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Crystal structure and Hirshfeld surface analysis of 5,5-difluoro-10-(5,6,7,8-tetrahydro-4*H*-cyclohepta[*b*]thiophen-2-yl)-5*H*-4λ^4,5λ^4-dipyrrolo[1,2-*c*:2′,1′-*f*][1,3,2]diazaborinine

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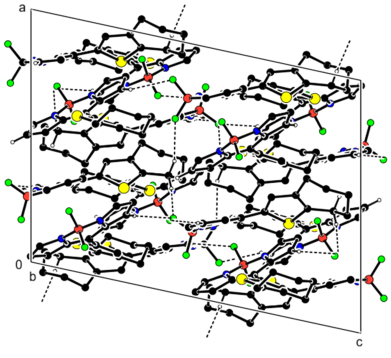
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In the title compound, $C_{18}H_{17}BF_2N_2S$, the asymmetric unit contains four independent molecules (*A*, *B*, *C* and *D*). In the crystal, molecules are linked to each other by C—H···F interactions, forming a three-dimensional network. Additionally, along the *a* axis, pairs of molecules are linked to each other by C—H···π interactions. In molecules *C* and *D*, the thiophene rings are disordered with the ratios of 0.7839 (15):0.2161 (15) for *C*, and of 0.7874 (16):0.2126 (16) for *D*, respectively, around the C—C bond that connects the thiophene rings, with a rotation of approximately 180° around the ring. The Hirshfeld surface analyses for the four molecules (*A*, *B*, *C* and *D*) in the asymmetric unit indicate that the most important contributions for the crystal packing are from H···H (*A*: 48.7%, *B*: 48.0%, *C*: 48.9% and *D*: 50.1%), F···H/H···F (*A*: 21.0%, *B*: 20.5%, *C*: 22.1% and *D*: 20.9%) and C···H/H···C (*A*: 17.0%, *B*: 17.2%, *C*: 15.9% and *D*: 15.9%) interactions.

1. Chemical context

The investigation and synthesis of new fluorescent organic molecules is one of the actively developing topics in research in the field of modern academic chemistry and one of the main molecular frameworks for synthesis of such compounds is the BODIPY (4,4-difluoro-4-bora-3a,4a-diaza-s-indacene) scaffold. The first derivative of this class was synthesized in 1968 (Treibs & Kreuzer, 1968), but the main BODIPY core was isolated and fully characterized only four decades later, in 2009 (Schmitt *et al.*, 2009). Since then, BODIPY derivatives have become widely used as functional dyes due to their possession of a number of properties: high fluorescence quantum yield, large molar absorption coefficient, narrow absorption and emission bands, and excellent photochemical stability (Bogomolec *et al.*, 2024). Due to the listed properties and the simplicity of synthetic construction of BODIPY target structures, they have become used as an innovative organic material in electronics (Zhao *et al.*, 2022; Zhang *et al.*, 2025; Mamedov *et al.*, 2024; Nie *et al.*, 2025), as well as fluorescent markers (Kowada *et al.*, 2015; Klymchenko, 2023) and agents for photodynamic therapy (PDT) (Nino-Suastegui & Abdelaziz, 2026; Javadzade *et al.*, 2026). This diversity of applications and properties of BODIPY scaffolds is achieved by



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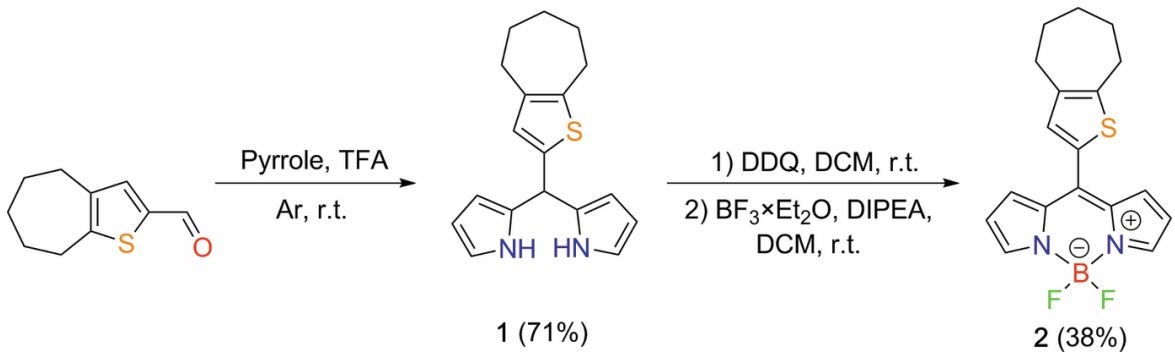
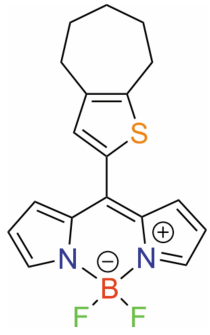


Figure 1
Synthesis of 5,5-difluoro-10-(5,6,7,8-tetrahydro-4*H*-cyclohepta[*b*]thiophen-2-yl)-5*H*-4λ^4,5λ^4-dipyrrolo[1,2-*c*:2′,1′-*f*][1,3,2]diazaborinine, **2**.

introducing substituents of various types into the structure of the original molecule. For example, modifications at specific positions of the BODIPY structure enable fine-tuning of photophysical properties, such as fluorescence efficiency and emission wavelength, strengthening the role of BODIPY in imaging and therapeutic applications in PDT (Malacarne *et al.*, 2022). However, a bibliographic review of the literature has shown that the introduction of aryl substituents, such as five-membered heterocycles (*e.g.* furan, thiophene, pyrrole, selenophene and its derivatives), into the meso-position remains poorly studied. Nevertheless, the available studies in this field show that attaching thienyl segments to the BODIPY core at the meso-position improves singlet oxygen generation compared to previous studies and could be considered as a promising photosensitizer agent for PDT applications (Karanlık *et al.*, 2023). Thus, to further study the effect of thiophene introduced into the *meso*-position on singlet oxygen generation ability, it is necessary to expand the range of such BODIPY derivatives. Herein, we report the synthesis of a novel BODIPY derivative functionalized with a thiophene ring, annulated with carbocycle, at the meso-position to investigate its influence on the structural, electronic and photophysical properties of the resultant fluorophore. A two-stage method for obtaining BODIPY-type structures, where various heterocyclic aldehydes were utilized as starting compounds, was previously described by our scientific group (Sadikhova *et al.*, 2024; Shchevnikov *et al.*, 2025; Polianskaia *et al.*, 2026; Polyanskaya *et al.*, 2026). In the present study, this general procedure was also utilized for 5,6,7,8-tetrahydro-4*H*-cyclohepta[*b*]thiophene-2-carbaldehyde, which was taken as the starting molecule. The target meso-thienyl-substituted BODIPY **2** was isolated in 38% yield (Fig. 1).

2. Structural commentary

In the title compound (Figs. 2 and 3), the asymmetric unit consists of four separate molecules (*A* with S1 atom, *B* with S2 atom, *C* with S3 atom and *D* with S4 atom). In molecule *A*, the mean plane of the 12-membered ring system [C1–C3/N4/B5/N6/C7–C9/C9*A*/C10/C10*A*; maximum deviation = 0.113 (2) Å for C1] makes a dihedral angle of 38.4 (1)° with the S1/C11/C12/C12*A*/C17*A* thiophene ring (Nardelli, 1983). In molecule *B*, the mean plane of the 12-membered ring system [C18–C20/N21/B22/N23/C24–C26/C26*A*/C27/C27*A*; maximum deviation = −0.125 (2) Å for C20] makes a dihedral angle of 41.0 (1)° with the S2/C28/C29/C29*A*/C34*A* thiophene ring. In molecule *C*, the mean plane of the 12-membered ring system [C35–C37/N38/B39/N40/C41–C43/C43*A*/C44/C44*A*; maximum deviation = −0.245 (2) Å for B39] makes a dihedral angle of 41.0 (1)° with the S3/C45/C46/C46*A*/C51*A* thiophene ring. In molecule *D*, the mean plane of the 12-membered ring system [C52–C54/N55/B56/N57/C58–C60/C60*A*/C61/C61*A*; maximum deviation = 0.176 (3) Å for B56] makes a dihedral angle of 42.8 (1)° with the S4/C62/C63/C63*A*/C68*A* thiophene ring. The puckering parameters (Cremer & Pople, 1975) of the seven-membered cycloheptene ring fused to the thiophene ring are *viz.* for *A* (C12/C13–C17/C17*A*) $\varphi(2)$ = 44.5 (7)° and $\varphi(3)$ = 77.1 (2)°; for *B* (C29*A*/C30–C34/C34*A*) $\varphi(2)$ = 45.3 (6)° and $\varphi(3)$ = 76.4 (2)°; for *C* (C46*A*/C47–C51/C51*A*) $\varphi(2)$ = 53.9 (5)° and $\varphi(3)$ = 77.5 (2)°; and for *D* (C63*A*/C64–C68/C68*A*) $\varphi(2)$ = −123.5 (5)° and $\varphi(3)$ = −102.3 (2)°. The cycloheptene ring in molecule *D* appears more puckered compared to the other three molecules (*A*, *B* and *C*) in the asymmetric unit. This may be due to the different molecular environment leading to greater interaction in molecule *D*.



3. Supramolecular features and Hirshfeld surface analysis

In the crystal, molecules are linked to each other by C—H···F interactions, forming a three-dimensional network (Table 1, and Figs. 4, 5 and 6). Additionally, along the *a* axis, pairs of molecules are linked to each other by C—H···π interactions (Table 1 and Fig. 7). π–π interactions have not been observed.

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···F6	0.95	2.53	3.055 (2)	115
C9—H9···S1	0.95	2.76	3.253 (2)	113
C17—H17A···F4^{i}	0.99	2.33	3.315 (3)	177
C19—H19···F8^{ii}	0.95	2.41	3.289 (3)	155
C26—H26···S2	0.95	2.79	3.258 (2)	112
C34—H34A···F2	0.99	2.47	3.388 (3)	154
C34—H34B···F3^{iii}	0.99	2.40	3.385 (3)	172
C35—H35···S3′	0.95	2.56	3.053 (3)	112
C35—H35···F3^{ii}	0.95	2.52	3.343 (2)	145
C43—H43···S3	0.95	2.69	3.214 (2)	115
C52—H52···S4′	0.95	2.62	3.116 (3)	113
C52—H52···F1	0.95	2.53	3.230 (2)	131
C60—H60···S4	0.95	2.67	3.187 (2)	115
C12—H12···$Cg5$^{iv}	0.95	2.95	3.477 (2)	116
C26—H26···$Cg6$	0.95	2.95	3.426 (2)	112
C26—H26···$Cg7$	0.95	2.95	3.466 (3)	116
C29—H29···$Cg10$	0.95	2.90	3.500 (2)	122
C43—H43···$Cg14$^{iv}	0.95	2.99	3.272 (2)	98

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

The Hirshfeld surface calculations and accompanying two-dimensional fingerprint plots for the title compound were performed using *CrystalExplorer21* (Spackman *et al.*, 2021) to investigate the impact of weak intermolecular interactions on molecular packing. Figs. 8(*a*)–(*d*) depict Hirshfeld surfaces mapped on d_{norm} with the fixed colour scales of −0.2466 (red) to +1.5438 a.u. (blue) for molecule *A*, of −0.2467 (red) to +1.5777 a.u. (blue) for molecule *B*, of −0.1027 (red) to +1.4830 a.u. (blue) for molecule *C* and of −0.2061 (red) to +1.4898 a.u. (blue) for molecule *D*. The few red dots represent intermolecular connections that participate in interactions (Tables 1 and 2).

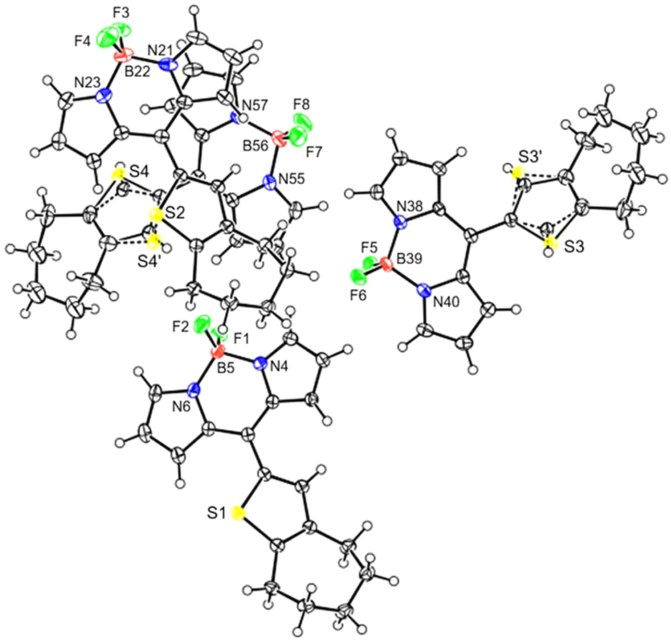


Figure 2
A view of the four independent molecules in the asymmetric unit. The major and minor components of the disorders are shown. Displacement ellipsoids are drawn at the 50% probability level. In the text, the molecules are named *A* (with S1 atoms), *B* (with S2 atoms), *C* (with S3 atoms) and *D* (with S4 atoms).

Table 2
Percentage contributions of interatomic contacts to the Hirshfeld surface for compounds A, B, C and D.

