Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Ethyl 1-(2,4-dichlorobenzyl)-4-oxo-7-trifluoromethyl-1,4-dihydroquinoline-3-carboxylate

Hoong-Kun Fun,[a]*‡ Chin Wei Ooi,[a] B. Garudachari,[b] Arun M. Isloor[b] and Gurumurthy Hegde[c]

[a]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, [b]Department of Chemistry, National Institute of Technology-Karnataka, Surathkal, Mangalore 575 025, India, and [c]Faculty of Industrial Science and Technology, Universiti Malaysia Pahang, Lebuhraya Tun Razak, 26300 Gambang Kuantan, Pahang Darul Makmur, Malaysia
Correspondence e-mail: hkfun@usm.my

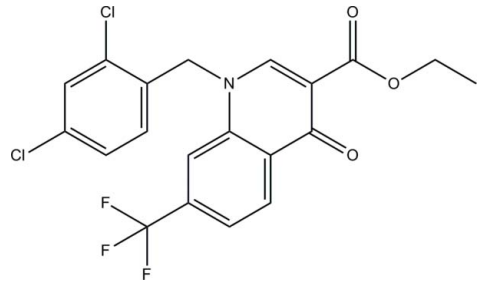
Received 5 January 2012; accepted 11 January 2012

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.056; wR factor = 0.179; data-to-parameter ratio = 17.6.

In the title compound, $C_{20}H_{14}Cl_2F_3NO_3$, the trifluromethyl group is disordered over two sets of sites in a 0.784 (10):0.216 (10) ratio. The quinoline ring system is essentially planar with a maximum deviation of 0.058 (2) Å for the N atom and forms dihedral angles of 89.23 (11) and 8.13 (17)°, respectively with the mean planes of the benzene ring and the carboxylate group. In the crystal, pairs of weak C—H···O and C—H···F hydrogen bonds link molecules into centrosymmetric dimers. The crystal structure is further stabilized by weak π–π [centroid–centroid distance = 3.624 (2) Å] interactions.

Related literature

For background to the properties and uses of quinoline derivatives, see: Kaur *et al.* (2010); Eswaran *et al.* (2010); Chou *et al.* (2010); Chen *et al.* (2004); Shingalapur *et al.* (2009). For a related structure, see: Fun *et al.* (2011). For standard bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{20}H_{14}Cl_2F_3NO_3$
M_r = 444.22
Triclinic, $P\overline{1}$
a = 8.090 (2) Å
b = 9.547 (3) Å
c = 14.047 (4) Å
α = 77.299 (6)°
β = 76.198 (5)°
γ = 67.488 (4)°
V = 963.3 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.39 mm^{-1}
T = 296 K
0.43 × 0.18 × 0.07 mm

Data collection

Bruker APEX DUO CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.852, T_{max} = 0.972
13916 measured reflections
5071 independent reflections
2759 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.179
S = 1.04
5071 reflections
288 parameters
7 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16A···O3^{i}	0.93	2.52	3.292 (5)	141
C18—H18A···F2^{i}	0.97	2.50	3.355 (7)	147

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

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: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

HKF and CWO thank Universiti Sains Malaysia (USM) for the Research University Grant (1001/PFIZIK/811160). CWO also thanks the Malaysian Government and USM for the award of the post of research assistant under the Research University Grant (1001/PFIZIK/811151). AMI is thankful to the Department of Atomic Energy, Board for Research in Nuclear Sciences, Government of India for the Young Scientist award.

‡ Visiting Professor, College of Pharmacy, King Saud University, Riyadh, Saudi Arabia. Thomson Reuters ResearcherID: A-3561-2009.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5400).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.

Bruker (2009). *SADABS*, *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Chen, Y. L., Hung, H. M., Lu, C. M., Li, K. C. & Tzeng, C. C. (2004). *Bioorg. Med. Chem.* **12**, 6539–6546.

