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Crystal structure and Hirshfeld surface analysis of (*Z*)-2-{[(2,4-dimethylphenyl)imino]methyl}-4-methylphenol

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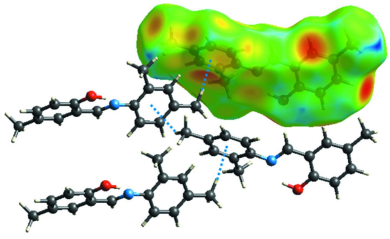
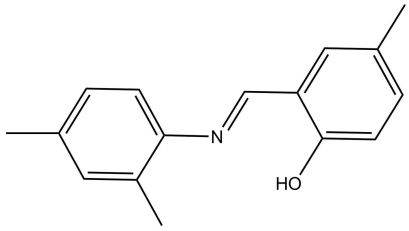
The title compound, $C_{16}H_{17}NO$, is a Schiff base that exists in the enol–imine tautomeric form and adopts a *Z* configuration. The molecule is non-planar, with the twisted rings making a dihedral angle of 39.92 (4)°. The intramolecular O—H···N hydrogen bond forms an *S*(6) ring motif. In the crystal, molecules are linked by C—H···π interactions and very weak π-π stacking interactions also help to consolidate the crystal packing. A Hirshfeld surface analysis was performed to investigate the contributions of different intermolecular contacts within the supramolecular structure. The major contributions are from H···H (65%), C···H (19.2%) and O···H (6.6%) interactions.

1. Chemical context

Schiff bases are well-known organic compounds widely used in many areas. These compounds can be easily synthesized by condensation of a primary aliphatic or aromatic amine with an aldehyde or ketone in different solvent media and they can easily be purified, since the amount of by-products is negligible (Tanak *et al.*, 2020). Schiff bases are in general more stable than the compounds from which they are synthesized (Wadher *et al.*, 2009). Nowadays, the possibility of molecular design is an important key for many research areas such as medicine or agriculture. In this respect, Schiff base formation provides an easy way to design new compounds, and biologically or chemically active compounds can be obtained using this method. As the structures of Schiff bases are generally similar to those of biological molecules, Schiff bases are valuable for understanding biological phenomena. As a result, Schiff bases are used in many studies. Various types of aldehydes or ketones have been used for their synthesis, but 2-hydroxybenzaldehyde and its derivatives are used especially often (Jeewoth *et al.*, 2000; Mazhar *et al.*, 2020). The basis of such preference is the tautomerism and stability provided by the hydroxyl group in conjunction with the imine group. Schiff bases with intramolecular hydrogen bonds can exhibit photochromic and thermochromic properties (Elerman *et al.*, 2002). Schiff bases obtained from 2-hydroxybenzaldehyde and its derivatives can also form complexes with various metal ions. The title compound is a Schiff base prepared from 2-hydroxy-5-methylbenzaldehyde.





2. Structural commentary

The title compound crystallizes in the phenol–imine tautomeric form with an *Z* configuration with respect to the imine bond. The asymmetric unit contains one molecule (Fig. 1), which is non-planar, two aromatic rings being twisted with respect to each other, subtending a dihedral angle of 39.92 (4)°. The hydroxy and imine groups are involved in a strong intramolecular O1—H1···N1 hydrogen bond forming an *S*(6) ring motif. The C1—O1 [1.353 (2) Å] and C7—N1 [1.282 (2) Å] bond distances indicate their single- and double-bond characters, respectively, being consistent with the phenol–imine tautomeric form.

3. Supramolecular features

In the crystal, molecules are linked by C16—H16*A*···π (C9–C14) interactions (Table 1, Fig. 2), and very weak π–π stacking interactions between the OH-substituted rings (C1–C6) related by the *a* glide plane [$Cg\cdots Cg$ ($-\frac{1}{2}+x$, y, $\frac{1}{2}-z$) = 4.0220 (9) Å] lead to additional stabilization of the crystal packing. A view of the crystal packing parallel to the *bc* plane is shown in Fig. 2.

