Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(1*Z*,1′*Z*,3*E*,3′*E*)-1,1′-Diphenyl-3,3′-[(1*S*,2*S*)-cyclohexane-1,2-diyldinitrilo]-dibut-1-en-1-ol

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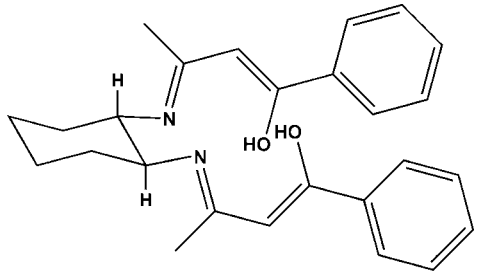
Received 29 April 2008; accepted 15 May 2008

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.061; wR factor = 0.160; data-to-parameter ratio = 9.8.

A new tetradentate chiral Schiff base ligand, $C_{26}H_{30}N_2O_2$, has been synthesized by the reaction of 1-phenylbutane-1,3-dione with (1*S*,2*S*)-(−)-1,2-diaminocyclohexane. The chiral centers in the molecule have the same *S* configuration, since the absolute configuration was determined by that of the starting reagent (1*S*,2*S*)-(−)-1,2-diaminohexane. The cyclohexane ring is in a chair conformation, and the substituents are equatorial in the most stable conformation (*trans*-cyclohexyl). The crystal structure is stabilized by two intramolecular O—H···N hydrogen bonds and a weak C—H···π interaction.

Related literature

For the chemistry of Schiff bases, see: Alemi & Shaabani (2000); Bandini *et al.* (1999, 2000); Belokon *et al.* (1997); Cozzi (2003); Jiang *et al.* (1995); Kureshy *et al.* (2001); Sasaki *et al.* (1991).



Experimental

Crystal data

$C_{26}H_{30}N_2O_2$ M_r = 402.52
Orthorhombic, $P2_12_12_1$
a = 8.9073 (11) Å
b = 10.1205 (13) Å
c = 26.476 (3) Å
V = 2386.7 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 293 (2) K
0.20 × 0.20 × 0.20 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.980, T_{max} = 0.990
22130 measured reflections
2683 independent reflections
1952 reflections with $I > 2\sigma(I)$
R_{int} = 0.062

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.159
S = 1.07
2683 reflections
275 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2*A*···N2	0.82	1.93	2.650 (3)	146
O1—H1···N1	0.82	1.91	2.629 (4)	145
C19—H19*A*···*Cg*3^{i}	0.97	2.96	3.795 (5)	144

Symmetry code: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, -z$. *Cg*3 is the centroid of the C10–C15 ring.

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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: *SHELXL97*.

This work was supported by a Start-up Grant from Southeast University to ZRQ.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2143).

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supplementary materials

Acta Cryst. (2008). E**64**, o1121 [**doi:10.1107/S1600536808014670**]

(1*Z*,1'*Z*,3*E*,3'*E*)-1,1'-Diphenyl-3,3'-[(1*S*,2*S*)-cyclohexane-1,2-diyldinitrilo]dibut-1-en-1-ol

X.-Z. Li and Z.-R. Qu

Comment

In recent years, research on Schiff bases has been intensified for the reason that some of them can form materials with non-linear optical (NLO) activity (Alemi & Shaabani, 2000), and some can be used for the asymmetric oxidation of methyl phenyl sulfides (Sasaki *et al.*, 1991). The search for new chiral ligands for asymmetric synthesis is an important task in organic chemistry. Various chiral Schiff bases are widely used in asymmetric reactions (Jiang *et al.*, 1995; Belokon *et al.*, 1997; Bandini *et al.*, 1999, 2000; Kureshy *et al.*, 2001; Cozzi, 2003). Herein, we report the synthesis and crystal structure of a new chiral Schiff base ligand (1*Z*,1'*Z*,3*E*,3'*E*)-3,3'-((1*S*,2*S*)-cyclohexane-1,2-diylbis(azan-1-yl-1-ylidene))bis(1-phenyl-but-1-en-1-ol). Fig. 1 show, the absolute configurations of the chiral centers and they have the same chirality (*S*-configuration). The cyclohexane ring is of chair conformation, and the substituents are equatorial in the most stable conformation of *trans*-cyclohexyl. The crystal structure is stabilized by two intramolecular O—H···N hydrogen bonds and a weak C—H···π interaction (Table 1).

