IUCrData

ISSN 2414-3146

(10-Ethyl-10*H*-phenothiazine-3,7-diyl)bis(*p*-tolylmethanone)

Karunakaran Hemanathan,[a] Mahalingam Ravivarma,[b] Chinnadurai Satheeshkumar,[b] Perumal Rajakumar[b] and K. Sakthi Murugesan[a]*

[a]Department of Physics, Presidency College (Autonomous), Chennai 600 005, India, and [b]Department of Organic Chemistry, University of Madras, Guindy Campus, Chennai 600 025, India. *Correspondence e-mail: ksakthimurugesan2492@gmail.com

Received 30 October 2016
Accepted 16 November 2016

Edited by H. Stoeckli-Evans, University of Neuchâtel, Switzerland

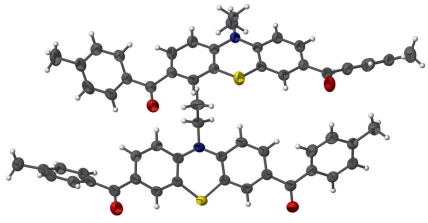
Keywords: crystal structure; phenothiazine derivative; C—H···O hydrogen bonding; C—H···π interactions.

CCDC reference: 1511272

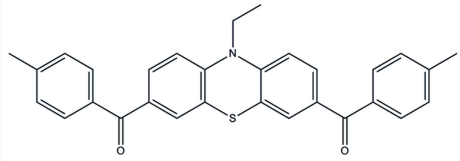
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{30}H_{25}NO_2S$, crystallizes with two independent molecules (*A* and *B*) having similar conformations in the asymmetric unit. Both phenothiazine units have a butterfly structure; the dihedral angles between the planes of the benzene rings are 17.95 (13) and 12.65 (14)° for molecules *A* and *B*, respectively. In the crystal, the *B* molecules are linked by pairs of C—H···O hydrogen bonds, forming inversion dimers with an $R_2^2(10)$ ring motif. The *A* molecules are linked by C—H···π interactions. Layers of *A* molecules and layers of *B* molecules are linked by a second C—H···π interaction, forming *A*–*B*–*B*–*A* slabs, which stack back-to-back and lie parallel to the *bc* plane.

3D view



Chemical scheme



Structure description

Phenothiazine is a well known heterocycle that occurs in many synthetic dyes, electroluminescent materials (Miller *et al.*, 1999) and drugs, especially various antipsychotic drugs, *e.g.* chlorpromazine, antihistaminic drugs and promethazine (Wermuth, 2003). Recently, new applications for phenothiazine derivatives in medicine have been developed, such as antitubercular (Wang *et al.*, 2008) and antitumor (Lam *et al.*, 2001). As part of our program devoted to new applications of phenothiazine derivatives in medicine, we report herein on the synthesis and crystal structure of the title compound.

The title compound, Fig. 1, crystallizes with two independent molecules (*A* and *B*) in the asymmetric unit. The molecular structures of *A* and *B* are similar (Fig. 2). The phenothiazine moieties have a butterfly structure, where the dihedral angles between the two benzene rings (C9–C14 and C17–C22 in *A*, and C9′–C14′ and C17′-C22′ in *B*) are 17.95 (13) and 12.65 (14)°, respectively. The thiazine rings in both molecules have a shallow boat-like conformation. The phenyl rings (C2–C7 and C24–C29) are inclined to

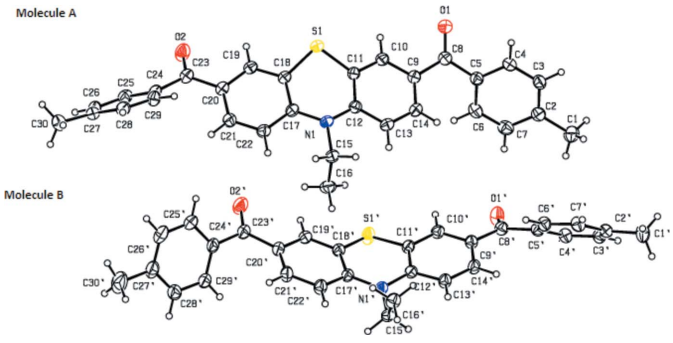


Figure 1
The molecular structure of the title compound, showing the atom labelling and 30% probability displacement ellipsoids.

