

## 2-(4-Hydroxyphenyl)acetamide

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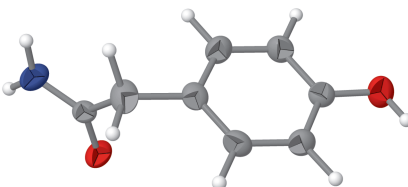
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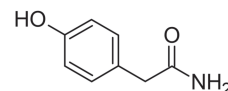
**Keywords:** crystal structure; atenolol; acetaminophen; DFT geometry optimization.**CCDC reference:** 2502168**Structural data:** full structural data are available from iucrdata.iucr.org

In the title molecule,  $C_8H_9NO_2$ , which is an isomer of acetaminophen [*N*-(4-hydroxyphenyl)acetamide], the acetamide group plane subtends a dihedral angle of  $89.95(5)^\circ$  with respect to the phenyl ring plane with the  $-NH_2$  group directed outward, in contrast to an *in vacuo* DFT geometry optimization in which the  $-NH_2$  group is directed inward. In the extended structure,  $N-H \cdots O$  hydrogen bonds organize molecules into stacks propagating along [100], with additional hydrogen bonding linking neighboring parallel stacks. A survey of known structures indicates that the structures of 2-phenylacetamide molecules with any substitution at the 4-position on the phenyl ring can demonstrate different orientations for the acetamide group ranging from the  $-NH_2$  group directed almost completely outward to the  $-NH_2$  group directed almost completely inward.

### 3D view

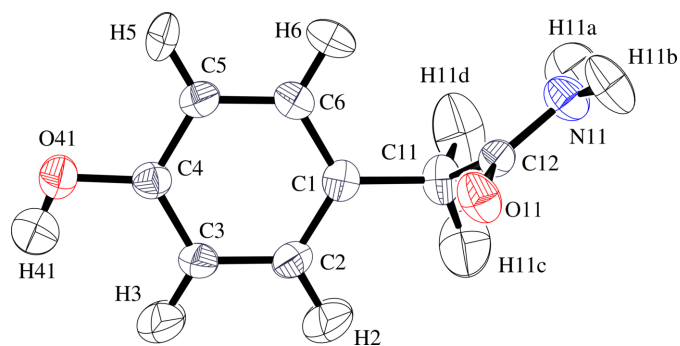


### Chemical scheme



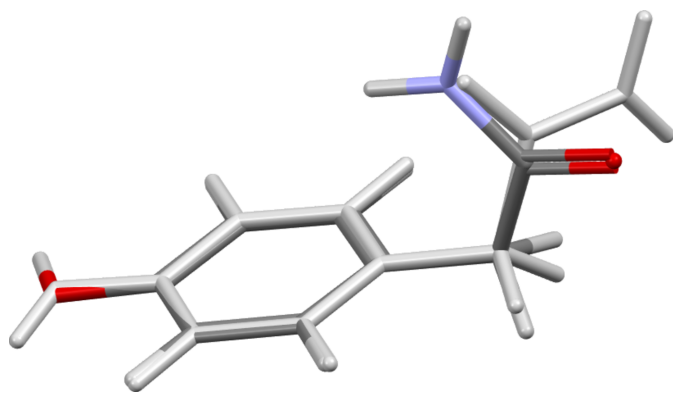
### Structure description

The title molecule,  $C_8H_9NO_2$  (**I**), is an isomer of *N*-(4-hydroxyphenyl)acetamide [Cambridge Structural Database (CSD) refcodes: HXACAN01–67], also known as acetaminophen or paracetamol in different countries. The mean  $C_a-N$  ( $a = \text{amide}$ ) bond length in structures of acetaminophen calculated from values in the CSD [ $1.346(25) \text{ \AA}$ ] is  $0.026 \text{ \AA}$  longer than in (**I**) (Fig. 1). The short  $C-N$  bond length in (**I**) is consistent with the well known ‘amide resonance’ effect (Kemnitz & Loewen, 2007). Bond lengths and angles within the amide group of (**I**) agree with mean values found for 2-substituted acetamide groups in the CSD [ $C-N=O$ :  $1.32(5)/1.23(5) \text{ \AA}$ ;  $N-C=O/C-C=O/C-C-N$ :  $122(5)/121(5)/116(5)^\circ$ ; 1620 hits, CSD Version 5.00, August 2025 updates, Groom *et al.*, 2016]. The  $-NH_2$  group in (**I**) is almost planar with slight pyramidalization [the N atom lies  $0.017 \text{ \AA}$  above the  $C12/N11/(H1a, H1b)$  mean plane] so that  $sp^2$  hybridization can be assigned to N11. The  $C_{ar}-OH$  ( $ar = \text{aromatic}$ ) bond length [ $1.381(3) \text{ \AA}$ ] found in the structure of the parent acid, 4-hydroxyphenylacetic acid (QAPBAL; Gracin & Fischer, 2005) is some  $0.019 \text{ \AA}$  longer than in (**I**). The  $C_{ar}-O-H$  angle agrees within 1 s.u. of  $109.5^\circ$  so that  $sp^3$  hybridization can be assumed for O41.

