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2,4-Bis[1-(trifluoromethylsulfonyl)-1,4-dihydropyridin-4-yl]benzene-1,3,5-triyl tris(trifluoromethanesulfonate)

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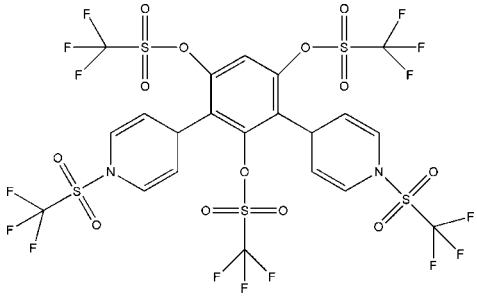
Key indicators: single-crystal X-ray study; T = 180 K; mean σ(C–C) = 0.006 Å; disorder in main residue; R factor = 0.061; wR factor = 0.212; data-to-parameter ratio = 11.4.

The title compound, $C_{21}H_{11}F_{15}N_2O_{13}S_5$, crystallizes with two unique molecules in the asymmetric unit. The dihydropyridine rings adopt highly distorted flattened boat conformations. An extensive series of C—H···O and C—H···F hydrogen bonds links the molecules into undulating rows along *c*. The molecules also form into columns down the *b* axis. The structure is further stabilized by a number of weak F···F, F···O and O···O interactions with distances in the range 2.5–3.0 Å. One of the trifluoromethylsulfonyl substituents in one molecule is disordered over two positions in a 0.57:0.43 ratio.

Related literature

For the activation of pyridine towards nucleophilic attack, see: Ito *et al.* (2003); Corey & Tian (2005). For related structures, see: Toscano *et al.* (1997); Katritsky *et al.* (2001); Vembu *et al.* (2003); Arnott *et al.* (2006).



Experimental

Crystal data

$C_{21}H_{11}F_{15}N_2O_{13}S_5$
M_r = 944.62
Triclinic, $P\overline{1}$
a = 12.0619 (5) Å
b = 14.1934 (6) Å
c = 20.3810 (6) Å
α = 99.280 (3)°
β = 100.780 (3)°
γ = 90.061 (2)°
V = 3381.0 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.49 mm^{-1}
T = 180 (2) K
0.14 × 0.12 × 0.10 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SORTAV*; Blessing 1995)
T_{min} = 0.814, T_{max} = 0.865
(expected range = 0.896–0.952)
35825 measured reflections
11802 independent reflections
8274 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.212
S = 1.05
11802 reflections
1039 parameters
12 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.96 e Å^{-3}
$\Delta\rho_{min}$ = −0.75 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5A—H5A···O9A^{i}	0.95	2.64	3.368 (6)	134
C18A—H18A···O6A^{i}	0.95	2.66	3.471 (5)	144
C18A—H18A···F7A^{i}	0.95	2.60	3.385 (6)	140
C2A—H2A···O13A^{ii}	0.95	2.48	3.176 (6)	130
C3A—H3A···O13A^{ii}	0.95	2.66	3.265 (6)	122
C6A—H6A···O12B^{iii}	0.95	2.51	3.356 (6)	148
C2B—H2B···O7A^{i}	0.95	2.55	3.501 (6)	179
C17B—H17B···O11B^{iv}	0.95	2.52	3.471 (6)	175
C5B—H5B···O7B^{iii}	0.95	2.38	3.293 (6)	162
C19B—H19B···O8B^{iii}	0.95	2.48	3.335 (6)	151

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

Data collection: *COLLECT* (Nonius 1998); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor 1997); data reduction: *HKL DENZO* (Otwinowski & Minor 1997) and *SCALEPACK*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*, *enCIFer* (Allen *et al.*, 2004) and *PLATON* (Spek, 2003).

We thank Dr John Davies, University of Cambridge, for the X-ray data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2662).

References

Allen, F. H., Johnson, O., Shields, G. P., Smith, B. R. & Towler, M. (2004). *J. Appl. Cryst.* **37**, 335–338.
Altomare, A., Cascarano, G., Giacovazzo, C. & Guagliardi, A. (1993). *J. Appl. Cryst.* **26**, 343–350.
Arnott, G., Clayden, J. & Hamilton, S. D. (2006). *Org. Lett.* **8**, 5325–5328.
Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Corey, E. J. & Tian, Y. (2005). *Org. Lett.* **7**, 5535–5537.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Ito, S., Yokoyama, R., Okujima, T., Terazono, T., Kubo, T., Tajiri, A., Watanabe, M. & Morita, N. (2003). *Org. Biomol. Chem.* **1**, 1947–1952.
Katritsky, A. R., Zhang, S., Kurz, T., Wand, M. & Steel, P. J. (2001). *Org. Lett.* **3**, 2807–2809.
Nonius (1998). *COLLECT*, Nonius BV, Delft, The Netherlands.

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Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Toscano, R. A., Hernadez-Gallindo, M. del C., Rosas, R., del Garcia-Mellado, O., Rio Portilla, F., Amabile-Cuevas, C. & Alvarez-Toledano, C. (1997). *Chem. Pharm. Bull.* **45**, 957–961.
Vembu, N., Nallu, M., Garrison, J. & Youngs, W. J. (2003). *Acta Cryst.* E**59**, o1019–o1021.

supplementary materials

Acta Cryst. (2007). E**63**, o4858-o4859 [**doi:10.1107/S1600536807060230**]

2,4-Bis[1-(trifluoromethylsulfonyl)-1,4-dihydropyridin-4-yl]benzene-1,3,5-triyl tris(trifluoromethanesulfonate)

A. R. Lister, S. C. Moratti and J. Simpson

Comment

Trifluoromethanesulfonates are a versatile class of functional group, and are often used as a halide equivalent in aliphatic and aromatic substitution and metal mediated coupling. They are usually formed from the reaction of triflic anhydride and a hydroxyl-group in the presence of a base. Pyridine is often employed as the base as it is usually quite inert. However, it has been occasionally found to be activated towards nucleophilic attack by electron rich arenes (Ito *et al.*, 2003; Corey & Tian, 2005). This is a potentially very useful way of making a wide range of pyridine-derivatives that are otherwise difficult to make (Corey & Tian, 2005). In the present case, attempted triflation of 1,3,5-trihydroxybenzene in the presence of pyridine gave a large mixture of products. However, the title compound (I) could be separated by column chromatography in moderate yield and we report its structure here.

Compound (I) crystallizes with two unique molecules in the asymmetric unit, Fig. 1 & 2. The central benzene ring carries trifluoromethylsulfonyl substituents at C7, C9 and C11 with 6-membered dihydropyridine rings at C8 and C12 each with an additional trifluoromethylsulfonyl substituent on the pyridine N1 and N2 atoms. Bond distances and angles in the trifluoromethyl sulphonate groups (I) are similar to those found in a related compound (Vembu *et al.*, 2003) The dihydropyridine rings adopt distorted, flattened boat conformations, similar to those reported for other dihydropyridine compounds with trifluoromethylsulfonyl substituents on the N atom (Toscano *et al.*, 1997; Katritzky *et al.*, 2001; Arnott, *et al.*, 2006). The dihedral angles between the benzene ring plane and the best fit meanplanes through the dihydropyridine rings are 83.0 (1)° and 81.0 (1)° for molecule *a* and 89.0 (2)° and 89.5 (2)° for molecule *b* respectively.

An extensive series of C—H···O and C—H···F hydrogen bonds link the molecules into undulating rows along *c* (Table 1). The molecules also form into colums down the *b* axis (Fig 2). The structure is further stabilized by a number of weak F···F, F···O and O···O interactions with distances in the range 2.50—3.00 Å.

Experimental

1,3,5-Trihydroxybenzene (0.75 g, 4.6 mmol) was dried *in vacuo* at 343 K for 5 h. Pyridine (15 ml) and trifluoromethanesulfonic anhydride (4.7 ml, 27.8 mmol) were then added under nitrogen at 0 °C. After 1 h the mixture was heated to room temperature, left for a further 24 h then added to ether (40 ml) and washed with HCl solution (10% in water, 3 × 30 ml). The mixture was then dried over magnesium sulfate, filtered and concentrated in vacuo. Column chromatography on silica gel, using 83:17 hexane:ethyl acetate and crystallization from ether layered with hexane yielded 0.39 g (10%) of a white solid as needles, 42: R_f (ethyl acetate:hexane 1:1) 0.80; m.p. 430–432 K; IR (KBr) 3100, 3000, 2370, 1700, 1600, 1410, 1235, 1140, 1050 cm^{-1}; ^{1}H NMR (400 MHz) δ ($CDCl_3$) 7.39 (s, 1H, H-1), 6.62 (d, 4H, H-7, ^{3}JHH = 10.0 Hz), 5.10 (d, 4H, H-6, ^{3}JHH = 10.0 Hz) 4.88 (s, 2H, H-5); 13 C NMR (100 MHz) δ ($CDCl_3$) 149.6, 148.8, 148.1, 129.4, 123.6, 119.9, 117.8, 116.8, 115.6, 106.8; m/*z* (ESI) 966.85280 [*M* + Na+. $C_{21}H_{11}O_{13}S_5N_2F_{15}Na$ requires *M* + Na, 966.85228]; m/*z* (ESI) 966.85 (*M* + Na+, 100); found C, 26.7% H, 1.2%. $C_{21}H_{11}O_{13}S_5N_2F_{15}$ requires C, 26.7%; H, 1.2%.

Refinement

In molecule *b* all atoms of the S2b trifluoromethylsulfonyl substituent were disordered over two positions. The respective occupancy factors refined to 0.57 and 0.43 and were fixed at those values in the final refinement cycles. A common, isotropic displacement parameter was assigned to the fluorine atoms of this disordered moiety.

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 and 1.00 Å, U_{iso} = 1.2U_{eq} (C) for CH groups.

Figures

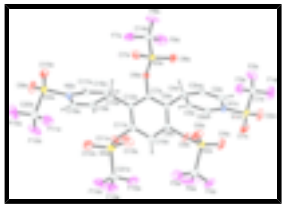


Fig. 1. The structure of molecule *a* of (I) with displacement parameters drawn at the 30% probability level.

