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9,9-Dimethyl-12-(4-nitrophenyl)-9,10-dihydro-12*H*-benzo[*a*]xanthen-11(8*H*)-one

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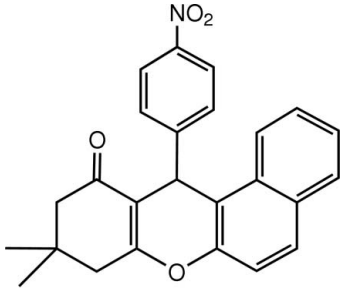
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.003 Å; R factor = 0.055; wR factor = 0.153; data-to-parameter ratio = 14.6.

In the molecular structure of the title compound, $C_{25}H_{21}NO_4$, the pyran ring adopts a flattened boat conformation, while the cyclohexenone ring is in an envelope conformation. The 4-nitrophenyl ring is almost perpendicular to the pyran ring [dihedral angle = 89.39 (1)°]. In the crystal, molecules are connected by intermolecular C—H···O hydrogen bonds.

Related literature

For the biological activity of xanthenes and benzoxanthenes, see: Lambert *et al.* (1997); Poupelin *et al.* (1978); Ion *et al.* (1998); Saint-Ruf *et al.* (1975).



Experimental

Crystal data

$C_{25}H_{21}NO_4$
M_r = 399.43
Monoclinic, $C2/c$
a = 24.178 (5) Å
b = 11.078 (2) Å
c = 17.481 (4) Å
β = 119.78 (3)°
V = 4063.9 (19) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 113 K
0.20 × 0.18 × 0.10 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.983, T_{max} = 0.999
14653 measured reflections
4007 independent reflections
3106 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.153
S = 1.03
4007 reflections
274 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O4^{i}	0.95	2.42	3.323 (3)	159
C6—H6···O2^{ii}	0.95	2.45	3.384 (3)	168
C18—H18*B*···O2^{iii}	0.98	2.43	3.355 (2)	158

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2257).

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supporting information

Acta Cryst. (2009). E**65**, o3141 [doi:10.1107/S1600536809048570]

9,9-Dimethyl-12-(4-nitrophenyl)-9,10-dihydro-12*H*-benzo[*a*]xanthen-11(8*H*)-one

De-Ling Li and Li-Hong Wang

S1. Comment

Xanthenes and benzoxanthenes are biologically important drug intermediates. They are cited as active oxygen heterocycles possessing anti-inflammatory (Poupelin *et al.*, 1978) and antiviral (Lambert *et al.*, 1997) activity. These compounds are also utilized as antagonists for paralyzing action of zoxazolamine (Saint-Ruf *et al.*, 1975) and in photodynamic therapy (Ion *et al.*, 1998). We report herein the crystal structure of the title compound, which belongs to this class of compounds.

The pyran ring of the title molecule (Fig. 1) adopts a flattened boat conformation. The cyclohexenone ring is in an envelope conformation with atom C15 at the flap. The 4-nitrophenyl ring and the planar part of the pyran ring (C1/C10/C12/C17) are nearly perpendicular to each other, with a dihedral angle of 89.39 (1)°. In the crystal, the molecules are connected by C—H···O hydrogen bonds (Fig. 2).

S2. Experimental

To a mixture of 2-naphthol (1.0 mmol), benzaldehyde (1.0 mmol), and 5,5-dimethylcyclohexane-1,3-dione (1.1 mmol) was added strontium trifluoromethanesulfonate (0.1 mmol) in 1,2-dichloroethane (2 ml). The mixture was stirred at 353 K for 5 h. The progress of the reaction was monitored by TLC. After completion of the reaction, water was added and the product was extracted with ethyl acetate (3×10 ml). The organic layer was dried ($MgSO_4$) and evaporated, and the crude product was purified by flash chromatography on silica gel. Pure product crystallized slowly at room temperature in ethanol. A single-crystal was obtained by slow evaporation of a solution in ethanol.

S3. Refinement

H atoms were included in the refinement in the riding and rotation model approximation, with C—H = 0.95–1.00 Å and U_{iso} (H) = 1.2 U_{eq}(Carrier atom). For the methyl H atoms, U_{iso}(H) = 1.5U_{eq}(C).

