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Bis[4-(2-hydroxybenzylamino)phenyl] ether

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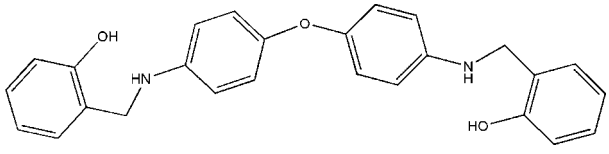
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.002 Å; R factor = 0.047; wR factor = 0.095; data-to-parameter ratio = 14.1.

The title compound, $C_{26}H_{24}N_2O_3$, was synthesized by reduction of the corresponding Schiff base. The molecule does not possess crystallographic or non-crystallographic symmetry. The dihedral angle between the oxygen-bridged benzene rings is 67.98 (8)°. Both hydroxyl groups are involved in O—H···O intramolecular hydrogen bonding. The molecules are linked into a two-dimensional network parallel to the (010) plane by N—H···O hydrogen bonds.

Related literature

For related literature, see: Ge, Zhang, Zhang, Guan *et al.* (2003); Ge, Zhang, Zhang, Guo *et al.* (2003).



Experimental

Crystal data

$C_{26}H_{24}N_2O_3$
M_r = 412.47
Monoclinic, $P2_1/n$
a = 5.8241 (5) Å
b = 43.960 (4) Å
c = 8.2874 (7) Å
β = 92.287 (1)°
V = 2120.1 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 295 (2) K
0.30 × 0.26 × 0.13 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.971, T_{max} = 0.982
11851 measured reflections
4170 independent reflections
2737 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.095
S = 0.93
4170 reflections
296 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.90 (2)	1.80 (2)	2.628 (2)	152 (2)
O3—H3···N2	0.94 (3)	1.82 (3)	2.670 (2)	150 (2)
N1—H1B···O3^{i}	0.88 (2)	2.00 (2)	2.876 (2)	179 (2)
N2—H2B···O1^{ii}	0.88 (2)	2.03 (2)	2.914 (2)	176 (2)

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2520).

References

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Ge, C. H., Zhang, X. D., Zhang, P., Guan, W., Guo, F. & Liu, Q. T. (2003). *Polyhedron*, **22**, 3493–3497.
Ge, C. H., Zhang, X. D., Zhang, P., Guo, F. & Liu, Q. T. (2003). *Inorg. Chem. Commun.* **6**, 1061–1064.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.

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supporting information

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Bis[4-(2-hydroxybenzylamino)phenyl] ether

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S1. Comment

The title compound has amino and hydroxyl groups which are good donor and acceptor for hydrogen bonding (Fig. 1). There are rigid phenyl rings and flexible methylene units in the same molecule which is similar to the ligands reported by Ge, Zhang, Zhang, Guan *et al.* (2003) and Ge, Zhang, Zhang, Guo *et al.* (2003). The molecule can be used as a semi-rigid ligand for metal complex formation or as a host for small molecule.

The dihedral angles formed by the C1—C6 (A), C8—C13 (B), C14—C19 (C) and C21—C26 (D) benzene rings are: A/B 66.36 (8)°, B/C 67.98 (8)° and C/D 67.68 (8)°. Both hydroxyl groups in the title molecule are involved in O—H···O intramolecular hydrogen bonding (Table 1). The molecules are linked into a two-dimensional network parallel to the (0 1 0) plane by N—H···O hydrogen bonds (Fig. 2).

S2. Experimental

A solution of 4,4′-diaminodiphenyl ether (0.1 mol) in ethanol (50 ml) was added dropwise to a solution of salicylaldehyde (0.21 mol) in ethanol (50 ml). The mixture was stirred for 4 h. The resulting solution was filtered to obtain a Schiff base, and it was dried. The title compound was obtained by the reaction of the Schiff base (0.05 mol) with a solution of $NaBH_4$ (0.4 mol) in ethanol (30 ml). Removal of the solvent under vacuum gave a white solid. Single crystals of the title compound were obtained by evaporating a solution of above-mentioned solid (0.2 mmol) in ethanol-water (30 ml, 2:1 *v*/*v*).

