Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

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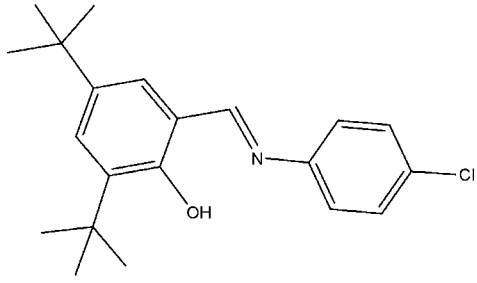
Received 10 November 2007; accepted 22 November 2007

Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.065; wR factor = 0.255; data-to-parameter ratio = 15.2.

In the title molecule, $C_{21}H_{26}ClNO$, the two benzene rings make a dihedral angle of 28.5 (5)°. The hydroxy group is involved in an intramolecular O—H···N hydrogen bond. One *tert*-butyl group exhibits rotational disorder between two orientations in a 0.64:0.36 ratio.

Related literature

For a related crystal structure, see: Li *et al.* (2007). For details of the crystallography and coordination chemistry of Schiff base compounds, see: Garnovskii *et al.* (1993).



Experimental

Crystal data

$C_{21}H_{26}ClNO$
M_r = 343.88
Monoclinic, $P2_1/c$
a = 17.920 (2) Å
b = 10.4888 (14) Å
c = 10.3660 (14) Å
β = 92.638 (2)°
V = 1946.4 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.20 mm^{-1}
T = 273 (2) K
0.18 × 0.15 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.964, T_{max} = 0.976
10040 measured reflections
3452 independent reflections
2335 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.255
S = 1.00
3452 reflections
227 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.88	2.615 (4)	150

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

The authors thank the Postgraduate Foundation of Taishan University (grant No. Y06–2-12) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2363).

References

Garnovskii, A. D., Nivorozhkin, A. L. & Minkin, V. I. (1993). *Coord. Chem. Rev.* **126**, 1–69.
Li, J., Ma, C. & He, G. (2007). *Acta Cryst.* E**63**, m2498.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

supplementary materials

Acta Cryst. (2007). E**63**, o4923 [**doi:10.1107/S1600536807062083**]

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

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Comment

Recently, a number of Schiff-bases have been investigated in terms of their crystallography and coordination chemistry (Garnovskii *et al.*, 1993). In continuation of our studies on Schiff-bases, we now report the synthesized and crystal structure of the title compound (I) (Fig. 1).

All the geometric parameters of (I) are in good agreement with those found in 2-((4-(Trimethylstannylthio)phenylimino)methyl)phenol (Li *et al.*, 2007). The mean planes of the two benzene rings in (I) make a dihedral angle of 28.5 (5)° showing that the Schiff-base ligand adopts a non-planar conformation.

Experimental

The Schiff-base compound was synthesized by the reaction of 3,5-di-*t*-butyl-2-hydroxybenzaldehyde (0.344 g, 1 mmol) and 4-chloroaniline (0.128 g, 1 mmol) in ethanol solution and stirred under reflux conditions (353 K) for 6 h. When cooled to room temperature the solution was filtered and after a week yellow crystals suitable for X-ray diffraction study were obtained. Yield, 0.387 g, 82%. m.p. 375–377 K.

Analysis found: C 72.30, H 7.65, N 4.04%; $C_{21}H_{26}ClNO$ requires: C 73.34, H 7.62, N 4.07%.

Refinement

The H-atoms were included in the riding-model approximation with C—H = 0.93 Å, C—H = 0.96 Å and O—H = 0.82 Å, and with U_{iso}(H) = 1.2U_{eq}(C-aromatic) and U_{iso}(H) = 1.5U_{eq}(*C*-methyl and O).

Figures

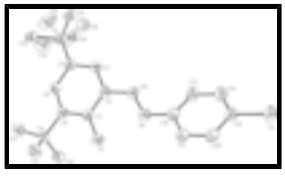


Fig. 1. The molecular structure of (I) showing 30% probability displacement ellipsoids and the atom-numbering scheme. The H atoms are omitted for clarity.

