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3,5-Dimethyl-2,6-diphenylpiperidine

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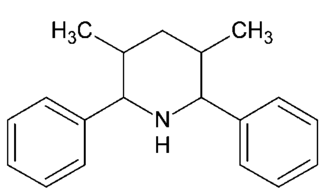
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.051; wR factor = 0.216; data-to-parameter ratio = 21.5.

In the title compound, $C_{19}H_{23}N$, the piperidine ring has a chair conformation. The phenyl rings are inclined to one another by 52.76 (16)°. One of the methyl substituents on the piperidine ring is axial while the other is equatorial, like the phenyl rings. In the crystal, molecules are linked *via* C—H$\cdots\pi$ interactions, forming zigzag chains along [001].

Related literature

For the biological activity of piperidine derivatives, see: Parthiban *et al.* (2005, 2009*a*,*b*, 2011); Aridoss *et al.* (2007). For related structures, see: Aravindhan *et al.* (2009); Sugumar *et al.* (2013). For ring puckering analysis, see: Cremer & Pople (1975); Nardelli (1983).



Experimental

Crystal data

$C_{19}H_{23}N$
M_r = 265.38
Orthorhombic, $Iba2$
a = 10.1689 (8) Å
b = 43.141 (3) Å
c = 7.2658 (5) Å
V = 3187.5 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.06 mm^{-1}
T = 293 K
0.35 × 0.30 × 0.25 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.978, T_{max} = 0.984
8658 measured reflections
3900 independent reflections
2652 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.216
S = 0.78
3900 reflections
181 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of rings C1–C6 and C12–C17, respectively.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C5—H5$\cdots Cg1^{i}$	0.93	2.90	3.187 (2)	170
C18—H18C$\cdots Cg2^{ii}$	0.96	2.99	3.762 (5)	139

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97*.

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Supporting information for this paper is available from the IUCr electronic archives (Reference: SU2706).

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Acta Cryst. (2014). E**70**, o404 [doi:10.1107/S160053681400470X]

3,5-Dimethyl-2,6-diphenylpiperidine

S. Sathya, K. Prathebha, G. Usha, S. Abdul Basheer and S. Ponnuswamy

S1. Comment

Piperidone molecules exhibit a broad-spectrum of biological activities ranging from anti-bacterial to anti-cancer (Parthiban *et al.*, 2005, 2009*b*, 2011). Isolation from natural products as well as synthesis of new molecules and the stereochemical analysis of this class of compounds are important in the field of medicinal chemistry. 2,6-disubstituted piperidones and their N-substituted derivatives are of great importance due to their significant pharmacological properties (Parthiban *et al.*, 2009*a*; Aridoss *et al.*, 2007).

The molecular structure of the title molecule is illustrated in Fig. 1. The bond distances and angles are normal and close to those observed previously for similar compounds (Aravindhan *et al.*, 2009; Sugumar *et al.*, 2013).

The piperidine ring adopts a chair conformation as defined by the puckering parameters (Cremer & Pople, 1975) and the smallest displacement asymmetry parameters (Nardelli, 1983) for the piperidine ring are q2 = 0. 0326 (3) Å, q3 = -0.579 (3) Å, QT = 0.5803 (3) Å,Theta2 $_2$ = 176.78 (3)° and D2(C7—N1) = 0.0050 (1) Å. The dihedral angle between the two phenyl rings is 52.80 (2)°.

In the crystal, molecules are linked *via* C—H···π interactions forming zigzag chains along [001]; see Table 1 and Fig. 2.

S2. Experimental

A mixture of 3,5-dimethyl-2,6-diphenylpiperidin-4-one (10 mmol) and 80% hydrazine hydrate (3.1 ml) in diethylene glycol (40 ml) was heated on a steam bath for 2 h. Potassium hydroxide pellets (2.8 g) were added to the mixture and the contents were refluxed vigorously on a heating mantle for another 2 h and then the reaction mixture was cooled. The product was filtered and recrystallized from ethanol yielding block-like colourless crystals.

S3. Refinement

H atoms were positioned geometrically and treated as riding atoms: C—H = 0.93–0.98 Å, N—H =0.86 Å with $U_{\rm iso}$(H)= 1.5$U_{\rm eq}$(*C*-methyl) and = 1.2$U_{\rm eq}$(N,*C*) for other H atoms.

