Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

Crystal structure of (*E*)-2,6-dimethoxy-4-{[(4-methoxyphenyl)imino]methyl}phenol

Md. Serajul Haque Faizi,[a] Mohamad Nadeem Lone,[b] Necmi Dege,[c] Sergey Malinkin[d]* and Tatiana Yu. Sliva[d]

[a]Department of Chemistry, Langat Singh College, Babasaheb Bhimrao Ambedkar Bihar University, Muzaffarpur, Bihar, India, [b]Department of Chemistry, Govt. College For Women, Udhampur, Jammu and Kashmir 182 101, India, [c]Ondokuz Mayıs University, Arts and Sciences Faculty, Department of Physics, Atakum 55139 Samsun, Turkey, and [d]Department of Chemistry, National Taras Shevchenko University of Kiev, 64/13, Volodymyrska Street, City of Kyiv, 01601, Ukraine. *Correspondence e-mail: malinachem88@gmail.com

Received 20 August 2018
Accepted 26 September 2018

Edited by S. V. Lindeman, Marquette University, USA

Keywords: crystal structure; syringaldehyde; 4-methoxyaniline; 4-hydroxy-3,5-dimethoxybenzaldehyde.

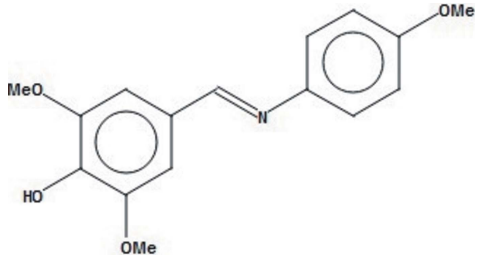
CCDC reference: 1843910

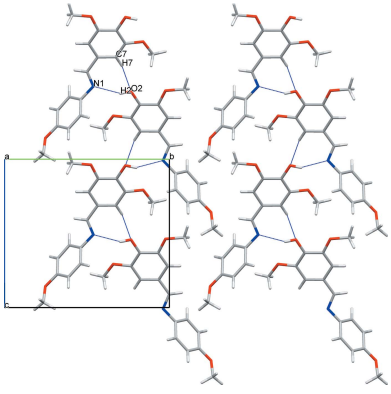
Supporting information: this article has supporting information at journals.iucr.org/e

In the title compound, $C_{16}H_{17}NO_4$, the dihedral angle between benzene rings is 72.7 (2)°. The methoxy groups are rotated by 2.4 (2) and −4.9 (2) (benzilidene moiety) and by 5.6 (3)° (aniline moiety) relative to the adjacent benzene ring. In the crystal, the molecules are linked into chains along [101] through C—H···O and O—H···N hydrogen bonds.

1. Chemical context

Syringaldehyde is a product of the catalytic decomposition of lignin (Crestini *et al.*, 2010). Syringaldehyde is widely used as a molecular marker to monitor pollution sources and detect the extent of combustion (Robinson *et al.*, 2006). It is also known to be an antioxidant (Ibrahim *et al.*, 2012), anticancer, anti-inflammatory (Duke, 2003) and antifungal agent (Gurpilhares *et al.*, 2006). In addition, its Schiff bases are known to exhibit a wide range of biological activities (Shi & Zhou, 2011; da Silva *et al.*, 2011).





2. Structural commentary

The molecular structure of the title molecule is shown on Fig. 1. The compound has a *trans*-configuration of the C9═N1 double bond. The molecule has a non-planar conformation with the two benzene rings forming a dihedral angle of 72.7 (2)°. The methoxy groups are almost co-planar with the planes of the adjacent aromatic rings [the C1—O1—C4—C3, C2—O3—C6—C7 and C16—O4—C13—C12 torsion angles are −4.9 (2), 2.4 (2) and 5.6 (3)°, respectively].

3. Supramolecular features

In the crystal, the molecules are connected *via* C7—H7···O2^{ii} and O2—H2···N1^{i} hydrogen bonding (Table 1), forming chains along the [101] direction (Fig. 2).

