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4,6-Di-*tert*-butyl-2-{(*E*)-[4-(dimethylamino)phenylimino]methyl}phenol

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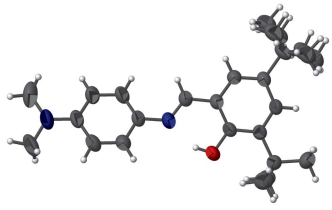
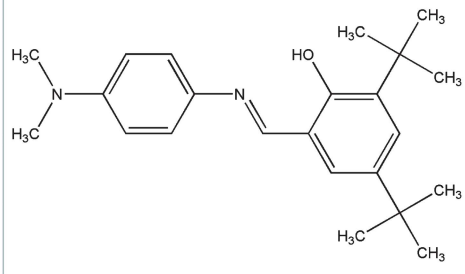
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{23}H_{32}N_2O$, adopts an *E* conformation about the C=N bond. The dihedral angle between the aromatic rings is 25.39 (14)°. One of the *tert*-butyl groups has rotational disorder, with site occupancies of 0.716 (3) and 0.284 (3). An intramolecular O—H···N hydrogen bond is present, forming an S(6) ring motif.

3D view



Chemical scheme



Structure description

Schiff bases have attracted much attention for their biological properties such as antibacterial, anti-cancer and antitumor (Ida Malarselvi *et al.*, 2016; Khattab, 2005; Karthikeyan *et al.*, 2006). We herein report the crystal structure of title compound, which contains a C=N bond (Fig. 1).

Bond lengths in the title compound are comparable with those in a similar structure (Fun *et al.*, 2013). The dihedral angle between the aromatic rings (C3–C8 and C10–C15) is 25.39 (14)°. The conformation of the C=N (C9=N2) bond of this Schiff base is *E* and the intramolecular O1—H1···N2 hydrogen bond forms an *S*(6) ring-motif (Fig. 1 and Table 1). There are no significant intermolecular interactions beyond normal van der Waals contacts present in the crystal structure.

Synthesis and crystallization

An ethanolic solution of *N*,*N*–dimethyl-1,4-phenylenediamine (5 mmol) was stirred magnetically 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 stirred for 1 h and then refluxed for 2–3 h. Upon cooling to room

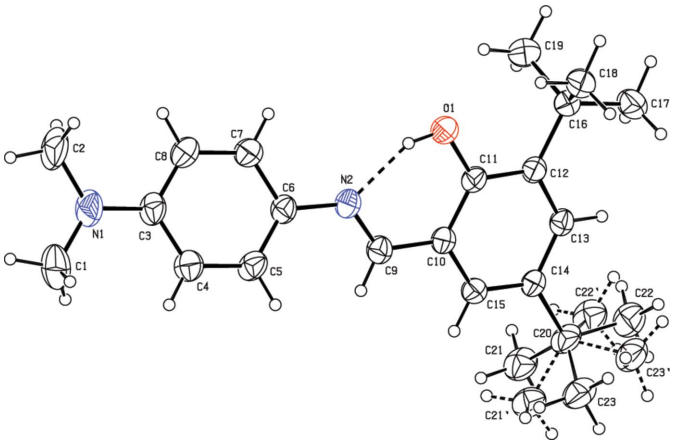


Figure 1
The molecular structure of the title compound, with the atom labelling and 30% probability displacement ellipsoids. The intramolecular O1—H1···N2 hydrogen bond is shown as a dashed line.

temperature, the yellow precipitate formed was filtered and dried *in vacuo* over anhydrous calcium chloride. Single crystals suitable for *X*–ray diffraction were obtained by slow evaporation of a solution of the title compound in dimethylformamide at room temperature.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. One of the *tert*-butyl groups shows rotational disorder with major components of C21, C22 and C23 having site occupancies 0.716 (3) and minor components of C21′, C22′ and C23′ site occupancies of 0.284 (3). The anisotropic displacement parameters of the disordered C atoms were restrained by SIMU instructions within 0.001 as standard deviations. Rigid-bond restraints were applied for bonds C20—C21, C20—C21′, C20—C22, C20—C22′, C20—C23 and C20—C23′ with a standard deviation of 0.001 using the DELU instruction during the final cycles of the *SHELXL* refinement.