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

Crystal data

$C_{21}H_{26}ClNO$	F_{000} = 736
M_r = 343.88	D_x = 1.174 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation

	λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2391 reflections
a = 17.920 (2) Å	θ = 2.3–26.4º
b = 10.4888 (14) Å	μ = 0.20 mm^{-1}
c = 10.3660 (14) Å	T = 273 (2) K
β = 92.638 (2)º	Block, yellow
V = 1946.4 (4) $Å^3$	0.18 × 0.15 × 0.12 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	3452 independent reflections
Radiation source: sealed tube	2335 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.028
T = 273(2) K	θ_{max} = 25.1º
phi and ω scans	θ_{min} = 1.1º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -20 \rightarrow 21$
T_{min} = 0.964, T_{max} = 0.976	$k = -12 \rightarrow 9$
10040 measured reflections	$l = -12 \rightarrow 11$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.065	H-atom parameters constrained
$wR(F^2)$ = 0.255	$w = 1/[\sigma^2(F_o^2) + (0.175P)^2 + 0.475P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.00	$(\Delta/\sigma)_{max} < 0.001$
3452 reflections	$\Delta\rho_{max}$ = 0.62 e $Å^{-3}$
227 parameters	$\Delta\rho_{min}$ = −0.42 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 $F^2 > 2\text{sigma}(F^2)$ 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}	Occ. (<1)
Cl1	0.36868 (6)	0.55951 (11)	0.21937 (11)	0.0845 (5)	
O1	0.67840 (12)	0.9894 (2)	0.6559 (2)	0.0627 (7)	
H1	0.6481	0.9500	0.6095	0.094*	
N1	0.61348 (15)	0.7948 (3)	0.5399 (3)	0.0598 (7)	
C1	0.73053 (16)	0.9078 (3)	0.7064 (3)	0.0483 (7)	
C2	0.72582 (17)	0.7775 (3)	0.6732 (3)	0.0515 (7)	
C3	0.77991 (17)	0.6935 (3)	0.7248 (3)	0.0538 (8)	
H3	0.7765	0.6075	0.7033	0.065*	
C4	0.83794 (16)	0.7334 (3)	0.8062 (3)	0.0498 (7)	
C5	0.83960 (17)	0.8633 (3)	0.8370 (3)	0.0500 (7)	
H5	0.8782	0.8921	0.8925	0.060*	
C6	0.78783 (16)	0.9519 (3)	0.7906 (3)	0.0466 (7)	
C7	0.8979 (2)	0.6405 (3)	0.8603 (3)	0.0650 (8)	
C8	0.9511 (5)	0.6169 (11)	0.7612 (9)	0.0650 (8)	0.360 (5)
H8A	0.9894	0.5603	0.7944	0.097*	0.360 (5)
H8B	0.9732	0.6961	0.7365	0.097*	0.360 (5)
H8C	0.9257	0.5788	0.6873	0.097*	0.360 (5)
C8'	0.9185 (4)	0.5397 (7)	0.7616 (7)	0.090 (2)	0.640 (5)
H8D	0.9326	0.5808	0.6837	0.135*	0.640 (5)
H8E	0.8762	0.4854	0.7429	0.135*	0.640 (5)
H8F	0.9595	0.4894	0.7961	0.135*	0.640 (5)
C9	0.8550 (5)	0.5117 (9)	0.8926 (10)	0.0650 (8)	0.360 (5)
H9A	0.8491	0.4607	0.8159	0.097*	0.360 (5)
H9B	0.8068	0.5319	0.9237	0.097*	0.360 (5)
H9C	0.8834	0.4650	0.9577	0.097*	0.360 (5)
C9'	0.8727 (5)	0.5791 (9)	0.9789 (7)	0.110 (2)	0.640 (5)
H9D	0.8272	0.5330	0.9593	0.165*	0.640 (5)
H9E	0.8639	0.6431	1.0425	0.165*	0.640 (5)
H9F	0.9104	0.5212	1.0118	0.165*	0.640 (5)
C10	0.9297 (6)	0.6831 (9)	0.9918 (8)	0.0650 (8)	0.360 (5)
H10A	0.9613	0.6172	1.0285	0.097*	0.360 (5)
H10B	0.8895	0.6994	1.0477	0.097*	0.360 (5)
H10C	0.9584	0.7595	0.9823	0.097*	0.360 (5)
C10'	0.9736 (4)	0.7120 (7)	0.8890 (10)	0.111 (2)	0.640 (5)
H10D	1.0120	0.6511	0.9120	0.167*	0.640 (5)
H10E	0.9682	0.7705	0.9591	0.167*	0.640 (5)
H10F	0.9871	0.7580	0.8135	0.167*	0.640 (5)
C11	0.79405 (18)	1.0936 (3)	0.8288 (3)	0.0521 (8)	
C12	0.8016 (2)	1.1760 (3)	0.7066 (4)	0.0692 (10)	
H12A	0.8469	1.1538	0.6659	0.104*	
H12B	0.8031	1.2645	0.7303	0.104*	
H12C	0.7597	1.1608	0.6477	0.104*	
C13	0.7248 (2)	1.1341 (4)	0.8994 (4)	0.0703 (10)	
H13A	0.6811	1.1232	0.8433	0.105*	
H13B	0.7293	1.2220	0.9241	0.105*	

