Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-[(*E*)-4-Quinolylmethylideneamino]-phenol

Sema Öztürk Yıldırım,[a] Mehmet Akkurt,[a]* Mustafa Kemal Gümüş,[b] Mevlüde Canlıca,[b] Şeniz Kaban[b] and Vickie McKee[c]

[a]Department of Physics, Faculty of Arts and Sciences, Erciyes University, 38039 Kayseri, Turkey, [b]Chemistry Department, Yıldız Technical University, Davutpasa Campus, Esenler 34220, Istanbul, Turkey, and [c]Chemistry Department, Loughborough University, Loughborough, Leicestershire LE11 3TU, England
Correspondence e-mail: akkurt@erciyes.edu.tr

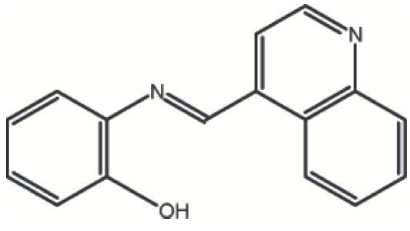
Received 25 September 2008; accepted 17 October 2008

Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.002 Å; R factor = 0.042; wR factor = 0.105; data-to-parameter ratio = 13.6.

In the title compound, $C_{16}H_{12}N_2O$, the dihedral angle between the two aromatic ring systems is 68.54 (5)°. The molecular packing is stabilized by intra- and intermolecular O—H···N and intramolecular C—H···N hydrogen-bond interactions.

Related literature

For bond-length data, see: Allen *et al.* (1987). For general background, see: Gao *et al.* (2005); Hagen *et al.* (1983); Lozytska *et al.* (2004); Sessler *et al.* (2004); Kuz'min *et al.* (2000). For related structures, see: Räisänen, Elo *et al.* (2007); Räisänen Leskelä & Repo (2007). For experimental procedures, see: Gümüş (2002).



Experimental

Crystal data

$C_{16}H_{12}N_2O$
M_r = 248.28
Monoclinic, $P2_1/n$
a = 6.7174 (6) Å
b = 23.931 (2) Å
c = 7.7495 (6) Å
β = 105.521 (1)°
V = 1200.33 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 150 (2) K
0.25 × 0.20 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.978, T_{max} = 0.991
12294 measured reflections
2991 independent reflections
2338 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.105
S = 1.05
2991 reflections
220 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.95 (2)	2.34 (2)	2.7766 (16)	107.5 (15)
O1—H1···N2^{i}	0.95 (2)	1.91 (2)	2.8085 (16)	156.4 (19)
C13—H13···N1	0.975 (15)	2.356 (14)	2.9776 (17)	121.0 (11)

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2807).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
Bruker (2005). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Gao, J., Ross Woolley, F. & Zingaro, R. A. (2005). *J. Med. Chem.* **48**, 7192–7197.
Gümüş, M. K. (2002). MSc thesis, Yıldız Technical University, Istanbul, Turkey.
Hagen, V., Dove, B., Morgenstern, E., Labes, D., Göres, E., Tomaschewski, G., Geisler, G. & Franke, C. (1983). *Pharmazie*, **38**, 437–439.
Kuz'min, V. E., Lozitsky, V. P., Kamalov, G. L., Lozitskaya, R. N., Zheltvay, A. I., Fedtchouk, A. S. & Kryzhanovsky, D. N. (2000). *Acta Biochim. Pol.* **47**, 867–875.
Lozytska, R., Kryzhanovsky, D., Mazepa, A., Gorodniuk, V., Kuz'min, V., Lozitsky, V., Fedchuck, A., Rybalko, S., Diadium, S. & Vanden Eynde, J. J. (2004). *Arkivoc*, **xix**, 118R.
Räisänen, M. T., Elo, P., Kettunen, M., Klinga, M., Leskelä, M. & Repo, T. (2007). *Synth. Commun.* **37**, 1765–1777.
Räisänen, M. T., Leskelä, M. & Repo, T. (2007). *Acta Cryst.* E**63**, o1816–o1817.
Sessler, J. L., Katayev, E., Pantos, G. D. & Ustynyuk, Yu. A. (2004). *J. Chem. Soc. Chem. Commun.* pp. 1276–1277.
Sheldrick, G. M. (2003). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2008). E**64**, o2168 [doi:10.1107/S1600536808033928]

