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5,13-Bis(4-methoxyphenyl)dinaphtho[2,3-*b*:2′,3′-*d*]-thiophene *S*,*S*-dioxide dichloromethane hemisolvate

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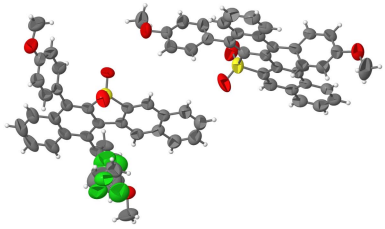
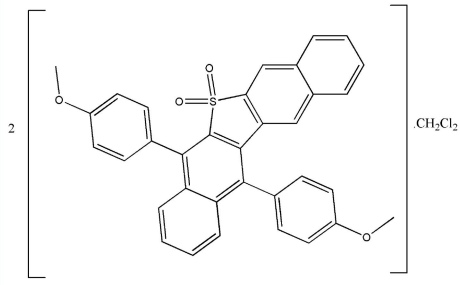
The title compound, $C_{34}H_{24}O_4S{\cdot}0.5CH_2Cl_2$, crystallizes with two independent molecules and one dichloromethane solvent molecule in the asymmetric unit. The crystal packing is consolidated by C—H···O hydrogen bonds.

3D view



Chemical scheme



Structure description

In order to ascertain the structure of the title compound, a crystallographic study has been carried out. The displacement ellipsoid plot of the molecule is shown in Fig. 1.

The asymmetric unit comprises two molecules of the dinaphthothiophene compound and one dichloromethane (DCM) solvent molecule. The solvent molecule is disordered over three sets of sites, with refined site occupancies of 0.279 (3), 0.330 (3) and 0.391 (3).

The central dinaphthothiophene ring system is essentially planar in both molecules, with maximum deviations of 0.010 (3) and 0.005 (3) Å.

The plane of the naphthalene ring (atoms C1–C10) makes dihedral angles of 72.43 (8) and 85.05 (7)° with the planes of phenyl rings C21–C26 and C27–C32, respectively. In the second molecule, these dihedral angles are 72.17 (8)° between C1′–C10′ and C21′–C26′, and 88.71 (7)° between C1′–C10′ and C27′-C32′.

The packing of the molecules in the unit cell is consolidated by C—H···O interactions (Table 1). The C34′—H34*B*···O2′ and C34—H34*E*···O1 interactions lead to the formation of a *C*(12) chain running along the *a*-axis direction, as shown in Fig. 2. Furthermore, the molecules are linked by pairs of C6—H6···O4 and C13′—H13′···O2′ hydrogen bonds, forming inversion dimers with $R_2^2(10)$ and $R_2^2(20)$ ring motifs (Fig. 3).

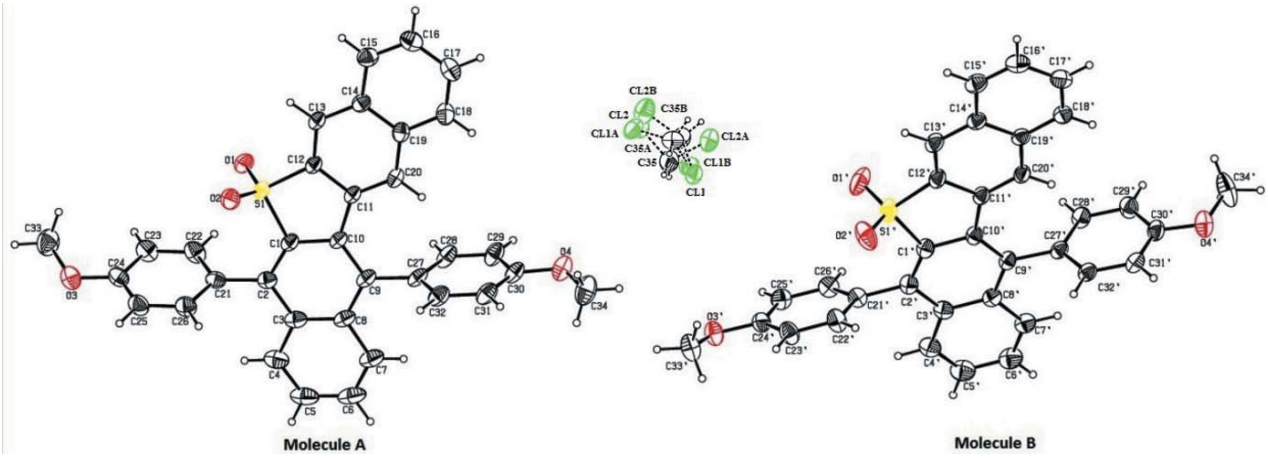


Figure 1
The molecular structure of the title compound, showing the atomic numbering and displacement ellipsoids drawn at the 30% probability level.

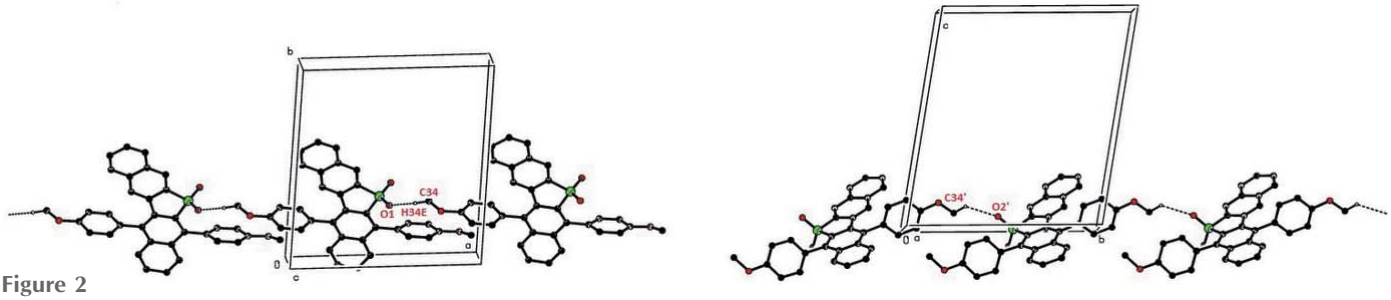


Figure 2
Part of the crystal structure, showing a $C(12)$ chain formed *via* C—H···O hydrogen-bond interactions. H atoms not involved in hydrogen bonding (dashed lines) have been omitted for clarity.

Synthesis and crystallization

To a solution of dianisylbenzo[*c*]furan (0.24 g, 0.72 mmol) in dry toluene (15 ml), naphtho[*b*]thiophene *S*,*S*-dioxide (0.25 g, 1.48 mmol) was added and the resulting solution refluxed until the disappearance of the fluorescent colour of the benzo[*c*]-furan (12 h). To this, *p*-toluenesulfonic acid (PTSA; 0.56 g, 2.90 mmol) was added and the solution further refluxed for 10 h. The reaction mixture was then poured into a saturated solution of $NaHCO_3$ (50 ml), extracted with ethyl acetate

