Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

t-3-Benzyl-*r*-2,*c*-6-di-2-furylpiperidin-4-one

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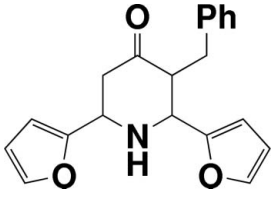
Received 23 April 2007; accepted 10 May 2007

Key indicators: single-crystal X-ray study; T = 160 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.071; wR factor = 0.226; data-to-parameter ratio = 14.5.

In the title molecule, $C_{20}H_{19}NO_3$, the piperidine ring adopts a chair conformation. The phenyl and furyl rings have equatorial orientations. Molecules are linked by C—H···O hydrogen bonds.

Related literature

For related literature, see: Balamurugan *et al.* (2006, 2007).



Experimental

Crystal data

$C_{20}H_{19}NO_3$
M_r = 321.36
Monoclinic, $P2_1/c$
a = 5.443 (5) Å
b = 21.437 (5) Å
c = 14.108 (5) Å
β = 91.037 (5)°
V = 1645.9 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 160 (1) K
0.25 × 0.25 × 0.13 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Absorption correction: none
30100 measured reflections
3254 independent reflections
2182 reflections with $I > 2\sigma(I)$
R_{int} = 0.086

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.226
S = 1.06
3254 reflections
225 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C23—H23···O4^{i}	0.95	2.38	3.266 (5)	155

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

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); 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).

The data collection was carried out by Dr A. Linden of the Institute of Organic Chemistry at the University of Zürich; his help is gratefully acknowledged by Dr A. Thiruvalluvar. AT also thanks Professor I. Brito for useful discussions.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2081).

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  doi:10.1107/S1600536807023112

supplementary materials

Acta Cryst. (2007). E**63**, o2910 [**doi:10.1107/S1600536807023112**]

t-3-Benzyl-*r*-2,*c*-6-di-2-furylpiperidin-4-one

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Comment

Piperidine heterocycles play an important role in the field of medicinal Chemistry (Balamurugan *et al.*, 2006,2007). In the title compound, (I), N1 shows a pyramidal geometry (Fig. 1). The piperidine ring adopts a chair conformation. The phenyl group at C3 and the furyl rings at C2 and C6 are in equatorial positions. In the solid state, the symmetry-related molecules are linked by C23—H23···O4 ($x + 1$, $-y + 1/2$, $z - 1/2$) hydrogen bonds to form chains along the *c* axis (Fig. 2).

Experimental

A mixture of ammonium acetate (38.5 g, 0.5 mol), furfuraldehyde (82.84 ml, 1 mol) and benzyl acetone (38.5 ml, 0.5 mol) in distilled ethanol was heated first to boiling. After cooling, the viscous liquid obtained was dissolved in ether (200 ml) and shaken with 10 ml of concentrated hydrochloric acid. The precipitated hydrochloride of 3-benzyl-2,6-di-furylpiperidin-4-one was removed by filtration and washed first with 40 ml mixture of ethanol and ether (1:1) and then with ether to remove most of the coloured impurities. The base was liberated from an alcoholic solution by adding aqueous ammonia and then diluted with water. It was recrystallized from mixture of petroleum ether. The yield of the compound was 70%.

Refinement

Atom H1 at N1 was located in a difference Fourier map and refined isotropically. Remaining H atoms were positioned geometrically and allowed to ride on their parent atoms with C–H = 0.93–1.00 Å and $U_{iso} = 1.2U_{eq}$(parent atom). The furyl ring at position 6 is disordered. The site occupancy of the two atom positions C65A and C65B were refined (0.604:0.396).