2-[(*E*)-4-Quinolylmethylideneamino]phenol

Sema Öztürk Yıldırım, Mehmet Akkurt, Mustafa Kemal Gümüş, Mevlüde Canlıca, Şeniz Kaban and Vickie McKee

S1. Comment

2- and 4-(*N*-arylimino)quinolines have been investigated to their clinical efficacy for use as an analgetic drug (Hagen *et al.*, 1983). A number of azomethines and their complexes possess high biological activity, including antineoplastic (Kuz'min *et al.*, 2000; Gao *et al.*, 2005) and antiviral (Lozytska *et al.*, 2004). It has been recently shown that the macrocyclic Schiff bases can selectively bind different anions acting as artificial anionic receptors (Sessler *et al.*, 2004).

In the title compound, (I), (Fig. 1), all bond lengths and angles are within normal ranges (Räisänen, Elo *et al.*, 2007; Räisänen Leskelä, & Repo 2007; Allen *et al.*, 1987). The molecule has a non-planar conformation. The dihedral angle between its two aromatic ring systems (C1–C6) and (N2/C8—C16) is 68.54 (5)°. The C6—N1—C7—C8 torsion angle is -179.98 (13)° and the N1—C6—C1—O1 angle deviates from zero only by -7.27 (18)°.

The molecular packing of the compound is stabilized by O—H···N and C—H···N hydrogen bonds (Table 1, Fig. 2).

S2. Experimental

Quinoline-4-carboxaldehyde (1.0 mmol) was dissolved in hot absolute ethanol (5 ml) and an equimolar amount of 2-aminophenol dissolved in hot absolute ethanol (10 ml) was added. The mixture was refluxed at reaction temperature for 2 h. The progress of the reaction was monitored by TLC using n-hexane/ethylacetate (1:1 *v*/*v*) as eluent. Upon completion of the reaction, the crude product which precipitated on cooling was collected by filtration. Further purification was accomplished by recrystallization from ethanol to yield yellow blocks of (I). [yield 80%, m.p. 475–476 K]. UV ($CHCl_3$): λ_{max}248, 343, 377 nm. IR (KBr): 3029, 2851, 1625, 1574 and1472, 1293–1165, 830 and 757 $cm^{-1.}$ ^{1}H NMR ($CDCl_3$, 200 MHz): δ(p.p.m.) 6.95–9.08 (m, ArH and CH, 11H), 9.41(s, OH, 1H). MS: m/*z* 249 (*M*+1), 248 (*M*+), 247 (*M*-1), 128 (*M*-120), 120 (*M*-128). Analysis calculated for $C_{16}H_{12}N_2O$: C 77.40, H 4.87, N 11.28%; found: C 77.62, H 4.96, N 11.12% (Gümüş, 2002).

S3. Refinement

The H atoms were found from a difference map and refined freely.

