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(*E*)-3-[4-(Benzo[*d*]oxazol-2-yl)styryl]-1-methylpyridin-1-ium trifluoroacetate

Ying Xia,[a,b] Haiyan Wang,[a,b]* Jianhua Yu[a,b] and Zhichao Wu[a,b]

[a]Department of Chemistry, Anhui University, Hefei 230601, People's Republic of China, and [b]Key Laboratory of Functional Inorganic Materials Chemistry, Hefei 230601, People's Republic of China. *Correspondence e-mail: 24886084@qq.com

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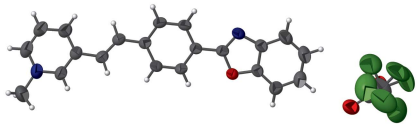
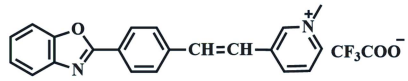
Structural data: full structural data are available from iucrdata.iucr.org

In the title molecular salt, $C_{21}H_{17}N_2O^+\cdot CF_3CO_2^-$, the dihedral angles between the benzene ring and pendant pyridyl and benzoxazole substituents of the cation are 15.35 (10) and 2.55 (9)°, respectively. In the crystal, the components are linked by weak C—H···O hydrogen bonds, C—F···π interactions and aromatic π–π stacking interactions. The F atoms of the anion are disordered over two set of sites in a 0.536 (6):0.464 (6) ratio.

3D view



Chemical scheme



Structure description

In the title molecular salt (Fig. 1), the dihedral angles between the benzene ring and pendant pyridyl and benzoxazole substituents of the cation are 15.35 (10) and 2.55 (9)°, respectively. The near co-planarity of the ring systems was also found in a similar structure (Centore *et al.*, 2013).

In the crystal (Figs. 2 and 3), the components are linked by weak C—H···O hydrogen bonds, C—F···π interactions (Table 1) and aromatic π–π stacking interactions [shortest centroid-centroid separation = 3.7709 (11) Å].

Synthesis and crystallization

Silver trifluoroacetate (0.15 g, 0.68 mmol) was added to a solution of 3-(4-(benzo[*d*]ox-]oxazol-2-yl)styryl)-1-methylpyridin-1-ium iodide (0.3 g, 0.68 mmol) in acetonitrile. The reaction mixture was refluxed for 4 h, then filtered and evaporated, and concentrated *in vacuo* to give an off-yellow solid. Yellow single crystals were obtained in 15% yield by recrystallization from acetonitrile solution.

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

*Cg*2 is the centroid of the C1–C5/N2 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···O2^{i}	0.93	2.49	3.375 (3)	158
C3—H3···O2^{ii}	0.93	2.40	3.213 (3)	146
C11—H11*A*···O1^{i}	0.96	2.34	3.245 (5)	157
C22—F2···*Cg*2^{iii}	1.35 (1)	3.24 (1)	4.072 (4)	120 (1)

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+1, -y, -z+1$; (iii) $-x+1, -y+1, -z+1$.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The F atoms of the anion are disordered over two set of sites in a 0.536 (6):0.464 (6) ratio.

Funding information

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References

Bruker (2000). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{21}H_{17}N_2O^+\cdot C_2F_3O_2^-$
M_r	426.39
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	19.817 (2), 8.4268 (9), 12.4459 (14)
β (°)	101.220 (1)
V (Å^3)	2038.6 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.11
Crystal size (mm)	0.2 × 0.2 × 0.2
Data collection	
Diffractometer	Bruker SMART CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2000)
T_{min}, T_{max}	0.950, 0.966
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14029, 3593, 2798
R_{int}	0.037
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.050, 0.161, 1.12
No. of reflections	3593
No. of parameters	311
No. of restraints	92
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.37, −0.23

Computer programs: *SMART* and *SAINT* (Bruker, 2000), *SHELXTL* (Sheldrick, 2008) and *SHELXL2014* (Sheldrick, 2015).

Centore, R., Piccialli, V. & Tuzi, A. (2013). *Acta Cryst.* E**69**, o667–o668.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.