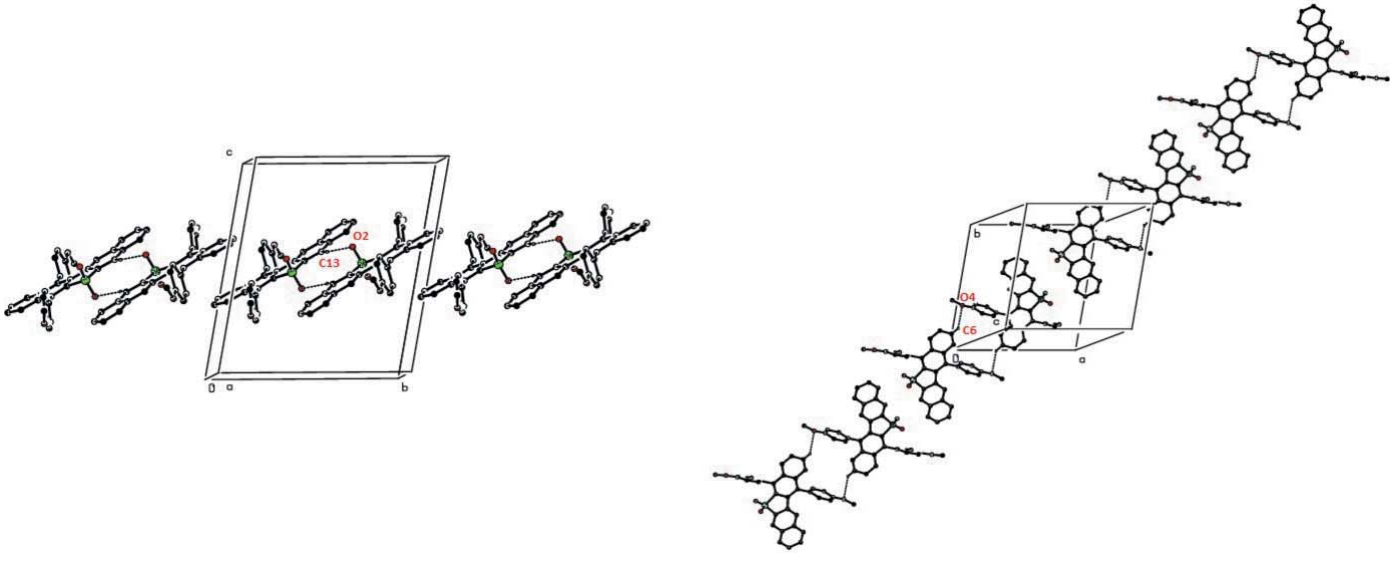


Figure 3
Part of the crystal structure, showing the $R_2^2(10)$ and $R_2^2(20)$ dimers. H atoms not involved in hydrogen bonding (dashed lines) have been omitted for clarity.

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

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13···O2^{i}	0.93	2.46	3.330 (3)	156
C26′—H26′···O2^{i}	0.93	2.59	3.329 (4)	137
C6—H6···O4^{ii}	0.93	2.56	3.304 (4)	137
C13′—H13′···O1′^{iii}	0.93	2.59	3.500 (3)	165
C34′—H34B···O2′^{iv}	0.96	2.45	3.191 (4)	134
C34—H34E···O1^{v}	0.96	2.60	3.177 (4)	119

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

(3 × 20 ml) and dried (Na_2SO_4). Removal of the solvent was followed by column chromatographic purification (silica gel; 10% ethyl acetate in hexane), affording dibenzothiophene *S*,*S*-dioxide as a brown solid.

Refinement

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

Acknowledgements

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Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Table 2
Experimental details.

Crystal data	
Chemical formula	$2C_{34}H_{24}O_4S{\cdot}CH_2Cl_2$
M_r	1142.11
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	293
a, b, c (Å)	13.7369 (5), 13.8077 (5), 16.4824 (6)
α, β, γ (°)	78.442 (2), 68.211 (2), 80.216 (2)
V (Å^3)	2828.35 (18)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.25
Crystal size (mm)	0.30 × 0.30 × 0.25
Data collection	
Diffractometer	Bruker SMART APEXII area-detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	41656, 11698, 6066
R_{int}	0.042
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.631
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.053, 0.169, 1.01
No. of reflections	11698
No. of parameters	791
No. of restraints	52
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.28, −0.26

Computer programs: *APEX2* (Bruker, 2008), *SAINT* (Bruker, 2008), *SHELXS97* (Sheldrick, 2008), *SHELXL2018* (Sheldrick, 2015), *ORTEP-3* (Farrugia, 2012), *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
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full crystallographic data

IUCrData (2019). **4**, x191394 [https://doi.org/10.1107/S2414314619013944]

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5,13-Bis(4-methoxyphenyl)dinaphtho[2,3-*b*:2′,3′-*d*]thiophene *S*,*S*-dioxide dichloromethane hemisolvate

Crystal data

$2C_{34}H_{24}O_4S·CH_2Cl_2$
M_r = 1142.11
Triclinic, $P\overline{1}$
a = 13.7369 (5) Å
b = 13.8077 (5) Å
c = 16.4824 (6) Å
α = 78.442 (2)°
β = 68.211 (2)°
γ = 80.216 (2)°
V = 2828.35 (18) Å^3
Z = 2
$F(000)$ = 1188
D_x = 1.341 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6066 reflections
θ = 0.9–0.9°
μ = 0.25 mm^{-1}
T = 293 K
Block, brown
0.30 × 0.30 × 0.25 mm

Data collection

Bruker SMART APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
ω and φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2008)

41656 measured reflections

11698 independent reflections
6066 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 26.7°, θ_{min} = 1.4°
h = −15→17
k = −17→17
l = −19→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.169
S = 1.01
11698 reflections
791 parameters
52 restraints

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.071P)^2 + 0.6749P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 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 C—Cl bond lengths were restrained to a distance of 1.72 (1) Å. Atomic displacement parameters of the disordered atoms were made similar in each moiety using similarity restraints (SIMU) with an effective s.u. of 0.01 Å^2. In addition, a rigid bond restraint (DELU) with an effective s.u. of 0.01 Å^2 was applied for bonded atoms in the dichloromethane solvent molecules.
H atoms were allowed to ride on the parent atoms, with a C—H distance of 0.96 Å for methyl, 0.97 Å for methylene and 0.93 Å for aromatic H atoms, and with U_{iso}(H) = 1.5U_{eq}(C$_{methyl}$) and U_{iso}(H) = 1.2U_{eq}(C) for the remaining H atoms.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.3976 (2)	0.23726 (19)	0.45563 (17)	0.0597 (7)	
C1′	0.2493 (2)	0.64646 (19)	0.97637 (17)	0.0622 (7)	
C2′	0.3509 (2)	0.62006 (19)	0.92568 (17)	0.0632 (7)	
C2	0.4515 (2)	0.16277 (19)	0.40718 (17)	0.0621 (7)	
C3	0.3888 (3)	0.1006 (2)	0.39185 (18)	0.0698 (8)	
C3′	0.4244 (2)	0.6913 (2)	0.90502 (18)	0.0636 (7)	
C4′	0.5306 (2)	0.6720 (2)	0.8519 (2)	0.0787 (9)	
H4′	0.553996	0.611161	0.831331	0.094*	
C4	0.4361 (3)	0.0182 (2)	0.34648 (19)	0.0880 (10)	
H4	0.509136	0.005689	0.324138	0.106*	
C5	0.3750 (4)	−0.0431 (3)	0.3352 (2)	0.1040 (13)	
H5	0.406686	−0.098564	0.307445	0.125*	
C5′	0.5994 (3)	0.7407 (3)	0.8302 (2)	0.0930 (10)	
H5′	0.669191	0.726683	0.794710	0.112*	
C6′	0.5664 (3)	0.8318 (3)	0.8608 (2)	0.0897 (10)	
H6′	0.614068	0.878651	0.845177	0.108*	
C6	0.2665 (4)	−0.0230 (3)	0.3651 (2)	0.1059 (13)	
H6	0.226129	−0.063755	0.354999	0.127*	
C7	0.2182 (3)	0.0549 (2)	0.4085 (2)	0.0855 (10)	
H7	0.145069	0.066531	0.428226	0.103*	
C7′	0.4651 (2)	0.8528 (2)	0.91310 (19)	0.0728 (8)	
H7′	0.444316	0.913691	0.933680	0.087*	
C8	0.2772 (3)	0.1193 (2)	0.42465 (18)	0.0678 (8)	
C8′	0.3900 (2)	0.78333 (19)	0.93714 (17)	0.0620 (7)	
C9	0.2252 (2)	0.19790 (19)	0.47470 (18)	0.0627 (7)	
C9′	0.2837 (2)	0.80587 (17)	0.99138 (16)	0.0577 (7)	
C10	0.2864 (2)	0.25688 (18)	0.49045 (17)	0.0574 (6)	
C10′	0.2124 (2)	0.73788 (17)	1.01103 (17)	0.0571 (6)	
C11′	0.0990 (2)	0.74440 (18)	1.06453 (17)	0.0565 (6)	
C11	0.2513 (2)	0.34299 (18)	0.53960 (17)	0.0559 (6)	
C12	0.33786 (19)	0.38690 (18)	0.53821 (17)	0.0571 (6)	
C12′	0.0523 (2)	0.65912 (18)	1.06699 (18)	0.0636 (7)	
C13′	−0.0509 (2)	0.6466 (2)	1.11355 (19)	0.0697 (8)	
H13′	−0.078079	0.589475	1.113350	0.084*	
C13	0.3276 (2)	0.46544 (19)	0.58033 (17)	0.0621 (7)	
H13	0.386912	0.491894	0.577352	0.075*	
C14	0.2265 (2)	0.50587 (19)	0.62817 (18)	0.0633 (7)	
C14′	−0.1161 (2)	0.7211 (2)	1.16213 (18)	0.0637 (7)	

