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N,*N*′-[Oxybis(benzene-4,1-diyl)]diacetamide

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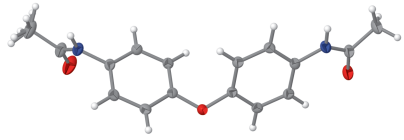
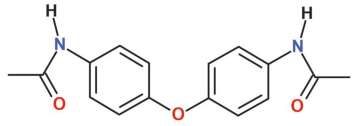
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{16}H_{16}N_2O_3$, the phenyl groups are twisted away from coplanarity with the ether linkage, forming a dihedral angle of 59.49 (4)° with each other. The ether oxygen atom lies somewhat out of both phenyl planes, by 0.066 (2) and 0.097 (2) Å. The acetamide substituents have quite different conformations with respect to the phenyl groups on either side of the molecule. On one side, the C—C—N—C torsion angle is 21.0 (2)°, while on the other side it is 76.4 (2)°. In the crystal, the acetamide N—H groups form intermolecular N—H···O hydrogen bonds to acetamide O atom, with both NH groups donating to the same molecule. Thus, ladder-like chains exist in the [101] direction. One of the methyl groups has its H atoms disordered into two orientations, and the crystal chosen for data collection was found to be twinned.

3D view



Chemical scheme



Structure description

Acetaminophen (*N*-[4-hydroxyphenyl]acetamide, $C_8H_9NO_2$), also known by various brand names such as Tylenol or Panadol in different countries, ranks among the most widely used pain relievers and fever reducers worldwide (Bertolini *et al.*, 2006; Ohashi & Kohno, 2020). Introduced in the 1950s, current estimates show that over 25 billion doses are sold each year in the United States alone (Yoon *et al.*, 2016). While this underscores the importance of acetaminophen in over-the-counter pain management, as with most medications, the focus extends beyond the safety and efficacy of the active pharmaceutical ingredient (API). Regulatory agencies also pay close attention to impurities, particularly those present in small amounts but still capable of raising concerns (ICH, 2006*a*,*b*). Although these impurities are generally not expected to cause immediate harm, about 50,000 emergency room visits in the United States each year are linked to acetaminophen toxicity, which can result in severe liver damage (specifically, centrilobular necrosis) and, in some cases, death (Stravitz & Lee, 2019; Yoon *et al.*, 2016). In

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O3^{i}	0.88 (2)	1.96 (2)	2.834 (2)	169.5 (19)
N2—H2N···O2^{i}	0.88 (2)	2.03 (2)	2.9066 (18)	170 (2)

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

recent years, the emphasis on monitoring even trace levels of impurities has increased, given their potential impact on both effectiveness of the drug and its long-term safety (ICH, 2006*a*, 2021).

The title compound, *N*,*N*′-(oxydibenzene-4,1-diyl)diacetamide ($C_{16}H_{16}N_2O_3$), commonly known as Impurity N, is one of over a dozen potential byproducts that can occur in acetaminophen. Typically present at levels below 0.1% of the active pharmaceutical ingredient (API) (Arıkan *et al.*, 2023), Impurity N forms when 4-aminophenol undergoes oxidative coupling during the manufacturing process. In standard industrial practice, 4-aminophenol is acetylated to produce acetaminophen; however, if two 4-aminophenol molecules couple oxidatively, they form 4,4′-oxydianiline, which then becomes Impurity N upon acetylation (NCBI, 2025). Even minimal traces of 4-aminophenol that dimerize or incomplete reduction of 4-nitrophenol can introduce this impurity. Additionally, under certain oxidizing conditions during storage, two acetaminophen molecules can theoretically couple *via* their phenolic –OH groups, creating the same ether-linked dimer (Rao & Narasaraju, 2006). These pathways are generally minor, and robust process controls combined with proper storage conditions typically keep Impurity N at trace levels (Kamberi *et al.*, 2004). Various analytical methods, such as reversed-phase HPLC or UPLC coupled with UV–Vis spectroscopy, photodiode array, or mass spectrometry detection are used to detect Impurity N with sensitivity down to p.p.m. or sub-p.p.m., ensuring that its presence remains within acceptable limits in the final acetaminophen batches (Arıkan *et al.*, 2023).