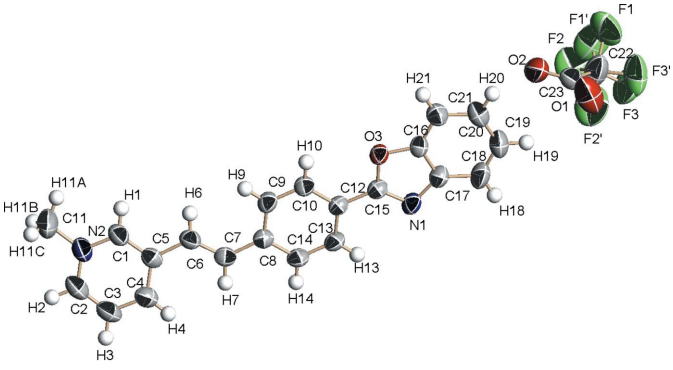

Figure 1
The molecular structure, with displacement ellipsoids drawn at the 50% probability level.

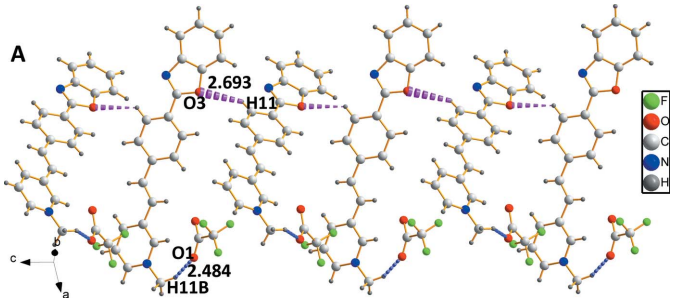

Figure 2
Hydrogen-bonded chain in the crystal.

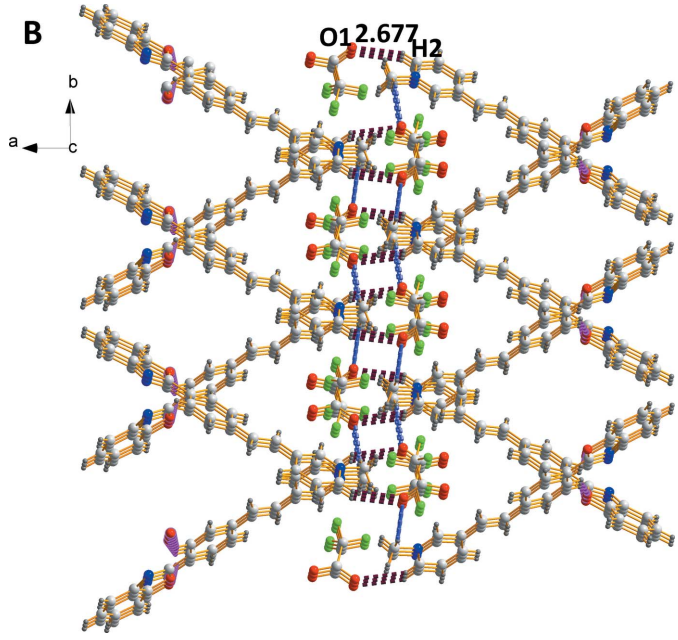

Figure 3
The unit-cell packing.

full crystallographic data

IUCrData (2017). **2**, x171733 [https://doi.org/10.1107/S2414314617017333]

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Crystal data

$C_{21}H_{17}N_2O^+\cdot C_2F_3O_2^-$
M_r = 426.39
Monoclinic, $P2_1/c$
a = 19.817 (2) Å
b = 8.4268 (9) Å
c = 12.4459 (14) Å
β = 101.220 (1)°
V = 2038.6 (4) Å^3
Z = 4
$F(000)$ = 880
D_x = 1.389 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4829 reflections
θ = 2.6–26.7°
μ = 0.11 mm^{-1}
T = 296 K
Block, yellow
0.2 × 0.2 × 0.2 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: sealed tube
phi and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2000)
T_{min} = 0.950, T_{max} = 0.966
14029 measured reflections
3593 independent reflections
2798 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 25.0°, θ_{min} = 1.1°
h = −22→23
k = −10→9
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.161
S = 1.12
3593 reflections
311 parameters
92 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
$w = 1/[\sigma^2(F_o^2) + (0.0891P)^2 + 0.3359P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Extinction correction: SHELXL2014 (Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.011 (2)