Acknowledgements

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N2	0.83 (1)	1.78 (2)	2.544 (3)	153 (4)

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{23}H_{32}N_2O$
M_r	352.50
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	295
a, b, c (Å)	22.8029 (15), 9.9908 (7), 9.3304 (6)
β (°)	90.247 (2)
V (Å^3)	2125.6 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.07
Crystal size (mm)	0.34 × 0.28 × 0.24
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.917, 0.980
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	35692, 4143, 2643
R_{int}	0.041
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.615
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.070, 0.215, 1.03
No. of reflections	4143
No. of parameters	277
No. of restraints	49
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.48, −0.40

Computer programs: *APEX2* and *SAINT* (Bruker, 2004), *SHELXS97* (Sheldrick, 2008), *SHELXL2016/4* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

full crystallographic data

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4,6-Di-*tert*-butyl-2-{(*E*)-[4-(dimethylamino)phenylimino]methyl}phenol

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4,6-Di-*tert*-butyl-2-{(*E*)-[4-(dimethylamino)phenylimino]methyl}phenol

Crystal data

$C_{23}H_{32}N_2O$
M_r = 352.50
Monoclinic, $P2_1/c$
a = 22.8029 (15) Å
b = 9.9908 (7) Å
c = 9.3304 (6) Å
β = 90.247 (2)°
V = 2125.6 (2) Å^3
Z = 4
$F(000)$ = 768
D_x = 1.102 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5165 reflections
θ = 2.4–22.4°
μ = 0.07 mm^{-1}
T = 295 K
Block, colourless
0.34 × 0.28 × 0.24 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
ω and φ scan
Absorption correction: multi-scan (SADABS; Bruker, 2004)
T_{min} = 0.917, T_{max} = 0.980
35692 measured reflections
4143 independent reflections
2643 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 25.9°, θ_{min} = 2.2°
h = −27→28
k = −12→11
l = −11→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.215
S = 1.03
4143 reflections
277 parameters
49 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0826P)^2 + 1.5721P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	1.08947 (15)	0.2191 (4)	0.4437 (5)	0.1011 (13)	

H1A	1.058733	0.210591	0.373632	0.152*	
H1B	1.126262	0.195125	0.401163	0.152*	
H1C	1.091260	0.310001	0.476835	0.152*	
C2	1.12567 (14)	0.0568 (6)	0.6207 (4)	0.1144 (16)	
H2A	1.133763	0.086893	0.716527	0.172*	
H2B	1.159763	0.069731	0.562351	0.172*	
H2C	1.115647	−0.036493	0.622452	0.172*	
C3	1.02298 (11)	0.1250 (3)	0.6223 (3)	0.0639 (8)	
C4	0.97629 (11)	0.2029 (3)	0.5733 (3)	0.0680 (8)	
H4	0.982342	0.261991	0.497808	0.082*	
C5	0.92141 (11)	0.1945 (3)	0.6339 (3)	0.0636 (8)	
H5	0.891252	0.248087	0.598714	0.076*	
C6	0.91044 (10)	0.1079 (3)	0.7460 (3)	0.0551 (7)	
C7	0.95692 (12)	0.0327 (4)	0.7962 (3)	0.0718 (9)	
H7	0.950977	−0.024917	0.873017	0.086*	
C8	1.01151 (12)	0.0404 (4)	0.7364 (4)	0.0760 (9)	
H8	1.041600	−0.012404	0.773195	0.091*	
C9	0.80644 (11)	0.1125 (3)	0.7538 (3)	0.0558 (7)	
H9	0.805782	0.152980	0.664084	0.067*	
C10	0.75150 (10)	0.0801 (3)	0.8222 (3)	0.0506 (6)	
C11	0.75054 (10)	0.0212 (3)	0.9600 (3)	0.0513 (6)	
C12	0.69728 (11)	−0.0174 (3)	1.0215 (3)	0.0495 (6)	
C13	0.64680 (11)	0.0056 (2)	0.9426 (3)	0.0498 (6)	
H13	0.611210	−0.019559	0.982777	0.060*	
C14	0.64568 (10)	0.0639 (3)	0.8067 (3)	0.0485 (6)	
C15	0.69883 (11)	0.1005 (3)	0.7497 (3)	0.0518 (6)	
H15	0.699573	0.140223	0.659533	0.062*	
C16	0.69585 (11)	−0.0847 (3)	1.1696 (3)	0.0571 (7)	
C17	0.63306 (13)	−0.1193 (4)	1.2142 (3)	0.0757 (9)	
H17A	0.610419	−0.038620	1.221550	0.114*	
H17B	0.633754	−0.163897	1.305361	0.114*	
H17C	0.615673	−0.177120	1.143687	0.114*	
C18	0.72105 (13)	0.0092 (3)	1.2834 (3)	0.0706 (8)	
H18A	0.697327	0.088351	1.288946	0.106*	
H18B	0.760412	0.033375	1.258066	0.106*	
H18C	0.721271	−0.035210	1.374642	0.106*	
C19	0.73069 (15)	−0.2162 (3)	1.1661 (4)	0.0806 (10)	
H19A	0.714146	−0.274631	1.094936	0.121*	
H19B	0.728853	−0.258575	1.258316	0.121*	
H19C	0.770836	−0.197624	1.142814	0.121*	
C20	0.58838 (12)	0.0852 (3)	0.7249 (3)	0.0675 (7)	
C21	0.5923 (2)	0.0156 (6)	0.5802 (5)	0.0822 (9)	0.716 (3)
H21A	0.597545	−0.078832	0.594498	0.123*	0.716 (3)
H21B	0.624950	0.050732	0.527729	0.123*	0.716 (3)
H21C	0.556754	0.030864	0.527023	0.123*	0.716 (3)
C22	0.53550 (19)	0.0335 (6)	0.8033 (6)	0.0861 (9)	0.716 (3)
H22A	0.532518	0.077576	0.894448	0.129*	0.716 (3)
H22B	0.539395	−0.061207	0.817945	0.129*	0.716 (3)