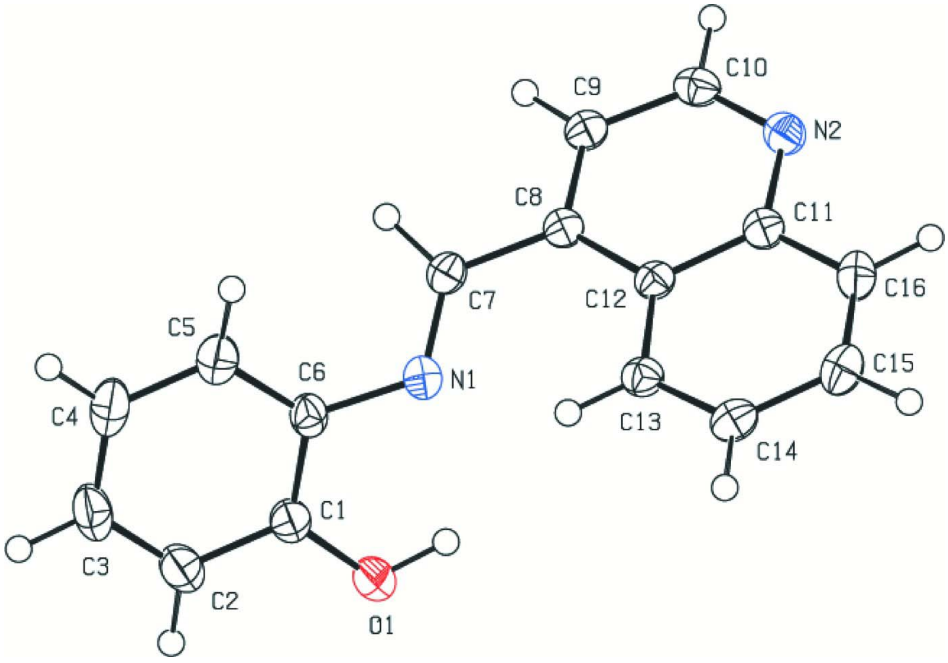


Figure 1

View of (I): displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

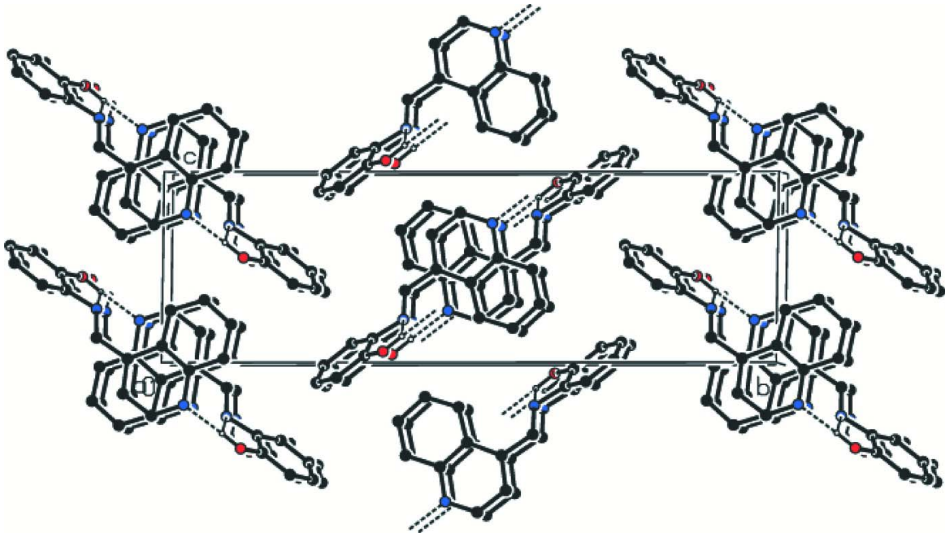


Figure 2

The hydrogen bonding interactions of (I) viewed down the *a* axis. For clarity, H atoms not involved in hydrogen bonding have been omitted.

2-[(E)-4-Quinolylmethylideneamino]phenol

Crystal data

$C_{16}H_{12}N_2O$	a = 6.7174 (6) Å
M_r = 248.28	b = 23.931 (2) Å
Monoclinic, $P2_1/n$	c = 7.7495 (6) Å
Hall symbol: -P 2yn	β = 105.521 (1)°