Contact	Percentage contribution			
	A	*B*	*C*	*D*
H···H	48.7	48.0	48.9	50.1
F···H/H···F	21.0	20.5	22.1	20.9
C···H/H···C	17.0	17.2	15.9	15.9
C···C	4.7	4.9	4.8	4.7
N···H/H···N	3.6	3.9	3.2	3.2
S···H/H···S	2.9	3.4	3.0	2.7
S···C/C···S	1.4	1.1	1.2	1.3
N···C/C···N	0.5	0.6	0.5	0.6
F···C/C···F	0.1	0.3	0.4	0.4
F···S/S···F	–	0.1	–	–

The two-dimensional fingerprint plots provide quantitative information about the non-covalent interactions and the crystal packing in terms of the percentage contribution of the interatomic contacts. The overall two-dimensional fingerprint plot is shown in Fig. 9(*a*). The most important interactions for the four molecules (*A*, *B*, *C* and *D*) in the asymmetric unit are H···H (*A*: 48.7%, *B*: 48.0%, *C*: 48.9% and *D*: 50.1%), F···H/H···F (*A*: 21.0%, *B*: 20.5%, *C*: 22.1% and *D*: 20.9%) and C···H/H···C (*A*: 17.0%, *B*: 17.2%, *C*: 15.9% and *D*: 15.9%) interactions. The percentage contributions for the all interactions of the molecules *A*, *B*, *C* and *D* are listed in Table 2. Upon examining the table, some deviations are observed. These deviations may be due to different environments in the crystal structures of molecules *A*, *B*, *C* and *D*.

4. Database survey

A search in the Cambridge Structural Database (CSD, Version 6.00, updated April 2025; Groom *et al.*, 2016) for a thiophene-substituted BODIPY revealed six compounds: {2-[([2,3′-bithiophen]-5′-yl)(2*H*-pyrrol-2-ylidene)methyl]-1*H*-pyrrolato}(difluoro)boron (XAWHIR: Polyanskaya *et al.*, 2026), 10-(5-bromothiophen-2-yl)-5,5-difluoro-5*H*-4,5-dipyrrolo[1,2-*c*:2′,1′-*f*][1,3,2]diazaborinine (ROHXEV: Farfán–Paredes *et al.*, 2023), 21-[5-(5,5-difluoro-5*H*-4λ^5,5λ^5-dipyrrolo[1,2-*c*:2′,1′-*f*][1,3,2]diazaborinin-10-yl)thiophen-2-yl]-19-norpregna-1,3,5(10)-trien-20-yne-3,17-diol acetone solvate (ZEQKEP: Martínez-Bourget *et al.*, 2022), 7-(diethylamino)-3-{[5-(5,5-difluoro-5*H*-6,5-dipyrrolo[1,2-*c*:2′,1′-*f*][1,3,2]diazaborinin-10-yl)thiophen-2-yl]ethynyl}-2*H*-1-benzopyran-2-one (IQOTAM: Ordóñez-Hernández *et al.*, 2021), 4-((5-(5,5-difluoro-5*H*-4λ^5,5λ^5-dipyrrolo[1,2-*c*:2′,1′-*f*][1,3,2]diazaborinin-10-yl)-2-thienyl)ethynyl)benzaldehyde (XAHZEO: Xochitiotzi-Flores *et al.*, 2016) and *N*,*N*′-difluoroboryl-5-(2-thienyl)-dipyrrin (DICJOP: Choi *et al.*, 2007).

XAWHIR, IQOTAM and ZEQKEP crystallize in the monoclinic space group $P2_1$. DICJOP crystallizes in the orthorhombic space group $P2_12_12_1$, while ROHXEV and XAHZEO crystallize in the triclinic space group $P\overline{1}$.

In the crystal of XAWHIR, molecules are linked by C—H···F interactions, forming a three-dimensional framework. C—H···π and π–π interactions are not observed. In ROHXEV, molecules are linked along the *a* axis by C—H···F interactions, forming *C*(8) zigzag chains. These chains are linked along the *b* axis by C—H···π interactions, forming layers parallel to the (002) plane. In ZEQKEP, C—H···F interactions form zigzag layers parallel to the plane (001) along the *b* axis. In IQOTAM, there are two molecules in the asymmetric unit. The molecules form a three-dimensional network with C—H···F and other C—H···O, C—H···S, C—H···π and π–π interactions. In XAHZEO, molecules form ribbons extending along the *a* axis with C—H···F interactions. In DICJOP, molecules form layers parallel to the plane (002) with the motif $R_4^4(26)$ along the *c* axis by C—H···F interactions.

In summary, the detection of C—H···F interactions in structures indicates that this interaction might play a significant role in the control of the molecular packing.

5. Synthesis and crystallization

The BODIPY general synthesis procedure was reported previously (Polyanskaya *et al.*, 2026). The earlier obtained starting 5,6,7,8-tetrahydro-4*H*-cyclohepta[*b*]thiophene-2-carbaldehyde (Yakovleva *et al.*, 2024) (810 mg, 4.49 mmol) and pyrrole (7.78 ml, 112.25 mmol) were placed in a two-necked flask. The reaction mixture was purged with argon for 10 min. Trifluoroacetic acid (TFA, 51.2 mg, 0.45 mmol) was added dropwise to the reaction under stirring at room temperature. After that, the reaction mixture was stirred for 1 h under argon. Et_3N (45 µl) was then added to pH ∼7. The reaction

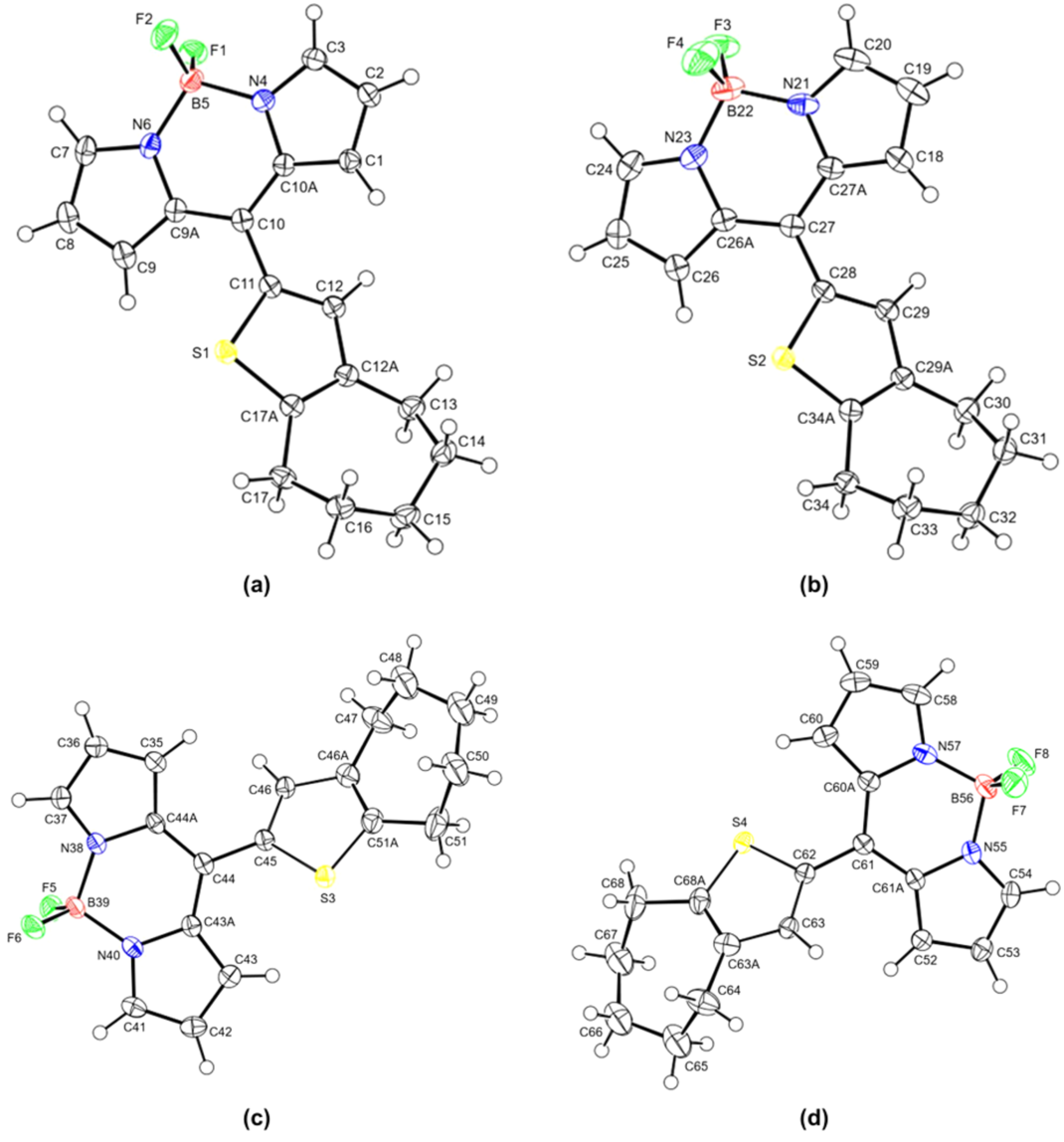


Figure 3
The molecular structures of the four independent molecules in an asymmetric unit, plotted with 50% probability displacement ellipsoids, showing (*a*) molecule *A* (S1 atom), (*b*) molecule *B* (S2 atom), (*c*) molecule *C* (S3 atom) and (*d*) molecule *D* (S4 atom). The minor components of the disorder are not shown for clarity.

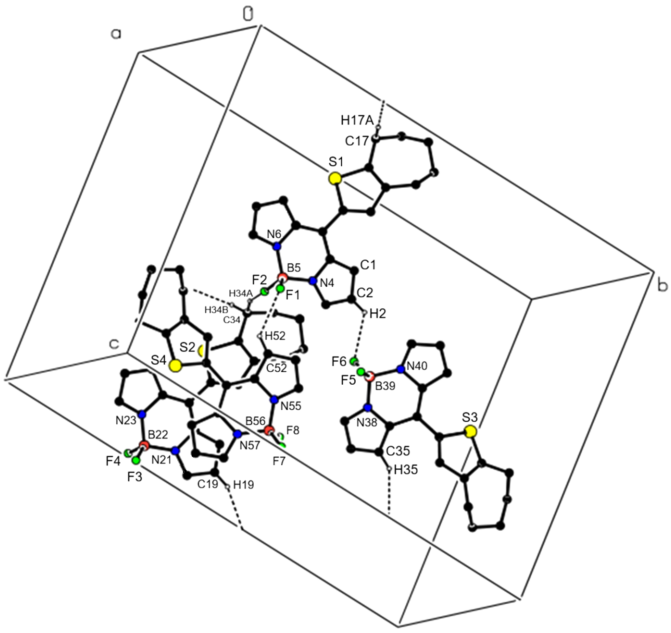


Figure 4
A general view of the C—H···F and C—H···S interactions in the unit cell. Minor components of the disorder and H atoms not involved in hydrogen bonding have been omitted for clarity.

mixture was poured into water (100 ml) and extracted with ethyl acetate (3 × 30 ml). The target product was purified by column chromatography [eluent: heptane/ethyl acetate 10:1, thin-layer chromatography (TLC): heptane/ethyl acetate 4:1]; beige powdery crystals, yield 71%, 939 mg (3.17 mmol), m.p. 425–426 K. ^{1}H NMR (700.2 MHz, $CDCl_3$) (J, Hz): δ 8.06 (*br s*, 2H, NH), 6.70 (*br s*, 2H, H-5,5′ Pyr), 6.52 (*s*, 1H, H-3 Thien), 6.18 (*q*, J = 2.7 Hz, 2H, H-4,4′ Pyr), 6.07 (*br s*, 2H, H-3,3′ Pyr), 5.75 (*s*, 1H, CH), 2.77–2.72 (*m*, 2H, CH_2), 2.64–2.60 (*m*, 2H, CH_2), 1.84 (quin, J = 5.7 Hz, 2H, CH_2), 1.68 (quin, J = 5.7 Hz, 2H, CH_2), 1.63 (quin, J = 5.7 Hz, 2H, CH_2). ^{13}C NMR (176.1 MHz, $CDCl_3$): δ 140.1, 139.0, 138.6, 132.2 (2C), 129.1, 117.2 (2C), 108.3 (2C), 106.8 (2C), 38.9, 32.3, 30.8, 29.9, 28.3, 27.8. GC–MS (EI, 70 eV): m/z (%) = 297 (19), 296 (98) [M^+], 295 (100), 281 (16), 253 (36), 230 (10), 229 (17), 228 (14), 200 (10), 145 (10), 144 (19), 143 (11). Dipyrromethane **1** (327 mg, 1.1 mmol) was dissolved in dry DCM (10 ml), after 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ, 752 mg, 3.3 mmol) was added; the reaction mixture was stirred for 30 min (TLC control), poured into water (100 ml) and extracted with DCM (3 × 30 ml). The organic layer was dried with anhydrous Na_2SO_4, concentrated *in vacuo* and the residue was dissolved in dry DCM (20 ml) without further purification. Boron trifluoride etherate (2.76 ml, 22.0 mmol) and an equal volume of diisopropylethylamine (DIPEA, 2.76 ml) were added. The solution was stirred under room temperature for 1 h (TLC control) and then poured into water (100 ml), extracted with DCM (3 × 30 ml) and washed with saturated Na_2CO_3 (3 × 30 ml). The organic layer was dried with anhydrous Na_2SO_4, the target product **2** was purified by column chromatography (eluent: ethyl acetate/hexane 1:10); orange crystals, yield 38%, 142 mg (0.41 mmol), m.p. 419–420 K. Single crystals of the title compound were grown from a mixture of ethyl acetate/hexane at 298 K. ^{1}H NMR (700.2 MHz, $CDCl_3$) (J, Hz): δ 7.89 (*s*, 2H, H-5,5′ Pyr), 7.35 (*d*, J = 4.0 Hz, 2H, H-4,4′ Pyr), 7.31 (*s*, 1H, H-3 Thien), 6.57 (*d*, J = 2.6 Hz, 2H, H-3,3′ Pyr), 2.96–2.92 (*m*, 2H, CH_2), 2.82–2.79 (*m*, 2H, CH_2), 1.94 (*m*, 2H, CH_2), 1.79 (*m*, 2H, CH_2), 1.73 (*m*, 2H, CH_2). ^{13}C NMR (176.1 MHz, $CDCl_3$): δ 149.3, 143.2 (2C), 142.6 (2C), 140.1, 136.9 (2C), 133.9, 131.2, 129.1, 118.0 (2C),

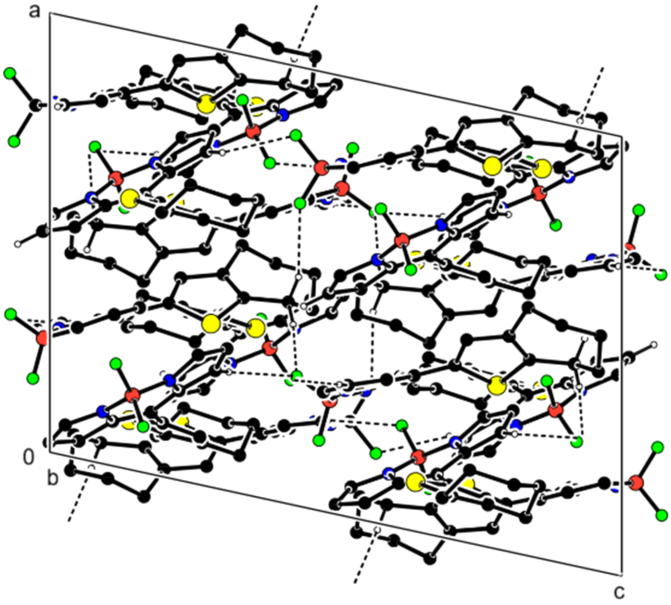


Figure 5
A view of C—H···F and C—H···S interactions along the *b* axis.

