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3,3,5,5-Tetramethyl-*r*-2,*c*-6-diphenylpiperidin-4-one

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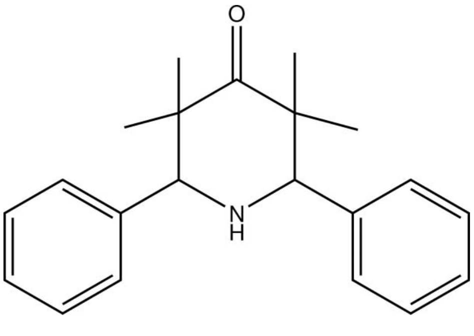
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.056; wR factor = 0.152; data-to-parameter ratio = 12.3.

The piperidone ring of the title compound, $C_{21}H_{25}NO$, adopts a chair conformation with the two phenyl groups equatorially oriented and *cis* to each other. In the crystal, molecules are linked by weak N—H···O hydrogen bonds, forming chains parallel to [100].

Related literature

For some bioactive properties of piperidones, see: Mobio *et al.* (1989). For piperidone ring conformations in related compounds, see: Parthiban *et al.* (2008); Lakshminarayana *et al.* (2009); Ravichandran *et al.* (2010). For the synthesis, see: Noller & Baliah (1948). For ring puckering parameters, see: Nardelli (1983); Cremer & Pople (1975).



Experimental

Crystal data

$C_{21}H_{25}NO$	α = 64.771 (4)°
M_r = 307.42	β = 80.755 (5)°
Triclinic, $P\overline{1}$	γ = 72.675 (4)°
a = 6.9227 (11) Å	V = 859.8 (3) Å^3
b = 11.540 (2) Å	Z = 2
c = 12.472 (2) Å	Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}	0.30 × 0.25 × 0.20 mm
T = 295 K	

Data collection

Bruker Kappa APEXII CCD diffractometer	12752 measured reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)	2659 independent reflections
$T_{\min}$ = 0.919, $T_{\max}$ = 0.986	2123 reflections with $I > 2\sigma(I)$
	$R_{\rm int}$ = 0.032
	$\theta_{\max}$ = 24.0°

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.152	$\Delta\rho_{\max}$ = 0.23 e Å^{-3}
S = 1.15	$\Delta\rho_{\min}$ = −0.18 e Å^{-3}
2659 reflections	
217 parameters	

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1$^{\rm i}$	0.94 (3)	2.39 (3)	3.258 (3)	153 (2)

Symmetry code: (i) $x - 1, y, z$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus* 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* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LR2058).

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supplementary materials

Acta Cryst. (2012). E**68**, o2097 [doi:10.1107/S1600536812018983]

3,3,5,5-Tetramethyl-*r*-2,*c*-6-diphenylpiperidin-4-one

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Comment

Aryl substituted piperidine-4-ones are important heterocyclic entities present in natural products like alkaloids.The piperidones exhibit diverse bioactivities such as bactericidal, fungicidal and herbicidal activities (Mobio *et al.*, 1989).The six-membered ring of piperidones adopts, predominantly, a chair conformation (Parthiban *et al.*, 2008) but many often the conformation depends on the substitution in the piperidone ring (Lakshminarayana *et al.*, 2009; Ravichandran *et al.*, 2010). The determination of the crystal structure of the title compound was mainly undertaken to evaluate the impact of four methyl groups at C2 and C4 carbon atoms. The *ORTEP* diagram of the title compound is shown in Fig. 1. In the title compound $C_{21}H_{25}NO$, the piperidone ring adopts a chair conformation with ring puckering parameters (Nardelli, 1983; Cremer & Pople, 1975) of Q=0.543 (2)°, θ = 155.55 (3)° and φ=136.72 (2)°. The two phenyl groups are equatorial oriented and *cis* to each other. The crystal packing is stabilized by a week N—H···O hydrogen bond [*d*(N—O)=3.257 (4) Å and angle N—H···O= 151.11 (2)°]. The N—H···O hydrogen bond connects the adjacent molecule into a head to tail fashion to generate a one dimensional chain extending parallel to the [1 0 0] direction.

Experimental

The title compound was prepared by one pot synthesis from 3,4-dimethy-3-pentanone, benzaldehyde and ammonium acetate at 1:2:1 proportion in ethanol as solvent by adopting the literature procedure reported by (Noller & Baliah, 1948). Crystals suitable for single-crystal X-raydiffraction were grown by slow evaporation of a solution in benzene (m.p. 467–469 K).

