

N-[(*R*)-(2-Chlorophenyl)(cyclopentyl)-methyl]-*N*-[(*R*)-(2-hydroxy-5-methylphenyl)(phenyl)methyl]acetamide

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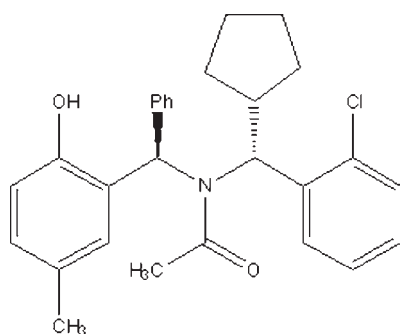
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.008$ Å; R factor = 0.060; wR factor = 0.186; data-to-parameter ratio = 15.4.

In the title compound, $\text{C}_{28}\text{H}_{30}\text{ClNO}_2$, the cyclopentane ring adopts an envelope conformation. In the crystal structure, molecules are linked by intermolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds, forming chains running along the a axis.

Related literature

For general background to amides, see: Calligaris *et al.* (1972); Ali *et al.* (2002); Cukurovali *et al.* (2002); Sriram *et al.* (2006); Kargar *et al.* (2009); Takenaka *et al.* (2002); Varlamov *et al.* (2003); Zhang *et al.* (2003). For the synthesis, see: Yang *et al.* (2005).



Experimental

Crystal data

$\text{C}_{28}\text{H}_{30}\text{ClNO}_2$

$M_r = 447.98$

Orthorhombic, $P2_12_12_1$

$a = 8.8038$ (8) Å

$b = 11.3417$ (10) Å

$c = 25.485$ (2) Å

$V = 2544.7$ (4) Å³

$Z = 4$

Mo $K\alpha$ radiation
 $\mu = 0.17$ mm⁻¹

$T = 298$ K
 $0.24 \times 0.16 \times 0.12$ mm

Data collection

Bruker SMART CCD area-detector diffractometer

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.960$, $T_{\max} = 0.980$

13334 measured reflections
4452 independent reflections
2845 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.034$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.060$

$wR(F^2) = 0.186$

$S = 1.05$

4452 reflections

290 parameters

H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.33$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.37$ e Å⁻³

Absolute structure: Flack (1983),

1871 Friedel pairs

Flack parameter: 0.04 (16)

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1}-\text{H1}\cdots\text{O2}^i$	0.82	1.82	2.637 (3)	172

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

Data collection: SMART (Bruker, 1999); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2646).

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supplementary materials

Acta Cryst. (2009). E65, o2948 [doi:10.1107/S1600536809044808]

***N*-[(*R*)-(2-Chlorophenyl)(cyclopentyl)methyl]-*N*-[(*R*)-(2-hydroxy-5-methylphenyl)(phenyl)methyl]acetamide**

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Comment

The Schiff base compounds have been widely used in organic and bioinorganic chemistry due to their significant biological activities (Ali *et al.*, 2002; Sriram *et al.*, 2006; Cukurovali *et al.*, 2002). These compounds have also been used as versatile ligands in coordination chemistry (Kargar *et al.*, 2009; Calligaris *et al.*, 1972). Therefore, the design and synthesis of Schiff bases with various functionalities has become an important field of research nowadays (Takenaka *et al.*, 2002; Varlamov *et al.*, 2003; Zhang *et al.*, 2003). As part of our continuing research of Schiff bases, we report the crystal structure of the title compound, which was acetylated from the corresponding aminophenol.

As shown in Fig. 1, the configuration at the new chiral center (C8) is *R*. The C9—C14 and C18—C23 aromatic rings are approximately vertical, the dihedral angle between their planes being 83.59 (17)°; the dihedral angle between the planes of the C1—C6 and C18—C23 aromatic rings is 17.45 (19)°, while that between the C1—C6 and C9—C14 planes is 78.89 (16)°. The intermolecular O1—H1...O2 hydrogen-bonding interactions are present in the crystal packing (Table 1 and Fig. 2).