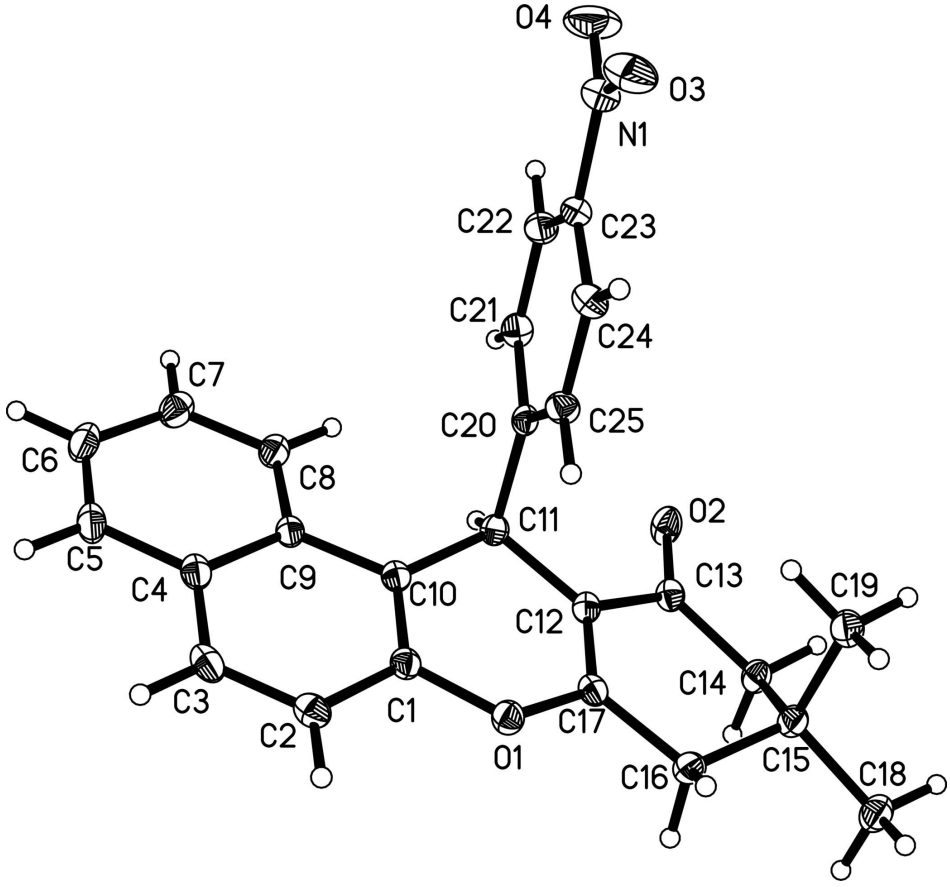

Figure 1

A view of the molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

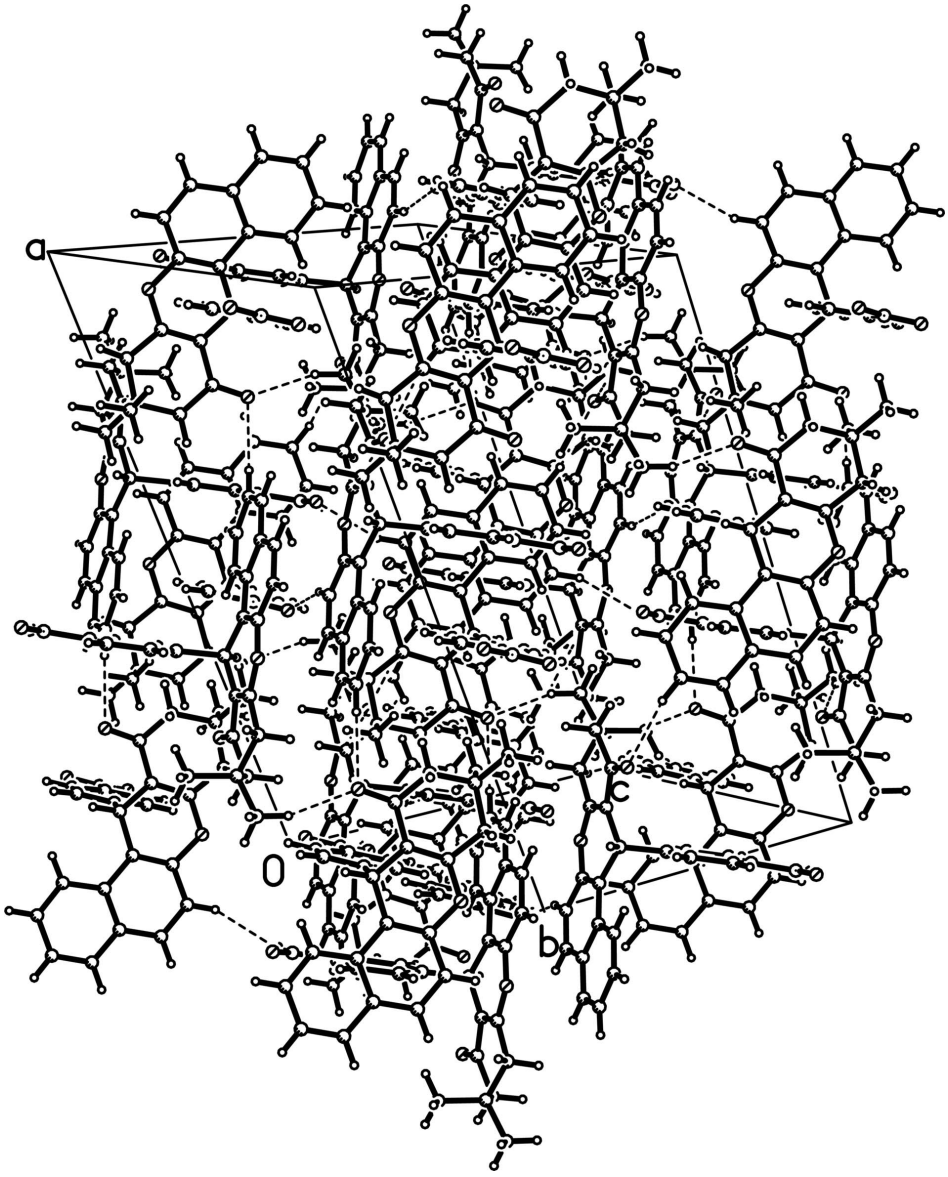

Figure 2

The packing, showing hydrogen-bond interactions as dashed lines; H atoms are shown as small spheres of arbitrary radii.

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Crystal data

$C_{25}H_{21}NO_4$
M_r = 399.43
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 24.178 (5) Å
b = 11.078 (2) Å
c = 17.481 (4) Å
β = 119.78 (3)°
V = 4063.9 (19) Å^3
Z = 8
F(000) = 1680
D_x = 1.306 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 4847 reflections
θ = 2.1–27.9°
μ = 0.09 mm^{-1}
T = 113 K
Prism, yellow
0.20 × 0.18 × 0.10 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Radiation source: rotating anode
Confocal monochromator
Detector resolution: 7.31 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.983, T_{max} = 0.999
14653 measured reflections
4007 independent reflections
3106 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 26.0°, θ_{min} = 2.1°
h = −29→26
k = −13→12
l = −18→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.153
S = 1.03
4007 reflections
274 parameters
0 restraints
