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Synthesis, crystal structure and Hirshfeld surface analysis of (*E*)-5-methoxy-2-[(*p*-tolylimino)methyl]-phenol

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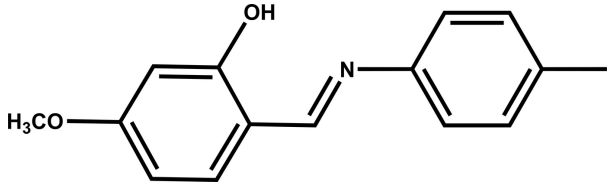
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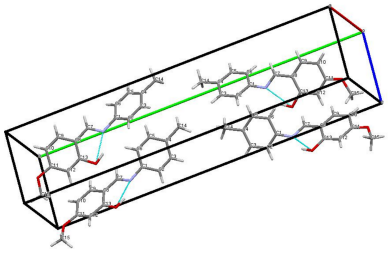
Single-crystal X-ray diffraction has been used to elucidate the molecular and crystal structures of (*E*)-5-methoxy-2-[(*p*-tolylimino)methyl]phenol {systematic name: (*E*)-5-methoxy-2-[*N*-(4-methylphenyl)carboximidoyl]-phenol}, $C_{15}H_{15}NO_2$. The Schiff base crystallizes in the orthorhombic space group $Pca2_1$ and the molecular structure is stabilized by an intramolecular O—H···N hydrogen bond, with an O···N separation of 2.605 (4) Å and an O—H···N angle of 146°. The crystal packing was examined using Hirshfeld surface analysis, which reveals dominant H···H contacts make the largest contribution to the intermolecular contacts (51.4%) of the surface, followed by H···C/C···H (30.9%), H···O/O···H (12.0%) and H···N/N···H (2.5%) contacts. The combined crystallographic and Hirshfeld surface analyses provide insight into the molecular organization and intermolecular forces governing the solid-state structure.

1. Chemical context

Schiff bases derived from salicylaldehyde are an important class of compounds owing to their structural diversity and applications in coordination chemistry, molecular recognition and materials chemistry. The azomethine group together with the appropriately positioned phenolic hydroxyl group provides a useful molecular scaffold for structural modification and metal coordination (Govindaraj & Ramanathan, 2014). This class of compounds has also attracted attention because of the reported biological potential of Schiff base derivatives, including antimicrobial and antioxidant properties (Govindaraj V *et al.*, 2026*c*).



In the present work, (*E*)-5-methoxy-2-[(*p*-tolylimino)-methyl]phenol was synthesized by condensation of 2-hydroxy-4-methoxybenzaldehyde with *p*-toluidine. The *p*-methyl substituent was introduced to provide an electron-donating group while minimizing steric effects near the azomethine linkage. The molecular and crystal structures were determined by single-crystal X-ray diffraction. Hirshfeld surface analysis



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and energy-framework calculations were subsequently employed to characterize the intermolecular contacts and to assess their contributions to the consolidation of the crystal structure.

2. Structural commentary

The molecular structure of the title compound, together with the atom-numbering scheme, is shown in Fig. 1. The molecule consists of two benzene rings connected through an azomethine (—CH=N—) linkage. Related Schiff-base structures have been characterized by single-crystal X-ray diffraction (Govindaraj *et al.*, 2026*a*,*b*). The C1–C6 ring corresponds to the *p*-tolyl ring, whereas the C8–C13 ring bears the phenolic hydroxyl and methoxy substituents. The two benzene ring mean planes are inclined at a dihedral angle 49.46 (16)°, indicating a non-planar molecular conformation. The azomethine group adopts a *trans* configuration, as indicated by the C8—C7—N1—C1 torsion angle of −172.9 (3)°. The torsion angles C2—C1—N1—C7 [−144.2 (3)°] and C6—C1—N1—C7 [41.6 (5)°] further describe the orientation of the *p*-tolyl ring relative to the imine group. The principal bond lengths are consistent with the expected geometry of the Schiff-base framework. In particular, the N1═C7 bond is 1.284 (4) Å, while the C1—N1 and C7—C8 bonds are 1.420 (4) and 1.432 (5) Å, respectively. The phenolic C13—O2 bond length is 1.345 (4) Å, and the methoxy group is characterized by C11—O1 = 1.358 (4) Å and O-1–C15 = 1.406 (5) Å.

