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A second tricilinc polymorph of 6,6′-diethoxy-2,2′-[propane-1,2-diylbis(nitrilomethylidyne)]diphenol

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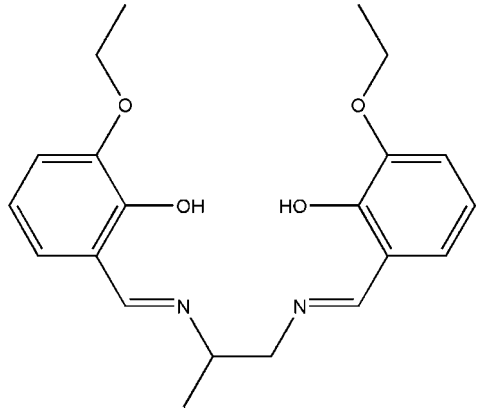
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.045; wR factor = 0.136; data-to-parameter ratio = 22.2.

The title Schiff base compound, $C_{21}H_{26}N_2O_4$, is a second triclinic polymorph of a previously reported room-temperature structure [Jia (2009). *Acta Cryst.* E**65**, o646]. Strong intramolecular O—H···N hydrogen bonds generate S(6) ring motifs. Intermolecular C—H···O interactions link neighbouring molecules into dimers with an $R_2^2(16)$ ring motif. The mean planes of the two benzene rings are almost perpendicular to each other, making a dihedral angle of 88.24 (5)°. An interesting feature of the crystal structure is the intermolecular short C···O [3.1878 (13) Å] contact which is shorter than the sum of the van der Waals radii of the relevant atoms. The crystal structure is further stabilized by intermolecular C—H···π and π–π interactions [centroid–centroid distance = 3.7414 (6) Å]. The structure has a stereogenic centre but the space group is centrosymmetric, so the molecule exists as a racemate.

Related literature

For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For information on Schiff base ligands, complexes and their applications, see: Calligaris & Randaccio (1987). For the other polymorph, see: Jia, (2009). For related structures, see: Li *et al.* (2005); Bomfim *et al.* (2005); Glidewell *et al.* (2005, 2006); Sun *et al.* (2004); Fun *et al.* (2008). For bond-length data, see: Allen *et al.* (1987). For stability of the temperature controller used for data collection, see: Cosier & Glazer (1986).



Experimental

Crystal data

$C_{21}H_{26}N_2O_4$
M_r = 370.44
Triclinic, $P\overline{1}$
a = 8.9729 (2) Å
b = 10.7008 (4) Å
c = 11.3633 (2) Å
α = 107.432 (1)°
β = 108.487 (1)°
γ = 95.979 (1)°
V = 963.03 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 K
0.56 × 0.27 × 0.25 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.952, T_{max} = 0.978
19581 measured reflections
5527 independent reflections
4721 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.136
S = 1.05
5527 reflections
249 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.84	1.83	2.5752 (13)	146
O2—H2···N2	0.84	1.88	2.6178 (13)	147
C9—H9A···O1^{i}	0.99	2.49	3.4293 (14)	159
C18—H18b···$Cg1^{ii}$	0.99	2.98	3.8340 (12)	142
C7—H7A···$Cg2^{iii}$	0.96	2.72	3.5554 (12)	176

Symmetry codes: (i) $-x+1, -y+1, -z+2$; (ii) $-x, -y+1, -z+1$; (iii) $-x+1, -y+2, -z+2$. $Cg1$ and $Cg2$ are the centroids of the C1–C6 and C11–C16 benzene rings, respectively.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2736).

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supplementary materials

Acta Cryst. (2009). E**65**, o722-o723 [**doi:10.1107/S1600536809008137**]

A second tricilinc polymorph of 6,6'-diethoxy-2,2'-[propane-1,2-diylbis(nitrilomethylidyne)]diphenol

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Comment

Schiff bases are one of the most prevalent mixed-donor ligands in the field of coordination chemistry. They play an important role in the development of coordination chemistry related to catalysis and enzymatic reactions, magnetism, and supramolecular architectures (Calligaris & Randaccio, 1987). Structures of Schiff bases derived from substituted benzaldehydes and closely related to the title compound have been reported earlier (Li *et al.*, 2005; Bomfim *et al.*, 2005; Glidewell *et al.*, 2006; Sun *et al.*, 2004; Fun *et al.,* 2008).