0 constraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0882P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}
Extinction correction: *SHELXS97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0043 (6)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.07668 (6)	−0.09846 (11)	0.23338 (8)	0.0274 (3)
O2	0.23273 (6)	0.17081 (12)	0.24963 (8)	0.0360 (4)
O3	0.06051 (8)	0.52066 (14)	0.42025 (11)	0.0504 (5)
O4	0.08357 (10)	0.64016 (14)	0.34280 (11)	0.0625 (5)
N1	0.07521 (9)	0.53889 (15)	0.36366 (11)	0.0385 (5)
C1	0.02775 (9)	−0.03873 (17)	0.16146 (11)	0.0247 (4)
C2	−0.03123 (9)	−0.09880 (17)	0.12366 (12)	0.0295 (5)
H2	−0.0351	−0.1738	0.1469	0.035*
C3	−0.08261 (9)	−0.04833 (18)	0.05346 (12)	0.0321 (5)
H3	−0.1227	−0.0880	0.0283	0.038*
C4	−0.07735 (9)	0.06226 (18)	0.01731 (12)	0.0292 (5)
C5	−0.13056 (10)	0.1170 (2)	−0.05572 (13)	0.0365 (5)
H5	−0.1710	0.0787	−0.0805	0.044*
C6	−0.12508 (10)	0.2230 (2)	−0.09105 (13)	0.0397 (6)
H6	−0.1615	0.2591	−0.1388	0.048*
C7	−0.06498 (10)	0.2782 (2)	−0.05608 (12)	0.0370 (5)
H7	−0.0607	0.3505	−0.0819	0.044*
C8	−0.01239 (9)	0.22896 (17)	0.01486 (11)	0.0295 (5)
H8	0.0277	0.2683	0.0378	0.035*
C9	−0.01689 (8)	0.12084 (17)	0.05423 (11)	0.0243 (4)
C10	0.03670 (8)	0.06891 (16)	0.13055 (11)	0.0230 (4)
C11	0.10058 (8)	0.13313 (16)	0.17849 (11)	0.0233 (4)

