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Diethyl 4-(3-chlorophenyl)-2,6-diphenyl-1,4-dihydropyridine-3,5-dicarboxylate

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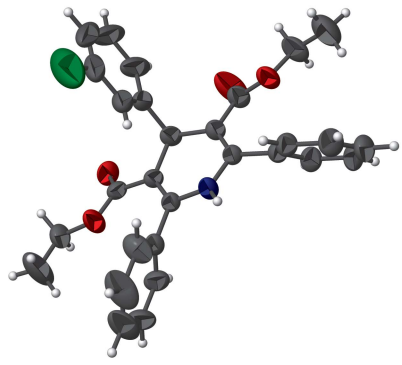
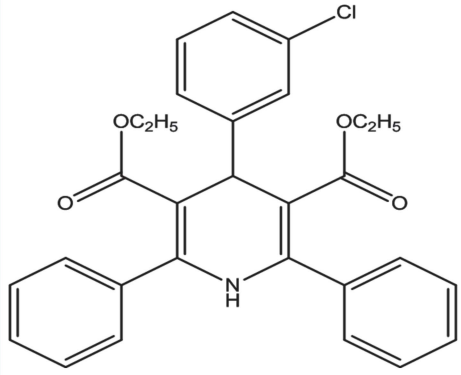
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{29}H_{26}ClNO_4$, the dihydropyridine ring adopts a shallow boat conformation. The mean plane of the dihydropyridine ring (all atoms) subtends dihedral angles of 66.54 (1), 73.71 (1) and 79.47 (1)° with the two phenyl rings and the chlorophenyl ring, respectively. In the crystal, N—H···O hydrogen bonds link the molecules into [001] chains.

3D view



Chemical scheme



Structure description

The geometric parameters of the title molecule (Fig. 1) agree well with those of reported similar structures (Wang *et al.*, 2013; Ahamed *et al.*, 2016). The dihydropyridine ring adopts a flattened boat conformation: atoms N1 and C12 are displaced out of the C7/C8/C19/C23 plane (r.m.s. deviation = 0.019 Å) by 0.124 (1) and 0.220 (2) Å, respectively. The mean plane of the pyridine ring (all atoms) subtends dihedral angles of 66.54 (1), 73.71 (1) and 79.47 (1)° with the 2- and 6-phenyl rings and the chlorophenyl ring, respectively. In the crystal, N—H···O hydrogen bonds (Fig. 2, Table 1) link the molecules into [001] chains.

Synthesis and crystallization

To an ethanolic solution of ammonium acetate (7.7 g, 0.1 mol), was added ethyl benzoylacetate (17.3 ml, 0.1 mol) followed by 3-chloro benzaldehyde (14 g, 0.1 mol). The reaction mixture was refluxed for 8 h and the turbid solution obtained was stirred for 10 min. The product separated out was washed, filtered and recrystallized from ethanol solution as yellow blocks (m.p. = 144°C, yield = 98%).

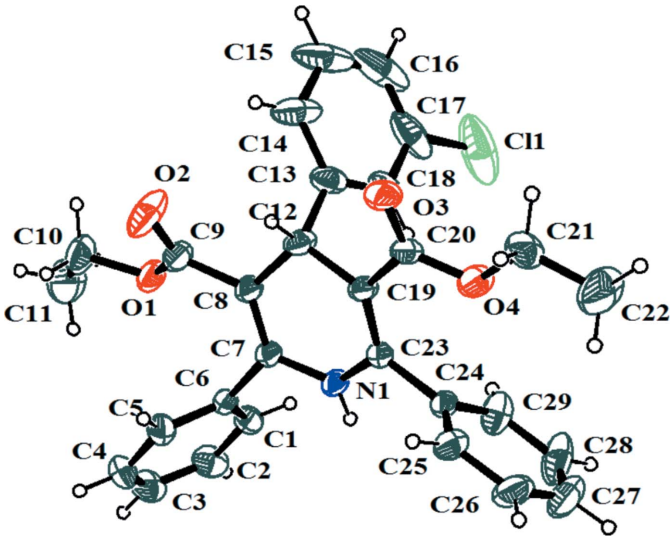


Figure 1
The molecular structure, with 30% probability displacement ellipsoids for non-H atoms.

