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Crystal structure of *N*-{4-[(6-chloropyridin-3-yl)methoxy]phenyl}-2,6-difluorobenzamide

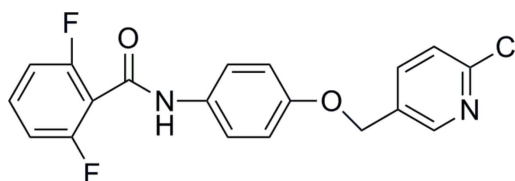
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In the title compound, $C_{19}H_{13}ClF_2N_2O_2$, the conformation of the N—H bond in the amide segment is *anti* to the C=O bond. The molecule is not planar, with dihedral angles between the central benzene ring and the outer benzene and pyridyl rings of 73.35 (7) and 81.26 (6)°, respectively. A weak intramolecular C—H \cdots O hydrogen bond occurs. In the crystal, N—H \cdots N, C—H \cdots O and C—H \cdots F hydrogen bonds lead to the formation of dimers. The N—H \cdots N inversion dimers are linked by π - π contacts between adjacent pyridine rings [centroid-centroid = 3.8541 (12) Å] and C—H \cdots π interactions. These contacts combine to stack the molecules along the *a* axis.

1. Chemical context

Amide derivatives show diverse biological properties, acting as insecticides (Liu *et al.*, 2004a), fungicides (Liu *et al.*, 2004b) and acaricides (Shiga *et al.*, 2003). Amides in regular commercial use include benzamide (flutolanil, fluopicolide), nicotinamide (boscalid) and thiazole carboxamide (thifluzamide, ethaboxam). As a part of our work on the synthesis of novel fluorine-containing compounds with good biological activities, we report herein on the crystal structure of the title compound, (I), Fig. 1.



2. Structural commentary

The conformation of the N—H and the C=O bonds in the amide segment are *anti* to one another, similar to the

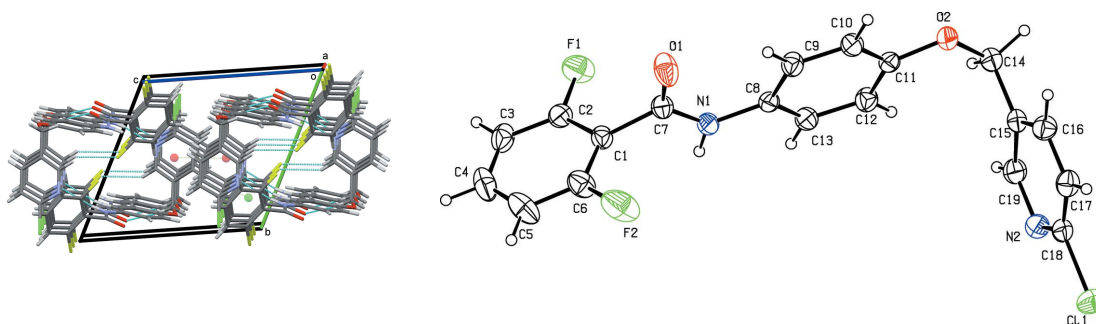


Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

Table 1

Hydrogen-bond geometry (Å, °).

Cg2 is the centroid of the C1–C6 benzene ring.

