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2,6-Bis(trifluoromethyl)benzoic acid

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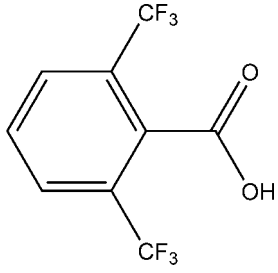
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.039; wR factor = 0.112; data-to-parameter ratio = 10.4.

The title compound, $C_9H_4F_6O_2$, contains two molecules in the asymmetric unit, one of which exhibits disorder in both of its trifluoromethyl groups. The dihedral angles between the benzene ring and the carboxyl group are 71.5 (2) and 99.3 (2)° in the two independent molecules. The compound exhibits a catemeric structure resulting from intermolecular O—H···O hydrogen bonding between the carboxyl groups.

Related literature

There is only one example in the literature of a crystallographically characterized benzoic acid with trifluoromethyl groups in the *ortho* position, namely 2-trifluoromethyl-3-pyrrole benzoic acid (see Faigl *et al.*, 1999). For a recent example of crystal engineering to promote the formation of dimeric or catemeric structures in benzoic acids, see: Moorthy *et al.* (2002). For synthesis details, see: Dmowski & Piasecka-Macieiewska (1998).



Experimental

Crystal data

$C_9H_4F_6O_2$ M_r = 258.12
Monoclinic, $P2_1/c$
a = 10.873 (2) Å
b = 15.755 (3) Å
c = 11.561 (2) Å
β = 94.961 (2)°
V = 1973.0 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.20 mm^{-1}
T = 296 K
0.39 × 0.31 × 0.26 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.834, T_{max} = 0.951
12904 measured reflections
3438 independent reflections
2889 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.112
S = 1.02
3438 reflections
331 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···O4^{i}	0.82	1.82	2.6340 (19)	169
O3—H3A···O1	0.82	1.88	2.6951 (18)	176

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2369).

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supporting information

Acta Cryst. (2009). E**65**, o1217 [doi:10.1107/S1600536809016468]

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S1. Comment

The title molecule crystallizes in a catemer motif, a relatively rare form compared to the typical dimeric motif exhibited by benzoic acids resulting from intermolecular hydrogen bonding between the carboxylic acid groups (Moorthy *et al.*, 2002). The sterically bulky *o*-CF_3 groups result in the carboxylic acid fragments being twisted with respect to the aryl ring. This results in dihedral angles between the aryl ring and carboxylic acid fragments of C7—C2—C1—O1 = 71.5 (2)° and C12—C11—C10—O4 = 99.3 (2)°.

S2. Experimental

The title compound was prepared following the literature methods (Dmowski & Piasecka-Macieiewska, 1998) with a slight modification. The compound crystallized from the oily reaction mixture that remained after acidification of the potassium benzoate salt with concentrated HCl, extraction of the organic components with toluene, drying of the organic fraction with magnesium sulfate and concentration by rotary evaporation.

S3. Refinement

H atoms were placed in geometrically idealized positions with C—H = 0.93 Å and O—H = 0.82 Å and constrained to ride on the parent atom with U_{iso}(H) = 1.2 U_{eq}(C) or 1.5 U_{eq}(O). The trifluoromethyl groups belonging to C17 and C18 were modeled with a two-site disorder of the F atoms with refined site occupancy factors of 0.569 (5):0.431 (5) and 0.689 (5):0.311 (5), respectively.

