2-[(*E*)-(Morpholin-4-ylimino)methyl]-6-(morpholin-4-ylmethyl)phenol

Mehmet Akkurt,[a]* Aliasghar Jarrahpour,[b] Mehdi Mohammadi Chermahini,[b] Mahdi Aberi[b] and Orhan Büyükgüngör[c]

[a]Department of Physics, Faculty of Sciences, Erciyes University, 38039 Kayseri, Turkey, [b]Department of Chemistry, College of Sciences, Shiraz University, 71454 Shiraz, Iran, and [c]Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, 55139 Samsun, Turkey
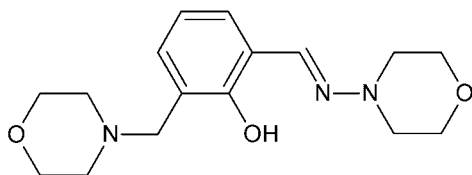Correspondence e-mail: akkurt@erciyes.edu.tr

The title compound, $C_{16}H_{23}N_3O_3$, contains two morpholine rings, each of which adopts a chair conformation. The molecular conformation is stabilized by an intramolecular O—H⋯N hydrogen bond, leading to a $S(6)$ ring. In the crystal, molecules are linked into zigzag chains along the c-axis direction by C—H⋯O and C—H⋯π interactions.

Related literature

For background to Schiff bases and their applications, see: Dhar & Taploo (1982); Nelson *et al.* (2004); Silva *et al.* (2011). For ring puckering parameters, see: Cremer & Pople (1975). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).

Experimental

Crystal data

$C_{16}H_{23}N_3O_3$	a = 9.0074 (6) Å
M_r = 305.37	b = 15.7781 (14) Å
Monoclinic, $P2_1/c$	c = 11.3083 (7) Å
β = 99.052 (5)°	μ = 0.09 mm^{-1}
V = 1587.1 (2) Å^3	T = 296 K
Z = 4	$0.51 \times 0.32 \times 0.09$ mm
Mo $K\alpha$ radiation	

Data collection

STOE IPDS 2 diffractometer	23637 measured reflections
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)	3289 independent reflections
T_{min} = 0.961, T_{max} = 0.990	1955 reflections with $I > 2\sigma(I)$
	R_{int} = 0.089

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058	199 parameters
$wR(F^2)$ = 0.123	H-atom parameters constrained
S = 1.03	$\Delta\rho_{max}$ = 0.13 e Å^{-3}
3289 reflections	$\Delta\rho_{min}$ = −0.12 e Å^{-3}

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

$Cg3$ is the centroid of the C6–C11 benzene ring.

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O2—H2⋯N2	0.82	1.91	2.636 (2)	146
C13—H13A⋯O3[i]	0.97	2.55	3.416 (3)	149
C4—H4A⋯$Cg3$[i]	0.97	2.87	3.646 (3)	138

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

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

References

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
Dhar, D. N. & Taploo, C. L. (1982). *J. Sci. Ind. Res.* **41**, 501–506.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Nelson, T. D., Rosen, J. D., Brands, K. M. J., Craig, B., Huffman, M. A. & McNamara, J. M. (2004). *Tetrahedron Lett.* **45**, 8917–8920.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Silva, C. M., da Silva, D. L., Modolo, L. V., Alves, R. B., de Resende, M. A., Martins, C. V. B. & de Fatima, A. (2011). *J. Adv. Res.* **2**, 1–8.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Stoe & Cie (2002). *X-AREA* and *X-RED32*. Stoe & Cie, Darmstadt, Germany.

supporting information

2-[(*E*)-(Morpholin-4-ylimino)methyl]-6-(morpholin-4-ylmethyl)phenol

Mehmet Akkurt, Aliasghar Jarrahpour, Mehdi Mohammadi Chermahini, Mahdi Aberi and Orhan Büyükgüngör

