

2,4-Di-*tert*-butyl-6-(4-nitrophenylimino-methyl)phenol

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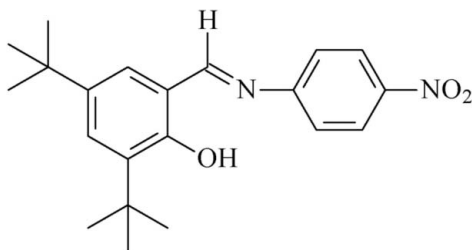
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 Key indicators: single-crystal X-ray study; $T = 291$ K; mean $\sigma(\text{C}-\text{C}) = 0.008$ Å; R factor = 0.078; wR factor = 0.176; data-to-parameter ratio = 12.8.

In the title compound, $\text{C}_{21}\text{H}_{26}\text{N}_2\text{O}_3$, the molecule adopts an *E* configuration about the central $\text{C}=\text{N}$ double bond and exists in the phenol-imine tautomeric form. The two benzene rings make a dihedral angle of 38.5 (4)°. Intramolecular $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonding is present.

Related literature

For general literature concerning applications of benzothiazole compounds, see: Siddiqui *et al.* (2006); Unver *et al.* (2002); Selvakumar *et al.* (2007); Oter *et al.* (2007). Similar tautomerism has also been observed in related Schiff bases reported by Sun *et al.* (2007) and Aazam *et al.* (2006). Other reported Schiff bases exist in the enamine-keto tautomeric form (Hokelek *et al.*, 2000).



Experimental

Crystal data

 $\text{C}_{21}\text{H}_{26}\text{N}_2\text{O}_3$
 $M_r = 354.44$
 Monoclinic, $P2_1/c$
 $a = 17.937$ (4) Å
 $b = 6.4674$ (13) Å
 $c = 19.047$ (4) Å

 $\beta = 113.31$ (3)°
 $V = 2029.2$ (7) Å³
 $Z = 4$
 Mo $K\alpha$ radiation

 $\mu = 0.08$ mm⁻¹
 $T = 291$ (2) K
 $0.20 \times 0.18 \times 0.16$ mm

Data collection

 Rigaku R-Axis-IV diffractometer
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.985$, $T_{\max} = 0.988$

 4678 measured reflections
 3066 independent reflections
 1226 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.074$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.078$
 $wR(F^2) = 0.176$
 $S = 0.97$
 3066 reflections
 240 parameters

 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.19$ e Å⁻³
 $\Delta\rho_{\min} = -0.15$ e Å⁻³
Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1}-\text{H1E}\cdots\text{N1}$	1.00 (7)	1.65 (7)	2.609 (5)	159 (6)

Data collection: *R-Axis* (Rigaku, 1996); cell refinement: *R-Axis*; data reduction: *R-Axis*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *TEXSAN* (Molecular Structure Corporation, 1999); software used to prepare material for publication: *TEXSAN*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2274).

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supplementary materials

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2,4-Di-*tert*-butyl-6-(4-nitrophenyliminomethyl)phenol

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Comment

Schiff bases have demonstrated significant biological activities and new examples are being tested for their antitumor, antimicrobial and antiviral activities (Siddiqui *et al.*, 2006). Moreover, Schiff base compounds can be classified by their photochromic and thermochromic characteristics (Unver *et al.*, 2002). Schiff bases have also been employed as ligands for metal complexes (Selvakumar *et al.*, 2007) and as optical sensor (Oter *et al.*, 2007). We herein report the synthesis and crystal structure of the title compound, (I), (Fig.1). The molecule of (I) is not planar and possesses normal geometric parameters. The molecule has E-configuration, across the C=N double bond. A dihedral angle of 38.5 (4)° is found between the mean planes of the two benzene rings. Also, while C14, C17, C18 and C21 are approximately coplanar with their attached benzene ring, C15, C16, C19 and C20 deviate by -1.1043 (5), 1.3469 (5), -1.2082 (6) and 1.3013 (5) Å, respectively. In addition, there is an intramolecular N···H—O hydrogen bond between the N1 and O1 atoms, which makes the phenol-imine form. Similar tautomerism has also been observed in related Schiff bases reported by Sun *et al.* (2007) and Aazam *et al.* (2006). However, this is obviously different from other reported Schiff base, in which the Schiff base exist in enamine-keto tautomeric form (Hokelek *et al.*, 2000).

