Crystal structure, DFT and Hirshfeld surface analysis of \( N \)-acetyl-\( t \)-3-methyl-\( r \)-2,\( c \)-6-diphenylpiperidine

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In the title compound [systematic name: 1-(3-methyl-2,6-diphenylpiperidin-1-yl)ethanone], \( \text{C}_{20}\text{H}_{23}\text{NO} \), the piperidine ring adopts a distorted boat conformation, while the phenyl rings subtend a dihedral angle 65.1 (2)°. In the crystal, molecules are linked by \( \text{C}^{-}\cdot\cdot\cdot\text{H} \) hydrogen bonds into chains extending along the \( b \)-axis direction. The DFT/B3LYP/6–311 G(d,p) method was used to determine the HOMO–LUMO energy levels. A Hirshfeld surface analysis was conducted to verify the contributions of the different intermolecular interactions, indicating that the important contributions to the crystal packing are from \( \text{H} \cdot\cdot\cdot\text{H} \) (73.2%), \( \text{C} \cdot\cdot\cdot\text{H} \) (18.4%) and \( \text{O} \cdot\cdot\cdot\text{H} \) (8.4%) interactions.

1. Chemical context

The structures of a wide array of heterocyclic derivatives have been analysed for their pharma-potentiality over the past three decades (Katritzky, 2010). Among these, derivatives of the six-membered heterocyclic base piperidine have proven to be successful pharmacophores. 2,6-Substituted piperidine derivatives have been found to be useful as tranquilizers and possess a wide range of biological activities such as anti-tumor (Vinaya et al., 2009), antiviral, antimalarial, antibacterial and antifungal activities (Aridoss et al., 2009; Mobio et al., 1989). These have spurred considerable awareness of the synthetic arena based on their structure, reactivity, synthesis and biological properties. We report herein the crystal structure, Hirshfeld surface analysis and DFT computational calculations of the title compound.

2. Structural commentary

The methyl-substituted piperidine title compound crystallizes in the monoclinic space group \( P2_1 \). A perspective view of the
molecule is shown in Fig. 1. The bond lengths and angles are well within the expected limits (Roques et al., 1981), and agree with values observed in related structures (Sekar et al., 1990).

The piperidine ring adopts a distorted boat conformation with puckering parameters (Cremer & Pople, 1975) and asymmetry parameters (Nardelli, 1983): \( q_2 = 0.720 (2) \) Å, \( q_3 = -0.004 (3) \) Å, \( \Phi(2) = 108.5 (2) \)^°, \( \Delta C(C3) \) and \( \Delta C(C6) = 14.5 (2) \)^°, and with maximum deviations of 0.406 (3) and 0.409 (2) Å, respectively, for atoms C3 and C6 from the best plane of the piperidine ring. The title molecule contains three chiral centres viz., C2, C5 and C6. The absolute configuration of the chiral centres is assigned as C2 (R), C5 (S) and C6 (S). The parent molecule itself is chiral and the configuration cannot be changed during the substitution of acetyl group at the nitrogen.

The sum of the bond angles (358.2°) at atom N1 of the piperidine ring is in accordance with the \( sp^2 \) hybridization state (Beddoes et al., 1986). The phenyl rings at the 2 and 6-positions of the piperidine ring occupy equatorial and axial orientations. The corresponding torsion angles are C4—C3—C2—C13 = -178.8 (2)^° and C4—C5—C6—C7 = -74.5 (3)^°.

The piperidine ring [N1/C2—C6] makes dihedral angles of 82.0 (1) and 58.4 (1)^°, respectively, with the C13—C18 and C7—C12 phenyl rings, and confirms the fact that the moieties are in axial and equatorial orientations. It is to be noted that there is a possibility of resonance between atoms N1, C19 and O1 as a result of the delocalization of the hetero \( \pi \) electrons of the carbonyl group, which is also confirmed by the torsion angles C2—N1—C19—O1 = 177.7 (2)^° and C6—N1—C19—O1 = 13.0 (3)^°.

