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# Crystal structure and Hirshfeld surface analysis of 6,6′-((1*E*,1′*E*)-{[1,4-phenylenebis(methylene)]bis(azanylylidene)}bis(methaneylylidene))bis(2-methoxyphenol)

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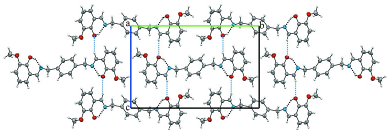
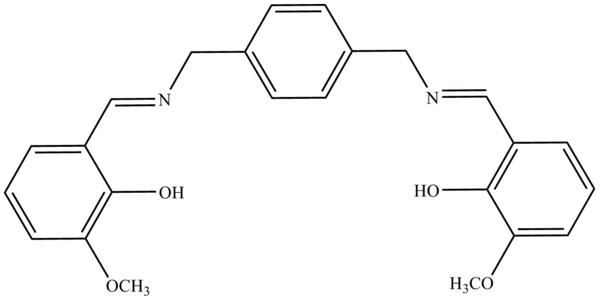
The Schiff base compound, $C_{24}H_{24}N_2O_4$, was synthesized by the interaction of 2-hydroxy-3-methoxy benzaldehyde and 1,4-benzene dimethanamine in ethanol, and crystallizes in the monoclinic space group $P2_1/n$ with $Z' = 0.5$. The molecule is not planar, the 1,4-diethylbenzene and the phenol rings are twisted with respect to each other, making a dihedral angle of 74.27 (5)°. The molecular structure is stabilized by an O—H⋯N hydrogen bond, forming an *S*(6) ring motif. In the crystal, molecules are linked by C—H⋯O hydrogen bonds, resulting in the formation of sheets parallel to the *bc* plane. A Hirshfeld surface analysis was undertaken to investigate the various intermolecular contacts controlling the supramolecular topology, suggesting the H⋯O (18%) contacts to be the most significant interactions, whereas the H⋯H (50.5%) and C⋯H (24.3%) interactions are less significant.



## 1. Chemical context

Schiff bases are used as pigments and dyes, catalysts, intermediates in organic synthesis, and as polymer stabilizers (Supuran *et al.*, 1996). In azomethine derivatives, the C═N linkage is essential for biological activity and several azomethines have been reported to possess remarkable antibacterial, antifungal, anticancer and diuretic activities (Gaur, 2003). Schiff bases having an azomethine group of general formula C═N– contain various substituted groups (Schiff, 1864). Of particular interest are the two different tautomeric structures for *o*-hydroxy Schiff bases, which are expressed as keto-amine and phenol-imine, with intrinsic N—H⋯O or O—H⋯N hydrogen bonds, (Filarowski *et al.*, 2004). There are many studies in the literature on the synthesis of Schiff bases and investigation of tautomeric structures. Phenol-imine and keto-amine tautomeric structures exhibit features of photochromism and thermochromism (Hadjoudis *et al.*, 2004). Tetradentate salen-type ligands have been used in almost all areas of coordination chemistry to prepare complexes that have catalytic and biological activity or which feature interesting structural, electrochemical or magnetic properties (Abd El-Hamid *et al.*, 2019). In this study, a symmetrical tetradentate Schiff base ligand bearing ONNO donor atoms, 6,6′-((1*E*,1′*E*)-{[1,4-phenylenebis(methylene)]bis(azanylylidene)}bis(methaneylylidene))bis(2-methoxyphenol) was synthesized by the interaction of 2-hydroxy-3-methoxy benzaldehyde and 1,4-benzene dimethanamine in ethanol and its crystal structure determined by single-crystal X-ray diffraction.