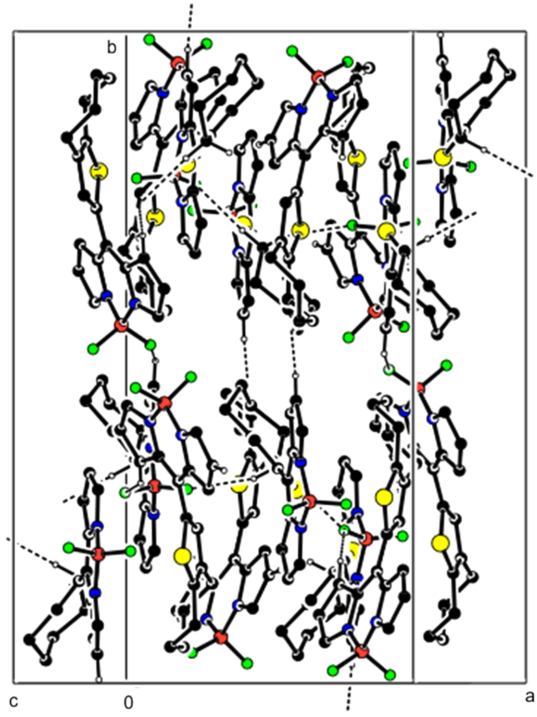


Figure 6
A view of C—H···F and C—H···S interactions along the *c* axis.

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{17}BF_2N_2S$
M_r	342.21
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	14.54911 (8), 23.71611 (13), 19.41866 (11)
β (°)	102.1987 (6)
V (Å^3)	6549.09 (7)
Z	16
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.95
Crystal size (mm)	0.15 × 0.10 × 0.10
Data collection	
Diffractometer	Rigaku XtaLAB Synergy-S HyPix-6000HE area-detector
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2021)
T_{min}, T_{max}	0.827, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	81021, 14098, 12698
R_{int}	0.041
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.639
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.054, 0.145, 1.05
No. of reflections	14098
No. of parameters	843
No. of restraints	18
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.18, −0.83

Computer programs: *CrysAlis PRO* (Rigaku OD, 2021), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2020).

32.3, 30.8, 30.4, 28.0, 27.7. ^{19}F NMR (658.8 MHz, $CDCl_3$): δ −145.3 to −145.5 (*m*, 2F). GC–MS (EI, 70 eV): *m*/*z* (%) = 343 (17), 342 (90) [M^+], 341 (100), 340 (15), 313 (10), 281 (10), 207 (13), 44 (24), 40 (15).

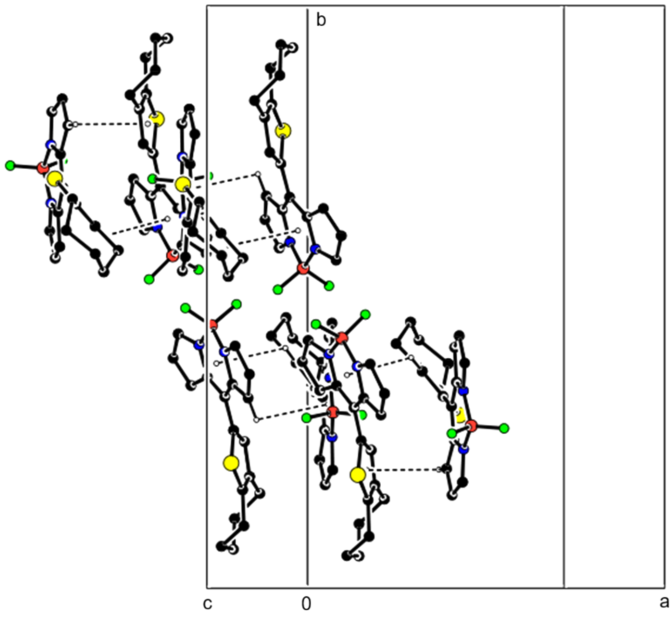


Figure 7
Views of the C—H···π interactions along the *c* axis.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All C-bound H atoms were positioned geometrically (C—H = 0.95 and 0.99 Å) and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C). In molecules *C* and *D*, the thiophene rings (S3/C45/C46/C46*A*/C51*A* and S4/C62/C63/C63*A*/C68*A*) were disordered by a 180° rotation over two positions about the C44—C45 bond with a ratio of 0.7839 (15):0.2161 (15) for *C*, and about the C61—C62 bond with a ratio of 0.7874 (16):0.2126 (16) for *D*. The DFIX command was used to restrain the S—C distances which are S3—C45, S3—C51*A*, S3′—C45 and S3′—C46*A* for the S3/C45/C46/C46*A*/C51*A* thiophene ring, and S4—C62, S4—C68*A*, S4′—C62 and S4′—C63*A* for the S4/C62/C63/C63*A*/C68*A* thiophene ring, to fix their bond lengths to 1.71 Å. In the disordered thiophene rings of the molecules *C* and *D*, the C—C bond lengths (for *C*: C46—C46*A*, C46′—C51*A*, and for *D*: C63—C63*A* and C63′—C68*A*) were restrained to fix these bond lengths to 1.42 Å, while the C=C bond lengths (for *C*: C46*A*—C51*A*, C45—C46, C45—C46′, and for *D*: C63*A*—C68*A*, C62—C63 and C62—C63′) were restrained to

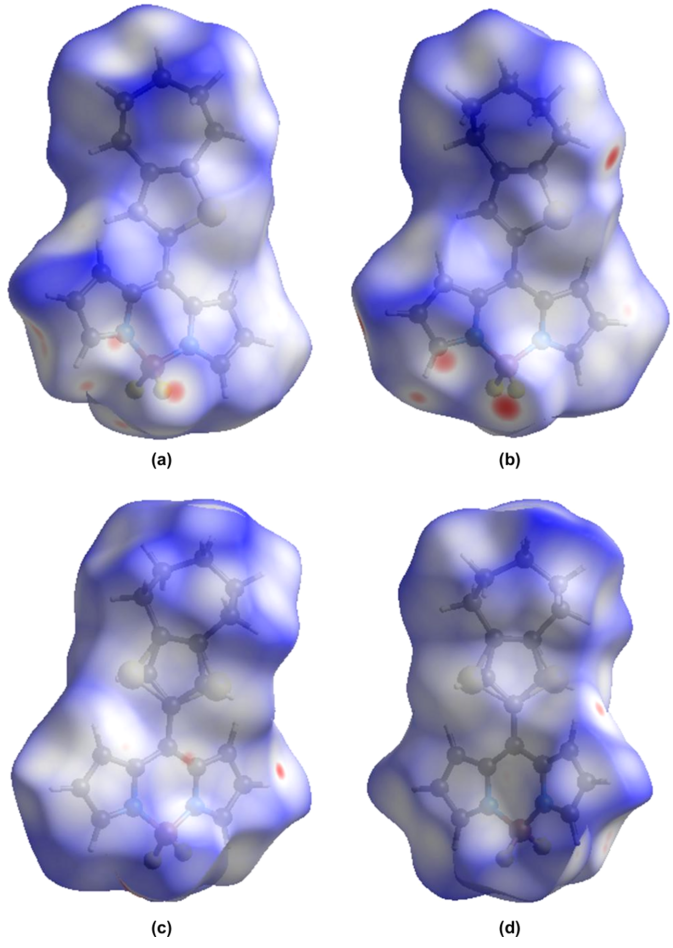


Figure 8
Three-dimensional Hirshfeld surface analyses of the four independent molecules in the asymmetric unit mapped over d_{norm}. (*a*) For molecule *A*, (*b*) for molecule *B*, (*c*) for molecule *C* and (*d*) for molecule *D*.

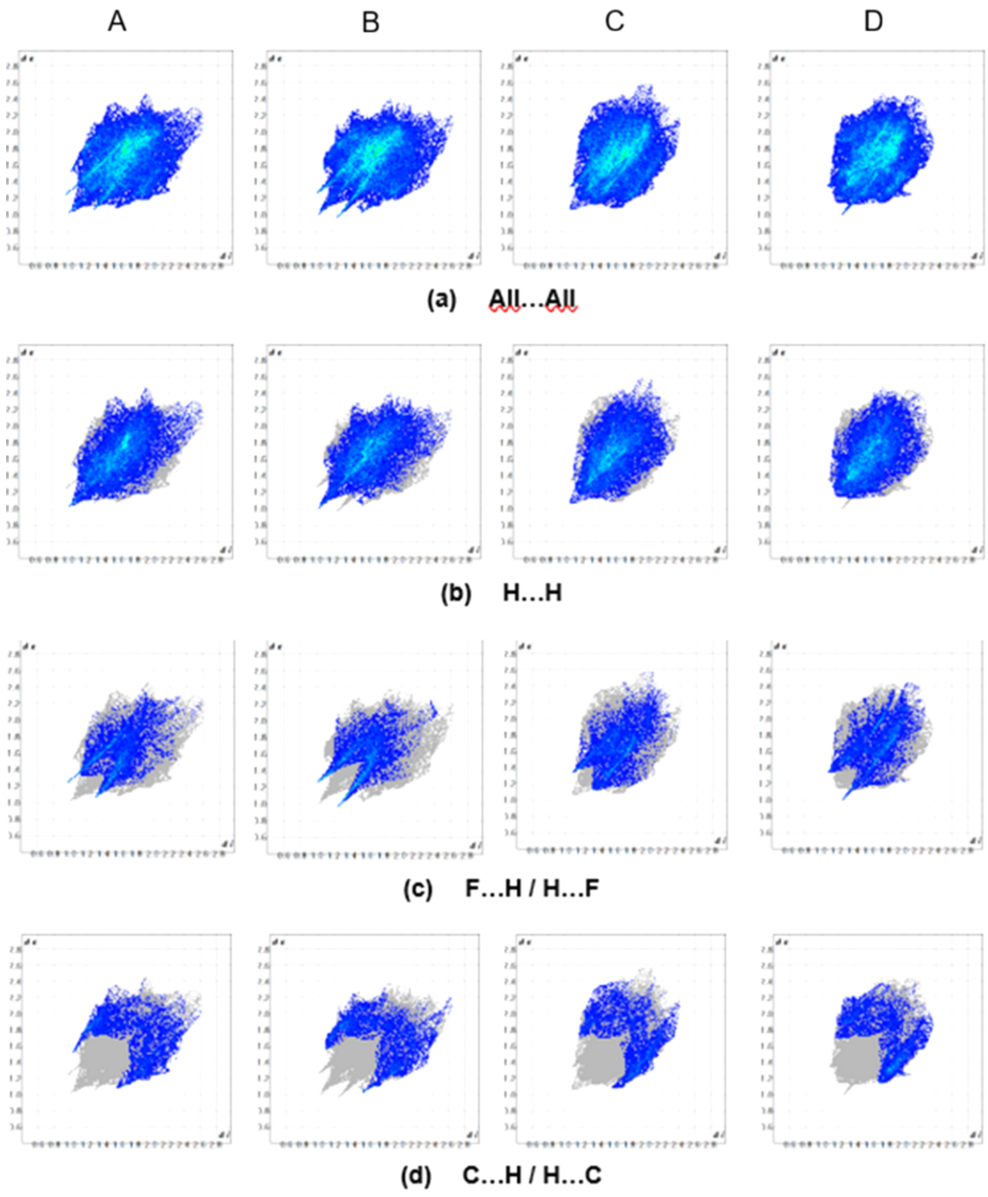


Figure 9
The two-dimensional fingerprint plots of the four independent molecules (*A*, *B*, *C* and *D*) in the asymmetric unit showing (*a*) all interactions, and those delineated into (*b*) H···H, (*c*) F···H/H···F and (*d*) C···H/H···C interactions. The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

fix these bond lengths to 1.37 Å. In the disordered thiophene rings, the displacement parameters of the corresponding atoms (S3 C46′ S3′ C46, S4 C63′ S4′ C63, C48 C49 C50 and C65 C66 C67) were made identical using the EADP command. Owing to poor agreement between the observed and calculated intensities, 59 outliers (−15 1 16, −14 1 17, −16 1 15, −15 2 17, −11 4 18, −14 2 17, −14 2 18, −13 5 16, −12 4 18, −15 6 16, −16 3 14, −15 5 16, −15 7 17, −16 7 15, −14 3 19, −17 4 13, −17 3 14, −13 2 20, −15 2 15, −15 0 16, −16 3 15, −15 4 15, −14 1 18, −16 2 15, −2 7 6, −14 0 16, −14 6 15, −15 2 16, −3 22 6, −14 1 16, −15 6 14, −15 3 17, −6 8 4, 1 10 5, −17 1 13, −17 4 14, −2 7 4, −1 1 7, −2 10 6, 4 20 9, 7 20 9, −14 3 17, −5 9 17, −2 12 4, −5 9 1, −9 5 1, −1 5 11, −17 3 13, 0 0 10, 0 12 0, −6 9 10, −2 2 8, −9 22 14, −9 23 6, −3 8 5, −2 2 14, −1 7 17, −3 5 7, −4 4 6) were omitted in the final cycles of refinement.