The methyl group substituted at the 5-position of the piperidine ring is axially oriented, as confirmed by the torsion angles N1—C6—C5—C21 = -68.0 (3)^° and C3—C4—C5—C21 = 112.4 (3)^°, whereas the methyl group substituted at C19...
is oriented equatorially with torsion angle $\text{C20—C19—N1—C6} = 166.3 (2)^\circ$ and $\text{C20—C19—N1—C2} = 1.7 (3)^\circ$.

3. Supramolecular features

The crystal packing features C—H···O interactions (Table 1). Atom C20 of the molecule at $(x, y, z)$ donates a proton to atom O1 of the molecule at $(x + 1, y + \frac{1}{2}, z + 1)$, forming a C4 zigzag chain (Bernstein et al., 1995) running along the $b$-axis direction as shown in Fig. 2. The overall packing is shown in Fig. 3.

4. Density functional theory (DFT) study

The optimized molecular structure and frontier molecular orbitals (FMOs) (Figs. 4 and 5, respectively) were calculated using the DFT/B3LYP/6-311G(d,p) basis set implemented in the GAUSSIAN09 program package (Frisch et al., 2009). The highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) are called frontier molecular orbitals (FMOs) as they lie at the outermost boundaries of the electrons of the molecule. The electron distribution (ED) of the HOMO, HOMO, LUMO and LUMO+1 energy levels and the energy values are shown in Fig. 5. The positive and negative phases are represented in green and red, respectively.

The HOMO of the title molecule is localized on one aromatic ring and the $\text{C=O}$ group, while the LUMO is located over the whole molecule with the exception of the CH$_3$ group and some carbon and hydrogen atoms in the piperidine ring. Thus the HOMO/LUMO implies an ED transfer to the $\text{C=O}$ group from the ring. The energy band gap ($\Delta E = E_{\text{HOMO}} - E_{\text{LUMO}}$) of the molecule is 3.165 eV and the calculated frontier molecular orbital energies, $E_{\text{HOMO}}$ and $E_{\text{LUMO}}$, are $-5.212$ and $-2.047$ eV, respectively. The title compound has a small frontier orbital gap, hence the molecule has high chemical reactivity and low kinetic stability. The electron affinity ($A$) and ionization potential ($I$) of the molecule were calculated using the DFT/B3LYP/6-311++G(d,p) basis set. The values of the hardness ($\eta$), softness ($\sigma$), electronegativity ($\mu$) and electrophilicity index ($\chi$) for the title compound are given in Table 2.

5. Hirshfeld surface analysis

In order to visualize the intermolecular interactions in the crystal of the title compound, a Hirshfeld surface (HS) analysis (Spackman & Jayatilaka, 2009) was carried out and the associated two-dimensional fingerprint plots (McKinnon et al., 2007) were generated using CrystalExplorer17 (Turner et al., 2017). The Hirshfeld surface mapped over $d$norm using a standard surface resolution with a fixed colour scale of $0.2$ (red) to $1.3$ (blue) a.u. is shown in Fig. 6a. The shorter and

![Figure 4](image1.png)
**Figure 4**
The optimized molecular structure of the title compound.

![Figure 5](image2.png)
**Figure 5**
The frontier molecular orbitals (FMOs) of the title compound.

| Parameter | Value |
|-----------|-------|
| $E_{\text{HOMO}}$ (eV) | $-5.212$ |
| $E_{\text{LUMO}}$ (eV) | $-2.047$ |
| $E_{\text{HOMO}} - E_{\text{LUMO}}$ energy gap (eV) | $3.165$ |
| $E_{\text{HOMO}}$ (eV) | $-5.851$ |
| $E_{\text{LUMO}}$ (eV) | $-2.248$ |
| Ionization potential ($I$) (eV) | $5.212$ |
| Electron affinity ($A$) | $2.047$ |
| Electrophilicity Index ($\chi$) | $4.163$ |
| Chemical Potential ($\mu$) | $3.629$ |
| Electro negativity ($\mu$) | $-3.630$ |
| Hardness ($\eta$) | $1.583$ |
| Softness ($\sigma$) | $0.316$ |

### Table 1

Hydrogen-bond geometry (Å, °).

