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4,6-Di-*tert*-butyl-2-({[4-(diethylamino)phenyl]-imino}methyl)phenol

C. Vidya Rani,[a] L. Mitu,[b] G. Chakkaravarthi[c]* and G. Rajagopal[d]*

[a]Department of Chemistry, Vaigai College of Engineering, Madurai 625 122, Tamil Nadu, India, [b]Department of Chemistry, University of Pitesti, Pitesti 11040, Romania, [c]Department of Physics, CPCL Polytechnic College, Chennai 600 068, India, and [d]PG & Research Department of Chemistry, Chikkanna Government Arts College, Tiruppur 641 602, Tamil Nadu, India. *Correspondence e-mail: chakkaravarthi_2005@yahoo.com, rajagopal18@yahoo.com

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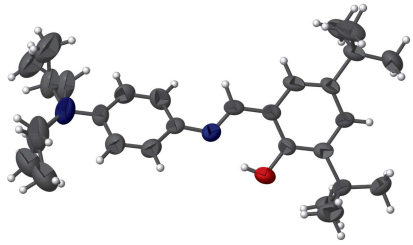
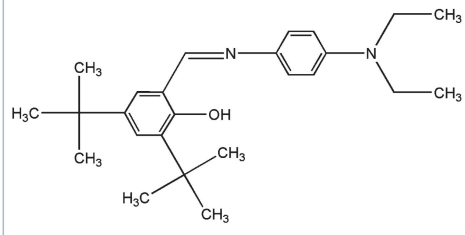
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{25}H_{36}N_2O$, adopts an *E* conformation about the C=N bond. The dihedral angle between the aromatic rings is 35.6 (6)°. The molecular structure is stabilized by an O—H···N hydrogen bond, which forms an *S*(6) loop, and weak C—H···O contacts. Weak intermolecular C—H···π interactions are observed in the crystal packing. The diethylamino group has rotational disorder with site occupancies of 0.85 (2) and 0.15 (2) for the major and minor components, respectively. The structure was refined as a three-component twin.

3D view



Chemical scheme



Structure description

Schiff base derivatives are a biologically versatile class of compounds possessing diverse activities, such as anti-inflammatory (Alam *et al.*, 2012), anti-bacterial (Sondhi *et al.*, 2006), anti-fungal (Jarrahpour *et al.*, 2007). We herein, report the synthesis and crystal structure of the title compound (Fig. 1). The bond distances are comparable with similar structures (Rani *et al.*, 2015, 2017).

The dihedral angle between the best planes through the aromatic rings (C5–C10 and C12–C17) is 35.6 (6)°. The C11=N2 bond adopts the *E* conformation, which allows formation of an intramolecular O1—H1···N2 hydrogen bond, resulting in an *S*(6) ring-motif (Fig. 1 and Table 1). The molecular structure is stabilized by an O—H···N hydrogen bond and weak C—H···O contacts (Table 1). Weak intermolecular C—H···π interactions are also observed in the crystal packing (Table 1).

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

*Cg*2 is the centroid of the C12–C17 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2	0.83 (7)	1.82 (11)	2.591 (12)	155 (14)
C23—H23*A*···O1	0.96	2.27	2.947 (17)	127
C24—H24*A*···O1	0.96	2.46	3.071 (16)	121
C2—H2*B*···*Cg*2^{i}	0.97	2.87	3.810 (19)	166
C2′—H2′1···*Cg*2^{i}	0.97	2.60	3.39 (11)	139

Symmetry code: (i) $x-1, y, z-1$.

Synthesis and crystallization

An ethanolic solution of N^1,N^1-diethylbenzene-1,4-diamine (5 mmol) was magnetically stirred in a round-bottom flask followed by dropwise addition of 3,5-di-*tert*-butyl-2-hydroxybenzaldehyde (5 mmol) containing 2–3 drops of glacial acetic acid. The reaction mixture was then refluxed for 3 h and upon cooling to room temperature, a yellow precipitate was separated out from the mixture. The precipitate was washed with ethanol and dried *in vacuo* over anhydrous $CaCl_2$. Single crystals suitable for X–ray diffraction were obtained by slow evaporation of a solution of the title compound in DMF at room temperature.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The diethylamine group has rotational disorder with occupancies of 0.85 (2) for the major component (atoms C1–C4) and 0.15 (2) for the minor component (atoms C1′–C4′). The command *DFIX* was used to restrain the N—C and C—C bond lengths involving these atoms to 1.43 (1) and 1.55 (1) Å, respectively. The same anisotropic displacement parameters were used for the disordered equivalent C atoms (C1 & C1′, C2 & C2′, C3 & C3′ and C4 & C4′) using the *EADP* command. Rigid bond restraints were used for N1—C2′, N1—C4′, N1—C2, N1—C4, N2—C8, C3′-C4′, C5—C6, C3—C4, C6—C7, C18—C21, C15—C16, and C1—C2 bonds, using the *DELU* command. The structure was refined as a three-component twin. In the absence of significant anomalous scattering effects, the absolute structure parameter is meaningless. Reflections $(20\bar{5})$, $(10\bar{5})$ and $(\bar{1}05)$ were omitted in the final cycles of refinement.

