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(6-Fluoro-2-oxo-2*H*-chromen-4-yl)methyl diethylcarbamodithioate

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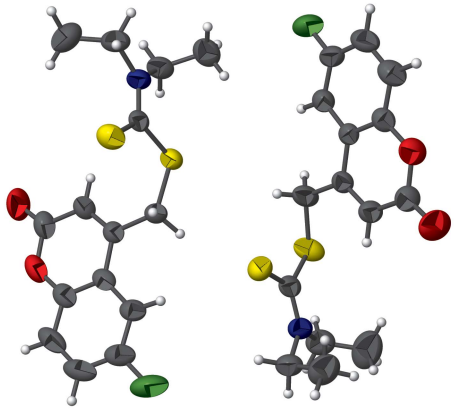
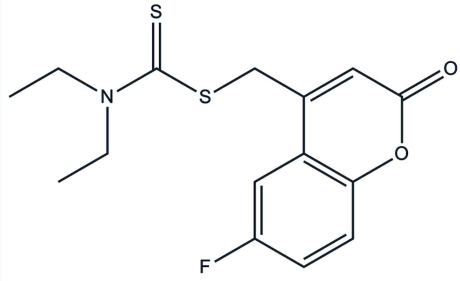
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{15}H_{16}FNO_2S_2$, crystallizes with two independent molecules (*A* and *B*) in the asymmetric unit. They differ essentially in the orientation of the ethyl groups. The chromene rings are planar (r.m.s. deviations = 0.013 Å for both molecules), with the maximum deviation from the ring planes being 0.014 (2) and 0.018 (2) Å for atoms C9*A* and C9*B*, respectively. The mean plane of the chromene ring makes dihedral angles of 80.01 (7) and 76.97 (8)° with the carbamodithioate moiety [(N—C(=S)—S] of molecules *A* and *B*, respectively. In the crystal, the two molecules are linked by C—H···S hydrogen bonds, forming a ladder-like arrangement propagating along the *a*-axis direction. Within the ladders there are offset π–π interactions involving the coumarins rings of the *B* molecules [intercentroid distances vary from 3.705 (2) to 3.860 (1) Å]. Neighbouring ladders are linked *via* offset π–π interactions involving the coumarins rings of the *A* molecules [intercentroid distances vary from 3.539 (1) to 3.601 (1) Å]. These latter interactions lead to the formation of layers parallel to the *ac* plane.

3D view



Chemical scheme



Structure description

Coumarins and their derivatives represent an interesting class of heterocyclic compounds, which have attracted attention because of their biological and medicinal properties, such as anti-bacterial (Basanagouda *et al.*, 2009), anti-oxidant (Vukovic *et al.*, 2010) and anti-inflammatory (Emmanuel-Giota *et al.*, 2001). As part of our ongoing studies of coumarin derivatives (El-Khatatneh *et al.*, 2016), the title compound was synthesized and we report herein on its crystal structure.

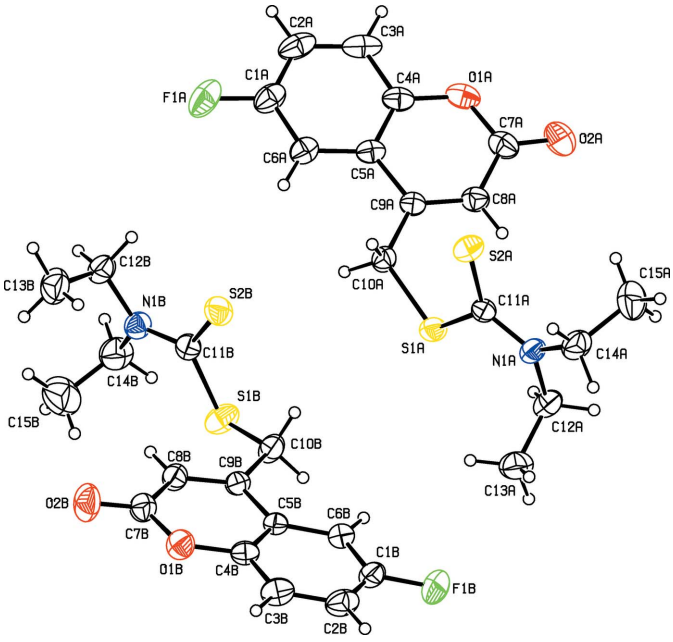


Figure 1
The molecular structure of the two independent molecules of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

The title compound, Fig. 1, crystallized with two independent molecules (*A* and *B*) in the asymmetric unit. The coumarin units are planar with their maximum deviations being 0.014 (2) and 0.018 (2) Å, for atoms C9*A* and C9*B*, respectively. The mean plane of the chromene rings make dihedral angles of 80.01 (7) and 76.97 (8)° with the carbamodithioate moiety [(N—C(=S)—S] of molecules *A* and *B*, respectively. The AutoMolFit drawing, Fig. 2 (*PLATON*; Spek, 2009), illustrates that the main difference in the conformation of the two molecules concerns the orientation of the ethyl groups. They are present in *-anti-periplanar* (C14*A*–N1*A*–C11*A*–S1*A*) and *-syn-periplanar* (C14*B*–N1*B*–C11*B*–S1*B*) conformations with respect to the carbamodithioate moiety [(N—C(=S)—S].