H11	0.1119	0.1628	0.1340	0.028*
C12	0.15111 (8)	0.04569 (16)	0.23939 (11)	0.0237 (4)
C13	0.21800 (9)	0.07594 (17)	0.27101 (11)	0.0263 (4)
C14	0.26749 (9)	−0.01679 (17)	0.32757 (12)	0.0291 (5)
H14A	0.3089	0.0244	0.3635	0.035*
H14B	0.2727	−0.0752	0.2887	0.035*
C15	0.25060 (9)	−0.08591 (16)	0.38902 (11)	0.0278 (4)
C16	0.18478 (9)	−0.14376 (17)	0.33158 (12)	0.0276 (4)
H16A	0.1893	−0.2140	0.3001	0.033*
H16B	0.1686	−0.1736	0.3701	0.033*
C17	0.13742 (9)	−0.05788 (16)	0.26568 (11)	0.0241 (4)
C18	0.30005 (10)	−0.18485 (18)	0.43696 (13)	0.0361 (5)
H18A	0.3425	−0.1484	0.4702	0.054*
H18B	0.2995	−0.2421	0.3938	0.054*
H18C	0.2899	−0.2275	0.4776	0.054*
C19	0.24992 (10)	0.00103 (19)	0.45700 (12)	0.0350 (5)
H19A	0.2913	0.0418	0.4892	0.052*
H19B	0.2418	−0.0445	0.4985	0.052*
H19C	0.2163	0.0613	0.4266	0.052*
C20	0.09628 (8)	0.24126 (16)	0.22956 (11)	0.0232 (4)
C21	0.10351 (9)	0.35856 (17)	0.20785 (12)	0.0285 (4)
H21	0.1129	0.3716	0.1617	0.034*
C22	0.09739 (10)	0.45691 (18)	0.25190 (12)	0.0323 (5)
H22	0.1023	0.5369	0.2366	0.039*
C23	0.08393 (9)	0.43547 (16)	0.31859 (12)	0.0276 (4)
C24	0.07792 (9)	0.32046 (17)	0.34403 (12)	0.0293 (5)
H24	0.0698	0.3081	0.3914	0.035*
C25	0.08398 (9)	0.22379 (17)	0.29877 (11)	0.0270 (4)
H25	0.0797	0.1440	0.3151	0.032*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0245 (7)	0.0279 (7)	0.0284 (7)	−0.0022 (5)	0.0120 (6)	0.0018 (5)
O2	0.0243 (7)	0.0399 (9)	0.0376 (8)	−0.0038 (6)	0.0108 (6)	0.0098 (6)
O3	0.0587 (11)	0.0439 (10)	0.0597 (10)	−0.0063 (8)	0.0378 (9)	−0.0174 (8)
O4	0.1033 (16)	0.0236 (9)	0.0641 (11)	0.0058 (9)	0.0444 (11)	−0.0003 (8)
N1	0.0419 (11)	0.0297 (10)	0.0373 (10)	0.0006 (8)	0.0146 (8)	−0.0073 (8)
C1	0.0236 (10)	0.0268 (10)	0.0230 (9)	0.0009 (7)	0.0110 (7)	−0.0040 (7)
C2	0.0292 (11)	0.0291 (10)	0.0342 (10)	−0.0044 (8)	0.0189 (8)	−0.0061 (8)
C3	0.0240 (11)	0.0381 (12)	0.0352 (11)	−0.0068 (8)	0.0155 (8)	−0.0149 (9)
C4	0.0229 (10)	0.0370 (11)	0.0268 (10)	0.0015 (8)	0.0116 (8)	−0.0099 (8)
C5	0.0223 (10)	0.0499 (14)	0.0295 (10)	0.0035 (9)	0.0070 (8)	−0.0131 (9)
C6	0.0316 (12)	0.0508 (14)	0.0271 (10)	0.0158 (10)	0.0073 (8)	−0.0033 (10)
C7	0.0407 (13)	0.0418 (13)	0.0253 (10)	0.0114 (10)	0.0140 (9)	0.0018 (9)
C8	0.0288 (11)	0.0347 (11)	0.0238 (9)	0.0054 (8)	0.0123 (8)	−0.0012 (8)
C9	0.0198 (10)	0.0301 (10)	0.0230 (9)	0.0025 (8)	0.0106 (7)	−0.0062 (7)
C10	0.0214 (10)	0.0268 (10)	0.0224 (9)	0.0006 (7)	0.0120 (7)	−0.0037 (7)