H22C	0.500839	0.051151	0.747706	0.129*	0.716 (3)
C23	0.5796 (2)	0.2327 (5)	0.6985 (6)	0.0825 (8)	0.716 (3)
H23A	0.543995	0.246161	0.645121	0.124*	0.716 (3)
H23B	0.612123	0.267189	0.645041	0.124*	0.716 (3)
H23C	0.577039	0.278641	0.788643	0.124*	0.716 (3)
C21′	0.5948 (5)	0.1512 (14)	0.5788 (13)	0.0814 (10)	0.284 (3)
H21D	0.610243	0.239913	0.590714	0.122*	0.284 (3)
H21E	0.557136	0.155938	0.532713	0.122*	0.284 (3)
H21F	0.621063	0.099402	0.520875	0.122*	0.284 (3)
C22′	0.5506 (5)	−0.0439 (14)	0.7261 (14)	0.0827 (10)	0.284 (3)
H22D	0.568456	−0.110274	0.666051	0.124*	0.284 (3)
H22E	0.511993	−0.023911	0.690690	0.124*	0.284 (3)
H22F	0.547980	−0.077336	0.822303	0.124*	0.284 (3)
C23′	0.5480 (5)	0.1814 (14)	0.8104 (14)	0.0835 (10)	0.284 (3)
H23D	0.532563	0.135513	0.892300	0.125*	0.284 (3)
H23E	0.516296	0.210602	0.750055	0.125*	0.284 (3)
H23F	0.570293	0.257690	0.841582	0.125*	0.284 (3)
N1	1.07772 (10)	0.1318 (4)	0.5625 (3)	0.0886 (9)	
N2	0.85586 (9)	0.0874 (2)	0.8129 (2)	0.0592 (6)	
O1	0.80132 (8)	0.0006 (2)	1.0312 (2)	0.0705 (6)	
H1	0.8283 (12)	0.023 (4)	0.977 (3)	0.106*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.074 (2)	0.102 (3)	0.127 (3)	−0.029 (2)	0.037 (2)	−0.010 (3)
C2	0.0412 (17)	0.202 (5)	0.100 (3)	0.016 (2)	0.0014 (17)	−0.016 (3)
C3	0.0391 (14)	0.083 (2)	0.0700 (18)	−0.0094 (13)	0.0000 (12)	−0.0063 (16)
C4	0.0483 (16)	0.073 (2)	0.083 (2)	−0.0119 (14)	0.0013 (14)	0.0103 (16)
C5	0.0416 (14)	0.0618 (17)	0.087 (2)	−0.0043 (12)	−0.0048 (13)	0.0078 (15)
C6	0.0401 (13)	0.0642 (17)	0.0610 (16)	−0.0062 (12)	−0.0004 (11)	0.0003 (13)
C7	0.0488 (16)	0.096 (2)	0.0704 (19)	0.0013 (15)	−0.0033 (14)	0.0174 (17)
C8	0.0433 (16)	0.101 (2)	0.083 (2)	0.0071 (16)	−0.0050 (14)	0.0108 (19)
C9	0.0453 (14)	0.0645 (17)	0.0576 (15)	−0.0033 (12)	0.0020 (12)	0.0026 (13)
C10	0.0414 (13)	0.0557 (15)	0.0546 (15)	−0.0011 (11)	0.0015 (11)	0.0016 (12)
C11	0.0398 (13)	0.0596 (16)	0.0545 (15)	0.0038 (11)	−0.0031 (11)	0.0009 (12)
C12	0.0442 (13)	0.0511 (14)	0.0532 (14)	0.0035 (11)	0.0023 (11)	−0.0002 (11)
C13	0.0409 (13)	0.0522 (15)	0.0564 (15)	−0.0003 (11)	0.0036 (11)	−0.0003 (12)
C14	0.0404 (13)	0.0507 (14)	0.0542 (14)	0.0012 (11)	−0.0009 (10)	−0.0031 (12)
C15	0.0468 (14)	0.0579 (15)	0.0509 (14)	0.0004 (12)	−0.0007 (11)	0.0049 (12)
C16	0.0509 (15)	0.0645 (17)	0.0560 (15)	0.0050 (12)	0.0022 (12)	0.0095 (13)
C17	0.0686 (19)	0.090 (2)	0.0683 (19)	−0.0068 (17)	0.0074 (15)	0.0199 (17)
C18	0.0682 (19)	0.087 (2)	0.0563 (16)	0.0071 (16)	−0.0006 (14)	0.0030 (16)
C19	0.086 (2)	0.071 (2)	0.085 (2)	0.0158 (17)	0.0063 (18)	0.0200 (17)
C20	0.0441 (13)	0.0855 (16)	0.0729 (14)	0.0065 (11)	−0.0171 (11)	−0.0013 (12)
C21	0.0651 (17)	0.1021 (19)	0.0793 (16)	0.0051 (16)	−0.0191 (14)	−0.0090 (15)
C22	0.0555 (16)	0.110 (2)	0.0928 (19)	−0.0010 (15)	−0.0086 (14)	0.0015 (17)
C23	0.0651 (17)	0.0909 (16)	0.0915 (19)	0.0160 (15)	−0.0152 (15)	0.0033 (14)