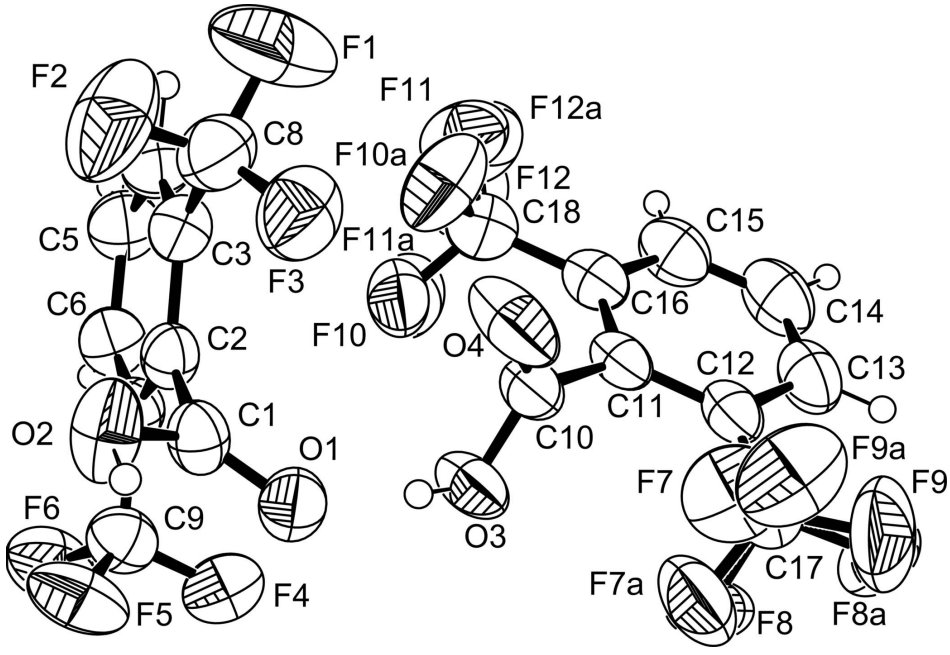

Figure 1

The two molecules in the asymmetric unit with displacement ellipsoids shown at 50% probability for non-H atoms. For the disordered CF_3 groups, both disorder components are shown.

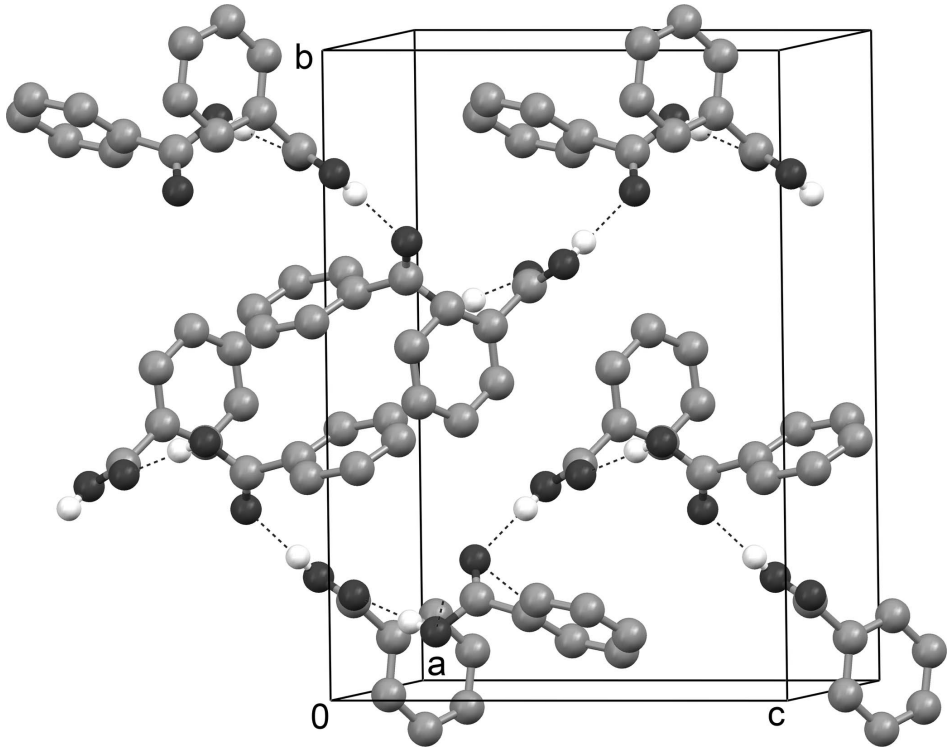

Figure 2

Ball and stick representation featuring the catemeric structure formed through O—H···O hydrogen bonding. H atoms not involved in H-bonding and the CF_3 groups have been omitted for clarity.

