Acta Cryst E
CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

The crystal structure and Hirshfeld surface analysis of 1-(2,5-dimethoxyphenyl)-2,2,6,6-tetramethylpiperidine

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Received 29 April 2020
Accepted 30 April 2020

Edited by G. Diaz de Delgado, Universidad de Los Andes, Venezuela

Keywords: crystal structure; piperidine; hydrogen bonding; Hirshfeld surface analysis; energy frameworks.

CCDC reference: 2000223

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

In the title compound, $C_{17}H_{27}NO_2$, the piperidine ring has a chair conformation and is positioned normal to the benzene ring. In the crystal, molecules are linked by C—H$\cdots$O hydrogen bonds, forming chains propagating along the *c*-axis direction.

1. Chemical context

During research on phytotoxins produced by the *Ceratocystis fimbriata* species (Tiouabi, 2005), the pathogenic agents responsible for the infections of plane, coffee and elm trees, analytical and spectroscopic studies enabled the isolation of a number of isocoumarins in small quantities. In order to confirm their molecular structures and especially to study their phytotoxicity and pathogenicity it was necessary to develop efficient methods for the total syntheses of these various isocoumarins. The title compound (**3**) was synthesized as a side product during the synthesis of the intermediate, methyl 3,6-dimethoxy-2-(2-methoxy-2-oxoethyl)benzoate (**2**) (see Fig. 1), necessary for the total synthesis of the isocoumarin 5,8-dimethoxy-3-methyl-1*H*-isochromen-1-one (Tiouabi, 2005).

2. Structural commentary

The molecular structure of the title compound, 1-(2,5-dimethoxyphenyl)-2,2,6,6-tetramethylpiperidine (**3**), is illustrated in Fig. 2. The piperidine ring has a chair conformation with atoms N1 and C11 being displaced by −0.5171 (12) and 0.6876 (15) Å, respectively, from the mean plane of the

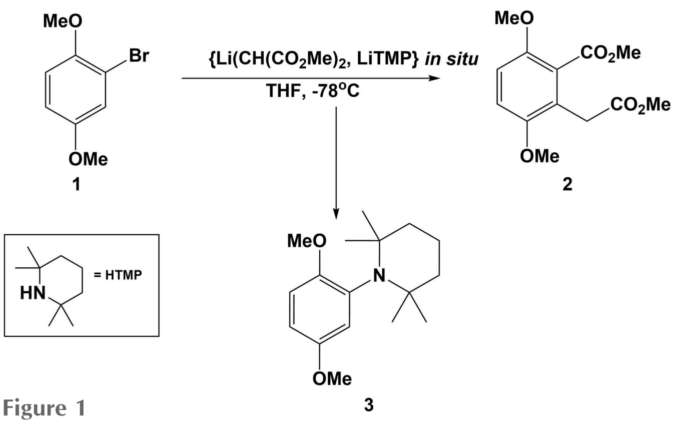
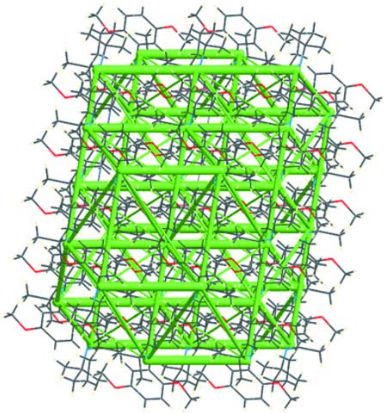
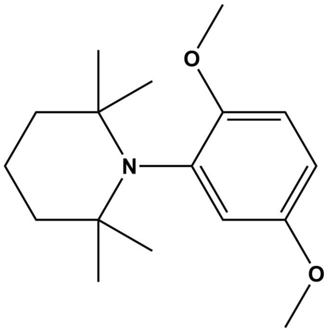


Figure 1
The reaction scheme resulting in the formation of the title compound, **3**.



remaining four C atoms (C9/C10/C12/C13). This mean plane is normal to the plane of the benzene ring (C1–C6), with a dihedral angle of 88.34 (9)°. Planes C2/O1/C7 and C5/O2/C8, involving the methoxy groups, are inclined to the benzene ring by 13.23 (15) and 10.45 (15)°, respectively.



3. Supramolecular features

In the crystal of **3**, molecules related by the glide plane are linked by C—H⋯O hydrogen bonds, forming chains propagating along the *c*-axis direction (Fig. 3 and Table 1). There are no other significant intermolecular interactions present in the crystal.

