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Crystal structure of chlorfluazuron

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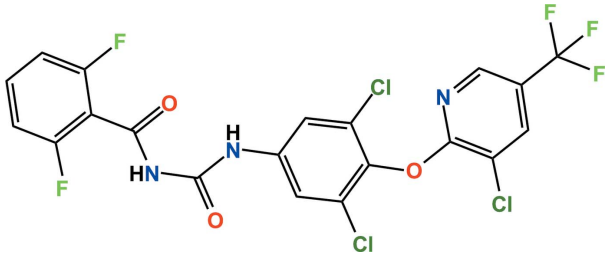
The title compound (systematic name: 1-{3,5-dichloro-4-[3-chloro-5-(trifluoromethyl)pyridin-2-yloxy]phenyl}-3-(2,6-difluorobenzoyl)urea), $C_{20}H_9Cl_3F_5N_3O_3$, is a benzoylphenylurea insecticide. The dihedral angles between the planes of the central dichlorophenyl and the terminal difluorophenyl and chloropyridyl rings are 79.51 (6) and 78.84 6)°, respectively. In the crystal, pairs of N—H···O hydrogen bonds link adjacent molecules, forming $R_2^2(8)$ inversion dimers. In addition, the dimers are linked by short F···Cl [3.1060 (16) Å] and Cl···Cl [3.2837 (7) Å] contacts, as well as weak intermolecular π–π interactions [ring centroid separation = 3.6100 (11) and 3.7764 (13) Å], resulting in a two-dimensional architecture parallel to (111).

Keywords: crystal structure; chlorfluazuron; urea; insecticidal properties; Cl···Cl contacts.

CCDC reference: 1037499

1. Related literature

For information on the insecticidal properties of the title compound, see: Choi *et al.* (2011); Lee *et al.* (2013). For a related crystal structure, see: Jeon *et al.* (2014).



2. Experimental

2.1. Crystal data

$C_{20}H_9Cl_3F_5N_3O_3$
M_r = 540.65
Triclinic, $P\overline{1}$
a = 8.5805 (3) Å
b = 10.1281 (4) Å
c = 12.5883 (4) Å
α = 79.498 (2)°
β = 82.930 (2)°
γ = 83.485 (2)°
V = 1062.82 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.51 mm^{-1}
T = 173 K
0.28 × 0.12 × 0.05 mm

2.2. Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.872, T_{max} = 0.975
19710 measured reflections
5259 independent reflections
4090 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.127
S = 1.06
5259 reflections
307 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.88	1.96	2.837 (2)	175

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *DIAMOND* (Brandenburg, 2010); software used to prepare material for publication: *SHELXTL*.

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: SJ5431).

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supporting information

Acta Cryst. (2015). E**71**, o55 [https://doi.org/10.1107/S2056989014026632]

Crystal structure of chlorfluazuron

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S1. Comment

Chlorfluazuron, $C_{20}H_9Cl_3F_5N_3O_3$, is a benzoylphenylurea which has been recognized as one of the promising insecticides with great potential for use in controlling insect attack on a broad range of fruits and vegetables (Lee *et al.*, 2013; Choi *et al.*, 2011). Its crystal structure is reported herein. In this compound (Scheme 1, Fig. 1), the dihedral angles between the central dichlorophenyl and the terminal difluorophenyland chloropyridyl rings are 79.51 (6) and 78.84 (6)°, respectively. All bond lengths and bond angles are normal and comparable to those observed in the crystal structure of a similar compound (Jeon *et al.*, 2014).

The crystal structure, (Fig. 2), is stabilized by N—H···O hydrogen bonds (Table 1), forming $R_2^2(8)$ inversion dimers. In addition, the dimers are linked by short F2···Cl3^{ii} [3.1060 (16) Å] and Cl1···Cl1^{iii} [3.2837 (7) Å] contacts as well as two weak intermolecular offset π–π stacking interactions [*Cg*1···*Cg*3^{iv} = 3.7764 (13)Å. *Cg*1 and *Cg*3 are the centroids of the C1—C2—C3—C4—C5—C6 and C15—C16—C17—C18—C19—N3 rings, respectively. *Cg*2···*Cg*2^{ii} = 3.6100 (11) Å. *Cg*2 is the centroid of the C9—C10—C11—C12—C13—C14 ring. (Symmetry codes: (ii), -*x* + 1, -*y* + 2, -*z* + 1; (iii) -*x* + 1, -*y* + 1, -*z* + 1 and (iv) *x*, *y* + 1, *z* - 1)], resulting in a two-dimensional architecture parallel to the (111) plane.