Chou, L. C., Tsai, M. T., Hsu, M. H., Wang, S. H., Way, T. D., Huang, C. H., Lin, H. Y., Qian, K., Dong, Y., Lee, K. H., Huang, L. J. & Kuo, S. C. (2010). *J. Med. Chem.* **53**, 8047–8058.

Eswaran, S., Adhikari, A. V., Chowdhury, I. H., Pal, N. K. & Thomas, K. D. (2010). *Eur. J. Med. Chem.* **45**, 3374–3383.

Fun, H.-K., Arshad, S., Garudachari, B., Isloor, A. M. & Satyanarayan, M. N. (2011). *Acta Cryst.* E**67**, o3117–o3118.

Kaur, K., Jain, M., Reddy, R. P. & Jain, R. (2010). *Eur. J. Med. Chem.* **45**, 3245–3264.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Shingalapur, R. V., Hosamani, K. M. & Keri, R. S. (2009). *Eur. J. Med. Chem.* **44**, 4244–4248.

Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supporting information

Acta Cryst. (2012). E**68**, o435–o436 [doi:10.1107/S1600536812001249]

Ethyl 1-(2,4-dichlorobenzyl)-4-oxo-7-trifluoromethyl-1,4-dihydroquinoline-3-carboxylate

Hoong-Kun Fun, Chin Wei Ooi, B. Garudachari, Arun M. Isloor and Gurumurthy Hegde

S1. Comment

The quinoline moiety is of great importance to chemists as well as biologists as it is one of the key building elements for many naturally occurring compounds. Members of this family have wide range of applications as pharmaceuticals as antimalarial (Kaur *et al.*, 2010), anti-tuberculosis (Eswaran *et al.*, 2010), antitumor (Chou *et al.*, 2010), anticancer (Chen *et al.*, 2004) and antiviral (Shingalapur *et al.*, 2009) agents. Some of the present day drugs such as chloroquine, mefloquine, tafenoquine and primaquine contain quinoline as the basic unit in their structures. In view of the biological importance, we have synthesized the title compound to study its crystal structure.

In the molecular structure (Fig. 1), the trifluromethyl group is disordered over two sets of sites in a ratio of 0.784 (10):0.216 (10). The quinoline ring (N1/C1–C9) is essentially planar with a maximum deviation of 0.058 (2) Å at atom N1. The quinoline ring makes dihedral angles of 89.23 (11) and 8.13 (17)°, respectively with the chloro-substituted benzene ring (C11–C16) and the carboxylate group (O1/O2/C17–C19). The bond lengths (Allen *et al.*, 1987) and angles are within normal ranges and are comparable to a related structure (Fun *et al.*, 2011).

In the crystal (Fig. 2), intermolecular C16—H16A···O3^{i} and C18—H18A···F2^{i} hydrogen bonds (Table 1) link molecules to form dimers. The crystal is further stabilized by weak π–π interactions between the quinoline (N1/C1–C9) and the benzene ring (C4–C9) [centroid-to-centroid (-*x*, 1 - *y*, -*z*); distance = 3.624 (2) Å].

S2. Experimental

A mixture of ethyl 4-hydroxy-7-(trifluoromethyl)quinoline-3-carboxylate (0.10 g, 0.00035 mol), potassium carbonate (0.053 g, 0.00038 mol) and 1-(bromomethyl)-2,4-dichlorobenzene (0.091 g, 0.00038 mol) in dimethylformamide (5 ml) was stirred at 353K for 3 h. After completion of the reaction, the reaction mixture was poured into ice-cold water. The solid product obtained was filtered, washed with water and recrystallized using ethanol. Yield: 0.150 g, 96.77%. *M. p.*: 428–429 K.

S3. Refinement

All H atoms were positioned geometrically and refined using a riding model with U_{iso}(H) = 1.2 or 1.5U_{eq}(C) (C—H = 0.93, 0.96 or 0.97 Å). A rotating group model was applied to the methyl group. In the final refinement, the outliners (-4 - 6 1), (3 2 0), (5 0 6), (5 1 8) were omitted. A bond-distance restraint was applied to C20A–C7. The same U_{ij} parameters were used for atom pairs F3A/F1A and C20A/C7.