4. Database survey

A search of the Cambridge Structural Database (CSD, version 5.42, update of May 2021; Groom *et al.*, 2016) for the (*Z*)-2-{[(2,4-dimethylphenyl)imino]methyl}-4-methylphenol unit, revealed ten hits where this fragment adopts the enol–imine tautomeric form. The imine bond length (N1—C7) in the title compound is the same within standard uncertainties as the corresponding bond lengths in the structures of 2-(diphenylmethyl)-6-[(mesitylimino)methyl]-4-methylphenol (DEHQIS; Zhou *et al.*, 2012), (*R*)-*N*,*N*′-bis(3,5-di-*t*-butylsalicylidene)-5,5′,6,6′,7,7′,8,8′-octahydro-1,1′-binaphthyl-2,2′-diamine (MIFXAA; Jia *et al.*, 2002), acetonitrile-bis{2-(mesitylcarbonoimidoyl)-6-[(mesitylimino)methyl]-4-methylphenolato}magnesium acetonitrile solvate (QUDZAS; Ghosh *et al.*, 2015), bis{2,4-di-*t*-butyl-6-[(mesitylimino)methyl]phenolato}tetrahydrofuranmagnesium (QUDZIA; Ghosh *et al.*, 2015) and 2,4-di-*t*-butyl-6-{[(2,4,6-tri-*t*-butylphenyl)imino]methyl}phenol (YADZOV; Ma *et al.*, 2016). As for the C1—O1 bond [1.353 (2) Å], its length compares well with 1.352 (2) Å for YADZOV and 1.359 (5) Å for DEHQIS. All other bond dimensions in the title structure agree well with those in previous literature reports. In NUGWES, NUGWIW and NUGWOC (Xu *et al.*, 2009) and in YADZOV (Ma *et al.*, 2016), the lengths of intramolecular O—H···N hydrogen bonds are especially short, being within the range 1.81–1.88 Å.

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

*Cg*2 is the centroid of the C9–C14 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.89	2.618 (2)	147
C16—H16*A*···*Cg*2^{i}	0.96	2.93 (3)	3.73	143

Symmetry code: (i) $x+\frac{1}{2}$, $-y+\frac{1}{2}$, $-z$.

5. Hirshfeld surface analysis

We have performed a Hirshfeld surface analysis and generated the associated two-dimensional fingerprint plots (Spackman & Jayatilaka, 2009) with *CrystalExplorer17* (Turner *et al.*, 2017). Hirshfeld surface analysis is an important way of determining the location of atoms with potential to form hydrogen bonds and other intermolecular contacts, and the quantitative ratio of these interactions (Demircioğlu *et al.*, 2019). The Hirshfeld

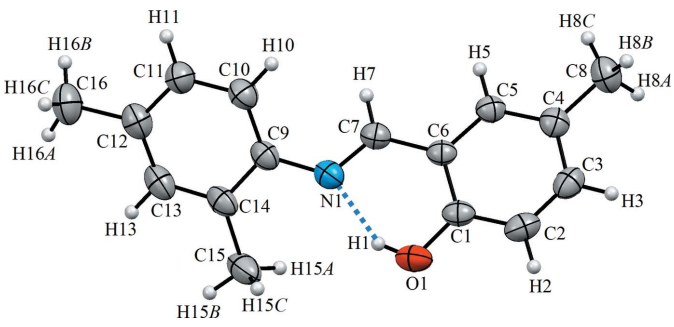


Figure 1
The molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 40% probability level. Dashed lines denote the intramolecular O—H···N hydrogen bond forming an *S*(6) ring motif.

