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N-[1-(Silatran-1-yl)propyl]pentafluorobenzamide

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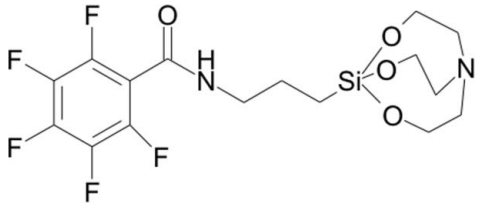
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.004 Å; R factor = 0.039; wR factor = 0.092; data-to-parameter ratio = 12.2.

In the title compound {systematic name: *N*-[3-(5-aza-2,8,9-trioxa-1-silabicyclo[3.3.3]undecan-1-yl)propyl]pentafluorobenzamide}, $C_{16}H_{19}F_5N_2O_4Si$, unexpected weak anion$\cdots\pi$-type C$=$O$\cdots$C(aromatic) interactions form a dimer [O$\cdots$C distances of 3.096 (3) and 3.036 (3) Å]. These dimers are further connected by a normal N—H$\cdots$O hydrogen bond [2.955 (2) Å], from the amide H atom to one of the silatrane O atoms. Also, four intermolecular contacts between CH groups and silatrane O and F atoms [3.101(3)–3.406 (3) Å] are observed.

Related literature

For related literature, see: Russo *et al.* (2007); Semenov *et al.* (2002).



Experimental

Crystal data

$C_{16}H_{19}F_5N_2O_4Si$
M_r = 426.42
Monoclinic, $P2_1/n$
a = 15.2027 (4) Å
b = 7.6207 (2) Å
c = 16.2411 (4) Å
β = 110.568 (1)°
V = 1761.67 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 173.0 (1) K
0.3 × 0.2 × 0.1 mm

Data collection

Nonius KappaCCD diffractometer with APEXII detector
Absorption correction: none
5912 measured reflections
3099 independent reflections
2456 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.092
S = 1.05
3099 reflections
253 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N9—H9$\cdots$O20^{i}	0.88	2.08	2.955 (2)	172
C15—H15$B\cdots$O20^{ii}	0.99	2.51	3.406 (3)	150
C16—H16$B\cdots$F6^{iii}	0.99	2.43	3.101 (3)	125
C18—H18$B\cdots$F6^{iii}	0.99	2.53	3.320 (3)	136
C23—H23$B\cdots$F3^{iv}	0.99	2.43	3.229 (3)	137

Symmetry codes: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+2, -y+2, -z+2$; (iii) $-x+2, -y+1, -z+2$; (iv) $x+1, y, z$.

Data collection: *COLLECT* (Nonius, 2004); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor 1997); data reduction: *HKL DENZO* (Otwinowski & Minor 1997) and *SCALEPACK*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2508).

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supplementary materials

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N-[1-(Silatran-1-yl)propyl]pentafluorobenzamide

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Comment

The title compound is a perfluorobenzamide derivative including a silatrane group (Fig. 1). A weak anion-π-type of interaction between the electron pair of the carbonyl oxygen O(8) and the two carbon atoms C(3) and C(4) of the perfluorobenzoic acid moiety creates a dimer. The interaction distances are 3.096 (3) and 3.036 (3) Å for the O(8)···C(3) and O(8)···C(4), respectively. Similar interaction but between the polarized iodine atoms in diiodotetrafluorobenzene and carbonyl oxygen has recently been observed in a study of halogen bonding (Russo *et al.*, 2007). In addition a normal hydrogen bond, N···O = 2.954 (2) Å with angle of 172.45°, exists from the amide hydrogen to one of the silatrane O atoms, O(20). Also two short intermolecular contacts ranging from 3.027 to 3.406 Å between C—H and silatrane O atoms and three to the fluorine atoms, from 3.101 to 3.229 Å are observed.

Experimental

Analytical grade reagents were used. 1-(3'-Amino)propylsilatrane (Semenov *et al.*, 2002) (400 mg, 1.72 mmol) was mixed in 30 ml dry dichloromethane under inert gas atmosphere. Triethylamine (470 µl, 3.44 mmol) was added. The reaction mixture was cooled (ice salt bath). Mixture of 2,3,4,5,6-pentafluorobenzoylchloride (240 µl, 1.72 mmol) and dry dichloromethane was added dropwise to the reaction flask. The reaction mixture was stirred at 0° C for 1 h and at the room temperature for 18 h. After that the mixture was washed with water, dried with $MgSO_4$, filtered and evaporated. Yield 460 mg (63%). Colorless crystals were obtained from chloroform at room temperature *via* slow evaporation. (mp. 454.6–455.2 K). ^{1}H-NMR (500 MHz, $CDCl_3$)δ, p.p.m.: 0.509 (t. 2H), 1.736 (tt. 2H), 2.802 (t·6H), 3.454 (q. 2H), 3.718 (t. 6H), 6.923 (s. 1H). ^{13}C NMR (126 MHz, $CDCl_3$)δ, p.p.m.: −47.417, −38.863, −27.089, 12.856, 23.412, 43.013, 50.989, 57.550, 156.880. MS (ESI-TOF) 449 [*M*+Na].

