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Diethyl 2,6-dimethyl-4-(naphthalen-1-yl)-1,4-dihydropyridine-3,5-dicarboxylate

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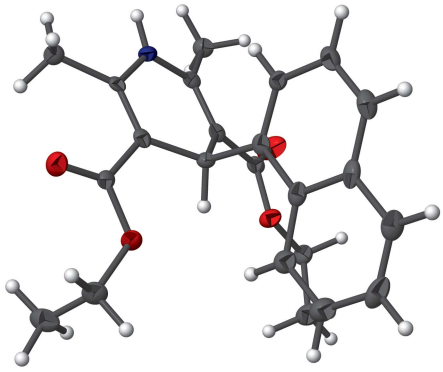
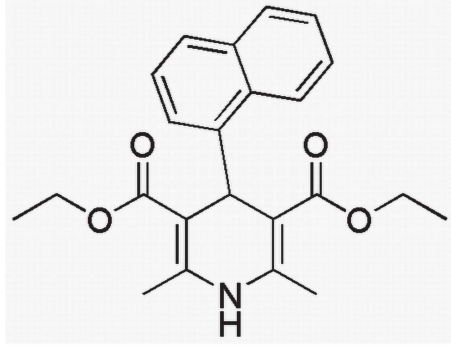
In the title compound, $C_{23}H_{25}NO_4$, the 1,4-dihydropyridine ring adopts a flattened boat conformation. The naphthalene ring system forms a dihedral angle of 88.59 (6)° with the pyridine ring. In the crystal, N—H···O and C—H···O hydrogen bonds generate an $R_2^1(6)$ ring motif and result in a zigzag chain along the *b* axis. Additional C—H···O hydrogen bonds form infinite chains along the *c*-axis direction.

3D view



Chemical scheme



Structure description

1,4-Dihydropyridines (1,4-DHPs) are an important class of chemicals widely used as drugs or their precursors (Giorgi *et al.*, 2010; Lavanya *et al.*, 2011; Datar & Pratibha, 2012). 1,4-Dihydropyridine compounds are prescribed for the treatment of hypertension and heart defibrilation (Metcalf & Holt, 2000). Dihydropyridines (DHPs), in particular 4-aryl-substituted 1,4-dihydropyridines (Hantzsch esters), have been recognized as an important class of organic calcium channel modulators for the treatment of cardiovascular diseases (Zonouz *et al.*, 2013). Herein, we report the crystal structure of the title 4-aryl-substituted 1,4-dihydropyridine compound, (Fig. 1).

The naphthalene substituent at C4 is positioned axially and is inclined to the pyridine ring at a dihedral angle of 88.590 (6)°. The pyridine ring with the naphthalene substituent at the C4 atom is significantly puckered and adopts a flattened boat conformation with atoms N1 and C4 displaced by 0.1444 (3) and 0.322 (6) Å, respectively, from the mean plane of the other four atoms C5/C6/C2/C3. Both ethylcarboxylate substituents on the dihydropyridine ring adopt *cis* orientations of the carbonyl O atoms and the adjacent methyl groups with respect to the C2═C3 and C5═C6 double bonds, respectively. This contrasts with two of three methoxy-substituted 4-phenyl-2,6-dimethyl-1,4-dihydropyridine-3,6-dicarboxylate compounds (Metcalf & Holt, 2000) where there is one *cis* and one *trans* conformation. This may be due to the presence of a bulky naphthalene group in