S2. Experimental

The title compound was purchased from the Dr. Ehrenstorfer GmbH Company. Slow evaporation of a solution in $CHCl_3$ gave single crystals suitable for X-ray analysis.

S3. Refinement

All H-atoms were positioned geometrically and refined using a riding model with d(C—H) = 0.95 Å, U_{iso} = 1.2U_{eq}(C) for aromatic C—H and d(N—H) = 0.88 Å, U_{iso} = 1.2U_{eq}(C) for urea group.

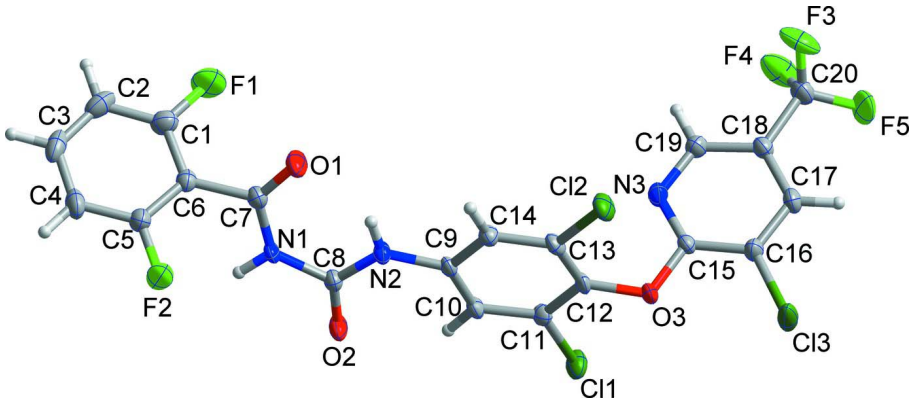

Figure 1

The asymmetric unit of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radius.

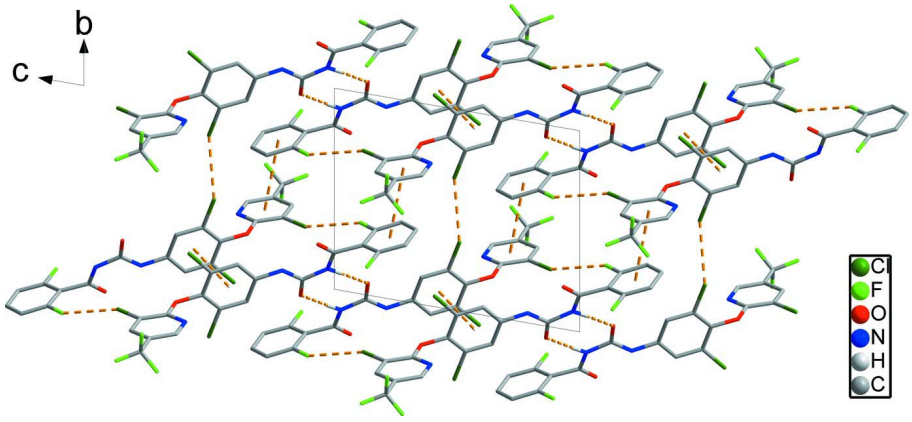

Figure 2

Crystal packing viewed along the *a* axis. The intermolecular N—H···O hydrogen bonds, short F···Cl, Cl···Cl contacts and π–π interactions are shown as dashed lines.

1-{3,5-Dichloro-4-[3-chloro-5-(trifluoromethyl)pyridin-2-yloxy]phenyl}-3-(2,6-difluorobenzoyl)urea