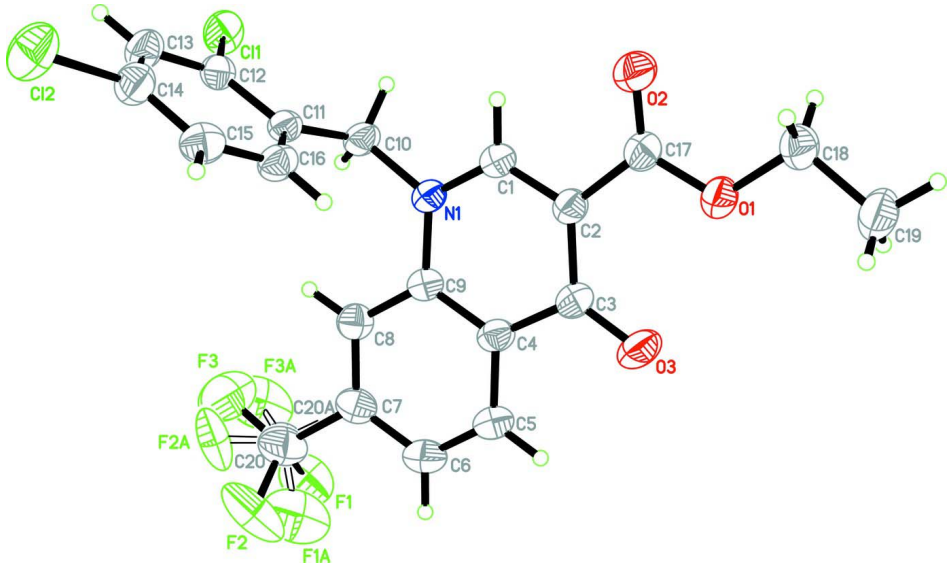


Figure 1

The molecular structure of the title compound, showing 30% probability displacement ellipsoids. Both disorder components are shown.

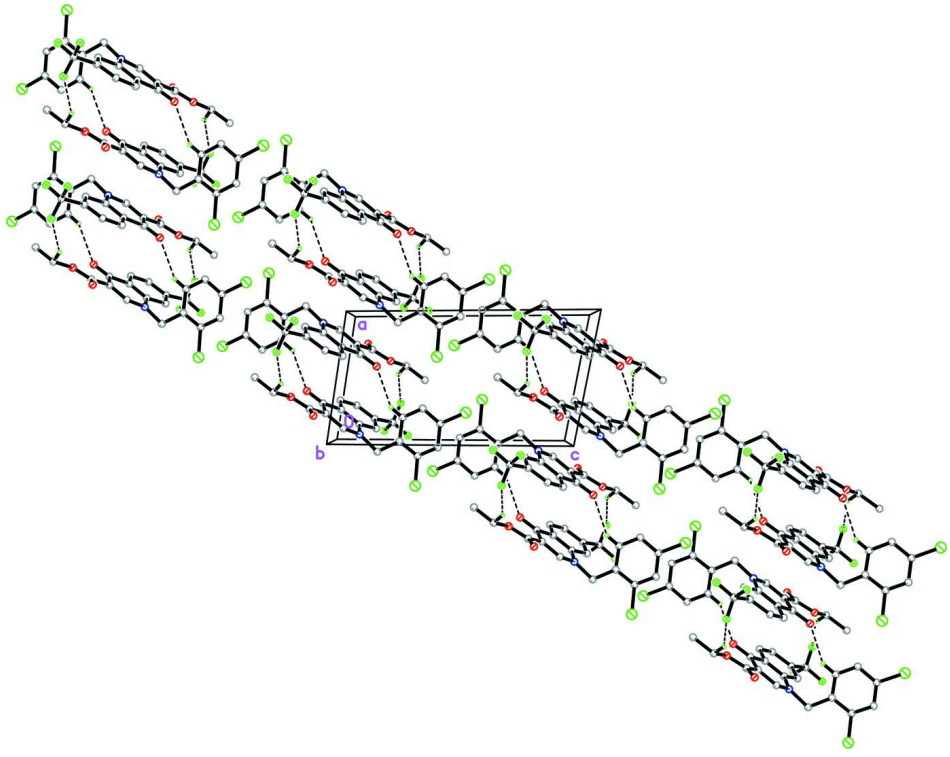


Figure 2

The crystal packing of the title compound. The dashed lines represent the hydrogen bonds. Only the major disordered component is shown.