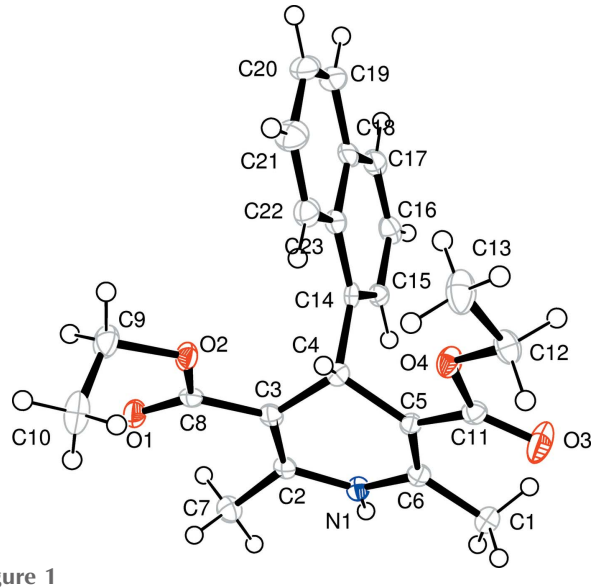


Figure 1
The molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are presented as small spheres of arbitrary radius.

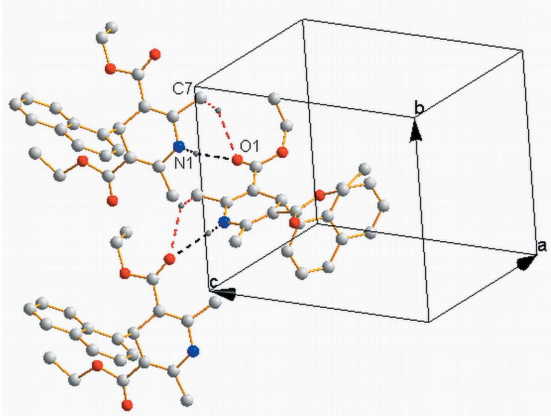


Figure 2
Fragment of an [010] chain in the title compound showing C—H···O and N—H···O interactions as dashed lines. H atoms not involved in hydrogen bonding have been excluded.

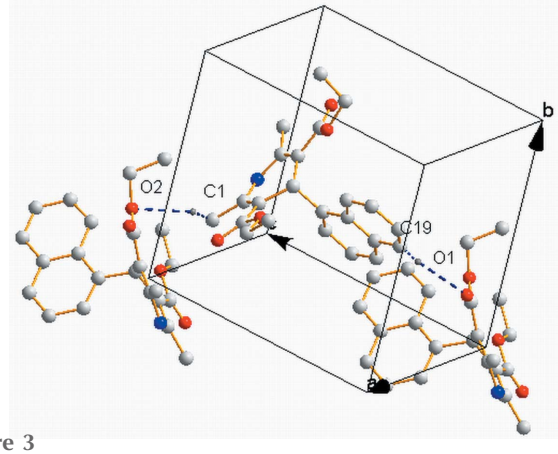


Figure 3
Fragment of an [001] chain in the title compound showing C—H···O interactions as dashed lines. H-atoms not involved in hydrogen bonding have been omitted.

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.88	2.13	2.985 (3)	164
C7—H7B···O1^{i}	0.98	2.58	3.378 (4)	138
C19—H19···O1^{ii}	0.95	2.59	3.503 (4)	161
C1—H1C···O2^{iii}	0.98	2.62	3.563 (3)	161

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{23}H_{25}NO_4$
M_r	379.44
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	100
a, b, c (Å)	8.7072 (17), 9.8740 (19), 11.221 (2)
β (°)	95.307 (6)
V (Å^3)	960.6 (3)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.18 × 0.16 × 0.16
Data collection	
Diffractometer	Bruker *SMART APEX* CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 1998)
T_{min}, T_{max}	0.984, 0.986
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7663, 3319, 3046
R_{int}	0.048
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.594
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.048, 0.123, 1.05
No. of reflections	3319
No. of parameters	257
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.30, −0.27

Computer programs: *SMART* and *SAINT-Plus* (Bruker, 1998), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows*and *WinGX* (Farrugia, 2012) and *CAMERON* (Watkin *et al.*, 1996).

the title compound. The bond lengths and angles in the title compound are in good agreement with the corresponding values in closely related structures (Fun *et al.*, 2012; Vrábel *et al.*, 2005; Giorgi *et al.*, 2010; Metcalf & Holt, 2000).

