.0113 (17) | 0.0065 (16)  | -0.002 (2)   |
| C7  | 0.0619 (19) | 0.050 (2)   | 0.0396 (18) | -0.0035 (16) | -0.0048 (16) | 0.0088 (17)  |
| C11 | 0.061 (2)   | 0.055 (2)   | 0.0422 (17) | -0.0058 (17) | -0.0002 (14) | -0.0092 (18) |
| C6  | 0.0438 (19) | 0.100 (3)   | 0.084 (3)   | 0.006 (2)    | 0.003 (2)    | 0.005 (3)    |
| C5  | 0.064 (2)   | 0.060 (2)   | 0.077 (3)   | 0.0036 (19)  | 0.003 (2)    | 0.021 (2)    |
| C2  | 0.075 (3)   | 0.064 (3)   | 0.083 (3)   | -0.020 (2)   | -0.012 (2)   | 0.032 (3)    |
| C8  | 0.064 (2)   | 0.067 (3)   | 0.048 (2)   | -0.0260 (19) | -0.0126 (16) | 0.010 (2)    |
| C3  | 0.059 (2)   | 0.061 (3)   | 0.084 (3)   | -0.0081 (19) | -0.019 (2)   | 0.028 (2)    |
| C9  | 0.076 (2)   | 0.0356 (18) | 0.0470 (18) | -0.0178 (18) | -0.0010 (16) | 0.0040 (18)  |
| C13 | 0.078 (3)   | 0.121 (4)   | 0.087 (3)   | -0.041 (3)   | 0.016 (3)    | -0.019 (3)   |

*Geometric parameters (Å, °)*

|         |           |          |           |
|---------|-----------|----------|-----------|
| O2—C10  | 1.401 (5) | C12—H12B | 0.9700    |
| O2—H2A  | 0.8200    | C11—H11A | 0.9700    |
| N1—C7   | 1.327 (5) | C11—H11B | 0.9700    |
| N1—C12  | 1.454 (5) | C6—C5    | 1.372 (6) |
| N1—C8   | 1.462 (4) | C6—H6    | 0.9300    |
| O1—C7   | 1.237 (5) | C5—H5    | 0.9300    |
| C10—C9  | 1.500 (5) | C2—C3    | 1.385 (5) |
| C10—C11 | 1.514 (5) | C2—H2    | 0.9300    |