Ethyl 1-(2,4-dichlorobenzyl)-4-oxo-7-trifluoromethyl-1,4-dihydroquinoline-3- carboxylate

Crystal data

$C_{20}H_{14}Cl_2F_3NO_3$
$M_r = 444.22$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.090$ (2) Å
$b = 9.547$ (3) Å
$c = 14.047$ (4) Å
$\alpha = 77.299$ (6)°
$\beta = 76.198$ (5)°
$\gamma = 67.488$ (4)°
$V = 963.3$ (5) Å^3
$Z = 2$
$F(000) = 452$
$D_x = 1.531$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3077 reflections
$\theta = 2.3$–$24.2°$
$\mu = 0.39$ mm^{-1}
$T = 296$ K
Block, colourless
0.43 × 0.18 × 0.07 mm

Data collection

Bruker APEX DUO CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.852$, $T_{max} = 0.972$
13916 measured reflections
5071 independent reflections
2759 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 29.1°$, $\theta_{min} = 1.5°$
$h = -10 \rightarrow 11$
$k = -13 \rightarrow 13$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.179$
$S = 1.04$
5071 reflections
288 parameters
7 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
$w = 1/[\sigma^2(F_o^2) + (0.0711P)^2 + 0.3522P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Cl1	−0.33323 (10)	0.73631 (10)	0.39029 (6)	0.0780 (3)	
Cl2	0.24014 (16)	0.66624 (13)	0.54781 (7)	0.1052 (4)	
C20	0.1448 (11)	0.0460 (8)	0.2381 (6)	0.0900 (15)	0.784 (10)

