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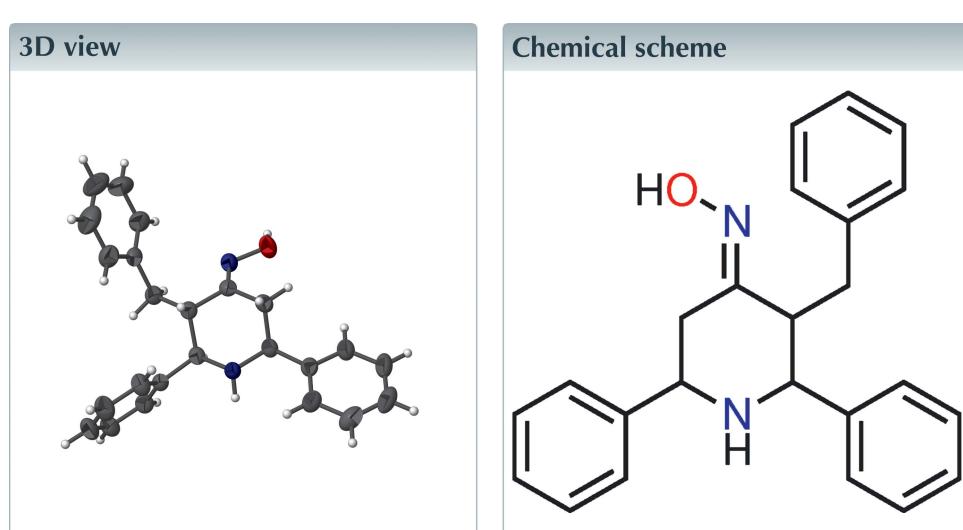
Structural data: full structural data are available from iucrdata.iucr.org

t-3-Benzyl-r-2,c-6-diphenylpiperidin-4-one oxime

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In the title compound, $C_{24}H_{24}N_2O$ [systematic name: (*E*)-3-benzyl-2,6-diphenylpiperidin-4-one oxime], the piperidine ring adopts a slightly distorted chair conformation and the phenyl rings and the benzyl group substituents are attached equatorially. The oxime group makes a dihedral angle of $42.88(12)^\circ$ with the piperidine ring. The dihedral angle between the phenyl rings is $71.96(8)^\circ$. The benzyl ring makes dihedral angles of $63.01(8)$ and $59.35(8)^\circ$ with the two phenyl rings. In the crystal, molecules are linked by O—H···N hydrogen bonds, forming *C*(7) chains along the *c* axis. The chains are linked by C—H···π interactions, forming slabs lying parallel to the *bc* plane.