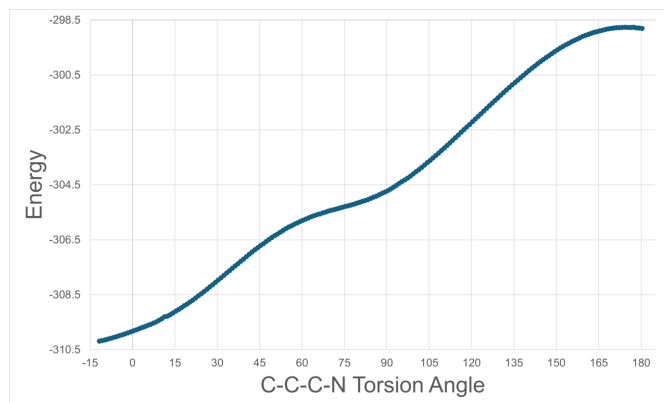


**Figure 1**  
Displacement ellipsoid plot of (**I**) at the 50% level with labels for all atoms.

The core atoms of (**I**) (C1–C6/C11/O41) are effectively planar [root-mean-square deviation (RMSD) = 0.003 Å] as are those of the acetamide group (C11, C12, O11, and N11; RMSD = 0.005 Å) with mean plane normals perpendicular [89.98 (5)°]. The –NH<sub>2</sub> group is directed outward from the phenyl ring and the carboxyl O-atom directed inward but not fully, as shown by the C1–C11–C12–N11 torsion angle of –135.91 (12)°. In contrast, since the N atom is bound to the phenyl ring in acetaminophen, the acetamide plane and the core atom plane are more closely aligned, *e.g.* with angles of 20.56 (5)° (monoclinic form I, HXACAN64) and 16.97 (5)° (orthorhombic form II, HXACAN65) between mean plane normals in recent structure determinations (Weatherston, 2024). In QAPBAL, the mean plane of the acid group is almost perpendicular to the phenyl ring mean plane [93.22 (14)°]. Here the carboxyl O-atom is directed inward, but with a larger torsion angle magnitude [159.8 (3)°]. A DFT geometry optimization [B3LYP, 6311+G(d,p); GAMESS (Schmidt *et al.*, 1993)] of (**I**) *in vacuo* results in the acetamide plane almost perpendicular (90.33°) to the plane of the core atoms, but with the carboxyl O atom directed outward, the –NH<sub>2</sub> group directed inward, and a torsion angle of –11.68° (Fig. 2). A semi-empirical, partially relaxed scan of this torsion angle (MOPAC2016, Version 19.255L, PM7 Hamiltonian;



**Figure 2**  
Capped stick plots of the DFT-optimized geometry (color scheme: C, gray; H, white; N, blue; O, red) superimposed on the experimental geometry (light gray) of (**I**).