Crystal data

$C_{20}H_9Cl_3F_5N_3O_3$
$M_r = 540.65$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.5805\ (3)$ Å
$b = 10.1281\ (4)$ Å
$c = 12.5883\ (4)$ Å
$\alpha = 79.498\ (2)°$
$\beta = 82.930\ (2)°$
$\gamma = 83.485\ (2)°$
$V = 1062.82\ (7)$ Å^3
$Z = 2$
$F(000) = 540$
$D_x = 1.689$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6417 reflections
$\theta = 2.4$–$28.1°$
$\mu = 0.51$ mm^{-1}
$T = 173$ K
Plate, colourless
0.28 × 0.12 × 0.05 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.872, T_{max} = 0.975
19710 measured reflections
5259 independent reflections
4090 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 28.3°, θ_{min} = 1.7°
h = −11→10
k = −13→13
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.127
S = 1.06
5259 reflections
307 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
$w = 1/[\sigma^2(F_o^2) + (0.0631P)^2 + 0.4257P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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	0.51049 (7)	0.65788 (5)	0.51055 (4)	0.03275 (16)
Cl2	0.82607 (7)	1.05194 (6)	0.59008 (4)	0.03172 (15)
Cl3	0.64381 (7)	0.71391 (8)	0.88086 (5)	0.0459 (2)
F1	1.05653 (18)	1.14118 (18)	−0.13423 (14)	0.0590 (5)
F2	0.54499 (16)	1.35343 (16)	−0.10772 (12)	0.0470 (4)
F3	1.33225 (17)	0.60959 (17)	0.78423 (15)	0.0549 (5)
F4	1.28741 (18)	0.43892 (17)	0.72279 (14)	0.0552 (5)
F5	1.2067 (2)	0.4572 (2)	0.88756 (14)	0.0753 (7)
O1	0.86100 (19)	1.20897 (17)	0.06450 (12)	0.0347 (4)
O2	0.51802 (19)	0.94182 (16)	0.13689 (12)	0.0323 (4)
O3	0.66744 (16)	0.79859 (14)	0.64590 (11)	0.0237 (3)
N1	0.6634 (2)	1.09625 (17)	0.02702 (13)	0.0229 (4)
H1	0.6120	1.0859	−0.0268	0.027*
N2	0.6858 (2)	1.04878 (17)	0.21206 (13)	0.0218 (4)
H2	0.7469	1.1153	0.1963	0.026*
N3	0.9237 (2)	0.70890 (17)	0.60728 (14)	0.0245 (4)