Refinement

The H atoms associated with the carbon atoms were fixed geometrically and allowed to ride on their parent carbon atoms with C–H distances in the range of 0.93 Å–0.98 Å and U_{iso}(H) set to either $1.2U_{equ}$(C) or $1.5U_{eqi}$(C) of the carrier atom. The H-atom bound to the N-atom is identified from a difference electron density map and restrained to a distance of 0.93 (3) Å

Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus* 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* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *PLATON* (Spek, 2009).

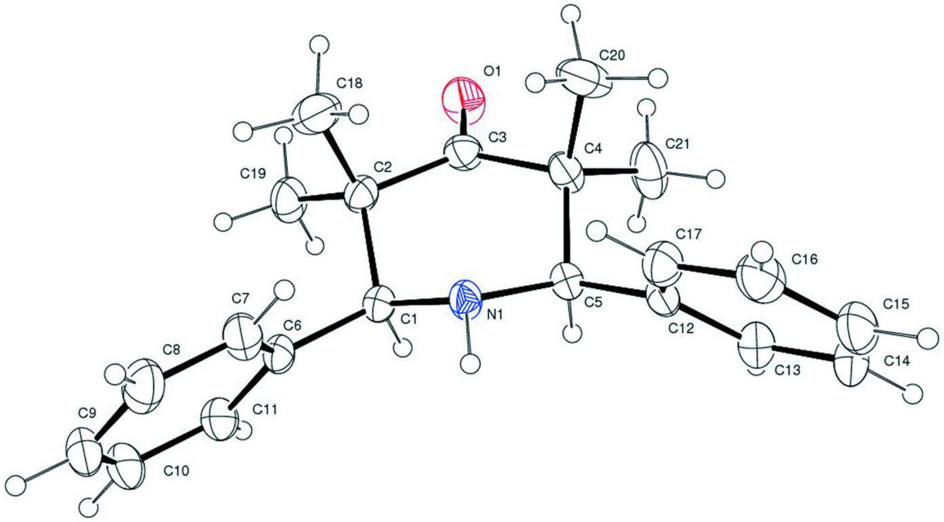

Figure 1

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 40% probability level.

