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3-Chloro-*r*-2,*c*-6-bis(4-fluorophenyl)-3-methylpiperidin-4-one

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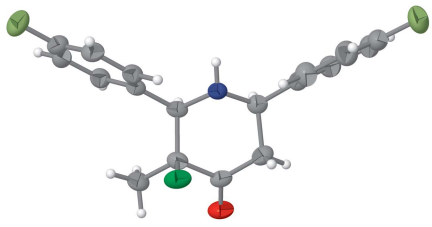
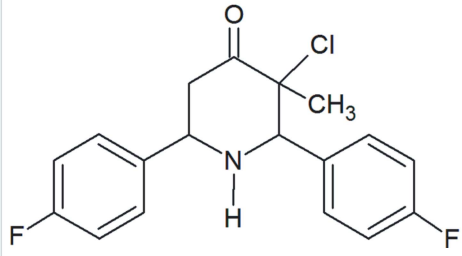
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{18}H_{16}ClF_2NO$, contains one independent molecule in the asymmetric unit, with the piperidin-4-one ring adopting a slightly distorted chair conformation and an equatorial orientation of all the substituents except chlorine. A single weak intermolecular C—H···O interaction influences the crystal packing, forming infinite one-dimensional zigzag chains along the *a* axis. The structure was refined as a two-component inversion twin.

3D view



Chemical scheme



Structure description

Piperidones are an important group of heterocyclic compounds in the field of medicinal chemistry due to their biological activities, which include cytotoxic properties (Dimmock *et al.*, 2001). They are also reported to possess analgesic, anti-inflammatory, central nervous system (CNS), local anaesthetic, anticancer, and antimicrobial activities (Perumal *et al.*, 2001). The synthesis and stereodynamics of piperidin-4-ones and their derivatives have been reported (Ponnuswamy *et al.*, 2002). The present investigation was undertaken to establish the molecular structure, the conformation of the heterocyclic ring and the orientation of the 4-fluorophenyl groups with respect to each other.

In the title compound, the piperidin-4-one ring is in a slightly distorted chair conformation [puckering parameters Q, θ, and φ = 0.548 (4) Å, 166.5 (4)°, and 182.7 (19)°, respectively] (Fig. 1), with an equatorial orientation of all the substituents except chlorine. The dihedral angle between the mean planes of the two fluoro-substituted benzene rings is 49.3 (3)°. Bond lengths are in normal ranges (Allen *et al.*, 1987). No classical hydrogen bonds are observed and all intermolecular π–π interactions are greater

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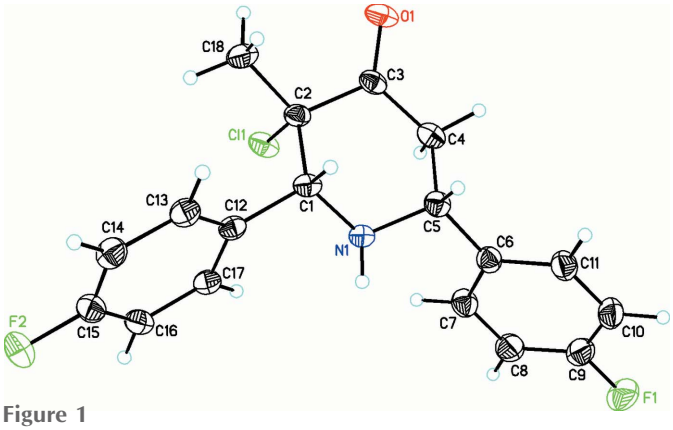

Figure 1
The molecular structure, showing the atom-labeling scheme and 30% probability displacement ellipsoids.

than 4 Å. A single weak intermolecular C5—H5···O1^{i} interaction influences the crystal packing, forming infinite one-dimensional zigzag chains along the *a* axis (Table 1 and Fig. 2).

Synthesis and crystallization

A mixture of ammonium acetate (0.1 mol, 7.71 g), 4-fluorobenzaldehyde (0.2 mol, 21.0 ml), and 3-chlorobutan-2-one (0.1 mol, 10.1 ml) in distilled ethanol was heated first to boiling. After cooling, the viscous liquid obtained was dissolved in ether (200 ml) and shaken with concentrated hydrochloric acid (100 ml). The precipitated hydrochloride of 3-chloro-*r*-2,*c*-6-bis(4-fluorophenyl)-3-methylpiperidin-4-one was removed by filtration and washed first with a 40 ml mixture of ethanol and ether (1:1 *v*/*v*) and then with ether to remove most of the coloured impurities. The base was liberated from an ethanol solution by adding aqueous ammonia and then diluting with water. It was recrystallized from ethanol yielding colourless rod-like crystals (yield 3.5 g).