C1	0.9398 (3)	1.2235 (2)	−0.1811 (2)	0.0323 (5)
C2	0.9644 (3)	1.2813 (3)	−0.2889 (2)	0.0382 (6)
H2A	1.0617	1.2633	−0.3309	0.046*
C3	0.8436 (3)	1.3662 (3)	−0.33402 (18)	0.0382 (6)
H3	0.8589	1.4080	−0.4080	0.046*
C4	0.7021 (3)	1.3915 (2)	−0.27473 (18)	0.0356 (6)
H4	0.6197	1.4502	−0.3066	0.043*
C5	0.6822 (3)	1.3296 (2)	−0.16762 (18)	0.0275 (5)
C6	0.7993 (2)	1.2441 (2)	−0.11733 (16)	0.0220 (4)
C7	0.7787 (2)	1.1828 (2)	0.00044 (16)	0.0228 (4)
C8	0.6163 (2)	1.0217 (2)	0.12916 (16)	0.0222 (4)
C9	0.6721 (2)	0.98326 (19)	0.32049 (15)	0.0190 (4)
C10	0.5976 (2)	0.86569 (19)	0.35643 (16)	0.0207 (4)
H10	0.5464	0.8274	0.3081	0.025*
C11	0.5998 (2)	0.80569 (19)	0.46473 (16)	0.0204 (4)
C12	0.6729 (2)	0.85890 (19)	0.53728 (15)	0.0202 (4)
C13	0.7419 (2)	0.9786 (2)	0.50062 (16)	0.0221 (4)
C14	0.7433 (2)	1.0399 (2)	0.39305 (16)	0.0221 (4)
H14	0.7929	1.1208	0.3685	0.026*
C15	0.8040 (2)	0.73051 (19)	0.67978 (16)	0.0192 (4)
C16	0.8070 (2)	0.6866 (2)	0.79131 (16)	0.0237 (4)
C17	0.9430 (2)	0.6189 (2)	0.82825 (17)	0.0258 (5)
H17	0.9492	0.5881	0.9037	0.031*
C18	1.0710 (2)	0.5965 (2)	0.75305 (17)	0.0235 (4)
C19	1.0565 (3)	0.6423 (2)	0.64440 (17)	0.0250 (4)
H19	1.1445	0.6262	0.5932	0.030*
C20	1.2233 (3)	0.5247 (2)	0.78821 (19)	0.0321 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0441 (3)	0.0284 (3)	0.0261 (3)	−0.0152 (2)	−0.0103 (2)	0.0063 (2)
Cl2	0.0376 (3)	0.0384 (3)	0.0237 (3)	−0.0096 (2)	−0.0131 (2)	−0.0067 (2)
Cl3	0.0296 (3)	0.0784 (5)	0.0193 (3)	0.0167 (3)	0.0006 (2)	0.0036 (3)
F1	0.0343 (8)	0.0660 (11)	0.0626 (11)	0.0190 (8)	0.0036 (8)	0.0059 (9)
F2	0.0289 (7)	0.0586 (9)	0.0402 (8)	0.0124 (7)	0.0018 (6)	0.0122 (7)
F3	0.0285 (8)	0.0604 (10)	0.0824 (13)	−0.0001 (7)	−0.0263 (8)	−0.0180 (9)
F4	0.0402 (9)	0.0576 (10)	0.0721 (12)	0.0233 (8)	−0.0194 (8)	−0.0305 (9)
F5	0.0415 (9)	0.1138 (16)	0.0434 (10)	0.0300 (10)	−0.0047 (8)	0.0351 (10)
O1	0.0393 (9)	0.0434 (9)	0.0243 (8)	−0.0195 (8)	−0.0120 (7)	0.0024 (7)
O2	0.0392 (9)	0.0394 (9)	0.0200 (8)	−0.0185 (7)	−0.0128 (7)	0.0059 (6)
O3	0.0189 (7)	0.0334 (8)	0.0160 (7)	0.0013 (6)	−0.0054 (6)	0.0030 (6)
N1	0.0234 (9)	0.0305 (9)	0.0154 (8)	−0.0070 (7)	−0.0089 (7)	0.0019 (7)
N2	0.0266 (9)	0.0222 (8)	0.0167 (8)	−0.0069 (7)	−0.0071 (7)	0.0022 (6)
N3	0.0261 (9)	0.0269 (9)	0.0188 (9)	0.0010 (7)	−0.0039 (7)	−0.0006 (7)
C1	0.0271 (12)	0.0321 (12)	0.0354 (13)	−0.0008 (9)	0.0004 (10)	−0.0039 (10)
C2	0.0398 (14)	0.0443 (14)	0.0311 (13)	−0.0145 (11)	0.0123 (11)	−0.0124 (11)
C3	0.0571 (16)	0.0417 (14)	0.0184 (11)	−0.0247 (12)	−0.0026 (11)	−0.0002 (10)

C4	0.0447 (14)	0.0369 (13)	0.0243 (12)	−0.0093 (11)	−0.0131 (11)	0.0071 (10)
C5	0.0247 (11)	0.0326 (11)	0.0233 (11)	−0.0045 (9)	−0.0030 (9)	0.0016 (9)
C6	0.0250 (11)	0.0219 (10)	0.0196 (10)	−0.0056 (8)	−0.0039 (8)	−0.0017 (8)
C7	0.0223 (10)	0.0246 (10)	0.0208 (10)	−0.0009 (8)	−0.0049 (8)	−0.0011 (8)
C8	0.0226 (10)	0.0248 (10)	0.0185 (10)	−0.0024 (8)	−0.0058 (8)	0.0006 (8)
C9	0.0181 (9)	0.0221 (9)	0.0159 (9)	0.0020 (7)	−0.0060 (7)	−0.0007 (7)
C10	0.0226 (10)	0.0225 (10)	0.0176 (10)	−0.0019 (8)	−0.0085 (8)	−0.0013 (8)
C11	0.0214 (10)	0.0177 (9)	0.0210 (10)	−0.0013 (7)	−0.0043 (8)	0.0008 (7)
C12	0.0202 (10)	0.0246 (10)	0.0142 (9)	0.0028 (8)	−0.0068 (8)	0.0015 (8)
C13	0.0219 (10)	0.0266 (10)	0.0200 (10)	−0.0006 (8)	−0.0090 (8)	−0.0063 (8)
C14	0.0229 (10)	0.0236 (10)	0.0201 (10)	−0.0052 (8)	−0.0056 (8)	−0.0009 (8)
C15	0.0180 (9)	0.0213 (9)	0.0185 (10)	−0.0019 (7)	−0.0065 (8)	−0.0007 (7)
C16	0.0231 (10)	0.0298 (11)	0.0168 (10)	0.0009 (8)	−0.0020 (8)	−0.0021 (8)
C17	0.0272 (11)	0.0321 (11)	0.0178 (10)	−0.0016 (9)	−0.0079 (9)	−0.0004 (8)
C18	0.0218 (10)	0.0251 (10)	0.0233 (10)	−0.0007 (8)	−0.0067 (8)	−0.0015 (8)
C19	0.0230 (10)	0.0295 (11)	0.0216 (10)	−0.0006 (8)	−0.0018 (8)	−0.0035 (8)
C20	0.0264 (11)	0.0389 (13)	0.0287 (12)	0.0045 (10)	−0.0069 (9)	−0.0020 (10)

