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t-3-Benzyl-1-formyl-*r*-2,*c*-6-diphenylpiperidin-4-one

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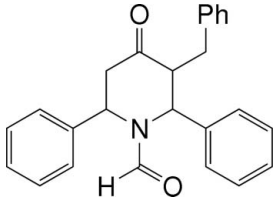
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.002 Å; R factor = 0.048; wR factor = 0.142; data-to-parameter ratio = 27.2.

The piperidine ring of the title compound, $C_{25}H_{23}NO_2$, is in a distorted boat form. The phenyl ring at position 2 makes a dihedral angle of 80.6 (1)° with the phenyl ring of the benzyl group at position 3, and 61.2 (1)° with the phenyl ring at position 6. The dihedral angle between the phenyl ring of the benzyl group and the phenyl ring at position 6 is 84.2 (1)°. The formyl group and the phenyl ring at position 6 have equatorial orientations. The phenyl ring at position 2 and the benzyl group at position 3 have axial orientations. C—H···O and C—H···π hydrogen bonds are found in the crystal structure.

Related literature

For a related crystal structure, see: Balamurugan *et al.* (2007). For applications of piperidines, see: Jayabharathi *et al.* (2007).



Experimental

Crystal data

$C_{25}H_{23}NO_2$
M_r = 369.44
Monoclinic, $P2_1/c$
a = 10.5355 (3) Å
b = 9.3464 (2) Å
c = 21.0493 (5) Å
β = 101.520 (3)°
V = 2030.95 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 200 (2) K
0.41 × 0.37 × 0.29 mm

Data collection

Oxford Diffraction Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.969, T_{max} = 1.000 (expected range = 0.948–0.978)
29482 measured reflections
6871 independent reflections
3596 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.142
S = 1.00
6871 reflections
253 parameters
H-atom parameters contsrained
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

*Cg*1 is the centroid of the C31–C36 ring and *Cg*2 is the centroid of the C21–C26 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C24—H24···*Cg*1^{i}	0.93	2.81	3.651 (1)	151
C34—H34···*Cg*2^{ii}	0.93	2.97	3.890 (2)	172
C2—H2···O1	0.98	2.41	2.8175 (15)	105
C3—H3···O4^{iii}	0.98	2.44	3.4093 (15)	170
C6—H6···O1^{iv}	0.98	2.29	3.2576 (16)	168

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003).

RJB acknowledges the NSF–MRI program for funding to purchase the X-ray CCD diffractometer. JJ is grateful to UGC F. No. 30-71/2004(SR), New Delhi, for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2335).

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supplementary materials

Acta Cryst. (2007). E**63**, o4533 [**doi:10.1107/S1600536807053846**]

t-3-Benzyl-1-formyl-*r*-2,*c*-6-diphenylpiperidin-4-one

A. Thiruvalluvar, S. Balamurugan, R. J. Butcher, A. Manimekalai and J. Jayabharathi

Comment

Jayabharathi *et al.* (2007) have reported synthesis, stereochemistry and antimicrobial evaluation of t3-benzyl-r2,c6-di-arylpiperidin- 4-one and its derivatives. Balamurugan *et al.* (2007) have reported a crystal structure of t3,t5-Dimethyl-r2,c-6-diphenylpiperidin-4-one wherein the piperidine ring is in chair form. The piperidine ring of the title molecule, $C_{25}H_{23}NO_2$, is in distorted boat form. The phenyl ring at position 2 makes a dihedral angle of 80.6 (1)° with the phenyl ring of benzyl moiety at 3, and 61.2 (1)° with the phenyl ring at 6. The dihedral angle between the phenyl ring of the benzyl moiety and the phenyl ring at 6 is 84.2 (1)°. The formyl group at N, is nearly co-planar with the adjacent C2 and C6 atoms. The phenyl ring at 6 is in equatorial orientations. The phenyl ring at 2, the benzyl group at 3 have axial orientations. C—H···O and C—H···π intra- and inter- molecular hydrogen bonds are found in the crystal structure (see Fig. 2, and hydrogen bonding table).

Experimental

Jayabharathi *et al.* (2007) have reported the synthesis of the title compound.

Refinement

H atoms were positioned geometrically and allowed to ride on their parent atoms with C—H = 0.93–0.98 Å and U_{iso} = 1.2U_{eq}(C).

