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2,5,8,11-Tetramethyl-2,5,8,11-tetraazadodecane-2,11-diium bis[hydroxytris(pentafluorophenyl)-borate] benzene 2.5-solvate

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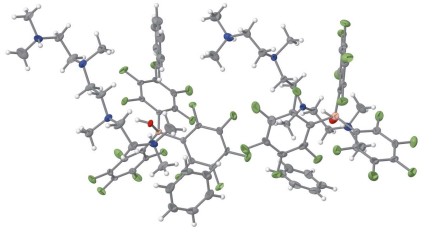
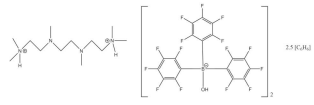
Structural data: full structural data are available from iucrdata.iucr.org

The title compound of overall stoichiometry, $C_{12}H_{32}N_4^{2+}\cdot 2C_{18}HBF_{15}O^{-}\cdot 2.5C_6H_6$, crystallizes in the triclinic space group $P\overline{1}$ and the stoichiometry of the asymmetric unit consists of two $[C_{12}H_{32}N_4]^{2+}$ dications, two $[C_{18}HBF_{15}O]^{-}$ anions, and 2.5 molecules of benzene as solvate. The dications are both at half occupancy and located on a center of inversion, as is one of the benzene solvate molecules. In the two anions the O—H groups participate in different hydrogen-bonding schemes. In anion *A*, the OH group participates in a bifurcated $2R_2^2(6)$ scheme with F atoms on different rings of an adjacent hydroxy[tris(pentafluorophenyl)]borate moiety with an additional N—H···O hydrogen bond with a dication. For anion *B*, the OH group participates in a single O—H···F $R_2^2(6)$ scheme. In addition, there are both O—H···N and N—H···O hydrogen bonds involving dication *D* and anion *B* in an $R_2^2(7)$ motif. There are numerous C—H···π interactions between the dications and all the three benzene solvate molecules. For solvate 3, the C—H···π interactions are on both sides of the benzene ring and link both dications and solvate into a linear chain in the *c*-axis direction.

3D view



Chemical scheme



Structure description

The title compound crystallizes in the triclinic space group $P\overline{1}$ and the stoichiometry of the asymmetric unit consists of two half $[C_{12}H_{32}N_4]^{2+}$ dications, two $[C_{18}HBF_{15}O]^{-}$ anions, and 2.5 molecules of benzene as solvate (see Fig. 1). Both dications are located on a center of inversion, as is one of the benzene solvate molecules. Tris(pentafluorophenyl)-borane is a well-known strong Lewis acid and is used extensively to promote the

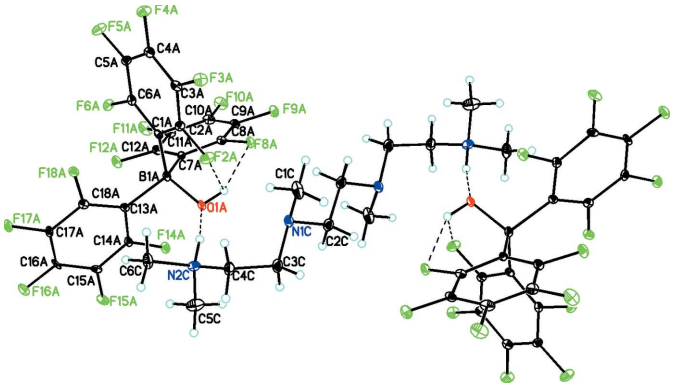


Figure 1
Diagram showing the structure of the $[C_{12}H_{32}N_4]^{2+}$ dication (*C*) and two $[C_{18}HBF_{15}O]^{+}$ anions (*A*). Only symmetry-independent atoms are labelled. Benzene solvate molecules are omitted for clarity. Hydrogen bonds are shown with dashed lines. Atomic displacement parameters are at the 30% probability level.

formation of highly active cationic catalysts for olefin polymerization (Chen & Marks, 2000) as well as a Lewis acid partner for making frustrated Lewis pairs (FLPs) (Berkefeld *et al.*, 2010). As a strong Lewis acid, it readily forms salts with bases such as amines. A search of the Cambridge Structural Database (CSD version 5.41, November 2019; Groom *et al.*, 2016) for structures containing amine salts of hydroxy[tris-(pentafluorophenyl)]borate gave 13 hits [DOJSAX (Peters *et al.*, 2008); GIZZIZ (Focante, Mercandelli *et al.*, 2006); ITULOA (Tao *et al.*, 2016); KERLUO (Duchateau *et al.*, 2000); MUQMUG (Drewitt *et al.*, 2002); OFAFUZ (Schneider *et al.*, 2018); OZUBUH (Kelsen *et al.*, 2011); PEGCUA (Focante, Camurati *et al.*, 2006); QIMKUS (Stibrany & Brant, 2001); RAQWAI (Saverio *et al.*, 2005); SEFDIR (Hewavitharanage *et al.*, 2005); UXIJIW, UXIJUI (Thakur *et al.*, 2016)]. However, there were no hits for the dication.

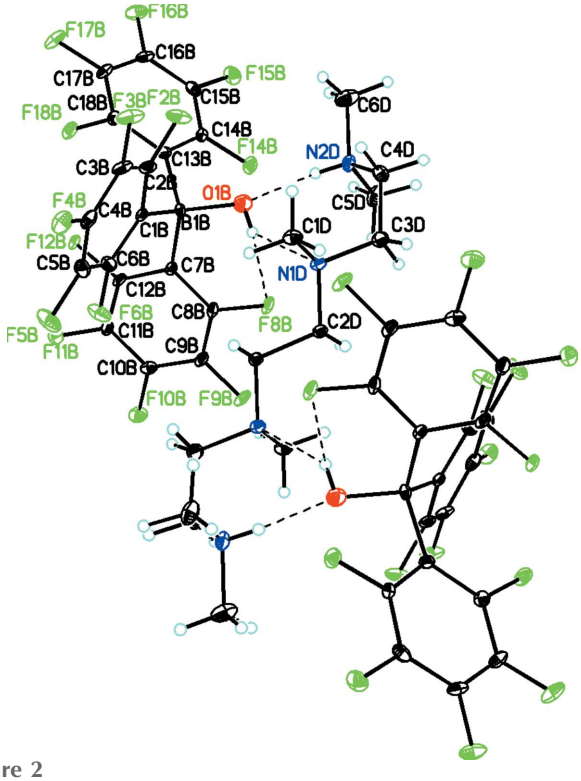


Figure 2
Diagram showing the structure of the $[C_{12}H_{32}N_4]^{2+}$ dication (*D*) and two $[C_{18}HBF_{15}O]^{+}$ anions (*B*). Only symmetry-independent atoms are labelled. Benzene solvate molecules are omitted for clarity. Hydrogen bonds are shown with dashed lines. Atomic displacement parameters are at the 30% probability level.

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

*Cg*4, *Cg*7–*Cg*9 are the centroids of the C1*B*–C6*B*, C11*S*–C16*S*, C21*S*–C26*S* and C31*S*–C33*S*/C31*S*′–C31*S*′ rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*A*—H1*A*···F8*A*	0.84	2.16	2.731 (3)	125
O1*B*—H1*B*···N1*D*	0.84	2.12	2.846 (4)	144
N2*C*—H2*C*···O1*A*	1.05 (4)	1.60 (4)	2.632 (4)	169 (3)
N2*D*—H2*D*···O1*B*	0.80 (4)	1.76 (4)	2.554 (5)	171 (4)
C2*C*—H2*CB*···F8*A*^{i}	0.99	2.46	3.435 (5)	168
C4*C*—H4*CA*···F6*A*^{ii}	0.99	2.40	3.191 (5)	137
C5*D*—H5*DC*···F14*B*	0.98	2.54	3.284 (5)	133
C32*S*—H32*A*···F10*B*^{iii}	0.95	2.52	3.133 (5)	123
C14*S*—H14*A*···*Cg*4^{iv}	0.95	2.95	3.779 (5)	147
C4*D*—H4*DA*···*Cg*7	0.99	2.73	3.620 (4)	150
C6*C*—H6*CB*···*Cg*9	0.98	2.74	3.689 (4)	163
C6*C*—H6*CB*···*Cg*9^{v}	0.98	2.74	3.689 (4)	163

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

In the present structure, the metrical parameters of both the 2-[(2-{[2-(dimethylammonio)ethyl]amino}ethyl)amino]-*N*,*N*,*N*-trimethylethan-1-aminium dications and hydroxy-[tris(pentafluorophenyl)]borate anions are in their usual ranges. The B—O distances for the two anions are 1.484 (5) and 1.487 (5) Å, which are in the normal range observed. In the two anions, the O—H groups participate in different hydrogen-bonding schemes (Table 1). In anion *A*, the OH group participates in a bifurcated $R_2^2(6)$ (Etter *et al.*, 1990) scheme with F atoms on different rings of an adjacent hydroxy[tris(pentafluorophenyl)]borate moiety with an additional N—H···O hydrogen bond with a dication (see Fig. 1). For anion *B*, the OH group participates in a single O—H···F $R_2^2(6)$ scheme (see Fig. 2). In addition, there are both O—

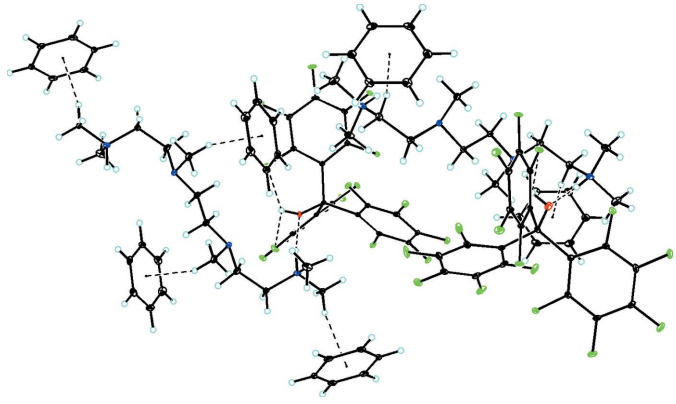


Figure 3
Diagram showing the numerous C—H···π interactions between the $[C_{12}H_{32}N_4]^{2+}$ dications and all the three benzene solvate molecules, also including the $[C_{18}HBF_{15}O]^{-}$ anions.