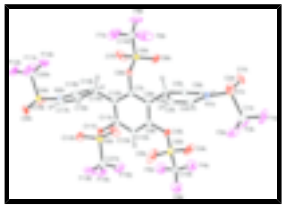


Fig. 2. The structure of molecule *b* of (I) with displacement parameters drawn at the 30% probability level. For clarity, atoms of the minor disorder component have been omitted.

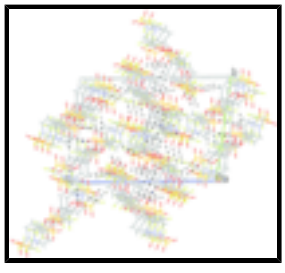


Fig. 3. Crystal packing of (I) viewed down the *a* axis with hydrogen bonds drawn as dashed lines. For clarity, atoms of the minor disorder component of molecule *b* have been omitted.

2,4-Bis[1-(trifluoromethylsulfonyl)-1,4-dihydropyridin-4-yl]benzene-1,3,5-triyl tris(trifluoromethanesulfonate)

Crystal data

$C_{21}H_{11}F_{15}N_2O_{13}S_5$	Z = 4
M_r = 944.62	F_{000} = 1880
Triclinic, $P\overline{1}$	D_x = 1.856 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 12.0619 (5) Å	Cell parameters from 30655 reflections
b = 14.1934 (6) Å	θ = 1.0–25.0º
c = 20.3810 (6) Å	μ = 0.49 mm^{-1}
α = 99.280 (3)º	T = 180 (2) K
β = 100.780 (3)º	Block, colourless

γ = 90.061 (2)º	0.14 × 0.12 × 0.10 mm
V = 3381.0 (2) Å^3	

Data collection

Nonius Kappa CCD diffractometer	8274 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.050
T = 180(2) K	θ_{max} = 25.0º
Thin slice ω and φ scans	θ_{min} = 1.5º
Absorption correction: multi-scan (SORTAV; Blessing 1995)	h = −14→14
T_{min} = 0.814, T_{max} = 0.865	k = −16→16
35825 measured reflections	l = −22→24
11802 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.061	H-atom parameters constrained
$wR(F^2)$ = 0.212	$w = 1/[\sigma^2(F_o^2) + (0.124P)^2 + 4.7285P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max}$ = <0.001
11802 reflections	$\Delta\rho_{max}$ = 0.96 e Å^{-3}
1039 parameters	$\Delta\rho_{min}$ = −0.75 e Å^{-3}
12 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\text{sigma}(F^2)$ 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)
N1B	0.0853 (3)	0.5106 (3)	0.77343 (19)	0.0348 (9)	
C2B	0.0947 (4)	0.4103 (3)	0.7563 (2)	0.0349 (11)	

H2B	0.0435	0.3759	0.7189	0.042*	
C3B	0.1726 (4)	0.3644 (3)	0.7910 (2)	0.0350 (11)	
H3B	0.1730	0.2968	0.7799	0.042*	
C4B	0.2619 (4)	0.4143 (3)	0.8481 (2)	0.0337 (11)	
H4B	0.3303	0.4249	0.8287	0.040*	
C5B	0.2211 (4)	0.5116 (3)	0.8743 (2)	0.0379 (12)	
H5B	0.2544	0.5421	0.9186	0.045*	
C6B	0.1417 (4)	0.5556 (3)	0.8385 (2)	0.0382 (12)	
H6B	0.1219	0.6180	0.8563	0.046*	
C7B	0.4060 (4)	0.3235 (3)	0.9223 (2)	0.0272 (10)	
C8B	0.2966 (4)	0.3548 (3)	0.9041 (2)	0.0299 (10)	
C9B	0.2200 (4)	0.3273 (4)	0.9417 (3)	0.0386 (12)	
C10B	0.2481 (4)	0.2714 (4)	0.9913 (3)	0.0431 (13)	
H10B	0.1937	0.2541	1.0158	0.052*	
C11B	0.3567 (4)	0.2415 (3)	1.0041 (2)	0.0355 (11)	
C12B	0.4407 (4)	0.2645 (3)	0.9704 (2)	0.0283 (10)	
N2B	0.6884 (3)	0.1114 (3)	1.0744 (2)	0.0362 (9)	
C15B	0.5604 (4)	0.2277 (3)	0.9841 (2)	0.0332 (11)	
H15B	0.6033	0.2535	0.9530	0.040*	
C16B	0.5643 (4)	0.1213 (3)	0.9696 (2)	0.0340 (11)	
H16B	0.5208	0.0891	0.9283	0.041*	
C17B	0.6239 (4)	0.0696 (3)	1.0102 (3)	0.0367 (11)	
H17B	0.6242	0.0024	0.9966	0.044*	
C18B	0.6793 (4)	0.2106 (4)	1.0953 (3)	0.0392 (12)	
H18B	0.7167	0.2392	1.1393	0.047*	
C19B	0.6205 (4)	0.2642 (4)	1.0556 (3)	0.0374 (11)	
H19B	0.6155	0.3300	1.0729	0.045*	
S1B	0.00953 (11)	0.57192 (10)	0.72241 (6)	0.0429 (3)	
O1B	0.0468 (4)	0.6684 (3)	0.7394 (2)	0.0609 (11)	
O2B	−0.0056 (4)	0.5199 (3)	0.65574 (17)	0.0598 (11)	
C1B	−0.1299 (5)	0.5686 (5)	0.7458 (3)	0.0621 (17)	
F1B	−0.2000 (4)	0.6177 (4)	0.7068 (3)	0.1122 (18)	
F2B	−0.1689 (3)	0.4800 (3)	0.7380 (2)	0.0772 (11)	
F3B	−0.1222 (3)	0.6101 (3)	0.8099 (2)	0.0823 (12)	
O3B	0.1096 (3)	0.3635 (3)	0.9276 (2)	0.0624 (12)	
S2B	0.0043 (2)	0.3075 (2)	0.90363 (13)	0.0496 (6)	0.57
O4B	−0.0650 (6)	0.3499 (8)	0.8552 (4)	0.085 (3)	0.57
O5B	0.0315 (7)	0.2098 (6)	0.8931 (7)	0.113 (4)	0.57
C13B	−0.0663 (8)	0.3289 (9)	0.9791 (7)	0.081 (5)	0.57
F4B	−0.0927 (7)	0.4154 (6)	0.9874 (4)	0.0876 (11)*	0.57
F5B	0.0072 (7)	0.3104 (6)	1.0306 (5)	0.0876 (11)*	0.57
F6B	−0.1517 (7)	0.2809 (6)	0.9749 (4)	0.0876 (11)*	0.57
S2B'	0.0048 (3)	0.3630 (3)	0.9605 (2)	0.0655 (12)	0.43
O4B'	−0.0629 (10)	0.4351 (8)	0.9343 (9)	0.110 (6)	0.43
O5B'	0.0414 (11)	0.3654 (9)	1.0343 (6)	0.088 (5)	0.43
C13'	−0.0744 (11)	0.2496 (11)	0.9277 (7)	0.060 (4)	0.43
F4B'	−0.1600 (9)	0.2417 (8)	0.9502 (5)	0.0876 (11)*	0.43
F5B'	−0.0116 (9)	0.1820 (8)	0.9433 (5)	0.0876 (11)*	0.43
F6B'	−0.1113 (9)	0.2418 (7)	0.8643 (5)	0.0876 (11)*	0.43

O6B	0.4868 (3)	0.3482 (2)	0.88441 (14)	0.0292 (7)
S3B	0.56148 (10)	0.44335 (8)	0.91179 (6)	0.0320 (3)
O7B	0.6467 (4)	0.4306 (3)	0.9675 (2)	0.0752 (15)
O8B	0.4953 (3)	0.5237 (3)	0.9145 (3)	0.0734 (14)
C14B	0.6314 (5)	0.4349 (5)	0.8396 (3)	0.0551 (15)
F7B	0.6833 (4)	0.3576 (3)	0.8313 (3)	0.118 (2)
F8B	0.7045 (4)	0.5076 (3)	0.8526 (2)	0.0901 (14)
F9B	0.5570 (5)	0.4409 (5)	0.7856 (2)	0.128 (2)
S4B	0.78150 (11)	0.05013 (10)	1.11614 (7)	0.0447 (4)
O9B	0.7511 (4)	−0.0478 (3)	1.0976 (3)	0.0729 (14)
O10B	0.8090 (4)	0.0959 (3)	1.1838 (2)	0.0662 (12)
C20B	0.9070 (5)	0.0679 (6)	1.0810 (4)	0.066 (2)
F10B	0.9335 (3)	0.1604 (4)	1.0900 (3)	0.1079 (19)
F11B	0.8864 (4)	0.0363 (5)	1.0153 (2)	0.120 (2)
F12B	0.9929 (3)	0.0232 (3)	1.1098 (2)	0.0899 (14)
O11B	0.3835 (3)	0.1740 (2)	1.04950 (17)	0.0390 (8)
S5B	0.39739 (12)	0.20251 (11)	1.12870 (7)	0.0465 (4)
O12B	0.4821 (4)	0.1449 (4)	1.1574 (2)	0.0776 (15)
O13B	0.3947 (5)	0.3014 (3)	1.1474 (2)	0.0785 (15)
C21B	0.2672 (5)	0.1494 (5)	1.1423 (3)	0.0550 (16)
F13B	0.2607 (4)	0.0585 (3)	1.1195 (2)	0.0895 (13)
F14B	0.2668 (4)	0.1616 (3)	1.20734 (19)	0.0845 (13)
F15B	0.1787 (3)	0.1907 (4)	1.1127 (2)	0.0951 (16)
N1A	0.3789 (3)	1.0465 (3)	0.69424 (19)	0.0341 (9)
C2A	0.3304 (4)	1.0516 (3)	0.6260 (2)	0.0332 (11)
H2A	0.3358	1.1103	0.6099	0.040*
C3A	0.2781 (4)	0.9779 (3)	0.5843 (2)	0.0329 (11)
H3A	0.2466	0.9860	0.5393	0.039*
C4A	0.2655 (4)	0.8807 (3)	0.6043 (2)	0.0290 (10)
H4A	0.3062	0.8344	0.5756	0.035*
C5A	0.3214 (4)	0.8818 (3)	0.6770 (2)	0.0309 (10)
H5A	0.3197	0.8242	0.6950	0.037*
C6A	0.3725 (4)	0.9574 (3)	0.7170 (2)	0.0329 (11)
H6A	0.4060	0.9525	0.7623	0.039*
C7A	0.0981 (4)	0.7677 (3)	0.5408 (2)	0.0241 (9)
C8A	0.1414 (4)	0.8457 (3)	0.5906 (2)	0.0268 (10)
C9A	0.0649 (4)	0.8864 (3)	0.6289 (2)	0.0296 (10)
C10A	−0.0435 (4)	0.8495 (3)	0.6232 (2)	0.0341 (11)
H10A	−0.0915	0.8765	0.6528	0.041*
C11A	−0.0794 (4)	0.7726 (3)	0.5733 (2)	0.0306 (10)
C12A	−0.0118 (4)	0.7289 (3)	0.5294 (2)	0.0255 (9)
N2A	−0.2422 (3)	0.5283 (3)	0.39497 (19)	0.0326 (9)
C15A	−0.0553 (4)	0.6451 (3)	0.4732 (2)	0.0258 (9)
H15A	0.0110	0.6191	0.4540	0.031*
C16A	−0.1384 (4)	0.6763 (3)	0.4163 (2)	0.0290 (10)
H16A	−0.1302	0.7390	0.4068	0.035*
C17A	−0.2218 (4)	0.6204 (3)	0.3794 (2)	0.0298 (10)
H17A	−0.2689	0.6416	0.3421	0.036*
C18A	−0.1916 (4)	0.5101 (3)	0.4604 (2)	0.0319 (11)