Figures

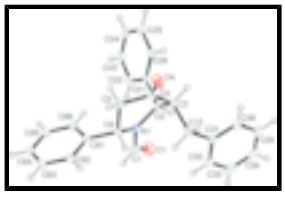

Fig. 1. The molecular structure of the title compound with the atomic numbering and 50% probability displacement ellipsoids. H atoms are shown as small spheres of arbitrary radius.

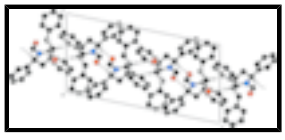

Fig. 2. The molecular packing of the title compound, viewed down the *b* axis showing the C—H···O (dashed lines) hydrogen bonds.

t-3-Benzyl-1-formyl-r-2,c-6-diphenylpiperidin-4-one

Crystal data

$C_{25}H_{23}NO_2$	F_{000} = 784
M_r = 369.44	D_x = 1.208 Mg m^{-3}

Monoclinic, $P2_1/c$	Melting point: 355.5 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 10.5355$ (3) Å	Cell parameters from 7426 reflections
$b = 9.3464$ (2) Å	$\theta = 4.4$–32.4°
$c = 21.0493$ (5) Å	$\mu = 0.08$ mm^{-1}
$\beta = 101.520$ (3)°	$T = 200$ (2) K
$V = 2030.95$ (9) Å^3	Prism, colourless
$Z = 4$	0.41 × 0.37 × 0.29 mm

Data collection

Oxford Diffraction Gemini diffractometer	6871 independent reflections
Radiation source: fine-focus sealed tube	3596 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.041$
$T = 200$(2) K	$\theta_{max} = 32.5^\circ$
phi and ω scans	$\theta_{min} = 4.5^\circ$
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)	$h = -15 \rightarrow 15$
$T_{min} = 0.969$, $T_{max} = 1.000$	$k = -14 \rightarrow 14$
29482 measured reflections	$l = -28 \rightarrow 31$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.048$	H-atom parameters constrained
$wR(F^2) = 0.142$	$w = 1/[\sigma^2(F_o^2) + (0.0708P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} = <0.001$
6871 reflections	$\Delta\rho_{max} = 0.47$ e Å^{-3}
253 parameters	$\Delta\rho_{min} = -0.21$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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 $F^2 > 2$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}
O1	0.54289 (11)	0.47782 (12)	0.30209 (5)	0.0663 (4)
O4	0.38017 (9)	−0.07286 (10)	0.42653 (5)	0.0494 (3)
N1	0.41809 (9)	0.29206 (10)	0.32395 (5)	0.0291 (3)
C1	0.46406 (13)	0.38370 (16)	0.28479 (7)	0.0476 (5)
C2	0.47899 (11)	0.28447 (12)	0.39350 (5)	0.0272 (3)
C3	0.51165 (10)	0.12848 (12)	0.41163 (5)	0.0280 (3)
C4	0.39016 (11)	0.03862 (13)	0.39836 (6)	0.0315 (3)
C5	0.28084 (11)	0.09412 (13)	0.34687 (6)	0.0322 (3)
C6	0.32664 (11)	0.17928 (13)	0.29375 (5)	0.0288 (3)
C13	0.61104 (12)	0.06259 (13)	0.37492 (6)	0.0356 (4)
C21	0.39739 (10)	0.35930 (12)	0.43612 (6)	0.0290 (3)
C22	0.34968 (13)	0.49578 (14)	0.41958 (7)	0.0408 (4)
C23	0.27833 (13)	0.56808 (15)	0.45821 (8)	0.0493 (5)
C24	0.25355 (13)	0.50590 (16)	0.51372 (8)	0.0494 (5)
C25	0.30142 (14)	0.37287 (17)	0.53101 (7)	0.0504 (5)
C26	0.37350 (12)	0.29960 (14)	0.49291 (6)	0.0391 (4)
C31	0.74256 (11)	0.13162 (13)	0.38979 (6)	0.0348 (4)
C32	0.78627 (14)	0.21533 (17)	0.34426 (8)	0.0521 (5)
C33	0.90858 (16)	0.27711 (19)	0.35832 (10)	0.0648 (7)
C34	0.98829 (15)	0.25635 (17)	0.41737 (10)	0.0599 (6)
C35	0.94666 (14)	0.17417 (17)	0.46316 (8)	0.0538 (5)
C36	0.82463 (12)	0.11224 (15)	0.44955 (7)	0.0417 (4)
C61	0.21206 (11)	0.23797 (13)	0.24538 (5)	0.0306 (3)
C62	0.16524 (12)	0.15946 (15)	0.18996 (6)	0.0417 (4)
C63	0.05711 (14)	0.20545 (18)	0.14556 (7)	0.0539 (5)
C64	−0.00269 (14)	0.33176 (17)	0.15558 (7)	0.0522 (5)
C65	0.04473 (13)	0.41193 (16)	0.21036 (7)	0.0477 (4)
C66	0.15077 (13)	0.36482 (14)	0.25539 (6)	0.0411 (4)
H1	0.43269	0.37417	0.24045	0.0572*
H2	0.56131	0.33633	0.39900	0.0326*
H3	0.54830	0.12422	0.45820	0.0336*
H5A	0.22560	0.15468	0.36716	0.0386*
H5B	0.22916	0.01382	0.32721	0.0386*
H6	0.37396	0.11376	0.27050	0.0345*
H13A	0.62061	−0.03829	0.38562	0.0427*
H13B	0.57690	0.06996	0.32870	0.0427*
H22	0.36573	0.53916	0.38222	0.0489*
H23	0.24701	0.65933	0.44646	0.0592*
H24	0.20469	0.55407	0.53917	0.0593*
H25	0.28567	0.33070	0.56870	0.0605*
H26	0.40615	0.20936	0.50567	0.0469*
H32	0.73320	0.23031	0.30388	0.0625*
H33	0.93655	0.33313	0.32728	0.0777*
H34	1.07021	0.29772	0.42641	0.0718*
H35	1.00038	0.15992	0.50343	0.0646*

