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N-Benzoyl-*r*-2,*c*-6-di-2-furyl-*t*-3-methylpiperidin-4-one

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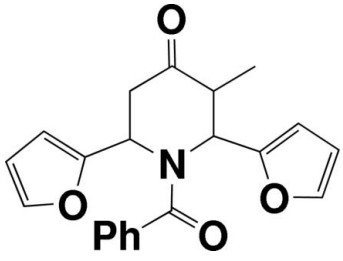
Key indicators: single-crystal X-ray study; T = 160 K; mean σ(C–C) = 0.003 Å; R factor = 0.056; wR factor = 0.156; data-to-parameter ratio = 17.1.

In the title molecule, $C_{21}H_{19}NO_4$, the piperidine ring adopts a chair conformation. The benzoyl group has a bisectional orientation. The planar furyl rings and the methyl group each have an axial orientation. The structure is stabilized by inter- and intramolecular C—H···O hydrogen bonds.

Related literature

For related literature, see: Balamurugan *et al.* (2006, 2007); Kumar & Pillay (1993).



Experimental

Crystal data

$C_{21}H_{19}NO_4$
M_r = 349.37
Monoclinic, $C2/c$
a = 20.5162 (5) Å
b = 8.9727 (3) Å
c = 19.0466 (6) Å
β = 91.395 (2)°
V = 3505.17 (18) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 160 (1) K
0.30 × 0.20 × 0.15 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Absorption correction: none
37792 measured reflections
4025 independent reflections
2961 reflections with $I > 2\sigma(I)$
R_{int} = 0.076

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.156
S = 1.06
4025 reflections
235 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O11	0.98	2.25	2.730 (2)	109
C5—H5B···O11^{i}	0.97	2.58	3.508 (2)	161
C24—H24···O4^{ii}	0.93	2.52	3.452 (3)	176
C116—H116···O62	0.93	2.55	3.305 (2)	139

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

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 Zurich; his help is gratefully acknowledged by AT.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2288).

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supplementary materials

Acta Cryst. (2007). E**63**, o2909 [**doi:10.1107/S1600536807022398**]

N-Benzoyl-*r*-2,*c*-6-di-2-furyl-*t*-3-methylpiperidin-4-one

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Comment

The title compound, (I), has been analysed as part of our crystallographic studies on substitued piperidines (Balamurugan *et al.*, 2006; 2007). The present X-ray diffraction study was undertaken to determine how the conformation of the system is affected by the substitution of a benzoyl group at the first position (N), furyl rings at 2 and 6 and a methyl group at 3 of the piperidin-4-one.

In the title molecule, (I), the piperidine ring adopts a chair conformation. The furyl rings at positons 2,6, and the methyl group at position 3 have an axial orientation. The benzoyl group at N has a bisectional orientation. The dihedral angle between the two planar furyl rings is 25.6 (1)°. The phenyl ring makes dihedral angles of 55.2 (1)° and 63.6 (1)° between the furyl ring at 2 and 6 respectively. In the solid state, the molecules are linked by inter- and intramolecular C–H···O hydrogen bonds.

Experimental

The title compound was prepared by following the general procedure reported by Kumar & Pillay (1993). A mixture of t(3)-methyl-r(2),c(6)-(2'-furyl)piperidin-4-one (2.45 g, 0.01 mol) benzoylchoride (1.16 ml, 0.01 mol) and triethylamine (3 ml, 0.03 mol) in benzene were refluxed for 8–10 h. The precipitated ammonium salt was filtered off and the solvent was washed with dilute HCl (2 N) followed by water and then removed at low pressure. The solid mass filtered off, dried and recrystallized from petroleum-ether (333–353 K). The yield of the isolated product was 2.44 g (70%).

Refinement

All the H atoms were positioned geometrically and allowed to ride on their parent atoms with C—H = 0.93–0.98 Å and U_{iso}(H) = 1.2–1.5U_{eq}(parent atom).

Figures

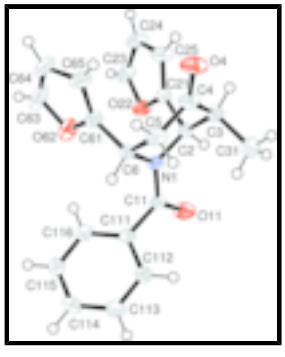
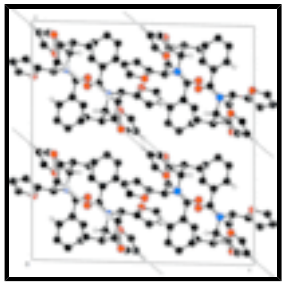


Figure 1 View of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.



