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Crystal structure and Hirshfeld surface analysis of 4-(3-methoxyphenyl)-2,6-diphenylpyridine

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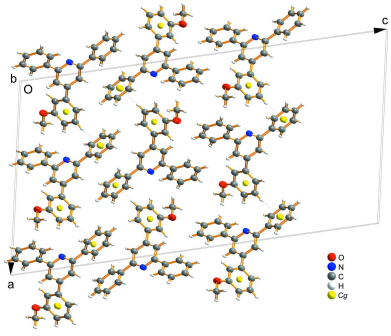
The title compound, $C_{24}H_{19}NO$, was obtained *via* the reaction of (1*E*,2*E*)-3-(3-methoxyphenyl)-1-phenylprop-2-en-1-one with ethyl 2-oxopropanoate, using NH_4I as a catalyst. The compound crystallizes in the monoclinic space group *I*2/*a*. In the molecule, the four rings are not in the same plane, the pyridine ring being inclined to the benzene rings by 17.26 (6), 56.16 (3) and 24.50 (6)°. In the crystal, molecules are linked by C—H···π interactions into a three-dimensional network. To further analyse the intermolecular interactions, a Hirshfeld surface analysis was performed. Hirshfeld surface analysis indicates that the most abundant contributions to the crystal packing are from H···H (50.4%), C···H/H···C (37.9%) and O···H/H···O (5.1%) interactions.

1. Chemical context

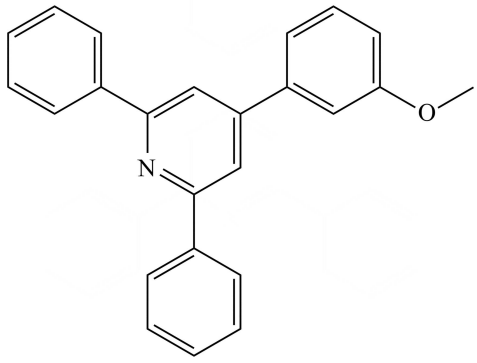
Substituted pyridines are privileged scaffolds in medicinal chemistry and are versatile building blocks for the construction of natural products (Haghighijoo *et al.*, 2020; Gujjarappa *et al.*, 2020; Nirogi *et al.*, 2015; De Rycke *et al.*, 2011; Chan *et al.*, 2010; Bora *et al.*, 2010), Accordingly, great effort has been devoted to developing efficient approaches to these scaffolds (Guin *et al.*, 2020; Wu *et al.*, 2019; Pandolfi *et al.*, 2017; Shen *et al.*, 2015). Ketoxime acetates have been demonstrated to be exceptionally advantaged and versatile building blocks for the synthesis and derivatization of nitrogen-containing heterocycles through N—O bond cleavage (Zhang *et al.*, 2020; Mao *et al.*, 2019; Xie *et al.*, 2018). Thus far, many synthetic approaches have been developed to access nitrogen-containing heterocycles through ketoxime acetates under metal-free conditions. For example, Duan *et al.* (2020) have successfully developed the NH_4I-triggered formal [4 + 2] annulation of α,β-unsaturated ketoxime acetates with *N*-acetyl enamides, providing efficient access to valuable highly substituted pyridines in moderate to good yields. Gao *et al.* (2018) have developed a facile and efficient I_2-triggered [3 + 2 + 1] annulation of aryl ketoxime acetates and 3-formylindoles to produce diverse 3-(4-pyridyl)indoles that are challenging to prepare by traditional methods. Given this background, we report herein the synthesis and crystal structure of the title compound, which was synthesized by NH_4I-triggered annulation of α,β-unsaturated ketoxime acetates.

2. Structural commentary

The title compound crystallizes in the monoclinic crystal system in space group *I*2/*a*. Its molecular structure is shown in Fig. 1. The methoxy group lies close to the mean plane of the



C12–C17 phenyl ring, as indicated by the C17—C16—O1—C24 torsion angle of −170.59 (10)°, and atom C24 deviating by 0.250 (2) Å from the mean plane through the C12–C17 ring. In the molecule, the four rings are not in the same plane, the pyridine ring being inclined to the C6–C11, C12–C17 and C18–C23 benzene rings by 17.26 (6), 56.16 (3) and 24.50 (6)°, respectively. There is a strong intramolecular hydrogen bond (C7—H7···N1; Table 1), forming an *S*(5) ring motif.