S3. Refinement

O– and N-bound H atoms were located in a difference map and refined freely. C-bound H atoms were placed in geometrically idealized positions (Csp^2—H = 0.93 and Csp^3—H = 0.97 Å) and refined in a riding model, with U_{iso}(H) = 1.2U_{eq}(C).

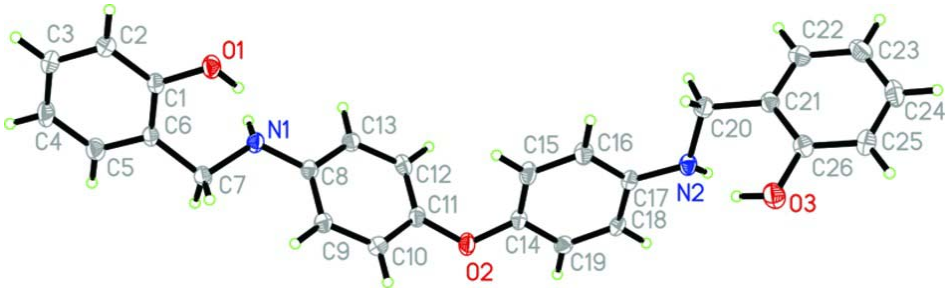

Figure 1

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

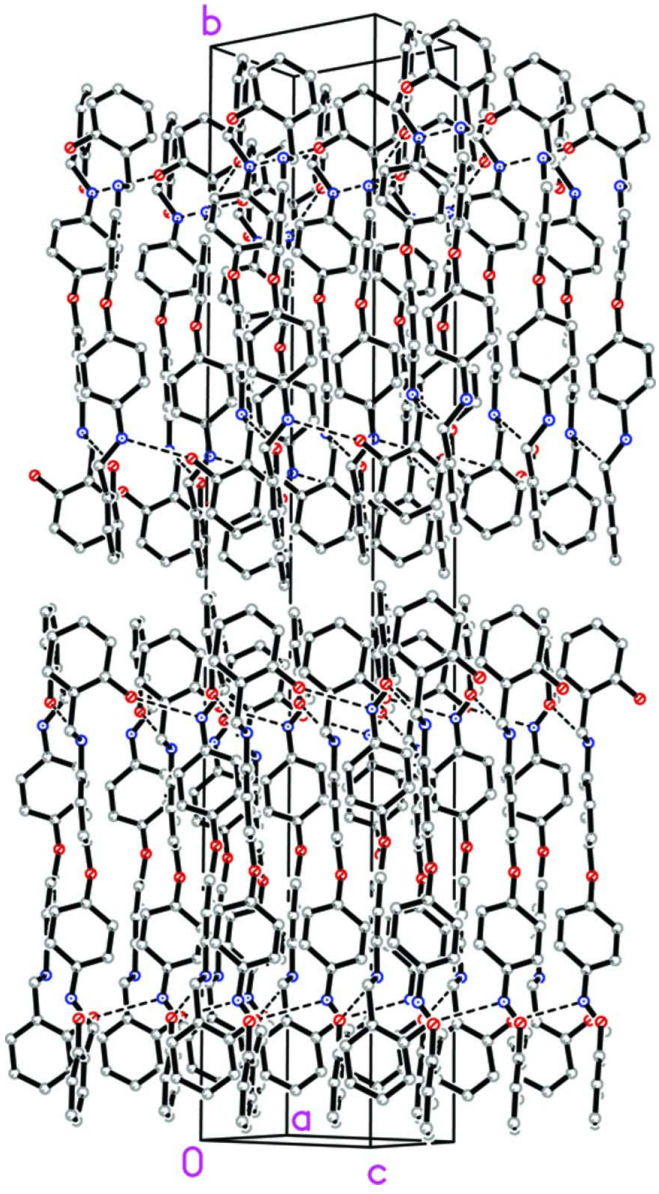

Figure 2

Crystal packing of the title compound.