Experimental

The chiral aminophenol was prepared by a condensation reaction of (*R*)-1-(2-chlorophenyl)-1-cyclopentylmethanamine and (2-hydroxy-5-methylphenyl)(phenyl)methanone followed by reduction with NaBH₄. The detailed procedure is similar to that reported by Yang *et al.* (2005). Then the aminophenol was reacted with acetic anhydride (5 equivalents) in a THF solution (10 ml) at room temperature for 12 h to obtain the title compound. After removal of the solvent, water (20 ml) was added to the residue, stirred and filtrated. Further purification of the filter cake was carried out by thin-layer silica-gel chromatography (chloroform) to give a colorless solid (yield 70.1%). Single crystals of the title compound suitable for X-ray analysis were obtained by slow evaporation of the n-hexane/ethyl acetate solution (3:2 v/v).

Refinement

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93–0.98 Å and O—H = 0.82 Å, and refined in riding mode with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C}, \text{O})$ for methyl H atoms and hydroxy-H atoms, and $1.2U_{\text{eq}}(\text{C})$ for the others.

Figures

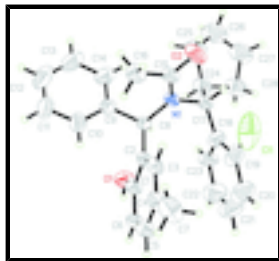


Fig. 1. The structure of the title compound with 30% probability ellipsoids. H atoms are shown as spheres of arbitrary radii.

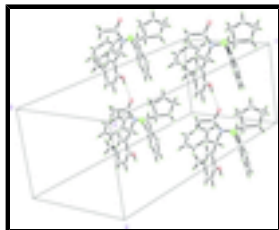


Fig. 2. A packing diagram of (I), dashed lines represent hydrogen bonding.

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Orthorhombic, $P2_12_12_1$

Hall symbol: P 2ac 2ab

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$b = 11.3417$ (10) Å

$c = 25.485$ (2) Å

$V = 2544.7$ (4) Å³

$Z = 4$

$F_{000} = 952$

$D_x = 1.169$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2267 reflections

$\theta = 2.5$ – 19.1°

$\mu = 0.17$ mm⁻¹

$T = 298$ K

Block, colourless

$0.24 \times 0.16 \times 0.12$ mm

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298$ K

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.960$, $T_{\max} = 0.980$

13334 measured reflections

4452 independent reflections

2845 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.034$

$\theta_{\text{max}} = 25.1^\circ$

$\theta_{\text{min}} = 2.0^\circ$

$h = -7 \rightarrow 10$

$k = -12 \rightarrow 13$

$l = -26 \rightarrow 30$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.060$	$w = 1/[\sigma^2(F_o^2) + (0.1097P)^2]$
$wR(F^2) = 0.186$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{\max} < 0.001$
4452 reflections	$\Delta\rho_{\max} = 0.33 \text{ e } \text{\AA}^{-3}$
290 parameters	$\Delta\rho_{\min} = -0.36 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none
Secondary atom site location: difference Fourier map	Absolute structure: Flack (1983), 1871 Friedel pairs
	Flack parameter: 0.04 (16)

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	0.8441 (4)	1.17857 (19)	0.06402 (7)	0.1811 (11)
O1	0.2924 (3)	0.8872 (3)	0.12767 (13)	0.0864 (9)
H1	0.2020	0.9041	0.1256	0.130*
O2	1.0028 (3)	0.9464 (3)	0.13070 (14)	0.0927 (10)
N1	0.7501 (3)	0.9350 (2)	0.13768 (11)	0.0520 (7)
C1	0.3627 (4)	0.9125 (3)	0.08087 (15)	0.0626 (9)
C2	0.5208 (3)	0.9060 (3)	0.08034 (14)	0.0536 (9)
C3	0.5941 (4)	0.9335 (3)	0.03418 (15)	0.0628 (10)
H3	0.6996	0.9297	0.0333	0.075*
C4	0.5179 (5)	0.9666 (4)	-0.01089 (15)	0.0746 (12)
C5	0.3620 (6)	0.9721 (4)	-0.00895 (17)	0.0834 (13)
H5	0.3081	0.9942	-0.0387	0.100*
C6	0.2852 (4)	0.9457 (4)	0.03610 (19)	0.0769 (12)
H6	0.1797	0.9501	0.0366	0.092*
C7	0.6058 (8)	0.9962 (6)	-0.06040 (18)	0.125 (2)
H7A	0.6982	0.9512	-0.0613	0.188*
H7B	0.6297	1.0788	-0.0607	0.188*

