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Crystal structures of two new 3-(2-chloroethyl)-*r*(2),*c*(6)-diarylpiperidin-4-ones

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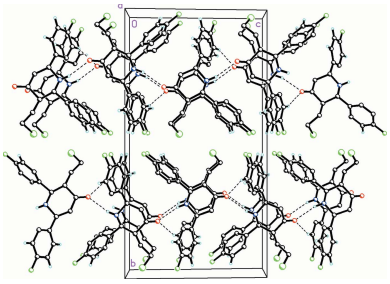
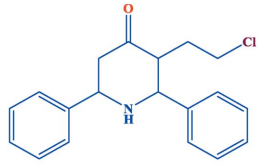
The syntheses and crystal structures of 3-(2-chloroethyl)-*r*-2,*c*-6-diphenylpiperidin-4-one, $C_{19}H_{20}ClNO$, (I), and 3-(2-chloroethyl)-*r*-2,*c*-6-bis(4-fluorophenyl)piperidin-4-one, $C_{19}H_{18}ClF_2NO$, (II), are described. The piperidone ring adopts a chair conformation in (I), whereas a slightly distorted chair conformation is formed in (II). The dihedral angle between the mean plane of the phenyl rings is 59.1 (1)° in (I) and 76.1 (1)° in (II). The crystal packing features weak intermolecular N—H···O hydrogen bonds in each structure.

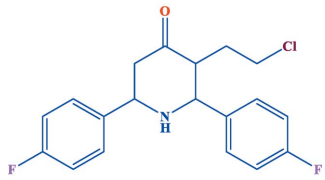
1. Chemical context

Piperidone molecules exhibit a wide spectrum of biological activities ranging from anti-bacterial to anti-cancer (Parthiban *et al.*, 2005, 2009, 2011). Most of the 2,6-diaryl-substituted piperidones and their derivatives are of significant pharmacological importance (Aridoss *et al.*, 2007). Some novel 3,5-dichloro-2,6-diarylpiperidin-4-ones are also reported to possess antimicrobial activity (Bhakiaraj *et al.*, 2014). Piperidones also display analgesic, anti-inflammatory, central nervous system (CNS), local anaesthetic, anticancer and antimicrobial activity (Perumal *et al.*, 2001). In view of the relevance of piperidone derivatives to a variety of ongoing health and pharmalogical issues, we have synthesized the title compounds and report their crystal structures here. Arulraj *et al.* (2017) has reported the crystal structure of three related 3-chloro-3-methyl-2,6-diarylpiperidin-4-ones. In each of these structures, the piperidine rings adopt chair conformations similar to what we have observed in the title compounds.





(I)



(II)

2. Structural commentary

Two new 3-(2-chloroethyl)-*r*-2,*c*-6-diarylpiperidin-4-one compounds, $C_{19}H_{20}ClNO$ (I) and $C_{19}H_{18}ClF_2NO$ (II), each crystallize in the $P2_1/c$ space group with one independent molecule in the asymmetric unit. The piperidone ring adopts a chair conformation in (I), (Fig. 1), whereas it forms a slightly distorted chair conformation in (II), (Fig. 2), with puckering parameters $Q = 0.576$ (2) Å, $\theta = 164.2$ (2)°, $\varphi = 179.4$ (8)° in (I) and $Q = 0.601$ (2) Å, $\theta = 4.93$ (19)°, $\varphi = 356$ (2)° in (II). The dihedral angle between the mean planes of the phenyl rings is 59.1 (1)° in (I) and 76.1 (1)° in (II). The increase in this dihedral angle in (II) could be attributed to steric repulsion from the substituent fluorine atoms. The sum of the bond angles around N1 in each structure [332.5° in (I) and 331.9° in (II)] is consistent with sp^3 hybridization (Beddoes *et al.*, 1986).

The substituents on the piperidine ring in both (I) and (II) adopt equatorial orientations with the keto oxygen atom being anti-clinal [O1—C3—C4—C5 = 136.1 (2)°] in (I) and anti-periplanar [O1—C1—C5—C4 = −120.4 (2)°] in (II). The 2-chloroethyl group lies in a syn-clinal orientation in both (I) [C3—C2—C18—C19 = 75.6 (3)°] and (II) [C1—C5—C6—C7 = 76.4 (2)°]. The two diaryl groups are both anti-clinal [N1—C5—C6—C11 = 54.5 (3)° and N1—C1—C12—C13 = 123.97 (18)°] in (I) whereas in (II) they are both syn-clinal [N1—C4—C14—C15 = −78.4 (2)° and N1—C3—C8—C13 = 35.4 (2)°].

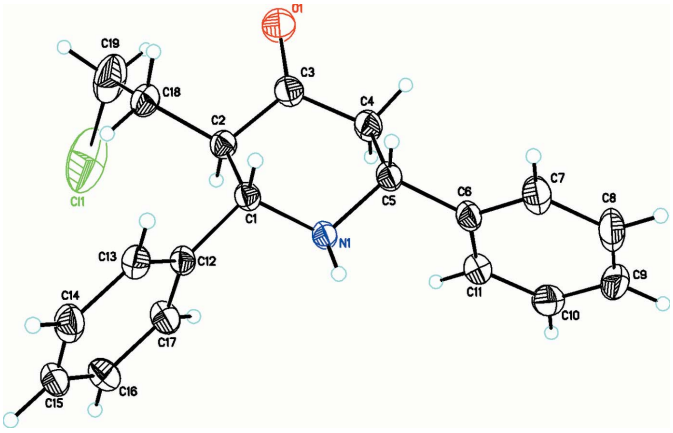


Figure 1
A view of the molecular structure of (I), showing displacement ellipsoids drawn at the 30% probability level.