Refinement

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

Acknowledgements

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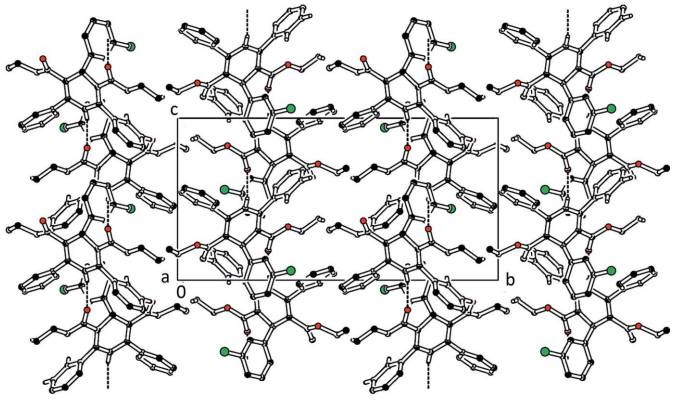

Figure 2
The packing viewed down [100]. Hydrogen bonds are shown as dashed lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O3^{i}	0.86	2.10	2.910 (2)	158

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{29}H_{26}ClNO_4$
M_r	487.96
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	295
a, b, c (Å)	10.519 (5), 22.059 (5), 11.246 (5)
β (°)	97.867 (5)
V (Å^3)	2584.9 (18)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.18
Crystal size (mm)	0.20 × 0.15 × 0.15
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Sheldrick, 1996)
T_{min}, T_{max}	0.968, 0.975
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	24505, 6384, 3478
R_{int}	0.029
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.668
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.060, 0.192, 1.06
No. of reflections	6384
No. of parameters	318
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.28, −0.40

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *SHELXL2018* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

References

Ahamed, F. M. M., Padusha, M. S. A. & Gunasekaran, B. (2016). *IUCrData*, **1**, x160155.
Bruker (2008). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst*. C**71**, 3–8.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Wang, K., Wang, Y., Yao, M. & Xu, D. (2013). *Acta Cryst.* E**69**, o785.

full crystallographic data

IUCrData (2019). **4**, x191644 [https://doi.org/10.1107/S2414314619016444]

Diethyl 4-(3-chlorophenyl)-2,6-diphenyl-1,4-dihydropyridine-3,5-dicarboxylate

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Diethyl 4-(3-chlorophenyl)-2,6-diphenyl-1,4-dihydropyridine-3,5-dicarboxylate

Crystal data

$C_{29}H_{26}ClNO_4$
M_r = 487.96
Monoclinic, $P2_1/n$
a = 10.519 (5) Å
b = 22.059 (5) Å
c = 11.246 (5) Å
β = 97.867 (5)°
V = 2584.9 (18) Å^3
Z = 4
$F(000)$ = 1024
D_x = 1.254 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6384 reflections
θ = 1.9–28.4°
μ = 0.18 mm^{-1}
T = 295 K
Block, yellow
0.20 × 0.15 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
ω and φ scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.968, T_{max} = 0.975
24505 measured reflections
6384 independent reflections
3478 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 28.4°, θ_{min} = 1.9°
h = −14→13
k = −29→22
l = −10→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.192
S = 1.06
6384 reflections
318 parameters
1 restraint
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0826P)^2 + 0.5988P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 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.