In the crystal, the O1 atom acts as a double-acceptor for the N1—H1···O1 and C7—H7···O1 hydrogen bonds (Table 1), generating an $R_2^1(6)$ ring motif and linking the molecules into zigzag chains running along the b axis (Fig. 2). C1—H1···O2 and C19—H19···O1 hydrogen bonds form infinite chains along the c-axis direction (Fig. 3).

Synthesis and crystallization

A mixture of naphthaldehyde (1 mmol), ethyl acetoacetate (2 mmol) and aqueous ammonia (1.5 mmol), was refluxed in dry ethanol (20 mmol) for 12 h. The progress of the reaction was monitored by TLC. After confirming that the reaction was complete, the reaction mixture was cooled to room tempera-

ture and allowed to stand for two days to allow the formation of a solid. The resulting solid product was washed with methanol and recrystallized from ethanol solution to yield single crystals suitable for X-ray diffraction studies (Yield: 78%; m.p. 192–194°C). The absolute structure of this compound was indeterminate in the present experiment.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The compound, crystallizes in a non-centric monoclinic space group with one molecule in the asymmetric unit but the absolute structure cannot be determined reliably by refinement of the Flack parameter because of insufficient anomalous scattering effects.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x160722 [doi:10.1107/S2414314616007227]

Diethyl 2,6-dimethyl-4-(naphthalen-1-yl)-1,4-dihydropyridine-3,5-dicarboxylate

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Diethyl 2,6-dimethyl-4-(naphthalen-1-yl)-1,4-dihydropyridine-3,5-dicarboxylate

Crystal data

$C_{23}H_{25}NO_4$
M_r = 379.44
Monoclinic, $P2_1$
Hall symbol: P 2yb
a = 8.7072 (17) Å
b = 9.8740 (19) Å
c = 11.221 (2) Å
β = 95.307 (6)°
V = 960.6 (3) Å^3
Z = 2
$F(000)$ = 404
D_x = 1.312 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3319 reflections
θ = 2.4–25.0°
μ = 0.09 mm^{-1}
T = 100 K
Block, colorless
0.18 × 0.16 × 0.16 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.984, T_{max} = 0.986
7663 measured reflections