the phenothiazine ring mean plane by 52.24 (10) and 61.61 (11)°, respectively, for molecule *A* and by 51.3 (1) and 59.07 (10)°, respectively, for the corresponding dihedral angles in molecule *B*. The two phenyl rings are inclined to one another by 71.65 (14)° in molecule *A* and by 76.67 (13)° in molecule *B*. The oxygen atoms, O1 and O2, in molecule *A* deviate from the mean plane of the phenothiazine ring by 0.109 (3) and −1.044 (2) Å, respectively. In molecule *B*, oxygen atoms, O1′ and O2′, deviate by −0.236 (2) and 0.783 (3) Å, respectively, from the phenothiazine ring mean plane.

In the crystal, the *B* molecules are linked by pairs of C—H···O hydrogen bonds, forming inversion dimers with an $R_2^2(10)$ ring motif (Fig. 3 and Table 1). The *A* molecules are linked by C—H···π interactions (Fig. 3 and Table 1). Layers of *A* molecules and layers of *B* molecules are linked by a second C—H···π interaction, forming *A*–*B*–*B*–*A* slabs, stacking back-to-back, and lying parallel to the *bc* plane (Fig. 3 and Table 1).

Synthesis and crystallization

To 10-ethyl-10*H*-phenothiazine (1 g, 4.4 mmol) in DCM (75 ml) was added $AlCl_3$ (1.76 g, 13.2 mmol) in a three-necked flask under a nitrogen atmosphere. *p*-Tolouyl chloride (1.2 ml, 9.25 mmol) was added dropwise to the reaction mixture, which was then refluxed gently. Thereafter, it was stirred at room temperature for another 8 h. The reaction mixture was taken up in DCM (200 ml), brine (100 ml) and dried with Na_2SO_4. The organic layer was concentrated under vacuum and the residue was purified by column chromatography on silica gel

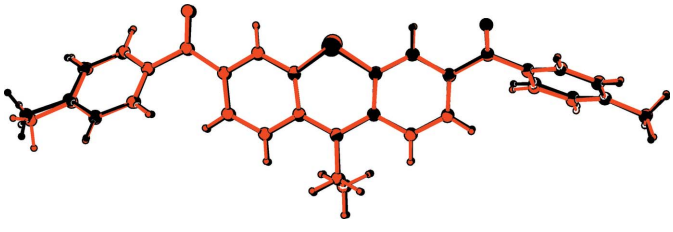


Figure 2
AutoMolFit (*PLATON*; Spek, 2009) of molecule *B* (red) inverted on molecule *A* (black).

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

*Cg*2 and *Cg*3 are the centroids of rings C2–C7 (molecule *A*) and C2′–C7′ (molecule *B*), respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4′—H4′···O1′^{i}	0.93	2.55	3.325 (3)	141
C30—H30*F*···*Cg*2^{ii}	0.96	2.98	3.716 (3)	134
C1—H1*A*···*Cg*3	0.96	2.91	3.667 (4)	137

Symmetry codes: (i) $-x, -y, -z+1$; (ii) $x, -y+\frac{3}{2}, z-\frac{1}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{30}H_{25}NO_2S$
M_r	463.57
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, *b*, *c* (Å)	19.6758 (8), 12.9382 (5), 21.1306 (9)
β (°)	117.513 (1)
V (Å^3)	4770.8 (3)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.16
Crystal size (mm)	0.30 × 0.25 × 0.20
Data collection	
Diffractometer	Bruker SMART APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.949, 0.966
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	57343, 8414, 5992
R_{int}	0.039
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.141, 1.03
No. of reflections	8414
No. of parameters	613
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.80, −0.59