S1. Comment

Schiff bases are formed by the condensation of a primary amine with a carbonyl compound (Dhar & Taploo, 1982). They are widely used for industrial purposes and also exhibit a broad range of biological activities (Silva *et al.*, 2011). The morpholine moiety has been utilized extensively by the pharmaceutical industry in drug design, often because of the improvement in pharmacokinetic properties it can confer. The World Drug Index contains well over 100 drugs incorporating this structural feature, including its presence as a side-chain, scaffold, and within fused-ring systems. The biological utility of molecules containing the morpholine moiety is wide-ranging (Nelson *et al.*, 2004). Therefore, Schiff base (I), which has the two morpholine rings, was synthesized and its X-ray structure is reported here.

The two morpholine rings (N1/O1/C1–C4 and N3/O3/C13–C16) of (I), Fig. 1, adopt a chair conformation with puckering parameters (Cremer & Pople, 1975) of $Q_T = 0.564$ (3) Å, $\theta = 180.0$ (2)°, $\varphi = 163$ (33)° and $Q_T = 0.553$ (2) Å, $\theta = 4.6$ (2)°, $\varphi = 19$ (3)°, respectively. The N1–C5–C6–C7, C5–C6–C7–O2, O2–C7–C8–C12 and C8–C12–N2–N3 torsion angles are -158.0 (2), 0.6 (3), -1.0 (3) and 179.97 (19)°, respectively.

An intramolecular O—H⋯N hydrogen bond (Table 1) stabilizes the molecular conformation of (I), forming a pseudo six-membered ring with a graph set motif *S*(6) (Bernstein *et al.*, 1995). In the crystal structure, C—H⋯O hydrogen bonds link the molecules into infinite one-dimensional chains along [001], with a C(4) graph-set motif (Table 1, Fig. 2). Additional C—H⋯π interactions also assist in the stabilization of the chain.

S2. Experimental

A mixture of 2-hydroxy-3-(morpholinomethyl)benzaldehyde (1.0 mmol) and morpholin-4-amine (1.0 mmol) was refluxed in EtOH for 4 h. After cooling the solution, the precipitate formed was filtered and recrystallized from ethanol to give yellow crystals in 82% yield. M. pt: 407–409 K. IR (KBr) cm^{-1}: 1612 (C=N). ^{1}H-NMR (250 MHz, CDCl$_3$), δ (p.p.m.): 2.57, 3.15 (CH$_2$N, t, 8H, J=5 Hz), 3.66 (CH$_2$, s, 2H), 3.75, 3.88 (CH$_2$O, t, 8H, J=5 Hz), 6.84 (aromatic H, t, 1H, J=7.5 Hz), 7.23 (aromatic H, d, 2H, J=7.5 Hz), 7.80 (HC=N, s, 1H), 11.71 (OH, s, 1H). ^{13}C-NMR (62.9 MHz, CDCl$_3$), δ (p.p.m): 51.8, 53.3 (CH$_2$N), 57.6 (CH$_2$), 66.2, 66.7 (CH$_2$O), 118.8–139.1 (aromatic carbons), 156.0 (C=N).

