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7-Pivaloyl-5,6-dihydro-4*H*-naphtho-[3,2,1-*de*]isoquinoline-4,6-dione

Hai-Tao Yu,* Yi Wei and Yan Zhang

School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210093, People's Republic of China
Correspondence e-mail: njubilly@gmail.com

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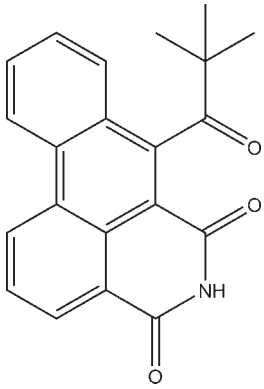
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.066; wR factor = 0.077; data-to-parameter ratio = 13.1.

In the crystal structure of the title compound, $C_{21}H_{17}NO_3$, the dibenzo–isoquinoline–dione unit has a planar structure, the maximum atomic deviation being 0.091 (3) Å. The crystal structure is stabilized by π–π stacking [centroid–centroid distance = 3.851 (2) Å] and intermolecular N—H···O hydrogen bonding.

Related literature

The title compound is an azonafide analogue. For the biological activity of 1,3,4(2*H*)-isoquinolinetrione derivatives, see: Malamas *et al.* (1994); Hall *et al.* (1994). For the antitumor properties of azonafide and analogues, see: Sami *et al.* (2000); Hutchings *et al.* (1988). For the synthesis, see: Zhang *et al.* (2000).



Experimental

Crystal data

$C_{21}H_{17}NO_3$
M_r = 331.36
Monoclinic, $P2_1/c$
a = 11.569 (2) Å
b = 9.1150 (18) Å
c = 15.746 (3) Å
β = 101.12 (3)°
V = 1629.3 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 K
0.10 × 0.10 × 0.05 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (*CAD-4 EXPRESS*; Enraf–Nonius, 1994)
T_{min} = 0.991, T_{max} = 0.996
3103 measured reflections
2950 independent reflections
1264 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.077
S = 1.00
2950 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N—H0A···O2^{i}	0.86	2.05	2.911 (3)	174

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

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2713).

References

Enraf–Nonius (1994). *CAD-4 EXPRESS*. Enraf–Nonius, Delft, The Netherlands.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Hall, I. H., Chapman, J. M. & Wong, O. T. (1994). *Anticancer Drugs*, **5**, 75–82.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
Hutchings, M. G., Chippendale, A. M. & Ferguson, I. (1988). *Tetrahedron*, **44**, 3727–3734.
Malamas, M. S., Hohman, T. C. & Millen, J. (1994). *J. Med. Chem.* **37**, 2043–2058.
Sami, S. M., Dorr, R. T., Alberts, D. S., Solyom, A. M. & Remers, W. A. (2000). *J. Med. Chem.* **43**, 3067–3073.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zhang, Y., Qian, S.-P., Fun, H.-K. & Xu, J.-H. (2000). *Tetrahedron Lett.* **41**, 8141–8145.

supporting information

Acta Cryst. (2010). E**66**, o836 [doi:10.1107/S1600536810008378]

7-Pivaloyl-5,6-dihydro-4*H*-naphtho[3,2,1-*de*]isoquinoline-4,6-dione

Hai-Tao Yu, Yi Wei and Yan Zhang

S1. Comment

1,3,4(2*H*)-Isoquinolinetrione derivatives have a variety of biological activities and are synthetic precursors for many naturally occurring alkaloids (Malamas *et al.* 1994; Hall *et al.* 1994). Moreover, many 2-[2′-(dimethyl-amino)ethyl]-1,2-dihydro-3*H*-dibenz[*de*, *h*]- isoquinoline-1,3-dione(azonafide) analogues with structural variations in the side chain and the bent phenanthrene nucleus have shown significant antitumor properties (Sami *et al.* 2000; Hutchings *et al.* 1988). As part of our work involving the synthesis of a series of azonafide analogues from 1,3,4(2*H*)-isoquinolinetrione we report herein the crystal structure of the title compound (Fig. 1).

