Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(3-Chloro-4-fluorophenyl)-2,2-diphenylacetamide

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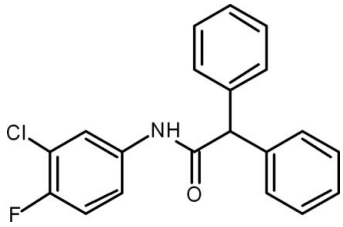
Received 21 June 2011; accepted 5 September 2011

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.004 Å; R factor = 0.042; wR factor = 0.109; data-to-parameter ratio = 17.2.

In the title compound, $C_{20}H_{15}ClFNO$, the dihedral angles between the mean planes of the acetamide group and the chlorofluoro-substituted benzene ring and the two phenyl rings are 10.8 (8), 81.9 (7) and 85.8 (5)°, respectively. The crystal packing is stabilized by N—H···O hydrogen bonds and weak C—H···O intermolecular interactions, forming infinite chains along the *c* axis.

Related literature

For the structural similarity of *N*-substituted 2-arylacetamides to the lateral chain of natural benzylpenicillin, see: Mijin & Marinkovic (2006); Mijin *et al.* (2008). For their coordination abilities, see: Wu *et al.* (2008, 2010). For related structures, see: Davis & Healy (2010); Li *et al.* (2010); Li & Wu (2010); Wang *et al.* (2010); Xiao *et al.* (2010).



Experimental

Crystal data

$C_{20}H_{15}ClFNO$
M_r = 339.78
Monoclinic, *Pc*
a = 9.3665 (17) Å
b = 10.2069 (12) Å
c = 9.7774 (16) Å
β = 114.42 (2)°
V = 851.1 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 173 K
0.35 × 0.12 × 0.12 mm

Data collection

Oxford Diffractio Xcalibur Eos Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2010)
T_{min} = 0.921, T_{max} = 0.972
7456 measured reflections
3794 independent reflections
3265 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.109
S = 1.01
3794 reflections
220 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Absolute structure: Flack (1983), 1668 Friedel pairs
Flack parameter: −0.06 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1*A*···O1^{i}	0.95	2.49	3.256 (3)	138
N1—H1*N*···O1^{i}	0.85 (2)	2.09 (2)	2.895 (2)	158 (2)

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2010); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

ASP thanks the UOM for research facilities. JPJ acknowledges the NSF–MRI program (grant No. CHE1039027) for funds to purchase the X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: YA2145).

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supporting information

Acta Cryst. (2011). E**67**, o2604 [https://doi.org/10.1107/S1600536811036075]

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S1. Comment

Amides are extensively used as ligands due to their excellent coordination abilities (Wu *et al.*, 2008; 2010). N-Substituted 2-arylacetamides are especially remarkable due to their structural similarity to the lateral chain of natural benzylpenicillin (Mijin & Marinkovic, 2006; Mijin *et al.*, 2008). Crystal structures of some acetamide derivatives, viz., 2-(4-bromophenyl)-N-(2-methoxyphenyl)acetamide (Xiao *et al.*, 2010), N-benzyl-2-(3-chloro-4-hydroxyphenyl)acetamide (Davis & Healy, 2010), 2-(2,2-dimethyl-2,3-dihydro-1-benzofuran-7-yloxy)-N- (o-tolyl)acetamide (Li *et al.*, 2010), N-benzyl-2-(2-bromophenyl)-2- (2-nitrophenoxy)acetamide (Li & Wu, 2010) and N-(4-chlorophenyl)-2-(8-quinolyloxy)acetamide monohydrate (Wang *et al.*, 2010) have been reported. In view of the importance of amides, we report herein the crystal structure of the title compound, $C_{20}H_{15}ClFNO$.

In the title compound, the dihedral angles between the mean planes of the acetamide group 01/N1/C6/C7/C8 and the chloro, fluoro substituted benzene ring C1-C6 and two phenyl rings C9-C14 and C15-C20 are 10.8 (8)°, 81.9 (7)° and 85.8 (5)°, respectively (Fig. 2). Crystal packing is stabilized by N1—H1N···O1^{i} hydrogen bonds and weak C1—H1A···O1^{i} (symmetry code i: x, 1-y, z+1/2) intermolecular interactions forming infinite one-dimensional chains along the *c* axis (Fig. 3, Table 1).