Experimental

A mixture of 4-nitroaniline (1 mmol) and 3,5-di-*tert*-butyl-2-hydroxybenzaldehyde (1 mmol) in anhydrous ethanol (30 ml) was refluxed for 3 hr, and then cooled to room temperature. The precipitate was filtered and dried. The crude product was recrystallized from ethanol. Red crystals were thus obtained in 79% yield. Analysis calculated for C₂₁H₂₆N₂O₃: C, 71.16; H, 7.39; N, 7.90. Found (%): C, 71.33; H, 7.28; N, 7.76. A single-crystal suitable for an X-ray structural analysis was obtained by slowly evaporating a ethanolic solution at room temperature.

Refinement

All H atoms were initially located in a difference Fourier map. The methyl H atoms were then constrained to an ideal geometry with C—H distances of 0.96 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$. The hydroxyl H atoms were refined freely along with an isotropic displacement parameter. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H distances of 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

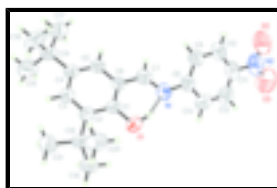


Fig. 1. View of the molecule of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radii. The dashed lines indicate hydrogen bonds.

2,4-Di-*tert*-butyl-6-(4-nitrophenyliminomethyl)phenol

Crystal data

$C_{21}H_{26}N_2O_3$	$F_{000} = 760$
$M_r = 354.44$	$D_x = 1.160 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
Hall symbol: -P 2ybc	$\lambda = 0.71073 \text{ \AA}$
$a = 17.937 (4) \text{ \AA}$	Cell parameters from 389 reflections
$b = 6.4674 (13) \text{ \AA}$	$\theta = 2-25.1^\circ$
$c = 19.047 (4) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$\beta = 113.31 (3)^\circ$	$T = 291 (2) \text{ K}$
$V = 2029.2 (7) \text{ \AA}^3$	Prismatic, red
$Z = 4$	$0.20 \times 0.18 \times 0.16 \text{ mm}$

Data collection

Rigaku R-AXIS-IV diffractometer	3066 independent reflections
Radiation source: fine-focus sealed tube	1226 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.074$
$T = 291(2) \text{ K}$	$\theta_{\text{max}} = 25.0^\circ$
Oscillation frames scans	$\theta_{\text{min}} = 1.2^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = 0 \rightarrow 21$
$T_{\text{min}} = 0.985, T_{\text{max}} = 0.988$	$k = -7 \rightarrow 7$
4678 measured reflections	$l = -22 \rightarrow 20$

Refinement

Refinement on F^2	Hydrogen site location: difference Fourier map
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.078$	$w = 1/[\sigma^2(F_o^2) + (0.062P)^2]$
$wR(F^2) = 0.176$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.97$	$(\Delta/\sigma)_{\text{max}} < 0.001$
3066 reflections	$\Delta\rho_{\text{max}} = 0.19 \text{ e \AA}^{-3}$
240 parameters	$\Delta\rho_{\text{min}} = -0.15 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: SHELXL97
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.0059 (13)

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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.1937 (2)	0.6463 (6)	0.0192 (2)	0.0652 (12)
N2	-0.0060 (3)	1.3225 (9)	-0.1296 (4)	0.0959 (18)
O1	0.3061 (2)	0.3763 (5)	0.03105 (19)	0.0711 (11)
O2	-0.0154 (3)	1.4634 (7)	-0.0908 (3)	0.1241 (18)
O3	-0.0361 (4)	1.3241 (9)	-0.1982 (3)	0.177 (3)
C1	0.3001 (3)	0.3053 (7)	0.0964 (3)	0.0533 (13)
C2	0.3475 (3)	0.1359 (7)	0.1350 (3)	0.0517 (13)
C3	0.3358 (3)	0.0701 (7)	0.1993 (2)	0.0555 (13)
H3A	0.3667	-0.0413	0.2262	0.067*
C4	0.2812 (3)	0.1577 (8)	0.2269 (2)	0.0531 (13)
C5	0.2370 (3)	0.3253 (7)	0.1876 (3)	0.0580 (14)
H5A	0.2010	0.3896	0.2048	0.070*
C6	0.2454 (3)	0.4011 (7)	0.1219 (3)	0.0503 (13)
C7	0.1950 (3)	0.5732 (8)	0.0823 (3)	0.0626 (15)
H7A	0.1619	0.6341	0.1036	0.075*
C8	0.1424 (3)	0.8192 (8)	-0.0155 (3)	0.0612 (14)
C9	0.1280 (3)	0.9791 (8)	0.0259 (3)	0.0711 (15)
H9A	0.1512	0.9751	0.0791	0.085*
C10	0.0792 (3)	1.1455 (8)	-0.0111 (4)	0.0720 (16)
H10A	0.0691	1.2521	0.0167	0.086*
C11	0.0464 (3)	1.1489 (10)	-0.0892 (4)	0.0708 (16)
C12	0.0606 (3)	0.9961 (11)	-0.1317 (3)	0.0850 (18)
H12A	0.0376	1.0026	-0.1848	0.102*
C13	0.1093 (3)	0.8326 (9)	-0.0950 (3)	0.0799 (17)
H13A	0.1203	0.7295	-0.1236	0.096*
C14	0.2742 (3)	0.0730 (8)	0.2992 (3)	0.0622 (14)
C15	0.2590 (4)	-0.1590 (8)	0.2925 (3)	0.117 (2)
H15A	0.3016	-0.2263	0.2827	0.175*
H15B	0.2078	-0.1865	0.2512	0.175*
H15C	0.2579	-0.2105	0.3394	0.175*
C16	0.3554 (4)	0.1089 (9)	0.3677 (3)	0.105 (2)
H16A	0.3982	0.0398	0.3587	0.158*
H16B	0.3520	0.0548	0.4133	0.158*