3. Supramolecular features

The phenolic hydroxyl group forms an intramolecular O2—H2*A*···N1 hydrogen bond, with an O2···N1 distance of 2.605 (4) Å and an O2—H2*A*···N1 angle of 146° (Table 1). This interaction generates a six-membered pseudo-ring and contributes to the stabilization of the molecular conformation. The crystal packing, shown in Fig. 2, is governed mainly by weak intermolecular contacts between neighboring molecules.

Hirshfeld surface analysis was used to quantify the intermolecular contacts (Dey *et al.*, 2024; Spackman & Jayatilaka, 2009). The Hirshfeld surface has a volume of 311.57 Å^3 and a surface area of 299.40 Å^3. The surface mappings are shown in Fig. 3. The two-dimensional fingerprint plots (Fig. 4) show that H···H contacts make the largest contribution 51.4%), followed by H···C/C···H contacts (30.9%). The H···O/O···H contacts contribute 12.0%, while H···N/N···H contacts contribute 2.5%. Smaller contributions arise from C···O/O···C (2.4%), C···C (0.4%) and N···O/O···N (0.2%) contacts.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*A*···N1	0.92	1.79	2.605 (4)	146

4. Database survey

A search of the Cambridge Structural Database (CSD, version 6.01, July 2026 update; Groom *et al.*, 2016) identified the closely related Schiff-base compound (*E*)-2-[(*p*-tolylimino)-methyl]phenol (refcode CULPOO01; Nieger, 2012). Both compounds exhibit a *trans* configuration of the azomethine group, with C6—C7—N8—C9 and C8—C7—N1—C1 torsion angles of 179.41 (11) and −172.9 (3)°, respectively. The aromatic rings of the reference compound are nearly coplanar, as indicated by the C7—N8—C9—C10 torsion angle of 172.26 (12)°, whereas the title compound exhibits a more

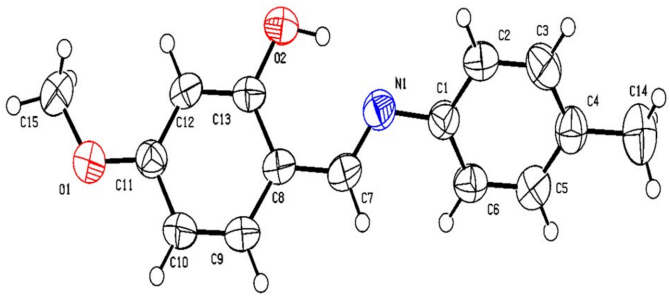


Figure 1
The molecular structure of the title compound, showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level.

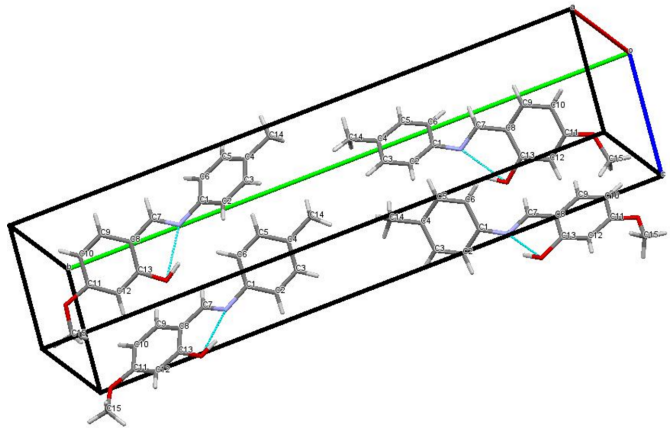


Figure 2
Crystal packing of the title compound, showing the arrangement of molecules in the crystal viewed along the *a* axis.

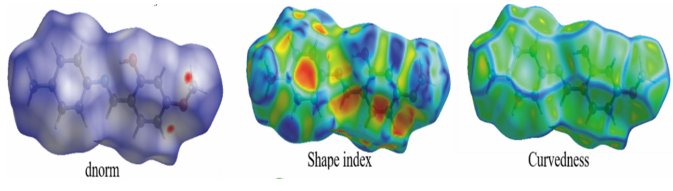


Figure 3
Hirshfeld surfaces of the title compound mapped over d_{norm}, shape-index and curvedness.

twisted arrangement, with a C2—C1—N1—C7 torsion angle of −144.2 (3)°. Both structures retain an intramolecular O–H···N hydrogen bond, with donor–acceptor distances of 2.5963 (14) and 2.605 (4) Å, respectively. The methoxy substituent in the title compound may influence its conformational preferences and crystal packing.