Figures

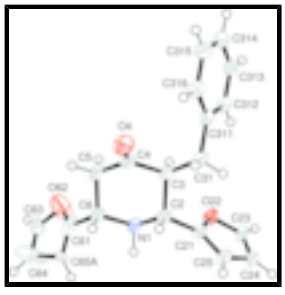

Fig. 1. View of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

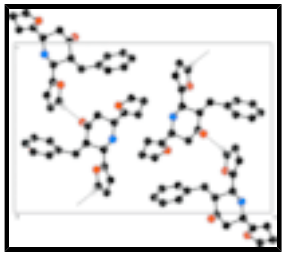

Fig. 2. The molecular packing of (I), viewed down the *a* axis showing the C–H···O(dashed lines) interactions.

t-3-Benzyl-r-2,c-6-di-2-furylpiperidin-4-one

Crystal data

$C_{20}H_{19}NO_3$	F_{000} = 680
M_r = 321.36	D_x = 1.297 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 463 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 5.443 (5) Å	Cell parameters from 3346 reflections
b = 21.437 (5) Å	θ = 2.0–26.0º
c = 14.108 (5) Å	μ = 0.09 mm^{-1}
β = 91.037 (5)º	T = 160 (1) K
V = 1645.9 (17) Å^3	Platelike, light-brown
Z = 4	0.25 × 0.25 × 0.13 mm

Data collection

Nonius KappaCCD area-detector diffractometer	3254 independent reflections
Radiation source: Nonius FR590 sealed tube generator	2182 reflections with $I > 2\sigma(I)$
Monochromator: horizontally mounted graphite crystal	R_{int} = 0.086
Detector resolution: 9 pixels mm^{-1}	θ_{max} = 26.0º
T = 160(1) K	θ_{min} = 2.4º
φ and ω scans with κ offsets	h = −6→6
Absorption correction: none	k = −26→26
30100 measured reflections	l = −17→17

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.071	$w = 1/[\sigma^2(F_o^2) + (0.1215P)^2 + 1.0322P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.226	$(\Delta/\sigma)_{max} < 0.001$
S = 1.06	$\Delta\rho_{max}$ = 0.49 e Å^{-3}

3254 reflections	$\Delta\rho_{min} = -0.50$ e Å^{-3}
225 parameters	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.040 (6)
Secondary atom site location: difference Fourier map	

Special details

Experimental. Solvent used: petroleum ether Cooling Device: Oxford Cryosystems Cryostream 700 Crystal mount: glued on a glass fibre Mosaicity (°.): 0.421 (1) Frames collected: 637 Seconds exposure per frame: 15 Degrees rotation per frame: 1.0 Crystal-Detector distance (mm): 35.0

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 $F^2 > 2\text{sigma}(F^2)$ 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}	Occ. (<1)
O4	−0.3321 (4)	0.26535 (11)	0.53493 (16)	0.0545 (9)	
O22	0.2807 (3)	0.31977 (9)	0.25411 (13)	0.0342 (7)	
O62	0.4497 (5)	0.40526 (14)	0.6315 (2)	0.0796 (11)	
N1	0.1558 (4)	0.38238 (11)	0.43396 (16)	0.0326 (8)	
C2	−0.0170 (5)	0.34803 (13)	0.37281 (19)	0.0309 (9)	
C3	−0.0465 (5)	0.27982 (13)	0.40998 (19)	0.0318 (9)	
C4	−0.1353 (6)	0.28604 (14)	0.5105 (2)	0.0384 (10)	
C5	0.0277 (6)	0.32360 (15)	0.5754 (2)	0.0437 (10)	
C6	0.0689 (5)	0.38847 (14)	0.53178 (19)	0.0337 (9)	
C21	0.0650 (5)	0.34981 (13)	0.27285 (19)	0.0290 (8)	
C23	0.3166 (5)	0.32621 (14)	0.1585 (2)	0.0348 (9)	
C24	0.1344 (5)	0.35883 (14)	0.11844 (19)	0.0350 (9)	
C25	−0.0293 (5)	0.37395 (14)	0.1926 (2)	0.0359 (10)	
C31	−0.2129 (5)	0.23934 (14)	0.3473 (2)	0.0351 (9)	
C61	0.2441 (5)	0.42625 (17)	0.5899 (2)	0.0410 (12)	
C63	0.5666 (6)	0.45457 (16)	0.6754 (2)	0.0424 (10)	
C64	0.4392 (7)	0.50353 (18)	0.6585 (4)	0.085 (2)	
C65A	0.2486 (2)	0.48141 (5)	0.57868 (8)	0.0265 (17)	0.604 (11)
C311	−0.1902 (2)	0.17066 (5)	0.36974 (8)	0.0291 (8)	
C312	0.0109 (2)	0.13637 (5)	0.33918 (8)	0.0325 (9)	
C313	0.0333 (2)	0.07361 (5)	0.35848 (8)	0.0387 (10)	
C314	−0.1458 (2)	0.04334 (5)	0.40948 (8)	0.0424 (11)	
C315	−0.3433 (2)	0.07662 (5)	0.44198 (8)	0.0419 (11)	
C316	−0.3665 (2)	0.13937 (5)	0.42228 (8)	0.0360 (9)	