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supporting information

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Crystal structure and Hirshfeld surface analysis of 5,5-difluoro-10-(5,6,7,8-tetrahydro-4*H*-cyclohepta[*b*]thiophen-2-yl)-5*H*-4λ^4,5λ^4-dipyrrolo[1,2-*c*:2′,1′-*f*][1,3,2]diazaborinine

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Computing details

5,5-Difluoro-10-(5,6,7,8-tetrahydro-4*H*-cyclohepta[*b*]thiophen-2-yl)-5*H*-4λ^4,5λ^4-dipyrrolo[1,2-*c*:2′,1′-*f*][1,3,2]diazaborinine

Crystal data

$C_{18}H_{17}BF_2N_2S$
M_r = 342.21
Monoclinic, $P2_1/c$
a = 14.54911 (8) Å
b = 23.71611 (13) Å
c = 19.41866 (11) Å
β = 102.1987 (6)°
V = 6549.09 (7) Å^3
Z = 16
$F(000)$ = 2848
D_x = 1.388 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 52697 reflections
θ = 3.0–79.9°
μ = 1.95 mm^{-1}
T = 100 K
Prism, colourless
0.15 × 0.10 × 0.10 mm

Data collection

Rigaku XtaLAB Synergy-S HyPix-6000HE area-detector diffractometer
Radiation source: micro-focus sealed X-ray tube
φ and ω scans
Absorption correction: multi-scan (CrysAlis PRO; Rigaku OD, 2021)
T_{min} = 0.827, T_{max} = 1.000
81021 measured reflections
14098 independent reflections
12698 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 80.0°, θ_{min} = 3.0°
h = −18→17
k = −29→29
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.145
S = 1.05
14098 reflections
843 parameters
18 restraints
Primary atom site location: difference Fourier map
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0713P)^2 + 6.8865P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.83 e Å^{-3}

Special details

Experimental. CrysAlisPro 1.171.43.143a (Rigaku OD, 2021). Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.13053 (3)	0.30670 (2)	0.22618 (2)	0.02069 (11)	
F1	0.15783 (9)	0.29231 (5)	0.56991 (6)	0.0301 (3)	
F2	0.31054 (9)	0.29741 (6)	0.56256 (8)	0.0376 (3)	
C1	0.17558 (14)	0.43127 (8)	0.40954 (10)	0.0224 (4)	
H1	0.1613	0.4508	0.3658	0.027*	
C2	0.20272 (14)	0.45536 (8)	0.47574 (11)	0.0252 (4)	
H2	0.2099	0.4945	0.4861	0.030*	
C3	0.21752 (13)	0.41122 (9)	0.52437 (10)	0.0237 (4)	
H3	0.2362	0.4157	0.5740	0.028*	
N4	0.20146 (11)	0.36136 (7)	0.49080 (8)	0.0207 (3)	
B5	0.21891 (16)	0.30216 (9)	0.52468 (12)	0.0240 (4)	
N6	0.19896 (11)	0.25959 (7)	0.46268 (9)	0.0217 (3)	
C7	0.20271 (15)	0.20310 (8)	0.46932 (11)	0.0260 (4)	
H7	0.2284	0.1835	0.5117	0.031*	
C8	0.16355 (15)	0.17753 (8)	0.40518 (12)	0.0273 (4)	
H8	0.1579	0.1382	0.3962	0.033*	
C9	0.13437 (14)	0.22044 (8)	0.35703 (11)	0.0240 (4)	
H9	0.1041	0.2160	0.3090	0.029*	
C9A	0.15801 (13)	0.27191 (8)	0.39276 (10)	0.0195 (3)	
C10	0.14643 (12)	0.32843 (8)	0.37022 (10)	0.0182 (3)	
C10A	0.17304 (13)	0.37229 (8)	0.41918 (10)	0.0195 (3)	
C11	0.10630 (13)	0.34328 (8)	0.29735 (10)	0.0192 (3)	
C12	0.04509 (13)	0.38690 (8)	0.27404 (10)	0.0201 (4)	
H12	0.0237	0.4123	0.3051	0.024*	
C12A	0.01676 (13)	0.39059 (8)	0.19967 (10)	0.0202 (4)	
C13	−0.05475 (15)	0.43318 (9)	0.16457 (10)	0.0281 (4)	
H13A	−0.0634	0.4613	0.2003	0.034*	
H13B	−0.1156	0.4136	0.1486	0.034*	
C14	−0.03148 (18)	0.46479 (10)	0.10137 (11)	0.0330 (5)	
H14A	−0.0778	0.4955	0.0880	0.040*	
H14B	0.0312	0.4824	0.1164	0.040*	
C15	−0.03112 (16)	0.42885 (10)	0.03628 (11)	0.0313 (5)	
H15A	−0.0310	0.4543	−0.0041	0.038*	
H15B	−0.0903	0.4069	0.0254	0.038*	
C16	0.05124 (15)	0.38797 (9)	0.04223 (11)	0.0278 (4)	
H16A	0.1103	0.4086	0.0611	0.033*	
H16B	0.0540	0.3746	−0.0056	0.033*	

C17	0.04624 (15)	0.33675 (9)	0.08907 (10)	0.0260 (4)	
H17A	−0.0155	0.3182	0.0728	0.031*	
H17B	0.0954	0.3095	0.0828	0.031*	
C17A	0.05869 (13)	0.34960 (8)	0.16636 (10)	0.0207 (4)	
S2	0.62810 (3)	0.29699 (2)	0.71817 (2)	0.02114 (11)	
F3	0.70570 (12)	0.26558 (7)	1.06851 (7)	0.0446 (4)	
F4	0.84073 (10)	0.27454 (7)	1.02956 (9)	0.0501 (4)	
C18	0.66894 (15)	0.41348 (9)	0.91142 (11)	0.0288 (4)	
H18	0.6470	0.4355	0.8704	0.035*	
C19	0.70090 (17)	0.43364 (11)	0.97927 (13)	0.0357 (5)	
H19	0.7036	0.4719	0.9939	0.043*	
C20	0.72831 (16)	0.38659 (11)	1.02191 (12)	0.0339 (5)	
H20	0.7538	0.3881	1.0711	0.041*	
N21	0.71374 (12)	0.33891 (8)	0.98388 (9)	0.0270 (4)	
B22	0.74362 (18)	0.27882 (12)	1.01058 (13)	0.0317 (5)	
N23	0.70440 (11)	0.23883 (8)	0.94867 (9)	0.0246 (3)	
C24	0.70266 (14)	0.18224 (9)	0.95181 (12)	0.0288 (4)	
H24	0.7299	0.1605	0.9920	0.035*	
C25	0.65510 (15)	0.15996 (9)	0.88746 (11)	0.0272 (4)	
H25	0.6442	0.1212	0.8763	0.033*	
C26	0.62693 (13)	0.20549 (8)	0.84311 (11)	0.0229 (4)	
H26	0.5925	0.2037	0.7958	0.027*	
C26A	0.65868 (13)	0.25499 (8)	0.88103 (10)	0.0209 (4)	
C27	0.64647 (13)	0.31229 (8)	0.86296 (10)	0.0204 (4)	
C27A	0.67510 (13)	0.35411 (9)	0.91459 (10)	0.0229 (4)	
C28	0.60253 (13)	0.32975 (8)	0.79169 (10)	0.0200 (3)	
C29	0.53892 (13)	0.37251 (8)	0.77108 (10)	0.0210 (4)	
H29	0.5165	0.3960	0.8036	0.025*	
C29A	0.50963 (13)	0.37861 (8)	0.69703 (10)	0.0209 (4)	
C30	0.43514 (15)	0.41988 (9)	0.66370 (11)	0.0270 (4)	
H30A	0.4212	0.4448	0.7011	0.032*	
H30B	0.3770	0.3986	0.6439	0.032*	
C31	0.45930 (16)	0.45703 (9)	0.60503 (11)	0.0295 (4)	
H31A	0.4116	0.4873	0.5939	0.035*	
H31B	0.5209	0.4753	0.6232	0.035*	
C32	0.46390 (15)	0.42596 (9)	0.53709 (11)	0.0289 (4)	
H32A	0.4050	0.4042	0.5220	0.035*	
H32B	0.4662	0.4543	0.5001	0.035*	
C33	0.54654 (15)	0.38575 (10)	0.54098 (11)	0.0291 (4)	
H33A	0.6052	0.4059	0.5625	0.035*	
H33B	0.5508	0.3752	0.4924	0.035*	
C34	0.54076 (15)	0.33180 (9)	0.58306 (10)	0.0255 (4)	
H34A	0.4788	0.3139	0.5652	0.031*	
H34B	0.5896	0.3052	0.5744	0.031*	
C34A	0.55332 (13)	0.34047 (8)	0.66135 (10)	0.0216 (4)	
S3	0.11212 (4)	0.78515 (2)	0.63947 (3)	0.02130 (14)	0.7839 (15)
S3′	0.11463 (17)	0.74133 (8)	0.78378 (11)	0.02130 (14)	0.2161 (15)
F5	0.10400 (9)	0.51249 (5)	0.66313 (7)	0.0334 (3)	

F6	0.23367 (10)	0.51912 (6)	0.61545 (7)	0.0362 (3)	
C35	0.26685 (14)	0.65190 (8)	0.78904 (10)	0.0217 (4)	
H35	0.2704	0.6871	0.8129	0.026*	
C36	0.32286 (14)	0.60504 (8)	0.80973 (10)	0.0243 (4)	
H36	0.3717	0.6020	0.8506	0.029*	
C37	0.29416 (14)	0.56310 (8)	0.75933 (10)	0.0233 (4)	
H37	0.3212	0.5266	0.7601	0.028*	
N38	0.22217 (11)	0.58231 (7)	0.70932 (8)	0.0204 (3)	
B39	0.16973 (16)	0.54913 (9)	0.64457 (12)	0.0238 (4)	
N40	0.11796 (11)	0.59398 (7)	0.59265 (9)	0.0219 (3)	
C41	0.06937 (14)	0.58412 (9)	0.52680 (10)	0.0262 (4)	
H41	0.0679	0.5492	0.5027	0.031*	
C42	0.02146 (14)	0.63258 (9)	0.49897 (11)	0.0269 (4)	
H42	−0.0166	0.6367	0.4530	0.032*	
C43	0.03960 (14)	0.67347 (9)	0.55070 (10)	0.0239 (4)	
H43	0.0153	0.7108	0.5473	0.029*	
C43A	0.10100 (13)	0.64956 (8)	0.60978 (10)	0.0203 (4)	
C44	0.14068 (13)	0.67139 (8)	0.67700 (10)	0.0196 (3)	
C44A	0.20332 (13)	0.63751 (8)	0.72572 (10)	0.0191 (3)	
C45	0.12177 (13)	0.72881 (7)	0.69741 (8)	0.0203 (4)	
C46	0.1092 (2)	0.74832 (9)	0.76209 (14)	0.02130 (14)	0.7839 (15)
H46	0.1092	0.7239	0.8009	0.026*	0.7839 (15)
C46′	0.1184 (8)	0.78117 (13)	0.6668 (3)	0.02130 (14)	0.2161 (15)
H46A	0.1299	0.7844	0.6206	0.026*	0.2161 (15)
C46A	0.09616 (14)	0.80800 (7)	0.76599 (10)	0.0272 (4)	
C47	0.08602 (17)	0.83715 (12)	0.83180 (14)	0.0401 (6)	
H47A	0.0876	0.8088	0.8695	0.048*	
H47B	0.0243	0.8564	0.8237	0.048*	
C48	0.1638 (2)	0.88034 (12)	0.85594 (18)	0.0509 (4)	
H48A	0.1640	0.8911	0.9053	0.061*	
H48B	0.2251	0.8625	0.8553	0.061*	
C49	0.1543 (2)	0.93311 (12)	0.81156 (17)	0.0509 (4)	
H49A	0.2014	0.9606	0.8358	0.061*	
H49B	0.0914	0.9494	0.8107	0.061*	
C50	0.1661 (2)	0.92786 (12)	0.73410 (17)	0.0509 (4)	
H50A	0.1662	0.9662	0.7139	0.061*	
H50B	0.2281	0.9106	0.7341	0.061*	
C51	0.0896 (2)	0.89278 (11)	0.68616 (17)	0.0474 (7)	
H51A	0.0271	0.9061	0.6916	0.057*	
H51B	0.0939	0.8988	0.6365	0.057*	
C51A	0.09801 (14)	0.83099 (8)	0.70241 (10)	0.0287 (4)	
S4	0.38348 (4)	0.19475 (2)	0.85986 (3)	0.02105 (14)	0.7874 (16)
S4′	0.38505 (18)	0.24452 (8)	0.72148 (10)	0.02105 (14)	0.2126 (16)
F7	0.40679 (11)	0.46975 (6)	0.86891 (8)	0.0439 (4)	
F8	0.28310 (11)	0.45317 (7)	0.92107 (8)	0.0458 (4)	
C52	0.23935 (13)	0.33984 (8)	0.72680 (10)	0.0214 (4)	
H52	0.2331	0.3069	0.6983	0.026*	
C53	0.18662 (14)	0.38874 (8)	0.71292 (11)	0.0253 (4)	

