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## Structure Reports

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## 6,6'-Diethoxy-2,2'-[propane-1,2-diyl-bis(nitrilomethylidene)]diphenol

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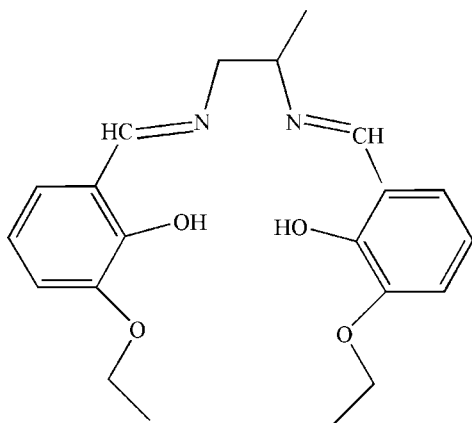
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Key indicators: single-crystal X-ray study;  $T = 273$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.066;  $wR$  factor = 0.193; data-to-parameter ratio = 13.9.

In the title molecule,  $\text{C}_{21}\text{H}_{26}\text{N}_2\text{O}_4$ , the dihedral angle between the two benzene rings is  $88.4(3)^\circ$ . Two fairly strong intramolecular  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bonds may, in part, influence the molecular conformation.

## Related literature

For background information on the coordination ability of tetradentate Schiff-base ligands, see: Bermejo *et al.* (2007); Ni *et al.* (2005); Nayak *et al.*, 2006; Mohanta *et al.*, 2002; Saha *et al.* (2007); Wang *et al.* (2008); Yu *et al.* (2007).



## Experimental

## Crystal data

 $\text{C}_{21}\text{H}_{26}\text{N}_2\text{O}_4$   
 $M_r = 370.44$ 

 Triclinic,  $P\bar{1}$   
 $a = 9.140(3)$  Å

 $b = 11.451(4)$  Å  
 $c = 13.013(5)$  Å  
 $\alpha = 113.845(5)^\circ$   
 $\beta = 109.628(6)^\circ$   
 $\gamma = 108.812(5)^\circ$   
 $V = 993.5(6)$  Å<sup>3</sup>
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.09$  mm<sup>-1</sup>  
 $T = 273(2)$  K  
 $0.12 \times 0.11 \times 0.09$  mm

## Data collection

 Bruker APEXII CCD area-detector diffractometer  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.990$ ,  $T_{\max} = 0.992$ 

 4894 measured reflections  
 3451 independent reflections  
 2325 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.030$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.066$   
 $wR(F^2) = 0.193$   
 $S = 1.00$   
 3451 reflections

 249 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.26$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.26$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O3}-\text{H3}\cdots\text{N2}$	0.82	1.89	2.614 (3)	147
$\text{O1}-\text{H1}\cdots\text{N1}$	0.82	1.85	2.576 (2)	146

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT-Plus (Bruker, 2001); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2762).

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## supporting information

*Acta Cryst.* (2009). E65, o646 [doi:10.1107/S1600536809003328]

**6,6'-Diethoxy-2,2'-[propane-1,2-diybis(nitrilomethylidene)]diphenol****Zhen Jia****S1. Comment**

Among the tetradentate schiff-base ligands studied intensely during the past several decades, the planar, salen types and their complexes (with interesting magnetic properties) have been given much attention due to their excellent coordination ability, utilizing two N atoms and two O atoms (Ni *et al.*, 2005; Wang *et al.*, 2008; Yu *et al.*, 2007; Nayak *et al.*, 2006; Mohanta *et al.*, 2002; Saha *et al.*, 2007).