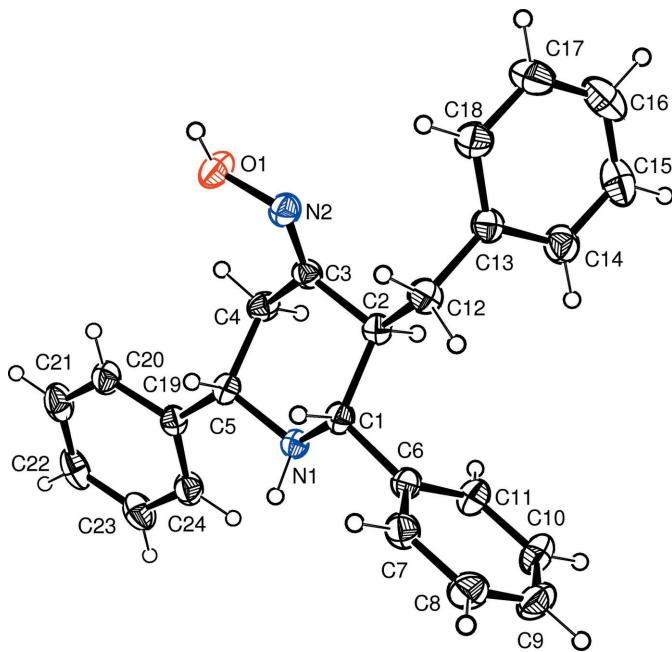


Structure description

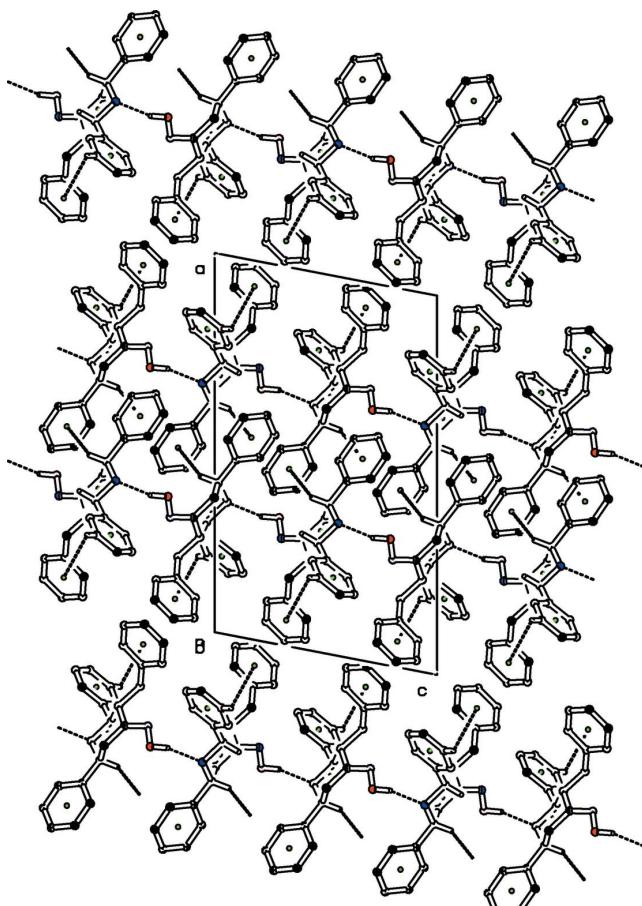
In the title compound, Fig. 1, the piperidine ring adopts a slightly distorted chair conformation [puckering parameters: $q_2 = 0.0698(13) \text{ \AA}$, $q_3 = 0.6086(13) \text{ \AA}$, $Q = 0.6125(13) \text{ \AA}$, $\theta = 6.50(12)^\circ$ and $\varphi = 300.5(11)^\circ$]. The phenyl rings at positions 2 and 6 and the benzyl group at position 3 are attached equatorially. The dihedral angle between the phenyl rings (C6—C11 and C19—C24) at positions 2 and 6, respectively, is $71.96(8)^\circ$. The benzyl ring (C13—C18) makes dihedral angles of $63.01(8)$ and $59.35(8)^\circ$, respectively, with the C6—C11 and C19—C24 phenyl rings.

In the crystal, molecules are linked by O1—H1O···N1 hydrogen bonds, forming *C*(7) chains along the *c*-axis direction (Table 1 and Fig. 2). In addition, there are two C—H···π interactions present, linking the chains to form slabs parallel to the *bc* plane (Table 1 and Fig. 2).

Jayabharathi *et al.* (2008) have reported the crystal structure of the bis(4-methoxyphenyl) derivative of the title compound, in which the piperidine ring adopts a chair

**Figure 1**

A view of the molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level, showing the atom labelling.

**Figure 2**

The crystal packing of the title compound, viewed along the b axis. The hydrogen bonds and $C-H\cdots\pi$ interactions (see Table 1) are shown as dashed lines. H atoms not involved in these interactions have been omitted for clarity.

Table 1
Hydrogen-bond geometry (\AA , $^\circ$).

$Cg3$ and $Cg4$ are the centroids of the C13–C18 and C19–C24 rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O1-H1O\cdots N1^i$	0.90 (2)	2.00 (2)	2.8682 (16)	163 (2)
$C5-H5\cdots Cg4^{ii}$	0.98	2.95	3.7424 (14)	139
$C8-H8\cdots Cg3^{iii}$	0.93	2.99	3.6890 (18)	133