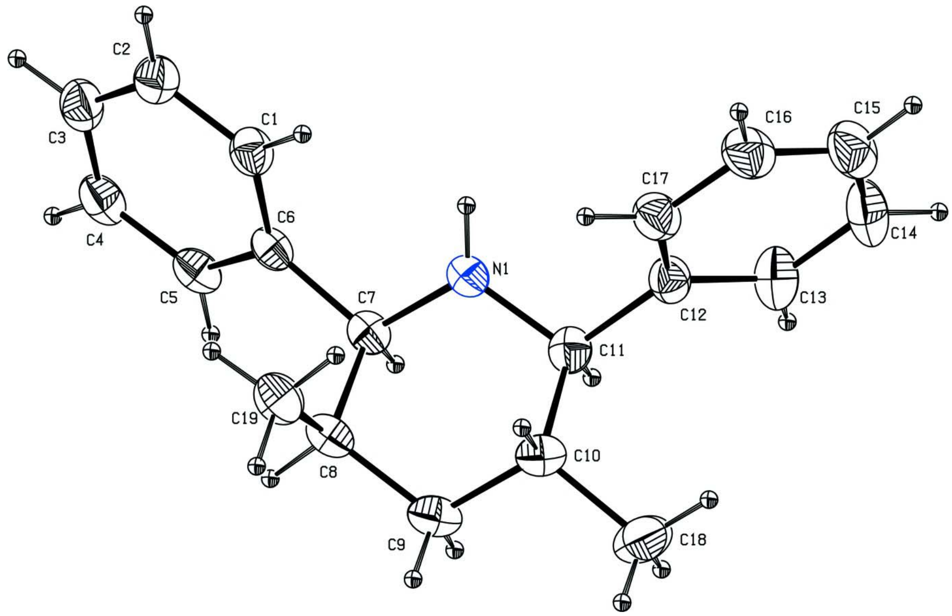

Figure 1

The molecular structure of the title molecule, with atom labelling. Displacement ellipsoids are drawn at the 30% probability level.

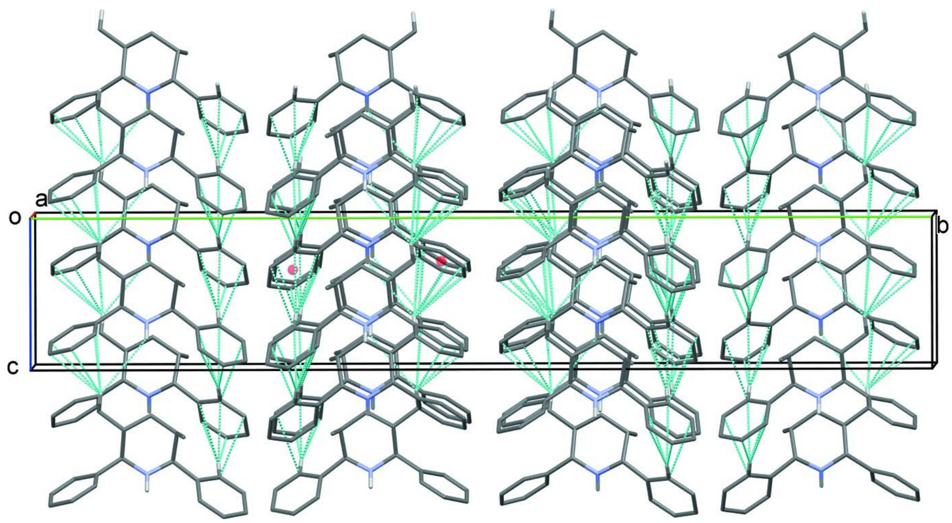

Figure 2

A view along the *a* axis of the crystal packing of the title compound. The centroids of phenyl rings C1—C6 and C12—C17 are marked with red dots and the dashed lines indicate the C—H···π interactions (see Table 1).

c-3,*t*-5-Dimethyl-*r*-2,*c*-6-diphenylpiperidine

Crystal data

$C_{19}H_{23}N$	b = 43.141 (3) Å
M_r = 265.38	c = 7.2658 (5) Å
Orthorhombic, *Iba*2	V = 3187.5 (4) Å^3
Hall symbol: I 2 -2 c	Z = 8
a = 10.1689 (8) Å	F(000) = 1152