In the crystal, the two molecules are linked by a C—H···S hydrogen bond, and these units are linked by further C—H···S hydrogen bonds, forming a ladder-like arrangement propagating along the *a*-axis direction (Fig. 3 and Table 1).

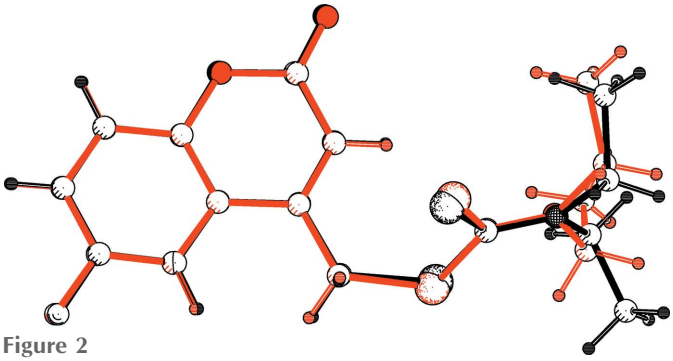


Figure 2
AutoMolFit drawing of molecule *B* (red) on molecule *A* (black) [*PLATON*; Spek, 2009].

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10*A*—H10*A*···S2*B*	0.97	2.87	3.621 (2)	135
C12*A*—H13*C*···O2*B*^{i}	0.97	2.60	3.368 (3)	136
C2*B*—H2*B*···S2*B*^{ii}	0.93	2.87	3.693 (3)	148
C10*B*—H10*C*···S2*A*^{iii}	0.97	2.82	3.660 (2)	145

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{16}FNO_2S_2$
M_r	325.41
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	293
a, b, c (Å)	7.1284 (2), 12.2818 (3), 18.3709 (5)
α, β, γ (°)	75.625 (2), 88.538 (2), 86.553 (2)
V (Å^3)	1555.10 (7)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.36
Crystal size (mm)	0.30 × 0.25 × 0.20
Data collection	
Diffractometer	Bruker APEXII CCD diffractometer
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	18765, 4555, 3711
R_{int}	0.029
θ_{max} (°)	23.5
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.560
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.036, 0.094, 1.03
No. of reflections	4555
No. of parameters	383
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.30, −0.16

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS2016/6* (Sheldrick, 2008), *SHELXL2016/6* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2008) and *PLATON* (Spek, 2009).

Within the ladders there are offset π-π interactions involving the coumarin rings of the *B* molecules [intercentroid distances vary from 3.705 (2) to 3.860 (1) Å]. Neighbouring ladders are

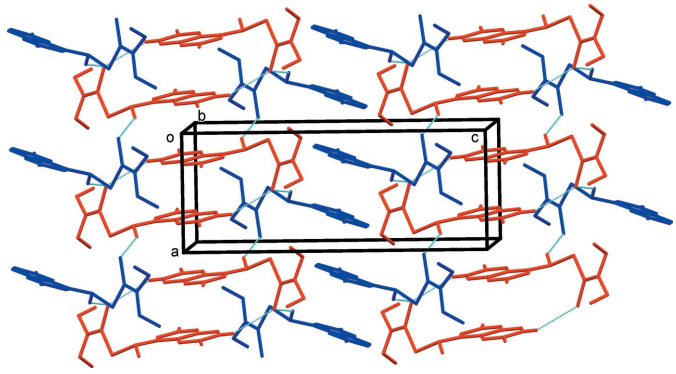


Figure 3
A view along the *b* axis of the crystal packing of the title compound, showing the hydrogen bonds as dashed lines (see Table 1; molecule *A* blue, molecule *B* red). The H atoms not involved in hydrogen bonding have been omitted for clarity.

linked by offset π–π interactions involving the coumarin rings of the *A* molecules [intercentroid distances vary from 3.539 (1) to 3.601 (1) Å], leading to the formation of layers parallel to the *ac* plane (Fig. 3 and Table 1).