Bis[4-(2-hydroxybenzylamino)phenyl] ether

Crystal data

$C_{26}H_{24}N_2O_3$
$M_r = 412.47$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 5.8241\ (5)$ Å
$b = 43.960\ (4)$ Å
$c = 8.2874\ (7)$ Å
$\beta = 92.287\ (1)°$
$V = 2120.1\ (3)$ Å^3
$Z = 4$
$F(000) = 872$
$D_x = 1.292$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 774 reflections
$\theta = 2.5–22.7°$
$\mu = 0.09$ mm^{-1}
$T = 295$ K
Block, colourless
0.30 × 0.26 × 0.13 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.971, T_{max} = 0.982
11851 measured reflections
4170 independent reflections
2737 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{max} = 26.1°, θ_{min} = 1.9°
$h = -7 \rightarrow 7$
$k = -49 \rightarrow 54$
$l = -9 \rightarrow 10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.095
S = 0.93
4170 reflections
296 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0352P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and 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 threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	−0.1278 (2)	0.10829 (3)	0.88351 (16)	0.0397 (3)
O2	0.5755 (2)	0.23713 (3)	0.53721 (16)	0.0457 (4)
N1	0.1605 (3)	0.12562 (3)	0.66554 (19)	0.0330 (4)
N2	0.2491 (3)	0.35409 (3)	0.65634 (19)	0.0343 (4)
C17	0.3126 (3)	0.32377 (4)	0.6221 (2)	0.0300 (4)
C19	0.5823 (3)	0.28987 (4)	0.4995 (2)	0.0336 (4)
H19	0.7096	0.2870	0.4369	0.040*
C6	0.1360 (3)	0.07358 (4)	0.7657 (2)	0.0305 (4)
C18	0.5022 (3)	0.31878 (4)	0.5268 (2)	0.0323 (4)
H18	0.5753	0.3353	0.4812	0.039*
C1	−0.0656 (3)	0.07893 (4)	0.8465 (2)	0.0313 (4)
O3	0.3648 (2)	0.39237 (3)	0.89618 (17)	0.0507 (4)
C12	0.2522 (3)	0.20261 (4)	0.5023 (2)	0.0367 (5)
H12	0.1763	0.2162	0.4325	0.044*
C16	0.2036 (3)	0.29862 (4)	0.6834 (2)	0.0401 (5)

