Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-Ethyl-2,6-bis(4-methoxyphenyl)-piperidin-4-one

T. Kavitha,[a] S. Ponnuswamy,[b] V. Mohanraj,[b] S. S. Ilango[b] and M. N. Ponnuswamy[a]*

[a]Centre of Advanced Study in Crystallography and Biophysics, University of Madras, Guindy Campus, Chennai 600025, India, and [b]Department of Chemistry, Government Arts College (Autonomous), Coimbatore 641018, India
Correspondence e-mail: mnpsy2004@yahoo.com

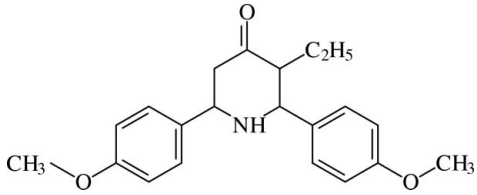
Received 20 August 2007; accepted 22 August 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.066; wR factor = 0.220; data-to-parameter ratio = 14.2.

In the title molecule, $C_{21}H_{25}NO_3$, the piperidine ring is in a chair conformation. The dihedral angle between the two benzene rings is 48.4 (1)°. The methoxy groups are almost coplanar with the attached benzene rings. The molecular and crystal structures are stabilized by C—H$\cdots\pi$ interactions.

Related literature

For related literature, see: Desiraju (1989); Dimmock *et al.* (1990); Sekar *et al.* (1990); Mutus *et al.* (1989).



Experimental

Crystal data

$C_{21}H_{25}NO_3$
M_r = 339.42
Monoclinic, $P2_1/c$
a = 14.012 (2) Å
b = 7.8060 (14) Å
c = 17.655 (3) Å
β = 110.401 (5)°
V = 1810.0 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
0.15 × 0.13 × 0.10 mm

Data collection

Bruker Kappa APEX II area-detector diffractometer
Absorption correction: none
15103 measured reflections
3270 independent reflections
2348 reflections with $I > 2\sigma(I)$
R_{int} = 0.060

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.220
S = 1.10
3270 reflections
230 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the C9–C14 and C15–C20 rings, respectively.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C8—H8*B*$\cdots$*Cg*1	0.96	2.79	3.662 (4)	152
C10—H10$\cdots$*Cg*2^{i}	0.93	2.87	3.647 (3)	142
C22—H22*C*$\cdots$*Cg*2^{ii}	0.96	2.77	3.637 (4)	151

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1995).

SP thanks UGC, Government of India, for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2447).

References

Bruker (2004). *APEX2* (Version 1.22) and *SAINT* (Version 6.0a). Bruker AXS Inc., Madison, Wisconsin, USA.
Desiraju, G. R. (1989). *Materials Science Monographs*, No. 54, *Crystal Engineering – The Design of Organic Solids*, edited by G. R. Desiraju, pp. 85–113. New York: Elsevier Science Publishers.
Dimmock, J. R., Arora, V. K., Wonko, S. L., Hamon, N. W., Quail, J. W., Jia, Z., Warrington, R. C., Fang, W. D. & Lee, J. S. (1990). *Drug Des. Deliv.* **6**, 183–194.
Mutus, B., Wagner, J. D., Talpas, C. J., Dimmock, J. R., Phillips, O. A. & Reid, R. S. (1989). *Anal. Biochem.* pp. 237–243.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Sekar, K., Parthasarathy, S. & Rajalingam, P. (1990). *Acta Cryst.* C**46**, 1153–1155.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

supplementary materials

Acta Cryst. (2007). E**63**, o3985 [**doi:10.1107/S1600536807041475**]

3-Ethyl-2,6-bis(4-methoxyphenyl)piperidin-4-one

T. Kavitha, S. Ponnuswamy, V. Mohanraj, S. S. Ilango and M. N. Ponnuswamy

Comment

Nitrogen heterocycles, in particular piperidone alkaloids, occur in both plants and animals and some of them possess a variety of biological activities, including cytotoxic and anti-cancer properties (Dimmock *et al.*, 1990; Mutus *et al.*, 1989). In view of the above importance, the X-ray crystal structure determination of the title compound has been undertaken.