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$C_9H_4F_6O_2$
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Hall symbol: -P 2ybc
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$b = 15.755$ (3) Å
$c = 11.561$ (2) Å
$\beta = 94.961$ (2)°
$V = 1973.0$ (6) Å^3
$Z = 8$
$F(000) = 1024$
$D_x = 1.738$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6970 reflections
$\theta = 2.3$–$28.0°$
$\mu = 0.20$ mm^{-1}
$T = 296$ K
Block, colorless
0.39 × 0.31 × 0.26 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, 2008)
$T_{min} = 0.834$, $T_{max} = 0.951$
12904 measured reflections
3438 independent reflections
2889 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.2°$
$h = -12 \rightarrow 12$
$k = -18 \rightarrow 18$
$l = -13 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.112$
$S = 1.02$
3438 reflections
331 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
$w = 1/[\sigma^2(F_o^2) + (0.058P)^2 + 0.5224P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ 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)
C1	0.25273 (16)	0.14562 (11)	0.00186 (14)	0.0532 (4)	
C2	0.34011 (15)	0.08652 (10)	0.07069 (14)	0.0490 (4)	
C3	0.43893 (16)	0.11687 (12)	0.14433 (16)	0.0564 (4)	
C4	0.51596 (17)	0.06028 (14)	0.20807 (17)	0.0666 (5)	