|               |           |               |            |
|---------------|-----------|---------------|------------|
| C10—H10       | 0.9800    | C8—C9         | 1.496 (5)  |
| C4—C3         | 1.363 (6) | C8—H8A        | 0.9700     |
| C4—C5         | 1.386 (5) | C8—H8B        | 0.9700     |
| C4—C7         | 1.487 (5) | C3—H3         | 0.9300     |
| C1—C2         | 1.358 (6) | C9—H9A        | 0.9700     |
| C1—C6         | 1.373 (7) | C9—H9B        | 0.9700     |
| C1—C13        | 1.514 (6) | C13—H13A      | 0.9600     |
| C12—C11       | 1.509 (5) | C13—H13B      | 0.9600     |
| C12—H12A      | 0.9700    | C13—H13C      | 0.9600     |
|               |           |               |            |
| C10—O2—H2A    | 109.5     | C5—C6—C1      | 122.0 (4)  |
| C7—N1—C12     | 126.1 (3) | C5—C6—H6      | 119.0      |
| C7—N1—C8      | 121.3 (3) | C1—C6—H6      | 119.0      |
| C12—N1—C8     | 112.6 (3) | C6—C5—C4      | 120.9 (4)  |
| O2—C10—C9     | 108.7 (3) | C6—C5—H5      | 119.6      |
| O2—C10—C11    | 110.4 (3) | C4—C5—H5      | 119.6      |
| C9—C10—C11    | 110.2 (3) | C1—C2—C3      | 121.8 (4)  |
| O2—C10—H10    | 109.1     | C1—C2—H2      | 119.1      |
| C9—C10—H10    | 109.1     | C3—C2—H2      | 119.1      |
| C11—C10—H10   | 109.1     | N1—C8—C9      | 109.4 (3)  |
| C3—C4—C5      | 117.0 (3) | N1—C8—H8A     | 109.8      |
| C3—C4—C7      | 121.7 (3) | C9—C8—H8A     | 109.8      |
| C5—C4—C7      | 121.2 (3) | N1—C8—H8B     | 109.8      |
| C2—C1—C6      | 116.9 (3) | C9—C8—H8B     | 109.8      |
| C2—C1—C13     | 121.1 (4) | H8A—C8—H8B    | 108.2      |
| C6—C1—C13     | 122.0 (4) | C4—C3—C2      | 121.3 (4)  |
| N1—C12—C11    | 111.1 (3) | C4—C3—H3      | 119.3      |
| N1—C12—H12A   | 109.4     | C2—C3—H3      | 119.3      |
| C11—C12—H12A  | 109.4     | C8—C9—C10     | 111.9 (3)  |
| N1—C12—H12B   | 109.4     | C8—C9—H9A     | 109.2      |
| C11—C12—H12B  | 109.4     | C10—C9—H9A    | 109.2      |
| H12A—C12—H12B | 108.0     | C8—C9—H9B     | 109.2      |
| O1—C7—N1      | 121.2 (3) | C10—C9—H9B    | 109.2      |
| O1—C7—C4      | 119.7 (3) | H9A—C9—H9B    | 107.9      |
| N1—C7—C4      | 119.0 (3) | C1—C13—H13A   | 109.5      |
| C12—C11—C10   | 110.6 (3) | C1—C13—H13B   | 109.5      |
| C12—C11—H11A  | 109.5     | H13A—C13—H13B | 109.5      |
| C10—C11—H11A  | 109.5     | C1—C13—H13C   | 109.5      |
| C12—C11—H11B  | 109.5     | H13A—C13—H13C | 109.5      |
| C10—C11—H11B  | 109.5     | H13B—C13—H13C | 109.5      |
| H11A—C11—H11B | 108.1     |               |            |
|               |           |               |            |
| C7—N1—C12—C11 | 117.5 (4) | C13—C1—C6—C5  | 179.5 (5)  |
| C8—N1—C12—C11 | -58.2 (4) | C1—C6—C5—C4   | 0.5 (7)    |
| C12—N1—C7—O1  | 175.6 (4) | C3—C4—C5—C6   | -0.6 (6)   |
| C8—N1—C7—O1   | -9.0 (6)  | C7—C4—C5—C6   | -177.1 (4) |
| C12—N1—C7—C4  | -1.3 (6)  | C6—C1—C2—C3   | 3.5 (7)    |
| C8—N1—C7—C4   | 174.1 (3) | C13—C1—C2—C3  | -177.9 (5) |



|                |            |               |            |
|----------------|------------|---------------|------------|
| C3—C4—C7—O1    | -74.8 (5)  | C7—N1—C8—C9   | -117.4 (4) |
| C5—C4—C7—O1    | 101.5 (5)  | C12—N1—C8—C9  | 58.6 (4)   |
| C3—C4—C7—N1    | 102.2 (4)  | C5—C4—C3—C2   | 2.2 (7)    |
| C5—C4—C7—N1    | -81.6 (5)  | C7—C4—C3—C2   | 178.7 (4)  |
| N1—C12—C11—C10 | 54.7 (4)   | C1—C2—C3—C4   | -3.8 (8)   |
| O2—C10—C11—C12 | -173.3 (3) | N1—C8—C9—C10  | -57.0 (4)  |
| C9—C10—C11—C12 | -53.1 (4)  | O2—C10—C9—C8  | 176.3 (3)  |
| C2—C1—C6—C5    | -1.9 (7)   | C11—C10—C9—C8 | 55.1 (5)   |

*Hydrogen-bond geometry (Å, °)*

| <i>D</i> —H $\cdots$ <i>A</i>           | <i>D</i> —H | H $\cdots$ <i>A</i> | <i>D</i> $\cdots$ <i>A</i> | <i>D</i> —H $\cdots$ <i>A</i> |
|---|-------------|---------------------|----------------------------|-------------------------------|
| O2—H2 <i>A</i> $\cdots$ O1 <sup>i</sup> | 0.82        | 1.97                | 2.741 (4)                  | 156                           |
| C8—H8 <i>B</i> $\cdots$ O1              | 0.97        | 2.33                | 2.740 (5)                  | 105                           |

Symmetry code: (i) *x*, *y*, *z*-1.