H16	0.0741	0.3013	0.7439	0.048*
C14	0.4741 (3)	0.26513 (4)	0.5647 (2)	0.0326 (4)
C13	0.1566 (3)	0.17455 (4)	0.5332 (2)	0.0339 (4)
H13	0.0145	0.1695	0.4853	0.041*
C11	0.4610 (3)	0.21042 (4)	0.5755 (2)	0.0348 (5)
C15	0.2846 (3)	0.26944 (4)	0.6559 (2)	0.0412 (5)
H15	0.2106	0.2528	0.6994	0.049*
C10	0.5729 (3)	0.19037 (4)	0.6786 (2)	0.0376 (5)
H10	0.7122	0.1958	0.7294	0.045*
C20	0.0224 (3)	0.36069 (4)	0.7182 (2)	0.0402 (5)
H20A	0.0016	0.3493	0.8169	0.048*
H20B	−0.0964	0.3545	0.6396	0.048*
C26	0.1751 (3)	0.40877 (4)	0.8431 (2)	0.0361 (5)
C21	0.0020 (3)	0.39425 (4)	0.7514 (2)	0.0331 (4)
C2	−0.2046 (3)	0.05532 (4)	0.8928 (2)	0.0395 (5)
H2	−0.3369	0.0593	0.9483	0.047*
C8	0.2693 (3)	0.15367 (4)	0.6348 (2)	0.0300 (4)
C5	0.1885 (3)	0.04368 (4)	0.7293 (2)	0.0445 (5)
H5	0.3207	0.0395	0.6740	0.053*
C3	−0.1467 (3)	0.02578 (4)	0.8566 (2)	0.0458 (5)
H3A	−0.2396	0.0098	0.8882	0.055*
C7	0.2944 (3)	0.09951 (4)	0.7283 (2)	0.0372 (5)
H7A	0.3815	0.1054	0.8255	0.045*
H7B	0.4021	0.0931	0.6488	0.045*
C9	0.4781 (3)	0.16194 (4)	0.7071 (2)	0.0365 (5)
H9	0.5560	0.1483	0.7756	0.044*
C25	0.1609 (3)	0.43923 (4)	0.8814 (2)	0.0455 (5)
H25	0.2769	0.4486	0.9438	0.055*
C22	−0.1831 (3)	0.41142 (4)	0.6961 (2)	0.0447 (5)
H22	−0.2991	0.4022	0.6331	0.054*
C24	−0.0287 (4)	0.45572 (5)	0.8255 (2)	0.0501 (6)
H24	−0.0403	0.4762	0.8510	0.060*
C4	0.0490 (3)	0.01987 (4)	0.7735 (3)	0.0524 (6)
H4	0.0869	0.0000	0.7473	0.063*
C23	−0.1999 (4)	0.44200 (5)	0.7326 (2)	0.0513 (6)
H23	−0.3261	0.4532	0.6945	0.062*
H1	−0.051 (3)	0.1201 (5)	0.815 (2)	0.065 (7)*
H3	0.369 (4)	0.3753 (6)	0.828 (3)	0.105 (10)*
H1B	0.071 (3)	0.1200 (4)	0.583 (2)	0.037 (6)*
H2B	0.283 (3)	0.3663 (4)	0.576 (2)	0.042 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0467 (9)	0.0271 (8)	0.0462 (9)	0.0022 (6)	0.0127 (7)	−0.0026 (6)
O2	0.0470 (9)	0.0249 (8)	0.0666 (10)	−0.0008 (6)	0.0198 (7)	0.0036 (6)
N1	0.0368 (10)	0.0274 (9)	0.0341 (10)	−0.0040 (7)	−0.0070 (8)	0.0043 (7)
N2	0.0420 (10)	0.0268 (9)	0.0345 (10)	−0.0023 (7)	0.0082 (8)	0.0037 (7)

