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# Crystal structure of *N*-(2-hydroxy-5-methylphenyl)benzamide

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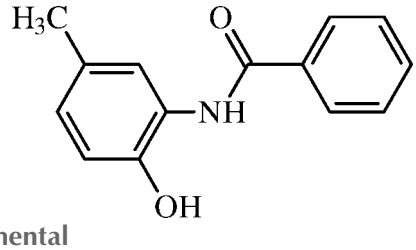
In the title compound, $C_{14}H_{13}NO_2$, the mean plane of the non-H atoms of the central amide fragment C—N—C(=O)—C (r.m.s. deviation = 0.029 Å) forms dihedral angles of 5.63 (6) and 10.20 (5)° with the phenyl and hydroxyphenyl rings, respectively. A short intramolecular N—H···O contact is present. In the crystal, the molecules are linked by O—H···O hydrogen bonds to generate *C*(7) chains along [100]. The chains are reinforced by weak C—H···O contacts, which together with the O—H···O bonds lead to $R_2^2(7)$ loops. Very weak N—H···O interactions link the molecules into inversion dimers.

**Keywords:** crystal structure; benzamide; benzanilide derivatives; biological activity.

**CCDC reference**: 1434264

## 1. Related literature

For the biological activity of benzanilide derivatives, see Calderone *et al.* (2006). For related structures, see: Gowda *et al.* (2008); Rodrigues *et al.* (2011).




## 2. Experimental

### 2.1. Crystal data

$C_{14}H_{13}NO_2$ $M_r$ = 227.25

Monoclinic, $P2_1/n$
$a$ = 7.2263 (3) Å
$b$ = 21.7442 (7) Å
$c$ = 7.4747 (3) Å
$\beta$ = 110.280 (5)°
$V$ = 1101.69 (8) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 123 K
0.40 × 0.35 × 0.25 mm

### 2.2. Data collection

Oxford Diffraction Gemini S CCD diffractometer
10254 measured reflections
2795 independent reflections
2332 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.032

### 2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.109
$S$ = 1.03
2795 reflections
163 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.33 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.27 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O2 | 0.889 (18) | 2.173 (16) | 2.6153 (15) | 110.0 (13) |
| N1—H1···O2$^{i}$ | 0.889 (18) | 2.518 (17) | 3.1928 (14) | 133.1 (14) |
| O2—H20···O1$^{ii}$ | 0.89 (2) | 1.75 (2) | 2.6390 (12) | 171.3 (19) |
| C6—H6···O2$^{iii}$ | 0.95 | 2.59 | 3.4197 (15) | 146 |

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $x+1, y, z$; (iii) $x-1, y, z$.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

## Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7532).

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# supporting information

*Acta Cryst.* (2015). E**71**, o943 [https://doi.org/10.1107/S2056989015020575]

## Crystal structure of *N*-(2-hydroxy-5-methylphenyl)benzamide

**Rodolfo Moreno-Fuquen, Nory J. Mariño and Alan R. Kennedy**

### S1. Comment

The crystal structure determination of N-(2-hydroxy-5-methylphenyl)benzamide (I), is part of a study on phenyl-benzamides carried out in our research group, and it was synthesized from the reaction between of 2-amino-4-methyl-phenol and benzoyl chloride in acetonitrile. Benzanilide systems have a wide range of biological properties such as potassium channel activators (Calderone *et al.*, 2006). Similar compounds to (I) have been reported in the literature: 2-Methyl-N-(m-tolyl)benzamide (II) (Gowda *et al.*, 2008) and N-(3,5-Dimethylphenyl)-4-methylbenzamide (III) (Rodrigues *et al.*, 2011). The molecular structure of (I) is shown in Fig. 1. The central amide moiety, C8—N1-C7(═O1)—C1, is close to planar (r.m.s. deviation for all non-H atoms = 0.0291 Å) and it forms dihedral angles of 5.63 (6)° with the C1-C6 and 10.20 (5)° with the C8-C13 rings respectively. Bond lengths and bond angles in the molecule are in a good agreement with those found in the related compounds (II) and (III). The conformation of the N—H group is *syn* to the –OH substituent in the benzoyl ring, which results in a short intramolecular N—H···O contact. In the crystal (Fig. 2), molecules are linked by strong O-H···O hydrogen bonds and weak C-H···O intermolecular contacts. Indeed, the O2-H20 at (x,y,z) acts as a hydrogen-bond donor to O1 atom of the carbonyl group at (x+1,+y,+z) and the C6-H6 acts as a hydrogen-bond donor to O2 atom of the hydroxyl group at (x-1,+y,+z). These interactions generate C(7) chains of molecules and $R_2^2(7)$ rings (See Fig. 2), running along [100]. Additionally, the molecules are linked by N-H···O interactions. N1-H1 acts as a hydrogen-bond donor to O2 atom of the hydroxyl group at (-x+1,-y,-z+1), forming inversion dimers (Fig. 3).