C15′	−0.2237 (2)	0.7130 (2)	1.2117 (2)	0.0785 (9)
H15′	−0.253655	0.656941	1.212795	0.094*
C15	0.2095 (3)	0.5854 (2)	0.6759 (2)	0.0803 (9)
H15	0.266702	0.614576	0.673975	0.096*
C16	0.1107 (3)	0.6193 (3)	0.7243 (2)	0.0911 (10)
H16	0.100634	0.670955	0.756043	0.109*
C16′	−0.2841 (3)	0.7864 (3)	1.2580 (2)	0.0848 (9)
H16′	−0.354801	0.779792	1.290961	0.102*
C17′	−0.2411 (3)	0.8713 (3)	1.2566 (2)	0.0815 (9)
H17′	−0.283234	0.921016	1.288334	0.098*
C17	0.0237 (3)	0.5777 (3)	0.7272 (2)	0.0936 (10)
H17	−0.043739	0.601285	0.761275	0.112*
C18′	−0.1384 (2)	0.8819 (2)	1.20922 (19)	0.0693 (8)
H18′	−0.110881	0.939186	1.208625	0.083*
C18	0.0370 (2)	0.5031 (2)	0.6808 (2)	0.0834 (9)
H18	−0.021942	0.477382	0.681913	0.100*
C19	0.1384 (2)	0.4635 (2)	0.63067 (19)	0.0660 (7)
C19′	−0.0721 (2)	0.80730 (19)	1.16051 (17)	0.0599 (7)
C20′	0.0352 (2)	0.81714 (19)	1.11112 (18)	0.0604 (7)
H20′	0.063344	0.874249	1.110149	0.073*
C20	0.1529 (2)	0.3834 (2)	0.58504 (19)	0.0657 (7)
H20	0.094327	0.357395	0.585884	0.079*
C21	0.5687 (2)	0.14822 (19)	0.37220 (17)	0.0633 (7)
C21′	0.3850 (2)	0.5212 (2)	0.89553 (18)	0.0659 (7)
C22′	0.3929 (3)	0.4370 (2)	0.9547 (2)	0.0825 (9)
H22′	0.376868	0.442919	1.013611	0.099*
C22	0.6268 (3)	0.1139 (2)	0.4259 (2)	0.0844 (9)
H22	0.591667	0.096895	0.486196	0.101*
C23′	0.4241 (3)	0.3443 (2)	0.9290 (2)	0.0836 (9)
H23′	0.429490	0.288728	0.970255	0.100*
C23	0.7358 (3)	0.1035 (2)	0.3938 (2)	0.0863 (10)
H23	0.772816	0.079422	0.432085	0.104*
C24	0.7886 (3)	0.1289 (2)	0.3057 (2)	0.0750 (8)
C24′	0.4471 (2)	0.3341 (2)	0.8426 (2)	0.0707 (8)
C25′	0.4396 (2)	0.4170 (2)	0.78204 (19)	0.0756 (8)
H25′	0.455261	0.410423	0.723340	0.091*
C25	0.7320 (3)	0.1628 (2)	0.2507 (2)	0.0857 (9)
H25	0.767323	0.179904	0.190480	0.103*
C26	0.6247 (3)	0.1717 (2)	0.2831 (2)	0.0821 (9)
H26	0.588126	0.194157	0.244274	0.098*
C26′	0.4092 (2)	0.5096 (2)	0.80782 (19)	0.0732 (8)
H26′	0.404728	0.565034	0.766242	0.088*
C27′	0.2519 (2)	0.90197 (18)	1.02690 (17)	0.0579 (7)
C27	0.1087 (2)	0.2121 (2)	0.51208 (19)	0.0663 (7)
C28	0.0558 (2)	0.1720 (2)	0.5987 (2)	0.0810 (9)
H28	0.094351	0.135005	0.632512	0.097*
C28′	0.2169 (2)	0.9864 (2)	0.98020 (19)	0.0733 (8)
H28′	0.213183	0.982787	0.925706	0.088*

C29′	0.1875 (3)	1.0754 (2)	1.0120 (2)	0.0787 (9)	
H29′	0.163312	1.130924	0.979579	0.094*	
C29	−0.0521 (3)	0.1857 (2)	0.6359 (2)	0.0846 (9)	
H29	−0.085705	0.157702	0.694000	0.102*	
C30	−0.1108 (3)	0.2408 (2)	0.5873 (2)	0.0773 (9)	
C30′	0.1939 (2)	1.0821 (2)	1.0913 (2)	0.0705 (8)	
C31	−0.0605 (3)	0.2810 (2)	0.5012 (2)	0.0827 (9)	
H31	−0.099461	0.317832	0.467639	0.099*	
C31′	0.2278 (2)	0.9990 (2)	1.13941 (19)	0.0697 (8)	
H31′	0.231465	1.003081	1.193826	0.084*	
C32	0.0480 (3)	0.2665 (2)	0.4646 (2)	0.0784 (9)	
H32	0.081214	0.294220	0.406281	0.094*	
C32′	0.2562 (2)	0.9101 (2)	1.10755 (18)	0.0637 (7)	
H32′	0.278820	0.854404	1.140804	0.076*	
C33	0.9578 (3)	0.1065 (3)	0.3238 (3)	0.1202 (14)	
H33A	0.933329	0.155347	0.362963	0.180*	
H33B	1.030616	0.112093	0.288367	0.180*	
H33C	0.950581	0.041249	0.357768	0.180*	
C33′	0.4654 (3)	0.1576 (2)	0.8741 (3)	0.1088 (13)	
H33D	0.513821	0.151873	0.904887	0.163*	
H33E	0.479073	0.100799	0.844653	0.163*	
H33F	0.394505	0.160847	0.915617	0.163*	
C34′	0.1305 (4)	1.2547 (3)	1.0821 (3)	0.1463 (19)	
H34A	0.180483	1.267951	1.023273	0.219*	
H34B	0.120568	1.310036	1.112460	0.219*	
H34C	0.064431	1.244754	1.079147	0.219*	
C34	−0.2836 (3)	0.2993 (3)	0.5812 (3)	0.1273 (15)	
H34D	−0.273084	0.368529	0.564753	0.191*	
H34E	−0.356130	0.292600	0.617010	0.191*	
H34F	−0.265899	0.269568	0.529006	0.191*	
O1	0.51147 (15)	0.27997 (17)	0.54193 (14)	0.0872 (6)	
O1′	0.1225 (2)	0.5637 (2)	0.93012 (17)	0.1185 (9)	
O2′	0.15741 (19)	0.48388 (14)	1.06430 (17)	0.1143 (9)	
O2	0.51534 (16)	0.38610 (15)	0.40331 (14)	0.0903 (7)	
O3′	0.47846 (18)	0.24479 (16)	0.81125 (15)	0.0913 (7)	
O3	0.89614 (19)	0.12260 (17)	0.26712 (16)	0.0995 (7)	
O4′	0.1691 (2)	1.16739 (16)	1.12854 (16)	0.0991 (7)	
O4	−0.21771 (18)	0.25056 (17)	0.63039 (17)	0.0976 (7)	
S1	0.45820 (5)	0.32462 (5)	0.48161 (5)	0.0654 (2)	
S1′	0.14417 (7)	0.57256 (6)	1.00631 (6)	0.0797 (3)	
C35	0.288 (3)	0.5232 (14)	0.2124 (14)	0.189 (9)	0.279 (3)
H35A	0.276327	0.489135	0.171144	0.226*	0.279 (3)
H35B	0.362506	0.529511	0.194021	0.226*	0.279 (3)
Cl1	0.2157 (5)	0.6368 (5)	0.2187 (5)	0.165 (2)	0.279 (3)
Cl2	0.2420 (10)	0.4615 (13)	0.3172 (13)	0.148 (5)	0.279 (3)
C35A	0.2299 (12)	0.5629 (17)	0.2512 (11)	0.151 (6)	0.330 (3)
H35C	0.196133	0.527954	0.225065	0.181*	0.330 (3)
H35D	0.182391	0.622144	0.267183	0.181*	0.330 (3)