F1	0.0710 (8)	−0.0345 (4)	0.2048 (3)	0.1144 (17)	0.784 (10)
F2	0.2991 (6)	−0.0610 (5)	0.2577 (5)	0.137 (2)	0.784 (10)
F3	0.0375 (13)	0.0915 (6)	0.3154 (4)	0.197 (5)	0.784 (10)
C20A	0.134 (3)	0.055 (2)	0.2391 (13)	0.0638 (7)	0.216 (10)
F1A	0.207 (3)	−0.0777 (17)	0.2083 (14)	0.149 (7)	0.216 (10)
F2A	0.204 (2)	0.042 (2)	0.3172 (9)	0.103 (6)	0.216 (10)
F3A	−0.026 (2)	0.078 (2)	0.2781 (19)	0.149 (7)	0.216 (10)
O1	0.3593 (3)	0.7747 (2)	−0.19081 (13)	0.0747 (6)	
O2	0.2188 (3)	0.9285 (2)	−0.07639 (15)	0.0818 (6)	
O3	0.4032 (4)	0.4757 (3)	−0.14202 (17)	0.0992 (8)	
N1	0.0638 (3)	0.5929 (2)	0.11707 (14)	0.0525 (5)	
C1	0.1139 (3)	0.6989 (3)	0.04830 (18)	0.0538 (6)	
H1A	0.0652	0.7997	0.0611	0.065*	
C2	0.2309 (3)	0.6694 (3)	−0.03871 (18)	0.0519 (6)	
C3	0.3065 (4)	0.5147 (3)	−0.0630 (2)	0.0614 (7)	
C4	0.2558 (3)	0.4008 (3)	0.01455 (19)	0.0546 (6)	
C5	0.3257 (4)	0.2471 (3)	−0.0008 (2)	0.0668 (7)	
H5A	0.4018	0.2206	−0.0600	0.080*	
C6	0.2850 (4)	0.1353 (3)	0.0693 (2)	0.0726 (8)	
H6A	0.3294	0.0344	0.0570	0.087*	
C7	0.1763 (4)	0.1747 (3)	0.1588 (2)	0.0638 (7)	
C8	0.1019 (4)	0.3237 (3)	0.1768 (2)	0.0580 (6)	
H8A	0.0275	0.3481	0.2369	0.070*	
C9	0.1394 (3)	0.4388 (3)	0.10383 (18)	0.0506 (6)	
C10	−0.0705 (3)	0.6443 (3)	0.20509 (18)	0.0570 (6)	
H10A	−0.1461	0.5812	0.2247	0.068*	
H10B	−0.1484	0.7490	0.1876	0.068*	
C11	0.0122 (3)	0.6370 (3)	0.29170 (17)	0.0497 (6)	
C12	−0.0999 (3)	0.6848 (3)	0.37876 (18)	0.0546 (6)	
C13	−0.0312 (4)	0.6930 (3)	0.4573 (2)	0.0692 (8)	
H13A	−0.1089	0.7262	0.5148	0.083*	
C14	0.1529 (4)	0.6517 (3)	0.4499 (2)	0.0680 (8)	
C15	0.2693 (4)	0.5999 (3)	0.3659 (2)	0.0651 (7)	
H15A	0.3942	0.5695	0.3619	0.078*	
C16	0.1983 (4)	0.5938 (3)	0.2878 (2)	0.0580 (6)	
H16A	0.2769	0.5598	0.2307	0.070*	
C17	0.2670 (3)	0.8046 (3)	−0.10207 (19)	0.0566 (6)	
C18	0.3971 (5)	0.9011 (3)	−0.2582 (2)	0.0729 (8)	
H18A	0.4611	0.9439	−0.2290	0.087*	
H18B	0.2848	0.9811	−0.2730	0.087*	
C19	0.5111 (6)	0.8397 (4)	−0.3499 (2)	0.1007 (13)	
H19A	0.5278	0.9226	−0.3993	0.151*	
H19B	0.4521	0.7878	−0.3740	0.151*	
H19C	0.6271	0.7691	−0.3356	0.151*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0572 (4)	0.0910 (6)	0.0667 (5)	−0.0187 (4)	0.0125 (3)	−0.0118 (4)
Cl2	0.1179 (8)	0.1260 (8)	0.0906 (7)	−0.0464 (7)	−0.0256 (6)	−0.0378 (6)
C20	0.091 (4)	0.062 (3)	0.116 (4)	−0.028 (3)	−0.016 (3)	−0.010 (3)
