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

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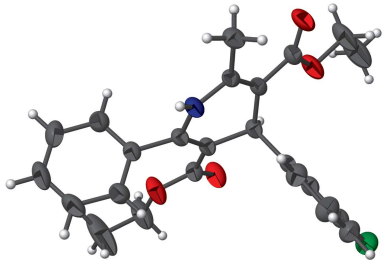
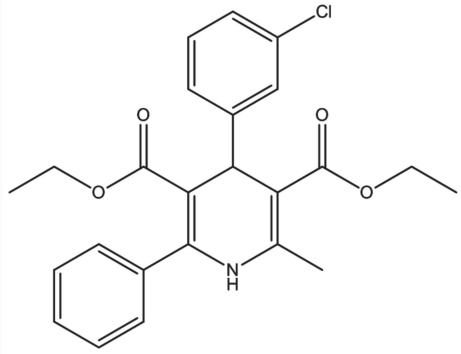
In the title compound, $C_{24}H_{24}ClNO_4$, the dihydropyridine ring adopts a flattened boat conformation. The plane of the pyridine ring subtends dihedral angles of 74.54 (6) and 85.69 (5)° with those of the phenyl and chlorophenyl rings, respectively. The dihedral angle between the planes of the chlorophenyl and phenyl rings is 72.20 (7)°. In the crystal, molecules are linked into [100] $C(6)$ chains by N—H···O hydrogen bonds. The chains are cross-linked by weak C—H···O interactions to generate a three-dimensional network.

3D view



Chemical scheme



Structure description

Heterocyclic compounds containing pyridine rings are associated with diverse pharmacological properties such as antimicrobial (Patel *et al.*, 2011), anticancer (Srivastava & Pandeya 2011), anticonvulsant (Paronikyan *et al.*, 2002) and antimycobacterial activities (Mamolo *et al.*, 2004). As part of our studies in this area, we now report the synthesis and structure of the title compound.

The geometric parameters of the title molecule (Fig. 1) agree well with reported similar structure (Steiger *et al.*, 2014; Wang *et al.*, 2013). The pyridine ring makes dihedral angles of 74.54 (6) and 85.69 (5)° with the phenyl and chlorophenyl rings, respectively. The dihedral angle between chlorophenyl and phenyl rings is 72.20 (7)°.

In the crystal, molecules are linked into [100] $C(6)$ chains by N—H···O hydrogen bonds. The chains are cross-linked by weak C—H···O interactions to generate a three-dimensional network (Table 1 and Fig. 2).

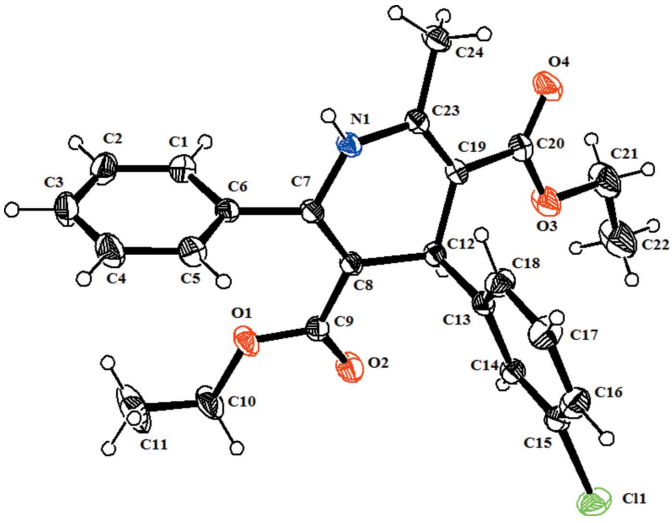


Figure 1
The molecular structure of (I), with 30% probability displacement ellipsoids for non-H atoms.

Synthesis and crystallization

To an ethanolic solution of ammonium acetate (1.92 g, 0.025 *M*), ethyl benzoylacetate (4.32 ml, 0.025 *M*) was added followed by 3-chloro benzaldehyde (3.51 g, 0.025 *M*) and ethyl acetoacetate (3.18ml, 0.025 *M*). The reaction mixture was taken in a round-bottom flask and refluxed for 24 h at 80° C and allowed to cool. The turbid solution obtained was kept over a magnetic stirrer and stirred for four h. The precipitate obtained was filtered, dried and recrystallized using absolute ethanol to obtain yellow blocks with a melting point of 160° C and a yield of 70%.