Synthesis and crystallization

4-Bromomethyl-6,7-dimethyl-chromen-2-one (3.9 g, 0.015 mol) and the potassium salt of morpholine-4-carboxylate 2.5 g (0.015 mol) were dissolved in 35 ml of absolute ethanol and stirred at room temperature for 14 h. After completion of the reaction (monitored by TLC), the ethanol was removed under reduced pressure. The solid obtained was extracted in ethyl acetate, washed with water, and the collected organic extract was dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure and the obtained solid product was recrystallized from an ethanol:chloroform mixture (7:3) by slow evaporation, giving colourless block-like crystals.

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x162069 [https://doi.org/10.1107/S2414314616020691]

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Crystal data

$C_{15}H_{16}FNO_2S_2$
M_r = 325.41
Triclinic, $P\overline{1}$
a = 7.1284 (2) Å
b = 12.2818 (3) Å
c = 18.3709 (5) Å
α = 75.625 (2)°
β = 88.538 (2)°
γ = 86.553 (2)°
V = 1555.10 (7) Å^3
Z = 4
$F(000)$ = 680
D_x = 1.390 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4557 reflections
θ = 1.1–23.5°
μ = 0.36 mm^{-1}
T = 293 K
Block, colourless
0.30 × 0.25 × 0.20 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: Bruker MicroStar microfocus rotating anode
Detector resolution: 18.4 pixels mm^{-1}
φ and ω scans
18765 measured reflections
4555 independent reflections
3711 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 23.5°, θ_{min} = 1.7°
h = −7→7
k = −13→13
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.094
S = 1.03
4555 reflections
383 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0413P)^2 + 0.5771P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1A	0.51933 (9)	0.66040 (5)	0.25174 (3)	0.05364 (19)
S2A	0.93545 (9)	0.68645 (6)	0.22242 (4)	0.0602 (2)
F1A	0.7749 (3)	0.18127 (14)	0.52266 (10)	0.0948 (6)
O1A	0.7712 (2)	0.62091 (17)	0.53152 (9)	0.0640 (5)
O2A	0.7301 (3)	0.80267 (19)	0.48010 (12)	0.0914 (7)
N1A	0.6629 (3)	0.83708 (15)	0.16329 (10)	0.0512 (5)
C1A	0.7756 (4)	0.2917 (2)	0.52380 (16)	0.0655 (7)
C2A	0.8280 (4)	0.3182 (3)	0.58777 (16)	0.0738 (9)
H2A	0.864836	0.261871	0.629689	0.089*
C3A	0.8258 (3)	0.4291 (3)	0.58945 (14)	0.0683 (8)
H3A	0.860317	0.449019	0.632678	0.082*
C4A	0.7714 (3)	0.5115 (2)	0.52580 (13)	0.0529 (6)
C5A	0.7216 (3)	0.4849 (2)	0.46005 (12)	0.0458 (6)
C6A	0.7236 (3)	0.3709 (2)	0.45985 (13)	0.0531 (6)
H6A	0.690296	0.349303	0.417061	0.064*
C7A	0.7241 (4)	0.7092 (2)	0.47157 (15)	0.0609 (7)
C8A	0.6733 (3)	0.6818 (2)	0.40312 (13)	0.0518 (6)
H8A	0.639944	0.740508	0.362011	0.062*
C9A	0.6715 (3)	0.57683 (19)	0.39565 (12)	0.0431 (5)
C10A	0.6263 (3)	0.54884 (18)	0.32320 (12)	0.0502 (6)
H10A	0.543009	0.487043	0.334541	0.060*
H10B	0.741791	0.522131	0.302691	0.060*
C11A	0.7138 (3)	0.73768 (18)	0.20824 (12)	0.0449 (5)
C12A	0.4672 (4)	0.8847 (2)	0.15371 (14)	0.0628 (7)
H13C	0.466889	0.965963	0.144464	0.075*
H13D	0.396879	0.856713	0.199792	0.075*
C13A	0.3726 (4)	0.8549 (3)	0.09011 (16)	0.0780 (8)
H14A	0.443735	0.880548	0.044619	0.117*
H14B	0.248238	0.890242	0.084249	0.117*
H14C	0.365089	0.774673	0.100622	0.117*
C14A	0.8042 (4)	0.9084 (2)	0.11895 (15)	0.0683 (7)
H15A	0.747783	0.953265	0.072877	0.082*
H15B	0.906248	0.861024	0.105437	0.082*
C15A	0.8818 (5)	0.9854 (3)	0.1617 (2)	0.0991 (11)
H16A	0.781020	1.032186	0.175377	0.149*
H16B	0.971273	1.031883	0.130680	0.149*
H16C	0.942355	0.941205	0.206303	0.149*
S1B	0.08922 (10)	0.33784 (6)	0.27010 (4)	0.0689 (2)
S2B	0.50869 (10)	0.28748 (6)	0.28251 (4)	0.0635 (2)
F1B	0.2068 (3)	0.76498 (13)	−0.04352 (10)	0.0965 (6)
O1B	0.2887 (2)	0.31283 (14)	−0.01045 (9)	0.0630 (5)
O2B	0.2880 (3)	0.13736 (16)	0.05644 (11)	0.0860 (6)
N1B	0.2507 (3)	0.15756 (16)	0.35756 (11)	0.0536 (5)
C1B	0.2303 (4)	0.6518 (2)	−0.03385 (16)	0.0628 (7)
C2B	0.2720 (4)	0.6108 (3)	−0.09550 (15)	0.0683 (8)