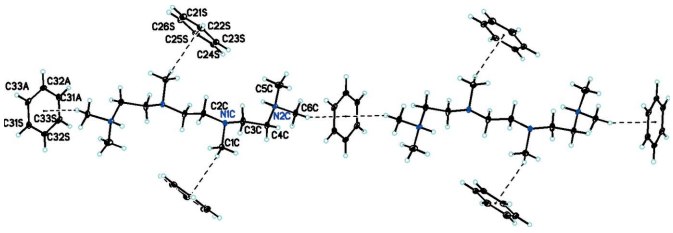


Figure 4
Diagram showing how the C—H···π interactions between the third benzene solvate molecule and cation *C*.

H···N and N—H···O hydrogen bonds involving cation *D* and anion *B* in a $R_2^2(7)$ motif.

While this structure contains numerous phenyl rings, there does not appear to be any π–π stacking. The closest is for the ring C7*A*–C12*A* with itself (symmetry code $1-x, 2-y, -z$) where the *CgI*_Perp distance is 2.8921 (15) Å but the slippage is 4.685 Å so there appears to be no stacking. However, there are numerous C—H···π interactions between the cations and all the three benzene solvate molecules (see Fig. 3). For solvate 3, the C—H···π interactions are on both sides of the benzene ring and link both cation and solvate into a linear chain in the *c*-axis direction (see Fig. 4). The packing is shown in Fig. 5.

Synthesis and crystallization

In a reaction bulb, hexamethyltriethylenetetramine (0.050 g, 0.22 mmol) was mixed with tris(pentafluorophenyl)borane (0.44 g, 0.86 mmol) in ~10 mL dry toluene in an argon-filled drybox. A yellowish brown mixture with two liquid phases resulted. On a vacuum line, the mixture was frozen and 1.72 mmol CO_2 was condensed in. After a day, solids began to form and the reaction was continued for several weeks. Some of the solids were flame sealed in an NMR tube with C_6D_6, but it was not soluble enough to obtain a spectrum. When the NMR tube was opened, crystals of the title compound were isolated. The oxygen atom must have come from the CO_2 and the proton must have come from either the toluene or the amine.

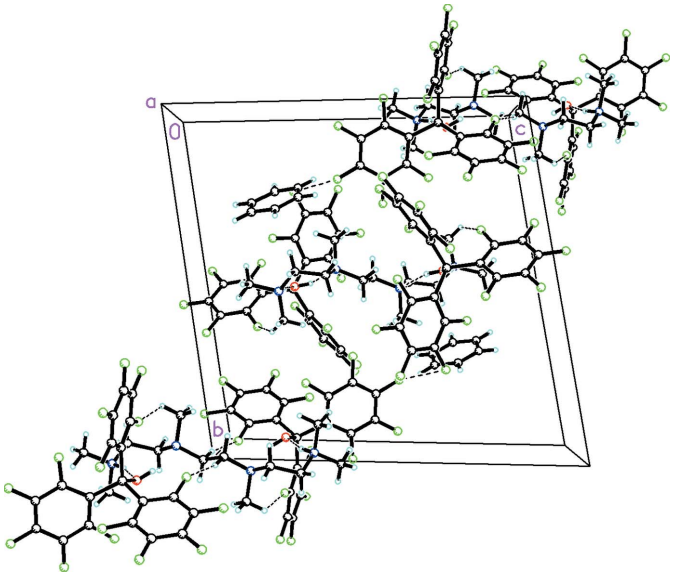


Figure 5
Packing diagram of the title compound.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{12}H_{32}N_4^{2+}\cdot 2C_{18}HBF_{15}O^-\cdot 2.5C_6H_6$
M_r	1485.68
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, b, c (Å)	10.4436 (5), 17.3961 (9), 17.8229 (9)
α, β, γ (°)	79.729 (3), 77.923 (3), 83.103 (3)
V (Å^3)	3104.1 (3)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.16
Crystal size (mm)	0.28 × 0.10 × 0.08
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.591, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	29409, 11027, 6339
R_{int}	0.097
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.600
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.061, 0.132, 1.00
No. of reflections	11027
No. of parameters	922
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.30, −0.39

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*) and *SHELXTL* (Sheldrick 2008).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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full crystallographic data

IUCrData (2022). **7**, x221049 [https://doi.org/10.1107/S2414314622010495]

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Crystal data

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M_r = 1485.68
Triclinic, $P\overline{1}$
a = 10.4436 (5) Å
b = 17.3961 (9) Å
c = 17.8229 (9) Å
α = 79.729 (3)°
β = 77.923 (3)°
γ = 83.103 (3)°
V = 3104.1 (3) Å^3
Z = 2
$F(000)$ = 1502
D_x = 1.590 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5245 reflections
θ = 2.8–28.3°
μ = 0.16 mm^{-1}
T = 100 K
Needle, colourless
0.28 × 0.10 × 0.08 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.591, T_{max} = 0.746
29409 measured reflections
11027 independent reflections
6339 reflections with $I > 2\sigma(I)$
R_{int} = 0.097
θ_{max} = 25.3°, θ_{min} = 2.5°
h = −12→12
k = −20→20
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.132
S = 1.00
11027 reflections
922 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0515P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

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. The structure was solved using SHELXT (Sheldrick, 2015*a*) and refined with *SHELXL2018*/3 (Sheldrick, 2015*b*). All hydrogen atoms were located in difference Fourier maps and the coordinates of those attached to N were refined with U_{iso}(H) = 1.2U_{eq}(N). For H atoms bonded to O the H—O—B—C torsion angles were refined with U_{iso}(H) = 1.2U_{eq}(O). Those attached to carbons were refined in idealized geometry using a riding model with with atomic displacement parameters of U_{iso}(H) = 1.2U_{eq}(C) [for CH_3, 1.5U_{eq}(C)] with C—H distances of 0.95 to 0.99 Å

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

	x	*y*	*z*	U_{iso}*/U_{eq}
F2A	0.7105 (2)	1.11156 (12)	0.17203 (14)	0.0324 (6)
F2B	0.5387 (2)	0.62060 (14)	0.75957 (12)	0.0414 (7)
F3A	0.5993 (2)	1.25327 (12)	0.13367 (13)	0.0291 (5)
F3B	0.5888 (3)	0.76050 (14)	0.67718 (13)	0.0449 (7)
F4A	0.3319 (2)	1.28043 (12)	0.15297 (13)	0.0330 (6)
F4B	0.7778 (2)	0.77305 (13)	0.54644 (14)	0.0405 (6)
F5A	0.1813 (2)	1.15904 (12)	0.21360 (14)	0.0357 (6)
F5B	0.9170 (3)	0.64057 (14)	0.50088 (15)	0.0538 (8)
F6A	0.2911 (2)	1.01481 (11)	0.25229 (12)	0.0244 (5)
F6B	0.8696 (2)	0.50149 (13)	0.58037 (14)	0.0438 (7)
F8A	0.6442 (2)	0.97021 (12)	0.05773 (11)	0.0238 (5)
F8B	0.5578 (2)	0.35383 (13)	0.63917 (13)	0.0316 (6)
F9A	0.5476 (2)	0.89899 (13)	−0.03480 (11)	0.0318 (6)
F9B	0.7125 (2)	0.24269 (12)	0.57213 (12)	0.0341 (6)
F10A	0.3411 (2)	0.80871 (13)	0.02350 (13)	0.0384 (6)
F10B	0.9676 (2)	0.21649 (12)	0.58371 (14)	0.0379 (6)
F11A	0.2427 (2)	0.78790 (13)	0.17925 (13)	0.0386 (6)
F11B	1.0673 (2)	0.30024 (14)	0.67035 (14)	0.0388 (6)
F12A	0.3429 (2)	0.85375 (12)	0.27384 (12)	0.0269 (5)
F12B	0.9160 (2)	0.41616 (13)	0.73518 (13)	0.0320 (6)
F14A	0.6558 (2)	0.80080 (12)	0.27730 (11)	0.0247 (5)
F14B	0.4976 (2)	0.35871 (13)	0.84276 (13)	0.0350 (6)
F15A	0.6257 (2)	0.72352 (12)	0.42236 (12)	0.0291 (5)
F15B	0.4775 (2)	0.33929 (14)	0.99533 (13)	0.0403 (6)
F16A	0.4870 (2)	0.79401 (13)	0.54272 (12)	0.0317 (6)
F16B	0.6233 (3)	0.42111 (14)	1.05999 (12)	0.0425 (7)
F17A	0.3939 (2)	0.94697 (13)	0.51587 (11)	0.0292 (6)
F17B	0.7857 (3)	0.52384 (13)	0.96620 (13)	0.0431 (7)
F18A	0.4322 (2)	1.02808 (12)	0.37335 (11)	0.0249 (5)
F18B	0.8016 (2)	0.54823 (13)	0.81312 (12)	0.0324 (6)
O1A	0.7149 (2)	0.95384 (14)	0.19924 (13)	0.0177 (6)
H1A	0.735166	0.978692	0.154103	0.021*
O1B	0.5064 (3)	0.4770 (2)	0.71571 (16)	0.0441 (8)
H1B	0.502930	0.486210	0.668244	0.053*
N1C	0.9782 (3)	1.03371 (19)	0.09770 (17)	0.0252 (8)
N1D	0.3776 (3)	0.52751 (17)	0.58736 (17)	0.0222 (8)
N2C	0.8851 (3)	0.98584 (18)	0.27692 (19)	0.0236 (8)
H2C	0.821 (4)	0.979 (2)	0.241 (2)	0.028*
N2D	0.2596 (3)	0.4640 (2)	0.7571 (2)	0.0286 (9)