C11	0.0208 (9)	0.0258 (10)	0.0237 (9)	0.0000 (7)	0.0113 (7)	0.0006 (7)
C12	0.0216 (10)	0.0270 (10)	0.0213 (9)	0.0005 (7)	0.0097 (7)	−0.0005 (7)
C13	0.0243 (10)	0.0308 (11)	0.0232 (9)	−0.0001 (8)	0.0113 (8)	−0.0012 (8)
C14	0.0213 (10)	0.0326 (11)	0.0305 (10)	0.0031 (8)	0.0107 (8)	0.0007 (8)
C15	0.0262 (11)	0.0280 (10)	0.0263 (10)	0.0051 (8)	0.0108 (8)	0.0006 (8)
C16	0.0293 (11)	0.0257 (10)	0.0270 (9)	0.0017 (8)	0.0134 (8)	0.0018 (8)
C17	0.0210 (10)	0.0269 (10)	0.0238 (9)	−0.0024 (7)	0.0106 (7)	−0.0046 (7)
C18	0.0330 (12)	0.0374 (12)	0.0334 (10)	0.0082 (9)	0.0130 (8)	0.0046 (9)
C19	0.0327 (11)	0.0378 (12)	0.0289 (10)	0.0044 (9)	0.0112 (8)	−0.0031 (9)
C20	0.0174 (9)	0.0247 (10)	0.0235 (9)	−0.0005 (7)	0.0069 (7)	0.0009 (7)
C21	0.0286 (10)	0.0297 (10)	0.0271 (9)	−0.0025 (8)	0.0137 (8)	0.0025 (8)
C22	0.0361 (12)	0.0223 (10)	0.0314 (10)	−0.0022 (8)	0.0115 (9)	0.0028 (8)
C23	0.0263 (10)	0.0225 (10)	0.0276 (10)	0.0003 (8)	0.0084 (8)	−0.0042 (8)
C24	0.0317 (11)	0.0301 (11)	0.0279 (10)	−0.0041 (8)	0.0162 (8)	−0.0051 (8)
C25	0.0301 (10)	0.0232 (10)	0.0276 (10)	−0.0033 (8)	0.0143 (8)	0.0010 (8)

Geometric parameters (Å, º)

O1—C17	1.362 (2)	C12—C13	1.465 (3)
O1—C1	1.393 (2)	C13—C14	1.513 (3)
O2—C13	1.226 (2)	C14—C15	1.531 (3)
O3—N1	1.223 (2)	C14—H14A	0.9900
O4—N1	1.227 (2)	C14—H14B	0.9900
N1—C23	1.464 (2)	C15—C18	1.529 (2)
C1—C10	1.370 (2)	C15—C19	1.536 (3)
C1—C2	1.406 (3)	C15—C16	1.538 (3)
C2—C3	1.359 (3)	C16—C17	1.494 (3)
C2—H2	0.9500	C16—H16A	0.9900
C3—C4	1.413 (3)	C16—H16B	0.9900
C3—H3	0.9500	C18—H18A	0.9800
C4—C5	1.422 (3)	C18—H18B	0.9800
C4—C9	1.427 (3)	C18—H18C	0.9800
C5—C6	1.364 (3)	C19—H19A	0.9800
C5—H5	0.9500	C19—H19B	0.9800
C6—C7	1.406 (3)	C19—H19C	0.9800
C6—H6	0.9500	C20—C21	1.389 (2)
C7—C8	1.373 (3)	C20—C25	1.395 (3)
C7—H7	0.9500	C21—C22	1.384 (3)
C8—C9	1.412 (3)	C21—H21	0.9500
C8—H8	0.9500	C22—C23	1.378 (3)
C9—C10	1.440 (2)	C22—H22	0.9500
C10—C11	1.519 (2)	C23—C24	1.381 (3)
C11—C12	1.507 (2)	C24—C25	1.382 (2)
C11—C20	1.528 (2)	C24—H24	0.9500
C11—H11	1.0000	C25—H25	0.9500
C12—C17	1.337 (2)		
C17—O1—C1	118.36 (14)	C13—C14—H14B	108.9