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

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C8—H8*B*⋯O2$^{\rm i}$	0.98	2.51	3.495 (2)	180

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

Table 2
Short interatomic contacts (Å)[a] in the crystal of compound **3**.

Atom1⋯Atom2	Length	Length − vdW
O2⋯H8*B*$^{\rm ii}$	2.515	−0.205
C4⋯H15*C*$^{\rm iii}$	2.830	−0.070
O2⋯H15*B*$^{\rm ii}$	2.686	−0.034
C2⋯H8*A*$^{\rm iv}$	2.918	0.018
C3⋯H14*C*$^{\rm iii}$	2.977	0.077
H7*C*⋯H17*A*$^{\rm iv}$	2.484	0.084
O1⋯H16*A*$^{\rm iv}$	2.814	0.094

Note: (*a*) Calculated using *Mercury* (Macrae *et al.*, 2020). Symmetry codes: (ii) $x, -y + \frac{1}{2}, z - \frac{1}{2}$; (iii) $x, y, z - 1$; (iv) $x - 1, y, z$.

4. Hirshfeld surface analysis and two-dimensional fingerprint plots

The Hirshfeld surface analysis (Spackman & Jayatilaka, 2009) and the associated two-dimensional fingerprint plots (McKinnon *et al.*, 2007) were performed with *CrystalExplorer17.5* (Turner *et al.*, 2017). For an excellent explanation of the use of Hirshfeld surface analysis and other calculations, such as energy frameworks, to study the molecular packing see the recent article by Tiekink and collaborators (Tan *et al.*, 2019). The Hirshfeld surface is colour-mapped with the normalized contact distance, $d_{\rm norm}$, from red (distances shorter than the sum of the van der Waals radii) through white to blue (distances longer than the sum of the van der Waals radii). The energy frameworks (Turner *et al.*, 2015; Tan *et al.*, 2019) are represented by cylinders joining the centroids of molecular pairs using red, green and blue colour codes for the $E_{\rm electrostatic}$,

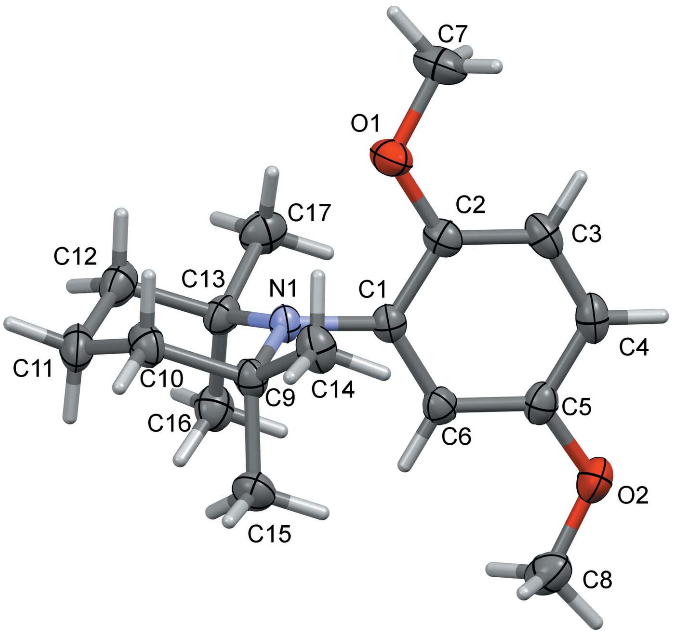


Figure 2
The molecular structure of compound **3**, with atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