Symmetry codes: (i) $x, -y + \frac{3}{2}, z + \frac{1}{2}$; (ii) $-x + 1, -y + 1, -z + 1$; (iii) $x, y - 1, z$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{24}H_{24}N_2O$
M_r	356.45
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	19.5024 (9), 8.7503 (4), 11.6500 (6)
β ($^\circ$)	100.846 (2)
V (Å 3)	1952.58 (16)
Z	4
Radiation type	$Cu K\alpha$
μ (mm $^{-1}$)	0.58
Crystal size (mm)	0.22 × 0.10 × 0.04
Data collection	
Diffractometer	Bruker Kappa APEX3 CCD area detector
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2015)
T_{\min}, T_{\max}	0.75, 0.98
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	29419, 3448, 2981
R_{int}	0.055
(sin θ/λ) $_{\text{max}}$ (Å $^{-1}$)	0.597
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.124, 1.04
No. of reflections	3448
No. of parameters	252
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å $^{-3}$)	0.16, -0.22

Computer programs: *APEX3* and *SAINT* (Bruker, 2015), *SHELXT2014* (Sheldrick, 2015a), *ORTEP-3* for Windows (Farrugia, 2012), *SHELXL2016* (Sheldrick, 2015b), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

conformation, with equatorial orientation of all substituents except the oxime group at position 4, which has a bisectinal orientation as in the title compound.

Synthesis and crystallization

A mixture of *t*-3-benzyl-*r*-2,6-diphenylpiperidin-4-one (0.1 mol, 7.71 g), hydroxilamine hydrochloride (0.1 mol) and sodium acetate trihydrate (0.3 mol) in methanol was refluxed until completion of reaction (monitored by TLC). After completion of the reaction, water was added and extracted with diethyl ether, dried with anhydrous sodium sulfate and the solvent evaporated. The residue obtained was dissolved in ether to get solid crystals. It was recrystallized twice in distilled ethanol to obtain good-quality single white crystals. Yield 2.6 g, m.p. 364 K.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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References

- Bruker (2015). *APEX3, SAINT and SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Jayabharathi, J., Thangamani, A., Balamurugan, S., Thiruvalluvar, A. & Linden, A. (2008). *Acta Cryst.* **E64**, o1211.
Sheldrick, G. M. (2015a). *Acta Cryst.* **A71**, 3–8.
Sheldrick, G. M. (2015b). *Acta Cryst.* **C71**, 3–8.
Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

full crystallographic data

IUCrData (2016). **1**, x161982 [https://doi.org/10.1107/S2414314616019829]

t-3-Benzyl-r-2,c-6-diphenylpiperidin-4-one oxime

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3-Benzyl-2,6-diphenylpiperidin-4-one oxime

Crystal data

C₂₄H₂₄N₂O
 $M_r = 356.45$
Monoclinic, $P2_1/c$
 $a = 19.5024 (9)$ Å
 $b = 8.7503 (4)$ Å
 $c = 11.6500 (6)$ Å
 $\beta = 100.846 (2)^\circ$
 $V = 1952.58 (16)$ Å³
 $Z = 4$

$F(000) = 760$
 $D_x = 1.213$ Mg m⁻³
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 9891 reflections
 $\theta = 2.3\text{--}66.7^\circ$
 $\mu = 0.58$ mm⁻¹
 $T = 296$ K
Plate, colourless
0.22 × 0.10 × 0.04 mm

Data collection

Bruker Kappa APEX3 CCD area detector
diffractometer
Radiation source: Incoatec Microfocus Source,
Bruker Kappa Duo APEX3
Multilayer Mirror monochromator
Detector resolution: 8.3333 pixels mm⁻¹
 φ and ω scans
Absorption correction: multi-scan
(SADABS; Bruker, 2015)

$T_{\min} = 0.75, T_{\max} = 0.98$
29419 measured reflections
3448 independent reflections
2981 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.055$
 $\theta_{\max} = 66.9^\circ, \theta_{\min} = 2.3^\circ$
 $h = -23\text{--}23$
 $k = -10\text{--}10$
 $l = -12\text{--}13$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.124$
 $S = 1.04$
3448 reflections
252 parameters
0 restraints

Secondary atom site location: difference Fourier
map
Hydrogen site location: mixed
H atoms treated by a mixture of independent
and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0692P)^2 + 0.371P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.16$ e Å⁻³
 $\Delta\rho_{\min} = -0.22$ e Å⁻³