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H7C	0.5453	0.9773	-0.0906	0.188*
C8	0.6007 (3)	0.8750 (3)	0.13155 (14)	0.0512 (8)
H8	0.5365	0.9094	0.1590	0.061*
C9	0.6029 (4)	0.7431 (4)	0.14369 (18)	0.0672 (11)
C10	0.5359 (5)	0.6629 (4)	0.1108 (3)	0.0967 (16)
H10	0.4909	0.6891	0.0799	0.116*
C11	0.5336 (7)	0.5430 (5)	0.1227 (4)	0.127 (2)
H11	0.4850	0.4906	0.1003	0.152*
C12	0.6012 (8)	0.5029 (6)	0.1664 (4)	0.135 (3)
H12	0.6032	0.4224	0.1733	0.162*
C13	0.6684 (7)	0.5812 (6)	0.2016 (3)	0.121 (2)
H13	0.7133	0.5534	0.2322	0.146*
C14	0.6677 (5)	0.7034 (5)	0.1903 (2)	0.0923 (14)
H14	0.7102	0.7568	0.2139	0.111*
C15	0.8845 (4)	0.8931 (4)	0.12091 (16)	0.0655 (10)
C16	0.8935 (4)	0.7808 (4)	0.0899 (2)	0.0860 (14)
H16A	0.9720	0.7875	0.0639	0.129*
H16B	0.7979	0.7666	0.0729	0.129*
H16C	0.9162	0.7163	0.1130	0.129*
C17	0.7476 (4)	1.0531 (3)	0.16311 (13)	0.0566 (8)
H17	0.8468	1.0892	0.1564	0.068*
C18	0.6322 (6)	1.1299 (4)	0.13737 (15)	0.0781 (12)
C19	0.6669 (10)	1.1861 (4)	0.0904 (2)	0.127 (2)
C20	0.5516 (12)	1.2498 (6)	0.0618 (3)	0.149 (2)
H20	0.5730	1.2880	0.0304	0.179*
C21	0.4125 (12)	1.2510 (7)	0.0828 (4)	0.156 (3)
H21	0.3363	1.2890	0.0640	0.187*
C22	0.3740 (9)	1.2019 (6)	0.1287 (4)	0.152 (3)
H22	0.2755	1.2079	0.1416	0.182*
C23	0.4846 (6)	1.1424 (5)	0.1564 (3)	0.1053 (17)
H23	0.4599	1.1095	0.1887	0.126*
C24	0.7295 (5)	1.0460 (4)	0.22294 (17)	0.0842 (12)
H24	0.6317	1.0095	0.2316	0.101*
C25	0.8582 (7)	0.9781 (6)	0.24986 (19)	0.1152 (16)
H25A	0.8233	0.8997	0.2591	0.138*
H25B	0.9432	0.9701	0.2259	0.138*
C26	0.9037 (9)	1.0362 (7)	0.2938 (3)	0.150 (2)
H26A	1.0137	1.0356	0.2958	0.180*
H26B	0.8646	0.9959	0.3246	0.180*
C27	0.8506 (8)	1.1554 (7)	0.2936 (2)	0.1364 (19)
H27A	0.9355	1.2091	0.2893	0.164*
H27B	0.8008	1.1733	0.3266	0.164*
C28	0.7391 (7)	1.1699 (5)	0.24837 (19)	0.1022 (14)
H28A	0.7759	1.2276	0.2233	0.123*
H28B	0.6404	1.1948	0.2611	0.123*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.303 (3)	0.1376 (15)	0.1031 (11)	-0.0737 (18)	0.0624 (16)	0.0110 (10)
O1	0.0368 (13)	0.119 (3)	0.103 (2)	0.0043 (13)	0.0143 (14)	0.021 (2)