Bond lengths and angles (Fig. 1) are comparable to those observed for 3-methyl-2,6-diphenyl-4-piperidone (Sekar *et al.*, 1990). The piperidine ring adopts a chair conformation, with a puckering amplitude Q_T of 0.577 (3) Å (Nardelli, 1995). The two benzene rings are in equatorial orientation with respect to the piperidine ring which is evidenced from the torsion angles C15—C6—C5—C4 of 174.7 (3)° and C4—C3—C2—C9 of −178.6 (2)°. The ethyl group substitued at C3 is also oriented equatorially with the N1—C2—C3—C7 torsion angle being 178.4 (2)°. The dihedral angle between the two benzene rings is 48.4 (1)°. The methoxy groups are almost coplanar with the attached benzene rings.

The molecular structure is stabilized by a C—H···π interaction involving the C9—C14 benzene ring (centroid *Cg*1). The crystal structure is stabilized by C—H···π interactions (Desiraju, 1989) involving the C15—C20 benzene ring (centroid *Cg*2). The packing of the molecules viewed down the *a* axis is shown in Fig.2. In addition to the above-mentioned interactions, the structure is also stabilized by van der Waals forces

Experimental

The condensation reaction involving anisaldehyde (24.3 ml, 200 mmol), ammonium acetate (7.7 g, 100 mmol) and pentan-2-one (10.7 ml, 100 mmol) afforded the title compound. Single crystals of the title compound were obtained by slow evaporation of a benzene-petroleum ether (8:1) solution.

Refinement

The N-bound H atom was located in a difference map and refined isotropically. C-bound H atoms were included in calculated positions [C—H = 0.93–0.98 Å] and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C_{methyl}).

Figures

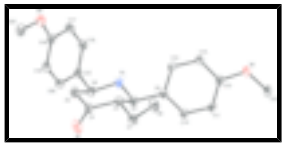


Fig. 1. The molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 20% probability level. For the sake of clarity, H atoms have been omitted.

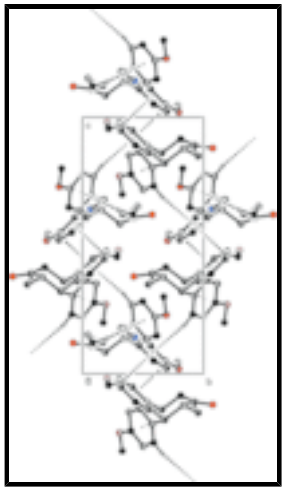


Fig. 2. Crystal packing viewed down the *a* axis.

3-Ethyl-2,6-bis(4-methoxyphenyl)piperidin-4-one

Crystal data

$C_{21}H_{25}NO_3$	F_{000} = 728
M_r = 339.42	D_x = 1.246 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3270 reflections
a = 14.012 (2) Å	θ = 1.6–25.3º
b = 7.8060 (14) Å	μ = 0.08 mm^{-1}
c = 17.655 (3) Å	T = 293 (2) K
β = 110.401 (5)º	Block, colourless
V = 1810.0 (5) Å^3	0.15 × 0.13 × 0.10 mm
Z = 4	