H2D	0.335 (4)	0.473 (2)	0.745 (2)	0.034*
C1A	0.5071 (4)	1.0538 (2)	0.21085 (19)	0.0161 (8)
C1B	0.7007 (4)	0.5520 (2)	0.6760 (2)	0.0211 (9)
C1C	0.9686 (5)	1.1192 (2)	0.0720 (2)	0.0424 (12)
H1CA	0.914079	1.132322	0.032137	0.064*
H1CB	0.928582	1.145717	0.116399	0.064*
H1CC	1.056664	1.136272	0.050297	0.064*
C1D	0.3899 (4)	0.6127 (2)	0.5776 (2)	0.0285 (10)
H1DA	0.356395	0.631234	0.627421	0.043*
H1DB	0.482598	0.622785	0.559864	0.043*
H1DC	0.339031	0.640405	0.539067	0.043*
C2A	0.5773 (4)	1.1184 (2)	0.1820 (2)	0.0190 (9)
C2B	0.6337 (4)	0.6222 (3)	0.6959 (2)	0.0286 (10)
C2C	1.0396 (4)	0.9929 (3)	0.0316 (2)	0.0310 (10)
H2CA	1.050134	0.935836	0.050561	0.037*
H2CB	1.128212	1.010768	0.009930	0.037*
C2D	0.4266 (3)	0.4965 (2)	0.5142 (2)	0.0216 (9)
H2DA	0.378658	0.525592	0.473974	0.026*
H2DB	0.409050	0.440680	0.521906	0.026*
C3A	0.5223 (4)	1.1940 (2)	0.1618 (2)	0.0201 (9)
C3B	0.6588 (4)	0.6955 (2)	0.6541 (2)	0.0292 (10)
C3C	1.0591 (4)	1.0147 (3)	0.1568 (2)	0.0389 (12)
H3CA	1.140205	1.042282	0.138414	0.047*
H3CB	1.085336	0.957650	0.163651	0.047*
C3D	0.2396 (4)	0.5108 (2)	0.6169 (2)	0.0298 (10)
H3DA	0.229914	0.456406	0.611045	0.036*
H3DB	0.183639	0.546404	0.584778	0.036*
C4A	0.3897 (4)	1.2077 (2)	0.1709 (2)	0.0209 (9)
C4B	0.7529 (4)	0.7022 (2)	0.5885 (2)	0.0283 (10)
C4C	0.9902 (4)	1.0370 (3)	0.2352 (2)	0.0292 (10)
H4CA	1.056339	1.034358	0.268293	0.035*
H4CB	0.951338	1.091878	0.227026	0.035*
C4D	0.1909 (4)	0.5203 (2)	0.7008 (2)	0.0272 (10)
H4DA	0.201919	0.574466	0.706740	0.033*
H4DB	0.095728	0.513150	0.714618	0.033*
C5A	0.3139 (4)	1.1462 (2)	0.2016 (2)	0.0195 (9)
C5B	0.8222 (4)	0.6353 (2)	0.5657 (2)	0.0329 (11)
C5C	0.9390 (5)	0.9046 (3)	0.3016 (3)	0.0479 (13)
H5CA	0.974656	0.879499	0.255631	0.072*
H5CB	0.868891	0.874795	0.335160	0.072*
H5CC	1.009091	0.905802	0.330194	0.072*
C5D	0.2446 (4)	0.3805 (2)	0.7559 (3)	0.0389 (12)
H5DA	0.282930	0.367635	0.704079	0.058*
H5DB	0.151083	0.371605	0.768439	0.058*
H5DC	0.289957	0.347029	0.794372	0.058*
C6A	0.3731 (4)	1.0723 (2)	0.2208 (2)	0.0175 (8)
C6B	0.7953 (4)	0.5634 (2)	0.6091 (2)	0.0270 (10)
C6C	0.8078 (4)	1.0198 (3)	0.3449 (2)	0.0362 (11)

H6CA	0.766412	1.071544	0.327195	0.054*
H6CB	0.866289	1.024951	0.379852	0.054*
H6CC	0.739774	0.985228	0.372679	0.054*
C6D	0.2130 (5)	0.4841 (3)	0.8370 (3)	0.0516 (14)
H6DA	0.237918	0.536374	0.838303	0.077*
H6DB	0.253322	0.445397	0.874215	0.077*
H6DC	0.117127	0.483852	0.850991	0.077*
C7A	0.5026 (3)	0.9146 (2)	0.17160 (19)	0.0144 (8)
C7B	0.7300 (4)	0.3920 (2)	0.6903 (2)	0.0185 (9)
C8A	0.5459 (4)	0.9237 (2)	0.0917 (2)	0.0178 (9)
C8B	0.6841 (4)	0.3441 (2)	0.6493 (2)	0.0226 (9)
C9A	0.4964 (4)	0.8883 (2)	0.0418 (2)	0.0218 (9)
C9B	0.7614 (4)	0.2858 (2)	0.6137 (2)	0.0256 (10)
C10A	0.3933 (4)	0.8429 (2)	0.0713 (2)	0.0240 (9)
C10B	0.8899 (4)	0.2720 (2)	0.6202 (2)	0.0255 (10)
C11A	0.3446 (4)	0.8325 (2)	0.1497 (2)	0.0233 (9)
C11B	0.9399 (4)	0.3145 (2)	0.6636 (2)	0.0266 (10)
C11S	0.2153 (5)	0.7509 (2)	0.7240 (3)	0.0428 (13)
H11A	0.297417	0.769195	0.723967	0.051*
C12A	0.3994 (4)	0.8671 (2)	0.1976 (2)	0.0198 (9)
C12B	0.8586 (4)	0.3721 (2)	0.6971 (2)	0.0221 (9)
C12S	0.1699 (4)	0.7591 (2)	0.6553 (3)	0.0378 (11)
H12A	0.219079	0.784327	0.608214	0.045*
C13A	0.5449 (3)	0.9188 (2)	0.3166 (2)	0.0157 (8)
C13B	0.6458 (4)	0.4561 (2)	0.8193 (2)	0.0215 (9)
C13S	0.0512 (4)	0.7299 (2)	0.6560 (3)	0.0372 (11)
H13A	0.019426	0.734348	0.609073	0.045*
C14A	0.5924 (4)	0.8407 (2)	0.3351 (2)	0.0176 (8)
C14B	0.5693 (4)	0.4032 (2)	0.8704 (2)	0.0238 (9)
C14S	−0.0198 (4)	0.6948 (2)	0.7243 (3)	0.0337 (11)
H14A	−0.100896	0.675021	0.724618	0.040*
C15A	0.5772 (4)	0.7994 (2)	0.4091 (2)	0.0199 (9)
C15B	0.5596 (4)	0.3908 (2)	0.9500 (2)	0.0271 (10)
C15S	0.0255 (4)	0.6878 (2)	0.7925 (3)	0.0380 (11)
H15A	−0.023930	0.663223	0.839835	0.046*
C16A	0.5090 (4)	0.8345 (2)	0.4701 (2)	0.0212 (9)
C16B	0.6309 (4)	0.4318 (2)	0.9827 (2)	0.0279 (10)
C16S	0.1428 (5)	0.7166 (3)	0.7920 (3)	0.0426 (12)
H16A	0.173495	0.712687	0.839190	0.051*
C17A	0.4607 (4)	0.9114 (2)	0.4561 (2)	0.0198 (9)
C17B	0.7123 (4)	0.4842 (2)	0.9345 (2)	0.0273 (10)
C18A	0.4806 (4)	0.9515 (2)	0.3808 (2)	0.0180 (9)
C18B	0.7181 (4)	0.4955 (2)	0.8556 (2)	0.0238 (9)
C21S	0.9916 (5)	0.6712 (3)	0.0254 (3)	0.0466 (13)
H21A	1.043861	0.633966	−0.003693	0.056*
C22S	1.0436 (5)	0.7020 (3)	0.0769 (3)	0.0436 (12)
H22A	1.130774	0.685267	0.084246	0.052*
C23S	0.9694 (5)	0.7570 (2)	0.1179 (2)	0.0357 (11)