Impurity N currently lacks any toxicological or pharmacological characterization. However, by analogy to the metabolism of acetaminophen and other 4-alkoxyanilides, this impurity is likely to undergo partial or complete deacetylation (Nohmi *et al.*, 1984; Ohashi & Kohno, 2020; Prescott, 1980). Such metabolism would yield aromatic amine derivatives, notably *N*[4-(4-aminophenoxy)phenyl]acetamide (the mono-deacetylated product) and 4,4′-oxydianiline (the fully de-acetylated diamine). In turn, these aromatic amines could undergo further biotransformations analogous to those of 4-aminophenol and 4-alkoxyaniline, potentially forming *N*-arachidonoylphenolamine (AM404)-like anandamide analogues or 4-alkoxynitrosophenol derivatives (Ohashi & Kohno, 2020; Zygmunt *et al.*, 2000). Metabolites of this type are known to elicit diverse pharmacological and pathophysiological effects. For example, certain 4-alkoxyaniline metabolites can inhibit cyclooxygenase-1 (COX-1) and have demonstrated carcinogenic and nephrotoxic effects (Kankuri *et al.*, 2003; NTP, 1990; Togei *et al.*, 1987). These metabolic considerations suggest that Impurity N could similarly give rise to bioactive or toxic species, warranting further toxicological evaluation, despite the current lack of direct data. To better understand the molecular structure and to inform studies of its potential biological interactions, we crystallized Impurity N from aqueous solution and determined its structure *via* single-crystal X-ray diffraction.

The title compound, $C_{16}H_{16}N_2O_3$ crystallizes with one molecule in the asymmetric unit (Fig. 1) in space group $P2_1/n$. The C1–C6 and C9–C14 phenyl groups are twisted out of coplanarity with the ether linkage, forming a dihedral angle of 59.49 (4)° with each other. The ether oxygen atom, O1, lies slightly out of the planes of both phenyl rings, by 0.066 (2) and 0.097 (2) Å, respectively. The acetamide substituents adopt markedly different conformations relative to the adjacent phenyl groups. On one side of the molecule, the C3—C4—N1—C7 torsion angle is 21.0 (2)°, while on the opposite side, the C13—C12—N2—C15 angle is 76.4 (2)°.

In the extended structure, the acetamide N—H groups participate in N—H···O hydrogen bonds (Table 1), each donating to the carbonyl oxygen atom of another acetamide group. Both N—H donors interact with the same acceptor molecule at $x+\frac{1}{2}, \frac{3}{2}-y, \frac{1}{2}+z$, resulting in the formation of ladder-like chains extending along the [101] direction, as shown in Fig. 2. The N···O distances in these hydrogen bonds are 2.834 (2) and 2.9066 (18) Å. One of the methyl groups exhibits hydrogen-atom disorder over two orientations, and

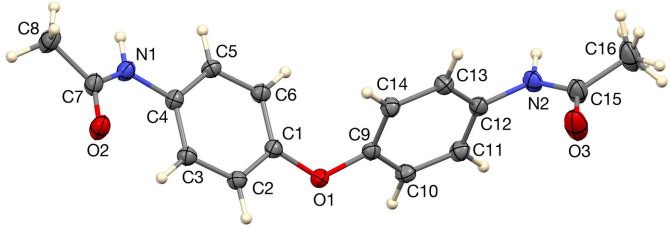


Figure 1
The asymmetric unit of the title compound with 50% ellipsoids.

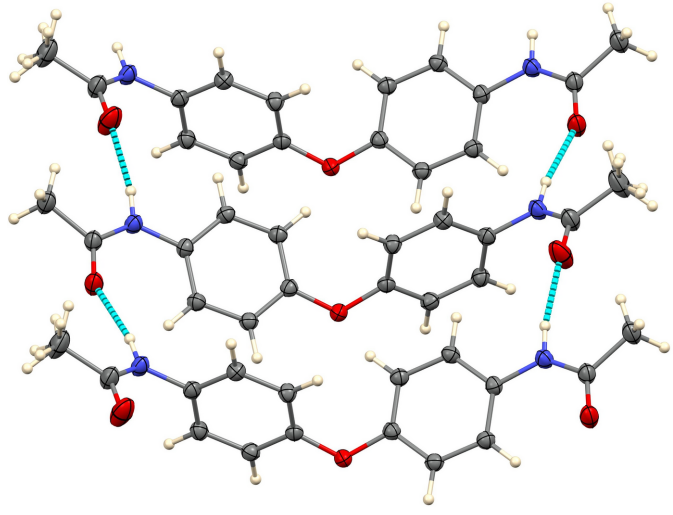


Figure 2
Detail of the the hydrogen bonding with 50% ellipsoids.