_N_-Benzoyl-r-2,c-6-di-2-furyl-t-3-methylpiperidin-4-one

Crystal data

$C_{21}H_{19}NO_4$	F_{000} = 1472
M_r = 349.37	D_x = 1.324 Mg m^{-3}
Monoclinic, *C*2/*c*	Melting point: 427 K
Hall symbol: -C 2yc	Mo *K*α radiation λ = 0.71073 Å
a = 20.5162 (5) Å	Cell parameters from 4257 reflections
b = 8.9727 (3) Å	θ = 2.0–27.5º
c = 19.0466 (6) Å	μ = 0.09 mm^{-1}
β = 91.395 (2)º	*T* = 160 (1) K
V = 3505.17 (18) Å^3	Tiny_blocks, colourless
Z = 8	0.30 × 0.20 × 0.15 mm

Data collection

Nonius KappaCCD area-detector diffractometer	4025 independent reflections
Radiation source: Nonius FR590 sealed tube generator	2961 reflections with $I > 2\sigma(I)$
Monochromator: horizontally mounted graphite crystal	R_{int} = 0.076
Detector resolution: 9 pixels mm^{-1}	θ_{max} = 27.5º
T = 160(1) K	θ_{min} = 2.1º
φ and ω scans with κ offsets	*h* = −26→26
Absorption correction: none	*k* = −11→11
37792 measured reflections	*l* = −24→24

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.056	H-atom parameters constrained
$wR(F^2)$ = 0.156	$w = 1/[\sigma^2(F_o^2) + (0.0737P)^2 + 3.1099P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.06	$(\Delta/\sigma)_{max} < 0.001$

4025 reflections	$\Delta\rho_{max} = 0.25$ e Å^{-3}
235 parameters	$\Delta\rho_{min} = -0.24$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. Solvent used: Mixture of Petroleum-ether Cooling Device: Oxford Cryosystems Cryostream 700 Crystal mount: glued on a glass fibre Mosaicity (°.): 0.995 (2) Frames collected: 456 Seconds exposure per frame: 41 Degrees rotation per frame: 1.3 Crystal-Detector distance (mm): 30.0

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}
O4	0.44450 (7)	0.31744 (17)	0.09889 (9)	0.0463 (5)
O11	0.26740 (7)	−0.08170 (18)	0.25095 (7)	0.0433 (5)
O22	0.36694 (6)	−0.23026 (15)	0.10441 (7)	0.0319 (4)
O62	0.26918 (7)	−0.03856 (17)	0.00725 (7)	0.0408 (5)
N1	0.30183 (7)	0.03966 (16)	0.15425 (7)	0.0218 (4)
C2	0.37023 (8)	−0.0006 (2)	0.17102 (9)	0.0236 (5)
C3	0.41222 (9)	0.1392 (2)	0.18472 (10)	0.0307 (6)
C4	0.40042 (9)	0.2555 (2)	0.12821 (11)	0.0315 (6)
C5	0.32971 (9)	0.2907 (2)	0.11244 (11)	0.0321 (6)
C6	0.28968 (8)	0.1487 (2)	0.09787 (9)	0.0245 (5)
C11	0.25465 (8)	−0.0072 (2)	0.19834 (9)	0.0260 (5)
C21	0.39848 (8)	−0.09842 (19)	0.11577 (9)	0.0232 (5)
C23	0.40031 (10)	−0.3035 (2)	0.05332 (10)	0.0347 (6)
C24	0.45082 (10)	−0.2228 (2)	0.03307 (11)	0.0367 (6)
C25	0.44997 (10)	−0.0897 (2)	0.07390 (11)	0.0363 (6)
C31	0.39855 (11)	0.2062 (3)	0.25692 (12)	0.0440 (7)
C61	0.30274 (9)	0.0875 (2)	0.02632 (9)	0.0292 (6)
C63	0.28507 (13)	−0.0700 (3)	−0.06067 (11)	0.0532 (9)
C64	0.32643 (12)	0.0321 (3)	−0.08387 (11)	0.0551 (9)
C65	0.33858 (11)	0.1355 (3)	−0.02753 (11)	0.0422 (7)
C111	0.18492 (8)	0.0335 (2)	0.18188 (9)	0.0250 (5)
C112	0.15183 (9)	0.1149 (2)	0.23184 (10)	0.0315 (6)
C113	0.08644 (9)	0.1474 (3)	0.22100 (11)	0.0376 (7)
C114	0.05335 (9)	0.0957 (3)	0.16204 (11)	0.0391 (7)
C115	0.08574 (9)	0.0133 (3)	0.11304 (11)	0.0386 (7)
C116	0.15167 (9)	−0.0167 (2)	0.12244 (10)	0.0328 (6)