Refinement. The H atoms were positioned geometrically (N—H = 0.86, C—H = 0.93–0.98 Å) and refined as riding atoms with U_{iso}(H) = 1.2U_{eq}(carrier) or 1.5U_{eq}(methyl carrier).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.3290 (2)	0.12025 (10)	0.47589 (19)	0.0522 (5)
H1	0.364970	0.156592	0.455041	0.063*
C2	0.4059 (2)	0.07648 (12)	0.5367 (2)	0.0707 (7)
H2	0.493445	0.083358	0.556614	0.085*
C3	0.3535 (3)	0.02293 (13)	0.5679 (2)	0.0757 (8)
H3	0.405875	−0.006916	0.607098	0.091*
C4	0.2245 (3)	0.01329 (11)	0.5414 (2)	0.0722 (7)
H4	0.188850	−0.022728	0.564405	0.087*
C5	0.1469 (2)	0.05674 (10)	0.4807 (2)	0.0582 (6)
H5	0.059071	0.049997	0.463143	0.070*
C6	0.19914 (19)	0.11043 (9)	0.44583 (17)	0.0428 (5)
C7	0.11605 (18)	0.15741 (9)	0.37990 (17)	0.0420 (5)
C8	0.0443 (2)	0.15097 (9)	0.27198 (18)	0.0463 (5)
C9	0.0366 (2)	0.09426 (11)	0.2012 (2)	0.0582 (6)
C10	0.1382 (3)	0.00161 (12)	0.1628 (3)	0.0837 (9)
H10A	0.114087	0.004609	0.076599	0.100*
H10B	0.075277	−0.023292	0.195352	0.100*
C11	0.2675 (4)	−0.02572 (15)	0.1905 (4)	0.1229 (14)
H11A	0.327992	−0.002317	0.152983	0.184*
H11B	0.265646	−0.066509	0.160525	0.184*
H11C	0.292792	−0.026027	0.275777	0.184*
C12	−0.0380 (2)	0.20264 (10)	0.21539 (18)	0.0519 (5)
H12	−0.122409	0.185946	0.184374	0.062*
C13	0.0185 (3)	0.22981 (12)	0.1105 (2)	0.0680 (7)
C14	−0.0232 (3)	0.21119 (17)	−0.0070 (2)	0.1011 (12)
H14	−0.085904	0.181396	−0.021709	0.121*
C15	0.0287 (5)	0.2370 (3)	−0.1013 (3)	0.145 (2)
H15	0.000901	0.223983	−0.179177	0.173*
C16	0.1202 (6)	0.2813 (2)	−0.0823 (5)	0.144 (3)
H16	0.153730	0.298948	−0.146468	0.173*
C17	0.1613 (4)	0.29910 (15)	0.0329 (4)	0.1202 (16)
C18	0.1107 (3)	0.27333 (12)	0.1287 (3)	0.0807 (8)
H18	0.140264	0.285992	0.206414	0.097*
C19	−0.05774 (18)	0.25090 (9)	0.30708 (16)	0.0436 (5)
C20	−0.1629 (2)	0.29297 (10)	0.26751 (18)	0.0472 (5)
C21	−0.2648 (3)	0.38644 (12)	0.3016 (2)	0.0739 (8)
H21A	−0.344665	0.368346	0.317869	0.089*
H21B	−0.273729	0.397671	0.217502	0.089*
C22	−0.2347 (5)	0.43973 (18)	0.3772 (4)	0.155 (2)
H22A	−0.239300	0.429377	0.459385	0.232*
H22B	−0.295244	0.471344	0.352380	0.232*
H22C	−0.149612	0.453524	0.369464	0.232*
C23	0.02010 (18)	0.25477 (8)	0.41280 (17)	0.0406 (4)
C24	0.0185 (2)	0.30256 (9)	0.50681 (18)	0.0441 (5)
C25	−0.0794 (3)	0.30666 (11)	0.5760 (2)	0.0629 (6)