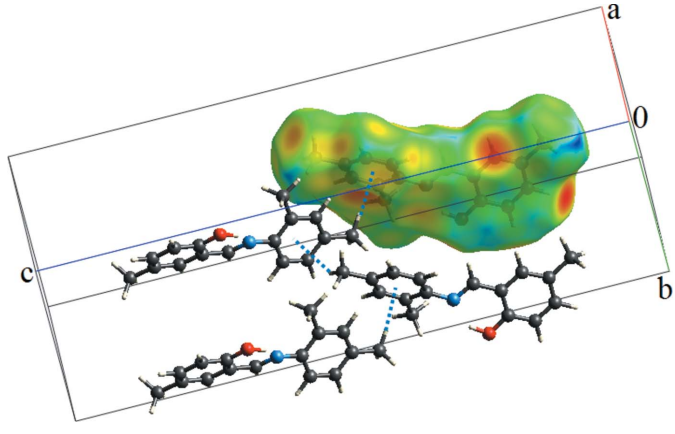


Figure 2
A view of the crystal packing of the title compound. The C16—H16*A*···*Cg*2 interactions are denoted as dashed lines and as a red spot on the d_e surface.

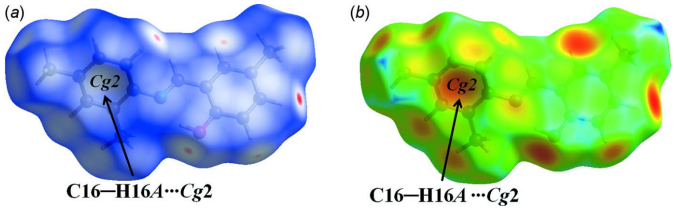


Figure 3
The red spots on the d_{norm} *and* d_e surfaces of the title molecule represent the C—H···π interactions.

surface was generated using a standard (high) surface resolution with the three-dimensional d_{norm} surface mapped over a fixed colour scale of −0.1168 (red) to 1.1632 Å (blue) (the fixed colour scale is 1.0201 to 2.4894 Å for the d_e surface). In Figs. 2 and 3, the red spots on the d_{norm} and d_e surfaces represent the C—H···*Cg* interactions. The most important interaction is H···H, contributing 65% to the overall crystal packing, which is illustrated in the 2D fingerprint (Fig. 4). Two symmetrical wings on the left and right sides are seen in the fingerprint plot for C···H/H···C interactions, the second most important contributor to the total Hirshfeld surface (19%). The O···H/H···O interactions provide a 6.6% contribution to the total Hirshfeld surface. Much weaker C···C (5.3%), N···H/H···N (2.3%) and C···O/O···C (1.3%) contacts are also present.

6. Synthesis and crystallization

(*Z*)-2-{[(2,4-dimethylphenyl)imino]methyl}-4-methylphenol was synthesized by condensation of 2-hydroxy-5-methylbenzaldehyde and 2,4-dimethylaniline (Fig. 5). For this purpose, a mixture of a solution containing 2-hydroxy-5-methylbenzaldehyde (0.04 mmol) in ethanol (20 mL) and a solution containing 2,4-dimethylaniline (0.04 mmol) in ethanol (20 mL) was refluxed for 6 h under stirring. The obtained crystalline product was washed with ethanol and dried at room temperature. Single crystals were obtained by slow evaporation of ethanol solution at room temperature.