## 2. Structural commentary

The molecular structure of the title Schiff base derivative is illustrated in Fig. 1. The asymmetric unit of the title compound contains one-half of the centrosymmetric molecule ($Z' = 0.5$). There is an intramolecular O2—H2···N1 hydrogen bond (Table 1 and Fig. 1); this is a common feature also observed in related phenol-imine Schiff bases. It forms an $S(6)$ ring motif and also induces the phenol ring and the Schiff base to be nearly coplanar, as indicated by the C6—C8—N1—C9 torsion angle of 178.54 (13)°. The molecule is non-planar, the 1,4-diethylbenzene ring being inclined to the phenol ring by 74.27 (5)°. The C7—C6—C8—N1 torsion angle [3.8 (2)°] further supports the co-planarity of the phenol ring and the Schiff base. The C7—O2 distance is 1.3438 (17) Å, which is close to normal values reported for single C—O bonds in phenols and salicylideneamines (Kaştaş & Albayrak Kaştaş, 2019). The N1—C8 bond is short at 1.2717 (17) Å, strongly indicating a C═N double bond, while the long C6—C8 bond [1.451 (2) Å] implies a single bond. All of these data support the existence of the phenol–imine tautomer for the title compound in the crystalline state.

## 3. Supramolecular features

In the crystal, molecules are connected into sheets extending in the *bc* plane by C8—H8···O2$^{i}$ hydrogen bonds (Table 1; Fig. 2).

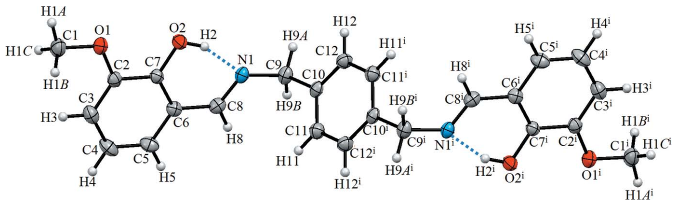


**Figure 1**
The molecular structure of the title compound with displacement ellipsoids drawn at the 40% probability level. Symmetry code: (i) $-x + 2, -y + 1, -z + 1$.

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O2—H2···N1 | 0.86 (1) | 1.79 (2) | 2.5877 (18) | 154 (2) |
| C8—H8···O2$^{i}$ | 0.93 | 2.51 | 3.410 (2) | 162 |

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

## 4. Database survey

A search of the Cambridge Structural Database (CSD Version 5.42, update of May 2021; Groom *et al.*, 2016) for the (1,4-phenylene)bis(*N*-ethylidenemethanamine) moiety revealed some related structures. The most similar structures are 1,4-bis(2-pyridylmethyleneaminomethyl)benzene (GOLJUN; Li *et al.*, 2009), 1,4-bis(3-pyridylmethyleneaminomethyl)benzene (GOLJOH; He *et al.*, 2009) and 1,4-bis(3,5-di-*t*-butyl-2-hydroxybenzylideneaminomethyl)benzene (OCAPAK; Tooke *et al.*, 2004). In GOLJUN and GOLJOH, the molecules have similar shapes to the title compound. The C—N bond lengths [1.253 (2) Å in GOLJOH and 1.256 (2) Å in GOLJUN] are typical for an azomethine C=N bond and shorter than in the title compound [1.2717 (19) Å]. The torsion angles involving the C—C═N—C units are −177.26 (11)° and 115.21 (13)° in GOLJUN. These values are similar to those observed in the title compound. In OCAPAK, a *t*-butyl group is present, different from the title compound. In addition, there is an intramolecular O—H···N contact in the title compound. Similarly, in OCAPAK, the hydroxyl H atom is involved in an intramolecular O—H···N hydrogen bond, forming an $S(6)$ ring motif as in the title compound. The length of intramolecular O—H···N hydrogen bond in OCAPAK is especially short [1.65 (2) Å] compared to that in the title compound [1.789 (15) Å].