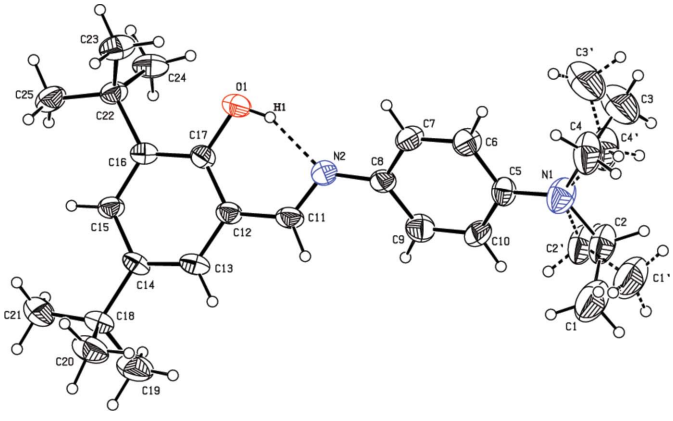


Figure 1
The molecular structure of the title compound, with atom labelling and 30% probability displacement ellipsoids. The O—H···N hydrogen bond is shown as a dashed line.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{25}H_{36}N_2O$
M_r	380.56
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	295
a, b, c (Å)	8.9303 (15), 15.572 (3), 9.4824 (16)
β (°)	117.320 (8)
V (Å^3)	1171.6 (3)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.07
Crystal size (mm)	0.30 × 0.28 × 0.24
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.921, 0.984
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8432, 8432, 6509
R_{int}	0.000
θ_{max} (°)	22.9
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.547
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.062, 0.189, 1.05
No. of reflections	8432
No. of parameters	277
No. of restraints	26
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.20, −0.22

Computer programs: *APEX2* and *SAINT* (Bruker, 2004), *SHELXS97* (Sheldrick, 2008), *SHELXL2016* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

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full crystallographic data

IUCrData (2017). **2**, x170572 [https://doi.org/10.1107/S2414314617005727]

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Crystal data

$C_{25}H_{36}N_2O$
M_r = 380.56
Monoclinic, $P2_1$
a = 8.9303 (15) Å
b = 15.572 (3) Å
c = 9.4824 (16) Å
β = 117.320 (8)°
V = 1171.6 (3) Å^3
Z = 2
$F(000)$ = 416
D_x = 1.079 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3084 reflections
θ = 2.4–20.5°
μ = 0.07 mm^{-1}
T = 295 K
Block, yellow
0.30 × 0.28 × 0.24 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (SADABS; Bruker, 2004)
T_{min} = 0.921, T_{max} = 0.984
8432 measured reflections
8432 independent reflections
6509 reflections with $I > 2\sigma(I)$
R_{int} = 0.000
θ_{max} = 22.9°, θ_{min} = 2.4°
h = −9→9
k = −17→17
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.189
S = 1.05
8432 reflections
277 parameters
26 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0973P)^2 + 0.2985P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Special details