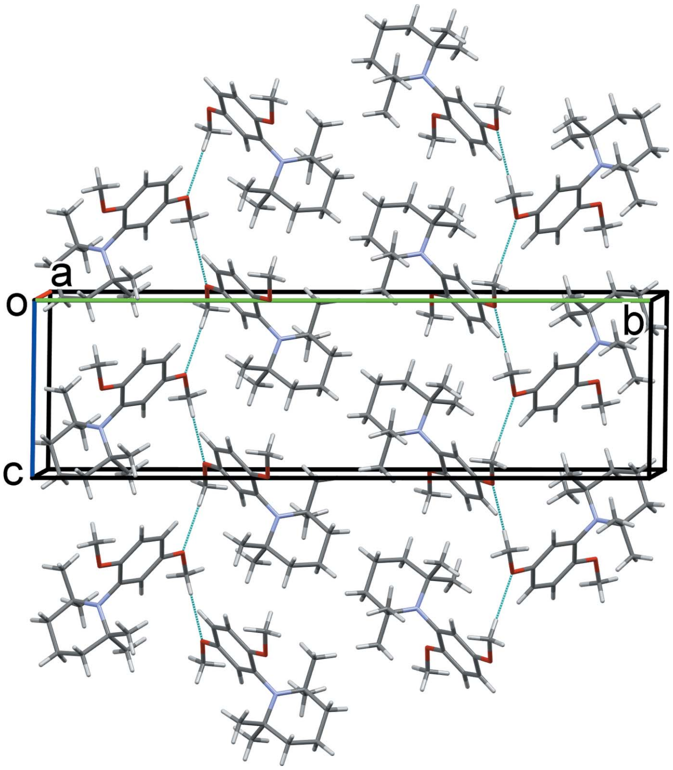


Figure 3
A view along the *a* axis of the crystal packing of compound **3**. The hydrogen bonds (Table 1) are shown as dashed lines.

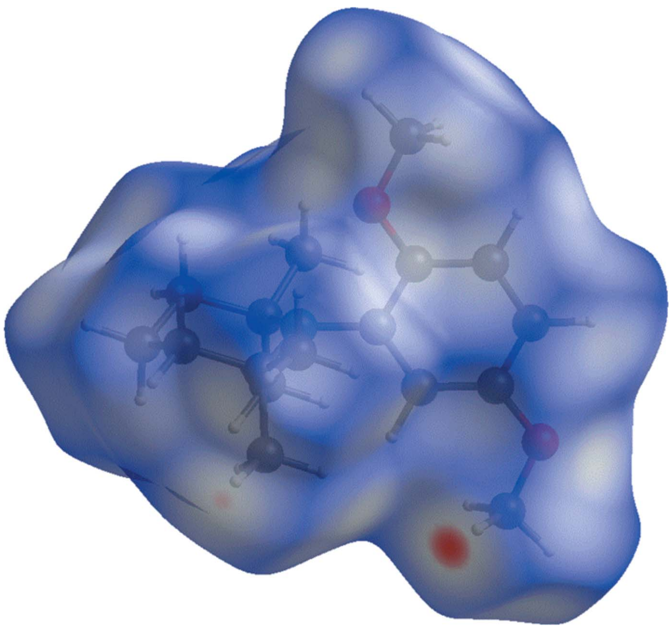


Figure 4
The Hirshfeld surface of compound **3** mapped over $d_{\rm norm}$, in the colour range −0.1434 to 1.2136 a.u..

$E_{\rm dispersion}$ and $E_{\rm total}$ energy components, respectively. The radius of the cylinder is proportional to the magnitude of the interaction energy.

A view of the Hirshfeld surface of **3** mapped over $d_{\rm norm}$ is shown in Fig. 4. The short interatomic O···H/H···O contacts are indicated by the faint red spots. A full list of short interatomic contacts in the crystal of **3** are given in Table 2. The most significant contacts, apart from H···H contacts, are O···H and C···H contacts as confirmed by the two-dimensional fingerprint plots (Fig. 5). The principal intermolecular contacts for **3**, are delineated into H···H at 84.1% (Fig. 5*b*), O···H/H···O at 8.3% (Fig. 5*c*) and C···H/H···C at 7.6% (Fig. 5*d*) contacts. The intermolecular contacts are therefore dominated by dispersion forces (H···H at 84.1%; Fig. 5*b*). This is confirmed by the energy frameworks shown in Fig. 6. The energy frameworks were adjusted to the same scale factor of 80 with a cut-off value of 5 kJ mol^{-1} within 2 × 2 × 2 unit cells, and obtained using the wave function calculated at the HF/3-21G level of theory.