H53	0.1378	0.3958	0.6729	0.030*	
C54	0.21879 (14)	0.42563 (8)	0.76882 (11)	0.0258 (4)	
H54	0.1941	0.4622	0.7732	0.031*	
N55	0.28981 (12)	0.40187 (7)	0.81564 (9)	0.0226 (3)	
B56	0.34499 (18)	0.42917 (10)	0.88430 (13)	0.0290 (5)	
N57	0.40074 (12)	0.38075 (7)	0.92726 (9)	0.0251 (3)	
C58	0.45530 (16)	0.38494 (10)	0.99240 (11)	0.0314 (5)	
H58	0.4616	0.4179	1.0208	0.038*	
C59	0.50113 (16)	0.33423 (11)	1.01221 (11)	0.0322 (5)	
H59	0.5424	0.3263	1.0560	0.039*	
C60	0.47533 (14)	0.29741 (9)	0.95619 (10)	0.0262 (4)	
H60	0.4964	0.2597	0.9540	0.031*	
C60A	0.41166 (13)	0.32655 (8)	0.90278 (10)	0.0218 (4)	
C61	0.36546 (13)	0.31003 (8)	0.83440 (10)	0.0195 (3)	
C61A	0.30423 (13)	0.34807 (8)	0.79141 (10)	0.0197 (3)	
C62	0.37820 (13)	0.25363 (7)	0.80766 (8)	0.0202 (4)	
C63	0.3869 (2)	0.23717 (9)	0.74048 (14)	0.02105 (14)	0.7874 (16)
H63	0.3873	0.2634	0.7035	0.025*	0.7874 (16)
C63′	0.3786 (8)	0.19974 (12)	0.8338 (3)	0.02105 (14)	0.2126 (16)
H63B	0.3689	0.1944	0.8802	0.025*	0.2126 (16)
C63A	0.39525 (14)	0.17738 (7)	0.73155 (10)	0.0284 (4)	
C64	0.40178 (17)	0.15307 (13)	0.66228 (14)	0.0416 (6)	
H64A	0.4634	0.1342	0.6666	0.050*	
H64B	0.3982	0.1839	0.6274	0.050*	
C65	0.3234 (2)	0.11058 (12)	0.63570 (18)	0.0498 (4)	
H65A	0.2625	0.1277	0.6391	0.060*	
H65B	0.3215	0.1028	0.5853	0.060*	
C66	0.3344 (2)	0.05551 (12)	0.67540 (17)	0.0498 (4)	
H66A	0.3976	0.0404	0.6748	0.060*	
H66B	0.2879	0.0286	0.6490	0.060*	
C67	0.3226 (2)	0.05602 (12)	0.75372 (17)	0.0498 (4)	
H67A	0.2606	0.0725	0.7553	0.060*	
H67B	0.3229	0.0166	0.7706	0.060*	
C68	0.39919 (18)	0.08920 (10)	0.80439 (17)	0.0457 (6)	
H68A	0.3941	0.0809	0.8534	0.055*	
H68B	0.4616	0.0760	0.7986	0.055*	
C68A	0.39327 (14)	0.15146 (8)	0.79318 (10)	0.0280 (4)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0242 (2)	0.0194 (2)	0.0205 (2)	0.00095 (16)	0.00950 (17)	−0.00113 (16)
F1	0.0424 (7)	0.0283 (6)	0.0212 (5)	−0.0049 (5)	0.0103 (5)	0.0017 (5)
F2	0.0299 (6)	0.0308 (7)	0.0442 (8)	0.0007 (5)	−0.0098 (6)	0.0069 (6)
C1	0.0256 (9)	0.0200 (9)	0.0224 (9)	0.0002 (7)	0.0068 (7)	0.0004 (7)
C2	0.0283 (10)	0.0205 (9)	0.0264 (9)	0.0002 (7)	0.0052 (8)	−0.0042 (7)
C3	0.0227 (9)	0.0265 (10)	0.0215 (9)	0.0004 (7)	0.0035 (7)	−0.0034 (7)
N4	0.0201 (7)	0.0218 (8)	0.0203 (7)	−0.0003 (6)	0.0046 (6)	0.0011 (6)

B5	0.0258 (10)	0.0222 (10)	0.0226 (10)	−0.0005 (8)	0.0019 (8)	0.0038 (8)
N6	0.0226 (7)	0.0195 (8)	0.0240 (8)	0.0023 (6)	0.0074 (6)	0.0044 (6)
C7	0.0287 (10)	0.0211 (9)	0.0320 (10)	0.0054 (7)	0.0149 (8)	0.0067 (8)
C8	0.0337 (10)	0.0183 (9)	0.0361 (11)	0.0010 (8)	0.0212 (9)	0.0014 (8)
C9	0.0260 (9)	0.0209 (9)	0.0293 (10)	−0.0014 (7)	0.0158 (8)	−0.0008 (7)
C9A	0.0184 (8)	0.0202 (9)	0.0220 (8)	0.0004 (7)	0.0092 (7)	0.0018 (7)
C10	0.0165 (8)	0.0194 (8)	0.0212 (8)	−0.0007 (6)	0.0095 (7)	0.0006 (7)
C10A	0.0195 (8)	0.0197 (9)	0.0203 (8)	0.0001 (7)	0.0066 (7)	0.0012 (7)
C11	0.0204 (8)	0.0186 (8)	0.0206 (8)	−0.0021 (7)	0.0087 (7)	−0.0009 (7)
C12	0.0219 (8)	0.0205 (9)	0.0197 (8)	−0.0013 (7)	0.0086 (7)	−0.0001 (7)
C12A	0.0209 (8)	0.0224 (9)	0.0189 (8)	−0.0019 (7)	0.0077 (7)	0.0010 (7)
C13	0.0291 (10)	0.0350 (11)	0.0212 (9)	0.0086 (8)	0.0075 (8)	0.0017 (8)
C14	0.0438 (12)	0.0323 (11)	0.0239 (10)	0.0102 (9)	0.0095 (9)	0.0062 (8)
C15	0.0347 (11)	0.0404 (12)	0.0201 (9)	0.0053 (9)	0.0083 (8)	0.0047 (8)
C16	0.0288 (10)	0.0359 (11)	0.0210 (9)	0.0000 (8)	0.0103 (8)	0.0004 (8)
C17	0.0304 (10)	0.0288 (10)	0.0204 (9)	−0.0018 (8)	0.0092 (8)	−0.0040 (8)
C17A	0.0211 (8)	0.0222 (9)	0.0206 (9)	−0.0025 (7)	0.0081 (7)	0.0006 (7)
S2	0.0234 (2)	0.0217 (2)	0.0197 (2)	0.00325 (16)	0.00776 (17)	−0.00065 (16)
F3	0.0645 (10)	0.0491 (8)	0.0195 (6)	−0.0218 (7)	0.0069 (6)	0.0015 (6)
F4	0.0293 (7)	0.0548 (9)	0.0568 (9)	−0.0086 (6)	−0.0125 (6)	0.0088 (8)
C18	0.0309 (10)	0.0277 (10)	0.0288 (10)	−0.0051 (8)	0.0085 (8)	−0.0071 (8)
C19	0.0363 (12)	0.0378 (12)	0.0347 (12)	−0.0089 (9)	0.0111 (9)	−0.0150 (10)
C20	0.0322 (11)	0.0469 (13)	0.0237 (10)	−0.0138 (10)	0.0084 (8)	−0.0109 (9)
N21	0.0251 (8)	0.0368 (10)	0.0195 (8)	−0.0097 (7)	0.0057 (6)	−0.0026 (7)
B22	0.0283 (11)	0.0417 (14)	0.0231 (11)	−0.0094 (10)	0.0006 (9)	0.0045 (10)
N23	0.0202 (7)	0.0316 (9)	0.0229 (8)	−0.0004 (6)	0.0066 (6)	0.0058 (7)
C24	0.0236 (9)	0.0332 (11)	0.0320 (10)	0.0036 (8)	0.0111 (8)	0.0109 (9)
C25	0.0274 (10)	0.0247 (10)	0.0336 (10)	0.0017 (8)	0.0155 (8)	0.0042 (8)
C26	0.0208 (8)	0.0244 (9)	0.0263 (9)	−0.0009 (7)	0.0114 (7)	0.0001 (7)
C26A	0.0171 (8)	0.0271 (9)	0.0202 (8)	−0.0014 (7)	0.0075 (7)	0.0012 (7)
C27	0.0170 (8)	0.0252 (9)	0.0207 (9)	−0.0024 (7)	0.0079 (7)	−0.0002 (7)
C27A	0.0221 (9)	0.0280 (10)	0.0199 (9)	−0.0044 (7)	0.0073 (7)	−0.0012 (7)
C28	0.0207 (8)	0.0206 (9)	0.0202 (8)	−0.0030 (7)	0.0077 (7)	−0.0026 (7)
C29	0.0221 (9)	0.0224 (9)	0.0202 (9)	−0.0017 (7)	0.0082 (7)	−0.0018 (7)
C29A	0.0209 (8)	0.0224 (9)	0.0210 (9)	−0.0007 (7)	0.0080 (7)	−0.0005 (7)
C30	0.0279 (10)	0.0314 (10)	0.0237 (9)	0.0080 (8)	0.0099 (8)	0.0030 (8)
C31	0.0347 (11)	0.0250 (10)	0.0296 (10)	0.0047 (8)	0.0087 (9)	0.0039 (8)
C32	0.0318 (10)	0.0314 (10)	0.0249 (10)	0.0023 (8)	0.0095 (8)	0.0064 (8)
C33	0.0293 (10)	0.0373 (11)	0.0234 (9)	0.0019 (9)	0.0116 (8)	0.0027 (8)
C34	0.0290 (10)	0.0294 (10)	0.0200 (9)	0.0044 (8)	0.0090 (7)	−0.0013 (7)
C34A	0.0219 (8)	0.0231 (9)	0.0215 (9)	0.0004 (7)	0.0082 (7)	0.0007 (7)
S3	0.0235 (3)	0.0196 (3)	0.0225 (3)	0.00073 (19)	0.0088 (3)	0.0021 (2)
S3′	0.0235 (3)	0.0196 (3)	0.0225 (3)	0.00073 (19)	0.0088 (3)	0.0021 (2)
F5	0.0371 (7)	0.0207 (6)	0.0387 (7)	−0.0074 (5)	−0.0003 (5)	0.0012 (5)
F6	0.0382 (7)	0.0363 (7)	0.0323 (7)	0.0149 (6)	0.0028 (5)	−0.0139 (5)
C35	0.0254 (9)	0.0202 (9)	0.0214 (9)	−0.0042 (7)	0.0094 (7)	−0.0019 (7)
C36	0.0243 (9)	0.0254 (9)	0.0234 (9)	−0.0041 (7)	0.0054 (7)	0.0000 (7)
C37	0.0235 (9)	0.0207 (9)	0.0264 (9)	0.0002 (7)	0.0070 (7)	0.0009 (7)