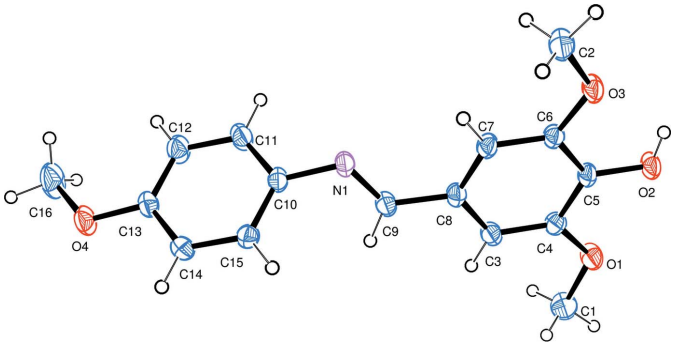


Figure 1
A view of the molecular structure of the title compound, with the atom labelling. Displacement ellipsoids are drawn at the 40% probability level.

4. Database survey

A search of the Cambridge Structural Database (CSD version 5.39, update of May 2018; Groom *et al.*, 2016) revealed the structures of five similar Schiff bases based on *p*-methoxyaniline and *p*-hydroxybenzaldehyde: 4-[(4-methoxyphenylimino)methyl]phenol, (I) (VUKDEK; Yeap *et al.*, 1992), (*E*)-5-methoxy-2-[(4-methoxyphenylimino)methyl]phenol, (II) (NURNAQ; Sahin *et al.*, 2010), 2-methoxy-4-{[(4-methoxyphenyl)imino]methyl}phenol, (III) (MOTLIR; Singh *et al.*, 2008), 2,6-di-*tert*-butyl-4-[(4-methoxyphenylimino)methyl]-phenol, (IV) (WEFTEH; Xin *et al.*, 2006) and 5-bromo-2-methoxy-4-{[(4-methoxyphenyl)imino]methyl}phenol monohydrate, (V) (GAPFEK; Mao *et al.*, 2012). The dihedral angle between the benzene rings in the title compound [72.7 (2)°] is larger than those in compounds (I), (III) and (IV) (49.75–53.63°). Compounds (II) and (V) are almost planar. In all of the compounds, the methoxy groups deviate from the plane of aromatic system. There are no C—H···π or π–π interactions in the crystal structure of the title compound, in contrast to what is observed for compounds (I), (IV) and (V).

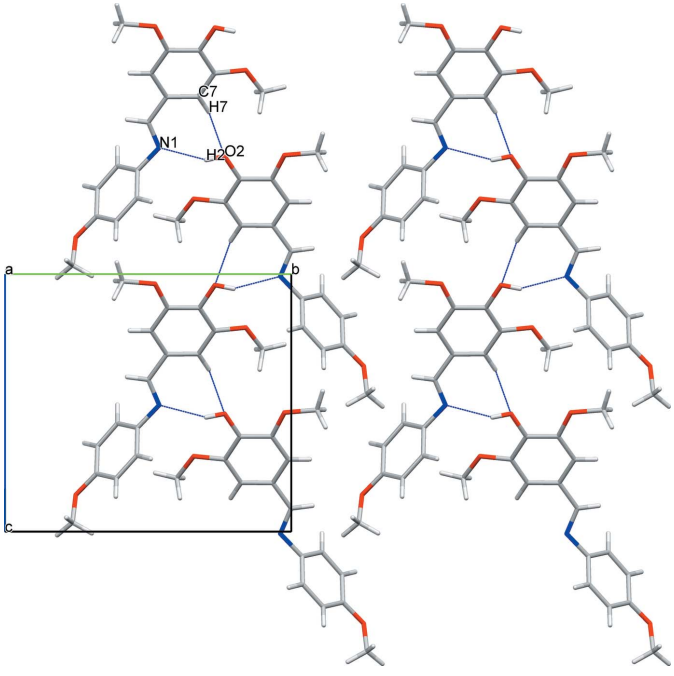


Figure 2
A view along the *a* axis of the crystal packing. Dashed lines indicate hydrogen bonds (see Table 1).

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···N1^{i}	0.82	2.21	2.9415 (18)	149
C7—H7···O2^{ii}	0.93	2.29	3.2043 (18)	167

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (ii) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$.