C65B	0.2195 (2)	0.49251 (5)	0.62338 (8)	0.0146 (19)	0.396 (11)
H1	0.19817	0.42561	0.40918	0.14 (2)*	
H3	0.12038	0.25992	0.41242	0.043 (8)*	
H5A	−0.04851	0.32791	0.63815	0.042 (8)*	
H2	−0.18116	0.36889	0.37523	0.026 (7)*	
H6	−0.09249	0.41072	0.52994	0.046 (9)*	
H23	0.45350	0.30988	0.12556	0.060 (10)*	
H24	0.11708	0.36973	0.05344	0.041 (9)*	
H25	−0.17804	0.39655	0.18610	0.055 (10)*	
H31A	−0.17119	0.24592	0.28005	0.044 (9)*	
H31B	−0.38559	0.25222	0.35555	0.038 (8)*	
H63	0.71196	0.45263	0.71091	0.0511*	
H64	0.45432	0.54271	0.68633	0.1024*	
H65A	0.16234	0.50540	0.53437	0.29 (9)*	0.604 (11)
H312	0.13517	0.15671	0.30425	0.044 (9)*	
H313	0.17167	0.05110	0.33673	0.049 (9)*	
H314	−0.13247	−0.00008	0.42201	0.050 (10)*	
H315	−0.46468	0.05620	0.47832	0.053 (10)*	
H316	−0.50465	0.16163	0.44485	0.045 (9)*	
H5B	0.18809	0.30210	0.58442	0.054 (10)*	
H65B	0.08362	0.51877	0.61995	0.019 (16)*	0.396 (11)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O4	0.0649 (16)	0.0520 (14)	0.0476 (15)	−0.0018 (12)	0.0306 (12)	0.0033 (11)
O22	0.0327 (11)	0.0453 (12)	0.0247 (11)	0.0100 (9)	0.0041 (8)	0.0015 (9)
O62	0.0713 (19)	0.0724 (19)	0.094 (2)	0.0224 (15)	−0.0269 (16)	−0.0344 (16)
N1	0.0429 (14)	0.0321 (13)	0.0230 (12)	0.0010 (10)	0.0083 (10)	0.0038 (10)
C2	0.0322 (15)	0.0348 (16)	0.0259 (15)	0.0072 (12)	0.0064 (12)	0.0055 (12)
C3	0.0361 (15)	0.0335 (15)	0.0261 (15)	0.0085 (12)	0.0056 (12)	0.0072 (12)
C4	0.0517 (19)	0.0335 (16)	0.0305 (17)	0.0105 (14)	0.0155 (14)	0.0087 (13)
C5	0.065 (2)	0.0458 (19)	0.0206 (15)	0.0083 (16)	0.0096 (14)	0.0061 (13)
C6	0.0369 (16)	0.0420 (17)	0.0225 (15)	0.0067 (13)	0.0059 (12)	0.0040 (12)
C21	0.0281 (14)	0.0330 (15)	0.0262 (15)	0.0054 (11)	0.0072 (11)	0.0040 (12)
C23	0.0375 (16)	0.0439 (18)	0.0234 (15)	−0.0011 (13)	0.0088 (12)	−0.0045 (12)
C24	0.0419 (17)	0.0415 (17)	0.0217 (15)	−0.0032 (13)	0.0028 (12)	0.0023 (12)
C25	0.0341 (16)	0.0457 (18)	0.0279 (16)	0.0047 (13)	0.0027 (12)	0.0073 (13)
C31	0.0354 (16)	0.0421 (17)	0.0279 (15)	0.0070 (13)	0.0026 (12)	0.0111 (13)
C61	0.0250 (15)	0.076 (3)	0.0220 (15)	0.0042 (15)	0.0013 (12)	0.0074 (15)
C63	0.0353 (16)	0.056 (2)	0.0358 (18)	−0.0001 (15)	−0.0048 (13)	−0.0097 (15)
C64	0.047 (2)	0.036 (2)	0.173 (6)	−0.0051 (17)	0.005 (3)	0.004 (3)
C65A	0.029 (3)	0.014 (3)	0.036 (3)	0.0025 (18)	−0.011 (2)	−0.003 (2)
C311	0.0268 (14)	0.0384 (16)	0.0221 (14)	0.0012 (11)	−0.0026 (11)	0.0024 (12)
C312	0.0315 (15)	0.0425 (17)	0.0233 (14)	−0.0001 (12)	−0.0019 (12)	−0.0007 (12)
C313	0.0393 (17)	0.0424 (18)	0.0339 (17)	0.0089 (14)	−0.0119 (13)	−0.0063 (13)
C314	0.052 (2)	0.0369 (18)	0.0376 (18)	−0.0052 (14)	−0.0155 (15)	0.0016 (13)
C315	0.0428 (18)	0.0457 (19)	0.0371 (18)	−0.0079 (14)	−0.0024 (14)	0.0074 (14)