3. Supramolecular features

In the crystal (Fig. 2), the molecules are linked by weak C—H···π interactions (C14—H14···*Cg*2^{i} and C24—H24···*Cg*3^{ii}, *Cg*2 and *Cg*3 are the centroids of the C6–C11 and C12–C17 rings, respectively, symmetry codes as in Table 1). The C24—H24···*Cg*3 interactions generate stacks along the *b*-axis direction. These stacks are linked by the C14—H14···*Cg*2 interactions. The packing is strengthened by van der Waals interactions between parallel molecular layers.

In order to investigate the intermolecular interactions in a visual manner, a Hirshfeld surface analysis was performed using *Crystal Explorer* (Spackman & Jayatilaka, 2009; Turner *et al.*, 2017). Fig. 3 shows the d_{norm} surface together with two adjacent molecules. The bright-red spots on the Hirshfeld surface mapped over d_{norm} correspond to H24*B*···H20 ($x-\frac{1}{2}$, $2-y$, z) close contacts. Fig. 4*a* is the fingerprint plot showing all intermolecular interactions while Fig. 4*b–d* show these resolved into C···H/H···C (37.9%), H···H (50.4%) and O···H/H···O (5.1%) contributions, respectively. As a result, van der Waals interactions are dominant in the crystal packing.

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

*Cg*2 and *Cg*3 are the centroids of the C6–C11 and C12–C17 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···N1	0.93	2.49	2.8025 (13)	100
C14—H14···*Cg*2^{i}	0.93	2.74	3.5482 (12)	146
C24—H24*A*···*Cg*3^{ii}	0.93	2.81	3.6787 (13)	150

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

4. Database survey

A search of the Cambridge Structural Database (Version 2021.1; Groom *et al.*, 2016) for the 2,4,6-triphenylpyridine moiety revealed seven structures closely related to the title compound, *viz*. 4-(4-fluorophenyl)-2,6-diphenylpyridine [(I) SURGER01; Zhang *et al.*, 2021], 4-[4-(azidomethyl)phenyl]-2,6-diphenylpyridine [(II) DOCLIT; Cheng *et al.*, 2019], 4-(4-chlorophenyl)-2,6-diphenylpyridine [(III) GISGEV; Lv & Huang, 2008], 2,4,6-triphenylpyridine [(IV) HEVVAF, Ondráček *et al.*, 1994; HEVVAF01, Ren *et al.*, 2011; HEVVAF02, Mao *et al.*, 2017], 2-(4-methylphenyl)-4,6-diphenylpyridine [(V) REMHOJ; Stivanin *et al.*, 2017], 4-(4-bromophenyl)-2,6-diphenylpyridine [(VI) AJEZOF; Cao *et al.*, 2009], 4-(2,6-diphenylpyridin-4-yl) phenol [(VII) KIDBIL; Kannan *et al.*, 2018].

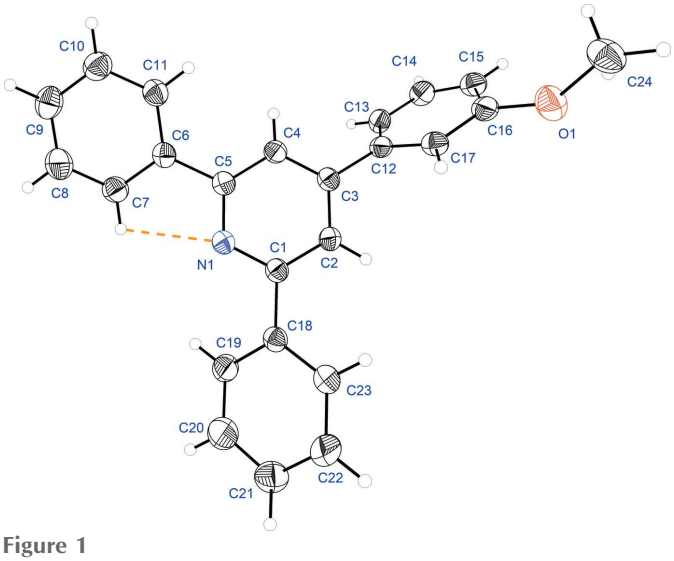


Figure 1
The molecular structure of the title compound, with the atom labelling and displacement ellipsoids drawn at the 50% probability level. H atoms are shown as small circles of arbitrary radii.