C17	0.0382 (11)	0.0248 (10)	0.0268 (10)	−0.0034 (8)	−0.0024 (8)	0.0000 (8)
C19	0.0323 (11)	0.0345 (11)	0.0343 (11)	−0.0036 (8)	0.0043 (8)	−0.0014 (8)
C6	0.0351 (11)	0.0236 (10)	0.0327 (11)	0.0013 (8)	−0.0007 (8)	0.0012 (8)
C18	0.0361 (11)	0.0268 (11)	0.0341 (11)	−0.0078 (8)	0.0019 (9)	0.0031 (8)
C1	0.0376 (11)	0.0231 (10)	0.0331 (11)	0.0011 (8)	−0.0008 (8)	−0.0004 (8)
O3	0.0562 (10)	0.0435 (9)	0.0507 (9)	0.0096 (7)	−0.0195 (7)	−0.0059 (7)
C12	0.0444 (12)	0.0294 (11)	0.0364 (11)	0.0078 (9)	0.0041 (9)	0.0043 (8)
C16	0.0479 (13)	0.0339 (12)	0.0395 (12)	−0.0022 (9)	0.0156 (9)	0.0003 (9)
C14	0.0382 (11)	0.0254 (11)	0.0343 (11)	−0.0015 (8)	0.0030 (9)	0.0004 (8)
C13	0.0355 (11)	0.0313 (11)	0.0346 (11)	0.0003 (8)	−0.0012 (9)	0.0004 (8)
C11	0.0404 (12)	0.0248 (11)	0.0400 (12)	−0.0003 (9)	0.0116 (9)	−0.0017 (8)
C15	0.0530 (13)	0.0258 (11)	0.0460 (12)	−0.0051 (9)	0.0161 (10)	0.0048 (9)
C10	0.0334 (11)	0.0362 (12)	0.0432 (12)	−0.0027 (9)	0.0013 (9)	−0.0008 (9)
C20	0.0412 (12)	0.0353 (12)	0.0444 (12)	−0.0022 (9)	0.0058 (9)	−0.0016 (9)
C26	0.0427 (12)	0.0346 (12)	0.0309 (11)	0.0040 (9)	0.0002 (9)	0.0030 (8)
C21	0.0362 (11)	0.0306 (11)	0.0328 (11)	−0.0008 (8)	0.0047 (8)	0.0014 (8)
C2	0.0366 (12)	0.0351 (12)	0.0468 (13)	−0.0008 (9)	0.0043 (9)	0.0025 (9)
C8	0.0349 (11)	0.0272 (10)	0.0280 (10)	0.0003 (8)	0.0037 (8)	−0.0019 (8)
C5	0.0472 (13)	0.0308 (12)	0.0564 (14)	0.0040 (9)	0.0138 (10)	−0.0008 (10)
C3	0.0469 (13)	0.0285 (12)	0.0620 (15)	−0.0067 (9)	0.0026 (11)	0.0034 (10)
C7	0.0389 (12)	0.0286 (11)	0.0444 (12)	0.0030 (8)	0.0070 (9)	0.0035 (9)
C9	0.0375 (12)	0.0314 (11)	0.0402 (12)	0.0003 (9)	−0.0012 (9)	0.0067 (9)
C25	0.0575 (15)	0.0345 (12)	0.0443 (13)	−0.0048 (10)	−0.0008 (10)	−0.0042 (9)
C22	0.0374 (12)	0.0460 (14)	0.0505 (13)	0.0030 (10)	−0.0001 (10)	−0.0027 (10)
C24	0.0648 (16)	0.0311 (12)	0.0552 (14)	0.0071 (11)	0.0124 (12)	−0.0003 (10)
C4	0.0619 (15)	0.0228 (11)	0.0732 (16)	0.0014 (10)	0.0101 (12)	−0.0034 (10)
C23	0.0451 (14)	0.0485 (14)	0.0605 (15)	0.0134 (11)	0.0035 (11)	0.0038 (11)

Geometric parameters (Å, º)

O1—C1	1.3784 (19)	C13—H13	0.93
O1—H1	0.90 (2)	C11—C10	1.374 (2)
O2—C14	1.3883 (19)	C15—H15	0.93
O2—C11	1.394 (2)	C10—C9	1.390 (2)
N1—C8	1.414 (2)	C10—H10	0.93
N1—C7	1.471 (2)	C20—C21	1.506 (2)
N1—H1B	0.877 (17)	C20—H20A	0.97
N2—C17	1.415 (2)	C20—H20B	0.97
N2—C20	1.465 (2)	C26—C25	1.379 (2)
N2—H2B	0.882 (17)	C26—C21	1.393 (2)
C17—C16	1.381 (2)	C21—C22	1.379 (2)
C17—C18	1.400 (2)	C2—C3	1.378 (2)
C19—C18	1.375 (2)	C2—H2	0.93
C19—C14	1.378 (2)	C8—C9	1.383 (2)
C19—H19	0.93	C5—C4	1.383 (2)
C6—C5	1.385 (2)	C5—H5	0.93
C6—C1	1.395 (2)	C3—C4	1.380 (3)
C6—C7	1.507 (2)	C3—H3A	0.93

C18—H18	0.93	C7—H7A	0.97
C1—C2	1.380 (2)	C7—H7B	0.97
O3—C26	1.377 (2)	C9—H9	0.93
O3—H3	0.94 (3)	C25—C24	1.385 (3)
C12—C11	1.381 (2)	C25—H25	0.93
C12—C13	1.382 (2)	C22—C23	1.382 (3)
C12—H12	0.93	C22—H22	0.93
C16—C15	1.389 (2)	C24—C23	1.374 (3)
C16—H16	0.93	C24—H24	0.93
C14—C15	1.376 (2)	C4—H4	0.93
C13—C8	1.392 (2)	C23—H23	0.93