The carbonyl group forms a dihedral angle of 78.8 (3)° with the phenanthrene moiety. The crystal structure is stabilized by intermolecular π-π stacking; centroids distance between nearly parallel C6-benzene and C17^{ii}-benzene rings is 3.851 (2) Å (symmetry code: (ii) 2-x, -y, 1-z]. In addition the intermolecular N—H···O hydrogen bonding further stabilize the crystal structure.

S2. Experimental

A solution of 1,3,4(2*H*)-isoquinolinetriones (175 mg, 1 mmol) and *tert*-butyl phenyl acetylene (316 mg, 2 mmol) in anhydrous acetonitrile (50 ml) was purged with dry argon for 10 min and then irradiated for 24 h under continuous argon purging. The single crystals of the title compound were obtained from the reaction mixture. The light source was a medium-pressure mercury lamp (500 W) in a cooling water jacket that was further surrounded by a layer of filter solution (1 cm thick, 20% aqueous sodium nitrite) to cut off light of wavelength shorter than 400 nm (Zhang *et al.*, 2000).

S3. Refinement

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å for the aromatic atoms, 0.96 Å for the CH_3 groups and 0.86 Å for the N—H group, and U_{iso}(H) = 1.2U_{eq}(C).

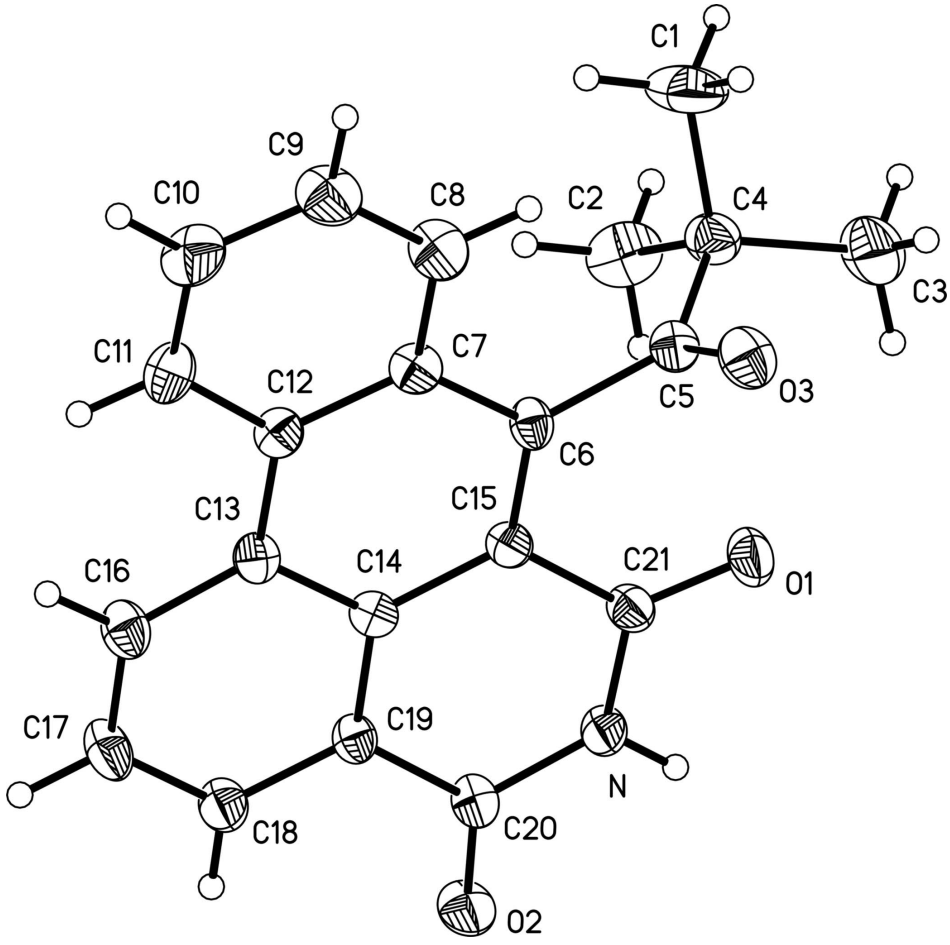

Figure 1

The molecular structure of the title compound with displacement ellipsoids shown at 30% probability ellipsoids for non-H atoms.