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. Refined as a 3-component twin. The H atom for the hydroxy group was located in a difference-Fourier map and refined with a distance restraint of 0.82 (1) Å, with U_{iso}(H) = 1.5U_{eq}(O). All other H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic CH, C—H = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for CH_2 and C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for CH_3.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	−0.077 (3)	0.5191 (13)	−0.506 (3)	0.150 (9)	0.85 (2)
H1A	−0.177280	0.485250	−0.557143	0.225*	0.85 (2)
H1B	−0.010074	0.512597	−0.560645	0.225*	0.85 (2)
H1C	−0.012806	0.500182	−0.397779	0.225*	0.85 (2)
C2	−0.1242 (18)	0.6139 (12)	−0.507 (2)	0.094 (5)	0.85 (2)
H2A	−0.190115	0.632881	−0.616152	0.113*	0.85 (2)
H2B	−0.192852	0.620445	−0.453017	0.113*	0.85 (2)
C3	−0.016 (4)	0.7921 (17)	−0.593 (3)	0.186 (12)	0.85 (2)
H3A	0.015996	0.820295	−0.665562	0.278*	0.85 (2)
H3B	−0.134618	0.780981	−0.645328	0.278*	0.85 (2)
H3C	0.011559	0.828409	−0.502735	0.278*	0.85 (2)
C4	0.081 (2)	0.7066 (14)	−0.5381 (18)	0.107 (6)	0.85 (2)
H4A	0.054761	0.669186	−0.628333	0.128*	0.85 (2)
H4B	0.201674	0.716854	−0.485022	0.128*	0.85 (2)
C1′	−0.175 (19)	0.563 (10)	−0.587 (14)	0.150 (9)	0.15 (2)
H1′1	−0.271543	0.530082	−0.598955	0.225*	0.15 (2)
H1′2	−0.205138	0.598040	−0.678834	0.225*	0.15 (2)
H1′3	−0.085701	0.524662	−0.574063	0.225*	0.15 (2)
C2′	−0.116 (11)	0.621 (8)	−0.438 (12)	0.094 (5)	0.15 (2)
H2′1	−0.205060	0.660315	−0.448596	0.113*	0.15 (2)
H2′2	−0.084905	0.586495	−0.343194	0.113*	0.15 (2)
C3′	0.08 (3)	0.818 (8)	−0.517 (19)	0.186 (12)	0.15 (2)
H3′1	0.043755	0.849312	−0.613457	0.278*	0.15 (2)
H3′2	0.035306	0.847736	−0.451956	0.278*	0.15 (2)
H3′3	0.196242	0.813633	−0.460255	0.278*	0.15 (2)
C4′	−0.002 (14)	0.727 (6)	−0.556 (9)	0.107 (6)	0.15 (2)
H4′1	−0.123560	0.733489	−0.616586	0.128*	0.15 (2)
H4′2	0.036441	0.699583	−0.624836	0.128*	0.15 (2)
C5	0.1139 (15)	0.6770 (9)	−0.2706 (11)	0.057 (3)	
C6	0.2514 (14)	0.7334 (8)	−0.2004 (12)	0.067 (3)	
H6	0.286148	0.764161	−0.264162	0.080*	
C7	0.3341 (14)	0.7435 (8)	−0.0403 (12)	0.063 (3)	
H7	0.425305	0.780968	0.001366	0.075*	
C8	0.2911 (14)	0.7014 (7)	0.0652 (11)	0.052 (3)	
C9	0.1524 (15)	0.6488 (9)	−0.0054 (13)	0.070 (3)	
H9	0.115149	0.620270	0.058848	0.084*	
C10	0.0672 (13)	0.6366 (8)	−0.1654 (14)	0.066 (3)	
H10	−0.025512	0.600110	−0.206012	0.079*	
C11	0.4023 (13)	0.6582 (7)	0.3275 (12)	0.057 (3)	
H11	0.354071	0.604812	0.289394	0.069*	
C12	0.4924 (14)	0.6693 (7)	0.4952 (12)	0.051 (3)	
C13	0.5096 (14)	0.6016 (7)	0.5958 (13)	0.060 (3)	
H13	0.460269	0.549358	0.550738	0.072*	
C14	0.5948 (13)	0.6069 (7)	0.7577 (13)	0.051 (3)	
C15	0.6630 (15)	0.6864 (7)	0.8231 (11)	0.052 (2)	