3319 independent reflections
3046 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 25.0°, θ_{min} = 2.4°
h = −10→10
k = −11→11
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.123
S = 1.05
3319 reflections
257 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0552P)^2 + 0.5392P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.006
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.0444 (2)	0.6473 (2)	0.85079 (17)	0.0229 (5)
O3	0.6369 (2)	0.1373 (2)	0.9159 (2)	0.0363 (6)
O2	0.2555 (2)	0.6312 (2)	0.75134 (16)	0.0206 (4)
O4	0.6092 (2)	0.3009 (2)	0.77744 (16)	0.0216 (5)
C18	0.1941 (3)	0.2709 (3)	0.4733 (2)	0.0223 (6)
C6	0.3320 (3)	0.2149 (3)	0.9818 (2)	0.0165 (6)
C11	0.5595 (3)	0.2253 (3)	0.8650 (2)	0.0180 (6)
N1	0.1949 (3)	0.2706 (2)	1.00885 (18)	0.0167 (5)
H1	0.1399	0.2262	1.0580	0.020*
C5	0.4022 (3)	0.2669 (3)	0.8886 (2)	0.0159 (6)
C23	0.2732 (3)	0.3409 (3)	0.5723 (3)	0.0200 (6)
C15	0.1469 (3)	0.1912 (3)	0.7039 (2)	0.0170 (6)
H15	0.1301	0.1621	0.7823	0.020*
C4	0.3184 (3)	0.3685 (3)	0.8039 (2)	0.0161 (6)
H4	0.3960	0.4350	0.7790	0.019*
C2	0.1386 (3)	0.3929 (3)	0.9629 (2)	0.0152 (6)
C14	0.2448 (3)	0.2979 (3)	0.6911 (2)	0.0168 (6)
C19	0.2202 (4)	0.3115 (3)	0.3546 (3)	0.0266 (7)
H19	0.1682	0.2658	0.2881	0.032*
C16	0.0703 (3)	0.1230 (3)	0.6056 (2)	0.0221 (6)
H16	0.0037	0.0491	0.6177	0.026*
C8	0.1561 (3)	0.5826 (3)	0.8255 (2)	0.0159 (6)
C1	0.3898 (3)	0.1038 (3)	1.0646 (2)	0.0220 (6)
H1A	0.4127	0.0237	1.0178	0.033*
H1B	0.3109	0.0811	1.1182	0.033*
H1C	0.4839	0.1337	1.1120	0.033*
C17	0.0929 (3)	0.1642 (3)	0.4929 (3)	0.0235 (7)
H17	0.0392	0.1201	0.4263	0.028*
C7	0.0198 (3)	0.4559 (3)	1.0338 (2)	0.0223 (6)
H7A	0.0550	0.5458	1.0614	0.033*
H7B	0.0044	0.3987	1.1031	0.033*
H7C	−0.0778	0.4645	0.9834	0.033*
C3	0.1992 (3)	0.4460 (3)	0.8674 (2)	0.0167 (6)
C9	0.2391 (4)	0.7720 (3)	0.7145 (3)	0.0269 (7)
H9A	0.1285	0.7966	0.7048	0.032*
H9B	0.2814	0.7843	0.6362	0.032*
C12	0.7675 (3)	0.2790 (3)	0.7500 (3)	0.0241 (7)
H12A	0.7793	0.1872	0.7166	0.029*
H12B	0.8395	0.2884	0.8231	0.029*
C22	0.3751 (3)	0.4470 (3)	0.5484 (3)	0.0231 (7)