H18A	−0.2189	0.4574	0.4768	0.038*
C19A	−0.1082 (4)	0.5644 (3)	0.4985 (2)	0.0276 (10)
H19A	−0.0803	0.5527	0.5431	0.033*
S1A	0.45187 (11)	1.13625 (9)	0.74180 (6)	0.0408 (3)
O1A	0.4573 (4)	1.1282 (3)	0.81034 (18)	0.0576 (11)
O2A	0.4215 (4)	1.2210 (2)	0.7156 (2)	0.0566 (11)
C1A	0.5959 (5)	1.1115 (4)	0.7252 (4)	0.0622 (18)
F1A	0.6676 (4)	1.1795 (3)	0.7601 (3)	0.1100 (18)
F2A	0.5977 (4)	1.1049 (3)	0.6608 (2)	0.0895 (13)
F3A	0.6274 (3)	1.0291 (3)	0.7454 (2)	0.0764 (11)
O3A	0.1011 (3)	0.9669 (2)	0.67929 (16)	0.0356 (8)
S2A	0.06102 (11)	1.07021 (9)	0.66863 (7)	0.0401 (3)
O4A	0.1483 (4)	1.1345 (3)	0.7045 (3)	0.0776 (15)
O5A	0.0132 (4)	1.0716 (3)	0.60091 (19)	0.0616 (12)
C13A	−0.0501 (6)	1.0857 (4)	0.7194 (3)	0.0575 (16)
F4A	−0.0750 (3)	1.1747 (2)	0.73006 (17)	0.0641 (10)
F5A	−0.1454 (4)	1.0399 (3)	0.6819 (3)	0.1082 (17)
F6A	−0.0251 (6)	1.0531 (5)	0.7728 (3)	0.166 (3)
O6A	0.1741 (2)	0.7197 (2)	0.50144 (14)	0.0256 (7)
S3A	0.18713 (9)	0.75272 (8)	0.43232 (5)	0.0290 (3)
O7A	0.0934 (3)	0.7187 (3)	0.38060 (16)	0.0429 (9)
O8A	0.2274 (3)	0.8481 (2)	0.44326 (18)	0.0469 (9)
C14A	0.3057 (5)	0.6758 (5)	0.4189 (3)	0.0495 (14)
F7A	0.2743 (4)	0.5850 (3)	0.41384 (19)	0.0731 (11)
F8A	0.3318 (3)	0.6890 (3)	0.3614 (2)	0.0801 (13)
F9A	0.3902 (3)	0.6959 (4)	0.4684 (2)	0.0949 (15)
S4A	−0.32403 (11)	0.44909 (9)	0.34168 (6)	0.0401 (3)
O9A	−0.2986 (4)	0.3583 (3)	0.3597 (2)	0.0599 (11)
O10A	−0.3298 (3)	0.4687 (3)	0.27565 (17)	0.0493 (9)
C20A	−0.4632 (5)	0.4758 (5)	0.3625 (3)	0.0567 (16)
F10A	−0.5413 (3)	0.4191 (3)	0.3193 (2)	0.0895 (14)
F11A	−0.4871 (3)	0.5646 (3)	0.3573 (2)	0.0695 (10)
F12A	−0.4645 (3)	0.4608 (4)	0.4247 (2)	0.0864 (13)
O11A	−0.1878 (3)	0.7298 (2)	0.57024 (17)	0.0384 (8)
S5A	−0.29834 (11)	0.77148 (11)	0.53323 (7)	0.0462 (4)
O12A	−0.3684 (3)	0.6925 (4)	0.4971 (2)	0.0772 (15)
O13A	−0.2718 (3)	0.8505 (4)	0.5054 (2)	0.0699 (13)
C21A	−0.3640 (5)	0.8142 (5)	0.6058 (3)	0.0541 (15)
F13A	−0.4587 (3)	0.8536 (4)	0.5855 (2)	0.0911 (14)
F14A	−0.3824 (4)	0.7453 (4)	0.6375 (2)	0.0987 (15)
F15A	−0.2979 (3)	0.8791 (3)	0.6494 (2)	0.0907 (14)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1B	0.036 (2)	0.035 (2)	0.029 (2)	0.0068 (18)	−0.0058 (17)	0.0076 (17)
C2B	0.038 (3)	0.036 (3)	0.026 (2)	−0.001 (2)	−0.002 (2)	0.000 (2)
C3B	0.049 (3)	0.032 (3)	0.022 (2)	0.000 (2)	0.002 (2)	0.003 (2)

C4B	0.039 (3)	0.031 (3)	0.029 (2)	0.001 (2)	−0.002 (2)	0.009 (2)
C5B	0.046 (3)	0.030 (3)	0.030 (2)	−0.004 (2)	−0.011 (2)	0.002 (2)
C6B	0.049 (3)	0.027 (3)	0.031 (3)	0.002 (2)	−0.008 (2)	0.001 (2)
C7B	0.028 (2)	0.026 (2)	0.026 (2)	0.0009 (19)	0.0029 (18)	0.0045 (18)
C8B	0.030 (3)	0.031 (2)	0.027 (2)	0.002 (2)	−0.0013 (19)	0.0091 (19)
C9B	0.028 (3)	0.047 (3)	0.042 (3)	0.009 (2)	0.003 (2)	0.018 (2)
C10B	0.037 (3)	0.051 (3)	0.051 (3)	0.012 (2)	0.013 (2)	0.030 (3)
C11B	0.040 (3)	0.036 (3)	0.035 (3)	0.006 (2)	0.005 (2)	0.020 (2)
C12B	0.029 (2)	0.025 (2)	0.031 (2)	0.0043 (19)	0.0025 (19)	0.0065 (19)
N2B	0.032 (2)	0.033 (2)	0.045 (2)	0.0081 (17)	0.0025 (18)	0.0135 (19)
C15B	0.032 (3)	0.030 (3)	0.039 (3)	0.005 (2)	0.003 (2)	0.012 (2)
C16B	0.032 (3)	0.034 (3)	0.034 (3)	0.008 (2)	0.002 (2)	0.004 (2)
C17B	0.036 (3)	0.028 (3)	0.045 (3)	0.004 (2)	0.005 (2)	0.003 (2)
C18B	0.032 (3)	0.043 (3)	0.038 (3)	0.001 (2)	−0.003 (2)	0.006 (2)
C19B	0.034 (3)	0.029 (3)	0.045 (3)	0.004 (2)	−0.001 (2)	0.002 (2)
S1B	0.0423 (8)	0.0577 (9)	0.0321 (7)	0.0167 (6)	0.0045 (5)	0.0201 (6)
O1B	0.076 (3)	0.049 (3)	0.064 (3)	0.011 (2)	0.009 (2)	0.031 (2)
O2B	0.068 (3)	0.087 (3)	0.0250 (18)	0.030 (2)	0.0033 (17)	0.0163 (19)
C1B	0.050 (4)	0.081 (5)	0.054 (4)	0.020 (4)	0.013 (3)	0.004 (3)
F1B	0.056 (3)	0.151 (5)	0.124 (4)	0.054 (3)	−0.007 (3)	0.037 (3)
F2B	0.048 (2)	0.103 (3)	0.076 (3)	−0.011 (2)	0.0130 (18)	0.000 (2)
F3B	0.071 (3)	0.102 (3)	0.073 (3)	0.010 (2)	0.037 (2)	−0.015 (2)
O3B	0.035 (2)	0.089 (3)	0.081 (3)	0.024 (2)	0.018 (2)	0.061 (3)
S2B	0.0296 (13)	0.0647 (17)	0.0498 (15)	0.0094 (11)	0.0003 (10)	0.0040 (13)
O4B	0.032 (4)	0.173 (10)	0.055 (5)	0.027 (5)	0.000 (3)	0.048 (6)
O5B	0.046 (5)	0.068 (6)	0.179 (11)	0.014 (4)	−0.024 (6)	−0.060 (7)
C13B	0.027 (6)	0.112 (12)	0.119 (12)	−0.024 (7)	−0.011 (6)	0.093 (11)
S2B'	0.052 (2)	0.061 (2)	0.067 (3)	0.027 (2)	−0.0168 (19)	−0.007 (2)
O4B'	0.068 (8)	0.056 (7)	0.191 (16)	0.020 (6)	−0.037 (9)	0.051 (9)
O5B'	0.084 (9)	0.078 (8)	0.062 (7)	0.036 (7)	−0.042 (6)	−0.040 (6)
C13'	0.040 (8)	0.083 (11)	0.071 (10)	0.023 (8)	0.020 (7)	0.043 (9)
O6B	0.0346 (18)	0.0268 (17)	0.0251 (16)	−0.0016 (13)	0.0033 (13)	0.0036 (13)
S3B	0.0361 (7)	0.0287 (6)	0.0307 (6)	−0.0036 (5)	0.0074 (5)	0.0024 (5)
O7B	0.098 (4)	0.072 (3)	0.041 (2)	−0.045 (3)	−0.033 (2)	0.022 (2)
O8B	0.044 (2)	0.029 (2)	0.146 (5)	0.0010 (18)	0.036 (3)	−0.009 (2)
C14B	0.052 (4)	0.059 (4)	0.057 (4)	−0.015 (3)	0.023 (3)	0.001 (3)
F7B	0.096 (3)	0.071 (3)	0.188 (6)	−0.006 (3)	0.087 (4)	−0.049 (3)
F8B	0.090 (3)	0.077 (3)	0.114 (3)	−0.034 (2)	0.067 (3)	−0.008 (2)
F9B	0.141 (5)	0.205 (6)	0.041 (2)	−0.066 (4)	0.006 (3)	0.043 (3)
S4B	0.0324 (7)	0.0574 (9)	0.0539 (8)	0.0138 (6)	0.0108 (6)	0.0346 (7)
O9B	0.060 (3)	0.052 (3)	0.115 (4)	0.015 (2)	0.007 (3)	0.050 (3)
O10B	0.056 (3)	0.100 (3)	0.050 (3)	0.026 (2)	0.007 (2)	0.036 (2)
C20B	0.034 (3)	0.107 (6)	0.074 (5)	0.024 (3)	0.015 (3)	0.056 (4)
F10B	0.051 (2)	0.122 (4)	0.174 (5)	−0.006 (2)	0.022 (3)	0.091 (4)
F11B	0.069 (3)	0.232 (7)	0.079 (3)	0.052 (4)	0.041 (2)	0.048 (4)
F12B	0.039 (2)	0.134 (4)	0.115 (3)	0.036 (2)	0.020 (2)	0.068 (3)
O11B	0.040 (2)	0.041 (2)	0.0427 (19)	0.0134 (15)	0.0106 (15)	0.0249 (16)
S5B	0.0453 (8)	0.0568 (9)	0.0396 (7)	0.0031 (6)	0.0005 (6)	0.0236 (6)
O12B	0.049 (3)	0.126 (4)	0.074 (3)	0.019 (3)	0.005 (2)	0.072 (3)