### S2. Experimental

The title molecule was synthesized taking 0.100 g (0.812 mmol) of 2-amino-4-methylphenol dissolved in acetonitrile (10 mL), and then was added benzoyl chloride (0.100 mL, 0.860 mmol). The solution was placed under reflux and constant stirring for 3 hours at 150°C. The solid was filtered and recrystallized from methanol. The solvent was evaporated at room temperature and pink crystals were obtained (m.p. 448 (1)K).

### S3. Refinement

All H-atoms were positioned in geometrically idealized positions, C—H = 0.95 Å, and were refined using a riding-model approximation with $U_{iso}$(H) constrained to 1.2 times $U_{eq}$ of the respective parent atom. H1 atom was found from the Fourier maps and its coordinates were refined freely.

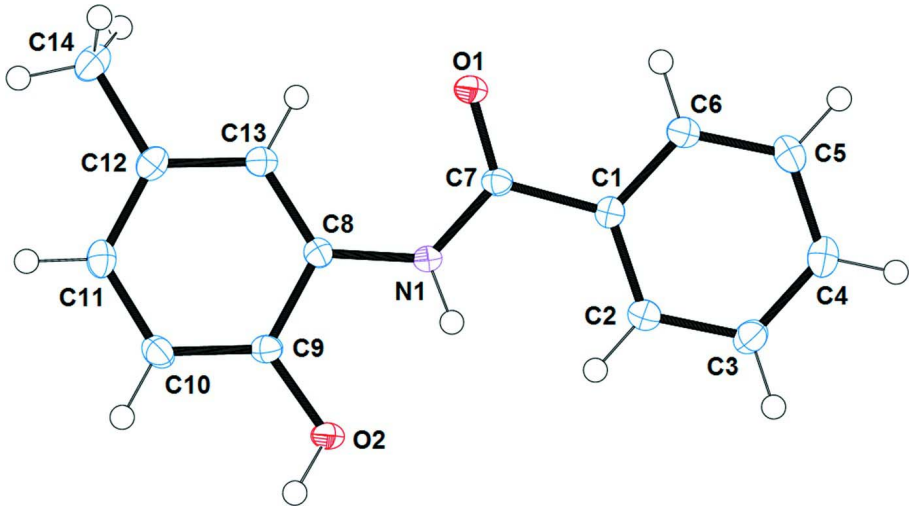


**Figure 1**

The molecular structure of (I) with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radius.