V = 1200.33 (17) Å^3
Z = 4
F(000) = 520
D_x = 1.374 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2762 reflections
θ = 2.9–26.4°
μ = 0.09 mm^{-1}
T = 150 K
Block, yellow
0.25 × 0.20 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.978, T_{max} = 0.991
12294 measured reflections
2991 independent reflections
2338 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 28.4°, θ_{min} = 1.7°
h = −8→8
k = −31→31
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.105
S = 1.05
2991 reflections
220 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difmap and geom
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0424P)^2 + 0.3303P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -R-factor-obs *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}
O1	1.06305 (16)	0.13183 (4)	0.54890 (14)	0.0340 (3)
N1	0.76446 (16)	0.10349 (4)	0.72156 (14)	0.0243 (3)
N2	0.80975 (16)	−0.03956 (5)	1.22446 (15)	0.0258 (3)
C1	0.8930 (2)	0.16414 (5)	0.52971 (17)	0.0264 (4)
C2	0.8697 (3)	0.20982 (6)	0.41486 (19)	0.0340 (4)
C3	0.6997 (3)	0.24448 (6)	0.3910 (2)	0.0372 (5)
C4	0.5529 (3)	0.23493 (6)	0.4839 (2)	0.0370 (5)
C5	0.5745 (2)	0.18955 (6)	0.59862 (19)	0.0313 (4)
C6	0.7433 (2)	0.15362 (5)	0.62205 (17)	0.0242 (4)
C7	0.72483 (19)	0.10243 (5)	0.87303 (17)	0.0235 (3)
C8	0.74355 (18)	0.05168 (5)	0.98390 (16)	0.0215 (3)

C9	0.78135 (19)	0.05904 (6)	1.16557 (17)	0.0236 (3)
C10	0.81518 (19)	0.01260 (6)	1.28017 (17)	0.0260 (4)
C11	0.76319 (18)	−0.04841 (5)	1.04285 (17)	0.0233 (3)
C12	0.72937 (18)	−0.00427 (5)	0.91566 (16)	0.0212 (3)
C13	0.67854 (19)	−0.01837 (6)	0.73121 (17)	0.0240 (4)
C14	0.6654 (2)	−0.07303 (6)	0.67751 (18)	0.0278 (4)
C15	0.7014 (2)	−0.11657 (6)	0.8042 (2)	0.0308 (4)
C16	0.7487 (2)	−0.10454 (5)	0.98290 (19)	0.0282 (4)
H1	1.068 (3)	0.1013 (9)	0.628 (3)	0.072 (6)*
H2	0.976 (3)	0.2161 (7)	0.350 (2)	0.044 (5)*