N38	0.0232 (7)	0.0173 (7)	0.0222 (7)	−0.0005 (6)	0.0077 (6)	−0.0021 (6)
B39	0.0270 (10)	0.0187 (10)	0.0255 (10)	0.0015 (8)	0.0052 (8)	−0.0059 (8)
N40	0.0227 (7)	0.0215 (8)	0.0226 (8)	−0.0006 (6)	0.0074 (6)	−0.0046 (6)
C41	0.0253 (9)	0.0313 (10)	0.0228 (9)	−0.0023 (8)	0.0066 (8)	−0.0069 (8)
C42	0.0234 (9)	0.0363 (11)	0.0214 (9)	−0.0019 (8)	0.0059 (7)	−0.0010 (8)
C43	0.0217 (9)	0.0275 (10)	0.0242 (9)	0.0011 (7)	0.0088 (7)	0.0025 (8)
C43A	0.0205 (8)	0.0202 (9)	0.0225 (9)	0.0003 (7)	0.0093 (7)	−0.0005 (7)
C44	0.0202 (8)	0.0184 (8)	0.0231 (9)	−0.0023 (7)	0.0114 (7)	−0.0012 (7)
C44A	0.0221 (8)	0.0166 (8)	0.0213 (8)	−0.0021 (7)	0.0103 (7)	−0.0028 (7)
C45	0.0226 (8)	0.0195 (9)	0.0209 (8)	−0.0001 (7)	0.0096 (7)	0.0001 (7)
C46	0.0235 (3)	0.0196 (3)	0.0225 (3)	0.00073 (19)	0.0088 (3)	0.0021 (2)
C46′	0.0235 (3)	0.0196 (3)	0.0225 (3)	0.00073 (19)	0.0088 (3)	0.0021 (2)
C46A	0.0213 (9)	0.0312 (10)	0.0301 (10)	0.0023 (8)	0.0076 (8)	−0.0041 (8)
C47	0.0313 (11)	0.0512 (15)	0.0399 (13)	0.0020 (10)	0.0123 (10)	−0.0189 (11)
C48	0.0461 (8)	0.0370 (8)	0.0673 (11)	0.0005 (7)	0.0069 (8)	−0.0157 (7)
C49	0.0461 (8)	0.0370 (8)	0.0673 (11)	0.0005 (7)	0.0069 (8)	−0.0157 (7)
C50	0.0461 (8)	0.0370 (8)	0.0673 (11)	0.0005 (7)	0.0069 (8)	−0.0157 (7)
C51	0.0436 (14)	0.0272 (12)	0.0645 (17)	−0.0014 (10)	−0.0040 (12)	0.0127 (11)
C51A	0.0248 (9)	0.0233 (10)	0.0363 (11)	−0.0021 (8)	0.0027 (8)	0.0007 (8)
S4	0.0222 (2)	0.0207 (3)	0.0214 (3)	0.00025 (19)	0.0072 (3)	0.0047 (2)
S4′	0.0222 (2)	0.0207 (3)	0.0214 (3)	0.00025 (19)	0.0072 (3)	0.0047 (2)
F7	0.0449 (8)	0.0265 (7)	0.0540 (9)	−0.0131 (6)	−0.0040 (7)	0.0024 (6)
F8	0.0458 (8)	0.0433 (8)	0.0467 (8)	0.0109 (7)	0.0063 (7)	−0.0240 (7)
C52	0.0227 (9)	0.0210 (9)	0.0215 (9)	−0.0027 (7)	0.0072 (7)	0.0007 (7)
C53	0.0236 (9)	0.0233 (9)	0.0290 (10)	−0.0014 (7)	0.0055 (8)	0.0052 (8)
C54	0.0250 (9)	0.0193 (9)	0.0346 (10)	0.0014 (7)	0.0097 (8)	0.0044 (8)
N55	0.0239 (8)	0.0179 (7)	0.0273 (8)	−0.0006 (6)	0.0079 (7)	−0.0015 (6)
B56	0.0315 (11)	0.0225 (11)	0.0329 (12)	−0.0023 (9)	0.0063 (10)	−0.0077 (9)
N57	0.0267 (8)	0.0277 (9)	0.0222 (8)	−0.0047 (7)	0.0082 (7)	−0.0055 (6)
C58	0.0325 (11)	0.0410 (12)	0.0224 (9)	−0.0083 (9)	0.0097 (8)	−0.0096 (9)
C59	0.0289 (10)	0.0474 (13)	0.0200 (9)	−0.0045 (9)	0.0048 (8)	−0.0005 (9)
C60	0.0227 (9)	0.0349 (11)	0.0222 (9)	−0.0009 (8)	0.0077 (7)	0.0033 (8)
C60A	0.0226 (9)	0.0246 (9)	0.0203 (9)	−0.0021 (7)	0.0091 (7)	−0.0010 (7)
C61	0.0195 (8)	0.0211 (9)	0.0203 (8)	−0.0023 (7)	0.0097 (7)	−0.0003 (7)
C61A	0.0212 (8)	0.0173 (8)	0.0224 (9)	−0.0018 (7)	0.0090 (7)	−0.0012 (7)
C62	0.0201 (8)	0.0211 (9)	0.0205 (8)	0.0007 (7)	0.0068 (7)	0.0017 (7)
C63	0.0222 (2)	0.0207 (3)	0.0214 (3)	0.00025 (19)	0.0072 (3)	0.0047 (2)
C63′	0.0222 (2)	0.0207 (3)	0.0214 (3)	0.00025 (19)	0.0072 (3)	0.0047 (2)
C63A	0.0192 (9)	0.0387 (11)	0.0282 (10)	0.0005 (8)	0.0071 (8)	−0.0047 (9)
C64	0.0308 (11)	0.0587 (16)	0.0382 (13)	−0.0021 (11)	0.0136 (10)	−0.0163 (11)
C65	0.0404 (8)	0.0409 (8)	0.0666 (11)	−0.0001 (6)	0.0078 (7)	−0.0166 (8)
C66	0.0404 (8)	0.0409 (8)	0.0666 (11)	−0.0001 (6)	0.0078 (7)	−0.0166 (8)
C67	0.0404 (8)	0.0409 (8)	0.0666 (11)	−0.0001 (6)	0.0078 (7)	−0.0166 (8)
C68	0.0378 (13)	0.0248 (11)	0.0689 (18)	0.0012 (9)	−0.0016 (12)	0.0110 (11)
C68A	0.0207 (9)	0.0234 (10)	0.0386 (11)	0.0006 (7)	0.0036 (8)	0.0024 (8)

Geometric parameters (Å, º)

S1—C17A	1.721 (2)	F6—B39	1.384 (2)
S1—C11	1.7301 (18)	C35—C36	1.386 (3)
F1—B5	1.395 (3)	C35—C44A	1.415 (3)
F2—B5	1.384 (3)	C35—H35	0.9500
C1—C2	1.386 (3)	C36—C37	1.396 (3)
C1—C10A	1.413 (3)	C36—H36	0.9500
C1—H1	0.9500	C37—N38	1.348 (3)
C2—C3	1.396 (3)	C37—H37	0.9500
C2—H2	0.9500	N38—C44A	1.388 (2)
C3—N4	1.347 (3)	N38—B39	1.542 (3)
C3—H3	0.9500	B39—N40	1.547 (3)
N4—C10A	1.389 (2)	N40—C41	1.344 (3)
N4—B5	1.549 (3)	N40—C43A	1.394 (2)
B5—N6	1.551 (3)	C41—C42	1.393 (3)
N6—C7	1.346 (3)	C41—H41	0.9500
N6—C9A	1.394 (2)	C42—C43	1.381 (3)
C7—C8	1.394 (3)	C42—H42	0.9500
C7—H7	0.9500	C43—C43A	1.415 (3)
C8—C9	1.386 (3)	C43—H43	0.9500
C8—H8	0.9500	C43A—C44	1.409 (3)
C9—C9A	1.410 (3)	C44—C44A	1.417 (3)
C9—H9	0.9500	C44—C45	1.460 (2)
C9A—C10	1.409 (3)	C45—C46′	1.373 (3)
C10—C10A	1.407 (3)	C45—C46	1.387 (2)
C10—C11	1.455 (3)	C46—C46A	1.432 (2)
C11—C12	1.378 (3)	C46—H46	0.9500
C12—C12A	1.418 (3)	C46′—C51A	1.432 (3)
C12—H12	0.9500	C46′—H46A	0.9500
C12A—C17A	1.379 (3)	C46A—C51A	1.355 (2)
C12A—C13	1.506 (3)	C46A—C47	1.487 (3)
C13—C14	1.536 (3)	C47—C48	1.525 (4)
C13—H13A	0.9900	C47—H47A	0.9900
C13—H13B	0.9900	C47—H47B	0.9900
C14—C15	1.525 (3)	C48—C49	1.509 (4)
C14—H14A	0.9900	C48—H48A	0.9900
C14—H14B	0.9900	C48—H48B	0.9900
C15—C16	1.527 (3)	C49—C50	1.554 (4)
C15—H15A	0.9900	C49—H49A	0.9900
C15—H15B	0.9900	C49—H49B	0.9900
C16—C17	1.529 (3)	C50—C51	1.536 (4)
C16—H16A	0.9900	C50—H50A	0.9900
C16—H16B	0.9900	C50—H50B	0.9900
C17—C17A	1.504 (3)	C51—C51A	1.499 (3)
C17—H17A	0.9900	C51—H51A	0.9900
C17—H17B	0.9900	C51—H51B	0.9900
S2—C34A	1.720 (2)	S4—C68A	1.6821 (18)

S2—C28	1.7335 (18)	S4—C62	1.7177 (16)
F3—B22	1.389 (3)	S4′—C63A	1.607 (2)
F4—B22	1.387 (3)	S4′—C62	1.711 (2)
C18—C19	1.386 (3)	F7—B56	1.392 (3)
C18—C27A	1.411 (3)	F8—B56	1.384 (3)
C18—H18	0.9500	C52—C53	1.385 (3)
C19—C20	1.397 (4)	C52—C61A	1.415 (3)
C19—H19	0.9500	C52—H52	0.9500
C20—N21	1.343 (3)	C53—C54	1.396 (3)
C20—H20	0.9500	C53—H53	0.9500
N21—C27A	1.392 (3)	C54—N55	1.347 (3)
N21—B22	1.547 (3)	C54—H54	0.9500
B22—N23	1.543 (3)	N55—C61A	1.391 (2)
N23—C24	1.344 (3)	N55—B56	1.546 (3)
N23—C26A	1.395 (2)	B56—N57	1.545 (3)
C24—C25	1.398 (3)	N57—C58	1.348 (3)
C24—H24	0.9500	N57—C60A	1.391 (3)
C25—C26	1.388 (3)	C58—C59	1.389 (3)
C25—H25	0.9500	C58—H58	0.9500
C26—C26A	1.411 (3)	C59—C60	1.383 (3)
C26—H26	0.9500	C59—H59	0.9500
C26A—C27	1.405 (3)	C60—C60A	1.416 (3)
C27—C27A	1.409 (3)	C60—H60	0.9500
C27—C28	1.457 (3)	C60A—C61	1.411 (3)
C28—C29	1.374 (3)	C61—C61A	1.411 (3)
C29—C29A	1.418 (3)	C61—C62	1.461 (2)
C29—H29	0.9500	C62—C63′	1.375 (3)
C29A—C34A	1.374 (3)	C62—C63	1.393 (2)
C29A—C30	1.502 (3)	C63—C63A	1.437 (2)
C30—C31	1.539 (3)	C63—H63	0.9500
C30—H30A	0.9900	C63′—C68A	1.432 (3)
C30—H30B	0.9900	C63′—H63B	0.9500
C31—C32	1.525 (3)	C63A—C68A	1.351 (2)
C31—H31A	0.9900	C63A—C64	1.485 (3)
C31—H31B	0.9900	C64—C65	1.527 (4)
C32—C33	1.524 (3)	C64—H64A	0.9900
C32—H32A	0.9900	C64—H64B	0.9900
C32—H32B	0.9900	C65—C66	1.508 (4)
C33—C34	1.530 (3)	C65—H65A	0.9900
C33—H33A	0.9900	C65—H65B	0.9900
C33—H33B	0.9900	C66—C67	1.566 (4)
C34—C34A	1.507 (3)	C66—H66A	0.9900
C34—H34A	0.9900	C66—H66B	0.9900
C34—H34B	0.9900	C67—C68	1.538 (4)
S3—C51A	1.6804 (18)	C67—H67A	0.9900
S3—C45	1.7334 (16)	C67—H67B	0.9900
S3′—C46A	1.629 (2)	C68—C68A	1.492 (3)
S3′—C45	1.728 (2)	C68—H68A	0.9900

F5—B39	1.395 (3)	C68—H68B	0.9900
C17A—S1—C11	92.61 (9)	C37—N38—C44A	108.34 (16)
C2—C1—C10A	107.19 (17)	C37—N38—B39	126.17 (16)
C2—C1—H1	126.4	C44A—N38—B39	125.49 (16)
C10A—C1—H1	126.4	F6—B39—F5	110.01 (17)
C1—C2—C3	106.94 (17)	F6—B39—N38	109.65 (17)
C1—C2—H2	126.5	F5—B39—N38	110.82 (17)
C3—C2—H2	126.5	F6—B39—N40	111.34 (17)
N4—C3—C2	110.18 (17)	F5—B39—N40	109.31 (17)
N4—C3—H3	124.9	N38—B39—N40	105.64 (15)
C2—C3—H3	124.9	C41—N40—C43A	107.90 (17)
C3—N4—C10A	107.78 (16)	C41—N40—B39	125.88 (17)
C3—N4—B5	126.47 (16)	C43A—N40—B39	125.50 (16)
C10A—N4—B5	125.58 (16)	N40—C41—C42	110.20 (18)
F2—B5—F1	108.78 (17)	N40—C41—H41	124.9
F2—B5—N4	110.64 (17)	C42—C41—H41	124.9
F1—B5—N4	110.50 (17)	C43—C42—C41	107.10 (18)
F2—B5—N6	111.15 (18)	C43—C42—H42	126.4
F1—B5—N6	109.89 (16)	C41—C42—H42	126.4
N4—B5—N6	105.87 (16)	C42—C43—C43A	107.41 (18)
C7—N6—C9A	107.61 (17)	C42—C43—H43	126.3
C7—N6—B5	125.20 (17)	C43A—C43—H43	126.3
C9A—N6—B5	126.24 (16)	N40—C43A—C44	120.65 (17)
N6—C7—C8	110.28 (18)	N40—C43A—C43	107.37 (17)
N6—C7—H7	124.9	C44—C43A—C43	131.95 (18)
C8—C7—H7	124.9	C43A—C44—C44A	119.33 (17)
C9—C8—C7	107.01 (18)	C43A—C44—C45	122.01 (17)
C9—C8—H8	126.5	C44A—C44—C45	118.63 (16)
C7—C8—H8	126.5	N38—C44A—C35	107.59 (16)
C8—C9—C9A	107.18 (18)	N38—C44A—C44	120.81 (17)
C8—C9—H9	126.4	C35—C44A—C44	130.80 (17)
C9A—C9—H9	126.4	C46′—C45—C44	135.8 (2)
N6—C9A—C10	120.05 (17)	C46—C45—C44	128.72 (16)
N6—C9A—C9	107.91 (16)	C46′—C45—S3′	105.1 (2)
C10—C9A—C9	132.05 (18)	C44—C45—S3′	118.49 (14)
C10A—C10—C9A	119.70 (17)	C46—C45—S3	108.82 (15)
C10A—C10—C11	118.33 (16)	C44—C45—S3	122.46 (12)
C9A—C10—C11	121.97 (17)	C45—C46—C46A	115.0 (2)
N4—C10A—C10	121.32 (17)	C45—C46—H46	122.5
N4—C10A—C1	107.87 (16)	C46A—C46—H46	122.5
C10—C10A—C1	130.80 (18)	C45—C46′—C51A	121.9 (4)
C12—C11—C10	126.87 (17)	C45—C46′—H46A	119.0
C12—C11—S1	109.92 (14)	C51A—C46′—H46A	119.0
C10—C11—S1	123.21 (14)	C51A—C46A—C46	108.74 (19)
C11—C12—C12A	114.17 (17)	C51A—C46A—C47	128.34 (19)
C11—C12—H12	122.9	C46—C46A—C47	122.9 (2)
C12A—C12—H12	122.9	C51A—C46A—S3′	123.35 (17)