Experimental

1-phenylbutane-1,3-dione (3.89 g, 0.024 mol) in 6 ml of chloroform was added dropwise to a solution of chloroform (20 ml) containing (1*S*, 2*S*)-(–)-1,2-diaminocyclohexane (1.14 g, 0.01 mol), which was kept at 0–5°C with vigorous stirring during the reaction. After complete addition which took approximately 30 min, the mixture was stirred for another 1 h at room temperature. After the evaporation of the solvent under reduced pressure, the crude product was recrystallized by slowly evaporating with petroleum ether to yield colorless crystals.

Refinement

Positional parameters of all the H atoms were calculated geometrically and were allowed to ride on the C, O atoms to which they are bonded, with C—H = 0.93 to 0.98Å, O—H = 0.82 Å , with U_{iso} (H) = 1.2U_{eq} ($C_{aromatic}$, $C_{methylene}$), U_{iso}(H) = 1.5U_{eq} (C_{methyl}) or 1.5 U_{eq}(O). In the absence of significant anomalous scattering effects, 2006 Friedel pairs were merged.

Figures

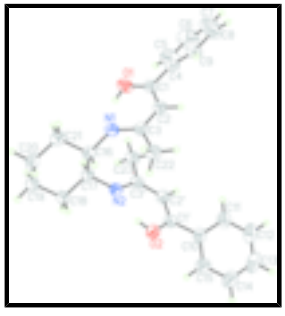


Fig. 1. A view of the compound with the atomic numbering scheme. Displacement ellipsoids were drawn at the 30% probability level.

(1*Z*,1'*Z*,3*E*,3'*E*)-1,1'-Diphenyl-3,3'- [(1*S*,2*S*)-cyclohexane-1,2-diyldinitrilo]dibut-1-en-1-ol

Crystal data

$C_{26}H_{30}N_2O_2$	F_{000} = 864
M_r = 402.52	D_x = 1.120 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 4136 reflections
a = 8.9073 (11) Å	θ = 3.1–27.5º
b = 10.1205 (13) Å	μ = 0.07 mm^{-1}
c = 26.476 (3) Å	T = 293 (2) K
V = 2386.7 (5) Å^3	Block, colorless
Z = 4	0.20 × 0.20 × 0.20 mm

