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3-*tert*-Butyl-4-oxo-3,4-dihydrophthalazin-1-yl 3,5-dimethylbenzoate

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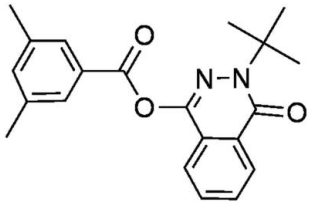
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.043; wR factor = 0.137; data-to-parameter ratio = 15.8.

The title compound, $C_{21}H_{22}N_2O_3$, was synthesized by the reaction of *tert*-butylhydrazine with phthalic anhydride and further *O*-benzoylation of the resulting intermediate by 3,5-dimethylbenzoyl chloride. Intermolecular C—H···O=C interactions link the molecules into layers.

Related literature

For ecdysone agonists, see: Wing (1988). For the synthesis, see: Hou *et al.* (2002). For C—N bond lengths, see: Sasada (1984).



Experimental

Crystal data

$C_{21}H_{22}N_2O_3$
M_r = 350.41
Monoclinic, $P2_1/n$
a = 8.7974 (2) Å
b = 18.7622 (4) Å
c = 11.7405 (3) Å
β = 92.634 (2)°
V = 1935.82 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 296 (2) K
0.54 × 0.52 × 0.48 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: none
14969 measured reflections
3804 independent reflections
2879 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.137
S = 1.06
3804 reflections
241 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···O1^{i}	0.93	2.56	3.391 (2)	149
C12—H12···O3^{ii}	0.93	2.27	3.149 (2)	157

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); 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: LN2004).

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3-*tert*-Butyl-4-oxo-3,4-dihydrophthalazin-1-yl 3,5-dimethylbenzoate

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S1. Comment

DibendzoyIhydrazines insect growth regulators are well known as nonsteroidal ecdysone agonists, which induce prematurely abnormal and ultimately lethal larval molting (Wing, 1988). The title compound, (I), was obtained unintentionally as the product of an attempted synthesis of a dibendzoylhydrazine and we present its crystal structure here. The molecular structure of (I) is shown in Fig.1. The bond length of C18—N2 [1.517 (2) Å] is slightly greater than the normal value of C—N [1.47 Å; Sasada, 1984] because of the larger terminal group *tert*-butyl moiety. The crystal structure of (I) also involves two weak C—H···O?C hydrogen-bonding interactions, which link the molecules into layers which lie parallel to the (101) plane. (Fig. 2 and Table 1).

S2. Experimental

Phthalic anhydride (0.015 mol) was heated to 323 K in acetic acid, *tert*-butyldrazine (0.015 mol) was added dropwise, the solution was stirred for 3 h at 383 K. Then the mixture was condensed and washed with water and filtered, which afforded 2-*tert*-butyl-4-hydroxyphthalazin-1(2*H*)-one (m.p. 391–393 K). This compound (0.01 mol) was heated to 333 K in butyl acetate (30 ml) and water (20 ml) in the presence of DMPA catalyst (0.1 g), 3,5-Dimethylbenzoyl chloride (0.01 mol) and a saturated solution of Na_2CO_3(0.02 mol) which were added dropwise, then the mixture reacted for 4 h (Hou *et al.*, 2002). The solution was cooled, washed with water and dried. The product was concentrated and purified by column chromatography (silica gel, petroleum ether-acetate 10:1) to give the title compound, (I) (yield 46%, m.p. 421–422 K). 1H NMR (CDCl3, *δ*, p.p.m): 1.71 (9*H*, s), 2.43 (6*H*, s), 7.33–7.26 (1*H*, s), 7.74–7.57 (1*H*, s), 7.79–7.75 (2*H*, m), 7.90–7.89 (2*H*, s), 8.46–8.43 (1*H*, m). Compound (I) was recrystallized from ethyl acetate. Single crystals of (I), suitable for X-ray analysis, were grown by natural evaporation of the solvent.