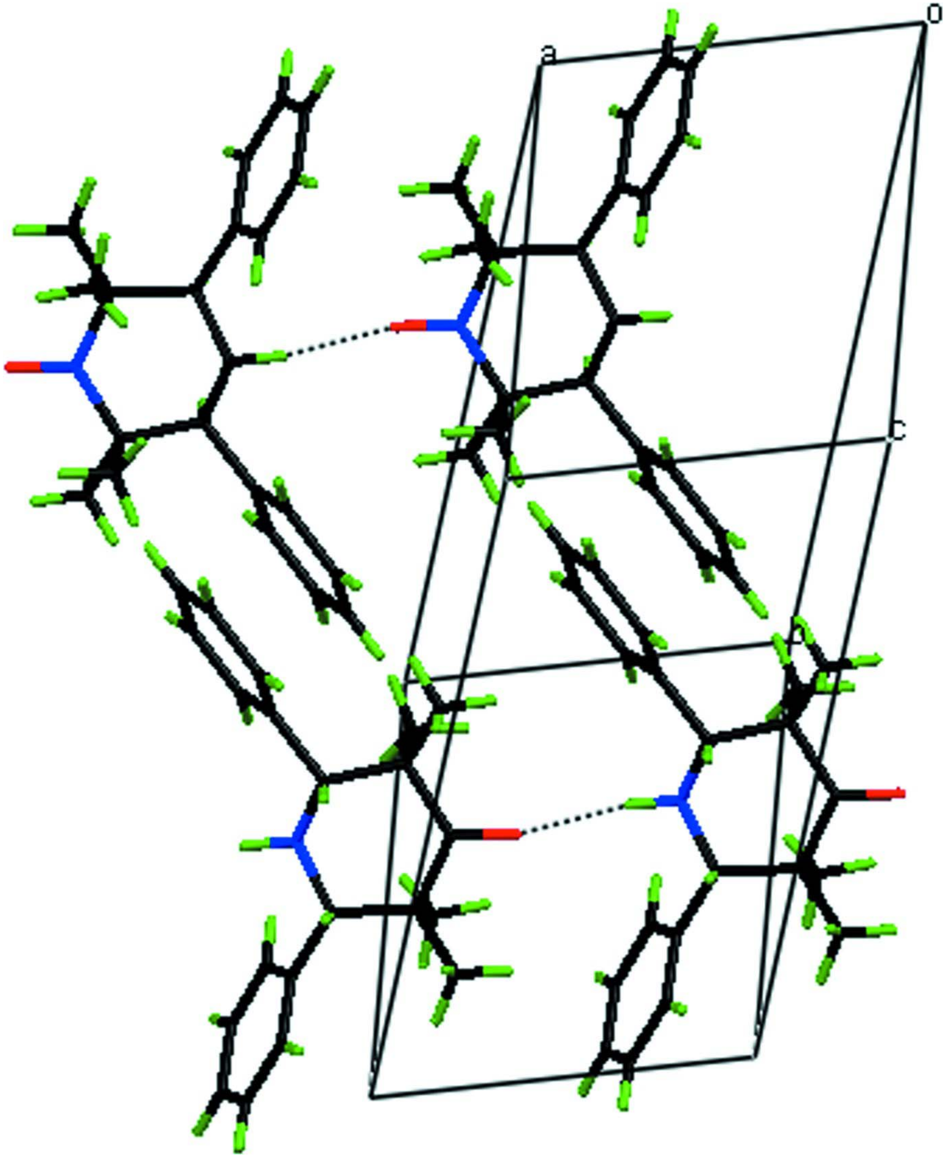

Figure 2

Part of crystal structure showing the packing of the molecules in the unit cell and formation of N1—H1A···O1 hydrogen bond.

3,3,5,5-Tetramethyl-*r*-2,*c*-6-diphenylpiperidin-4-one

Crystal data

$C_{21}H_{25}NO$
$M_r = 307.42$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.9227\ (11)$ Å
$b = 11.540\ (2)$ Å
$c = 12.472\ (2)$ Å
$\alpha = 64.771\ (4)°$
$\beta = 80.755\ (5)°$
$\gamma = 72.675\ (4)°$
$V = 859.8\ (3)$ Å^3
$Z = 2$
$F(000) = 332$
$D_x = 1.187$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4779 reflections
$\theta = 2.1–23.8°$
$\mu = 0.07$ mm^{-1}

T = 295 K
Block, colourless

0.30 × 0.25 × 0.20 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)
$T_{\min} = 0.919$, $T_{\max} = 0.986$

12752 measured reflections
2659 independent reflections
2123 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.032$
$\theta_{\max} = 24.0°$, $\theta_{\min} = 2.1°$
$h = -7 \rightarrow 7$
$k = -13 \rightarrow 13$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.152$
$S = 1.15$
2659 reflections
217 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0562P)^2 + 0.4957P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.23$ e Å^{-3}
$\Delta\rho_{\min} = -0.18$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.020 (4)

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	0.7201 (4)	0.4000 (2)	0.1945 (2)	0.0372 (6)
H1	0.7165	0.4280	0.1087	0.045*
C2	0.9321 (4)	0.3963 (2)	0.2220 (2)	0.0407 (6)
C3	1.0898 (4)	0.2903 (2)	0.1901 (2)	0.0435 (6)
C4	1.0442 (4)	0.1603 (2)	0.2102 (2)	0.0446 (6)
C5	0.8169 (4)	0.1810 (2)	0.1951 (2)	0.0386 (6)
H5	0.7920	0.2263	0.1100	0.046*
C6	0.5498 (4)	0.4960 (2)	0.2302 (2)	0.0394 (6)
C7	0.4653 (4)	0.4602 (3)	0.3438 (2)	0.0496 (7)
H7	0.5133	0.3750	0.4003	0.059*
C8	0.3102 (5)	0.5492 (3)	0.3749 (3)	0.0633 (8)
H8	0.2544	0.5234	0.4518	0.076*
C9	0.2383 (5)	0.6751 (3)	0.2932 (3)	0.0657 (9)