H3	0.686 (3)	0.2753 (7)	0.307 (2)	0.046 (5)*
H4	0.433 (3)	0.2587 (7)	0.469 (2)	0.042 (5)*
H5	0.468 (2)	0.1808 (6)	0.657 (2)	0.033 (4)*
H7	0.689 (2)	0.1376 (6)	0.929 (2)	0.031 (4)*
H9	0.788 (2)	0.0966 (6)	1.214 (2)	0.031 (4)*
H10	0.844 (2)	0.0186 (6)	1.409 (2)	0.024 (4)*
H13	0.653 (2)	0.0114 (6)	0.642 (2)	0.025 (4)*
H14	0.632 (2)	−0.0822 (6)	0.550 (2)	0.032 (4)*
H15	0.693 (2)	−0.1566 (7)	0.765 (2)	0.035 (4)*
H16	0.772 (2)	−0.1340 (7)	1.074 (2)	0.033 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0385 (6)	0.0322 (5)	0.0359 (6)	0.0058 (4)	0.0181 (4)	0.0097 (4)
N1	0.0246 (5)	0.0223 (5)	0.0254 (6)	0.0006 (4)	0.0055 (4)	0.0023 (4)
N2	0.0220 (5)	0.0295 (6)	0.0259 (6)	0.0025 (4)	0.0062 (4)	0.0040 (5)
C1	0.0343 (7)	0.0221 (6)	0.0214 (6)	−0.0012 (5)	0.0049 (5)	−0.0020 (5)
C2	0.0475 (9)	0.0274 (7)	0.0272 (7)	−0.0040 (6)	0.0100 (6)	0.0022 (6)
C3	0.0549 (10)	0.0214 (7)	0.0308 (8)	−0.0020 (6)	0.0037 (7)	0.0037 (6)
C4	0.0436 (9)	0.0238 (7)	0.0383 (8)	0.0074 (6)	0.0018 (7)	0.0010 (6)
C5	0.0335 (7)	0.0257 (7)	0.0328 (7)	0.0021 (6)	0.0057 (6)	0.0002 (6)
C6	0.0303 (7)	0.0185 (6)	0.0217 (6)	−0.0016 (5)	0.0036 (5)	−0.0009 (5)
C7	0.0226 (6)	0.0221 (6)	0.0249 (6)	0.0003 (5)	0.0050 (5)	−0.0017 (5)
C8	0.0168 (6)	0.0238 (6)	0.0238 (6)	−0.0003 (5)	0.0052 (4)	0.0004 (5)
C9	0.0211 (6)	0.0251 (6)	0.0248 (6)	−0.0007 (5)	0.0064 (5)	−0.0023 (5)
C10	0.0227 (6)	0.0345 (7)	0.0210 (6)	0.0009 (5)	0.0060 (5)	0.0005 (5)
C11	0.0173 (6)	0.0259 (6)	0.0269 (6)	0.0004 (5)	0.0062 (5)	0.0017 (5)
C12	0.0166 (6)	0.0234 (6)	0.0241 (6)	0.0000 (4)	0.0064 (4)	−0.0004 (5)
C13	0.0212 (6)	0.0266 (7)	0.0247 (6)	0.0006 (5)	0.0070 (5)	0.0001 (5)
C14	0.0249 (6)	0.0297 (7)	0.0285 (7)	−0.0002 (5)	0.0068 (5)	−0.0056 (5)
C15	0.0282 (7)	0.0240 (7)	0.0388 (8)	0.0006 (5)	0.0064 (6)	−0.0036 (6)
C16	0.0257 (7)	0.0224 (6)	0.0358 (7)	0.0012 (5)	0.0071 (5)	0.0036 (6)