5. Synthesis

4-Hydroxy-3,5-dimethoxybenzaldehyde (syringaldehyde) (0.05 mol) was added to a mixture of 50 ml of methanol and *p*-methoxyaniline (PMA) (5 ml, 0.05 mol) and 50 ml of distilled water. The reaction mixture was taken in a clean 250 ml round-bottom flask and stirred well with a magnetic stirrer. It was then refluxed for 7 h. The dark-yellow product that formed was separated by filtration, dried under vacuum and recrystallized from methanol solution upon slow evaporation for two days (yield 65%, m.p. 353–357 K).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were positioned geom-

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{17}NO_4$
M_r	287.30
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	296
a, b, c (Å)	10.4996 (15), 12.4896 (18), 11.8128 (17)
β (°)	107.936 (5)
V (Å^3)	1473.8 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.45 × 0.33 × 0.21
Data collection	
Diffractometer	Bruker APEXII CCD
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	19289, 2887, 2306
R_{int}	0.035
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.116, 1.05
No. of reflections	2887
No. of parameters	194
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.17, −0.21

Computer programs: *APEX2* and *SAINT* (Bruker, 2004), *SHELXS97* (Sheldrick 2008), *SHELXL2017* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008) and *PLATON* (Spek, 2009).

etrically and refined using a riding model: O—H = 0.82–0.96 Å and C—H = 0.93–0.96 Å with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(O, Cmethyl).

Acknowledgements

The authors are grateful to the Department of Chemistry, Langat Singh College, Babasaheb Bhimrao Ambedkar Bihar University, Muzaffarpur, Bihar, India for the research lab and National Taras Shevchenko University, Department of Chemistry, Volodymyrska Str. 64, 01601 Kyiv, Ukraine, for financial support.

References

Bruker (2004). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Crestini, C., Crucianelli, M., Orlandi, M. & Saladino, R. (2010). *Catal. Today*, **156**, 8–22.
Duke, J. A. (2003). CRC book of medicinal spices. Boca Raton, Florida: CRC Press LLC.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.
Gurpilhares, D. B., Pessoa, A. Jr & Roberto, I. C. (2006). *Process Biochem.* **41**, 631–637.
Ibrahim, M. N., Sriprasanthi, R. B., Shamsudeen, S., Adam, F. & Bhawani, S. A. (2012). *BioResources J.* **7**, 4377–4399.
Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
Mao, C.-G., Wang, S.-S., Su, D.-C. & Qian, S.-S. (2012). *Acta Cryst.* E**68**, o249.
Robinson, A. L., Subramanian, R., Donahue, N. M., Bernardo-Bricker, A. & Rogge, W. F. (2006). *Environ. Sci. Technol.* **40**, 7811–7819.
Sahin, O., Buyukgungor, O., Albayrak, C. & Odabasoglu, M. (2010). *Chin. J. Struct. Chem.(Jiegou Huaxue)*, **29**, 359–361.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* A**71**, 3–8.
Shi, Y. & Zhou, C. H. (2011). *Bioorg. Med. Chem. Lett.* **21**, 956–960.
Silva, C. M. da, da Silva, D. L., Modolo, L. V., Alves, R. B., de Resende, M. A., Martins, C. V. B., de Fátima, A. & Ângelo, (2011). *J. Adv. Res.* **2**, 1–8.
Singh, N. B., Das, S. S., Gupta, P., Gupta, A. & Fröhlich, R. (2008). *Mol. Cryst. Liq. Cryst.* **490**, 106–123.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Xin, C.-W., Zeng, T. & Li, J.-S. (2006). *Acta Cryst.* E**62**, o1560–o1561.
Yeap, G.-Y., Fun, H.-K., Teoh, S.-G., Teo, S.-B., Chinnakali, K. & Yip, B.-C. (1992). *Acta Cryst.* C**48**, 2257–2258.

supporting information

Acta Cryst. (2018). E**74**, 1540-1542 [https://doi.org/10.1107/S2056989018013713]

Crystal structure of (*E*)-2,6-dimethoxy-4-{[(4-methoxyphenyl)imino]methyl}-phenol

Md. Serajul Haque Faizi, Mohamad Nadeem Lone, Necmi Dege, Sergey Malinkin and Tatiana Yu. Sliva

Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick 2008); program(s) used to refine structure: *SHELXL2017* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL2017* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