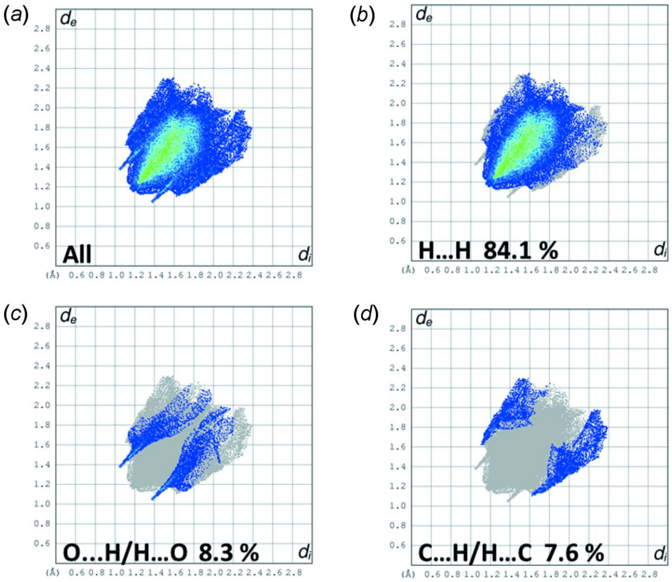


Figure 5
(*a*) The full two-dimensional fingerprint plot for compound **3**, and fingerprint plots delineated into (*b*) H···H at 84.1%, (*c*) O···H/H···O at 8.3% and (*d*) C···H/H···C at 7.6% contacts.

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{27}NO_2$
M_r	277.39
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	173
a, b, c (Å)	6.8817 (10), 28.249 (4), 8.1369 (13)
β (°)	99.649 (12)
V (Å^3)	1559.4 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.40 × 0.10 × 0.10
Data collection	
Diffractometer	STOE IPDS 2
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10596, 2770, 1695
$R_{\rm int}$	0.085
$(\sin \theta/\lambda)_{\rm max}$ (Å^{-1})	0.599
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.037, 0.073, 0.83
No. of reflections	2770
No. of parameters	188
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\rm max}$, $\Delta\rho_{\rm min}$ (e Å^{-3})	0.13, −0.13

Computer programs: *X-AREA* and *X-RED32* (Stoe & Cie, 2005), *SHELXS97* (Sheldrick, 2008), *SHELXL2018/3* (Sheldrick, 2015), *PLATON* (Spek, 2020), *Mercury* (Macrae *et al.*, 2020) and *publCIF* (Westrip, 2010).

5. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.41, last update March 2020; Groom *et al.*, 2016) for 1-(phenyl)-2,2,6,6-tetramethylpiperidines gave 26 hits (see file S1 in the supporting information). A number of these structures involve heteroaryl and heterocyclic aluminium compounds, see for example CSD refcodes CEGLUY, CEGMF, CEGMEJ, CEGMIN, CEGMOT and CEGMUZ (Chen *et al.*, 2017). They also include a number of borohydride derivatives, see for example CSD refcodes JAKZON, JAKZUT, JALBAC and JALBEG (Chernichenko *et al.*, 2017). Only one compound has a methoxy substituent, *viz*. 1-(2-iodo-3-methoxyphenyl)-2,2,6,6-tetramethylpiperidine (VAPCUM; Crosbie *et al.*, 2012). In these eleven compounds, the piperidine ring has a chair conformation with the mean plane of the four planar C atoms being inclined to the plane of the benzene ring by dihedral angles varying from *ca* 83.0 to 90.0°. In compound **3** this dihedral angle is similar at 88.34 (9)°.