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.71287 (6)	0.48150 (14)	0.53698 (11)	0.0344 (3)
H1	0.696340	0.448499	0.607433	0.041*
C2	0.75685 (6)	0.62853 (14)	0.56741 (11)	0.0351 (3)
H2	0.774300	0.660421	0.497550	0.042*
C3	0.70827 (6)	0.75152 (14)	0.59598 (11)	0.0355 (3)
C4	0.64540 (7)	0.77889 (15)	0.50245 (12)	0.0395 (3)
H4A	0.659495	0.809454	0.430283	0.047*
H4B	0.616634	0.859130	0.525988	0.047*
C5	0.60474 (6)	0.62797 (15)	0.48523 (11)	0.0364 (3)
H5	0.596166	0.595063	0.561691	0.044*
C6	0.75469 (6)	0.35187 (14)	0.49844 (11)	0.0362 (3)
C7	0.76226 (7)	0.21623 (16)	0.56053 (13)	0.0454 (3)
H7	0.739392	0.203561	0.623105	0.054*
C8	0.80339 (9)	0.09896 (17)	0.53092 (16)	0.0569 (4)
H8	0.808004	0.008403	0.573471	0.068*
C9	0.83739 (9)	0.11667 (19)	0.43848 (16)	0.0585 (4)
H9	0.865520	0.038605	0.419148	0.070*
C10	0.82978 (9)	0.2496 (2)	0.37481 (14)	0.0564 (4)
H10	0.852402	0.260936	0.311817	0.068*
C11	0.78851 (8)	0.36688 (17)	0.40403 (13)	0.0467 (3)
H11	0.783376	0.456359	0.360170	0.056*
C12	0.81996 (7)	0.59761 (15)	0.66502 (13)	0.0424 (3)
H12A	0.804277	0.595180	0.739226	0.051*
H12B	0.838663	0.497506	0.652662	0.051*
C13	0.87751 (7)	0.71372 (15)	0.67239 (12)	0.0398 (3)
C14	0.91929 (8)	0.7167 (2)	0.58864 (14)	0.0532 (4)
H14	0.911404	0.646502	0.527649	0.064*
C15	0.97260 (9)	0.8224 (3)	0.59409 (18)	0.0722 (5)
H15	0.999760	0.823739	0.536488	0.087*
C16	0.98532 (10)	0.9249 (2)	0.6844 (2)	0.0799 (6)
H16	1.020921	0.996431	0.688086	0.096*
C17	0.94536 (10)	0.9215 (2)	0.7691 (2)	0.0768 (6)
H17	0.954393	0.989848	0.831266	0.092*
C18	0.89179 (8)	0.81725 (19)	0.76293 (15)	0.0568 (4)
H18	0.864818	0.816768	0.820813	0.068*
C19	0.53459 (6)	0.64409 (15)	0.40399 (12)	0.0378 (3)
C20	0.48520 (7)	0.73866 (17)	0.43985 (15)	0.0487 (4)
H20	0.496318	0.789015	0.511231	0.058*
C21	0.41999 (8)	0.75889 (19)	0.37115 (17)	0.0587 (4)
H21	0.388035	0.824205	0.395815	0.070*
C22	0.40208 (8)	0.6831 (2)	0.26665 (16)	0.0588 (5)
H22	0.358067	0.696256	0.220566	0.071*
C23	0.45010 (8)	0.5872 (2)	0.23073 (15)	0.0592 (4)
H23	0.438208	0.534715	0.160376	0.071*
C24	0.51617 (7)	0.56853 (18)	0.29906 (13)	0.0488 (4)