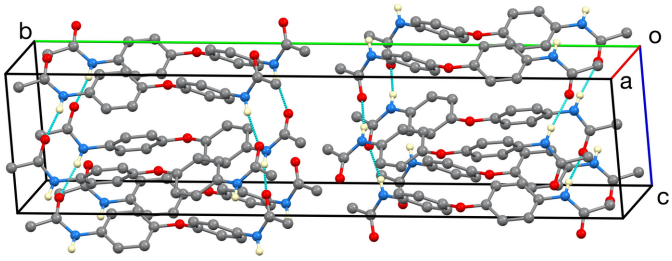


Figure 3
The unit-cell packing. Only NH hydrogen atoms are shown.

the crystal was a pseudomerohedral twin. The unit-cell packing is illustrated in Fig. 3.

Synthesis and crystallization

N,*N*′-(Oxydibenzene-4,1-diyl)diacetamide, $C_{16}H_{16}N_2O_3$ (CAS 3070–86-8) was obtained from AmBeed (Arlington Heights, Illinois, USA) and was used without further purification. Crystals in the form of colorless laths were prepared by slow cooling of a nearly saturated solution of the title compound in boiling deionized water (resistance *ca*. 18 *M*Ω cm^{-1}).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The crystal was a slight pseudomerohedral twin with twin law [1 0 0, 0 −1 0, 0 0 −1] and refined BASF parameter of 0.0053 (5). All H atoms were located in difference maps and those on C were thereafter treated as riding in geometrically idealized positions with C—H distances 0.95 Å for phenyl and 0.98 Å for methyl. Coordinates of the N—H atom were refined. U_{iso}(H) values were assigned as 1.2U_{eq} for the attached atom (1.5 for methyl). The H atoms on methyl group C16 were disordered into two conformations and were treated as two half-occupied sets related by a 60° torsional rotation. A residual density peak of 0.90 e Å^{-3} lies 0.95 Å from the O atom (O3) of the acetamide containing the disordered methyl group, perhaps indicative of further disorder in this substituent or imperfect handling of the twinning. The 0 4 0 reflection was omitted from the refinement, having negative F_o and large F_c.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{16}N_2O_3$
M_r	284.31
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	100
a, b, c (Å)	5.5676 (5), 33.185 (3), 7.6949 (5)
β (°)	90.325 (2)
V (Å^3)	1421.68 (19)
Z	4
Radiation type	Ag $K\alpha$, λ = 0.56086 Å
μ (mm^{-1})	0.06
Crystal size (mm)	0.32 × 0.27 × 0.09
Data collection	
Diffractometer	Bruker D8 Venture DUO with Photon III C14
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.933, 0.995
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22399, 4306, 3468
R_{int}	0.065
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.714
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.065, 0.179, 1.05
No. of reflections	4306
No. of parameters	198
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.90, −0.43

Computer programs: *APEX5* and *SAINT* (Bruker, 2016), *SHELXT2018/2* (Sheldrick, 2015a), *SHELXL2019/1* (Sheldrick, 2015b), *Mercury* (Macrae *et al.*, 2020) and *publCIF* (Westrip, 2010).

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full crystallographic data

IUCrData (2025). **10**, x250384 [https://doi.org/10.1107/S2414314625003840]

N,*N*′-[Oxybis(benzene-4,1-diyl)]diacetamide

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Crystal data

$C_{16}H_{16}N_2O_3$
M_r = 284.31
Monoclinic, $P2_1/n$
a = 5.5676 (5) Å
b = 33.185 (3) Å
c = 7.6949 (5) Å
β = 90.325 (2)°
V = 1421.68 (19) Å^3
Z = 4
$F(000)$ = 600
D_x = 1.328 Mg m^{-3}
Ag $K\alpha$ radiation, λ = 0.56086 Å
Cell parameters from 4722 reflections
θ = 2.5–23.6°
μ = 0.06 mm^{-1}
T = 100 K
Plate, colourless
0.32 × 0.27 × 0.09 mm