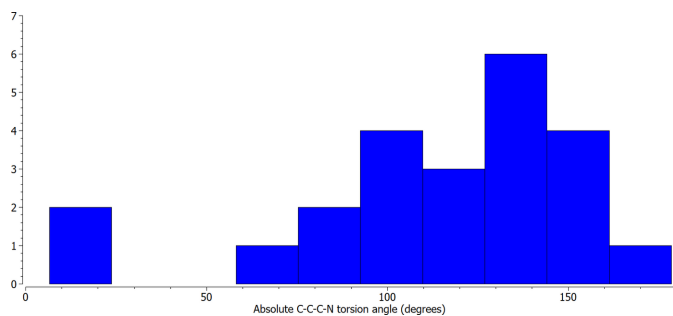


**Figure 3**  
Plot of a semiempirical, partially relaxed scan in 1° increments of the C1–C11–C12–N11 torsion angle in (**I**) starting at the DFT-optimized value to a value of 180.3°. The acetamide group is constrained to be approximately planar and to be approximately perpendicular to the phenyl ring during the scan. Energy (kJ mol<sup>-1</sup>) is plotted on the vertical axis with the torsion angle (°) plotted on the horizontal axis.

Stewart, 2016) shows a steady rise in energy from its optimized value to a maximum value as the torsion angle approaches 180° (Fig. 3). A MOL file of the optimized geometry has been placed in the supporting information.

A search of the CSD for 2-phenylacetamide molecules with any substitution at the 4-position on the phenyl ring yielded 21 hits that are dominated by pharmaceutically related compounds or natural products. Ten of these are structures of atenolol (CEZVIN and CIDHAZ; de Castro *et al.*, 2007), a  $\beta$  blocker medication for treatment of high blood pressure (Heel *et al.*, 1979), or its salts or cocrystal: [succinate (DETHIU; Cai *et al.*, 2006), nicotinate and isonicotinate (GUJBOG and GUJCAT; Botes *et al.*, 2024), fumarate and adipate (IGUWUG and UHOGUX; Shajan *et al.*, 2024), 4-aminobenzoate (JIRWIR; Lou *et al.*, 2007), chloride (WEWLOC; Rama Kumar *et al.*, 2018), and binaphthylphosphate (QAJYIL; Wang & Chen, 2011)]. The atenolol molecule possesses a substituted propoxy group at the 4-position and, as a result, (**I**) is a common reagent in its synthetic preparation (Procopio *et al.*, 2024).

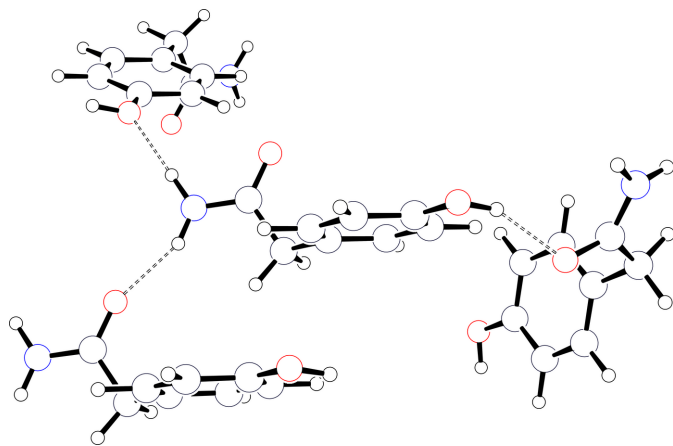
The crystal structures of atenolol show an orientation for the acetamide group similar to that in (**I**), *i.e.*, approximately perpendicular interplanar angles [86.01 (9)° for CEZVIN, 90.43 (11) and 86.74 (11)° for CIDHAZ] and similar torsion angle magnitudes [141.24 (19)° for CEZVIN, 135.0 (3) and 142.1 (2)° for CIDHAZ]. The acetamide groups in the salts and cocrystal show a range of orientations. For GUJBOG, JIRWIR, UHOGUX, and WEWLOC, the –NH<sub>2</sub> group is directed more outward, for DETHIEU, GUJCAT, and IGUWUG neither the –NH<sub>2</sub> nor –C=O groups are directed outward significantly, while for QAJYIL the –NH<sub>2</sub> group is directed more inward. In the structures of two other compounds, the natural product millingtonanine A (BAKWUJ; Jumai *et al.*, 2021) and 2-carboxamidomethyl-4,5-dimethoxy-phenyl-*N,N*-diethylsulfonamide (CXMESX; Hamdrakas *et al.*, 1977), the amide group is directed almost



**Figure 4**  
Histogram of the C—C—C—N torsion angle magnitude frequency for 2-phenylacetamide molecules with any substitution at the 4-position on the phenyl ring.