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. All hydrogen atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 Å and and U_{iso}(H) = 1.5U_{eq}(C) for the methyl H atoms and 1.2U_{eq}(C) for the others.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O3	0.43709 (6)	0.38309 (16)	0.38049 (9)	0.0493 (4)	
C12	0.49287 (9)	0.2408 (2)	0.54155 (13)	0.0443 (4)	
C15	0.43415 (9)	0.3313 (2)	0.48389 (14)	0.0462 (4)	
N1	0.37833 (8)	0.3688 (2)	0.51762 (13)	0.0555 (4)	
C7	0.66050 (10)	−0.0328 (2)	0.71466 (15)	0.0508 (5)	
H7	0.6525	−0.0861	0.7764	0.061*	
C8	0.60374 (9)	0.0606 (2)	0.65363 (14)	0.0459 (4)	
C5	0.77889 (10)	−0.1425 (2)	0.75259 (15)	0.0507 (5)	
C10	0.54997 (10)	0.2117 (2)	0.49481 (14)	0.0514 (5)	
H10	0.5513	0.2518	0.4256	0.062*	
C14	0.54614 (10)	0.0900 (2)	0.69936 (15)	0.0515 (5)	
H14	0.5443	0.0482	0.7679	0.062*	
C13	0.49192 (10)	0.1796 (2)	0.64546 (14)	0.0507 (5)	
H13	0.4545	0.1994	0.6784	0.061*	
C6	0.72239 (10)	−0.0490 (2)	0.69052 (16)	0.0538 (5)	
H6	0.7306	0.0037	0.6287	0.065*	
C16	0.37561 (9)	0.4620 (2)	0.34662 (15)	0.0476 (5)	
C9	0.60454 (10)	0.1243 (2)	0.54981 (14)	0.0524 (5)	
H9	0.6425	0.1073	0.5177	0.063*	
N2	0.89569 (9)	−0.2225 (2)	0.77180 (15)	0.0688 (5)	
C1	0.84123 (11)	−0.1384 (3)	0.71989 (17)	0.0597 (5)	
H1	0.8459	−0.0759	0.6602	0.072*	
C3	0.83135 (13)	−0.3201 (3)	0.89581 (19)	0.0718 (6)	
H3	0.8282	−0.3819	0.9565	0.086*	
C2	0.89154 (13)	−0.3125 (3)	0.8594 (2)	0.0714 (6)	
H2	0.9297	−0.3693	0.8949	0.086*	
C20	0.28822 (12)	0.6107 (3)	0.23782 (19)	0.0676 (6)	
H20	0.2697	0.6628	0.1729	0.081*	
C17	0.33959 (10)	0.4538 (2)	0.43082 (16)	0.0527 (5)	
C21	0.35254 (11)	0.5396 (3)	0.24913 (17)	0.0602 (5)	
H21	0.3783	0.5442	0.1943	0.072*	
C4	0.77489 (12)	−0.2364 (3)	0.84290 (17)	0.0623 (6)	
H4	0.7337	−0.2428	0.8679	0.075*	
C18	0.27540 (12)	0.5279 (3)	0.4186 (2)	0.0721 (7)	
H18	0.2500	0.5251	0.4740	0.087*	
C19	0.25131 (12)	0.6053 (3)	0.3212 (2)	0.0723 (7)	
H19	0.2088	0.6556	0.3113	0.087*	
C11	0.96006 (15)	−0.2176 (5)	0.7288 (3)	0.1203 (13)	
H11A	0.9543	−0.1482	0.6666	0.180*	
H11B	0.9968	−0.1792	0.7847	0.180*	
H11C	0.9710	−0.3225	0.7073	0.180*	
O2	0.17618 (10)	0.6468 (2)	−0.02605 (16)	0.0915 (6)	