The molecule of the title compound (Fig. 1), is a potentially tetradentate Schiff base ligand. The bond lengths (Allen *et al.,* 1987) and angles are comparable to the earlier room-temperature polymorph which was published previously (Jia, 2009). Strong intramolecular O—H···N hydrogen bonds generate *S(6)* ring motifs (Bernstein *et al.*, 1995). Intermolecular C—H···O interactions link neighbouring molecules into dimers with a $R_2^2(16)$ ring motif (Bernstein *et al.,* 1995). The mean planes of the two benzene rings are almost perpendicular to each other making a dihedral angle of 88.24 (5)°. The interesting feature of the crystal structure is the short C18···O2 [3.1878 (13) Å, symmetry code: 1 - x, 1 - y, 1 - z] contact which is shorter than the sum of the van der Waals radii of the relevant atoms. The crystal structure, is further stabilizd by intermolecular C—H···π and π-π interactions [centroid to centroid distance of 3.7414 (6) Å]. The structure has a stereogenic centre but the space group is centrosymmetric, so the molecule exists as racemate.

Experimental

The synthetic method has been described earlier (Fun *et al.,* 2008), except that 3-ethoxy salicylaldehyde and 2-methyl-2,3-propanediamine were used as starting materials. Single crystals suitable for *X*-ray diffraction were obtained by evaporation of an ethanol solution at room temperature.

Refinement

H atoms of the hydroxy groups were positioned by a freely rotating O—H bond and constrained with a fixed distance of 0.84 Å. The rest of the hydrogen atoms were positioned geometrically and refined using a riding model with C—H = 0.95–1.00 Å and U_{iso}(H) = 1.2 or 1.5 U_{eq}(C). A rotating-group model was applied for the methyl groups.

Figures

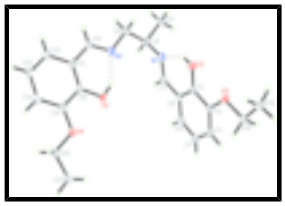

Fig. 1. The molecular structure of the title compound with atom labels and 50% probability ellipsoids for non-H atoms. Dashed lines indicate intramolecular O—H···N hydrogen bonds.

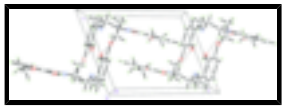

Fig. 2. The crystal structure of the title compound, viewed down the *b*-axis, showing dimer formation by $R_2^2(16)$ ring motif.

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

Crystal data

$C_{21}H_{26}N_2O_4$	$Z = 2$
$M_r = 370.44$	$F_{000} = 396$
Triclinic, $P\overline{1}$	$D_x = 1.277$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.9729$ (2) Å	Cell parameters from 9912 reflections
$b = 10.7008$ (4) Å	$\theta = 2.5$–33.9º
$c = 11.3633$ (2) Å	$\mu = 0.09$ mm^{-1}
$\alpha = 107.432$ (1)º	$T = 100$ K
$\beta = 108.487$ (1)º	Block, yellow
$\gamma = 95.979$ (1)º	0.56 × 0.27 × 0.25 mm
$V = 963.03$ (5) Å^3	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	5527 independent reflections
Radiation source: fine-focus sealed tube	4721 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.026$
$T = 100$ K	$\theta_{max} = 30.0$º
φ and ω scans	$\theta_{min} = 2.0$º
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)	$h = -12 \rightarrow 12$
$T_{min} = 0.952$, $T_{max} = 0.978$	$k = -15 \rightarrow 15$
19581 measured reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.045$	H-atom parameters constrained
$wR(F^2) = 0.136$	$w = 1/[\sigma^2(F_o^2) + (0.0795P)^2 + 0.2658P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.001$
5527 reflections	$\Delta\rho_{max} = 0.53$ e Å^{-3}
249 parameters	$\Delta\rho_{min} = -0.23$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cyrosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1)K.

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.