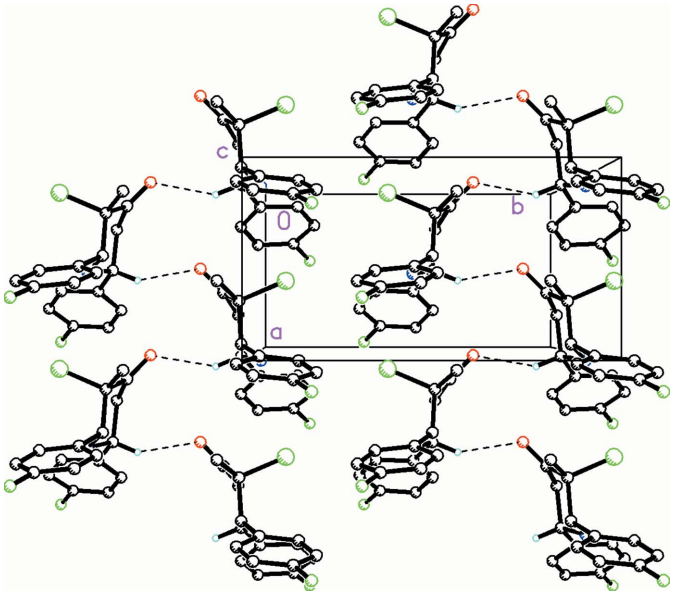

Figure 2
The molecular packing, viewed along the *c* axis. Dashed lines indicate weak intermolecular C—H···O interactions. H atoms not involved in hydrogen bonding have been removed for clarity.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O1^{i}	1.00	2.44	3.328 (5)	148

Symmetry code: (i) $x+\frac{1}{2}, -y+\frac{3}{2}, z$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{16}ClF_2NO$
M_r	335.77
Crystal system, space group	Orthorhombic, $Pna2_1$
Temperature (K)	173
a, *b*, *c* (Å)	6.2844 (2), 11.7141 (5), 21.6006 (10)
V (Å^3)	1590.15 (11)
Z	4
Radiation type	Cu *Kα*
μ (mm^{-1})	2.35
Crystal size (mm)	0.48 × 0.15 × 0.14
Data collection	
Diffractometer	Rigaku Oxford Diffraction
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.441, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10608, 2341, 2207
R_{int}	0.052
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.614
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.049, 0.122, 1.08
No. of reflections	2341
No. of parameters	210
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.56, −0.20
Absolute structure	Flack *x* determined using 650 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.02 (3)

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The structure was refined as a two-component inversion twin (TWIN Law = −1 0 0 0 1 0 0 0 −1; BASF = 0.37605).

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The authors would like to acknowledge the Sophisticated Analytical Instrument Facility (SAIF), IITM, Chennai, for recording the NMR spectra. We extend our thanks to the Principal Dr N. Seraman, Chairman Mr R. Sattanathan and Treasurer Mr T. Ramalingam of Thiruvalluvar Arts and

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full crystallographic data

IUCrData (2016). **1**, x161580 [https://doi.org/10.1107/S2414314616015807]

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Crystal data

$C_{18}H_{16}ClF_2NO$
M_r = 335.77
Orthorhombic, $Pna2_1$
a = 6.2844 (2) Å
b = 11.7141 (5) Å
c = 21.6006 (10) Å
V = 1590.15 (11) Å^3
Z = 4
$F(000)$ = 696
D_x = 1.403 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 3685 reflections
θ = 3.8–71.6°
μ = 2.35 mm^{-1}
T = 173 K
Needle, colourless
0.48 × 0.15 × 0.14 mm

Data collection

Rigaku Oxford Diffraction diffractometer
Radiation source: fine-focus sealed X-ray tube, Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 16.0416 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Rigaku OD, 2015)
T_{min} = 0.441, T_{max} = 1.000
10608 measured reflections
2341 independent reflections
2207 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
θ_{max} = 71.3°, θ_{min} = 3.8°
h = −7→7
k = −14→14
l = −22→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.122
S = 1.08
2341 reflections
210 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0862P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Absolute structure: Flack x determined using 650 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: 0.02 (3)

Special details

Experimental. IR (KBr): 3325.34 (N-H), 3075.55, 3008.86 (υC-H), 1716.35 (υC=O), 1609.56, 1508.41 (υC=C), 767.12 (υC-Cl) cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.54 - 7.03 (m, Aromatic protons), 4.06 - 4.03 (dd, H(6) proton), 3.94 (s, H(2) proton), 3.45 - 3.40 (dd, H(5e) proton), 2.53-2.49 (dd, H(5a) proton), 2.07 (s, NH proton), 1.42 (s, CH_3 proton).