H25	−0.146413	0.278868	0.564751	0.075*
C26	−0.0796 (3)	0.35092 (14)	0.6608 (2)	0.0842 (9)
H26	−0.147338	0.353369	0.705811	0.101*
C27	0.0169 (4)	0.39077 (16)	0.6798 (3)	0.0992 (11)
H27	0.014864	0.421235	0.736649	0.119*
C28	0.1178 (4)	0.38710 (14)	0.6167 (4)	0.1079 (12)
H28	0.186047	0.414051	0.631768	0.129*
C29	0.1177 (3)	0.34263 (12)	0.5293 (3)	0.0770 (8)
H29	0.186363	0.340110	0.485386	0.092*
N1	0.11284 (16)	0.21111 (7)	0.44327 (14)	0.0462 (4)
H1A	0.170700	0.217468	0.503767	0.055*
O1	0.14323 (16)	0.06147 (7)	0.21670 (14)	0.0619 (4)
O2	−0.0565 (2)	0.07963 (10)	0.1336 (2)	0.1071 (8)
O3	−0.24413 (15)	0.28243 (7)	0.18351 (14)	0.0628 (4)
O4	−0.16058 (17)	0.34422 (8)	0.32941 (14)	0.0711 (5)
Cl1	0.28030 (17)	0.35347 (5)	0.05870 (16)	0.1984 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0512 (13)	0.0519 (13)	0.0526 (13)	0.0048 (10)	0.0046 (10)	0.0055 (10)
C2	0.0581 (15)	0.0794 (18)	0.0730 (17)	0.0181 (13)	0.0034 (12)	0.0111 (14)
C3	0.092 (2)	0.0653 (17)	0.0690 (17)	0.0340 (15)	0.0064 (15)	0.0140 (13)
C4	0.102 (2)	0.0452 (14)	0.0692 (17)	0.0037 (14)	0.0108 (15)	0.0105 (12)
C5	0.0644 (14)	0.0484 (13)	0.0596 (14)	−0.0065 (11)	0.0007 (11)	0.0016 (11)
C6	0.0506 (12)	0.0378 (11)	0.0388 (11)	0.0021 (9)	0.0020 (9)	−0.0025 (8)
C7	0.0449 (11)	0.0408 (11)	0.0385 (11)	0.0007 (8)	−0.0001 (8)	−0.0020 (9)
C8	0.0507 (12)	0.0455 (12)	0.0403 (11)	0.0044 (9)	−0.0022 (9)	−0.0040 (9)
C9	0.0644 (15)	0.0546 (14)	0.0524 (13)	0.0029 (12)	−0.0039 (11)	−0.0124 (11)
C10	0.104 (2)	0.0551 (15)	0.092 (2)	0.0035 (15)	0.0138 (17)	−0.0272 (15)
C11	0.159 (4)	0.082 (2)	0.128 (3)	0.041 (2)	0.021 (3)	−0.018 (2)
C12	0.0555 (13)	0.0601 (13)	0.0364 (11)	0.0111 (10)	−0.0068 (9)	−0.0072 (10)
C13	0.0911 (18)	0.0708 (15)	0.0426 (13)	0.0412 (11)	0.0110 (12)	0.0098 (12)
C14	0.118 (3)	0.143 (3)	0.0401 (15)	0.069 (2)	0.0038 (15)	−0.0026 (17)
C15	0.185 (5)	0.209 (6)	0.0444 (18)	0.129 (4)	0.033 (3)	0.029 (3)
C16	0.199 (5)	0.150 (4)	0.106 (4)	0.124 (4)	0.101 (4)	0.076 (3)
C17	0.168 (4)	0.078 (2)	0.138 (3)	0.066 (2)	0.104 (3)	0.053 (2)
C18	0.111 (2)	0.0641 (16)	0.0769 (18)	0.0324 (12)	0.0474 (17)	0.0209 (14)
C19	0.0483 (11)	0.0482 (12)	0.0327 (10)	0.0067 (9)	−0.0002 (8)	−0.0019 (9)
C20	0.0525 (12)	0.0559 (13)	0.0328 (10)	0.0070 (10)	0.0050 (9)	0.0042 (10)
C21	0.0843 (19)	0.0685 (16)	0.0691 (16)	0.0350 (14)	0.0107 (14)	0.0115 (14)
C22	0.221 (5)	0.117 (3)	0.110 (3)	0.104 (3)	−0.036 (3)	−0.041 (2)
C23	0.0440 (11)	0.0396 (10)	0.0373 (10)	0.0006 (8)	0.0022 (8)	−0.0002 (8)
C24	0.0490 (12)	0.0406 (11)	0.0389 (11)	0.0031 (9)	−0.0072 (9)	−0.0024 (9)
C25	0.0761 (17)	0.0670 (15)	0.0465 (13)	−0.0036 (12)	0.0120 (12)	−0.0082 (11)
C26	0.113 (2)	0.094 (2)	0.0462 (15)	0.024 (2)	0.0122 (15)	−0.0156 (15)
C27	0.120 (3)	0.084 (2)	0.083 (2)	0.030 (2)	−0.025 (2)	−0.0421 (18)
C28	0.097 (2)	0.0656 (19)	0.149 (3)	−0.0134 (17)	−0.027 (2)	−0.042 (2)