Cl1A	0.2223 (12)	0.4901 (9)	0.3503 (8)	0.185 (4)	0.330 (3)
Cl2A	0.3358 (3)	0.6060 (3)	0.1648 (2)	0.1120 (13)	0.330 (3)
C35B	0.2897 (13)	0.5696 (10)	0.2624 (7)	0.120 (3)	0.391 (3)
H35E	0.363026	0.581348	0.243436	0.144*	0.391 (3)
H35F	0.245011	0.622199	0.294236	0.144*	0.391 (3)
Cl1B	0.2545 (4)	0.5556 (5)	0.1757 (3)	0.166 (2)	0.391 (3)
Cl2B	0.2670 (11)	0.4546 (10)	0.3227 (7)	0.180 (4)	0.391 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0622 (17)	0.0607 (16)	0.0629 (16)	−0.0212 (13)	−0.0272 (14)	−0.0012 (13)
C1′	0.0718 (19)	0.0561 (16)	0.0575 (16)	−0.0154 (13)	−0.0213 (15)	−0.0009 (13)
C2′	0.077 (2)	0.0568 (16)	0.0542 (16)	−0.0102 (14)	−0.0253 (15)	0.0010 (13)
C2	0.0761 (19)	0.0593 (16)	0.0522 (15)	−0.0147 (14)	−0.0245 (14)	−0.0010 (13)
C3	0.103 (2)	0.0577 (17)	0.0558 (16)	−0.0222 (16)	−0.0347 (17)	0.0005 (13)
C3′	0.0668 (18)	0.0620 (17)	0.0570 (16)	−0.0072 (14)	−0.0230 (14)	0.0052 (13)
C4′	0.073 (2)	0.080 (2)	0.076 (2)	−0.0056 (16)	−0.0233 (17)	−0.0015 (16)
C4	0.130 (3)	0.070 (2)	0.0641 (19)	−0.0239 (19)	−0.029 (2)	−0.0089 (16)
C5	0.174 (4)	0.076 (2)	0.071 (2)	−0.040 (3)	−0.038 (3)	−0.0147 (17)
C5′	0.072 (2)	0.103 (3)	0.090 (2)	−0.017 (2)	−0.0181 (19)	0.004 (2)
C6′	0.080 (2)	0.087 (2)	0.096 (2)	−0.0325 (18)	−0.027 (2)	0.014 (2)
C6	0.172 (4)	0.094 (3)	0.079 (2)	−0.061 (3)	−0.057 (3)	−0.007 (2)
C7	0.123 (3)	0.079 (2)	0.074 (2)	−0.0439 (19)	−0.049 (2)	0.0014 (17)
C7′	0.074 (2)	0.0700 (18)	0.0735 (19)	−0.0228 (15)	−0.0286 (17)	0.0095 (15)
C8	0.095 (2)	0.0622 (17)	0.0616 (17)	−0.0311 (16)	−0.0411 (17)	0.0039 (14)
C8′	0.0692 (18)	0.0595 (16)	0.0589 (16)	−0.0156 (13)	−0.0289 (15)	0.0075 (13)
C9	0.0734 (18)	0.0626 (16)	0.0644 (17)	−0.0275 (14)	−0.0374 (15)	0.0063 (14)
C9′	0.0753 (19)	0.0474 (14)	0.0554 (15)	−0.0165 (13)	−0.0302 (15)	0.0040 (12)
C10	0.0610 (16)	0.0597 (16)	0.0604 (16)	−0.0203 (12)	−0.0299 (13)	0.0002 (13)
C10′	0.0687 (17)	0.0481 (14)	0.0567 (15)	−0.0141 (12)	−0.0250 (14)	−0.0002 (12)
C11′	0.0647 (17)	0.0493 (14)	0.0594 (16)	−0.0141 (12)	−0.0255 (14)	−0.0026 (12)
C11	0.0554 (16)	0.0565 (15)	0.0620 (16)	−0.0184 (12)	−0.0265 (13)	−0.0003 (13)
C12	0.0555 (15)	0.0578 (15)	0.0621 (16)	−0.0192 (12)	−0.0230 (13)	−0.0022 (13)
C12′	0.0752 (19)	0.0509 (15)	0.0713 (18)	−0.0194 (13)	−0.0309 (15)	−0.0030 (13)
C13′	0.0732 (19)	0.0604 (17)	0.082 (2)	−0.0262 (15)	−0.0317 (17)	−0.0005 (15)
C13	0.0568 (17)	0.0641 (17)	0.0706 (18)	−0.0203 (13)	−0.0247 (14)	−0.0051 (14)
C14	0.0693 (18)	0.0577 (16)	0.0666 (17)	−0.0144 (13)	−0.0275 (15)	−0.0037 (13)
C14′	0.0625 (17)	0.0638 (17)	0.0679 (17)	−0.0149 (14)	−0.0291 (15)	0.0024 (14)
C15′	0.071 (2)	0.085 (2)	0.082 (2)	−0.0244 (17)	−0.0306 (18)	0.0045 (18)
C15	0.089 (2)	0.0696 (19)	0.089 (2)	−0.0086 (17)	−0.0357 (19)	−0.0186 (17)
C16	0.102 (3)	0.082 (2)	0.087 (2)	0.002 (2)	−0.030 (2)	−0.0241 (19)
C16′	0.0628 (19)	0.104 (3)	0.081 (2)	−0.0104 (19)	−0.0248 (17)	0.001 (2)
C17′	0.070 (2)	0.094 (2)	0.080 (2)	0.0040 (18)	−0.0314 (18)	−0.0144 (18)
C17	0.082 (2)	0.095 (3)	0.086 (2)	0.004 (2)	−0.0123 (19)	−0.018 (2)
C18′	0.071 (2)	0.0726 (18)	0.0707 (19)	−0.0028 (15)	−0.0327 (16)	−0.0133 (15)
C18	0.065 (2)	0.087 (2)	0.092 (2)	−0.0092 (16)	−0.0191 (18)	−0.0122 (19)
C19	0.0591 (17)	0.0650 (17)	0.0698 (18)	−0.0102 (13)	−0.0210 (15)	−0.0011 (14)