Data collection

Bruker Kappa APEX II area-detector diffractometer	2348 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.060
Monochromator: graphite	θ_{max} = 25.3º
T = 293(2) K	θ_{min} = 1.6º
ω and φ scans	h = −15→16
Absorption correction: none	k = −9→9
15103 measured reflections	l = −21→21
3270 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.066$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.220$	$w = 1/[\sigma^2(F_o^2) + (0.1169P)^2 + 0.8076P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.10$	$(\Delta/\sigma)_{max} = 0.001$
3270 reflections	$\Delta\rho_{max} = 0.26$ e Å^{-3}
230 parameters	$\Delta\rho_{min} = -0.27$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
H1	0.465 (2)	0.530 (5)	0.1687 (19)	0.057 (9)*
C2	0.54806 (18)	0.3215 (4)	0.17902 (16)	0.0411 (7)
H2	0.5470	0.2782	0.2308	0.049*
C3	0.54152 (19)	0.1662 (4)	0.12238 (16)	0.0422 (7)
H3	0.5390	0.2119	0.0700	0.051*
C4	0.4410 (2)	0.0763 (4)	0.10928 (18)	0.0462 (7)
C5	0.3484 (2)	0.1890 (4)	0.08452 (18)	0.0492 (7)
H5A	0.2904	0.1234	0.0863	0.059*
H5B	0.3337	0.2270	0.0293	0.059*
C6	0.36336 (19)	0.3454 (4)	0.13980 (17)	0.0418 (7)
H6	0.3705	0.3066	0.1943	0.050*
C7	0.6321 (2)	0.0451 (4)	0.1516 (2)	0.0544 (8)
H7A	0.6594	0.0486	0.2102	0.065*
H7B	0.6082	−0.0706	0.1358	0.065*
C8	0.7175 (3)	0.0832 (5)	0.1204 (2)	0.0678 (10)
H8A	0.7712	0.0011	0.1421	0.102*
H8B	0.7433	0.1963	0.1368	0.102*
H8C	0.6923	0.0763	0.0625	0.102*
C9	0.64449 (19)	0.4237 (4)	0.19468 (16)	0.0400 (6)
C10	0.7234 (2)	0.4118 (4)	0.26803 (16)	0.0427 (7)
H10	0.7151	0.3450	0.3089	0.051*
C11	0.81529 (19)	0.4977 (4)	0.28201 (16)	0.0446 (7)
H11	0.8680	0.4867	0.3314	0.054*
C12	0.8272 (2)	0.5987 (4)	0.22232 (17)	0.0429 (7)
C13	0.7491 (2)	0.6126 (4)	0.14879 (17)	0.0484 (7)
H13	0.7576	0.6795	0.1080	0.058*
C14	0.6584 (2)	0.5277 (4)	0.13550 (17)	0.0472 (7)
H14	0.6057	0.5402	0.0862	0.057*

C15	0.27395 (19)	0.4669 (4)	0.11000 (16)	0.0399 (6)
C16	0.2672 (2)	0.5889 (4)	0.05091 (17)	0.0478 (7)
H16	0.3198	0.5993	0.0306	0.057*
C17	0.1835 (2)	0.6948 (4)	0.02204 (17)	0.0481 (7)
H17	0.1804	0.7759	−0.0173	0.058*
C18	0.10395 (19)	0.6814 (4)	0.05126 (16)	0.0422 (7)
C19	0.10883 (19)	0.5612 (4)	0.10976 (17)	0.0447 (7)
H19	0.0558	0.5508	0.1297	0.054*
C20	0.1939 (2)	0.4555 (4)	0.13862 (17)	0.0438 (7)