Data collection

Bruker D8 Venture DUO with Photon III C14 diffractometer
Radiation source: IμS 3.0 microfocus
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.933, T_{max} = 0.995
22399 measured reflections
4306 independent reflections
3468 reflections with $I > 2\sigma(I)$
R_{int} = 0.065
θ_{max} = 23.6°, θ_{min} = 2.1°
h = −7→5
k = −47→47
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.179
S = 1.05
4306 reflections
198 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0799P)^2 + 0.725P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.90 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

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. Refined as a 2-component twin.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.1938 (2)	0.75069 (3)	0.64144 (15)	0.0233 (2)	
O2	0.4346 (2)	0.56780 (3)	0.40229 (16)	0.0333 (3)	
O3	0.5307 (3)	0.91576 (5)	0.3437 (2)	0.0510 (4)	
N1	0.6286 (3)	0.59932 (4)	0.62577 (17)	0.0247 (3)	
H1N	0.756 (4)	0.5980 (6)	0.695 (3)	0.030*	
N2	0.6478 (3)	0.90044 (4)	0.61679 (18)	0.0263 (3)	
H2N	0.744 (4)	0.9074 (6)	0.703 (3)	0.032*	
C1	0.3149 (3)	0.71413 (4)	0.63352 (18)	0.0209 (3)	
C2	0.1942 (3)	0.68320 (4)	0.54986 (19)	0.0222 (3)	
H2A	0.045052	0.688389	0.493585	0.027*	
C3	0.2906 (3)	0.64448 (4)	0.54791 (19)	0.0228 (3)	
H3	0.205855	0.623136	0.492738	0.027*	
C4	0.5119 (3)	0.63719 (4)	0.62715 (19)	0.0215 (3)	
C5	0.6302 (3)	0.66855 (4)	0.71332 (19)	0.0218 (3)	
H5	0.779782	0.663529	0.769297	0.026*	
C6	0.5316 (3)	0.70702 (4)	0.71806 (19)	0.0223 (3)	
H6	0.611423	0.728157	0.778366	0.027*	
C7	0.5930 (3)	0.56846 (4)	0.5137 (2)	0.0261 (3)	
C8	0.7694 (4)	0.53426 (5)	0.5312 (3)	0.0348 (4)	
H8A	0.893903	0.541497	0.616144	0.052*	
H8B	0.843772	0.529005	0.418365	0.052*	
H8C	0.685113	0.510015	0.570580	0.052*	
C9	0.3190 (3)	0.78663 (4)	0.63494 (18)	0.0204 (3)	
C10	0.2098 (3)	0.81915 (5)	0.7162 (2)	0.0234 (3)	
H10	0.063804	0.815553	0.777608	0.028*	
C11	0.3159 (3)	0.85704 (4)	0.7068 (2)	0.0246 (3)	
H11	0.240517	0.879529	0.759981	0.030*	
C12	0.5310 (3)	0.86207 (4)	0.62024 (19)	0.0228 (3)	
C13	0.6378 (3)	0.82935 (4)	0.53787 (19)	0.0230 (3)	
H13	0.784291	0.832953	0.477080	0.028*	
C14	0.5318 (3)	0.79144 (4)	0.54388 (19)	0.0222 (3)	
H14	0.603747	0.769176	0.486610	0.027*	
C15	0.6455 (4)	0.92400 (5)	0.4754 (2)	0.0335 (4)	
C16	0.8005 (4)	0.96122 (6)	0.4857 (3)	0.0458 (5)	
H16A	0.877402	0.962618	0.600446	0.069*	0.5
H16B	0.924151	0.960014	0.395741	0.069*	0.5
H16C	0.700668	0.985194	0.467726	0.069*	0.5
H16D	0.790745	0.975933	0.375496	0.069*	0.5
H16E	0.743996	0.978537	0.580201	0.069*	0.5
H16F	0.967479	0.953357	0.508215	0.069*	0.5

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0205 (5)	0.0192 (5)	0.0303 (6)	0.0009 (4)	−0.0001 (4)	0.0008 (4)