H2	0.37034	−0.05811	0.21475	0.0283*
H3	0.45821	0.10989	0.18408	0.0368*
H5A	0.32655	0.35584	0.07184	0.0385*
H5B	0.31167	0.34319	0.15204	0.0385*
H6	0.24347	0.17604	0.09874	0.0294*
H23	0.38914	−0.39661	0.03533	0.0416*
H24	0.48070	−0.24809	−0.00089	0.0440*
H25	0.47959	−0.01144	0.07188	0.0435*
H31A	0.40609	0.13207	0.29256	0.0660*
H31B	0.35402	0.23878	0.25798	0.0660*
H31C	0.42698	0.28954	0.26544	0.0660*
H63	0.26932	−0.15067	−0.08665	0.0639*
H64	0.34415	0.03583	−0.12831	0.0661*
H65	0.36565	0.21860	−0.02810	0.0506*
H112	0.17357	0.14731	0.27244	0.0377*
H113	0.06465	0.20459	0.25371	0.0450*
H114	0.00922	0.11643	0.15544	0.0469*
H115	0.06337	−0.02233	0.07345	0.0463*
H116	0.17359	−0.07083	0.08869	0.0394*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O4	0.0396 (8)	0.0398 (9)	0.0606 (10)	−0.0118 (7)	0.0212 (7)	−0.0038 (7)
O11	0.0345 (8)	0.0630 (10)	0.0327 (8)	0.0069 (7)	0.0083 (6)	0.0233 (7)
O22	0.0355 (7)	0.0296 (7)	0.0311 (7)	−0.0072 (6)	0.0087 (6)	−0.0048 (5)
O62	0.0544 (9)	0.0388 (8)	0.0291 (8)	0.0037 (7)	−0.0012 (6)	−0.0043 (6)
N1	0.0218 (7)	0.0230 (8)	0.0206 (7)	0.0012 (6)	0.0033 (5)	0.0028 (6)
C2	0.0215 (8)	0.0275 (9)	0.0219 (9)	0.0002 (7)	0.0015 (7)	0.0004 (7)
C3	0.0248 (9)	0.0326 (11)	0.0347 (10)	−0.0013 (8)	0.0008 (8)	−0.0085 (8)
C4	0.0309 (10)	0.0242 (10)	0.0399 (11)	−0.0056 (8)	0.0120 (8)	−0.0107 (8)
C5	0.0363 (10)	0.0228 (10)	0.0376 (11)	0.0012 (8)	0.0115 (8)	0.0021 (8)
C6	0.0245 (8)	0.0260 (9)	0.0231 (9)	0.0028 (7)	0.0042 (7)	0.0054 (7)
C11	0.0271 (9)	0.0293 (10)	0.0219 (9)	−0.0009 (7)	0.0045 (7)	0.0023 (7)
C21	0.0233 (8)	0.0209 (9)	0.0255 (9)	0.0012 (7)	0.0002 (7)	0.0009 (7)
C23	0.0458 (12)	0.0277 (10)	0.0308 (10)	0.0018 (9)	0.0050 (9)	−0.0080 (8)
C24	0.0396 (11)	0.0325 (11)	0.0386 (11)	0.0072 (9)	0.0154 (9)	−0.0035 (9)
C25	0.0341 (10)	0.0264 (10)	0.0491 (12)	−0.0026 (8)	0.0173 (9)	−0.0025 (9)
C31	0.0426 (12)	0.0492 (13)	0.0402 (12)	−0.0045 (10)	−0.0004 (9)	−0.0159 (10)
C61	0.0313 (10)	0.0318 (10)	0.0245 (9)	0.0081 (8)	0.0040 (7)	0.0056 (7)
C63	0.0726 (17)	0.0608 (16)	0.0260 (11)	0.0274 (14)	−0.0054 (11)	−0.0113 (11)
C64	0.0580 (15)	0.086 (2)	0.0217 (11)	0.0368 (14)	0.0086 (10)	0.0035 (12)
C65	0.0410 (11)	0.0548 (14)	0.0312 (11)	0.0118 (10)	0.0122 (9)	0.0132 (10)
C111	0.0239 (9)	0.0273 (9)	0.0241 (9)	−0.0032 (7)	0.0050 (7)	0.0029 (7)
C112	0.0260 (9)	0.0361 (11)	0.0324 (10)	−0.0051 (8)	0.0040 (8)	−0.0076 (8)
C113	0.0273 (10)	0.0419 (12)	0.0438 (12)	−0.0024 (8)	0.0082 (8)	−0.0115 (10)
C114	0.0228 (9)	0.0523 (13)	0.0424 (12)	−0.0009 (9)	0.0032 (8)	−0.0035 (10)
C115	0.0309 (10)	0.0545 (14)	0.0303 (11)	−0.0062 (9)	−0.0022 (8)	−0.0063 (9)

