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Diethyl 4-(1*H*-indol-3-yl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate

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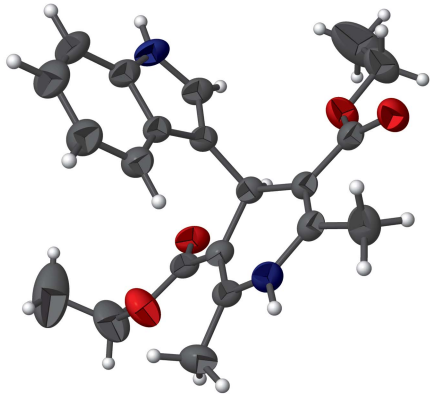
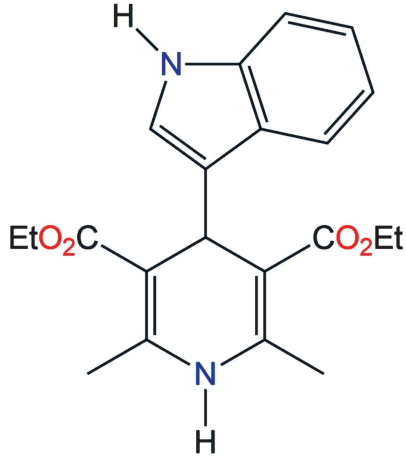
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{21}H_{24}N_2O_4$, the 1,4-dihydropyridine ring adopts a very flattened boat conformation, with the 3-pyridine substituent in an axial orientation. The pyridine ring is almost orthogonally twisted relative to the 1,4-dihydropyridine skeleton by 85.97 (2)°. In the crystal, pairs of N—H···O hydrogen bonds form inversion dimers enclosing $R_2^2(16)$ rings. Pairs of intermolecular N—H···O hydrogen bonds link the dimers into chains along [100].

3D view



Chemical scheme



Structure description

1,4-dihydropyridine (1,4-DHP) derivatives are known as Hantzsch compounds. According to our recent report, they show anti-cancer activities against the HCT116 human colon cancer cell lines (Ahn *et al.*, 2018). Their biological activities include anticonvulsant (Prasanthi *et al.*, 2014), calcium channel modulator (Budriesi *et al.*, 2005), anti-tubercular (Khoshneviszadeh *et al.*, 2009) and antimycobacterial activities (Lentz *et al.*, 2016).

The molecular structure of the title compound is shown in Fig. 1. The 1,4-dihydropyridine (C1–C5/N1) ring is slightly twisted from planarity, with a maximum deviation of 0.138 (1) Å at C3 (r.m.s. deviation = 0.091 Å). The dihedral angle formed between the plane of the 1,4-dihydropyridine (C1–C5/N1) ring and the indole (C10–C17/N2; r.m.s. deviation = 0.011 Å) ring is 85.97 (2)°. One of the carbonyl groups (C7═O1) lies on the same side of the plane as the methyl group at C6, while the other carbonyl group (C18═O3) lies on the opposite side to the methyl group at C21.

In the crystal structure, pairs of N2—H2···O3^{ii} hydrogen bonds form inversion dimers enclosing $R^2_2(16)$ rings (Table 1, Fig. 2). The dimers are linked into chains along the *a*-axis direction by pairs of N1—H1···O1^{i} hydrogen bonds (Table 1, Fig. 3).

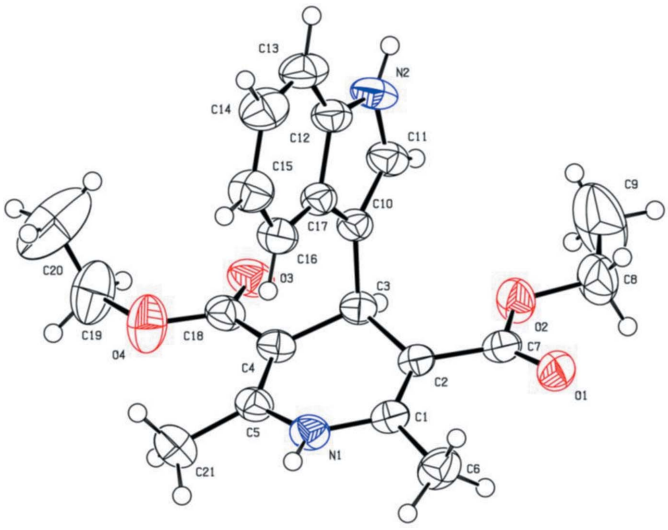


Figure 1
The molecular structure of the title compound, showing the atom-labelling scheme with displacement ellipsoids drawn at the 30% probability level.