H24	0.548246	0.504319	0.273591	0.059*
N1	0.65090 (5)	0.51402 (12)	0.44530 (9)	0.0347 (3)
N2	0.71857 (6)	0.80763 (13)	0.69892 (10)	0.0409 (3)
O1	0.66591 (5)	0.91461 (13)	0.71101 (10)	0.0533 (3)
H1N	0.6278 (8)	0.4224 (18)	0.4301 (13)	0.045 (4)*
H1O	0.6709 (10)	0.935 (2)	0.7877 (19)	0.068 (6)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0352 (6)	0.0339 (6)	0.0355 (7)	0.0025 (5)	0.0100 (5)	0.0046 (5)
C2	0.0354 (6)	0.0349 (7)	0.0352 (7)	0.0010 (5)	0.0072 (5)	0.0033 (5)
C3	0.0363 (7)	0.0318 (6)	0.0384 (7)	-0.0014 (5)	0.0071 (5)	0.0017 (5)
C4	0.0426 (7)	0.0343 (7)	0.0399 (7)	0.0059 (5)	0.0037 (6)	-0.0002 (5)
C5	0.0362 (7)	0.0381 (7)	0.0361 (7)	0.0048 (5)	0.0094 (5)	0.0017 (5)
C6	0.0331 (6)	0.0345 (7)	0.0401 (7)	0.0018 (5)	0.0047 (5)	-0.0006 (5)
C7	0.0432 (7)	0.0397 (7)	0.0539 (9)	0.0009 (6)	0.0107 (6)	0.0066 (6)
C8	0.0567 (9)	0.0356 (8)	0.0759 (11)	0.0088 (7)	0.0059 (8)	0.0047 (7)
C9	0.0549 (9)	0.0518 (9)	0.0664 (11)	0.0185 (7)	0.0051 (8)	-0.0131 (8)
C10	0.0565 (9)	0.0677 (10)	0.0477 (9)	0.0158 (8)	0.0163 (7)	-0.0063 (7)
C11	0.0500 (8)	0.0472 (8)	0.0446 (8)	0.0101 (6)	0.0135 (6)	0.0042 (6)
C12	0.0406 (7)	0.0395 (7)	0.0448 (8)	0.0042 (6)	0.0024 (6)	0.0049 (6)
C13	0.0341 (6)	0.0404 (7)	0.0420 (7)	0.0057 (5)	-0.0005 (5)	0.0027 (6)
C14	0.0448 (8)	0.0654 (10)	0.0484 (9)	0.0013 (7)	0.0058 (6)	-0.0032 (7)
C15	0.0468 (9)	0.0985 (15)	0.0727 (12)	-0.0091 (9)	0.0145 (8)	0.0130 (11)
C16	0.0558 (11)	0.0794 (14)	0.0983 (16)	-0.0246 (10)	-0.0016 (10)	0.0029 (11)
C17	0.0664 (11)	0.0716 (13)	0.0866 (14)	-0.0156 (9)	-0.0009 (10)	-0.0255 (10)
C18	0.0509 (9)	0.0639 (10)	0.0542 (9)	-0.0015 (7)	0.0063 (7)	-0.0130 (8)
C19	0.0339 (6)	0.0382 (7)	0.0426 (7)	0.0004 (5)	0.0103 (5)	0.0046 (5)
C20	0.0393 (7)	0.0477 (8)	0.0606 (9)	0.0049 (6)	0.0131 (7)	-0.0003 (7)
C21	0.0361 (8)	0.0526 (9)	0.0886 (13)	0.0075 (7)	0.0153 (8)	0.0151 (8)
C22	0.0329 (7)	0.0702 (11)	0.0708 (11)	-0.0039 (7)	0.0033 (7)	0.0277 (9)
C23	0.0457 (8)	0.0794 (12)	0.0497 (9)	-0.0137 (8)	0.0020 (7)	0.0041 (8)
C24	0.0376 (7)	0.0600 (9)	0.0489 (9)	-0.0021 (6)	0.0083 (6)	-0.0036 (7)
N1	0.0317 (5)	0.0329 (6)	0.0400 (6)	0.0009 (4)	0.0080 (4)	-0.0011 (4)
N2	0.0379 (6)	0.0413 (6)	0.0437 (7)	0.0039 (5)	0.0081 (5)	-0.0019 (5)
O1	0.0510 (6)	0.0622 (7)	0.0456 (6)	0.0185 (5)	0.0067 (5)	-0.0107 (5)

Geometric parameters (\AA , $^\circ$)

C1—N1	1.4820 (16)	C12—H12A	0.9700
C1—C6	1.5138 (17)	C12—H12B	0.9700
C1—C2	1.5499 (17)	C13—C18	1.379 (2)
C1—H1	0.9800	C13—C14	1.384 (2)
C2—C3	1.5116 (17)	C14—C15	1.384 (2)
C2—C12	1.5344 (18)	C14—H14	0.9300
C2—H2	0.9800	C15—C16	1.369 (3)
C3—N2	1.2764 (17)	C15—H15	0.9300