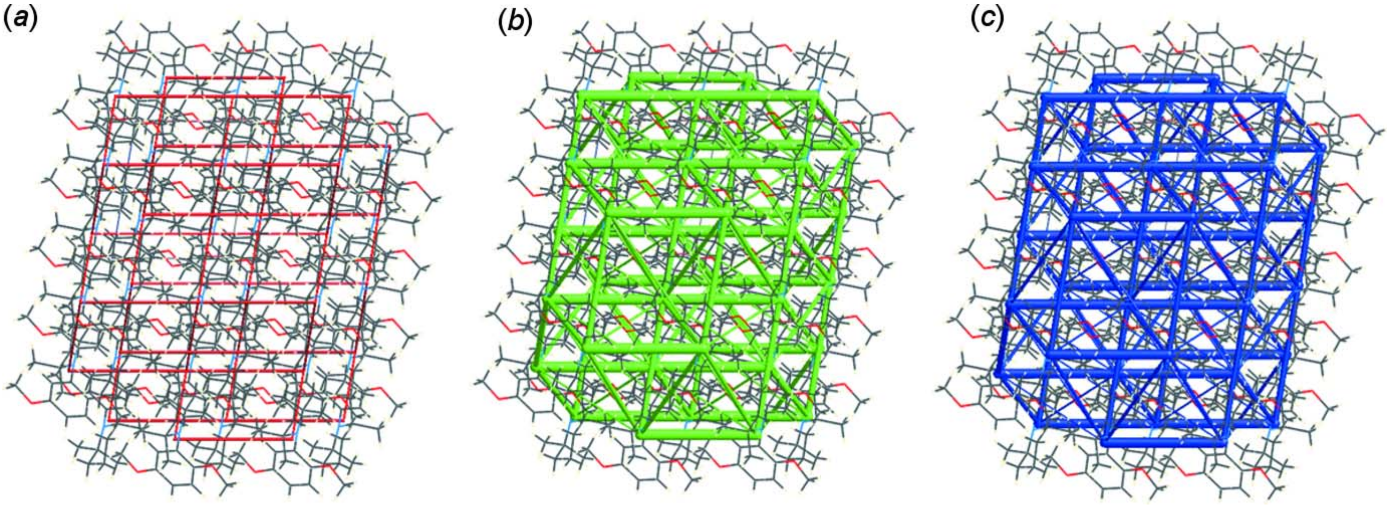


Figure 6
The energy frameworks viewed down the *b*-axis direction comprising (*a*) electrostatic potential forces, (*b*) dispersion forces and (*c*) total energy for a cluster about a reference molecule of **3**. The energy frameworks were adjusted to the same scale factor of 80 with a cut-off value of 5 kJ mol^{-1} within 2 × 2 × 2 unit cells.

6. Synthesis and crystallization

The synthesis of compound **3** is illustrated in Fig. 1. It arises as a result of the condensation of 2-bromo-1,4-dimethoxybenzene (**1**) with tetramethylpiperidene (HTMP). It is a side product obtained during the synthesis of methyl 3,6-dimethoxy-2-(2-methoxy-2-oxoethyl)benzoate (**2**) (Tiouabi, 2005). Colourless rod-like crystals of **3** were obtained by slow evaporation at room temperature of a solution in acetone.There are no analytical or spectroscopic data available for compound **3**.

7. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 3. The hydrogen atoms were fixed geometrically (C—H = 0.95–0.99 Å) and allowed to ride on their parent atoms with $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C-methyl) and 1.2$U_{\rm eq}$(C) for other H atoms.

Acknowledgements

RT and HSE are grateful to the University of Neuchâtel for their support over the years.

Funding information

Funding for this research was provided by: Swiss National Science Foundation and the University of Neuchâtel.

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supporting information

Acta Cryst. (2020). E**76**, 794-797   [https://doi.org/10.1107/S2056989020005952]

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Computing details

Data collection: *X-AREA* (Stoe & Cie, 2005); cell refinement: *X-AREA* (Stoe & Cie, 2005); data reduction: *X-RED32* (Stoe & Cie, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015); molecular graphics: *PLATON* (Spek, 2020) and *Mercury* (Macrae *et al.*, 2020); software used to prepare material for publication: *SHELXL2018/3* (Sheldrick, 2015), *PLATON* (Spek, 2020) and *publCIF* (Westrip, 2010).

1-(2,5-Dimethoxyphenyl)-2,2,6,6-tetramethylpiperidine

Crystal data

$C_{17}H_{27}NO_2$
$M_r = 277.39$
Monoclinic, $P2_1/c$
$a = 6.8817$ (10) Å
$b = 28.249$ (4) Å
$c = 8.1369$ (13) Å
$\beta = 99.649$ (12)°
$V = 1559.4$ (4) Å^3
$Z = 4$
$F(000) = 608$
$D_x = 1.182$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4940 reflections
$\theta = 1.4$–25.5°
$\mu = 0.08$ mm^{-1}
$T = 173$ K
Rod, colourless
0.40 × 0.10 × 0.10 mm

Data collection

STOE IPDS 2 diffractometer
Radiation source: fine-focus sealed tube
Plane graphite monochromator
$\varphi + \omega$ scans
10596 measured reflections
2770 independent reflections
1695 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.085$
$\theta_{\max} = 25.2°$, $\theta_{\min} = 1.4°$
$h = -8\rightarrow8$
$k = -33\rightarrow33$
$l = -9\rightarrow9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.073$
$S = 0.83$
2770 reflections
188 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0237P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.13$ e Å^{-3}
$\Delta\rho_{\min} = -0.13$ e Å^{-3}

Extinction correction: (*SHELXL2018/3*; Sheldrick, 2015), $Fc^{*}=kFc[1+0.001xFc^{2}\lambda^{3}/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0127 (13)