| D—H···A | D—H | H···A | D···A | D—H···A |
|----------|------|-------|-------|---------|
| C20—H20B···O1' | 0.96 | 2.44 | 3.292 (3) | 148 |

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

### Table 2

Physico-chemical properties.

| Parameter | Value |
|-----------|-------|
| $E_{\text{HOMO}}$ (eV) | $-5.212$ |
| $E_{\text{LUMO}}$ (eV) | $-2.047$ |
| $E_{\text{HOMO}} - E_{\text{LUMO}}$ energy gap (eV) | $3.165$ |
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| Softness ($\sigma$) | $0.316$ |
longer contacts are indicated as red and blue spots, respectively, on the Hirshfeld surfaces, and contacts with distances approximately equal to the sum of the van der Waals radii are represented as white spots. The most important red spots on the $d_{\text{norm}}$ surface represent C–H···O interactions.

The HS mapped over curvedness and shape-index, introduced by Koenderink (Koenderink, 1990; Koenderink & van Doorn, 1992), give further chemical insight into molecular packing. A surface with low curvedness designates a flat region and may be indicative of $\pi$–$\pi$ stacking in the crystal. A surface with high curvedness is highlighted as dark blue edges, and is indicative of the absence of $\pi$–$\pi$ stacking (Fig. 6). The nearest neighbour coordination environment of a molecule is identified from the colour patches on the Hirshfeld surface, depending on their closeness to adjacent molecules (Mohamooda Sumaya et al., 2017).

The two-dimensional fingerprint plots of $(d_i, d_e)$ points of all the contacts contributing to the Hirshfeld surface analysis in normal mode for all the atoms are shown in Fig. 7. The most important intermolecular interactions are H···H contacts, contributing 73.2% to the overall crystal packing. Other interactions and their respective contributions are C···H/ H···C (18.4%) and O···H/H···O (8.4%), respectively.

The Hirshfeld surface analysis confirms the importance of H-atom contacts in establishing the packing. The large number of H···H and C···H/C···C interactions suggest that van der Waals interactions and hydrogen bonding play the major roles in the crystal packing (Hathwar et al., 2015).

6. Database survey
A search of the Cambridge Structural Database (CSD, version 5.39, update August 2018; Groom et al., 2016) for the 3-methyl-2,6-diphenylpiperidine skeleton yielded two hits, methyl 4-oxo-r-2,c-6-diphenylpiperidine-3-carboxylate (BIHZYEY; Sampath et al., 2004) and r-2,c-6-diphenylpiperidine (NIKYEN; Maheshwaran et al., 2013). The piperidine ring has a boat-shaped conformation in both compounds, as in the title compound. The benzene ring and the mean plane of the piperidine ring are inclined to each other by dihedral angles ranging from 19.95 to 29.16°, compared to 22.05 (6)° in the title compound.

7. Synthesis and crystallization
The compound t-3-methyl-r-2,c-6-diphenylpiperidin-4-one was reduced to the corresponding piperidine using the Wolf–Kishner reduction (Ravindran & Jeyaraman, 1992). The piperidine-4-one (10 mmol) was treated with diethylene glycol (40 ml), hydrazine hydrate (10 mmol) and KOH pellets (10 mmol) to give t-3-methyl-r-2,c-6-diphenylpiperidine. N-Acetyl piperidine was synthesized by the acetylation of the above piperidine. To t-3-methyl-r-2,c-6-diphenylpiperidine (5 mmol) dissolved in benzene (50 ml) were added triethylamine (20 mmol) and acetyl chloride (20 mmol) to give N-acetyl-t-3-methyl-r-2,c-6-diphenylpiperidine, which was crystallized by slow evaporation from a benzene and petroleum ether solution.

8. Refinement
Crystal data, data collection and structure refinement details are summarized in Table 3. H atoms were positioned geometrically (N–H = 0.88–0.90 Å and C–H = 0.93–0.98 Å) and
allowed to ride on their parent atoms, with $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H and $1.2U_{eq}(C)$ for other H atoms.