C316	0.0304 (15)	0.0434 (18)	0.0341 (16)	−0.0007 (13)	0.0004 (12)	0.0033 (13)
C65B	0.015 (3)	0.011 (3)	0.018 (4)	−0.001 (2)	0.007 (3)	−0.002 (2)

Geometric parameters (Å, °)

O4—C4	1.215 (4)	C3—H3	1.0000
O22—C21	1.369 (3)	C5—H5A	0.9900
O22—C23	1.373 (4)	C5—H5B	0.9900
O62—C61	1.333 (4)	C6—H6	1.0000
O62—C63	1.375 (5)	C23—H23	0.9500
N1—C2	1.464 (4)	C24—H24	0.9500
N1—C6	1.473 (4)	C25—H25	0.9500
N1—H1	1.0200	C31—H31B	0.9900
C2—C21	1.487 (4)	C31—H31A	0.9900
C2—C3	1.563 (4)	C63—H63	0.9300
C3—C4	1.512 (4)	C64—H64	0.9300
C3—C31	1.525 (4)	C65A—H65A	0.9300
C4—C5	1.498 (5)	C65B—H65B	0.9300
C5—C6	1.539 (5)	C311—C312	1.393 (2)
C6—C61	1.486 (4)	C311—C316	1.395 (2)
C21—C25	1.339 (4)	C312—C313	1.378 (2)
C23—C24	1.331 (4)	C313—C314	1.384 (2)
C24—C25	1.424 (4)	C314—C315	1.376 (2)
C31—C311	1.511 (3)	C315—C316	1.379 (2)
C61—C65A	1.193 (4)	C312—H312	0.9500
C61—C65B	1.504 (4)	C313—H313	0.9500
C63—C64	1.278 (5)	C314—H314	0.9500
C64—C65A	1.590 (5)	C315—H315	0.9500
C64—C65B	1.308 (4)	C316—H316	0.9500
C2—H2	1.0000		
O4···C311	3.196 (4)	H1···H65A^{iv}	2.5900
O4···C316	3.137 (4)	H1···C64^{viii}	2.6800
O4···C23^{i}	3.266 (5)	H1···C65B^{iv}	2.9000
O22···N1	2.960 (4)	H2···H6	2.4000
O62···N1	3.226 (5)	H2···H64^{iv}	2.5500
O4···H5B^{ii}	2.8300	H2···C65B^{iv}	2.9800
O4···H23^{i}	2.3800	H2···H65B^{iv}	2.4700
O4···H316	2.7200	H3···C312	2.9000
O4···H31B	2.5600	H3···O22	2.7300
O22···H3	2.7300	H5A···H312^{x}	2.5500
O22···H31B^{iii}	2.7100	H5A···C312^{x}	2.9500
O62···H5B	2.7100	H5B···O4^{iii}	2.8300
O62···H6^{iii}	2.9000	H5B···O62	2.7100
N1···O22	2.960 (4)	H5B···C23^{x}	3.0200
N1···O62	3.226 (5)	H6···C65A^{iv}	2.8900
N1···H65B^{iv}	2.5900	H6···H65A^{iv}	2.0500