S3. Refinement

The C—H atoms were constrained to an ideal geometry, with *C*(methyl)—H distances of 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C), and *C*(phenyl)—H distances of 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

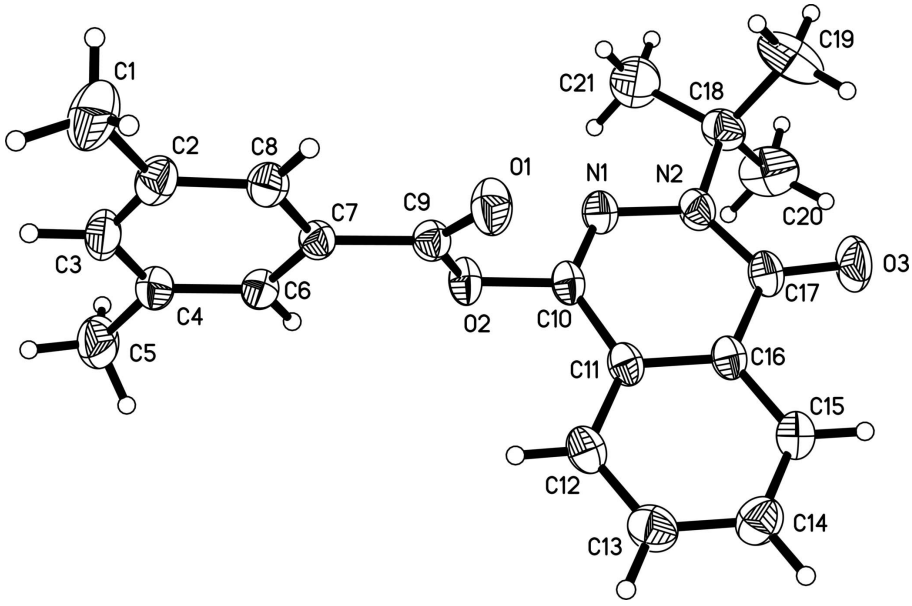

Figure 1

The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

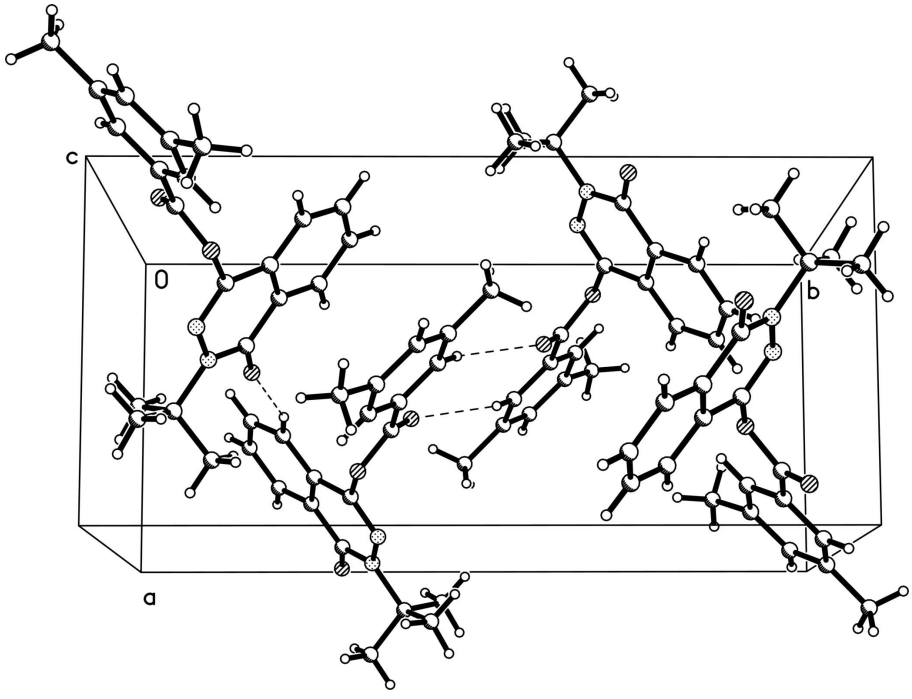

Figure 2

The crystal structure of (I), viewed along the *a* axis. The dashed lines indicate C—H···O interations.