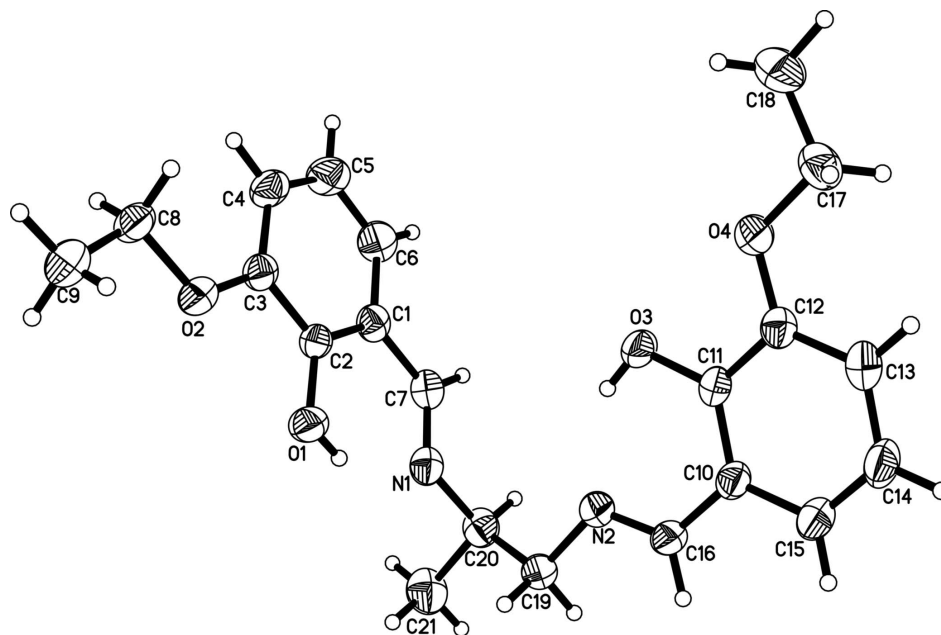
Herein, we report the synthesis and crystal structure of a new tetradentate Schiff base ligand, *N,N'*-bis(2-hydroxy-3-ethoxybenzylidene)-1,2-diaminopropane. The molecular structure of the title compound is shown in Fig. 1. The molecule possesses an O<sub>2</sub>N<sub>2</sub> donor set affording a potentially tetradentate ligand. The imide bond lengths 1.262 (3) for N1—C7 and 1.263 (3) Å for N2—C16 are slightly shorter than that of *N,N'*-bis(2-hydroxy-3-methoxybenzylidene)ethylenediamine (1.272 Å) (Bermejo, *et al.*, 2007). The C—N bond distance of 1.461 (3) Å is in agreement well with that found in the same compound. Two fairly strong intramolecular O···H—N hydrogen bonds may in part influence the molecular conformation.

**S2. Experimental**

The Schiff base ligand was synthesized by condensation 1,2-diaminopropane and 2-hydroxy-3-ethoxybenzaldehyde with molar ratio 1:2 in ethanol. The mixture formed was allowed to partially evaporate in air for several days to produce crystals suitable for X-ray diffraction with a yield about 65%.

**S3. Refinement**

H atoms were placed in calculated positions with C—H distances of 0.93, 0.96, 0.97 Å and O—H 0.82 Å, and were allowed for as riding atoms with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$  for methyl H atoms,  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for all other C bound H atoms and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$ .

**Figure 1**

The molecular structure of the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

### 6,6'-Diethoxy-2,2'-[propane-1,2-diylbis(nitrilomethylidyne)]diphenol

#### Crystal data

$C_{21}H_{26}N_2O_4$

$M_r = 370.44$

Triclinic,  $P\bar{1}$

Hall symbol:  $-P\ 1$

$a = 9.140\ (3)\ \text{\AA}$

$b = 11.451\ (4)\ \text{\AA}$

$c = 13.013\ (5)\ \text{\AA}$

$\alpha = 113.845\ (5)^\circ$

$\beta = 109.628\ (6)^\circ$

$\gamma = 108.812\ (5)^\circ$

$V = 993.5\ (6)\ \text{\AA}^3$

$Z = 2$

$F(000) = 396$

$D_x = 1.238\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 1361 reflections

$\theta = 2.4\text{--}23.9^\circ$

$\mu = 0.09\ \text{mm}^{-1}$

$T = 273\ \text{K}$

Block, yellow

$0.12 \times 0.11 \times 0.09\ \text{mm}$

#### Data collection

Bruker APEXII CCD area-detector  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.990$ ,  $T_{\max} = 0.992$

4894 measured reflections

3451 independent reflections

2325 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.030$

$\theta_{\max} = 25.0^\circ$ ,  $\theta_{\min} = 2.0^\circ$

$h = -10 \rightarrow 10$

$k = -13 \rightarrow 11$

$l = -15 \rightarrow 13$

Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.066$   
 $wR(F^2) = 0.193$   
 $S = 1.00$   
 3451 reflections  
 249 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-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.1202P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.26 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.26 \text{ e } \text{\AA}^{-3}$