Data collection

Rigaku SCXmini diffractometer	2683 independent reflections
Radiation source: fine-focus sealed tube	1952 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.062
Detector resolution: 13.6612 pixels mm^{-1}	θ_{max} = 26.0º
T = 293(2) K	θ_{min} = 2.4º
ω scans	h = −10→10
Absorption correction: multi-scan (CrystalClear; Rigaku, 2005)	k = −12→12
T_{min} = 0.980, T_{max} = 0.990	l = −32→32
22130 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.061	H-atom parameters constrained
$wR(F^2)$ = 0.159	$w = 1/[\sigma^2(F_o^2) + (0.0753P)^2 + 0.2595P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max} < 0.001$
2683 reflections	$\Delta\rho_{max}$ = 0.29 e Å^{-3}
275 parameters	$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N2	0.8242 (3)	0.2435 (3)	0.96116 (10)	0.0576 (7)
C17	0.8209 (4)	0.1345 (3)	0.92486 (12)	0.0562 (8)
H17	0.9072	0.1434	0.9021	0.067*
N1	0.6697 (4)	0.2620 (3)	0.86429 (10)	0.0618 (8)
O2	0.7103 (3)	0.3353 (2)	1.04671 (9)	0.0684 (7)
H2A	0.7189	0.2838	1.0230	0.103*
C1'	0.7786 (4)	0.4406 (3)	1.03675 (13)	0.0582 (8)
C18	0.8342 (5)	0.0039 (3)	0.95283 (14)	0.0669 (10)
H18A	0.9290	0.0014	0.9708	0.080*
H18B	0.7541	−0.0025	0.9776	0.080*
C2	0.6168 (4)	0.4861 (4)	0.84749 (13)	0.0597 (9)
H2	0.5630	0.5613	0.8564	0.072*
C3'	0.8907 (4)	0.3615 (4)	0.95676 (13)	0.0571 (8)
C3	0.5973 (4)	0.3737 (4)	0.87611 (13)	0.0597 (9)
C21	0.6703 (6)	0.0219 (4)	0.85724 (15)	0.0776 (12)
H21A	0.5761	0.0238	0.8389	0.093*
H21B	0.7512	0.0291	0.8329	0.093*
O1	0.7936 (4)	0.3983 (3)	0.79076 (10)	0.0852 (9)
H1	0.7875	0.3376	0.8112	0.128*
C16	0.6767 (4)	0.1386 (3)	0.89317 (13)	0.0584 (9)
H16	0.5899	0.1345	0.9159	0.070*
C4	0.7242 (4)	0.6191 (4)	0.77629 (13)	0.0653 (10)
C2'	0.8698 (4)	0.4569 (4)	0.99355 (13)	0.0618 (9)
H2'	0.9192	0.5372	0.9896	0.074*
C10	0.7610 (4)	0.5522 (4)	1.07347 (14)	0.0648 (9)
C23	0.9890 (5)	0.3907 (4)	0.91182 (14)	0.0684 (10)
H23A	0.9330	0.3765	0.8813	0.103*
H23B	1.0747	0.3332	0.9123	0.103*
H23C	1.0219	0.4809	0.9132	0.103*
C1	0.7137 (4)	0.4938 (4)	0.80549 (13)	0.0629 (9)
C22	0.4918 (5)	0.3766 (4)	0.92075 (15)	0.0778 (12)
H22A	0.5438	0.3469	0.9504	0.117*
H22B	0.4079	0.3194	0.9143	0.117*