O3—N1—O4	123.25 (17)	C15—C14—H14B	108.9
O3—N1—C23	118.92 (17)	H14A—C14—H14B	107.7
O4—N1—C23	117.82 (18)	C18—C15—C14	109.56 (16)
C10—C1—O1	122.67 (16)	C18—C15—C19	109.35 (15)
C10—C1—C2	123.27 (17)	C14—C15—C19	109.78 (15)
O1—C1—C2	114.06 (16)	C18—C15—C16	109.46 (15)
C3—C2—C1	119.24 (19)	C14—C15—C16	107.49 (15)
C3—C2—H2	120.4	C19—C15—C16	111.18 (16)
C1—C2—H2	120.4	C17—C16—C15	112.73 (15)
C2—C3—C4	121.03 (18)	C17—C16—H16A	109.0
C2—C3—H3	119.5	C15—C16—H16A	109.0
C4—C3—H3	119.5	C17—C16—H16B	109.0
C3—C4—C5	121.93 (19)	C15—C16—H16B	109.0
C3—C4—C9	119.44 (17)	H16A—C16—H16B	107.8
C5—C4—C9	118.62 (19)	C12—C17—O1	122.74 (16)
C6—C5—C4	121.7 (2)	C12—C17—C16	125.83 (17)
C6—C5—H5	119.1	O1—C17—C16	111.42 (16)
C4—C5—H5	119.1	C15—C18—H18A	109.5
C5—C6—C7	119.32 (19)	C15—C18—H18B	109.5
C5—C6—H6	120.3	H18A—C18—H18B	109.5
C7—C6—H6	120.3	C15—C18—H18C	109.5
C8—C7—C6	120.9 (2)	H18A—C18—H18C	109.5
C8—C7—H7	119.6	H18B—C18—H18C	109.5
C6—C7—H7	119.6	C15—C19—H19A	109.5
C7—C8—C9	121.07 (19)	C15—C19—H19B	109.5
C7—C8—H8	119.5	H19A—C19—H19B	109.5
C9—C8—H8	119.5	C15—C19—H19C	109.5
C8—C9—C4	118.34 (17)	H19A—C19—H19C	109.5
C8—C9—C10	122.60 (17)	H19B—C19—H19C	109.5
C4—C9—C10	119.05 (18)	C21—C20—C25	118.47 (16)
C1—C10—C9	117.88 (17)	C21—C20—C11	121.29 (16)
C1—C10—C11	120.43 (16)	C25—C20—C11	120.23 (16)
C9—C10—C11	121.63 (16)	C22—C21—C20	121.44 (17)
C12—C11—C10	109.51 (15)	C22—C21—H21	119.3
C12—C11—C20	110.94 (14)	C20—C21—H21	119.3
C10—C11—C20	110.11 (14)	C23—C22—C21	118.07 (17)
C12—C11—H11	108.7	C23—C22—H22	121.0
C10—C11—H11	108.7	C21—C22—H22	121.0
C20—C11—H11	108.7	C22—C23—C24	122.59 (17)
C17—C12—C13	118.81 (16)	C22—C23—N1	118.57 (17)
C17—C12—C11	122.81 (17)	C24—C23—N1	118.85 (17)
C13—C12—C11	118.38 (16)	C23—C24—C25	118.20 (17)
O2—C13—C12	120.95 (17)	C23—C24—H24	120.9
O2—C13—C14	121.74 (17)	C25—C24—H24	120.9
C12—C13—C14	117.25 (16)	C24—C25—C20	121.19 (17)
C13—C14—C15	113.47 (16)	C24—C25—H25	119.4
C13—C14—H14A	108.9	C20—C25—H25	119.4
C15—C14—H14A	108.9		