H13C	0.7204	1.0824	0.9751	0.105*
C14	0.8621 (2)	1.1200 (4)	0.9182 (4)	0.0714 (10)
H14A	0.8585	1.0718	0.9963	0.107*
H14B	0.8643	1.2093	0.9385	0.107*
H14C	0.9066	1.0957	0.8761	0.107*
C15	0.66569 (18)	0.7270 (3)	0.5914 (3)	0.0592 (8)
H15	0.6650	0.6398	0.5753	0.071*
C16	0.55663 (17)	0.7359 (3)	0.4608 (3)	0.0562 (8)
C17	0.56777 (19)	0.6271 (4)	0.3906 (4)	0.0726 (10)
H17	0.6147	0.5892	0.3931	0.087*
C18	0.5100 (2)	0.5734 (4)	0.3162 (4)	0.0768 (11)
H18	0.5182	0.5000	0.2686	0.092*
C19	0.44063 (18)	0.6289 (4)	0.3130 (3)	0.0609 (8)
C20	0.42850 (19)	0.7374 (4)	0.3819 (4)	0.0682 (9)
H20	0.3814	0.7748	0.3794	0.082*
C21	0.48642 (19)	0.7913 (4)	0.4551 (4)	0.0681 (9)
H21	0.4782	0.8657	0.5012	0.082*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0689 (7)	0.0875 (8)	0.0941 (8)	−0.0176 (5)	−0.0274 (5)	0.0014 (5)
O1	0.0573 (13)	0.0529 (13)	0.0759 (15)	0.0090 (10)	−0.0178 (12)	0.0024 (11)
N1	0.0537 (16)	0.0618 (17)	0.0626 (17)	0.0002 (13)	−0.0106 (13)	0.0010 (14)
C1	0.0439 (15)	0.0489 (16)	0.0517 (16)	0.0027 (12)	−0.0017 (12)	0.0084 (13)
C2	0.0473 (15)	0.0491 (16)	0.0573 (17)	−0.0008 (13)	−0.0066 (13)	0.0028 (13)
C3	0.0544 (16)	0.0461 (15)	0.0599 (17)	0.0043 (13)	−0.0076 (14)	0.0002 (13)
C4	0.0490 (15)	0.0502 (16)	0.0496 (15)	0.0074 (13)	−0.0050 (13)	0.0008 (13)
C5	0.0488 (15)	0.0525 (16)	0.0479 (15)	0.0018 (13)	−0.0050 (12)	0.0003 (13)
C6	0.0455 (15)	0.0468 (16)	0.0474 (15)	0.0015 (12)	0.0001 (12)	0.0010 (12)
C7	0.0654 (16)	0.0644 (17)	0.0638 (16)	0.0219 (13)	−0.0124 (13)	0.0034 (13)
C8	0.0654 (16)	0.0644 (17)	0.0638 (16)	0.0219 (13)	−0.0124 (13)	0.0034 (13)
C8'	0.094 (4)	0.081 (4)	0.092 (4)	0.032 (3)	−0.023 (3)	−0.020 (3)
C9	0.0654 (16)	0.0644 (17)	0.0638 (16)	0.0219 (13)	−0.0124 (13)	0.0034 (13)
C9'	0.112 (4)	0.129 (5)	0.089 (4)	0.056 (4)	0.012 (4)	0.038 (4)
C10	0.0654 (16)	0.0644 (17)	0.0638 (16)	0.0219 (13)	−0.0124 (13)	0.0034 (13)
C10'	0.072 (4)	0.095 (4)	0.163 (6)	0.022 (3)	−0.039 (4)	−0.001 (4)
C11	0.0601 (18)	0.0444 (16)	0.0517 (17)	0.0007 (13)	0.0001 (14)	−0.0007 (13)
C12	0.085 (2)	0.0534 (19)	0.069 (2)	−0.0085 (17)	0.0026 (19)	0.0078 (16)
C13	0.079 (2)	0.062 (2)	0.070 (2)	0.0080 (18)	0.0105 (19)	−0.0090 (18)
C14	0.076 (2)	0.056 (2)	0.081 (2)	−0.0048 (18)	−0.0125 (19)	−0.0083 (18)
C15	0.0567 (17)	0.0521 (17)	0.0674 (18)	−0.0004 (14)	−0.0126 (15)	0.0029 (15)
C16	0.0470 (16)	0.0616 (18)	0.0589 (17)	0.0021 (14)	−0.0074 (14)	0.0003 (15)
C17	0.0503 (17)	0.089 (2)	0.077 (2)	0.0143 (17)	−0.0123 (16)	−0.0184 (19)
C18	0.064 (2)	0.082 (2)	0.083 (2)	0.0112 (18)	−0.0128 (18)	−0.0247 (19)
C19	0.0508 (17)	0.069 (2)	0.0615 (19)	−0.0052 (15)	−0.0116 (15)	0.0046 (16)
C20	0.0497 (17)	0.071 (2)	0.082 (2)	0.0094 (16)	−0.0143 (17)	−0.0031 (18)
C21	0.0579 (19)	0.065 (2)	0.080 (2)	0.0102 (16)	−0.0149 (17)	−0.0084 (17)