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Crystal structure, DFT and Hirshfeld surface analysis of N-acetyl-t-3-methyl-r-2,c-6-diphenylpiperidine

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Computing details

Data collection: APEX2 (Bruker, 2016); cell refinement: SAINT (Bruker, 2016); data reduction: SAINT (Bruker, 2016); program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL-2018/3 (Sheldrick, 2015); molecular graphics: ORTEP-3 for Windows (Farrugia, 2012); software used to prepare material for publication: SHELXL97 and PLATON (Spek, 2020).

1-(3-Methyl-2,6-diphenylpiperidin-1-yl)ethanone

Crystal data

C$_{20}$H$_{23}$NO  
$F(000) = 316$  
$D_x = 1.153$ Mg m$^{-3}$  
Monoclinic, $P2_1$  
$D = 1.153$ Mg m$^{-3}$  
a = 8.3063 (4) Å  
b = 7.5842 (4) Å  
c = 13.8410 (7) Å  
$\alpha = 104.174 (2)^\circ$  
$V = 845.39 (7)$ Å$^3$  
$Z = 2$  

Data collection

Bruker SMART APEXII CCD  
diffractometer  
Radiation source: fine-focus sealed tube  
$\omega$ and $\phi$ scans  
Absorption correction: multi-scan (SADABS; Bruker, 2016)  
$T_{\text{min}} = 0.697, T_{\text{max}} = 0.745$  
15383 measured reflections  

Refinement

Refinement on $F^2$  
$R[F^2 > 2\sigma(F^2)] = 0.037$  
$wR(F^2) = 0.101$  
$S = 1.03$  
3447 reflections  
201 parameters  
1 restraint  

Hydrogen site location: inferred from neighbouring sites  

$R_{\text{int}} = 0.024$  
$\theta_{\text{max}} = 26.4^\circ, \theta_{\text{min}} = 2.6^\circ$  
$h = -10$→$9$  
k = $-9$→$9$  
l = $-17$→$17$  

$\Delta(\sigma)_{\text{max}} < 0.001$  
$\Delta \rho_{\text{max}} = 0.22$ e Å$^{-3}$  
$\Delta \rho_{\text{min}} = -0.13$ e Å$^{-3}$
Absolute structure: Flack $x$ determined using 1136 quotients $[(I^-)-(I^+)]/[(I^-)+(I^+)]$ (Parsons et al., 2013)
Absolute structure parameter: 0.0 (5)