H22C	0.4565	0.4652	0.9259	0.117*
C19	0.8253 (5)	−0.1133 (4)	0.91717 (15)	0.0772 (11)
H19A	0.9126	−0.1136	0.8953	0.093*
H19B	0.8262	−0.1946	0.9366	0.093*
C20	0.6840 (6)	−0.1081 (4)	0.88527 (18)	0.0847 (12)
H20A	0.6855	−0.1801	0.8611	0.102*
H20B	0.5971	−0.1197	0.9069	0.102*
C15	0.7371 (5)	0.5242 (4)	1.12405 (15)	0.0771 (11)
H15	0.7328	0.4368	1.1348	0.093*
C9	0.6005 (5)	0.6985 (4)	0.76822 (16)	0.0787 (12)
H9	0.5080	0.6744	0.7817	0.094*
C11	0.7644 (5)	0.6836 (4)	1.05852 (18)	0.0824 (13)
H11	0.7793	0.7047	1.0247	0.099*
C12	0.7458 (6)	0.7824 (5)	1.0933 (2)	0.1040 (17)
H12	0.7483	0.8701	1.0828	0.125*
C8	0.6128 (7)	0.8127 (5)	0.74050 (19)	0.1055 (17)
H8	0.5290	0.8658	0.7352	0.127*
C14	0.7197 (7)	0.6255 (5)	1.15854 (18)	0.1006 (16)
H14	0.7049	0.6065	1.1925	0.121*
C5	0.8588 (5)	0.6560 (6)	0.75543 (18)	0.1002 (16)
H5	0.9425	0.6022	0.7597	0.120*
C13	0.7242 (6)	0.7548 (6)	1.1424 (2)	0.1062 (18)
H13	0.7123	0.8232	1.1655	0.127*
C6	0.8718 (8)	0.7720 (7)	0.7282 (3)	0.133 (2)
H6	0.9640	0.7979	0.7150	0.160*
C7	0.7471 (11)	0.8477 (6)	0.7210 (2)	0.126 (2)
H7	0.7546	0.9251	0.7023	0.152*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N2	0.0638 (17)	0.0557 (16)	0.0532 (15)	−0.0045 (15)	0.0003 (14)	−0.0004 (14)
C17	0.061 (2)	0.0553 (19)	0.0528 (17)	0.0016 (18)	0.0041 (16)	0.0009 (16)
N1	0.0690 (19)	0.0633 (18)	0.0531 (15)	0.0081 (17)	−0.0017 (15)	0.0041 (14)
O2	0.0813 (18)	0.0624 (15)	0.0614 (14)	−0.0075 (15)	0.0111 (14)	−0.0046 (12)
C1'	0.062 (2)	0.0504 (18)	0.0618 (19)	−0.0020 (18)	−0.0071 (18)	0.0042 (17)
C18	0.077 (3)	0.059 (2)	0.065 (2)	0.003 (2)	−0.006 (2)	0.0059 (18)
C2	0.063 (2)	0.061 (2)	0.0551 (18)	0.0043 (18)	0.0048 (17)	0.0030 (17)
C3'	0.0552 (19)	0.0579 (19)	0.0582 (19)	−0.0051 (17)	−0.0012 (17)	0.0089 (17)
C3	0.059 (2)	0.070 (2)	0.0505 (18)	0.006 (2)	0.0025 (16)	0.0044 (18)
C21	0.091 (3)	0.073 (3)	0.069 (2)	−0.002 (2)	−0.013 (2)	−0.011 (2)
O1	0.091 (2)	0.097 (2)	0.0675 (16)	0.0300 (19)	0.0233 (16)	0.0236 (15)
C16	0.065 (2)	0.0539 (19)	0.0566 (18)	0.0023 (19)	0.0052 (18)	0.0011 (16)
C4	0.065 (2)	0.077 (2)	0.0537 (18)	−0.010 (2)	−0.0035 (18)	0.0070 (19)
C2'	0.067 (2)	0.0527 (19)	0.066 (2)	−0.0099 (18)	0.0021 (18)	0.0005 (18)
C10	0.061 (2)	0.061 (2)	0.072 (2)	0.0020 (19)	−0.0050 (19)	−0.0072 (19)
C23	0.067 (2)	0.072 (2)	0.066 (2)	−0.007 (2)	0.0063 (19)	0.008 (2)
C1	0.058 (2)	0.074 (2)	0.0565 (18)	0.009 (2)	0.0001 (17)	0.0050 (19)

C22	0.080 (3)	0.083 (3)	0.070 (2)	0.014 (2)	0.026 (2)	0.014 (2)
C19	0.090 (3)	0.056 (2)	0.086 (3)	0.006 (2)	0.004 (2)	0.001 (2)
C20	0.100 (3)	0.060 (2)	0.094 (3)	−0.001 (2)	−0.003 (3)	−0.015 (2)
C15	0.082 (3)	0.083 (3)	0.067 (2)	0.004 (2)	−0.005 (2)	−0.008 (2)
C9	0.078 (3)	0.083 (3)	0.076 (3)	0.001 (2)	−0.012 (2)	0.020 (2)
C11	0.088 (3)	0.064 (2)	0.095 (3)	0.000 (2)	0.007 (3)	−0.001 (2)
C12	0.106 (4)	0.064 (3)	0.142 (5)	0.002 (3)	0.016 (4)	−0.023 (3)
C8	0.136 (5)	0.090 (3)	0.090 (3)	−0.001 (4)	−0.018 (3)	0.031 (3)
C14	0.110 (4)	0.114 (4)	0.078 (3)	0.014 (4)	−0.010 (3)	−0.030 (3)
C5	0.077 (3)	0.124 (4)	0.100 (3)	−0.017 (3)	0.012 (3)	0.031 (3)
C13	0.096 (4)	0.091 (4)	0.131 (5)	0.001 (3)	0.001 (4)	−0.054 (4)
C6	0.120 (5)	0.149 (6)	0.130 (5)	−0.056 (5)	0.021 (4)	0.039 (5)
C7	0.180 (7)	0.099 (4)	0.100 (4)	−0.037 (5)	−0.006 (5)	0.034 (3)

Geometric parameters (Å, °)