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 $F^2 > 2$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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.45973 (9)	0.68396 (7)	1.04387 (8)	0.02067 (16)
H1	0.3996	0.6074	0.9989	0.031*
O2	0.23678 (10)	0.61221 (7)	0.56112 (7)	0.02165 (17)
H2	0.2199	0.5617	0.6018	0.032*
O3	0.60593 (9)	0.93704 (7)	1.19014 (7)	0.02040 (16)
O4	0.30071 (10)	0.74269 (7)	0.41348 (7)	0.02157 (17)
N1	0.20357 (10)	0.51029 (9)	0.87252 (9)	0.01932 (18)
N2	0.22170 (11)	0.39204 (9)	0.61688 (9)	0.01981 (18)
C1	0.37342 (12)	0.77863 (10)	1.03131 (9)	0.01695 (19)
C2	0.45003 (12)	0.91483 (10)	1.10727 (10)	0.01745 (19)
C3	0.36454 (13)	1.01381 (10)	1.09335 (10)	0.0202 (2)
H3A	0.4165	1.1055	1.1421	0.024*
C4	0.20267 (13)	0.98033 (11)	1.00838 (11)	0.0230 (2)
H4A	0.1456	1.0492	1.0003	0.028*
C5	0.12610 (12)	0.84751 (11)	0.93638 (11)	0.0218 (2)
H5A	0.0158	0.8249	0.8801	0.026*
C6	0.21104 (12)	0.74568 (10)	0.94623 (10)	0.01782 (19)
C7	0.13033 (12)	0.60568 (10)	0.86605 (10)	0.0193 (2)
H7A	0.0211	0.5852	0.8079	0.023*
C8	0.11726 (12)	0.37212 (10)	0.78846 (10)	0.0197 (2)
H8A	0.0055	0.3712	0.7325	0.024*

C9	0.20882 (13)	0.31383 (10)	0.70025 (10)	0.0209 (2)
H9A	0.3182	0.3127	0.7564	0.025*
H9B	0.1525	0.2200	0.6432	0.025*
C10	0.25539 (12)	0.33633 (10)	0.51501 (10)	0.0195 (2)
H10A	0.2624	0.2448	0.4936	0.023*
C11	0.28343 (12)	0.40753 (10)	0.43059 (10)	0.01798 (19)
C12	0.32606 (13)	0.34087 (11)	0.32285 (10)	0.0224 (2)
H12A	0.3319	0.2492	0.3041	0.027*
C13	0.35938 (13)	0.40746 (11)	0.24449 (10)	0.0236 (2)
H13A	0.3881	0.3617	0.1721	0.028*
C14	0.35108 (12)	0.54260 (11)	0.27131 (10)	0.0211 (2)
H14A	0.3732	0.5880	0.2165	0.025*
C15	0.31054 (12)	0.61053 (10)	0.37785 (10)	0.01799 (19)
C16	0.27562 (11)	0.54322 (10)	0.45865 (9)	0.01716 (19)
C17	0.11095 (14)	0.29050 (11)	0.87711 (11)	0.0251 (2)
H17A	0.0583	0.3321	0.9376	0.038*
H17B	0.2207	0.2884	0.9286	0.038*
H17C	0.0497	0.1987	0.8220	0.038*
C18	0.68435 (13)	1.07531 (10)	1.27022 (10)	0.0207 (2)
H18A	0.6284	1.1129	1.3306	0.025*
H18B	0.6818	1.1295	1.2129	0.025*
C19	0.85652 (13)	1.07880 (11)	1.34933 (11)	0.0250 (2)
H19A	0.9117	1.1714	1.4071	0.038*
H19B	0.9119	1.0446	1.2887	0.038*
H19C	0.8576	1.0226	1.4036	0.038*
C20	0.32265 (13)	0.81235 (11)	0.32824 (11)	0.0228 (2)
H20A	0.2482	0.7626	0.2357	0.027*
H20B	0.4345	0.8213	0.3305	0.027*
C21	0.28754 (16)	0.94927 (12)	0.37877 (13)	0.0284 (2)
H21A	0.3039	1.0011	0.3242	0.043*
H21B	0.3602	0.9965	0.4710	0.043*
H21C	0.1757	0.9390	0.3739	0.043*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0213 (3)	0.0161 (3)	0.0204 (4)	0.0042 (3)	0.0039 (3)	0.0045 (3)
O2	0.0338 (4)	0.0181 (3)	0.0173 (3)	0.0072 (3)	0.0154 (3)	0.0053 (3)
O3	0.0215 (3)	0.0164 (3)	0.0181 (3)	0.0023 (3)	0.0042 (3)	0.0027 (3)
O4	0.0309 (4)	0.0184 (3)	0.0173 (3)	0.0041 (3)	0.0113 (3)	0.0066 (3)
N1	0.0206 (4)	0.0199 (4)	0.0153 (4)	0.0007 (3)	0.0065 (3)	0.0044 (3)
N2	0.0234 (4)	0.0187 (4)	0.0165 (4)	0.0036 (3)	0.0070 (3)	0.0059 (3)
C1	0.0202 (4)	0.0180 (4)	0.0139 (4)	0.0042 (3)	0.0082 (3)	0.0053 (3)
C2	0.0204 (4)	0.0183 (4)	0.0145 (4)	0.0037 (3)	0.0085 (3)	0.0049 (3)
C3	0.0257 (5)	0.0191 (4)	0.0187 (5)	0.0064 (4)	0.0124 (4)	0.0055 (4)
C4	0.0251 (5)	0.0247 (5)	0.0240 (5)	0.0110 (4)	0.0132 (4)	0.0090 (4)
C5	0.0199 (4)	0.0271 (5)	0.0209 (5)	0.0080 (4)	0.0096 (4)	0.0087 (4)
C6	0.0191 (4)	0.0202 (4)	0.0153 (4)	0.0039 (3)	0.0084 (3)	0.0057 (3)