S3. Refinement

All H atoms were located geometrically with O—H = 0.82 Å, and C—H = 0.93 and 0.97 Å, and refined using a riding model with U_{iso}(H) = 1.2U_{eq}(C) for the aromatic- and methylene-H atoms, and U_{iso}(H) = 1.5U_{eq}(O) for the hydroxyl-H atom.
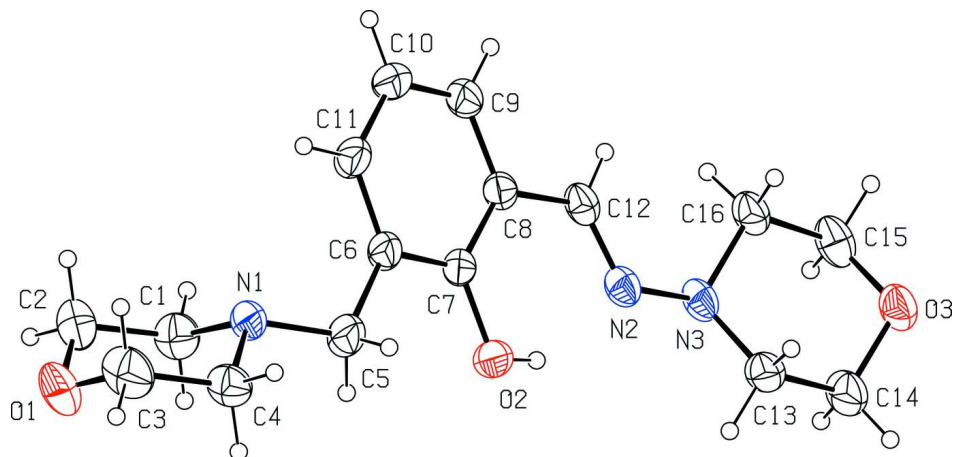
Figure 1

The molecular structure of (I) with the atom-labelling scheme and 30% probability displacement ellipsoids.
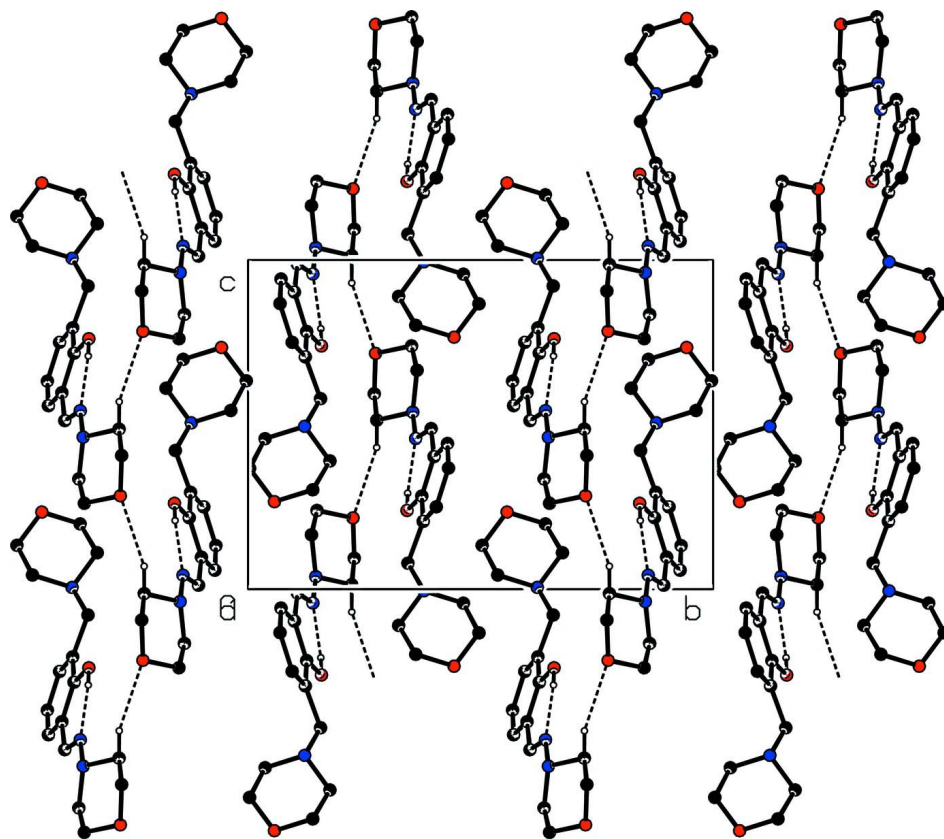
Figure 2

Packing diagram of (I) viewed down the *a* axis. Hydrogen bonds are indicated by broken lines. H atoms not participating in hydrogen bonding have been omitted for clarity.