C116	0.0315 (10)	0.0404 (11)	0.0268 (10)	−0.0010 (8)	0.0059 (8)	−0.0043 (8)

Geometric parameters (Å, °)

O4—C4	1.210 (2)	C3—H3	0.9800
O11—C11	1.227 (2)	C5—H5A	0.9700
O22—C21	1.363 (2)	C5—H5B	0.9700
O22—C23	1.371 (2)	C6—H6	0.9800
O62—C61	1.369 (2)	C111—C112	1.390 (3)
O62—C63	1.371 (3)	C111—C116	1.383 (3)
N1—C2	1.477 (2)	C112—C113	1.384 (3)
N1—C6	1.470 (2)	C113—C114	1.378 (3)
N1—C11	1.363 (2)	C114—C115	1.375 (3)
C2—C3	1.540 (3)	C115—C116	1.387 (3)
C2—C21	1.498 (2)	C23—H23	0.9300
C3—C4	1.514 (3)	C24—H24	0.9300
C3—C31	1.533 (3)	C25—H25	0.9300
C4—C5	1.508 (3)	C31—H31A	0.9600
C5—C6	1.538 (3)	C31—H31B	0.9600
C6—C61	1.499 (2)	C31—H31C	0.9600
C11—C111	1.502 (2)	C63—H63	0.9300
C21—C25	1.341 (3)	C64—H64	0.9300
C23—C24	1.329 (3)	C65—H65	0.9300
C24—C25	1.426 (3)	C112—H112	0.9300
C61—C65	1.347 (3)	C113—H113	0.9300
C63—C64	1.332 (4)	C114—H114	0.9300
C64—C65	1.436 (3)	C115—H115	0.9300
C2—H2	0.9800	C116—H116	0.9300
O4···C115^{i}	3.394 (3)	C65···H6^{v}	2.7200
O11···C112^{ii}	3.200 (2)	C111···H31B^{ii}	3.0000
O11···C64^{iii}	3.373 (3)	C111···H6	2.3800
O22···O62	3.1977 (19)	C113···H2^{vii}	3.0400
O22···N1	2.9348 (19)	C114···H31C^{ii}	3.1000
O62···C116	3.305 (2)	C114···H113^{xii}	3.1000
O62···O22	3.1977 (19)	C115···H65^{v}	3.0800
O62···C21	3.366 (2)	C115···H23^{xi}	3.0700
O62···N1	2.9477 (19)	C115···H31C^{ii}	3.0800
O4···H115^{i}	2.8800	C116···H6	2.6000
O4···H24^{iv}	2.5200	H2···O11	2.2500
O11···H2	2.2500	H2···H31A	2.3700
O11···H5B^{ii}	2.5800	H2···C113^{ii}	3.0400
O11···H64^{iii}	2.7900	H2···H113^{ii}	2.5800
O11···H112	2.8500	H3···C25	2.7600
O11···H112^{ii}	2.7600	H3···H25	2.4500
O22···H112^{ii}	2.7400	H5A···C65	2.7500
O62···H116	2.5500	H5A···H65	2.4200