C21′	0.0663 (19)	0.098 (2)	0.0800 (17)	0.0095 (18)	−0.0167 (16)	0.0046 (16)
C22′	0.0594 (19)	0.0997 (19)	0.089 (2)	−0.0054 (15)	−0.0166 (18)	−0.0035 (16)
C23′	0.0588 (19)	0.100 (2)	0.0918 (19)	0.0149 (16)	−0.0090 (16)	−0.0028 (18)
N1	0.0407 (13)	0.133 (3)	0.092 (2)	−0.0062 (15)	0.0079 (13)	0.0055 (19)
N2	0.0405 (12)	0.0713 (15)	0.0658 (14)	−0.0034 (10)	0.0007 (10)	0.0042 (12)
O1	0.0411 (10)	0.1058 (17)	0.0646 (13)	0.0038 (10)	−0.0043 (9)	0.0183 (11)

Geometric parameters (Å, º)

C1—N1	1.437 (5)	C16—C19	1.536 (4)
C1—H1A	0.9600	C17—H17A	0.9600
C1—H1B	0.9600	C17—H17B	0.9600
C1—H1C	0.9600	C17—H17C	0.9600
C2—N1	1.431 (5)	C18—H18A	0.9600
C2—H2A	0.9600	C18—H18B	0.9600
C2—H2B	0.9600	C18—H18C	0.9600
C2—H2C	0.9600	C19—H19A	0.9600
C3—N1	1.371 (3)	C19—H19B	0.9600
C3—C8	1.385 (4)	C19—H19C	0.9600
C3—C4	1.394 (4)	C20—C22	1.505 (6)
C4—C5	1.378 (4)	C20—C23	1.507 (6)
C4—H4	0.9300	C20—C21	1.522 (6)
C5—C6	1.381 (4)	C20—C21′	1.522 (12)
C5—H5	0.9300	C20—C22′	1.551 (13)
C6—C7	1.379 (4)	C20—C23′	1.554 (12)
C6—N2	1.410 (3)	C21—H21A	0.9600
C7—C8	1.368 (4)	C21—H21B	0.9600
C7—H7	0.9300	C21—H21C	0.9600
C8—H8	0.9300	C22—H22A	0.9600
C9—N2	1.277 (3)	C22—H22B	0.9600
C9—C10	1.445 (3)	C22—H22C	0.9600
C9—H9	0.9300	C23—H23A	0.9600
C10—C15	1.391 (3)	C23—H23B	0.9600
C10—C11	1.414 (4)	C23—H23C	0.9600
C11—O1	1.348 (3)	C21′—H21D	0.9600
C11—C12	1.400 (3)	C21′—H21E	0.9600
C12—C13	1.383 (3)	C21′—H21F	0.9600
C12—C16	1.537 (4)	C22′—H22D	0.9600
C13—C14	1.395 (4)	C22′—H22E	0.9600
C13—H13	0.9300	C22′—H22F	0.9600
C14—C15	1.375 (3)	C23′—H23D	0.9600
C14—C20	1.526 (3)	C23′—H23E	0.9600
C15—H15	0.9300	C23′—H23F	0.9600
C16—C18	1.527 (4)	O1—H1	0.830 (10)
C16—C17	1.532 (4)		
N1—C1—H1A	109.5	C16—C18—H18B	109.5
N1—C1—H1B	109.5	H18A—C18—H18B	109.5

