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Crystal structure of (*E*)-2-{{(4-anilinophenyl)imino}-methyl}-4-nitrophenol

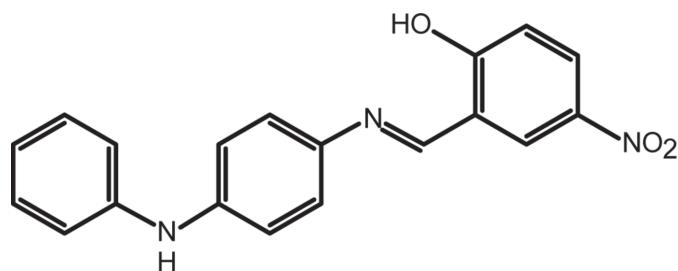
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In the title compound, $C_{19}H_{15}N_3O_3$, which crystallizes as the phenol-imine tautomer, the dihedral angle between the aromatic rings bridged by the NH unit is $47.16(16)^\circ$. The dihedral angle between the rings bridged by the imine unit is $6.24(15)^\circ$; this near coplanarity is reinforced by an intramolecular O—H···N hydrogen bond, which generates an S(6) ring. In the crystal, N—H···O hydrogen bonds generate [201] $C(13)$ chains. The chains are reinforced and cross-linked by C—H···O interactions to generate (001) sheets.

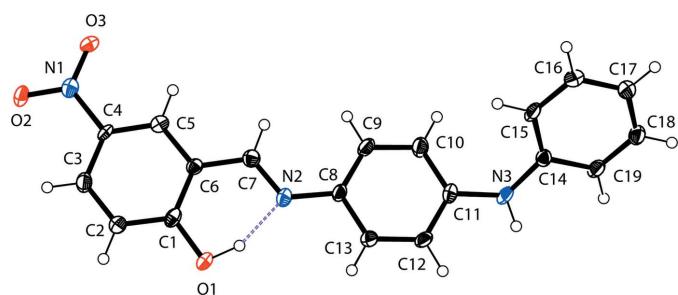
1. Chemical context

Schiff bases derived from 2-hydroxy-5-nitrobenzaldehyde are widely used either as materials or as intermediates in explosives, dyestuffs, pesticides and organic synthesis (Yan *et al.*, 2006). Intramolecular hydrogen-atom transfer (tautomerism) from the *o*-hydroxy group to the imine-N atom is of prime importance with respect to the solvato-, thermo- and photochromic properties exhibited by *o*-hydroxy Schiff bases (Filarowski, 2005; Hadjoudis *et al.*, 2004). Such proton-exchanging materials can be utilized for the design of various molecular electronic devices (Alarcón *et al.*, 1999). As part of our ongoing studies of Schiff bases and their complexes (Faizi *et al.*, 2016), we now report the synthesis (from 2-hydroxy-5-nitrobenzaldehyde and *N*-phenyl-*p*-phenylenediamine) and crystal structure of the title compound, (I).



2. Structural commentary

The molecular structure of the title compound, (I), is illustrated in Fig. 1. There is an intramolecular O—H···N hydrogen bond (Table 1), which is a common feature in related imine-phenol compounds. The imine group displays a C6—C7—N2—C8 torsion angle of $177.1(3)^\circ$ and the nitro phenol ring (C1—C6) is inclined to the central benzene ring

**Figure 1**

The molecular structure of the title compound, with displacement ellipsoids drawn at the 40% probability level. The intramolecular O—H···N hydrogen bond is shown as a dashed line.

(C8—C13) by 6.24 (4)°. The overall twisted conformation of the molecule is largely determined by the orientation of the terminal aminophenyl ring (C14—C19) with respect to the central benzene ring (C8—C13); the dihedral angle between them is 47.18 (4)°. The two outer aromatic rings (C1—C6 and C14—C19) are inclined to one another by 42.08 (4)°. The C1—O1 distance [1.351 (4) Å] is close to normal values reported for single C—O bonds in phenols and salicylideneamines (Ozeryanskii *et al.*, 2006). The N2—C7 bond is short at 1.287 (4) Å, strongly indicating the existence of a conjugated C=N bond, while the long C6—C7 bond [1.445 (4) Å] implies a single bond. All these data support the existence of the phenol-imine tautomer for (I) in its crystalline state. These features are similar to those observed in related 4-dimethylamino-N-salicylideneanilines (Filipenko *et al.*, 1983; Aldoshin *et al.*, 1984; Wozniak *et al.*, 1995; Pizzala *et al.*, 2000).