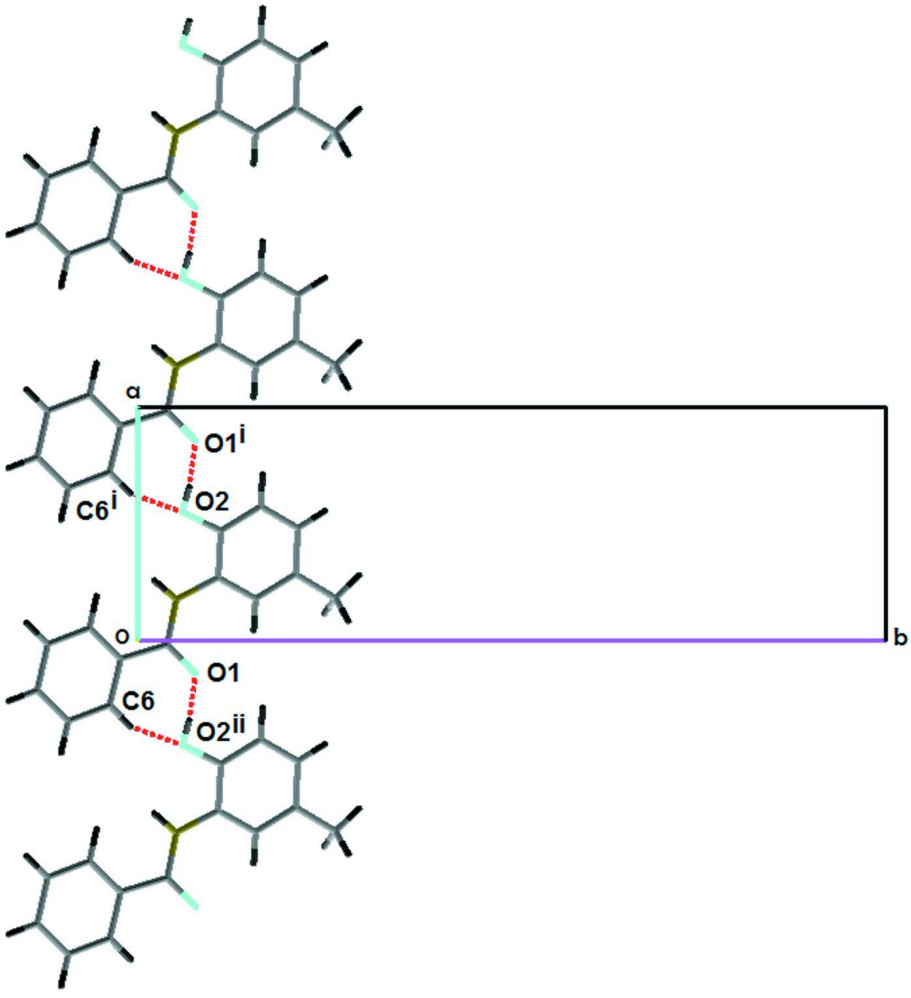


**Figure 2**

Part of the crystal structure of (I), showing the formation of C(7) chains of molecules along [100] [Symmetry codes: (i) *x* + 1, +*y*, +*z*; (ii) *x* - 1, +*y*, +*z*].

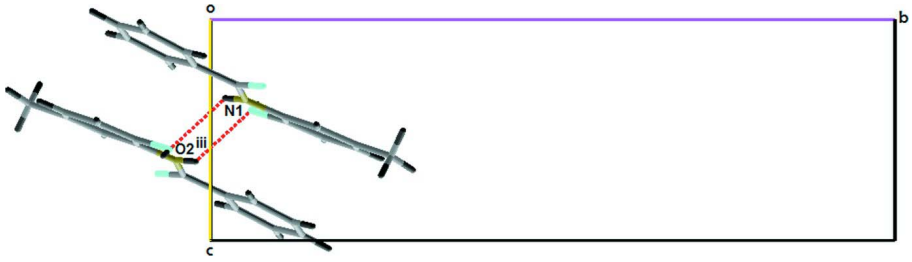


**Figure 3**

Part of the crystal structure of (I), showing the formation of dimers along [001]. [Symmetry codes: (iii) -*x* + 1, -*y*, -*z* + 1].

## *N*-(2-Hydroxy-5-methylphenyl)benzamide

*Crystal data*

$C_{14}H_{13}NO_2$
$M_r$ = 227.25

Monoclinic, $P2_1/n$
*a* = 7.2263 (3) Å

$b$ = 21.7442 (7) Å
$c$ = 7.4747 (3) Å
$\beta$ = 110.280 (5)°
$V$ = 1101.69 (8) Å$^3$
$Z$ = 4
$F(000)$ = 480
$D_x$ = 1.370 Mg m$^{-3}$
Melting point: 448(1) K

Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 10254 reflections
$\theta$ = 3.4–29.4°
$\mu$ = 0.09 mm$^{-1}$
$T$ = 123 K
Block, pink
0.40 × 0.35 × 0.25 mm

*Data collection*

Oxford Diffraction Gemini S CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
10254 measured reflections
2795 independent reflections

2332 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.032
$\theta_{max}$ = 29.4°, $\theta_{min}$ = 3.4°
$h$ = −9→9
$k$ = −30→30
$l$ = −9→10

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.109
$S$ = 1.03
2795 reflections
163 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0448P)^2 + 0.5141P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.33 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.27 e Å$^{-3}$

*Special details*

**Experimental**. The IR spectrum was recorded on a FT—IR SHIMADZU IR-Affinity-1 spectrophotometer. IR (KBr), cm$^{-1}$, 3395 (amide N-H); 3073 (Hydroxyl O-H), 1643 (amide, C=O); 1593 (C=C).