Geometric parameters (Å, º)

Cl1—C11	1.7315 (19)	C2—H2A	0.9500
Cl2—C13	1.723 (2)	C3—C4	1.368 (4)
Cl3—C16	1.716 (2)	C3—H3	0.9500
F1—C1	1.350 (3)	C4—C5	1.378 (3)
F2—C5	1.340 (3)	C4—H4	0.9500
F3—C20	1.331 (3)	C5—C6	1.385 (3)
F4—C20	1.333 (3)	C6—C7	1.497 (3)
F5—C20	1.311 (3)	C9—C10	1.392 (3)
O1—C7	1.217 (2)	C9—C14	1.394 (3)
O2—C8	1.217 (2)	C10—C11	1.389 (3)
O3—C15	1.365 (2)	C10—H10	0.9500
O3—C12	1.390 (2)	C11—C12	1.384 (3)
N1—C7	1.366 (3)	C12—C13	1.387 (3)
N1—C8	1.405 (2)	C13—C14	1.382 (3)
N1—H1	0.8800	C14—H14	0.9500
N2—C8	1.347 (3)	C15—C16	1.396 (3)
N2—C9	1.402 (2)	C16—C17	1.373 (3)
N2—H2	0.8800	C17—C18	1.386 (3)
N3—C15	1.314 (3)	C17—H17	0.9500
N3—C19	1.347 (3)	C18—C19	1.378 (3)
C1—C2	1.377 (3)	C18—C20	1.497 (3)
C1—C6	1.381 (3)	C19—H19	0.9500
C2—C3	1.379 (4)		

C15—O3—C12	116.53 (15)	C11—C10—H10	120.8
C7—N1—C8	128.40 (17)	C9—C10—H10	120.8
C7—N1—H1	115.8	C12—C11—C10	122.32 (18)
C8—N1—H1	115.8	C12—C11—Cl1	118.64 (15)

C8—N2—C9	127.54 (17)	C10—C11—Cl1	119.03 (15)
C8—N2—H2	116.2	C11—C12—C13	118.40 (17)
C9—N2—H2	116.2	C11—C12—O3	120.52 (17)
C15—N3—C19	117.22 (17)	C13—C12—O3	120.94 (17)
F1—C1—C2	119.5 (2)	C14—C13—C12	120.64 (18)
F1—C1—C6	117.4 (2)	C14—C13—Cl2	119.64 (15)
C2—C1—C6	123.2 (2)	C12—C13—Cl2	119.72 (15)
C1—C2—C3	118.0 (2)	C13—C14—C9	120.16 (18)
C1—C2—H2A	121.0	C13—C14—H14	119.9
C3—C2—H2A	121.0	C9—C14—H14	119.9
C4—C3—C2	121.5 (2)	N3—C15—O3	119.22 (17)
C4—C3—H3	119.2	N3—C15—C16	123.69 (18)
C2—C3—H3	119.2	O3—C15—C16	117.09 (18)
C3—C4—C5	118.4 (2)	C17—C16—C15	118.60 (19)
C3—C4—H4	120.8	C17—C16—Cl3	120.33 (16)
C5—C4—H4	120.8	C15—C16—Cl3	121.07 (16)
F2—C5—C4	119.4 (2)	C16—C17—C18	118.51 (19)
F2—C5—C6	117.64 (18)	C16—C17—H17	120.7
C4—C5—C6	122.9 (2)	C18—C17—H17	120.7
C1—C6—C5	116.01 (19)	C19—C18—C17	118.80 (19)
C1—C6—C7	121.58 (19)	C19—C18—C20	120.08 (19)
C5—C6—C7	122.35 (19)	C17—C18—C20	121.11 (19)
O1—C7—N1	124.57 (19)	N3—C19—C18	123.18 (19)
O1—C7—C6	121.15 (18)	N3—C19—H19	118.4
N1—C7—C6	114.27 (17)	C18—C19—H19	118.4
O2—C8—N2	125.62 (18)	F5—C20—F3	107.5 (2)
O2—C8—N1	119.61 (18)	F5—C20—F4	108.0 (2)
N2—C8—N1	114.76 (17)	F3—C20—F4	104.67 (19)
C10—C9—C14	120.10 (18)	F5—C20—C18	112.37 (19)
C10—C9—N2	123.68 (18)	F3—C20—C18	111.92 (19)
C14—C9—N2	116.18 (17)	F4—C20—C18	112.02 (19)
C11—C10—C9	118.32 (18)		