3. Supramolecular features

In the crystal, molecules are connected by N—H···O hydrogen bonds, generating *C*(13) chains propagating in the

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>
O1—H1O1···N2	0.97 (4)	1.67 (4)	2.573 (4)	155 (4)
N3—H1N3···O3 ⁱ	0.85 (3)	2.40 (3)	3.140 (4)	147 (3)
C3—H3···O2 ⁱⁱ	0.93	2.48	3.217 (4)	136
C12—H12···O2 ^j	0.93	2.55	3.470 (4)	173

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

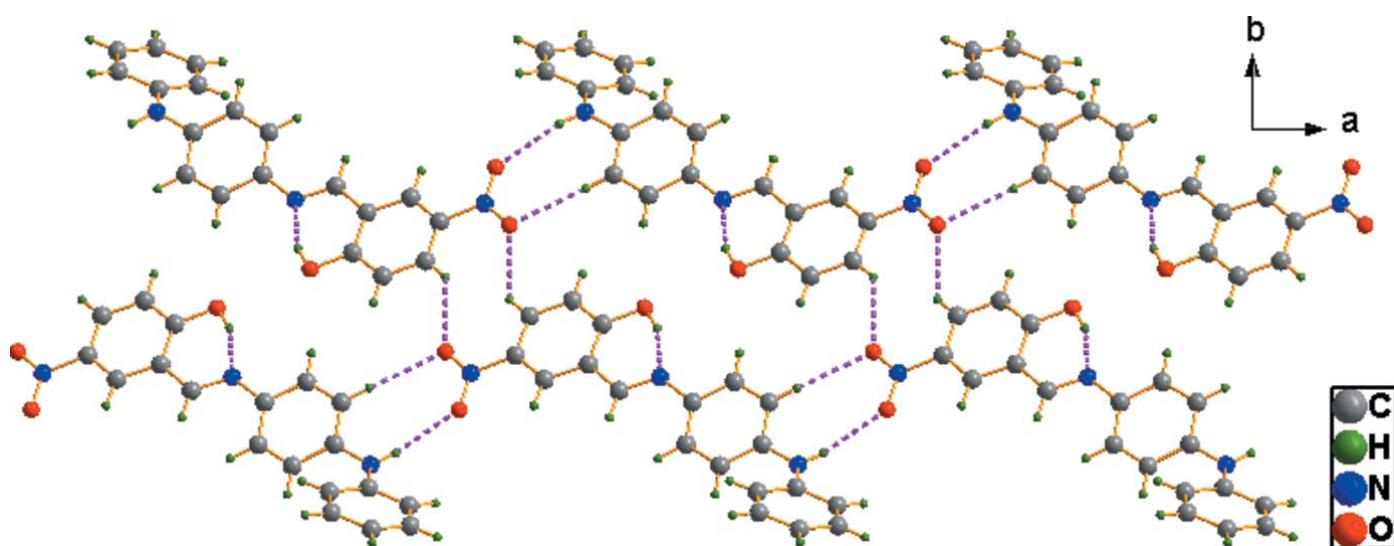
[001] direction. The chains are reinforced by the C12—H12···O2 link and cross-linked by the C3—H3···O2 bond [which in its own right generates a *C*(5) chain] (Table 1), resulting in (001) sheets (Fig. 2).

4. Database survey

A search of the Cambridge Structural Database (Groom *et al.*, 2016) revealed the structure of one very similar compound, *viz.* (*E*)-2-((4-(dialkylamino)phenyl)imino)methyl)-4-nitrophenol (II) (Valkonen *et al.*, 2012), in which the 4-alkylamino-substituted benzene ring in the title compound is replaced by a 4-*N*-phenylbenzene ring. In (II), the 4-alkylamino-substituted ring makes a dihedral angle of 13.44 (19)° with the 4-nitro-substituted phenol ring. The equivalent dihedral angle is smaller in the title compound [6.24 (4)°] owing to the presence of the intramolecular O—H···N hydrogen bond.

5. Synthesis and crystallization

100 mg (1 mmol) of *N*-phenyl-*p*-phenylenediamine was dissolved in 10 ml of absolute ethanol. To this solution, 90 mg (1 mmol) of 2-hydroxy-5-nitrobenzaldehyde in 5 ml of absolute ethanol was added dropwise with stirring. The mixture was stirred for 10 min, two drops of glacial acetic acid were

**Figure 2**

A view down [001] of the N—H···O and C—H···O interactions (shown as dashed lines) in the crystal of the title compound.