H23A	1.005813	0.779091	0.152968	0.043*
C24S	0.8423 (5)	0.7803 (2)	0.1083 (2)	0.0350 (11)
H24A	0.791058	0.818470	0.136606	0.042*
C25S	0.7897 (4)	0.7483 (2)	0.0575 (3)	0.0364 (11)
H25A	0.701581	0.763818	0.051432	0.044*
C26S	0.8645 (5)	0.6936 (3)	0.0153 (3)	0.0399 (12)
H26A	0.828636	0.671768	−0.020117	0.048*
C31S	1.1011 (4)	1.0345 (3)	0.4477 (2)	0.0347 (11)
H31A	1.171195	1.058454	0.411630	0.042*
C32S	1.0012 (5)	1.0798 (2)	0.4862 (3)	0.0359 (11)
H32A	1.001603	1.135257	0.476554	0.043*
C33S	0.9005 (4)	1.0453 (3)	0.5385 (2)	0.0338 (11)
H33A	0.831688	1.076925	0.565297	0.041*
B1A	0.5700 (4)	0.9616 (2)	0.2250 (2)	0.0164 (10)
B1B	0.6459 (4)	0.4690 (3)	0.7248 (3)	0.0215 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F2A	0.0216 (14)	0.0231 (13)	0.0543 (16)	−0.0061 (10)	−0.0116 (12)	−0.0030 (12)
F2B	0.0527 (17)	0.0439 (16)	0.0188 (12)	0.0177 (13)	0.0006 (12)	−0.0050 (12)
F3A	0.0334 (14)	0.0165 (12)	0.0396 (14)	−0.0089 (10)	−0.0093 (11)	−0.0031 (11)
F3B	0.072 (2)	0.0369 (15)	0.0274 (13)	0.0209 (14)	−0.0196 (13)	−0.0149 (12)
F4A	0.0381 (15)	0.0153 (12)	0.0440 (15)	0.0055 (11)	−0.0093 (12)	−0.0040 (11)
F4B	0.0545 (18)	0.0217 (13)	0.0486 (16)	−0.0116 (12)	−0.0171 (13)	−0.0006 (12)
F5A	0.0229 (14)	0.0249 (13)	0.0584 (16)	0.0036 (11)	−0.0071 (12)	−0.0086 (12)
F5B	0.0494 (18)	0.0358 (16)	0.0578 (18)	−0.0131 (13)	0.0263 (15)	0.0042 (14)
F6A	0.0201 (13)	0.0188 (12)	0.0334 (13)	−0.0060 (10)	−0.0008 (10)	−0.0042 (10)
F6B	0.0478 (17)	0.0227 (13)	0.0479 (16)	−0.0039 (12)	0.0210 (13)	−0.0056 (12)
F8A	0.0242 (13)	0.0330 (13)	0.0142 (11)	−0.0096 (10)	−0.0012 (9)	−0.0022 (10)
F8B	0.0308 (15)	0.0355 (14)	0.0360 (14)	−0.0142 (11)	−0.0152 (11)	−0.0071 (11)
F9A	0.0380 (15)	0.0448 (15)	0.0152 (11)	0.0000 (12)	−0.0059 (10)	−0.0128 (11)
F9B	0.0516 (17)	0.0271 (13)	0.0321 (13)	−0.0177 (12)	−0.0145 (12)	−0.0106 (11)
F10A	0.0533 (17)	0.0383 (15)	0.0359 (14)	−0.0112 (12)	−0.0227 (13)	−0.0170 (12)
F10B	0.0492 (17)	0.0233 (13)	0.0425 (15)	−0.0007 (12)	−0.0052 (13)	−0.0142 (12)
F11A	0.0491 (17)	0.0366 (14)	0.0382 (14)	−0.0311 (13)	−0.0164 (12)	0.0000 (12)
F11B	0.0276 (15)	0.0470 (16)	0.0452 (15)	0.0021 (12)	−0.0094 (12)	−0.0173 (13)
F12A	0.0315 (14)	0.0309 (13)	0.0205 (12)	−0.0192 (11)	−0.0040 (10)	0.0003 (10)
F12B	0.0241 (14)	0.0440 (15)	0.0365 (13)	−0.0115 (11)	−0.0081 (11)	−0.0207 (12)
F14A	0.0344 (14)	0.0200 (12)	0.0193 (11)	0.0006 (10)	−0.0021 (10)	−0.0078 (10)
F14B	0.0359 (15)	0.0414 (15)	0.0305 (13)	−0.0208 (12)	−0.0063 (11)	−0.0014 (12)
F15A	0.0407 (15)	0.0198 (13)	0.0279 (12)	−0.0043 (11)	−0.0140 (11)	0.0035 (10)
F15B	0.0389 (16)	0.0458 (16)	0.0302 (13)	−0.0126 (13)	0.0021 (12)	0.0057 (12)
F16A	0.0360 (15)	0.0407 (14)	0.0183 (12)	−0.0123 (12)	−0.0083 (10)	0.0050 (11)
F16B	0.0685 (19)	0.0398 (15)	0.0178 (12)	0.0000 (13)	−0.0095 (12)	−0.0029 (11)
F17A	0.0310 (14)	0.0430 (14)	0.0147 (11)	−0.0028 (11)	−0.0025 (10)	−0.0098 (11)
F17B	0.073 (2)	0.0325 (14)	0.0346 (14)	−0.0135 (13)	−0.0267 (14)	−0.0077 (12)
F18A	0.0327 (14)	0.0239 (13)	0.0183 (11)	0.0040 (10)	−0.0062 (10)	−0.0065 (10)

F18B	0.0429 (16)	0.0320 (14)	0.0271 (12)	−0.0199 (12)	−0.0102 (11)	−0.0021 (11)
O1A	0.0194 (15)	0.0213 (15)	0.0120 (13)	−0.0067 (11)	−0.0021 (11)	0.0006 (11)
O1B	0.044 (2)	0.061 (2)	0.0281 (17)	−0.0146 (17)	−0.0045 (15)	−0.0067 (18)
N1C	0.027 (2)	0.031 (2)	0.0174 (17)	−0.0041 (16)	−0.0011 (15)	−0.0063 (15)
N1D	0.030 (2)	0.0195 (18)	0.0173 (17)	−0.0076 (15)	−0.0021 (15)	−0.0024 (14)
N2C	0.023 (2)	0.0220 (19)	0.0302 (19)	−0.0009 (15)	−0.0112 (16)	−0.0089 (16)
N2D	0.023 (2)	0.026 (2)	0.041 (2)	−0.0028 (17)	−0.0111 (18)	−0.0087 (17)
C1A	0.021 (2)	0.018 (2)	0.0109 (18)	−0.0033 (17)	−0.0063 (16)	−0.0032 (16)
C1B	0.019 (2)	0.028 (2)	0.021 (2)	−0.0018 (18)	−0.0087 (18)	−0.0100 (18)
C1C	0.060 (3)	0.038 (3)	0.026 (2)	−0.015 (2)	0.006 (2)	−0.007 (2)
C1D	0.040 (3)	0.020 (2)	0.024 (2)	−0.0040 (19)	−0.003 (2)	−0.0037 (19)
C2A	0.017 (2)	0.024 (2)	0.020 (2)	−0.0031 (18)	−0.0069 (17)	−0.0085 (18)
C2B	0.030 (3)	0.043 (3)	0.016 (2)	0.006 (2)	−0.0109 (19)	−0.012 (2)
C2C	0.025 (3)	0.046 (3)	0.023 (2)	0.001 (2)	−0.0013 (18)	−0.016 (2)
C2D	0.025 (2)	0.023 (2)	0.017 (2)	−0.0062 (18)	−0.0036 (18)	−0.0034 (18)
C3A	0.026 (2)	0.017 (2)	0.019 (2)	−0.0078 (18)	−0.0076 (18)	−0.0010 (17)
C3B	0.043 (3)	0.025 (2)	0.026 (2)	0.013 (2)	−0.021 (2)	−0.013 (2)
C3C	0.028 (3)	0.069 (3)	0.022 (2)	0.000 (2)	−0.002 (2)	−0.016 (2)
C3D	0.032 (3)	0.030 (2)	0.028 (2)	−0.005 (2)	−0.005 (2)	−0.006 (2)
C4A	0.031 (3)	0.016 (2)	0.018 (2)	0.0012 (18)	−0.0072 (18)	−0.0081 (17)
C4B	0.038 (3)	0.017 (2)	0.035 (2)	−0.007 (2)	−0.019 (2)	−0.003 (2)
C4C	0.022 (2)	0.047 (3)	0.022 (2)	−0.010 (2)	−0.0022 (18)	−0.011 (2)
C4D	0.024 (2)	0.022 (2)	0.032 (2)	0.0028 (18)	−0.0034 (19)	−0.0015 (19)
C5A	0.017 (2)	0.023 (2)	0.021 (2)	0.0007 (17)	−0.0058 (17)	−0.0074 (18)
C5B	0.029 (3)	0.034 (3)	0.035 (3)	−0.012 (2)	0.000 (2)	−0.003 (2)
C5C	0.043 (3)	0.035 (3)	0.070 (4)	0.003 (2)	−0.026 (3)	−0.008 (3)
C5D	0.041 (3)	0.026 (2)	0.056 (3)	−0.003 (2)	−0.026 (2)	−0.004 (2)
C6A	0.019 (2)	0.020 (2)	0.0149 (19)	−0.0076 (17)	−0.0016 (17)	−0.0049 (17)
C6B	0.026 (2)	0.020 (2)	0.034 (2)	−0.0047 (19)	0.002 (2)	−0.009 (2)
C6C	0.033 (3)	0.056 (3)	0.022 (2)	−0.017 (2)	0.002 (2)	−0.014 (2)
C6D	0.074 (4)	0.050 (3)	0.036 (3)	0.009 (3)	−0.023 (3)	−0.015 (3)
C7A	0.015 (2)	0.0149 (19)	0.0137 (18)	−0.0011 (16)	−0.0029 (16)	−0.0031 (16)
C7B	0.023 (2)	0.019 (2)	0.0140 (19)	−0.0107 (17)	−0.0049 (17)	0.0018 (17)
C8A	0.022 (2)	0.014 (2)	0.020 (2)	−0.0015 (17)	−0.0077 (17)	−0.0032 (17)
C8B	0.022 (2)	0.025 (2)	0.023 (2)	−0.0107 (18)	−0.0103 (18)	0.0036 (19)
C9A	0.031 (2)	0.021 (2)	0.014 (2)	0.0071 (18)	−0.0072 (18)	−0.0065 (17)
C9B	0.034 (3)	0.025 (2)	0.023 (2)	−0.015 (2)	−0.0091 (19)	−0.0023 (19)
C10A	0.034 (3)	0.018 (2)	0.029 (2)	−0.0041 (19)	−0.019 (2)	−0.0104 (19)
C10B	0.040 (3)	0.013 (2)	0.022 (2)	−0.0031 (19)	−0.003 (2)	−0.0020 (18)
C11A	0.025 (2)	0.017 (2)	0.030 (2)	−0.0086 (18)	−0.0094 (19)	−0.0001 (18)
C11B	0.025 (3)	0.033 (2)	0.026 (2)	−0.009 (2)	−0.0087 (19)	−0.003 (2)
C11S	0.034 (3)	0.029 (3)	0.073 (4)	−0.003 (2)	−0.013 (3)	−0.025 (3)
C12A	0.023 (2)	0.021 (2)	0.017 (2)	−0.0059 (18)	−0.0051 (18)	−0.0025 (17)
C12B	0.031 (3)	0.020 (2)	0.019 (2)	−0.0121 (18)	−0.0067 (18)	−0.0055 (18)
C12S	0.038 (3)	0.027 (2)	0.047 (3)	−0.002 (2)	0.000 (2)	−0.011 (2)
C13A	0.015 (2)	0.018 (2)	0.0161 (19)	−0.0057 (16)	−0.0063 (16)	−0.0013 (16)
C13B	0.023 (2)	0.022 (2)	0.019 (2)	−0.0033 (18)	−0.0022 (18)	−0.0059 (18)
C13S	0.037 (3)	0.027 (3)	0.048 (3)	0.003 (2)	−0.016 (2)	−0.003 (2)