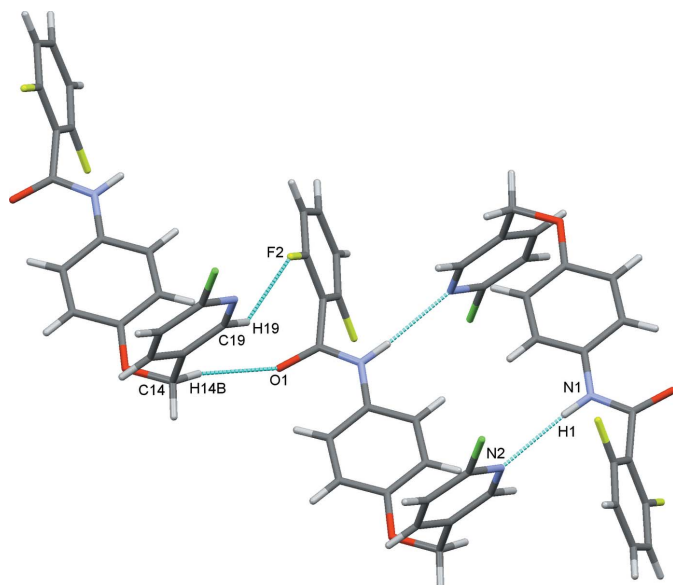
<i>D</i> –H... <i>A</i>	<i>D</i> –H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> –H... <i>A</i>
C9–H9...O1	0.93	2.27	2.863 (2)	121
N1–H1...N2 ⁱ	0.88 (2)	2.24 (2)	3.109 (2)	170.6 (18)
C19–H19...F2 ⁱⁱ	0.93	2.54	3.309 (2)	140
C14–H14B...O1 ⁱⁱ	0.97	2.42	3.344 (3)	160
C16–H16...Cg2 ⁱⁱⁱ	0.93	2.99	3.912 (2)	173

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

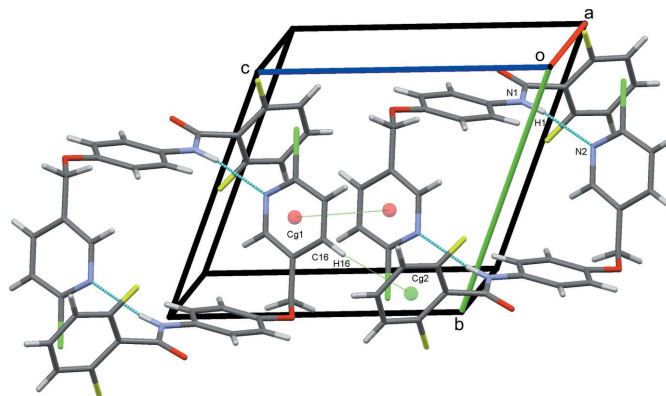
conformation observed in another amide compound (Gowda *et al.*, 2010). The dihedral angle between the two benzene rings is 73.35 (6)° while that between the central benzene ring and the chloro-substituted pyridine ring is 81.26 (6). The amide residue C1/N1/C7/O1 lies close to the plane of the central benzene ring, making a dihedral angle of 8.73 (6)°. A weak intramolecular C9–H9...O1 hydrogen bond (Table 1) contributes to the planarity of this part of the molecule.

3. Supramolecular features

In the crystal structure, pairs of classical N1–H1...N2ⁱ hydrogen bonds, Table 1, link the molecules into inversion dimers and generate $R_2^2(22)$ rings (Bernstein *et al.*, 1995). C14–H14B...O1ⁱⁱ and C19–H19...F2ⁱⁱ hydrogen bonds also form dimers, which enclose an $R_2^2(10)$ ring motif, Fig. 2. The N–H...N dimers are linked into chains along the *c*-axis direction by π – π stacking interactions between adjacent pyridyl rings [$Cg1...Cg1^{iv} = 3.8541$ (12) Å; symmetry code: (iv) $1 - x, 1 - y, 1 - z$] augmented by a weak C16–H16...Cg2 contact (Cg2 is the centroid of the C1–C6 benzene ring), Table 1, Fig. 3. These contacts combine to stack the molecules along the *a* axis, Fig. 4.


Figure 2

A pair of dimers with hydrogen bonds drawn as blue dashed lines.