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	$U_{\rm iso}$*/$U_{\rm eq}$
O1	−0.15231 (15)	0.11464 (4)	0.48898 (14)	0.0359 (3)
O2	0.47503 (17)	0.23289 (4)	0.44354 (15)	0.0389 (3)
N1	0.17336 (17)	0.10517 (4)	0.72612 (15)	0.0239 (3)
C1	0.1701 (2)	0.14010 (5)	0.59863 (18)	0.0240 (4)
C2	0.0023 (2)	0.14458 (5)	0.4777 (2)	0.0274 (4)
C3	−0.0050 (2)	0.17837 (6)	0.3529 (2)	0.0320 (4)
H3	−0.120713	0.181465	0.271592	0.038*
C4	0.1545 (2)	0.20752 (6)	0.3461 (2)	0.0326 (4)
H4	0.148437	0.230424	0.259885	0.039*
C5	0.3219 (2)	0.20347 (5)	0.4637 (2)	0.0286 (4)
C6	0.3285 (2)	0.17020 (5)	0.58934 (19)	0.0264 (4)
H6	0.443892	0.167808	0.671343	0.032*
C7	−0.3053 (2)	0.11190 (7)	0.3485 (2)	0.0420 (5)
H7C	−0.398183	0.086893	0.366432	0.063*
H7B	−0.248449	0.104630	0.248721	0.063*
H7A	−0.374711	0.142279	0.333365	0.063*
C8	0.6384 (3)	0.23518 (6)	0.5748 (2)	0.0407 (5)
H8A	0.703032	0.204187	0.588607	0.061*
H8B	0.592985	0.244041	0.678454	0.061*
H8C	0.732223	0.258909	0.548061	0.061*
C9	0.1554 (2)	0.12313 (5)	0.89467 (19)	0.0269 (4)
C10	0.0977 (2)	0.08181 (6)	0.9977 (2)	0.0342 (4)
H10A	0.103522	0.092378	1.114443	0.041*
H10B	−0.040201	0.072692	0.954118	0.041*
C11	0.2287 (2)	0.03873 (6)	0.9958 (2)	0.0381 (5)
H11A	0.365874	0.046683	1.046272	0.046*
H11B	0.182345	0.012857	1.061593	0.046*
C12	0.2215 (3)	0.02299 (6)	0.8172 (2)	0.0364 (4)
H12B	0.084985	0.013326	0.770843	0.044*
H12A	0.307259	−0.005084	0.815714	0.044*
C13	0.2870 (2)	0.06129 (5)	0.7049 (2)	0.0294 (4)
C14	−0.0136 (2)	0.15863 (6)	0.8748 (2)	0.0352 (4)
H14C	−0.039727	0.167933	0.985055	0.053*
H14B	−0.132032	0.144135	0.810935	0.053*
H14A	0.022371	0.186676	0.815626	0.053*

C15	0.3403 (2)	0.14765 (6)	0.9888 (2)	0.0361 (4)
H15C	0.316036	0.157724	1.098873	0.054*
H15B	0.371277	0.175361	0.925566	0.054*
H15A	0.451420	0.125506	1.002183	0.054*
C16	0.5112 (2)	0.06636 (6)	0.7429 (2)	0.0350 (4)
H16C	0.572685	0.036915	0.713805	0.053*
H16B	0.552574	0.072901	0.861923	0.053*
H16A	0.552219	0.092519	0.677366	0.053*
C17	0.2301 (2)	0.04478 (6)	0.5248 (2)	0.0387 (5)
H17A	0.280543	0.067303	0.450547	0.058*
H17B	0.086213	0.042978	0.495777	0.058*
H17C	0.287008	0.013449	0.512256	0.058*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0285 (6)	0.0478 (7)	0.0295 (7)	−0.0066 (5)	−0.0007 (5)	0.0043 (6)
O2	0.0453 (7)	0.0328 (7)	0.0391 (7)	−0.0084 (6)	0.0085 (6)	0.0091 (6)
N1	0.0296 (7)	0.0217 (7)	0.0205 (7)	0.0021 (6)	0.0045 (6)	0.0027 (6)
C1	0.0292 (9)	0.0225 (8)	0.0210 (9)	0.0038 (7)	0.0058 (7)	−0.0006 (7)
C2	0.0276 (9)	0.0319 (9)	0.0233 (9)	0.0011 (7)	0.0063 (8)	−0.0023 (7)
C3	0.0353 (10)	0.0384 (10)	0.0218 (9)	0.0095 (8)	0.0032 (8)	0.0026 (8)
C4	0.0465 (11)	0.0275 (9)	0.0256 (9)	0.0094 (8)	0.0111 (9)	0.0059 (7)
C5	0.0362 (9)	0.0229 (8)	0.0283 (9)	0.0011 (7)	0.0098 (8)	0.0005 (7)
C6	0.0304 (9)	0.0230 (8)	0.0251 (8)	0.0027 (7)	0.0024 (7)	−0.0004 (7)
C7	0.0308 (10)	0.0594 (12)	0.0329 (10)	−0.0019 (9)	−0.0032 (8)	−0.0076 (9)
C8	0.0476 (11)	0.0392 (11)	0.0374 (11)	−0.0115 (9)	0.0136 (10)	−0.0044 (8)
C9	0.0334 (9)	0.0276 (9)	0.0197 (8)	0.0020 (7)	0.0045 (7)	0.0017 (7)
C10	0.0368 (10)	0.0400 (10)	0.0266 (9)	0.0011 (8)	0.0082 (8)	0.0080 (8)
C11	0.0397 (10)	0.0337 (10)	0.0409 (11)	0.0013 (8)	0.0068 (9)	0.0146 (8)
C12	0.0379 (10)	0.0248 (9)	0.0472 (11)	0.0019 (8)	0.0088 (9)	0.0065 (8)
C13	0.0318 (9)	0.0225 (8)	0.0340 (10)	0.0007 (7)	0.0063 (8)	0.0014 (7)
C14	0.0428 (10)	0.0355 (10)	0.0284 (10)	0.0095 (8)	0.0093 (8)	0.0006 (8)
C15	0.0427 (10)	0.0369 (10)	0.0270 (9)	−0.0030 (8)	0.0010 (8)	−0.0032 (8)
C16	0.0343 (9)	0.0309 (9)	0.0403 (10)	0.0064 (8)	0.0076 (8)	0.0036 (8)
C17	0.0426 (11)	0.0301 (9)	0.0437 (11)	0.0007 (8)	0.0085 (9)	−0.0079 (9)