S2. Experimental

Diphenylacetyl chloride (0.230 g, 1 mmol) and 3-chloro-4-fluoroaniline (0.145 g, 1 mmol) were dissolved in dichloromethane (20 mL). The mixture was stirred in the presence of triethylamine at 273 K for about 3 h (Fig. 1). The contents were poured into 100 ml of ice-cold aqueous hydrochloric acid with stirring, which was extracted three times with dichloromethane. The organic layer was washed with saturated $NaHCO_3$ and brine solutions, dried and concentrated under reduced pressure to give the title compound. Single crystals were grown from toluene by the slow evaporation method (M.P.: 427 K).

S3. Refinement

The N–H atom bonded to N1 was located in the diference Fourier map and refined isotropically with N-H distance constrained to 0.86 (2) Å. All C-bound H atoms were placed in their calculated positions and included in the refinement in the riding model approximation with C–H lengths of 0.95 Å for aromatic and 1.00 Å for methyne H atoms and temperature factors set to 1.2 times U_{eq} of the parent atom. 1668 Friedel pairs were measured.

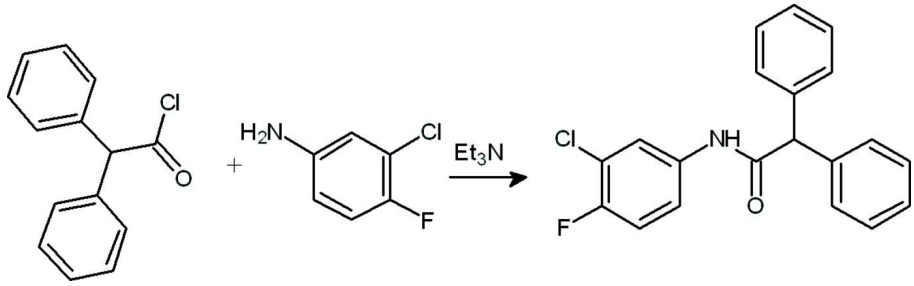

Figure 1

Synthesis of the title compound; reaction scheme.

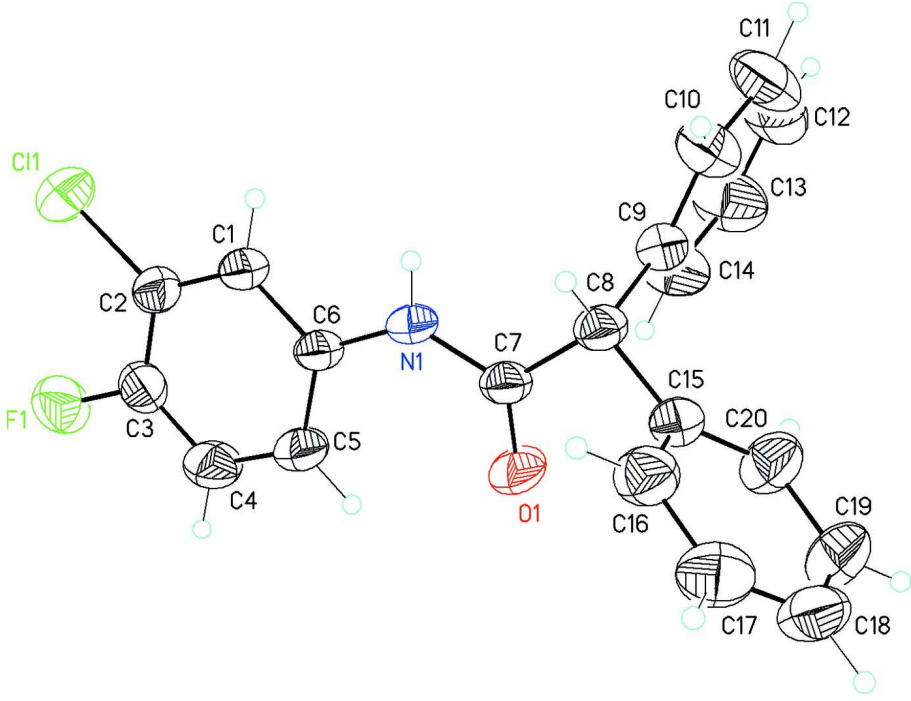

Figure 2

Molecular structure of the title compound; thermal displacement ellipsoids are drawn at the 50° probability level.