Figure 3

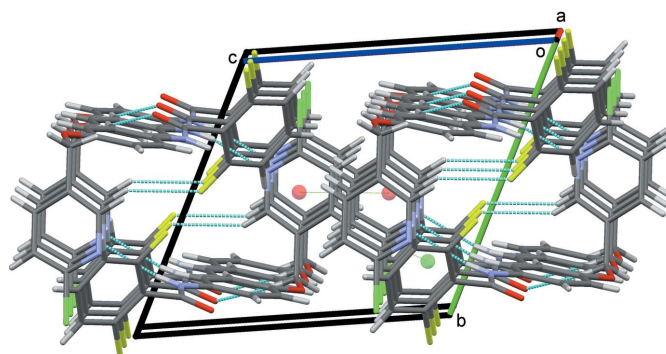
 Chains of inversion dimers along the *c*-axis direction. Hydrogen bonds are drawn as dashed lines with π – π and C–H... π contacts shown as green dotted lines.

4. Synthesis and crystallization

Triethylamine (6mmol) was added dropwise to a stirred solution of 4-(6-chloropyridin-3-yl) methoxy aniline (5mmol) and 2,6-difluorobenzoyl chloride (5mmol) in dry dichloromethane (20ml) at 275–277 K. The mixture was stirred at 283–288 K for 2 h, then washed with 0.5% hydrochloric acid solution, and a saturated aqueous solution of sodium hydrogen carbonate, dried and evaporated. The residue was recrystallized from dichloromethane, giving colourless blocks of the title compound after three weeks.

5. Database survey

A search of the Cambridge Structural Database (Version 5.36 with three updates) (Groom & Allen, 2014) for *N*-(4-(pyridin-3-ylmethoxy)phenyl)benzamide or its substituted derivatives gave no hits. However, structures of eight substituted 2,6-difluoro-*N*-phenylbenzamide derivatives were found, see for example Cockcroft *et al.* (2007); Spitaleri *et al.* (2004); Fun *et al.* (2010). Two structures of purely organic 3-(phenoxy)methylpyridine derivatives have also been reported (Lakshminarayana *et al.*, 2009; Liu *et al.*, 2010) together with that of a cadmium complex of 4-[(6-chloropyridin-3-yl)methoxy]benzoate, Li *et al.* (2007).


Figure 4

 The overall packing for (I) viewed along the *a*-axis direction.

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₁₉ H ₁₃ ClF ₂ N ₂ O ₂
<i>M</i> _r	374.76
Crystal system, space group	Triclinic, <i>P</i> $\bar{1}$
Temperature (K)	298
<i>a</i> , <i>b</i> , <i>c</i> (Å)	8.8173 (11), 10.7036 (13), 10.8452 (14)
α , β , γ (°)	61.939 (2), 77.597 (2), 69.636 (2)
<i>V</i> (Å ³)	845.15 (18)
<i>Z</i>	2
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.26
Crystal size (mm)	0.16 × 0.12 × 0.10
Data collection	
Diffractometer	Bruker SMART APEX CCD area detector
Absorption correction	Multi-scan (<i>SADABS</i> ; Sheldrick, 2001)
<i>T</i> _{min} , <i>T</i> _{max}	0.959, 0.974
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	5474, 3271, 2886
<i>R</i> _{int}	0.029
(sin θ/λ) _{max} (Å ⁻¹)	0.617
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.045, 0.116, 1.06
No. of reflections	3271
No. of parameters	239
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.21, -0.23

Computer programs: *SMART* and *SAINT* (Bruker, 2000), *SHELXS97*, *SHELXL97* and *SHELXTL* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2008).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The NH H atom was located in a difference Fourier map and freely refined. The C-bound H atoms were positioned geometrically and refined using a riding model with *d*(C–H) = 0.93–0.97 Å and *U*_{iso}(H) = 1.2*U*_{eq}(C).