N1···O22	2.9348 (19)	H5A···C63^{v}	2.9900
N1···O62	2.9477 (19)	H5B···C31	2.9200
N1···H31B	2.8500	H5B···H31B	2.3700
C4···C25	3.428 (3)	H5B···O11^{vii}	2.5800
C4···C65	3.374 (3)	H6···C111	2.3800
C5···C63^{v}	3.562 (3)	H6···C116	2.6000
C6···C116	3.241 (2)	H6···C64^{v}	3.0000
C6···C65^{v}	3.507 (3)	H6···C65^{v}	2.7200
C21···C61	3.063 (2)	H23···C115^{xi}	3.0700
C21···O62	3.366 (2)	H23···H115^{xi}	2.4200
C24···C114^{vi}	3.586 (3)	H24···O4^{iv}	2.5200
C25···C65	3.581 (3)	H25···C3	2.9200
C25···C4	3.428 (3)	H25···H3	2.4500
C25···C61	3.513 (3)	H31A···H2	2.3700
C31···C116^{vii}	3.555 (3)	H31A···H64^{iii}	2.5000
C61···C21	3.063 (2)	H31B···N1	2.8500
C61···C25	3.513 (3)	H31B···C5	2.8400
C63···C5^{v}	3.562 (3)	H31B···H5B	2.3700
C64···O11^{viii}	3.373 (3)	H31B···C111^{vii}	3.0000
C65···C4	3.374 (3)	H31C···C114^{vii}	3.1000
C65···C6^{v}	3.507 (3)	H31C···C115^{vii}	3.0800
C65···C25	3.581 (3)	H64···O11^{viii}	2.7900
C3···H25	2.9200	H64···H31A^{viii}	2.5000
C4···H65	3.0600	H65···C4	3.0600
C5···H31B	2.8400	H65···C5	2.8700
C5···H65	2.8700	H65···H5A	2.4200
C6···H116	3.0900	H65···C115^{v}	3.0800
C112···O11^{vii}	3.200 (2)	H112···O11	2.8500
C114···C24^{ix}	3.586 (3)	H112···O11^{vii}	2.7600
C115···O4^{x}	3.394 (3)	H112···O22^{vii}	2.7400
C116···O62	3.305 (2)	H113···C114^{xii}	3.1000
C116···C6	3.241 (2)	H113···H114^{xii}	2.4600
C116···C31^{ii}	3.555 (3)	H113···H2^{vii}	2.5800
C23···H115^{xi}	2.9900	H114···H113^{xii}	2.4600
C23···H114^{vi}	3.0100	H114···C23^{ix}	3.0100
C24···H115^{xi}	3.0700	H114···C24^{ix}	2.9700
C24···H114^{vi}	2.9700	H115···O4^{x}	2.8800
C25···H3	2.7600	H115···C23^{xi}	2.9900
C31···H5B	2.9200	H115···C24^{xi}	3.0700
C63···H5A^{v}	2.9900	H115···H23^{xi}	2.4200
C64···H6^{v}	3.0000	H116···O62	2.5500
C65···H5A	2.7500	H116···C6	3.0900
C21—O22—C23	106.58 (14)	C6—C5—H5B	109.00