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Crystal data

$C_{21}H_{22}N_2O_3$
$M_r = 350.41$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 8.7974$ (2) Å
$b = 18.7622$ (4) Å
$c = 11.7405$ (3) Å
$\beta = 92.634$ (2)°
$V = 1935.82$ (8) Å^3
$Z = 4$
$F(000) = 744$
$D_x = 1.202$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4673 reflections
$\theta = 2.6$–$26.8°$
$\mu = 0.08$ mm^{-1}
$T = 296$ K
Block, colourless
0.54 × 0.52 × 0.48 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
14969 measured reflections
3804 independent reflections
2879 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.2°$
$h = -8 \rightarrow 10$
$k = -23 \rightarrow 23$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.137$
$S = 1.06$
3804 reflections
241 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
$w = 1/[\sigma^2(F_o^2) + (0.0654P)^2 + 0.3695P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ e Å^{-3}
Extinction correction: *SHELXL97*, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.020 (2)

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}
C1	−0.1890 (3)	−0.01591 (13)	0.3028 (2)	0.0934 (7)
H1A	−0.2610	−0.0137	0.2389	0.140*
H1B	−0.2406	−0.0080	0.3720	0.140*

H1C	−0.1417	−0.0620	0.3055	0.140*
C2	−0.06900 (19)	0.04061 (9)	0.29032 (15)	0.0586 (4)
C3	−0.0157 (2)	0.08071 (10)	0.38294 (14)	0.0628 (5)
H3	−0.0547	0.0720	0.4539	0.075*
C4	0.0936 (2)	0.13334 (9)	0.37380 (13)	0.0563 (4)
C5	0.1455 (3)	0.17747 (12)	0.47572 (16)	0.0809 (6)
H5A	0.0757	0.1714	0.5354	0.121*
H5B	0.1487	0.2268	0.4543	0.121*
H5C	0.2452	0.1623	0.5022	0.121*
C6	0.15174 (18)	0.14558 (8)	0.26761 (13)	0.0484 (4)
H6	0.2263	0.1801	0.2594	0.058*
C7	0.09907 (16)	0.10652 (8)	0.17396 (12)	0.0438 (3)
C8	−0.01108 (17)	0.05444 (9)	0.18535 (14)	0.0509 (4)
H8	−0.0461	0.0287	0.1218	0.061*
C9	0.15521 (17)	0.11830 (8)	0.05858 (13)	0.0463 (4)
C10	0.33337 (17)	0.17600 (8)	−0.04896 (12)	0.0468 (4)
C11	0.26329 (16)	0.22905 (8)	−0.12040 (12)	0.0463 (4)
C12	0.14226 (19)	0.27236 (10)	−0.09065 (14)	0.0578 (4)
H12	0.1017	0.2681	−0.0192	0.069*
C13	0.0840 (2)	0.32105 (11)	−0.16753 (17)	0.0676 (5)
H13	0.0035	0.3500	−0.1478	0.081*
C14	0.1433 (2)	0.32802 (10)	−0.27457 (17)	0.0662 (5)
H14	0.1015	0.3610	−0.3262	0.079*
C15	0.26313 (19)	0.28648 (9)	−0.30426 (14)	0.0561 (4)
H15	0.3034	0.2916	−0.3757	0.067*
C16	0.32475 (16)	0.23645 (8)	−0.22752 (12)	0.0465 (4)
C17	0.45363 (18)	0.19228 (9)	−0.25804 (13)	0.0536 (4)
C18	0.65359 (19)	0.10239 (10)	−0.19097 (16)	0.0624 (5)
C19	0.6200 (3)	0.04906 (15)	−0.2852 (2)	0.1083 (9)
H19A	0.7114	0.0237	−0.3011	0.163*