## 5. Hirshfeld surface analysis

Hirshfeld surface analysis was used to analyse the various intermolecular interactions in the title compound, through mapping of the normalized contact distance ($d_{\rm norm}$) using *CrystalExplorer17* (Turner *et al.*, 2017; Spackman & Jayatilaka, 2009). Hirshfeld surface analysis is a valuable tool for assessing the strength of intermolecular interactions, predicting the properties of a crystal and its potential applications (Al-Resayes *et al.*, 2020). The Hirshfeld surface was generated using a standard (high) surface resolution with the three-dimensional $d_{\rm norm}$ surface mapped over a fixed color scale of

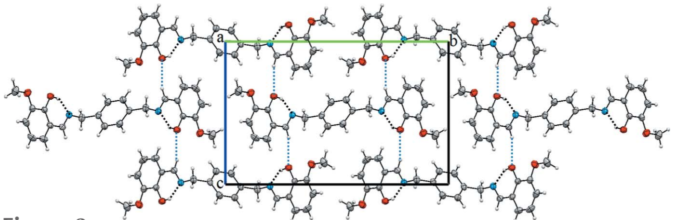


**Figure 2**
A view of the crystal packing of the title compound in a view parallel to the *bc* plane. C—H···O hydrogen bonds are shown as dashed blue lines.

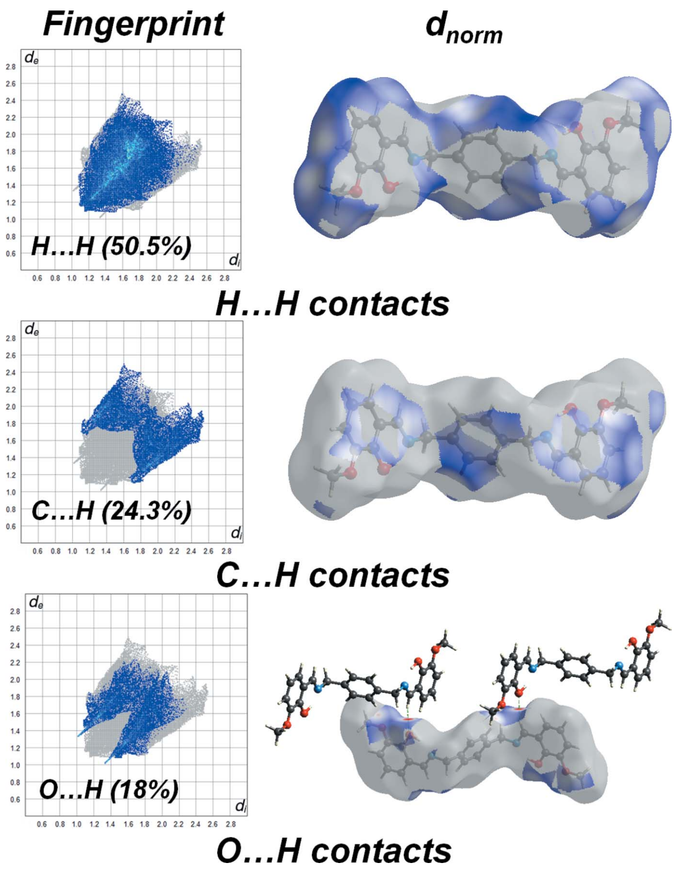


**Figure 3**
The Hirshfeld surface analysis of the title compound mapped with $d_{norm}$ over −0.175 to 1.404 a.u. showing the C—H⋯O hydrogen-bonded contacts.

−0.175 (red) to 1.404 a.u. (blue). The packing of molecules is mainly dependent on H⋯H (50.5%) and C⋯H (24.3%) interactions and the significant C—H⋯O interactions (18%). Blue regions in the $d_{norm}$ map indicate intermolecular interactions with distances longer than van der Waals radius sum of the interacting elements (Fig. 3). The C—H⋯O interactions, which appear as red spots in the $d_{norm}$ map, have contact distances shorter than the sum of the van der Waals radii of the oxygen and hydrogen atoms

## 6. Synthesis and crystallization

0.0225 g (0.148 mmol) of 2-hydroxy-3-methoxy benzaldehyde was dissolved in 20 mL of ethanol and mixed with 0.0100 g (0.074 mmol) of 1,4-benzene dimethanamine dissolved in 20 mL of ethanol (Fig. 4). The reaction mixture was refluxed for 6 h and at the end of the reaction, the solution was allowed to cool. The yellow product obtained was washed with ether and crystallized in ethanol at room temperature (m.p. = 431–434 K, yield 85%).