H20	0.1970	0.3750	0.1782	0.053*
C21	0.9997 (2)	0.6714 (5)	0.3003 (2)	0.0695 (10)
H21A	1.0539	0.7436	0.2977	0.104*
H21B	1.0213	0.5540	0.3051	0.104*
H21C	0.9822	0.7024	0.3465	0.104*
C22	−0.0592 (2)	0.7846 (5)	0.0444 (2)	0.0583 (9)
H22A	−0.1079	0.8711	0.0175	0.087*
H22B	−0.0376	0.8016	0.1018	0.087*
H22C	−0.0899	0.6735	0.0311	0.087*
N1	0.45796 (16)	0.4296 (3)	0.14268 (15)	0.0451 (6)
O1	0.43561 (17)	−0.0761 (3)	0.12028 (19)	0.0785 (8)
O2	0.91367 (15)	0.6923 (3)	0.22939 (13)	0.0614 (6)
O3	0.02622 (15)	0.7956 (3)	0.01916 (13)	0.0572 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C2	0.0278 (13)	0.0504 (16)	0.0437 (14)	0.0004 (12)	0.0109 (11)	0.0018 (12)
C3	0.0321 (14)	0.0487 (16)	0.0465 (15)	0.0016 (12)	0.0145 (12)	0.0041 (12)
C4	0.0365 (15)	0.0428 (17)	0.0587 (18)	−0.0027 (12)	0.0160 (13)	−0.0059 (13)
C5	0.0323 (15)	0.0490 (17)	0.0615 (18)	−0.0029 (12)	0.0102 (13)	−0.0046 (14)
C6	0.0290 (13)	0.0486 (16)	0.0475 (15)	0.0016 (11)	0.0129 (11)	−0.0004 (12)
C7	0.0368 (15)	0.0480 (18)	0.080 (2)	0.0054 (13)	0.0223 (15)	0.0078 (15)
C8	0.0468 (18)	0.060 (2)	0.107 (3)	0.0027 (15)	0.0401 (19)	−0.0070 (19)
C9	0.0292 (13)	0.0446 (15)	0.0437 (14)	0.0004 (11)	0.0094 (11)	−0.0019 (12)
C10	0.0336 (14)	0.0506 (16)	0.0433 (15)	−0.0004 (12)	0.0124 (11)	0.0045 (12)
C11	0.0280 (13)	0.0567 (18)	0.0435 (15)	0.0014 (12)	0.0056 (11)	0.0035 (13)
C12	0.0317 (14)	0.0445 (16)	0.0511 (16)	−0.0017 (12)	0.0125 (12)	−0.0010 (13)
C13	0.0435 (16)	0.0490 (17)	0.0496 (16)	−0.0021 (13)	0.0124 (13)	0.0087 (13)
C14	0.0346 (15)	0.0544 (18)	0.0449 (15)	0.0006 (13)	0.0040 (12)	0.0060 (13)
C15	0.0266 (13)	0.0485 (16)	0.0428 (14)	−0.0004 (11)	0.0099 (11)	−0.0020 (12)
C16	0.0325 (14)	0.0616 (19)	0.0550 (17)	−0.0008 (13)	0.0226 (13)	0.0010 (14)
C17	0.0392 (15)	0.0566 (18)	0.0528 (16)	0.0026 (13)	0.0213 (13)	0.0106 (14)
C18	0.0303 (14)	0.0456 (15)	0.0490 (15)	−0.0002 (12)	0.0118 (11)	−0.0025 (12)
C19	0.0274 (13)	0.0550 (17)	0.0561 (17)	−0.0013 (12)	0.0201 (12)	−0.0013 (14)
C20	0.0329 (14)	0.0506 (17)	0.0496 (16)	−0.0029 (12)	0.0165 (12)	0.0033 (13)
C21	0.0327 (16)	0.082 (2)	0.081 (2)	−0.0140 (16)	0.0043 (15)	0.0105 (19)
C22	0.0329 (15)	0.066 (2)	0.076 (2)	0.0050 (14)	0.0195 (14)	−0.0070 (17)
N1	0.0272 (12)	0.0445 (14)	0.0599 (15)	−0.0008 (10)	0.0106 (10)	−0.0070 (12)