H19B	0.5830	0.0736	−0.3526	0.163*
H19C	0.5443	0.0160	−0.2618	0.163*
C20	0.7848 (2)	0.15067 (13)	−0.2199 (3)	0.0987 (8)
H20A	0.8019	0.1851	−0.1602	0.148*
H20B	0.7603	0.1749	−0.2904	0.148*
H20C	0.8750	0.1226	−0.2275	0.148*
C21	0.6985 (3)	0.06425 (15)	−0.0799 (2)	0.1006 (8)
H21A	0.7924	0.0391	−0.0883	0.151*
H21B	0.6202	0.0310	−0.0619	0.151*
H21C	0.7112	0.0986	−0.0196	0.151*
N1	0.44872 (15)	0.13807 (7)	−0.07117 (11)	0.0521 (3)
N2	0.51350 (15)	0.14770 (7)	−0.17419 (11)	0.0531 (4)
O1	0.10477 (15)	0.09179 (7)	−0.02755 (9)	0.0687 (4)
O2	0.27700 (12)	0.16353 (6)	0.05844 (8)	0.0525 (3)
O3	0.50744 (16)	0.19522 (9)	−0.35226 (10)	0.0811 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0836 (15)	0.1065 (17)	0.0913 (15)	−0.0374 (13)	0.0168 (12)	0.0187 (13)
C2	0.0530 (9)	0.0635 (10)	0.0599 (10)	−0.0050 (8)	0.0100 (8)	0.0118 (8)
C3	0.0667 (11)	0.0748 (12)	0.0481 (9)	0.0025 (9)	0.0174 (8)	0.0133 (9)
C4	0.0660 (11)	0.0594 (10)	0.0438 (8)	0.0052 (8)	0.0057 (7)	0.0035 (7)
C5	0.1118 (17)	0.0858 (14)	0.0454 (10)	−0.0070 (12)	0.0064 (10)	−0.0040 (9)
C6	0.0504 (9)	0.0490 (8)	0.0461 (8)	−0.0003 (7)	0.0052 (6)	0.0036 (7)
C7	0.0421 (8)	0.0469 (8)	0.0428 (7)	0.0039 (6)	0.0067 (6)	0.0030 (6)
C8	0.0482 (9)	0.0533 (9)	0.0516 (9)	−0.0023 (7)	0.0051 (7)	0.0016 (7)
C9	0.0461 (8)	0.0484 (8)	0.0448 (8)	−0.0023 (6)	0.0054 (6)	−0.0002 (7)
C10	0.0441 (8)	0.0591 (9)	0.0379 (7)	−0.0071 (7)	0.0091 (6)	−0.0019 (7)
C11	0.0410 (8)	0.0560 (9)	0.0423 (8)	−0.0064 (6)	0.0072 (6)	−0.0055 (7)
C12	0.0516 (9)	0.0696 (11)	0.0533 (9)	0.0013 (8)	0.0153 (7)	−0.0044 (8)
C13	0.0540 (10)	0.0737 (12)	0.0757 (12)	0.0110 (9)	0.0101 (9)	−0.0027 (10)
C14	0.0611 (11)	0.0718 (11)	0.0650 (11)	0.0046 (9)	−0.0037 (9)	0.0100 (9)
C15	0.0551 (10)	0.0677 (10)	0.0459 (8)	−0.0044 (8)	0.0046 (7)	0.0018 (8)
C16	0.0420 (8)	0.0576 (9)	0.0401 (7)	−0.0058 (7)	0.0060 (6)	−0.0031 (7)
C17	0.0480 (9)	0.0685 (10)	0.0452 (8)	−0.0028 (8)	0.0126 (7)	−0.0021 (8)
C18	0.0509 (10)	0.0663 (11)	0.0710 (11)	0.0090 (8)	0.0148 (8)	−0.0055 (9)
C19	0.0810 (16)	0.1075 (18)	0.136 (2)	0.0210 (14)	0.0026 (15)	−0.0579 (17)
C20	0.0515 (12)	0.0989 (17)	0.148 (2)	0.0077 (11)	0.0250 (13)	0.0081 (16)
C21	0.0916 (17)	0.1129 (19)	0.0984 (17)	0.0488 (15)	0.0183 (13)	0.0172 (14)
N1	0.0488 (8)	0.0610 (8)	0.0472 (7)	−0.0021 (6)	0.0103 (6)	0.0013 (6)
N2	0.0481 (8)	0.0622 (8)	0.0501 (7)	0.0044 (6)	0.0150 (6)	0.0003 (6)
O1	0.0797 (9)	0.0804 (9)	0.0463 (6)	−0.0271 (7)	0.0065 (6)	−0.0067 (6)
O2	0.0512 (6)	0.0686 (7)	0.0383 (5)	−0.0120 (5)	0.0102 (4)	−0.0012 (5)
O3	0.0777 (9)	0.1161 (11)	0.0520 (7)	0.0211 (8)	0.0310 (6)	0.0112 (7)