## 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 with $U_{iso}$(H) = 1.5$U_{eq}$(O) and a distance restraint. The C-bound H atoms

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{24}H_{24}N_2O_4$ |
| $M_r$ | 404.45 |
| Crystal system, space group | Monoclinic, $P2_1/n$ |
| Temperature (K) | 296 |
| $a, b, c$ (Å) | 4.7339 (10), 18.406 (4), 11.880 (2) |
| $\beta$ (°) | 98.47 (3) |
| $V$ (Å$^3$) | 1023.8 (4) |
| $Z$ | 2 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.09 |
| Crystal size (mm) | 0.61 × 0.45 × 0.23 |
| Data collection | |
| Diffractometer | Stoe IPDS 2 |
| Absorption correction | Integration (*X-RED32*; Stoe & Cie, 2002) |
| $T_{min}$, $T_{max}$ | 0.963, 0.992 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 6766, 1863, 1315 |
| $R_{int}$ | 0.034 |
| $(\sin \theta/\lambda)_{max}$ (Å$^{-1}$) | 0.600 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.037, 0.092, 1.01 |
| No. of reflections | 1863 |
| No. of parameters | 140 |
| 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$^{-3}$) | 0.11, −0.09 |

Computer programs: *X-AREA* and *X-RED* (Stoe & Cie, 2002), *SHELXT2014/5* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*) and *PLATON* (Spek, 2020).

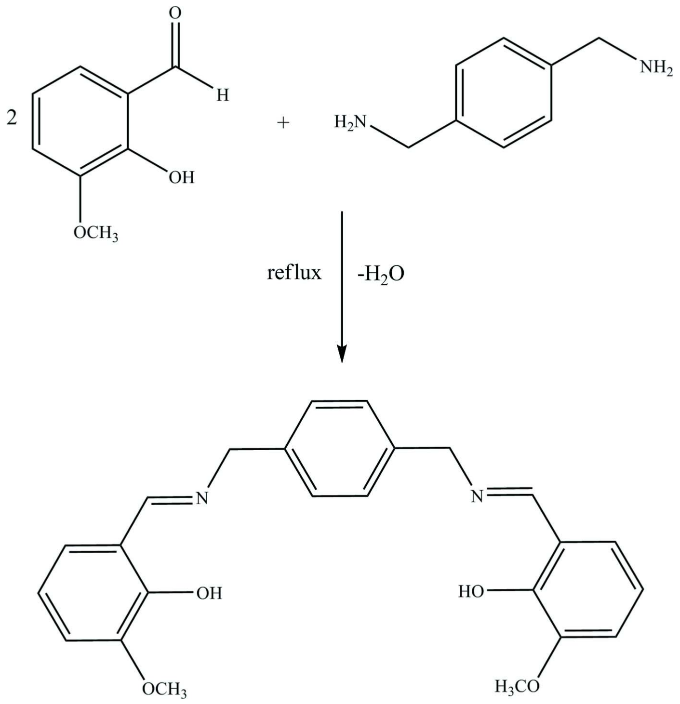


**Figure 4**
The synthesis of the title compound.

were positioned geometrically (C—H = 0.93, 0.96 and 0.97 Å) and refined using a riding model, with $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C) for methyl H atoms and 1.2$U_{\rm eq}$(C) for other H atoms.

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Author contributions are as follows. Conceptualization, SK, EA and ES; synthesis, SY and EA; writing (review and editing of the manuscript) SK and SY; formal analysis, SY, EA, ND and SK; crystal-structure determination, SY, SK and ND; validation, SY, EA and ES; project administration, EA, SY and SK.

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# supporting information

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## Crystal structure and Hirshfeld surface analysis of 6,6′-((1*E*,1′*E*)-{[1,4-phenylenebis(methylene)]bis(azanylylidene)}bis(methaneylylidene))bis(2-methoxyphenol)

**Sevgi Kansiz, Semanur Yesilbag, Necmi Dege, Eiad Saif and Erbil Agar**

### 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: *SHELXT2014/5* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015b); molecular graphics: *PLATON* (Spek, 2020).