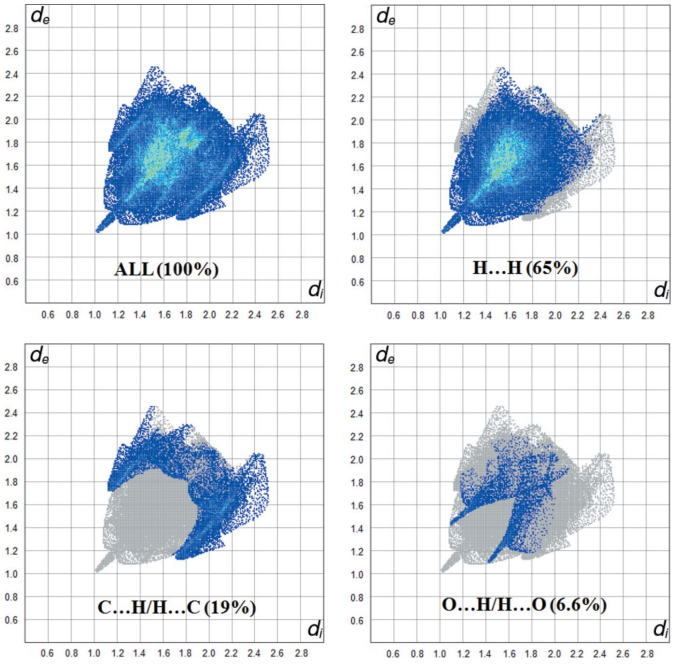


Figure 4
Fingerprint plots showing all intermolecular interactions and resolved into H···H, C···H/H···C and O···H/H···O contacts.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{17}NO$
M_r	239.30
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	296
a, *b*, *c* (Å)	7.6699 (4), 11.6080 (6), 30.1431 (17)
V (Å^3)	2683.7 (2)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.07
Crystal size (mm)	0.68 × 0.48 × 0.18
Data collection	
Diffractometer	Stoe IPDS 2
Absorption correction	Integration (*X-RED32*; Stoe & Cie, 2002)
T_{min}, T_{max}	0.953, 0.990
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14869, 2213, 1451
R_{int}	0.081
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.583
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.042, 0.125, 1.00
No. of reflections	2213
No. of parameters	168
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.11, −0.11

Computer programs: *X-AREA* (Stoe & Cie, 2002), *X-RED* (Stoe & Cie, 2002), *SHELXT2017/1* (Sheldrick, 2015*a*), *SHELXL2017/1* (Sheldrick, 2015*b*), *PLATON* (Spek, 2020), *WinGX* (Farrugia, 2012).

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The O-bound H atom was located in a difference-Fourier map and refined with O—H = 0.82 Å, and with U_{iso}(H) = 1.5U_{eq}(O). The C-bound H atoms were positioned geometrically and refined using a riding model with C—H = 0.93 and U_{iso}(H) = 1.2U_{eq}(C) for sp^2-hybridized C atoms and with C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl groups.

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Author contributions are as follows. Conceptualization, SK, ND and ES; synthesis, AG and EA; writing (review and

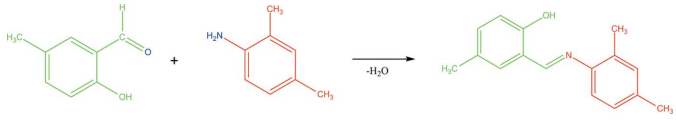

Figure 5
The scheme of synthesis of the title compound.

editing of the manuscript) SK, EA and AG; formal analysis, SK and ND; crystal-structure determination, ND; validation, SK, ND and EA; project administration, SK, ND and ES.

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supporting information

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Crystal structure and Hirshfeld surface analysis of (*Z*)-2-{[(2,4-dimethylphenyl)-imino]methyl}-4-methylphenol

Sevgi Kansiz, Adem Gul, Necmi Dege, Erbil Agar and Eiad Saif

Computing details

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA* (Stoe & Cie, 2002); data reduction: *X-RED* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXT2017/1* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2017/1* (Sheldrick, 2015b); molecular graphics: *PLATON* (Spek, 2020); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

(*Z*)-2-{[(2,4-Dimethylphenyl)imino]methyl}-4-methylphenol

Crystal data

$C_{16}H_{17}NO$
$M_r = 239.30$
Orthorhombic, *Pbca*
$a = 7.6699$ (4) Å
$b = 11.6080$ (6) Å
$c = 30.1431$ (17) Å
$V = 2683.7$ (2) Å^3
$Z = 8$
$F(000) = 1024$
$D_x = 1.185$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 13620 reflections
$\theta = 1.4$–$24.9°$
$\mu = 0.07$ mm^{-1}
$T = 296$ K
Plate, orange
0.68 × 0.48 × 0.18 mm