(*E*)-2,6-Dimethoxy-4-{[(4-methoxyphenyl)imino]methyl}phenol

Crystal data

$C_{16}H_{17}NO_4$
$M_r = 287.30$
Monoclinic, $P2_1/n$
$a = 10.4996$ (15) Å
$b = 12.4896$ (18) Å
$c = 11.8128$ (17) Å
$\beta = 107.936$ (5)°
$V = 1473.8$ (4) Å^3
$Z = 4$
$F(000) = 608$
$D_x = 1.295$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6353 reflections
$\theta = 2.3$–$28.3°$
$\mu = 0.09$ mm^{-1}
$T = 296$ K
Prism, colorless
0.45 × 0.33 × 0.21 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
19289 measured reflections
2887 independent reflections
2306 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.3°$
$h = -12 \rightarrow 12$
$k = -15 \rightarrow 15$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.116$
$S = 1.05$
2887 reflections
194 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0509P)^2 + 0.4295P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O2	0.34000 (12)	0.73324 (9)	0.04196 (10)	0.0465 (3)
H2	0.347012	0.797633	0.056037	0.070*
O3	0.52685 (12)	0.84064 (9)	0.20703 (10)	0.0473 (3)
O1	0.32775 (12)	0.52385 (9)	0.03728 (11)	0.0530 (4)
O4	1.04377 (13)	0.24711 (10)	0.85736 (10)	0.0524 (3)
N1	0.76944 (13)	0.53851 (10)	0.50837 (11)	0.0388 (3)
C10	0.83876 (15)	0.46251 (12)	0.59633 (13)	0.0350 (4)
C15	0.93325 (16)	0.39274 (12)	0.57930 (14)	0.0369 (4)
H15	0.951974	0.392859	0.507304	0.044*
C8	0.61237 (15)	0.56465 (13)	0.31098 (13)	0.0355 (4)
C4	0.42672 (15)	0.56804 (13)	0.12973 (13)	0.0371 (4)
C6	0.53028 (15)	0.73189 (12)	0.21930 (13)	0.0344 (4)
C14	1.00014 (16)	0.32282 (12)	0.66827 (14)	0.0384 (4)
H14	1.064957	0.277361	0.656291	0.046*
C7	0.61974 (15)	0.67549 (13)	0.30970 (13)	0.0361 (4)
H7	0.684472	0.711472	0.369303	0.043*
C9	0.69704 (15)	0.50052 (13)	0.40957 (14)	0.0377 (4)
H9	0.697878	0.426753	0.399120	0.045*
C5	0.43155 (15)	0.67913 (13)	0.13033 (13)	0.0345 (4)
C3	0.51728 (16)	0.51059 (13)	0.21959 (14)	0.0386 (4)
H3	0.514739	0.436151	0.219040	0.046*
C13	0.97179 (16)	0.31969 (13)	0.77481 (14)	0.0380 (4)
C11	0.81296 (18)	0.46051 (15)	0.70406 (15)	0.0486 (5)
H11	0.751385	0.508458	0.717490	0.058*
C12	0.87678 (18)	0.38867 (16)	0.79243 (16)	0.0505 (5)
H12	0.855831	0.386815	0.863378	0.061*
C2	0.6266 (2)	0.90036 (14)	0.29204 (16)	0.0546 (5)
H2B	0.615906	0.975079	0.272312	0.082*
H2C	0.713615	0.877111	0.291596	0.082*
H2D	0.617836	0.889302	0.369713	0.082*
C1	0.3232 (2)	0.41090 (15)	0.02729 (18)	0.0603 (5)
H1A	0.255752	0.390654	−0.044946	0.090*
H1B	0.302110	0.380713	0.094094	0.090*
H1C	0.408703	0.384713	0.025963	0.090*
C16	1.0104 (2)	0.2356 (2)	0.96441 (19)	0.0743 (7)
H16A	0.918409	0.214220	0.945995	0.111*
H16B	1.023357	0.302705	1.006081	0.111*
H16C	1.066751	0.182152	1.013549	0.111*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0477 (7)	0.0351 (6)	0.0389 (6)	0.0019 (5)	−0.0128 (5)	0.0021 (5)
O3	0.0525 (7)	0.0317 (6)	0.0402 (6)	−0.0019 (5)	−0.0114 (5)	0.0026 (5)
O1	0.0521 (7)	0.0372 (7)	0.0488 (7)	−0.0005 (5)	−0.0152 (6)	−0.0056 (5)
O4	0.0602 (8)	0.0525 (8)	0.0453 (7)	0.0195 (6)	0.0174 (6)	0.0221 (6)
N1	0.0403 (7)	0.0353 (7)	0.0342 (7)	0.0050 (6)	0.0017 (6)	0.0049 (6)
C10	0.0353 (8)	0.0315 (8)	0.0324 (8)	−0.0008 (6)	0.0019 (6)	0.0039 (6)
C15	0.0442 (9)	0.0333 (8)	0.0314 (8)	0.0013 (7)	0.0091 (7)	0.0009 (6)
C8	0.0328 (8)	0.0371 (8)	0.0322 (8)	0.0034 (6)	0.0036 (6)	0.0025 (6)
C4	0.0341 (8)	0.0375 (9)	0.0337 (8)	−0.0001 (7)	0.0016 (6)	−0.0034 (6)
C6	0.0354 (8)	0.0323 (8)	0.0308 (8)	−0.0002 (6)	0.0034 (6)	0.0008 (6)
C14	0.0418 (9)	0.0317 (8)	0.0413 (9)	0.0055 (7)	0.0121 (7)	0.0022 (7)
C7	0.0339 (8)	0.0380 (9)	0.0291 (8)	−0.0018 (7)	−0.0011 (6)	−0.0006 (6)
C9	0.0368 (8)	0.0333 (8)	0.0389 (9)	0.0028 (7)	0.0056 (7)	0.0049 (7)
C5	0.0319 (8)	0.0373 (9)	0.0285 (8)	0.0033 (6)	0.0007 (6)	0.0030 (6)
C3	0.0402 (9)	0.0314 (8)	0.0394 (9)	0.0030 (7)	0.0052 (7)	0.0017 (7)
C13	0.0378 (9)	0.0348 (9)	0.0380 (9)	0.0031 (7)	0.0066 (7)	0.0080 (7)
C11	0.0460 (10)	0.0548 (11)	0.0458 (10)	0.0201 (8)	0.0156 (8)	0.0111 (8)
C12	0.0529 (11)	0.0624 (12)	0.0400 (9)	0.0154 (9)	0.0198 (8)	0.0145 (8)
C2	0.0591 (12)	0.0363 (10)	0.0509 (11)	−0.0115 (8)	−0.0089 (9)	0.0027 (8)
C1	0.0658 (13)	0.0427 (11)	0.0568 (11)	−0.0089 (9)	−0.0042 (10)	−0.0113 (9)
C16	0.0816 (16)	0.0896 (17)	0.0569 (13)	0.0299 (13)	0.0291 (11)	0.0395 (12)