F1	0.120 (4)	0.097 (2)	0.156 (3)	−0.073 (3)	−0.038 (2)	0.003 (2)
F2	0.099 (3)	0.099 (3)	0.207 (5)	−0.048 (2)	−0.072 (3)	0.069 (3)
F3	0.325 (11)	0.088 (3)	0.129 (4)	−0.094 (5)	0.092 (6)	−0.020 (3)
C20A	0.0626 (17)	0.0525 (15)	0.0778 (19)	−0.0208 (13)	−0.0151 (14)	−0.0079 (13)
F1A	0.096 (9)	0.116 (10)	0.226 (15)	−0.066 (7)	0.006 (8)	0.010 (9)
F2A	0.083 (9)	0.145 (15)	0.076 (8)	−0.057 (10)	−0.038 (7)	0.053 (8)
F3A	0.096 (9)	0.116 (10)	0.226 (15)	−0.066 (7)	0.006 (8)	0.010 (9)
O1	0.0975 (15)	0.0655 (12)	0.0540 (11)	−0.0334 (11)	0.0120 (10)	−0.0122 (9)
O2	0.1094 (17)	0.0645 (13)	0.0696 (13)	−0.0377 (12)	0.0106 (12)	−0.0200 (10)
O3	0.1143 (19)	0.0721 (14)	0.0803 (15)	−0.0225 (13)	0.0394 (13)	−0.0285 (12)
N1	0.0536 (12)	0.0498 (11)	0.0481 (11)	−0.0138 (9)	0.0006 (9)	−0.0124 (9)
C1	0.0558 (15)	0.0509 (14)	0.0526 (14)	−0.0154 (11)	−0.0049 (11)	−0.0139 (11)
C2	0.0520 (14)	0.0529 (14)	0.0486 (13)	−0.0178 (11)	−0.0027 (11)	−0.0103 (11)
C3	0.0539 (15)	0.0601 (16)	0.0569 (15)	−0.0089 (12)	0.0025 (12)	−0.0153 (12)
C4	0.0477 (13)	0.0523 (14)	0.0582 (15)	−0.0091 (11)	−0.0061 (11)	−0.0153 (11)
C5	0.0615 (17)	0.0576 (16)	0.0692 (18)	−0.0067 (13)	−0.0025 (13)	−0.0198 (14)
C6	0.0751 (19)	0.0515 (16)	0.087 (2)	−0.0132 (14)	−0.0137 (16)	−0.0176 (15)
C7	0.0626 (17)	0.0525 (15)	0.0778 (19)	−0.0208 (13)	−0.0151 (14)	−0.0079 (13)
C8	0.0548 (15)	0.0585 (16)	0.0601 (15)	−0.0212 (12)	−0.0063 (12)	−0.0087 (12)
C9	0.0476 (13)	0.0481 (13)	0.0553 (14)	−0.0139 (11)	−0.0070 (11)	−0.0131 (11)
C10	0.0511 (14)	0.0554 (14)	0.0551 (15)	−0.0129 (11)	0.0065 (11)	−0.0168 (12)
C11	0.0544 (14)	0.0411 (12)	0.0491 (13)	−0.0184 (10)	0.0034 (10)	−0.0076 (10)
C12	0.0558 (14)	0.0498 (14)	0.0491 (14)	−0.0196 (11)	0.0069 (11)	−0.0039 (11)
C13	0.078 (2)	0.0700 (18)	0.0518 (16)	−0.0258 (15)	0.0095 (14)	−0.0156 (13)
C14	0.081 (2)	0.0682 (18)	0.0591 (16)	−0.0310 (16)	−0.0091 (15)	−0.0132 (14)
C15	0.0621 (17)	0.0616 (17)	0.0757 (19)	−0.0261 (14)	−0.0078 (14)	−0.0140 (14)
C16	0.0562 (15)	0.0569 (15)	0.0578 (15)	−0.0208 (12)	0.0045 (12)	−0.0156 (12)
C17	0.0541 (15)	0.0618 (16)	0.0529 (14)	−0.0210 (12)	−0.0026 (11)	−0.0119 (12)
C18	0.084 (2)	0.0724 (19)	0.0620 (17)	−0.0388 (16)	0.0061 (15)	−0.0073 (14)
C19	0.137 (3)	0.100 (3)	0.064 (2)	−0.058 (3)	0.023 (2)	−0.0218 (18)