Synthesis and crystallization

Methyl acetoacetate (20 mmol) and indole-3-carbaldehyde (10 mmol) were dissolved in 30 ml of ethanol to give a clear solution. To the mixture, ammonium acetate (10 mmol) was added and the reaction mixture was heated at 363 K for 2 h. After completion of the reaction (monitored by TLC), the mixture was cooled to room temperature to produce a solid product. This solid was recrystallized from ethanol solution to obtain single-crystal of the title the compound in 51% yield.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.90 (2)	2.18 (2)	3.009 (2)	153 (2)
N2—H2···O3^{ii}	0.91 (2)	2.00 (2)	2.906 (3)	173 (3)
C6—H6B···O1^{i}	0.97	2.49	3.296 (3)	140
C13—H13···O1^{iii}	0.94	2.58	3.357 (3)	140

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{21}H_{24}N_2O_4$
M_r	368.42
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	223
a, b, c (Å)	10.6258 (5), 10.2217 (5), 18.0993 (8)
β (°)	90.798 (2)
V (Å^3)	1965.64 (16)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.24 × 0.18 × 0.14
Data collection	
Diffractometer	PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2012)
T_{min}, T_{max}	0.686, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	83213, 4908, 3123
R_{int}	0.096
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.063, 0.198, 1.03
No. of reflections	4908
No. of parameters	254
No. of restraints	4
H-atom treatment	H-atom parameters not refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.54, −0.48

Computer programs: *APEX2* and *SAINT* (Bruker, 2012), *SHELXS* and *SHELXTL* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *publCIF* (Westrip, 2010).

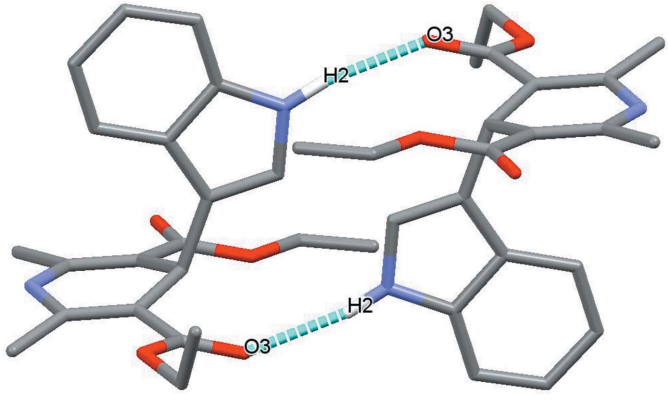


Figure 2
Part of the structure showing a dimer formed by N—H···N hydrogen bonds (shown as blue dashed lines).

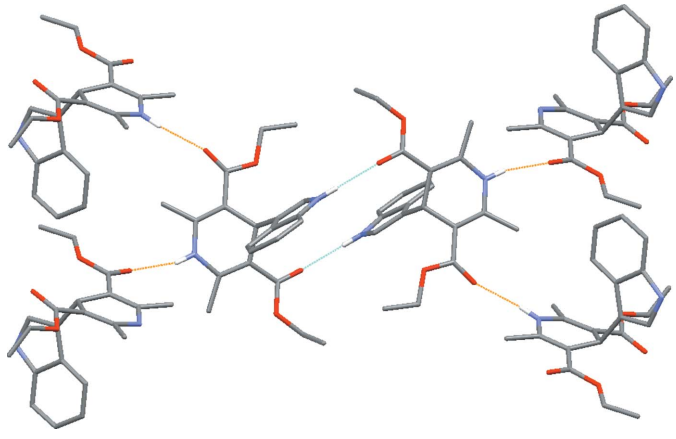


Figure 3
Part of the crystal structure showing N—H···N hydrogen bonds as orange dash lines. For clarity only those H atoms involved in hydrogen bonding are shown.