2-[(*E*)-(Morpholin-4-ylimino)methyl]-6-(morpholin-4-ylmethyl)phenol

Crystal data

$C_{16}H_{23}N_3O_3$	$F(000) = 656$
$M_r = 305.37$	$D_x = 1.278$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 17755 reflections
$a = 9.0074$ (6) Å	$\theta = 2.2$–27.3°
$b = 15.7781$ (14) Å	$\mu = 0.09$ mm^{-1}
$c = 11.3083$ (7) Å	$T = 296$ K
$\beta = 99.052$ (5)°	Shapeless, yellow
$V = 1587.1$ (2) Å^3	$0.51 \times 0.32 \times 0.09$ mm
$Z = 4$	

Data collection

STOE IPDS 2 diffractometer	$T_{min} = 0.961$, $T_{max} = 0.990$
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus	23637 measured reflections
	3289 independent reflections
Plane graphite monochromator	1955 reflections with $I > 2\sigma(I)$
Detector resolution: 6.67 pixels mm^{-1}	$R_{int} = 0.089$
ω–scans	$\theta_{max} = 26.5°$, $\theta_{min} = 2.2°$
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)	$h = -11 \rightarrow 11$
	$k = -19 \rightarrow 19$
	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.058$	W = $1/[\Sigma^2(FO^2) + (0.0519P)^2]$ WHERE $P = (FO^2 + 2FC^2)/3$
$wR(F^2) = 0.123$	
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
3289 reflections	$\Delta\rho_{max} = 0.13$ e Å^{-3}
199 parameters	$\Delta\rho_{min} = -0.12$ e Å^{-3}
0 restraints	

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 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 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	0.7886 (2)	0.05694 (15)	0.26574 (16)	0.0912 (9)
O2	0.46117 (17)	0.15800 (11)	0.73906 (12)	0.0586 (5)
O3	0.15802 (19)	0.22570 (11)	1.21636 (13)	0.0659 (6)
N1	0.7555 (2)	0.12192 (11)	0.49469 (14)	0.0497 (6)
N2	0.3995 (2)	0.13953 (12)	0.95782 (15)	0.0500 (6)