H1A—C1—H1B	109.5	C16—C18—H18C	109.5
N1—C1—H1C	109.5	H18A—C18—H18C	109.5
H1A—C1—H1C	109.5	H18B—C18—H18C	109.5
H1B—C1—H1C	109.5	C16—C19—H19A	109.5
N1—C2—H2A	109.5	C16—C19—H19B	109.5
N1—C2—H2B	109.5	H19A—C19—H19B	109.5
H2A—C2—H2B	109.5	C16—C19—H19C	109.5
N1—C2—H2C	109.5	H19A—C19—H19C	109.5
H2A—C2—H2C	109.5	H19B—C19—H19C	109.5
H2B—C2—H2C	109.5	C22—C20—C23	108.0 (3)
N1—C3—C8	121.2 (3)	C22—C20—C21	109.0 (3)
N1—C3—C4	122.3 (3)	C23—C20—C21	108.1 (4)
C8—C3—C4	116.5 (2)	C22—C20—C14	113.3 (3)
C5—C4—C3	121.7 (3)	C23—C20—C14	109.3 (3)
C5—C4—H4	119.2	C21—C20—C14	109.1 (3)
C3—C4—H4	119.2	C21′—C20—C14	115.0 (5)
C4—C5—C6	121.1 (3)	C21′—C20—C22′	115.0 (7)
C4—C5—H5	119.5	C14—C20—C22′	110.8 (5)
C6—C5—H5	119.5	C21′—C20—C23′	104.5 (7)
C7—C6—C5	117.2 (2)	C14—C20—C23′	109.7 (5)
C7—C6—N2	116.7 (3)	C22′—C20—C23′	100.4 (7)
C5—C6—N2	126.1 (2)	C20—C21—H21A	109.5
C8—C7—C6	122.0 (3)	C20—C21—H21B	109.5
C8—C7—H7	119.0	H21A—C21—H21B	109.5
C6—C7—H7	119.0	C20—C21—H21C	109.5
C7—C8—C3	121.5 (3)	H21A—C21—H21C	109.5
C7—C8—H8	119.3	H21B—C21—H21C	109.5
C3—C8—H8	119.3	C20—C22—H22A	109.5
N2—C9—C10	122.1 (3)	C20—C22—H22B	109.5
N2—C9—H9	119.0	H22A—C22—H22B	109.5
C10—C9—H9	119.0	C20—C22—H22C	109.5
C15—C10—C11	119.1 (2)	H22A—C22—H22C	109.5
C15—C10—C9	120.1 (2)	H22B—C22—H22C	109.5
C11—C10—C9	120.8 (2)	C20—C23—H23A	109.5
O1—C11—C12	120.0 (2)	C20—C23—H23B	109.5
O1—C11—C10	119.7 (2)	H23A—C23—H23B	109.5
C12—C11—C10	120.3 (2)	C20—C23—H23C	109.5
C13—C12—C11	117.2 (2)	H23A—C23—H23C	109.5
C13—C12—C16	122.0 (2)	H23B—C23—H23C	109.5
C11—C12—C16	120.7 (2)	C20—C21′—H21D	109.5
C12—C13—C14	124.4 (2)	C20—C21′—H21E	109.5
C12—C13—H13	117.8	H21D—C21′—H21E	109.5
C14—C13—H13	117.8	C20—C21′—H21F	109.5
C15—C14—C13	116.8 (2)	H21D—C21′—H21F	109.5
C15—C14—C20	121.5 (2)	H21E—C21′—H21F	109.5
C13—C14—C20	121.7 (2)	C20—C22′—H22D	109.5
C14—C15—C10	122.2 (2)	C20—C22′—H22E	109.5
C14—C15—H15	118.9	H22D—C22′—H22E	109.5