C29	0.0648 (16)	0.0627 (16)	0.103 (2)	−0.0076 (13)	0.0079 (15)	−0.0216 (15)
N1	0.0510 (10)	0.0421 (9)	0.0407 (9)	0.0060 (8)	−0.0105 (7)	−0.0062 (7)
O1	0.0737 (11)	0.0501 (9)	0.0595 (10)	0.0076 (8)	0.0005 (8)	−0.0173 (7)
O2	0.0845 (14)	0.0985 (15)	0.1233 (17)	0.0145 (12)	−0.0388 (13)	−0.0616 (14)
O3	0.0619 (10)	0.0706 (11)	0.0497 (9)	0.0097 (8)	−0.0143 (8)	0.0042 (8)
O4	0.0870 (12)	0.0666 (11)	0.0532 (10)	0.0368 (9)	−0.0139 (8)	−0.0104 (8)
Cl1	0.2676 (17)	0.0805 (7)	0.2945 (19)	0.0159 (8)	0.2084 (16)	0.0452 (8)

Geometric parameters (Å, º)

C1—C6	1.379 (3)	C15—C16	1.369 (7)
C1—C2	1.380 (3)	C15—H15	0.9300
C1—H1	0.9300	C16—C17	1.366 (7)
C2—C3	1.369 (4)	C16—H16	0.9300
C2—H2	0.9300	C17—C18	1.387 (4)
C3—C4	1.366 (4)	C17—Cl1	1.729 (5)
C3—H3	0.9300	C18—H18	0.9300
C4—C5	1.378 (3)	C19—C23	1.351 (3)
C4—H4	0.9300	C19—C20	1.465 (3)
C5—C6	1.385 (3)	C20—O3	1.207 (2)
C5—H5	0.9300	C20—O4	1.326 (3)
C6—C7	1.487 (3)	C21—O4	1.440 (3)
C7—C8	1.346 (3)	C21—C22	1.460 (5)
C7—N1	1.385 (2)	C21—H21A	0.9700
C8—C9	1.479 (3)	C21—H21B	0.9700
C8—C12	1.518 (3)	C22—H22A	0.9600
C9—O2	1.199 (3)	C22—H22B	0.9600
C9—O1	1.326 (3)	C22—H22C	0.9600
C10—O1	1.451 (3)	C23—N1	1.380 (2)
C10—C11	1.481 (4)	C23—C24	1.495 (3)
C10—H10A	0.9700	C24—C29	1.365 (3)
C10—H10B	0.9700	C24—C25	1.375 (3)
C11—H11A	0.9600	C25—C26	1.366 (4)
C11—H11B	0.9600	C25—H25	0.9300
C11—H11C	0.9600	C26—C27	1.338 (5)
C12—C13	1.516 (3)	C26—H26	0.9300
C12—C19	1.516 (3)	C27—C28	1.357 (5)
C12—H12	0.9800	C27—H27	0.9300
C13—C18	1.360 (4)	C28—C29	1.389 (4)
C13—C14	1.395 (4)	C28—H28	0.9300
C14—C15	1.380 (6)	C29—H29	0.9300
C14—H14	0.9300	N1—H1A	0.8600
C6—C1—C2	120.4 (2)	C17—C16—C15	118.5 (4)
C6—C1—H1	119.8	C17—C16—H16	120.8
C2—C1—H1	119.8	C15—C16—H16	120.8
C3—C2—C1	120.1 (3)	C16—C17—C18	120.9 (5)
C3—C2—H2	119.9	C16—C17—Cl1	119.1 (3)