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

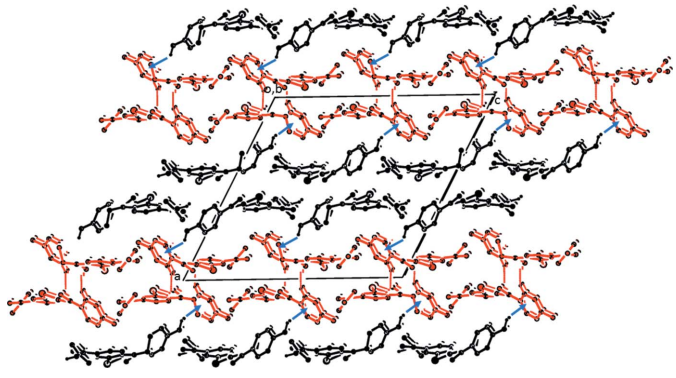


Figure 3
The crystal structure of the title compound, viewed along the *b* axis. Hydrogen bonds are illustrated by dashed lines and C—H···π interactions by blue arrows (see Table 1; colour code: molecule *A* black and molecule *B* red). For clarity, only the H atoms involved in these interactions have been included.

using chloroform–hexane (1:1 *v*/*v*) to give the title compound as orange–red block-like crystals.

Refinement

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

Acknowledgements

KH and KSM thank the Department of SAIF, IIT, Chennai, India, for the X-ray intensity data collection. MR thanks the DST for NMR facilities.

References

Bruker (2008). *APEX2*, *SADABS* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Lam, M., Oleinick, N. L. & Nieminen, A. L. (2001). *J. Biol. Chem.* **276**, 47379–47386.
Miller, M. T., Gantzel, P. K. & Karpishin, T. B. (1999). *J. Am. Chem. Soc.* **121**, 4292–4293.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Wang, J., Dong, M., Liang, J., Chang, Z., Feng, S., Wang, H. & Ding, N. (2008). *Chin. J. Lab. Diagn*, **12**, 381–382.
Wermuth, C. G. (2003). In *The Practice of Medicinal Chemistry*, 2nd ed. London: Academic Press.

full crystallographic data

IUCrData (2016). **1**, x161838 [https://doi.org/10.1107/S2414314616018381]

(10-Ethyl-10*H*-phenothiazine-3,7-diyl)bis(*p*-tolylmethanone)

Karunakaran Hemanathan, Mahalingam Ravivarma, Chinnadurai Satheeshkumar, Perumal Rajakumar and K. Sakthi Murugesan

(10-Ethyl-10*H*-phenothiazine-3,7-diyl)bis(*p*-tolylmethanone)

Crystal data

$C_{30}H_{25}NO_2S$
M_r = 463.57
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 19.6758 (8) Å
b = 12.9382 (5) Å
c = 21.1306 (9) Å
β = 117.513 (1)°
V = 4770.8 (3) Å^3
Z = 8
$F(000)$ = 1952
D_x = 1.291 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5992 reflections
θ = 1.2–25.0°
μ = 0.16 mm^{-1}
T = 293 K
Block, orange–red
0.30 × 0.25 × 0.20 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.949, T_{max} = 0.966
57343 measured reflections
8414 independent reflections
5992 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 25.0°, θ_{min} = 1.2°
h = −23→23
k = −15→15
l = −25→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.141
S = 1.03
8414 reflections
613 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
$w = 1/[\sigma^2(F_o^2) + (0.0639P)^2 + 2.3313P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.80 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}
Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0023 (4)