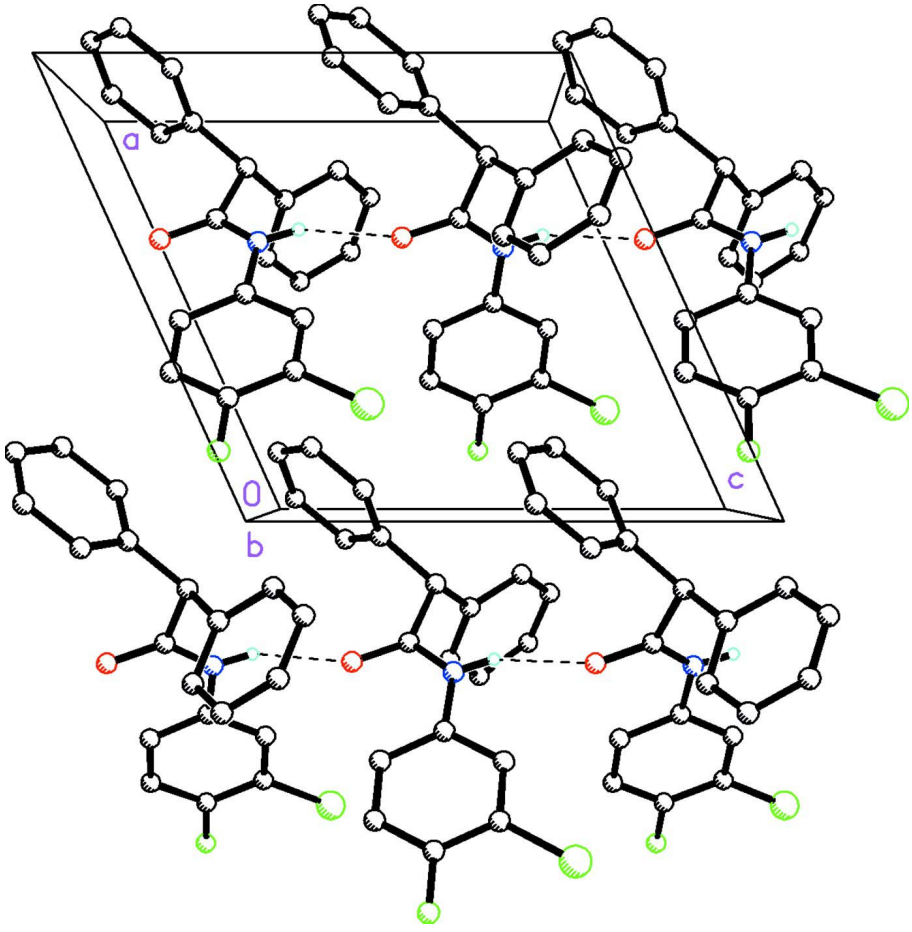

Figure 3

Packing diagram of the title compound viewed down the *b* axis. Dashed lines represent N—H···O hydrogen bonds forming infinite one-dimensional chains along the *c* axis; weak C-H···O interactions are not shown.

N-(3-Chloro-4-fluorophenyl)-2,2-diphenylacetamide

Crystal data

$C_{20}H_{15}ClFNO$
$M_r = 339.78$
Monoclinic, *Pc*
Hall symbol: P -2yc
$a = 9.3665\ (17)$ Å
$b = 10.2069\ (12)$ Å
$c = 9.7774\ (16)$ Å
$\beta = 114.42\ (2)°$
$V = 851.1\ (2)$ Å^3
$Z = 2$
$F(000) = 352$
$D_x = 1.326$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3667 reflections
$\theta = 3.0–32.4°$
$\mu = 0.24$ mm^{-1}
$T = 173$ K
Block, colorless
0.35 × 0.12 × 0.12 mm

Data collection

Oxford Diffractio Xcalibur Eos Gemini diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.1500 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2010)
$T_{min} = 0.921$, $T_{max} = 0.972$
7456 measured reflections

3794 independent reflections
3265 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 28.3°$, $\theta_{min} = 3.0°$
$h = -12 \rightarrow 12$
$k = -13 \rightarrow 13$
$l = -12 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.109$
$S = 1.01$
3794 reflections
220 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0597P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}
Absolute structure: Flack (1983), 1668 Friedel pairs
Absolute structure parameter: −0.06 (6)