N3	0.2980 (2)	0.14585 (12)	1.03797 (14)	0.0514 (6)
C1	0.7095 (3)	0.03684 (16)	0.4572 (2)	0.0669 (9)
C2	0.8012 (4)	0.00352 (19)	0.3670 (2)	0.0838 (11)
C3	0.8362 (4)	0.1393 (2)	0.3018 (2)	0.0859 (13)
C4	0.7453 (3)	0.17607 (16)	0.38952 (19)	0.0614 (8)
C5	0.6625 (3)	0.15608 (18)	0.57868 (19)	0.0667 (9)
C6	0.7055 (3)	0.12328 (14)	0.70585 (18)	0.0523 (8)
C7	0.5991 (2)	0.12627 (13)	0.78287 (18)	0.0467 (7)
C8	0.6357 (2)	0.09994 (13)	0.90283 (18)	0.0452 (7)
C9	0.7809 (3)	0.07110 (14)	0.9425 (2)	0.0562 (8)
C10	0.8869 (3)	0.06887 (16)	0.8678 (2)	0.0629 (9)
C11	0.8489 (3)	0.09507 (15)	0.7501 (2)	0.0600 (9)
C12	0.5296 (3)	0.10624 (14)	0.98800 (18)	0.0501 (8)
C13	0.2093 (3)	0.22298 (16)	1.01350 (19)	0.0584 (9)
C14	0.0910 (3)	0.22850 (19)	1.0939 (2)	0.0691 (10)
C15	0.2348 (3)	0.14835 (18)	1.2391 (2)	0.0707 (10)
C16	0.3593 (3)	0.13650 (15)	1.16513 (18)	0.0566 (8)
H1A	0.60400	0.03710	0.42230	0.0800*
H1B	0.72160	−0.00030	0.52650	0.0800*
H2	0.40790	0.15670	0.79150	0.0880*
H2A	0.90580	−0.00040	0.40360	0.1010*
H2B	0.76680	−0.05290	0.34220	0.1010*
H3A	0.82770	0.17570	0.23190	0.1030*
H3B	0.94120	0.13770	0.33800	0.1030*
H4A	0.78230	0.23230	0.41320	0.0740*
H4B	0.64110	0.18110	0.35220	0.0740*
H5A	0.55830	0.14180	0.55030	0.0800*
H5B	0.67080	0.21740	0.57950	0.0800*
H9	0.80660	0.05290	1.02130	0.0670*
H10	0.98380	0.04990	0.89600	0.0750*
H11	0.92120	0.09370	0.69980	0.0720*
H12	0.55720	0.08570	1.06540	0.0600*
H13A	0.16130	0.22320	0.93050	0.0700*
H13B	0.27480	0.27200	1.02640	0.0700*
H14A	0.03510	0.28090	1.07820	0.0830*
H14B	0.02110	0.18170	1.07680	0.0830*
H15A	0.16360	0.10220	1.22240	0.0850*
H15B	0.27740	0.14560	1.32330	0.0850*
H16A	0.43750	0.17840	1.18800	0.0680*
H16B	0.40340	0.08060	1.17960	0.0680*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.1117 (17)	0.1190 (17)	0.0446 (10)	0.0059 (13)	0.0173 (10)	−0.0190 (11)
O2	0.0528 (9)	0.0838 (11)	0.0411 (8)	0.0177 (8)	0.0129 (7)	0.0064 (8)
O3	0.0724 (12)	0.0822 (12)	0.0457 (9)	0.0009 (9)	0.0178 (8)	−0.0106 (8)
N1	0.0550 (11)	0.0584 (12)	0.0378 (9)	0.0049 (9)	0.0141 (8)	0.0022 (8)

N2	0.0553 (12)	0.0586 (11)	0.0379 (9)	−0.0038 (9)	0.0128 (8)	−0.0032 (8)
N3	0.0578 (11)	0.0657 (12)	0.0339 (9)	−0.0087 (10)	0.0168 (8)	−0.0046 (8)
C1	0.0723 (17)	0.0674 (16)	0.0628 (15)	−0.0028 (13)	0.0164 (13)	0.0056 (13)
C2	0.101 (2)	0.085 (2)	0.0652 (17)	0.0133 (17)	0.0121 (16)	−0.0203 (16)
C3	0.086 (2)	0.122 (3)	0.0555 (16)	−0.0115 (19)	0.0288 (15)	0.0107 (17)
C4	0.0664 (15)	0.0706 (16)	0.0480 (13)	−0.0028 (13)	0.0118 (11)	0.0105 (12)
C5	0.0764 (17)	0.0838 (17)	0.0434 (13)	0.0302 (14)	0.0202 (12)	0.0073 (12)
C6	0.0625 (15)	0.0575 (14)	0.0383 (11)	0.0173 (11)	0.0119 (10)	0.0016 (10)
C7	0.0533 (14)	0.0458 (12)	0.0409 (11)	0.0097 (10)	0.0070 (10)	−0.0036 (9)
C8	0.0555 (14)	0.0405 (11)	0.0396 (11)	0.0037 (10)	0.0075 (10)	−0.0008 (9)
C9	0.0722 (16)	0.0564 (14)	0.0390 (12)	0.0141 (12)	0.0053 (11)	0.0014 (10)
C10	0.0619 (16)	0.0742 (16)	0.0509 (14)	0.0248 (13)	0.0036 (12)	0.0025 (12)
C11	0.0608 (16)	0.0727 (16)	0.0494 (13)	0.0222 (12)	0.0177 (11)	0.0032 (12)
C12	0.0702 (17)	0.0460 (12)	0.0352 (11)	−0.0021 (11)	0.0122 (11)	−0.0006 (9)
C13	0.0563 (15)	0.0766 (17)	0.0433 (12)	0.0045 (12)	0.0110 (11)	0.0012 (12)
C14	0.0611 (16)	0.099 (2)	0.0503 (14)	−0.0016 (14)	0.0181 (12)	−0.0086 (14)
C15	0.094 (2)	0.0805 (18)	0.0419 (13)	−0.0078 (16)	0.0245 (13)	−0.0040 (13)
C16	0.0771 (16)	0.0586 (15)	0.0355 (11)	0.0008 (12)	0.0129 (11)	0.0013 (10)