C19′	0.0634 (17)	0.0637 (16)	0.0603 (16)	−0.0103 (13)	−0.0327 (14)	−0.0018 (13)
C20′	0.0690 (18)	0.0518 (15)	0.0696 (17)	−0.0152 (13)	−0.0322 (15)	−0.0062 (13)
C20	0.0537 (17)	0.0697 (18)	0.0790 (19)	−0.0171 (13)	−0.0271 (15)	−0.0065 (15)
C21	0.080 (2)	0.0594 (16)	0.0518 (16)	−0.0055 (14)	−0.0250 (15)	−0.0075 (13)
C21′	0.0709 (18)	0.0666 (18)	0.0558 (17)	−0.0058 (14)	−0.0191 (14)	−0.0064 (14)
C22′	0.116 (3)	0.069 (2)	0.0587 (18)	0.0057 (17)	−0.0326 (18)	−0.0098 (15)
C22	0.090 (2)	0.095 (2)	0.0557 (18)	0.0063 (18)	−0.0246 (18)	0.0023 (16)
C23′	0.111 (3)	0.0659 (19)	0.068 (2)	0.0078 (17)	−0.0321 (19)	−0.0084 (15)
C23	0.090 (3)	0.094 (2)	0.070 (2)	0.0131 (19)	−0.0366 (19)	−0.0050 (17)
C24	0.081 (2)	0.0654 (18)	0.073 (2)	0.0043 (15)	−0.0206 (19)	−0.0190 (15)
C24′	0.0713 (19)	0.0720 (19)	0.0687 (19)	−0.0017 (15)	−0.0222 (16)	−0.0192 (16)
C25′	0.079 (2)	0.091 (2)	0.0548 (17)	−0.0079 (17)	−0.0188 (16)	−0.0149 (17)
C25	0.088 (2)	0.103 (2)	0.0553 (18)	−0.0130 (19)	−0.0135 (19)	−0.0065 (17)
C26	0.089 (2)	0.098 (2)	0.0572 (18)	−0.0088 (18)	−0.0285 (18)	−0.0025 (16)
C26′	0.078 (2)	0.076 (2)	0.0600 (18)	−0.0103 (15)	−0.0206 (16)	−0.0019 (15)
C27′	0.0655 (16)	0.0527 (15)	0.0619 (16)	−0.0230 (12)	−0.0292 (14)	0.0051 (13)
C27	0.0761 (19)	0.0662 (17)	0.0730 (19)	−0.0336 (14)	−0.0423 (16)	0.0065 (14)
C28	0.081 (2)	0.092 (2)	0.084 (2)	−0.0394 (17)	−0.0499 (18)	0.0240 (17)
C28′	0.104 (2)	0.0570 (17)	0.0688 (18)	−0.0156 (15)	−0.0462 (18)	0.0044 (14)
C29′	0.106 (2)	0.0509 (17)	0.083 (2)	−0.0090 (15)	−0.0447 (19)	0.0032 (15)
C29	0.078 (2)	0.095 (2)	0.086 (2)	−0.0395 (17)	−0.0394 (19)	0.0212 (18)
C30	0.074 (2)	0.0717 (19)	0.099 (2)	−0.0304 (16)	−0.043 (2)	0.0022 (17)
C30′	0.078 (2)	0.0541 (17)	0.082 (2)	−0.0194 (14)	−0.0246 (17)	−0.0103 (15)
C31	0.084 (2)	0.084 (2)	0.096 (2)	−0.0185 (17)	−0.057 (2)	0.0080 (18)
C31′	0.083 (2)	0.0712 (19)	0.0655 (18)	−0.0239 (15)	−0.0327 (16)	−0.0062 (15)
C32	0.089 (2)	0.083 (2)	0.075 (2)	−0.0275 (17)	−0.0455 (18)	0.0107 (16)
C32′	0.0729 (18)	0.0570 (16)	0.0683 (18)	−0.0185 (13)	−0.0343 (15)	0.0031 (14)
C33	0.091 (3)	0.120 (3)	0.152 (4)	0.007 (2)	−0.051 (3)	−0.023 (3)
C33′	0.135 (3)	0.072 (2)	0.111 (3)	0.002 (2)	−0.033 (3)	−0.025 (2)
C34′	0.211 (5)	0.054 (2)	0.141 (4)	0.008 (3)	−0.031 (4)	−0.018 (2)
C34	0.082 (3)	0.136 (3)	0.170 (4)	0.000 (2)	−0.067 (3)	−0.002 (3)
O1	0.0653 (12)	0.1178 (17)	0.0988 (15)	0.0044 (11)	−0.0479 (12)	−0.0362 (13)
O1′	0.1149 (19)	0.148 (2)	0.1134 (19)	−0.0487 (16)	−0.0227 (16)	−0.0702 (17)
O2′	0.1077 (18)	0.0480 (12)	0.141 (2)	−0.0151 (11)	0.0039 (16)	0.0020 (13)
O2	0.0857 (14)	0.0934 (14)	0.0819 (14)	−0.0497 (12)	0.0016 (12)	−0.0172 (12)
O3′	0.1037 (17)	0.0791 (15)	0.0862 (15)	0.0017 (12)	−0.0220 (13)	−0.0324 (13)
O3	0.0783 (16)	0.1057 (17)	0.1039 (18)	0.0073 (13)	−0.0199 (14)	−0.0292 (14)
O4′	0.1255 (19)	0.0648 (14)	0.1042 (17)	−0.0168 (13)	−0.0299 (15)	−0.0207 (13)
O4	0.0757 (15)	0.1009 (16)	0.1211 (19)	−0.0234 (12)	−0.0422 (14)	−0.0003 (14)
S1	0.0543 (4)	0.0764 (5)	0.0716 (5)	−0.0222 (3)	−0.0194 (4)	−0.0168 (4)
S1′	0.0862 (6)	0.0602 (5)	0.0895 (6)	−0.0262 (4)	−0.0144 (5)	−0.0202 (4)
C35	0.160 (13)	0.169 (11)	0.168 (12)	0.014 (10)	−0.019 (13)	0.026 (11)
Cl1	0.192 (6)	0.134 (4)	0.152 (5)	−0.012 (4)	−0.060 (4)	0.017 (4)
Cl2	0.073 (4)	0.139 (8)	0.174 (10)	−0.022 (5)	−0.001 (5)	0.033 (6)
C35A	0.139 (11)	0.120 (10)	0.151 (11)	−0.032 (10)	−0.017 (9)	0.024 (9)
Cl1A	0.192 (11)	0.168 (8)	0.186 (8)	−0.047 (7)	−0.075 (7)	0.037 (6)
Cl2A	0.098 (2)	0.118 (2)	0.115 (3)	−0.0189 (19)	−0.044 (2)	0.0132 (19)
C35B	0.100 (7)	0.157 (8)	0.118 (8)	−0.028 (7)	−0.038 (6)	−0.038 (6)

Cl1B	0.158 (4)	0.219 (5)	0.108 (3)	0.050 (4)	−0.061 (3)	−0.026 (3)
Cl2B	0.164 (9)	0.204 (6)	0.112 (4)	0.019 (5)	−0.025 (5)	0.036 (4)

Geometric parameters (Å, º)

C1—C2	1.369 (4)	C21—C26	1.381 (4)
C1—C10	1.417 (4)	C21′—C22′	1.377 (4)
C1—S1	1.773 (3)	C21′—C26′	1.394 (4)
C1′—C2′	1.364 (4)	C22′—C23′	1.378 (4)
C1′—C10′	1.426 (3)	C22′—H22′	0.9300
C1′—S1′	1.772 (3)	C22—C23	1.382 (4)
C2′—C3′	1.432 (4)	C22—H22	0.9300
C2′—C21′	1.487 (4)	C23′—C24′	1.372 (4)
C2—C3	1.429 (4)	C23′—H23′	0.9300
C2—C21	1.487 (4)	C23—C24	1.364 (4)
C3—C4	1.415 (4)	C23—H23	0.9300
C3—C8	1.420 (4)	C24—C25	1.368 (4)
C3′—C4′	1.407 (4)	C24—O3	1.370 (4)
C3′—C8′	1.414 (4)	C24′—O3′	1.371 (3)
C4′—C5′	1.356 (4)	C24′—C25′	1.377 (4)
C4′—H4′	0.9300	C25′—C26′	1.376 (4)
C4—C5	1.369 (5)	C25′—H25′	0.9300
C4—H4	0.9300	C25—C26	1.362 (4)
C5—C6	1.382 (5)	C25—H25	0.9300
C5—H5	0.9300	C26—H26	0.9300
C5′—C6′	1.391 (5)	C26′—H26′	0.9300
C5′—H5′	0.9300	C27′—C32′	1.380 (4)
C6′—C7′	1.355 (4)	C27′—C28′	1.381 (3)
C6′—H6′	0.9300	C27—C32	1.382 (4)
C6—C7	1.350 (5)	C27—C28	1.387 (4)
C6—H6	0.9300	C28—C29	1.373 (4)
C7—C8	1.420 (4)	C28—H28	0.9300
C7—H7	0.9300	C28′—C29′	1.370 (4)
C7′—C8′	1.422 (4)	C28′—H28′	0.9300
C7′—H7′	0.9300	C29′—C30′	1.366 (4)
C8—C9	1.424 (4)	C29′—H29′	0.9300
C8′—C9′	1.420 (4)	C29—C30	1.376 (4)
C9—C10	1.385 (3)	C29—H29	0.9300
C9—C27	1.479 (4)	C30—O4	1.370 (4)
C9′—C10′	1.379 (3)	C30—C31	1.374 (4)
C9′—C27′	1.490 (3)	C30′—O4′	1.370 (3)
C10—C11	1.484 (4)	C30′—C31′	1.375 (4)
C10′—C11′	1.475 (4)	C31—C32	1.380 (4)
C11′—C20′	1.370 (3)	C31—H31	0.9300
C11′—C12′	1.421 (3)	C31′—C32′	1.370 (4)
C11—C20	1.363 (3)	C31′—H31′	0.9300
C11—C12	1.415 (3)	C32—H32	0.9300
C12—C13	1.362 (3)	C32′—H32′	0.9300