Acknowledgements

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Crystal structure of *N*-{4-[(6-chloropyridin-3-yl)methoxy]phenyl}-2,6-difluorobenzamide

Ying Liang, Li-Qiao Shi and Zi-Wen Yang

Computing details

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINTE* (Bruker, 2000); data reduction: *SAINTE* (Bruker, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

N-{4-[(6-Chloropyridin-3-yl)methoxy]phenyl}-2,6-difluorobenzamide

Crystal data

C₁₉H₁₃ClF₂N₂O₂

M_r = 374.76

Triclinic, *P*1

Hall symbol: -P 1

a = 8.8173 (11) Å

b = 10.7036 (13) Å

c = 10.8452 (14) Å

α = 61.939 (2)°

β = 77.597 (2)°

γ = 69.636 (2)°

V = 845.15 (18) Å³

Z = 2

F(000) = 384

D_x = 1.473 Mg m⁻³

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 2810 reflections

θ = 2.3–28.3°

μ = 0.26 mm⁻¹

T = 298 K

Block, colorless

0.16 × 0.12 × 0.10 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 2001)

T_{min} = 0.959, *T_{max}* = 0.974

5474 measured reflections

3271 independent reflections

2886 reflections with *I* > 2σ(*I*)

R_{int} = 0.029

θ_{max} = 26.0°, θ_{min} = 2.1°

h = -10→10

k = -13→13

l = -12→13

Refinement

Refinement on *F*²

Least-squares matrix: full

R[*F*² > 2σ(*F*²)] = 0.045

wR(*F*²) = 0.116

S = 1.06

3271 reflections

239 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 atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0526P)^2 + 0.196P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$

$$\Delta\rho_{\max} = 0.21 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.23 \text{ e } \text{\AA}^{-3}$$

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. 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 $F^2 > 2\text{sigma}(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.7630 (2)	0.2167 (2)	-0.02643 (18)	0.0427 (4)
C2	0.8270 (2)	0.1167 (2)	-0.08394 (19)	0.0478 (4)
C3	0.9422 (3)	0.1317 (3)	-0.1918 (2)	0.0611 (6)
H3	0.9816	0.0618	-0.2276	0.073*
C4	0.9982 (3)	0.2526 (3)	-0.2461 (2)	0.0706 (7)
H4	1.0773	0.2644	-0.3195	0.085*
C5	0.9403 (3)	0.3566 (3)	-0.1949 (2)	0.0750 (7)
H5	0.9787	0.4388	-0.2327	0.090*
C6	0.8239 (3)	0.3360 (2)	-0.0861 (2)	0.0602 (5)
C7	0.6521 (2)	0.1886 (2)	0.10413 (18)	0.0432 (4)
C8	0.3644 (2)	0.21024 (17)	0.18987 (17)	0.0391 (4)
C9	0.3813 (2)	0.1688 (2)	0.32952 (18)	0.0462 (4)
H9	0.4817	0.1503	0.3590	0.055*
C10	0.2489 (2)	0.1551 (2)	0.42425 (18)	0.0461 (4)
H10	0.2609	0.1273	0.5176	0.055*
C11	0.0990 (2)	0.18196 (17)	0.38294 (18)	0.0408 (4)
C12	0.0809 (2)	0.2233 (2)	0.24416 (19)	0.0470 (4)
H12	-0.0198	0.2422	0.2149	0.056*
C13	0.2140 (2)	0.2363 (2)	0.14935 (18)	0.0461 (4)
H13	0.2019	0.2631	0.0563	0.055*
C14	-0.1851 (2)	0.2030 (2)	0.4525 (2)	0.0497 (5)
H14A	-0.2488	0.1521	0.5341	0.060*
H14B	-0.1861	0.1737	0.3806	0.060*
C15	-0.2607 (2)	0.36755 (19)	0.40005 (18)	0.0414 (4)
C16	-0.2680 (2)	0.4370 (2)	0.4829 (2)	0.0498 (5)
H16	-0.2264	0.3819	0.5710	0.060*
C17	-0.3362 (2)	0.5864 (2)	0.4347 (2)	0.0506 (5)
H17	-0.3418	0.6348	0.4885	0.061*
C18	-0.3961 (2)	0.6622 (2)	0.3043 (2)	0.0479 (4)
C19	-0.3260 (2)	0.4551 (2)	0.2721 (2)	0.0503 (5)
H19	-0.3230	0.4098	0.2161	0.060*
Cl1	-0.48341 (8)	0.85162 (6)	0.23999 (7)	0.0783 (2)