O2	0.0339 (12)	0.114 (2)	0.130 (3)	-0.0049 (14)	0.0073 (15)	-0.034 (2)
N1	0.0335 (12)	0.0595 (17)	0.0629 (16)	0.0023 (12)	-0.0005 (13)	-0.0064 (13)
C1	0.0391 (18)	0.074 (2)	0.075 (2)	-0.0015 (17)	0.0032 (18)	0.0019 (19)
C2	0.0383 (17)	0.056 (2)	0.067 (2)	-0.0048 (14)	0.0028 (15)	-0.0060 (16)
C3	0.053 (2)	0.071 (2)	0.065 (2)	-0.0095 (17)	0.0037 (18)	-0.0108 (18)
C4	0.080 (3)	0.084 (3)	0.060 (2)	-0.031 (2)	0.003 (2)	-0.009 (2)
C5	0.091 (3)	0.087 (3)	0.071 (3)	-0.012 (3)	-0.024 (3)	-0.003 (2)
C6	0.049 (2)	0.088 (3)	0.093 (3)	-0.0030 (19)	-0.020 (2)	-0.005 (2)
C7	0.149 (5)	0.164 (6)	0.063 (3)	-0.065 (4)	0.003 (3)	0.010 (3)
C8	0.0328 (15)	0.057 (2)	0.064 (2)	0.0000 (13)	0.0049 (15)	0.0002 (16)
C9	0.0408 (17)	0.060 (2)	0.101 (3)	-0.0027 (16)	0.0080 (19)	0.008 (2)
C10	0.073 (3)	0.066 (3)	0.151 (5)	-0.008 (2)	0.007 (3)	-0.002 (3)
C11	0.109 (4)	0.060 (3)	0.212 (7)	-0.004 (3)	0.001 (5)	-0.004 (4)
C12	0.109 (5)	0.074 (4)	0.221 (8)	0.019 (4)	0.044 (5)	0.028 (5)
C13	0.103 (4)	0.103 (5)	0.157 (6)	0.023 (4)	0.021 (4)	0.058 (5)
C14	0.075 (3)	0.093 (4)	0.109 (3)	0.009 (2)	0.010 (3)	0.030 (3)
C15	0.0380 (19)	0.079 (3)	0.080 (2)	0.0035 (18)	0.0028 (17)	-0.008 (2)
C16	0.049 (2)	0.093 (3)	0.116 (3)	0.013 (2)	0.022 (2)	-0.024 (3)
C17	0.0516 (18)	0.060 (2)	0.058 (2)	0.0015 (18)	-0.0008 (17)	-0.0073 (16)
C18	0.113 (3)	0.055 (2)	0.066 (2)	0.020 (2)	-0.028 (2)	-0.0157 (19)
C19	0.227 (6)	0.063 (3)	0.091 (3)	0.020 (4)	-0.053 (4)	-0.011 (3)
C20	0.237 (7)	0.098 (4)	0.111 (4)	0.032 (5)	-0.063 (5)	-0.011 (3)
C21	0.215 (7)	0.099 (4)	0.153 (6)	0.060 (5)	-0.088 (6)	-0.031 (4)
C22	0.152 (5)	0.115 (5)	0.187 (6)	0.066 (4)	-0.051 (5)	-0.060 (4)
C23	0.085 (3)	0.088 (3)	0.143 (4)	0.044 (3)	-0.048 (3)	-0.046 (3)
C24	0.082 (3)	0.106 (3)	0.065 (2)	0.003 (2)	-0.019 (2)	-0.016 (2)
C25	0.129 (4)	0.132 (4)	0.084 (3)	0.010 (3)	-0.048 (3)	-0.006 (3)
C26	0.147 (4)	0.177 (5)	0.126 (4)	0.022 (4)	-0.053 (3)	-0.028 (4)
C27	0.133 (4)	0.156 (4)	0.120 (3)	0.000 (4)	-0.044 (3)	-0.042 (3)
C28	0.102 (3)	0.126 (3)	0.078 (3)	0.010 (3)	-0.015 (3)	-0.037 (3)