Geometric parameters (Å, º)

C1—C2	1.508 (3)	C12—C13	1.367 (3)
C1—H1A	0.9600	C12—H12	0.9300
C1—H1B	0.9600	C13—C14	1.389 (3)
C1—H1C	0.9600	C13—H13	0.9300
C2—C8	1.380 (2)	C14—C15	1.369 (2)
C2—C3	1.386 (3)	C14—H14	0.9300
C3—C4	1.386 (2)	C15—C16	1.393 (2)
C3—H3	0.9300	C15—H15	0.9300
C4—C6	1.388 (2)	C16—C17	1.462 (2)
C4—C5	1.509 (3)	C17—O3	1.2243 (18)
C5—H5A	0.9600	C17—N2	1.378 (2)
C5—H5B	0.9600	C18—C19	1.511 (3)
C5—H5C	0.9600	C18—N2	1.517 (2)
C6—C7	1.383 (2)	C18—C20	1.518 (3)
C6—H6	0.9300	C18—C21	1.523 (3)
C7—C8	1.387 (2)	C19—H19A	0.9600

C7—C9	1.4796 (19)	C19—H19B	0.9600
C8—H8	0.9300	C19—H19C	0.9600
C9—O1	1.1939 (18)	C20—H20A	0.9600
C9—O2	1.3668 (18)	C20—H20B	0.9600
C10—N1	1.276 (2)	C20—H20C	0.9600
C10—O2	1.3958 (17)	C21—H21A	0.9600
C10—C11	1.424 (2)	C21—H21B	0.9600
C11—C16	1.3985 (19)	C21—H21C	0.9600
C11—C12	1.397 (2)	N1—N2	1.3725 (17)

C2—C1—H1A	109.5	C12—C13—H13	119.5
C2—C1—H1B	109.5	C14—C13—H13	119.5
H1A—C1—H1B	109.5	C15—C14—C13	120.16 (17)
C2—C1—H1C	109.5	C15—C14—H14	119.9
H1A—C1—H1C	109.5	C13—C14—H14	119.9
H1B—C1—H1C	109.5	C14—C15—C16	120.01 (15)
C8—C2—C3	118.23 (15)	C14—C15—H15	120.0
C8—C2—C1	120.53 (17)	C16—C15—H15	120.0
C3—C2—C1	121.24 (16)	C15—C16—C11	119.56 (14)
C2—C3—C4	122.48 (15)	C15—C16—C17	120.42 (14)
C2—C3—H3	118.8	C11—C16—C17	120.02 (14)
C4—C3—H3	118.8	O3—C17—N2	121.47 (15)
C3—C4—C6	118.23 (15)	O3—C17—C16	122.15 (16)
C3—C4—C5	121.03 (16)	N2—C17—C16	116.37 (13)
C6—C4—C5	120.73 (16)	C19—C18—N2	109.48 (15)
C4—C5—H5A	109.5	C19—C18—C20	110.88 (19)
C4—C5—H5B	109.5	N2—C18—C20	108.96 (15)
H5A—C5—H5B	109.5	C19—C18—C21	110.5 (2)
C4—C5—H5C	109.5	N2—C18—C21	109.42 (14)
H5A—C5—H5C	109.5	C20—C18—C21	107.58 (19)
H5B—C5—H5C	109.5	C18—C19—H19A	109.5
C7—C6—C4	120.15 (15)	C18—C19—H19B	109.5
C7—C6—H6	119.9	H19A—C19—H19B	109.5
C4—C6—H6	119.9	C18—C19—H19C	109.5
C6—C7—C8	120.43 (14)	H19A—C19—H19C	109.5
C6—C7—C9	122.33 (13)	H19B—C19—H19C	109.5
C8—C7—C9	117.24 (13)	C18—C20—H20A	109.5
C2—C8—C7	120.47 (15)	C18—C20—H20B	109.5
C2—C8—H8	119.8	H20A—C20—H20B	109.5
C7—C8—H8	119.8	C18—C20—H20C	109.5
O1—C9—O2	121.23 (13)	H20A—C20—H20C	109.5
O1—C9—C7	125.91 (14)	H20B—C20—H20C	109.5
O2—C9—C7	112.86 (12)	C18—C21—H21A	109.5
N1—C10—O2	114.20 (14)	C18—C21—H21B	109.5
N1—C10—C11	126.62 (13)	H21A—C21—H21B	109.5
O2—C10—C11	119.16 (13)	C18—C21—H21C	109.5
C16—C11—C12	119.86 (15)	H21A—C21—H21C	109.5
C16—C11—C10	115.11 (13)	H21B—C21—H21C	109.5