C14A	0.019 (2)	0.022 (2)	0.0139 (19)	−0.0064 (17)	−0.0032 (16)	−0.0055 (17)
C14B	0.019 (2)	0.030 (2)	0.025 (2)	−0.0067 (19)	−0.0040 (18)	−0.008 (2)
C14S	0.025 (3)	0.025 (2)	0.051 (3)	0.0007 (19)	−0.009 (2)	−0.003 (2)
C15A	0.021 (2)	0.019 (2)	0.022 (2)	−0.0030 (17)	−0.0127 (18)	0.0005 (18)
C15B	0.024 (2)	0.023 (2)	0.027 (2)	−0.0023 (19)	0.0045 (19)	0.0024 (19)
C15S	0.039 (3)	0.034 (3)	0.042 (3)	−0.001 (2)	−0.003 (2)	−0.016 (2)
C16A	0.026 (2)	0.033 (2)	0.0075 (18)	−0.0131 (19)	−0.0080 (17)	0.0036 (18)
C16B	0.040 (3)	0.027 (2)	0.018 (2)	0.006 (2)	−0.008 (2)	−0.0091 (19)
C16S	0.048 (3)	0.041 (3)	0.046 (3)	0.006 (2)	−0.014 (3)	−0.026 (3)
C17A	0.017 (2)	0.033 (2)	0.0122 (19)	−0.0056 (18)	−0.0010 (16)	−0.0090 (18)
C17B	0.041 (3)	0.020 (2)	0.027 (2)	−0.003 (2)	−0.016 (2)	−0.0084 (19)
C18A	0.018 (2)	0.018 (2)	0.021 (2)	−0.0062 (17)	−0.0079 (17)	−0.0038 (17)
C18B	0.027 (2)	0.019 (2)	0.026 (2)	−0.0075 (18)	−0.0038 (19)	−0.0030 (18)
C21S	0.050 (4)	0.034 (3)	0.051 (3)	0.012 (2)	−0.004 (3)	−0.012 (2)
C22S	0.034 (3)	0.041 (3)	0.053 (3)	−0.002 (2)	−0.014 (2)	0.005 (3)
C23S	0.047 (3)	0.033 (3)	0.030 (2)	−0.014 (2)	−0.007 (2)	−0.006 (2)
C24S	0.044 (3)	0.026 (2)	0.028 (2)	−0.004 (2)	0.007 (2)	−0.001 (2)
C25S	0.032 (3)	0.029 (3)	0.044 (3)	−0.004 (2)	−0.007 (2)	0.004 (2)
C26S	0.048 (3)	0.036 (3)	0.041 (3)	−0.007 (2)	−0.015 (2)	−0.012 (2)
C31S	0.035 (3)	0.052 (3)	0.022 (2)	−0.023 (2)	−0.003 (2)	−0.007 (2)
C32S	0.055 (3)	0.023 (2)	0.039 (3)	−0.008 (2)	−0.027 (3)	−0.006 (2)
C33S	0.030 (3)	0.041 (3)	0.038 (3)	0.007 (2)	−0.016 (2)	−0.024 (2)
B1A	0.019 (3)	0.021 (2)	0.012 (2)	−0.0066 (19)	−0.0021 (18)	−0.0053 (19)
B1B	0.014 (2)	0.027 (3)	0.024 (2)	−0.009 (2)	−0.001 (2)	−0.004 (2)

Geometric parameters (Å, º)

F2A—C2A	1.359 (4)	C4B—C5B	1.374 (6)
F2B—C2B	1.341 (4)	C4C—H4CA	0.9900
F3A—C3A	1.344 (4)	C4C—H4CB	0.9900
F3B—C3B	1.351 (4)	C4D—H4DA	0.9900
F4A—C4A	1.349 (4)	C4D—H4DB	0.9900
F4B—C4B	1.346 (4)	C5A—C6A	1.376 (5)
F5A—C5A	1.354 (4)	C5B—C6B	1.376 (5)
F5B—C5B	1.352 (5)	C5C—H5CA	0.9800
F6A—C6A	1.361 (4)	C5C—H5CB	0.9800
F6B—C6B	1.362 (4)	C5C—H5CC	0.9800
F8A—C8A	1.357 (4)	C5D—H5DA	0.9800
F8B—C8B	1.356 (4)	C5D—H5DB	0.9800
F9A—C9A	1.346 (4)	C5D—H5DC	0.9800
F9B—C9B	1.350 (4)	C6C—H6CA	0.9800
F10A—C10A	1.353 (4)	C6C—H6CB	0.9800
F10B—C10B	1.353 (4)	C6C—H6CC	0.9800
F11A—C11A	1.353 (4)	C6D—H6DA	0.9800
F11B—C11B	1.351 (4)	C6D—H6DB	0.9800
F12A—C12A	1.353 (4)	C6D—H6DC	0.9800
F12B—C12B	1.369 (4)	C7A—C8A	1.387 (5)
F14A—C14A	1.357 (4)	C7A—C12A	1.388 (5)

F14B—C14B	1.355 (4)	C7A—B1A	1.663 (5)
F15A—C15A	1.354 (4)	C7B—C12B	1.371 (5)
F15B—C15B	1.352 (4)	C7B—C8B	1.385 (5)
F16A—C16A	1.347 (4)	C7B—B1B	1.650 (6)
F16B—C16B	1.344 (4)	C8A—C9A	1.379 (5)
F17A—C17A	1.351 (4)	C8B—C9B	1.378 (5)
F17B—C17B	1.352 (4)	C9A—C10A	1.371 (5)
F18A—C18A	1.360 (4)	C9B—C10B	1.360 (6)
F18B—C18B	1.357 (4)	C10A—C11A	1.371 (5)
O1A—B1A	1.484 (5)	C10B—C11B	1.372 (5)
O1A—H1A	0.8400	C11A—C12A	1.375 (5)
O1B—B1B	1.487 (5)	C11B—C12B	1.371 (5)
O1B—H1B	0.8400	C11S—C16S	1.365 (6)
N1C—C3C	1.454 (5)	C11S—C12S	1.382 (6)
N1C—C1C	1.473 (5)	C11S—H11A	0.9500
N1C—C2C	1.475 (5)	C12S—C13S	1.393 (6)
N1D—C2D	1.470 (4)	C12S—H12A	0.9500
N1D—C3D	1.472 (5)	C13A—C18A	1.380 (5)
N1D—C1D	1.478 (4)	C13A—C14A	1.395 (5)
N2C—C5C	1.483 (5)	C13A—B1A	1.649 (5)
N2C—C6C	1.483 (5)	C13B—C14B	1.374 (5)
N2C—C4C	1.485 (5)	C13B—C18B	1.395 (5)
N2C—H2C	1.04 (4)	C13B—B1B	1.659 (6)
N2D—C5D	1.485 (5)	C13S—C14S	1.367 (6)
N2D—C6D	1.495 (5)	C13S—H13A	0.9500
N2D—C4D	1.503 (5)	C14A—C15A	1.372 (5)
N2D—H2D	0.80 (4)	C14B—C15B	1.380 (5)
C1A—C6A	1.379 (5)	C14S—C15S	1.376 (6)
C1A—C2A	1.379 (5)	C14S—H14A	0.9500
C1A—B1A	1.656 (5)	C15A—C16A	1.367 (5)
C1B—C6B	1.381 (5)	C15B—C16B	1.364 (5)
C1B—C2B	1.397 (5)	C15S—C16S	1.375 (6)
C1B—B1B	1.646 (6)	C15S—H15A	0.9500
C1C—H1CA	0.9800	C16A—C17A	1.370 (5)
C1C—H1CB	0.9800	C16B—C17B	1.375 (6)
C1C—H1CC	0.9800	C16S—H16A	0.9500
C1D—H1DA	0.9800	C17A—C18A	1.384 (5)
C1D—H1DB	0.9800	C17B—C18B	1.376 (5)
C1D—H1DC	0.9800	C21S—C22S	1.370 (6)
C2A—C3A	1.387 (5)	C21S—C26S	1.378 (6)
C2B—C3B	1.382 (6)	C21S—H21A	0.9500
C2C—C2C^{i}	1.503 (7)	C22S—C23S	1.373 (6)
C2C—H2CA	0.9900	C22S—H22A	0.9500
C2C—H2CB	0.9900	C23S—C24S	1.378 (6)
C2D—C2D^{ii}	1.522 (7)	C23S—H23A	0.9500
C2D—H2DA	0.9900	C24S—C25S	1.375 (6)
C2D—H2DB	0.9900	C24S—H24A	0.9500
C3A—C4A	1.357 (5)	C25S—C26S	1.383 (6)