O13B	0.125 (4)	0.059 (3)	0.045 (2)	−0.015 (3)	−0.002 (3)	0.012 (2)
C21B	0.059 (4)	0.068 (4)	0.048 (3)	0.015 (3)	0.016 (3)	0.031 (3)
F13B	0.113 (4)	0.073 (3)	0.093 (3)	−0.021 (3)	0.046 (3)	0.017 (2)
F14B	0.102 (3)	0.116 (3)	0.052 (2)	0.019 (3)	0.041 (2)	0.033 (2)
F15B	0.052 (2)	0.166 (4)	0.092 (3)	0.026 (3)	0.024 (2)	0.080 (3)
N1A	0.043 (2)	0.028 (2)	0.027 (2)	−0.0061 (17)	−0.0031 (17)	0.0026 (16)
C2A	0.039 (3)	0.029 (3)	0.029 (2)	−0.006 (2)	−0.004 (2)	0.007 (2)
C3A	0.037 (3)	0.033 (3)	0.027 (2)	−0.002 (2)	0.000 (2)	0.008 (2)
C4A	0.027 (2)	0.030 (2)	0.030 (2)	0.0017 (19)	0.0034 (19)	0.0055 (19)
C5A	0.030 (2)	0.030 (3)	0.032 (2)	0.001 (2)	−0.001 (2)	0.010 (2)
C6A	0.030 (3)	0.037 (3)	0.029 (2)	0.000 (2)	−0.003 (2)	0.010 (2)
C7A	0.024 (2)	0.025 (2)	0.023 (2)	0.0040 (18)	0.0042 (17)	0.0039 (18)
C8A	0.027 (2)	0.024 (2)	0.028 (2)	−0.0008 (18)	−0.0009 (18)	0.0051 (18)
C9A	0.031 (3)	0.025 (2)	0.030 (2)	0.0046 (19)	−0.0017 (19)	0.0026 (19)
C10A	0.031 (3)	0.035 (3)	0.035 (3)	0.007 (2)	0.006 (2)	0.003 (2)
C11A	0.026 (2)	0.031 (3)	0.033 (2)	−0.0024 (19)	0.0037 (19)	0.002 (2)
C12A	0.026 (2)	0.025 (2)	0.024 (2)	0.0023 (18)	0.0020 (18)	0.0016 (18)
N2A	0.030 (2)	0.031 (2)	0.032 (2)	−0.0058 (17)	−0.0045 (17)	0.0064 (17)
C15A	0.021 (2)	0.025 (2)	0.029 (2)	0.0020 (18)	0.0022 (18)	0.0002 (18)
C16A	0.030 (2)	0.028 (2)	0.030 (2)	0.001 (2)	0.0052 (19)	0.0080 (19)
C17A	0.033 (3)	0.029 (2)	0.028 (2)	0.000 (2)	0.002 (2)	0.0084 (19)
C18A	0.032 (3)	0.030 (3)	0.035 (3)	0.002 (2)	0.005 (2)	0.012 (2)
C19A	0.031 (2)	0.026 (2)	0.025 (2)	0.0050 (19)	0.0017 (19)	0.0064 (18)
S1A	0.0458 (8)	0.0316 (7)	0.0371 (7)	−0.0008 (6)	−0.0025 (6)	−0.0061 (5)
O1A	0.076 (3)	0.052 (2)	0.034 (2)	0.002 (2)	−0.0038 (19)	−0.0076 (17)
O2A	0.068 (3)	0.028 (2)	0.063 (3)	−0.0024 (18)	−0.008 (2)	0.0017 (18)
C1A	0.043 (3)	0.047 (4)	0.084 (5)	−0.008 (3)	−0.001 (3)	−0.013 (3)
F1A	0.056 (3)	0.074 (3)	0.172 (5)	−0.025 (2)	−0.008 (3)	−0.028 (3)
F2A	0.084 (3)	0.101 (3)	0.094 (3)	−0.012 (2)	0.045 (3)	0.015 (3)
F3A	0.052 (2)	0.061 (2)	0.112 (3)	0.0147 (18)	0.008 (2)	0.008 (2)
O3A	0.0374 (19)	0.0274 (17)	0.0331 (17)	0.0081 (14)	−0.0058 (14)	−0.0067 (14)
S2A	0.0467 (8)	0.0291 (7)	0.0425 (7)	0.0083 (6)	0.0107 (6)	−0.0025 (5)
O4A	0.055 (3)	0.036 (2)	0.125 (4)	−0.005 (2)	0.011 (3)	−0.029 (2)
O5A	0.093 (3)	0.051 (2)	0.043 (2)	0.031 (2)	0.015 (2)	0.0100 (19)
C13A	0.077 (5)	0.046 (4)	0.057 (4)	0.023 (3)	0.029 (3)	0.009 (3)
F4A	0.091 (3)	0.048 (2)	0.057 (2)	0.0323 (18)	0.0291 (19)	0.0014 (16)
F5A	0.082 (3)	0.079 (3)	0.169 (5)	0.002 (3)	0.070 (3)	−0.019 (3)
F6A	0.271 (8)	0.178 (5)	0.120 (4)	0.176 (6)	0.140 (5)	0.114 (4)
O6A	0.0242 (16)	0.0284 (16)	0.0243 (15)	0.0034 (12)	0.0052 (12)	0.0042 (12)
S3A	0.0275 (6)	0.0340 (6)	0.0257 (6)	0.0021 (5)	0.0058 (4)	0.0046 (5)
O7A	0.0339 (19)	0.066 (2)	0.0262 (17)	−0.0070 (17)	−0.0019 (14)	0.0080 (16)
O8A	0.065 (3)	0.037 (2)	0.040 (2)	−0.0072 (18)	0.0124 (18)	0.0071 (16)
C14A	0.039 (3)	0.066 (4)	0.050 (3)	0.020 (3)	0.023 (3)	0.012 (3)
F7A	0.107 (3)	0.052 (2)	0.077 (3)	0.037 (2)	0.052 (2)	0.0204 (19)
F8A	0.090 (3)	0.096 (3)	0.083 (3)	0.039 (2)	0.068 (2)	0.040 (2)
F9A	0.030 (2)	0.161 (4)	0.090 (3)	0.026 (2)	0.005 (2)	0.017 (3)
S4A	0.0362 (7)	0.0382 (7)	0.0406 (7)	−0.0056 (5)	0.0002 (5)	−0.0013 (6)
O9A	0.068 (3)	0.031 (2)	0.071 (3)	−0.0063 (19)	−0.007 (2)	0.0021 (19)
O10A	0.048 (2)	0.062 (2)	0.0307 (19)	−0.0090 (19)	−0.0002 (16)	−0.0046 (17)