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₁₉ H ₁₅ N ₃ O ₃
M _r	333.34
Crystal system, space group	Monoclinic, P2 ₁ /n
Temperature (K)	293
a, b, c (Å)	6.4243 (12), 31.818 (6), 7.6595 (14)
β (°)	100.736 (5)
V (Å ³)	1538.2 (5)
Z	4
Radiation type	Mo Kα
μ (mm ⁻¹)	0.10
Crystal size (mm)	0.20 × 0.15 × 0.10
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (SADABS; Sheldrick, 2014)
T _{min} , T _{max}	0.954, 0.983
No. of measured, independent and observed [I > 2σ(I)] reflections	18286, 2760, 1365
R _{int}	0.113
(sin θ/λ) _{max} (Å ⁻¹)	0.599
Refinement	
R[F ² > 2σ(F ²)], wR(F ²), S	0.067, 0.125, 1.01
No. of reflections	2760
No. of parameters	233
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.25, -0.21

Computer programs: APEX2 and SAINT (Bruker, 2003), SHELXS97 (Sheldrick, 2008), SHELXL-2014/7 (Sheldrick, 2014) and DIAMOND (Brandenberg & Putz, 2006).

then added and the mixture was refluxed for 2 h. The resulting reddish yellow precipitate was recovered by filtration, washed several times with small portions of EtOH and then with diethyl ether to give 150 mg (83%) of the title compound. Colourless blocks of (I) were obtained within three days by slow evaporation of a solution in methanol.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The O—H, N—H and H atoms

were located in a difference-Fourier map and freely refined. All C-bound H atoms were positioned geometrically and refined using a riding model with C—H = 0.93–0.97 Å and with U_{iso}(H) = 1.2–1.5U_{eq}(C).

Acknowledgements

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Crystal structure of (*E*)-2-{{(4-anilinophenyl)imino)methyl}-4-nitrophenol

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Computing details

Data collection: *APEX2* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT* (Bruker, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL-2014/7* (Sheldrick, 2014); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2006); software used to prepare material for publication: *DIAMOND* (Brandenberg & Putz, 2006).

(*E*)-2-{{(4-Anilinophenyl)imino)methyl}-4-nitrophenol

Crystal data

$C_{19}H_{15}N_3O_3$
 $M_r = 333.34$
Monoclinic, $P2_1/n$
 $a = 6.4243 (12)$ Å
 $b = 31.818 (6)$ Å
 $c = 7.6595 (14)$ Å
 $\beta = 100.736 (5)^\circ$
 $V = 1538.2 (5)$ Å³
 $Z = 4$

$F(000) = 696$
 $D_x = 1.439 \text{ Mg m}^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1374 reflections
 $\theta = 2.7\text{--}25.0^\circ$
 $\mu = 0.10 \text{ mm}^{-1}$
 $T = 293 \text{ K}$
Block, colourless
 $0.20 \times 0.15 \times 0.10$ mm

Data collection

Bruker APEXII CCD
diffractometer
Radiation source: fine-focus sealed tube
Horizontally mounted graphite crystal
monochromator
Detector resolution: 9 pixels mm⁻¹
 φ scans and ω scans with κ offset
Absorption correction: multi-scan
(SADABS; Sheldrick, 2014)

$T_{\min} = 0.954, T_{\max} = 0.983$
18286 measured reflections
2760 independent reflections
1365 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.113$
 $\theta_{\max} = 25.2^\circ, \theta_{\min} = 2.6^\circ$
 $h = -7 \rightarrow 7$
 $k = -37 \rightarrow 38$
 $l = -9 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.067$
 $wR(F^2) = 0.125$
 $S = 1.01$
2760 reflections
233 parameters
0 restraints
Primary atom site location: structure-invariant
direct methods

Hydrogen site location: inferred from
neighbouring sites
H atoms treated by a mixture of independent
and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.040P)^2 + 0.4218P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.25 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.21 \text{ e } \text{\AA}^{-3}$