5. Synthesis and crystallization

The title compound was prepared according to the reported procedure of Kudernac *et al.* (2009) *p*-toluidine (0.106 g, 1 mmol) and 2-hydroxy-4-methoxybenzaldehyde (0.152 g, 1 mmol) were dissolved in 15 ml of ethanol and the reaction mixture was refluxed for 3 h. After cooling to room temperature, the resulting yellow crystals were collected by filtration and dried under vacuum to give the product in approximately 0.186 g (77%) yield. Single crystals suitable for X-ray diffraction were obtained by allowing the solution to stand at room temperature for approximately 2 days, affording clear light-yellow plate-shaped crystals.

FT–IR (KBr, cm^{-1}): 3546 [ν(O—H)], 1618 [ν(C═N)], 1522 [ν(C═C)], 3021 [ν(C—H)], 2922 [ν(aliphatic C—H, CH_3)] and 1288 [ν(C—O)]. ^{1}H NMR (500 MHz, DMSO-d_6, δ ppm): 6.54 (*d*, 1H), 7.28 (*d*, 1H), 7.25 (*d*, 1H), 6.56 (*d*, 1H), 8.85 (*s*, 1H), 7.51 (*d*, 1H), 6.48 (*d*, 1H), 7.23 (*s*, 1H), 3.80 (*s*, 3H), 2.32 (*s*, 3H, Ar–CH_3) and 13.81 (*s*, 1H, OH). HRMS (CH_2Cl_2): *m*/*z* 242.11 [*M* + H]$^+$·Elemental analysis: calculated for $C_{15}H_{15}NO_2$: C, 74.67; H, 6.27; N, 5.81; O, 13.26%; found: C, 74.66; H, 6.25; N, 5.80; O, 13.26%.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{15}NO_2$
M_r	241.28
Crystal system, space group	Orthorhombic, $Pca2_1$
Temperature (K)	300
a, *b*, *c* (Å)	7.2146 (7), 28.256 (3), 6.2413 (6)
V (Å^3)	1272.3 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.34 × 0.22 × 0.08
Data collection	
Diffractometer	Bruker D8 QUEST
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.972, 0.994
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	29157, 3164, 2247
R_{int}	0.061
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.057, 0.151, 1.06
No. of reflections	3164
No. of parameters	167
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.19, −0.17
Absolute structure	Flack *x* determined using 786 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.2 (6)

Computer programs: *Instrument Service* and *SAINT* V8.41 (Bruker, 2016), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2019/2* (Sheldrick, 2015*b*) and *ShelXle* (Hübschle *et al.*, 2011).