C20A	0.041 (3)	0.074 (5)	0.058 (4)	−0.005 (3)	0.012 (3)	0.017 (3)
F10A	0.045 (2)	0.117 (4)	0.096 (3)	−0.041 (2)	−0.016 (2)	0.021 (3)
F11A	0.0407 (19)	0.086 (3)	0.081 (3)	0.0167 (18)	0.0092 (17)	0.014 (2)
F12A	0.060 (2)	0.143 (4)	0.068 (3)	−0.014 (2)	0.0227 (19)	0.040 (3)
O11A	0.0231 (17)	0.043 (2)	0.048 (2)	0.0000 (15)	0.0086 (15)	0.0026 (16)
S5A	0.0281 (7)	0.0715 (10)	0.0387 (7)	0.0071 (6)	0.0075 (5)	0.0067 (7)
O12A	0.033 (2)	0.105 (4)	0.076 (3)	−0.009 (2)	0.005 (2)	−0.032 (3)
O13A	0.047 (2)	0.098 (4)	0.079 (3)	0.020 (2)	0.014 (2)	0.053 (3)
C21A	0.037 (3)	0.064 (4)	0.061 (4)	0.007 (3)	0.023 (3)	−0.003 (3)
F13A	0.045 (2)	0.125 (4)	0.103 (3)	0.038 (2)	0.025 (2)	0.003 (3)
F14A	0.104 (3)	0.112 (4)	0.108 (4)	0.008 (3)	0.069 (3)	0.042 (3)
F15A	0.064 (3)	0.113 (3)	0.081 (3)	0.000 (2)	0.029 (2)	−0.043 (3)

Geometric parameters (Å, °)

N1B—C2B	1.420 (6)	C21B—F13B	1.296 (8)
N1B—C6B	1.421 (6)	C21B—F14B	1.310 (7)
N1B—S1B	1.616 (4)	C21B—F15B	1.312 (7)
C2B—C3B	1.308 (7)	N1A—C2A	1.419 (6)
C2B—H2B	0.9500	N1A—C6A	1.422 (6)
C3B—C4B	1.510 (6)	N1A—S1A	1.618 (4)
C3B—H3B	0.9500	C2A—C3A	1.313 (7)
C4B—C5B	1.515 (7)	C2A—H2A	0.9500
C4B—C8B	1.525 (6)	C3A—C4A	1.516 (6)
C4B—H4B	1.0000	C3A—H3A	0.9500
C5B—C6B	1.313 (6)	C4A—C5A	1.506 (6)
C5B—H5B	0.9500	C4A—C8A	1.538 (6)
C6B—H6B	0.9500	C4A—H4A	1.0000
C7B—C8B	1.395 (6)	C5A—C6A	1.313 (7)
C7B—C12B	1.397 (6)	C5A—H5A	0.9500
C7B—O6B	1.427 (5)	C6A—H6A	0.9500
C8B—C9B	1.398 (7)	C7A—C12A	1.399 (6)
C9B—C10B	1.377 (6)	C7A—C8A	1.401 (6)
C9B—O3B	1.424 (6)	C7A—O6A	1.432 (5)
C10B—C11B	1.369 (7)	C8A—C9A	1.385 (7)
C10B—H10B	0.9500	C9A—C10A	1.385 (7)
C11B—C12B	1.391 (7)	C9A—O3A	1.416 (5)
C11B—O11B	1.433 (5)	C10A—C11A	1.373 (7)
C12B—C15B	1.528 (6)	C10A—H10A	0.9500
N2B—C18B	1.415 (7)	C11A—C12A	1.394 (7)
N2B—C17B	1.427 (6)	C11A—O11A	1.427 (6)
N2B—S4B	1.620 (4)	C12A—C15A	1.529 (6)
C15B—C16B	1.494 (7)	N2A—C18A	1.422 (6)
C15B—C19B	1.509 (7)	N2A—C17A	1.427 (6)
C15B—H15B	1.0000	N2A—S4A	1.619 (4)
C16B—C17B	1.310 (6)	C15A—C16A	1.509 (6)
C16B—H16B	0.9500	C15A—C19A	1.516 (6)
C17B—H17B	0.9500	C15A—H15A	1.0000
C18B—C19B	1.312 (7)	C16A—C17A	1.315 (6)

C18B—H18B	0.9500	C16A—H16A	0.9500
C19B—H19B	0.9500	C17A—H17A	0.9500
S1B—O1B	1.409 (4)	C18A—C19A	1.312 (6)
S1B—O2B	1.417 (4)	C18A—H18A	0.9500
S1B—C1B	1.834 (7)	C19A—H19A	0.9500
C1B—F2B	1.316 (8)	S1A—O1A	1.409 (4)
C1B—F1B	1.327 (7)	S1A—O2A	1.415 (4)
C1B—F3B	1.331 (7)	S1A—C1A	1.854 (7)
O3B—S2B	1.458 (5)	C1A—F2A	1.305 (8)
O3B—S2B'	1.539 (6)	C1A—F1A	1.316 (7)
S2B—O4B	1.386 (7)	C1A—F3A	1.335 (7)
S2B—O5B	1.416 (9)	O3A—S2A	1.579 (3)
S2B—C13B	1.878 (15)	S2A—O5A	1.396 (4)
C13B—F6B	1.216 (11)	S2A—O4A	1.404 (4)
C13B—F4B	1.262 (13)	S2A—C13A	1.833 (6)
C13B—F5B	1.302 (11)	C13A—F6A	1.236 (7)
S2B'—O4B'	1.420 (10)	C13A—F4A	1.293 (6)
S2B'—O5B'	1.481 (12)	C13A—F5A	1.355 (8)
S2B'—C13'	1.832 (17)	O6A—S3A	1.589 (3)
C13'—F4B'	1.218 (13)	S3A—O8A	1.407 (4)
C13'—F5B'	1.267 (13)	S3A—O7A	1.418 (3)
C13'—F6B'	1.273 (14)	S3A—C14A	1.834 (5)
O6B—S3B	1.585 (3)	C14A—F9A	1.288 (7)
S3B—O8B	1.393 (4)	C14A—F8A	1.310 (6)
S3B—O7B	1.417 (4)	C14A—F7A	1.325 (7)
S3B—C14B	1.815 (6)	S4A—O10A	1.407 (4)
C14B—F7B	1.268 (8)	S4A—O9A	1.415 (4)
C14B—F9B	1.298 (8)	S4A—C20A	1.832 (6)
C14B—F8B	1.317 (7)	C20A—F11A	1.311 (7)
S4B—O10B	1.405 (5)	C20A—F12A	1.321 (7)
S4B—O9B	1.410 (5)	C20A—F10A	1.330 (7)
S4B—C20B	1.825 (6)	O11A—S5A	1.571 (3)
C20B—F12B	1.310 (6)	S5A—O13A	1.398 (4)
C20B—F11B	1.318 (9)	S5A—O12A	1.419 (5)
C20B—F10B	1.327 (9)	S5A—C21A	1.825 (6)
O11B—S5B	1.577 (4)	C21A—F14A	1.297 (7)
S5B—O13B	1.397 (5)	C21A—F13A	1.299 (7)
S5B—O12B	1.409 (4)	C21A—F15A	1.320 (7)
S5B—C21B	1.828 (6)		
C2B—N1B—C6B	117.7 (4)	O11B—S5B—C21B	100.5 (2)
C2B—N1B—S1B	121.8 (3)	F13B—C21B—F14B	108.3 (5)
C6B—N1B—S1B	120.5 (3)	F13B—C21B—F15B	109.9 (6)
C3B—C2B—N1B	121.1 (4)	F14B—C21B—F15B	108.2 (5)
C3B—C2B—H2B	119.4	F13B—C21B—S5B	110.6 (4)
N1B—C2B—H2B	119.4	F14B—C21B—S5B	109.2 (5)
C2B—C3B—C4B	122.7 (4)	F15B—C21B—S5B	110.7 (4)
C2B—C3B—H3B	118.6	C2A—N1A—C6A	118.2 (4)
C4B—C3B—H3B	118.6	C2A—N1A—S1A	120.4 (3)
C3B—C4B—C5B	109.1 (4)	C6A—N1A—S1A	121.1 (3)

C3B—C4B—C8B	112.7 (4)	C3A—C2A—N1A	122.1 (4)
C5B—C4B—C8B	112.4 (4)	C3A—C2A—H2A	118.9
C3B—C4B—H4B	107.5	N1A—C2A—H2A	118.9
C5B—C4B—H4B	107.5	C2A—C3A—C4A	123.4 (4)
C8B—C4B—H4B	107.5	C2A—C3A—H3A	118.3
C6B—C5B—C4B	123.0 (4)	C4A—C3A—H3A	118.3
C6B—C5B—H5B	118.5	C5A—C4A—C3A	110.5 (4)
C4B—C5B—H5B	118.5	C5A—C4A—C8A	111.9 (4)
C5B—C6B—N1B	120.5 (4)	C3A—C4A—C8A	112.0 (4)
C5B—C6B—H6B	119.7	C5A—C4A—H4A	107.4
N1B—C6B—H6B	119.7	C3A—C4A—H4A	107.4
C8B—C7B—C12B	125.7 (4)	C8A—C4A—H4A	107.4
C8B—C7B—O6B	116.6 (4)	C6A—C5A—C4A	124.1 (4)
C12B—C7B—O6B	117.5 (4)	C6A—C5A—H5A	118.0
C7B—C8B—C9B	114.5 (4)	C4A—C5A—H5A	118.0
C7B—C8B—C4B	123.5 (4)	C5A—C6A—N1A	121.7 (4)
C9B—C8B—C4B	122.1 (4)	C5A—C6A—H6A	119.2
C10B—C9B—C8B	123.4 (4)	N1A—C6A—H6A	119.2
C10B—C9B—O3B	120.8 (4)	C12A—C7A—C8A	125.2 (4)
C8B—C9B—O3B	115.8 (4)	C12A—C7A—O6A	117.0 (4)
C11B—C10B—C9B	118.0 (5)	C8A—C7A—O6A	117.7 (4)
C11B—C10B—H10B	121.0	C9A—C8A—C7A	114.8 (4)
C9B—C10B—H10B	121.0	C9A—C8A—C4A	122.2 (4)
C10B—C11B—C12B	124.1 (4)	C7A—C8A—C4A	122.9 (4)
C10B—C11B—O11B	118.4 (4)	C8A—C9A—C10A	123.6 (4)
C12B—C11B—O11B	117.1 (4)	C8A—C9A—O3A	118.5 (4)
C11B—C12B—C7B	114.3 (4)	C10A—C9A—O3A	117.9 (4)
C11B—C12B—C15B	123.1 (4)	C11A—C10A—C9A	117.8 (5)
C7B—C12B—C15B	122.6 (4)	C11A—C10A—H10A	121.1
C18B—N2B—C17B	117.6 (4)	C9A—C10A—H10A	121.1
C18B—N2B—S4B	121.3 (3)	C10A—C11A—C12A	123.5 (4)
C17B—N2B—S4B	120.5 (3)	C10A—C11A—O11A	118.2 (4)
C16B—C15B—C19B	110.0 (4)	C12A—C11A—O11A	118.0 (4)
C16B—C15B—C12B	113.1 (4)	C11A—C12A—C7A	114.8 (4)
C19B—C15B—C12B	111.7 (4)	C11A—C12A—C15A	122.3 (4)
C16B—C15B—H15B	107.3	C7A—C12A—C15A	122.9 (4)
C19B—C15B—H15B	107.3	C18A—N2A—C17A	117.3 (4)
C12B—C15B—H15B	107.3	C18A—N2A—S4A	121.2 (3)
C17B—C16B—C15B	124.1 (5)	C17A—N2A—S4A	121.4 (3)
C17B—C16B—H16B	118.0	C16A—C15A—C19A	109.4 (3)
C15B—C16B—H16B	118.0	C16A—C15A—C12A	111.8 (3)
C16B—C17B—N2B	121.9 (4)	C19A—C15A—C12A	113.1 (4)
C16B—C17B—H17B	119.0	C16A—C15A—H15A	107.5
N2B—C17B—H17B	119.0	C19A—C15A—H15A	107.5
C19B—C18B—N2B	121.7 (5)	C12A—C15A—H15A	107.5
C19B—C18B—H18B	119.2	C17A—C16A—C15A	122.8 (4)
N2B—C18B—H18B	119.2	C17A—C16A—H16A	118.6
C18B—C19B—C15B	124.1 (5)	C15A—C16A—H16A	118.6
C18B—C19B—H19B	118.0	C16A—C17A—N2A	120.4 (4)