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H16C	0.3667	0.2544	0.3738	0.158*
C17	0.2078 (3)	0.1812 (9)	0.3168 (3)	0.106 (2)
H17A	0.2182	0.3272	0.3217	0.160*
H17B	0.2073	0.1281	0.3637	0.160*
H17C	0.1560	0.1563	0.2759	0.160*
C18	0.4088 (3)	0.0318 (8)	0.1086 (3)	0.0594 (14)
C19	0.3662 (3)	-0.0516 (7)	0.0269 (3)	0.0775 (17)
H19A	0.3270	-0.1540	0.0257	0.116*
H19B	0.4057	-0.1128	0.0109	0.116*
H19C	0.3394	0.0598	-0.0069	0.116*
C20	0.4737 (3)	0.1925 (8)	0.1101 (3)	0.0867 (18)
H20A	0.4476	0.3068	0.0775	0.130*
H20B	0.5114	0.1288	0.0924	0.130*
H20C	0.5023	0.2413	0.1614	0.130*
C21	0.4521 (4)	-0.1499 (9)	0.1605 (3)	0.112 (2)
H21A	0.4128	-0.2518	0.1596	0.168*
H21B	0.4804	-0.1010	0.2118	0.168*
H21C	0.4901	-0.2105	0.1425	0.168*
H1E	0.264 (4)	0.487 (11)	0.015 (4)	0.17 (3)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.068 (3)	0.056 (3)	0.069 (3)	0.001 (3)	0.023 (3)	0.007 (3)
N2	0.082 (4)	0.086 (5)	0.119 (6)	0.010 (4)	0.039 (4)	0.030 (5)
O1	0.093 (3)	0.072 (3)	0.064 (2)	0.006 (2)	0.048 (2)	0.011 (2)
O2	0.110 (4)	0.097 (4)	0.166 (5)	0.030 (3)	0.054 (3)	0.033 (3)
O3	0.211 (6)	0.175 (6)	0.105 (4)	0.071 (4)	0.021 (4)	0.057 (4)
C1	0.063 (4)	0.056 (3)	0.049 (3)	-0.004 (3)	0.031 (3)	-0.005 (3)
C2	0.055 (3)	0.056 (3)	0.046 (3)	-0.001 (3)	0.021 (3)	0.000 (3)
C3	0.060 (3)	0.057 (3)	0.053 (3)	0.004 (3)	0.026 (3)	0.001 (3)
C4	0.058 (3)	0.058 (4)	0.049 (3)	-0.004 (3)	0.029 (3)	-0.007 (3)
C5	0.071 (4)	0.057 (3)	0.062 (3)	0.000 (3)	0.042 (3)	-0.007 (3)
C6	0.054 (3)	0.042 (3)	0.056 (3)	0.000 (3)	0.023 (3)	0.000 (3)
C7	0.065 (4)	0.059 (4)	0.069 (4)	-0.009 (3)	0.033 (3)	-0.008 (3)
C8	0.064 (4)	0.056 (4)	0.059 (4)	-0.011 (3)	0.020 (3)	0.000 (3)
C9	0.077 (4)	0.058 (4)	0.063 (4)	-0.006 (3)	0.012 (3)	-0.004 (4)
C10	0.066 (4)	0.055 (4)	0.081 (5)	-0.003 (3)	0.015 (4)	0.001 (4)
C11	0.049 (4)	0.066 (4)	0.091 (5)	0.004 (3)	0.021 (4)	0.017 (4)
C12	0.085 (5)	0.092 (5)	0.071 (4)	0.012 (4)	0.023 (4)	0.019 (4)
C13	0.095 (5)	0.087 (5)	0.068 (4)	0.007 (4)	0.044 (4)	-0.001 (4)
C14	0.075 (4)	0.069 (4)	0.052 (3)	-0.008 (3)	0.035 (3)	-0.007 (3)
C15	0.189 (7)	0.083 (5)	0.124 (5)	-0.023 (5)	0.110 (5)	0.000 (4)
C16	0.116 (5)	0.149 (6)	0.067 (4)	-0.001 (5)	0.054 (4)	0.007 (4)
C17	0.120 (5)	0.135 (5)	0.103 (5)	0.033 (4)	0.086 (5)	0.030 (4)
C18	0.063 (4)	0.069 (4)	0.059 (3)	0.001 (3)	0.038 (3)	-0.007 (3)
C19	0.095 (4)	0.072 (4)	0.085 (4)	-0.002 (3)	0.057 (4)	-0.016 (3)
C20	0.067 (4)	0.118 (5)	0.085 (4)	-0.014 (4)	0.040 (3)	-0.022 (4)