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. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1′	0.21978 (17)	−0.0743 (2)	0.78932 (16)	0.0668 (8)
H1′1	0.2682	−0.0466	0.8235	0.100*
H1′2	0.2266	−0.1443	0.7783	0.100*
H1′3	0.1844	−0.0729	0.8089	0.100*
C1	0.27952 (18)	−0.0687 (2)	0.59268 (17)	0.0669 (8)
H1A	0.2293	−0.0445	0.5824	0.100*
H1B	0.3132	−0.0619	0.6429	0.100*
H1C	0.2767	−0.1400	0.5791	0.100*
C2	0.30984 (14)	−0.00555 (18)	0.55147 (14)	0.0471 (6)
C2′	0.18861 (13)	−0.01010 (18)	0.72228 (13)	0.0441 (6)
C3′	0.11942 (14)	−0.03427 (18)	0.66442 (14)	0.0449 (6)
H3′	0.0928	−0.0927	0.6662	0.054*
C3	0.38131 (15)	−0.02495 (19)	0.55703 (14)	0.0494 (6)
H3	0.4094	−0.0808	0.5843	0.059*
C4′	0.08915 (14)	0.02664 (17)	0.60415 (13)	0.0444 (6)
H4′	0.0429	0.0083	0.5656	0.053*
C4	0.41231 (15)	0.03576 (18)	0.52354 (14)	0.0487 (6)
H4	0.4605	0.0203	0.5281	0.058*
C5	0.37177 (14)	0.12036 (18)	0.48281 (13)	0.0458 (6)
C5′	0.12708 (13)	0.11525 (17)	0.60039 (12)	0.0400 (5)
C6′	0.19735 (13)	0.13937 (18)	0.65853 (13)	0.0459 (6)
H6′	0.2239	0.1981	0.6571	0.055*
C6	0.29903 (14)	0.1388 (2)	0.47541 (14)	0.0523 (6)
H6	0.2706	0.1940	0.4477	0.063*
C7	0.26833 (15)	0.0765 (2)	0.50845 (15)	0.0540 (7)
H7	0.2190	0.0895	0.5019	0.065*
C7′	0.22756 (14)	0.07683 (19)	0.71786 (14)	0.0499 (6)
H7′	0.2750	0.0931	0.7557	0.060*
C8	0.40814 (15)	0.1840 (2)	0.44764 (14)	0.0524 (6)
C8′	0.09327 (14)	0.17748 (18)	0.53355 (13)	0.0448 (6)
C9	0.39953 (14)	0.29850 (18)	0.44435 (13)	0.0455 (6)
C9′	0.10108 (13)	0.29161 (17)	0.53681 (12)	0.0414 (5)
C10′	0.08842 (14)	0.34462 (18)	0.47499 (13)	0.0439 (6)
H10′	0.0818	0.3071	0.4350	0.053*
C10	0.41756 (14)	0.35455 (18)	0.39779 (12)	0.0448 (6)

H10	0.4285	0.3189	0.3654	0.054*
C11	0.41968 (13)	0.46085 (18)	0.39826 (12)	0.0407 (5)
C11′	0.08532 (13)	0.45108 (17)	0.47120 (12)	0.0411 (5)
C12′	0.09787 (13)	0.51072 (17)	0.53132 (12)	0.0393 (5)
C12	0.40114 (13)	0.51805 (18)	0.44485 (12)	0.0397 (5)
C13′	0.11327 (14)	0.45661 (18)	0.59384 (13)	0.0460 (6)
H13′	0.1237	0.4934	0.6351	0.055*
C13	0.38083 (15)	0.46127 (19)	0.48976 (13)	0.0495 (6)
H13	0.3664	0.4964	0.5201	0.059*
C14	0.38146 (15)	0.35449 (19)	0.49045 (13)	0.0496 (6)
H14	0.3695	0.3195	0.5225	0.059*
C14′	0.11335 (14)	0.35002 (18)	0.59575 (13)	0.0457 (6)
H14′	0.1219	0.3167	0.6378	0.055*
C15	0.38786 (14)	0.67828 (19)	0.50153 (13)	0.0459 (6)
H15A	0.4125	0.7455	0.5122	0.055*
H15B	0.4105	0.6377	0.5450	0.055*
C15′	0.10342 (14)	0.67352 (18)	0.59412 (12)	0.0416 (5)
H15C	0.0797	0.6333	0.6174	0.050*
H15D	0.0774	0.7397	0.5809	0.050*
C16′	0.18679 (15)	0.6915 (2)	0.64643 (13)	0.0530 (6)
H16A	0.1902	0.7266	0.6878	0.079*
H16B	0.2103	0.7331	0.6243	0.079*
H16C	0.2128	0.6263	0.6604	0.079*
C16	0.30322 (15)	0.6925 (2)	0.47868 (15)	0.0594 (7)
H16D	0.2969	0.7261	0.5161	0.089*
H16E	0.2786	0.6262	0.4691	0.089*
H16F	0.2806	0.7341	0.4363	0.089*
C17′	0.09416 (13)	0.67828 (17)	0.47387 (12)	0.0397 (5)
C17	0.40185 (13)	0.68766 (18)	0.39154 (12)	0.0395 (5)
C18	0.41822 (13)	0.64591 (17)	0.33849 (12)	0.0398 (5)
C18′	0.08166 (14)	0.63426 (17)	0.40819 (12)	0.0425 (6)
C19′	0.08529 (14)	0.69365 (19)	0.35596 (13)	0.0473 (6)
H19′	0.0783	0.6621	0.3138	0.057*
C19	0.41100 (13)	0.70532 (18)	0.28176 (12)	0.0429 (6)
H19	0.4192	0.6747	0.2460	0.051*
C20′	0.09912 (15)	0.79945 (18)	0.36410 (13)	0.0483 (6)
C20	0.39191 (13)	0.80970 (18)	0.27601 (13)	0.0438 (6)
C21	0.37872 (15)	0.85238 (19)	0.32956 (14)	0.0496 (6)
H21	0.3673	0.9224	0.3281	0.060*
C21′	0.10987 (15)	0.84357 (19)	0.42761 (14)	0.0520 (6)
H21′	0.1189	0.9142	0.4345	0.062*
C22′	0.10749 (15)	0.78442 (18)	0.48115 (13)	0.0495 (6)
H22′	0.1150	0.8165	0.5233	0.059*
C22	0.38233 (15)	0.79241 (18)	0.38507 (13)	0.0487 (6)
H22	0.3714	0.8227	0.4193	0.058*
C23	0.38333 (14)	0.8663 (2)	0.21178 (13)	0.0482 (6)
C23′	0.10651 (17)	0.8552 (2)	0.30615 (15)	0.0579 (7)
C24	0.38274 (14)	0.98162 (19)	0.20998 (13)	0.0458 (6)