H22	0.4292	0.4943	0.6130	0.028*
C13	0.8000 (4)	0.3842 (4)	0.6602 (3)	0.0344 (8)
H13A	0.7254	0.3758	0.5896	0.052*
H13B	0.9046	0.3716	0.6366	0.052*
H13C	0.7913	0.4744	0.6955	0.052*
C21	0.3965 (4)	0.4823 (4)	0.4328 (3)	0.0299 (8)
H21	0.4655	0.5536	0.4182	0.036*
C20	0.3175 (4)	0.4139 (4)	0.3359 (3)	0.0304 (8)
H20	0.3328	0.4401	0.2563	0.036*
C10	0.3226 (4)	0.8625 (3)	0.8053 (3)	0.0317 (8)
H10A	0.2740	0.8570	0.8805	0.047*
H10B	0.3180	0.9560	0.7760	0.047*
H10C	0.4305	0.8338	0.8189	0.047*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0252 (11)	0.0204 (11)	0.0234 (10)	0.0072 (9)	0.0043 (8)	0.0025 (9)
O3	0.0269 (12)	0.0407 (14)	0.0427 (13)	0.0166 (11)	0.0096 (10)	0.0209 (12)
O2	0.0248 (10)	0.0155 (10)	0.0224 (10)	0.0042 (9)	0.0065 (8)	0.0050 (8)
O4	0.0167 (9)	0.0236 (11)	0.0252 (10)	0.0042 (9)	0.0053 (8)	0.0062 (9)
C18	0.0204 (14)	0.0267 (16)	0.0197 (13)	0.0118 (14)	0.0005 (11)	−0.0056 (13)
C6	0.0155 (14)	0.0156 (14)	0.0176 (14)	−0.0034 (12)	−0.0024 (11)	−0.0020 (11)
C11	0.0203 (14)	0.0169 (15)	0.0166 (13)	−0.0024 (12)	−0.0003 (11)	−0.0008 (12)
N1	0.0174 (12)	0.0154 (12)	0.0177 (11)	−0.0014 (10)	0.0044 (9)	0.0027 (10)
C5	0.0175 (13)	0.0136 (14)	0.0156 (12)	0.0005 (12)	−0.0032 (10)	−0.0017 (11)
C23	0.0198 (14)	0.0215 (16)	0.0188 (14)	0.0077 (12)	0.0017 (11)	−0.0011 (12)
C15	0.0164 (14)	0.0171 (15)	0.0179 (14)	0.0035 (12)	0.0033 (11)	0.0004 (11)
C4	0.0154 (13)	0.0157 (14)	0.0174 (13)	−0.0022 (11)	0.0025 (11)	0.0011 (12)
C2	0.0163 (13)	0.0120 (14)	0.0171 (13)	−0.0052 (12)	0.0005 (10)	−0.0024 (11)
C14	0.0156 (13)	0.0139 (14)	0.0208 (13)	0.0077 (12)	0.0009 (10)	0.0009 (12)
C19	0.0294 (17)	0.0312 (18)	0.0184 (14)	0.0082 (15)	−0.0016 (12)	−0.0014 (13)
C16	0.0193 (14)	0.0185 (16)	0.0281 (15)	0.0011 (13)	0.0005 (12)	−0.0059 (13)
C8	0.0183 (14)	0.0172 (14)	0.0120 (12)	−0.0022 (13)	0.0002 (10)	−0.0017 (11)
C1	0.0215 (14)	0.0218 (16)	0.0224 (14)	0.0017 (13)	−0.0001 (11)	0.0029 (13)
C17	0.0200 (15)	0.0242 (16)	0.0247 (15)	0.0053 (13)	−0.0062 (12)	−0.0083 (13)
C7	0.0230 (15)	0.0211 (16)	0.0235 (14)	−0.0005 (13)	0.0057 (12)	−0.0005 (13)
C3	0.0156 (13)	0.0157 (14)	0.0183 (13)	−0.0028 (12)	−0.0021 (11)	−0.0042 (12)
C9	0.0329 (17)	0.0193 (15)	0.0292 (15)	0.0031 (14)	0.0068 (13)	0.0078 (14)
C12	0.0188 (14)	0.0238 (16)	0.0308 (15)	0.0024 (14)	0.0080 (12)	−0.0023 (14)
C22	0.0212 (15)	0.0238 (17)	0.0245 (14)	0.0033 (13)	0.0027 (12)	0.0011 (13)
C13	0.0286 (17)	0.0296 (19)	0.047 (2)	0.0078 (16)	0.0163 (15)	0.0084 (17)
C21	0.0305 (18)	0.0326 (18)	0.0274 (16)	−0.0009 (15)	0.0071 (14)	0.0040 (14)
C20	0.0335 (17)	0.041 (2)	0.0170 (15)	0.0142 (16)	0.0065 (12)	0.0047 (14)
C10	0.0250 (16)	0.0201 (16)	0.050 (2)	0.0036 (13)	0.0044 (15)	0.0081 (15)