H36	0.79730	0.05679	0.48096	0.0501*
H62	0.20653	0.07507	0.18234	0.0500*
H63	0.02515	0.15064	0.10899	0.0647*
H64	−0.07459	0.36310	0.12570	0.0627*
H65	0.00517	0.49808	0.21701	0.0573*
H66	0.18099	0.41853	0.29252	0.0494*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0586 (7)	0.0752 (8)	0.0630 (7)	−0.0297 (6)	0.0070 (6)	0.0227 (6)
O4	0.0559 (6)	0.0402 (5)	0.0461 (5)	−0.0080 (4)	−0.0044 (5)	0.0154 (4)
N1	0.0267 (5)	0.0356 (5)	0.0253 (5)	−0.0036 (4)	0.0056 (4)	0.0048 (4)
C1	0.0425 (8)	0.0609 (9)	0.0394 (7)	−0.0103 (7)	0.0081 (6)	0.0160 (7)
C2	0.0221 (5)	0.0320 (6)	0.0264 (6)	0.0005 (4)	0.0024 (4)	0.0001 (5)
C3	0.0272 (6)	0.0320 (6)	0.0232 (5)	0.0035 (5)	0.0009 (4)	0.0002 (5)
C4	0.0343 (6)	0.0322 (6)	0.0277 (6)	0.0008 (5)	0.0054 (5)	0.0013 (5)
C5	0.0267 (6)	0.0353 (6)	0.0324 (6)	−0.0047 (5)	0.0008 (5)	0.0032 (5)
C6	0.0264 (6)	0.0345 (6)	0.0244 (5)	0.0021 (5)	0.0025 (4)	−0.0001 (5)
C13	0.0335 (6)	0.0394 (7)	0.0323 (6)	0.0087 (5)	0.0027 (5)	−0.0069 (5)
C21	0.0227 (5)	0.0329 (6)	0.0295 (6)	0.0000 (5)	0.0010 (4)	−0.0052 (5)
C22	0.0425 (7)	0.0350 (7)	0.0437 (8)	0.0013 (6)	0.0058 (6)	−0.0030 (6)
C23	0.0405 (8)	0.0370 (7)	0.0665 (10)	0.0092 (6)	0.0013 (7)	−0.0161 (7)
C24	0.0345 (7)	0.0592 (9)	0.0552 (9)	0.0053 (6)	0.0106 (7)	−0.0239 (8)
C25	0.0470 (8)	0.0666 (10)	0.0411 (8)	0.0051 (7)	0.0170 (6)	−0.0077 (7)
C26	0.0376 (7)	0.0454 (8)	0.0354 (7)	0.0075 (6)	0.0099 (5)	0.0000 (6)
C31	0.0289 (6)	0.0395 (7)	0.0369 (7)	0.0102 (5)	0.0088 (5)	−0.0056 (6)
C32	0.0415 (8)	0.0699 (10)	0.0483 (8)	0.0140 (7)	0.0171 (7)	0.0110 (8)
C33	0.0499 (9)	0.0666 (11)	0.0873 (14)	0.0055 (8)	0.0365 (10)	0.0123 (9)
C34	0.0335 (8)	0.0563 (9)	0.0925 (14)	0.0016 (7)	0.0191 (8)	−0.0149 (9)
C35	0.0341 (8)	0.0657 (10)	0.0584 (10)	0.0081 (7)	0.0016 (7)	−0.0175 (8)
C36	0.0341 (7)	0.0504 (8)	0.0396 (7)	0.0060 (6)	0.0050 (5)	−0.0042 (6)
C61	0.0273 (6)	0.0414 (7)	0.0230 (5)	0.0037 (5)	0.0048 (4)	0.0048 (5)
C62	0.0404 (7)	0.0514 (8)	0.0305 (7)	0.0116 (6)	0.0005 (5)	−0.0036 (6)
C63	0.0469 (8)	0.0779 (11)	0.0310 (7)	0.0146 (8)	−0.0066 (6)	−0.0097 (7)
C64	0.0404 (8)	0.0774 (10)	0.0346 (7)	0.0211 (7)	−0.0026 (6)	0.0058 (7)
C65	0.0398 (7)	0.0539 (8)	0.0469 (8)	0.0176 (6)	0.0025 (6)	0.0031 (7)
C66	0.0374 (7)	0.0470 (8)	0.0366 (7)	0.0087 (6)	0.0016 (5)	−0.0037 (6)