H2B	0.287050	0.659402	−0.142680	0.082*
C3B	0.2911 (4)	0.4965 (2)	−0.08610 (14)	0.0642 (7)
H3B	0.318233	0.466425	−0.127166	0.077*
C4B	0.2698 (3)	0.4262 (2)	−0.01553 (13)	0.0498 (6)
C5B	0.2303 (3)	0.46786 (18)	0.04738 (12)	0.0444 (5)
C6B	0.2095 (3)	0.5847 (2)	0.03657 (14)	0.0554 (6)
H6B	0.181708	0.616144	0.076986	0.067*
C7B	0.2686 (4)	0.2351 (2)	0.05671 (15)	0.0592 (7)
C8B	0.2283 (3)	0.2784 (2)	0.12185 (13)	0.0533 (6)
H8B	0.213405	0.227154	0.168002	0.064*
C9B	0.2111 (3)	0.38798 (19)	0.11955 (12)	0.0467 (6)
C10B	0.1792 (4)	0.4326 (2)	0.18835 (13)	0.0625 (7)
H10C	0.092746	0.498300	0.175431	0.075*
H10D	0.297740	0.457461	0.201271	0.075*
C11B	0.2913 (3)	0.25121 (19)	0.30801 (12)	0.0492 (6)
C12B	0.3993 (4)	0.0731 (2)	0.39041 (14)	0.0639 (7)
H13A	0.354027	0.026564	0.437468	0.077*
H13B	0.506735	0.111039	0.401320	0.077*
C13B	0.4604 (4)	−0.0008 (2)	0.33904 (19)	0.0854 (9)
H14D	0.355637	−0.040849	0.329730	0.128*
H14E	0.559207	−0.053535	0.362242	0.128*
H14F	0.505236	0.044952	0.292356	0.128*
C14B	0.0577 (4)	0.1330 (3)	0.38627 (17)	0.0811 (9)
H15C	0.062020	0.100211	0.440021	0.097*
H15D	−0.018925	0.202902	0.377820	0.097*
C15B	−0.0283 (5)	0.0566 (3)	0.3502 (3)	0.1224 (14)
H16D	−0.049498	0.093084	0.298224	0.184*
H16E	−0.146040	0.035520	0.374573	0.184*
H16F	0.053583	−0.009453	0.353828	0.184*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1A	0.0565 (4)	0.0556 (4)	0.0454 (4)	−0.0069 (3)	−0.0087 (3)	−0.0041 (3)
S2A	0.0540 (4)	0.0632 (4)	0.0590 (4)	0.0101 (3)	−0.0035 (3)	−0.0097 (3)
F1A	0.1031 (13)	0.0625 (11)	0.0965 (13)	0.0007 (9)	0.0064 (10)	0.0206 (9)
O1A	0.0563 (11)	0.0928 (15)	0.0476 (10)	−0.0056 (10)	−0.0059 (8)	−0.0255 (10)
O2A	0.1197 (18)	0.0826 (15)	0.0881 (15)	−0.0025 (13)	−0.0183 (13)	−0.0506 (13)
N1A	0.0553 (12)	0.0455 (12)	0.0472 (11)	0.0008 (9)	−0.0059 (9)	−0.0015 (9)
C1A	0.0523 (16)	0.0660 (19)	0.0640 (18)	−0.0004 (13)	0.0059 (13)	0.0094 (14)
C2A	0.0516 (16)	0.091 (2)	0.0579 (18)	0.0019 (15)	0.0000 (13)	0.0195 (16)
C3A	0.0397 (14)	0.115 (3)	0.0403 (14)	−0.0060 (15)	−0.0021 (11)	−0.0011 (15)
C4A	0.0336 (12)	0.0764 (19)	0.0464 (14)	−0.0044 (12)	0.0021 (10)	−0.0112 (13)
C5A	0.0317 (12)	0.0623 (16)	0.0395 (13)	−0.0027 (10)	0.0037 (9)	−0.0057 (11)
C6A	0.0464 (14)	0.0574 (16)	0.0490 (14)	−0.0022 (11)	0.0060 (11)	−0.0016 (12)
C7A	0.0554 (16)	0.074 (2)	0.0613 (17)	−0.0032 (13)	−0.0038 (13)	−0.0307 (15)
C8A	0.0528 (14)	0.0580 (16)	0.0452 (14)	0.0011 (12)	−0.0044 (11)	−0.0146 (12)
C9A	0.0369 (12)	0.0501 (14)	0.0425 (13)	−0.0020 (10)	0.0010 (9)	−0.0118 (11)