**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 $F^2 > \sigma(F^2)$ 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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O2 | 0.55117 (13) | 0.05937 (4) | 0.41236 (14) | 0.0204 (2) |
| O1 | −0.14306 (13) | 0.07692 (4) | 0.30232 (14) | 0.0214 (2) |
| N1 | 0.17579 (15) | 0.05132 (5) | 0.36397 (15) | 0.0166 (2) |
| C1 | −0.07846 (17) | −0.02289 (5) | 0.20522 (16) | 0.0153 (2) |
| C2 | 0.05257 (19) | −0.06486 (6) | 0.17363 (18) | 0.0192 (3) |
| H2 | 0.1892 | −0.0554 | 0.2136 | 0.023* |
| C3 | −0.0159 (2) | −0.12053 (6) | 0.08386 (19) | 0.0222 (3) |
| H3 | 0.0743 | −0.1490 | 0.0632 | 0.027* |

| | | | | |
|---|---|---|---|---|
| C4 | −0.2145 (2) | −0.13469 (6) | 0.02438 (18) | 0.0217 (3) |
| H4 | −0.2607 | −0.1728 | −0.0371 | 0.026* |
| C5 | −0.34605 (19) | −0.09320 (6) | 0.05467 (19) | 0.0224 (3) |
| H5 | −0.4827 | −0.1028 | 0.0136 | 0.027* |
| C6 | −0.27845 (18) | −0.03785 (6) | 0.14471 (18) | 0.0193 (3) |
| H6 | −0.3693 | −0.0097 | 0.1656 | 0.023* |
| C7 | −0.01844 (17) | 0.03897 (5) | 0.29485 (17) | 0.0150 (2) |
| C8 | 0.26922 (17) | 0.10733 (5) | 0.43855 (17) | 0.0149 (2) |
| C13 | 0.17867 (18) | 0.15716 (6) | 0.48997 (17) | 0.0172 (3) |
| H13 | 0.0430 | 0.1547 | 0.4756 | 0.021* |
| C12 | 0.28408 (19) | 0.21075 (6) | 0.56243 (18) | 0.0186 (3) |
| C11 | 0.48182 (19) | 0.21370 (6) | 0.58174 (18) | 0.0202 (3) |
| H11 | 0.5548 | 0.2501 | 0.6301 | 0.024* |
| C10 | 0.57479 (18) | 0.16395 (6) | 0.53108 (18) | 0.0195 (3) |
| H10 | 0.7104 | 0.1666 | 0.5452 | 0.023* |
| C9 | 0.46985 (17) | 0.11075 (5) | 0.46028 (17) | 0.0157 (2) |
| C14 | 0.1817 (2) | 0.26392 (6) | 0.6182 (2) | 0.0258 (3) |
| H141 | 0.2788 | 0.2956 | 0.6812 | 0.039* |
| H142 | 0.1168 | 0.2495 | 0.7059 | 0.039* |