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. Refined as a 2-component twin.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.08854 (13)	0.40538 (7)	0.52705 (7)	0.0446 (3)
F1	0.9527 (6)	0.3396 (4)	0.23545 (15)	0.0731 (10)
F2	0.6850 (5)	0.3219 (3)	0.76478 (13)	0.0620 (8)
O1	0.0162 (5)	0.6728 (2)	0.46516 (17)	0.0479 (8)
N1	0.5435 (5)	0.4835 (3)	0.49061 (14)	0.0317 (6)
H1	0.6721	0.4620	0.4976	0.038*
C1	0.4464 (5)	0.5400 (3)	0.54363 (19)	0.0321 (7)
H1A	0.5031	0.6197	0.5451	0.038*
C2	0.2029 (5)	0.5480 (3)	0.5335 (2)	0.0347 (8)
C3	0.1544 (6)	0.6011 (3)	0.4701 (2)	0.0353 (8)
C4	0.2845 (7)	0.5591 (4)	0.4168 (2)	0.0435 (9)
H4A	0.2677	0.6123	0.3815	0.052*
H4B	0.2310	0.4834	0.4037	0.052*
C5	0.5239 (6)	0.5493 (3)	0.43340 (19)	0.0357 (8)
H5	0.5827	0.6275	0.4404	0.043*
C6	0.6454 (6)	0.4932 (4)	0.38161 (19)	0.0377 (8)
C7	0.6428 (8)	0.3745 (4)	0.3746 (2)	0.0445 (9)
H7	0.5686	0.3288	0.4038	0.053*
C8	0.7467 (9)	0.3231 (4)	0.3258 (2)	0.0520 (10)
H8	0.7455	0.2424	0.3212	0.062*
C9	0.8523 (8)	0.3909 (5)	0.2838 (2)	0.0517 (11)
C10	0.8613 (8)	0.5067 (5)	0.2891 (2)	0.0541 (11)
H10	0.9369	0.5514	0.2597	0.065*
C11	0.7571 (8)	0.5577 (4)	0.3385 (2)	0.0462 (9)
H11	0.7623	0.6383	0.3430	0.055*
C12	0.5098 (6)	0.4818 (3)	0.60302 (18)	0.0324 (7)
C13	0.5488 (7)	0.5447 (4)	0.6568 (2)	0.0397 (9)
H13	0.5356	0.6254	0.6557	0.048*
C14	0.6059 (7)	0.4923 (4)	0.7111 (2)	0.0438 (9)
H14	0.6301	0.5357	0.7475	0.053*
C15	0.6271 (7)	0.3753 (4)	0.7115 (2)	0.0447 (9)
C16	0.5943 (6)	0.3102 (4)	0.6598 (2)	0.0405 (9)
H16	0.6126	0.2297	0.6612	0.049*
C17	0.5340 (6)	0.3637 (3)	0.60545 (19)	0.0359 (8)
H17	0.5088	0.3194	0.5694	0.043*
C18	0.0902 (7)	0.6093 (5)	0.5858 (2)	0.0495 (12)
H18A	−0.0600	0.6199	0.5750	0.074*
H18B	0.1569	0.6839	0.5925	0.074*
H18C	0.1007	0.5637	0.6237	0.074*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0329 (4)	0.0338 (4)	0.0673 (6)	−0.0052 (3)	−0.0073 (4)	0.0127 (4)
F1	0.071 (2)	0.104 (3)	0.0439 (15)	0.0193 (18)	0.0142 (14)	−0.0073 (16)
F2	0.0677 (18)	0.076 (2)	0.0426 (14)	0.0096 (14)	−0.0129 (13)	0.0101 (14)
O1	0.0387 (14)	0.0370 (14)	0.068 (2)	0.0091 (12)	−0.0078 (14)	0.0069 (14)
N1	0.0281 (14)	0.0305 (14)	0.0364 (17)	0.0024 (11)	−0.0015 (11)	−0.0010 (12)
C1	0.0264 (15)	0.0243 (14)	0.046 (2)	−0.0016 (11)	−0.0007 (14)	−0.0024 (14)
C2	0.0306 (16)	0.0272 (13)	0.046 (2)	0.0017 (11)	0.0021 (16)	0.0038 (15)
C3	0.0302 (18)	0.0279 (18)	0.048 (2)	−0.0026 (13)	−0.0069 (16)	0.0062 (15)
C4	0.043 (2)	0.043 (2)	0.044 (2)	0.0059 (17)	−0.0089 (17)	0.0057 (17)
C5	0.0354 (17)	0.0298 (17)	0.042 (2)	−0.0033 (14)	−0.0013 (16)	0.0013 (15)
C6	0.0366 (18)	0.0403 (19)	0.036 (2)	−0.0017 (16)	−0.0024 (15)	0.0034 (16)
C7	0.054 (2)	0.0347 (19)	0.045 (2)	−0.0015 (17)	0.0019 (19)	0.0008 (18)
C8	0.059 (3)	0.051 (2)	0.047 (2)	0.008 (2)	0.002 (2)	−0.002 (2)
C9	0.043 (2)	0.074 (3)	0.038 (2)	0.007 (2)	−0.0007 (19)	0.000 (2)
C10	0.049 (2)	0.074 (3)	0.040 (2)	0.000 (2)	0.0026 (18)	0.015 (2)
C11	0.046 (2)	0.046 (2)	0.047 (2)	−0.0040 (17)	−0.0002 (19)	0.0101 (18)
C12	0.0256 (15)	0.0325 (16)	0.0390 (18)	−0.0012 (13)	0.0022 (13)	−0.0025 (15)
C13	0.039 (2)	0.039 (2)	0.042 (2)	0.0005 (17)	0.0014 (16)	−0.0049 (18)
C14	0.039 (2)	0.055 (3)	0.037 (2)	−0.0006 (17)	−0.0026 (16)	−0.0086 (19)
C15	0.0363 (19)	0.057 (3)	0.041 (2)	0.0039 (18)	−0.0053 (17)	0.0046 (19)
C16	0.037 (2)	0.037 (2)	0.048 (2)	0.0057 (15)	−0.0024 (16)	0.0034 (18)
C17	0.0340 (17)	0.0339 (18)	0.0397 (19)	0.0027 (14)	0.0010 (15)	−0.0049 (15)
C18	0.041 (2)	0.057 (3)	0.051 (3)	0.0173 (18)	0.0040 (19)	−0.003 (2)