H15	0.721045	0.691959	0.932885	0.063*
C16	0.6464 (12)	0.7588 (6)	0.7274 (11)	0.050 (3)
C17	0.5607 (12)	0.7496 (7)	0.5649 (11)	0.049 (3)
C18	0.6143 (16)	0.5287 (8)	0.8651 (13)	0.065 (3)
C19	0.4436 (17)	0.4872 (10)	0.8153 (16)	0.094 (4)
H19A	0.395662	0.470994	0.705493	0.141*
H19B	0.370156	0.527204	0.829953	0.141*
H19C	0.456973	0.437040	0.878934	0.141*
C20	0.7227 (17)	0.4621 (10)	0.8346 (17)	0.093 (4)
H20A	0.675752	0.451327	0.722708	0.140*
H20B	0.724633	0.409644	0.888660	0.140*
H20C	0.835444	0.483593	0.873406	0.140*
C21	0.693 (2)	0.5511 (10)	1.0374 (14)	0.113 (6)
H21A	0.708759	0.499740	1.098732	0.170*
H21B	0.620636	0.589810	1.056491	0.170*
H21C	0.800130	0.578005	1.067742	0.170*
C22	0.7209 (14)	0.8462 (7)	0.8094 (12)	0.055 (3)
C23	0.8412 (17)	0.8824 (9)	0.7467 (17)	0.084 (4)
H23A	0.781027	0.888380	0.633457	0.126*
H23B	0.934110	0.843646	0.773981	0.126*
H23C	0.882885	0.937421	0.794029	0.126*
C24	0.5703 (16)	0.9104 (9)	0.7627 (16)	0.078 (4)
H24A	0.519704	0.921425	0.650623	0.117*
H24B	0.611075	0.963319	0.819554	0.117*
H24C	0.487803	0.885891	0.789197	0.117*
C25	0.8121 (18)	0.8411 (8)	0.9828 (13)	0.079 (4)
H25A	0.863737	0.895478	1.024963	0.119*
H25B	0.897574	0.797584	1.013385	0.119*
H25C	0.734835	0.826746	1.023648	0.119*
N1	0.0275 (13)	0.6674 (8)	−0.4291 (11)	0.088 (3)
N2	0.3832 (11)	0.7164 (6)	0.2262 (10)	0.058 (2)
O1	0.5431 (11)	0.8175 (5)	0.4662 (9)	0.072 (2)
H1	0.488 (16)	0.799 (9)	0.375 (7)	0.107*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.14 (2)	0.143 (15)	0.113 (16)	−0.027 (15)	0.016 (16)	−0.044 (15)
C2	0.072 (8)	0.149 (12)	0.057 (10)	−0.021 (7)	0.027 (8)	−0.018 (10)
C3	0.27 (4)	0.139 (16)	0.107 (18)	−0.010 (10)	0.05 (2)	0.043 (13)
C4	0.073 (10)	0.182 (14)	0.064 (8)	−0.016 (9)	0.029 (7)	0.005 (7)
C1′	0.14 (2)	0.143 (15)	0.113 (16)	−0.027 (15)	0.016 (16)	−0.044 (15)
C2′	0.072 (8)	0.149 (12)	0.057 (10)	−0.021 (7)	0.027 (8)	−0.018 (10)
C3′	0.27 (4)	0.139 (16)	0.107 (18)	−0.010 (10)	0.05 (2)	0.043 (13)
C4′	0.073 (10)	0.182 (14)	0.064 (8)	−0.016 (9)	0.029 (7)	0.005 (7)
C5	0.061 (5)	0.070 (8)	0.044 (5)	0.000 (5)	0.026 (4)	−0.004 (5)
C6	0.078 (7)	0.071 (9)	0.060 (4)	−0.011 (5)	0.040 (5)	−0.005 (6)
C7	0.068 (6)	0.058 (8)	0.064 (4)	−0.016 (6)	0.031 (5)	−0.011 (6)