O1	0.0477 (14)	0.0490 (15)	0.141 (2)	−0.0038 (11)	0.0357 (14)	−0.0003 (14)
O2	0.0366 (11)	0.0731 (16)	0.0672 (14)	−0.0154 (10)	0.0090 (10)	0.0132 (11)
O3	0.0362 (11)	0.0648 (14)	0.0737 (14)	0.0122 (10)	0.0231 (10)	0.0125 (11)

Geometric parameters (Å, °)

C2—N1	1.468 (3)	C11—H11	0.93
C2—C9	1.509 (4)	C12—C13	1.380 (4)
C2—C3	1.554 (4)	C12—O2	1.382 (3)
C2—H2	0.98	C13—C14	1.379 (4)
C3—C4	1.517 (4)	C13—H13	0.93
C3—C7	1.521 (4)	C14—H14	0.93
C3—H3	0.98	C15—C20	1.384 (4)
C4—O1	1.212 (4)	C15—C16	1.391 (4)
C4—C5	1.502 (4)	C16—C17	1.379 (4)
C5—C6	1.531 (4)	C16—H16	0.93
C5—H5A	0.97	C17—C18	1.385 (4)
C5—H5B	0.97	C17—H17	0.93
C6—N1	1.464 (3)	C18—O3	1.368 (3)
C6—C15	1.512 (4)	C18—C19	1.379 (4)
C6—H6	0.98	C19—C20	1.392 (4)
C7—C8	1.511 (4)	C19—H19	0.93
C7—H7A	0.97	C20—H20	0.93
C7—H7B	0.97	C21—O2	1.413 (4)
C8—H8A	0.96	C21—H21A	0.96
C8—H8B	0.96	C21—H21B	0.96
C8—H8C	0.96	C21—H21C	0.96
C9—C10	1.382 (4)	C22—O3	1.418 (3)
C9—C14	1.389 (4)	C22—H22A	0.96
C10—C11	1.395 (4)	C22—H22B	0.96
C10—H10	0.93	C22—H22C	0.96
C11—C12	1.372 (4)	N1—H1	0.90 (3)
N1—C2—C9	110.8 (2)	C12—C11—H11	120.3
N1—C2—C3	108.6 (2)	C10—C11—H11	120.3
C9—C2—C3	112.2 (2)	C11—C12—C13	119.9 (3)
N1—C2—H2	108.4	C11—C12—O2	124.9 (2)
C9—C2—H2	108.4	C13—C12—O2	115.2 (2)
C3—C2—H2	108.4	C14—C13—C12	120.3 (3)
C4—C3—C7	112.6 (2)	C14—C13—H13	119.9
C4—C3—C2	107.6 (2)	C12—C13—H13	119.9
C7—C3—C2	114.3 (2)	C13—C14—C9	121.0 (2)
C4—C3—H3	107.3	C13—C14—H14	119.5
C7—C3—H3	107.3	C9—C14—H14	119.5
C2—C3—H3	107.3	C20—C15—C16	117.7 (2)
O1—C4—C5	121.7 (3)	C20—C15—C6	120.7 (2)
O1—C4—C3	122.4 (3)	C16—C15—C6	121.5 (2)
C5—C4—C3	115.8 (2)	C17—C16—C15	121.0 (3)
C4—C5—C6	111.7 (2)	C17—C16—H16	119.5
C4—C5—H5A	109.3	C15—C16—H16	119.5

C6—C5—H5A	109.3	C16—C17—C18	120.5 (3)
C4—C5—H5B	109.3	C16—C17—H17	119.7
C6—C5—H5B	109.3	C18—C17—H17	119.7
H5A—C5—H5B	107.9	O3—C18—C19	125.3 (2)
N1—C6—C15	111.1 (2)	O3—C18—C17	115.1 (3)
N1—C6—C5	107.5 (2)	C19—C18—C17	119.6 (3)
C15—C6—C5	111.4 (2)	C18—C19—C20	119.3 (2)
N1—C6—H6	108.9	C18—C19—H19	120.3
C15—C6—H6	108.9	C20—C19—H19	120.3
C5—C6—H6	108.9	C15—C20—C19	121.9 (3)
C8—C7—C3	115.3 (3)	C15—C20—H20	119.1
C8—C7—H7A	108.5	C19—C20—H20	119.1
C3—C7—H7A	108.5	O2—C21—H21A	109.5
C8—C7—H7B	108.5	O2—C21—H21B	109.5
C3—C7—H7B	108.5	H21A—C21—H21B	109.5
H7A—C7—H7B	107.5	O2—C21—H21C	109.5
C7—C8—H8A	109.5	H21A—C21—H21C	109.5
C7—C8—H8B	109.5	H21B—C21—H21C	109.5
H8A—C8—H8B	109.5	O3—C22—H22A	109.5
C7—C8—H8C	109.5	O3—C22—H22B	109.5
H8A—C8—H8C	109.5	H22A—C22—H22B	109.5
H8B—C8—H8C	109.5	O3—C22—H22C	109.5
C10—C9—C14	117.9 (2)	H22A—C22—H22C	109.5
C10—C9—C2	120.6 (2)	H22B—C22—H22C	109.5
C14—C9—C2	121.5 (2)	C6—N1—C2	112.8 (2)
C9—C10—C11	121.4 (3)	C6—N1—H1	110 (2)
C9—C10—H10	119.3	C2—N1—H1	111 (2)
C11—C10—H10	119.3	C12—O2—C21	117.9 (2)
C12—C11—C10	119.5 (2)	C18—O3—C22	117.9 (2)
N1—C2—C3—C4	−55.8 (3)	C12—C13—C14—C9	−1.5 (5)
C9—C2—C3—C4	−178.6 (2)	C10—C9—C14—C13	1.7 (4)
N1—C2—C3—C7	178.4 (2)	C2—C9—C14—C13	−176.1 (3)
C9—C2—C3—C7	55.5 (3)	N1—C6—C15—C20	−146.8 (3)
C7—C3—C4—O1	−1.0 (4)	C5—C6—C15—C20	93.3 (3)
C2—C3—C4—O1	−127.8 (3)	N1—C6—C15—C16	35.8 (4)
C7—C3—C4—C5	176.9 (3)	C5—C6—C15—C16	−84.1 (3)
C2—C3—C4—C5	50.1 (3)	C20—C15—C16—C17	0.1 (4)
O1—C4—C5—C6	128.2 (3)	C6—C15—C16—C17	177.6 (3)
C3—C4—C5—C6	−49.7 (3)	C15—C16—C17—C18	−0.2 (5)
C4—C5—C6—N1	52.6 (3)	C16—C17—C18—O3	178.7 (3)
C4—C5—C6—C15	174.6 (2)	C16—C17—C18—C19	0.1 (4)
C4—C3—C7—C8	144.8 (3)	O3—C18—C19—C20	−178.4 (3)
C2—C3—C7—C8	−92.0 (3)	C17—C18—C19—C20	0.2 (4)
N1—C2—C9—C10	133.4 (3)	C16—C15—C20—C19	0.2 (4)
C3—C2—C9—C10	−105.0 (3)	C6—C15—C20—C19	−177.3 (2)
N1—C2—C9—C14	−48.8 (4)	C18—C19—C20—C15	−0.3 (4)
C3—C2—C9—C14	72.8 (3)	C15—C6—N1—C2	174.2 (2)
C14—C9—C10—C11	−1.5 (4)	C5—C6—N1—C2	−63.6 (3)
C2—C9—C10—C11	176.3 (3)	C9—C2—N1—C6	−169.6 (2)