Geometric parameters (Å, º)

O1—C2	1.3743 (19)	C9—C15	1.536 (2)
O1—C7	1.4204 (18)	C10—C11	1.516 (2)
O2—C5	1.3732 (19)	C10—H10A	0.9900
O2—C8	1.416 (2)	C10—H10B	0.9900
N1—C1	1.4293 (19)	C11—C12	1.513 (2)
N1—C9	1.4867 (19)	C11—H11A	0.9900
N1—C13	1.4908 (19)	C11—H11B	0.9900
C1—C2	1.392 (2)	C12—C13	1.532 (2)
C1—C6	1.394 (2)	C12—H12B	0.9900

C2—C3	1.388 (2)	C12—H12A	0.9900
C3—C4	1.381 (2)	C13—C17	1.526 (2)
C3—H3	0.9500	C13—C16	1.529 (2)
C4—C5	1.374 (2)	C14—H14C	0.9800
C4—H4	0.9500	C14—H14B	0.9800
C5—C6	1.384 (2)	C14—H14A	0.9800
C6—H6	0.9500	C15—H15C	0.9800
C7—H7C	0.9800	C15—H15B	0.9800
C7—H7B	0.9800	C15—H15A	0.9800
C7—H7A	0.9800	C16—H16C	0.9800
C8—H8A	0.9800	C16—H16B	0.9800
C8—H8B	0.9800	C16—H16A	0.9800
C8—H8C	0.9800	C17—H17A	0.9800
C9—C14	1.524 (2)	C17—H17B	0.9800
C9—C10	1.528 (2)	C17—H17C	0.9800