C8	0.066 (6)	0.036 (7)	0.054 (4)	0.004 (6)	0.028 (5)	−0.005 (5)
C9	0.069 (7)	0.079 (10)	0.070 (8)	−0.008 (7)	0.038 (6)	0.009 (7)
C10	0.052 (6)	0.069 (10)	0.069 (8)	−0.019 (6)	0.022 (6)	−0.005 (6)
C11	0.077 (7)	0.032 (7)	0.064 (7)	0.001 (6)	0.033 (6)	0.000 (6)
C12	0.065 (6)	0.036 (7)	0.055 (6)	0.003 (5)	0.029 (5)	0.001 (5)
C13	0.076 (8)	0.035 (7)	0.076 (8)	0.005 (6)	0.041 (6)	0.010 (6)
C14	0.066 (7)	0.038 (7)	0.058 (7)	0.014 (6)	0.036 (6)	0.015 (5)
C15	0.066 (6)	0.037 (6)	0.056 (6)	−0.004 (5)	0.030 (5)	−0.005 (4)
C16	0.057 (6)	0.040 (6)	0.062 (6)	−0.003 (6)	0.036 (5)	−0.001 (4)
C17	0.061 (6)	0.044 (7)	0.048 (6)	0.002 (6)	0.028 (5)	0.003 (5)
C18	0.079 (8)	0.043 (7)	0.074 (5)	0.002 (7)	0.037 (6)	0.015 (6)
C19	0.100 (9)	0.080 (12)	0.117 (10)	−0.010 (8)	0.062 (8)	0.029 (8)
C20	0.092 (10)	0.062 (10)	0.127 (11)	0.020 (8)	0.053 (9)	0.033 (8)
C21	0.160 (15)	0.089 (12)	0.069 (5)	−0.024 (11)	0.034 (9)	0.022 (7)
C22	0.070 (7)	0.044 (8)	0.056 (7)	−0.011 (6)	0.034 (6)	−0.010 (5)
C23	0.093 (9)	0.067 (10)	0.106 (10)	−0.027 (8)	0.057 (8)	−0.009 (7)
C24	0.099 (10)	0.041 (8)	0.108 (9)	0.000 (7)	0.059 (8)	−0.004 (6)
C25	0.103 (10)	0.061 (9)	0.069 (8)	−0.025 (8)	0.035 (7)	−0.021 (6)
N1	0.081 (5)	0.121 (9)	0.063 (6)	−0.019 (6)	0.035 (5)	−0.017 (5)
N2	0.065 (5)	0.049 (6)	0.056 (4)	−0.001 (5)	0.024 (4)	−0.004 (5)
O1	0.096 (6)	0.046 (5)	0.067 (5)	−0.006 (5)	0.033 (5)	0.008 (4)

Geometric parameters (Å, º)

C1—C2	1.53 (2)	C11—C12	1.425 (14)
C1—H1A	0.9600	C11—H11	0.9300
C1—H1B	0.9600	C12—C13	1.383 (15)
C1—H1C	0.9600	C12—C17	1.416 (14)
C2—N1	1.468 (15)	C13—C14	1.368 (12)
C2—H2A	0.9700	C13—H13	0.9300
C2—H2B	0.9700	C14—C15	1.393 (15)
C3—C4	1.54 (2)	C14—C18	1.545 (16)
C3—H3A	0.9600	C15—C16	1.411 (15)
C3—H3B	0.9600	C15—H15	0.9300
C3—H3C	0.9600	C16—C17	1.377 (12)
C4—N1	1.458 (16)	C16—C22	1.557 (14)
C4—H4A	0.9700	C17—O1	1.372 (12)
C4—H4B	0.9700	C18—C21	1.493 (17)
C1′—C2′	1.55 (2)	C18—C19	1.518 (17)
C1′—H1′1	0.9600	C18—C20	1.534 (18)
C1′—H1′2	0.9600	C19—H19A	0.9600
C1′—H1′3	0.9600	C19—H19B	0.9600
C2′—N1	1.44 (2)	C19—H19C	0.9600
C2′—H2′1	0.9700	C20—H20A	0.9600
C2′—H2′2	0.9700	C20—H20B	0.9600
C3′—C4′	1.55 (2)	C20—H20C	0.9600
C3′—H3′1	0.9600	C21—H21A	0.9600
C4′—N1	1.44 (2)	C21—H21B	0.9600

C4′—H4′1	0.9700	C21—H21C	0.9600
C4′—H4′2	0.9700	C22—C25	1.464 (14)
C5—N1	1.346 (12)	C22—C23	1.553 (16)
C5—C10	1.394 (16)	C22—C24	1.569 (17)
C5—C6	1.404 (17)	C23—H23A	0.9600
C6—C7	1.359 (14)	C23—H23B	0.9600
C6—H6	0.9300	C23—H23C	0.9600
C7—C8	1.389 (15)	C24—H24A	0.9600
C7—H7	0.9300	C24—H24B	0.9600
C8—C9	1.375 (15)	C24—H24C	0.9600
C8—N2	1.382 (12)	C25—H25A	0.9600
C9—C10	1.363 (15)	C25—H25B	0.9600
C9—H9	0.9300	C25—H25C	0.9600
C10—H10	0.9300	O1—H1	0.83 (2)
C11—N2	1.273 (12)		