Geometric parameters (\AA , $^\circ$)

C11—C19	1.701 (9)	C14—H14	0.9300
O1—C1	1.374 (5)	C15—C16	1.501 (6)
O1—H1	0.8200	C16—H16A	0.9600
O2—C15	1.230 (4)	C16—H16B	0.9600
N1—C15	1.345 (4)	C16—H16C	0.9600
N1—C17	1.488 (4)	C17—C18	1.490 (5)
N1—C8	1.489 (4)	C17—C24	1.535 (6)
C1—C6	1.382 (6)	C17—H17	0.9800
C1—C2	1.394 (5)	C18—C19	1.391 (8)
C2—C3	1.377 (5)	C18—C23	1.394 (7)

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C2—C8	1.524 (5)	C19—C20	1.443 (9)
C3—C4	1.382 (6)	C20—C21	1.337 (12)
C3—H3	0.9300	C20—H20	0.9300
C4—C5	1.374 (7)	C21—C22	1.340 (11)
C4—C7	1.518 (6)	C21—H21	0.9300
C5—C6	1.366 (6)	C22—C23	1.379 (9)
C5—H5	0.9300	C22—H22	0.9300
C6—H6	0.9300	C23—H23	0.9300
C7—H7A	0.9600	C24—C25	1.532 (7)
C7—H7B	0.9600	C24—C28	1.550 (7)
C7—H7C	0.9600	C24—H24	0.9800
C8—C9	1.528 (5)	C25—C26	1.361 (8)
C8—H8	0.9800	C25—H25A	0.9700
C9—C10	1.370 (7)	C25—H25B	0.9700
C9—C14	1.394 (6)	C26—C27	1.430 (10)
C10—C11	1.393 (8)	C26—H26A	0.9700
C10—H10	0.9300	C26—H26B	0.9700
C11—C12	1.343 (11)	C27—C28	1.523 (8)
C11—H11	0.9300	C27—H27A	0.9700
C12—C13	1.394 (10)	C27—H27B	0.9700
C12—H12	0.9300	C28—H28A	0.9700
C13—C14	1.415 (8)	C28—H28B	0.9700
C13—H13	0.9300		
C1—O1—H1	109.5	C15—C16—H16C	109.5
C15—N1—C17	118.0 (3)	H16A—C16—H16C	109.5
C15—N1—C8	125.6 (3)	H16B—C16—H16C	109.5
C17—N1—C8	116.3 (2)	N1—C17—C18	110.2 (3)
O1—C1—C6	123.5 (3)	N1—C17—C24	112.8 (3)
O1—C1—C2	116.6 (3)	C18—C17—C24	113.4 (3)
C6—C1—C2	119.9 (4)	N1—C17—H17	106.7
C3—C2—C1	117.7 (3)	C18—C17—H17	106.7
C3—C2—C8	124.6 (3)	C24—C17—H17	106.7
C1—C2—C8	117.7 (3)	C19—C18—C23	117.2 (5)
C2—C3—C4	122.9 (3)	C19—C18—C17	119.8 (5)
C2—C3—H3	118.5	C23—C18—C17	122.8 (4)
C4—C3—H3	118.5	C18—C19—C20	120.6 (8)
C5—C4—C3	117.9 (4)	C18—C19—C11	121.2 (5)
C5—C4—C7	122.0 (4)	C20—C19—C11	118.1 (6)
C3—C4—C7	120.2 (4)	C21—C20—C19	116.6 (8)
C6—C5—C4	121.0 (4)	C21—C20—H20	121.7
C6—C5—H5	119.5	C19—C20—H20	121.7
C4—C5—H5	119.5	C20—C21—C22	125.2 (8)
C5—C6—C1	120.6 (4)	C20—C21—H21	117.4
C5—C6—H6	119.7	C22—C21—H21	117.4
C1—C6—H6	119.7	C21—C22—C23	118.2 (8)
C4—C7—H7A	109.5	C21—C22—H22	120.9
C4—C7—H7B	109.5	C23—C22—H22	120.9
H7A—C7—H7B	109.5	C22—C23—C18	122.0 (7)
C4—C7—H7C	109.5	C22—C23—H23	119.0