C2···C65B^{iv}	3.592 (4)	H6···H65A	2.4600
C23···O4^{v}	3.266 (5)	H6···O62^{ii}	2.9000
C65A···C65A^{iv}	3.560 (4)	H6···C63^{ii}	2.9500
C65B···C2^{iv}	3.592 (4)	H6···H2	2.4000
C2···H65B^{iv}	2.8800	H6···C65B^{iv}	3.0700
C6···H65B^{iv}	3.0300	H23···O4^{v}	2.3800
C6···H65A^{iv}	2.7500	H24···C313^{vi}	3.0300
C21···H31A	2.5700	H24···C314^{vi}	3.0900
C23···H5B^{vi}	3.0200	H24···C312^{vi}	3.0700
C24···H314^{vii}	3.0800	H31A···H312	2.5600
C63···H6^{iii}	2.9500	H31A···C21	2.5700
C64···H1^{viii}	2.6800	H31B···O4	2.5600
C65A···H6^{iv}	2.8900	H31B···O22^{ii}	2.7100
C65A···H65A^{iv}	2.7400	H31B···H316	2.4100
C65A···H1	2.6800	H63···C312^{xii}	3.0800
C65B···H1^{iv}	2.9000	H63···C313^{xii}	2.7500
C65B···H2^{iv}	2.9800	H63···C314^{xii}	2.8900
C65B···H6^{iv}	3.0700	H64···H2^{iv}	2.5500
C311···O4	3.196 (4)	H64···H1^{viii}	2.4400
C312···C316^{iii}	3.566 (4)	H65A···H1	2.4700
C313···C315^{iii}	3.572 (4)	H65A···H6^{iv}	2.0500
C314···C314^{ix}	3.514 (4)	H65A···H65A^{iv}	2.0100
C315···C313^{ii}	3.572 (4)	H65A···C6^{iv}	2.7500
C316···C312^{ii}	3.566 (4)	H65A···C65A^{iv}	2.7400
C316···O4	3.137 (4)	H65A···H6	2.4600
C312···H5A^{vi}	2.9500	H65A···H1^{iv}	2.5900
C312···H24^{x}	3.0700	H65B···C6^{iv}	3.0300
C312···H316^{iii}	3.0500	H65B···H1^{iv}	1.9800
C312···H3	2.9000	H65B···N1^{iv}	2.5900
C312···H63^{xi}	3.0800	H65B···C2^{iv}	2.8800
C313···H63^{xi}	2.7500	H65B···H2^{iv}	2.4700
C313···H24^{x}	3.0300	H312···H31A	2.5600
C314···H63^{xi}	2.8900	H312···H5A^{vi}	2.5500
C314···H314^{ix}	2.9500	H313···C315^{iii}	3.0500
C314···H24^{x}	3.0900	H314···C314^{ix}	2.9500
C315···H313^{ii}	3.0500	H314···C24^{xiii}	3.0800
H1···C65A	2.6800	H315···H315^{xiv}	2.5200
H1···H65A	2.4700	H316···H31B	2.4100
H1···H65B^{iv}	1.9800	H316···O4	2.7200
H1···H64^{viii}	2.4400	H316···C312^{ii}	3.0500
C21—O22—C23	106.3 (2)	C6—C5—H5B	110.00