Geometric parameters (Å, º)

O1—C2^{i}	3.159 (2)	C6—C7	1.379 (2)
O2—C5	1.3610 (17)	C6—C5	1.394 (2)
O2—H2	0.8200	C14—C13	1.380 (2)
O3—C6	1.3652 (19)	C14—H14	0.9300
O3—C2	1.4193 (19)	C7—H7	0.9300
O1—C4	1.3704 (18)	C9—H9	0.9300
O1—C1	1.415 (2)	C3—H3	0.9300
O4—C13	1.3748 (18)	C13—C12	1.382 (2)
O4—C16	1.420 (2)	C11—C12	1.383 (2)
N1—C9	1.2722 (19)	C11—H11	0.9300
N1—C10	1.4299 (19)	C12—H12	0.9300
C10—C11	1.380 (2)	C2—H2B	0.9600
C10—C15	1.381 (2)	C2—H2C	0.9600
C15—C14	1.381 (2)	C2—H2D	0.9600
C15—H15	0.9300	C1—H1A	0.9600
C8—C7	1.387 (2)	C1—H1B	0.9600
C8—C3	1.398 (2)	C1—H1C	0.9600
C8—C9	1.466 (2)	C16—H16A	0.9600
C4—C3	1.387 (2)	C16—H16B	0.9600
C4—C5	1.388 (2)	C16—H16C	0.9600