H7A—C7—H7C	109.5	C18—C23—H23	119.0
H7B—C7—H7C	109.5	C25—C24—C17	113.2 (4)
N1—C8—C2	113.1 (3)	C25—C24—C28	103.2 (4)
N1—C8—C9	114.5 (3)	C17—C24—C28	111.2 (4)
C2—C8—C9	113.9 (3)	C25—C24—H24	109.7
N1—C8—H8	104.6	C17—C24—H24	109.7
C2—C8—H8	104.6	C28—C24—H24	109.7
C9—C8—H8	104.6	C26—C25—C24	110.1 (5)
C10—C9—C14	118.9 (4)	C26—C25—H25A	109.6
C10—C9—C8	121.4 (4)	C24—C25—H25A	109.6
C14—C9—C8	119.6 (4)	C26—C25—H25B	109.6
C9—C10—C11	121.4 (6)	C24—C25—H25B	109.6
C9—C10—H10	119.3	H25A—C25—H25B	108.2
C11—C10—H10	119.3	C25—C26—C27	111.0 (6)
C12—C11—C10	120.3 (7)	C25—C26—H26A	109.4
C12—C11—H11	119.8	C27—C26—H26A	109.4
C10—C11—H11	119.8	C25—C26—H26B	109.4
C11—C12—C13	120.4 (6)	C27—C26—H26B	109.4
C11—C12—H12	119.8	H26A—C26—H26B	108.0
C13—C12—H12	119.8	C26—C27—C28	108.4 (5)
C12—C13—C14	119.5 (6)	C26—C27—H27A	110.0
C12—C13—H13	120.3	C28—C27—H27A	110.0
C14—C13—H13	120.3	C26—C27—H27B	110.0
C9—C14—C13	119.4 (6)	C28—C27—H27B	110.0
C9—C14—H14	120.3	H27A—C27—H27B	108.4
C13—C14—H14	120.3	C27—C28—C24	104.7 (4)
O2—C15—N1	120.4 (3)	C27—C28—H28A	110.8
O2—C15—C16	118.6 (3)	C24—C28—H28A	110.8
N1—C15—C16	120.9 (3)	C27—C28—H28B	110.8
C15—C16—H16A	109.5	C24—C28—H28B	110.8
C15—C16—H16B	109.5	H28A—C28—H28B	108.9
H16A—C16—H16B	109.5		
O1—C1—C2—C3	-178.6 (3)	C8—N1—C15—O2	-175.7 (4)
C6—C1—C2—C3	-0.1 (5)	C17—N1—C15—C16	-173.5 (4)
O1—C1—C2—C8	-1.6 (5)	C8—N1—C15—C16	4.4 (6)
C6—C1—C2—C8	176.9 (3)	C15—N1—C17—C18	127.5 (4)
C1—C2—C3—C4	-0.1 (6)	C8—N1—C17—C18	-50.6 (4)
C8—C2—C3—C4	-176.9 (3)	C15—N1—C17—C24	-104.7 (4)
C2—C3—C4—C5	0.1 (6)	C8—N1—C17—C24	77.2 (4)
C2—C3—C4—C7	179.8 (4)	N1—C17—C18—C19	-80.3 (5)
C3—C4—C5—C6	0.0 (7)	C24—C17—C18—C19	152.2 (4)
C7—C4—C5—C6	-179.7 (5)	N1—C17—C18—C23	95.1 (4)
C4—C5—C6—C1	-0.1 (7)	C24—C17—C18—C23	-32.4 (5)
O1—C1—C6—C5	178.6 (4)	C23—C18—C19—C20	-2.8 (7)
C2—C1—C6—C5	0.2 (6)	C17—C18—C19—C20	172.9 (5)
C15—N1—C8—C2	-89.0 (4)	C23—C18—C19—C11	179.0 (4)
C17—N1—C8—C2	88.9 (3)	C17—C18—C19—C11	-5.3 (6)
C15—N1—C8—C9	43.7 (5)	C18—C19—C20—C21	-0.2 (9)
C17—N1—C8—C9	-138.3 (3)	C11—C19—C20—C21	178.1 (6)