C12—C11—C10	125.03 (14)	C10—N1—N2	118.22 (13)
C13—C12—C11	119.38 (15)	N1—N2—C17	123.30 (13)
C13—C12—H12	120.3	N1—N2—C18	114.41 (13)
C11—C12—H12	120.3	C17—N2—C18	122.24 (13)
C12—C13—C14	121.03 (17)	C9—O2—C10	114.60 (11)

C8—C2—C3—C4	−0.5 (3)	C12—C11—C16—C15	−0.8 (2)
C1—C2—C3—C4	−179.50 (18)	C10—C11—C16—C15	179.37 (14)
C2—C3—C4—C6	−0.4 (3)	C12—C11—C16—C17	178.66 (14)
C2—C3—C4—C5	178.11 (18)	C10—C11—C16—C17	−1.1 (2)
C3—C4—C6—C7	0.9 (2)	C15—C16—C17—O3	−3.2 (3)
C5—C4—C6—C7	−177.60 (16)	C11—C16—C17—O3	177.35 (16)
C4—C6—C7—C8	−0.6 (2)	C15—C16—C17—N2	175.80 (14)
C4—C6—C7—C9	178.92 (14)	C11—C16—C17—N2	−3.7 (2)
C3—C2—C8—C7	0.9 (2)	O2—C10—N1—N2	−178.84 (12)
C1—C2—C8—C7	179.90 (17)	C11—C10—N1—N2	−0.7 (2)
C6—C7—C8—C2	−0.4 (2)	C10—N1—N2—C17	−5.0 (2)
C9—C7—C8—C2	−179.87 (14)	C10—N1—N2—C18	177.70 (14)
C6—C7—C9—O1	−172.15 (16)	O3—C17—N2—N1	−174.04 (16)
C8—C7—C9—O1	7.3 (2)	C16—C17—N2—N1	7.0 (2)
C6—C7—C9—O2	8.7 (2)	O3—C17—N2—C18	3.0 (3)
C8—C7—C9—O2	−171.80 (13)	C16—C17—N2—C18	−175.93 (14)
N1—C10—C11—C16	3.6 (2)	C19—C18—N2—N1	113.71 (19)
O2—C10—C11—C16	−178.33 (13)	C20—C18—N2—N1	−124.88 (18)
N1—C10—C11—C12	−176.22 (16)	C21—C18—N2—N1	−7.5 (2)
O2—C10—C11—C12	1.9 (2)	C19—C18—N2—C17	−63.6 (2)
C16—C11—C12—C13	0.8 (2)	C20—C18—N2—C17	57.8 (2)
C10—C11—C12—C13	−179.44 (16)	C21—C18—N2—C17	175.19 (18)
C11—C12—C13—C14	0.0 (3)	O1—C9—O2—C10	0.8 (2)
C12—C13—C14—C15	−0.8 (3)	C7—C9—O2—C10	179.99 (12)
C13—C14—C15—C16	0.8 (3)	N1—C10—O2—C9	−97.91 (16)
C14—C15—C16—C11	0.1 (2)	C11—C10—O2—C9	83.76 (17)
C14—C15—C16—C17	−179.44 (16)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···O1^{i}	0.93	2.56	3.391 (2)	149
C12—H12···O3^{ii}	0.93	2.27	3.149 (2)	157

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