completely inward and similar to the orientation found in the DFT geometry optimization. At the opposite extreme is the structure of 2-(4-chlorophenyl)acetamide (OCETAT; Ma *et al.*, 2011) in which the  $\text{-NH}_2$  group is directed almost completely outward [torsion angle =  $178.6(2)^\circ$ ]. A histogram of torsion angle magnitudes for these compounds (Fig. 4) shows the full range of  $\text{-NH}_2$  group orientations with a mean value of  $115^\circ$  (standard deviation =  $42^\circ$ ) and a median of  $121.7^\circ$ . The orientation of the acetamide group appears to depend on competition between minimizing the molecular energy and optimizing the intermolecular hydrogen-bonding interactions, *e.g.*, an outward-directed  $\text{-NH}_2$  group may be more available as a hydrogen-bond donor if a suitable acceptor atom is present.

The  $\text{-NH}_2$  group in **(I)** is a hydrogen-bond donor to carboxyl and to hydroxyl O atoms while the hydroxyl group is a hydrogen-bond donor to a carboxyl O atom, each to different molecules (Fig. 5). The  $\text{N-H}\cdots\text{O}=\text{C}$  interaction links molecules into stacks along *a* with the other interactions linking neighboring parallel stacks (Fig. 6). By comparison, OCETAT is found in the same space group as **(I)** and with a slightly larger molecular volume [ $197.9(2)\text{ \AA}^3$  versus  $186.12(2)\text{ \AA}^3$  in **(I)**], but with the chloro substituent not



**Figure 5**  
Donor hydrogen-bond interactions by a given molecule in **(I)** to three neighboring molecules. Atoms are drawn as circles of arbitrary radii and hydrogen bonds are indicated by dashed lines.

**Table 1**  
Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D\text{-H}\cdots A$	$D\text{-H}$	$\text{H}\cdots A$	$D\cdots A$	$D\text{-H}\cdots A$
$\text{O41-H41}\cdots\text{O11}^{\text{i}}$	0.914 (18)	1.92 (2)	2.7703 (13)	154.1 (16)
$\text{N11-H11a}\cdots\text{O11}^{\text{ii}}$	0.947 (16)	2.041 (16)	2.9365 (16)	157.1 (13)
$\text{N11-H11b}\cdots\text{O41}^{\text{iii}}$	1.000 (15)	1.965 (16)	2.9646 (19)	178.0 (13)

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

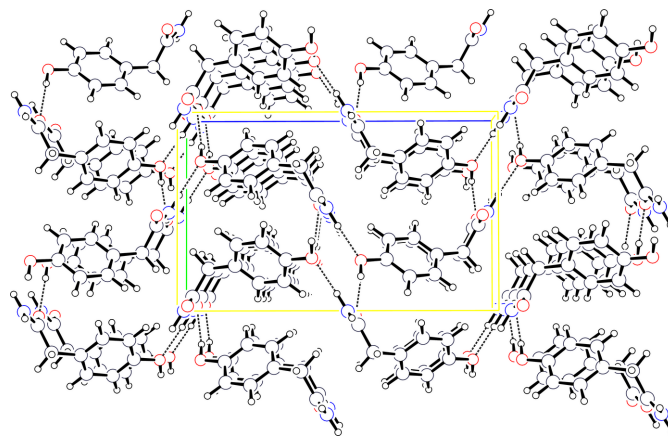
involved in N—H hydrogen bonding. In this case, the extended structure consists of herringbone bilayers with the acetamide groups linked by  $\text{N-H}\cdots\text{O}$  hydrogen bonding on the outside of the bilayer while the 4-chloro substituents abut each other in the middle. Hydrogen-bond geometrical data for **(I)** are presented in Table 1.

### Synthesis and crystallization

2-(4-Hydroxyphenyl)acetamide (Aldrich, 99%) was dissolved in methanol and diffraction-quality crystals grown by slow evaporation at room temperature.

### Refinement

Crystal data, data collection, and structure refinement details are listed in Table 2. Structure solution and initial refinement using an independent atom model occurred within the Bruker *APEX3* software package (Version 2019/11-0; Bruker 2019) followed by Hirshfeld atom refinement within the *OLEX2-1.5* system using *NoSpherA2* (Kleemiss *et al.*, 2021; Midgley *et al.*, 2021). Non-spherical atomic form factors were derived from electron density determined by DFT calculations using *ORCA 5.0* (B3LYP functional, def2-SVP basis set; Neese, 2022). All atoms were refined anisotropically. Two low angle reflections with  $F_o \ll F_c$  were presumed to be blocked by the beam catcher and omitted from the refinement. A secondary extinction correction coefficient was refined to a value of 0.017 (2).