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. 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 $F^2 > \sigma(F^2)$ 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}
Cl1	0.25355 (8)	0.11734 (7)	0.82272 (8)	0.0727 (2)
F1	0.15076 (18)	0.07394 (14)	0.50254 (19)	0.0658 (4)
O1	0.6516 (2)	0.52072 (16)	0.54006 (16)	0.0550 (4)
N1	0.6367 (2)	0.42807 (16)	0.74325 (18)	0.0431 (4)
H1N	0.665 (3)	0.433 (2)	0.837 (2)	0.052*
C1	0.4496 (3)	0.28097 (19)	0.7678 (2)	0.0446 (4)
H1A	0.4915	0.3022	0.8716	0.053*
C2	0.3294 (3)	0.19290 (18)	0.7097 (3)	0.0454 (5)
C3	0.2684 (2)	0.16238 (19)	0.5588 (3)	0.0461 (5)
C4	0.3265 (3)	0.2195 (2)	0.4665 (3)	0.0543 (5)
H4A	0.2836	0.1976	0.3628	0.065*
C5	0.4470 (3)	0.3086 (2)	0.5227 (2)	0.0506 (5)
H5A	0.4865	0.3489	0.4579	0.061*
C6	0.5107 (2)	0.33973 (18)	0.6746 (2)	0.0387 (4)
C7	0.6985 (2)	0.51195 (18)	0.6763 (2)	0.0390 (4)
C8	0.8312 (2)	0.59755 (18)	0.7841 (2)	0.0393 (4)
H8A	0.8897	0.5446	0.8765	0.047*
C9	0.7663 (3)	0.71731 (18)	0.8311 (2)	0.0433 (4)
C10	0.8448 (3)	0.7672 (2)	0.9741 (3)	0.0582 (6)

H10A	0.9365	0.7245	1.0431	0.070*
C11	0.7909 (4)	0.8791 (3)	1.0177 (4)	0.0751 (8)
H11A	0.8460	0.9124	1.1165	0.090*
C12	0.6600 (4)	0.9418 (3)	0.9208 (4)	0.0796 (9)
H12A	0.6245	1.0189	0.9515	0.096*
C13	0.5799 (4)	0.8935 (3)	0.7795 (4)	0.0767 (8)
H13A	0.4882	0.9370	0.7117	0.092*
C14	0.6317 (3)	0.7811 (3)	0.7341 (3)	0.0628 (6)
H14A	0.5745	0.7476	0.6357	0.075*
C15	0.9445 (2)	0.62793 (18)	0.7125 (2)	0.0416 (4)
C16	1.0589 (3)	0.5378 (2)	0.7245 (3)	0.0532 (5)
H16A	1.0688	0.4600	0.7810	0.064*
C17	1.1594 (3)	0.5589 (3)	0.6554 (3)	0.0649 (6)
H17A	1.2372	0.4956	0.6645	0.078*
C18	1.1470 (3)	0.6703 (3)	0.5742 (3)	0.0662 (7)
H18A	1.2167	0.6854	0.5277	0.079*
C19	1.0328 (3)	0.7606 (3)	0.5601 (3)	0.0662 (7)
H19A	1.0229	0.8377	0.5024	0.079*
C20	0.9324 (3)	0.7403 (2)	0.6290 (3)	0.0570 (6)
H20A	0.8545	0.8038	0.6191	0.068*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0985 (5)	0.0717 (4)	0.0713 (4)	−0.0219 (4)	0.0586 (4)	−0.0035 (3)
F1	0.0645 (8)	0.0659 (8)	0.0738 (10)	−0.0204 (7)	0.0356 (7)	−0.0198 (7)
O1	0.0727 (10)	0.0649 (9)	0.0269 (7)	−0.0149 (8)	0.0200 (7)	0.0038 (6)
N1	0.0602 (10)	0.0470 (8)	0.0244 (7)	−0.0089 (8)	0.0197 (8)	−0.0019 (7)
C1	0.0650 (12)	0.0413 (9)	0.0328 (10)	−0.0007 (9)	0.0257 (9)	0.0003 (7)
C2	0.0594 (12)	0.0392 (9)	0.0494 (12)	0.0018 (9)	0.0342 (10)	0.0011 (8)
C3	0.0482 (11)	0.0405 (9)	0.0520 (13)	−0.0027 (8)	0.0232 (10)	−0.0059 (9)
C4	0.0603 (13)	0.0646 (13)	0.0345 (10)	−0.0093 (10)	0.0161 (10)	−0.0079 (9)
C5	0.0651 (13)	0.0580 (11)	0.0328 (10)	−0.0110 (10)	0.0242 (10)	−0.0025 (9)
C6	0.0514 (10)	0.0391 (8)	0.0298 (9)	0.0015 (8)	0.0208 (8)	0.0004 (7)
C7	0.0512 (10)	0.0387 (9)	0.0299 (9)	0.0038 (7)	0.0196 (8)	0.0012 (7)
C8	0.0477 (10)	0.0413 (9)	0.0305 (9)	0.0021 (8)	0.0177 (8)	0.0030 (7)
C9	0.0516 (10)	0.0440 (9)	0.0401 (10)	−0.0048 (9)	0.0248 (9)	−0.0031 (8)
C10	0.0589 (14)	0.0617 (13)	0.0506 (13)	−0.0039 (11)	0.0193 (11)	−0.0142 (11)
C11	0.0766 (17)	0.0792 (17)	0.0691 (19)	−0.0120 (15)	0.0299 (15)	−0.0369 (14)
C12	0.088 (2)	0.0621 (14)	0.101 (3)	0.0039 (15)	0.0507 (19)	−0.0263 (16)
C13	0.0832 (18)	0.0728 (17)	0.076 (2)	0.0251 (15)	0.0355 (16)	−0.0065 (15)
C14	0.0691 (15)	0.0664 (13)	0.0487 (13)	0.0169 (12)	0.0202 (12)	−0.0032 (11)
C15	0.0491 (10)	0.0435 (10)	0.0333 (10)	−0.0019 (8)	0.0181 (8)	0.0004 (7)
C16	0.0645 (13)	0.0484 (11)	0.0518 (13)	0.0084 (10)	0.0293 (11)	0.0037 (9)
C17	0.0640 (14)	0.0715 (15)	0.0666 (17)	0.0085 (12)	0.0344 (13)	−0.0051 (13)
C18	0.0688 (15)	0.0879 (18)	0.0563 (16)	−0.0157 (14)	0.0403 (14)	−0.0130 (13)
C19	0.0809 (17)	0.0669 (14)	0.0597 (16)	−0.0054 (13)	0.0381 (14)	0.0155 (12)
C20	0.0653 (14)	0.0548 (12)	0.0586 (15)	0.0061 (11)	0.0332 (12)	0.0135 (10)