O2	0.0427 (7)	0.0221 (5)	0.0349 (6)	0.0029 (5)	−0.0140 (5)	−0.0010 (4)
O3	0.0667 (11)	0.0395 (8)	0.0464 (8)	−0.0211 (7)	−0.0289 (8)	0.0121 (6)
N1	0.0271 (7)	0.0211 (6)	0.0257 (6)	0.0031 (5)	−0.0055 (5)	0.0009 (5)
N2	0.0302 (7)	0.0218 (6)	0.0269 (7)	−0.0051 (5)	−0.0066 (5)	−0.0020 (5)
C1	0.0207 (7)	0.0202 (6)	0.0219 (6)	0.0009 (5)	0.0003 (5)	0.0019 (5)
C2	0.0203 (7)	0.0236 (7)	0.0228 (7)	−0.0002 (5)	−0.0016 (5)	0.0006 (5)
C3	0.0225 (7)	0.0225 (7)	0.0235 (7)	−0.0012 (5)	−0.0025 (5)	0.0003 (5)
C4	0.0235 (7)	0.0198 (6)	0.0212 (7)	0.0013 (5)	−0.0003 (5)	0.0014 (5)
C5	0.0209 (7)	0.0231 (7)	0.0215 (6)	0.0012 (5)	−0.0023 (5)	0.0011 (5)
C6	0.0227 (7)	0.0221 (7)	0.0219 (7)	−0.0002 (5)	−0.0017 (5)	−0.0003 (5)
C7	0.0313 (8)	0.0194 (6)	0.0275 (7)	0.0011 (6)	−0.0039 (6)	0.0013 (5)
C8	0.0406 (10)	0.0238 (7)	0.0399 (9)	0.0080 (7)	−0.0109 (8)	−0.0036 (6)
C9	0.0201 (6)	0.0201 (6)	0.0210 (6)	0.0003 (5)	−0.0035 (5)	−0.0001 (5)
C10	0.0211 (7)	0.0244 (7)	0.0247 (7)	0.0022 (5)	−0.0006 (5)	−0.0021 (5)
C11	0.0256 (7)	0.0221 (7)	0.0261 (7)	0.0029 (5)	−0.0020 (6)	−0.0043 (5)
C12	0.0249 (7)	0.0201 (6)	0.0231 (7)	−0.0007 (5)	−0.0052 (5)	−0.0014 (5)
C13	0.0226 (7)	0.0226 (7)	0.0237 (7)	−0.0005 (5)	0.0001 (5)	0.0000 (5)
C14	0.0230 (7)	0.0213 (6)	0.0224 (7)	0.0009 (5)	0.0013 (5)	−0.0010 (5)
C15	0.0399 (10)	0.0250 (8)	0.0355 (9)	−0.0077 (7)	−0.0111 (7)	0.0029 (6)
C16	0.0603 (13)	0.0322 (9)	0.0446 (11)	−0.0202 (9)	−0.0143 (10)	0.0058 (8)

Geometric parameters (Å, º)

O1—C9	1.3827 (17)	C8—H8A	0.9800
O1—C1	1.3896 (17)	C8—H8B	0.9800
O2—C7	1.227 (2)	C8—H8C	0.9800
O3—C15	1.226 (2)	C9—C10	1.389 (2)
N1—C7	1.353 (2)	C9—C14	1.389 (2)
N1—C4	1.4150 (19)	C10—C11	1.392 (2)
N1—H1N	0.88 (2)	C10—H10	0.9500
N2—C15	1.340 (2)	C11—C12	1.384 (2)
N2—C12	1.4299 (19)	C11—H11	0.9500
N2—H2N	0.88 (2)	C12—C13	1.392 (2)
C1—C2	1.384 (2)	C13—C14	1.391 (2)
C1—C6	1.388 (2)	C13—H13	0.9500
C2—C3	1.393 (2)	C14—H14	0.9500
C2—H2A	0.9500	C15—C16	1.508 (2)
C3—C4	1.392 (2)	C16—H16A	0.9800
C3—H3	0.9500	C16—H16B	0.9800
C4—C5	1.397 (2)	C16—H16C	0.9800
C5—C6	1.390 (2)	C16—H16D	0.9800
C5—H5	0.9500	C16—H16E	0.9800
C6—H6	0.9500	C16—H16F	0.9800
C7—C8	1.506 (2)		
C9—O1—C1	120.45 (12)	H8A—C8—H8C	109.5
C7—N1—C4	127.70 (13)	H8B—C8—H8C	109.5
C7—N1—H1N	117.3 (14)	O1—C9—C10	115.59 (13)