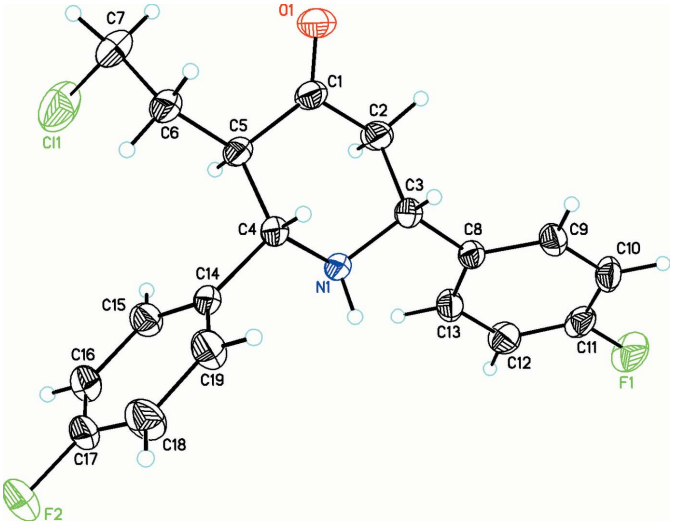


Figure 2
A view of the molecular structure of (II), showing displacement ellipsoids drawn at the 30% probability level.

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

*Cg*3 is the centroid of the C12–C17 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.86 (2)	2.52 (2)	3.335 (2)	158 (2)
C4—H4*A*···*Cg*3^{ii}	0.97	2.79	3.665 (2)	150

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

3. Supramolecular features

The crystal packing features very weak N1—H1···O1 hydrogen bonds in (I), forming infinite *C*(6) chains along the *b*-axis direction, with the molecules rotating in a 180° spiral motif along the axis (Table 1, Fig. 3). In addition, a weak C—H···π interaction between the piperdine ring and a diaryl group in (I) also occurs.

In (II), weak N—H···O hydrogen bonds (Fig. 4, Table 2) are again observed, also forming infinite *C*(6) chains but along the *c* axis in this case. Weak C—H···O and C—H···F interactions (Table 2) are also observed and contribute to the packing stability. In (II), the keto oxygen, O1, acts as the

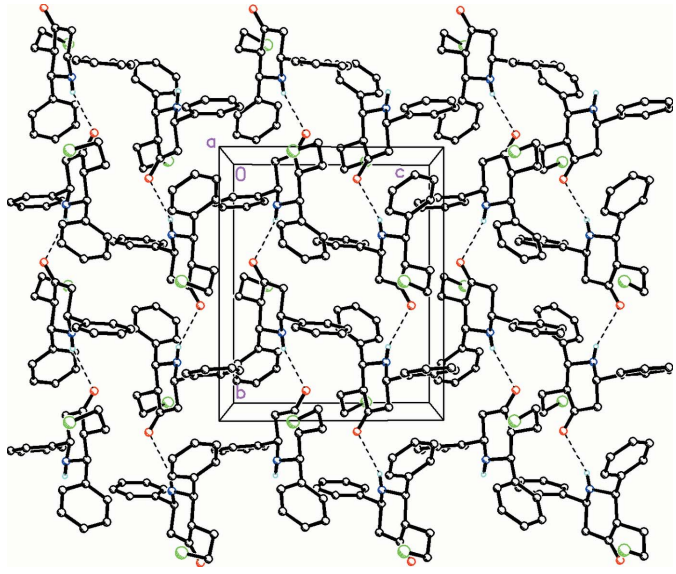


Figure 3
A partial view along the *a* axis of the crystal packing for (I), showing infinite chains formed along [010] by weak N1—H1···O1 hydrogen bonds with the molecules rotating in a 180° spiral motif along the axis. H atoms not involved in this interaction have been omitted for clarity.

Table 2
Hydrogen-bond geometry (Å, °) for (II).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.89 (2)	2.32 (2)	3.189 (2)	165 (2)
C9—H9···F2^{ii}	0.93	2.61	3.378 (2)	140
C10—H10···F2^{iii}	0.93	2.58	3.343 (2)	139
C12—H12···O1^{iv}	0.93	2.57	3.412 (3)	150
C16—H16···F1^{v}	0.93	2.62	3.379 (2)	139

Symmetry codes: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (iii) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$; (iv) $x-1, -y+\frac{1}{2}, z+\frac{1}{2}$; (v) $-x, y+\frac{1}{2}, -z+\frac{3}{2}$.

acceptor of weak hydrogen bonds involving atom N1 from a piperdine ring in the same plane and with atom C12 from one of the diaryl groups of a molecule in an adjacent plane along the *a* axis. An unusual weak C1—O1···π [O1···π = 3.8263 (19) Å, C1···π = 4.377 (2) Å, C1—O1···π = 109°; x, $\frac{1}{2}-y$, $-\frac{1}{2}+z$; centroid of the C8–C13 ring] interaction also between the piperidine ring and a diaryl group is observed.

4. Database survey

A search in the Cambridge Crystallographic Database (CSD version 5.38 of Nov, 2016, updates May, 2017; Groom *et al.*, 2016) for the 2,6-diphenylpiperidin-4-one skeleton resulted in 229 hits, which was further refined to 50 hits by removing those structures in which the title skeleton substructure was combined with larger molecules. The two most closely related remaining structures based on the pendant arms of the 2,6-diphenylpiperidine-4-one central substructure, *viz*. 2,6-diphenyl-3-isopropylpiperidin-4-one (ACEZUD; Nilofar Nissa *et al.*, 2001) and *t*-3-pentyl-r-2,c-6-diphenylpiperidin-4-one (RUGLOV; Gayathri *et al.*, 2009) were then compared with the two reported here. The piperidone ring in compounds

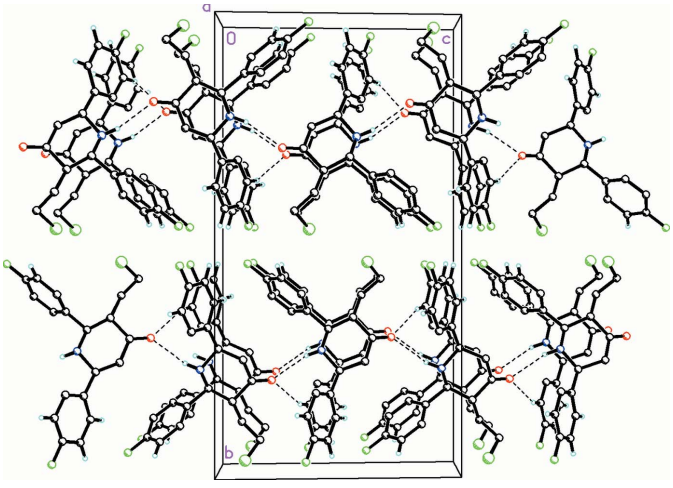


Figure 4
A partial view along the *a* axis of the crystal packing for (II), showing infinite chains formed along [001] by weak N1—H1···O1 and C12—H12···O1 hydrogen-bonding interactions. The keto oxygen, O1, forms a weak hydrogen bond with N1 from a piperdine ring in the same plane and with C12 from one of the diaryl groups of a molecule in an adjacent plane along the *a* axis. H atoms not involved in these interactions have been omitted for clarity.