C12—S1	1.742 (3)	C33—O3	1.442 (4)
C12′—C13′	1.360 (4)	C33—H33A	0.9600
C12′—S1′	1.747 (3)	C33—H33B	0.9600
C13′—C14′	1.410 (4)	C33—H33C	0.9600
C13′—H13′	0.9300	C33′—O3′	1.411 (4)
C13—C14	1.400 (4)	C33′—H33D	0.9600
C13—H13	0.9300	C33′—H33E	0.9600
C14—C15	1.415 (4)	C33′—H33F	0.9600
C14—C19	1.416 (4)	C34′—O4′	1.427 (4)
C14′—C15′	1.410 (4)	C34′—H34A	0.9600
C14′—C19′	1.415 (4)	C34′—H34B	0.9600
C15′—C16′	1.362 (4)	C34′—H34C	0.9600
C15′—H15′	0.9300	C34—O4	1.431 (4)
C15—C16	1.352 (4)	C34—H34D	0.9600
C15—H15	0.9300	C34—H34E	0.9600
C16—C17	1.392 (5)	C34—H34F	0.9600
C16—H16	0.9300	O1—S1	1.430 (2)
C16′—C17′	1.392 (4)	O1′—S1′	1.426 (3)
C16′—H16′	0.9300	O2′—S1′	1.425 (2)
C17′—C18′	1.351 (4)	O2—S1	1.427 (2)
C17′—H17′	0.9300	C35—Cl2	1.700 (10)
C17—C18	1.352 (5)	C35—Cl1	1.707 (10)
C17—H17	0.9300	C35—H35A	0.9700
C18′—C19′	1.416 (4)	C35—H35B	0.9700
C18′—H18′	0.9300	C35A—Cl2A	1.708 (9)
C18—C19	1.410 (4)	C35A—Cl1A	1.714 (9)
C18—H18	0.9300	C35A—H35C	0.9700
C19—C20	1.406 (4)	C35A—H35D	0.9700
C19′—C20′	1.409 (4)	C35B—Cl2B	1.707 (9)
C20′—H20′	0.9300	C35B—Cl1B	1.722 (8)
C20—H20	0.9300	C35B—H35E	0.9700
C21—C22	1.369 (4)	C35B—H35F	0.9700

C2—C1—C10	125.2 (2)	C26′—C21′—C2′	122.1 (3)
C2—C1—S1	124.4 (2)	C21′—C22′—C23′	121.8 (3)
C10—C1—S1	110.45 (19)	C21′—C22′—H22′	119.1
C2′—C1′—C10′	124.9 (2)	C23′—C22′—H22′	119.1
C2′—C1′—S1′	124.5 (2)	C21—C22—C23	122.4 (3)
C10′—C1′—S1′	110.5 (2)	C21—C22—H22	118.8
C1′—C2′—C3′	116.7 (2)	C23—C22—H22	118.8
C1′—C2′—C21′	122.0 (2)	C24′—C23′—C22′	119.9 (3)
C3′—C2′—C21′	121.3 (3)	C24′—C23′—H23′	120.1
C1—C2—C3	116.3 (3)	C22′—C23′—H23′	120.1
C1—C2—C21	121.6 (2)	C24—C23—C22	119.6 (3)
C3—C2—C21	122.1 (3)	C24—C23—H23	120.2
C4—C3—C8	119.0 (3)	C22—C23—H23	120.2
C4—C3—C2	121.0 (3)	C23—C24—C25	118.9 (3)
C8—C3—C2	119.9 (3)	C23—C24—O3	124.4 (3)

C4′—C3′—C8′	119.1 (3)	C25—C24—O3	116.7 (3)
C4′—C3′—C2′	121.1 (3)	O3′—C24′—C23′	123.8 (3)
C8′—C3′—C2′	119.8 (2)	O3′—C24′—C25′	116.7 (3)
C5′—C4′—C3′	121.0 (3)	C23′—C24′—C25′	119.5 (3)
C5′—C4′—H4′	119.5	C26′—C25′—C24′	120.4 (3)
C3′—C4′—H4′	119.5	C26′—C25′—H25′	119.8
C5—C4—C3	120.5 (4)	C24′—C25′—H25′	119.8
C5—C4—H4	119.8	C26—C25—C24	120.9 (3)
C3—C4—H4	119.8	C26—C25—H25	119.6
C4—C5—C6	120.3 (4)	C24—C25—H25	119.6
C4—C5—H5	119.9	C25—C26—C21	121.7 (3)
C6—C5—H5	119.9	C25—C26—H26	119.1
C4′—C5′—C6′	120.5 (3)	C21—C26—H26	119.1
C4′—C5′—H5′	119.7	C25′—C26′—C21′	120.8 (3)
C6′—C5′—H5′	119.7	C25′—C26′—H26′	119.6
C7′—C6′—C5′	120.3 (3)	C21′—C26′—H26′	119.6
C7′—C6′—H6′	119.9	C32′—C27′—C28′	117.5 (2)
C5′—C6′—H6′	119.9	C32′—C27′—C9′	121.4 (2)
C7—C6—C5	121.2 (3)	C28′—C27′—C9′	121.1 (2)
C7—C6—H6	119.4	C32—C27—C28	117.0 (3)
C5—C6—H6	119.4	C32—C27—C9	122.7 (3)
C6—C7—C8	121.1 (4)	C28—C27—C9	120.3 (3)
C6—C7—H7	119.4	C29—C28—C27	121.6 (3)
C8—C7—H7	119.4	C29—C28—H28	119.2
C6′—C7′—C8′	121.2 (3)	C27—C28—H28	119.2
C6′—C7′—H7′	119.4	C29′—C28′—C27′	121.8 (3)
C8′—C7′—H7′	119.4	C29′—C28′—H28′	119.1
C3—C8—C7	117.9 (3)	C27′—C28′—H28′	119.1
C3—C8—C9	121.5 (2)	C30′—C29′—C28′	119.8 (3)
C7—C8—C9	120.6 (3)	C30′—C29′—H29′	120.1
C3′—C8′—C9′	121.1 (2)	C28′—C29′—H29′	120.1
C3′—C8′—C7′	117.9 (3)	C28—C29—C30	120.2 (3)
C9′—C8′—C7′	121.1 (3)	C28—C29—H29	119.9
C10—C9—C8	118.3 (3)	C30—C29—H29	119.9
C10—C9—C27	121.5 (3)	O4—C30—C31	124.8 (3)
C8—C9—C27	120.2 (2)	O4—C30—C29	115.8 (3)
C10′—C9′—C8′	119.4 (2)	C31—C30—C29	119.5 (3)
C10′—C9′—C27′	121.3 (2)	C29′—C30′—O4′	124.9 (3)
C8′—C9′—C27′	119.3 (2)	C29′—C30′—C31′	119.6 (3)
C9—C10—C1	118.9 (2)	O4′—C30′—C31′	115.6 (3)
C9—C10—C11	128.4 (2)	C30—C31—C32	119.7 (3)
C1—C10—C11	112.7 (2)	C30—C31—H31	120.1
C9′—C10′—C1′	118.1 (2)	C32—C31—H31	120.1
C9′—C10′—C11′	129.5 (2)	C32′—C31′—C30′	120.3 (3)
C1′—C10′—C11′	112.4 (2)	C32′—C31′—H31′	119.8
C20′—C11′—C12′	117.3 (2)	C30′—C31′—H31′	119.8
C20′—C11′—C10′	130.6 (2)	C31—C32—C27	121.9 (3)
C12′—C11′—C10′	112.2 (2)	C31—C32—H32	119.0