Geometric parameters (Å, º)

O1—C2	1.412 (3)	C15—C16	1.512 (4)
O1—C3	1.409 (4)	C1—H1A	0.9700
O2—C7	1.359 (2)	C1—H1B	0.9700
O3—C14	1.422 (3)	C2—H2A	0.9700
O3—C15	1.406 (3)	C2—H2B	0.9700
O2—H2	0.8200	C3—H3A	0.9700
N1—C1	1.449 (3)	C3—H3B	0.9700
N1—C5	1.465 (3)	C4—H4A	0.9700
N1—C4	1.456 (3)	C4—H4B	0.9700
N2—N3	1.389 (2)	C5—H5A	0.9700
N2—C12	1.281 (3)	C5—H5B	0.9700
N3—C16	1.464 (3)	C9—H9	0.9300
N3—C13	1.458 (3)	C10—H10	0.9300
C1—C2	1.505 (4)	C11—H11	0.9300
C3—C4	1.499 (4)	C12—H12	0.9300
C5—C6	1.520 (3)	C13—H13A	0.9700
C6—C7	1.394 (3)	C13—H13B	0.9700
C6—C11	1.383 (4)	C14—H14A	0.9700
C7—C8	1.407 (3)	C14—H14B	0.9700
C8—C12	1.463 (3)	C15—H15A	0.9700
C8—C9	1.391 (3)	C15—H15B	0.9700
C9—C10	1.371 (4)	C16—H16A	0.9700
C10—C11	1.384 (3)	C16—H16B	0.9700
C13—C14	1.508 (4)		
C2—O1—C3	109.51 (19)	O1—C3—H3B	109.00
C14—O3—C15	109.05 (18)	C4—C3—H3A	109.00