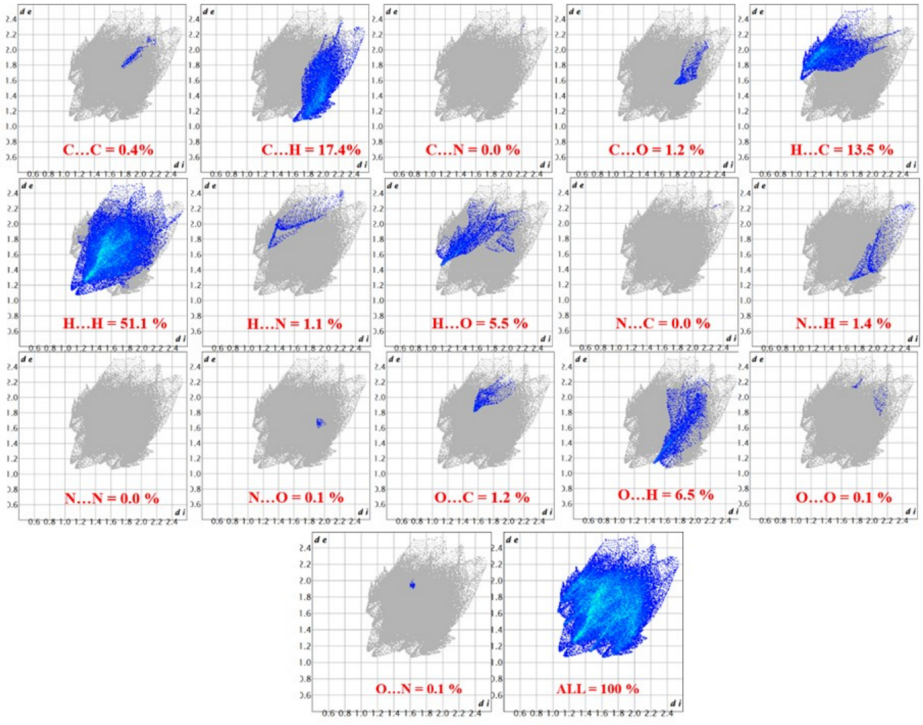


Figure 4
Two-dimensional fingerprint plots showing the contributions of the intermolecular contacts in the crystal structure of the title compound.

6. Refinement

Details of the crystal data, data collection and refinement are given in Table 2. C-bound H atoms were placed in calculated positions and refined using a riding model, while the O-bound H atom was refined independently.

Acknowledgements

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Computing details

(*E*)-5-Methoxy-2-[*N*-(4-methylphenyl)carboximidoyl]phenol

Crystal data

$C_{15}H_{15}NO_2$
M_r = 241.28
Orthorhombic, $Pca2_1$
a = 7.2146 (7) Å
b = 28.256 (3) Å
c = 6.2413 (6) Å
V = 1272.3 (2) Å^3
Z = 4
$F(000)$ = 512
D_x = 1.26 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6384 reflections
θ = 2.9–23.7°
μ = 0.08 mm^{-1}
T = 300 K
Plate, clear light yellow
0.34 × 0.22 × 0.08 mm

Data collection

Bruker D8 QUEST diffractometer
Radiation source: microfocus sealed tube, INCOATEC IμS 3.0
Multilayer mirror monochromator
Detector resolution: 7.391 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.972, T_{max} = 0.994
29157 measured reflections
3164 independent reflections
2247 reflections with $I > 2\sigma(I)$
R_{int} = 0.061
θ_{max} = 28.3°, θ_{min} = 2.2°
h = −9→9
k = −36→37
l = −8→8

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.151
S = 1.06
3164 reflections
167 parameters
1 restraint
Primary atom site location: Intrinsic Phasing
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0623P)^2 + 0.323P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.007
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Absolute structure: Flack x determined using 786 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.2 (6)

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.