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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.2732 (2)	0.85334 (19)	0.31097 (15)	0.0615 (5)
H1	0.2881	0.8851	0.3848	0.092*
O2	0.1699 (2)	0.75251 (19)	0.06238 (15)	0.0625 (5)
O3	0.1229 (2)	0.44342 (19)	0.38472 (16)	0.0658 (5)
H3	0.1614	0.5336	0.4307	0.099*
O4	0.0549 (2)	0.16836 (19)	0.25933 (17)	0.0666 (5)
N1	0.1898 (3)	0.8527 (2)	0.4813 (2)	0.0553 (5)
N2	0.3270 (3)	0.7183 (2)	0.60118 (19)	0.0571 (5)
C1	-0.0337 (3)	0.6987 (3)	0.2479 (2)	0.0521 (6)
C2	0.0950 (3)	0.7499 (2)	0.2166 (2)	0.0477 (6)
C3	0.0365 (3)	0.6931 (3)	0.0830 (2)	0.0514 (6)
C4	-0.1454 (3)	0.5848 (3)	-0.0147 (3)	0.0621 (7)
H4	-0.1842	0.5446	-0.1036	0.075*
C5	-0.2713 (4)	0.5348 (3)	0.0171 (3)	0.0717 (8)
H5	-0.3937	0.4618	-0.0504	0.086*
C6	-0.2174 (3)	0.5916 (3)	0.1466 (3)	0.0673 (7)
H6	-0.3033	0.5588	0.1674	0.081*
C7	0.0251 (4)	0.7553 (3)	0.3859 (3)	0.0554 (6)
H7	-0.0619	0.7182	0.4045	0.067*
C8	0.1151 (4)	0.6978 (3)	-0.0732 (2)	0.0642 (7)
H8A	0.0269	0.7214	-0.1103	0.077*
H8B	0.0583	0.5892	-0.1270	0.077*
C9	0.2824 (4)	0.7724 (3)	-0.0729 (3)	0.0811 (9)
H9A	0.3376	0.8797	-0.0192	0.122*
H9B	0.2492	0.7382	-0.1626	0.122*

H9C	0.3681	0.7475	-0.0369	0.122*
C10	0.3713 (3)	0.5196 (3)	0.5889 (2)	0.0523 (6)
C11	0.2296 (3)	0.4113 (3)	0.4549 (2)	0.0509 (6)
C12	0.1958 (3)	0.2656 (3)	0.3898 (2)	0.0543 (6)
C13	0.3036 (4)	0.2294 (3)	0.4590 (3)	0.0641 (7)
H13	0.2816	0.1324	0.4161	0.077*
C14	0.4442 (4)	0.3374 (3)	0.5920 (3)	0.0722 (8)
H14	0.5158	0.3124	0.6379	0.087*
C15	0.4778 (4)	0.4803 (3)	0.6557 (3)	0.0687 (7)
H15	0.5728	0.5520	0.7446	0.082*
C16	0.4133 (3)	0.6729 (3)	0.6564 (2)	0.0563 (6)
H16	0.5092	0.7418	0.7454	0.068*
C17	0.0096 (4)	0.0166 (3)	0.1890 (3)	0.0718 (8)
H17A	-0.0139	-0.0273	0.2360	0.086*
H17B	0.1100	0.0128	0.1810	0.086*
C18	-0.1577 (5)	-0.0678 (3)	0.0545 (3)	0.0911 (10)
H18A	-0.2550	-0.0608	0.0637	0.137*
H18B	-0.1943	-0.1717	0.0050	0.137*
H18C	-0.1316	-0.0253	0.0079	0.137*
C19	0.3894 (4)	0.8780 (3)	0.6768 (2)	0.0609 (7)
H19A	0.4958	0.9345	0.6779	0.073*
H19B	0.4262	0.9145	0.7681	0.073*
C20	0.2425 (4)	0.9054 (3)	0.6181 (2)	0.0606 (7)
H20	0.1354	0.8498	0.6181	0.073*
C21	0.3133 (5)	1.0728 (3)	0.6992 (3)	0.0823 (9)
H21A	0.4190	1.1274	0.7001	0.123*
H21B	0.3464	1.1076	0.7889	0.123*
H21C	0.2192	1.0891	0.6599	0.123*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0559 (10)	0.0630 (11)	0.0471 (9)	0.0206 (9)	0.0246 (9)	0.0290 (9)
O2	0.0652 (11)	0.0655 (11)	0.0460 (9)	0.0286 (9)	0.0262 (8)	0.0316 (9)
O3	0.0776 (12)	0.0552 (11)	0.0516 (10)	0.0405 (10)	0.0184 (9)	0.0305 (9)
O4	0.0835 (12)	0.0521 (10)	0.0561 (11)	0.0391 (10)	0.0296 (10)	0.0292 (9)
N1	0.0655 (13)	0.0568 (12)	0.0575 (12)	0.0359 (11)	0.0376 (11)	0.0371 (11)
N2	0.0645 (12)	0.0497 (12)	0.0481 (12)	0.0273 (10)	0.0254 (10)	0.0279 (10)
C1	0.0525 (13)	0.0543 (14)	0.0617 (15)	0.0350 (12)	0.0305 (12)	0.0374 (13)
C2	0.0481 (13)	0.0457 (13)	0.0480 (13)	0.0267 (11)	0.0205 (11)	0.0290 (11)
C3	0.0581 (14)	0.0496 (14)	0.0507 (14)	0.0336 (12)	0.0263 (12)	0.0305 (12)
C4	0.0612 (16)	0.0656 (17)	0.0531 (15)	0.0383 (14)	0.0199 (13)	0.0346 (13)
C5	0.0499 (15)	0.0744 (19)	0.0703 (19)	0.0333 (14)	0.0175 (14)	0.0382 (16)
C6	0.0514 (15)	0.0750 (18)	0.0800 (19)	0.0363 (14)	0.0324 (15)	0.0483 (16)
C7	0.0610 (15)	0.0584 (15)	0.0669 (16)	0.0367 (13)	0.0408 (14)	0.0419 (14)
C8	0.0781 (17)	0.0652 (16)	0.0425 (13)	0.0379 (14)	0.0274 (13)	0.0302 (13)
C9	0.095 (2)	0.085 (2)	0.0584 (17)	0.0396 (18)	0.0421 (16)	0.0423 (16)
C10	0.0522 (13)	0.0598 (15)	0.0498 (13)	0.0284 (12)	0.0264 (12)	0.0370 (12)