C10A	0.0648 (15)	0.0426 (13)	0.0411 (13)	−0.0041 (11)	−0.0027 (11)	−0.0062 (10)
C11A	0.0560 (14)	0.0460 (14)	0.0349 (12)	−0.0011 (11)	−0.0044 (10)	−0.0142 (10)
C12A	0.0674 (17)	0.0550 (16)	0.0600 (16)	0.0104 (13)	−0.0074 (13)	−0.0053 (13)
C13A	0.0691 (18)	0.084 (2)	0.079 (2)	0.0074 (16)	−0.0180 (15)	−0.0169 (16)
C14A	0.0732 (18)	0.0617 (17)	0.0591 (16)	−0.0083 (14)	−0.0017 (14)	0.0069 (13)
C15A	0.113 (3)	0.070 (2)	0.113 (3)	−0.0313 (19)	0.000 (2)	−0.0137 (19)
S1B	0.0736 (5)	0.0745 (5)	0.0507 (4)	0.0198 (4)	0.0048 (3)	−0.0070 (3)
S2B	0.0661 (4)	0.0624 (4)	0.0603 (4)	−0.0193 (3)	−0.0007 (3)	−0.0083 (3)
F1B	0.1369 (16)	0.0513 (10)	0.0896 (12)	−0.0101 (10)	−0.0252 (11)	0.0084 (9)
O1B	0.0764 (12)	0.0585 (12)	0.0570 (11)	0.0061 (9)	0.0007 (9)	−0.0222 (9)
O2B	0.1241 (18)	0.0530 (12)	0.0868 (15)	0.0044 (11)	0.0041 (12)	−0.0310 (11)
N1B	0.0550 (12)	0.0524 (12)	0.0496 (12)	−0.0057 (10)	0.0022 (9)	−0.0049 (10)
C1B	0.0637 (17)	0.0488 (16)	0.0674 (19)	−0.0073 (12)	−0.0173 (14)	0.0045 (14)
C2B	0.0614 (17)	0.080 (2)	0.0524 (17)	−0.0100 (15)	−0.0029 (13)	0.0064 (15)
C3B	0.0597 (16)	0.080 (2)	0.0492 (15)	0.0024 (14)	0.0032 (12)	−0.0117 (14)
C4B	0.0409 (13)	0.0590 (16)	0.0486 (14)	0.0002 (11)	−0.0027 (10)	−0.0119 (12)
C5B	0.0394 (12)	0.0443 (14)	0.0486 (14)	−0.0018 (10)	−0.0085 (10)	−0.0093 (11)
C6B	0.0592 (15)	0.0508 (15)	0.0548 (15)	−0.0022 (12)	−0.0127 (12)	−0.0093 (12)
C7B	0.0660 (17)	0.0523 (17)	0.0610 (17)	0.0010 (13)	−0.0027 (13)	−0.0179 (14)
C8B	0.0639 (16)	0.0459 (15)	0.0489 (14)	−0.0005 (12)	−0.0024 (12)	−0.0102 (11)
C9B	0.0485 (13)	0.0459 (14)	0.0454 (13)	0.0021 (11)	−0.0061 (10)	−0.0111 (11)
C10B	0.093 (2)	0.0445 (14)	0.0479 (14)	0.0116 (13)	−0.0083 (13)	−0.0102 (12)
C11B	0.0638 (15)	0.0485 (14)	0.0370 (12)	−0.0019 (11)	0.0012 (11)	−0.0142 (11)
C12B	0.0710 (17)	0.0528 (16)	0.0603 (16)	−0.0026 (13)	−0.0061 (13)	0.0008 (13)
C13B	0.087 (2)	0.0594 (18)	0.111 (3)	0.0054 (16)	−0.0021 (19)	−0.0241 (18)
C14B	0.077 (2)	0.085 (2)	0.075 (2)	−0.0137 (17)	0.0029 (16)	−0.0034 (17)
C15B	0.083 (2)	0.120 (3)	0.170 (4)	−0.020 (2)	−0.015 (3)	−0.042 (3)