Refinement. The diffraction data were processed using SAINT (Bruker, 2016) and absorption correction was applied using SADABS (Krause *et al.*, 2015). The structure was solved by intrinsic phasing using SHELXT 2018/2 and refined by full-matrix least-squares methods against F^2 using SHELXL-2019/3 (Sheldrick, 2015a,b). All non-H atoms were refined anisotropically.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.5091 (4)	0.31881 (12)	0.3712 (6)	0.0444 (8)
C2	0.5694 (5)	0.35917 (12)	0.4749 (6)	0.0518 (9)
H2	0.618437	0.356993	0.612401	0.062*
C3	0.5574 (5)	0.40250 (13)	0.3759 (8)	0.0585 (10)
H3	0.601158	0.429228	0.446663	0.070*
C4	0.4811 (5)	0.40729 (12)	0.1718 (7)	0.0558 (10)
C5	0.4216 (5)	0.36685 (12)	0.0713 (7)	0.0545 (9)
H5	0.372322	0.368988	−0.066013	0.065*
C6	0.4329 (4)	0.32304 (13)	0.1688 (6)	0.0491 (8)
H6	0.389169	0.296313	0.098084	0.059*
C7	0.5508 (4)	0.23666 (12)	0.3821 (6)	0.0463 (8)
H7	0.590493	0.238534	0.240619	0.056*
C8	0.5352 (4)	0.19109 (11)	0.4809 (5)	0.0433 (8)
C9	0.5914 (4)	0.15020 (12)	0.3729 (6)	0.0474 (8)
H9	0.639037	0.153035	0.234987	0.057*
C10	0.5789 (4)	0.10639 (12)	0.4623 (6)	0.0481 (8)
H10	0.622562	0.080033	0.388681	0.058*
C11	0.5001 (4)	0.10124 (12)	0.6659 (6)	0.0445 (8)
C12	0.4384 (5)	0.14066 (11)	0.7776 (6)	0.0462 (8)
H12	0.383505	0.137234	0.911506	0.055*
C13	0.4595 (4)	0.18514 (11)	0.6879 (6)	0.0441 (8)
C14	0.4622 (7)	0.45488 (14)	0.0664 (10)	0.0826 (14)
H14A	0.536888	0.477583	0.141530	0.124*
H14B	0.334792	0.464653	0.070195	0.124*
H14C	0.502843	0.452796	−0.079713	0.124*
C15	0.4117 (7)	0.04730 (15)	0.9405 (7)	0.0764 (13)
H15A	0.285977	0.058395	0.938838	0.115*
H15B	0.479579	0.063565	1.050459	0.115*
H15C	0.413186	0.013907	0.968858	0.115*
N1	0.5117 (4)	0.27501 (10)	0.4827 (5)	0.0481 (7)
O1	0.4944 (4)	0.05613 (9)	0.7406 (4)	0.0580 (7)
O2	0.4075 (4)	0.22284 (9)	0.8050 (4)	0.0624 (8)
H2A	0.428 (6)	0.2502 (14)	0.727 (5)	0.094*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0395 (16)	0.049 (2)	0.044 (2)	0.0026 (13)	0.0062 (17)	0.0003 (15)
C2	0.0496 (18)	0.061 (2)	0.0447 (19)	−0.0015 (15)	−0.0016 (17)	−0.0056 (19)
C3	0.0531 (19)	0.053 (2)	0.070 (3)	−0.0063 (16)	−0.002 (2)	−0.009 (2)
C4	0.051 (2)	0.054 (2)	0.063 (3)	−0.0020 (16)	0.004 (2)	0.0060 (19)
C5	0.0487 (19)	0.063 (2)	0.052 (2)	0.0035 (16)	0.0005 (16)	0.0035 (18)
C6	0.0488 (17)	0.055 (2)	0.044 (2)	−0.0037 (15)	−0.0008 (16)	−0.0053 (15)
C7	0.0419 (16)	0.060 (2)	0.0370 (18)	0.0005 (14)	−0.0018 (14)	−0.0006 (16)
C8	0.0412 (16)	0.0533 (19)	0.0354 (18)	0.0018 (13)	−0.0003 (15)	−0.0039 (16)
C9	0.0445 (17)	0.060 (2)	0.0376 (17)	0.0017 (15)	0.0043 (15)	−0.0076 (17)
C10	0.0480 (17)	0.0534 (19)	0.0429 (18)	0.0049 (14)	0.0013 (16)	−0.0088 (17)
C11	0.0450 (17)	0.0473 (19)	0.0412 (19)	−0.0006 (14)	−0.0057 (16)	−0.0037 (15)
C12	0.0481 (17)	0.057 (2)	0.0332 (17)	0.0024 (15)	0.0029 (15)	0.0009 (15)
C13	0.0422 (16)	0.052 (2)	0.0381 (18)	0.0042 (14)	0.0011 (15)	−0.0061 (15)
C14	0.085 (3)	0.063 (3)	0.100 (4)	0.002 (2)	−0.009 (3)	0.015 (3)
C15	0.115 (4)	0.062 (2)	0.052 (2)	0.005 (2)	0.018 (2)	0.010 (2)
N1	0.0457 (14)	0.0526 (17)	0.0461 (16)	0.0012 (12)	0.0017 (15)	0.0001 (14)
O1	0.0721 (18)	0.0509 (14)	0.0510 (15)	0.0016 (12)	0.0041 (12)	−0.0008 (12)
O2	0.0848 (19)	0.0548 (14)	0.0474 (16)	0.0107 (14)	0.0176 (14)	−0.0056 (13)

Geometric parameters (Å, º)