7-Pivaloyl-5,6-dihydro-4*H*-naphtho[3,2,1-*de*]isoquinoline-4,6-dione

Crystal data

$C_{21}H_{17}NO_3$
$M_r = 331.36$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 11.569\ (2)$ Å
$b = 9.1150\ (18)$ Å
$c = 15.746\ (3)$ Å
$\beta = 101.12\ (3)°$
$V = 1629.3\ (6)$ Å^3
$Z = 4$
$F(000) = 696$
$D_x = 1.351$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 9–12°$
$\mu = 0.09$ mm^{-1}
$T = 298$ K
Block, light-yellow
0.10 × 0.10 × 0.05 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: ψ scan (*CAD-4 EXPRESS*; Enraf–Nonius, 1994)
$T_{min} = 0.991$, $T_{max} = 0.996$

3103 measured reflections
2950 independent reflections
1264 reflections with $I > 2\sigma(I)$
$R_{int} = 0.056$
$\theta_{max} = 25.3°$, $\theta_{min} = 1.8°$

$h = 0 \rightarrow 13$
$k = 0 \rightarrow 10$
$l = -18 \rightarrow 18$
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.066$
$wR(F^2) = 0.077$
$S = 1.00$
2950 reflections
226 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.001P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

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.

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 $F^2 > \sigma(F^2)$ 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}
N	0.9224 (2)	0.3212 (3)	0.52319 (16)	0.0380 (8)
H0A	0.9433	0.4046	0.5467	0.046*
O1	0.7998 (2)	−0.0308 (3)	0.72692 (14)	0.0517 (7)
O2	0.9979 (2)	0.3921 (2)	0.40785 (14)	0.0494 (7)
O3	0.8470 (2)	0.2652 (2)	0.64021 (14)	0.0508 (7)
C1	0.5388 (3)	−0.0139 (4)	0.6829 (2)	0.0769 (14)
H1A	0.5228	−0.0812	0.6352	0.115*
H1B	0.4670	0.0333	0.6897	0.115*
H1C	0.5713	−0.0664	0.7349	0.115*
C2	0.5766 (3)	0.1815 (4)	0.5817 (2)	0.0675 (13)
H2A	0.5630	0.1123	0.5349	0.101*
H2B	0.6310	0.2552	0.5704	0.101*
H2C	0.5035	0.2271	0.5870	0.101*
C3	0.6483 (3)	0.2081 (4)	0.7420 (2)	0.0781 (15)
H3A	0.7027	0.2832	0.7326	0.117*
H3B	0.6803	0.1551	0.7939	0.117*
H3C	0.5750	0.2524	0.7478	0.117*
C4	0.6277 (3)	0.1027 (4)	0.6652 (2)	0.0461 (10)
C5	0.7422 (3)	0.0215 (4)	0.6623 (2)	0.0358 (9)
C6	0.7748 (3)	−0.0144 (4)	0.5757 (2)	0.0337 (9)