Geometric parameters (Å, º)

Cl1—C2	1.824 (3)	C7—C8	1.379 (7)
F1—C9	1.360 (6)	C8—H8	0.9500
F2—C15	1.360 (5)	C8—C9	1.376 (7)
O1—C3	1.213 (5)	C9—C10	1.363 (8)
N1—H1	0.8599	C10—H10	0.9500
N1—C1	1.457 (5)	C10—C11	1.388 (7)
N1—C5	1.461 (5)	C11—H11	0.9500
C1—H1A	1.0000	C12—C13	1.397 (5)
C1—C2	1.548 (4)	C12—C17	1.392 (5)
C1—C12	1.507 (5)	C13—H13	0.9500
C2—C3	1.535 (6)	C13—C14	1.372 (7)
C2—C18	1.515 (6)	C14—H14	0.9500
C3—C4	1.495 (6)	C14—C15	1.376 (7)
C4—H4A	0.9900	C15—C16	1.368 (6)
C4—H4B	0.9900	C16—H16	0.9500
C4—C5	1.551 (5)	C16—C17	1.384 (6)
C5—H5	1.0000	C17—H17	0.9500
C5—C6	1.505 (6)	C18—H18A	0.9800
C6—C7	1.399 (6)	C18—H18B	0.9800

C6—C11	1.389 (6)	C18—H18C	0.9800
C7—H7	0.9500		

C1—N1—H1	112.9	C7—C8—H8	120.6
C1—N1—C5	112.9 (3)	C9—C8—C7	118.7 (4)
C5—N1—H1	112.5	C9—C8—H8	120.6
N1—C1—H1A	107.5	F1—C9—C8	118.4 (5)
N1—C1—C2	109.3 (3)	F1—C9—C10	119.0 (5)
N1—C1—C12	110.7 (3)	C10—C9—C8	122.7 (4)
C2—C1—H1A	107.5	C9—C10—H10	120.9
C12—C1—H1A	107.5	C9—C10—C11	118.2 (4)
C12—C1—C2	114.1 (3)	C11—C10—H10	120.9
C1—C2—Cl1	110.2 (2)	C6—C11—C10	121.3 (4)
C3—C2—Cl1	103.0 (2)	C6—C11—H11	119.3
C3—C2—C1	110.3 (3)	C10—C11—H11	119.3
C18—C2—Cl1	107.9 (3)	C13—C12—C1	121.0 (3)
C18—C2—C1	112.7 (3)	C17—C12—C1	120.7 (3)
C18—C2—C3	112.4 (3)	C17—C12—C13	118.3 (4)
O1—C3—C2	120.1 (4)	C12—C13—H13	119.3
O1—C3—C4	123.4 (4)	C14—C13—C12	121.4 (4)
C4—C3—C2	116.5 (3)	C14—C13—H13	119.3
C3—C4—H4A	109.2	C13—C14—H14	120.8
C3—C4—H4B	109.2	C13—C14—C15	118.4 (4)
C3—C4—C5	112.1 (3)	C15—C14—H14	120.8
H4A—C4—H4B	107.9	F2—C15—C14	119.3 (4)
C5—C4—H4A	109.2	F2—C15—C16	118.3 (4)
C5—C4—H4B	109.2	C16—C15—C14	122.4 (4)
N1—C5—C4	108.5 (3)	C15—C16—H16	120.6