C15B—C19B—H19B	118.0	C16A—C17A—H17A	119.8
O1B—S1B—O2B	123.3 (3)	N2A—C17A—H17A	119.8
O1B—S1B—N1B	109.2 (2)	C19A—C18A—N2A	121.6 (4)
O2B—S1B—N1B	108.7 (2)	C19A—C18A—H18A	119.2
O1B—S1B—C1B	105.4 (3)	N2A—C18A—H18A	119.2
O2B—S1B—C1B	104.9 (3)	C18A—C19A—C15A	121.7 (4)
N1B—S1B—C1B	103.3 (3)	C18A—C19A—H19A	119.1
F2B—C1B—F1B	109.8 (6)	C15A—C19A—H19A	119.1
F2B—C1B—F3B	109.8 (6)	O1A—S1A—O2A	123.0 (3)
F1B—C1B—F3B	108.4 (6)	O1A—S1A—N1A	109.3 (2)
F2B—C1B—S1B	110.9 (4)	O2A—S1A—N1A	109.6 (2)
F1B—C1B—S1B	108.6 (5)	O1A—S1A—C1A	105.5 (3)
F3B—C1B—S1B	109.3 (5)	O2A—S1A—C1A	105.4 (3)
C9B—O3B—S2B	126.6 (4)	N1A—S1A—C1A	101.8 (3)
C9B—O3B—S2B'	134.3 (3)	F2A—C1A—F1A	109.7 (6)
S2B—O3B—S2B'	51.0 (2)	F2A—C1A—F3A	109.2 (6)
O4B—S2B—O5B	123.1 (7)	F1A—C1A—F3A	108.4 (5)
O4B—S2B—O3B	109.5 (5)	F2A—C1A—S1A	110.9 (4)
O5B—S2B—O3B	107.8 (4)	F1A—C1A—S1A	110.1 (5)
O4B—S2B—C13B	104.2 (5)	F3A—C1A—S1A	108.5 (5)
O5B—S2B—C13B	107.7 (7)	C9A—O3A—S2A	120.9 (3)
O3B—S2B—C13B	102.6 (4)	O5A—S2A—O4A	122.2 (3)
F6B—C13B—F4B	107.4 (11)	O5A—S2A—O3A	110.9 (2)
F6B—C13B—F5B	108.2 (9)	O4A—S2A—O3A	106.7 (2)
F4B—C13B—F5B	111.3 (12)	O5A—S2A—C13A	109.1 (3)
F6B—C13B—S2B	115.8 (11)	O4A—S2A—C13A	104.7 (3)
F4B—C13B—S2B	107.4 (7)	O3A—S2A—C13A	100.9 (2)
F5B—C13B—S2B	106.7 (9)	F6A—C13A—F4A	111.8 (6)
O4B'—S2B'—O5B'	121.6 (9)	F6A—C13A—F5A	108.9 (7)
O4B'—S2B'—O3B	104.0 (8)	F4A—C13A—F5A	105.2 (5)
O5B'—S2B'—O3B	109.2 (6)	F6A—C13A—S2A	112.6 (5)
O4B'—S2B'—C13'	106.4 (7)	F4A—C13A—S2A	109.8 (4)
O5B'—S2B'—C13'	106.3 (8)	F5A—C13A—S2A	108.2 (4)
O3B—S2B'—C13'	108.7 (5)	C7A—O6A—S3A	119.7 (2)
F4B'—C13'—F5B'	107.2 (12)	O8A—S3A—O7A	121.6 (2)
F4B'—C13'—F6B'	102.9 (12)	O8A—S3A—O6A	111.22 (19)
F5B'—C13'—F6B'	112.9 (13)	O7A—S3A—O6A	110.36 (19)
F4B'—C13'—S2B'	114.3 (12)	O8A—S3A—C14A	107.6 (3)
F5B'—C13'—S2B'	108.6 (10)	O7A—S3A—C14A	107.5 (3)
F6B'—C13'—S2B'	110.9 (10)	O6A—S3A—C14A	95.0 (2)
C7B—O6B—S3B	118.6 (3)	F9A—C14A—F8A	111.5 (5)
O8B—S3B—O7B	121.0 (3)	F9A—C14A—F7A	108.8 (5)
O8B—S3B—O6B	111.5 (2)	F8A—C14A—F7A	108.7 (5)
O7B—S3B—O6B	110.4 (2)	F9A—C14A—S3A	110.9 (4)
O8B—S3B—C14B	109.6 (3)	F8A—C14A—S3A	106.9 (4)
O7B—S3B—C14B	105.7 (3)	F7A—C14A—S3A	109.9 (4)
O6B—S3B—C14B	95.3 (2)	O10A—S4A—O9A	123.2 (3)
F7B—C14B—F9B	109.9 (6)	O10A—S4A—N2A	109.5 (2)
F7B—C14B—F8B	109.3 (5)	O9A—S4A—N2A	108.2 (2)

F9B—C14B—F8B	110.1 (6)	O10A—S4A—C20A	105.8 (3)
F7B—C14B—S3B	111.6 (5)	O9A—S4A—C20A	105.5 (3)
F9B—C14B—S3B	109.3 (5)	N2A—S4A—C20A	102.7 (3)
F8B—C14B—S3B	106.6 (4)	F11A—C20A—F12A	110.0 (6)
O10B—S4B—O9B	123.1 (3)	F11A—C20A—F10A	108.4 (5)
O10B—S4B—N2B	109.0 (2)	F12A—C20A—F10A	109.2 (5)
O9B—S4B—N2B	109.2 (2)	F11A—C20A—S4A	110.2 (4)
O10B—S4B—C20B	104.7 (3)	F12A—C20A—S4A	109.8 (4)
O9B—S4B—C20B	106.2 (3)	F10A—C20A—S4A	109.4 (5)
N2B—S4B—C20B	102.7 (2)	C11A—O11A—S5A	121.3 (3)
F12B—C20B—F11B	109.2 (6)	O13A—S5A—O12A	124.5 (3)
F12B—C20B—F10B	109.1 (6)	O13A—S5A—O11A	110.2 (2)
F11B—C20B—F10B	107.6 (6)	O12A—S5A—O11A	107.0 (3)
F12B—C20B—S4B	111.2 (4)	O13A—S5A—C21A	108.2 (3)
F11B—C20B—S4B	110.0 (5)	O12A—S5A—C21A	104.2 (3)
F10B—C20B—S4B	109.7 (5)	O11A—S5A—C21A	99.9 (2)
C11B—O11B—S5B	122.8 (3)	F14A—C21A—F13A	109.6 (5)
O13B—S5B—O12B	124.4 (3)	F14A—C21A—F15A	107.6 (6)
O13B—S5B—O11B	110.9 (2)	F13A—C21A—F15A	108.0 (5)
O12B—S5B—O11B	106.5 (3)	F14A—C21A—S5A	111.4 (4)
O13B—S5B—C21B	108.3 (3)	F13A—C21A—S5A	109.6 (4)
O12B—S5B—C21B	103.5 (3)	F15A—C21A—S5A	110.6 (4)
C6B—N1B—C2B—C3B	−16.1 (7)	C11B—O11B—S5B—C21B	106.7 (4)
S1B—N1B—C2B—C3B	166.1 (4)	O13B—S5B—C21B—F13B	173.8 (4)
N1B—C2B—C3B—C4B	−4.2 (8)	O12B—S5B—C21B—F13B	−52.5 (5)
C2B—C3B—C4B—C5B	21.5 (7)	O11B—S5B—C21B—F13B	57.5 (4)
C2B—C3B—C4B—C8B	147.0 (5)	O13B—S5B—C21B—F14B	−67.1 (5)
C3B—C4B—C5B—C6B	−21.0 (7)	O12B—S5B—C21B—F14B	66.6 (5)
C8B—C4B—C5B—C6B	−146.7 (5)	O11B—S5B—C21B—F14B	176.5 (4)
C4B—C5B—C6B—N1B	3.3 (8)	O13B—S5B—C21B—F15B	51.8 (6)
C2B—N1B—C6B—C5B	16.5 (7)	O12B—S5B—C21B—F15B	−174.5 (5)
S1B—N1B—C6B—C5B	−165.7 (4)	O11B—S5B—C21B—F15B	−64.5 (5)
C12B—C7B—C8B—C9B	3.9 (7)	C6A—N1A—C2A—C3A	1.6 (7)
O6B—C7B—C8B—C9B	178.8 (4)	S1A—N1A—C2A—C3A	174.6 (4)
C12B—C7B—C8B—C4B	−176.1 (4)	N1A—C2A—C3A—C4A	−0.7 (8)
O6B—C7B—C8B—C4B	−1.3 (6)	C2A—C3A—C4A—C5A	−0.4 (7)
C3B—C4B—C8B—C7B	118.3 (5)	C2A—C3A—C4A—C8A	125.0 (5)
C5B—C4B—C8B—C7B	−118.0 (5)	C3A—C4A—C5A—C6A	0.7 (7)
C3B—C4B—C8B—C9B	−61.8 (6)	C8A—C4A—C5A—C6A	−124.8 (5)
C5B—C4B—C8B—C9B	61.9 (6)	C4A—C5A—C6A—N1A	0.1 (8)
C7B—C8B—C9B—C10B	−2.0 (8)	C2A—N1A—C6A—C5A	−1.3 (7)
C4B—C8B—C9B—C10B	178.1 (5)	S1A—N1A—C6A—C5A	−174.3 (4)
C7B—C8B—C9B—O3B	175.9 (4)	C12A—C7A—C8A—C9A	−1.8 (6)
C4B—C8B—C9B—O3B	−4.0 (7)	O6A—C7A—C8A—C9A	−177.3 (3)
C8B—C9B—C10B—C11B	0.0 (9)	C12A—C7A—C8A—C4A	175.3 (4)
O3B—C9B—C10B—C11B	−177.8 (5)	O6A—C7A—C8A—C4A	−0.2 (6)
C9B—C10B—C11B—C12B	0.4 (9)	C5A—C4A—C8A—C9A	53.5 (5)
C9B—C10B—C11B—O11B	−172.6 (5)	C3A—C4A—C8A—C9A	−71.2 (5)
C10B—C11B—C12B—C7B	1.2 (7)	C5A—C4A—C8A—C7A	−123.4 (4)