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.7180 (4)	0.01793 (8)	1.0878 (3)	0.0290 (6)
H1O1	0.657 (6)	0.0376 (13)	0.997 (5)	0.070 (14)*
O2	1.6498 (3)	0.05876 (7)	1.4408 (3)	0.0322 (7)
O3	1.5860 (3)	0.11239 (8)	1.2643 (3)	0.0299 (6)
N1	1.5327 (4)	0.07871 (10)	1.3227 (4)	0.0255 (7)
N2	0.6467 (4)	0.08236 (9)	0.8823 (3)	0.0241 (7)
N3	0.0003 (4)	0.16368 (10)	0.4069 (4)	0.0306 (8)
H1N3	-0.118 (5)	0.1527 (10)	0.413 (4)	0.037*
C1	0.9164 (5)	0.03312 (11)	1.1387 (4)	0.0235 (9)
C2	1.0557 (5)	0.01128 (11)	1.2681 (4)	0.0289 (9)
H2	1.0110	-0.0133	1.3159	0.035*
C3	1.2570 (5)	0.02547 (11)	1.3255 (4)	0.0286 (9)
H3	1.3498	0.0107	1.4115	0.034*
C4	1.3215 (5)	0.06199 (11)	1.2546 (4)	0.0214 (8)
C5	1.1882 (5)	0.08439 (11)	1.1266 (4)	0.0229 (9)
H5	1.2358	0.1088	1.0801	0.027*
C6	0.9819 (5)	0.07046 (10)	1.0666 (4)	0.0206 (8)
C7	0.8378 (5)	0.09492 (11)	0.9384 (4)	0.0247 (9)
H7	0.8837	0.1200	0.8961	0.030*
C8	0.4951 (5)	0.10551 (11)	0.7634 (4)	0.0226 (9)
C9	0.5258 (5)	0.14469 (11)	0.6939 (5)	0.0286 (9)
H9	0.6565	0.1579	0.7261	0.034*
C10	0.3657 (5)	0.16458 (11)	0.5776 (4)	0.0296 (9)
H10	0.3885	0.1912	0.5347	0.035*
C11	0.1687 (5)	0.14472 (11)	0.5240 (4)	0.0235 (9)
C12	0.1366 (5)	0.10576 (11)	0.5961 (4)	0.0266 (9)
H12	0.0058	0.0925	0.5656	0.032*
C13	0.2985 (5)	0.08666 (11)	0.7131 (4)	0.0247 (9)
H13	0.2751	0.0604	0.7593	0.030*
C14	0.0098 (5)	0.18488 (10)	0.2476 (5)	0.0233 (9)
C15	0.1924 (5)	0.18889 (11)	0.1768 (5)	0.0280 (9)
H15	0.3206	0.1787	0.2394	0.034*
C16	0.1843 (6)	0.20790 (11)	0.0138 (5)	0.0342 (10)
H16	0.3076	0.2103	-0.0326	0.041*
C17	-0.0036 (5)	0.22338 (11)	-0.0815 (5)	0.0329 (10)
H17	-0.0080	0.2357	-0.1921	0.039*
C18	-0.1849 (5)	0.22024 (11)	-0.0099 (5)	0.0314 (10)
H18	-0.3118	0.2310	-0.0724	0.038*
C19	-0.1803 (5)	0.20138 (10)	0.1532 (5)	0.0275 (9)