**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 ($Å^2$)**

|   | $x$          | $y$          | $z$             | $U_{eq}$/$U_{eq}$ |
|---|-------------|-------------|-----------------|-------------------|
| C2| 0.3371 (3)  | 0.2057 (3)  | 0.31568 (16)   | 0.0457 (5)        |
| H2| 0.377220    | 0.270737    | 0.378151        | 0.055*            |
| C3| 0.1580 (3)  | 0.2626 (4)  | 0.2699 (2)      | 0.0565 (6)        |
| H3A| 0.155366   | 0.388579    | 0.257504        | 0.068*            |
| H3B| 0.117951   | 0.203547    | 0.206358        | 0.068*            |
| C4| 0.0435 (3)  | 0.2199 (4)  | 0.3367 (2)      | 0.0679 (7)        |
| H4A| −0.070712  | 0.231457    | 0.298638        | 0.081*            |
| H4B| 0.061680   | 0.304992    | 0.390657        | 0.081*            |
| C5| 0.0700 (3)  | 0.0344 (4)  | 0.38074 (17)    | 0.0567 (6)        |
| H5| −0.038621  | −0.023553   | 0.368498        | 0.068*            |
| C6| 0.1821 (3)  | −0.0774 (3) | 0.33117 (17)    | 0.0481 (5)        |
| H6| 0.209751    | −0.182736   | 0.372930        | 0.058*            |
| C7| 0.1060 (3)  | −0.1457 (3) | 0.22655 (17)    | 0.0502 (5)        |
| C8| −0.0600 (3) | −0.1247 (4) | 0.1781 (2)      | 0.0659 (7)        |
| H8| −0.129032  | −0.058009   | 0.207568        | 0.079*            |
| C9| −0.1240 (5) | −0.2032 (5) | 0.0855 (2)      | 0.0812 (10)       |
| H9| −0.235412  | −0.188306   | 0.053477        | 0.097*            |
| C10| −0.0235 (6)| −0.3020 (5) | 0.0415 (2)      | 0.0890 (11)       |
| H10| −0.066947  | −0.354500   | −0.020068       | 0.107*            |
| C11| 0.1404 (5) | −0.3236 (4) | 0.0881 (2)      | 0.0824 (10)       |
| H11| 0.208456   | −0.390605   | 0.058133        | 0.099*            |
| C12| 0.2053 (4) | −0.2460 (4) | 0.1796 (2)      | 0.0637 (7)        |
| H12| 0.317158   | −0.260974   | 0.210498        | 0.076*            |
| C13| 0.4446 (3) | 0.2557 (3)  | 0.24606 (16)    | 0.0471 (5)        |
| C14| 0.4544 (3) | 0.1539 (4)  | 0.16487 (19)    | 0.0584 (6)        |
| H14| 0.395691   | 0.048462    | 0.152879        | 0.070*            |
| C15| 0.5502 (4) | 0.2063 (5)  | 0.1012 (2)      | 0.0715 (8)        |
| H15| 0.555322   | 0.136101    | 0.047006        | 0.086*            |
| C16| 0.6372 (4) | 0.3607 (5)  | 0.1175 (2)      | 0.0783 (9)        |
| H16| 0.701865   | 0.395466    | 0.074701        | 0.094*            |
| C17| 0.6289 (4) | 0.4638 (4)  | 0.1971 (3)      | 0.0775 (9)        |
| H17| 0.688101   | 0.568970    | 0.208368        | 0.093*            |
| C18| 0.5326 (3) | 0.4126 (4)  | 0.2611 (2)      | 0.0632 (7)        |
| H18| 0.526974   | 0.484386    | 0.314655        | 0.076*            |
| C19| 0.4825 (3) | −0.0674 (3) | 0.39016 (16)    | 0.0476 (5)        |
| Atomic displacement parameters (Å²) |
|-----------------------------------|
|                                  |
| $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
| C2      | 0.0422 (11) | 0.0485 (13) | 0.0457 (11) | 0.0023 (10) | 0.0097 (9) | −0.0057 (10) |
| C3      | 0.0478 (13) | 0.0552 (14) | 0.0642 (14) | 0.0106 (11) | 0.0097 (11) | 0.0003 (12) |
| C4      | 0.0484 (14) | 0.0814 (19) | 0.0771 (17) | 0.0154 (14) | 0.0216 (13) | −0.0054 (15) |
| C5      | 0.0388 (12) | 0.0813 (18) | 0.0536 (13) | −0.0051 (12) | 0.0180 (10) | −0.0059 (13) |
| C6      | 0.0379 (11) | 0.0585 (13) | 0.0484 (11) | −0.0038 (10) | 0.0117 (9) | 0.0029 (11) |
| C7      | 0.0493 (13) | 0.0504 (12) | 0.0509 (12) | −0.0083 (11) | 0.0123 (10) | 0.0014 (11) |
| C8      | 0.0556 (15) | 0.0738 (19) | 0.0623 (15) | −0.0092 (14) | 0.0029 (12) | −0.0028 (14) |
| C9      | 0.080 (2)   | 0.085 (2)   | 0.0654 (17) | −0.0241 (17) | −0.0076 (16) | 0.0078 (16) |
| C10     | 0.122 (3)   | 0.086 (2)   | 0.0541 (16) | −0.035 (2)   | 0.0132 (19) | −0.0097 (16) |
| C11     | 0.109 (3)   | 0.071 (2)   | 0.0726 (19) | −0.0196 (18) | 0.0327 (19) | −0.0186 (16) |
| C12     | 0.0700 (17) | 0.0594 (15) | 0.0644 (15) | −0.0064 (13) | 0.0217 (13) | −0.0078 (13) |
| C13     | 0.0420 (12) | 0.0468 (12) | 0.0502 (12) | 0.0015 (10)  | 0.0068 (9)  | 0.0034 (10)  |
| C14     | 0.0599 (14) | 0.0624 (15) | 0.0547 (14) | −0.0057 (12) | 0.0173 (12) | −0.0007 (11) |
| C15     | 0.0708 (17) | 0.082 (2)   | 0.0616 (15) | 0.0017 (16)  | 0.0277 (14) | 0.0080 (15)  |
| C16     | 0.0658 (18) | 0.092 (2)   | 0.083 (2)   | −0.0003 (17) | 0.0287 (15) | 0.0310 (19)  |
| C17     | 0.0677 (17) | 0.0639 (18) | 0.102 (2)   | −0.0122 (14) | 0.0221 (17) | 0.0219 (17)  |
| C18     | 0.0586 (15) | 0.0526 (14) | 0.0755 (16) | −0.0018 (12) | 0.0110 (13) | 0.0047 (13)  |
| C19     | 0.0417 (12) | 0.0580 (14) | 0.0444 (11) | 0.0082 (11)  | 0.0129 (9)  | 0.0067 (10)  |
| C20     | 0.0361 (11) | 0.0821 (18) | 0.0650 (14) | 0.0069 (12)  | 0.0085 (10) | 0.0051 (14)  |
| C21     | 0.0709 (18) | 0.091 (2)   | 0.0638 (15) | −0.0030 (16) | 0.0278 (13) | 0.0006 (16)  |
| N1      | 0.0335 (9)  | 0.0520 (10) | 0.0445 (9)  | 0.0014 (8)   | 0.0100 (7)  | 0.0023 (8)   |
| O1      | 0.0595 (12) | 0.0657 (12) | 0.0843 (13) | 0.0117 (9)   | 0.0125 (10) | 0.0206 (10)  |