C2—C1—H1A	109.5	C12—C13—H13	118.1
C2—C1—H1B	109.5	C13—C14—C15	117.2 (9)
H1A—C1—H1B	109.5	C13—C14—C18	121.9 (10)
C2—C1—H1C	109.5	C15—C14—C18	120.9 (9)
H1A—C1—H1C	109.5	C14—C15—C16	121.9 (9)
H1B—C1—H1C	109.5	C14—C15—H15	119.1
N1—C2—C1	110.7 (15)	C16—C15—H15	119.1
N1—C2—H2A	109.5	C17—C16—C15	118.5 (9)
C1—C2—H2A	109.5	C17—C16—C22	122.7 (8)
N1—C2—H2B	109.5	C15—C16—C22	118.8 (8)
C1—C2—H2B	109.5	O1—C17—C16	120.9 (9)
H2A—C2—H2B	108.1	O1—C17—C12	118.2 (8)
C4—C3—H3A	109.5	C16—C17—C12	120.9 (9)
C4—C3—H3B	109.5	C21—C18—C19	109.9 (11)
H3A—C3—H3B	109.5	C21—C18—C20	110.1 (11)
C4—C3—H3C	109.5	C19—C18—C20	106.5 (11)
H3A—C3—H3C	109.5	C21—C18—C14	113.0 (11)
H3B—C3—H3C	109.5	C19—C18—C14	109.7 (9)
N1—C4—C3	106.6 (19)	C20—C18—C14	107.4 (10)
N1—C4—H4A	110.4	C18—C19—H19A	109.5
C3—C4—H4A	110.4	C18—C19—H19B	109.5
N1—C4—H4B	110.4	H19A—C19—H19B	109.5
C3—C4—H4B	110.4	C18—C19—H19C	109.5
H4A—C4—H4B	108.6	H19A—C19—H19C	109.5
C2′—C1′—H1′1	109.5	H19B—C19—H19C	109.5
C2′—C1′—H1′2	109.5	C18—C20—H20A	109.5
H1′1—C1′—H1′2	109.5	C18—C20—H20B	109.5
C2′—C1′—H1′3	109.5	H20A—C20—H20B	109.5
H1′1—C1′—H1′3	109.5	C18—C20—H20C	109.5
H1′2—C1′—H1′3	109.5	H20A—C20—H20C	109.5
N1—C2′—C1′	105 (8)	H20B—C20—H20C	109.5
N1—C2′—H2′1	110.6	C18—C21—H21A	109.5

C1′—C2′—H2′1	110.6	C18—C21—H21B	109.5
N1—C2′—H2′2	110.6	H21A—C21—H21B	109.5
C1′—C2′—H2′2	110.6	C18—C21—H21C	109.5
H2′1—C2′—H2′2	108.8	H21A—C21—H21C	109.5
C4′—C3′—H3′1	109.5	H21B—C21—H21C	109.5
C4′—C3′—H3′3	109.5	C25—C22—C23	108.9 (10)
H3′2—C3′—H3′3	109.5	C25—C22—C16	113.8 (9)
N1—C4′—C3′	120 (9)	C23—C22—C16	109.7 (8)
N1—C4′—H4′1	107.3	C25—C22—C24	108.4 (10)
N1—C4′—H4′2	107.3	C23—C22—C24	108.3 (9)
C3′—C4′—H4′2	107.3	C16—C22—C24	107.6 (9)
H4′1—C4′—H4′2	106.9	C22—C23—H23A	109.5
N1—C5—C10	122.8 (11)	C22—C23—H23B	109.5
N1—C5—C6	121.8 (10)	H23A—C23—H23B	109.5
C10—C5—C6	115.2 (9)	C22—C23—H23C	109.5
C7—C6—C5	120.8 (11)	H23A—C23—H23C	109.5
C7—C6—H6	119.6	H23B—C23—H23C	109.5
C5—C6—H6	119.6	C22—C24—H24A	109.5
C6—C7—C8	124.1 (11)	C22—C24—H24B	109.5
C6—C7—H7	117.9	H24A—C24—H24B	109.5
C8—C7—H7	117.9	C22—C24—H24C	109.5
C9—C8—N2	125.8 (9)	H24A—C24—H24C	109.5
C9—C8—C7	114.6 (9)	H24B—C24—H24C	109.5
N2—C8—C7	119.6 (10)	C22—C25—H25A	109.5
C10—C9—C8	122.8 (10)	C22—C25—H25B	109.5
C10—C9—H9	118.6	H25A—C25—H25B	109.5
C8—C9—H9	118.6	C22—C25—H25C	109.5
C9—C10—C5	122.5 (11)	H25A—C25—H25C	109.5
C9—C10—H10	118.8	H25B—C25—H25C	109.5
C5—C10—H10	118.8	C5—N1—C4′	131 (5)
N2—C11—C12	124.6 (10)	C5—N1—C2′	99 (4)
N2—C11—H11	117.7	C4′—N1—C2′	117 (7)
C12—C11—H11	117.7	C5—N1—C4	122.6 (11)
C13—C12—C17	117.6 (9)	C5—N1—C2	123.4 (11)
C13—C12—C11	120.3 (10)	C4—N1—C2	114.0 (11)
C17—C12—C11	122.0 (9)	C11—N2—C8	121.3 (9)
C14—C13—C12	123.8 (11)	C17—O1—H1	106 (10)
C14—C13—H13	118.1		