### 6,6′-((1*E*,1′*E*)-{[1,4-Phenylenebis(methylene)]bis(azanylylidene)}bis(methaneylylidene))bis(2-methoxyphenol)

*Crystal data*

$C_{24}H_{24}N_2O_4$
$M_r = 404.45$
Monoclinic, $P2_1/n$
$a = 4.7339$ (10) Å
$b = 18.406$ (4) Å
$c = 11.880$ (2) Å
$\beta = 98.47$ (3)°
$V = 1023.8$ (4) Å$^3$
$Z = 2$
$F(000) = 428$
$D_x = 1.312$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7423 reflections
$\theta = 1.7$–31.5°
$\mu = 0.09$ mm$^{-1}$
$T = 296$ K
Plate, yellow
0.61 × 0.45 × 0.23 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)
$T_{min} = 0.963$, $T_{max} = 0.992$
6766 measured reflections
1863 independent reflections
1315 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 25.3°$, $\theta_{min} = 2.1°$
$h = -5 \rightarrow 5$
$k = -22 \rightarrow 22$
$l = -13 \rightarrow 14$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.092$
$S = 1.01$
1863 reflections
140 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement

| | |
|---|---|
| $w = 1/[\sigma^2(F_o^2) + (0.049P)^2]$<br>where $P = (F_o^2 + 2F_c^2)/3$ | $\Delta\rho_{max} = 0.11$ e Å$^{-3}$ |
| $(\Delta/\sigma)_{max} < 0.001$ | $\Delta\rho_{min} = -0.09$ e Å$^{-3}$ |