F1—C1—C2—C3	−179.2 (2)	Cl1—C11—C12—O3	−3.3 (3)
C6—C1—C2—C3	1.5 (4)	C15—O3—C12—C11	107.5 (2)
C1—C2—C3—C4	−0.9 (4)	C15—O3—C12—C13	−77.0 (2)
C2—C3—C4—C5	−0.1 (4)	C11—C12—C13—C14	−2.7 (3)
C3—C4—C5—F2	179.6 (2)	O3—C12—C13—C14	−178.30 (18)
C3—C4—C5—C6	0.6 (4)	C11—C12—C13—Cl2	177.03 (16)
F1—C1—C6—C5	179.7 (2)	O3—C12—C13—Cl2	1.5 (3)
C2—C1—C6—C5	−1.0 (3)	C12—C13—C14—C9	1.4 (3)
F1—C1—C6—C7	2.6 (3)	Cl2—C13—C14—C9	−178.39 (15)
C2—C1—C6—C7	−178.1 (2)	C10—C9—C14—C13	0.8 (3)
F2—C5—C6—C1	−179.1 (2)	N2—C9—C14—C13	−177.08 (18)
C4—C5—C6—C1	−0.1 (3)	C19—N3—C15—O3	179.44 (17)
F2—C5—C6—C7	−2.0 (3)	C19—N3—C15—C16	−1.0 (3)
C4—C5—C6—C7	177.0 (2)	C12—O3—C15—N3	−9.7 (3)
C8—N1—C7—O1	0.0 (4)	C12—O3—C15—C16	170.78 (18)

C8—N1—C7—C6	179.18 (19)	N3—C15—C16—C17	1.1 (3)
C1—C6—C7—O1	60.5 (3)	O3—C15—C16—C17	−179.40 (18)
C5—C6—C7—O1	−116.5 (2)	N3—C15—C16—Cl3	−177.88 (16)
C1—C6—C7—N1	−118.8 (2)	O3—C15—C16—Cl3	1.6 (3)
C5—C6—C7—N1	64.3 (3)	C15—C16—C17—C18	−0.4 (3)
C9—N2—C8—O2	6.7 (4)	Cl3—C16—C17—C18	178.62 (16)
C9—N2—C8—N1	−174.42 (18)	C16—C17—C18—C19	−0.3 (3)
C7—N1—C8—O2	−175.0 (2)	C16—C17—C18—C20	179.3 (2)
C7—N1—C8—N2	6.1 (3)	C15—N3—C19—C18	0.3 (3)
C8—N2—C9—C10	8.7 (3)	C17—C18—C19—N3	0.3 (3)
C8—N2—C9—C14	−173.53 (19)	C20—C18—C19—N3	−179.2 (2)
C14—C9—C10—C11	−1.6 (3)	C19—C18—C20—F5	−163.0 (2)
N2—C9—C10—C11	176.18 (18)	C17—C18—C20—F5	17.4 (3)
C9—C10—C11—C12	0.1 (3)	C19—C18—C20—F3	76.0 (3)
C9—C10—C11—Cl1	−178.97 (15)	C17—C18—C20—F3	−103.6 (2)
C10—C11—C12—C13	2.0 (3)	C19—C18—C20—F4	−41.2 (3)
Cl1—C11—C12—C13	−178.89 (16)	C17—C18—C20—F4	139.2 (2)
C10—C11—C12—O3	177.58 (18)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.88	1.96	2.837 (2)	175

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