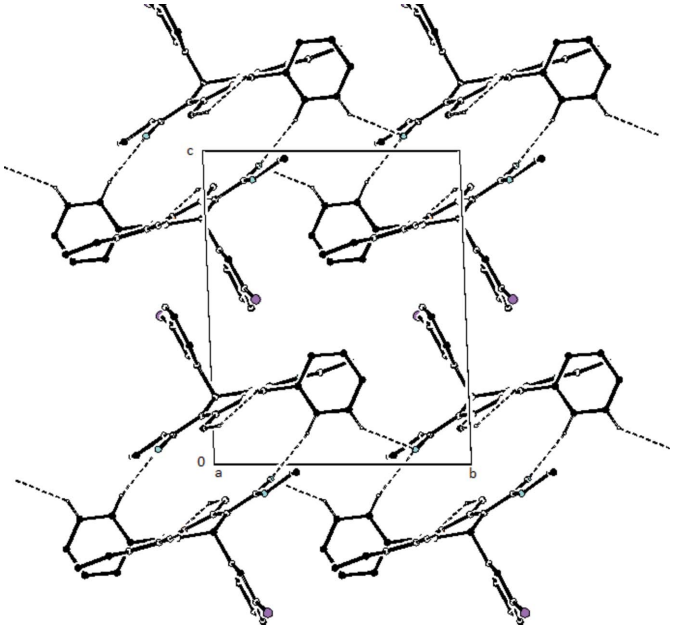


Figure 2
The packing of (I), viewed down the *a* axis. Hydrogen bonds are shown as dashed lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.86	2.20	3.037 (3)	166
C24—H24*B*···O2^{i}	0.96	2.51	3.365 (3)	148
C2—H2···O4^{ii}	0.93	2.59	3.330 (3)	137
C1—H1*A*···O4^{iii}	0.93	2.53	3.412 (3)	159

Symmetry codes: (i) $x+1, y, z$; (ii) $x, y+1, z$; (iii) $-x+1, -y, -z$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{24}H_{24}ClNO_4$
M_r	425.89
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	295
a, *b*, *c* (Å)	7.621 (5), 10.753 (5), 13.138 (5)
α, β, γ (°)	92.102 (5), 93.806 (5), 91.275 (5)
V (Å^3)	1073.2 (10)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	0.21
Crystal size (mm)	0.23 × 0.17 × 0.11
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Sheldrick, 1996)
T_{min}, T_{max}	0.958, 0.977
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	15576, 4480, 3491
R_{int}	0.022
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.630
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.044, 0.122, 1.02
No. of reflections	4480
No. of parameters	274
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.29, −0.25

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

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x160155 [doi:10.1107/S2414314616001553]

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Crystal data

$C_{24}H_{24}ClNO_4$
M_r = 425.89
Triclinic, $P\overline{1}$
a = 7.621 (5) Å
b = 10.753 (5) Å
c = 13.138 (5) Å
α = 92.102 (5)°
β = 93.806 (5)°
γ = 91.275 (5)°
V = 1073.2 (10) Å^3
Z = 2
$F(000)$ = 448
D_x = 1.318 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4480 reflections
θ = 1.6–26.6°
μ = 0.21 mm^{-1}
T = 295 K
Block, yellow
0.23 × 0.17 × 0.11 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.958, T_{max} = 0.977
15576 measured reflections
4480 independent reflections
3491 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 26.6°, θ_{min} = 1.6°
h = −9→9
k = −13→13
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.122
S = 1.02
4480 reflections
274 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
$w = 1/[\sigma^2(F_o^2) + (0.0532P)^2 + 0.5427P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.5155 (3)	0.40545 (18)	0.16421 (16)	0.0429 (4)