*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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O2 | 0.6966 (3) | 0.21666 (6) | 0.38262 (9) | 0.0633 (3) |
| H2 | 0.817 (4) | 0.2501 (10) | 0.4060 (16) | 0.095* |
| O1 | 0.3093 (3) | 0.11352 (6) | 0.35977 (10) | 0.0722 (4) |
| N1 | 1.0411 (3) | 0.30049 (6) | 0.51303 (11) | 0.0550 (3) |
| C7 | 0.6181 (3) | 0.18967 (7) | 0.47846 (12) | 0.0499 (4) |
| C6 | 0.7362 (3) | 0.21470 (8) | 0.58611 (12) | 0.0528 (4) |
| C10 | 1.1273 (3) | 0.43140 (8) | 0.51623 (13) | 0.0533 (4) |
| C8 | 0.9571 (3) | 0.26998 (8) | 0.59825 (13) | 0.0561 (4) |
| H8 | 1.040345 | 0.283593 | 0.671014 | 0.067* |
| C2 | 0.4103 (3) | 0.13480 (8) | 0.46848 (13) | 0.0560 (4) |
| C12 | 1.1668 (4) | 0.47353 (9) | 0.42431 (14) | 0.0620 (4) |
| H12 | 1.279589 | 0.456251 | 0.372334 | 0.074* |
| C9 | 1.2603 (4) | 0.35690 (8) | 0.53440 (15) | 0.0629 (4) |
| H9A | 1.400552 | 0.350226 | 0.483419 | 0.075* |
| H9B | 1.357488 | 0.352833 | 0.611939 | 0.075* |
| C11 | 0.9593 (4) | 0.45861 (9) | 0.59194 (14) | 0.0634 (4) |
| H11 | 0.930241 | 0.431002 | 0.654796 | 0.076* |
| C5 | 0.6416 (4) | 0.18568 (10) | 0.68255 (14) | 0.0697 (5) |
| H5 | 0.719087 | 0.202247 | 0.754451 | 0.084* |
| C3 | 0.3230 (4) | 0.10710 (9) | 0.56514 (17) | 0.0702 (5) |
| H3 | 0.186333 | 0.070445 | 0.558980 | 0.084* |
| C4 | 0.4365 (4) | 0.13326 (11) | 0.67187 (16) | 0.0786 (5) |
| H4 | 0.372061 | 0.114863 | 0.736433 | 0.094* |
| C1 | 0.0961 (4) | 0.05885 (10) | 0.34579 (18) | 0.0816 (6) |
| H1A | 0.044148 | 0.048311 | 0.266297 | 0.122* |
| H1B | −0.068976 | 0.075560 | 0.376457 | 0.122* |
| H1C | 0.168648 | 0.015654 | 0.385164 | 0.122* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O2 | 0.0715 (8) | 0.0674 (7) | 0.0513 (6) | −0.0180 (6) | 0.0096 (5) | 0.0000 (5) |
| O1 | 0.0729 (8) | 0.0703 (7) | 0.0742 (8) | −0.0230 (6) | 0.0139 (6) | −0.0124 (6) |
| N1 | 0.0550 (8) | 0.0453 (7) | 0.0626 (8) | 0.0025 (6) | 0.0021 (6) | −0.0016 (6) |
| C7 | 0.0525 (8) | 0.0459 (7) | 0.0519 (8) | 0.0048 (7) | 0.0102 (7) | 0.0047 (6) |
| C6 | 0.0519 (9) | 0.0532 (8) | 0.0523 (8) | 0.0089 (7) | 0.0044 (7) | 0.0069 (6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C10 | 0.0448 (9) | 0.0483 (8) | 0.0641 (9) | −0.0039 (6) | −0.0012 (7) | −0.0083 (7) |
| C8 | 0.0562 (9) | 0.0560 (9) | 0.0532 (9) | 0.0104 (7) | −0.0019 (7) | −0.0021 (7) |
| C2 | 0.0540 (9) | 0.0503 (8) | 0.0644 (10) | 0.0024 (7) | 0.0110 (8) | 0.0020 (7) |
| C12 | 0.0607 (10) | 0.0598 (9) | 0.0670 (10) | 0.0024 (8) | 0.0146 (8) | −0.0071 (8) |
| C9 | 0.0535 (9) | 0.0523 (9) | 0.0805 (11) | 0.0008 (7) | 0.0022 (8) | −0.0051 (8) |
| C11 | 0.0675 (11) | 0.0570 (9) | 0.0665 (10) | 0.0020 (8) | 0.0128 (9) | 0.0029 (7) |
| C5 | 0.0690 (11) | 0.0868 (12) | 0.0527 (9) | 0.0083 (10) | 0.0066 (8) | 0.0126 (8) |
| C3 | 0.0629 (11) | 0.0631 (10) | 0.0865 (13) | −0.0018 (8) | 0.0170 (10) | 0.0180 (9) |
| C4 | 0.0742 (12) | 0.0940 (14) | 0.0699 (12) | 0.0043 (11) | 0.0188 (10) | 0.0333 (10) |
| C1 | 0.0695 (12) | 0.0710 (12) | 0.1064 (15) | −0.0183 (9) | 0.0202 (11) | −0.0169 (10) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O2—C7 | 1.3438 (17) | C2—C3 | 1.375 (2) |
| O2—H2 | 0.858 (13) | C12—C11$^{\text{i}}$ | 1.386 (2) |
| O1—C2 | 1.3668 (19) | C12—H12 | 0.9300 |
| O1—C1 | 1.418 (2) | C9—H9A | 0.9700 |
| N1—C8 | 1.2717 (19) | C9—H9B | 0.9700 |
| N1—C9 | 1.463 (2) | C11—H11 | 0.9300 |
| C7—C6 | 1.396 (2) | C5—C4 | 1.361 (3) |
| C7—C2 | 1.403 (2) | C5—H5 | 0.9300 |
| C6—C5 | 1.396 (2) | C3—C4 | 1.388 (3) |
| C6—C8 | 1.451 (2) | C3—H3 | 0.9300 |
| C10—C12 | 1.374 (2) | C4—H4 | 0.9300 |
| C10—C11 | 1.379 (2) | C1—H1A | 0.9600 |
| C10—C9 | 1.511 (2) | C1—H1B | 0.9600 |
| C8—H8 | 0.9300 | C1—H1C | 0.9600 |