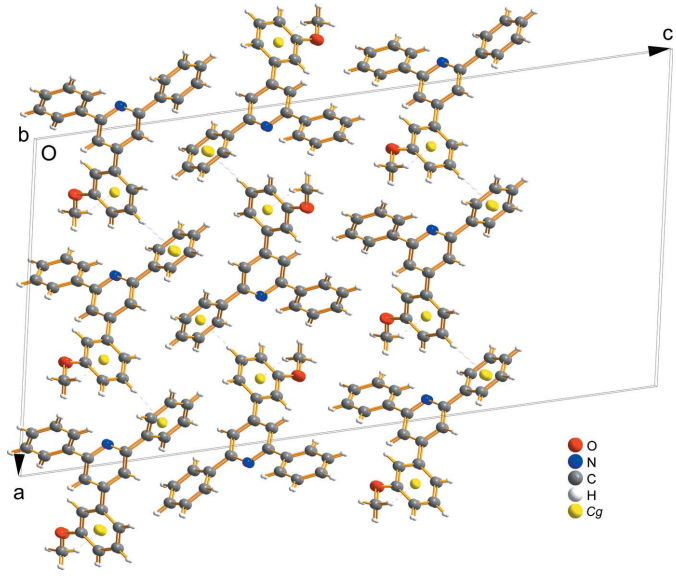


Figure 2
A packing diagram of the title compound. The C—H···π interactions are shown as dashed lines. Yellow spheres denoted *Cg* represent the centroids of the 3-methoxyphenyl rings.

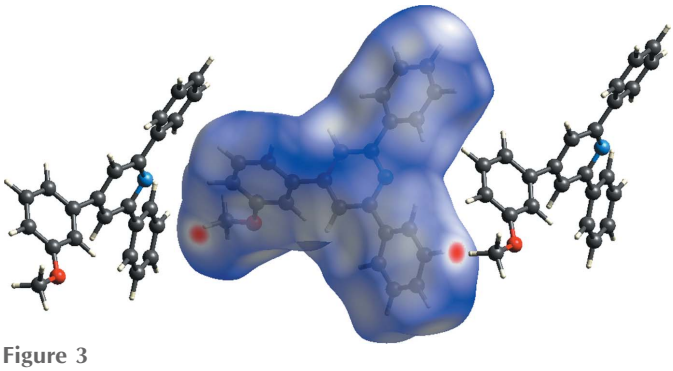


Figure 3
The Hirshfeld surface mapped over d_{norm} together with two adjacent molecules.

As in the title compound, in (I), (II), (III), (IV) and (V), C—H···π (ring) interactions connect the molecules, forming tri-periodic networks. In (VI), molecules are linked by weak intermolecular C—H···Br hydrogen bonds, and weak intermolecular C—H···π (ring) interactions are also observed. In (VII), molecules are linked by weak intermolecular C—H···O hydrogen bonds, and there are also weak intermolecular C—H···π (ring) interactions.