Refinement

All H atoms were visible in electron density maps, but were placed in idealized positions and allowed to ride on their parent atoms at C—H distances of 0.99 Å (methylene) and 0.88 Å for H—N with U_{iso}(H) of 1.2 times U_{eq}(C) and U_{eq}(N).

Figures

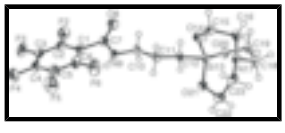


Fig. 1. View of the molecule of (I) showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary size.

N-[3-(5-aza-2,8,9-trioxa-1-silabicyclo[3.3.3]undecan-1-yl)propyl] pentafluorobenzamide

Crystal data

$C_{16}H_{19}F_5N_2O_4Si$
$M_r = 426.42$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 15.2027$ (4) Å
$b = 7.6207$ (2) Å
$c = 16.2411$ (4) Å
$\beta = 110.568$ (1)º
$V = 1761.67$ (8) Å^3
$Z = 4$
$F_{000} = 880$
$D_x = 1.608$ Mg m^{-3}
Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 15147 reflections
$\theta = 2.6$–27.1º
$\mu = 0.21$ mm^{-1}
$T = 173.0$ (1) K
Prism, colourless
0.3 × 0.2 × 0.1 mm

Data collection

Nonius KappaCCD with APEXII detector diffractometer
Radiation source: fine-focus sealed tube
Monochromator: graphite
Detector resolution: 9 pixels mm^{-1}
$T = 173.0(1)$ K
φ and ω scans
Absorption correction: none
5912 measured reflections
3099 independent reflections
2456 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 25$º
$\theta_{min} = 2.7$º
$h = -17\rightarrow18$
$k = -9\rightarrow8$
$l = -19\rightarrow19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.092$
$S = 1.05$
3099 reflections
253 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0296P)^2 + 1.504P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}
Extinction correction: none

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
Si13	0.97532 (4)	0.78594 (8)	0.86902 (4)	0.02310 (16)
F2	0.40578 (10)	0.6889 (2)	0.84279 (11)	0.0522 (4)
F3	0.27692 (10)	0.4350 (3)	0.82441 (11)	0.0594 (5)
F4	0.33118 (12)	0.0976 (2)	0.86283 (11)	0.0614 (5)
F5	0.51698 (13)	0.0127 (2)	0.91677 (13)	0.0692 (5)
F6	0.64535 (10)	0.2641 (2)	0.93287 (12)	0.0594 (5)
O8	0.65323 (12)	0.6813 (3)	0.96762 (11)	0.0464 (5)
O14	0.97348 (10)	0.7809 (2)	0.97124 (9)	0.0269 (4)
O20	1.01580 (10)	0.9657 (2)	0.83334 (10)	0.0269 (4)
O21	0.97836 (10)	0.5987 (2)	0.81759 (10)	0.0312 (4)
N9	0.61017 (12)	0.6639 (3)	0.81880 (12)	0.0278 (4)
H9	0.5708	0.6143	0.7712	0.033*
N17	1.12283 (12)	0.7347 (3)	0.93537 (12)	0.0262 (4)
C1	0.52963 (15)	0.4837 (3)	0.88953 (14)	0.0309 (6)
C2	0.43490 (16)	0.5230 (4)	0.86223 (15)	0.0341 (6)
C3	0.36870 (16)	0.3938 (4)	0.85321 (16)	0.0382 (6)
C4	0.39591 (18)	0.2229 (4)	0.87225 (17)	0.0413 (7)
C5	0.48958 (19)	0.1797 (4)	0.89961 (18)	0.0427 (7)
C6	0.55422 (16)	0.3103 (4)	0.90777 (16)	0.0378 (6)
C7	0.60408 (16)	0.6221 (3)	0.89642 (15)	0.0312 (6)
C10	0.67912 (15)	0.7881 (3)	0.80927 (15)	0.0288 (5)
H10A	0.679	0.8942	0.8444	0.035*
H10B	0.6598	0.824	0.7468	0.035*
C11	0.77909 (14)	0.7152 (3)	0.83832 (15)	0.0295 (5)
H11A	0.8026	0.6978	0.9028	0.035*
H11B	0.7778	0.5991	0.8105	0.035*
C12	0.84674 (14)	0.8355 (3)	0.81418 (14)	0.0257 (5)
H12A	0.8355	0.9576	0.8289	0.031*
H12B	0.8313	0.8298	0.7497	0.031*
C15	1.05262 (14)	0.7340 (3)	1.04586 (14)	0.0282 (5)
H15A	1.0516	0.6064	1.0571	0.034*
H15B	1.0509	0.7976	1.0984	0.034*
C16	1.14112 (15)	0.7814 (3)	1.02816 (14)	0.0307 (5)
H16A	1.1546	0.9083	1.0378	0.037*
H16B	1.1955	0.7146	1.0675	0.037*
C18	1.17155 (16)	0.8512 (3)	0.89244 (16)	0.0329 (6)
H18A	1.1762	0.7947	0.8392	0.04*
H18B	1.2357	0.8788	0.9332	0.04*
C19	1.11278 (15)	1.0158 (3)	0.86826 (16)	0.0305 (5)
H19A	1.1245	1.0904	0.9209	0.037*
H19B	1.1295	1.0835	0.8239	0.037*
C22	1.06325 (17)	0.5059 (3)	0.83005 (16)	0.0354 (6)
H22A	1.0898	0.5422	0.7851	0.042*
H22B	1.0507	0.3782	0.8239	0.042*
C23	1.13256 (16)	0.5461 (3)	0.92118 (16)	0.0330 (6)