O11B—C11B—C12B—C7B	174.3 (4)	C3A—C4A—C8A—C7A	111.9 (5)
C10B—C11B—C12B—C15B	−178.1 (5)	C7A—C8A—C9A—C10A	5.1 (6)
O11B—C11B—C12B—C15B	−5.0 (7)	C4A—C8A—C9A—C10A	−172.0 (4)
C8B—C7B—C12B—C11B	−3.6 (7)	C7A—C8A—C9A—O3A	−178.6 (4)
O6B—C7B—C12B—C11B	−178.4 (4)	C4A—C8A—C9A—O3A	4.3 (6)
C8B—C7B—C12B—C15B	175.7 (4)	C8A—C9A—C10A—C11A	−5.0 (7)
O6B—C7B—C12B—C15B	0.9 (6)	O3A—C9A—C10A—C11A	178.6 (4)
C11B—C12B—C15B—C16B	60.9 (6)	C9A—C10A—C11A—C12A	1.4 (7)
C7B—C12B—C15B—C16B	−118.3 (5)	C9A—C10A—C11A—O11A	175.5 (4)
C11B—C12B—C15B—C19B	−63.8 (6)	C10A—C11A—C12A—C7A	1.6 (6)
C7B—C12B—C15B—C19B	117.0 (5)	O11A—C11A—C12A—C7A	−172.5 (4)
C19B—C15B—C16B—C17B	−8.2 (7)	C10A—C11A—C12A—C15A	−178.4 (4)
C12B—C15B—C16B—C17B	−133.8 (5)	O11A—C11A—C12A—C15A	7.5 (6)
C15B—C16B—C17B—N2B	2.4 (8)	C8A—C7A—C12A—C11A	−1.4 (6)
C18B—N2B—C17B—C16B	4.7 (7)	O6A—C7A—C12A—C11A	174.1 (4)
S4B—N2B—C17B—C16B	−166.7 (4)	C8A—C7A—C12A—C15A	178.6 (4)
C17B—N2B—C18B—C19B	−4.8 (7)	O6A—C7A—C12A—C15A	−5.9 (6)
S4B—N2B—C18B—C19B	166.5 (4)	C11A—C12A—C15A—C16A	71.9 (5)
N2B—C18B—C19B—C15B	−1.9 (8)	C7A—C12A—C15A—C16A	−108.1 (5)
C16B—C15B—C19B—C18B	8.0 (7)	C11A—C12A—C15A—C19A	−52.1 (5)
C12B—C15B—C19B—C18B	134.4 (5)	C7A—C12A—C15A—C19A	128.0 (4)
C2B—N1B—S1B—O1B	−158.4 (4)	C19A—C15A—C16A—C17A	−23.1 (6)
C6B—N1B—S1B—O1B	23.9 (5)	C12A—C15A—C16A—C17A	−149.1 (4)
C2B—N1B—S1B—O2B	−21.3 (5)	C15A—C16A—C17A—N2A	4.4 (7)
C6B—N1B—S1B—O2B	161.0 (4)	C18A—N2A—C17A—C16A	16.9 (7)
C2B—N1B—S1B—C1B	89.8 (5)	S4A—N2A—C17A—C16A	−165.9 (4)
C6B—N1B—S1B—C1B	−87.9 (5)	C17A—N2A—C18A—C19A	−16.8 (7)
O1B—S1B—C1B—F2B	−174.1 (4)	S4A—N2A—C18A—C19A	165.9 (4)
O2B—S1B—C1B—F2B	54.4 (5)	N2A—C18A—C19A—C15A	−4.5 (7)
N1B—S1B—C1B—F2B	−59.5 (5)	C16A—C15A—C19A—C18A	23.1 (6)
O1B—S1B—C1B—F1B	65.2 (5)	C12A—C15A—C19A—C18A	148.3 (4)
O2B—S1B—C1B—F1B	−66.4 (6)	C2A—N1A—S1A—O1A	159.8 (4)
N1B—S1B—C1B—F1B	179.8 (5)	C6A—N1A—S1A—O1A	−27.4 (5)
O1B—S1B—C1B—F3B	−52.9 (5)	C2A—N1A—S1A—O2A	22.3 (5)
O2B—S1B—C1B—F3B	175.5 (5)	C6A—N1A—S1A—O2A	−164.9 (4)
N1B—S1B—C1B—F3B	61.7 (5)	C2A—N1A—S1A—C1A	−88.9 (5)
C10B—C9B—O3B—S2B	−61.6 (7)	C6A—N1A—S1A—C1A	83.9 (5)
C8B—C9B—O3B—S2B	120.4 (5)	O1A—S1A—C1A—F2A	171.9 (4)
C10B—C9B—O3B—S2B'	6.5 (9)	O2A—S1A—C1A—F2A	−56.7 (5)
C8B—C9B—O3B—S2B'	−171.4 (5)	N1A—S1A—C1A—F2A	57.7 (5)
C9B—O3B—S2B—O4B	−139.5 (6)	O1A—S1A—C1A—F1A	−66.5 (6)
S2B'—O3B—S2B—O4B	99.3 (5)	O2A—S1A—C1A—F1A	65.0 (6)
C9B—O3B—S2B—O5B	−3.3 (8)	N1A—S1A—C1A—F1A	179.4 (5)
S2B'—O3B—S2B—O5B	−124.4 (7)	O1A—S1A—C1A—F3A	51.9 (5)
C9B—O3B—S2B—C13B	110.2 (5)	O2A—S1A—C1A—F3A	−176.6 (4)
S2B'—O3B—S2B—C13B	−10.9 (4)	N1A—S1A—C1A—F3A	−62.2 (5)
O4B—S2B—C13B—F6B	73.8 (10)	C8A—C9A—O3A—S2A	106.1 (4)
O5B—S2B—C13B—F6B	−58.5 (9)	C10A—C9A—O3A—S2A	−77.4 (5)
O3B—S2B—C13B—F6B	−172.1 (8)	C9A—O3A—S2A—O5A	−14.4 (4)