C3B—C4B	1.359 (6)	C25S—H25A	0.9500
C3C—C4C	1.526 (5)	C26S—H26A	0.9500
C3C—H3CA	0.9900	C31S—C33S^{iii}	1.369 (6)
C3C—H3CB	0.9900	C31S—C32S	1.369 (6)
C3D—C4D	1.507 (5)	C31S—H31A	0.9500
C3D—H3DA	0.9900	C32S—C33S	1.369 (6)
C3D—H3DB	0.9900	C32S—H32A	0.9500
C4A—C5A	1.372 (5)	C33S—H33A	0.9500

B1A—O1A—H1A	109.5	C8A—C7A—B1A	119.9 (3)
B1B—O1B—H1B	109.5	C12A—C7A—B1A	126.9 (3)
C3C—N1C—C1C	109.1 (3)	C12B—C7B—C8B	113.2 (3)
C3C—N1C—C2C	108.8 (3)	C12B—C7B—B1B	121.3 (3)
C1C—N1C—C2C	110.2 (3)	C8B—C7B—B1B	125.5 (3)
C2D—N1D—C3D	109.6 (3)	F8A—C8A—C9A	115.4 (3)
C2D—N1D—C1D	111.8 (3)	F8A—C8A—C7A	119.7 (3)
C3D—N1D—C1D	110.3 (3)	C9A—C8A—C7A	124.9 (3)
C5C—N2C—C6C	110.5 (3)	F8B—C8B—C9B	114.9 (3)
C5C—N2C—C4C	111.9 (3)	F8B—C8B—C7B	121.1 (4)
C6C—N2C—C4C	110.0 (3)	C9B—C8B—C7B	124.0 (4)
C5C—N2C—H2C	104 (2)	F9A—C9A—C10A	120.5 (3)
C6C—N2C—H2C	109 (2)	F9A—C9A—C8A	120.5 (3)
C4C—N2C—H2C	112 (2)	C10A—C9A—C8A	118.9 (3)
C5D—N2D—C6D	111.1 (4)	F9B—C9B—C10B	119.4 (4)
C5D—N2D—C4D	113.5 (3)	F9B—C9B—C8B	121.4 (4)
C6D—N2D—C4D	109.5 (3)	C10B—C9B—C8B	119.2 (3)
C5D—N2D—H2D	111 (3)	F10A—C10A—C11A	120.7 (3)
C6D—N2D—H2D	106 (3)	F10A—C10A—C9A	120.3 (3)
C4D—N2D—H2D	105 (3)	C11A—C10A—C9A	119.0 (3)
C6A—C1A—C2A	112.6 (3)	F10B—C10B—C9B	119.7 (3)
C6A—C1A—B1A	121.2 (3)	F10B—C10B—C11B	120.4 (4)
C2A—C1A—B1A	125.9 (3)	C9B—C10B—C11B	119.8 (4)
C6B—C1B—C2B	112.6 (4)	F11A—C11A—C10A	119.4 (3)
C6B—C1B—B1B	128.4 (3)	F11A—C11A—C12A	120.5 (3)
C2B—C1B—B1B	118.3 (3)	C10A—C11A—C12A	120.1 (3)
N1C—C1C—H1CA	109.5	F11B—C11B—C12B	122.0 (3)
N1C—C1C—H1CB	109.5	F11B—C11B—C10B	119.7 (4)
H1CA—C1C—H1CB	109.5	C12B—C11B—C10B	118.3 (4)
N1C—C1C—H1CC	109.5	C16S—C11S—C12S	120.4 (4)
H1CA—C1C—H1CC	109.5	C16S—C11S—H11A	119.8
H1CB—C1C—H1CC	109.5	C12S—C11S—H11A	119.8
N1D—C1D—H1DA	109.5	F12A—C12A—C11A	115.2 (3)
N1D—C1D—H1DB	109.5	F12A—C12A—C7A	120.9 (3)
H1DA—C1D—H1DB	109.5	C11A—C12A—C7A	123.9 (3)
N1D—C1D—H1DC	109.5	F12B—C12B—C7B	118.7 (3)
H1DA—C1D—H1DC	109.5	F12B—C12B—C11B	115.7 (3)
H1DB—C1D—H1DC	109.5	C7B—C12B—C11B	125.4 (3)
F2A—C2A—C1A	120.6 (3)	C11S—C12S—C13S	119.0 (5)

F2A—C2A—C3A	114.5 (3)	C11S—C12S—H12A	120.5
C1A—C2A—C3A	124.9 (4)	C13S—C12S—H12A	120.5
F2B—C2B—C3B	116.1 (4)	C18A—C13A—C14A	113.1 (3)
F2B—C2B—C1B	119.6 (4)	C18A—C13A—B1A	127.5 (3)
C3B—C2B—C1B	124.3 (4)	C14A—C13A—B1A	119.4 (3)
N1C—C2C—C2C^{i}	112.7 (4)	C14B—C13B—C18B	113.1 (3)
N1C—C2C—H2CA	109.1	C14B—C13B—B1B	120.9 (3)
C2C^{i}—C2C—H2CA	109.1	C18B—C13B—B1B	126.0 (3)
N1C—C2C—H2CB	109.1	C14S—C13S—C12S	120.0 (4)
C2C^{i}—C2C—H2CB	109.1	C14S—C13S—H13A	120.0
H2CA—C2C—H2CB	107.8	C12S—C13S—H13A	120.0
N1D—C2D—C2D^{ii}	111.9 (3)	F14A—C14A—C15A	116.2 (3)
N1D—C2D—H2DA	109.2	F14A—C14A—C13A	119.4 (3)
C2D^{ii}—C2D—H2DA	109.2	C15A—C14A—C13A	124.4 (3)
N1D—C2D—H2DB	109.2	F14B—C14B—C13B	119.4 (3)
C2D^{ii}—C2D—H2DB	109.2	F14B—C14B—C15B	115.9 (3)
H2DA—C2D—H2DB	107.9	C13B—C14B—C15B	124.7 (3)
F3A—C3A—C4A	120.2 (3)	C13S—C14S—C15S	120.4 (4)
F3A—C3A—C2A	120.5 (3)	C13S—C14S—H14A	119.8
C4A—C3A—C2A	119.4 (3)	C15S—C14S—H14A	119.8
F3B—C3B—C4B	119.6 (4)	F15A—C15A—C16A	119.4 (3)
F3B—C3B—C2B	120.5 (4)	F15A—C15A—C14A	120.9 (3)
C4B—C3B—C2B	119.8 (4)	C16A—C15A—C14A	119.7 (3)
N1C—C3C—C4C	113.4 (3)	F15B—C15B—C16B	120.2 (4)
N1C—C3C—H3CA	108.9	F15B—C15B—C14B	119.9 (4)
C4C—C3C—H3CA	108.9	C16B—C15B—C14B	119.8 (4)
N1C—C3C—H3CB	108.9	C16S—C15S—C14S	119.7 (5)
C4C—C3C—H3CB	108.9	C16S—C15S—H15A	120.2
H3CA—C3C—H3CB	107.7	C14S—C15S—H15A	120.2
N1D—C3D—C4D	113.8 (3)	F16A—C16A—C15A	120.8 (3)
N1D—C3D—H3DA	108.8	F16A—C16A—C17A	120.1 (3)
C4D—C3D—H3DA	108.8	C15A—C16A—C17A	119.0 (3)
N1D—C3D—H3DB	108.8	F16B—C16B—C15B	121.2 (4)
C4D—C3D—H3DB	108.8	F16B—C16B—C17B	120.4 (3)
H3DA—C3D—H3DB	107.7	C15B—C16B—C17B	118.4 (3)
F4A—C4A—C3A	121.4 (3)	C11S—C16S—C15S	120.4 (5)
F4A—C4A—C5A	120.0 (4)	C11S—C16S—H16A	119.8
C3A—C4A—C5A	118.6 (4)	C15S—C16S—H16A	119.8
F4B—C4B—C3B	120.8 (4)	F17A—C17A—C16A	119.7 (3)
F4B—C4B—C5B	120.5 (4)	F17A—C17A—C18A	120.8 (3)
C3B—C4B—C5B	118.7 (4)	C16A—C17A—C18A	119.5 (3)
N2C—C4C—C3C	113.6 (3)	F17B—C17B—C16B	118.9 (3)
N2C—C4C—H4CA	108.8	F17B—C17B—C18B	121.1 (4)
C3C—C4C—H4CA	108.8	C16B—C17B—C18B	120.0 (3)
N2C—C4C—H4CB	108.8	F18A—C18A—C13A	120.7 (3)
C3C—C4C—H4CB	108.8	F18A—C18A—C17A	115.0 (3)
H4CA—C4C—H4CB	107.7	C13A—C18A—C17A	124.3 (3)
N2D—C4D—C3D	114.4 (3)	F18B—C18B—C17B	115.5 (3)