(I) and (II) reported here adopt chair or distorted chair conformations, unlike in ACEZUD and RUGLOV. The crystal packing is stabilized by N—H···O intermolecular hydrogen bonds in both (I) and (II), as well as in ACEZUD. In contrast, the crystal packing in RUGLOV is influenced only by weak C—H···O and C—H···π intermolecular interactions.

5. Synthesis and crystallization

A mixture of ammonium acetate (0.1 mol, 7.71 g), the respective aldehyde (0.2 mol), benzaldehyde/*p*-fluorobenzaldehyde (20.4 ml/21.0 ml) and 5-chloro-2-pentanone (0.1 mol, 11.4 ml) in distilled ethanol was heated first to boiling. After cooling, the viscous liquid obtained was dissolved in diethyl ether (200 ml) and shaken with 100 ml of concentrated hydrochloric acid. The precipitated hydrochlorides of the 3-(2-chloroethyl)-*r*-2,*c*-6-diarylpiperidin-4-ones were removed by filtration and washed first with a 40 ml mixture of ethanol and diethyl ether (1:1) and then with diethyl ether to remove most of the coloured impurities. The base was liberated from an alcoholic solution by adding aqueous ammonia and then diluted with water. Each compound was recrystallized twice from a distilled ethanol solution: single crystals of (I) and (II) were obtained after two days. The yield of the isolated product was 3.0 g (I) and 2.5 g (II).

3-(2-Chloroethyl)-*r*-2,*c*-6-diphenylpiperidin-4-one, ($C_{19}H_{20}ClNO$), (I):

IR (KBr): 3311.07 (νN—H), 3067.56, 3033.34 (νC—H), 1697.03 (νC═O), 1605.39, 1493.90 (νC═C), 769.33 (νC—Cl) $cm^{-1.}$ ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.42–7.19 (*m*, aromatic protons), 4.03 (*d*, H6 proton), 3.64 (*d*, H2 proton), 3.36–3.33 (m, H5a proton), 2.61 (*dd*, H5e proton), 2.18–2.09 (*m*, H3 proton, 1.99 (*s*, NH proton), 2.94 (*s*, CH_2Cl proton), 2.75 (*t*, CH_2 proton). ^{13}C NMR ($CDCl_3$, 400 MHz): δ 208.60 (C═O), 140.67 (aromatic *ipso* carbon atoms), 128.81–126.63 (aromatic carbon atoms), 67.27 (C-3 carbon), 61.92 (C-2 carbon), 53.76 (C-6 carbon), 51.27 (C-5 carbon), 28.18 (methylene carbon), 43.49 (CH_2Cl Carbon). Melting point: 371 K.

3-(2-Chloroethyl)-*r*-2,*c*-6-bis(p-fluorophenyl)piperidin-4-one, ($C_{19}H_{18}ClF_2NO$), (II):

IR (KBr): 3292.53 (νN—H), 3078.27, 3077.86 (νC—H), 1702.32 (νC═O), 1605.79, 1511.47 (νC═C), 760.50 (νC—Cl) $cm^{-1.}$ ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39–7.02 (*m*, aromatic protons), 3.99 (*dd*, H6 proton), 3.61 (*d*, H2 proton), 3.36 (*dd*, H5a proton), 2.52 (*dd*, H5e proton), 2.16–2.08 (*m*, H3 proton), 1.99 (*s*, NH proton), 2.84 (*t*, CH_2Cl proton), 2.67 (*t*, CH_2 proton). ^{13}C NMR ($CDCl_3$, 400 MHz): δ 208.09 (C═O), (aromatic *ipso* carbon atoms), 115.84–115.51 (aromatic carbon atoms), 55.77 (C-3 carbon), 66.34 (C-2 carbon), 61.09 (C-6 carbon), 51.41 (C-5 carbon), 28.06 (methylene carbon), 43.45 (CH_2Cl Carbon). Melting point: 375 K.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The N1-bound H atoms in both

Table 3
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	$C_{19}H_{20}ClNO$	$C_{19}H_{18}ClF_2NO$
M_r	313.81	349.79
Crystal system, space group	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/c$
Temperature (K)	293	293
a, b, c (Å)	11.3306 (3), 13.3638 (4), 10.9821 (3)	5.5105 (2), 24.2612 (6), 12.8622 (3)
β (°)	91.996 (2)	93.809 (3)
V (Å^3)	1661.90 (8)	1715.77 (9)
Z	4	4
Radiation type	Cu $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	2.03	2.20
Crystal size (mm)	0.42 × 0.38 × 0.14	0.34 × 0.16 × 0.14
Data collection		
Diffractometer	Rigaku Oxford Diffraction	Rigaku Oxford Diffraction
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2015)	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.535, 1.000	0.524, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6237, 3168, 2545	6548, 3267, 2702
R_{int}	0.028	0.020
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.615	0.614
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.055, 0.158, 1.05	0.046, 0.131, 1.04
No. of reflections	3168	3267
No. of parameters	204	222
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.56, −0.44	0.34, −0.38

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

molecules were located in a difference-Fourier map and their coordinates and displacement parameters freely refined. All C-bound H atoms were refined using a riding model with d(C—H) = 0.93 Å for aromatic, 0.97 Å for methylene and 0.98 Å for methine H atoms, all with $U_{iso} = 1.2U_{eq}$ (C)