C20—C11—C12	117.2 (2)	C27—C32—H32	119.0
C20—C11—C10	131.1 (2)	C31′—C32′—C27′	121.1 (3)
C12—C11—C10	111.6 (2)	C31′—C32′—H32′	119.5
C13—C12—C11	123.6 (2)	C27′—C32′—H32′	119.5
C13—C12—S1	124.3 (2)	O3—C33—H33A	109.5
C11—C12—S1	112.09 (19)	O3—C33—H33B	109.5
C13′—C12′—C11′	123.3 (3)	H33A—C33—H33B	109.5
C13′—C12′—S1′	125.0 (2)	O3—C33—H33C	109.5
C11′—C12′—S1′	111.7 (2)	H33A—C33—H33C	109.5
C12′—C13′—C14′	119.4 (2)	H33B—C33—H33C	109.5
C12′—C13′—H13′	120.3	O3′—C33′—H33D	109.5
C14′—C13′—H13′	120.3	O3′—C33′—H33E	109.5
C12—C13—C14	119.2 (2)	H33D—C33′—H33E	109.5
C12—C13—H13	120.4	O3′—C33′—H33F	109.5
C14—C13—H13	120.4	H33D—C33′—H33F	109.5
C13—C14—C15	122.5 (3)	H33E—C33′—H33F	109.5
C13—C14—C19	118.5 (2)	O4′—C34′—H34A	109.5
C15—C14—C19	119.0 (3)	O4′—C34′—H34B	109.5
C13′—C14′—C15′	122.3 (3)	H34A—C34′—H34B	109.5
C13′—C14′—C19′	118.7 (2)	O4′—C34′—H34C	109.5
C15′—C14′—C19′	119.0 (3)	H34A—C34′—H34C	109.5
C16′—C15′—C14′	120.5 (3)	H34B—C34′—H34C	109.5
C16′—C15′—H15′	119.7	O4—C34—H34D	109.5
C14′—C15′—H15′	119.7	O4—C34—H34E	109.5
C16—C15—C14	120.5 (3)	H34D—C34—H34E	109.5
C16—C15—H15	119.8	O4—C34—H34F	109.5
C14—C15—H15	119.8	H34D—C34—H34F	109.5
C15—C16—C17	120.8 (3)	H34E—C34—H34F	109.5
C15—C16—H16	119.6	C24′—O3′—C33′	117.4 (2)
C17—C16—H16	119.6	C24—O3—C33	118.2 (3)
C15′—C16′—C17′	120.6 (3)	C30′—O4′—C34′	117.3 (3)
C15′—C16′—H16′	119.7	C30—O4—C34	118.5 (3)
C17′—C16′—H16′	119.7	O2—S1—O1	117.46 (14)
C18′—C17′—C16′	120.4 (3)	O2—S1—C12	111.10 (13)
C18′—C17′—H17′	119.8	O1—S1—C12	109.52 (13)
C16′—C17′—H17′	119.8	O2—S1—C1	110.65 (13)
C18—C17—C16	120.3 (3)	O1—S1—C1	112.36 (13)
C18—C17—H17	119.9	C12—S1—C1	93.13 (12)
C16—C17—H17	119.9	O2′—S1′—O1′	117.94 (17)
C17′—C18′—C19′	121.2 (3)	O2′—S1′—C12′	109.59 (14)
C17′—C18′—H18′	119.4	O1′—S1′—C12′	111.38 (16)
C19′—C18′—H18′	119.4	O2′—S1′—C1′	111.66 (15)
C17—C18—C19	121.3 (3)	O1′—S1′—C1′	110.40 (14)
C17—C18—H18	119.4	C12′—S1′—C1′	93.13 (13)
C19—C18—H18	119.4	Cl2—C35—Cl1	103.8 (10)
C20—C19—C18	121.6 (3)	Cl2—C35—H35A	111.0
C20—C19—C14	120.2 (3)	Cl1—C35—H35A	111.0
C18—C19—C14	118.1 (3)	Cl2—C35—H35B	111.0

C20′—C19′—C14′	119.9 (2)	Cl1—C35—H35B	111.0
C20′—C19′—C18′	121.8 (2)	H35A—C35—H35B	109.0
C14′—C19′—C18′	118.3 (3)	Cl2A—C35A—Cl1A	130.9 (12)
C11′—C20′—C19′	121.4 (2)	Cl2A—C35A—H35C	104.5
C11′—C20′—H20′	119.3	Cl1A—C35A—H35C	104.5
C19′—C20′—H20′	119.3	Cl2A—C35A—H35D	104.5
C11—C20—C19	121.3 (2)	Cl1A—C35A—H35D	104.5
C11—C20—H20	119.4	H35C—C35A—H35D	105.7
C19—C20—H20	119.4	Cl2B—C35B—Cl1B	98.2 (7)
C22—C21—C26	116.4 (3)	Cl2B—C35B—H35E	112.1
C22—C21—C2	122.4 (3)	Cl1B—C35B—H35E	112.1
C26—C21—C2	121.1 (3)	Cl2B—C35B—H35F	112.1
C22′—C21′—C26′	117.5 (3)	Cl1B—C35B—H35F	112.1
C22′—C21′—C2′	120.3 (2)	H35E—C35B—H35F	109.8

C10′—C1′—C2′—C3′	−1.2 (4)	C13′—C14′—C19′—C20′	−0.2 (4)
S1′—C1′—C2′—C3′	177.4 (2)	C15′—C14′—C19′—C20′	−179.8 (3)
C10′—C1′—C2′—C21′	176.8 (2)	C13′—C14′—C19′—C18′	179.7 (2)
S1′—C1′—C2′—C21′	−4.6 (4)	C15′—C14′—C19′—C18′	0.1 (4)
C10—C1—C2—C3	−0.4 (4)	C17′—C18′—C19′—C20′	−179.7 (3)
S1—C1—C2—C3	−179.0 (2)	C17′—C18′—C19′—C14′	0.4 (4)
C10—C1—C2—C21	179.3 (2)	C12′—C11′—C20′—C19′	0.9 (4)
S1—C1—C2—C21	0.6 (4)	C10′—C11′—C20′—C19′	−178.2 (3)
C1—C2—C3—C4	−176.7 (2)	C14′—C19′—C20′—C11′	−0.4 (4)
C21—C2—C3—C4	3.6 (4)	C18′—C19′—C20′—C11′	179.7 (2)
C1—C2—C3—C8	1.4 (4)	C12—C11—C20—C19	−1.8 (4)
C21—C2—C3—C8	−178.3 (2)	C10—C11—C20—C19	177.0 (3)
C1′—C2′—C3′—C4′	−178.9 (3)	C18—C19—C20—C11	−177.4 (3)
C21′—C2′—C3′—C4′	3.0 (4)	C14—C19—C20—C11	1.8 (4)
C1′—C2′—C3′—C8′	0.1 (4)	C1—C2—C21—C22	70.3 (4)
C21′—C2′—C3′—C8′	−178.0 (2)	C3—C2—C21—C22	−110.1 (3)
C8′—C3′—C4′—C5′	−1.0 (4)	C1—C2—C21—C26	−107.8 (3)
C2′—C3′—C4′—C5′	178.0 (3)	C3—C2—C21—C26	71.8 (4)
C8—C3—C4—C5	−0.7 (4)	C1′—C2′—C21′—C22′	−71.8 (4)
C2—C3—C4—C5	177.4 (3)	C3′—C2′—C21′—C22′	106.2 (3)
C3—C4—C5—C6	2.6 (5)	C1′—C2′—C21′—C26′	107.7 (3)
C3′—C4′—C5′—C6′	0.5 (5)	C3′—C2′—C21′—C26′	−74.3 (4)
C4′—C5′—C6′—C7′	0.5 (5)	C26′—C21′—C22′—C23′	0.3 (5)
C4—C5—C6—C7	−2.5 (6)	C2′—C21′—C22′—C23′	179.9 (3)
C5—C6—C7—C8	0.4 (5)	C26—C21—C22—C23	0.5 (5)
C5′—C6′—C7′—C8′	−0.8 (5)	C2—C21—C22—C23	−177.7 (3)
C4—C3—C8—C7	−1.3 (4)	C21′—C22′—C23′—C24′	−0.6 (5)
C2—C3—C8—C7	−179.4 (2)	C21—C22—C23—C24	0.6 (5)
C4—C3—C8—C9	176.7 (2)	C22—C23—C24—C25	−1.0 (5)
C2—C3—C8—C9	−1.4 (4)	C22—C23—C24—O3	179.3 (3)
C6—C7—C8—C3	1.4 (4)	C22′—C23′—C24′—O3′	−179.9 (3)
C6—C7—C8—C9	−176.6 (3)	C22′—C23′—C24′—C25′	0.5 (5)
C4′—C3′—C8′—C9′	−179.6 (3)	O3′—C24′—C25′—C26′	−179.7 (3)