Data collection

Stoe IPDS 2 diffractometer
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus
Detector resolution: 6.67 pixels mm^{-1}
rotation method scans
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)
$T_{min} = 0.953$, $T_{max} = 0.990$
14869 measured reflections
2213 independent reflections
1451 reflections with $I > 2\sigma(I)$
$R_{int} = 0.081$
$\theta_{max} = 24.5°$, $\theta_{min} = 1.4°$
$h = -8 \rightarrow 8$
$k = -13 \rightarrow 13$
$l = -34 \rightarrow 34$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.125$
$S = 1.00$
2213 reflections
168 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0725P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.11$ e Å^{-3}

$\Delta\rho_{min}$ = −0.11 e Å^{-3}

Extinction correction:
file:///iucrfs/e/yk2157/yk2157.cif,
$Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0094 (14)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.3099 (2)	0.58146 (10)	0.30727 (4)	0.0844 (4)
H1	0.330751	0.540427	0.328769	0.127*
N1	0.42492 (18)	0.40012 (12)	0.34984 (5)	0.0663 (4)
C6	0.4130 (2)	0.40987 (13)	0.27056 (6)	0.0569 (4)
C5	0.4477 (2)	0.35487 (14)	0.23014 (5)	0.0595 (4)
H5	0.495649	0.281288	0.230684	0.071*
C7	0.4516 (2)	0.35261 (15)	0.31204 (6)	0.0611 (5)
H7	0.497415	0.278473	0.311267	0.073*
C1	0.3426 (2)	0.52223 (13)	0.26953 (6)	0.0630 (5)
C9	0.4629 (2)	0.33967 (15)	0.38970 (6)	0.0633 (5)
C4	0.4139 (2)	0.40502 (16)	0.18961 (6)	0.0648 (5)
C14	0.5297 (2)	0.40228 (16)	0.42555 (6)	0.0692 (5)
C10	0.4302 (2)	0.22231 (16)	0.39438 (6)	0.0724 (5)
H10	0.383752	0.180914	0.370760	0.087*
C2	0.3077 (2)	0.57301 (15)	0.22917 (7)	0.0739 (5)
H2	0.259857	0.646596	0.228269	0.089*
C3	0.3428 (2)	0.51607 (16)	0.19032 (7)	0.0736 (5)
H3	0.318475	0.552460	0.163539	0.088*
C12	0.5363 (2)	0.22599 (19)	0.46974 (6)	0.0759 (6)
C13	0.5668 (2)	0.34303 (19)	0.46426 (6)	0.0771 (6)
H13	0.614731	0.383787	0.487863	0.093*
C11	0.4663 (3)	0.16695 (17)	0.43391 (6)	0.0774 (5)
H11	0.443232	0.088594	0.436544	0.093*
C8	0.4528 (3)	0.34410 (19)	0.14659 (6)	0.0893 (6)
H8A	0.524423	0.392488	0.128285	0.134*
H8B	0.345600	0.327600	0.131447	0.134*
H8C	0.513250	0.273397	0.152645	0.134*
C15	0.5618 (3)	0.53050 (18)	0.42172 (7)	0.0970 (7)
H15A	0.638745	0.545186	0.397253	0.145*
H15B	0.613945	0.558242	0.448631	0.145*
H15C	0.453020	0.569432	0.416857	0.145*
C16	0.5729 (3)	0.1666 (2)	0.51352 (7)	0.1014 (7)
H16A	0.650363	0.213308	0.530910	0.152*
H16B	0.625932	0.093075	0.508055	0.152*
H16C	0.465487	0.155857	0.529352	0.152*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0935 (10)	0.0608 (7)	0.0990 (10)	0.0078 (7)	0.0082 (9)	−0.0177 (7)
N1	0.0658 (9)	0.0681 (9)	0.0649 (10)	−0.0063 (7)	0.0056 (8)	−0.0106 (8)
C6	0.0514 (9)	0.0516 (9)	0.0676 (10)	−0.0051 (7)	−0.0008 (8)	−0.0042 (8)
C5	0.0546 (9)	0.0567 (9)	0.0673 (11)	−0.0019 (7)	−0.0042 (9)	−0.0018 (9)
C7	0.0588 (10)	0.0572 (10)	0.0672 (11)	−0.0014 (8)	0.0001 (9)	−0.0053 (9)
C1	0.0544 (9)	0.0532 (9)	0.0813 (12)	−0.0049 (7)	0.0020 (10)	−0.0063 (10)
C9	0.0585 (10)	0.0731 (12)	0.0582 (10)	−0.0035 (8)	0.0057 (9)	−0.0098 (9)
C4	0.0552 (10)	0.0704 (12)	0.0686 (12)	−0.0072 (8)	−0.0058 (9)	0.0003 (9)
C14	0.0639 (11)	0.0820 (12)	0.0618 (11)	−0.0096 (9)	0.0138 (9)	−0.0186 (10)
C10	0.0748 (12)	0.0757 (12)	0.0667 (12)	−0.0056 (9)	−0.0078 (10)	−0.0093 (9)
C2	0.0638 (11)	0.0548 (10)	0.1032 (15)	−0.0006 (8)	−0.0073 (11)	0.0066 (11)
C3	0.0672 (12)	0.0713 (12)	0.0822 (14)	−0.0090 (10)	−0.0129 (10)	0.0163 (10)
C12	0.0647 (11)	0.0989 (15)	0.0642 (12)	0.0014 (10)	−0.0002 (9)	−0.0072 (10)
C13	0.0672 (12)	0.1049 (16)	0.0593 (11)	−0.0127 (11)	0.0051 (9)	−0.0186 (10)
C11	0.0842 (13)	0.0762 (12)	0.0716 (12)	0.0001 (10)	−0.0075 (11)	−0.0006 (10)
C8	0.0923 (15)	0.1077 (16)	0.0680 (13)	0.0019 (12)	−0.0081 (11)	−0.0041 (11)
C15	0.1220 (19)	0.0904 (15)	0.0785 (13)	−0.0314 (13)	0.0196 (13)	−0.0273 (11)
C16	0.1019 (17)	0.130 (2)	0.0727 (14)	−0.0012 (14)	−0.0154 (12)	0.0056 (13)