C7	0.7494 (3)	−0.1610 (4)	0.5410 (2)	0.0358 (9)
C8	0.7003 (3)	−0.2677 (4)	0.5887 (2)	0.0504 (11)
H8A	0.6861	−0.2445	0.6433	0.061*
C9	0.6734 (3)	−0.4046 (4)	0.5553 (3)	0.0584 (12)
H9A	0.6409	−0.4736	0.5874	0.070*
C10	0.6942 (3)	−0.4420 (4)	0.4742 (2)	0.0560 (12)
H10A	0.6738	−0.5346	0.4514	0.067*
C11	0.7448 (3)	−0.3419 (4)	0.4277 (2)	0.0457 (11)
H11A	0.7606	−0.3690	0.3742	0.055*
C12	0.7736 (3)	−0.1988 (4)	0.4589 (2)	0.0351 (9)
C13	0.8287 (3)	−0.0921 (4)	0.4115 (2)	0.0361 (9)
C14	0.8587 (3)	0.0469 (4)	0.4492 (2)	0.0314 (9)
C15	0.8305 (3)	0.0825 (4)	0.5310 (2)	0.0320 (9)
C16	0.8571 (3)	−0.1202 (4)	0.3306 (2)	0.0430 (10)
H16A	0.8379	−0.2110	0.3048	0.052*
C17	0.9120 (3)	−0.0188 (4)	0.2882 (2)	0.0480 (11)
H17A	0.9299	−0.0415	0.2346	0.058*
C18	0.9412 (3)	0.1181 (4)	0.3250 (2)	0.0417 (10)
H18A	0.9782	0.1872	0.2959	0.050*
C19	0.9154 (3)	0.1513 (4)	0.4046 (2)	0.0324 (9)
C20	0.9491 (3)	0.2966 (4)	0.4427 (2)	0.0358 (9)
C21	0.8659 (3)	0.2269 (4)	0.5700 (2)	0.0364 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N	0.052 (2)	0.0271 (19)	0.0377 (18)	−0.0090 (16)	0.0150 (16)	−0.0042 (15)
O1	0.0629 (19)	0.0489 (18)	0.0445 (16)	0.0042 (15)	0.0135 (14)	0.0078 (14)
O2	0.070 (2)	0.0339 (16)	0.0499 (16)	−0.0110 (14)	0.0247 (14)	0.0060 (13)
O3	0.073 (2)	0.0420 (17)	0.0425 (15)	−0.0127 (15)	0.0247 (15)	−0.0123 (13)
C1	0.061 (3)	0.071 (3)	0.109 (4)	−0.017 (3)	0.044 (3)	0.007 (3)
C2	0.058 (3)	0.052 (3)	0.090 (3)	0.008 (2)	0.009 (3)	0.009 (3)
C3	0.079 (3)	0.070 (3)	0.094 (3)	0.002 (3)	0.040 (3)	−0.031 (3)
C4	0.046 (3)	0.041 (3)	0.054 (3)	−0.001 (2)	0.017 (2)	−0.004 (2)
C5	0.050 (3)	0.024 (2)	0.035 (2)	−0.004 (2)	0.011 (2)	0.0057 (18)
C6	0.044 (2)	0.027 (2)	0.030 (2)	0.0027 (19)	0.0083 (18)	−0.0013 (18)
C7	0.044 (3)	0.022 (2)	0.042 (2)	0.0019 (19)	0.010 (2)	0.0068 (19)
C8	0.067 (3)	0.032 (2)	0.056 (3)	0.002 (2)	0.020 (2)	0.005 (2)
C9	0.074 (3)	0.040 (3)	0.067 (3)	−0.005 (3)	0.027 (3)	0.007 (2)
C10	0.069 (3)	0.026 (2)	0.073 (3)	−0.008 (2)	0.014 (3)	0.000 (2)
C11	0.057 (3)	0.027 (2)	0.052 (3)	0.000 (2)	0.005 (2)	−0.007 (2)
C12	0.037 (2)	0.028 (2)	0.040 (2)	0.0029 (19)	0.0064 (19)	−0.0003 (19)
C13	0.039 (2)	0.035 (2)	0.034 (2)	0.002 (2)	0.0067 (19)	−0.0011 (19)
C14	0.032 (2)	0.029 (2)	0.034 (2)	0.0041 (18)	0.0072 (18)	0.0045 (18)
C15	0.036 (2)	0.026 (2)	0.036 (2)	0.0004 (18)	0.0107 (18)	−0.0004 (18)
C16	0.055 (3)	0.034 (2)	0.041 (2)	0.006 (2)	0.014 (2)	−0.004 (2)
C17	0.069 (3)	0.046 (3)	0.033 (2)	0.001 (2)	0.020 (2)	0.000 (2)
C18	0.052 (3)	0.036 (2)	0.039 (2)	−0.003 (2)	0.013 (2)	−0.001 (2)

C19	0.037 (2)	0.027 (2)	0.034 (2)	0.0038 (19)	0.0084 (18)	−0.0022 (18)
C20	0.046 (3)	0.029 (2)	0.033 (2)	0.004 (2)	0.0090 (19)	0.0032 (18)
C21	0.038 (2)	0.037 (2)	0.037 (2)	0.001 (2)	0.0119 (19)	−0.002 (2)