Geometric parameters (Å, °)

| Geometric parameters (Å, °) |
|----------------------------|
|                            |
| C2—N1  | 1.481 (3) | C11—C12 | 1.381 (4) |
| C2—C13 | 1.513 (3) | C11—H11 | 0.9300 |
| C2—C3  | 1.530 (3) | C12—H12 | 0.9300 |
| C2—H2  | 0.9800   | C13—C14 | 1.382 (4) |
| C3—C4  | 1.515 (4) | C13—C18 | 1.386 (4) |
| C3—H3A | 0.9700   | C14—C15 | 1.382 (4) |
| C3—H3B | 0.9700   | C14—H14 | 0.9300 |
| C4—C5  | 1.528 (4) | C15—C16 | 1.366 (5) |
| C4—H4A | 0.9700   | C15—H15 | 0.9300 |

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C4—H4B  0.9700  C16—C17  1.366 (5)
C5—C21  1.511 (4)  C16—H16  0.9300
C5—C6   1.539 (3)  C17—C18  1.386 (4)
C5—H5   0.9800  C17—H17  0.9300
C6—N1   1.475 (3)  C18—H18  0.9300
C6—C7   1.522 (3)  C19—O1  1.230 (3)
C6—H6   0.9800  C19—N1  1.364 (3)
C7—C8   1.387 (3)  C19—C20  1.499 (4)
C7—C12  1.394 (4)  C20—H20A  0.9600
C8—C9   1.395 (4)  C20—H20B  0.9600
C8—H8   0.9300  C20—H20C  0.9600
C9—C10  1.371 (6)  C21—H21A  0.9600
C9—H9   0.9300  C21—H21B  0.9600
C10—C11 1.366 (5)  C21—H21C  0.9600
C10—H10 0.9300