C1—C2	1.381 (5)	C9—C10	1.361 (5)
C1—C6	1.383 (5)	C9—H9	0.9300
C1—N1	1.420 (4)	C10—C11	1.399 (5)
C2—C3	1.374 (5)	C10—H10	0.9300
C2—H2	0.9300	C11—O1	1.358 (4)
C3—C4	1.394 (6)	C11—C12	1.387 (4)
C3—H3	0.9300	C12—C13	1.384 (4)
C4—C5	1.372 (5)	C12—H12	0.9300
C4—C14	1.503 (5)	C13—O2	1.345 (4)
C5—C6	1.382 (5)	C14—H14A	0.9600
C5—H5	0.9300	C14—H14B	0.9600
C6—H6	0.9300	C14—H14C	0.9600
C7—N1	1.284 (4)	C15—O1	1.406 (5)
C7—C8	1.432 (5)	C15—H15A	0.9600
C7—H7	0.9300	C15—H15B	0.9600
C8—C9	1.398 (4)	C15—H15C	0.9600
C8—C13	1.412 (4)	O2—H2A	0.92 (5)
C2—C1—C6	118.8 (3)	C9—C10—C11	119.6 (3)
C2—C1—N1	119.0 (3)	C9—C10—H10	120.2
C6—C1—N1	121.9 (3)	C11—C10—H10	120.2
C3—C2—C1	120.3 (4)	O1—C11—C12	124.8 (3)
C3—C2—H2	119.8	O1—C11—C10	114.9 (3)
C1—C2—H2	119.8	C12—C11—C10	120.2 (3)

C2—C3—C4	121.5 (4)	C13—C12—C11	119.4 (3)
C2—C3—H3	119.3	C13—C12—H12	120.3
C4—C3—H3	119.3	C11—C12—H12	120.3
C5—C4—C3	117.4 (3)	O2—C13—C12	117.9 (3)
C5—C4—C14	121.1 (4)	O2—C13—C8	120.7 (3)
C3—C4—C14	121.5 (4)	C12—C13—C8	121.4 (3)
C4—C5—C6	121.8 (4)	C4—C14—H14A	109.5
C4—C5—H5	119.1	C4—C14—H14B	109.5
C6—C5—H5	119.1	H14A—C14—H14B	109.5
C5—C6—C1	120.2 (3)	C4—C14—H14C	109.5
C5—C6—H6	119.9	H14A—C14—H14C	109.5
C1—C6—H6	119.9	H14B—C14—H14C	109.5
N1—C7—C8	122.1 (3)	O1—C15—H15A	109.5
N1—C7—H7	119.0	O1—C15—H15B	109.5
C8—C7—H7	119.0	H15A—C15—H15B	109.5
C9—C8—C13	117.1 (3)	O1—C15—H15C	109.5
C9—C8—C7	120.8 (3)	H15A—C15—H15C	109.5
C13—C8—C7	122.1 (3)	H15B—C15—H15C	109.5
C10—C9—C8	122.3 (3)	C7—N1—C1	119.9 (3)
C10—C9—H9	118.8	C11—O1—C15	119.0 (3)
C8—C9—H9	118.8	C13—O2—H2A	109.5
C6—C1—C2—C3	−1.4 (5)	C9—C10—C11—O1	−179.9 (3)
N1—C1—C2—C3	−175.8 (3)	C9—C10—C11—C12	−1.3 (5)
C1—C2—C3—C4	1.4 (6)	O1—C11—C12—C13	177.1 (3)
C2—C3—C4—C5	−1.3 (6)	C10—C11—C12—C13	−1.4 (5)
C2—C3—C4—C14	178.0 (4)	C11—C12—C13—O2	−176.5 (3)
C3—C4—C5—C6	1.2 (6)	C11—C12—C13—C8	2.8 (5)
C14—C4—C5—C6	−178.0 (4)	C9—C8—C13—O2	177.9 (3)
C4—C5—C6—C1	−1.3 (5)	C7—C8—C13—O2	−3.4 (4)
C2—C1—C6—C5	1.4 (5)	C9—C8—C13—C12	−1.3 (4)
N1—C1—C6—C5	175.6 (3)	C7—C8—C13—C12	177.3 (3)
N1—C7—C8—C9	−175.3 (3)	C8—C7—N1—C1	−172.9 (3)
N1—C7—C8—C13	6.1 (5)	C2—C1—N1—C7	−144.2 (3)
C13—C8—C9—C10	−1.5 (4)	C6—C1—N1—C7	41.6 (5)
C7—C8—C9—C10	179.8 (3)	C12—C11—O1—C15	3.6 (5)
C8—C9—C10—C11	2.8 (5)	C10—C11—O1—C15	−177.8 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*A*···N1	0.92	1.79	2.605 (4)	146