Geometric parameters (Å, °)

O1—C1	1.2147 (18)	C62—C63	1.390 (2)
O4—C4	1.2138 (16)	C63—C64	1.374 (2)
N1—C1	1.3443 (18)	C64—C65	1.382 (2)
N1—C2	1.4781 (15)	C65—C66	1.3847 (19)
N1—C6	1.4829 (15)	C1—H1	0.9300
C2—C3	1.5288 (16)	C2—H2	0.9800
C2—C21	1.5301 (16)	C3—H3	0.9800
C3—C4	1.5096 (16)	C5—H5A	0.9700

C3—C13	1.5479 (17)	C5—H5B	0.9700
C4—C5	1.5072 (17)	C6—H6	0.9800
C5—C6	1.5271 (17)	C13—H13A	0.9700
C6—C61	1.5178 (16)	C13—H13B	0.9700
C13—C31	1.5037 (17)	C22—H22	0.9300
C21—C22	1.3897 (17)	C23—H23	0.9300
C21—C26	1.3870 (17)	C24—H24	0.9300
C22—C23	1.388 (2)	C25—H25	0.9300
C23—C24	1.376 (2)	C26—H26	0.9300
C24—C25	1.364 (2)	C32—H32	0.9300
C25—C26	1.390 (2)	C33—H33	0.9300
C31—C32	1.385 (2)	C34—H34	0.9300
C31—C36	1.3886 (19)	C35—H35	0.9300
C32—C33	1.389 (2)	C36—H36	0.9300
C33—C34	1.368 (3)	C62—H62	0.9300
C34—C35	1.371 (2)	C63—H63	0.9300
C35—C36	1.387 (2)	C64—H64	0.9300
C61—C62	1.3830 (17)	C65—H65	0.9300
C61—C66	1.3861 (18)	C66—H66	0.9300
O1···C6^{i}	3.2576 (16)	C66···H33^{iv}	2.9700
O4···C3^{ii}	3.4093 (15)	H1···C61	2.6700
O1···H22	2.8100	H1···C66	3.0500
O1···H6^{i}	2.2900	H1···C13^{i}	2.9600
O1···H13B^{i}	2.9200	H1···H13B^{i}	2.3300
O1···H62^{i}	2.7500	H2···O1	2.4100
O1···H2	2.4100	H2···C31	2.7400
O4···H13A	2.8500	H2···C32	3.0500
O4···H3^{ii}	2.4400	H2···C24^{v}	2.8100
O4···H26^{ii}	2.7300	H3···C26	2.6700
N1···H13B	2.6600	H3···C36	2.9600
N1···H22	2.7200	H3···H26	2.1100
N1···H66	2.7200	H3···O4^{ii}	2.4400
C1···C22	3.459 (2)	H5A···C2	2.8800
C1···C66	3.239 (2)	H5A···C21	2.8300
C3···O4^{ii}	3.4093 (15)	H5A···C34^{iv}	3.0500
C4···C26	3.1751 (18)	H5A···C66	3.0500
C5···C21	3.2029 (17)	H5B···C64^{ix}	3.0100
C5···C26	3.5906 (18)	H5B···C65^{ix}	2.9900
C6···C13	3.3229 (17)	H5B···H64^{ix}	2.5000
C6···O1^{iii}	3.2576 (16)	H5B···H65^{ix}	2.4600
C13···C6	3.3229 (17)	H6···C3	3.0400
C21···C5	3.2029 (17)	H6···C13	3.0200
C22···C1	3.459 (2)	H6···H13B	2.2800
C26···C4	3.1751 (18)	H6···H62	2.3200
C26···C5	3.5906 (18)	H6···O1^{iii}	2.2900
C66···C1	3.239 (2)	H13A···O4	2.8500