C1—C2—H2	119.9	C18—C17—Cl1	120.0 (4)
C4—C3—C2	120.1 (2)	C13—C18—C17	120.9 (4)
C4—C3—H3	120.0	C13—C18—H18	119.5
C2—C3—H3	120.0	C17—C18—H18	119.5
C3—C4—C5	120.2 (2)	C23—C19—C20	124.64 (18)
C3—C4—H4	119.9	C23—C19—C12	121.34 (18)
C5—C4—H4	119.9	C20—C19—C12	113.96 (16)
C4—C5—C6	120.3 (2)	O3—C20—O4	122.37 (19)
C4—C5—H5	119.8	O3—C20—C19	122.7 (2)
C6—C5—H5	119.8	O4—C20—C19	114.95 (18)
C1—C6—C5	118.9 (2)	O4—C21—C22	107.3 (2)
C1—C6—C7	120.52 (18)	O4—C21—H21A	110.3
C5—C6—C7	120.57 (19)	C22—C21—H21A	110.3
C8—C7—N1	120.27 (17)	O4—C21—H21B	110.3
C8—C7—C6	126.50 (18)	C22—C21—H21B	110.3
N1—C7—C6	113.18 (16)	H21A—C21—H21B	108.5
C7—C8—C9	123.88 (19)	C21—C22—H22A	109.5
C7—C8—C12	121.08 (18)	C21—C22—H22B	109.5
C9—C8—C12	115.03 (17)	H22A—C22—H22B	109.5
O2—C9—O1	122.6 (2)	C21—C22—H22C	109.5
O2—C9—C8	123.3 (2)	H22A—C22—H22C	109.5
O1—C9—C8	114.02 (19)	H22B—C22—H22C	109.5
O1—C10—C11	107.6 (2)	C19—C23—N1	119.80 (17)
O1—C10—H10A	110.2	C19—C23—C24	127.08 (17)
C11—C10—H10A	110.2	N1—C23—C24	113.12 (16)
O1—C10—H10B	110.2	C29—C24—C25	117.7 (2)
C11—C10—H10B	110.2	C29—C24—C23	120.3 (2)
H10A—C10—H10B	108.5	C25—C24—C23	121.89 (19)
C10—C11—H11A	109.5	C26—C25—C24	121.0 (3)
C10—C11—H11B	109.5	C26—C25—H25	119.5
H11A—C11—H11B	109.5	C24—C25—H25	119.5
C10—C11—H11C	109.5	C27—C26—C25	120.5 (3)
H11A—C11—H11C	109.5	C27—C26—H26	119.8
H11B—C11—H11C	109.5	C25—C26—H26	119.8
C13—C12—C19	110.89 (19)	C26—C27—C28	120.5 (3)
C13—C12—C8	111.17 (18)	C26—C27—H27	119.7
C19—C12—C8	111.44 (16)	C28—C27—H27	119.7
C13—C12—H12	107.7	C27—C28—C29	119.2 (3)
C19—C12—H12	107.7	C27—C28—H28	120.4
C8—C12—H12	107.7	C29—C28—H28	120.4
C18—C13—C14	118.4 (3)	C24—C29—C28	120.9 (3)
C18—C13—C12	120.7 (2)	C24—C29—H29	119.5
C14—C13—C12	121.0 (3)	C28—C29—H29	119.5
C15—C14—C13	120.0 (4)	C23—N1—C7	122.35 (16)
C15—C14—H14	120.0	C23—N1—H1A	118.8
C13—C14—H14	120.0	C7—N1—H1A	118.8
C16—C15—C14	121.2 (5)	C9—O1—C10	117.38 (19)
C16—C15—H15	119.4	C20—O4—C21	118.62 (19)