C5—O2—H2	109.5	C4—C5—C6	119.60 (13)
C6—O3—C2	117.27 (12)	C4—C3—C8	119.96 (15)
C4—O1—C1	117.75 (13)	C4—C3—H3	120.0
C13—O4—C16	117.76 (14)	C8—C3—H3	120.0
C9—N1—C10	116.47 (13)	O4—C13—C14	116.08 (14)
C11—C10—C15	118.47 (14)	O4—C13—C12	124.69 (15)
C11—C10—N1	118.78 (14)	C14—C13—C12	119.22 (14)
C15—C10—N1	122.73 (14)	C10—C11—C12	121.36 (16)
C14—C15—C10	120.54 (15)	C10—C11—H11	119.3
C14—C15—H15	119.7	C12—C11—H11	119.3
C10—C15—H15	119.7	C13—C12—C11	119.69 (16)
C7—C8—C3	120.18 (14)	C13—C12—H12	120.2
C7—C8—C9	122.12 (14)	C11—C12—H12	120.2
C3—C8—C9	117.62 (14)	O3—C2—H2B	109.5
O1—C4—C3	125.06 (15)	O3—C2—H2C	109.5
O1—C4—C5	115.09 (13)	H2B—C2—H2C	109.5
C3—C4—C5	119.85 (14)	O3—C2—H2D	109.5
O3—C6—C7	125.44 (13)	H2B—C2—H2D	109.5
O3—C6—C5	113.65 (13)	H2C—C2—H2D	109.5
C7—C6—C5	120.91 (14)	O1—C1—H1A	109.5
C13—C14—C15	120.67 (15)	O1—C1—H1B	109.5
C13—C14—H14	119.7	H1A—C1—H1B	109.5
C15—C14—H14	119.7	O1—C1—H1C	109.5
C6—C7—C8	119.44 (14)	H1A—C1—H1C	109.5
C6—C7—H7	120.3	H1B—C1—H1C	109.5
C8—C7—H7	120.3	O4—C16—H16A	109.5
N1—C9—C8	124.73 (15)	O4—C16—H16B	109.5
N1—C9—H9	117.6	H16A—C16—H16B	109.5
C8—C9—H9	117.6	O4—C16—H16C	109.5
O2—C5—C4	118.44 (13)	H16A—C16—H16C	109.5
O2—C5—C6	121.96 (14)	H16B—C16—H16C	109.5

C9—N1—C10—C11	−120.05 (18)	C3—C4—C5—C6	2.1 (2)
C9—N1—C10—C15	61.7 (2)	O3—C6—C5—O2	−1.2 (2)
C11—C10—C15—C14	0.0 (2)	C7—C6—C5—O2	178.26 (15)
N1—C10—C15—C14	178.20 (15)	O3—C6—C5—C4	177.70 (14)
C1—O1—C4—C3	−4.9 (3)	C7—C6—C5—C4	−2.8 (2)
C1—O1—C4—C5	175.89 (16)	O1—C4—C3—C8	−178.61 (15)
C2—O3—C6—C7	2.4 (2)	C5—C4—C3—C8	0.5 (2)
C2—O3—C6—C5	−178.17 (15)	C7—C8—C3—C4	−2.4 (2)
C10—C15—C14—C13	1.4 (2)	C9—C8—C3—C4	174.26 (15)
O3—C6—C7—C8	−179.66 (15)	C16—O4—C13—C14	−175.25 (18)
C5—C6—C7—C8	0.9 (2)	C16—O4—C13—C12	5.6 (3)
C3—C8—C7—C6	1.7 (2)	C15—C14—C13—O4	179.86 (15)
C9—C8—C7—C6	−174.84 (15)	C15—C14—C13—C12	−1.0 (3)
C10—N1—C9—C8	176.30 (14)	C15—C10—C11—C12	−1.8 (3)
C7—C8—C9—N1	10.4 (3)	N1—C10—C11—C12	179.89 (16)
C3—C8—C9—N1	−166.23 (16)	O4—C13—C12—C11	178.25 (17)

O1—C4—C5—O2	0.2 (2)	C14—C13—C12—C11	−0.8 (3)
C3—C4—C5—O2	−178.98 (14)	C10—C11—C12—C13	2.2 (3)
O1—C4—C5—C6	−178.72 (14)		

Symmetry code: (i) $x-1/2, -y+3/2, z-1/2$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···N1^{i}	0.82	2.21	2.9415 (18)	149
C7—H7···O2^{ii}	0.93	2.29	3.2043 (18)	167

Symmetry codes: (i) $x-1/2, -y+3/2, z-1/2$; (ii) $x+1/2, -y+3/2, z+1/2$.