Geometric parameters (Å, º)

N—C21	1.376 (4)	C7—C12	1.417 (4)
N—C20	1.379 (3)	C8—C9	1.366 (4)
N—H0A	0.8600	C8—H8A	0.9300
O1—C5	1.201 (3)	C9—C10	1.387 (4)
O2—C20	1.224 (3)	C9—H9A	0.9300
O3—C21	1.219 (3)	C10—C11	1.369 (4)
C1—C4	1.541 (4)	C10—H10A	0.9300
C1—H1A	0.9600	C11—C12	1.410 (4)
C1—H1B	0.9600	C11—H11A	0.9300
C1—H1C	0.9600	C12—C13	1.447 (4)
C2—C4	1.514 (4)	C13—C16	1.399 (4)
C2—H2A	0.9600	C13—C14	1.413 (4)
C2—H2B	0.9600	C14—C19	1.416 (4)
C2—H2C	0.9600	C14—C15	1.426 (4)
C3—C4	1.527 (4)	C15—C21	1.476 (4)
C3—H3A	0.9600	C16—C17	1.366 (4)
C3—H3B	0.9600	C16—H16A	0.9300
C3—H3C	0.9600	C17—C18	1.390 (4)
C4—C5	1.526 (4)	C17—H17A	0.9300
C5—C6	1.520 (4)	C18—C19	1.378 (4)
C6—C15	1.365 (4)	C18—H18A	0.9300
C6—C7	1.452 (4)	C19—C20	1.475 (4)
C7—C8	1.413 (4)		
C21—N—C20	127.1 (3)	C8—C9—C10	120.8 (4)
C21—N—H0A	116.4	C8—C9—H9A	119.6
C20—N—H0A	116.4	C10—C9—H9A	119.6
C4—C1—H1A	109.5	C11—C10—C9	119.7 (4)
C4—C1—H1B	109.5	C11—C10—H10A	120.1
H1A—C1—H1B	109.5	C9—C10—H10A	120.1
C4—C1—H1C	109.5	C10—C11—C12	121.8 (4)
H1A—C1—H1C	109.5	C10—C11—H11A	119.1
H1B—C1—H1C	109.5	C12—C11—H11A	119.1
C4—C2—H2A	109.5	C11—C12—C7	117.8 (3)
C4—C2—H2B	109.5	C11—C12—C13	122.7 (3)
H2A—C2—H2B	109.5	C7—C12—C13	119.4 (3)
C4—C2—H2C	109.5	C16—C13—C14	117.7 (3)
H2A—C2—H2C	109.5	C16—C13—C12	123.4 (3)
H2B—C2—H2C	109.5	C14—C13—C12	118.9 (3)
C4—C3—H3A	109.5	C13—C14—C19	119.6 (3)
C4—C3—H3B	109.5	C13—C14—C15	120.2 (3)
H3A—C3—H3B	109.5	C19—C14—C15	120.2 (3)

C4—C3—H3C	109.5	C6—C15—C14	122.1 (3)
H3A—C3—H3C	109.5	C6—C15—C21	118.9 (3)
H3B—C3—H3C	109.5	C14—C15—C21	119.0 (3)
C2—C4—C5	113.6 (3)	C17—C16—C13	122.3 (3)
C2—C4—C3	111.3 (3)	C17—C16—H16A	118.8
C5—C4—C3	108.9 (3)	C13—C16—H16A	118.8
C2—C4—C1	108.8 (3)	C16—C17—C18	120.1 (3)
C5—C4—C1	106.5 (3)	C16—C17—H17A	120.0
C3—C4—C1	107.4 (3)	C18—C17—H17A	120.0
O1—C5—C6	118.8 (3)	C19—C18—C17	119.9 (3)
O1—C5—C4	120.7 (3)	C19—C18—H18A	120.0
C6—C5—C4	119.9 (3)	C17—C18—H18A	120.0
C15—C6—C7	118.9 (3)	C18—C19—C14	120.4 (3)
C15—C6—C5	123.1 (3)	C18—C19—C20	118.7 (3)
C7—C6—C5	117.9 (3)	C14—C19—C20	120.9 (3)
C8—C7—C12	119.2 (3)	O2—C20—N	120.0 (3)
C8—C7—C6	120.4 (3)	O2—C20—C19	124.4 (3)
C12—C7—C6	120.4 (3)	N—C20—C19	115.5 (3)
C9—C8—C7	120.6 (4)	O3—C21—N	119.6 (3)
C9—C8—H8A	119.7	O3—C21—C15	123.3 (3)
C7—C8—H8A	119.7	N—C21—C15	117.2 (3)