Acknowledgements

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supporting information

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Crystal structures of two new 3-(2-chloroethyl)-*r*(2),*c*(6)-diarylpiperidin-4-ones

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Computing details

For both structures, data collection: *CrysAlis PRO* (Rigaku OD, 2015); cell refinement: *CrysAlis PRO* (Rigaku OD, 2015); data reduction: *CrysAlis PRO* (Rigaku OD, 2015); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

3-(2-Chloroethyl)-*r*-2,*c*-6-diphenylpiperidin-4-one (I)

Crystal data

$C_{19}H_{20}ClNO$
$M_r = 313.81$
Monoclinic, $P2_1/c$
$a = 11.3306$ (3) Å
$b = 13.3638$ (4) Å
$c = 10.9821$ (3) Å
$\beta = 91.996$ (2)°
$V = 1661.90$ (8) Å^3
$Z = 4$
$F(000) = 664$
$D_x = 1.254$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 2185 reflections
$\theta = 5.1$–$71.2°$
$\mu = 2.03$ mm^{-1}
$T = 293$ K
Prism, colourless
0.42 × 0.38 × 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)
$T_{min} = 0.535$, $T_{max} = 1.000$
6237 measured reflections
3168 independent reflections
2545 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 71.4°$, $\theta_{min} = 3.9°$
$h = -13 \rightarrow 13$
$k = -14 \rightarrow 16$
$l = -13 \rightarrow 8$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.158$
$S = 1.05$
3168 reflections
204 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.075P)^2 + 0.5181P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.56$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ e Å^{-3}

Extinction correction: SHELXL2018 (Sheldrick, 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0026 (4)

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}
Cl1	0.08089 (8)	0.50912 (12)	0.17386 (10)	0.1402 (6)
O1	0.44751 (18)	0.41543 (13)	0.1217 (2)	0.0771 (6)
N1	0.48661 (13)	0.69143 (12)	0.26049 (15)	0.0370 (4)
H1	0.511 (2)	0.7523 (19)	0.270 (2)	0.045 (6)*
C1	0.41112 (15)	0.67867 (13)	0.15013 (17)	0.0356 (4)
H1A	0.460437	0.682251	0.078697	0.043*
C2	0.35356 (16)	0.57351 (14)	0.15481 (18)	0.0393 (4)
H2	0.303654	0.572734	0.225915	0.047*
C3	0.44765 (19)	0.49404 (15)	0.1762 (2)	0.0479 (5)
C4	0.5424 (2)	0.51707 (15)	0.2711 (2)	0.0509 (5)
H4A	0.607257	0.470401	0.262937	0.061*
H4B	0.511036	0.508140	0.351412	0.061*
C5	0.58905 (17)	0.62451 (15)	0.25931 (18)	0.0410 (4)
H5	0.627033	0.631318	0.180923	0.049*
C6	0.67816 (17)	0.64909 (15)	0.3605 (2)	0.0447 (5)
C7	0.79567 (19)	0.66364 (18)	0.3344 (2)	0.0557 (6)
H7	0.819078	0.661112	0.254103	0.067*
C8	0.8789 (2)	0.6821 (2)	0.4283 (3)	0.0711 (8)
H8	0.957634	0.691906	0.410133	0.085*
C9	0.8460 (2)	0.6858 (2)	0.5464 (3)	0.0744 (8)
H9	0.902038	0.697968	0.608508	0.089*
C10	0.7293 (3)	0.6715 (2)	0.5735 (3)	0.0688 (7)
H10	0.706558	0.673952	0.654000	0.083*
C11	0.6462 (2)	0.65346 (19)	0.4813 (2)	0.0575 (6)
H11	0.567619	0.644106	0.500381	0.069*
C12	0.31935 (15)	0.76066 (14)	0.14123 (16)	0.0361 (4)
C13	0.30967 (17)	0.82110 (15)	0.03920 (18)	0.0420 (4)
H13	0.362040	0.812853	−0.023373	0.050*
C14	0.2224 (2)	0.89410 (17)	0.0292 (2)	0.0514 (5)
H14	0.216607	0.933973	−0.040138	0.062*
C15	0.14510 (19)	0.90767 (17)	0.1206 (2)	0.0544 (6)
H15	0.086504	0.956250	0.113438	0.065*
C16	0.1547 (2)	0.84889 (19)	0.2234 (2)	0.0574 (6)
H16	0.102923	0.858368	0.286259	0.069*
C17	0.24084 (19)	0.77582 (18)	0.23368 (19)	0.0488 (5)