C14—C15—H15	119.4		
C6—C1—C2—C3	−0.1 (4)	C16—C17—C18—C13	−0.2 (5)
C1—C2—C3—C4	−1.6 (4)	Cl1—C17—C18—C13	−179.0 (2)
C2—C3—C4—C5	1.6 (4)	C13—C12—C19—C23	−106.0 (2)
C3—C4—C5—C6	0.2 (4)	C8—C12—C19—C23	18.4 (3)
C2—C1—C6—C5	1.8 (3)	C13—C12—C19—C20	71.5 (2)
C2—C1—C6—C7	−179.8 (2)	C8—C12—C19—C20	−164.12 (18)
C4—C5—C6—C1	−1.9 (3)	C23—C19—C20—O3	−166.5 (2)
C4—C5—C6—C7	179.7 (2)	C12—C19—C20—O3	16.2 (3)
C1—C6—C7—C8	120.3 (2)	C23—C19—C20—O4	14.9 (3)
C5—C6—C7—C8	−61.3 (3)	C12—C19—C20—O4	−162.47 (18)
C1—C6—C7—N1	−62.4 (2)	C20—C19—C23—N1	177.24 (18)
C5—C6—C7—N1	116.0 (2)	C12—C19—C23—N1	−5.6 (3)
N1—C7—C8—C9	−176.6 (2)	C20—C19—C23—C24	−2.3 (3)
C6—C7—C8—C9	0.5 (3)	C12—C19—C23—C24	174.84 (19)
N1—C7—C8—C12	2.0 (3)	C19—C23—C24—C29	−111.8 (3)
C6—C7—C8—C12	179.1 (2)	N1—C23—C24—C29	68.6 (3)
C7—C8—C9—O2	150.2 (3)	C19—C23—C24—C25	70.4 (3)
C12—C8—C9—O2	−28.4 (4)	N1—C23—C24—C25	−109.2 (2)
C7—C8—C9—O1	−31.4 (3)	C29—C24—C25—C26	2.6 (4)
C12—C8—C9—O1	150.0 (2)	C23—C24—C25—C26	−179.5 (2)
C7—C8—C12—C13	107.7 (2)	C24—C25—C26—C27	−1.1 (4)
C9—C8—C12—C13	−73.6 (3)	C25—C26—C27—C28	−1.3 (5)
C7—C8—C12—C19	−16.6 (3)	C26—C27—C28—C29	2.1 (5)
C9—C8—C12—C19	162.14 (18)	C25—C24—C29—C28	−1.8 (4)
C19—C12—C13—C18	39.7 (3)	C23—C24—C29—C28	−179.7 (3)
C8—C12—C13—C18	−84.9 (3)	C27—C28—C29—C24	−0.4 (5)
C19—C12—C13—C14	−139.9 (2)	C19—C23—N1—C7	−11.5 (3)
C8—C12—C13—C14	95.6 (3)	C24—C23—N1—C7	168.13 (17)
C18—C13—C14—C15	−0.2 (4)	C8—C7—N1—C23	13.4 (3)
C12—C13—C14—C15	179.3 (3)	C6—C7—N1—C23	−164.10 (17)
C13—C14—C15—C16	−0.6 (6)	O2—C9—O1—C10	−9.3 (4)
C14—C15—C16—C17	1.0 (7)	C8—C9—O1—C10	172.2 (2)
C15—C16—C17—C18	−0.6 (6)	C11—C10—O1—C9	179.2 (3)
C15—C16—C17—Cl1	178.1 (3)	O3—C20—O4—C21	5.3 (3)
C14—C13—C18—C17	0.7 (4)	C19—C20—O4—C21	−176.1 (2)
C12—C13—C18—C17	−178.9 (2)	C22—C21—O4—C20	−176.8 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O3^{i}	0.86	2.10	2.910 (2)	158

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