C61—O62—C63	108.5 (3)	H5A—C5—H5B	108.00
C2—N1—C6	112.5 (2)	N1—C6—H6	108.00
C2—N1—H1	114.00	C5—C6—H6	108.00
C6—N1—H1	109.00	C61—C6—H6	108.00
C3—C2—C21	112.1 (2)	O22—C23—H23	125.00
N1—C2—C3	110.0 (2)	C24—C23—H23	125.00
N1—C2—C21	110.2 (2)	C25—C24—H24	127.00
C2—C3—C4	105.6 (2)	C23—C24—H24	127.00
C2—C3—C31	113.7 (2)	C24—C25—H25	126.00
C4—C3—C31	113.4 (2)	C21—C25—H25	126.00
O4—C4—C3	122.2 (3)	C3—C31—H31B	109.00
C3—C4—C5	115.1 (3)	C311—C31—H31A	109.00
O4—C4—C5	122.6 (3)	C311—C31—H31B	109.00
C4—C5—C6	109.3 (2)	H31A—C31—H31B	108.00
N1—C6—C61	110.6 (2)	C3—C31—H31A	109.00
C5—C6—C61	111.6 (2)	C64—C63—H63	126.00
N1—C6—C5	110.3 (2)	O62—C63—H63	126.00
C2—C21—C25	134.0 (3)	C63—C64—H64	128.00
O22—C21—C2	116.4 (2)	C65A—C64—H64	128.00
O22—C21—C25	109.6 (2)	C65B—C64—H64	113.00
O22—C23—C24	110.6 (2)	C61—C65A—H65A	129.00
C23—C24—C25	106.2 (2)	C64—C65A—H65A	129.00
C21—C25—C24	107.3 (2)	C61—C65B—H65B	129.00
C3—C31—C311	112.8 (2)	C64—C65B—H65B	129.00
O62—C61—C65B	105.0 (2)	C31—C311—C316	121.71 (14)
O62—C61—C6	125.8 (3)	C31—C311—C312	120.74 (14)
O62—C61—C65A	112.0 (3)	C312—C311—C316	117.55 (10)
C6—C61—C65B	128.9 (2)	C311—C312—C313	121.42 (10)
C6—C61—C65A	118.8 (3)	C312—C313—C314	120.01 (10)
O62—C63—C64	107.6 (3)	C313—C314—C315	119.49 (10)
C63—C64—C65B	114.3 (3)	C314—C315—C316	120.53 (10)
C63—C64—C65A	103.4 (3)	C311—C316—C315	120.99 (10)
C61—C65A—C64	102.5 (2)	C311—C312—H312	119.00
C61—C65B—C64	101.8 (2)	C313—C312—H312	119.00
C21—C2—H2	108.00	C312—C313—H313	120.00
N1—C2—H2	109.00	C314—C313—H313	120.00
C3—C2—H2	108.00	C315—C314—H314	120.00
C4—C3—H3	108.00	C313—C314—H314	120.00
C2—C3—H3	108.00	C314—C315—H315	120.00
C31—C3—H3	108.00	C316—C315—H315	120.00
C4—C5—H5A	110.00	C315—C316—H316	119.00
C4—C5—H5B	110.00	C311—C316—H316	120.00
C6—C5—H5A	110.00		
C23—O22—C21—C2	178.7 (2)	C31—C3—C4—C5	177.9 (2)
C23—O22—C21—C25	−0.1 (3)	C2—C3—C31—C311	165.7 (2)
C21—O22—C23—C24	0.3 (3)	C4—C3—C31—C311	−73.6 (3)
C63—O62—C61—C6	177.6 (3)	O4—C4—C5—C6	−120.3 (3)
C63—O62—C61—C65A	19.2 (3)	C3—C4—C5—C6	55.3 (3)
C61—O62—C63—C64	−1.7 (4)	C4—C5—C6—N1	−52.6 (3)

C6—N1—C2—C3	−62.6 (3)	C4—C5—C6—C61	−175.9 (2)
C6—N1—C2—C21	173.3 (2)	N1—C6—C61—O62	−82.1 (4)
C2—N1—C6—C5	58.8 (3)	N1—C6—C61—C65A	74.9 (3)
C2—N1—C6—C61	−177.2 (2)	C5—C6—C61—O62	41.0 (4)
N1—C2—C3—C4	58.3 (3)	C5—C6—C61—C65A	−161.9 (2)
N1—C2—C3—C31	−176.8 (2)	O22—C21—C25—C24	−0.2 (3)
C21—C2—C3—C4	−178.7 (2)	C2—C21—C25—C24	−178.6 (3)
C21—C2—C3—C31	−53.8 (3)	O22—C23—C24—C25	−0.4 (3)
N1—C2—C21—O22	65.6 (3)	C23—C24—C25—C21	0.3 (3)
N1—C2—C21—C25	−116.1 (4)	C3—C31—C311—C312	−76.9 (2)
C3—C2—C21—O22	−57.3 (3)	C3—C31—C311—C316	102.4 (2)
C3—C2—C21—C25	121.1 (3)	O62—C61—C65A—C64	−24.5 (3)
C2—C3—C4—O4	118.6 (3)	C6—C61—C65A—C64	175.5 (3)
C2—C3—C4—C5	−57.0 (3)	O62—C63—C64—C65A	−11.4 (4)
C31—C3—C4—O4	−6.5 (4)	C63—C64—C65A—C61	22.7 (4)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C23—H23···O4^{v}	0.95	2.38	3.266 (5)	155