C17A—C12A—C12	111.84 (17)	C47—C46A—S3′	108.11 (17)
C17A—C12A—C13	126.32 (17)	C46A—C47—C48	112.0 (2)
C12—C12A—C13	121.77 (17)	C46A—C47—H47A	109.2
C12A—C13—C14	116.19 (17)	C48—C47—H47A	109.2
C12A—C13—H13A	108.2	C46A—C47—H47B	109.2
C14—C13—H13A	108.2	C48—C47—H47B	109.2
C12A—C13—H13B	108.2	H47A—C47—H47B	107.9
C14—C13—H13B	108.2	C49—C48—C47	114.2 (3)
H13A—C13—H13B	107.4	C49—C48—H48A	108.7
C15—C14—C13	115.43 (19)	C47—C48—H48A	108.7
C15—C14—H14A	108.4	C49—C48—H48B	108.7
C13—C14—H14A	108.4	C47—C48—H48B	108.7
C15—C14—H14B	108.4	H48A—C48—H48B	107.6
C13—C14—H14B	108.4	C48—C49—C50	118.1 (2)
H14A—C14—H14B	107.5	C48—C49—H49A	107.8
C14—C15—C16	115.61 (18)	C50—C49—H49A	107.8
C14—C15—H15A	108.4	C48—C49—H49B	107.8
C16—C15—H15A	108.4	C50—C49—H49B	107.8
C14—C15—H15B	108.4	H49A—C49—H49B	107.1
C16—C15—H15B	108.4	C51—C50—C49	114.6 (3)
H15A—C15—H15B	107.4	C51—C50—H50A	108.6
C15—C16—C17	114.48 (17)	C49—C50—H50A	108.6
C15—C16—H16A	108.6	C51—C50—H50B	108.6
C17—C16—H16A	108.6	C49—C50—H50B	108.6
C15—C16—H16B	108.6	H50A—C50—H50B	107.6
C17—C16—H16B	108.6	C51A—C51—C50	112.7 (2)
H16A—C16—H16B	107.6	C51A—C51—H51A	109.1
C17A—C17—C16	114.96 (17)	C50—C51—H51A	109.1
C17A—C17—H17A	108.5	C51A—C51—H51B	109.1
C16—C17—H17A	108.5	C50—C51—H51B	109.1
C17A—C17—H17B	108.5	H51A—C51—H51B	107.8
C16—C17—H17B	108.5	C46A—C51A—C46′	98.9 (2)
H17A—C17—H17B	107.5	C46A—C51A—C51	124.7 (2)
C12A—C17A—C17	129.69 (18)	C46′—C51A—C51	136.2 (3)
C12A—C17A—S1	111.45 (14)	C46A—C51A—S3	115.55 (15)
C17—C17A—S1	118.78 (14)	C51—C51A—S3	119.77 (18)
C34A—S2—C28	92.46 (9)	C68A—S4—C62	92.42 (9)
C19—C18—C27A	107.3 (2)	C63A—S4′—C62	91.66 (13)
C19—C18—H18	126.4	C53—C52—C61A	107.18 (17)
C27A—C18—H18	126.4	C53—C52—H52	126.4
C18—C19—C20	106.5 (2)	C61A—C52—H52	126.4
C18—C19—H19	126.7	C52—C53—C54	107.01 (18)
C20—C19—H19	126.7	C52—C53—H53	126.5
N21—C20—C19	110.78 (19)	C54—C53—H53	126.5
N21—C20—H20	124.6	N55—C54—C53	110.25 (18)
C19—C20—H20	124.6	N55—C54—H54	124.9
C20—N21—C27A	107.34 (19)	C53—C54—H54	124.9
C20—N21—B22	126.22 (19)	C54—N55—C61A	107.71 (17)

C27A—N21—B22	126.17 (18)	C54—N55—B56	126.27 (17)
F4—B22—F3	108.96 (19)	C61A—N55—B56	126.01 (17)
F4—B22—N23	110.5 (2)	F8—B56—F7	110.27 (19)
F3—B22—N23	110.32 (18)	F8—B56—N55	109.96 (18)
F4—B22—N21	110.79 (19)	F7—B56—N55	110.22 (19)
F3—B22—N21	110.4 (2)	F8—B56—N57	110.59 (19)
N23—B22—N21	105.87 (17)	F7—B56—N57	109.91 (18)
C24—N23—C26A	107.90 (18)	N55—B56—N57	105.79 (16)
C24—N23—B22	125.86 (18)	C58—N57—C60A	107.56 (18)
C26A—N23—B22	126.10 (18)	C58—N57—B56	126.15 (18)
N23—C24—C25	110.33 (18)	C60A—N57—B56	125.96 (17)
N23—C24—H24	124.8	N57—C58—C59	110.42 (19)
C25—C24—H24	124.8	N57—C58—H58	124.8
C26—C25—C24	106.63 (19)	C59—C58—H58	124.8
C26—C25—H25	126.7	C60—C59—C58	107.10 (19)
C24—C25—H25	126.7	C60—C59—H59	126.4
C25—C26—C26A	107.59 (18)	C58—C59—H59	126.4
C25—C26—H26	126.2	C59—C60—C60A	107.14 (19)
C26A—C26—H26	126.2	C59—C60—H60	126.4
N23—C26A—C27	120.72 (18)	C60A—C60—H60	126.4
N23—C26A—C26	107.54 (17)	N57—C60A—C61	120.79 (18)
C27—C26A—C26	131.61 (18)	N57—C60A—C60	107.75 (17)
C26A—C27—C27A	120.01 (18)	C61—C60A—C60	131.43 (19)
C26A—C27—C28	121.28 (17)	C61A—C61—C60A	119.67 (17)
C27A—C27—C28	118.70 (17)	C61A—C61—C62	119.14 (16)
N21—C27A—C27	120.25 (18)	C60A—C61—C62	121.18 (17)
N21—C27A—C18	108.03 (18)	N55—C61A—C61	120.52 (17)
C27—C27A—C18	131.65 (19)	N55—C61A—C52	107.84 (16)
C29—C28—C27	128.31 (17)	C61—C61A—C52	131.00 (17)
C29—C28—S2	109.84 (14)	C63′—C62—C61	135.3 (2)
C27—C28—S2	121.85 (14)	C63—C62—C61	129.27 (16)
C28—C29—C29A	114.21 (17)	C63′—C62—S4′	104.3 (2)
C28—C29—H29	122.9	C61—C62—S4′	120.08 (14)
C29A—C29—H29	122.9	C63—C62—S4	108.87 (15)
C34A—C29A—C29	111.85 (17)	C61—C62—S4	121.86 (12)
C34A—C29A—C30	125.47 (17)	C62—C63—C63A	114.6 (2)
C29—C29A—C30	122.58 (17)	C62—C63—H63	122.7
C29A—C30—C31	115.81 (17)	C63A—C63—H63	122.7
C29A—C30—H30A	108.3	C62—C63′—C68A	122.0 (4)
C31—C30—H30A	108.3	C62—C63′—H63B	119.0
C29A—C30—H30B	108.3	C68A—C63′—H63B	119.0
C31—C30—H30B	108.3	C68A—C63A—C63	108.90 (19)
H30A—C30—H30B	107.4	C68A—C63A—C64	130.03 (19)
C32—C31—C30	115.00 (18)	C63—C63A—C64	121.0 (2)
C32—C31—H31A	108.5	C68A—C63A—S4′	122.67 (17)
C30—C31—H31A	108.5	C64—C63A—S4′	107.24 (18)
C32—C31—H31B	108.5	C63A—C64—C65	112.1 (2)
C30—C31—H31B	108.5	C63A—C64—H64A	109.2

H31A—C31—H31B	107.5	C65—C64—H64A	109.2
C33—C32—C31	115.96 (18)	C63A—C64—H64B	109.2
C33—C32—H32A	108.3	C65—C64—H64B	109.2
C31—C32—H32A	108.3	H64A—C64—H64B	107.9
C33—C32—H32B	108.3	C66—C65—C64	114.1 (3)
C31—C32—H32B	108.3	C66—C65—H65A	108.7
H32A—C32—H32B	107.4	C64—C65—H65A	108.7
C32—C33—C34	114.71 (17)	C66—C65—H65B	108.7
C32—C33—H33A	108.6	C64—C65—H65B	108.7
C34—C33—H33A	108.6	H65A—C65—H65B	107.6
C32—C33—H33B	108.6	C65—C66—C67	117.9 (2)
C34—C33—H33B	108.6	C65—C66—H66A	107.8
H33A—C33—H33B	107.6	C67—C66—H66A	107.8
C34A—C34—C33	114.59 (17)	C65—C66—H66B	107.8
C34A—C34—H34A	108.6	C67—C66—H66B	107.8
C33—C34—H34A	108.6	H66A—C66—H66B	107.2
C34A—C34—H34B	108.6	C68—C67—C66	114.4 (3)
C33—C34—H34B	108.6	C68—C67—H67A	108.7
H34A—C34—H34B	107.6	C66—C67—H67A	108.7
C29A—C34A—C34	128.92 (18)	C68—C67—H67B	108.7
C29A—C34A—S2	111.63 (14)	C66—C67—H67B	108.7
C34—C34A—S2	119.41 (14)	H67A—C67—H67B	107.6
C51A—S3—C45	91.85 (9)	C68A—C68—C67	113.7 (2)
C46A—S3′—C45	90.12 (13)	C68A—C68—H68A	108.8
C36—C35—C44A	107.13 (17)	C67—C68—H68A	108.8
C36—C35—H35	126.4	C68A—C68—H68B	108.8
C44A—C35—H35	126.4	C67—C68—H68B	108.8
C35—C36—C37	107.31 (18)	H68A—C68—H68B	107.7
C35—C36—H36	126.3	C63A—C68A—C63′	99.1 (2)
C37—C36—H36	126.3	C63A—C68A—C68	124.6 (2)
N38—C37—C36	109.62 (17)	C63′—C68A—C68	136.2 (2)
N38—C37—H37	125.2	C63A—C68A—S4	115.17 (15)
C36—C37—H37	125.2	C68—C68A—S4	120.21 (17)

C10A—C1—C2—C3	0.8 (2)	B39—N40—C41—C42	171.76 (18)
C1—C2—C3—N4	0.5 (2)	N40—C41—C42—C43	−1.6 (2)
C2—C3—N4—C10A	−1.7 (2)	C41—C42—C43—C43A	1.3 (2)
C2—C3—N4—B5	173.84 (18)	C41—N40—C43A—C44	177.97 (17)
C3—N4—B5—F2	−53.8 (3)	B39—N40—C43A—C44	7.3 (3)
C10A—N4—B5—F2	121.0 (2)	C41—N40—C43A—C43	−0.3 (2)
C3—N4—B5—F1	66.7 (2)	B39—N40—C43A—C43	−170.94 (17)
C10A—N4—B5—F1	−118.50 (19)	C42—C43—C43A—N40	−0.7 (2)
C3—N4—B5—N6	−174.32 (17)	C42—C43—C43A—C44	−178.7 (2)
C10A—N4—B5—N6	0.4 (3)	N40—C43A—C44—C44A	4.2 (3)
F2—B5—N6—C7	62.3 (3)	C43—C43A—C44—C44A	−178.05 (19)
F1—B5—N6—C7	−58.2 (3)	N40—C43A—C44—C45	−177.90 (16)
N4—B5—N6—C7	−177.55 (17)	C43—C43A—C44—C45	−0.2 (3)
F2—B5—N6—C9A	−130.34 (19)	C37—N38—C44A—C35	−0.4 (2)