C1···H22	2.8700	H13B···N1	2.6600
C1···H66	3.0400	H13B···C6	2.7900
C1···H13B^{i}	2.9200	H13B···H6	2.2800
C2···H5A	2.8800	H13B···H32	2.3600
C3···H6	3.0400	H13B···O1^{iii}	2.9200
C3···H26	2.5700	H13B···C1^{iii}	2.9200
C4···H26	2.7400	H13B···H1^{iii}	2.3300
C6···H13B	2.7900	H22···O1	2.8100
C13···H1^{iii}	2.9600	H22···N1	2.7200
C13···H6	3.0200	H22···C1	2.8700
C21···H5A	2.8300	H24···C33^{v}	3.1000
C22···H66	2.9900	H24···C34^{v}	2.9800
C24···H34^{iv}	3.0800	H24···C35^{v}	2.9900
C24···H2^{v}	2.8100	H25···C62^{x}	3.0700
C25···H34^{iv}	3.0200	H26···C3	2.5700
C26···H3	2.6700	H26···C4	2.7400
C31···H2	2.7400	H26···H3	2.1100
C32···H2	3.0500	H26···O4^{ii}	2.7300
C33···H62^{i}	3.0900	H32···H13B	2.3600
C33···H24^{v}	3.1000	H33···C65^{vi}	3.0000
C34···H5A^{vi}	3.0500	H33···C66^{vi}	2.9700
C34···H24^{v}	2.9800	H34···C24^{vi}	3.0800
C35···H24^{v}	2.9900	H34···C25^{vi}	3.0200
C36···H3	2.9600	H62···H6	2.3200
C61···H1	2.6700	H62···O1^{iii}	2.7500
C62···H25^{vii}	3.0700	H62···C33^{iii}	3.0900
C64···H5B^{viii}	3.0100	H64···H5B^{viii}	2.5000
C65···H33^{iv}	3.0000	H65···H5B^{viii}	2.4600
C65···H5B^{viii}	2.9900	H66···N1	2.7200
C66···H1	3.0500	H66···C1	3.0400
C66···H5A	3.0500	H66···C22	2.9900
C1—N1—C2	119.98 (10)	C2—C3—H3	108.00
C1—N1—C6	118.22 (10)	C4—C3—H3	108.00
C2—N1—C6	120.45 (9)	C13—C3—H3	108.00
O1—C1—N1	125.88 (13)	C4—C5—H5A	109.00
N1—C2—C3	108.94 (9)	C4—C5—H5B	109.00
N1—C2—C21	112.04 (9)	C6—C5—H5A	109.00
C3—C2—C21	114.48 (9)	C6—C5—H5B	109.00
C2—C3—C4	110.13 (9)	H5A—C5—H5B	108.00
C2—C3—C13	113.31 (9)	N1—C6—H6	108.00
C4—C3—C13	108.63 (9)	C5—C6—H6	108.00
O4—C4—C3	122.70 (11)	C61—C6—H6	108.00
O4—C4—C5	121.22 (11)	C3—C13—H13A	109.00
C3—C4—C5	116.07 (10)	C3—C13—H13B	109.00