Geometric parameters (Å, º)

S1A—C11A	1.785 (2)	S1B—C11B	1.787 (2)
S1A—C10A	1.793 (2)	S1B—C10B	1.787 (3)
S2A—C11A	1.668 (2)	S2B—C11B	1.662 (3)
F1A—C1A	1.362 (3)	F1B—C1B	1.357 (3)
O1A—C7A	1.373 (3)	O1B—C7B	1.370 (3)
O1A—C4A	1.374 (3)	O1B—C4B	1.371 (3)
O2A—C7A	1.200 (3)	O2B—C7B	1.202 (3)
N1A—C11A	1.329 (3)	N1B—C11B	1.320 (3)
N1A—C14A	1.468 (3)	N1B—C12B	1.467 (3)
N1A—C12A	1.477 (3)	N1B—C14B	1.481 (3)
C1A—C2A	1.362 (4)	C1B—C6B	1.360 (3)
C1A—C6A	1.369 (3)	C1B—C2B	1.369 (4)
C2A—C3A	1.368 (4)	C2B—C3B	1.371 (4)
C2A—H2A	0.9300	C2B—H2B	0.9300
C3A—C4A	1.389 (3)	C3B—C4B	1.378 (3)
C3A—H3A	0.9300	C3B—H3B	0.9300
C4A—C5A	1.387 (3)	C4B—C5B	1.391 (3)
C5A—C6A	1.400 (3)	C5B—C6B	1.399 (3)

C5A—C9A	1.453 (3)	C5B—C9B	1.449 (3)
C6A—H6A	0.9300	C6B—H6B	0.9300
C7A—C8A	1.440 (3)	C7B—C8B	1.441 (3)
C8A—C9A	1.331 (3)	C8B—C9B	1.334 (3)
C8A—H8A	0.9300	C8B—H8B	0.9300
C9A—C10A	1.502 (3)	C9B—C10B	1.504 (3)
C10A—H10A	0.9700	C10B—H10C	0.9700
C10A—H10B	0.9700	C10B—H10D	0.9700
C12A—C13A	1.496 (4)	C12B—C13B	1.503 (4)
C12A—H13C	0.9700	C12B—H13A	0.9700
C12A—H13D	0.9700	C12B—H13B	0.9700
C13A—H14A	0.9600	C13B—H14D	0.9600
C13A—H14B	0.9600	C13B—H14E	0.9600
C13A—H14C	0.9600	C13B—H14F	0.9600
C14A—C15A	1.507 (4)	C14B—C15B	1.448 (4)
C14A—H15A	0.9700	C14B—H15C	0.9700
C14A—H15B	0.9700	C14B—H15D	0.9700
C15A—H16A	0.9600	C15B—H16D	0.9600
C15A—H16B	0.9600	C15B—H16E	0.9600
C15A—H16C	0.9600	C15B—H16F	0.9600

C11A—S1A—C10A	103.59 (11)	C11B—S1B—C10B	103.50 (12)
C7A—O1A—C4A	121.12 (19)	C7B—O1B—C4B	121.61 (19)
C11A—N1A—C14A	120.6 (2)	C11B—N1B—C12B	120.9 (2)
C11A—N1A—C12A	124.3 (2)	C11B—N1B—C14B	123.2 (2)
C14A—N1A—C12A	115.09 (19)	C12B—N1B—C14B	115.9 (2)
C2A—C1A—F1A	118.9 (2)	F1B—C1B—C6B	118.3 (3)
C2A—C1A—C6A	123.3 (3)	F1B—C1B—C2B	118.4 (2)
F1A—C1A—C6A	117.8 (3)	C6B—C1B—C2B	123.2 (3)
C1A—C2A—C3A	119.0 (3)	C1B—C2B—C3B	118.5 (2)
C1A—C2A—H2A	120.5	C1B—C2B—H2B	120.8
C3A—C2A—H2A	120.5	C3B—C2B—H2B	120.8
C2A—C3A—C4A	119.2 (3)	C2B—C3B—C4B	119.7 (3)
C2A—C3A—H3A	120.4	C2B—C3B—H3B	120.2
C4A—C3A—H3A	120.4	C4B—C3B—H3B	120.2
O1A—C4A—C5A	121.9 (2)	O1B—C4B—C3B	116.5 (2)
O1A—C4A—C3A	116.2 (2)	O1B—C4B—C5B	121.6 (2)
C5A—C4A—C3A	121.9 (3)	C3B—C4B—C5B	121.9 (2)
C4A—C5A—C6A	117.8 (2)	C4B—C5B—C6B	117.6 (2)
C4A—C5A—C9A	118.1 (2)	C4B—C5B—C9B	118.3 (2)
C6A—C5A—C9A	124.1 (2)	C6B—C5B—C9B	124.1 (2)
C1A—C6A—C5A	118.8 (3)	C1B—C6B—C5B	119.1 (2)
C1A—C6A—H6A	120.6	C1B—C6B—H6B	120.4
C5A—C6A—H6A	120.6	C5B—C6B—H6B	120.4
O2A—C7A—O1A	117.6 (2)	O2B—C7B—O1B	117.5 (2)
O2A—C7A—C8A	125.3 (3)	O2B—C7B—C8B	125.8 (2)
O1A—C7A—C8A	117.1 (2)	O1B—C7B—C8B	116.7 (2)
C9A—C8A—C7A	123.4 (2)	C9B—C8B—C7B	123.6 (2)