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|---|---|---|---|
| C7—O2—H2 | 104.1 (13) | C10—C9—H9A | 109.6 |
| C2—O1—C1 | 117.26 (13) | N1—C9—H9B | 109.6 |
| C8—N1—C9 | 118.17 (14) | C10—C9—H9B | 109.6 |
| O2—C7—C6 | 122.05 (13) | H9A—C9—H9B | 108.1 |
| O2—C7—C2 | 118.20 (14) | C10—C11—C12$^{\text{i}}$ | 120.95 (15) |
| C6—C7—C2 | 119.75 (13) | C10—C11—H11 | 119.5 |
| C7—C6—C5 | 119.45 (15) | C12$^{\text{i}}$—C11—H11 | 119.5 |
| C7—C6—C8 | 120.53 (13) | C4—C5—C6 | 120.35 (17) |
| C5—C6—C8 | 120.02 (15) | C4—C5—H5 | 119.8 |
| C12—C10—C11 | 118.18 (14) | C6—C5—H5 | 119.8 |
| C12—C10—C9 | 121.52 (14) | C2—C3—C4 | 120.71 (17) |
| C11—C10—C9 | 120.30 (15) | C2—C3—H3 | 119.6 |
| N1—C8—C6 | 122.40 (14) | C4—C3—H3 | 119.6 |
| N1—C8—H8 | 118.8 | C5—C4—C3 | 120.38 (16) |
| C6—C8—H8 | 118.8 | C5—C4—H4 | 119.8 |
| O1—C2—C3 | 125.21 (15) | C3—C4—H4 | 119.8 |
| O1—C2—C7 | 115.45 (13) | O1—C1—H1A | 109.5 |
| C3—C2—C7 | 119.34 (16) | O1—C1—H1B | 109.5 |
| C10—C12—C11$^{\text{i}}$ | 120.88 (14) | H1A—C1—H1B | 109.5 |
| C10—C12—H12 | 119.6 | O1—C1—H1C | 109.5 |

| | | | |
|---|---|---|---|
| C11$^{i}$—C12—H12 | 119.6 | H1A—C1—H1C | 109.5 |
| N1—C9—C10 | 110.42 (13) | H1B—C1—H1C | 109.5 |
| N1—C9—H9A | 109.6 | | |
| | | | |
| O2—C7—C6—C5 | 178.60 (14) | C11—C10—C12—C11$^{i}$ | −0.1 (3) |
| C2—C7—C6—C5 | −1.3 (2) | C9—C10—C12—C11$^{i}$ | 179.25 (15) |
| O2—C7—C6—C8 | −1.9 (2) | C8—N1—C9—C10 | −102.38 (16) |
| C2—C7—C6—C8 | 178.27 (13) | C12—C10—C9—N1 | −108.69 (17) |
| C9—N1—C8—C6 | 178.54 (13) | C11—C10—C9—N1 | 70.69 (19) |
| C7—C6—C8—N1 | 3.8 (2) | C12—C10—C11—C12$^{i}$ | 0.1 (3) |
| C5—C6—C8—N1 | −176.65 (14) | C9—C10—C11—C12$^{i}$ | −179.26 (15) |
| C1—O1—C2—C3 | 0.4 (2) | C7—C6—C5—C4 | 0.2 (2) |
| C1—O1—C2—C7 | −179.17 (14) | C8—C6—C5—C4 | −179.33 (15) |
| O2—C7—C2—O1 | 0.7 (2) | O1—C2—C3—C4 | −179.08 (16) |
| C6—C7—C2—O1 | −179.47 (13) | C7—C2—C3—C4 | 0.5 (2) |
| O2—C7—C2—C3 | −178.96 (14) | C6—C5—C4—C3 | 1.2 (3) |
| C6—C7—C2—C3 | 0.9 (2) | C2—C3—C4—C5 | −1.6 (3) |

Symmetry code: (i) −*x*+2, −*y*+1, −*z*+1.

### *Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O2—H2···N1 | 0.86 (1) | 1.79 (2) | 2.5877 (18) | 154 (2) |
| C8—H8···O2$^{ii}$ | 0.93 | 2.51 | 3.410 (2) | 162 |

Symmetry code: (ii) *x*+1/2, −*y*+1/2, *z*+1/2.