C4—C5—C6	113.46 (10)	C31—C13—H13A	109.00
N1—C6—C5	109.26 (9)	C31—C13—H13B	109.00
N1—C6—C61	113.10 (10)	H13A—C13—H13B	108.00
C5—C6—C61	110.75 (10)	C21—C22—H22	120.00
C3—C13—C31	114.36 (10)	C23—C22—H22	120.00
C2—C21—C22	119.35 (11)	C22—C23—H23	120.00
C2—C21—C26	122.78 (10)	C24—C23—H23	120.00
C22—C21—C26	117.80 (11)	C23—C24—H24	120.00
C21—C22—C23	120.74 (13)	C25—C24—H24	120.00
C22—C23—C24	120.57 (13)	C24—C25—H25	120.00
C23—C24—C25	119.28 (14)	C26—C25—H25	120.00
C24—C25—C26	120.72 (14)	C21—C26—H26	120.00
C21—C26—C25	120.87 (12)	C25—C26—H26	120.00
C13—C31—C32	121.21 (12)	C31—C32—H32	120.00
C13—C31—C36	120.92 (11)	C33—C32—H32	120.00
C32—C31—C36	117.87 (12)	C32—C33—H33	120.00
C31—C32—C33	120.65 (15)	C34—C33—H33	120.00
C32—C33—C34	120.65 (17)	C33—C34—H34	120.00
C33—C34—C35	119.58 (16)	C35—C34—H34	120.00
C34—C35—C36	120.14 (15)	C34—C35—H35	120.00
C31—C36—C35	121.10 (13)	C36—C35—H35	120.00
C6—C61—C62	118.42 (11)	C31—C36—H36	119.00
C6—C61—C66	122.64 (10)	C35—C36—H36	119.00
C62—C61—C66	118.92 (11)	C61—C62—H62	120.00
C61—C62—C63	120.64 (13)	C63—C62—H62	120.00
C62—C63—C64	120.13 (14)	C62—C63—H63	120.00
C63—C64—C65	119.56 (14)	C64—C63—H63	120.00
C64—C65—C66	120.43 (13)	C63—C64—H64	120.00
C61—C66—C65	120.30 (12)	C65—C64—H64	120.00
O1—C1—H1	117.00	C64—C65—H65	120.00
N1—C1—H1	117.00	C66—C65—H65	120.00
N1—C2—H2	107.00	C61—C66—H66	120.00
C3—C2—H2	107.00	C65—C66—H66	120.00
C21—C2—H2	107.00		
C2—N1—C1—O1	−10.3 (2)	N1—C6—C61—C66	−38.97 (15)
C6—N1—C1—O1	−177.08 (13)	C5—C6—C61—C62	−94.24 (13)
C1—N1—C2—C3	−128.30 (11)	C5—C6—C61—C66	84.06 (14)
C1—N1—C2—C21	104.00 (13)	C3—C13—C31—C32	−109.37 (14)
C6—N1—C2—C3	38.20 (13)	C3—C13—C31—C36	71.24 (15)
C6—N1—C2—C21	−89.50 (12)	C2—C21—C22—C23	−178.23 (12)
C1—N1—C6—C5	−176.52 (11)	C26—C21—C22—C23	−1.27 (19)
C1—N1—C6—C61	−52.68 (14)	C2—C21—C26—C25	178.42 (12)
C2—N1—C6—C5	16.75 (14)	C22—C21—C26—C25	1.56 (19)
C2—N1—C6—C61	140.59 (10)	C21—C22—C23—C24	0.0 (2)
N1—C2—C3—C4	−59.37 (12)	C22—C23—C24—C25	0.9 (2)
N1—C2—C3—C13	62.53 (12)	C23—C24—C25—C26	−0.6 (2)
C21—C2—C3—C4	66.94 (12)	C24—C25—C26—C21	−0.6 (2)
C21—C2—C3—C13	−171.17 (9)	C13—C31—C32—C33	−179.22 (14)
N1—C2—C21—C22	−48.07 (14)	C36—C31—C32—C33	0.2 (2)