C9A—C8A—H8A	118.3	C9B—C8B—H8B	118.2
C7A—C8A—H8A	118.3	C7B—C8B—H8B	118.2
C8A—C9A—C5A	118.4 (2)	C8B—C9B—C5B	118.2 (2)
C8A—C9A—C10A	123.2 (2)	C8B—C9B—C10B	123.3 (2)
C5A—C9A—C10A	118.3 (2)	C5B—C9B—C10B	118.5 (2)
C9A—C10A—S1A	116.64 (16)	C9B—C10B—S1B	116.79 (18)
C9A—C10A—H10A	108.1	C9B—C10B—H10C	108.1
S1A—C10A—H10A	108.1	S1B—C10B—H10C	108.1
C9A—C10A—H10B	108.1	C9B—C10B—H10D	108.1
S1A—C10A—H10B	108.1	S1B—C10B—H10D	108.1
H10A—C10A—H10B	107.3	H10C—C10B—H10D	107.3
N1A—C11A—S2A	124.47 (18)	N1B—C11B—S2B	124.09 (19)
N1A—C11A—S1A	113.32 (17)	N1B—C11B—S1B	113.70 (18)
S2A—C11A—S1A	122.20 (13)	S2B—C11B—S1B	122.22 (14)
N1A—C12A—C13A	112.1 (2)	N1B—C12B—C13B	112.3 (2)
N1A—C12A—H13C	109.2	N1B—C12B—H13A	109.1
C13A—C12A—H13C	109.2	C13B—C12B—H13A	109.1
N1A—C12A—H13D	109.2	N1B—C12B—H13B	109.1
C13A—C12A—H13D	109.2	C13B—C12B—H13B	109.1
H13C—C12A—H13D	107.9	H13A—C12B—H13B	107.9
C12A—C13A—H14A	109.5	C12B—C13B—H14D	109.5
C12A—C13A—H14B	109.5	C12B—C13B—H14E	109.5
H14A—C13A—H14B	109.5	H14D—C13B—H14E	109.5
C12A—C13A—H14C	109.5	C12B—C13B—H14F	109.5
H14A—C13A—H14C	109.5	H14D—C13B—H14F	109.5
H14B—C13A—H14C	109.5	H14E—C13B—H14F	109.5
N1A—C14A—C15A	111.8 (2)	C15B—C14B—N1B	112.1 (3)
N1A—C14A—H15A	109.3	C15B—C14B—H15C	109.2
C15A—C14A—H15A	109.3	N1B—C14B—H15C	109.2
N1A—C14A—H15B	109.3	C15B—C14B—H15D	109.2
C15A—C14A—H15B	109.3	N1B—C14B—H15D	109.2
H15A—C14A—H15B	107.9	H15C—C14B—H15D	107.9
C14A—C15A—H16A	109.5	C14B—C15B—H16D	109.5
C14A—C15A—H16B	109.5	C14B—C15B—H16E	109.5
H16A—C15A—H16B	109.5	H16D—C15B—H16E	109.5
C14A—C15A—H16C	109.5	C14B—C15B—H16F	109.5
H16A—C15A—H16C	109.5	H16D—C15B—H16F	109.5
H16B—C15A—H16C	109.5	H16E—C15B—H16F	109.5