C21 0.130 (5) 0.124 (5) 0.116 (5) 0.073 (5) 0.086 (5) 0.047 (5)

Geometric parameters (Å, °)

N1—C7	1.283 (5)	C12—H12A	0.9300
N1—C8	1.432 (6)	C13—H13A	0.9300
N2—O3	1.200 (6)	C14—C15	1.521 (6)
N2—O2	1.226 (6)	C14—C17	1.529 (6)
N2—C11	1.471 (7)	C14—C16	1.541 (7)
O1—C1	1.371 (5)	C15—H15A	0.9600
O1—H1E	1.00 (7)	C15—H15B	0.9600
C1—C6	1.398 (5)	C15—H15C	0.9600
C1—C2	1.403 (6)	C16—H16A	0.9600
C2—C3	1.388 (5)	C16—H16B	0.9600
C2—C18	1.534 (5)	C16—H16C	0.9600
C3—C4	1.402 (5)	C17—H17A	0.9600
C3—H3A	0.9300	C17—H17B	0.9600
C4—C5	1.376 (5)	C17—H17C	0.9600
C4—C14	1.533 (6)	C18—C19	1.534 (6)
C5—C6	1.407 (5)	C18—C21	1.534 (6)
C5—H5A	0.9300	C18—C20	1.553 (6)
C6—C7	1.445 (6)	C19—H19A	0.9600
C7—H7A	0.9300	C19—H19B	0.9600
C8—C9	1.386 (6)	C19—H19C	0.9600
C8—C13	1.394 (6)	C20—H20A	0.9600
C9—C10	1.391 (6)	C20—H20B	0.9600
C9—H9A	0.9300	C20—H20C	0.9600
C10—C11	1.366 (6)	C21—H21A	0.9600
C10—H10A	0.9300	C21—H21B	0.9600
C11—C12	1.365 (7)	C21—H21C	0.9600
C12—C13	1.373 (6)		
C7—N1—C8	119.3 (4)	C17—C14—C4	112.4 (4)
O3—N2—O2	122.7 (7)	C15—C14—C16	107.3 (5)
O3—N2—C11	119.8 (7)	C17—C14—C16	107.7 (4)
O2—N2—C11	117.5 (6)	C4—C14—C16	108.7 (4)
C1—O1—H1E	101 (4)	C14—C15—H15A	109.5
O1—C1—C6	119.0 (4)	C14—C15—H15B	109.5
O1—C1—C2	119.2 (4)	H15A—C15—H15B	109.5
C6—C1—C2	121.8 (4)	C14—C15—H15C	109.5
C3—C2—C1	115.4 (4)	H15A—C15—H15C	109.5
C3—C2—C18	122.2 (4)	H15B—C15—H15C	109.5
C1—C2—C18	122.4 (4)	C14—C16—H16A	109.5
C2—C3—C4	125.4 (4)	C14—C16—H16B	109.5
C2—C3—H3A	117.3	H16A—C16—H16B	109.5
C4—C3—H3A	117.3	C14—C16—H16C	109.5
C5—C4—C3	116.8 (4)	H16A—C16—H16C	109.5
C5—C4—C14	122.5 (4)	H16B—C16—H16C	109.5
C3—C4—C14	120.7 (5)	C14—C17—H17A	109.5
C4—C5—C6	121.1 (4)	C14—C17—H17B	109.5