Geometric parameters (Å, º)

Cl1—C12	1.735 (3)	C5—H5A	0.9300
Cl2—C14	1.741 (3)	C6—C7	1.388 (4)
C20—F3	1.262 (8)	C6—H6A	0.9300
C20—F2	1.320 (7)	C7—C8	1.371 (4)
C20—F1	1.344 (8)	C8—C9	1.401 (4)
C20—C7	1.522 (8)	C8—H8A	0.9300
C20A—F3A	1.235 (16)	C10—C11	1.499 (4)
C20A—F1A	1.303 (16)	C10—H10A	0.9700
C20A—F2A	1.311 (16)	C10—H10B	0.9700

C20A—C7	1.494 (17)	C11—C12	1.387 (3)
O1—C17	1.320 (3)	C11—C16	1.391 (4)
O1—C18	1.445 (3)	C12—C13	1.377 (4)
O2—C17	1.204 (3)	C13—C14	1.371 (4)
O3—C3	1.236 (3)	C13—H13A	0.9300
N1—C1	1.349 (3)	C14—C15	1.376 (4)
N1—C9	1.396 (3)	C15—C16	1.375 (4)
N1—C10	1.472 (3)	C15—H15A	0.9300
C1—C2	1.365 (3)	C16—H16A	0.9300
C1—H1A	0.9300	C18—C19	1.485 (4)
C2—C3	1.450 (4)	C18—H18A	0.9700
C2—C17	1.484 (4)	C18—H18B	0.9700
C3—C4	1.465 (4)	C19—H19A	0.9600
C4—C5	1.401 (4)	C19—H19B	0.9600
C4—C9	1.402 (3)	C19—H19C	0.9600
C5—C6	1.367 (4)		

F3—C20—F2	112.3 (8)	N1—C9—C8	121.8 (2)
F3—C20—F1	105.5 (6)	N1—C9—C4	118.2 (2)
F2—C20—F1	101.2 (6)	C8—C9—C4	120.1 (2)
F3—C20—C7	113.9 (6)	N1—C10—C11	113.9 (2)
F2—C20—C7	111.8 (6)	N1—C10—H10A	108.8
F1—C20—C7	111.2 (6)	C11—C10—H10A	108.8
F3A—C20A—F1A	110.4 (17)	N1—C10—H10B	108.8
F3A—C20A—F2A	99.9 (16)	C11—C10—H10B	108.8
F1A—C20A—F2A	106.3 (18)	H10A—C10—H10B	107.7
F3A—C20A—C7	118.3 (17)	C12—C11—C16	117.1 (2)
F1A—C20A—C7	109.6 (14)	C12—C11—C10	119.6 (2)
F2A—C20A—C7	111.4 (13)	C16—C11—C10	123.2 (2)
C17—O1—C18	116.3 (2)	C13—C12—C11	121.8 (3)
C1—N1—C9	120.0 (2)	C13—C12—Cl1	118.4 (2)
C1—N1—C10	118.3 (2)	C11—C12—Cl1	119.8 (2)
C9—N1—C10	121.7 (2)	C14—C13—C12	119.3 (3)
N1—C1—C2	124.9 (2)	C14—C13—H13A	120.3
N1—C1—H1A	117.6	C12—C13—H13A	120.3
C2—C1—H1A	117.6	C13—C14—C15	120.8 (3)
C1—C2—C3	119.4 (2)	C13—C14—Cl2	119.5 (2)
C1—C2—C17	115.1 (2)	C15—C14—Cl2	119.7 (3)
C3—C2—C17	125.5 (2)	C16—C15—C14	119.1 (3)
O3—C3—C2	125.5 (3)	C16—C15—H15A	120.4
O3—C3—C4	120.0 (2)	C14—C15—H15A	120.4
C2—C3—C4	114.5 (2)	C15—C16—C11	121.8 (2)
C5—C4—C9	118.3 (2)	C15—C16—H16A	119.1
C5—C4—C3	118.9 (2)	C11—C16—H16A	119.1
C9—C4—C3	122.8 (2)	O2—C17—O1	122.9 (2)
C6—C5—C4	121.6 (3)	O2—C17—C2	124.4 (2)
C6—C5—H5A	119.2	O1—C17—C2	112.6 (2)
C4—C5—H5A	119.2	O1—C18—C19	107.1 (3)

C5—C6—C7	119.0 (3)	O1—C18—H18A	110.3
C5—C6—H6A	120.5	C19—C18—H18A	110.3
C7—C6—H6A	120.5	O1—C18—H18B	110.3
C8—C7—C6	121.6 (3)	C19—C18—H18B	110.3
C8—C7—C20A	117.5 (8)	H18A—C18—H18B	108.6
C6—C7—C20A	120.9 (8)	C18—C19—H19A	109.5
C8—C7—C20	120.7 (4)	C18—C19—H19B	109.5
C6—C7—C20	117.7 (4)	H19A—C19—H19B	109.5
C7—C8—C9	119.3 (3)	C18—C19—H19C	109.5
C7—C8—H8A	120.4	H19A—C19—H19C	109.5
C9—C8—H8A	120.4	H19B—C19—H19C	109.5