F1	0.77345 (18)	-0.00346 (13)	-0.02627 (13)	0.0741 (4)
F2	0.7661 (2)	0.43493 (16)	-0.03160 (16)	0.1031 (6)
N1	0.49454 (18)	0.22686 (16)	0.08547 (16)	0.0430 (4)
H1	0.468 (2)	0.265 (2)	-0.001 (2)	0.052*
N2	-0.3942 (2)	0.60203 (18)	0.22226 (16)	0.0537 (4)
O1	0.71012 (17)	0.1345 (2)	0.21658 (15)	0.0727 (5)
O2	-0.02172 (15)	0.16015 (14)	0.48849 (13)	0.0495 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0410 (9)	0.0482 (10)	0.0375 (9)	-0.0112 (8)	-0.0013 (7)	-0.0189 (8)
C2	0.0514 (11)	0.0483 (10)	0.0415 (10)	-0.0084 (8)	-0.0054 (8)	-0.0207 (8)
C3	0.0524 (12)	0.0763 (15)	0.0463 (11)	0.0010 (11)	-0.0033 (9)	-0.0335 (11)
C4	0.0484 (12)	0.116 (2)	0.0456 (12)	-0.0288 (13)	0.0066 (9)	-0.0342 (13)
C5	0.0860 (17)	0.1005 (19)	0.0517 (13)	-0.0615 (15)	0.0073 (12)	-0.0240 (13)
C6	0.0785 (15)	0.0630 (13)	0.0489 (11)	-0.0310 (11)	0.0043 (10)	-0.0278 (10)
C7	0.0470 (10)	0.0465 (9)	0.0385 (9)	-0.0125 (8)	-0.0001 (8)	-0.0220 (8)
C8	0.0434 (9)	0.0330 (8)	0.0364 (9)	-0.0069 (7)	0.0014 (7)	-0.0159 (7)
C9	0.0425 (10)	0.0540 (10)	0.0408 (10)	-0.0085 (8)	-0.0032 (8)	-0.0230 (8)
C10	0.0508 (11)	0.0483 (10)	0.0347 (9)	-0.0076 (8)	-0.0026 (8)	-0.0188 (8)
C11	0.0453 (10)	0.0322 (8)	0.0391 (9)	-0.0062 (7)	0.0016 (7)	-0.0160 (7)
C12	0.0423 (10)	0.0523 (10)	0.0444 (10)	-0.0092 (8)	-0.0041 (8)	-0.0219 (9)
C13	0.0512 (11)	0.0480 (10)	0.0355 (9)	-0.0090 (8)	-0.0030 (8)	-0.0188 (8)
C14	0.0457 (10)	0.0462 (10)	0.0515 (11)	-0.0141 (8)	0.0055 (8)	-0.0194 (9)
C15	0.0353 (9)	0.0447 (9)	0.0424 (9)	-0.0120 (7)	0.0045 (7)	-0.0198 (8)
C16	0.0479 (11)	0.0540 (11)	0.0457 (10)	-0.0101 (8)	-0.0079 (8)	-0.0214 (9)
C17	0.0483 (11)	0.0552 (11)	0.0573 (12)	-0.0160 (9)	0.0002 (9)	-0.0321 (10)
C18	0.0379 (9)	0.0427 (9)	0.0550 (11)	-0.0123 (7)	0.0062 (8)	-0.0179 (9)
C19	0.0544 (11)	0.0524 (11)	0.0444 (10)	-0.0118 (9)	0.0011 (8)	-0.0254 (9)
C11	0.0732 (4)	0.0415 (3)	0.0948 (5)	-0.0080 (2)	0.0032 (3)	-0.0186 (3)
F1	0.1111 (11)	0.0569 (7)	0.0632 (8)	-0.0301 (7)	0.0031 (7)	-0.0322 (6)
F2	0.1807 (18)	0.0716 (9)	0.0786 (10)	-0.0650 (11)	0.0283 (10)	-0.0444 (8)
N1	0.0453 (9)	0.0451 (8)	0.0327 (8)	-0.0082 (6)	-0.0008 (6)	-0.0161 (7)
N2	0.0541 (10)	0.0527 (9)	0.0428 (9)	-0.0079 (7)	-0.0019 (7)	-0.0173 (7)
O1	0.0500 (8)	0.1190 (14)	0.0444 (8)	-0.0210 (9)	-0.0008 (7)	-0.0348 (9)
O2	0.0436 (7)	0.0507 (7)	0.0411 (7)	-0.0063 (6)	0.0034 (5)	-0.0170 (6)