D_x = 1.106 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
μ = 0.06 mm^{-1}
T = 293 K
Block, colourless
0.35 × 0.30 × 0.25 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.978, T_{max} = 0.984
8658 measured reflections
3900 independent reflections
2652 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 28.3°, θ_{min} = 0.9°
$h = -9 \rightarrow 13$
$k = -57 \rightarrow 45$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.216
S = 0.78
3900 reflections
181 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.2P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
C1	0.2691 (3)	0.31401 (6)	0.3689 (4)	0.0682 (6)
H1	0.3282	0.3302	0.3853	0.082*
C2	0.2822 (3)	0.28735 (6)	0.4756 (5)	0.0776 (7)
H2	0.3496	0.2857	0.5614	0.093*
C3	0.1939 (3)	0.26338 (6)	0.4524 (5)	0.0800 (8)
H3	0.2025	0.2453	0.5211	0.096*
C4	0.0933 (3)	0.26627 (6)	0.3277 (4)	0.0763 (7)
H4	0.0329	0.2503	0.3138	0.092*
C5	0.0812 (2)	0.29289 (5)	0.2223 (3)	0.0661 (6)
H5	0.0121	0.2946	0.1391	0.079*
C6	0.1706 (2)	0.31695 (5)	0.2394 (3)	0.0562 (5)
C7	0.1597 (2)	0.34446 (5)	0.1132 (3)	0.0573 (5)
H7	0.0660	0.3479	0.0886	0.069*

C8	0.2284 (2)	0.33925 (6)	−0.0733 (3)	0.0670 (6)
H8	0.1847	0.3219	−0.1349	0.080*
C9	0.2068 (3)	0.36835 (7)	−0.1906 (4)	0.0779 (7)
H9A	0.2541	0.3660	−0.3058	0.093*
H9B	0.1140	0.3701	−0.2194	0.093*
C10	0.2518 (3)	0.39803 (6)	−0.0974 (4)	0.0702 (7)
H10	0.3471	0.3968	−0.0789	0.084*
C11	0.1862 (2)	0.40069 (5)	0.0914 (4)	0.0635 (6)
H11	0.0910	0.4027	0.0734	0.076*
C12	0.2343 (2)	0.42859 (5)	0.1987 (4)	0.0662 (6)
C13	0.1532 (3)	0.45364 (6)	0.2290 (6)	0.0918 (10)
H13	0.0681	0.4535	0.1821	0.110*
C14	0.1971 (4)	0.47910 (6)	0.3290 (8)	0.1080 (13)
H14	0.1413	0.4958	0.3498	0.130*
C15	0.3227 (4)	0.47958 (7)	0.3968 (6)	0.1008 (12)
H15	0.3521	0.4965	0.4651	0.121*
C16	0.4041 (4)	0.45530 (6)	0.3639 (5)	0.0914 (9)
H16	0.4902	0.4559	0.4070	0.110*
C17	0.3604 (3)	0.42965 (7)	0.2667 (4)	0.0780 (7)
H17	0.4168	0.4130	0.2474	0.094*
C18	0.2231 (5)	0.42606 (9)	−0.2189 (6)	0.1090 (12)
H18A	0.2522	0.4446	−0.1579	0.163*
H18B	0.1303	0.4274	−0.2414	0.163*
H18C	0.2688	0.4239	−0.3338	0.163*
C19	0.3720 (3)	0.33137 (7)	−0.0545 (5)	0.0794 (8)
H19A	0.4097	0.3285	−0.1745	0.119*
H19B	0.3813	0.3126	0.0154	0.119*
H19C	0.4167	0.3480	0.0075	0.119*
N1	0.21151 (19)	0.37261 (4)	0.1973 (3)	0.0599 (5)
H1A	0.2533	0.3727	0.3002	0.072*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0619 (13)	0.0621 (12)	0.0804 (17)	−0.0039 (9)	−0.0054 (12)	−0.0084 (12)
C2	0.0826 (18)	0.0710 (15)	0.0793 (18)	0.0082 (13)	−0.0061 (14)	−0.0033 (14)
C3	0.097 (2)	0.0625 (14)	0.0808 (18)	0.0029 (13)	0.0222 (16)	−0.0044 (13)
C4	0.0858 (17)	0.0669 (14)	0.0760 (16)	−0.0181 (12)	0.0179 (15)	−0.0179 (13)
C5	0.0602 (12)	0.0750 (13)	0.0630 (12)	−0.0131 (10)	0.0065 (11)	−0.0173 (11)
C6	0.0497 (10)	0.0601 (11)	0.0588 (11)	−0.0007 (8)	0.0057 (9)	−0.0152 (10)
C7	0.0464 (9)	0.0628 (11)	0.0628 (13)	−0.0018 (8)	−0.0011 (10)	−0.0086 (10)
C8	0.0657 (15)	0.0756 (14)	0.0598 (13)	−0.0068 (11)	0.0001 (11)	−0.0185 (11)
C9	0.0816 (16)	0.0959 (18)	0.0561 (13)	−0.0100 (14)	−0.0074 (12)	−0.0069 (13)
C10	0.0691 (14)	0.0829 (16)	0.0587 (14)	−0.0036 (12)	−0.0055 (11)	0.0032 (12)
C11	0.0549 (11)	0.0617 (13)	0.0740 (14)	0.0011 (9)	−0.0030 (12)	−0.0011 (11)
C12	0.0715 (14)	0.0552 (11)	0.0721 (15)	−0.0054 (10)	0.0068 (13)	−0.0006 (11)
C13	0.0821 (17)	0.0632 (14)	0.130 (3)	−0.0011 (12)	0.012 (2)	−0.0039 (17)
C14	0.126 (3)	0.0569 (15)	0.141 (3)	−0.0040 (16)	0.025 (3)	−0.0173 (19)