5. Synthesis and crystallization

(1*E*,2*E*)-3-(3-Methoxyphenyl)-1-phenylprop-2-en-1-one (3.0 mmol), ethyl 2-oxopropanoate (0.3 mmol), NH_4I (0.22 g, 0.15 mmol) and $NaHSO_3$ (0.31 g, 3.0 mmol) were loaded into a 20 mL tube under an N_2 atmosphere. The solvent toluene (15 mL) was added into the tube by syringe. The reaction mixture was stirred at 373 K for 12 h. Upon completion of the reaction, the mixture was then allowed to cool down to room temperature and flushed through a short column of silica gel with EtOAc (15 mL). After rotary evaporation, the residue was purified by column chromatography on silica gel (petroleum ether/EtOAc) to give the product as a white solid. Part of the purified product was redissolved in petroleum ether/ethyl acetate and colourless crystals suitable for X-ray diffraction were formed after slow evaporation for several days. Spectroscopic data: ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.20 (*d*, *J* = 7.8 Hz, 4H), 7.87 (*s*, 2H), 7.53–7.50 (*m*, 4H), 7.46–7.42 (*m*, 3H), 7.33–7.32 (*m*, 1H), 7.26–7.24 (*m*, 1H), 7.02–7.00 (*m*, 1H), 3.89 (*s*, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.2, 157.5, 150.2, 140.6, 139.5, 130.2, 129.1, 128.8, 127.2, 119.7, 117.3, 114.3, 113.1, 55.5.

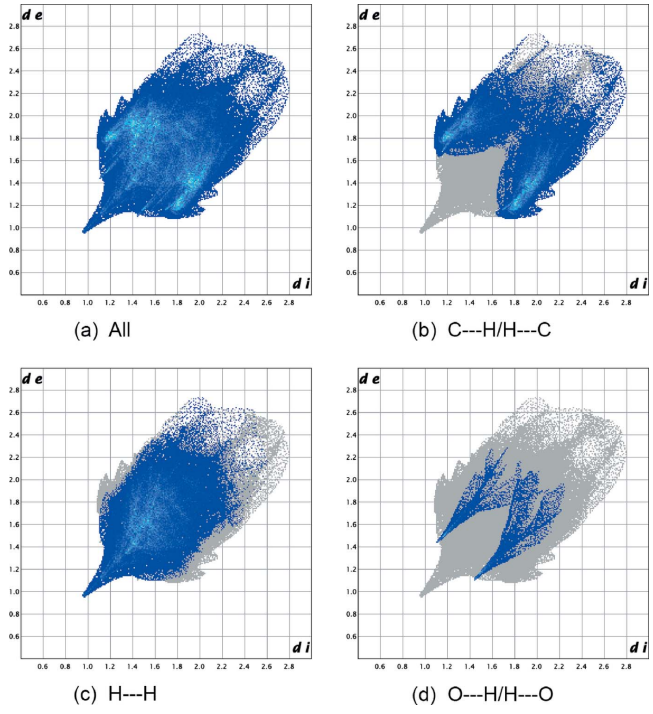


Figure 4
Fingerprint plots for the title molecule: (*a*) all intermolecular interactions, (*b*) C···H/H···C interactions, (*c*) H···H interactions and (*d*) O···H/H···O interactions.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{24}H_{19}NO$
M_r	337.40
Crystal system, space group	Monoclinic, *I*2/*a*
Temperature (K)	200
a, *b*, *c* (Å)	18.6588 (2), 5.4739 (1), 35.5689 (5)
β (°)	100.729 (1)
V (Å^3)	3569.37 (9)
Z	8
Radiation type	Cu *K*α
μ (mm^{-1})	0.59
Crystal size (mm)	0.15 × 0.11 × 0.1
Data collection	
Diffractometer	XtaLAB AFC12 (RINC): Kappa single
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2017)
T_{min}, T_{max}	0.747, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8525, 3417, 3189
R_{int}	0.016
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.615
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.034, 0.099, 1.00
No. of reflections	3417
No. of parameters	237
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.19, −0.15

Computer programs: *CrysAlis PRO* (Rigaku OD, 2017), *SHELXT2014/5* (Sheldrick, 2015*a*), *SHELXL2017/1* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms were positioned geometrically with C—H = 0.93–0.98 Å and refined as riding atoms. The constraint U_{iso}(H) = 1.2U_{eq} (C) or 1.5U_{eq}(C_{Me}) was applied in all cases.