H17	0.246249	0.736357	0.303402	0.059*
C18	0.2733 (2)	0.55077 (18)	0.0436 (2)	0.0510 (5)
H18A	0.232158	0.611677	0.019567	0.061*
H18B	0.322225	0.531314	−0.023166	0.061*
C19	0.1841 (3)	0.4707 (3)	0.0620 (4)	0.0939 (11)
H19A	0.223702	0.409828	0.088879	0.113*
H19B	0.142107	0.456775	−0.014624	0.113*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0686 (5)	0.2364 (16)	0.1155 (8)	−0.0747 (8)	−0.0010 (5)	0.0298 (8)
O1	0.0723 (12)	0.0455 (10)	0.1114 (15)	0.0094 (8)	−0.0271 (11)	−0.0258 (10)
N1	0.0310 (7)	0.0311 (8)	0.0486 (9)	0.0021 (6)	−0.0054 (6)	−0.0010 (6)
C1	0.0295 (8)	0.0354 (9)	0.0419 (9)	0.0005 (7)	0.0004 (7)	0.0006 (7)
C2	0.0343 (9)	0.0368 (10)	0.0466 (10)	−0.0024 (7)	−0.0015 (7)	−0.0015 (8)
C3	0.0436 (11)	0.0344 (10)	0.0654 (13)	−0.0010 (8)	−0.0037 (9)	−0.0017 (9)
C4	0.0487 (11)	0.0348 (10)	0.0681 (14)	0.0067 (9)	−0.0141 (10)	0.0006 (9)
C5	0.0335 (9)	0.0378 (10)	0.0514 (11)	0.0043 (8)	−0.0042 (8)	−0.0003 (8)
C6	0.0351 (9)	0.0359 (10)	0.0625 (12)	0.0061 (8)	−0.0092 (8)	−0.0008 (8)
C7	0.0397 (11)	0.0521 (13)	0.0747 (15)	0.0006 (9)	−0.0069 (10)	0.0069 (11)
C8	0.0377 (12)	0.0649 (16)	0.109 (2)	−0.0009 (11)	−0.0211 (13)	0.0024 (15)
C9	0.0599 (15)	0.0682 (17)	0.092 (2)	0.0121 (13)	−0.0366 (14)	−0.0202 (14)
C10	0.0685 (16)	0.0701 (17)	0.0666 (15)	0.0199 (13)	−0.0167 (12)	−0.0181 (12)
C11	0.0458 (11)	0.0591 (14)	0.0669 (14)	0.0107 (10)	−0.0083 (10)	−0.0125 (11)
C12	0.0297 (8)	0.0354 (9)	0.0428 (9)	−0.0003 (7)	−0.0044 (7)	−0.0007 (7)
C13	0.0375 (9)	0.0446 (11)	0.0435 (10)	−0.0029 (8)	−0.0051 (7)	0.0024 (8)
C14	0.0498 (12)	0.0439 (11)	0.0592 (12)	0.0003 (9)	−0.0152 (10)	0.0090 (9)
C15	0.0416 (11)	0.0439 (12)	0.0766 (15)	0.0103 (9)	−0.0150 (10)	−0.0058 (10)
C16	0.0446 (11)	0.0635 (14)	0.0643 (14)	0.0154 (11)	0.0036 (10)	−0.0086 (11)
C17	0.0438 (11)	0.0553 (12)	0.0474 (11)	0.0104 (9)	0.0026 (8)	0.0054 (9)
C18	0.0450 (11)	0.0517 (12)	0.0556 (12)	−0.0056 (9)	−0.0084 (9)	−0.0063 (10)
C19	0.082 (2)	0.078 (2)	0.119 (3)	−0.0299 (17)	−0.0414 (19)	0.0050 (19)

Geometric parameters (Å, º)

Cl1—C19	1.801 (4)	C8—C9	1.363 (4)
O1—C3	1.209 (3)	C9—H9	0.9300
N1—H1	0.86 (2)	C9—C10	1.379 (4)
N1—C1	1.469 (2)	C10—H10	0.9300
N1—C5	1.466 (2)	C10—C11	1.379 (3)
C1—H1A	0.9800	C11—H11	0.9300
C1—C2	1.551 (2)	C12—C13	1.382 (3)
C1—C12	1.511 (2)	C12—C17	1.388 (3)
C2—H2	0.9800	C13—H13	0.9300
C2—C3	1.517 (3)	C13—C14	1.391 (3)
C2—C18	1.528 (3)	C14—H14	0.9300
C3—C4	1.502 (3)	C14—C15	1.367 (3)

C4—H4A	0.9700	C15—H15	0.9300
C4—H4B	0.9700	C15—C16	1.376 (3)
C4—C5	1.537 (3)	C16—H16	0.9300
C5—H5	0.9800	C16—C17	1.383 (3)
C5—C6	1.512 (3)	C17—H17	0.9300
C6—C7	1.386 (3)	C18—H18A	0.9700
C6—C11	1.389 (3)	C18—H18B	0.9700
C7—H7	0.9300	C18—C19	1.490 (4)
C7—C8	1.395 (4)	C19—H19A	0.9700
C8—H8	0.9300	C19—H19B	0.9700

C1—N1—H1	112.3 (15)	C8—C9—H9	120.1
C5—N1—H1	109.1 (16)	C8—C9—C10	119.8 (2)
C5—N1—C1	111.13 (15)	C10—C9—H9	120.1
N1—C1—H1A	108.8	C9—C10—H10	120.0
N1—C1—C2	108.14 (15)	C9—C10—C11	120.1 (3)
N1—C1—C12	110.41 (15)	C11—C10—H10	120.0
C2—C1—H1A	108.8	C6—C11—H11	119.5
C12—C1—H1A	108.8	C10—C11—C6	121.0 (2)
C12—C1—C2	111.71 (15)	C10—C11—H11	119.5
C1—C2—H2	106.9	C13—C12—C1	120.73 (17)
C3—C2—C1	110.20 (15)	C13—C12—C17	118.22 (18)
C3—C2—H2	106.9	C17—C12—C1	121.04 (17)
C3—C2—C18	112.34 (17)	C12—C13—H13	119.7
C18—C2—C1	113.15 (17)	C12—C13—C14	120.66 (19)
C18—C2—H2	106.9	C14—C13—H13	119.7
O1—C3—C2	122.9 (2)	C13—C14—H14	119.8
O1—C3—C4	120.7 (2)	C15—C14—C13	120.5 (2)
C4—C3—C2	116.46 (17)	C15—C14—H14	119.8
C3—C4—H4A	109.2	C14—C15—H15	120.3
C3—C4—H4B	109.2	C14—C15—C16	119.5 (2)
C3—C4—C5	111.87 (17)	C16—C15—H15	120.3
H4A—C4—H4B	107.9	C15—C16—H16	119.8
C5—C4—H4A	109.2	C15—C16—C17	120.4 (2)
C5—C4—H4B	109.2	C17—C16—H16	119.8
N1—C5—C4	107.14 (16)	C12—C17—H17	119.6
N1—C5—H5	108.9	C16—C17—C12	120.8 (2)
N1—C5—C6	111.71 (16)	C16—C17—H17	119.6
C4—C5—H5	108.9	C2—C18—H18A	108.5
C6—C5—C4	111.33 (17)	C2—C18—H18B	108.5
C6—C5—H5	108.9	H18A—C18—H18B	107.5
C7—C6—C5	120.0 (2)	C19—C18—C2	115.0 (2)
C7—C6—C11	118.5 (2)	C19—C18—H18A	108.5
C11—C6—C5	121.46 (19)	C19—C18—H18B	108.5
C6—C7—H7	120.0	Cl1—C19—H19A	109.6
C6—C7—C8	120.1 (3)	Cl1—C19—H19B	109.6
C8—C7—H7	120.0	C18—C19—Cl1	110.3 (2)
C7—C8—H8	119.7	C18—C19—H19A	109.6