C7	0.0190 (4)	0.0231 (5)	0.0150 (4)	0.0018 (3)	0.0070 (3)	0.0058 (4)
C8	0.0195 (4)	0.0194 (4)	0.0169 (4)	0.0010 (3)	0.0047 (3)	0.0050 (4)
C9	0.0264 (5)	0.0188 (4)	0.0178 (4)	0.0055 (4)	0.0078 (4)	0.0070 (4)
C10	0.0226 (4)	0.0166 (4)	0.0164 (4)	0.0043 (3)	0.0055 (4)	0.0038 (3)
C11	0.0194 (4)	0.0181 (4)	0.0140 (4)	0.0041 (3)	0.0052 (3)	0.0033 (3)
C12	0.0276 (5)	0.0212 (5)	0.0169 (4)	0.0079 (4)	0.0088 (4)	0.0033 (4)
C13	0.0272 (5)	0.0277 (5)	0.0155 (4)	0.0083 (4)	0.0103 (4)	0.0037 (4)
C14	0.0218 (5)	0.0262 (5)	0.0152 (4)	0.0041 (4)	0.0075 (4)	0.0066 (4)
C15	0.0184 (4)	0.0188 (4)	0.0146 (4)	0.0026 (3)	0.0052 (3)	0.0043 (3)
C16	0.0185 (4)	0.0185 (4)	0.0125 (4)	0.0036 (3)	0.0059 (3)	0.0029 (3)
C17	0.0282 (5)	0.0245 (5)	0.0222 (5)	0.0000 (4)	0.0093 (4)	0.0096 (4)
C18	0.0247 (5)	0.0160 (4)	0.0181 (4)	0.0019 (3)	0.0081 (4)	0.0021 (3)
C19	0.0253 (5)	0.0213 (5)	0.0222 (5)	0.0020 (4)	0.0049 (4)	0.0042 (4)
C20	0.0276 (5)	0.0240 (5)	0.0205 (5)	0.0041 (4)	0.0116 (4)	0.0105 (4)
C21	0.0377 (6)	0.0249 (5)	0.0295 (6)	0.0082 (4)	0.0168 (5)	0.0140 (4)

Geometric parameters (Å, °)

O1—C1	1.3514 (12)	C9—H9B	0.9900
O1—H1	0.8400	C10—C11	1.4542 (15)
O2—C16	1.3484 (11)	C10—H10A	0.9500
O2—H2	0.8400	C11—C16	1.4046 (13)
O3—C2	1.3643 (12)	C11—C12	1.4087 (14)
O3—C18	1.4432 (12)	C12—C13	1.3765 (16)
O4—C15	1.3701 (12)	C12—H12A	0.9500
O4—C20	1.4338 (13)	C13—C14	1.4008 (15)
N1—C7	1.2780 (14)	C13—H13A	0.9500
N1—C8	1.4644 (13)	C14—C15	1.3905 (14)
N2—C10	1.2777 (13)	C14—H14A	0.9500
N2—C9	1.4614 (14)	C15—C16	1.4112 (14)
C1—C6	1.4062 (13)	C17—H17A	0.9800
C1—C2	1.4153 (13)	C17—H17B	0.9800
C2—C3	1.3885 (14)	C17—H17C	0.9800
C3—C4	1.4018 (15)	C18—C19	1.5110 (15)
C3—H3A	0.9500	C18—H18A	0.9900
C4—C5	1.3802 (15)	C18—H18B	0.9900
C4—H4A	0.9500	C19—H19A	0.9800
C5—C6	1.4046 (14)	C19—H19B	0.9800
C5—H5A	0.9500	C19—H19C	0.9800
C6—C7	1.4617 (14)	C20—C21	1.5107 (16)
C7—H7A	0.9500	C20—H20A	0.9900
C8—C9	1.5242 (15)	C20—H20B	0.9900
C8—C17	1.5277 (15)	C21—H21A	0.9800
C8—H8A	1.0000	C21—H21B	0.9800
C9—H9A	0.9900	C21—H21C	0.9800
C1—O1—H1	109.5	C13—C12—C11	120.54 (9)
C16—O2—H2	109.5	C13—C12—H12A	119.7
C2—O3—C18	116.03 (8)	C11—C12—H12A	119.7
C15—O4—C20	116.95 (8)	C12—C13—C14	120.13 (9)