Funding information

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full crystallographic data

IUCrData (2019). **4**, x190193 [https://doi.org/10.1107/S2414314619001937]

Diethyl 4-(1*H*-indol-3-yl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate

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Crystal data

$C_{21}H_{24}N_2O_4$
M_r = 368.42
Monoclinic, $P2_1/c$
a = 10.6258 (5) Å
b = 10.2217 (5) Å
c = 18.0993 (8) Å
β = 90.798 (2)°
V = 1965.64 (16) Å^3
Z = 4
$F(000)$ = 784
D_x = 1.245 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9897 reflections
θ = 2.3–25.4°
μ = 0.09 mm^{-1}
T = 223 K
Block, colourless
0.24 × 0.18 × 0.14 mm

Data collection

PHOTON 100 CMOS diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2012)
T_{min} = 0.686, T_{max} = 0.746
83213 measured reflections
4908 independent reflections
3123 reflections with $I > 2\sigma(I)$
R_{int} = 0.096
θ_{max} = 28.3°, θ_{min} = 1.9°
h = −14→14
k = −13→13
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.198
S = 1.02
4908 reflections
254 parameters
4 restraints
Hydrogen site location: mixed
H-atom parameters not refined
$w = 1/[\sigma^2(F_o^2) + (0.087P)^2 + 1.2621P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
N1	0.00309 (17)	0.61066 (19)	0.15703 (10)	0.0407 (4)

H1	−0.0613 (19)	0.648 (2)	0.1808 (13)	0.049*
C1	0.04291 (19)	0.4898 (2)	0.18142 (12)	0.0381 (5)
C2	0.13159 (19)	0.4253 (2)	0.14337 (11)	0.0358 (5)
C3	0.19820 (19)	0.4892 (2)	0.07873 (11)	0.0367 (5)
H3	0.2050	0.4229	0.0391	0.044*
C4	0.12181 (19)	0.6032 (2)	0.04792 (11)	0.0375 (5)
C5	0.0307 (2)	0.6611 (2)	0.08802 (12)	0.0394 (5)
C6	−0.0235 (3)	0.4445 (3)	0.24927 (14)	0.0536 (6)
H6A	−0.0521	0.3552	0.2422	0.080*
H6B	−0.0952	0.5007	0.2582	0.080*
H6C	0.0339	0.4482	0.2914	0.080*
C7	0.1697 (2)	0.2926 (2)	0.16465 (12)	0.0401 (5)
O1	0.14621 (16)	0.23585 (17)	0.22188 (10)	0.0525 (5)
O2	0.23841 (17)	0.23580 (16)	0.11138 (9)	0.0528 (5)
C8	0.2857 (3)	0.1066 (3)	0.12725 (17)	0.0689 (8)
H8A	0.2160	0.0440	0.1291	0.083*
H8B	0.3297	0.1059	0.1752	0.083*
C9	0.3752 (5)	0.0696 (5)	0.0667 (2)	0.131 (2)
H9A	0.3319	0.0747	0.0192	0.196*
H9B	0.4051	−0.0190	0.0747	0.196*
H9C	0.4462	0.1293	0.0672	0.196*
C10	0.33057 (19)	0.5307 (2)	0.10047 (11)	0.0366 (5)
C11	0.4375 (2)	0.4691 (3)	0.07841 (13)	0.0443 (5)
H11	0.4394	0.3950	0.0476	0.053*
N2	0.54168 (18)	0.5301 (2)	0.10733 (11)	0.0497 (5)
H2	0.6204 (18)	0.505 (3)	0.0940 (15)	0.060*
C12	0.5038 (2)	0.6340 (3)	0.14898 (12)	0.0434 (5)
C13	0.5751 (2)	0.7250 (3)	0.18868 (14)	0.0569 (7)
H13	0.6635	0.7225	0.1884	0.068*
C14	0.5125 (3)	0.8182 (3)	0.22819 (16)	0.0611 (7)
H14	0.5588	0.8798	0.2559	0.073*
C15	0.3812 (3)	0.8233 (3)	0.22806 (15)	0.0554 (6)
H15	0.3404	0.8879	0.2558	0.067*
C16	0.3107 (2)	0.7345 (2)	0.18760 (13)	0.0455 (5)
H16	0.2223	0.7396	0.1874	0.055*
C17	0.37063 (19)	0.6372 (2)	0.14690 (12)	0.0379 (5)
C18	0.1572 (2)	0.6424 (2)	−0.02674 (13)	0.0434 (5)
O3	0.21205 (15)	0.57075 (19)	−0.06892 (9)	0.0527 (5)
O4	0.1257 (2)	0.76502 (19)	−0.04444 (10)	0.0688 (6)
C19	0.1540 (3)	0.8084 (4)	−0.11777 (17)	0.0840 (10)
H19A	0.0812	0.8548	−0.1390	0.101*
H19B	0.1719	0.7328	−0.1492	0.101*
C20	0.2678 (5)	0.8993 (6)	−0.1152 (3)	0.144 (2)
H20A	0.2520	0.9706	−0.0812	0.215*
H20B	0.2823	0.9343	−0.1642	0.215*
H20C	0.3413	0.8508	−0.0986	0.215*
C21	−0.0505 (3)	0.7756 (3)	0.06674 (15)	0.0557 (7)
H21A	−0.0035	0.8561	0.0740	0.084*