H4A	0.5807	0.0808	0.2581	0.080*	
C5	0.49740 (19)	−0.02557 (14)	0.19783 (18)	0.0689 (5)	
H5A	0.5498	−0.0629	0.2405	0.083*	
C6	0.40178 (18)	−0.05640 (12)	0.12489 (16)	0.0614 (5)	
H6A	0.3900	−0.1147	0.1175	0.074*	
C7	0.32257 (15)	−0.00131 (10)	0.06209 (14)	0.0508 (4)	
C8	0.46743 (19)	0.20978 (14)	0.1562 (2)	0.0756 (6)	
F1	0.5244 (2)	0.22865 (11)	0.25885 (18)	0.1361 (7)	
F2	0.53907 (15)	0.23619 (9)	0.07602 (19)	0.1232 (7)	
F3	0.36850 (12)	0.25931 (8)	0.14440 (14)	0.0893 (4)	
C9	0.21830 (18)	−0.03876 (12)	−0.01534 (17)	0.0632 (5)	
F4	0.11518 (12)	−0.04286 (10)	0.03733 (13)	0.0975 (4)	
F5	0.19338 (14)	0.00483 (8)	−0.11254 (11)	0.0911 (4)	
F6	0.24344 (13)	−0.11707 (8)	−0.04877 (12)	0.0906 (4)	
C10	0.10257 (17)	0.15284 (11)	0.30263 (15)	0.0545 (4)	
C11	0.07034 (16)	0.13002 (10)	0.42282 (14)	0.0514 (4)	
C12	−0.04150 (17)	0.15569 (11)	0.46310 (15)	0.0561 (4)	
C13	−0.0643 (2)	0.14110 (13)	0.57757 (18)	0.0711 (5)	
H13A	−0.1380	0.1593	0.6045	0.085*	
C14	0.0220 (2)	0.09977 (15)	0.65140 (18)	0.0801 (6)	
H14A	0.0066	0.0906	0.7283	0.096*	
C15	0.1301 (2)	0.07212 (14)	0.61252 (17)	0.0730 (6)	
H15A	0.1869	0.0430	0.6626	0.088*	
C16	0.15558 (18)	0.08709 (12)	0.49899 (16)	0.0603 (5)	
O1	0.14736 (11)	0.15753 (8)	0.02411 (10)	0.0606 (3)	
O2	0.30404 (14)	0.18036 (9)	−0.08444 (12)	0.0751 (4)	
H2A	0.2549	0.2129	−0.1192	0.113*	
O3	0.05615 (13)	0.10397 (9)	0.22093 (11)	0.0684 (4)	
H3A	0.0818	0.1182	0.1592	0.103*	
O4	0.16936 (19)	0.21110 (11)	0.28586 (13)	0.0999 (6)	
C17	−0.13950 (10)	0.19782 (8)	0.38373 (10)	0.0726 (5)	
F7A	−0.09321 (12)	0.25255 (8)	0.31618 (10)	0.1010 (13)	0.569 (5)
F8A	−0.19164 (10)	0.13805 (10)	0.31178 (10)	0.0901 (11)	0.569 (5)
F9A	−0.22489 (10)	0.23045 (8)	0.43893 (12)	0.139 (2)	0.569 (5)
F7B	−0.17175 (10)	0.16347 (9)	0.28614 (11)	0.144 (3)	0.431 (5)
F9B	−0.10986 (11)	0.28028 (10)	0.35381 (9)	0.1164 (19)	0.431 (5)
F8B	−0.24254 (11)	0.21614 (8)	0.43317 (12)	0.0970 (19)	0.431 (5)
C18	0.27540 (10)	0.05569 (8)	0.46034 (11)	0.0751 (6)	
F10A	0.26369 (10)	0.01894 (8)	0.35789 (13)	0.0877 (11)	0.689 (5)
F11A	0.36230 (10)	0.11205 (10)	0.46284 (11)	0.1163 (14)	0.689 (5)
F12A	0.32020 (9)	−0.01015 (9)	0.52898 (13)	0.1142 (11)	0.689 (5)
F10B	0.33236 (9)	0.12165 (10)	0.40107 (11)	0.108 (2)	0.311 (5)
F12B	0.35672 (10)	0.03614 (8)	0.54011 (13)	0.125 (3)	0.311 (5)
F11B	0.26173 (10)	0.00490 (9)	0.37781 (12)	0.154 (5)	0.311 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0618 (10)	0.0542 (9)	0.0442 (9)	0.0104 (7)	0.0085 (7)	0.0040 (7)
C2	0.0497 (8)	0.0552 (9)	0.0428 (8)	0.0073 (7)	0.0077 (7)	0.0041 (7)
C3	0.0508 (9)	0.0623 (10)	0.0566 (10)	0.0011 (8)	0.0089 (8)	−0.0018 (8)
C4	0.0507 (10)	0.0864 (14)	0.0607 (11)	0.0064 (9)	−0.0062 (8)	−0.0020 (10)
C5	0.0631 (11)	0.0776 (13)	0.0641 (12)	0.0199 (10)	−0.0061 (9)	0.0105 (10)
C6	0.0689 (11)	0.0567 (10)	0.0582 (11)	0.0113 (8)	0.0025 (9)	0.0077 (8)
C7	0.0535 (9)	0.0551 (9)	0.0436 (9)	0.0056 (7)	0.0044 (7)	0.0031 (7)
C8	0.0608 (11)	0.0702 (12)	0.0965 (16)	−0.0044 (10)	0.0112 (11)	−0.0113 (11)
F1	0.1536 (16)	0.0987 (11)	0.1447 (15)	−0.0163 (10)	−0.0518 (13)	−0.0361 (10)
F2	0.1085 (11)	0.0773 (9)	0.1956 (19)	−0.0172 (8)	0.0813 (12)	−0.0035 (10)
F3	0.0828 (8)	0.0627 (7)	0.1245 (12)	0.0037 (6)	0.0221 (8)	−0.0124 (7)
C9	0.0672 (11)	0.0597 (11)	0.0615 (11)	0.0030 (9)	−0.0013 (9)	0.0003 (9)
F4	0.0628 (7)	0.1270 (12)	0.1024 (10)	−0.0164 (7)	0.0050 (7)	−0.0162 (9)
F5	0.1201 (11)	0.0832 (8)	0.0628 (7)	−0.0013 (7)	−0.0338 (7)	0.0035 (6)
F6	0.1079 (10)	0.0632 (7)	0.0972 (10)	0.0013 (6)	−0.0118 (8)	−0.0186 (6)
C10	0.0609 (10)	0.0574 (10)	0.0454 (9)	−0.0107 (8)	0.0059 (7)	−0.0075 (7)
C11	0.0640 (10)	0.0495 (9)	0.0408 (8)	−0.0136 (7)	0.0046 (7)	−0.0079 (7)
C12	0.0679 (11)	0.0526 (9)	0.0486 (9)	−0.0112 (8)	0.0089 (8)	−0.0117 (7)
C13	0.0839 (13)	0.0731 (12)	0.0591 (12)	−0.0128 (10)	0.0231 (10)	−0.0126 (10)
C14	0.1122 (18)	0.0860 (15)	0.0440 (10)	−0.0135 (13)	0.0171 (11)	0.0010 (10)
C15	0.0927 (15)	0.0781 (13)	0.0473 (10)	−0.0043 (11)	0.0009 (10)	0.0031 (9)
C16	0.0698 (11)	0.0606 (10)	0.0499 (10)	−0.0094 (9)	0.0017 (8)	−0.0042 (8)
O1	0.0575 (7)	0.0753 (8)	0.0490 (7)	0.0156 (6)	0.0041 (5)	0.0077 (6)
O2	0.0858 (9)	0.0756 (9)	0.0677 (8)	0.0301 (7)	0.0294 (7)	0.0303 (7)
O3	0.0850 (9)	0.0783 (9)	0.0420 (6)	−0.0259 (7)	0.0064 (6)	−0.0103 (6)
O4	0.1505 (15)	0.0963 (11)	0.0575 (9)	−0.0706 (11)	0.0357 (9)	−0.0223 (8)
C17	0.0723 (13)	0.0783 (14)	0.0675 (13)	0.0023 (11)	0.0087 (10)	−0.0092 (11)
F7A	0.115 (2)	0.088 (2)	0.099 (2)	0.0095 (16)	0.0008 (17)	0.0347 (18)
F8A	0.0718 (17)	0.0977 (19)	0.095 (2)	−0.0026 (14)	−0.0251 (14)	−0.0169 (16)
F9A	0.153 (4)	0.144 (3)	0.121 (4)	0.087 (3)	0.022 (3)	−0.030 (3)
F7B	0.156 (5)	0.187 (5)	0.079 (3)	0.090 (4)	−0.040 (3)	−0.064 (3)
F9B	0.100 (3)	0.097 (3)	0.151 (4)	0.009 (2)	0.005 (3)	0.039 (3)
F8B	0.055 (2)	0.146 (4)	0.092 (4)	0.006 (3)	0.018 (2)	0.007 (3)
C18	0.0736 (13)	0.0807 (15)	0.0699 (14)	−0.0014 (11)	0.0001 (11)	−0.0030 (11)
F10A	0.082 (2)	0.116 (2)	0.0655 (15)	0.0210 (16)	0.0119 (13)	−0.0152 (16)
F11A	0.0730 (14)	0.115 (2)	0.161 (3)	−0.0229 (14)	0.0114 (17)	−0.033 (2)
F12A	0.1041 (18)	0.130 (2)	0.107 (2)	0.0381 (17)	−0.0002 (15)	0.0232 (16)
F10B	0.076 (3)	0.109 (4)	0.146 (6)	0.006 (3)	0.039 (3)	0.029 (4)
F12B	0.084 (3)	0.204 (9)	0.081 (4)	0.039 (5)	−0.020 (3)	0.023 (4)
F11B	0.099 (7)	0.145 (7)	0.222 (11)	−0.022 (5)	0.038 (6)	−0.109 (7)