H9	0.1351	0.7354	0.3144	0.079*
C10	0.3196 (5)	0.7116 (3)	0.1799 (3)	0.0641 (9)
H10	0.2705	0.7970	0.1239	0.077*
C11	0.4734 (4)	0.6232 (2)	0.1478 (3)	0.0514 (7)
H11	0.5265	0.6493	0.0703	0.062*
C12	0.7552 (4)	0.0522 (2)	0.2417 (2)	0.0408 (6)
C13	0.7551 (4)	−0.0084 (3)	0.1664 (3)	0.0533 (7)
H13	0.7920	0.0311	0.0866	0.064*
C14	0.7008 (5)	−0.1267 (3)	0.2086 (3)	0.0647 (9)
H14	0.7004	−0.1655	0.1568	0.078*
C15	0.6482 (5)	−0.1867 (3)	0.3250 (3)	0.0655 (9)
H15	0.6137	−0.2669	0.3532	0.079*
C16	0.6461 (4)	−0.1284 (3)	0.4009 (3)	0.0597 (8)
H16	0.6098	−0.1689	0.4807	0.072*
C17	0.6982 (4)	−0.0093 (2)	0.3588 (2)	0.0483 (7)
H17	0.6945	0.0300	0.4108	0.058*
C18	0.9507 (5)	0.3605 (3)	0.3540 (3)	0.0632 (8)
H18A	0.9024	0.2832	0.4010	0.095*
H18B	0.8713	0.4332	0.3736	0.095*
H18C	1.0900	0.3429	0.3700	0.095*
C19	0.9807 (4)	0.5297 (3)	0.1504 (3)	0.0569 (8)
H19A	1.1159	0.5236	0.1653	0.085*
H19B	0.8867	0.5960	0.1733	0.085*
H19C	0.9702	0.5535	0.0675	0.085*
C20	1.1125 (5)	0.0629 (3)	0.3352 (3)	0.0691 (9)
H20A	1.2464	0.0646	0.3447	0.104*
H20B	1.1131	−0.0249	0.3467	0.104*
H20C	1.0207	0.0879	0.3927	0.104*
C21	1.1721 (5)	0.1079 (3)	0.1211 (3)	0.0707 (10)
H21A	1.1335	0.1695	0.0422	0.106*
H21B	1.1507	0.0238	0.1359	0.106*
H21C	1.3126	0.0973	0.1293	0.106*
N1	0.6901 (3)	0.26610 (18)	0.25244 (18)	0.0388 (5)
O1	1.2574 (3)	0.30563 (19)	0.1531 (2)	0.0641 (6)
H1A	0.554 (4)	0.268 (2)	0.251 (2)	0.042 (7)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0395 (14)	0.0324 (12)	0.0436 (14)	−0.0100 (10)	−0.0031 (10)	−0.0179 (11)
C2	0.0389 (14)	0.0400 (14)	0.0502 (15)	−0.0132 (11)	−0.0018 (11)	−0.0225 (12)
C3	0.0344 (15)	0.0428 (14)	0.0531 (15)	−0.0111 (11)	−0.0032 (11)	−0.0179 (12)
C4	0.0370 (15)	0.0330 (13)	0.0583 (16)	−0.0050 (10)	0.0008 (11)	−0.0169 (12)
C5	0.0393 (14)	0.0320 (12)	0.0441 (14)	−0.0047 (10)	−0.0036 (10)	−0.0171 (11)
C6	0.0391 (14)	0.0319 (13)	0.0546 (16)	−0.0104 (10)	−0.0028 (11)	−0.0230 (12)
C7	0.0482 (16)	0.0434 (15)	0.0598 (17)	−0.0111 (12)	0.0030 (13)	−0.0254 (13)
C8	0.0566 (19)	0.073 (2)	0.078 (2)	−0.0182 (16)	0.0122 (15)	−0.0510 (18)
C9	0.0520 (19)	0.0570 (19)	0.105 (3)	−0.0006 (14)	−0.0078 (17)	−0.055 (2)
C10	0.063 (2)	0.0361 (15)	0.094 (2)	0.0003 (13)	−0.0180 (18)	−0.0303 (16)
C11	0.0548 (17)	0.0365 (14)	0.0644 (18)	−0.0099 (12)	−0.0086 (13)	−0.0207 (13)