C24′	0.11282 (16)	0.97004 (19)	0.30765 (13)	0.0500 (6)
C25′	0.16577 (17)	1.0166 (2)	0.29121 (14)	0.0581 (7)
H25′	0.1993	0.9760	0.2821	0.070*
C25	0.33361 (15)	1.0323 (2)	0.14739 (14)	0.0512 (6)
H25	0.2982	0.9946	0.1088	0.061*
C26	0.33712 (15)	1.1381 (2)	0.14219 (14)	0.0537 (7)
H26	0.3027	1.1710	0.1005	0.064*
C26′	0.16950 (19)	1.1227 (2)	0.28817 (15)	0.0662 (8)
H26′	0.2063	1.1528	0.2780	0.079*
C27	0.39059 (15)	1.19654 (19)	0.19755 (15)	0.0508 (6)
C27′	0.1195 (2)	1.1851 (2)	0.29996 (15)	0.0656 (8)
C28	0.43847 (15)	1.14547 (19)	0.26014 (14)	0.0508 (6)
H28	0.4744	1.1832	0.2985	0.061*
C28′	0.06678 (18)	1.1383 (2)	0.31601 (15)	0.0617 (7)
H28′	0.0324	1.1790	0.3239	0.074*
C29′	0.06352 (16)	1.03236 (19)	0.32074 (14)	0.0534 (7)
H29′	0.0280	1.0026	0.3328	0.064*
C29	0.43398 (15)	1.04008 (19)	0.26688 (13)	0.0492 (6)
H29	0.4656	1.0080	0.3100	0.059*
C30′	0.1229 (3)	1.3012 (2)	0.2955 (2)	0.1176 (16)
H30A	0.1635	1.3199	0.2845	0.176*
H30B	0.1324	1.3311	0.3404	0.176*
H30C	0.0751	1.3264	0.2587	0.176*
C30	0.39930 (18)	1.3108 (2)	0.19008 (18)	0.0691 (8)
H30D	0.4393	1.3374	0.2339	0.104*
H30E	0.3520	1.3451	0.1795	0.104*
H30F	0.4122	1.3228	0.1521	0.104*
N1	0.40368 (11)	0.62686 (15)	0.44721 (10)	0.0417 (5)
N1′	0.09290 (11)	0.61911 (14)	0.52887 (10)	0.0409 (5)
O1′	0.05830 (12)	0.13384 (13)	0.47603 (9)	0.0621 (5)
O1	0.44698 (13)	0.14253 (15)	0.42364 (12)	0.0751 (6)
O2′	0.10905 (17)	0.80727 (16)	0.25741 (13)	0.0923 (8)
O2	0.37729 (13)	0.81890 (14)	0.15934 (10)	0.0689 (6)
S1	0.45355 (4)	0.51999 (5)	0.34352 (4)	0.05027 (19)
S1′	0.05463 (5)	0.50526 (5)	0.38606 (4)	0.0605 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1′	0.0627 (18)	0.0652 (18)	0.0595 (18)	0.0032 (14)	0.0172 (15)	0.0202 (15)
C1	0.078 (2)	0.0512 (16)	0.086 (2)	−0.0083 (15)	0.0501 (18)	0.0002 (15)
C2	0.0550 (15)	0.0374 (13)	0.0516 (15)	−0.0070 (11)	0.0269 (13)	−0.0092 (11)
C2′	0.0435 (13)	0.0421 (13)	0.0461 (14)	0.0054 (11)	0.0202 (12)	0.0038 (11)
C3′	0.0458 (14)	0.0354 (12)	0.0551 (16)	−0.0027 (10)	0.0245 (12)	0.0031 (11)
C3	0.0598 (16)	0.0388 (13)	0.0492 (15)	0.0062 (12)	0.0248 (13)	0.0026 (11)
C4′	0.0427 (13)	0.0396 (13)	0.0451 (14)	−0.0033 (10)	0.0154 (11)	−0.0021 (11)
C4	0.0523 (15)	0.0434 (14)	0.0548 (16)	0.0086 (11)	0.0285 (13)	0.0031 (12)
C5	0.0541 (15)	0.0412 (13)	0.0444 (14)	0.0035 (11)	0.0246 (12)	0.0007 (11)