N1—C2—C13 113.69 (18)  C10—C11—C12  120.1 (3)
N1—C2—C3  109.49 (19)  C10—C11—H11  119.9
C13—C2—C3 109.34 (19)  C12—C11—H11  119.9
N1—C2—H2  108.1  C11—C12—C7  121.2 (3)
C13—C2—H2 108.1  C11—C12—H12  119.4
C3—C2—H2  108.1  C7—C12—H12  119.4
C4—C3—C2  112.3 (2)  C14—C13—C18  117.9 (2)
C4—C3—H3A 109.2  C14—C13—C2  122.6 (2)
C2—C3—H3A 109.2  C18—C13—C2  119.4 (2)
C4—C3—H3B 109.2  C15—C14—C13  121.0 (3)
C2—C3—H3B 109.2  C15—C14—H14  119.5
H3A—C3—H3B 107.9  C13—C14—H14  119.5
C3—C4—C5  112.9 (2)  C16—C15—C14  120.4 (3)
C3—C4—H4A 109.0  C16—C15—H15  119.8
C5—C4—H4A 109.0  C14—C15—H15  119.8
C3—C4—H4B 109.0  C17—C16—C15  119.6 (3)
C5—C4—H4B 109.0  C17—C16—H16  120.2
H4A—C4—H4B 107.8  C15—C16—H16  120.2
C21—C5—C4 110.9 (2)  C16—C17—C18  120.4 (3)
C21—C5—C6 110.1 (2)  C16—C17—H17  119.8
C4—C5—C6  111.90 (19)  C18—C17—H17  119.8
C21—C5—H5  107.9  C13—C18—C17  120.7 (3)
C4—C5—H5  107.9  C13—C18—H18  119.7
C6—C5—H5  107.9  C17—C18—H18  119.7
N1—C6—C7  113.10 (17)  O1—C19—N1  121.4 (2)
N1—C6—C5  109.31 (19)  O1—C19—C20  120.0 (2)
C7—C6—C5  117.12 (19)  N1—C19—C20  118.5 (2)
N1—C6—H6  105.4  C19—C20—H20A  109.5
C7—C6—H6  105.4  C19—C20—H20B  109.5
C5—C6—H6  105.4  H20A—C20—H20B  109.5
C8—C7—C12 118.0 (2)  C19—C20—H20C  109.5
C8—C7—C6  123.5 (2)  H20A—C20—H20C  109.5
C12—C7—C6 118.3 (2) H20B—C20—H20C 109.5
C7—C8—C9 120.3 (3) C5—C21—H21A 109.5
C7—C8—H8 119.8 C5—C21—H21B 109.5
C9—C8—H8 119.8 H21A—C21—H21B 109.5
C10—C9—C8 120.3 (3) C5—C21—H21C 109.5
C10—C9—H9 119.8 H21A—C21—H21C 109.5
C8—C9—H9 119.8 H21B—C21—H21C 109.5
C11—C10—C9 120.1 (3) C19—N1—C6 117.61 (18)
C11—C10—H10 120.0 C19—N1—C2 122.16 (19)
C9—C10—H10 120.0 C6—N1—C2 118.46 (17)

N1—C2—C3—C4 56.0 (3) N1—C2—C13—C18 −141.6 (2)
C13—C2—C3—C4 −178.8 (2) C3—C2—C13—C18 95.7 (3)
C2—C3—C4—C5 −45.0 (3) C13—C14—C15—C16 0.0 (5)
C3—C4—C5—C6 −11.0 (3) C2—C13—C14—C15 −178.1 (2)
C21—C5—C6—N1 −68.0 (3) C14—C15—C16—C17 0.0 (5)
C4—C5—C6—C7 161.7 (2) C14—C15—C16—C17 0.0 (5)
C21—C5—C6—N1 −119.4 (2) C14—C15—C16—C17 0.0 (5)
C21—C5—C6—C7 161.7 (2) C14—C15—C16—C17 0.0 (5)
C4—C5—C6—C7 −119.4 (2) C14—C15—C16—C17 0.0 (5)
C13—C2—C13—C18 95.7 (3) C3—C2—N1—C19 64.0 (3)
C3—C2—C13—C14 −173.40 (18) C3—C2—N1—C6 −8.9 (3)
C3—C2—C13—C14 −81.8 (3)

Hydrogen-bond geometry (Å, °)

| D—H—A | D—H | H—A | D···A | D—H···A |
|--------|-----|-----|-------|--------|
| C20—H20B···O1
      | 0.96 | 2.44 | 3.292 (3) | 148 |

Symmetry code: (i) −x+1, y+1/2, −z+1.