N2D—C4D—H4DA	108.7	F18B—C18B—C13B	120.6 (3)
C3D—C4D—H4DA	108.7	C17B—C18B—C13B	123.9 (4)
N2D—C4D—H4DB	108.7	C22S—C21S—C26S	120.8 (4)
C3D—C4D—H4DB	108.7	C22S—C21S—H21A	119.6
H4DA—C4D—H4DB	107.6	C26S—C21S—H21A	119.6
F5A—C5A—C4A	119.6 (3)	C21S—C22S—C23S	119.8 (5)
F5A—C5A—C6A	120.5 (3)	C21S—C22S—H22A	120.1
C4A—C5A—C6A	119.8 (4)	C23S—C22S—H22A	120.1
F5B—C5B—C4B	119.8 (4)	C22S—C23S—C24S	120.1 (4)
F5B—C5B—C6B	120.4 (4)	C22S—C23S—H23A	119.9
C4B—C5B—C6B	119.8 (4)	C24S—C23S—H23A	119.9
N2C—C5C—H5CA	109.5	C25S—C24S—C23S	119.9 (4)
N2C—C5C—H5CB	109.5	C25S—C24S—H24A	120.1
H5CA—C5C—H5CB	109.5	C23S—C24S—H24A	120.1
N2C—C5C—H5CC	109.5	C24S—C25S—C26S	120.3 (4)
H5CA—C5C—H5CC	109.5	C24S—C25S—H25A	119.9
H5CB—C5C—H5CC	109.5	C26S—C25S—H25A	119.9
N2D—C5D—H5DA	109.5	C21S—C26S—C25S	119.1 (4)
N2D—C5D—H5DB	109.5	C21S—C26S—H26A	120.4
H5DA—C5D—H5DB	109.5	C25S—C26S—H26A	120.4
N2D—C5D—H5DC	109.5	C33S^{iii}—C31S—C32S	119.6 (4)
H5DA—C5D—H5DC	109.5	C33S^{iii}—C31S—H31A	120.2
H5DB—C5D—H5DC	109.5	C32S—C31S—H31A	120.2
F6A—C6A—C5A	116.3 (3)	C33S—C32S—C31S	120.2 (4)
F6A—C6A—C1A	119.1 (3)	C33S—C32S—H32A	119.9
C5A—C6A—C1A	124.6 (3)	C31S—C32S—H32A	119.9
F6B—C6B—C5B	114.4 (3)	C31S^{iii}—C33S—C32S	120.2 (4)
F6B—C6B—C1B	120.9 (3)	C31S^{iii}—C33S—H33A	119.9
C5B—C6B—C1B	124.7 (4)	C32S—C33S—H33A	119.9
N2C—C6C—H6CA	109.5	O1A—B1A—C13A	104.5 (3)
N2C—C6C—H6CB	109.5	O1A—B1A—C1A	112.3 (3)
H6CA—C6C—H6CB	109.5	C13A—B1A—C1A	114.6 (3)
N2C—C6C—H6CC	109.5	O1A—B1A—C7A	108.9 (3)
H6CA—C6C—H6CC	109.5	C13A—B1A—C7A	110.8 (3)
H6CB—C6C—H6CC	109.5	C1A—B1A—C7A	105.7 (3)
N2D—C6D—H6DA	109.5	O1B—B1B—C1B	103.1 (3)
N2D—C6D—H6DB	109.5	O1B—B1B—C7B	112.5 (3)
H6DA—C6D—H6DB	109.5	C1B—B1B—C7B	112.0 (3)
N2D—C6D—H6DC	109.5	O1B—B1B—C13B	107.2 (3)
H6DA—C6D—H6DC	109.5	C1B—B1B—C13B	114.5 (3)
H6DB—C6D—H6DC	109.5	C7B—B1B—C13B	107.6 (3)
C8A—C7A—C12A	113.1 (3)		

C6A—C1A—C2A—F2A	176.9 (3)	C8B—C7B—C12B—C11B	4.0 (6)
B1A—C1A—C2A—F2A	−9.0 (5)	B1B—C7B—C12B—C11B	−173.0 (4)
C6A—C1A—C2A—C3A	−2.3 (5)	F11B—C11B—C12B—F12B	2.4 (5)
B1A—C1A—C2A—C3A	171.8 (3)	C10B—C11B—C12B—F12B	−175.6 (3)
C6B—C1B—C2B—F2B	179.9 (3)	F11B—C11B—C12B—C7B	177.3 (3)

B1B—C1B—C2B—F2B	8.7 (5)	C10B—C11B—C12B—C7B	−0.6 (6)
C6B—C1B—C2B—C3B	−0.5 (6)	C16S—C11S—C12S—C13S	−1.9 (6)
B1B—C1B—C2B—C3B	−171.8 (4)	C11S—C12S—C13S—C14S	1.0 (6)
C3C—N1C—C2C—C2C^{i}	178.3 (5)	C18A—C13A—C14A—F14A	178.9 (3)
C1C—N1C—C2C—C2C^{i}	−62.1 (6)	B1A—C13A—C14A—F14A	−1.4 (5)
C3D—N1D—C2D—C2D^{ii}	−173.2 (4)	C18A—C13A—C14A—C15A	0.4 (5)
C1D—N1D—C2D—C2D^{ii}	64.2 (5)	B1A—C13A—C14A—C15A	−180.0 (3)
F2A—C2A—C3A—F3A	1.1 (5)	C18B—C13B—C14B—F14B	−177.6 (3)
C1A—C2A—C3A—F3A	−179.7 (3)	B1B—C13B—C14B—F14B	2.8 (6)
F2A—C2A—C3A—C4A	−178.7 (3)	C18B—C13B—C14B—C15B	2.0 (6)
C1A—C2A—C3A—C4A	0.6 (6)	B1B—C13B—C14B—C15B	−177.6 (4)
F2B—C2B—C3B—F3B	−0.7 (5)	C12S—C13S—C14S—C15S	−0.2 (6)
C1B—C2B—C3B—F3B	179.7 (3)	F14A—C14A—C15A—F15A	1.1 (5)
F2B—C2B—C3B—C4B	−179.5 (3)	C13A—C14A—C15A—F15A	179.7 (3)
C1B—C2B—C3B—C4B	0.9 (6)	F14A—C14A—C15A—C16A	−177.0 (3)
C1C—N1C—C3C—C4C	73.7 (4)	C13A—C14A—C15A—C16A	1.6 (6)
C2C—N1C—C3C—C4C	−166.0 (4)	F14B—C14B—C15B—F15B	−2.9 (5)
C2D—N1D—C3D—C4D	164.5 (3)	C13B—C14B—C15B—F15B	177.5 (4)
C1D—N1D—C3D—C4D	−72.1 (4)	F14B—C14B—C15B—C16B	178.5 (4)
F3A—C3A—C4A—F4A	−0.7 (5)	C13B—C14B—C15B—C16B	−1.1 (6)
C2A—C3A—C4A—F4A	179.1 (3)	C13S—C14S—C15S—C16S	0.2 (6)
F3A—C3A—C4A—C5A	−178.3 (3)	F15A—C15A—C16A—F16A	−1.6 (5)
C2A—C3A—C4A—C5A	1.5 (5)	C14A—C15A—C16A—F16A	176.6 (3)
F3B—C3B—C4B—F4B	0.5 (6)	F15A—C15A—C16A—C17A	179.8 (3)
C2B—C3B—C4B—F4B	179.3 (3)	C14A—C15A—C16A—C17A	−2.1 (5)
F3B—C3B—C4B—C5B	−179.5 (3)	F15B—C15B—C16B—F16B	1.2 (6)
C2B—C3B—C4B—C5B	−0.7 (6)	C14B—C15B—C16B—F16B	179.8 (4)
C5C—N2C—C4C—C3C	67.0 (4)	F15B—C15B—C16B—C17B	−179.4 (4)
C6C—N2C—C4C—C3C	−169.8 (4)	C14B—C15B—C16B—C17B	−0.8 (6)
N1C—C3C—C4C—N2C	71.9 (5)	C12S—C11S—C16S—C15S	1.9 (7)
C5D—N2D—C4D—C3D	−60.9 (5)	C14S—C15S—C16S—C11S	−1.1 (6)
C6D—N2D—C4D—C3D	174.3 (4)	F16A—C16A—C17A—F17A	1.8 (5)
N1D—C3D—C4D—N2D	−63.9 (4)	C15A—C16A—C17A—F17A	−179.6 (3)
F4A—C4A—C5A—F5A	0.2 (5)	F16A—C16A—C17A—C18A	−178.0 (3)
C3A—C4A—C5A—F5A	177.8 (3)	C15A—C16A—C17A—C18A	0.6 (5)
F4A—C4A—C5A—C6A	−179.2 (3)	F16B—C16B—C17B—F17B	0.9 (6)
C3A—C4A—C5A—C6A	−1.5 (5)	C15B—C16B—C17B—F17B	−178.5 (4)
F4B—C4B—C5B—F5B	0.5 (6)	F16B—C16B—C17B—C18B	−179.1 (4)
C3B—C4B—C5B—F5B	−179.5 (4)	C15B—C16B—C17B—C18B	1.5 (6)
F4B—C4B—C5B—C6B	−179.8 (4)	C14A—C13A—C18A—F18A	177.7 (3)
C3B—C4B—C5B—C6B	0.2 (6)	B1A—C13A—C18A—F18A	−1.9 (5)
F5A—C5A—C6A—F6A	−0.5 (5)	C14A—C13A—C18A—C17A	−1.9 (5)
C4A—C5A—C6A—F6A	178.8 (3)	B1A—C13A—C18A—C17A	178.5 (3)
F5A—C5A—C6A—C1A	−179.8 (3)	F17A—C17A—C18A—F18A	2.0 (5)
C4A—C5A—C6A—C1A	−0.5 (5)	C16A—C17A—C18A—F18A	−178.2 (3)
C2A—C1A—C6A—F6A	−177.0 (3)	F17A—C17A—C18A—C13A	−178.4 (3)
B1A—C1A—C6A—F6A	8.5 (5)	C16A—C17A—C18A—C13A	1.5 (6)
C2A—C1A—C6A—C5A	2.3 (5)	F17B—C17B—C18B—F18B	0.2 (6)