| H143 | 0.0827 | 0.2813 | 0.5038 | 0.039* |
| H1 | 0.258 (2) | 0.0217 (8) | 0.357 (2) | 0.031 (4)* |
| H20 | 0.658 (3) | 0.0685 (9) | 0.383 (3) | 0.047 (6)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O2 | 0.0158 (4) | 0.0173 (4) | 0.0316 (5) | 0.0009 (3) | 0.0126 (4) | −0.0013 (4) |
| O1 | 0.0150 (4) | 0.0177 (4) | 0.0333 (5) | 0.0005 (3) | 0.0108 (4) | −0.0022 (4) |
| N1 | 0.0129 (5) | 0.0147 (5) | 0.0224 (5) | 0.0010 (4) | 0.0063 (4) | −0.0027 (4) |
| C1 | 0.0170 (6) | 0.0148 (5) | 0.0142 (5) | −0.0004 (4) | 0.0056 (4) | 0.0008 (4) |
| C2 | 0.0161 (6) | 0.0200 (6) | 0.0210 (6) | 0.0009 (5) | 0.0056 (5) | −0.0008 (5) |
| C3 | 0.0235 (7) | 0.0188 (6) | 0.0240 (6) | 0.0027 (5) | 0.0078 (5) | −0.0030 (5) |
| C4 | 0.0267 (7) | 0.0172 (6) | 0.0190 (6) | −0.0028 (5) | 0.0051 (5) | −0.0012 (5) |
| C5 | 0.0186 (6) | 0.0230 (6) | 0.0238 (6) | −0.0047 (5) | 0.0051 (5) | −0.0013 (5) |
| C6 | 0.0162 (6) | 0.0197 (6) | 0.0220 (6) | 0.0008 (5) | 0.0065 (5) | −0.0002 (5) |
| C7 | 0.0143 (5) | 0.0156 (6) | 0.0164 (5) | 0.0010 (4) | 0.0069 (4) | 0.0014 (4) |
| C8 | 0.0145 (6) | 0.0150 (5) | 0.0146 (5) | −0.0003 (4) | 0.0043 (4) | 0.0009 (4) |
| C13 | 0.0161 (6) | 0.0180 (6) | 0.0180 (6) | 0.0012 (4) | 0.0065 (5) | −0.0001 (4) |
| C12 | 0.0227 (6) | 0.0155 (6) | 0.0178 (6) | 0.0015 (5) | 0.0073 (5) | 0.0006 (4) |
| C11 | 0.0230 (7) | 0.0149 (6) | 0.0222 (6) | −0.0034 (5) | 0.0071 (5) | 0.0006 (5) |
| C10 | 0.0152 (6) | 0.0195 (6) | 0.0238 (6) | −0.0019 (5) | 0.0069 (5) | 0.0027 (5) |
| C9 | 0.0153 (6) | 0.0156 (5) | 0.0172 (6) | 0.0022 (4) | 0.0070 (5) | 0.0022 (4) |
| C14 | 0.0297 (7) | 0.0184 (6) | 0.0308 (7) | 0.0023 (5) | 0.0125 (6) | −0.0044 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O2—C9 | 1.3667 (14) | C5—H5 | 0.9500 |
| O2—H20 | 0.89 (2) | C6—H6 | 0.9500 |