H23A	1.1179	0.476	0.9661	0.04*
H23B	1.1974	0.5186	0.9247	0.04*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Si13	0.0218 (3)	0.0238 (3)	0.0226 (3)	−0.0001 (3)	0.0064 (2)	0.0027 (3)
F2	0.0415 (9)	0.0471 (10)	0.0674 (11)	0.0108 (7)	0.0183 (8)	0.0011 (8)
F3	0.0238 (7)	0.0906 (14)	0.0646 (11)	0.0000 (8)	0.0166 (7)	−0.0068 (10)
F4	0.0566 (10)	0.0715 (12)	0.0621 (11)	−0.0332 (9)	0.0283 (9)	−0.0114 (9)
F5	0.0733 (12)	0.0416 (11)	0.0933 (14)	0.0003 (9)	0.0300 (11)	0.0161 (10)
F6	0.0306 (8)	0.0621 (11)	0.0797 (12)	0.0107 (8)	0.0122 (8)	0.0202 (10)
O8	0.0414 (10)	0.0700 (14)	0.0257 (9)	−0.0139 (10)	0.0090 (8)	−0.0094 (9)
O14	0.0209 (7)	0.0371 (9)	0.0214 (8)	0.0006 (7)	0.0059 (6)	0.0031 (7)
O20	0.0217 (8)	0.0279 (9)	0.0292 (8)	−0.0010 (7)	0.0067 (6)	0.0065 (7)
O21	0.0299 (8)	0.0278 (9)	0.0337 (9)	0.0019 (7)	0.0085 (7)	−0.0015 (7)
N9	0.0232 (9)	0.0344 (11)	0.0248 (10)	−0.0036 (8)	0.0073 (8)	−0.0029 (9)
N17	0.0219 (9)	0.0316 (11)	0.0248 (10)	0.0022 (8)	0.0080 (8)	0.0058 (8)
C1	0.0249 (11)	0.0446 (16)	0.0244 (12)	−0.0016 (11)	0.0101 (10)	0.0008 (11)
C2	0.0314 (13)	0.0432 (16)	0.0301 (13)	0.0017 (12)	0.0139 (11)	−0.0016 (11)
C3	0.0219 (12)	0.0628 (19)	0.0329 (13)	−0.0030 (12)	0.0136 (10)	−0.0076 (13)
C4	0.0407 (14)	0.0518 (18)	0.0383 (14)	−0.0169 (13)	0.0227 (12)	−0.0063 (13)
C5	0.0464 (15)	0.0397 (17)	0.0447 (15)	−0.0025 (13)	0.0192 (13)	0.0069 (13)
C6	0.0263 (12)	0.0483 (17)	0.0379 (14)	0.0043 (12)	0.0099 (11)	0.0086 (12)
C7	0.0253 (11)	0.0387 (15)	0.0297 (13)	−0.0004 (11)	0.0097 (10)	−0.0014 (11)
C10	0.0245 (11)	0.0292 (13)	0.0311 (12)	−0.0036 (10)	0.0078 (9)	−0.0005 (10)
C11	0.0230 (11)	0.0283 (13)	0.0330 (13)	−0.0022 (10)	0.0046 (10)	0.0020 (11)
C12	0.0232 (11)	0.0281 (13)	0.0241 (11)	−0.0019 (10)	0.0062 (9)	0.0007 (10)
C15	0.0263 (11)	0.0334 (14)	0.0225 (11)	0.0013 (10)	0.0056 (9)	0.0027 (10)
C16	0.0233 (11)	0.0390 (14)	0.0258 (12)	−0.0007 (10)	0.0038 (9)	0.0037 (11)
C18	0.0235 (11)	0.0415 (15)	0.0349 (13)	0.0012 (11)	0.0117 (10)	0.0103 (12)
C19	0.0232 (11)	0.0335 (14)	0.0337 (12)	−0.0057 (10)	0.0087 (10)	0.0045 (11)
C22	0.0399 (13)	0.0306 (14)	0.0389 (14)	0.0094 (11)	0.0178 (11)	0.0037 (11)
C23	0.0317 (12)	0.0338 (14)	0.0364 (13)	0.0110 (11)	0.0158 (11)	0.0091 (11)