Geometric parameters (Å, º)

O1—C8	1.219 (3)	C16—C17	1.359 (4)
O3—C11	1.210 (4)	C16—H16	0.9500
O2—C8	1.344 (3)	C8—C3	1.466 (4)
O2—C9	1.454 (4)	C1—H1A	0.9800
O4—C11	1.338 (3)	C1—H1B	0.9800
O4—C12	1.457 (3)	C1—H1C	0.9800
C18—C17	1.404 (5)	C17—H17	0.9500
C18—C19	1.428 (4)	C7—H7A	0.9800
C18—C23	1.430 (4)	C7—H7B	0.9800
C6—C5	1.360 (4)	C7—H7C	0.9800
C6—N1	1.373 (4)	C9—C10	1.492 (4)
C6—C1	1.495 (4)	C9—H9A	0.9900
C11—C5	1.477 (4)	C9—H9B	0.9900
N1—C2	1.384 (4)	C12—C13	1.492 (5)
N1—H1	0.8800	C12—H12A	0.9900
C5—C4	1.521 (4)	C12—H12B	0.9900
C23—C22	1.414 (4)	C22—C21	1.372 (4)
C23—C14	1.442 (4)	C22—H22	0.9500
C15—C14	1.371 (4)	C13—H13A	0.9800
C15—C16	1.407 (4)	C13—H13B	0.9800
C15—H15	0.9500	C13—H13C	0.9800
C4—C3	1.519 (4)	C21—C20	1.405 (5)
C4—C14	1.533 (4)	C21—H21	0.9500
C4—H4	1.0000	C20—H20	0.9500
C2—C3	1.344 (4)	C10—H10A	0.9800
C2—C7	1.497 (4)	C10—H10B	0.9800
C19—C20	1.349 (5)	C10—H10C	0.9800
C19—H19	0.9500		
C8—O2—C9	117.8 (2)	H1A—C1—H1C	109.5
C11—O4—C12	116.7 (2)	H1B—C1—H1C	109.5
C17—C18—C19	120.9 (3)	C16—C17—C18	121.2 (3)
C17—C18—C23	120.3 (3)	C16—C17—H17	119.4
C19—C18—C23	118.8 (3)	C18—C17—H17	119.4
C5—C6—N1	118.7 (3)	C2—C7—H7A	109.5
C5—C6—C1	127.2 (3)	C2—C7—H7B	109.5
N1—C6—C1	114.0 (2)	H7A—C7—H7B	109.5
O3—C11—O4	122.9 (3)	C2—C7—H7C	109.5
O3—C11—C5	126.9 (3)	H7A—C7—H7C	109.5
O4—C11—C5	110.2 (2)	H7B—C7—H7C	109.5
C6—N1—C2	123.5 (2)	C2—C3—C8	120.5 (2)
C6—N1—H1	118.2	C2—C3—C4	120.9 (3)
C2—N1—H1	118.2	C8—C3—C4	118.6 (2)
C6—C5—C11	121.5 (3)	O2—C9—C10	110.5 (2)
C6—C5—C4	120.4 (2)	O2—C9—H9A	109.6
C11—C5—C4	118.1 (2)	C10—C9—H9A	109.6

C22—C23—C18	118.4 (3)	O2—C9—H9B	109.6
C22—C23—C14	123.9 (3)	C10—C9—H9B	109.6
C18—C23—C14	117.7 (3)	H9A—C9—H9B	108.1
C14—C15—C16	122.7 (3)	O4—C12—C13	106.4 (2)
C14—C15—H15	118.7	O4—C12—H12A	110.5
C16—C15—H15	118.7	C13—C12—H12A	110.5
C3—C4—C5	110.4 (2)	O4—C12—H12B	110.5
C3—C4—C14	111.4 (2)	C13—C12—H12B	110.5
C5—C4—C14	110.9 (2)	H12A—C12—H12B	108.6
C3—C4—H4	108.0	C21—C22—C23	120.7 (3)
C5—C4—H4	108.0	C21—C22—H22	119.7
C14—C4—H4	108.0	C23—C22—H22	119.7
C3—C2—N1	119.0 (2)	C12—C13—H13A	109.5
C3—C2—C7	127.1 (3)	C12—C13—H13B	109.5
N1—C2—C7	113.8 (2)	H13A—C13—H13B	109.5
C15—C14—C23	119.0 (2)	C12—C13—H13C	109.5
C15—C14—C4	118.7 (2)	H13A—C13—H13C	109.5
C23—C14—C4	122.3 (2)	H13B—C13—H13C	109.5
C20—C19—C18	120.8 (3)	C22—C21—C20	120.7 (3)
C20—C19—H19	119.6	C22—C21—H21	119.7
C18—C19—H19	119.6	C20—C21—H21	119.7
C17—C16—C15	119.2 (3)	C19—C20—C21	120.6 (3)
C17—C16—H16	120.4	C19—C20—H20	119.7
C15—C16—H16	120.4	C21—C20—H20	119.7
O1—C8—O2	122.1 (3)	C9—C10—H10A	109.5
O1—C8—C3	126.4 (2)	C9—C10—H10B	109.5
O2—C8—C3	111.5 (2)	H10A—C10—H10B	109.5
C6—C1—H1A	109.5	C9—C10—H10C	109.5
C6—C1—H1B	109.5	H10A—C10—H10C	109.5
H1A—C1—H1B	109.5	H10B—C10—H10C	109.5
C6—C1—H1C	109.5		