Geometric parameters (Å, °)

Cl1—C19	1.738 (3)	C9'—H9E	0.9600
O1—C1	1.355 (3)	C9'—H9F	0.9600
O1—H1	0.8200	C10—H10A	0.9600
N1—C15	1.273 (4)	C10—H10B	0.9600
N1—C16	1.420 (4)	C10—H10C	0.9600
C1—C6	1.396 (4)	C10'—H10D	0.9600
C1—C2	1.411 (4)	C10'—H10E	0.9600
C2—C3	1.398 (4)	C10'—H10F	0.9600
C2—C15	1.441 (4)	C11—C14	1.523 (5)
C3—C4	1.373 (4)	C11—C13	1.530 (5)
C3—H3	0.9300	C11—C12	1.544 (5)
C4—C5	1.400 (4)	C12—H12A	0.9600
C4—C7	1.538 (4)	C12—H12B	0.9600
C5—C6	1.384 (4)	C12—H12C	0.9600
C5—H5	0.9300	C13—H13A	0.9600
C6—C11	1.541 (4)	C13—H13B	0.9600
C7—C8	1.454 (9)	C13—H13C	0.9600
C7—C9'	1.477 (7)	C14—H14A	0.9600
C7—C10	1.520 (9)	C14—H14B	0.9600
C7—C8'	1.528 (7)	C14—H14C	0.9600
C7—C10'	1.566 (7)	C15—H15	0.9300
C7—C9	1.598 (9)	C16—C17	1.373 (5)
C8—H8A	0.9600	C16—C21	1.385 (4)
C8—H8B	0.9600	C17—C18	1.382 (5)
C8—H8C	0.9600	C17—H17	0.9300
C8'—H8D	0.9600	C18—C19	1.372 (5)
C8'—H8E	0.9600	C18—H18	0.9300
C8'—H8F	0.9600	C19—C20	1.366 (5)
C9—H9A	0.9600	C20—C21	1.378 (5)
C9—H9B	0.9600	C20—H20	0.9300
C9—H9C	0.9600	C21—H21	0.9300
C9'—H9D	0.9600		
C1—O1—H1	109.5	C7—C10—H10B	109.5
C15—N1—C16	119.5 (3)	H10A—C10—H10B	109.5
O1—C1—C6	120.4 (3)	C7—C10—H10C	109.5
O1—C1—C2	119.0 (3)	H10A—C10—H10C	109.5
C6—C1—C2	120.5 (3)	H10B—C10—H10C	109.5
C3—C2—C1	119.0 (3)	C7—C10'—H10D	109.5
C3—C2—C15	118.7 (3)	C7—C10'—H10E	109.5
C1—C2—C15	122.3 (3)	H10D—C10'—H10E	109.5
C4—C3—C2	122.4 (3)	C7—C10'—H10F	109.5
C4—C3—H3	118.8	H10D—C10'—H10F	109.5
C2—C3—H3	118.8	H10E—C10'—H10F	109.5
C3—C4—C5	116.4 (3)	C14—C11—C13	107.7 (3)
C3—C4—C7	121.9 (3)	C14—C11—C6	112.2 (3)
C5—C4—C7	121.8 (3)	C13—C11—C6	109.9 (3)