C9—C8—C7	120.6 (2)	C18—C19—H19B	109.6
C9—C8—H8	119.7	H19A—C19—H19B	108.1

O1—C3—C4—C5	136.1 (2)	C4—C5—C6—C11	−65.2 (3)
N1—C1—C2—C3	−52.8 (2)	C5—N1—C1—C2	68.10 (18)
N1—C1—C2—C18	−179.46 (16)	C5—N1—C1—C12	−169.41 (15)
N1—C1—C12—C13	123.97 (18)	C5—C6—C7—C8	−177.2 (2)
N1—C1—C12—C17	−57.6 (2)	C5—C6—C11—C10	177.0 (2)
N1—C5—C6—C7	−128.3 (2)	C6—C7—C8—C9	0.1 (4)
N1—C5—C6—C11	54.5 (3)	C7—C6—C11—C10	−0.2 (4)
C1—N1—C5—C4	−67.8 (2)	C7—C8—C9—C10	−0.2 (4)
C1—N1—C5—C6	170.05 (16)	C8—C9—C10—C11	0.0 (4)
C1—C2—C3—O1	−137.1 (2)	C9—C10—C11—C6	0.2 (4)
C1—C2—C3—C4	43.6 (2)	C11—C6—C7—C8	0.1 (3)
C1—C2—C18—C19	−158.8 (2)	C12—C1—C2—C3	−174.45 (16)
C1—C12—C13—C14	177.64 (18)	C12—C1—C2—C18	58.8 (2)
C1—C12—C17—C16	−178.0 (2)	C12—C13—C14—C15	0.4 (3)
C2—C1—C12—C13	−115.65 (19)	C13—C12—C17—C16	0.5 (3)
C2—C1—C12—C17	62.8 (2)	C13—C14—C15—C16	0.4 (3)
C2—C3—C4—C5	−44.6 (3)	C14—C15—C16—C17	−0.8 (4)
C2—C18—C19—Cl1	64.5 (3)	C15—C16—C17—C12	0.3 (4)
C3—C2—C18—C19	75.6 (3)	C17—C12—C13—C14	−0.9 (3)
C3—C4—C5—N1	53.6 (2)	C18—C2—C3—O1	−9.9 (3)
C3—C4—C5—C6	176.03 (18)	C18—C2—C3—C4	170.81 (19)
C4—C5—C6—C7	112.0 (2)		

Hydrogen-bond geometry (Å, º)

Cg3 is the centroid of the C12–C17 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.86 (2)	2.52 (2)	3.335 (2)	158 (2)
C4—H4*A*···*Cg*3^{ii}	0.97	2.79	3.665 (2)	150

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

3-(2-chloroethyl)-*r*-2,*c*-6-bis(4-fluorophenyl)piperidin-4-one (II)

Crystal data

$C_{19}H_{18}ClF_2NO$	*F*(000) = 728
M_r = 349.79	D_x = 1.354 Mg m^{-3}
Monoclinic, $P2_1/c$	Cu *Kα* radiation, λ = 1.54184 Å
a = 5.5105 (2) Å	Cell parameters from 2364 reflections
b = 24.2612 (6) Å	θ = 3.4–71.3°
c = 12.8622 (3) Å	μ = 2.20 mm^{-1}
β = 93.809 (3)°	*T* = 293 K
V = 1715.77 (9) Å^3	Prism, colourless
Z = 4	0.34 × 0.16 × 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} = 0.524, T_{max} = 1.000
6548 measured reflections
3267 independent reflections
2702 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 71.3°, θ_{min} = 3.6°
h = −6→6
k = −29→16
l = −14→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.131
S = 1.04
3267 reflections
222 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0592P)^2 + 0.5453P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}
Extinction correction: SHELXL2018 (Sheldrick, 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0058 (5)

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cl1	0.15647 (18)	0.46455 (3)	0.38176 (8)	0.1057 (3)
F1	−0.2069 (3)	0.04268 (6)	0.63058 (13)	0.0854 (5)
F2	0.6123 (3)	0.45967 (6)	0.88365 (11)	0.0747 (4)
O1	0.4499 (4)	0.29713 (7)	0.28005 (11)	0.0702 (5)
N1	0.3190 (3)	0.27067 (6)	0.57146 (11)	0.0396 (4)
H1	0.366 (4)	0.2579 (9)	0.6346 (17)	0.043 (5)*
C1	0.3477 (4)	0.29649 (8)	0.36027 (14)	0.0489 (5)
C2	0.1985 (4)	0.24790 (9)	0.39147 (14)	0.0528 (5)
H2A	0.199144	0.219410	0.338582	0.063*
H2B	0.031521	0.259163	0.398695	0.063*
C3	0.3112 (4)	0.22560 (7)	0.49651 (14)	0.0414 (4)
H3	0.478176	0.213743	0.486823	0.050*
C4	0.4808 (3)	0.31538 (7)	0.54325 (13)	0.0384 (4)
H4	0.639887	0.299519	0.530846	0.046*
C5	0.3752 (4)	0.34225 (7)	0.44054 (13)	0.0431 (4)
H5	0.212671	0.356346	0.452333	0.052*
C6	0.5288 (4)	0.39034 (8)	0.40516 (16)	0.0530 (5)
H6A	0.582661	0.412091	0.465641	0.064*
H6B	0.672413	0.375749	0.375148	0.064*