| | | | |
|---|---|---|---|
| O1—C7 | 1.2369 (14) | C8—C13 | 1.3871 (16) |
| N1—C7 | 1.3440 (15) | C8—C9 | 1.4038 (16) |
| N1—C8 | 1.4103 (15) | C13—C12 | 1.3949 (17) |
| N1—H1 | 0.889 (18) | C13—H13 | 0.9500 |
| C1—C2 | 1.3929 (17) | C12—C11 | 1.3870 (18) |
| C1—C6 | 1.3949 (17) | C12—C14 | 1.5074 (17) |
| C1—C7 | 1.4984 (16) | C11—C10 | 1.3933 (18) |
| C2—C3 | 1.3893 (17) | C11—H11 | 0.9500 |
| C2—H2 | 0.9500 | C10—C9 | 1.3838 (17) |
| C3—C4 | 1.3818 (19) | C10—H10 | 0.9500 |
| C3—H3 | 0.9500 | C14—H141 | 0.9800 |
| C4—C5 | 1.3849 (19) | C14—H142 | 0.9800 |
| C4—H4 | 0.9500 | C14—H143 | 0.9800 |
| C5—C6 | 1.3829 (18) | | |

| | | | |
|---|---|---|---|
| C9—O2—H20 | 111.6 (12) | C13—C8—C9 | 119.61 (11) |
| C7—N1—C8 | 128.14 (10) | C13—C8—N1 | 125.23 (11) |
| C7—N1—H1 | 117.3 (11) | C9—C8—N1 | 115.16 (10) |
| C8—N1—H1 | 114.4 (11) | C8—C13—C12 | 120.90 (11) |
| C2—C1—C6 | 118.75 (11) | C8—C13—H13 | 119.5 |
| C2—C1—C7 | 123.75 (11) | C12—C13—H13 | 119.5 |
| C6—C1—C7 | 117.46 (10) | C11—C12—C13 | 118.90 (11) |
| C3—C2—C1 | 120.22 (12) | C11—C12—C14 | 121.51 (12) |
| C3—C2—H2 | 119.9 | C13—C12—C14 | 119.59 (11) |
| C1—C2—H2 | 119.9 | C12—C11—C10 | 120.82 (11) |
| C4—C3—C2 | 120.39 (12) | C12—C11—H11 | 119.6 |
| C4—C3—H3 | 119.8 | C10—C11—H11 | 119.6 |
| C2—C3—H3 | 119.8 | C9—C10—C11 | 120.07 (11) |
| C3—C4—C5 | 119.83 (12) | C9—C10—H10 | 120.0 |
| C3—C4—H4 | 120.1 | C11—C10—H10 | 120.0 |
| C5—C4—H4 | 120.1 | O2—C9—C10 | 123.73 (11) |
| C6—C5—C4 | 119.99 (12) | O2—C9—C8 | 116.55 (10) |
| C6—C5—H5 | 120.0 | C10—C9—C8 | 119.71 (11) |
| C4—C5—H5 | 120.0 | C12—C14—H141 | 109.5 |
| C5—C6—C1 | 120.81 (12) | C12—C14—H142 | 109.5 |
| C5—C6—H6 | 119.6 | H141—C14—H142 | 109.5 |
| C1—C6—H6 | 119.6 | C12—C14—H143 | 109.5 |
| O1—C7—N1 | 121.94 (11) | H141—C14—H143 | 109.5 |
| O1—C7—C1 | 121.11 (11) | H142—C14—H143 | 109.5 |
| N1—C7—C1 | 116.95 (10) | | |

| | | | |
|---|---|---|---|
| C6—C1—C2—C3 | −0.16 (18) | C7—N1—C8—C9 | −166.27 (11) |
| C7—C1—C2—C3 | −177.86 (11) | C9—C8—C13—C12 | 0.22 (18) |
| C1—C2—C3—C4 | 0.27 (19) | N1—C8—C13—C12 | −179.91 (11) |
| C2—C3—C4—C5 | −0.10 (19) | C8—C13—C12—C11 | 0.28 (18) |
| C3—C4—C5—C6 | −0.2 (2) | C8—C13—C12—C14 | −179.59 (12) |
| C4—C5—C6—C1 | 0.3 (2) | C13—C12—C11—C10 | −0.44 (19) |
| C2—C1—C6—C5 | −0.12 (18) | C14—C12—C11—C10 | 179.44 (12) |

| | | | |
|---|---|---|---|
| C7—C1—C6—C5 | 177.72 (11) | C12—C11—C10—C9 | 0.08 (19) |
| C8—N1—C7—O1 | −5.48 (19) | C11—C10—C9—O2 | −178.11 (11) |
| C8—N1—C7—C1 | 173.71 (10) | C11—C10—C9—C8 | 0.44 (18) |
| C2—C1—C7—O1 | 172.66 (12) | C13—C8—C9—O2 | 178.06 (11) |
| C6—C1—C7—O1 | −5.06 (17) | N1—C8—C9—O2 | −1.82 (15) |
| C2—C1—C7—N1 | −6.54 (17) | C13—C8—C9—C10 | −0.59 (17) |
| C6—C1—C7—N1 | 175.74 (11) | N1—C8—C9—C10 | 179.54 (11) |
| C7—N1—C8—C13 | 13.9 (2) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O2 | 0.889 (18) | 2.173 (16) | 2.6153 (15) | 110.0 (13) |
| N1—H1···O2$^{i}$ | 0.889 (18) | 2.518 (17) | 3.1928 (14) | 133.1 (14) |
| O2—H20···O1$^{ii}$ | 0.89 (2) | 1.75 (2) | 2.6390 (12) | 171.3 (19) |
| C6—H6···O2$^{iii}$ | 0.95 | 2.59 | 3.4197 (15) | 146 |

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