C15	0.132 (3)	0.0689 (18)	0.102 (2)	−0.0337 (18)	0.016 (2)	−0.0117 (17)
C16	0.099 (2)	0.0863 (18)	0.089 (2)	−0.0260 (16)	−0.0070 (18)	−0.0075 (15)
C17	0.0792 (16)	0.0765 (15)	0.0784 (17)	−0.0010 (13)	−0.0083 (14)	−0.0101 (13)
C18	0.138 (3)	0.107 (3)	0.081 (2)	−0.005 (2)	−0.019 (2)	0.026 (2)
C19	0.0694 (16)	0.0872 (17)	0.0817 (17)	0.0035 (13)	0.0160 (14)	−0.0152 (14)
N1	0.0650 (11)	0.0579 (10)	0.0569 (11)	−0.0023 (7)	−0.0026 (9)	−0.0064 (9)

Geometric parameters (Å, º)

C1—C6	1.380 (4)	C10—H10	0.9800
C1—C2	1.394 (4)	C11—N1	1.458 (3)
C1—H1	0.9300	C11—C12	1.516 (4)
C2—C3	1.380 (4)	C11—H11	0.9800
C2—H2	0.9300	C12—C17	1.374 (4)
C3—C4	1.372 (5)	C12—C13	1.378 (4)
C3—H3	0.9300	C13—C14	1.391 (5)
C4—C5	1.386 (4)	C13—H13	0.9300
C4—H4	0.9300	C14—C15	1.369 (6)
C5—C6	1.385 (3)	C14—H14	0.9300
C5—H5	0.9300	C15—C16	1.356 (5)
C6—C7	1.504 (3)	C15—H15	0.9300
C7—N1	1.458 (3)	C16—C17	1.386 (4)
C7—C8	1.541 (3)	C16—H16	0.9300
C7—H7	0.9800	C17—H17	0.9300
C8—C19	1.506 (4)	C18—H18A	0.9600
C8—C9	1.533 (4)	C18—H18B	0.9600
C8—H8	0.9800	C18—H18C	0.9600
C9—C10	1.519 (4)	C19—H19A	0.9600
C9—H9A	0.9700	C19—H19B	0.9600
C9—H9B	0.9700	C19—H19C	0.9600
C10—C18	1.525 (4)	N1—H1A	0.8600
C10—C11	1.530 (4)		
C6—C1—C2	121.6 (2)	C11—C10—H10	108.2
C6—C1—H1	119.2	N1—C11—C12	109.3 (2)
C2—C1—H1	119.2	N1—C11—C10	109.5 (2)
C3—C2—C1	119.2 (3)	C12—C11—C10	112.3 (2)
C3—C2—H2	120.4	N1—C11—H11	108.5
C1—C2—H2	120.4	C12—C11—H11	108.5
C4—C3—C2	119.8 (3)	C10—C11—H11	108.5
C4—C3—H3	120.1	C17—C12—C13	118.4 (3)
C2—C3—H3	120.1	C17—C12—C11	120.8 (2)
C3—C4—C5	120.5 (2)	C13—C12—C11	120.8 (3)
C3—C4—H4	119.8	C12—C13—C14	120.7 (3)
C5—C4—H4	119.8	C12—C13—H13	119.7
C6—C5—C4	120.8 (2)	C14—C13—H13	119.7
C6—C5—H5	119.6	C15—C14—C13	120.0 (3)
C4—C5—H5	119.6	C15—C14—H14	120.0