C12	0.0366 (14)	0.0295 (12)	0.0541 (16)	−0.0022 (10)	−0.0059 (11)	−0.0176 (11)
C13	0.0601 (19)	0.0417 (15)	0.0627 (18)	−0.0091 (13)	−0.0059 (14)	−0.0266 (14)
C14	0.070 (2)	0.0442 (17)	0.093 (2)	−0.0083 (14)	−0.0144 (18)	−0.0399 (17)
C15	0.0576 (19)	0.0381 (16)	0.102 (3)	−0.0130 (13)	−0.0099 (17)	−0.0264 (17)
C16	0.0537 (19)	0.0442 (16)	0.073 (2)	−0.0170 (13)	−0.0043 (14)	−0.0122 (15)
C17	0.0473 (16)	0.0415 (14)	0.0591 (17)	−0.0146 (12)	−0.0013 (12)	−0.0211 (13)
C18	0.0543 (19)	0.086 (2)	0.0630 (19)	−0.0170 (16)	−0.0097 (14)	−0.0406 (17)
C19	0.0506 (18)	0.0462 (16)	0.085 (2)	−0.0197 (13)	0.0024 (14)	−0.0335 (15)
C20	0.0489 (18)	0.0526 (18)	0.084 (2)	−0.0073 (14)	−0.0257 (16)	−0.0032 (16)
C21	0.0541 (19)	0.0559 (18)	0.108 (3)	−0.0136 (14)	0.0245 (17)	−0.0487 (18)
N1	0.0331 (12)	0.0320 (11)	0.0558 (13)	−0.0103 (8)	0.0015 (9)	−0.0217 (9)
O1	0.0380 (12)	0.0621 (13)	0.0986 (16)	−0.0187 (9)	0.0098 (10)	−0.0387 (12)

Geometric parameters (Å, º)

C1—N1	1.464 (3)	C11—H11	0.9300
C1—C6	1.513 (3)	C12—C17	1.375 (4)
C1—C2	1.545 (3)	C12—C13	1.390 (4)
C1—H1	0.9800	C13—C14	1.383 (4)
C2—C19	1.523 (3)	C13—H13	0.9300
C2—C3	1.525 (3)	C14—C15	1.359 (5)
C2—C18	1.534 (4)	C14—H14	0.9300
C3—O1	1.213 (3)	C15—C16	1.372 (4)
C3—C4	1.532 (3)	C15—H15	0.9300
C4—C21	1.523 (4)	C16—C17	1.383 (4)
C4—C20	1.531 (4)	C16—H16	0.9300
C4—C5	1.550 (3)	C17—H17	0.9300
C5—N1	1.460 (3)	C18—H18A	0.9600
C5—C12	1.514 (3)	C18—H18B	0.9600
C5—H5	0.9800	C18—H18C	0.9600
C6—C7	1.378 (4)	C19—H19A	0.9600
C6—C11	1.385 (3)	C19—H19B	0.9600
C7—C8	1.381 (4)	C19—H19C	0.9600
C7—H7	0.9300	C20—H20A	0.9600
C8—C9	1.367 (4)	C20—H20B	0.9600
C8—H8	0.9300	C20—H20C	0.9600
C9—C10	1.367 (5)	C21—H21A	0.9600
C9—H9	0.9300	C21—H21B	0.9600
C10—C11	1.378 (4)	C21—H21C	0.9600
C10—H10	0.9300	N1—H1A	0.94 (3)

N1—C1—C6	110.46 (19)	C17—C12—C13	117.6 (2)
N1—C1—C2	109.22 (19)	C17—C12—C5	121.9 (2)
C6—C1—C2	113.51 (18)	C13—C12—C5	120.5 (2)
N1—C1—H1	107.8	C14—C13—C12	120.9 (3)
C6—C1—H1	107.8	C14—C13—H13	119.6
C2—C1—H1	107.8	C12—C13—H13	119.6
C19—C2—C3	109.0 (2)	C15—C14—C13	120.5 (3)
C19—C2—C18	108.4 (2)	C15—C14—H14	119.8
C3—C2—C18	107.4 (2)	C13—C14—H14	119.8