C7—N1—C8	118.97 (9)	C12—C13—H13A	119.9
C10—N2—C9	117.69 (9)	C14—C13—H13A	119.9
O1—C1—C6	122.09 (9)	C15—C14—C13	120.23 (10)
O1—C1—C2	118.39 (8)	C15—C14—H14A	119.9
C6—C1—C2	119.52 (9)	C13—C14—H14A	119.9
O3—C2—C3	125.27 (9)	O4—C15—C14	124.90 (9)
O3—C2—C1	115.48 (9)	O4—C15—C16	114.95 (8)
C3—C2—C1	119.25 (9)	C14—C15—C16	120.15 (9)
C2—C3—C4	120.94 (9)	O2—C16—C11	122.22 (9)
C2—C3—H3A	119.5	O2—C16—C15	118.56 (9)
C4—C3—H3A	119.5	C11—C16—C15	119.22 (9)
C5—C4—C3	120.10 (10)	C8—C17—H17A	109.5
C5—C4—H4A	119.9	C8—C17—H17B	109.5
C3—C4—H4A	119.9	H17A—C17—H17B	109.5
C4—C5—C6	120.06 (10)	C8—C17—H17C	109.5
C4—C5—H5A	120.0	H17A—C17—H17C	109.5
C6—C5—H5A	120.0	H17B—C17—H17C	109.5
C5—C6—C1	120.10 (9)	O3—C18—C19	107.74 (8)
C5—C6—C7	119.59 (9)	O3—C18—H18A	110.2
C1—C6—C7	120.30 (9)	C19—C18—H18A	110.2
N1—C7—C6	121.39 (9)	O3—C18—H18B	110.2
N1—C7—H7A	119.3	C19—C18—H18B	110.2
C6—C7—H7A	119.3	H18A—C18—H18B	108.5
N1—C8—C9	108.28 (8)	C18—C19—H19A	109.5
N1—C8—C17	108.78 (8)	C18—C19—H19B	109.5
C9—C8—C17	109.96 (9)	H19A—C19—H19B	109.5
N1—C8—H8A	109.9	C18—C19—H19C	109.5
C9—C8—H8A	109.9	H19A—C19—H19C	109.5
C17—C8—H8A	109.9	H19B—C19—H19C	109.5
N2—C9—C8	111.50 (8)	O4—C20—C21	106.98 (9)
N2—C9—H9A	109.3	O4—C20—H20A	110.3
C8—C9—H9A	109.3	C21—C20—H20A	110.3
N2—C9—H9B	109.3	O4—C20—H20B	110.3
C8—C9—H9B	109.3	C21—C20—H20B	110.3
H9A—C9—H9B	108.0	H20A—C20—H20B	108.6
N2—C10—C11	122.60 (9)	C20—C21—H21A	109.5
N2—C10—H10A	118.7	C20—C21—H21B	109.5
C11—C10—H10A	118.7	H21A—C21—H21B	109.5
C16—C11—C12	119.72 (10)	C20—C21—H21C	109.5
C16—C11—C10	120.87 (9)	H21A—C21—H21C	109.5
C12—C11—C10	119.35 (9)	H21B—C21—H21C	109.5
C18—O3—C2—C3	1.11 (15)	C17—C8—C9—N2	−178.20 (8)
C18—O3—C2—C1	−178.73 (8)	C9—N2—C10—C11	−175.17 (9)
O1—C1—C2—O3	−1.69 (13)	N2—C10—C11—C16	0.46 (15)
C6—C1—C2—O3	177.98 (9)	N2—C10—C11—C12	177.59 (10)
O1—C1—C2—C3	178.45 (9)	C16—C11—C12—C13	−0.30 (15)
C6—C1—C2—C3	−1.88 (15)	C10—C11—C12—C13	−177.47 (9)
O3—C2—C3—C4	−177.92 (10)	C11—C12—C13—C14	−0.02 (16)
C1—C2—C3—C4	1.92 (15)	C12—C13—C14—C15	0.56 (16)