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C4—C5—H5A	119.4	H17A—C17—H17B	109.5
C6—C5—H5A	119.4	C14—C17—H17C	109.5
C1—C6—C5	119.4 (4)	H17A—C17—H17C	109.5
C1—C6—C7	122.7 (4)	H17B—C17—H17C	109.5
C5—C6—C7	117.9 (4)	C19—C18—C2	110.7 (4)
N1—C7—C6	123.3 (5)	C19—C18—C21	107.8 (4)
N1—C7—H7A	118.3	C2—C18—C21	111.8 (4)
C6—C7—H7A	118.3	C19—C18—C20	108.8 (3)
C9—C8—C13	118.5 (5)	C2—C18—C20	109.3 (4)
C9—C8—N1	123.4 (5)	C21—C18—C20	108.4 (4)
C13—C8—N1	118.0 (5)	C18—C19—H19A	109.5
C8—C9—C10	120.7 (5)	C18—C19—H19B	109.5
C8—C9—H9A	119.6	H19A—C19—H19B	109.5
C10—C9—H9A	119.6	C18—C19—H19C	109.5
C11—C10—C9	118.6 (5)	H19A—C19—H19C	109.5
C11—C10—H10A	120.7	H19B—C19—H19C	109.5
C9—C10—H10A	120.7	C18—C20—H20A	109.5
C12—C11—C10	122.3 (6)	C18—C20—H20B	109.5
C12—C11—N2	118.2 (6)	H20A—C20—H20B	109.5
C10—C11—N2	119.6 (6)	C18—C20—H20C	109.5
C11—C12—C13	119.1 (6)	H20A—C20—H20C	109.5
C11—C12—H12A	120.5	H20B—C20—H20C	109.5
C13—C12—H12A	120.5	C18—C21—H21A	109.5
C12—C13—C8	120.9 (5)	C18—C21—H21B	109.5
C12—C13—H13A	119.6	H21A—C21—H21B	109.5
C8—C13—H13A	119.6	C18—C21—H21C	109.5
C15—C14—C17	109.9 (4)	H21A—C21—H21C	109.5
C15—C14—C4	110.7 (4)	H21B—C21—H21C	109.5
O1—C1—C2—C3	-178.1 (4)	C9—C10—C11—C12	-0.7 (8)
C6—C1—C2—C3	0.5 (6)	C9—C10—C11—N2	179.6 (4)
O1—C1—C2—C18	2.5 (6)	O3—N2—C11—C12	1.7 (8)
C6—C1—C2—C18	-178.9 (4)	O2—N2—C11—C12	-176.8 (5)
C1—C2—C3—C4	0.5 (6)	O3—N2—C11—C10	-178.6 (6)
C18—C2—C3—C4	179.9 (4)	O2—N2—C11—C10	2.9 (8)
C2—C3—C4—C5	-1.4 (7)	C10—C11—C12—C13	0.3 (8)
C2—C3—C4—C14	-179.3 (4)	N2—C11—C12—C13	180.0 (5)
C3—C4—C5—C6	1.4 (7)	C11—C12—C13—C8	1.5 (8)
C14—C4—C5—C6	179.2 (4)	C9—C8—C13—C12	-2.7 (7)
O1—C1—C6—C5	178.1 (4)	N1—C8—C13—C12	-179.1 (4)
C2—C1—C6—C5	-0.5 (7)	C5—C4—C14—C15	129.0 (5)
O1—C1—C6—C7	-0.3 (6)	C3—C4—C14—C15	-53.3 (6)
C2—C1—C6—C7	-178.9 (4)	C5—C4—C14—C17	5.7 (7)
C4—C5—C6—C1	-0.5 (7)	C3—C4—C14—C17	-176.5 (4)
C4—C5—C6—C7	177.9 (4)	C5—C4—C14—C16	-113.4 (5)
C8—N1—C7—C6	-179.2 (4)	C3—C4—C14—C16	64.4 (6)
C1—C6—C7—N1	3.0 (7)	C3—C2—C18—C19	121.2 (5)
C5—C6—C7—N1	-175.3 (4)	C1—C2—C18—C19	-59.5 (6)
C7—N1—C8—C9	35.8 (7)	C3—C2—C18—C21	1.0 (6)
C7—N1—C8—C13	-148.0 (5)	C1—C2—C18—C21	-179.7 (4)

C13—C8—C9—C10	2.3 (7)	C3—C2—C18—C20	-119.0 (5)
N1—C8—C9—C10	178.4 (4)	C1—C2—C18—C20	60.3 (6)
C8—C9—C10—C11	-0.6 (7)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O1—H1E \cdots N1	1.00 (7)	1.65 (7)	2.609 (5)	159 (6)

Fig. 1