H1A	0.4998	0.3671	0.0996	0.051*
C2	0.5597 (3)	0.53110 (19)	0.17448 (19)	0.0537 (5)
H2	0.5705	0.5774	0.1167	0.064*
C3	0.5876 (3)	0.58753 (18)	0.2697 (2)	0.0570 (6)
H3	0.6159	0.6721	0.2765	0.068*
C4	0.5737 (3)	0.51907 (19)	0.35468 (19)	0.0550 (6)
H4	0.5964	0.5569	0.4192	0.066*
C5	0.5261 (3)	0.39396 (18)	0.34544 (16)	0.0436 (4)
H5	0.5152	0.3483	0.4035	0.052*
C6	0.4948 (2)	0.33704 (15)	0.24965 (14)	0.0322 (4)
C7	0.4397 (2)	0.20311 (15)	0.23494 (13)	0.0307 (4)
C8	0.2751 (2)	0.15345 (15)	0.23497 (13)	0.0311 (4)
C9	0.1176 (2)	0.22663 (16)	0.24928 (14)	0.0354 (4)
C10	0.0044 (3)	0.4246 (2)	0.2929 (2)	0.0683 (7)
H10A	−0.0696	0.3896	0.3425	0.082*
H10B	−0.0661	0.4326	0.2293	0.082*
C11	0.0763 (4)	0.5464 (3)	0.3303 (4)	0.1272 (17)
H11A	0.1455	0.5374	0.3932	0.191*
H11B	−0.0184	0.6016	0.3416	0.191*
H11C	0.1489	0.5802	0.2805	0.191*
C12	0.2418 (2)	0.01385 (14)	0.21610 (13)	0.0310 (4)
H12	0.1304	0.0021	0.1748	0.037*
C13	0.2234 (2)	−0.05196 (15)	0.31574 (13)	0.0316 (4)
C14	0.0581 (2)	−0.08508 (16)	0.34641 (14)	0.0354 (4)
H14	−0.0423	−0.0688	0.3054	0.042*
C15	0.0437 (2)	−0.14221 (16)	0.43803 (15)	0.0389 (4)
C16	0.1879 (3)	−0.16631 (19)	0.50181 (16)	0.0476 (5)
H16	0.1756	−0.2034	0.5639	0.057*
C17	0.3521 (3)	−0.1338 (2)	0.47086 (17)	0.0497 (5)
H17	0.4518	−0.1493	0.5127	0.060*
C18	0.3702 (2)	−0.07876 (18)	0.37911 (15)	0.0421 (4)
H18	0.4821	−0.0592	0.3592	0.051*
C19	0.3864 (2)	−0.04154 (15)	0.15517 (13)	0.0316 (4)
C20	0.3488 (2)	−0.15654 (16)	0.09419 (14)	0.0384 (4)
C21	0.1295 (3)	−0.3022 (2)	0.0290 (2)	0.0740 (8)
H21A	0.1847	−0.3744	0.0581	0.089*
H21B	0.1686	−0.2933	−0.0392	0.089*
C22	−0.0614 (4)	−0.3180 (3)	0.0247 (3)	0.0959 (11)
H22A	−0.0985	−0.3284	0.0924	0.144*
H22B	−0.0964	−0.3903	−0.0175	0.144*
H22C	−0.1148	−0.2458	−0.0035	0.144*
C23	0.5485 (2)	0.01250 (15)	0.15995 (13)	0.0310 (4)
C24	0.7087 (2)	−0.03756 (18)	0.11409 (15)	0.0416 (4)
H24A	0.7428	−0.1123	0.1471	0.062*
H24B	0.8030	0.0233	0.1233	0.062*
H24C	0.6828	−0.0558	0.0425	0.062*
N1	0.57631 (18)	0.12722 (13)	0.20987 (11)	0.0336 (3)
H1	0.6827	0.1526	0.2261	0.040*