C2—C3—C4—C5	−0.39 (17)	C20—O4—C15—C14	4.75 (14)
C3—C4—C5—C6	−1.17 (16)	C20—O4—C15—C16	−175.21 (8)
C4—C5—C6—C1	1.18 (16)	C13—C14—C15—O4	179.28 (9)
C4—C5—C6—C7	−177.88 (9)	C13—C14—C15—C16	−0.76 (15)
O1—C1—C6—C5	−179.99 (9)	C12—C11—C16—O2	−179.44 (9)
C2—C1—C6—C5	0.35 (15)	C10—C11—C16—O2	−2.33 (15)
O1—C1—C6—C7	−0.94 (15)	C12—C11—C16—C15	0.10 (14)
C2—C1—C6—C7	179.41 (9)	C10—C11—C16—C15	177.22 (9)
C8—N1—C7—C6	−179.15 (9)	O4—C15—C16—O2	−0.05 (13)
C5—C6—C7—N1	−179.86 (10)	C14—C15—C16—O2	179.99 (9)
C1—C6—C7—N1	1.08 (15)	O4—C15—C16—C11	−179.61 (8)
C7—N1—C8—C9	121.02 (10)	C14—C15—C16—C11	0.43 (14)
C7—N1—C8—C17	−119.50 (10)	C2—O3—C18—C19	−177.40 (9)
C10—N2—C9—C8	−161.52 (9)	C15—O4—C20—C21	173.58 (9)
N1—C8—C9—N2	−59.47 (11)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.84	1.83	2.5752 (13)	146
O2—H2···N2	0.84	1.88	2.6178 (13)	147
C9—H9A···O1^{i}	0.99	2.49	3.4293 (14)	159
C18—H18b···Cg1^{ii}	0.9900	2.9800	3.8340 (12)	142.00
C7—H7A···Cg2^{iii}	0.96	2.72	3.5554 (12)	176

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+2; (ii) −*x*, −*y*+1, −*z*+1; (iii) −*x*+1, −*y*+2, −*z*+2.

Fig. 1

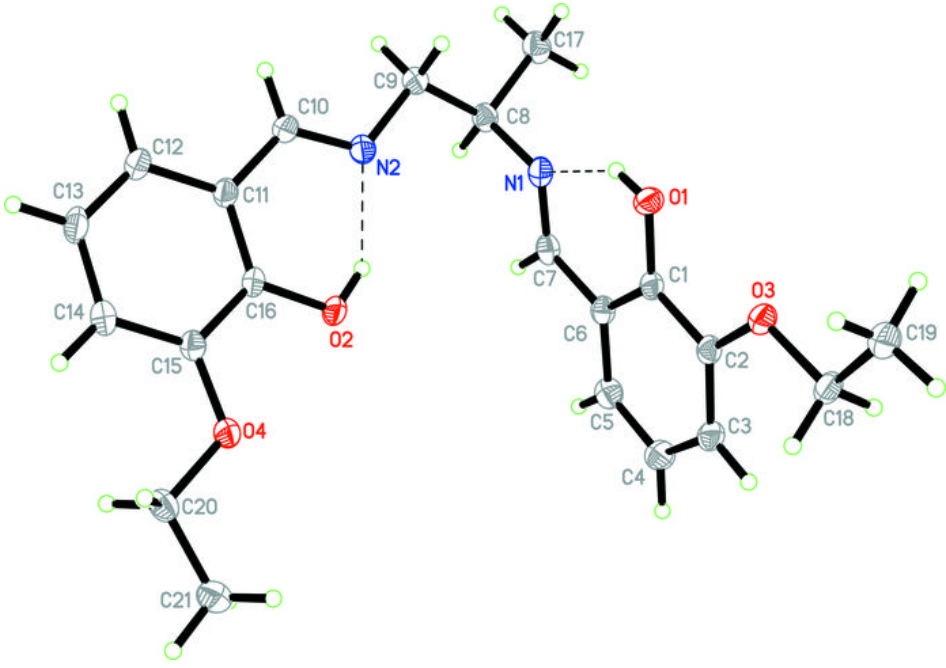
C17
C9
C10
C8
C12
N2
N1
O1
C13
C11
C7
C1
O3
C14
C16
O2
C6
C2
C19
C15
C5
C3
C18
O4
C4
C20
C21

Fig. 2