H21B	−0.1248	0.7768	0.0973	0.084*
H21C	−0.0756	0.7680	0.0152	0.084*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0359 (9)	0.0443 (11)	0.0421 (10)	0.0035 (8)	0.0093 (8)	−0.0045 (8)
C1	0.0335 (10)	0.0409 (12)	0.0400 (11)	−0.0048 (9)	0.0042 (9)	−0.0035 (9)
C2	0.0310 (10)	0.0386 (11)	0.0380 (11)	−0.0024 (8)	0.0031 (8)	−0.0007 (9)
C3	0.0333 (10)	0.0409 (12)	0.0361 (11)	0.0004 (9)	0.0038 (8)	−0.0014 (9)
C4	0.0308 (10)	0.0453 (12)	0.0362 (11)	−0.0004 (9)	−0.0004 (8)	−0.0025 (9)
C5	0.0349 (11)	0.0415 (12)	0.0417 (11)	0.0006 (9)	−0.0035 (9)	−0.0031 (9)
C6	0.0570 (15)	0.0502 (14)	0.0542 (14)	−0.0020 (12)	0.0224 (12)	−0.0021 (12)
C7	0.0323 (10)	0.0420 (12)	0.0461 (12)	−0.0039 (9)	0.0041 (9)	−0.0024 (10)
O1	0.0498 (10)	0.0510 (10)	0.0570 (10)	0.0044 (8)	0.0163 (8)	0.0125 (8)
O2	0.0616 (11)	0.0435 (9)	0.0536 (10)	0.0114 (8)	0.0154 (8)	0.0003 (8)
C8	0.079 (2)	0.0482 (16)	0.080 (2)	0.0195 (14)	0.0211 (16)	0.0032 (14)
C9	0.166 (5)	0.105 (3)	0.123 (3)	0.075 (3)	0.057 (3)	0.013 (3)
C10	0.0309 (10)	0.0454 (12)	0.0335 (10)	0.0019 (9)	0.0050 (8)	0.0062 (9)
C11	0.0351 (11)	0.0564 (14)	0.0414 (12)	0.0046 (10)	0.0052 (9)	0.0003 (11)
N2	0.0293 (9)	0.0713 (14)	0.0486 (11)	0.0064 (9)	0.0059 (8)	−0.0001 (10)
C12	0.0322 (11)	0.0590 (14)	0.0392 (11)	0.0001 (10)	0.0037 (9)	0.0073 (10)
C13	0.0368 (12)	0.0796 (19)	0.0540 (14)	−0.0115 (13)	−0.0055 (11)	0.0054 (14)
C14	0.0548 (16)	0.0669 (18)	0.0614 (16)	−0.0131 (14)	−0.0099 (13)	−0.0080 (14)
C15	0.0530 (15)	0.0546 (15)	0.0586 (15)	−0.0028 (12)	−0.0026 (12)	−0.0103 (12)
C16	0.0387 (12)	0.0481 (13)	0.0498 (13)	0.0004 (10)	0.0002 (10)	−0.0027 (11)
C17	0.0318 (10)	0.0455 (12)	0.0365 (10)	−0.0004 (9)	0.0016 (8)	0.0070 (9)
C18	0.0360 (11)	0.0508 (14)	0.0432 (12)	−0.0003 (10)	−0.0059 (9)	0.0014 (11)
O3	0.0418 (9)	0.0740 (12)	0.0424 (9)	0.0091 (8)	0.0071 (7)	0.0025 (8)
O4	0.1006 (16)	0.0565 (12)	0.0496 (11)	0.0063 (11)	0.0064 (10)	0.0113 (9)
C19	0.123 (3)	0.077 (2)	0.0526 (17)	−0.005 (2)	−0.0008 (18)	0.0205 (16)
C20	0.187 (5)	0.153 (5)	0.092 (3)	−0.089 (4)	0.022 (3)	0.004 (3)
C21	0.0513 (14)	0.0575 (16)	0.0581 (15)	0.0149 (12)	−0.0031 (12)	−0.0005 (13)