N2—C3'	1.338 (4)	C10—C15	1.385 (5)
N2—C17	1.463 (4)	C10—C11	1.388 (5)
C17—C18	1.520 (5)	C23—H23A	0.9600
C17—C16	1.535 (5)	C23—H23B	0.9600
C17—H17	0.9800	C23—H23C	0.9600
N1—C3	1.339 (5)	C22—H22A	0.9600
N1—C16	1.465 (4)	C22—H22B	0.9600
O2—C1'	1.255 (4)	C22—H22C	0.9600
O2—H2A	0.8200	C19—C20	1.517 (6)
C1'—C2'	1.413 (5)	C19—H19A	0.9700
C1'—C10	1.498 (5)	C19—H19B	0.9700
C18—C19	1.518 (5)	C20—H20A	0.9700
C18—H18A	0.9700	C20—H20B	0.9700
C18—H18B	0.9700	C15—C14	1.382 (6)
C2—C3	1.378 (5)	C15—H15	0.9300
C2—C1	1.409 (5)	C9—C8	1.374 (6)
C2—H2	0.9300	C9—H9	0.9300
C3'—C2'	1.384 (5)	C11—C12	1.370 (6)
C3'—C23	1.506 (5)	C11—H11	0.9300
C3—C22	1.510 (5)	C12—C13	1.341 (7)
C21—C20	1.515 (5)	C12—H12	0.9300
C21—C16	1.517 (5)	C8—C7	1.350 (8)
C21—H21A	0.9700	C8—H8	0.9300
C21—H21B	0.9700	C14—C13	1.377 (7)
O1—C1	1.262 (4)	C14—H14	0.9300
O1—H1	0.8200	C5—C6	1.382 (8)
C16—H16	0.9800	C5—H5	0.9300
C4—C5	1.372 (6)	C13—H13	0.9300
C4—C9	1.380 (5)	C6—C7	1.363 (9)
C4—C1	1.488 (5)	C6—H6	0.9300
C2'—H2'	0.9300	C7—H7	0.9300
C3'—N2—C17	128.6 (3)	H23A—C23—H23C	109.5
N2—C17—C18	109.5 (3)	H23B—C23—H23C	109.5

N2—C17—C16	110.8 (3)	O1—C1—C2	123.2 (3)
C18—C17—C16	110.8 (3)	O1—C1—C4	117.2 (3)
N2—C17—H17	108.6	C2—C1—C4	119.7 (3)
C18—C17—H17	108.6	C3—C22—H22A	109.5
C16—C17—H17	108.6	C3—C22—H22B	109.5
C3—N1—C16	128.2 (3)	H22A—C22—H22B	109.5
C1'—O2—H2A	109.5	C3—C22—H22C	109.5
O2—C1'—C2'	123.2 (3)	H22A—C22—H22C	109.5
O2—C1'—C10	116.9 (3)	H22B—C22—H22C	109.5
C2'—C1'—C10	119.8 (3)	C20—C19—C18	111.2 (3)
C19—C18—C17	111.9 (3)	C20—C19—H19A	109.4
C19—C18—H18A	109.2	C18—C19—H19A	109.4
C17—C18—H18A	109.2	C20—C19—H19B	109.4
C19—C18—H18B	109.2	C18—C19—H19B	109.4
C17—C18—H18B	109.2	H19A—C19—H19B	108.0
H18A—C18—H18B	107.9	C21—C20—C19	111.7 (4)
C3—C2—C1	123.8 (3)	C21—C20—H20A	109.3
C3—C2—H2	118.1	C19—C20—H20A	109.3
C1—C2—H2	118.1	C21—C20—H20B	109.3
N2—C3'—C2'	120.1 (3)	C19—C20—H20B	109.3
N2—C3'—C23	120.1 (3)	H20A—C20—H20B	107.9
C2'—C3'—C23	119.8 (3)	C14—C15—C10	120.3 (4)
N1—C3—C2	120.5 (3)	C14—C15—H15	119.9
N1—C3—C22	119.9 (3)	C10—C15—H15	119.9
C2—C3—C22	119.6 (3)	C8—C9—C4	120.6 (5)
C20—C21—C16	111.5 (3)	C8—C9—H9	119.7
C20—C21—H21A	109.3	C4—C9—H9	119.7
C16—C21—H21A	109.3	C12—C11—C10	120.3 (5)
C20—C21—H21B	109.3	C12—C11—H11	119.8
C16—C21—H21B	109.3	C10—C11—H11	119.8
H21A—C21—H21B	108.0	C13—C12—C11	121.1 (5)
C1—O1—H1	109.5	C13—C12—H12	119.4
N1—C16—C21	109.5 (3)	C11—C12—H12	119.4
N1—C16—C17	110.1 (3)	C7—C8—C9	119.7 (6)
C21—C16—C17	110.7 (3)	C7—C8—H8	120.2
N1—C16—H16	108.8	C9—C8—H8	120.2
C21—C16—H16	108.8	C13—C14—C15	119.8 (5)
C17—C16—H16	108.8	C13—C14—H14	120.1
C5—C4—C9	118.5 (4)	C15—C14—H14	120.1
C5—C4—C1	119.7 (4)	C4—C5—C6	120.9 (6)
C9—C4—C1	121.8 (4)	C4—C5—H5	119.5
C3'—C2'—C1'	124.5 (3)	C6—C5—H5	119.5
C3'—C2'—H2'	117.8	C12—C13—C14	120.2 (5)
C1'—C2'—H2'	117.8	C12—C13—H13	119.9
C15—C10—C11	118.3 (4)	C14—C13—H13	119.9
C15—C10—C1'	119.3 (3)	C7—C6—C5	118.8 (6)
C11—C10—C1'	122.3 (4)	C7—C6—H6	120.6
C3'—C23—H23A	109.5	C5—C6—H6	120.6
C3'—C23—H23B	109.5	C8—C7—C6	121.5 (5)