C9—N1—C1—C2	3.1 (4)	C20A—C7—C8—C9	179.4 (8)
C10—N1—C1—C2	−177.2 (2)	C20—C7—C8—C9	177.5 (4)
N1—C1—C2—C3	1.6 (4)	C1—N1—C9—C8	174.9 (2)
N1—C1—C2—C17	−179.3 (2)	C10—N1—C9—C8	−4.8 (4)
C1—C2—C3—O3	174.7 (3)	C1—N1—C9—C4	−5.0 (4)
C17—C2—C3—O3	−4.3 (5)	C10—N1—C9—C4	175.2 (2)
C1—C2—C3—C4	−3.8 (4)	C7—C8—C9—N1	178.3 (2)
C17—C2—C3—C4	177.2 (2)	C7—C8—C9—C4	−1.7 (4)
O3—C3—C4—C5	3.0 (4)	C5—C4—C9—N1	−177.3 (2)
C2—C3—C4—C5	−178.4 (3)	C3—C4—C9—N1	2.6 (4)
O3—C3—C4—C9	−176.8 (3)	C5—C4—C9—C8	2.7 (4)
C2—C3—C4—C9	1.8 (4)	C3—C4—C9—C8	−177.4 (2)
C9—C4—C5—C6	−0.8 (4)	C1—N1—C10—C11	−93.1 (3)
C3—C4—C5—C6	179.3 (3)	C9—N1—C10—C11	86.7 (3)
C4—C5—C6—C7	−2.1 (5)	N1—C10—C11—C12	178.9 (2)
C5—C6—C7—C8	3.2 (5)	N1—C10—C11—C16	3.4 (3)
C5—C6—C7—C20A	−177.6 (8)	C16—C11—C12—C13	1.6 (4)
C5—C6—C7—C20	−175.6 (4)	C10—C11—C12—C13	−174.2 (2)
F3A—C20A—C7—C8	49 (2)	C16—C11—C12—Cl1	−178.55 (18)
F1A—C20A—C7—C8	176.8 (13)	C10—C11—C12—Cl1	5.6 (3)
F2A—C20A—C7—C8	−65.8 (19)	C11—C12—C13—C14	−0.6 (4)
F3A—C20A—C7—C6	−130.1 (17)	Cl1—C12—C13—C14	179.5 (2)
F1A—C20A—C7—C6	−2.5 (18)	C12—C13—C14—C15	−1.1 (4)
F2A—C20A—C7—C6	114.9 (15)	C12—C13—C14—Cl2	178.5 (2)
F3A—C20A—C7—C20	−159 (16)	C13—C14—C15—C16	1.7 (4)
F1A—C20A—C7—C20	−31 (14)	Cl2—C14—C15—C16	−177.9 (2)
F2A—C20A—C7—C20	86 (15)	C14—C15—C16—C11	−0.7 (4)
F3—C20—C7—C8	4.5 (8)	C12—C11—C16—C15	−0.9 (4)
F2—C20—C7—C8	−124.1 (6)	C10—C11—C16—C15	174.7 (2)
F1—C20—C7—C8	123.6 (6)	C18—O1—C17—O2	−1.4 (4)
F3—C20—C7—C6	−176.7 (6)	C18—O1—C17—C2	178.7 (2)
F2—C20—C7—C6	54.7 (8)	C1—C2—C17—O2	9.3 (4)
F1—C20—C7—C6	−57.6 (8)	C3—C2—C17—O2	−171.8 (3)
F3—C20—C7—C20A	−24 (14)	C1—C2—C17—O1	−170.9 (2)
F2—C20—C7—C20A	−153 (15)	C3—C2—C17—O1	8.1 (4)
F1—C20—C7—C20A	95 (15)	C17—O1—C18—C19	176.4 (3)

C6—C7—C8—C9	−1.3 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16*A*···O3^{i}	0.93	2.52	3.292 (5)	141
C18—H18*A*···F2^{i}	0.97	2.50	3.355 (7)	147

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