Geometric parameters (Å, º)

O1—C1	1.353 (2)	C10—H10	0.9300
O1—H1	0.8200	C2—C3	1.371 (3)
N1—C7	1.2823 (19)	C2—H2	0.9300
N1—C9	1.421 (2)	C3—H3	0.9300
C6—C5	1.401 (2)	C12—C11	1.387 (3)
C6—C1	1.412 (2)	C12—C13	1.388 (3)
C6—C7	1.447 (2)	C12—C16	1.515 (3)
C5—C4	1.378 (2)	C13—H13	0.9300
C5—H5	0.9300	C11—H11	0.9300
C7—H7	0.9300	C8—H8A	0.9600
C1—C2	1.378 (2)	C8—H8B	0.9600
C9—C10	1.392 (2)	C8—H8C	0.9600
C9—C14	1.400 (2)	C15—H15A	0.9600
C4—C3	1.400 (3)	C15—H15B	0.9600
C4—C8	1.507 (3)	C15—H15C	0.9600
C14—C13	1.384 (3)	C16—H16A	0.9600
C14—C15	1.513 (3)	C16—H16B	0.9600
C10—C11	1.382 (2)	C16—H16C	0.9600
C1—O1—H1	109.5	C2—C3—H3	118.9
C7—N1—C9	120.40 (15)	C4—C3—H3	118.9
C5—C6—C1	118.32 (16)	C11—C12—C13	117.14 (18)
C5—C6—C7	120.23 (15)	C11—C12—C16	121.7 (2)
C1—C6—C7	121.44 (16)	C13—C12—C16	121.16 (18)