C12—O4—C11—O3	−3.9 (4)	C3—C4—C14—C23	110.4 (3)
C12—O4—C11—C5	175.4 (2)	C5—C4—C14—C23	−126.3 (3)
C5—C6—N1—C2	−13.3 (4)	C17—C18—C19—C20	−180.0 (3)
C1—C6—N1—C2	164.6 (2)	C23—C18—C19—C20	0.0 (4)
N1—C6—C5—C11	171.3 (2)	C14—C15—C16—C17	−0.3 (4)
C1—C6—C5—C11	−6.2 (4)	C9—O2—C8—O1	8.6 (4)
N1—C6—C5—C4	−9.9 (4)	C9—O2—C8—C3	−172.3 (2)
C1—C6—C5—C4	172.6 (3)	C15—C16—C17—C18	1.8 (4)
O3—C11—C5—C6	6.1 (5)	C19—C18—C17—C16	178.5 (3)
O4—C11—C5—C6	−173.2 (2)	C23—C18—C17—C16	−1.6 (4)
O3—C11—C5—C4	−172.8 (3)	N1—C2—C3—C8	−172.5 (2)
O4—C11—C5—C4	7.9 (3)	C7—C2—C3—C8	3.1 (4)
C17—C18—C23—C22	179.5 (3)	N1—C2—C3—C4	5.0 (4)
C19—C18—C23—C22	−0.5 (4)	C7—C2—C3—C4	−179.4 (3)
C17—C18—C23—C14	0.0 (4)	O1—C8—C3—C2	−17.1 (4)
C19—C18—C23—C14	179.9 (3)	O2—C8—C3—C2	163.9 (2)

C6—C5—C4—C3	26.8 (3)	O1—C8—C3—C4	165.3 (2)
C11—C5—C4—C3	−154.3 (2)	O2—C8—C3—C4	−13.7 (3)
C6—C5—C4—C14	−97.1 (3)	C5—C4—C3—C2	−24.4 (3)
C11—C5—C4—C14	81.8 (3)	C14—C4—C3—C2	99.2 (3)
C6—N1—C2—C3	15.9 (4)	C5—C4—C3—C8	153.2 (2)
C6—N1—C2—C7	−160.3 (2)	C14—C4—C3—C8	−83.2 (3)
C16—C15—C14—C23	−1.2 (4)	C8—O2—C9—C10	85.1 (3)
C16—C15—C14—C4	178.0 (3)	C11—O4—C12—C13	−173.9 (3)
C22—C23—C14—C15	−178.1 (3)	C18—C23—C22—C21	0.4 (4)
C18—C23—C14—C15	1.4 (4)	C14—C23—C22—C21	179.9 (3)
C22—C23—C14—C4	2.7 (4)	C23—C22—C21—C20	0.1 (5)
C18—C23—C14—C4	−177.8 (2)	C18—C19—C20—C21	0.5 (5)
C3—C4—C14—C15	−68.8 (3)	C22—C21—C20—C19	−0.6 (5)
C5—C4—C14—C15	54.5 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.88	2.13	2.985 (3)	164
C7—H7*B*···O1^{i}	0.98	2.58	3.378 (4)	138
C19—H19···O1^{ii}	0.95	2.59	3.503 (4)	161
C1—H1*C*···O2^{iii}	0.98	2.62	3.563 (3)	161

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