C23	0.11504 (13)	0.6724 (3)	−0.03020 (19)	0.0677 (6)	
O1	0.06594 (13)	0.5908 (3)	−0.0700 (2)	0.1265 (9)	
C22	0.09873 (16)	0.8216 (4)	0.0293 (3)	0.1014 (10)	
F2	0.1534 (4)	0.8663 (7)	0.1057 (5)	0.150 (3)	0.536 (6)
F3	0.0446 (5)	0.8467 (13)	0.0561 (8)	0.167 (3)	0.536 (6)
F1	0.1012 (3)	0.9471 (6)	−0.0515 (7)	0.150 (2)	0.536 (6)
F2′	0.1024 (4)	0.7737 (10)	0.1428 (4)	0.158 (3)	0.464 (6)
F1′	0.1287 (4)	0.9425 (9)	0.0258 (9)	0.155 (3)	0.464 (6)
F3′	0.0297 (4)	0.8498 (11)	0.0030 (8)	0.138 (3)	0.464 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.0469 (7)	0.0595 (8)	0.0440 (7)	0.0070 (6)	0.0151 (5)	0.0010 (6)
C12	0.0451 (10)	0.0481 (10)	0.0409 (9)	−0.0034 (8)	0.0114 (8)	−0.0060 (7)
C15	0.0493 (10)	0.0511 (11)	0.0400 (9)	−0.0028 (8)	0.0133 (8)	−0.0052 (8)
N1	0.0509 (9)	0.0703 (11)	0.0496 (9)	0.0083 (8)	0.0209 (7)	−0.0003 (8)
C7	0.0584 (12)	0.0512 (11)	0.0430 (10)	−0.0026 (9)	0.0103 (8)	0.0013 (8)
C8	0.0499 (10)	0.0465 (10)	0.0406 (9)	−0.0037 (8)	0.0076 (8)	−0.0028 (7)
C5	0.0575 (12)	0.0431 (10)	0.0487 (10)	0.0002 (8)	0.0038 (8)	−0.0003 (8)
C10	0.0540 (11)	0.0640 (12)	0.0387 (9)	0.0074 (9)	0.0156 (8)	0.0036 (8)
C14	0.0577 (12)	0.0586 (12)	0.0405 (9)	−0.0042 (9)	0.0151 (8)	0.0030 (8)
C13	0.0501 (11)	0.0607 (12)	0.0450 (9)	−0.0028 (9)	0.0183 (8)	−0.0004 (8)
C6	0.0602 (12)	0.0529 (11)	0.0486 (10)	0.0035 (9)	0.0113 (9)	0.0076 (9)
C16	0.0435 (10)	0.0494 (11)	0.0502 (10)	0.0036 (8)	0.0102 (8)	−0.0068 (8)
C9	0.0497 (11)	0.0667 (13)	0.0440 (10)	0.0066 (9)	0.0166 (8)	−0.0004 (9)
N2	0.0612 (11)	0.0721 (12)	0.0708 (11)	0.0161 (9)	0.0076 (9)	0.0102 (10)
C1	0.0627 (13)	0.0602 (13)	0.0548 (11)	0.0120 (10)	0.0080 (10)	0.0086 (9)
C3	0.0831 (17)	0.0618 (14)	0.0659 (13)	0.0016 (12)	0.0027 (12)	0.0180 (11)
C2	0.0772 (16)	0.0582 (13)	0.0710 (14)	0.0106 (12)	−0.0048 (12)	0.0103 (11)
C20	0.0672 (14)	0.0611 (13)	0.0688 (13)	0.0112 (11)	−0.0008 (11)	−0.0003 (11)
C17	0.0482 (11)	0.0575 (12)	0.0544 (11)	0.0037 (9)	0.0149 (9)	−0.0066 (9)
C21	0.0640 (13)	0.0633 (13)	0.0537 (11)	0.0078 (10)	0.0121 (10)	0.0012 (10)
C4	0.0668 (13)	0.0558 (12)	0.0622 (12)	−0.0027 (10)	0.0074 (10)	0.0080 (10)
C18	0.0557 (13)	0.0858 (17)	0.0798 (15)	0.0149 (12)	0.0252 (11)	−0.0055 (13)
C19	0.0540 (13)	0.0723 (15)	0.0882 (17)	0.0171 (11)	0.0081 (12)	−0.0074 (13)
C11	0.0751 (18)	0.162 (3)	0.131 (3)	0.048 (2)	0.0386 (18)	0.052 (2)
O2	0.0895 (13)	0.0849 (13)	0.1105 (14)	0.0171 (10)	0.0453 (11)	0.0163 (10)
C23	0.0698 (15)	0.0606 (14)	0.0690 (14)	−0.0011 (12)	0.0044 (12)	0.0095 (11)
O1	0.1061 (17)	0.0880 (15)	0.162 (2)	0.0031 (13)	−0.0307 (15)	−0.0219 (15)
C22	0.0757 (18)	0.080 (2)	0.155 (3)	0.0000 (16)	0.039 (2)	−0.0221 (17)
F2	0.181 (5)	0.116 (4)	0.131 (4)	0.011 (3)	−0.021 (4)	−0.066 (3)
F3	0.142 (5)	0.183 (5)	0.206 (7)	0.036 (4)	0.111 (5)	−0.010 (5)
F1	0.159 (5)	0.066 (2)	0.225 (6)	0.027 (3)	0.034 (4)	0.017 (3)
F2′	0.158 (5)	0.226 (6)	0.098 (3)	0.031 (5)	0.044 (3)	−0.031 (4)
F1′	0.152 (6)	0.102 (4)	0.226 (7)	−0.045 (4)	0.068 (5)	−0.065 (5)
F3′	0.096 (3)	0.119 (4)	0.197 (7)	0.036 (3)	0.024 (4)	−0.049 (5)