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supporting information

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Crystal structure and Hirshfeld surface analysis of 4-(3-methoxyphenyl)-2,6-diphenylpyridine

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Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2017); cell refinement: *CrysAlis PRO* (Rigaku OD, 2017); data reduction: *CrysAlis PRO* (Rigaku OD, 2017); program(s) used to solve structure: *SHELXT2014/5* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2017/1* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

4-(3-Methoxyphenyl)-2,6-diphenylpyridine

Crystal data

$C_{24}H_{19}NO$
M_r = 337.40
Monoclinic, *I*2/*a*
a = 18.6588 (2) Å
b = 5.4739 (1) Å
c = 35.5689 (5) Å
β = 100.729 (1)°
V = 3569.37 (9) Å^3
Z = 8
F(000) = 1424
D_x = 1.256 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54184 Å
Cell parameters from 6287 reflections
θ = 2.6–71.4°
μ = 0.59 mm^{-1}
T = 200 K
Block, clear light colourless
0.15 × 0.11 × 0.1 mm

Data collection

XtaLAB AFC12 (RINC): Kappa single diffractometer
Radiation source: Rotating-anode X-ray tube, Rigaku (Cu) X-ray Source
Mirror monochromator
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2017)
T_{min} = 0.747, T_{max} = 1.000
8525 measured reflections
3417 independent reflections
3189 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
θ_{max} = 71.5°, θ_{min} = 2.5°
h = −20→22
k = −4→6
l = −42→43

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.099
S = 1.00
3417 reflections
237 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0557P)^2 + 1.7292P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

Extinction correction: SHELXL-2017/1 (Sheldrick 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00128 (9)

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	0.31876 (5)	0.10179 (16)	0.43410 (2)	0.0435 (2)
N1	0.56039 (4)	0.98962 (16)	0.36511 (2)	0.0280 (2)
C1	0.52794 (5)	1.00634 (19)	0.39576 (3)	0.0275 (2)
C2	0.46613 (5)	0.87064 (19)	0.39895 (3)	0.0295 (2)
H2	0.445343	0.884525	0.420676	0.035*
C3	0.43587 (5)	0.71485 (19)	0.36952 (3)	0.0282 (2)
C4	0.46901 (5)	0.7006 (2)	0.33766 (3)	0.0296 (2)
H4	0.449647	0.600015	0.317211	0.036*
C5	0.53147 (5)	0.83820 (19)	0.33658 (3)	0.0276 (2)
C6	0.57027 (5)	0.8247 (2)	0.30363 (3)	0.0283 (2)
C7	0.62006 (6)	1.0059 (2)	0.29844 (3)	0.0349 (3)
H7	0.628023	1.137188	0.315289	0.042*
C8	0.65777 (7)	0.9923 (2)	0.26844 (3)	0.0416 (3)
H8	0.690790	1.114477	0.265319	0.050*
C9	0.64673 (6)	0.7985 (2)	0.24310 (3)	0.0409 (3)
H9	0.672523	0.789083	0.223154	0.049*
C10	0.59708 (6)	0.6193 (2)	0.24767 (3)	0.0398 (3)
H10	0.589029	0.489378	0.230547	0.048*
C11	0.55906 (6)	0.6315 (2)	0.27768 (3)	0.0349 (3)
H11	0.525773	0.509472	0.280488	0.042*
C12	0.37016 (5)	0.5655 (2)	0.37171 (3)	0.0288 (2)
C13	0.30860 (6)	0.5772 (2)	0.34262 (3)	0.0355 (3)
H13	0.307468	0.684207	0.322203	0.043*
C14	0.24943 (6)	0.4289 (2)	0.34437 (3)	0.0393 (3)
H14	0.208289	0.439001	0.325132	0.047*
C15	0.25003 (6)	0.2652 (2)	0.37419 (3)	0.0361 (3)
H15	0.210233	0.163835	0.374717	0.043*
C16	0.31115 (6)	0.2552 (2)	0.40329 (3)	0.0320 (2)
C17	0.37049 (5)	0.4078 (2)	0.40215 (3)	0.0301 (2)
H17	0.410674	0.403553	0.422021	0.036*
C18	0.56109 (5)	1.17960 (19)	0.42620 (3)	0.0289 (2)
C19	0.60256 (6)	1.3753 (2)	0.41768 (3)	0.0358 (3)
H19	0.609761	1.397731	0.392735	0.043*
C20	0.63323 (7)	1.5371 (2)	0.44594 (4)	0.0458 (3)
H20	0.661015	1.666984	0.439753	0.055*