**Figure 6**  
Unit-cell packing diagram for **(I)** viewed down *a* with *b* vertical and *c* horizontal. Atoms are drawn as circles of arbitrary radii and hydrogen bonds are indicated by dashed lines.

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Table 2

Experimental details.

Crystal data	
Chemical formula	C <sub>8</sub> H <sub>9</sub> NO <sub>2</sub>
<i>M<sub>r</sub></i>	151.17
Crystal system, space group	Orthorhombic, <i>P</i> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
Temperature (K)	295
<i>a</i> , <i>b</i> , <i>c</i> (Å)	5.0935 (2), 9.5089 (4), 15.3708 (7)
<i>V</i> (Å <sup>3</sup> )	744.46 (6)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm <sup>-1</sup> )	0.10
Crystal size (mm)	0.49 × 0.21 × 0.17
Data collection	
Diffractionmeter	Bruker D8 Quest Eco CCD
Absorption correction	Multi-scan ( <i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.689, 0.746
No. of measured, independent and observed [ <i>I</i> ≥ 2σ( <i>I</i> )] reflections	21517, 1908, 1483
<i>R<sub>int</sub></i>	0.057
(sin θ/λ) <sub>max</sub> (Å <sup>-1</sup> )	0.675
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.038, 0.048, 1.13
No. of reflections	1908
No. of parameters	182
H-atom treatment	All H-atom parameters refined
Δρ <sub>max</sub> , Δρ <sub>min</sub> (e Å <sup>-3</sup> )	0.20, −0.21
Absolute structure	Hooft <i>et al.</i> (2010)
Absolute structure parameter	−0.1 (5)

Computer programs: *SAINT* (Bruker, 2019), *SHELXT2018/2* (Sheldrick, 2015a), *OLEX2.refine* (Bourhis *et al.*, 2015), *SHELXL2018/3* (Sheldrick, 2015b), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2020) and *publCIF* (Westrip, 2010).

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## full crystallographic data

*IUCrData* (2025). **10**, x251007 [<https://doi.org/10.1107/S2414314625010077>]

## 2-(4-Hydroxyphenyl)acetamide

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## 2-(4-Hydroxyphenyl)acetamide

*Crystal data*

$C_8H_9NO_2$	$D_x = 1.349 \text{ Mg m}^{-3}$
$M_r = 151.17$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Orthorhombic, $P2_12_12_1$	Cell parameters from 6683 reflections
$a = 5.0935 (2) \text{ \AA}$	$\theta = 3.4\text{--}26.3^\circ$
$b = 9.5089 (4) \text{ \AA}$	$\mu = 0.10 \text{ mm}^{-1}$
$c = 15.3708 (7) \text{ \AA}$	$T = 295 \text{ K}$
$V = 744.46 (6) \text{ \AA}^3$	Rod, colourless
$Z = 4$	$0.49 \times 0.21 \times 0.17 \text{ mm}$
$F(000) = 320.229$	

*Data collection*

Bruker D8 Quest Eco CCD diffractometer	1908 independent reflections
$\varphi$ and $\omega$ scans	1483 reflections with $I \geq 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Krause <i>et al.</i> , 2015)	$R_{\text{int}} = 0.057$
$T_{\text{min}} = 0.689$ , $T_{\text{max}} = 0.746$	$\theta_{\text{max}} = 28.7^\circ$ , $\theta_{\text{min}} = 3.4^\circ$
21517 measured reflections	$h = -6 \rightarrow 6$
	$k = -12 \rightarrow 12$
	$l = -20 \rightarrow 20$

*Refinement*

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0163P)^2 + 0.0113P]$
Least-squares matrix: full	where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.038$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$wR(F^2) = 0.048$	$\Delta\rho_{\text{max}} = 0.20 \text{ e \AA}^{-3}$
$S = 1.13$	$\Delta\rho_{\text{min}} = -0.20 \text{ e \AA}^{-3}$
1908 reflections	Extinction correction: Zachariasen,
182 parameters	$F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
0 restraints	Extinction coefficient: 0.017 (2)
0 constraints	Absolute structure: Hooft <i>et al.</i> (2010)
Primary atom site location: dual	Absolute structure parameter: $-0.1 (5)$
All H-atom parameters refined	