H19	-0.3034	0.1997	0.2003	0.033*
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Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0164 (14)	0.0337 (16)	0.0344 (16)	-0.0028 (12)	-0.0019 (12)	0.0031 (14)
O2	0.0214 (14)	0.0425 (17)	0.0289 (15)	0.0020 (12)	-0.0052 (12)	0.0051 (13)
O3	0.0198 (14)	0.0313 (16)	0.0374 (16)	-0.0063 (12)	0.0025 (12)	0.0022 (13)
N1	0.0231 (18)	0.031 (2)	0.0225 (18)	0.0034 (16)	0.0046 (15)	-0.0032 (16)
N2	0.0206 (17)	0.0289 (19)	0.0211 (17)	0.0005 (14)	-0.0004 (14)	-0.0017 (14)
N3	0.0129 (17)	0.043 (2)	0.034 (2)	-0.0002 (15)	0.0010 (16)	0.0047 (17)
C1	0.016 (2)	0.031 (2)	0.023 (2)	0.0023 (18)	0.0026 (18)	-0.0068 (19)
C2	0.025 (2)	0.031 (2)	0.029 (2)	-0.0050 (18)	-0.0008 (19)	0.0034 (19)
C3	0.024 (2)	0.030 (2)	0.028 (2)	0.0033 (18)	-0.0022 (18)	0.0023 (19)
C4	0.0104 (19)	0.027 (2)	0.025 (2)	-0.0033 (16)	-0.0007 (17)	-0.0024 (19)
C5	0.022 (2)	0.023 (2)	0.024 (2)	-0.0007 (17)	0.0065 (18)	-0.0055 (17)
C6	0.018 (2)	0.023 (2)	0.021 (2)	0.0006 (17)	0.0054 (17)	-0.0009 (17)
C7	0.024 (2)	0.025 (2)	0.025 (2)	0.0013 (17)	0.0057 (19)	-0.0005 (18)
C8	0.018 (2)	0.029 (2)	0.019 (2)	-0.0015 (18)	-0.0022 (17)	-0.0009 (18)
C9	0.018 (2)	0.030 (2)	0.034 (2)	-0.0039 (17)	-0.0038 (19)	-0.0026 (19)
C10	0.029 (2)	0.025 (2)	0.031 (2)	-0.0006 (18)	-0.0049 (19)	-0.0001 (19)
C11	0.021 (2)	0.029 (2)	0.019 (2)	0.0040 (18)	0.0004 (18)	-0.0032 (18)
C12	0.016 (2)	0.039 (3)	0.025 (2)	-0.0060 (18)	0.0050 (18)	0.0006 (19)
C13	0.021 (2)	0.030 (2)	0.024 (2)	-0.0030 (17)	0.0043 (18)	0.0022 (18)
C14	0.022 (2)	0.020 (2)	0.026 (2)	0.0009 (17)	-0.0008 (18)	-0.0006 (17)
C15	0.015 (2)	0.030 (2)	0.036 (3)	-0.0006 (16)	-0.0029 (18)	-0.0017 (19)
C16	0.024 (2)	0.037 (3)	0.041 (3)	-0.0040 (18)	0.006 (2)	0.006 (2)
C17	0.030 (2)	0.030 (2)	0.036 (2)	-0.0031 (19)	-0.001 (2)	0.0081 (19)
C18	0.024 (2)	0.028 (2)	0.038 (3)	0.0015 (18)	-0.0034 (19)	0.005 (2)
C19	0.017 (2)	0.026 (2)	0.038 (2)	0.0001 (16)	0.0012 (18)	0.000 (2)

Geometric parameters (\AA , $^\circ$)

O1—C1	1.351 (4)	C8—C9	1.384 (4)
O1—H1O1	0.97 (4)	C8—C13	1.387 (4)
O2—N1	1.238 (3)	C9—C10	1.382 (4)
O3—N1	1.234 (3)	C9—H9	0.9300
N1—C4	1.460 (4)	C10—C11	1.406 (4)
N2—C7	1.287 (4)	C10—H10	0.9300
N2—C8	1.410 (4)	C11—C12	1.388 (4)
N3—C14	1.406 (4)	C12—C13	1.381 (4)
N3—C11	1.406 (4)	C12—H12	0.9300
N3—H1N3	0.85 (3)	C13—H13	0.9300
C1—C2	1.391 (4)	C14—C15	1.387 (4)
C1—C6	1.407 (4)	C14—C19	1.400 (4)
C2—C3	1.363 (4)	C15—C16	1.379 (4)
C2—H2	0.9300	C15—H15	0.9300
C3—C4	1.379 (4)	C16—C17	1.380 (4)