C21	0.62333 (7)	1.5093 (2)	0.48313 (4)	0.0467 (3)
H21	0.643968	1.619274	0.501995	0.056*
C22	0.58241 (8)	1.3160 (3)	0.49179 (4)	0.0542 (4)
H22	0.574972	1.295836	0.516738	0.065*
C23	0.55208 (7)	1.1507 (3)	0.46386 (3)	0.0456 (3)
H23	0.525391	1.018874	0.470363	0.055*
C24	0.26481 (7)	−0.0842 (2)	0.43386 (4)	0.0459 (3)
H24A	0.261990	−0.182605	0.411288	0.069*
H24B	0.218282	−0.009630	0.433972	0.069*
H24C	0.277951	−0.185138	0.456145	0.069*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0405 (5)	0.0415 (5)	0.0487 (5)	−0.0114 (4)	0.0090 (4)	0.0073 (4)
N1	0.0251 (4)	0.0288 (4)	0.0301 (4)	−0.0006 (3)	0.0050 (3)	0.0004 (3)
C1	0.0244 (5)	0.0279 (5)	0.0301 (5)	0.0010 (4)	0.0045 (4)	0.0005 (4)
C2	0.0263 (5)	0.0325 (5)	0.0305 (5)	−0.0010 (4)	0.0076 (4)	−0.0012 (4)
C3	0.0227 (5)	0.0294 (5)	0.0320 (5)	0.0006 (4)	0.0041 (4)	0.0009 (4)
C4	0.0261 (5)	0.0328 (5)	0.0292 (5)	−0.0019 (4)	0.0032 (4)	−0.0022 (4)
C5	0.0246 (5)	0.0286 (5)	0.0287 (5)	0.0019 (4)	0.0029 (4)	0.0024 (4)
C6	0.0239 (5)	0.0326 (5)	0.0274 (5)	0.0028 (4)	0.0025 (4)	0.0038 (4)
C7	0.0360 (6)	0.0339 (6)	0.0355 (6)	−0.0019 (5)	0.0087 (4)	0.0019 (5)
C8	0.0399 (6)	0.0449 (7)	0.0431 (6)	−0.0037 (5)	0.0156 (5)	0.0089 (5)
C9	0.0386 (6)	0.0546 (7)	0.0320 (6)	0.0077 (5)	0.0134 (5)	0.0072 (5)
C10	0.0369 (6)	0.0495 (7)	0.0333 (6)	0.0034 (5)	0.0072 (5)	−0.0070 (5)
C11	0.0301 (5)	0.0401 (6)	0.0347 (6)	−0.0027 (5)	0.0062 (4)	−0.0032 (5)
C12	0.0235 (5)	0.0309 (5)	0.0330 (5)	−0.0011 (4)	0.0080 (4)	−0.0063 (4)
C13	0.0294 (5)	0.0439 (6)	0.0328 (5)	−0.0032 (5)	0.0049 (4)	−0.0008 (5)
C14	0.0260 (5)	0.0517 (7)	0.0383 (6)	−0.0049 (5)	0.0009 (4)	−0.0056 (5)
C15	0.0254 (5)	0.0401 (6)	0.0442 (6)	−0.0085 (4)	0.0101 (4)	−0.0097 (5)
C16	0.0300 (5)	0.0310 (5)	0.0369 (5)	−0.0016 (4)	0.0114 (4)	−0.0045 (4)
C17	0.0235 (5)	0.0324 (5)	0.0340 (5)	−0.0012 (4)	0.0042 (4)	−0.0045 (4)
C18	0.0244 (5)	0.0291 (5)	0.0330 (5)	0.0011 (4)	0.0051 (4)	−0.0020 (4)
C19	0.0394 (6)	0.0317 (6)	0.0374 (6)	−0.0038 (5)	0.0097 (5)	−0.0009 (5)
C20	0.0525 (7)	0.0334 (6)	0.0522 (7)	−0.0136 (5)	0.0111 (6)	−0.0051 (5)
C21	0.0507 (7)	0.0425 (7)	0.0453 (7)	−0.0100 (6)	0.0047 (5)	−0.0145 (6)
C22	0.0642 (9)	0.0656 (9)	0.0341 (6)	−0.0236 (7)	0.0127 (6)	−0.0114 (6)
C23	0.0508 (7)	0.0512 (7)	0.0363 (6)	−0.0227 (6)	0.0118 (5)	−0.0058 (5)
C24	0.0394 (6)	0.0326 (6)	0.0703 (9)	−0.0040 (5)	0.0224 (6)	0.0034 (6)