C4—N1—H1N	114.1 (13)	O1—C9—C14	123.29 (13)
C15—N2—C12	122.17 (14)	C10—C9—C14	120.97 (13)
C15—N2—H2N	117.5 (14)	C9—C10—C11	119.45 (14)
C12—N2—H2N	119.5 (14)	C9—C10—H10	120.3
C2—C1—C6	120.72 (13)	C11—C10—H10	120.3
C2—C1—O1	115.69 (13)	C12—C11—C10	120.20 (14)
C6—C1—O1	123.27 (13)	C12—C11—H11	119.9
C1—C2—C3	120.20 (14)	C10—C11—H11	119.9
C1—C2—H2A	119.9	C11—C12—C13	119.87 (14)
C3—C2—H2A	119.9	C11—C12—N2	120.73 (13)
C4—C3—C2	119.72 (14)	C13—C12—N2	119.39 (14)
C4—C3—H3	120.1	C14—C13—C12	120.53 (14)
C2—C3—H3	120.1	C14—C13—H13	119.7
C3—C4—C5	119.48 (13)	C12—C13—H13	119.7
C3—C4—N1	123.81 (13)	C9—C14—C13	118.95 (13)
C5—C4—N1	116.72 (13)	C9—C14—H14	120.5
C6—C5—C4	120.73 (14)	C13—C14—H14	120.5
C6—C5—H5	119.6	O3—C15—N2	122.93 (16)
C4—C5—H5	119.6	O3—C15—C16	121.45 (16)
C1—C6—C5	119.09 (13)	N2—C15—C16	115.60 (16)
C1—C6—H6	120.5	C15—C16—H16A	109.5
C5—C6—H6	120.5	C15—C16—H16B	109.5
O2—C7—N1	124.15 (14)	H16A—C16—H16B	109.5
O2—C7—C8	120.98 (14)	C15—C16—H16C	109.5
N1—C7—C8	114.85 (14)	H16A—C16—H16C	109.5
C7—C8—H8A	109.5	H16B—C16—H16C	109.5
C7—C8—H8B	109.5	H16D—C16—H16E	109.5
H8A—C8—H8B	109.5	H16D—C16—H16F	109.5
C7—C8—H8C	109.5	H16E—C16—H16F	109.5

C9—O1—C1—C2	−146.40 (13)	C1—O1—C9—C10	−153.03 (13)
C9—O1—C1—C6	40.1 (2)	C1—O1—C9—C14	31.3 (2)
C6—C1—C2—C3	−0.7 (2)	O1—C9—C10—C11	−176.08 (13)
O1—C1—C2—C3	−174.44 (13)	C14—C9—C10—C11	−0.3 (2)
C1—C2—C3—C4	−1.4 (2)	C9—C10—C11—C12	−1.3 (2)
C2—C3—C4—C5	2.4 (2)	C10—C11—C12—C13	1.9 (2)
C2—C3—C4—N1	−177.33 (14)	C10—C11—C12—N2	−176.98 (14)
C7—N1—C4—C3	21.0 (2)	C15—N2—C12—C11	−104.7 (2)
C7—N1—C4—C5	−158.72 (16)	C15—N2—C12—C13	76.4 (2)
C3—C4—C5—C6	−1.1 (2)	C11—C12—C13—C14	−0.9 (2)
N1—C4—C5—C6	178.57 (13)	N2—C12—C13—C14	178.00 (13)
C2—C1—C6—C5	1.9 (2)	O1—C9—C14—C13	176.73 (13)
O1—C1—C6—C5	175.17 (13)	C10—C9—C14—C13	1.3 (2)
C4—C5—C6—C1	−1.0 (2)	C12—C13—C14—C9	−0.7 (2)
C4—N1—C7—O2	−6.5 (3)	C12—N2—C15—O3	5.1 (3)
C4—N1—C7—C8	171.91 (15)	C12—N2—C15—C16	−173.16 (17)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O3^{i}	0.88 (2)	1.96 (2)	2.834 (2)	169.5 (19)
N2—H2*N*···O2^{i}	0.88 (2)	2.03 (2)	2.9066 (18)	170 (2)

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