F1A—C1A—C2A—C3A	−178.9 (2)	F1B—C1B—C2B—C3B	−178.3 (2)
C6A—C1A—C2A—C3A	1.3 (4)	C6B—C1B—C2B—C3B	1.0 (4)
C1A—C2A—C3A—C4A	−0.4 (4)	C1B—C2B—C3B—C4B	−0.6 (4)
C7A—O1A—C4A—C5A	−1.0 (3)	C7B—O1B—C4B—C3B	−179.3 (2)
C7A—O1A—C4A—C3A	178.5 (2)	C7B—O1B—C4B—C5B	0.4 (3)
C2A—C3A—C4A—O1A	179.6 (2)	C2B—C3B—C4B—O1B	179.3 (2)
C2A—C3A—C4A—C5A	−0.9 (4)	C2B—C3B—C4B—C5B	−0.4 (4)
O1A—C4A—C5A—C6A	−179.19 (19)	O1B—C4B—C5B—C6B	−178.7 (2)
C3A—C4A—C5A—C6A	1.4 (3)	C3B—C4B—C5B—C6B	1.1 (3)

O1A—C4A—C5A—C9A	1.1 (3)	O1B—C4B—C5B—C9B	0.6 (3)
C3A—C4A—C5A—C9A	−178.3 (2)	C3B—C4B—C5B—C9B	−179.7 (2)
C2A—C1A—C6A—C5A	−0.9 (4)	F1B—C1B—C6B—C5B	179.0 (2)
F1A—C1A—C6A—C5A	179.4 (2)	C2B—C1B—C6B—C5B	−0.3 (4)
C4A—C5A—C6A—C1A	−0.5 (3)	C4B—C5B—C6B—C1B	−0.7 (3)
C9A—C5A—C6A—C1A	179.2 (2)	C9B—C5B—C6B—C1B	−179.9 (2)
C4A—O1A—C7A—O2A	−178.7 (2)	C4B—O1B—C7B—O2B	−179.8 (2)
C4A—O1A—C7A—C8A	0.6 (3)	C4B—O1B—C7B—C8B	−0.5 (3)
O2A—C7A—C8A—C9A	178.8 (3)	O2B—C7B—C8B—C9B	178.8 (3)
O1A—C7A—C8A—C9A	−0.5 (4)	O1B—C7B—C8B—C9B	−0.3 (4)
C7A—C8A—C9A—C5A	0.7 (3)	C7B—C8B—C9B—C5B	1.3 (4)
C7A—C8A—C9A—C10A	−177.4 (2)	C7B—C8B—C9B—C10B	−176.6 (2)
C4A—C5A—C9A—C8A	−0.9 (3)	C4B—C5B—C9B—C8B	−1.4 (3)
C6A—C5A—C9A—C8A	179.4 (2)	C6B—C5B—C9B—C8B	177.8 (2)
C4A—C5A—C9A—C10A	177.2 (2)	C4B—C5B—C9B—C10B	176.6 (2)
C6A—C5A—C9A—C10A	−2.5 (3)	C6B—C5B—C9B—C10B	−4.2 (3)
C8A—C9A—C10A—S1A	−14.5 (3)	C8B—C9B—C10B—S1B	−19.8 (3)
C5A—C9A—C10A—S1A	167.51 (16)	C5B—C9B—C10B—S1B	162.27 (17)
C11A—S1A—C10A—C9A	81.97 (19)	C11B—S1B—C10B—C9B	79.0 (2)
C14A—N1A—C11A—S2A	2.9 (3)	C12B—N1B—C11B—S2B	−4.5 (3)
C12A—N1A—C11A—S2A	−176.84 (18)	C14B—N1B—C11B—S2B	172.5 (2)
C14A—N1A—C11A—S1A	−175.79 (17)	C12B—N1B—C11B—S1B	175.80 (17)
C12A—N1A—C11A—S1A	4.4 (3)	C14B—N1B—C11B—S1B	−7.3 (3)
C10A—S1A—C11A—N1A	−167.43 (16)	C10B—S1B—C11B—N1B	−163.79 (17)
C10A—S1A—C11A—S2A	13.81 (17)	C10B—S1B—C11B—S2B	16.45 (18)
C11A—N1A—C12A—C13A	−91.7 (3)	C11B—N1B—C12B—C13B	−80.5 (3)
C14A—N1A—C12A—C13A	88.5 (3)	C14B—N1B—C12B—C13B	102.4 (3)
C11A—N1A—C14A—C15A	−89.1 (3)	C11B—N1B—C14B—C15B	101.2 (3)
C12A—N1A—C14A—C15A	90.7 (3)	C12B—N1B—C14B—C15B	−81.8 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10*A*—H10*A*···S2*B*	0.97	2.87	3.621 (2)	135
C12*A*—H13*C*···O2*B*^{i}	0.97	2.60	3.368 (3)	136
C2*B*—H2*B*···S2*B*^{ii}	0.93	2.87	3.693 (3)	148
C10*B*—H10*C*···S2*A*^{iii}	0.97	2.82	3.660 (2)	145

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