N1—C5—C6—C7	178.4 (11)	C13—C14—C18—C19	−49.8 (15)
C10—C5—C6—C7	2.6 (18)	C15—C14—C18—C19	129.6 (12)
C5—C6—C7—C8	−0.8 (18)	C13—C14—C18—C20	65.5 (13)
C6—C7—C8—C9	−1.6 (17)	C15—C14—C18—C20	−115.1 (12)
C6—C7—C8—N2	−179.8 (11)	C17—C16—C22—C25	−178.0 (10)
N2—C8—C9—C10	−179.9 (11)	C15—C16—C22—C25	3.9 (15)
C7—C8—C9—C10	2.1 (17)	C17—C16—C22—C23	−55.7 (13)
C8—C9—C10—C5	−0.2 (19)	C15—C16—C22—C23	126.1 (11)
N1—C5—C10—C9	−177.9 (13)	C17—C16—C22—C24	61.9 (12)

C6—C5—C10—C9	−2.2 (18)	C15—C16—C22—C24	−116.2 (10)
N2—C11—C12—C13	−178.5 (11)	C10—C5—N1—C4′	146 (7)
N2—C11—C12—C17	4.3 (17)	C6—C5—N1—C4′	−29 (7)
C17—C12—C13—C14	−3.1 (17)	C10—C5—N1—C2′	8 (6)
C11—C12—C13—C14	179.6 (11)	C6—C5—N1—C2′	−167 (6)
C12—C13—C14—C15	2.1 (16)	C10—C5—N1—C4	−177.2 (16)
C12—C13—C14—C18	−178.4 (11)	C6—C5—N1—C4	7 (2)
C13—C14—C15—C16	−0.4 (17)	C10—C5—N1—C2	0 (2)
C18—C14—C15—C16	−179.8 (10)	C6—C5—N1—C2	−175.3 (15)
C14—C15—C16—C17	−0.2 (16)	C3′—C4′—N1—C5	2 (19)
C14—C15—C16—C22	178.0 (9)	C3′—C4′—N1—C2′	134 (15)
C15—C16—C17—O1	−179.0 (9)	C1′—C2′—N1—C5	−149 (10)
C22—C16—C17—O1	2.9 (14)	C1′—C2′—N1—C4′	65 (13)
C15—C16—C17—C12	−0.8 (14)	C3—C4—N1—C5	−95 (2)
C22—C16—C17—C12	−178.9 (9)	C3—C4—N1—C2	87.3 (19)
C13—C12—C17—O1	−179.4 (10)	C1—C2—N1—C5	−82 (2)
C11—C12—C17—O1	−2.1 (15)	C1—C2—N1—C4	96 (2)
C13—C12—C17—C16	2.3 (15)	C12—C11—N2—C8	−178.7 (10)
C11—C12—C17—C16	179.6 (10)	C9—C8—N2—C11	33.1 (16)
C13—C14—C18—C21	−172.9 (12)	C7—C8—N2—C11	−149.0 (11)
C15—C14—C18—C21	6.5 (16)		

Hydrogen-bond geometry (Å, º)

Cg2 is the centroid of the C12–C17 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2	0.83 (7)	1.82 (11)	2.591 (12)	155 (14)
C23—H23*A*···O1	0.96	2.27	2.947 (17)	127
C24—H24*A*···O1	0.96	2.46	3.071 (16)	121
C2—H2*B*···*Cg*2^{i}	0.97	2.87	3.810 (19)	166
C2′—H2′1···*Cg*2^{i}	0.97	2.60	3.39 (11)	139

Symmetry code: (i) *x*−1, *y*, *z*−1.