C3—C4	1.4984 (18)	C16—C17	1.369 (3)
C4—C5	1.5340 (18)	C16—H16	0.9300
C4—H4A	0.9700	C17—C18	1.378 (3)
C4—H4B	0.9700	C17—H17	0.9300
C5—N1	1.4760 (16)	C18—H18	0.9300
C5—C19	1.5165 (18)	C19—C24	1.377 (2)
C5—H5	0.9800	C19—C20	1.3924 (19)
C6—C7	1.3833 (19)	C20—C21	1.381 (2)
C6—C11	1.3910 (19)	C20—H20	0.9300
C7—C8	1.385 (2)	C21—C22	1.373 (3)
C7—H7	0.9300	C21—H21	0.9300
C8—C9	1.375 (3)	C22—C23	1.380 (3)
C8—H8	0.9300	C22—H22	0.9300
C9—C10	1.372 (2)	C23—C24	1.391 (2)
C9—H9	0.9300	C23—H23	0.9300
C10—C11	1.386 (2)	C24—H24	0.9300
C10—H10	0.9300	N1—H1N	0.920 (16)
C11—H11	0.9300	N2—O1	1.4161 (14)
C12—C13	1.5044 (19)	O1—H1O	0.90 (2)
N1—C1—C6	110.00 (10)	C13—C12—H12A	108.7
N1—C1—C2	110.28 (10)	C2—C12—H12A	108.7
C6—C1—C2	112.58 (10)	C13—C12—H12B	108.7
N1—C1—H1	107.9	C2—C12—H12B	108.7
C6—C1—H1	107.9	H12A—C12—H12B	107.6
C2—C1—H1	107.9	C18—C13—C14	117.77 (14)
C3—C2—C12	114.26 (11)	C18—C13—C12	121.91 (13)
C3—C2—C1	107.37 (10)	C14—C13—C12	120.30 (13)
C12—C2—C1	110.81 (10)	C15—C14—C13	121.14 (16)
C3—C2—H2	108.1	C15—C14—H14	119.4
C12—C2—H2	108.1	C13—C14—H14	119.4
C1—C2—H2	108.1	C16—C15—C14	119.93 (18)
N2—C3—C4	125.76 (12)	C16—C15—H15	120.0
N2—C3—C2	119.10 (11)	C14—C15—H15	120.0
C4—C3—C2	114.50 (11)	C17—C16—C15	119.65 (18)
C3—C4—C5	106.84 (10)	C17—C16—H16	120.2
C3—C4—H4A	110.4	C15—C16—H16	120.2
C5—C4—H4A	110.4	C16—C17—C18	120.36 (18)
C3—C4—H4B	110.4	C16—C17—H17	119.8
C5—C4—H4B	110.4	C18—C17—H17	119.8
H4A—C4—H4B	108.6	C17—C18—C13	121.13 (16)
N1—C5—C19	113.47 (11)	C17—C18—H18	119.4
N1—C5—C4	106.96 (10)	C13—C18—H18	119.4
C19—C5—C4	112.64 (10)	C24—C19—C20	118.17 (13)
N1—C5—H5	107.8	C24—C19—C5	124.30 (12)
C19—C5—H5	107.8	C20—C19—C5	117.50 (12)
C4—C5—H5	107.8	C21—C20—C19	121.07 (15)
C7—C6—C11	118.34 (12)	C21—C20—H20	119.5