C9—C10—C11—C12	1.1 (4)	C3—C2—N1—C6	66.7 (3)
C10—C11—C12—C13	−0.9 (4)	C11—C12—O2—C21	5.9 (5)
C10—C11—C12—O2	178.8 (3)	C13—C12—O2—C21	−174.3 (3)
C11—C12—C13—C14	1.1 (5)	C19—C18—O3—C22	−3.6 (4)
O2—C12—C13—C14	−178.6 (3)	C17—C18—O3—C22	177.8 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8B···Cg1	0.96	2.79	3.662 (4)	152
C10—H10···Cg2^{i}	0.93	2.87	3.647 (3)	142
C22—H22C···Cg2^{ii}	0.96	2.77	3.637 (4)	151

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

Fig. 1

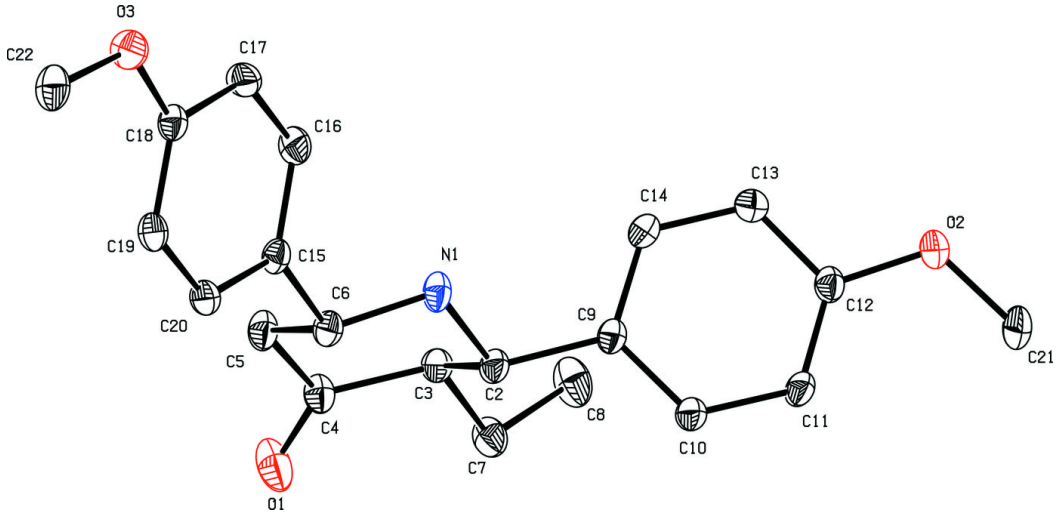

O3
C22
C17
C18
C16
C19
C15
N1
C6
C20
C5
C9
C14
C13
O2
C12
C21
C3
C2
C8
C4
C7
C10
C11
O1

Fig. 2