Geometric parameters (Å, º)

C1—O1	1.210 (2)	C11—C12	1.399 (3)
C1—O2	1.305 (2)	C12—C13	1.387 (3)

C1—C2	1.507 (2)	C12—C17	1.500 (2)
C2—C3	1.396 (2)	C13—C14	1.376 (3)
C2—C7	1.399 (2)	C13—H13A	0.930
C3—C4	1.390 (3)	C14—C15	1.365 (3)
C3—C8	1.500 (3)	C14—H14A	0.930
C4—C5	1.371 (3)	C15—C16	1.385 (3)
C4—H4A	0.930	C15—H15A	0.930
C5—C6	1.370 (3)	C16—C18	1.498 (2)
C5—H5A	0.930	O2—H2A	0.820
C6—C7	1.383 (2)	O3—H3A	0.820
C6—H6A	0.930	C17—F7B	1.2729 (11)
C7—C9	1.503 (3)	C17—F9A	1.2791 (11)
C8—F1	1.324 (3)	C17—F7A	1.2941 (11)
C8—F3	1.326 (3)	C17—F8B	1.3326 (12)
C8—F2	1.328 (3)	C17—F8A	1.3485 (12)
C9—F4	1.323 (2)	C17—F9B	1.3895 (12)
C9—F5	1.325 (2)	C18—F11B	1.2443 (10)
C9—F6	1.328 (2)	C18—F12B	1.2593 (11)
C10—O4	1.197 (2)	C18—F11A	1.2952 (11)
C10—O3	1.287 (2)	C18—F10A	1.3146 (11)
C10—C11	1.506 (2)	C18—F12A	1.3697 (11)
C11—C16	1.397 (3)	C18—F10B	1.4165 (12)