Geometric parameters (Å, °)

C1—C6	1.374 (3)	C11—O2	1.377 (2)
C1—C2	1.382 (2)	C11—C12	1.383 (2)
C1—C7	1.504 (2)	C12—C13	1.384 (2)
C2—F1	1.344 (2)	C12—H12	0.9300
C2—C3	1.361 (3)	C13—H13	0.9300
C3—C4	1.366 (3)	C14—O2	1.432 (2)
C3—H3	0.9300	C14—C15	1.508 (2)
C4—C5	1.368 (4)	C14—H14A	0.9700

C4—H4	0.9300	C14—H14B	0.9700
C5—C6	1.374 (3)	C15—C19	1.371 (3)
C5—H5	0.9300	C15—C16	1.391 (2)
C6—F2	1.347 (2)	C16—C17	1.368 (3)
C7—O1	1.217 (2)	C16—H16	0.9300
C7—N1	1.336 (2)	C17—C18	1.372 (3)
C8—C13	1.381 (3)	C17—H17	0.9300
C8—C9	1.390 (2)	C18—N2	1.316 (2)
C8—N1	1.423 (2)	C18—Cl1	1.7328 (19)
C9—C10	1.379 (2)	C19—N2	1.345 (2)
C9—H9	0.9300	C19—H19	0.9300
C10—C11	1.378 (3)	N1—H1	0.88 (2)
C10—H10	0.9300		
C6—C1—C2	115.21 (17)	C11—C12—C13	119.36 (17)
C6—C1—C7	121.35 (16)	C11—C12—H12	120.3
C2—C1—C7	122.93 (16)	C13—C12—H12	120.3
F1—C2—C3	119.06 (18)	C8—C13—C12	121.47 (16)
F1—C2—C1	117.06 (16)	C8—C13—H13	119.3
C3—C2—C1	123.86 (19)	C12—C13—H13	119.3
C2—C3—C4	118.0 (2)	O2—C14—C15	111.33 (15)
C2—C3—H3	121.0	O2—C14—H14A	109.4
C4—C3—H3	121.0	C15—C14—H14A	109.4
C3—C4—C5	121.5 (2)	O2—C14—H14B	109.4
C3—C4—H4	119.3	C15—C14—H14B	109.4
C5—C4—H4	119.3	H14A—C14—H14B	108.0
C4—C5—C6	118.1 (2)	C19—C15—C16	116.97 (17)
C4—C5—H5	121.0	C19—C15—C14	122.83 (17)
C6—C5—H5	121.0	C16—C15—C14	120.19 (16)
F2—C6—C1	116.98 (18)	C17—C16—C15	119.99 (17)
F2—C6—C5	119.7 (2)	C17—C16—H16	120.0
C1—C6—C5	123.4 (2)	C15—C16—H16	120.0
O1—C7—N1	125.21 (17)	C16—C17—C18	117.59 (17)
O1—C7—C1	118.93 (16)	C16—C17—H17	121.2
N1—C7—C1	115.86 (15)	C18—C17—H17	121.2
C13—C8—C9	118.73 (16)	N2—C18—C17	124.97 (17)
C13—C8—N1	117.80 (15)	N2—C18—Cl1	116.22 (15)
C9—C8—N1	123.47 (16)	C17—C18—Cl1	118.81 (15)
C10—C9—C8	119.84 (17)	N2—C19—C15	124.31 (17)
C10—C9—H9	120.1	N2—C19—H19	117.8
C8—C9—H9	120.1	C15—C19—H19	117.8
C11—C10—C9	121.11 (16)	C7—N1—C8	127.66 (15)
C11—C10—H10	119.4	C7—N1—H1	116.4 (13)
C9—C10—H10	119.4	C8—N1—H1	115.9 (13)
O2—C11—C10	115.23 (15)	C18—N2—C19	116.17 (17)
O2—C11—C12	125.25 (16)	C11—O2—C14	118.83 (14)
C10—C11—C12	119.49 (16)		