C1—C6—C5	118.0 (2)	C13—C14—H14	120.0
C1—C6—C7	122.80 (19)	C16—C15—C14	119.6 (3)
C5—C6—C7	119.2 (2)	C16—C15—H15	120.2
N1—C7—C6	112.05 (18)	C14—C15—H15	120.2
N1—C7—C8	109.02 (19)	C15—C16—C17	120.7 (3)
C6—C7—C8	112.79 (19)	C15—C16—H16	119.6
N1—C7—H7	107.6	C17—C16—H16	119.6
C6—C7—H7	107.6	C12—C17—C16	120.6 (3)
C8—C7—H7	107.6	C12—C17—H17	119.7
C19—C8—C9	112.0 (2)	C16—C17—H17	119.7
C19—C8—C7	113.1 (2)	C10—C18—H18A	109.5
C9—C8—C7	107.7 (2)	C10—C18—H18B	109.5
C19—C8—H8	107.9	H18A—C18—H18B	109.5
C9—C8—H8	107.9	C10—C18—H18C	109.5
C7—C8—H8	107.9	H18A—C18—H18C	109.5
C10—C9—C8	113.5 (2)	H18B—C18—H18C	109.5
C10—C9—H9A	108.9	C8—C19—H19A	109.5
C8—C9—H9A	108.9	C8—C19—H19B	109.5
C10—C9—H9B	108.9	H19A—C19—H19B	109.5
C8—C9—H9B	108.9	C8—C19—H19C	109.5
H9A—C9—H9B	107.7	H19A—C19—H19C	109.5
C9—C10—C18	110.7 (3)	H19B—C19—H19C	109.5
C9—C10—C11	109.4 (2)	C11—N1—C7	114.0 (2)
C18—C10—C11	112.1 (3)	C11—N1—H1A	123.0
C9—C10—H10	108.2	C7—N1—H1A	123.0
C18—C10—H10	108.2		

C6—C1—C2—C3	−0.5 (4)	C9—C10—C11—N1	54.0 (3)
C1—C2—C3—C4	−1.2 (5)	C18—C10—C11—N1	177.1 (2)
C2—C3—C4—C5	1.2 (4)	C9—C10—C11—C12	175.7 (2)
C3—C4—C5—C6	0.6 (4)	C18—C10—C11—C12	−61.2 (3)
C2—C1—C6—C5	2.2 (4)	N1—C11—C12—C17	52.2 (3)
C2—C1—C6—C7	−175.6 (2)	C10—C11—C12—C17	−69.6 (3)
C4—C5—C6—C1	−2.3 (3)	N1—C11—C12—C13	−128.4 (3)
C4—C5—C6—C7	175.7 (2)	C10—C11—C12—C13	109.8 (3)
C1—C6—C7—N1	−30.0 (3)	C17—C12—C13—C14	−1.2 (5)
C5—C6—C7—N1	152.2 (2)	C11—C12—C13—C14	179.4 (3)
C1—C6—C7—C8	93.5 (3)	C12—C13—C14—C15	0.7 (6)
C5—C6—C7—C8	−84.3 (2)	C13—C14—C15—C16	0.8 (7)
N1—C7—C8—C19	67.8 (3)	C14—C15—C16—C17	−1.8 (6)
C6—C7—C8—C19	−57.4 (3)	C13—C12—C17—C16	0.2 (5)
N1—C7—C8—C9	−56.5 (2)	C11—C12—C17—C16	179.6 (3)
C6—C7—C8—C9	178.34 (19)	C15—C16—C17—C12	1.3 (5)
C19—C8—C9—C10	−69.9 (3)	C12—C11—N1—C7	175.44 (19)
C7—C8—C9—C10	55.1 (3)	C10—C11—N1—C7	−61.1 (3)
C8—C9—C10—C18	−178.0 (3)	C6—C7—N1—C11	−171.69 (18)
C8—C9—C10—C11	−54.1 (3)	C8—C7—N1—C11	62.7 (2)

Hydrogen-bond geometry (Å, º)

Cg1 and Cg2 are the centroids of rings C1–C6 and C12–C17, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···*Cg*1^{i}	0.93	2.90	3.187 (2)	170
C18—H18*C*···*Cg*2^{ii}	0.96	2.99	3.762 (5)	139

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