O1—C1—O2	124.93 (16)	C13—C12—C17	118.76 (16)
O1—C1—C2	123.28 (15)	C11—C12—C17	121.09 (14)
O2—C1—C2	111.78 (14)	C14—C13—C12	120.1 (2)
C3—C2—C7	118.36 (15)	C14—C13—H13A	119.9
C3—C2—C1	121.80 (15)	C12—C13—H13A	119.9
C7—C2—C1	119.84 (15)	C15—C14—C13	120.45 (19)
C4—C3—C2	120.00 (17)	C15—C14—H14A	119.8
C4—C3—C8	117.85 (18)	C13—C14—H14A	119.8
C2—C3—C8	122.14 (17)	C14—C15—C16	120.4 (2)
C5—C4—C3	120.63 (18)	C14—C15—H15A	119.8
C5—C4—H4A	119.7	C16—C15—H15A	119.8
C3—C4—H4A	119.7	C15—C16—C11	120.24 (19)
C6—C5—C4	120.08 (17)	C15—C16—C18	118.50 (17)
C6—C5—H5A	120.0	C11—C16—C18	121.25 (15)
C4—C5—H5A	120.0	C1—O2—H2A	109.5
C5—C6—C7	120.36 (18)	C10—O3—H3A	109.5
C5—C6—H6A	119.8	F9A—C17—F7A	111.7
C7—C6—H6A	119.8	F7B—C17—F8B	107.2
C6—C7—C2	120.55 (16)	F9A—C17—F8A	107.7
C6—C7—C9	118.00 (16)	F7A—C17—F8A	104.9
C2—C7—C9	121.45 (15)	F7B—C17—F9B	103.2
F1—C8—F3	105.80 (19)	F8B—C17—F9B	97.2
F1—C8—F2	107.3 (2)	F7B—C17—C12	118.73 (8)
F3—C8—F2	105.3 (2)	F9A—C17—C12	112.38 (8)
F1—C8—C3	112.2 (2)	F7A—C17—C12	111.79 (8)

F3—C8—C3	113.92 (17)	F8B—C17—C12	114.37 (8)
F2—C8—C3	111.77 (18)	F8A—C17—C12	107.87 (8)
F4—C9—F5	107.23 (17)	F9B—C17—C12	113.47 (8)
F4—C9—F6	107.01 (17)	F11B—C18—F12B	115.7
F5—C9—F6	105.48 (16)	F11A—C18—F10A	109.6
F4—C9—C7	111.76 (16)	F11A—C18—F12A	106.5
F5—C9—C7	112.95 (16)	F10A—C18—F12A	101.0
F6—C9—C7	111.98 (16)	F11B—C18—F10B	97.4
O4—C10—O3	123.01 (17)	F12B—C18—F10B	103.0
O4—C10—C11	121.71 (15)	F11B—C18—C16	113.07 (8)
O3—C10—C11	115.25 (15)	F12B—C18—C16	115.85 (8)
C16—C11—C12	118.60 (16)	F11A—C18—C16	114.75 (8)
C16—C11—C10	120.19 (16)	F10A—C18—C16	113.29 (8)
C12—C11—C10	121.10 (16)	F12A—C18—C16	110.63 (9)
C13—C12—C11	120.14 (18)	F10B—C18—C16	109.27 (9)
C7—C2—C1—O1	71.5 (2)	C12—C11—C10—O4	99.3 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*A*···O4^{i}	0.82	1.82	2.6340 (19)	169
O3—H3*A*···O1	0.82	1.88	2.6951 (18)	176

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