O4B—S2B—C13B—F4B	−46.3 (9)	C9A—O3A—S2A—O4A	−149.7 (4)
O5B—S2B—C13B—F4B	−178.5 (7)	C9A—O3A—S2A—C13A	101.2 (4)
O3B—S2B—C13B—F4B	67.9 (7)	O5A—S2A—C13A—F6A	156.4 (6)
O4B—S2B—C13B—F5B	−165.7 (8)	O4A—S2A—C13A—F6A	−71.2 (7)
O5B—S2B—C13B—F5B	62.0 (9)	O3A—S2A—C13A—F6A	39.5 (7)
O3B—S2B—C13B—F5B	−51.6 (8)	O5A—S2A—C13A—F4A	−78.4 (5)
C9B—O3B—S2B'—O4B'	162.9 (8)	O4A—S2A—C13A—F4A	54.1 (5)
S2B—O3B—S2B'—O4B'	−90.8 (7)	O3A—S2A—C13A—F4A	164.8 (4)
C9B—O3B—S2B'—O5B'	31.6 (9)	O5A—S2A—C13A—F5A	35.9 (5)
S2B—O3B—S2B'—O5B'	137.9 (6)	O4A—S2A—C13A—F5A	168.4 (4)
C9B—O3B—S2B'—C13'	−84.0 (7)	O3A—S2A—C13A—F5A	−80.9 (4)
S2B—O3B—S2B'—C13'	22.3 (4)	C12A—C7A—O6A—S3A	93.0 (4)
O4B'—S2B'—C13'—F4B'	−68.0 (13)	C8A—C7A—O6A—S3A	−91.1 (4)
O5B'—S2B'—C13'—F4B'	63.0 (11)	C7A—O6A—S3A—O8A	61.3 (3)
O3B—S2B'—C13'—F4B'	−179.5 (8)	C7A—O6A—S3A—O7A	−76.8 (3)
O4B'—S2B'—C13'—F5B'	172.4 (12)	C7A—O6A—S3A—C14A	172.4 (3)
O5B'—S2B'—C13'—F5B'	−56.6 (11)	O8A—S3A—C14A—F9A	54.5 (5)
O3B—S2B'—C13'—F5B'	60.9 (10)	O7A—S3A—C14A—F9A	−172.8 (4)
O4B'—S2B'—C13'—F6B'	47.8 (13)	O6A—S3A—C14A—F9A	−59.6 (5)
O5B'—S2B'—C13'—F6B'	178.8 (9)	O8A—S3A—C14A—F8A	−67.3 (5)
O3B—S2B'—C13'—F6B'	−63.7 (9)	O7A—S3A—C14A—F8A	65.4 (5)
C8B—C7B—O6B—S3B	92.6 (4)	O6A—S3A—C14A—F8A	178.6 (4)
C12B—C7B—O6B—S3B	−92.1 (4)	O8A—S3A—C14A—F7A	174.9 (4)
C7B—O6B—S3B—O8B	−62.2 (4)	O7A—S3A—C14A—F7A	−52.5 (4)
C7B—O6B—S3B—O7B	75.4 (4)	O6A—S3A—C14A—F7A	60.8 (4)
C7B—O6B—S3B—C14B	−175.7 (3)	C18A—N2A—S4A—O10A	−159.2 (4)
O8B—S3B—C14B—F7B	−173.3 (5)	C17A—N2A—S4A—O10A	23.7 (4)
O7B—S3B—C14B—F7B	54.8 (5)	C18A—N2A—S4A—O9A	−22.4 (5)
O6B—S3B—C14B—F7B	−58.2 (5)	C17A—N2A—S4A—O9A	160.4 (4)
O8B—S3B—C14B—F9B	−51.5 (5)	C18A—N2A—S4A—C20A	88.8 (4)
O7B—S3B—C14B—F9B	176.6 (5)	C17A—N2A—S4A—C20A	−88.4 (4)
O6B—S3B—C14B—F9B	63.6 (5)	O10A—S4A—C20A—F11A	−57.6 (5)
O8B—S3B—C14B—F8B	67.5 (5)	O9A—S4A—C20A—F11A	170.4 (4)
O7B—S3B—C14B—F8B	−64.4 (5)	N2A—S4A—C20A—F11A	57.2 (5)
O6B—S3B—C14B—F8B	−177.4 (4)	O10A—S4A—C20A—F12A	−178.8 (4)
C18B—N2B—S4B—O10B	25.6 (5)	O9A—S4A—C20A—F12A	49.2 (5)
C17B—N2B—S4B—O10B	−163.4 (4)	N2A—S4A—C20A—F12A	−64.1 (5)
C18B—N2B—S4B—O9B	162.5 (4)	O10A—S4A—C20A—F10A	61.4 (5)
C17B—N2B—S4B—O9B	−26.4 (5)	O9A—S4A—C20A—F10A	−70.6 (5)
C18B—N2B—S4B—C20B	−85.1 (5)	N2A—S4A—C20A—F10A	176.2 (4)
C17B—N2B—S4B—C20B	86.0 (5)	C10A—C11A—O11A—S5A	83.5 (5)
O10B—S4B—C20B—F12B	65.6 (6)	C12A—C11A—O11A—S5A	−102.0 (4)
O9B—S4B—C20B—F12B	−66.0 (6)	C11A—O11A—S5A—O13A	1.0 (4)
N2B—S4B—C20B—F12B	179.4 (6)	C11A—O11A—S5A—O12A	139.1 (4)
O10B—S4B—C20B—F11B	−173.3 (5)	C11A—O11A—S5A—C21A	−112.7 (4)
O9B—S4B—C20B—F11B	55.1 (6)	O13A—S5A—C21A—F14A	−174.7 (4)
N2B—S4B—C20B—F11B	−59.5 (6)	O12A—S5A—C21A—F14A	51.0 (5)
O10B—S4B—C20B—F10B	−55.3 (5)	O11A—S5A—C21A—F14A	−59.5 (5)
O9B—S4B—C20B—F10B	173.2 (4)	O13A—S5A—C21A—F13A	63.8 (5)

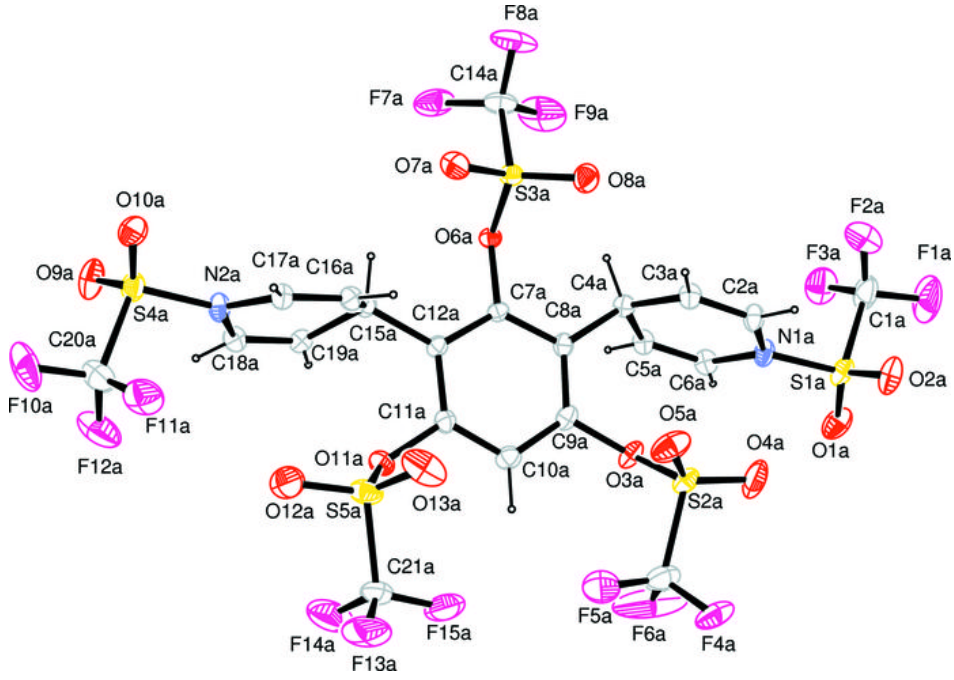
N2B—S4B—C20B—F10B	58.6 (5)	O12A—S5A—C21A—F13A	−70.4 (5)
C10B—C11B—O11B—S5B	−75.5 (6)	O11A—S5A—C21A—F13A	179.1 (4)
C12B—C11B—O11B—S5B	111.0 (4)	O13A—S5A—C21A—F15A	−55.2 (5)
C11B—O11B—S5B—O13B	−7.7 (5)	O12A—S5A—C21A—F15A	170.6 (5)
C11B—O11B—S5B—O12B	−145.7 (4)	O11A—S5A—C21A—F15A	60.1 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5A—H5A···O9A^{i}	0.95	2.64	3.368 (6)	134
C18A—H18A···O6A^{i}	0.95	2.66	3.471 (5)	144
C18A—H18A···F7A^{i}	0.95	2.60	3.385 (6)	140
C2A—H2A···O13A^{ii}	0.95	2.48	3.176 (6)	130
C3A—H3A···O13A^{ii}	0.95	2.66	3.265 (6)	122
C6A—H6A···O12B^{iii}	0.95	2.51	3.356 (6)	148
C2B—H2B···O7A^{i}	0.95	2.55	3.501 (6)	179
C17B—H17B···O11B^{iv}	0.95	2.52	3.471 (6)	175
C5B—H5B···O7B^{iii}	0.95	2.38	3.293 (6)	162
C19B—H19B···O8B^{iii}	0.95	2.48	3.335 (6)	151

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

Fig. 1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S3a
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C10a
O3a
S2a
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F5a
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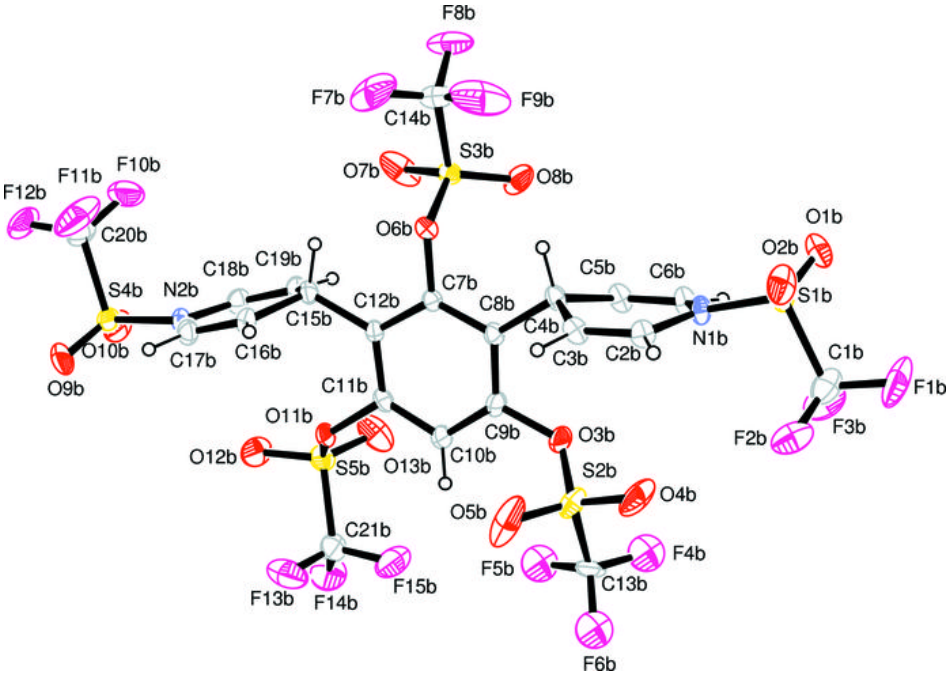
F14a
F15a
F13a

Fig. 2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C10b
S2b
O4b
O5b
C21b
F4b
F5b
C13b
F15b
F13b
F14b
F6b

Fig. 3