C2—C4—C5—O1	170.9 (3)	C12—C13—C14—C15	−2.5 (5)
C3—C4—C5—O1	46.3 (4)	C7—C6—C15—C14	3.4 (5)
C1—C4—C5—O1	−69.3 (4)	C5—C6—C15—C14	−179.1 (3)
C2—C4—C5—C6	−18.5 (5)	C7—C6—C15—C21	−174.6 (3)
C3—C4—C5—C6	−143.2 (3)	C5—C6—C15—C21	2.9 (5)
C1—C4—C5—C6	101.2 (4)	C13—C14—C15—C6	0.2 (5)
O1—C5—C6—C15	−105.0 (4)	C19—C14—C15—C6	179.3 (3)
C4—C5—C6—C15	84.3 (4)	C13—C14—C15—C21	178.3 (3)
O1—C5—C6—C7	72.5 (4)	C19—C14—C15—C21	−2.7 (5)
C4—C5—C6—C7	−98.2 (4)	C14—C13—C16—C17	0.1 (5)
C15—C6—C7—C8	175.1 (3)	C12—C13—C16—C17	−178.2 (3)
C5—C6—C7—C8	−2.5 (5)	C13—C16—C17—C18	−0.3 (6)
C15—C6—C7—C12	−4.9 (5)	C16—C17—C18—C19	0.4 (5)
C5—C6—C7—C12	177.5 (3)	C17—C18—C19—C14	−0.3 (5)
C12—C7—C8—C9	−1.7 (6)	C17—C18—C19—C20	179.0 (3)
C6—C7—C8—C9	178.3 (4)	C13—C14—C19—C18	0.1 (5)
C7—C8—C9—C10	0.2 (6)	C15—C14—C19—C18	−179.0 (3)
C8—C9—C10—C11	1.6 (6)	C13—C14—C19—C20	−179.2 (3)
C9—C10—C11—C12	−2.0 (6)	C15—C14—C19—C20	1.7 (5)
C10—C11—C12—C7	0.5 (5)	C21—N—C20—O2	178.6 (3)
C10—C11—C12—C13	179.0 (4)	C21—N—C20—C19	−1.6 (5)
C8—C7—C12—C11	1.3 (5)	C18—C19—C20—O2	0.9 (6)
C6—C7—C12—C11	−178.7 (3)	C14—C19—C20—O2	−179.8 (3)
C8—C7—C12—C13	−177.3 (3)	C18—C19—C20—N	−178.9 (3)
C6—C7—C12—C13	2.7 (5)	C14—C19—C20—N	0.4 (5)
C11—C12—C13—C16	0.7 (5)	C20—N—C21—O3	−179.0 (3)

C7—C12—C13—C16	179.3 (3)	C20—N—C21—C15	0.6 (5)
C11—C12—C13—C14	−177.6 (3)	C6—C15—C21—O3	−0.7 (5)
C7—C12—C13—C14	1.0 (5)	C14—C15—C21—O3	−178.8 (3)
C16—C13—C14—C19	0.0 (5)	C6—C15—C21—N	179.6 (3)
C12—C13—C14—C19	178.4 (3)	C14—C15—C21—N	1.6 (5)
C16—C13—C14—C15	179.1 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N—H0*A*···O2^{i}	0.86	2.05	2.911 (3)	174

Symmetry code: (i) −*x*+2, −*y*+1, −*z*+1.