Geometric parameters (Å, º)

Cl1—C2	1.723 (2)	C10—C11	1.385 (4)
F1—C3	1.353 (3)	C10—H10A	0.9500
O1—C7	1.221 (2)	C11—C12	1.360 (5)
N1—C7	1.346 (3)	C11—H11A	0.9500
N1—C6	1.414 (3)	C12—C13	1.363 (5)
N1—H1N	0.847 (17)	C12—H12A	0.9500
C1—C2	1.367 (3)	C13—C14	1.388 (4)
C1—C6	1.396 (3)	C13—H13A	0.9500
C1—H1A	0.9500	C14—H14A	0.9500
C2—C3	1.379 (3)	C15—C16	1.380 (3)
C3—C4	1.363 (3)	C15—C20	1.385 (3)
C4—C5	1.374 (3)	C16—C17	1.384 (4)
C4—H4A	0.9500	C16—H16A	0.9500
C5—C6	1.389 (3)	C17—C18	1.364 (4)
C5—H5A	0.9500	C17—H17A	0.9500
C7—C8	1.528 (3)	C18—C19	1.375 (4)
C8—C9	1.519 (3)	C18—H18A	0.9500
C8—C15	1.526 (3)	C19—C20	1.380 (4)
C8—H8A	1.0000	C19—H19A	0.9500
C9—C10	1.380 (3)	C20—H20A	0.9500
C9—C14	1.387 (3)		
C7—N1—C6	128.12 (17)	C9—C10—C11	120.4 (3)
C7—N1—H1N	118.9 (18)	C9—C10—H10A	119.8
C6—N1—H1N	112.4 (18)	C11—C10—H10A	119.8
C2—C1—C6	120.06 (19)	C12—C11—C10	120.8 (3)
C2—C1—H1A	120.0	C12—C11—H11A	119.6
C6—C1—H1A	120.0	C10—C11—H11A	119.6
C1—C2—C3	119.92 (19)	C11—C12—C13	119.7 (3)
C1—C2—Cl1	120.96 (17)	C11—C12—H12A	120.1
C3—C2—Cl1	119.12 (17)	C13—C12—H12A	120.1
F1—C3—C4	119.8 (2)	C12—C13—C14	120.3 (3)
F1—C3—C2	119.5 (2)	C12—C13—H13A	119.9
C4—C3—C2	120.61 (19)	C14—C13—H13A	119.9
C3—C4—C5	120.3 (2)	C9—C14—C13	120.6 (3)
C3—C4—H4A	119.8	C9—C14—H14A	119.7
C5—C4—H4A	119.8	C13—C14—H14A	119.7
C4—C5—C6	119.8 (2)	C16—C15—C20	118.3 (2)
C4—C5—H5A	120.1	C16—C15—C8	119.25 (18)
C6—C5—H5A	120.1	C20—C15—C8	122.37 (19)
C5—C6—C1	119.23 (19)	C15—C16—C17	121.1 (2)
C5—C6—N1	123.94 (18)	C15—C16—H16A	119.5
C1—C6—N1	116.83 (17)	C17—C16—H16A	119.5
O1—C7—N1	122.95 (18)	C18—C17—C16	120.2 (2)
O1—C7—C8	122.26 (17)	C18—C17—H17A	119.9
N1—C7—C8	114.79 (17)	C16—C17—H17A	119.9