C1—O1—H1	105.1 (13)	C21—C20—H20A	109.7
C14—O2—C11	119.95 (13)	N2—C20—H20B	109.7
C8—N1—C7	120.62 (15)	C21—C20—H20B	109.7
C8—N1—H1B	111.2 (11)	H20A—C20—H20B	108.2
C7—N1—H1B	110.2 (11)	O3—C26—C25	119.30 (18)
C17—N2—C20	120.24 (15)	O3—C26—C21	119.25 (17)
C17—N2—H2B	110.8 (12)	C25—C26—C21	121.45 (18)
C20—N2—H2B	112.1 (11)	C22—C21—C26	118.01 (18)
C16—C17—C18	117.79 (16)	C22—C21—C20	122.77 (17)
C16—C17—N2	123.51 (16)	C26—C21—C20	119.21 (16)
C18—C17—N2	118.64 (15)	C3—C2—C1	119.80 (17)
C18—C19—C14	120.09 (16)	C3—C2—H2	120.1
C18—C19—H19	120.0	C1—C2—H2	120.1
C14—C19—H19	120.0	C9—C8—C13	118.32 (16)
C5—C6—C1	117.52 (16)	C9—C8—N1	122.91 (16)
C5—C6—C7	122.06 (16)	C13—C8—N1	118.70 (16)
C1—C6—C7	120.34 (15)	C4—C5—C6	121.54 (18)
C19—C18—C17	121.18 (16)	C4—C5—H5	119.2
C19—C18—H18	119.4	C6—C5—H5	119.2
C17—C18—H18	119.4	C2—C3—C4	120.01 (18)
O1—C1—C2	118.68 (16)	C2—C3—H3A	120.0
O1—C1—C6	119.93 (15)	C4—C3—H3A	120.0
C2—C1—C6	121.39 (16)	N1—C7—C6	110.04 (14)
C26—O3—H3	105.5 (15)	N1—C7—H7A	109.7
C11—C12—C13	119.65 (17)	C6—C7—H7A	109.7
C11—C12—H12	120.2	N1—C7—H7B	109.7
C13—C12—H12	120.2	C6—C7—H7B	109.7
C17—C16—C15	120.99 (17)	H7A—C7—H7B	108.2
C17—C16—H16	119.5	C8—C9—C10	120.73 (17)
C15—C16—H16	119.5	C8—C9—H9	119.6
C15—C14—C19	119.76 (16)	C10—C9—H9	119.6
C15—C14—O2	124.64 (15)	C26—C25—C24	119.02 (19)
C19—C14—O2	115.55 (15)	C26—C25—H25	120.5
C12—C13—C8	121.12 (17)	C24—C25—H25	120.5
C12—C13—H13	119.4	C21—C22—C23	121.37 (19)
C8—C13—H13	119.4	C21—C22—H22	119.3

C10—C11—C12	120.12 (17)	C23—C22—H22	119.3
C10—C11—O2	117.58 (17)	C23—C24—C25	120.6 (2)
C12—C11—O2	122.03 (17)	C23—C24—H24	119.7
C14—C15—C16	120.15 (16)	C25—C24—H24	119.7
C14—C15—H15	119.9	C3—C4—C5	119.71 (18)
C16—C15—H15	119.9	C3—C4—H4	120.1
C11—C10—C9	120.03 (18)	C5—C4—H4	120.1
C11—C10—H10	120.0	C24—C23—C22	119.54 (19)
C9—C10—H10	120.0	C24—C23—H23	120.2
N2—C20—C21	109.67 (14)	C22—C23—H23	120.2
N2—C20—H20A	109.7		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.90 (2)	1.80 (2)	2.628 (2)	152 (2)
O3—H3···N2	0.94 (3)	1.82 (3)	2.670 (2)	150 (2)
N1—H1*B*···O3^{i}	0.88 (2)	2.00 (2)	2.876 (2)	179 (2)
N2—H2*B*···O1^{ii}	0.88 (2)	2.03 (2)	2.914 (2)	176 (2)

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