C61—O62—C63	106.91 (16)	H5A—C5—H5B	108.00
C2—N1—C6	117.67 (13)	N1—C6—H6	108.00
C2—N1—C11	118.47 (14)	C5—C6—H6	108.00
C6—N1—C11	123.03 (14)	C61—C6—H6	108.00
N1—C2—C3	111.23 (14)	C112—C111—C116	119.49 (16)
N1—C2—C21	111.92 (14)	C11—C111—C112	117.61 (15)
C3—C2—C21	111.83 (14)	C11—C111—C116	122.68 (16)
C2—C3—C4	111.20 (15)	C111—C112—C113	119.78 (18)
C2—C3—C31	110.95 (16)	C112—C113—C114	120.5 (2)
C4—C3—C31	109.74 (16)	C113—C114—C115	119.84 (18)
O4—C4—C3	122.44 (17)	C114—C115—C116	120.20 (19)
O4—C4—C5	122.57 (18)	C111—C116—C115	120.18 (18)
C3—C4—C5	114.98 (16)	O22—C23—H23	125.00
C4—C5—C6	111.69 (15)	C24—C23—H23	125.00
N1—C6—C5	109.85 (14)	C23—C24—H24	127.00
N1—C6—C61	112.92 (14)	C25—C24—H24	127.00
C5—C6—C61	111.17 (15)	C21—C25—H25	126.00
O11—C11—N1	122.04 (16)	C24—C25—H25	126.00
O11—C11—C111	119.06 (15)	C3—C31—H31A	109.00
N1—C11—C111	118.90 (15)	C3—C31—H31B	109.00
O22—C21—C2	115.45 (14)	C3—C31—H31C	109.00
O22—C21—C25	109.51 (15)	H31A—C31—H31B	109.00
C2—C21—C25	135.02 (16)	H31A—C31—H31C	109.00
O22—C23—C24	110.56 (16)	H31B—C31—H31C	110.00
C23—C24—C25	106.15 (18)	O62—C63—H63	125.00
C21—C25—C24	107.20 (17)	C64—C63—H63	125.00
O62—C61—C6	116.36 (15)	C63—C64—H64	126.00
O62—C61—C65	110.03 (17)	C65—C64—H64	126.00
C6—C61—C65	133.46 (18)	C61—C65—H65	127.00
O62—C63—C64	109.9 (2)	C64—C65—H65	127.00
C63—C64—C65	107.3 (2)	C111—C112—H112	120.00
C61—C65—C64	105.9 (2)	C113—C112—H112	120.00
C21—C2—H2	107.00	C112—C113—H113	120.00
N1—C2—H2	107.00	C114—C113—H113	120.00
C3—C2—H2	107.00	C113—C114—H114	120.00
C31—C3—H3	108.00	C115—C114—H114	120.00
C2—C3—H3	108.00	C114—C115—H115	120.00
C4—C3—H3	108.00	C116—C115—H115	120.00
C4—C5—H5B	109.00	C111—C116—H116	120.00
C4—C5—H5A	109.00	C115—C116—H116	120.00
C6—C5—H5A	109.00		
C23—O22—C21—C2	−179.24 (15)	C3—C2—C21—C25	−3.2 (3)
C23—O22—C21—C25	−0.5 (2)	C2—C3—C4—O4	−131.7 (2)
C21—O22—C23—C24	0.2 (2)	C2—C3—C4—C5	49.6 (2)
C63—O62—C61—C6	176.40 (17)	C31—C3—C4—O4	105.2 (2)
C63—O62—C61—C65	0.3 (2)	C31—C3—C4—C5	−73.5 (2)
C61—O62—C63—C64	−0.5 (3)	O4—C4—C5—C6	129.7 (2)
C6—N1—C2—C3	52.52 (19)	C3—C4—C5—C6	−51.6 (2)
C6—N1—C2—C21	−73.38 (19)	C4—C5—C6—N1	50.5 (2)

C11—N1—C2—C3	−117.37 (17)	C4—C5—C6—C61	−75.2 (2)
C11—N1—C2—C21	116.73 (17)	N1—C6—C61—O62	56.6 (2)
C2—N1—C6—C5	−53.57 (19)	N1—C6—C61—C65	−128.4 (2)
C2—N1—C6—C61	71.13 (19)	C5—C6—C61—O62	−179.38 (15)
C11—N1—C6—C5	115.82 (17)	C5—C6—C61—C65	−4.4 (3)
C11—N1—C6—C61	−119.47 (17)	O11—C11—C111—C112	58.9 (2)
C2—N1—C11—O11	−0.3 (3)	O11—C11—C111—C116	−115.8 (2)
C2—N1—C11—C111	179.83 (15)	N1—C11—C111—C112	−121.19 (18)
C6—N1—C11—O11	−169.58 (17)	N1—C11—C111—C116	64.1 (2)
C6—N1—C11—C111	10.5 (2)	O22—C21—C25—C24	0.7 (2)
N1—C2—C3—C4	−47.42 (19)	C2—C21—C25—C24	179.02 (19)
N1—C2—C3—C31	75.02 (19)	O22—C23—C24—C25	0.2 (2)
C21—C2—C3—C4	78.53 (18)	C23—C24—C25—C21	−0.5 (2)
C21—C2—C3—C31	−159.03 (16)	O62—C61—C65—C64	0.0 (3)
N1—C2—C21—O22	−59.31 (19)	C6—C61—C65—C64	−175.2 (2)
N1—C2—C21—C25	122.4 (2)	O62—C63—C64—C65	0.5 (3)
C3—C2—C21—O22	175.12 (14)	C63—C64—C65—C61	−0.3 (3)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O11	0.98	2.25	2.730 (2)	109
C5—H5B···O11^{vii}	0.97	2.58	3.508 (2)	161
C24—H24···O4^{iv}	0.93	2.52	3.452 (3)	176
C116—H116···O62	0.93	2.55	3.305 (2)	139