N1—C5—H5	108.9	C15—C16—C17	118.7 (4)
N1—C5—C6	110.8 (3)	C17—C16—H16	120.6
C4—C5—H5	108.9	C12—C17—H17	119.6
C6—C5—C4	110.7 (3)	C16—C17—C12	120.8 (4)
C6—C5—H5	108.9	C16—C17—H17	119.6
C7—C6—C5	120.5 (4)	C2—C18—H18A	109.5
C11—C6—C5	121.1 (4)	C2—C18—H18B	109.5
C11—C6—C7	118.3 (4)	C2—C18—H18C	109.5
C6—C7—H7	119.6	H18A—C18—H18B	109.5
C8—C7—C6	120.8 (4)	H18A—C18—H18C	109.5
C8—C7—H7	119.6	H18B—C18—H18C	109.5

Cl1—C2—C3—O1	106.0 (3)	C4—C5—C6—C11	98.1 (4)
Cl1—C2—C3—C4	−73.7 (4)	C5—N1—C1—C2	65.3 (3)
F1—C9—C10—C11	179.7 (4)	C5—N1—C1—C12	−168.2 (3)
F2—C15—C16—C17	179.6 (4)	C5—C6—C7—C8	177.4 (4)
O1—C3—C4—C5	136.3 (4)	C5—C6—C11—C10	−177.0 (4)
N1—C1—C2—Cl1	61.3 (3)	C6—C7—C8—C9	−0.3 (7)
N1—C1—C2—C3	−51.7 (3)	C7—C6—C11—C10	1.0 (7)
N1—C1—C2—C18	−178.1 (3)	C7—C8—C9—F1	−179.4 (4)

N1—C1—C12—C13	142.7 (3)	C7—C8—C9—C10	1.1 (8)
N1—C1—C12—C17	−36.4 (4)	C8—C9—C10—C11	−0.8 (7)
N1—C5—C6—C7	40.5 (5)	C9—C10—C11—C6	−0.3 (7)
N1—C5—C6—C11	−141.5 (4)	C11—C6—C7—C8	−0.7 (7)
C1—N1—C5—C4	−64.1 (4)	C12—C1—C2—Cl1	−63.2 (4)
C1—N1—C5—C6	174.3 (3)	C12—C1—C2—C3	−176.2 (3)
C1—C2—C3—O1	−136.4 (4)	C12—C1—C2—C18	57.4 (4)
C1—C2—C3—C4	43.9 (4)	C12—C13—C14—C15	0.9 (6)
C1—C12—C13—C14	179.8 (4)	C13—C12—C17—C16	0.3 (6)
C1—C12—C17—C16	179.3 (3)	C13—C14—C15—F2	179.5 (4)
C2—C1—C12—C13	−93.6 (4)	C13—C14—C15—C16	0.3 (7)
C2—C1—C12—C17	87.4 (4)	C14—C15—C16—C17	−1.1 (7)
C2—C3—C4—C5	−44.0 (4)	C15—C16—C17—C12	0.8 (6)
C3—C4—C5—N1	51.1 (4)	C17—C12—C13—C14	−1.2 (6)
C3—C4—C5—C6	172.9 (3)	C18—C2—C3—O1	−9.9 (5)
C4—C5—C6—C7	−79.9 (5)	C18—C2—C3—C4	170.4 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O1^{i}	1.00	2.44	3.328 (5)	148

Symmetry code: (i) *x*+1/2, −*y*+3/2, *z*.