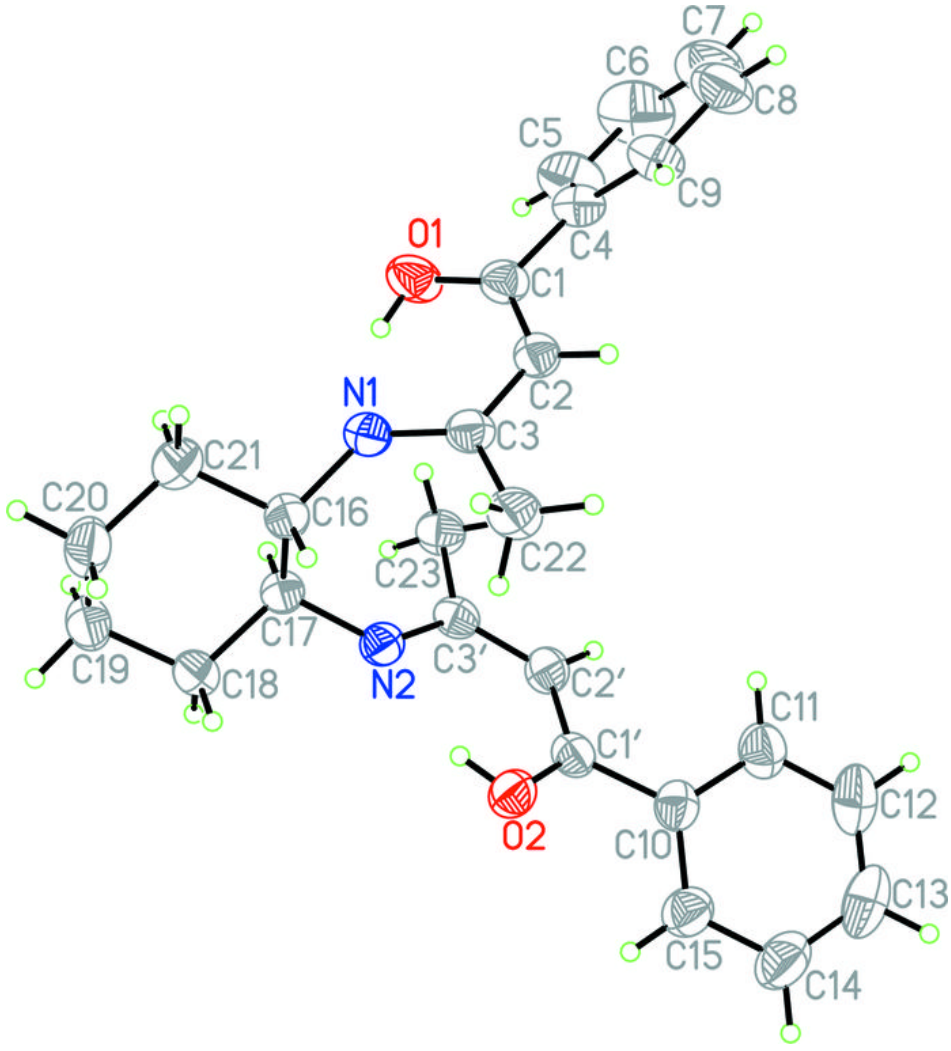
H23A—C23—H23B	109.5	C8—C7—H7	119.3
C3'—C23—H23C	109.5	C6—C7—H7	119.3
C3'—N2—C17—C18	141.4 (4)	C3—C2—C1—O1	−1.2 (6)
C3'—N2—C17—C16	−96.1 (4)	C3—C2—C1—C4	178.6 (3)
N2—C17—C18—C19	177.8 (3)	C5—C4—C1—O1	−34.7 (6)
C16—C17—C18—C19	55.2 (4)	C9—C4—C1—O1	143.5 (4)
C17—N2—C3'—C2'	174.1 (3)	C5—C4—C1—C2	145.5 (4)
C17—N2—C3'—C23	−6.1 (5)	C9—C4—C1—C2	−36.3 (5)
C16—N1—C3—C2	172.3 (3)	C17—C18—C19—C20	−54.6 (5)
C16—N1—C3—C22	−8.4 (6)	C16—C21—C20—C19	−55.7 (5)
C1—C2—C3—N1	−1.4 (6)	C18—C19—C20—C21	54.4 (5)
C1—C2—C3—C22	179.4 (4)	C11—C10—C15—C14	−1.0 (7)
C3—N1—C16—C21	141.4 (4)	C1'—C10—C15—C14	−179.6 (4)
C3—N1—C16—C17	−96.7 (4)	C5—C4—C9—C8	−0.9 (6)
C20—C21—C16—N1	177.5 (4)	C1—C4—C9—C8	−179.1 (4)
C20—C21—C16—C17	56.0 (5)	C15—C10—C11—C12	0.6 (7)
N2—C17—C16—N1	61.4 (3)	C1'—C10—C11—C12	179.1 (4)