Geometric parameters (Å, º)

O1—C16	1.3668 (14)	C12—C13	1.3970 (14)
O1—C24	1.4306 (14)	C12—C17	1.3839 (15)
N1—C1	1.3452 (13)	C13—H13	0.9300
N1—C5	1.3432 (13)	C13—C14	1.3811 (16)
C1—C2	1.3940 (14)	C14—H14	0.9300

C1—C18	1.4849 (14)	C14—C15	1.3868 (17)
C2—H2	0.9300	C15—H15	0.9300
C2—C3	1.3864 (14)	C15—C16	1.3913 (16)
C3—C4	1.3905 (14)	C16—C17	1.3936 (15)
C3—C12	1.4879 (14)	C17—H17	0.9300
C4—H4	0.9300	C18—C19	1.3876 (15)
C4—C5	1.3941 (14)	C18—C23	1.3897 (15)
C5—C6	1.4897 (14)	C19—H19	0.9300
C6—C7	1.3946 (15)	C19—C20	1.3812 (17)
C6—C11	1.3934 (15)	C20—H20	0.9300
C7—H7	0.9300	C20—C21	1.3778 (19)
C7—C8	1.3852 (16)	C21—H21	0.9300
C8—H8	0.9300	C21—C22	1.3730 (19)
C8—C9	1.3820 (18)	C22—H22	0.9300
C9—H9	0.9300	C22—C23	1.3845 (18)
C9—C10	1.3796 (18)	C23—H23	0.9300
C10—H10	0.9300	C24—H24A	0.9600
C10—C11	1.3890 (15)	C24—H24B	0.9600
C11—H11	0.9300	C24—H24C	0.9600

C16—O1—C24	117.66 (9)	C14—C13—C12	119.56 (11)
C5—N1—C1	118.45 (9)	C14—C13—H13	120.2
N1—C1—C2	122.25 (9)	C13—C14—H14	119.3
N1—C1—C18	116.44 (9)	C13—C14—C15	121.44 (10)
C2—C1—C18	121.31 (9)	C15—C14—H14	119.3
C1—C2—H2	120.2	C14—C15—H15	120.5
C3—C2—C1	119.54 (9)	C14—C15—C16	118.90 (10)
C3—C2—H2	120.2	C16—C15—H15	120.5
C2—C3—C4	118.00 (9)	O1—C16—C15	124.70 (10)
C2—C3—C12	121.48 (9)	O1—C16—C17	115.27 (9)
C4—C3—C12	120.51 (9)	C15—C16—C17	120.02 (10)
C3—C4—H4	120.2	C12—C17—C16	120.58 (10)
C3—C4—C5	119.54 (9)	C12—C17—H17	119.7
C5—C4—H4	120.2	C16—C17—H17	119.7
N1—C5—C4	122.19 (9)	C19—C18—C1	120.49 (10)
N1—C5—C6	116.07 (9)	C19—C18—C23	118.09 (10)
C4—C5—C6	121.73 (9)	C23—C18—C1	121.41 (10)
C7—C6—C5	120.13 (10)	C18—C19—H19	119.7
C11—C6—C5	121.59 (10)	C20—C19—C18	120.57 (11)
C11—C6—C7	118.28 (10)	C20—C19—H19	119.7
C6—C7—H7	119.7	C19—C20—H20	119.5
C8—C7—C6	120.67 (11)	C21—C20—C19	121.08 (12)
C8—C7—H7	119.7	C21—C20—H20	119.5
C7—C8—H8	119.7	C20—C21—H21	120.7
C9—C8—C7	120.54 (11)	C22—C21—C20	118.70 (11)
C9—C8—H8	119.7	C22—C21—H21	120.7
C8—C9—H9	120.3	C21—C22—H22	119.6
C10—C9—C8	119.40 (10)	C21—C22—C23	120.85 (12)