supplementary materials

C3—C2—C8—N1	30.9 (5)	C19—C20—C21—C22	2.6 (12)
C1—C2—C8—N1	-145.9 (3)	C20—C21—C22—C23	-1.8 (12)
C3—C2—C8—C9	-102.2 (4)	C21—C22—C23—C18	-1.5 (9)
C1—C2—C8—C9	81.0 (4)	C19—C18—C23—C22	3.7 (7)
N1—C8—C9—C10	-133.2 (4)	C17—C18—C23—C22	-171.8 (5)
C2—C8—C9—C10	-0.9 (5)	N1—C17—C24—C25	60.2 (5)
N1—C8—C9—C14	49.9 (5)	C18—C17—C24—C25	-173.7 (4)
C2—C8—C9—C14	-177.7 (3)	N1—C17—C24—C28	175.9 (3)
C14—C9—C10—C11	-1.1 (7)	C18—C17—C24—C28	-58.1 (5)
C8—C9—C10—C11	-177.9 (4)	C17—C24—C25—C26	136.6 (6)
C9—C10—C11—C12	-1.7 (9)	C28—C24—C25—C26	16.2 (7)
C10—C11—C12—C13	2.9 (10)	C24—C25—C26—C27	-16.4 (10)
C11—C12—C13—C14	-1.4 (10)	C25—C26—C27—C28	9.3 (10)
C10—C9—C14—C13	2.6 (7)	C26—C27—C28—C24	1.3 (8)
C8—C9—C14—C13	179.5 (4)	C25—C24—C28—C27	-9.9 (6)
C12—C13—C14—C9	-1.4 (8)	C17—C24—C28—C27	-131.6 (5)
C17—N1—C15—O2	6.4 (5)		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1 \cdots O2 ⁱ	0.82	1.82	2.637 (3)	172

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

Fig. 1

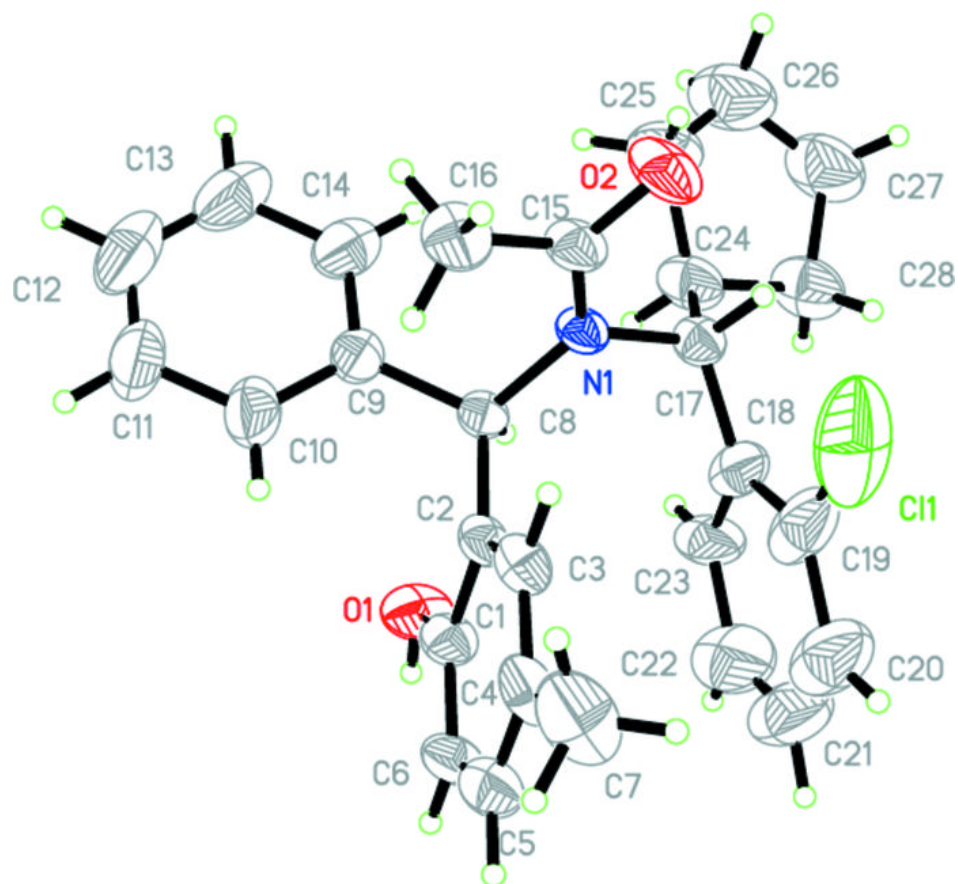


Fig. 2