C3—H3	0.9300	C16—H16	0.9300
C4—C5	1.375 (4)	C17—C18	1.380 (4)
C5—C6	1.392 (4)	C17—H17	0.9300
C5—H5	0.9300	C18—C19	1.381 (4)
C6—C7	1.445 (4)	C18—H18	0.9300
C7—H7	0.9300	C19—H19	0.9300
C1—O1—H1O1	102 (2)	C10—C9—H9	119.4
O3—N1—O2	122.6 (3)	C8—C9—H9	119.4
O3—N1—C4	119.2 (3)	C9—C10—C11	120.3 (3)
O2—N1—C4	118.2 (3)	C9—C10—H10	119.9
C7—N2—C8	123.7 (3)	C11—C10—H10	119.9
C14—N3—C11	127.3 (3)	C12—C11—N3	118.9 (3)
C14—N3—H1N3	116 (2)	C12—C11—C10	118.5 (3)
C11—N3—H1N3	112 (2)	N3—C11—C10	122.5 (3)
O1—C1—C2	118.3 (3)	C13—C12—C11	120.1 (3)
O1—C1—C6	121.6 (3)	C13—C12—H12	119.9
C2—C1—C6	120.1 (3)	C11—C12—H12	119.9
C3—C2—C1	120.7 (3)	C12—C13—C8	121.8 (3)
C3—C2—H2	119.7	C12—C13—H13	119.1
C1—C2—H2	119.7	C8—C13—H13	119.1
C2—C3—C4	119.3 (3)	C15—C14—C19	118.9 (3)
C2—C3—H3	120.4	C15—C14—N3	124.1 (3)
C4—C3—H3	120.4	C19—C14—N3	116.9 (3)
C5—C4—C3	121.7 (3)	C16—C15—C14	120.1 (3)
C5—C4—N1	118.7 (3)	C16—C15—H15	119.9
C3—C4—N1	119.6 (3)	C14—C15—H15	119.9
C4—C5—C6	119.9 (3)	C15—C16—C17	121.1 (3)
C4—C5—H5	120.0	C15—C16—H16	119.4
C6—C5—H5	120.0	C17—C16—H16	119.4
C5—C6—C1	118.4 (3)	C18—C17—C16	118.9 (3)
C5—C6—C7	120.2 (3)	C18—C17—H17	120.5
C1—C6—C7	121.4 (3)	C16—C17—H17	120.5
N2—C7—C6	120.7 (3)	C17—C18—C19	120.9 (3)
N2—C7—H7	119.6	C17—C18—H18	119.6
C6—C7—H7	119.6	C19—C18—H18	119.6
C9—C8—C13	118.1 (3)	C18—C19—C14	120.0 (3)
C9—C8—N2	126.0 (3)	C18—C19—H19	120.0
C13—C8—N2	115.9 (3)	C14—C19—H19	120.0
C10—C9—C8	121.2 (3)	 	
O1—C1—C2—C3	-179.4 (3)	C13—C8—C9—C10	-0.1 (5)
C6—C1—C2—C3	-0.5 (5)	N2—C8—C9—C10	179.8 (3)
C1—C2—C3—C4	0.4 (5)	C8—C9—C10—C11	-1.5 (5)
C2—C3—C4—C5	-0.4 (5)	C14—N3—C11—C12	-137.7 (4)
C2—C3—C4—N1	176.4 (3)	C14—N3—C11—C10	45.4 (5)
O3—N1—C4—C5	0.1 (4)	C9—C10—C11—C12	2.7 (5)
O2—N1—C4—C5	178.4 (3)	C9—C10—C11—N3	179.6 (3)

O3—N1—C4—C3	−176.8 (3)	N3—C11—C12—C13	−179.2 (3)
O2—N1—C4—C3	1.5 (4)	C10—C11—C12—C13	−2.2 (5)
C3—C4—C5—C6	0.5 (5)	C11—C12—C13—C8	0.6 (5)
N1—C4—C5—C6	−176.3 (3)	C9—C8—C13—C12	0.5 (5)
C4—C5—C6—C1	−0.7 (4)	N2—C8—C13—C12	−179.4 (3)
C4—C5—C6—C7	177.0 (3)	C11—N3—C14—C15	2.6 (5)
O1—C1—C6—C5	179.5 (3)	C11—N3—C14—C19	−179.8 (3)
C2—C1—C6—C5	0.7 (5)	C19—C14—C15—C16	−1.7 (5)
O1—C1—C6—C7	1.8 (5)	N3—C14—C15—C16	175.8 (3)
C2—C1—C6—C7	−177.0 (3)	C14—C15—C16—C17	0.3 (5)
C8—N2—C7—C6	177.1 (3)	C15—C16—C17—C18	1.1 (5)
C5—C6—C7—N2	−179.9 (3)	C16—C17—C18—C19	−1.0 (5)
C1—C6—C7—N2	−2.3 (5)	C17—C18—C19—C14	−0.5 (5)
C7—N2—C8—C9	−1.6 (5)	C15—C14—C19—C18	1.8 (5)
C7—N2—C8—C13	178.3 (3)	N3—C14—C19—C18	−175.9 (3)

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O1 ⁱ	0.97 (4)	1.67 (4)	2.573 (4)	155 (4)
N3—H1···O3 ⁱ	0.85 (3)	2.40 (3)	3.140 (4)	147 (3)
C3—H3···O2 ⁱⁱ	0.93	2.48	3.217 (4)	136
C12—H12···O2 ⁱ	0.93	2.55	3.470 (4)	173

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