B1A—C1A—C6A—C5A	−172.2 (3)	C16B—C17B—C18B—F18B	−179.8 (4)
F5B—C5B—C6B—F6B	−0.8 (6)	F17B—C17B—C18B—C13B	179.5 (4)
C4B—C5B—C6B—F6B	179.5 (4)	C16B—C17B—C18B—C13B	−0.5 (6)
F5B—C5B—C6B—C1B	179.9 (4)	C14B—C13B—C18B—F18B	178.1 (3)
C4B—C5B—C6B—C1B	0.2 (7)	B1B—C13B—C18B—F18B	−2.3 (6)
C2B—C1B—C6B—F6B	−179.4 (3)	C14B—C13B—C18B—C17B	−1.2 (6)
B1B—C1B—C6B—F6B	−9.2 (6)	B1B—C13B—C18B—C17B	178.4 (4)
C2B—C1B—C6B—C5B	0.0 (6)	C26S—C21S—C22S—C23S	−1.4 (7)
B1B—C1B—C6B—C5B	170.1 (4)	C21S—C22S—C23S—C24S	1.1 (7)
C12A—C7A—C8A—F8A	178.3 (3)	C22S—C23S—C24S—C25S	0.1 (6)
B1A—C7A—C8A—F8A	0.7 (5)	C23S—C24S—C25S—C26S	−0.9 (6)
C12A—C7A—C8A—C9A	−1.7 (5)	C22S—C21S—C26S—C25S	0.5 (7)
B1A—C7A—C8A—C9A	−179.3 (3)	C24S—C25S—C26S—C21S	0.6 (7)
C12B—C7B—C8B—F8B	177.9 (3)	C33S^{iii}—C31S—C32S—C33S	0.4 (7)
B1B—C7B—C8B—F8B	−5.2 (6)	C31S—C32S—C33S—C31S^{iii}	−0.4 (7)
C12B—C7B—C8B—C9B	−4.6 (5)	C18A—C13A—B1A—O1A	122.2 (4)
B1B—C7B—C8B—C9B	172.3 (4)	C14A—C13A—B1A—O1A	−57.4 (4)
F8A—C8A—C9A—F9A	1.8 (5)	C18A—C13A—B1A—C1A	−1.2 (5)
C7A—C8A—C9A—F9A	−178.1 (3)	C14A—C13A—B1A—C1A	179.2 (3)
F8A—C8A—C9A—C10A	−177.4 (3)	C18A—C13A—B1A—C7A	−120.6 (4)
C7A—C8A—C9A—C10A	2.7 (6)	C14A—C13A—B1A—C7A	59.8 (4)
F8B—C8B—C9B—F9B	0.1 (5)	C6A—C1A—B1A—O1A	170.8 (3)
C7B—C8B—C9B—F9B	−177.6 (3)	C2A—C1A—B1A—O1A	−2.8 (5)
F8B—C8B—C9B—C10B	179.5 (3)	C6A—C1A—B1A—C13A	−70.1 (4)
C7B—C8B—C9B—C10B	1.9 (6)	C2A—C1A—B1A—C13A	116.2 (4)
F9A—C9A—C10A—F10A	−0.5 (6)	C6A—C1A—B1A—C7A	52.2 (4)
C8A—C9A—C10A—F10A	178.7 (3)	C2A—C1A—B1A—C7A	−121.5 (4)
F9A—C9A—C10A—C11A	179.2 (3)	C8A—C7A—B1A—O1A	−44.7 (4)
C8A—C9A—C10A—C11A	−1.6 (6)	C12A—C7A—B1A—O1A	138.0 (4)
F9B—C9B—C10B—F10B	1.2 (5)	C8A—C7A—B1A—C13A	−159.2 (3)
C8B—C9B—C10B—F10B	−178.2 (3)	C12A—C7A—B1A—C13A	23.6 (5)
F9B—C9B—C10B—C11B	−178.7 (3)	C8A—C7A—B1A—C1A	76.2 (4)
C8B—C9B—C10B—C11B	1.9 (6)	C12A—C7A—B1A—C1A	−101.1 (4)
F10A—C10A—C11A—F11A	−0.4 (6)	C6B—C1B—B1B—O1B	−114.6 (4)
C9A—C10A—C11A—F11A	179.9 (3)	C2B—C1B—B1B—O1B	55.1 (4)
F10A—C10A—C11A—C12A	179.5 (3)	C6B—C1B—B1B—C7B	6.5 (6)
C9A—C10A—C11A—C12A	−0.2 (6)	C2B—C1B—B1B—C7B	176.2 (3)
F10B—C10B—C11B—F11B	−0.4 (6)	C6B—C1B—B1B—C13B	129.4 (4)
C9B—C10B—C11B—F11B	179.5 (4)	C2B—C1B—B1B—C13B	−60.9 (5)
F10B—C10B—C11B—C12B	177.6 (3)	C12B—C7B—B1B—O1B	−176.4 (3)
C9B—C10B—C11B—C12B	−2.5 (6)	C8B—C7B—B1B—O1B	7.0 (5)
F11A—C11A—C12A—F12A	−0.9 (5)	C12B—C7B—B1B—C1B	68.0 (4)
C10A—C11A—C12A—F12A	179.3 (3)	C8B—C7B—B1B—C1B	−108.6 (4)
F11A—C11A—C12A—C7A	−179.0 (3)	C12B—C7B—B1B—C13B	−58.7 (4)
C10A—C11A—C12A—C7A	1.2 (6)	C8B—C7B—B1B—C13B	124.8 (4)
C8A—C7A—C12A—F12A	−178.2 (3)	C14B—C13B—B1B—O1B	47.0 (5)
B1A—C7A—C12A—F12A	−0.8 (6)	C18B—C13B—B1B—O1B	−132.5 (4)
C8A—C7A—C12A—C11A	−0.2 (6)	C14B—C13B—B1B—C1B	160.6 (4)

B1A—C7A—C12A—C11A	177.2 (4)	C18B—C13B—B1B—C1B	−18.9 (5)
C8B—C7B—C12B—F12B	178.8 (3)	C14B—C13B—B1B—C7B	−74.2 (4)
B1B—C7B—C12B—F12B	1.9 (5)	C18B—C13B—B1B—C7B	106.3 (4)

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

Hydrogen-bond geometry (Å, º)

*Cg*4, *Cg*7–*Cg*9 are the centroids of the C1*B*–C6*B*, C11*S*–C16*S*, C21*S*–C26*S* and C31*S*–C33*S*/C31*S*′–C31*S*′ rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*A*—H1*A*···F8*A*	0.84	2.16	2.731 (3)	125
O1*B*—H1*B*···N1*D*	0.84	2.12	2.846 (4)	144
N2*C*—H2*C*···O1*A*	1.05 (4)	1.60 (4)	2.632 (4)	169 (3)
N2*D*—H2*D*···O1*B*	0.80 (4)	1.76 (4)	2.554 (5)	171 (4)
C2*C*—H2*CB*···F8*A*^{i}	0.99	2.46	3.435 (5)	168
C4*C*—H4*CA*···F6*A*^{iv}	0.99	2.40	3.191 (5)	137
C5*D*—H5*DC*···F14*B*	0.98	2.54	3.284 (5)	133
C32*S*—H32*A*···F10*B*^{v}	0.95	2.52	3.133 (5)	123
C14*S*—H14*A*···*Cg*4^{vi}	0.95	2.95	3.779 (5)	147
C4*D*—H4*DA*···*Cg*7	0.99	2.73	3.620 (4)	150
C6*C*—H6*CB*···*Cg*9	0.98	2.74	3.689 (4)	163
C6*C*—H6*CB*···*Cg*9^{iii}	0.98	2.74	3.689 (4)	163

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