C6—C1—C2—F1	178.43 (17)	C10—C11—C12—C13	0.3 (3)
C7—C1—C2—F1	6.5 (3)	C9—C8—C13—C12	0.6 (3)
C6—C1—C2—C3	0.0 (3)	N1—C8—C13—C12	-179.67 (16)
C7—C1—C2—C3	-171.90 (18)	C11—C12—C13—C8	-0.6 (3)
F1—C2—C3—C4	-178.15 (19)	O2—C14—C15—C19	123.96 (19)
C1—C2—C3—C4	0.2 (3)	O2—C14—C15—C16	-56.7 (2)
C2—C3—C4—C5	-0.4 (3)	C19—C15—C16—C17	-0.8 (3)
C3—C4—C5—C6	0.3 (4)	C14—C15—C16—C17	179.80 (17)
C2—C1—C6—F2	-179.11 (18)	C15—C16—C17—C18	0.3 (3)
C7—C1—C6—F2	-7.1 (3)	C16—C17—C18—N2	0.6 (3)
C2—C1—C6—C5	-0.1 (3)	C16—C17—C18—C11	179.99 (14)
C7—C1—C6—C5	171.9 (2)	C16—C15—C19—N2	0.7 (3)
C4—C5—C6—F2	178.9 (2)	C14—C15—C19—N2	-179.97 (17)
C4—C5—C6—C1	0.0 (4)	O1—C7—N1—C8	-1.5 (3)
C6—C1—C7—O1	-77.8 (3)	C1—C7—N1—C8	178.76 (15)
C2—C1—C7—O1	93.7 (2)	C13—C8—N1—C7	-170.21 (16)
C6—C1—C7—N1	102.0 (2)	C9—C8—N1—C7	9.5 (3)
C2—C1—C7—N1	-86.6 (2)	C17—C18—N2—C19	-0.7 (3)
C13—C8—C9—C10	-0.3 (3)	C11—C18—N2—C19	179.84 (14)
N1—C8—C9—C10	-179.98 (16)	C15—C19—N2—C18	0.1 (3)
C8—C9—C10—C11	0.0 (3)	C10—C11—O2—C14	172.31 (14)
C9—C10—C11—O2	178.18 (16)	C12—C11—O2—C14	-9.6 (2)
C9—C10—C11—C12	0.0 (3)	C15—C14—O2—C11	-78.49 (19)
O2—C11—C12—C13	-177.66 (16)		

Hydrogen-bond geometry (Å, °)

Cg2 is the centroid of the C1—C6 benzene ring.

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C9—H9...O1	0.93	2.27	2.863 (2)	121
N1—H1...N2 ⁱ	0.88 (2)	2.24 (2)	3.109 (2)	170.6 (18)
C19—H19...F2 ⁱⁱ	0.93	2.54	3.309 (2)	140
C14—H14B...O1 ⁱⁱ	0.97	2.42	3.344 (3)	160
C16—H16...Cg2 ⁱⁱⁱ	0.93	2.99	3.912 (2)	173

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