C2′—C3′—C8′—C9′	1.3 (4)	C23′—C24′—C25′—C26′	−0.1 (5)
C4′—C3′—C8′—C7′	0.6 (4)	C23—C24—C25—C26	0.4 (5)
C2′—C3′—C8′—C7′	−178.4 (3)	O3—C24—C25—C26	−179.9 (3)
C6′—C7′—C8′—C3′	0.3 (4)	C24—C25—C26—C21	0.7 (5)
C6′—C7′—C8′—C9′	−179.5 (3)	C22—C21—C26—C25	−1.1 (5)
C3—C8—C9—C10	0.4 (4)	C2—C21—C26—C25	177.1 (3)
C7—C8—C9—C10	178.3 (3)	C24′—C25′—C26′—C21′	−0.3 (5)
C3—C8—C9—C27	−176.7 (2)	C22′—C21′—C26′—C25′	0.2 (5)
C7—C8—C9—C27	1.2 (4)	C2′—C21′—C26′—C25′	−179.4 (3)
C3′—C8′—C9′—C10′	−1.8 (4)	C10′—C9′—C27′—C32′	88.6 (3)
C7′—C8′—C9′—C10′	178.0 (3)	C8′—C9′—C27′—C32′	−90.6 (3)
C3′—C8′—C9′—C27′	177.4 (2)	C10′—C9′—C27′—C28′	−91.5 (3)
C7′—C8′—C9′—C27′	−2.8 (4)	C8′—C9′—C27′—C28′	89.4 (3)
C8—C9—C10—C1	0.6 (4)	C10—C9—C27—C32	97.3 (3)
C27—C9—C10—C1	177.6 (2)	C8—C9—C27—C32	−85.7 (3)
C8—C9—C10—C11	179.4 (2)	C10—C9—C27—C28	−81.2 (3)
C27—C9—C10—C11	−3.5 (4)	C8—C9—C27—C28	95.8 (3)
C2—C1—C10—C9	−0.6 (4)	C32—C27—C28—C29	0.0 (4)
S1—C1—C10—C9	178.2 (2)	C9—C27—C28—C29	178.6 (3)
C2—C1—C10—C11	−179.6 (2)	C32′—C27′—C28′—C29′	0.1 (4)
S1—C1—C10—C11	−0.8 (3)	C9′—C27′—C28′—C29′	−179.9 (3)
C8′—C9′—C10′—C1′	0.7 (4)	C27′—C28′—C29′—C30′	0.9 (5)
C27′—C9′—C10′—C1′	−178.5 (2)	C27—C28—C29—C30	−0.4 (5)
C8′—C9′—C10′—C11′	−179.4 (3)	C28—C29—C30—O4	−179.7 (3)
C27′—C9′—C10′—C11′	1.4 (4)	C28—C29—C30—C31	0.7 (5)
C2′—C1′—C10′—C9′	0.9 (4)	C28′—C29′—C30′—O4′	178.4 (3)
S1′—C1′—C10′—C9′	−177.9 (2)	C28′—C29′—C30′—C31′	−1.3 (5)
C2′—C1′—C10′—C11′	−179.1 (3)	O4—C30—C31—C32	179.8 (3)
S1′—C1′—C10′—C11′	2.2 (3)	C29—C30—C31—C32	−0.6 (5)
C9′—C10′—C11′—C20′	−2.5 (5)	C29′—C30′—C31′—C32′	0.8 (4)
C1′—C10′—C11′—C20′	177.4 (3)	O4′—C30′—C31′—C32′	−179.0 (3)
C9′—C10′—C11′—C12′	178.4 (3)	C30—C31—C32—C27	0.2 (5)
C1′—C10′—C11′—C12′	−1.7 (3)	C28—C27—C32—C31	0.1 (4)
C9—C10—C11—C20	3.7 (5)	C9—C27—C32—C31	−178.4 (3)
C1—C10—C11—C20	−177.4 (3)	C30′—C31′—C32′—C27′	0.2 (4)
C9—C10—C11—C12	−177.5 (3)	C28′—C27′—C32′—C31′	−0.6 (4)
C1—C10—C11—C12	1.4 (3)	C9′—C27′—C32′—C31′	179.4 (2)
C20—C11—C12—C13	0.8 (4)	C23′—C24′—O3′—C33′	13.5 (5)
C10—C11—C12—C13	−178.2 (2)	C25′—C24′—O3′—C33′	−167.0 (3)
C20—C11—C12—S1	177.6 (2)	C23—C24—O3—C33	−12.4 (5)
C10—C11—C12—S1	−1.4 (3)	C25—C24—O3—C33	167.9 (3)
C20′—C11′—C12′—C13′	−0.7 (4)	C29′—C30′—O4′—C34′	2.1 (5)
C10′—C11′—C12′—C13′	178.5 (3)	C31′—C30′—O4′—C34′	−178.1 (3)
C20′—C11′—C12′—S1′	−178.8 (2)	C31—C30—O4—C34	5.1 (5)
C10′—C11′—C12′—S1′	0.4 (3)	C29—C30—O4—C34	−174.5 (3)
C11′—C12′—C13′—C14′	0.1 (4)	C13—C12—S1—O2	−68.9 (3)
S1′—C12′—C13′—C14′	178.0 (2)	C11—C12—S1—O2	114.3 (2)
C11—C12—C13—C14	0.2 (4)	C13—C12—S1—O1	62.5 (3)

S1—C12—C13—C14	−176.2 (2)	C11—C12—S1—O1	−114.3 (2)
C12—C13—C14—C15	178.0 (3)	C13—C12—S1—C1	177.5 (2)
C12—C13—C14—C19	−0.2 (4)	C11—C12—S1—C1	0.8 (2)
C12′—C13′—C14′—C15′	179.9 (3)	C2—C1—S1—O2	64.9 (3)
C12′—C13′—C14′—C19′	0.3 (4)	C10—C1—S1—O2	−113.9 (2)
C13′—C14′—C15′—C16′	179.8 (3)	C2—C1—S1—O1	−68.5 (3)
C19′—C14′—C15′—C16′	−0.6 (4)	C10—C1—S1—O1	112.7 (2)
C13—C14—C15—C16	−177.1 (3)	C2—C1—S1—C12	178.9 (2)
C19—C14—C15—C16	1.1 (5)	C10—C1—S1—C12	0.0 (2)
C14—C15—C16—C17	−0.9 (5)	C13′—C12′—S1′—O2′	−63.1 (3)
C14′—C15′—C16′—C17′	0.7 (5)	C11′—C12′—S1′—O2′	115.0 (2)
C15′—C16′—C17′—C18′	−0.2 (5)	C13′—C12′—S1′—O1′	69.3 (3)
C15—C16—C17—C18	−0.6 (5)	C11′—C12′—S1′—O1′	−112.7 (2)
C16′—C17′—C18′—C19′	−0.3 (5)	C13′—C12′—S1′—C1′	−177.4 (3)
C16—C17—C18—C19	2.0 (5)	C11′—C12′—S1′—C1′	0.7 (2)
C17—C18—C19—C20	177.4 (3)	C2′—C1′—S1′—O2′	67.1 (3)
C17—C18—C19—C14	−1.7 (5)	C10′—C1′—S1′—O2′	−114.2 (2)
C13—C14—C19—C20	−0.7 (4)	C2′—C1′—S1′—O1′	−66.2 (3)
C15—C14—C19—C20	−179.0 (3)	C10′—C1′—S1′—O1′	112.6 (2)
C13—C14—C19—C18	178.5 (3)	C2′—C1′—S1′—C12′	179.6 (3)
C15—C14—C19—C18	0.2 (4)	C10′—C1′—S1′—C12′	−1.6 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13···O2^{i}	0.93	2.46	3.330 (3)	156
C26′—H26′···O2^{i}	0.93	2.59	3.329 (4)	137
C6—H6···O4^{ii}	0.93	2.56	3.304 (4)	137
C13′—H13′···O1′^{iii}	0.93	2.59	3.500 (3)	165
C34′—H34*B*···O2′^{iv}	0.96	2.45	3.191 (4)	134
C34—H34*E*···O1^{v}	0.96	2.60	3.177 (4)	119

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