N1—C2—C21—C26	135.12 (11)	C13—C31—C36—C35	179.15 (13)
C3—C2—C21—C22	−172.75 (11)	C32—C31—C36—C35	−0.3 (2)
C3—C2—C21—C26	10.44 (16)	C31—C32—C33—C34	0.1 (3)
C2—C3—C4—O4	−155.25 (11)	C32—C33—C34—C35	−0.3 (3)
C2—C3—C4—C5	25.61 (13)	C33—C34—C35—C36	0.2 (2)
C13—C3—C4—O4	80.12 (14)	C34—C35—C36—C31	0.1 (2)
C13—C3—C4—C5	−99.03 (12)	C6—C61—C62—C63	177.20 (12)
C2—C3—C13—C31	63.87 (13)	C66—C61—C62—C63	−1.16 (19)
C4—C3—C13—C31	−173.40 (10)	C6—C61—C66—C65	−178.53 (12)
O4—C4—C5—C6	−148.61 (12)	C62—C61—C66—C65	−0.24 (19)
C3—C4—C5—C6	30.55 (14)	C61—C62—C63—C64	1.6 (2)
C4—C5—C6—N1	−52.04 (13)	C62—C63—C64—C65	−0.6 (2)
C4—C5—C6—C61	−177.26 (10)	C63—C64—C65—C66	−0.8 (2)
N1—C6—C61—C62	142.73 (11)	C64—C65—C66—C61	1.2 (2)

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+1/2; (ii) −*x*+1, −*y*, −*z*+1; (iii) −*x*+1, *y*−1/2, −*z*+1/2; (iv) *x*−1, *y*, *z*; (v) −*x*+1, −*y*+1, −*z*+1; (vi) *x*+1, *y*, *z*; (vii) *x*, −*y*+1/2, *z*−1/2; (viii) −*x*, *y*+1/2, −*z*+1/2; (ix) −*x*, *y*−1/2, −*z*+1/2; (x) *x*, −*y*+1/2, *z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C24—H24···Cg^{v}	0.93	2.81	3.651 (1)	151
C34—H34···Cg^{vi}	0.93	2.97	3.890 (2)	172
C2—H2···O1	0.98	2.41	2.8175 (15)	105
C3—H3···O4^{ii}	0.98	2.44	3.4093 (15)	170
C6—H6···O1^{iii}	0.98	2.29	3.2576 (16)	168

Symmetry codes: (v) −*x*+1, −*y*+1, −*z*+1; (vi) *x*+1, *y*, *z*; (ii) −*x*+1, −*y*, −*z*+1; (iii) −*x*+1, *y*−1/2, −*z*+1/2.

Fig. 1

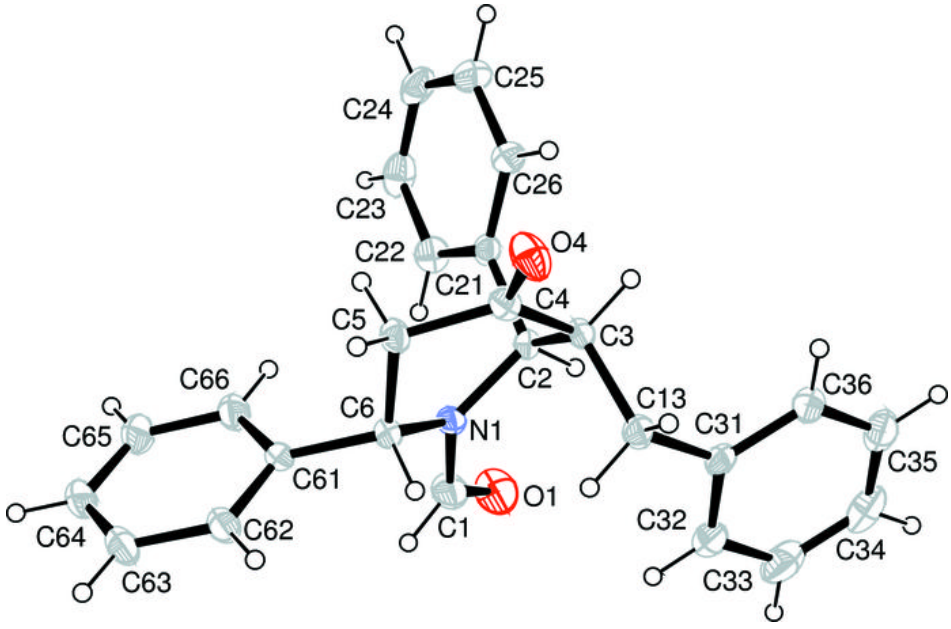
C25
C24
C26
C23
O4
C22
C21
C4
C5
C3
C2
C66
C6
N1
C13
C36
C31
C65
C61
O1
C35
C32
C64
C62
C1
C34
C63
C33

Fig. 2