C7	0.3962 (5)	0.42751 (11)	0.3263 (2)	0.0737 (7)
H7A	0.329082	0.405487	0.268405	0.088*
H7B	0.510404	0.453477	0.299551	0.088*
C8	0.1707 (3)	0.17694 (7)	0.53451 (13)	0.0389 (4)
C9	0.2447 (4)	0.12399 (8)	0.51246 (15)	0.0462 (4)
H9	0.382523	0.118931	0.475566	0.055*
C10	0.1180 (4)	0.07832 (8)	0.54414 (17)	0.0548 (5)
H10	0.166749	0.042824	0.527870	0.066*
C11	−0.0797 (4)	0.08699 (8)	0.59972 (16)	0.0534 (5)
C12	−0.1588 (4)	0.13849 (9)	0.62493 (17)	0.0552 (5)
H12	−0.294820	0.142967	0.663223	0.066*
C13	−0.0313 (4)	0.18376 (8)	0.59200 (16)	0.0480 (5)
H13	−0.081684	0.219075	0.608620	0.058*
C14	0.5130 (3)	0.35521 (7)	0.63374 (13)	0.0378 (4)
C15	0.3388 (4)	0.39397 (8)	0.65460 (15)	0.0488 (5)
H15	0.197012	0.396256	0.611350	0.059*
C16	0.3714 (4)	0.42936 (8)	0.73856 (16)	0.0534 (5)
H16	0.254041	0.455500	0.751883	0.064*
C17	0.5796 (4)	0.42507 (8)	0.80138 (15)	0.0513 (5)
C18	0.7540 (4)	0.38685 (10)	0.78520 (18)	0.0628 (6)
H18	0.892640	0.384155	0.830246	0.075*
C19	0.7201 (4)	0.35205 (9)	0.70008 (17)	0.0544 (5)
H19	0.838816	0.326106	0.687407	0.065*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1146 (7)	0.0738 (5)	0.1305 (7)	0.0231 (4)	0.0211 (5)	0.0356 (5)
F1	0.1086 (12)	0.0563 (8)	0.0919 (11)	−0.0353 (8)	0.0103 (9)	0.0197 (7)
F2	0.1015 (11)	0.0585 (8)	0.0632 (8)	−0.0144 (7)	−0.0006 (7)	−0.0275 (6)
O1	0.1093 (14)	0.0624 (9)	0.0408 (8)	−0.0254 (9)	0.0187 (8)	−0.0040 (7)
N1	0.0553 (9)	0.0310 (7)	0.0325 (7)	−0.0058 (6)	0.0018 (6)	0.0019 (6)
C1	0.0664 (12)	0.0454 (10)	0.0342 (9)	−0.0112 (9)	−0.0015 (8)	0.0048 (7)
C2	0.0737 (13)	0.0469 (10)	0.0371 (9)	−0.0191 (10)	−0.0017 (9)	−0.0026 (8)
C3	0.0506 (10)	0.0337 (8)	0.0401 (9)	−0.0062 (7)	0.0046 (7)	−0.0015 (7)
C4	0.0453 (9)	0.0328 (8)	0.0370 (8)	−0.0033 (7)	0.0019 (7)	−0.0006 (7)
C5	0.0549 (10)	0.0373 (9)	0.0369 (9)	−0.0093 (8)	0.0023 (7)	0.0048 (7)
C6	0.0693 (13)	0.0430 (10)	0.0472 (10)	−0.0153 (9)	0.0075 (9)	0.0045 (8)
C7	0.101 (2)	0.0561 (13)	0.0645 (14)	−0.0090 (13)	0.0123 (13)	0.0215 (11)
C8	0.0465 (9)	0.0325 (8)	0.0372 (8)	−0.0037 (7)	−0.0008 (7)	−0.0006 (6)
C9	0.0523 (10)	0.0370 (9)	0.0494 (10)	−0.0009 (8)	0.0038 (8)	−0.0060 (8)
C10	0.0726 (14)	0.0295 (9)	0.0611 (12)	−0.0003 (9)	−0.0048 (10)	−0.0018 (8)
C11	0.0662 (12)	0.0415 (10)	0.0514 (11)	−0.0176 (9)	−0.0049 (9)	0.0103 (8)
C12	0.0557 (12)	0.0545 (12)	0.0563 (11)	−0.0090 (9)	0.0105 (9)	0.0017 (9)
C13	0.0539 (11)	0.0356 (9)	0.0552 (11)	0.0002 (8)	0.0083 (9)	−0.0019 (8)
C14	0.0471 (9)	0.0305 (8)	0.0356 (8)	−0.0062 (7)	0.0024 (7)	0.0009 (6)
C15	0.0505 (10)	0.0478 (10)	0.0475 (10)	0.0012 (8)	−0.0016 (8)	−0.0052 (8)
C16	0.0641 (12)	0.0417 (10)	0.0550 (11)	0.0037 (9)	0.0085 (9)	−0.0073 (8)

C17	0.0715 (13)	0.0382 (9)	0.0443 (10)	−0.0151 (9)	0.0043 (9)	−0.0097 (8)
C18	0.0622 (13)	0.0659 (14)	0.0577 (12)	−0.0028 (11)	−0.0159 (10)	−0.0153 (11)
C19	0.0557 (11)	0.0492 (11)	0.0566 (11)	0.0074 (9)	−0.0079 (9)	−0.0108 (9)

Geometric parameters (Å, º)