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
O11	0.22820 (14)	0.47323 (8)	0.44521 (5)	0.0404 (2)
O41	-0.0450 (2)	0.24609 (10)	0.07225 (7)	0.0437 (3)
H41	-0.152 (3)	0.169 (2)	0.0717 (11)	0.069 (6)
N11	0.6580 (3)	0.49778 (15)	0.46884 (8)	0.0407 (3)

H11a	0.829 (3)	0.4650 (16)	0.4559 (9)	0.057 (4)
H11b	0.620 (3)	0.5855 (16)	0.5025 (10)	0.054 (5)
C1	0.3607 (2)	0.27802 (11)	0.30625 (6)	0.0329 (3)
C2	0.1609 (2)	0.18008 (13)	0.29703 (8)	0.0360 (3)
H2	0.111 (3)	0.1155 (13)	0.3516 (8)	0.065 (4)
C3	0.0224 (3)	0.16737 (13)	0.21944 (8)	0.0374 (3)
H3	-0.129 (3)	0.0902 (14)	0.2123 (7)	0.068 (4)
C4	0.0839 (2)	0.25385 (11)	0.14971 (7)	0.0326 (3)
C5	0.2843 (3)	0.35193 (14)	0.15763 (9)	0.0391 (3)
H5	0.332 (3)	0.4167 (14)	0.1032 (7)	0.064 (4)
C6	0.4203 (3)	0.36305 (14)	0.23543 (8)	0.0396 (3)
H6	0.573 (3)	0.4385 (14)	0.2415 (9)	0.076 (5)
C11	0.5106 (3)	0.29262 (15)	0.39025 (9)	0.0405 (3)
H11c	0.459 (3)	0.2104 (13)	0.4351 (9)	0.085 (6)
H11d	0.716 (3)	0.2869 (16)	0.3787 (9)	0.084 (5)
C12	0.4544 (2)	0.42959 (11)	0.43655 (7)	0.0283 (3)

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O11	0.0233 (4)	0.0482 (5)	0.0498 (5)	0.0059 (4)	-0.0030 (4)	-0.0130 (4)
O41	0.0497 (6)	0.0443 (6)	0.0370 (5)	-0.0048 (5)	-0.0088 (5)	0.0048 (5)
H41	0.054 (12)	0.097 (15)	0.055 (11)	-0.021 (11)	-0.004 (10)	0.011 (12)
N11	0.0260 (6)	0.0446 (8)	0.0517 (7)	0.0003 (6)	-0.0017 (6)	-0.0046 (6)
H11a	0.040 (9)	0.071 (10)	0.062 (10)	0.011 (9)	-0.003 (9)	0.008 (9)
H11b	0.043 (10)	0.042 (9)	0.077 (12)	-0.001 (8)	-0.013 (8)	-0.026 (8)
C1	0.0345 (6)	0.0314 (6)	0.0328 (6)	0.0065 (6)	0.0001 (5)	-0.0032 (5)
C2	0.0413 (7)	0.0353 (7)	0.0313 (7)	-0.0011 (6)	0.0057 (6)	0.0027 (6)
H2	0.088 (11)	0.057 (9)	0.050 (8)	-0.018 (9)	-0.001 (8)	0.020 (7)
C3	0.0400 (7)	0.0362 (8)	0.0360 (7)	-0.0103 (6)	0.0014 (6)	0.0010 (6)
H3	0.094 (11)	0.062 (10)	0.047 (8)	-0.035 (10)	-0.002 (8)	0.012 (7)
C4	0.0343 (7)	0.0295 (6)	0.0339 (6)	-0.0007 (6)	0.0023 (5)	-0.0003 (5)
C5	0.0460 (8)	0.0381 (7)	0.0332 (7)	-0.0083 (6)	0.0013 (6)	0.0050 (6)
H5	0.082 (10)	0.075 (10)	0.034 (7)	-0.025 (9)	-0.027 (8)	0.020 (7)
C6	0.0402 (8)	0.0379 (7)	0.0407 (8)	-0.0100 (6)	-0.0024 (6)	0.0005 (5)
H6	0.097 (12)	0.066 (9)	0.065 (9)	-0.057 (10)	-0.013 (9)	0.008 (8)
C11	0.0396 (9)	0.0395 (8)	0.0424 (8)	0.0136 (7)	-0.0090 (7)	-0.0042 (6)
H11c	0.137 (16)	0.037 (8)	0.080 (11)	-0.002 (9)	-0.042 (11)	0.015 (9)
H11d	0.071 (11)	0.091 (12)	0.090 (12)	0.038 (11)	-0.006 (9)	-0.059 (9)
C12	0.0237 (6)	0.0342 (6)	0.0270 (6)	0.0037 (5)	0.0007 (5)	0.0022 (5)