C18—C17—C16—N1	−176.9 (3)	C10—C11—C12—C13	0.0 (9)
N2—C17—C16—C21	−177.4 (3)	C4—C9—C8—C7	0.0 (7)
C18—C17—C16—C21	−55.6 (4)	C10—C15—C14—C13	0.8 (8)
N2—C3'—C2'—C1'	−1.1 (6)	C9—C4—C5—C6	1.9 (7)
C23—C3'—C2'—C1'	179.1 (3)	C1—C4—C5—C6	−179.9 (5)
O2—C1'—C2'—C3'	2.2 (6)	C11—C12—C13—C14	−0.3 (9)
C10—C1'—C2'—C3'	−178.4 (3)	C15—C14—C13—C12	−0.2 (9)
O2—C1'—C10—C15	30.0 (5)	C4—C5—C6—C7	−2.0 (9)
C2'—C1'—C10—C15	−149.4 (4)	C9—C8—C7—C6	0.0 (10)
O2—C1'—C10—C11	−148.5 (4)	C5—C6—C7—C8	1.0 (11)
C2'—C1'—C10—C11	32.1 (6)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2A···N2	0.82	1.93	2.650 (3)	146
O1—H1···N1	0.82	1.91	2.629 (4)	145
C19—H19A···Cg3^{i}	0.97	2.96	3.795 (5)	144

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

Fig. 1


C7
C6
C8
C5
C9
C4
O1
C1
C2
N1
C3
C21
C20
C16
C22
C23
C17
C19
C18
N2
C3′
C2′
C11
C1′
C12
O2
C10
C13
C15
C14