Geometric parameters (Å, º)

N1—C1	1.376 (3)	C11—N2	1.368 (3)
N1—C5	1.387 (3)	C11—H11	0.9400
N1—H1	0.899 (16)	N2—C12	1.366 (3)
C1—C2	1.348 (3)	N2—H2	0.911 (17)
C1—C6	1.498 (3)	C12—C13	1.393 (4)
C2—C7	1.465 (3)	C12—C17	1.416 (3)
C2—C3	1.523 (3)	C13—C14	1.369 (4)
C3—C10	1.516 (3)	C13—H13	0.9400
C3—C4	1.521 (3)	C14—C15	1.396 (4)
C3—H3	0.9900	C14—H14	0.9400
C4—C5	1.354 (3)	C15—C16	1.381 (3)
C4—C18	1.463 (3)	C15—H15	0.9400

C5—C21	1.501 (3)	C16—C17	1.397 (3)
C6—H6A	0.9700	C16—H16	0.9400
C6—H6B	0.9700	C18—O3	1.213 (3)
C6—H6C	0.9700	C18—O4	1.335 (3)
C7—O1	1.216 (3)	O4—C19	1.435 (3)
C7—O2	1.349 (3)	C19—C20	1.5250 (19)
O2—C8	1.440 (3)	C19—H19A	0.9800
C8—C9	1.509 (3)	C19—H19B	0.9800
C8—H8A	0.9800	C20—H20A	0.9700
C8—H8B	0.9800	C20—H20B	0.9700
C9—H9A	0.9700	C20—H20C	0.9700
C9—H9B	0.9700	C21—H21A	0.9700
C9—H9C	0.9700	C21—H21B	0.9700
C10—C11	1.364 (3)	C21—H21C	0.9700
C10—C17	1.436 (3)		

C1—N1—C5	123.70 (18)	C10—C11—N2	110.5 (2)
C1—N1—H1	117.4 (16)	C10—C11—H11	124.7
C5—N1—H1	116.5 (16)	N2—C11—H11	124.7
C2—C1—N1	119.32 (19)	C12—N2—C11	108.83 (19)
C2—C1—C6	127.5 (2)	C12—N2—H2	130.1 (18)
N1—C1—C6	113.22 (19)	C11—N2—H2	120.7 (18)
C1—C2—C7	120.77 (19)	N2—C12—C13	129.9 (2)
C1—C2—C3	121.2 (2)	N2—C12—C17	107.8 (2)
C7—C2—C3	117.99 (18)	C13—C12—C17	122.3 (2)
C10—C3—C4	111.69 (18)	C14—C13—C12	118.0 (2)
C10—C3—C2	111.10 (17)	C14—C13—H13	121.0
C4—C3—C2	111.04 (17)	C12—C13—H13	121.0
C10—C3—H3	107.6	C13—C14—C15	121.2 (3)
C4—C3—H3	107.6	C13—C14—H14	119.4
C2—C3—H3	107.6	C15—C14—H14	119.4
C5—C4—C18	124.7 (2)	C16—C15—C14	120.8 (3)
C5—C4—C3	121.34 (19)	C16—C15—H15	119.6
C18—C4—C3	113.93 (18)	C14—C15—H15	119.6
C4—C5—N1	118.8 (2)	C15—C16—C17	120.0 (2)
C4—C5—C21	128.0 (2)	C15—C16—H16	120.0
N1—C5—C21	113.2 (2)	C17—C16—H16	120.0
C1—C6—H6A	109.5	C16—C17—C12	117.7 (2)
C1—C6—H6B	109.5	C16—C17—C10	135.6 (2)
H6A—C6—H6B	109.5	C12—C17—C10	106.63 (19)
C1—C6—H6C	109.5	O3—C18—O4	122.4 (2)
H6A—C6—H6C	109.5	O3—C18—C4	123.2 (2)
H6B—C6—H6C	109.5	O4—C18—C4	114.3 (2)
O1—C7—O2	121.5 (2)	C18—O4—C19	117.2 (2)
O1—C7—C2	127.3 (2)	O4—C19—C20	109.6 (3)
O2—C7—C2	111.17 (19)	O4—C19—H19A	109.7
C7—O2—C8	116.30 (19)	C20—C19—H19A	109.7
O2—C8—C9	107.9 (3)	O4—C19—H19B	109.7