Geometric parameters (Å, º)

O3—C15	1.371 (2)	N2—C2	1.344 (3)
O3—C16	1.380 (2)	N2—C1	1.346 (3)
C12—C10	1.391 (3)	N2—C11	1.477 (3)
C12—C13	1.396 (2)	C3—C2	1.357 (4)
C12—C15	1.458 (3)	C3—C4	1.377 (3)
C15—N1	1.296 (2)	C20—C19	1.382 (3)
N1—C17	1.395 (3)	C20—C21	1.390 (3)
C7—C6	1.325 (3)	C17—C18	1.398 (3)
C7—C8	1.459 (3)	C18—C19	1.377 (4)
C8—C14	1.393 (3)	O2—C23	1.222 (3)
C8—C9	1.402 (3)	C23—O1	1.215 (3)
C5—C1	1.374 (3)	C23—C22	1.525 (4)
C5—C4	1.390 (3)	C22—F1′	1.184 (6)
C5—C6	1.461 (3)	C22—F3	1.203 (7)
C10—C9	1.375 (3)	C22—F2	1.348 (6)
C14—C13	1.376 (3)	C22—F3′	1.365 (8)
C16—C21	1.376 (3)	C22—F2′	1.456 (6)
C16—C17	1.380 (3)	C22—F1	1.467 (7)
C15—O3—C16	104.12 (13)	N2—C1—C5	121.8 (2)
C10—C12—C13	118.74 (17)	C2—C3—C4	120.1 (2)
C10—C12—C15	121.51 (16)	N2—C2—C3	119.6 (2)
C13—C12—C15	119.74 (16)	C19—C20—C21	121.2 (2)
N1—C15—O3	114.91 (16)	C16—C17—C18	119.3 (2)
N1—C15—C12	128.15 (16)	C16—C17—N1	109.01 (16)
O3—C15—C12	116.93 (14)	C18—C17—N1	131.69 (19)
C15—N1—C17	104.48 (15)	C16—C21—C20	115.8 (2)
C6—C7—C8	126.23 (18)	C3—C4—C5	120.6 (2)
C14—C8—C9	117.73 (17)	C19—C18—C17	117.3 (2)
C14—C8—C7	119.54 (17)	C20—C19—C18	122.2 (2)
C9—C8—C7	122.72 (17)	O1—C23—O2	128.7 (3)
C1—C5—C4	116.73 (19)	O1—C23—C22	115.8 (3)
C1—C5—C6	118.07 (17)	O2—C23—C22	115.3 (2)
C4—C5—C6	125.20 (19)	F3—C22—F2	113.1 (6)
C9—C10—C12	120.73 (17)	F1′—C22—F3′	109.1 (7)
C13—C14—C8	121.50 (17)	F1′—C22—F2′	110.1 (6)
C14—C13—C12	120.30 (17)	F3′—C22—F2′	98.1 (5)
C7—C6—C5	125.69 (18)	F3—C22—F1	102.3 (6)
C21—C16—C17	124.16 (19)	F2—C22—F1	98.7 (5)
C21—C16—O3	128.35 (17)	F1′—C22—C23	122.4 (4)
C17—C16—O3	107.47 (16)	F3—C22—C23	124.4 (6)
C10—C9—C8	120.99 (17)	F2—C22—C23	110.9 (3)
C2—N2—C1	121.1 (2)	F3′—C22—C23	108.9 (4)
C2—N2—C11	120.2 (2)	F2′—C22—C23	105.5 (4)
C1—N2—C11	118.7 (2)	F1—C22—C23	102.9 (4)

Hydrogen-bond geometry (Å, º)

Cg2 is the centroid of the C1–C5/N2 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···O2^{i}	0.93	2.49	3.375 (3)	158
C3—H3···O2^{ii}	0.93	2.40	3.213 (3)	146
C11—H11*A*···O1^{i}	0.96	2.34	3.245 (5)	157
C22—F2···*Cg*2^{iii}	1.35 (1)	3.24 (1)	4.072 (4)	120 (1)

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+1/2; (ii) −*x*+1, −*y*, −*z*+1; (iii) −*x*+1, −*y*+1, −*z*+1.