C11	0.0558 (13)	0.0574 (15)	0.0537 (14)	0.0337 (12)	0.0300 (12)	0.0394 (12)
C12	0.0609 (15)	0.0575 (15)	0.0559 (15)	0.0335 (13)	0.0342 (13)	0.0372 (13)
C13	0.0728 (17)	0.0681 (17)	0.0798 (19)	0.0450 (15)	0.0460 (16)	0.0538 (16)
C14	0.0699 (17)	0.083 (2)	0.083 (2)	0.0471 (16)	0.0342 (16)	0.0630 (18)
C15	0.0634 (16)	0.0759 (19)	0.0646 (16)	0.0350 (15)	0.0245 (14)	0.0484 (15)
C16	0.0538 (14)	0.0562 (15)	0.0439 (13)	0.0209 (12)	0.0201 (12)	0.0291 (12)
C17	0.0860 (19)	0.0567 (17)	0.079 (2)	0.0429 (16)	0.0472 (17)	0.0374 (15)
C18	0.106 (2)	0.0601 (18)	0.080 (2)	0.0436 (18)	0.041 (2)	0.0271 (17)
C19	0.0686 (15)	0.0513 (15)	0.0475 (14)	0.0251 (13)	0.0255 (12)	0.0271 (12)
C20	0.0739 (17)	0.0623 (16)	0.0578 (15)	0.0367 (14)	0.0445 (14)	0.0359 (13)
C21	0.114 (2)	0.0701 (19)	0.081 (2)	0.0571 (19)	0.063 (2)	0.0424 (17)