O1	0.15107 (17)	0.34518 (12)	0.27709 (14)	0.0575 (4)
O2	−0.03089 (16)	0.18390 (12)	0.23772 (13)	0.0522 (4)
O3	0.17836 (19)	−0.19126 (13)	0.09204 (13)	0.0574 (4)
O4	0.4528 (2)	−0.21604 (13)	0.04750 (12)	0.0564 (4)
Cl1	−0.16512 (7)	−0.18564 (5)	0.47366 (5)	0.05796 (18)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0436 (10)	0.0393 (10)	0.0461 (11)	−0.0009 (8)	0.0064 (8)	−0.0001 (8)
C2	0.0526 (12)	0.0374 (10)	0.0728 (15)	−0.0013 (9)	0.0114 (11)	0.0135 (10)
C3	0.0515 (12)	0.0284 (9)	0.0907 (18)	−0.0044 (8)	0.0097 (12)	−0.0068 (11)
C4	0.0566 (13)	0.0428 (11)	0.0636 (14)	−0.0034 (9)	0.0037 (10)	−0.0215 (10)
C5	0.0472 (11)	0.0390 (10)	0.0441 (11)	−0.0009 (8)	0.0036 (9)	−0.0045 (8)
C6	0.0238 (8)	0.0297 (8)	0.0434 (10)	0.0017 (6)	0.0049 (7)	−0.0023 (7)
C7	0.0290 (8)	0.0278 (8)	0.0352 (9)	0.0026 (6)	0.0026 (7)	−0.0031 (7)
C8	0.0284 (8)	0.0270 (8)	0.0377 (9)	0.0018 (6)	0.0031 (7)	−0.0022 (7)
C9	0.0289 (8)	0.0303 (8)	0.0475 (11)	0.0008 (7)	0.0059 (7)	−0.0003 (7)
C10	0.0391 (11)	0.0388 (11)	0.128 (2)	0.0119 (9)	0.0172 (13)	−0.0155 (13)
C11	0.0606 (17)	0.0581 (17)	0.259 (5)	0.0115 (14)	0.015 (2)	−0.065 (2)
C12	0.0255 (8)	0.0268 (8)	0.0401 (10)	0.0006 (6)	0.0003 (7)	−0.0030 (7)
C13	0.0303 (8)	0.0254 (8)	0.0389 (10)	−0.0004 (6)	0.0051 (7)	−0.0044 (7)
C14	0.0294 (8)	0.0324 (9)	0.0438 (10)	−0.0015 (7)	0.0017 (7)	−0.0039 (7)
C15	0.0361 (9)	0.0322 (9)	0.0487 (11)	−0.0044 (7)	0.0114 (8)	−0.0056 (8)
C16	0.0517 (12)	0.0473 (11)	0.0447 (11)	−0.0029 (9)	0.0068 (9)	0.0084 (9)
C17	0.0402 (10)	0.0580 (12)	0.0509 (12)	0.0014 (9)	−0.0024 (9)	0.0135 (10)
C18	0.0302 (9)	0.0469 (11)	0.0496 (11)	−0.0008 (8)	0.0032 (8)	0.0064 (9)
C19	0.0341 (8)	0.0263 (8)	0.0341 (9)	0.0037 (7)	0.0019 (7)	−0.0011 (7)
C20	0.0427 (10)	0.0312 (9)	0.0408 (10)	0.0011 (8)	0.0014 (8)	−0.0020 (8)
C21	0.0586 (14)	0.0497 (13)	0.110 (2)	−0.0095 (11)	0.0022 (14)	−0.0384 (14)
C22	0.0627 (16)	0.0712 (18)	0.148 (3)	−0.0094 (14)	−0.0013 (18)	−0.0498 (19)
C23	0.0328 (8)	0.0283 (8)	0.0322 (9)	0.0066 (6)	0.0022 (7)	0.0000 (7)
C24	0.0352 (9)	0.0406 (10)	0.0490 (11)	0.0076 (8)	0.0059 (8)	−0.0063 (8)
N1	0.0236 (7)	0.0311 (7)	0.0457 (9)	0.0014 (5)	0.0025 (6)	−0.0065 (6)
O1	0.0303 (7)	0.0326 (7)	0.1100 (13)	0.0042 (5)	0.0156 (7)	−0.0153 (7)
O2	0.0259 (6)	0.0417 (7)	0.0881 (11)	0.0017 (5)	0.0035 (6)	−0.0091 (7)
O3	0.0468 (8)	0.0430 (8)	0.0802 (11)	−0.0074 (6)	0.0055 (7)	−0.0257 (7)
O4	0.0597 (9)	0.0408 (8)	0.0683 (10)	0.0025 (7)	0.0141 (8)	−0.0208 (7)
Cl1	0.0443 (3)	0.0612 (3)	0.0697 (4)	−0.0131 (2)	0.0221 (2)	−0.0033 (3)

Geometric parameters (Å, º)

C1—C6	1.380 (3)	C13—C14	1.390 (2)
C1—C2	1.385 (3)	C13—C18	1.392 (3)
C1—H1A	0.9300	C14—C15	1.381 (3)
C2—C3	1.372 (3)	C14—H14	0.9300
C2—H2	0.9300	C15—C16	1.373 (3)
C3—C4	1.368 (3)	C15—Cl1	1.747 (2)