*Geometric parameters (Å, °)*

O11—C12	1.2319 (12)	C2—C3	1.3908 (16)
O41—H41	0.914 (18)	C3—H3	1.072 (13)
O41—C4	1.3618 (15)	C3—C4	1.3868 (15)
N11—H11a	0.947 (16)	C4—C5	1.3878 (16)
N11—H11b	1.000 (15)	C5—H5	1.067 (11)

N11—C12	1.3197 (16)	C5—C6	1.3862 (18)
C1—C2	1.3869 (16)	C6—H6	1.062 (13)
C1—C6	1.3895 (16)	C11—H11c	1.075 (14)
C1—C11	1.5063 (17)	C11—H11d	1.065 (15)
C2—H2	1.069 (11)	C11—C12	1.5115 (17)
C4—O41—H41	109.9 (11)	H5—C5—C4	119.1 (7)
H11b—N11—H11a	124.2 (14)	C6—C5—C4	119.63 (12)
C12—N11—H11a	118.8 (9)	C6—C5—H5	121.3 (7)
C12—N11—H11b	116.8 (9)	C5—C6—C1	121.48 (12)
C6—C1—C2	118.11 (11)	H6—C6—C1	118.9 (8)
C11—C1—C2	121.42 (11)	H6—C6—C5	119.6 (8)
C11—C1—C6	120.47 (12)	H11c—C11—C1	110.9 (7)
H2—C2—C1	118.6 (7)	H11d—C11—C1	110.6 (8)
C3—C2—C1	121.20 (12)	H11d—C11—H11c	108.2 (11)
C3—C2—H2	120.2 (7)	C12—C11—C1	112.78 (10)
H3—C3—C2	120.9 (6)	C12—C11—H11c	106.1 (7)
C4—C3—C2	119.78 (12)	C12—C11—H11d	108.0 (8)
C4—C3—H3	119.3 (6)	N11—C12—O11	121.91 (12)
C3—C4—O41	122.32 (11)	C11—C12—O11	121.20 (11)
C5—C4—O41	117.89 (11)	C11—C12—N11	116.86 (12)
C5—C4—C3	119.79 (11)		
O11—C12—C11—C1	45.69 (11)	C2—C1—C11—C12	-111.31 (12)
O41—C4—C3—C2	-179.97 (11)	C2—C3—C4—C5	0.39 (14)
O41—C4—C5—C6	-179.99 (11)	C3—C2—C1—C6	-0.34 (13)
N11—C12—C11—C1	-135.91 (12)	C3—C2—C1—C11	179.75 (11)
C1—C2—C3—C4	-0.05 (13)	C3—C4—C5—C6	-0.33 (13)
C1—C6—C5—C4	-0.07 (14)	C5—C6—C1—C11	-179.69 (11)
C2—C1—C6—C5	0.40 (13)	C6—C1—C11—C12	68.78 (12)

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O41—H41 $\cdots$ O11 <sup>i</sup>	0.914 (18)	1.92 (2)	2.7703 (13)	154.1 (16)
N11—H11a $\cdots$ O11 <sup>ii</sup>	0.947 (16)	2.041 (16)	2.9365 (16)	157.1 (13)
N11—H11b $\cdots$ O41 <sup>iii</sup>	1.000 (15)	1.965 (16)	2.9646 (19)	178.0 (13)

Symmetry codes: (i)  $-x, y-1/2, -z+1/2$ ; (ii)  $x+1, y, z$ ; (iii)  $-x+1/2, -y+1, z+1/2$ .