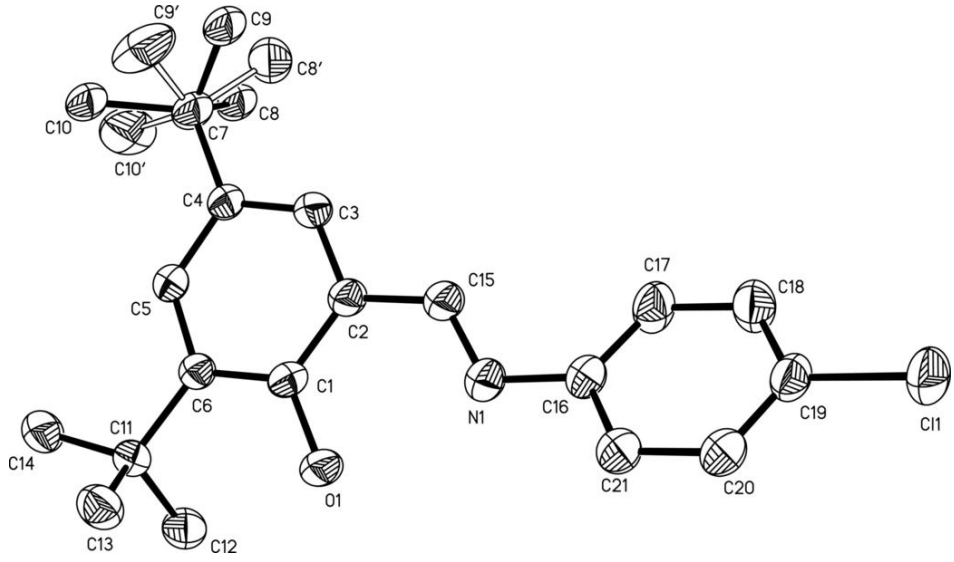
C6—C5—C4	124.6 (3)	C14—C11—C12	107.4 (3)
C6—C5—H5	117.7	C13—C11—C12	110.0 (3)
C4—C5—H5	117.7	C6—C11—C12	109.7 (3)
C5—C6—C1	117.2 (3)	C11—C12—H12A	109.5
C5—C6—C11	121.3 (3)	C11—C12—H12B	109.5
C1—C6—C11	121.5 (3)	H12A—C12—H12B	109.5
C8—C7—C10	117.0 (6)	C11—C12—H12C	109.5
C9'—C7—C8'	110.4 (5)	H12A—C12—H12C	109.5
C8—C7—C4	108.6 (4)	H12B—C12—H12C	109.5
C9'—C7—C4	110.1 (4)	C11—C13—H13A	109.5
C10—C7—C4	111.6 (4)	C11—C13—H13B	109.5
C8'—C7—C4	112.3 (3)	H13A—C13—H13B	109.5
C9'—C7—C10'	110.3 (5)	C11—C13—H13C	109.5
C8'—C7—C10'	103.0 (5)	H13A—C13—H13C	109.5
C4—C7—C10'	110.6 (4)	H13B—C13—H13C	109.5
C8—C7—C9	110.0 (6)	C11—C14—H14A	109.5
C10—C7—C9	103.0 (6)	C11—C14—H14B	109.5
C4—C7—C9	106.1 (4)	H14A—C14—H14B	109.5
C7—C8—H8A	109.5	C11—C14—H14C	109.5
C7—C8—H8B	109.5	H14A—C14—H14C	109.5
H8A—C8—H8B	109.5	H14B—C14—H14C	109.5
C7—C8—H8C	109.5	N1—C15—C2	123.8 (3)
H8A—C8—H8C	109.5	N1—C15—H15	118.1
H8B—C8—H8C	109.5	C2—C15—H15	118.1
C7—C8'—H8D	109.5	C17—C16—C21	118.7 (3)
C7—C8'—H8E	109.5	C17—C16—N1	123.4 (3)
H8D—C8'—H8E	109.5	C21—C16—N1	117.9 (3)
C7—C8'—H8F	109.5	C16—C17—C18	120.7 (3)
H8D—C8'—H8F	109.5	C16—C17—H17	119.6
H8E—C8'—H8F	109.5	C18—C17—H17	119.6
C7—C9—H9A	109.5	C19—C18—C17	119.7 (4)
C7—C9—H9B	109.5	C19—C18—H18	120.2
H9A—C9—H9B	109.5	C17—C18—H18	120.2
C7—C9—H9C	109.5	C20—C19—C18	120.4 (3)
H9A—C9—H9C	109.5	C20—C19—Cl1	120.6 (3)
H9B—C9—H9C	109.5	C18—C19—Cl1	119.0 (3)
C7—C9'—H9D	109.5	C19—C20—C21	119.7 (3)
C7—C9'—H9E	109.5	C19—C20—H20	120.2
H9D—C9'—H9E	109.5	C21—C20—H20	120.2
C7—C9'—H9F	109.5	C20—C21—C16	120.8 (3)
H9D—C9'—H9F	109.5	C20—C21—H21	119.6
H9E—C9'—H9F	109.5	C16—C21—H21	119.6
C7—C10—H10A	109.5		
O1—C1—C2—C3	179.6 (3)	C5—C4—C7—C10'	−28.0 (6)
C6—C1—C2—C3	−0.7 (5)	C3—C4—C7—C9	−39.1 (6)
O1—C1—C2—C15	−2.6 (5)	C5—C4—C7—C9	141.0 (5)
C6—C1—C2—C15	177.1 (3)	C5—C6—C11—C14	0.8 (4)
C1—C2—C3—C4	−0.5 (5)	C1—C6—C11—C14	−178.3 (3)
C15—C2—C3—C4	−178.4 (3)	C5—C6—C11—C13	−119.0 (3)