Cl1—C7	1.785 (3)	C7—H7A	0.9700
F1—C11	1.357 (2)	C7—H7B	0.9700
F2—C17	1.353 (2)	C8—C9	1.383 (3)
O1—C1	1.208 (2)	C8—C13	1.386 (3)
N1—H1	0.89 (2)	C9—H9	0.9300
N1—C3	1.457 (2)	C9—C10	1.385 (3)
N1—C4	1.465 (2)	C10—H10	0.9300
C1—C2	1.507 (3)	C10—C11	1.359 (3)
C1—C5	1.517 (3)	C11—C12	1.369 (3)
C2—H2A	0.9700	C12—H12	0.9300
C2—H2B	0.9700	C12—C13	1.385 (3)
C2—C3	1.547 (3)	C13—H13	0.9300
C3—H3	0.9800	C14—C15	1.383 (3)
C3—C8	1.511 (2)	C14—C19	1.381 (3)
C4—H4	0.9800	C15—H15	0.9300
C4—C5	1.551 (2)	C15—C16	1.382 (3)
C4—C14	1.514 (2)	C16—H16	0.9300
C5—H5	0.9800	C16—C17	1.363 (3)
C5—C6	1.528 (2)	C17—C18	1.361 (3)
C6—H6A	0.9700	C18—H18	0.9300
C6—H6B	0.9700	C18—C19	1.385 (3)
C6—C7	1.509 (3)	C19—H19	0.9300
C3—N1—H1	109.6 (14)	C6—C7—H7A	109.3
C3—N1—C4	112.57 (14)	C6—C7—H7B	109.3
C4—N1—H1	109.7 (14)	H7A—C7—H7B	107.9
O1—C1—C2	122.08 (19)	C9—C8—C3	119.67 (17)
O1—C1—C5	122.75 (18)	C9—C8—C13	118.58 (17)
C2—C1—C5	115.02 (16)	C13—C8—C3	121.75 (16)
C1—C2—H2A	110.1	C8—C9—H9	119.3
C1—C2—H2B	110.1	C8—C9—C10	121.42 (18)
C1—C2—C3	108.16 (16)	C10—C9—H9	119.3
H2A—C2—H2B	108.4	C9—C10—H10	121.0
C3—C2—H2A	110.1	C11—C10—C9	117.93 (18)
C3—C2—H2B	110.1	C11—C10—H10	121.0
N1—C3—C2	107.94 (15)	F1—C11—C10	118.6 (2)
N1—C3—H3	108.5	F1—C11—C12	118.4 (2)
N1—C3—C8	111.46 (14)	C10—C11—C12	123.02 (19)
C2—C3—H3	108.5	C11—C12—H12	120.8
C8—C3—C2	111.80 (15)	C11—C12—C13	118.36 (19)
C8—C3—H3	108.5	C13—C12—H12	120.8
N1—C4—H4	108.4	C8—C13—H13	119.7

N1—C4—C5	108.78 (14)	C12—C13—C8	120.67 (18)
N1—C4—C14	108.93 (13)	C12—C13—H13	119.7
C5—C4—H4	108.4	C15—C14—C4	122.38 (16)
C14—C4—H4	108.4	C19—C14—C4	119.30 (17)
C14—C4—C5	113.86 (14)	C19—C14—C15	118.29 (17)
C1—C5—C4	106.67 (15)	C14—C15—H15	119.4
C1—C5—H5	108.0	C16—C15—C14	121.19 (19)
C1—C5—C6	112.85 (16)	C16—C15—H15	119.4
C4—C5—H5	108.0	C15—C16—H16	120.8
C6—C5—C4	112.99 (16)	C17—C16—C15	118.48 (19)
C6—C5—H5	108.0	C17—C16—H16	120.8
C5—C6—H6A	108.8	F2—C17—C16	118.6 (2)
C5—C6—H6B	108.8	F2—C17—C18	118.92 (19)
H6A—C6—H6B	107.7	C18—C17—C16	122.44 (18)
C7—C6—C5	113.76 (19)	C17—C18—H18	120.8
C7—C6—H6A	108.8	C17—C18—C19	118.5 (2)
C7—C6—H6B	108.8	C19—C18—H18	120.8
Cl1—C7—H7A	109.3	C14—C19—C18	121.1 (2)
Cl1—C7—H7B	109.3	C14—C19—H19	119.4
C6—C7—Cl1	111.78 (17)	C18—C19—H19	119.4

F1—C11—C12—C13	−178.99 (19)	C4—C5—C6—C7	−162.48 (18)
F2—C17—C18—C19	−179.3 (2)	C4—C14—C15—C16	179.14 (18)
O1—C1—C2—C3	120.0 (2)	C4—C14—C19—C18	−178.5 (2)
O1—C1—C5—C4	−120.4 (2)	C5—C1—C2—C3	−55.6 (2)
O1—C1—C5—C6	4.2 (3)	C5—C4—C14—C15	43.2 (2)
N1—C3—C8—C9	−144.20 (17)	C5—C4—C14—C19	−138.73 (19)
N1—C3—C8—C13	35.4 (2)	C5—C6—C7—Cl1	67.6 (2)
N1—C4—C5—C1	−56.49 (19)	C8—C9—C10—C11	−1.3 (3)
N1—C4—C5—C6	178.94 (15)	C9—C8—C13—C12	−1.2 (3)
N1—C4—C14—C15	−78.4 (2)	C9—C10—C11—F1	179.48 (19)
N1—C4—C14—C19	99.7 (2)	C9—C10—C11—C12	0.4 (3)
C1—C2—C3—N1	56.4 (2)	C10—C11—C12—C13	0.1 (3)
C1—C2—C3—C8	179.37 (16)	C11—C12—C13—C8	0.3 (3)
C1—C5—C6—C7	76.4 (2)	C13—C8—C9—C10	1.7 (3)
C2—C1—C5—C4	55.1 (2)	C14—C4—C5—C1	−178.17 (15)
C2—C1—C5—C6	179.78 (18)	C14—C4—C5—C6	57.3 (2)
C2—C3—C8—C9	94.9 (2)	C14—C15—C16—C17	−0.4 (3)
C2—C3—C8—C13	−85.5 (2)	C15—C14—C19—C18	−0.3 (3)
C3—N1—C4—C5	65.35 (19)	C15—C16—C17—F2	179.98 (18)
C3—N1—C4—C14	−170.01 (15)	C15—C16—C17—C18	−0.9 (3)
C3—C8—C9—C10	−178.71 (18)	C16—C17—C18—C19	1.6 (4)
C3—C8—C13—C12	179.24 (18)	C17—C18—C19—C14	−1.0 (4)
C4—N1—C3—C2	−64.5 (2)	C19—C14—C15—C16	1.0 (3)
C4—N1—C3—C8	172.34 (15)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.89 (2)	2.32 (2)	3.189 (2)	165 (2)
C9—H9···F2^{ii}	0.93	2.61	3.378 (2)	140
C10—H10···F2^{iii}	0.93	2.58	3.343 (2)	139
C12—H12···O1^{iv}	0.93	2.57	3.412 (3)	150
C16—H16···F1^{v}	0.93	2.62	3.379 (2)	139

Symmetry codes: (i) *x*, −*y*+1/2, *z*+1/2; (ii) *x*, −*y*+1/2, *z*−1/2; (iii) −*x*+1, *y*−1/2, −*z*+3/2; (iv) *x*−1, −*y*+1/2, *z*+1/2; (v) −*x*, *y*+1/2, −*z*+3/2.