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

Fig. 1

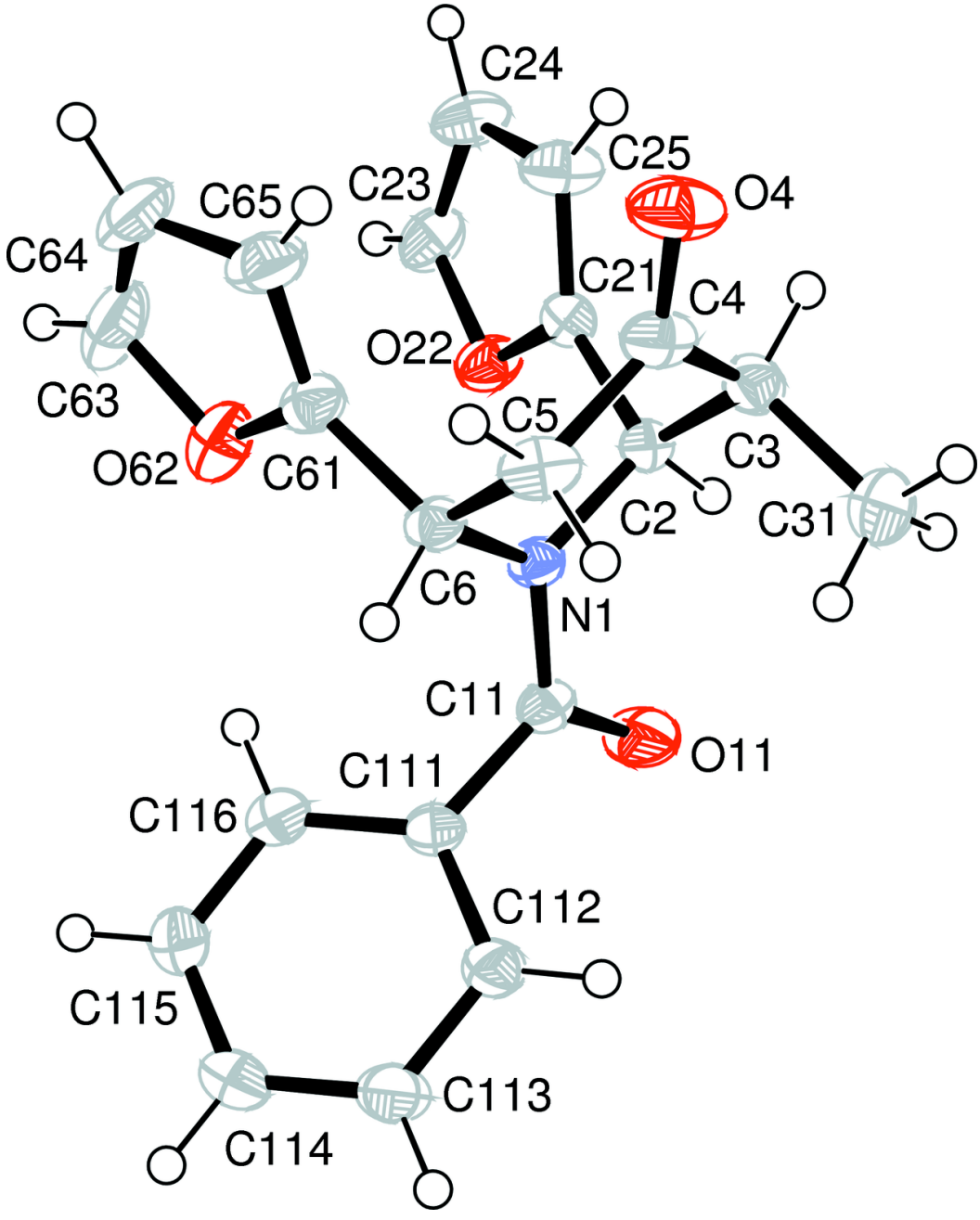

C24
C25
O4
C23
C65
C64
C21
C4
O22
C63
C5
C3
O62
C61
C2
C31
C6
N1
C11
O11
C111
C116
C112
C115
C113
C114

Fig. 2