C2—C3—C4—C5	1.1 (5)	C1—C6—C11—C13	62.0 (4)
C2—C3—C4—C7	−178.8 (3)	C5—C6—C11—C12	120.0 (3)
C3—C4—C5—C6	−0.5 (5)	C1—C6—C11—C12	−59.0 (4)
C7—C4—C5—C6	179.3 (3)	C16—N1—C15—C2	−179.9 (3)
C4—C5—C6—C1	−0.5 (5)	C3—C2—C15—N1	179.7 (3)
C4—C5—C6—C11	−179.6 (3)	C1—C2—C15—N1	1.9 (5)
O1—C1—C6—C5	−179.1 (3)	C15—N1—C16—C17	−29.1 (5)
C2—C1—C6—C5	1.1 (4)	C15—N1—C16—C21	150.7 (3)
O1—C1—C6—C11	0.0 (4)	C21—C16—C17—C18	−0.4 (6)
C2—C1—C6—C11	−179.8 (3)	N1—C16—C17—C18	179.4 (4)
C3—C4—C7—C8	79.1 (6)	C16—C17—C18—C19	−0.3 (7)
C5—C4—C7—C8	−100.8 (6)	C17—C18—C19—C20	0.6 (6)
C3—C4—C7—C9'	−86.0 (6)	C17—C18—C19—Cl1	−179.8 (3)
C5—C4—C7—C9'	94.2 (6)	C18—C19—C20—C21	0.0 (6)
C3—C4—C7—C10	−150.5 (6)	Cl1—C19—C20—C21	−179.7 (3)
C5—C4—C7—C10	29.6 (6)	C19—C20—C21—C16	−0.7 (6)
C3—C4—C7—C8'	37.4 (6)	C17—C16—C21—C20	1.0 (6)
C5—C4—C7—C8'	−142.4 (5)	N1—C16—C21—C20	−178.9 (3)
C3—C4—C7—C10'	151.9 (5)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.88	2.615 (4)	150

Fig. 1


C9′
C9
C8′
C10
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C3
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C18
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C6
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C16
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Cl1
C11
C14
O1
C21
C20
C13
C12