C10—C9—H9	120.3	C23—C22—H22	119.6
C9—C10—H10	119.8	C18—C23—H23	119.7
C9—C10—C11	120.43 (11)	C22—C23—C18	120.69 (12)
C11—C10—H10	119.8	C22—C23—H23	119.7
C6—C11—H11	119.7	O1—C24—H24A	109.5
C10—C11—C6	120.69 (11)	O1—C24—H24B	109.5
C10—C11—H11	119.7	O1—C24—H24C	109.5
C13—C12—C3	120.52 (10)	H24A—C24—H24B	109.5
C17—C12—C3	120.01 (9)	H24A—C24—H24C	109.5
C17—C12—C13	119.44 (10)	H24B—C24—H24C	109.5
C12—C13—H13	120.2		

O1—C16—C17—C12	177.88 (9)	C5—N1—C1—C18	−178.87 (9)
N1—C1—C2—C3	−0.90 (15)	C5—C6—C7—C8	178.44 (10)
N1—C1—C18—C19	24.21 (14)	C5—C6—C11—C10	−178.45 (10)
N1—C1—C18—C23	−155.42 (11)	C6—C7—C8—C9	−0.03 (18)
N1—C5—C6—C7	−16.90 (14)	C7—C6—C11—C10	0.57 (16)
N1—C5—C6—C11	162.10 (10)	C7—C8—C9—C10	0.69 (18)
C1—N1—C5—C4	0.54 (15)	C8—C9—C10—C11	−0.70 (18)
C1—N1—C5—C6	−179.20 (9)	C9—C10—C11—C6	0.07 (17)
C1—C2—C3—C4	0.02 (15)	C11—C6—C7—C8	−0.59 (16)
C1—C2—C3—C12	179.70 (9)	C12—C3—C4—C5	−178.60 (9)
C1—C18—C19—C20	179.78 (11)	C12—C13—C14—C15	−0.93 (18)
C1—C18—C23—C22	−179.00 (12)	C13—C12—C17—C16	2.26 (16)
C2—C1—C18—C19	−155.29 (10)	C13—C14—C15—C16	1.44 (18)
C2—C1—C18—C23	25.08 (16)	C14—C15—C16—O1	−179.69 (10)
C2—C3—C4—C5	1.09 (15)	C14—C15—C16—C17	−0.10 (16)
C2—C3—C12—C13	125.72 (11)	C15—C16—C17—C12	−1.75 (16)
C2—C3—C12—C17	−56.26 (14)	C17—C12—C13—C14	−0.93 (16)
C3—C4—C5—N1	−1.42 (15)	C18—C1—C2—C3	178.57 (9)
C3—C4—C5—C6	178.32 (9)	C18—C19—C20—C21	−0.2 (2)
C3—C12—C13—C14	177.10 (10)	C19—C18—C23—C22	1.37 (19)
C3—C12—C17—C16	−175.78 (9)	C19—C20—C21—C22	0.3 (2)
C4—C3—C12—C13	−54.60 (14)	C20—C21—C22—C23	0.5 (2)
C4—C3—C12—C17	123.41 (11)	C21—C22—C23—C18	−1.4 (2)
C4—C5—C6—C7	163.35 (10)	C23—C18—C19—C20	−0.59 (17)
C4—C5—C6—C11	−17.65 (15)	C24—O1—C16—C15	9.02 (16)
C5—N1—C1—C2	0.62 (15)	C24—O1—C16—C17	−170.59 (10)

Hydrogen-bond geometry (Å, º)

*Cg*2 and *Cg*3 are the centroids of the C6–C11 and C12–C17 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···N1	0.93	2.49	2.8025 (13)	100
C14—H14···*Cg*2^{i}	0.93	2.74	3.5482 (12)	146
C24—H24*A*···*Cg*3^{ii}	0.93	2.81	3.6787 (13)	150

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