*Geometric parameters (Å, °)*

O1—C2	1.341 (3)	C9—H9B	0.9600
O1—H1	0.8200	C9—H9C	0.9600
O2—C3	1.361 (3)	C10—C15	1.391 (3)
O2—C8	1.437 (3)	C10—C11	1.397 (3)
O3—C11	1.351 (3)	C10—C16	1.447 (3)
O3—H3	0.8200	C11—C12	1.394 (3)
O4—C12	1.364 (3)	C12—C13	1.387 (4)
O4—C17	1.423 (3)	C13—C14	1.388 (4)
N1—C7	1.262 (3)	C13—H13	0.9300
N1—C20	1.461 (3)	C14—C15	1.366 (4)
N2—C16	1.263 (3)	C14—H14	0.9300
N2—C19	1.461 (3)	C15—H15	0.9300
C1—C6	1.393 (3)	C16—H16	0.9300
C1—C2	1.401 (3)	C17—C18	1.489 (4)
C1—C7	1.456 (4)	C17—H17A	0.9700
C2—C3	1.404 (3)	C17—H17B	0.9700
C3—C4	1.376 (3)	C18—H18A	0.9600
C4—C5	1.382 (4)	C18—H18B	0.9600
C4—H4	0.9300	C18—H18C	0.9600
C5—C6	1.362 (4)	C19—C20	1.503 (4)
C5—H5	0.9300	C19—H19A	0.9700
C6—H6	0.9300	C19—H19B	0.9700
C7—H7	0.9300	C20—C21	1.521 (4)
C8—C9	1.490 (4)	C20—H20	0.9800
C8—H8A	0.9700	C21—H21A	0.9600
C8—H8B	0.9700	C21—H21B	0.9600
C9—H9A	0.9600	C21—H21C	0.9600
C2—O1—H1	109.5	O4—C12—C13	124.9 (2)
C3—O2—C8	116.92 (19)	O4—C12—C11	115.6 (2)
C11—O3—H3	109.5	C13—C12—C11	119.5 (2)
C12—O4—C17	118.2 (2)	C12—C13—C14	120.2 (3)
C7—N1—C20	120.5 (2)	C12—C13—H13	119.9
C16—N2—C19	118.7 (2)	C14—C13—H13	119.9

C6—C1—C2	119.9 (2)	C15—C14—C13	120.3 (2)
C6—C1—C7	120.0 (2)	C15—C14—H14	119.9
C2—C1—C7	120.1 (2)	C13—C14—H14	119.9
O1—C2—C1	122.0 (2)	C14—C15—C10	120.7 (3)
O1—C2—C3	118.7 (2)	C14—C15—H15	119.6
C1—C2—C3	119.4 (2)	C10—C15—H15	119.6
O2—C3—C4	125.7 (2)	N2—C16—C10	123.6 (2)
O2—C3—C2	115.3 (2)	N2—C16—H16	118.2
C4—C3—C2	119.1 (2)	C10—C16—H16	118.2
C3—C4—C5	121.1 (2)	O4—C17—C18	107.3 (2)
C3—C4—H4	119.4	O4—C17—H17A	110.3
C5—C4—H4	119.4	C18—C17—H17A	110.3
C6—C5—C4	120.5 (2)	O4—C17—H17B	110.3
C6—C5—H5	119.8	C18—C17—H17B	110.3
C4—C5—H5	119.8	H17A—C17—H17B	108.5
C5—C6—C1	120.0 (3)	C17—C18—H18A	109.5
C5—C6—H6	120.0	C17—C18—H18B	109.5
C1—C6—H6	120.0	H18A—C18—H18B	109.5
N1—C7—C1	122.4 (2)	C17—C18—H18C	109.5
N1—C7—H7	118.8	H18A—C18—H18C	109.5
C1—C7—H7	118.8	H18B—C18—H18C	109.5
O2—C8—C9	107.9 (2)	N2—C19—C20	112.0 (2)
O2—C8—H8A	110.1	N2—C19—H19A	109.2
C9—C8—H8A	110.1	C20—C19—H19A	109.2
O2—C8—H8B	110.1	N2—C19—H19B	109.2
C9—C8—H8B	110.1	C20—C19—H19B	109.2
H8A—C8—H8B	108.4	H19A—C19—H19B	107.9
C8—C9—H9A	109.5	N1—C20—C19	109.1 (2)
C8—C9—H9B	109.5	N1—C20—C21	109.2 (2)
H9A—C9—H9B	109.5	C19—C20—C21	110.2 (2)
C8—C9—H9C	109.5	N1—C20—H20	109.5
H9A—C9—H9C	109.5	C19—C20—H20	109.5
H9B—C9—H9C	109.5	C21—C20—H20	109.5
C15—C10—C11	119.3 (2)	C20—C21—H21A	109.5
C15—C10—C16	119.9 (2)	C20—C21—H21B	109.5
C11—C10—C16	120.8 (2)	H21A—C21—H21B	109.5
O3—C11—C12	118.1 (2)	C20—C21—H21C	109.5
O3—C11—C10	121.8 (2)	H21A—C21—H21C	109.5
C12—C11—C10	120.0 (2)	H21B—C21—H21C	109.5

*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>
O3—H3...N2	0.82	1.89	2.614 (3)	147
O1—H1...N1	0.82	1.85	2.576 (2)	146