Geometric parameters (Å, °)

Si13—O21	1.6625 (17)	C4—C5	1.374 (4)
Si13—O14	1.6706 (15)	C5—C6	1.372 (4)
Si13—O20	1.6860 (16)	C10—C11	1.529 (3)
Si13—C12	1.880 (2)	C10—H10A	0.99
Si13—N17	2.1551 (18)	C10—H10B	0.99
F2—C2	1.341 (3)	C11—C12	1.528 (3)
F3—C3	1.344 (3)	C11—H11A	0.99
F4—C4	1.341 (3)	C11—H11B	0.99
F5—C5	1.338 (3)	C12—H12A	0.99
F6—C6	1.346 (3)	C12—H12B	0.99
O8—C7	1.221 (3)	C15—C16	1.515 (3)
O14—C15	1.421 (2)	C15—H15A	0.99

O20—C19	1.433 (2)	C15—H15B	0.99
O21—C22	1.422 (3)	C16—H16A	0.99
N9—C7	1.335 (3)	C16—H16B	0.99
N9—C10	1.460 (3)	C18—C19	1.510 (3)
N9—H9	0.88	C18—H18A	0.99
N17—C23	1.472 (3)	C18—H18B	0.99
N17—C16	1.477 (3)	C19—H19A	0.99
N17—C18	1.478 (3)	C19—H19B	0.99
C1—C6	1.377 (4)	C22—C23	1.516 (3)
C1—C2	1.383 (3)	C22—H22A	0.99
C1—C7	1.522 (3)	C22—H22B	0.99
C2—C3	1.378 (4)	C23—H23A	0.99
C3—C4	1.368 (4)	C23—H23B	0.99
O21—Si13—O14	119.51 (9)	C12—C11—C10	112.86 (19)
O21—Si13—O20	116.55 (8)	C12—C11—H11A	109
O14—Si13—O20	119.73 (8)	C10—C11—H11A	109
O21—Si13—C12	98.18 (9)	C12—C11—H11B	109
O14—Si13—C12	95.62 (8)	C10—C11—H11B	109
O20—Si13—C12	96.79 (9)	H11A—C11—H11B	107.8
O21—Si13—N17	83.57 (8)	C11—C12—Si13	116.06 (15)
O14—Si13—N17	82.92 (7)	C11—C12—H12A	108.3
O20—Si13—N17	82.97 (7)	Si13—C12—H12A	108.3
C12—Si13—N17	178.12 (9)	C11—C12—H12B	108.3
C15—O14—Si13	123.26 (13)	Si13—C12—H12B	108.3
C19—O20—Si13	121.96 (14)	H12A—C12—H12B	107.4
C22—O21—Si13	122.63 (15)	O14—C15—C16	108.70 (17)
C7—N9—C10	123.05 (19)	O14—C15—H15A	110
C7—N9—H9	118.5	C16—C15—H15A	110
C10—N9—H9	118.5	O14—C15—H15B	110
C23—N17—C16	113.68 (18)	C16—C15—H15B	110
C23—N17—C18	114.70 (18)	H15A—C15—H15B	108.3
C16—N17—C18	113.02 (19)	N17—C16—C15	105.95 (17)
C23—N17—Si13	104.05 (14)	N17—C16—H16A	110.5
C16—N17—Si13	104.87 (13)	C15—C16—H16A	110.5
C18—N17—Si13	105.15 (13)	N17—C16—H16B	110.5
C6—C1—C2	116.7 (2)	C15—C16—H16B	110.5
C6—C1—C7	120.7 (2)	H16A—C16—H16B	108.7
C2—C1—C7	122.5 (2)	N17—C18—C19	105.81 (17)
F2—C2—C3	118.7 (2)	N17—C18—H18A	110.6
F2—C2—C1	120.0 (2)	C19—C18—H18A	110.6
C3—C2—C1	121.3 (2)	N17—C18—H18B	110.6
F3—C3—C4	119.7 (2)	C19—C18—H18B	110.6
F3—C3—C2	120.0 (3)	H18A—C18—H18B	108.7
C4—C3—C2	120.3 (2)	O20—C19—C18	108.34 (19)
F4—C4—C3	120.0 (2)	O20—C19—H19A	110
F4—C4—C5	120.1 (3)	C18—C19—H19A	110
C3—C4—C5	119.8 (2)	O20—C19—H19B	110
F5—C5—C6	120.7 (2)	C18—C19—H19B	110
F5—C5—C4	120.4 (2)	H19A—C19—H19B	108.4