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

Fig. 1

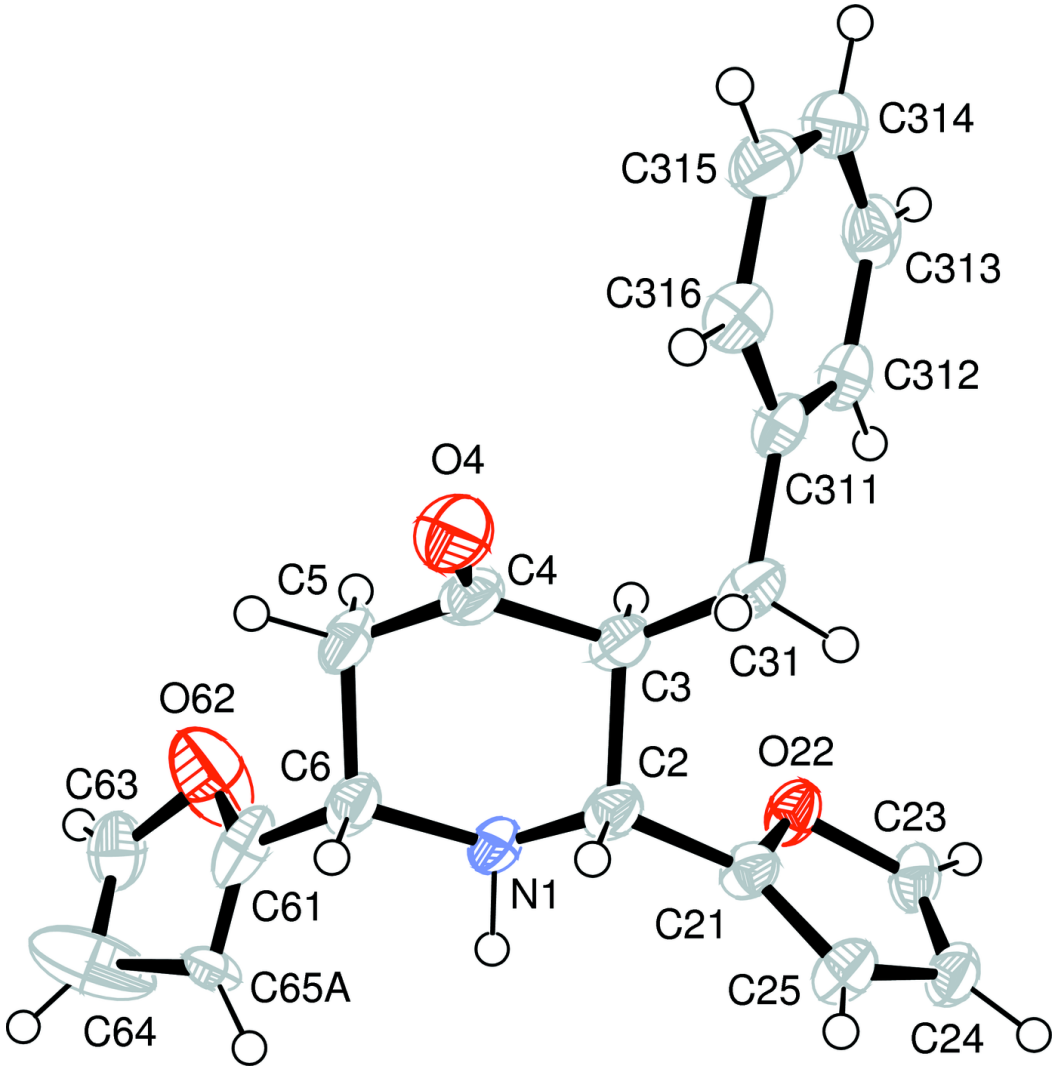
C314
C315
C313
C316
C312
C311
O4
C4
C5
C31
C3
O62
C6
C2
O22
C63
C23
C61
N1
C21
C65A
C25
C64
C24

Fig. 2