C3—H3	0.9300	C16—C17	1.383 (3)
C4—C5	1.384 (3)	C16—H16	0.9300
C4—H4	0.9300	C17—C18	1.376 (3)
C5—C6	1.383 (3)	C17—H17	0.9300
C5—H5	0.9300	C18—H18	0.9300
C6—C7	1.493 (2)	C19—C23	1.350 (2)
C7—C8	1.353 (2)	C19—C20	1.461 (2)
C7—N1	1.386 (2)	C20—O4	1.214 (2)
C8—C9	1.469 (2)	C20—O3	1.341 (2)
C8—C12	1.525 (2)	C21—O3	1.454 (2)
C9—O2	1.210 (2)	C21—C22	1.458 (4)
C9—O1	1.328 (2)	C21—H21A	0.9700
C10—O1	1.443 (2)	C21—H21B	0.9700
C10—C11	1.464 (3)	C22—H22A	0.9600
C10—H10A	0.9700	C22—H22B	0.9600
C10—H10B	0.9700	C22—H22C	0.9600
C11—H11A	0.9600	C23—N1	1.381 (2)
C11—H11B	0.9600	C23—C24	1.499 (2)
C11—H11C	0.9600	C24—H24A	0.9600
C12—C19	1.523 (2)	C24—H24B	0.9600
C12—C13	1.524 (2)	C24—H24C	0.9600
C12—H12	0.9800	N1—H1	0.8600

C6—C1—C2	120.19 (19)	C15—C14—C13	119.76 (16)
C6—C1—H1A	119.9	C15—C14—H14	120.1
C2—C1—H1A	119.9	C13—C14—H14	120.1
C3—C2—C1	120.2 (2)	C16—C15—C14	122.18 (17)
C3—C2—H2	119.9	C16—C15—Cl1	118.95 (16)
C1—C2—H2	119.9	C14—C15—Cl1	118.87 (14)
C4—C3—C2	119.85 (19)	C15—C16—C17	117.91 (19)
C4—C3—H3	120.1	C15—C16—H16	121.0
C2—C3—H3	120.1	C17—C16—H16	121.0
C3—C4—C5	120.5 (2)	C18—C17—C16	121.02 (18)
C3—C4—H4	119.7	C18—C17—H17	119.5
C5—C4—H4	119.7	C16—C17—H17	119.5
C6—C5—C4	119.9 (2)	C17—C18—C13	120.86 (17)
C6—C5—H5	120.1	C17—C18—H18	119.6
C4—C5—H5	120.1	C13—C18—H18	119.6
C1—C6—C5	119.33 (17)	C23—C19—C20	120.41 (16)
C1—C6—C7	118.40 (16)	C23—C19—C12	120.59 (15)
C5—C6—C7	122.26 (17)	C20—C19—C12	118.97 (15)
C8—C7—N1	119.19 (15)	O4—C20—O3	121.31 (17)
C8—C7—C6	127.54 (15)	O4—C20—C19	126.59 (17)
N1—C7—C6	113.00 (14)	O3—C20—C19	112.08 (15)
C7—C8—C9	124.08 (15)	O3—C21—C22	108.2 (2)
C7—C8—C12	120.59 (14)	O3—C21—H21A	110.1
C9—C8—C12	115.31 (14)	C22—C21—H21A	110.1
O2—C9—O1	122.04 (16)	O3—C21—H21B	110.1