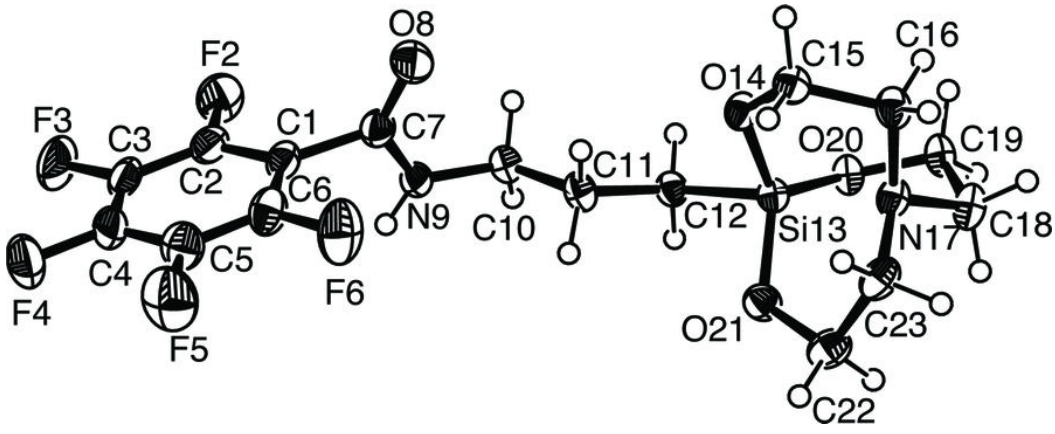
C6—C5—C4	118.9 (3)	O21—C22—C23	108.86 (19)
F6—C6—C5	117.7 (2)	O21—C22—H22A	109.9
F6—C6—C1	119.3 (2)	C23—C22—H22A	109.9
C5—C6—C1	123.0 (2)	O21—C22—H22B	109.9
O8—C7—N9	125.7 (2)	C23—C22—H22B	109.9
O8—C7—C1	121.2 (2)	H22A—C22—H22B	108.3
N9—C7—C1	113.11 (19)	N17—C23—C22	106.05 (19)
N9—C10—C11	113.86 (19)	N17—C23—H23A	110.5
N9—C10—H10A	108.8	C22—C23—H23A	110.5
C11—C10—H10A	108.8	N17—C23—H23B	110.5
N9—C10—H10B	108.8	C22—C23—H23B	110.5
C11—C10—H10B	108.8	H23A—C23—H23B	108.7
H10A—C10—H10B	107.7		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N9—H9···O20^{i}	0.88	2.08	2.955 (2)	172
C15—H15B···O20^{ii}	0.99	2.51	3.406 (3)	150
C16—H16B···F6^{iii}	0.99	2.43	3.101 (3)	125
C18—H18B···F6^{iii}	0.99	2.53	3.320 (3)	136
C23—H23B···F3^{iv}	0.99	2.43	3.229 (3)	137

Symmetry codes: (i) −*x*+3/2, *y*−1/2, −*z*+3/2; (ii) −*x*+2, −*y*+2, −*z*+2; (iii) −*x*+2, −*y*+1, −*z*+2; (iv) *x*+1, *y*, *z*.

Fig. 1


O8
F2
F3
C3
C1
C7
C2
C6
N9
C10
C11
C12
Si13
O14
C15
C16
O20
C19
N17
C18
C4
C5
F6
F4
F5
O21
C23
C22