C4—C5—C6	122.88 (16)	C14—C13—C12	123.48 (17)
C4—C5—H5	118.6	C14—C13—H13	118.3
C6—C5—H5	118.6	C12—C13—H13	118.3
N1—C7—C6	122.54 (16)	C10—C11—C12	121.27 (19)
N1—C7—H7	118.7	C10—C11—H11	119.4
C6—C7—H7	118.7	C12—C11—H11	119.4
O1—C1—C2	119.28 (16)	C4—C8—H8A	109.5
O1—C1—C6	121.45 (17)	C4—C8—H8B	109.5
C2—C1—C6	119.26 (17)	H8A—C8—H8B	109.5
C10—C9—C14	119.71 (17)	C4—C8—H8C	109.5
C10—C9—N1	122.14 (15)	H8A—C8—H8C	109.5
C14—C9—N1	118.12 (16)	H8B—C8—H8C	109.5
C5—C4—C3	116.66 (17)	C14—C15—H15A	109.5
C5—C4—C8	121.83 (17)	C14—C15—H15B	109.5
C3—C4—C8	121.50 (17)	H15A—C15—H15B	109.5
C13—C14—C9	117.93 (17)	C14—C15—H15C	109.5
C13—C14—C15	121.31 (17)	H15A—C15—H15C	109.5
C9—C14—C15	120.76 (18)	H15B—C15—H15C	109.5
C11—C10—C9	120.43 (17)	C12—C16—H16A	109.5
C11—C10—H10	119.8	C12—C16—H16B	109.5
C9—C10—H10	119.8	H16A—C16—H16B	109.5
C3—C2—C1	120.63 (17)	C12—C16—H16C	109.5
C3—C2—H2	119.7	H16A—C16—H16C	109.5
C1—C2—H2	119.7	H16B—C16—H16C	109.5
C2—C3—C4	122.24 (17)		

C1—C6—C5—C4	−0.9 (2)	N1—C9—C14—C15	−0.5 (3)
C7—C6—C5—C4	−179.97 (15)	C14—C9—C10—C11	−1.2 (3)
C9—N1—C7—C6	179.20 (14)	N1—C9—C10—C11	−178.95 (16)
C5—C6—C7—N1	178.78 (14)	O1—C1—C2—C3	178.64 (16)
C1—C6—C7—N1	−0.3 (2)	C6—C1—C2—C3	−0.8 (3)
C5—C6—C1—O1	−178.36 (15)	C1—C2—C3—C4	0.3 (3)
C7—C6—C1—O1	0.7 (2)	C5—C4—C3—C2	−0.1 (3)
C5—C6—C1—C2	1.1 (2)	C8—C4—C3—C2	−179.56 (17)
C7—C6—C1—C2	−179.83 (15)	C9—C14—C13—C12	−2.0 (3)
C7—N1—C9—C10	−38.6 (2)	C15—C14—C13—C12	178.60 (18)
C7—N1—C9—C14	143.67 (16)	C11—C12—C13—C14	0.6 (3)
C6—C5—C4—C3	0.4 (2)	C16—C12—C13—C14	−177.52 (18)
C6—C5—C4—C8	179.87 (15)	C9—C10—C11—C12	−0.3 (3)
C10—C9—C14—C13	2.3 (3)	C13—C12—C11—C10	0.6 (3)
N1—C9—C14—C13	−179.87 (15)	C16—C12—C11—C10	178.71 (19)
C10—C9—C14—C15	−178.33 (17)		

Hydrogen-bond geometry (Å, º)

*Cg*2 is the centroid of the C9–C14 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.89	2.618 (2)	147

C16—H16*A*···*Cg*2^{i}	0.96	2.93 (3)	3.73	143

Symmetry code: (i) $x+1/2, -y+1/2, -z$.