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 (1E,2E)-3-(3-methoxyphenyl)-1-phenylprop-2-en-1-one with ethyl 2-oxopropanoate, using NH_{4}I 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_{4}I-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_{4}I-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⋯Cg2 and C24—H24⋯Cg3), Cg2 and Cg3 are the centroids of the C6–C11 and C12–C17 rings, respectively, symmetry codes as in Table 1). The C24—H24⋯Cg3 interactions generate stacks along the b-axis direction. These stacks are linked by the C14—H14⋯Cg2 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 H24B⋯H20 ($x - \frac{1}{2}$, 2 − y, z) close contacts. Fig. 4a is the fingerprint plot showing all intermolecular interactions while Fig. 4b–d show these resolved into C⋯H/H—H (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.

### 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].
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

(1E,2E)-3-(3-Methoxyphenyl)-1-phenylprop-2-en-1-one (3.0 mmol), ethyl 2-oxopropanoate (0.3 mmol), NH₄I (0.22 g, 0.15 mmol) and NaHSO₃ (0.31 g, 3.0 mmol) were loaded into a 20 mL tube under an N₂ 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: ¹H NMR (600 MHz, CDCl₃) 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); ¹³C NMR (125 MHz, CDCl₃) 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.

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(eq)(H) = 1.2U(eq)(C) or 1.5U(eq)(CMe) was applied in all cases.

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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

C₂₄H₁₉NO

$M_r = 337.40$

Monoclinic, $I2/a$

$a = 18.6588$ (2) Å

$b = 5.4739$ (1) Å

$c = 35.5689$ (5) Å

$\beta = 100.729$ (1)°

$V = 3569.37$ (9) Å³

$Z = 8$

$F(000) = 1424$

$D_x = 1.256$ Mg m⁻³

Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å

Cell parameters from 6287 reflections

$\theta = 2.6$–$71.4$°

$\mu = 0.59$ 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

$\omega$ scans

Absorption correction: multi-scan

(CrysAlisPro; Rigaku OD, 2017)

$T_{\text{min}} = 0.747, T_{\text{max}} = 1.000$

8525 measured reflections

3417 independent reflections

3189 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.016$

$\theta_{\text{max}} = 71.5$°, $\theta_{\text{min}} = 2.5$°

$h = -20→22$

$k = -4→6$

$l = -42→43$

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 neighbour sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_c^2) + (0.0557P)^2 + 1.7292P]$

where $P = (F_c^2 + 2F_s^2)/3$
sup-2

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Supporting Information

\( \frac{\Delta(\sigma)}{\sigma} _{\text{max}} = 0.001 \)
\( \Delta \rho_{\text{max}} = 0.19 \, \text{e} \, \text{Å}^{-3} \)
\( \Delta \rho_{\text{min}} = -0.15 \, \text{e} \, \text{Å}^{-3} \)

Extinction correction: SHELXL-2017/1 (Sheldrick 2015b),
\[ Fc^2 = \text{KFC}[1 + 0.001xFc^2 \lambda^2 / \sin(2\theta)]^{-1/4} \]
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 (Å²)**

| X     | Y     | Z     | Uiso* / Ueq |
|-------|-------|-------|-------------|
| 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    | 0.445334    | 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)

|          | U₁₁   | U₂₂   | U₃₃   | U₁₂   | U₁₃   | U₂₃   |
|----------|-------|-------|-------|-------|-------|-------|
| 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, °)

|          | 1.3668 (14) | C12—C13 1.3970 (14) |
|----------|-------------|---------------------|
| O1—C16   | 1.3406 (14) | C12—C17 1.3839 (15) |
| O1—C24   | 1.3452 (13) | C13—H13 0.9300 |
| N1—C1    | 1.3432 (13) | C13—C14 1.3811 (16) |
| N1—C5    | 1.3432 (13) | C14—H14 0.9300 |
| C1—C2    | 1.3940 (14) |                       |

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| Bond          | Distance (Å) | Bond          | Distance (Å) | Bond          | Distance (Å) |
|--------------|--------------|--------------|--------------|--------------|--------------|
| 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—C15 | 121.44 (10)  |
| N1—C1—C18    | 116.44 (9)   | C13—C14—H14 | 119.3        |
| 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)  |
| Bond Description | Angle (°) | Bond Description | Angle (°) |
|------------------|----------|------------------|----------|
| 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     | 119.7    | C22—C23—H23     | 119.7    |
| C6—C11—C10—H10  | 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    |                  |          |

C7—H7···N1 0.93 2.49 2.8025 (13) 100
C14—H14···Cg2 0.93 2.74 3.5482 (12) 146
C24—H24A···Cg3 0.93 2.81 3.6787 (13) 150

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

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Hydrogen-bond geometry (Å, °)

Cg2 and Cg3 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···Cg2  | 0.93  | 2.74  | 3.5482 (12) | 146     |
| C24—H24A···Cg3 | 0.93  | 2.81  | 3.6787 (13) | 150     |

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