C10—C15—H15	118.9	C20—C22′—H22F	109.5
C18—C16—C17	107.4 (2)	H22D—C22′—H22F	109.5
C18—C16—C19	110.3 (2)	H22E—C22′—H22F	109.5
C17—C16—C19	107.3 (3)	C20—C23′—H23D	109.5
C18—C16—C12	110.3 (2)	C20—C23′—H23E	109.5
C17—C16—C12	111.5 (2)	H23D—C23′—H23E	109.5
C19—C16—C12	110.0 (2)	C20—C23′—H23F	109.5
C16—C17—H17A	109.5	H23D—C23′—H23F	109.5
C16—C17—H17B	109.5	H23E—C23′—H23F	109.5
H17A—C17—H17B	109.5	C3—N1—C2	121.0 (3)
C16—C17—H17C	109.5	C3—N1—C1	121.2 (3)
H17A—C17—H17C	109.5	C2—N1—C1	117.8 (3)
H17B—C17—H17C	109.5	C9—N2—C6	124.0 (2)
C16—C18—H18A	109.5	C11—O1—H1	107 (3)

N1—C3—C4—C5	179.6 (3)	C9—C10—C15—C14	176.1 (2)
C8—C3—C4—C5	−1.0 (5)	C13—C12—C16—C18	−119.7 (3)
C3—C4—C5—C6	−0.1 (5)	C11—C12—C16—C18	61.4 (3)
C4—C5—C6—C7	1.3 (4)	C13—C12—C16—C17	−0.5 (4)
C4—C5—C6—N2	−177.6 (3)	C11—C12—C16—C17	−179.4 (3)
C5—C6—C7—C8	−1.4 (5)	C13—C12—C16—C19	118.4 (3)
N2—C6—C7—C8	177.6 (3)	C11—C12—C16—C19	−60.5 (3)
C6—C7—C8—C3	0.3 (5)	C15—C14—C20—C22	177.7 (3)
N1—C3—C8—C7	−179.7 (3)	C13—C14—C20—C22	−1.8 (4)
C4—C3—C8—C7	0.9 (5)	C15—C14—C20—C23	−61.9 (4)
N2—C9—C10—C15	−175.4 (3)	C13—C14—C20—C23	118.6 (3)
N2—C9—C10—C11	1.4 (4)	C15—C14—C20—C21	56.2 (4)
C15—C10—C11—O1	179.8 (2)	C13—C14—C20—C21	−123.4 (3)
C9—C10—C11—O1	3.0 (4)	C15—C14—C20—C21′	−1.0 (7)
C15—C10—C11—C12	0.8 (4)	C13—C14—C20—C21′	179.5 (6)
C9—C10—C11—C12	−176.0 (2)	C15—C14—C20—C22′	131.6 (6)
O1—C11—C12—C13	−179.5 (2)	C13—C14—C20—C22′	−48.0 (7)
C10—C11—C12—C13	−0.5 (4)	C15—C14—C20—C23′	−118.5 (6)
O1—C11—C12—C16	−0.5 (4)	C13—C14—C20—C23′	62.0 (7)
C10—C11—C12—C16	178.5 (2)	C8—C3—N1—C2	−3.3 (5)
C11—C12—C13—C14	0.2 (4)	C4—C3—N1—C2	176.1 (3)
C16—C12—C13—C14	−178.8 (2)	C8—C3—N1—C1	179.7 (3)
C12—C13—C14—C15	−0.1 (4)	C4—C3—N1—C1	−0.9 (5)
C12—C13—C14—C20	179.4 (3)	C10—C9—N2—C6	175.0 (2)
C13—C14—C15—C10	0.4 (4)	C7—C6—N2—C9	−156.2 (3)
C20—C14—C15—C10	−179.1 (3)	C5—C6—N2—C9	22.8 (5)
C11—C10—C15—C14	−0.8 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2	0.83 (1)	1.78 (2)	2.544 (3)	153 (4)