Geometric parameters (Å, º)

O1—C1	1.3542 (17)	C11—C12	1.4210 (17)
O1—H1	0.95 (2)	C12—C13	1.4186 (18)

N1—C6	1.4126 (16)	C13—C14	1.368 (2)
N1—C7	1.2715 (17)	C14—C15	1.408 (2)
N2—C11	1.3740 (17)	C15—C16	1.366 (2)
N2—C10	1.3181 (19)	C2—H2	0.989 (19)
C1—C2	1.3918 (19)	C3—H3	0.972 (16)
C1—C6	1.4042 (19)	C4—H4	0.967 (19)
C2—C3	1.383 (3)	C5—H5	0.966 (14)
C3—C4	1.387 (3)	C7—H7	1.005 (15)
C4—C5	1.386 (2)	C9—H9	0.971 (15)
C5—C6	1.3957 (19)	C10—H10	0.975 (15)
C7—C8	1.4735 (17)	C13—H13	0.975 (15)
C8—C9	1.3734 (18)	C14—H14	0.978 (15)
C8—C12	1.4334 (17)	C15—H15	1.002 (17)
C9—C10	1.403 (2)	C16—H16	0.980 (16)
C11—C16	1.4161 (17)		

C1—O1—H1	113.2 (13)	C13—C14—C15	120.70 (13)
C6—N1—C7	120.37 (11)	C14—C15—C16	120.07 (13)
C10—N2—C11	117.40 (11)	C11—C16—C15	120.62 (12)
O1—C1—C2	117.77 (13)	C1—C2—H2	118.1 (10)
C2—C1—C6	119.56 (13)	C3—C2—H2	121.6 (10)
O1—C1—C6	122.67 (11)	C2—C3—H3	118.1 (12)
C1—C2—C3	120.27 (16)	C4—C3—H3	121.3 (12)
C2—C3—C4	120.54 (14)	C3—C4—H4	121.7 (10)
C3—C4—C5	119.68 (16)	C5—C4—H4	118.6 (10)
C4—C5—C6	120.53 (14)	C4—C5—H5	120.4 (9)
N1—C6—C1	116.70 (11)	C6—C5—H5	118.9 (9)
C1—C6—C5	119.40 (12)	N1—C7—H7	121.0 (8)
N1—C6—C5	123.63 (12)	C8—C7—H7	115.6 (8)
N1—C7—C8	123.26 (11)	C8—C9—H9	119.5 (9)
C7—C8—C12	124.61 (11)	C10—C9—H9	120.4 (9)
C9—C8—C12	118.28 (11)	N2—C10—H10	117.1 (9)
C7—C8—C9	117.10 (11)	C9—C10—H10	119.1 (9)
C8—C9—C10	120.11 (13)	C12—C13—H13	119.3 (9)
N2—C10—C9	123.87 (12)	C14—C13—H13	119.9 (9)
N2—C11—C16	117.33 (11)	C13—C14—H14	120.0 (9)
C12—C11—C16	119.56 (12)	C15—C14—H14	119.3 (9)
N2—C11—C12	123.11 (11)	C14—C15—H15	120.7 (9)
C8—C12—C13	124.63 (11)	C16—C15—H15	119.2 (9)
C11—C12—C13	118.22 (11)	C11—C16—H16	117.5 (9)
C8—C12—C11	117.13 (11)	C15—C16—H16	121.8 (9)
C12—C13—C14	120.82 (12)		

C7—N1—C6—C1	141.39 (13)	C7—C8—C9—C10	−175.57 (12)
C7—N1—C6—C5	−44.64 (19)	C12—C8—C9—C10	3.15 (19)
C6—N1—C7—C8	−179.98 (13)	C7—C8—C12—C11	176.39 (12)
C11—N2—C10—C9	−1.61 (19)	C7—C8—C12—C13	−5.5 (2)
C10—N2—C11—C12	2.52 (19)	C9—C8—C12—C11	−2.23 (18)

C10—N2—C11—C16	−177.36 (12)	C9—C8—C12—C13	175.91 (13)
O1—C1—C2—C3	−179.58 (13)	C8—C9—C10—N2	−1.3 (2)
C6—C1—C2—C3	−0.4 (2)	N2—C11—C12—C8	−0.62 (19)
O1—C1—C6—N1	−7.27 (18)	N2—C11—C12—C13	−178.87 (12)
O1—C1—C6—C5	178.49 (12)	C16—C11—C12—C8	179.26 (12)
C2—C1—C6—N1	173.54 (12)	C16—C11—C12—C13	1.00 (18)
C2—C1—C6—C5	−0.70 (19)	N2—C11—C16—C15	179.50 (13)
C1—C2—C3—C4	1.4 (2)	C12—C11—C16—C15	−0.4 (2)
C2—C3—C4—C5	−1.4 (2)	C8—C12—C13—C14	−179.03 (13)
C3—C4—C5—C6	0.4 (2)	C11—C12—C13—C14	−0.92 (19)
C4—C5—C6—N1	−173.12 (13)	C12—C13—C14—C15	0.2 (2)
C4—C5—C6—C1	0.7 (2)	C13—C14—C15—C16	0.4 (2)
N1—C7—C8—C9	153.65 (13)	C14—C15—C16—C11	−0.3 (2)
N1—C7—C8—C12	−25.0 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.95 (2)	2.34 (2)	2.7766 (16)	107.5 (15)
O1—H1···N2^{i}	0.95 (2)	1.91 (2)	2.8085 (16)	156.4 (19)
C13—H13···N1	0.975 (15)	2.356 (14)	2.9776 (17)	121.0 (11)

Symmetry code: (i) −*x*+2, −*y*, −*z*+2.