C17—O1—C1—C10	−10.1 (2)	C17—C12—C13—C14	3.6 (2)
C17—O1—C1—C2	169.76 (15)	C11—C12—C13—C14	−176.40 (15)
C10—C1—C2—C3	−0.7 (3)	O2—C13—C14—C15	146.74 (17)
O1—C1—C2—C3	179.44 (15)	C12—C13—C14—C15	−35.8 (2)
C1—C2—C3—C4	1.0 (3)	C13—C14—C15—C18	174.83 (15)
C2—C3—C4—C5	−179.58 (17)	C13—C14—C15—C19	−65.1 (2)
C2—C3—C4—C9	1.0 (3)	C13—C14—C15—C16	56.0 (2)
C3—C4—C5—C6	−179.19 (18)	C18—C15—C16—C17	−165.35 (15)
C9—C4—C5—C6	0.2 (3)	C14—C15—C16—C17	−46.4 (2)
C4—C5—C6—C7	1.8 (3)	C19—C15—C16—C17	73.74 (19)
C5—C6—C7—C8	−2.2 (3)	C13—C12—C17—O1	−173.81 (15)
C6—C7—C8—C9	0.7 (3)	C11—C12—C17—O1	6.2 (3)
C7—C8—C9—C4	1.3 (3)	C13—C12—C17—C16	5.4 (3)
C7—C8—C9—C10	−177.74 (17)	C11—C12—C17—C16	−174.52 (16)
C3—C4—C9—C8	177.69 (16)	C1—O1—C17—C12	9.3 (2)
C5—C4—C9—C8	−1.7 (3)	C1—O1—C17—C16	−170.01 (14)
C3—C4—C9—C10	−3.3 (3)	C15—C16—C17—C12	17.8 (3)
C5—C4—C9—C10	177.33 (16)	C15—C16—C17—O1	−162.89 (14)
O1—C1—C10—C9	178.31 (14)	C12—C11—C20—C21	123.51 (18)
C2—C1—C10—C9	−1.6 (3)	C10—C11—C20—C21	−115.09 (19)
O1—C1—C10—C11	−4.4 (3)	C12—C11—C20—C25	−57.4 (2)
C2—C1—C10—C11	175.71 (16)	C10—C11—C20—C25	64.0 (2)
C8—C9—C10—C1	−177.50 (16)	C25—C20—C21—C22	−1.4 (3)
C4—C9—C10—C1	3.5 (3)	C11—C20—C21—C22	177.65 (17)
C8—C9—C10—C11	5.3 (3)	C20—C21—C22—C23	0.1 (3)
C4—C9—C10—C11	−173.76 (15)	C21—C22—C23—C24	1.5 (3)
C1—C10—C11—C12	17.4 (2)	C21—C22—C23—N1	−177.96 (17)
C9—C10—C11—C12	−165.45 (15)	O3—N1—C23—C22	176.83 (18)
C1—C10—C11—C20	−104.88 (19)	O4—N1—C23—C22	−3.7 (3)
C9—C10—C11—C20	72.3 (2)	O3—N1—C23—C24	−2.7 (3)
C10—C11—C12—C17	−18.7 (2)	O4—N1—C23—C24	176.80 (19)
C20—C11—C12—C17	103.10 (19)	C22—C23—C24—C25	−1.8 (3)
C10—C11—C12—C13	161.39 (15)	N1—C23—C24—C25	177.68 (17)
C20—C11—C12—C13	−76.85 (19)	C23—C24—C25—C20	0.4 (3)
C17—C12—C13—O2	−178.88 (17)	C21—C20—C25—C24	1.1 (3)
C11—C12—C13—O2	1.1 (3)	C11—C20—C25—C24	−177.95 (16)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O4^{i}	0.95	2.42	3.323 (3)	159
C6—H6···O2^{ii}	0.95	2.45	3.384 (3)	168
C18—H18*B*···O2^{iii}	0.98	2.43	3.355 (2)	158

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