C7—O2—H2	109.00	C4—C3—H3B	109.00
C1—N1—C5	111.37 (19)	H3A—C3—H3B	108.00
C4—N1—C5	110.18 (18)	N1—C4—H4A	110.00
C1—N1—C4	109.06 (17)	N1—C4—H4B	110.00
N3—N2—C12	121.63 (17)	C3—C4—H4A	110.00
N2—N3—C16	116.65 (18)	C3—C4—H4B	110.00
C13—N3—C16	112.40 (17)	H4A—C4—H4B	108.00
N2—N3—C13	109.48 (17)	N1—C5—H5A	109.00
N1—C1—C2	111.1 (2)	N1—C5—H5B	109.00
O1—C2—C1	111.0 (2)	C6—C5—H5A	109.00
O1—C3—C4	112.1 (3)	C6—C5—H5B	109.00
N1—C4—C3	110.0 (2)	H5A—C5—H5B	108.00
N1—C5—C6	113.7 (2)	C8—C9—H9	119.00
C5—C6—C7	118.8 (2)	C10—C9—H9	119.00
C5—C6—C11	122.4 (2)	C9—C10—H10	120.00
C7—C6—C11	118.66 (19)	C11—C10—H10	120.00
O2—C7—C8	121.49 (17)	C6—C11—H11	119.00
C6—C7—C8	120.84 (18)	C10—C11—H11	119.00
O2—C7—C6	117.64 (18)	N2—C12—H12	119.00
C7—C8—C9	118.25 (18)	C8—C12—H12	119.00
C9—C8—C12	119.24 (19)	N3—C13—H13A	110.00
C7—C8—C12	122.43 (18)	N3—C13—H13B	110.00
C8—C9—C10	121.4 (2)	C14—C13—H13A	109.00
C9—C10—C11	119.6 (2)	C14—C13—H13B	110.00
C6—C11—C10	121.3 (2)	H13A—C13—H13B	108.00
N2—C12—C8	121.17 (18)	O3—C14—H14A	109.00
N3—C13—C14	110.6 (2)	O3—C14—H14B	109.00
O3—C14—C13	110.7 (2)	C13—C14—H14A	110.00
O3—C15—C16	113.1 (2)	C13—C14—H14B	110.00
N3—C16—C15	109.4 (2)	H14A—C14—H14B	108.00
N1—C1—H1A	109.00	O3—C15—H15A	109.00
N1—C1—H1B	109.00	O3—C15—H15B	109.00
C2—C1—H1A	109.00	C16—C15—H15A	109.00
C2—C1—H1B	109.00	C16—C15—H15B	109.00
H1A—C1—H1B	108.00	H15A—C15—H15B	108.00
O1—C2—H2A	109.00	N3—C16—H16A	110.00
O1—C2—H2B	109.00	N3—C16—H16B	110.00
C1—C2—H2A	109.00	C15—C16—H16A	110.00
C1—C2—H2B	109.00	C15—C16—H16B	110.00
H2A—C2—H2B	108.00	H16A—C16—H16B	108.00
O1—C3—H3A	109.00		
C2—O1—C3—C4	−59.1 (3)	N1—C5—C6—C7	−158.0 (2)
C3—O1—C2—C1	58.2 (3)	C5—C6—C11—C10	177.2 (2)
C14—O3—C15—C16	60.8 (3)	C11—C6—C7—O2	176.9 (2)
C15—O3—C14—C13	−61.0 (3)	C5—C6—C7—O2	0.6 (3)
C1—N1—C4—C3	−55.5 (3)	C7—C6—C11—C10	1.0 (3)
C4—N1—C1—C2	55.8 (3)	C11—C6—C7—C8	−1.0 (3)

C5—N1—C4—C3	−178.0 (2)	C5—C6—C7—C8	−177.3 (2)
C1—N1—C5—C6	78.8 (2)	O2—C7—C8—C9	−177.62 (19)
C4—N1—C5—C6	−160.1 (2)	O2—C7—C8—C12	−1.0 (3)
C5—N1—C1—C2	177.6 (2)	C6—C7—C8—C12	176.8 (2)
C12—N2—N3—C16	17.4 (3)	C6—C7—C8—C9	0.2 (3)
C12—N2—N3—C13	146.5 (2)	C7—C8—C12—N2	−2.9 (3)
N3—N2—C12—C8	−179.97 (19)	C12—C8—C9—C10	−176.1 (2)
C13—N3—C16—C15	50.3 (3)	C7—C8—C9—C10	0.6 (3)
N2—N3—C13—C14	176.21 (18)	C9—C8—C12—N2	173.7 (2)
C16—N3—C13—C14	−52.5 (3)	C8—C9—C10—C11	−0.6 (4)
N2—N3—C16—C15	177.92 (19)	C9—C10—C11—C6	−0.3 (4)
N1—C1—C2—O1	−58.0 (3)	N3—C13—C14—O3	57.5 (3)
O1—C3—C4—N1	58.4 (3)	O3—C15—C16—N3	−55.1 (3)
N1—C5—C6—C11	25.8 (3)		

Hydrogen-bond geometry (Å, º)

Cg3 is the centroid of the C6–C11 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···N2	0.82	1.91	2.636 (2)	146
C13—H13*A*···O3[i]	0.97	2.55	3.416 (3)	149
C4—H4*A*···Cg3[i]	0.97	2.87	3.646 (3)	138

Symmetry code: (i) *x*, −*y*+1/2, *z*−1/2.