O2—C9—C8	123.68 (16)	C22—C21—H21B	110.1
O1—C9—C8	114.28 (14)	H21A—C21—H21B	108.4
O1—C10—C11	107.45 (19)	C21—C22—H22A	109.5
O1—C10—H10A	110.2	C21—C22—H22B	109.5
C11—C10—H10A	110.2	H22A—C22—H22B	109.5
O1—C10—H10B	110.2	C21—C22—H22C	109.5
C11—C10—H10B	110.2	H22A—C22—H22C	109.5
H10A—C10—H10B	108.5	H22B—C22—H22C	109.5
C10—C11—H11A	109.5	C19—C23—N1	119.27 (15)
C10—C11—H11B	109.5	C19—C23—C24	126.90 (16)
H11A—C11—H11B	109.5	N1—C23—C24	113.82 (15)
C10—C11—H11C	109.5	C23—C24—H24A	109.5
H11A—C11—H11C	109.5	C23—C24—H24B	109.5
H11B—C11—H11C	109.5	H24A—C24—H24B	109.5
C19—C12—C13	111.77 (13)	C23—C24—H24C	109.5
C19—C12—C8	110.17 (13)	H24A—C24—H24C	109.5
C13—C12—C8	111.45 (14)	H24B—C24—H24C	109.5
C19—C12—H12	107.8	C23—N1—C7	122.66 (14)
C13—C12—H12	107.8	C23—N1—H1	118.7
C8—C12—H12	107.8	C7—N1—H1	118.7
C14—C13—C18	118.24 (17)	C9—O1—C10	118.31 (15)
C14—C13—C12	120.53 (15)	C20—O3—C21	115.18 (16)
C18—C13—C12	121.22 (15)		

C6—C1—C2—C3	1.7 (3)	C13—C14—C15—C16	1.0 (3)
C1—C2—C3—C4	0.7 (3)	C13—C14—C15—Cl1	−178.77 (13)
C2—C3—C4—C5	−2.1 (3)	C14—C15—C16—C17	−1.3 (3)
C3—C4—C5—C6	1.0 (3)	Cl1—C15—C16—C17	178.49 (16)
C2—C1—C6—C5	−2.8 (3)	C15—C16—C17—C18	0.1 (3)
C2—C1—C6—C7	177.45 (17)	C16—C17—C18—C13	1.3 (3)
C4—C5—C6—C1	1.5 (3)	C14—C13—C18—C17	−1.6 (3)
C4—C5—C6—C7	−178.78 (18)	C12—C13—C18—C17	177.41 (18)
C1—C6—C7—C8	−96.3 (2)	C13—C12—C19—C23	−97.89 (18)
C5—C6—C7—C8	83.9 (2)	C8—C12—C19—C23	26.6 (2)
C1—C6—C7—N1	77.6 (2)	C13—C12—C19—C20	80.00 (19)
C5—C6—C7—N1	−102.10 (19)	C8—C12—C19—C20	−155.52 (15)
N1—C7—C8—C9	−173.11 (16)	C23—C19—C20—O4	3.2 (3)
C6—C7—C8—C9	0.5 (3)	C12—C19—C20—O4	−174.65 (18)
N1—C7—C8—C12	4.9 (3)	C23—C19—C20—O3	−175.15 (16)
C6—C7—C8—C12	178.51 (16)	C12—C19—C20—O3	7.0 (2)
C7—C8—C9—O2	171.24 (19)	C20—C19—C23—N1	173.75 (15)
C12—C8—C9—O2	−6.8 (3)	C12—C19—C23—N1	−8.4 (2)
C7—C8—C9—O1	−9.2 (3)	C20—C19—C23—C24	−4.9 (3)
C12—C8—C9—O1	172.68 (16)	C12—C19—C23—C24	172.92 (16)
C7—C8—C12—C19	−24.8 (2)	C19—C23—N1—C7	−15.4 (2)
C9—C8—C12—C19	153.40 (15)	C24—C23—N1—C7	163.49 (16)
C7—C8—C12—C13	99.91 (18)	C8—C7—N1—C23	17.2 (3)
C9—C8—C12—C13	−81.93 (18)	C6—C7—N1—C23	−157.34 (15)

C19—C12—C13—C14	−135.33 (16)	O2—C9—O1—C10	−0.5 (3)
C8—C12—C13—C14	100.91 (17)	C8—C9—O1—C10	179.9 (2)
C19—C12—C13—C18	45.7 (2)	C11—C10—O1—C9	175.7 (3)
C8—C12—C13—C18	−78.08 (19)	O4—C20—O3—C21	−1.1 (3)
C18—C13—C14—C15	0.4 (2)	C19—C20—O3—C21	177.43 (19)
C12—C13—C14—C15	−178.58 (15)	C22—C21—O3—C20	−173.0 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.86	2.20	3.037 (3)	166
C24—H24*B*···O2^{i}	0.96	2.51	3.365 (3)	148
C2—H2···O4^{ii}	0.93	2.59	3.330 (3)	137
C1—H1*A*···O4^{iii}	0.93	2.53	3.412 (3)	159

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