C9—C8—C15	114.64 (16)	C17—C18—C19	119.5 (3)
C9—C8—C7	110.86 (16)	C17—C18—H18A	120.2
C15—C8—C7	108.75 (16)	C19—C18—H18A	120.2
C9—C8—H8A	107.4	C18—C19—C20	120.6 (2)
C15—C8—H8A	107.4	C18—C19—H19A	119.7
C7—C8—H8A	107.4	C20—C19—H19A	119.7
C10—C9—C14	118.2 (2)	C19—C20—C15	120.4 (2)
C10—C9—C8	119.4 (2)	C19—C20—H20A	119.8
C14—C9—C8	122.4 (2)	C15—C20—H20A	119.8

C6—C1—C2—C3	−0.1 (3)	C15—C8—C9—C14	88.2 (3)
C6—C1—C2—Cl1	179.12 (15)	C7—C8—C9—C14	−35.4 (3)
C1—C2—C3—F1	179.20 (19)	C14—C9—C10—C11	−0.9 (4)
Cl1—C2—C3—F1	−0.1 (3)	C8—C9—C10—C11	177.7 (3)
C1—C2—C3—C4	−0.2 (3)	C9—C10—C11—C12	0.0 (5)
Cl1—C2—C3—C4	−179.44 (18)	C10—C11—C12—C13	0.6 (5)
F1—C3—C4—C5	−179.4 (2)	C11—C12—C13—C14	−0.2 (6)
C2—C3—C4—C5	−0.1 (3)	C10—C9—C14—C13	1.2 (4)
C3—C4—C5—C6	0.6 (4)	C8—C9—C14—C13	−177.3 (3)
C4—C5—C6—C1	−0.9 (3)	C12—C13—C14—C9	−0.7 (5)
C4—C5—C6—N1	178.7 (2)	C9—C8—C15—C16	152.1 (2)
C2—C1—C6—C5	0.7 (3)	C7—C8—C15—C16	−83.2 (2)
C2—C1—C6—N1	−178.94 (18)	C9—C8—C15—C20	−31.1 (3)
C7—N1—C6—C5	12.1 (3)	C7—C8—C15—C20	93.6 (2)
C7—N1—C6—C1	−168.3 (2)	C20—C15—C16—C17	0.2 (3)
C6—N1—C7—O1	−1.1 (3)	C8—C15—C16—C17	177.0 (2)
C6—N1—C7—C8	177.97 (18)	C15—C16—C17—C18	0.2 (4)
O1—C7—C8—C9	95.3 (2)	C16—C17—C18—C19	−0.8 (4)
N1—C7—C8—C9	−83.8 (2)	C17—C18—C19—C20	0.9 (4)
O1—C7—C8—C15	−31.6 (2)	C18—C19—C20—C15	−0.5 (4)
N1—C7—C8—C15	149.28 (17)	C16—C15—C20—C19	0.0 (4)
C15—C8—C9—C10	−90.3 (3)	C8—C15—C20—C19	−176.8 (2)
C7—C8—C9—C10	146.1 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*A*···O1^{i}	0.95	2.49	3.256 (3)	138
N1—H1*N*···O1^{i}	0.85 (2)	2.09 (2)	2.895 (2)	158 (2)

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