C19—C2—C1	110.9 (2)	C14—C15—C16	119.7 (3)
C3—C2—C1	108.89 (19)	C14—C15—H15	120.2
C18—C2—C1	112.2 (2)	C16—C15—H15	120.2
O1—C3—C2	119.9 (2)	C15—C16—C17	120.0 (3)
O1—C3—C4	118.9 (2)	C15—C16—H16	120.0
C2—C3—C4	121.1 (2)	C17—C16—H16	120.0
C21—C4—C20	108.7 (2)	C12—C17—C16	121.4 (3)
C21—C4—C3	108.7 (2)	C12—C17—H17	119.3
C20—C4—C3	106.0 (2)	C16—C17—H17	119.3
C21—C4—C5	109.6 (2)	C2—C18—H18A	109.5
C20—C4—C5	112.4 (2)	C2—C18—H18B	109.5
C3—C4—C5	111.33 (19)	H18A—C18—H18B	109.5
N1—C5—C12	109.7 (2)	C2—C18—H18C	109.5
N1—C5—C4	110.6 (2)	H18A—C18—H18C	109.5
C12—C5—C4	113.06 (19)	H18B—C18—H18C	109.5
N1—C5—H5	107.7	C2—C19—H19A	109.5
C12—C5—H5	107.7	C2—C19—H19B	109.5
C4—C5—H5	107.7	H19A—C19—H19B	109.5
C7—C6—C11	118.1 (2)	C2—C19—H19C	109.5
C7—C6—C1	121.7 (2)	H19A—C19—H19C	109.5
C11—C6—C1	120.2 (2)	H19B—C19—H19C	109.5
C6—C7—C8	120.9 (3)	C4—C20—H20A	109.5
C6—C7—H7	119.5	C4—C20—H20B	109.5
C8—C7—H7	119.5	H20A—C20—H20B	109.5
C9—C8—C7	120.3 (3)	C4—C20—H20C	109.5
C9—C8—H8	119.8	H20A—C20—H20C	109.5
C7—C8—H8	119.8	H20B—C20—H20C	109.5
C8—C9—C10	119.4 (3)	C4—C21—H21A	109.5
C8—C9—H9	120.3	C4—C21—H21B	109.5
C10—C9—H9	120.3	H21A—C21—H21B	109.5
C9—C10—C11	120.7 (3)	C4—C21—H21C	109.5
C9—C10—H10	119.6	H21A—C21—H21C	109.5
C11—C10—H10	119.6	H21B—C21—H21C	109.5
C10—C11—C6	120.5 (3)	C5—N1—C1	111.10 (19)
C10—C11—H11	119.7	C5—N1—H1A	109.0 (15)
C6—C11—H11	119.7	C1—N1—H1A	111.2 (15)

N1—C1—C2—C19	172.5 (2)	N1—C1—C6—C11	−141.9 (2)
C6—C1—C2—C19	−63.7 (3)	C2—C1—C6—C11	95.1 (3)
N1—C1—C2—C3	52.6 (3)	C11—C6—C7—C8	−0.6 (4)
C6—C1—C2—C3	176.3 (2)	C1—C6—C7—C8	179.8 (2)
N1—C1—C2—C18	−66.1 (3)	C6—C7—C8—C9	−0.3 (4)
C6—C1—C2—C18	57.6 (3)	C7—C8—C9—C10	0.8 (5)
C19—C2—C3—O1	25.8 (3)	C8—C9—C10—C11	−0.4 (5)
C18—C2—C3—O1	−91.4 (3)	C9—C10—C11—C6	−0.5 (4)
C1—C2—C3—O1	146.9 (2)	C7—C6—C11—C10	1.0 (4)
C19—C2—C3—C4	−157.6 (2)	C1—C6—C11—C10	−179.4 (2)
C18—C2—C3—C4	85.2 (3)	N1—C5—C12—C17	−37.9 (3)
C1—C2—C3—C4	−36.5 (3)	C4—C5—C12—C17	86.1 (3)

O1—C3—C4—C21	−30.6 (3)	N1—C5—C12—C13	142.3 (2)
C2—C3—C4—C21	152.7 (2)	C4—C5—C12—C13	−93.7 (3)
O1—C3—C4—C20	86.0 (3)	C17—C12—C13—C14	−0.4 (4)
C2—C3—C4—C20	−90.6 (3)	C5—C12—C13—C14	179.4 (2)
O1—C3—C4—C5	−151.4 (2)	C12—C13—C14—C15	−0.6 (4)
C2—C3—C4—C5	31.9 (3)	C13—C14—C15—C16	0.9 (5)
C21—C4—C5—N1	−163.2 (2)	C14—C15—C16—C17	−0.2 (4)
C20—C4—C5—N1	75.8 (3)	C13—C12—C17—C16	1.2 (4)
C3—C4—C5—N1	−42.9 (3)	C5—C12—C17—C16	−178.6 (2)
C21—C4—C5—C12	73.3 (3)	C15—C16—C17—C12	−0.9 (4)
C20—C4—C5—C12	−47.7 (3)	C12—C5—N1—C1	−169.68 (19)
C3—C4—C5—C12	−166.4 (2)	C4—C5—N1—C1	64.9 (2)
N1—C1—C6—C7	37.7 (3)	C6—C1—N1—C5	163.89 (19)
C2—C1—C6—C7	−85.3 (3)	C2—C1—N1—C5	−70.6 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O1^{i}	0.94 (3)	2.39 (3)	3.258 (3)	153 (2)

Symmetry code: (i) *x*−1, *y*, *z*.