C7—C6—C1	119.88 (12)	C19—C20—H20	119.5
C11—C6—C1	121.73 (12)	C22—C21—C20	120.34 (15)
C6—C7—C8	121.00 (14)	C22—C21—H21	119.8
C6—C7—H7	119.5	C20—C21—H21	119.8
C8—C7—H7	119.5	C21—C22—C23	119.27 (14)
C9—C8—C7	119.90 (14)	C21—C22—H22	120.4
C9—C8—H8	120.1	C23—C22—H22	120.4
C7—C8—H8	120.1	C22—C23—C24	120.42 (16)
C10—C9—C8	119.98 (14)	C22—C23—H23	119.8
C10—C9—H9	120.0	C24—C23—H23	119.8
C8—C9—H9	120.0	C19—C24—C23	120.71 (15)
C9—C10—C11	120.24 (15)	C19—C24—H24	119.6
C9—C10—H10	119.9	C23—C24—H24	119.6
C11—C10—H10	119.9	C5—N1—C1	111.44 (10)
C10—C11—C6	120.53 (14)	C5—N1—H1N	110.1 (9)
C10—C11—H11	119.7	C1—N1—H1N	106.0 (10)
C6—C11—H11	119.7	C3—N2—O1	111.03 (11)
C13—C12—C2	114.15 (11)	N2—O1—H1O	106.4 (12)
N1—C1—C2—C3	52.80 (13)	C2—C12—C13—C14	-72.61 (16)
C6—C1—C2—C3	176.06 (10)	C18—C13—C14—C15	-1.5 (2)
N1—C1—C2—C12	178.22 (10)	C12—C13—C14—C15	-179.83 (14)
C6—C1—C2—C12	-58.53 (14)	C13—C14—C15—C16	0.9 (3)
C12—C2—C3—N2	-6.87 (17)	C14—C15—C16—C17	0.4 (3)
C1—C2—C3—N2	116.46 (13)	C15—C16—C17—C18	-1.1 (3)
C12—C2—C3—C4	-178.23 (11)	C16—C17—C18—C13	0.5 (3)
C1—C2—C3—C4	-54.90 (14)	C14—C13—C18—C17	0.7 (2)
N2—C3—C4—C5	-110.41 (14)	C12—C13—C18—C17	179.09 (16)
C2—C3—C4—C5	60.28 (14)	N1—C5—C19—C24	-3.99 (18)
C3—C4—C5—N1	-62.16 (13)	C4—C5—C19—C24	117.73 (14)
C3—C4—C5—C19	172.50 (10)	N1—C5—C19—C20	174.28 (12)
N1—C1—C6—C7	-116.50 (13)	C4—C5—C19—C20	-64.00 (15)
C2—C1—C6—C7	120.09 (13)	C24—C19—C20—C21	-1.3 (2)
N1—C1—C6—C11	66.07 (15)	C5—C19—C20—C21	-179.72 (13)
C2—C1—C6—C11	-57.35 (16)	C19—C20—C21—C22	1.4 (2)
C11—C6—C7—C8	1.1 (2)	C20—C21—C22—C23	-0.4 (2)
C1—C6—C7—C8	-176.45 (13)	C21—C22—C23—C24	-0.6 (2)
C6—C7—C8—C9	0.0 (2)	C20—C19—C24—C23	0.4 (2)
C7—C8—C9—C10	-0.9 (3)	C5—C19—C24—C23	178.62 (13)
C8—C9—C10—C11	0.7 (3)	C22—C23—C24—C19	0.6 (2)
C9—C10—C11—C6	0.4 (2)	C19—C5—N1—C1	-169.51 (10)
C7—C6—C11—C10	-1.3 (2)	C4—C5—N1—C1	65.66 (13)
C1—C6—C11—C10	176.22 (13)	C6—C1—N1—C5	173.66 (10)
C3—C2—C12—C13	-78.23 (14)	C2—C1—N1—C5	-61.59 (13)
C1—C2—C12—C13	160.32 (11)	C4—C3—N2—O1	-6.48 (18)
C2—C12—C13—C18	109.09 (16)	C2—C3—N2—O1	-176.78 (10)

Hydrogen-bond geometry (Å, °)

Cg3 and Cg4 are the centroids of the C13–C18 and C19–C24 rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1O \cdots N1 ⁱ	0.90 (2)	2.00 (2)	2.8682 (16)	163 (2)
C5—H5 \cdots Cg4 ⁱⁱ	0.98	2.95	3.7424 (14)	139
C8—H8 \cdots Cg3 ⁱⁱⁱ	0.93	2.99	3.6890 (18)	133

Symmetry codes: (i) $x, -y+3/2, z+1/2$; (ii) $-x+1, -y+1, -z+1$; (iii) $x, y-1, z$.