O2—C8—H8A	110.1	C20—C19—H19B	109.7
C9—C8—H8A	110.1	H19A—C19—H19B	108.2
O2—C8—H8B	110.1	C19—C20—H20A	109.5
C9—C8—H8B	110.1	C19—C20—H20B	109.5
H8A—C8—H8B	108.4	H20A—C20—H20B	109.5
C8—C9—H9A	109.5	C19—C20—H20C	109.5
C8—C9—H9B	109.5	H20A—C20—H20C	109.5
H9A—C9—H9B	109.5	H20B—C20—H20C	109.5
C8—C9—H9C	109.5	C5—C21—H21A	109.5
H9A—C9—H9C	109.5	C5—C21—H21B	109.5
H9B—C9—H9C	109.5	H21A—C21—H21B	109.5
C11—C10—C17	106.24 (19)	C5—C21—H21C	109.5
C11—C10—C3	124.7 (2)	H21A—C21—H21C	109.5
C17—C10—C3	129.07 (19)	H21B—C21—H21C	109.5

C5—N1—C1—C2	12.5 (3)	C4—C3—C10—C17	51.8 (3)
C5—N1—C1—C6	−166.3 (2)	C2—C3—C10—C17	−72.8 (3)
N1—C1—C2—C7	−175.62 (19)	C17—C10—C11—N2	−0.4 (3)
C6—C1—C2—C7	3.0 (4)	C3—C10—C11—N2	180.0 (2)
N1—C1—C2—C3	6.4 (3)	C10—C11—N2—C12	−0.2 (3)
C6—C1—C2—C3	−175.0 (2)	C11—N2—C12—C13	−179.6 (2)
C1—C2—C3—C10	104.3 (2)	C11—N2—C12—C17	0.8 (3)
C7—C2—C3—C10	−73.7 (2)	N2—C12—C13—C14	−177.9 (3)
C1—C2—C3—C4	−20.7 (3)	C17—C12—C13—C14	1.6 (4)
C7—C2—C3—C4	161.33 (18)	C12—C13—C14—C15	−0.8 (4)
C10—C3—C4—C5	−105.6 (2)	C13—C14—C15—C16	−0.3 (4)
C2—C3—C4—C5	19.0 (3)	C14—C15—C16—C17	0.8 (4)
C10—C3—C4—C18	73.9 (2)	C15—C16—C17—C12	−0.1 (3)
C2—C3—C4—C18	−161.51 (18)	C15—C16—C17—C10	179.2 (2)
C18—C4—C5—N1	177.33 (19)	N2—C12—C17—C16	178.5 (2)
C3—C4—C5—N1	−3.2 (3)	C13—C12—C17—C16	−1.1 (3)
C18—C4—C5—C21	−1.1 (4)	N2—C12—C17—C10	−1.1 (2)
C3—C4—C5—C21	178.4 (2)	C13—C12—C17—C10	179.3 (2)
C1—N1—C5—C4	−14.2 (3)	C11—C10—C17—C16	−178.5 (3)
C1—N1—C5—C21	164.4 (2)	C3—C10—C17—C16	1.1 (4)
C1—C2—C7—O1	−13.3 (4)	C11—C10—C17—C12	0.9 (2)
C3—C2—C7—O1	164.7 (2)	C3—C10—C17—C12	−179.5 (2)
C1—C2—C7—O2	167.0 (2)	C5—C4—C18—O3	−159.2 (2)
C3—C2—C7—O2	−15.0 (3)	C3—C4—C18—O3	21.3 (3)
O1—C7—O2—C8	−2.1 (3)	C5—C4—C18—O4	21.9 (3)
C2—C7—O2—C8	177.6 (2)	C3—C4—C18—O4	−157.6 (2)
C7—O2—C8—C9	−171.5 (3)	O3—C18—O4—C19	3.1 (4)
C4—C3—C10—C11	−128.8 (2)	C4—C18—O4—C19	−178.0 (2)
C2—C3—C10—C11	106.7 (2)	C18—O4—C19—C20	−104.9 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.90 (2)	2.18 (2)	3.009 (2)	153 (2)
N2—H2···O3^{ii}	0.91 (2)	2.00 (2)	2.906 (3)	173 (3)
C6—H6*B*···O1^{i}	0.97	2.49	3.296 (3)	140
C13—H13···O1^{iii}	0.94	2.58	3.357 (3)	140

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