C2—O1—C7	117.22 (13)	C9—C10—H10B	108.9
C5—O2—C8	117.75 (13)	H10A—C10—H10B	107.7
C1—N1—C9	116.13 (11)	C12—C11—C10	108.78 (14)
C1—N1—C13	115.76 (12)	C12—C11—H11A	109.9
C9—N1—C13	121.11 (11)	C10—C11—H11A	109.9
C2—C1—C6	118.02 (14)	C12—C11—H11B	109.9
C2—C1—N1	119.07 (14)	C10—C11—H11B	109.9
C6—C1—N1	122.90 (13)	H11A—C11—H11B	108.3
O1—C2—C3	122.57 (14)	C11—C12—C13	113.56 (14)
O1—C2—C1	117.18 (14)	C11—C12—H12B	108.9
C3—C2—C1	120.24 (15)	C13—C12—H12B	108.9
C4—C3—C2	120.51 (15)	C11—C12—H12A	108.9
C4—C3—H3	119.7	C13—C12—H12A	108.9
C2—C3—H3	119.7	H12B—C12—H12A	107.7
C5—C4—C3	120.13 (15)	N1—C13—C17	108.08 (12)
C5—C4—H4	119.9	N1—C13—C16	115.46 (12)
C3—C4—H4	119.9	C17—C13—C16	108.10 (14)
O2—C5—C4	115.91 (14)	N1—C13—C12	107.81 (13)
O2—C5—C6	124.65 (14)	C17—C13—C12	107.65 (13)
C4—C5—C6	119.42 (15)	C16—C13—C12	109.49 (13)
C5—C6—C1	121.67 (14)	C9—C14—H14C	109.5
C5—C6—H6	119.2	C9—C14—H14B	109.5
C1—C6—H6	119.2	H14C—C14—H14B	109.5
O1—C7—H7C	109.5	C9—C14—H14A	109.5
O1—C7—H7B	109.5	H14C—C14—H14A	109.5
H7C—C7—H7B	109.5	H14B—C14—H14A	109.5
O1—C7—H7A	109.5	C9—C15—H15C	109.5
H7C—C7—H7A	109.5	C9—C15—H15B	109.5
H7B—C7—H7A	109.5	H15C—C15—H15B	109.5
O2—C8—H8A	109.5	C9—C15—H15A	109.5
O2—C8—H8B	109.5	H15C—C15—H15A	109.5
H8A—C8—H8B	109.5	H15B—C15—H15A	109.5

O2—C8—H8C	109.5	C13—C16—H16C	109.5
H8A—C8—H8C	109.5	C13—C16—H16B	109.5
H8B—C8—H8C	109.5	H16C—C16—H16B	109.5
N1—C9—C14	107.86 (12)	C13—C16—H16A	109.5
N1—C9—C10	108.36 (12)	H16C—C16—H16A	109.5
C14—C9—C10	107.30 (14)	H16B—C16—H16A	109.5
N1—C9—C15	115.10 (13)	C13—C17—H17A	109.5
C14—C9—C15	108.04 (13)	C13—C17—H17B	109.5
C10—C9—C15	109.90 (13)	H17A—C17—H17B	109.5
C11—C10—C9	113.44 (14)	C13—C17—H17C	109.5
C11—C10—H10A	108.9	H17A—C17—H17C	109.5
C9—C10—H10A	108.9	H17B—C17—H17C	109.5
C11—C10—H10B	108.9		

C9—N1—C1—C2	−106.25 (16)	C1—N1—C9—C14	46.76 (17)
C13—N1—C1—C2	102.61 (16)	C13—N1—C9—C14	−163.75 (13)
C9—N1—C1—C6	73.77 (19)	C1—N1—C9—C10	162.62 (12)
C13—N1—C1—C6	−77.38 (18)	C13—N1—C9—C10	−47.89 (17)
C7—O1—C2—C3	13.5 (2)	C1—N1—C9—C15	−73.91 (16)
C7—O1—C2—C1	−166.84 (14)	C13—N1—C9—C15	75.58 (17)
C6—C1—C2—O1	−179.96 (14)	N1—C9—C10—C11	50.81 (17)
N1—C1—C2—O1	0.1 (2)	C14—C9—C10—C11	167.03 (14)
C6—C1—C2—C3	−0.3 (2)	C15—C9—C10—C11	−75.74 (17)
N1—C1—C2—C3	179.71 (14)	C9—C10—C11—C12	−57.94 (18)
O1—C2—C3—C4	−179.64 (15)	C10—C11—C12—C13	58.42 (18)
C1—C2—C3—C4	0.7 (2)	C1—N1—C13—C17	−46.30 (16)
C2—C3—C4—C5	−0.4 (2)	C9—N1—C13—C17	164.11 (13)
C8—O2—C5—C4	170.51 (15)	C1—N1—C13—C16	74.85 (17)
C8—O2—C5—C6	−11.2 (2)	C9—N1—C13—C16	−74.74 (18)
C3—C4—C5—O2	177.94 (15)	C1—N1—C13—C12	−162.40 (12)
C3—C4—C5—C6	−0.4 (2)	C9—N1—C13—C12	48.01 (17)
O2—C5—C6—C1	−177.36 (15)	C11—C12—C13—N1	−51.42 (17)
C4—C5—C6—C1	0.9 (2)	C11—C12—C13—C17	−167.79 (14)
C2—C1—C6—C5	−0.5 (2)	C11—C12—C13—C16	74.93 (18)
N1—C1—C6—C5	179.49 (14)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8*B*···O2^{i}	0.98	2.51	3.495 (2)	180

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