F1—B5—N6—C9A	109.2 (2)	B39—N38—C44A—C35	179.93 (17)
N4—B5—N6—C9A	−10.1 (3)	C37—N38—C44A—C44	170.36 (17)
C9A—N6—C7—C8	−0.9 (2)	B39—N38—C44A—C44	−9.3 (3)
B5—N6—C7—C8	168.44 (18)	C36—C35—C44A—N38	−0.1 (2)
N6—C7—C8—C9	−0.1 (2)	C36—C35—C44A—C44	−169.59 (19)
C7—C8—C9—C9A	1.0 (2)	C43A—C44—C44A—N38	−3.3 (3)
C7—N6—C9A—C10	−179.01 (17)	C45—C44—C44A—N38	178.75 (16)
B5—N6—C9A—C10	11.8 (3)	C43A—C44—C44A—C35	165.08 (19)
C7—N6—C9A—C9	1.5 (2)	C45—C44—C44A—C35	−12.9 (3)
B5—N6—C9A—C9	−167.67 (17)	C43A—C44—C45—C46′	−44.8 (8)
C8—C9—C9A—N6	−1.6 (2)	C44A—C44—C45—C46′	133.1 (7)
C8—C9—C9A—C10	179.06 (19)	C43A—C44—C45—C46	142.3 (2)
N6—C9A—C10—C10A	−2.5 (3)	C44A—C44—C45—C46	−39.8 (3)
C9—C9A—C10—C10A	176.83 (19)	C43A—C44—C45—S3′	145.24 (18)
N6—C9A—C10—C11	178.37 (16)	C44A—C44—C45—S3′	−36.9 (2)
C9—C9A—C10—C11	−2.3 (3)	C43A—C44—C45—S3	−38.1 (2)
C3—N4—C10A—C10	−176.81 (17)	C44A—C44—C45—S3	139.85 (15)
B5—N4—C10A—C10	7.6 (3)	C46A—S3′—C45—C46′	6.3 (5)
C3—N4—C10A—C1	2.2 (2)	C46A—S3′—C45—C44	179.04 (17)
B5—N4—C10A—C1	−173.42 (17)	C51A—S3—C45—C46	2.70 (18)
C9A—C10—C10A—N4	−6.8 (3)	C51A—S3—C45—C44	−177.03 (17)
C11—C10—C10A—N4	172.40 (16)	C44—C45—C46—C46A	177.1 (2)
C9A—C10—C10A—C1	174.50 (19)	S3—C45—C46—C46A	−2.6 (3)
C11—C10—C10A—C1	−6.3 (3)	C44—C45—C46′—C51A	−179.3 (4)
C2—C1—C10A—N4	−1.8 (2)	S3′—C45—C46′—C51A	−8.5 (10)
C2—C1—C10A—C10	177.02 (19)	C45—C46—C46A—C51A	1.0 (3)
C10A—C10—C11—C12	−38.5 (3)	C45—C46—C46A—C47	−177.1 (2)
C9A—C10—C11—C12	140.72 (19)	C45—S3′—C46A—C51A	−4.1 (2)
C10A—C10—C11—S1	141.60 (15)	C45—S3′—C46A—C47	−179.47 (17)
C9A—C10—C11—S1	−39.2 (2)	C51A—C46A—C47—C48	−58.6 (3)
C17A—S1—C11—C12	−0.24 (14)	C46—C46A—C47—C48	119.1 (3)
C17A—S1—C11—C10	179.70 (16)	S3′—C46A—C47—C48	116.4 (2)
C10—C11—C12—C12A	−179.15 (17)	C46A—C47—C48—C49	73.2 (3)
S1—C11—C12—C12A	0.8 (2)	C47—C48—C49—C50	−66.7 (3)
C11—C12—C12A—C17A	−1.1 (2)	C48—C49—C50—C51	65.6 (3)
C11—C12—C12A—C13	175.95 (18)	C49—C50—C51—C51A	−71.6 (3)
C17A—C12A—C13—C14	−47.7 (3)	C47—C46A—C51A—C46′	174.6 (5)
C12—C12A—C13—C14	135.7 (2)	S3′—C46A—C51A—C46′	0.2 (5)
C12A—C13—C14—C15	67.3 (3)	C46—C46A—C51A—C51	−178.1 (2)
C13—C14—C15—C16	−71.8 (3)	C47—C46A—C51A—C51	−0.1 (4)
C14—C15—C16—C17	73.2 (3)	S3′—C46A—C51A—C51	−174.5 (2)
C15—C16—C17—C17A	−68.6 (2)	C46—C46A—C51A—S3	1.2 (2)
C12—C12A—C17A—C17	177.53 (18)	C47—C46A—C51A—S3	179.15 (18)
C13—C12A—C17A—C17	0.7 (3)	C45—C46′—C51A—C46A	5.7 (10)
C12—C12A—C17A—S1	0.9 (2)	C45—C46′—C51A—C51	179.4 (4)
C13—C12A—C17A—S1	−176.01 (16)	C50—C51—C51A—C46A	58.0 (3)
C16—C17—C17A—C12A	47.7 (3)	C50—C51—C51A—C46′	−114.4 (7)
C16—C17—C17A—S1	−135.79 (16)	C50—C51—C51A—S3	−121.3 (2)

C11—S1—C17A—C12A	−0.36 (15)	C45—S3—C51A—C46A	−2.30 (18)
C11—S1—C17A—C17	−177.44 (15)	C45—S3—C51A—C51	177.01 (19)
C27A—C18—C19—C20	1.7 (3)	C61A—C52—C53—C54	−0.6 (2)
C18—C19—C20—N21	−0.7 (3)	C52—C53—C54—N55	1.0 (2)
C19—C20—N21—C27A	−0.5 (2)	C53—C54—N55—C61A	−1.0 (2)
C19—C20—N21—B22	173.9 (2)	C53—C54—N55—B56	179.41 (19)
C20—N21—B22—F4	−64.2 (3)	C54—N55—B56—F8	47.1 (3)
C27A—N21—B22—F4	109.1 (2)	C61A—N55—B56—F8	−132.3 (2)
C20—N21—B22—F3	56.5 (3)	C54—N55—B56—F7	−74.6 (3)
C27A—N21—B22—F3	−130.1 (2)	C61A—N55—B56—F7	105.9 (2)
C20—N21—B22—N23	175.92 (19)	C54—N55—B56—N57	166.58 (18)
C27A—N21—B22—N23	−10.7 (3)	C61A—N55—B56—N57	−12.9 (3)
F4—B22—N23—C24	69.8 (3)	F8—B56—N57—C58	−57.7 (3)
F3—B22—N23—C24	−50.8 (3)	F7—B56—N57—C58	64.3 (3)
N21—B22—N23—C24	−170.21 (18)	N55—B56—N57—C58	−176.74 (18)
F4—B22—N23—C26A	−115.1 (2)	F8—B56—N57—C60A	129.6 (2)
F3—B22—N23—C26A	124.4 (2)	F7—B56—N57—C60A	−108.4 (2)
N21—B22—N23—C26A	5.0 (3)	N55—B56—N57—C60A	10.6 (3)
C26A—N23—C24—C25	−0.9 (2)	C60A—N57—C58—C59	−1.0 (2)
B22—N23—C24—C25	175.03 (19)	B56—N57—C58—C59	−174.76 (19)
N23—C24—C25—C26	0.2 (2)	N57—C58—C59—C60	1.3 (3)
C24—C25—C26—C26A	0.6 (2)	C58—C59—C60—C60A	−1.1 (2)
C24—N23—C26A—C27	177.59 (17)	C58—N57—C60A—C61	−177.72 (18)
B22—N23—C26A—C27	1.7 (3)	B56—N57—C60A—C61	−3.9 (3)
C24—N23—C26A—C26	1.2 (2)	C58—N57—C60A—C60	0.3 (2)
B22—N23—C26A—C26	−174.68 (18)	B56—N57—C60A—C60	174.05 (18)
C25—C26—C26A—N23	−1.1 (2)	C59—C60—C60A—N57	0.5 (2)
C25—C26—C26A—C27	−176.93 (19)	C59—C60—C60A—C61	178.2 (2)
N23—C26A—C27—C27A	−4.1 (3)	N57—C60A—C61—C61A	−2.8 (3)
C26—C26A—C27—C27A	171.26 (19)	C60—C60A—C61—C61A	179.75 (19)
N23—C26A—C27—C28	177.28 (16)	N57—C60A—C61—C62	178.59 (16)
C26—C26A—C27—C28	−7.3 (3)	C60—C60A—C61—C62	1.1 (3)
C20—N21—C27A—C27	−175.88 (18)	C54—N55—C61A—C61	−171.11 (17)
B22—N21—C27A—C27	9.7 (3)	B56—N55—C61A—C61	8.4 (3)
C20—N21—C27A—C18	1.6 (2)	C54—N55—C61A—C52	0.7 (2)
B22—N21—C27A—C18	−172.83 (19)	B56—N55—C61A—C52	−179.79 (18)
C26A—C27—C27A—N21	−1.3 (3)	C60A—C61—C61A—N55	0.7 (3)
C28—C27—C27A—N21	177.33 (17)	C62—C61—C61A—N55	179.31 (16)
C26A—C27—C27A—C18	−178.1 (2)	C60A—C61—C61A—C52	−168.96 (19)
C28—C27—C27A—C18	0.6 (3)	C62—C61—C61A—C52	9.7 (3)
C19—C18—C27A—N21	−2.0 (2)	C53—C52—C61A—N55	−0.1 (2)
C19—C18—C27A—C27	175.0 (2)	C53—C52—C61A—C61	170.56 (19)
C26A—C27—C28—C29	139.0 (2)	C61A—C61—C62—C63′	−133.1 (7)
C27A—C27—C28—C29	−39.6 (3)	C60A—C61—C62—C63′	45.5 (8)
C26A—C27—C28—S2	−42.0 (2)	C61A—C61—C62—C63	40.7 (3)
C27A—C27—C28—S2	139.37 (16)	C60A—C61—C62—C63	−140.6 (2)
C34A—S2—C28—C29	−0.30 (15)	C61A—C61—C62—S4′	39.6 (2)
C34A—S2—C28—C27	−179.45 (16)	C60A—C61—C62—S4′	−141.74 (18)

C27—C28—C29—C29A	179.96 (18)	C61A—C61—C62—S4	−138.54 (15)
S2—C28—C29—C29A	0.9 (2)	C60A—C61—C62—S4	40.1 (2)
C28—C29—C29A—C34A	−1.2 (2)	C63A—S4′—C62—C63′	−4.0 (6)
C28—C29—C29A—C30	175.29 (18)	C63A—S4′—C62—C61	−178.75 (17)
C34A—C29A—C30—C31	−52.0 (3)	C68A—S4—C62—C63	−1.60 (18)
C29—C29A—C30—C31	132.0 (2)	C68A—S4—C62—C61	177.82 (16)
C29A—C30—C31—C32	69.5 (3)	C61—C62—C63—C63A	−177.9 (2)
C30—C31—C32—C33	−70.0 (2)	S4—C62—C63—C63A	1.5 (3)
C31—C32—C33—C34	71.6 (2)	C61—C62—C63′—C68A	179.8 (4)
C32—C33—C34—C34A	−70.0 (2)	S4′—C62—C63′—C68A	6.3 (10)
C29—C29A—C34A—C34	178.46 (19)	C62—C63—C63A—C68A	−0.5 (3)
C30—C29A—C34A—C34	2.1 (3)	C62—C63—C63A—C64	177.9 (2)
C29—C29A—C34A—S2	0.9 (2)	C62—S4′—C63A—C68A	1.6 (2)
C30—C29A—C34A—S2	−175.43 (16)	C62—S4′—C63A—C64	179.03 (17)
C33—C34—C34A—C29A	49.5 (3)	C68A—C63A—C64—C65	56.0 (3)
C33—C34—C34A—S2	−133.08 (16)	C63—C63A—C64—C65	−122.1 (3)
C28—S2—C34A—C29A	−0.36 (15)	S4′—C63A—C64—C65	−121.2 (2)
C28—S2—C34A—C34	−178.18 (16)	C63A—C64—C65—C66	−72.1 (3)
C44A—C35—C36—C37	0.5 (2)	C64—C65—C66—C67	68.3 (3)
C35—C36—C37—N38	−0.8 (2)	C65—C66—C67—C68	−66.1 (3)
C36—C37—N38—C44A	0.8 (2)	C66—C67—C68—C68A	70.0 (3)
C36—C37—N38—B39	−179.61 (18)	C64—C63A—C68A—C63′	−175.4 (5)
C37—N38—B39—F6	−42.0 (3)	S4′—C63A—C68A—C63′	1.4 (5)
C44A—N38—B39—F6	137.59 (18)	C63—C63A—C68A—C68	179.3 (2)
C37—N38—B39—F5	79.6 (2)	C64—C63A—C68A—C68	1.1 (4)
C44A—N38—B39—F5	−100.8 (2)	S4′—C63A—C68A—C68	177.8 (2)
C37—N38—B39—N40	−162.08 (17)	C63—C63A—C68A—S4	−0.7 (2)
C44A—N38—B39—N40	17.5 (2)	C64—C63A—C68A—S4	−179.00 (19)
F6—B39—N40—C41	55.5 (3)	C62—C63′—C68A—C63A	−5.1 (10)
F5—B39—N40—C41	−66.3 (2)	C62—C63′—C68A—C68	179.1 (4)
N38—B39—N40—C41	174.45 (17)	C67—C68—C68A—C63A	−56.7 (3)
F6—B39—N40—C43A	−135.49 (18)	C67—C68—C68A—C63′	118.2 (7)
F5—B39—N40—C43A	102.8 (2)	C67—C68—C68A—S4	123.4 (2)
N38—B39—N40—C43A	−16.5 (2)	C62—S4—C68A—C63A	1.40 (17)
C43A—N40—C41—C42	1.1 (2)	C62—S4—C68A—C68	−178.66 (18)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···F6	0.95	2.53	3.055 (2)	115
C9—H9···S1	0.95	2.76	3.253 (2)	113
C17—H17*A*···F4^{i}	0.99	2.33	3.315 (3)	177
C19—H19···F8^{ii}	0.95	2.41	3.289 (3)	155
C26—H26···S2	0.95	2.79	3.258 (2)	112
C34—H34*A*···F2	0.99	2.47	3.388 (3)	154
C34—H34*B*···F3^{iii}	0.99	2.40	3.385 (3)	172
C35—H35···S3′	0.95	2.56	3.053 (3)	112
C35—H35···F3^{ii}	0.95	2.52	3.343 (2)	145

C43—H43···S3	0.95	2.69	3.214 (2)	115
C52—H52···S4′	0.95	2.62	3.116 (3)	113
C52—H52···F1	0.95	2.53	3.230 (2)	131
C60—H60···S4	0.95	2.67	3.187 (2)	115
C12—H12···Cg5^{iv}	0.95	2.95	3.477 (2)	116
C26—H26···Cg6	0.95	2.95	3.426 (2)	112
C26—H26···Cg7	0.95	2.95	3.466 (3)	116
C29—H29···Cg10	0.95	2.90	3.500 (2)	122
C43—H43···Cg14^{iv}	0.95	2.99	3.272 (2)	98

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