C5′	0.0416 (13)	0.0339 (12)	0.0443 (14)	0.0007 (10)	0.0198 (11)	−0.0011 (10)
C6′	0.0409 (13)	0.0405 (13)	0.0540 (16)	−0.0050 (10)	0.0200 (12)	0.0015 (12)
C6	0.0485 (15)	0.0469 (14)	0.0538 (16)	0.0074 (12)	0.0170 (13)	0.0044 (12)
C7	0.0424 (14)	0.0518 (15)	0.0659 (18)	−0.0019 (12)	0.0235 (13)	−0.0048 (13)
C7′	0.0376 (13)	0.0517 (15)	0.0510 (16)	−0.0011 (11)	0.0125 (12)	0.0020 (12)
C8	0.0639 (17)	0.0504 (15)	0.0497 (16)	0.0113 (13)	0.0320 (14)	0.0066 (12)
C8′	0.0458 (14)	0.0427 (13)	0.0457 (15)	−0.0030 (11)	0.0209 (12)	−0.0011 (11)
C9	0.0497 (14)	0.0463 (14)	0.0446 (14)	0.0070 (11)	0.0253 (12)	0.0061 (11)
C9′	0.0445 (13)	0.0379 (13)	0.0411 (13)	−0.0005 (10)	0.0191 (11)	0.0011 (10)
C10′	0.0529 (14)	0.0431 (13)	0.0385 (13)	−0.0030 (11)	0.0235 (11)	−0.0042 (11)
C10	0.0519 (14)	0.0483 (14)	0.0376 (13)	0.0085 (11)	0.0234 (11)	0.0025 (11)
C11	0.0423 (13)	0.0449 (13)	0.0349 (13)	0.0060 (10)	0.0179 (11)	0.0049 (10)
C11′	0.0481 (14)	0.0406 (13)	0.0377 (13)	−0.0029 (10)	0.0225 (11)	0.0001 (10)
C12′	0.0436 (13)	0.0377 (12)	0.0390 (13)	−0.0018 (10)	0.0210 (11)	−0.0008 (10)
C12	0.0410 (13)	0.0448 (13)	0.0324 (12)	0.0030 (10)	0.0162 (10)	0.0002 (10)
C13′	0.0609 (16)	0.0415 (13)	0.0354 (13)	−0.0020 (11)	0.0221 (12)	−0.0013 (10)
C13	0.0622 (16)	0.0520 (15)	0.0456 (15)	0.0048 (12)	0.0345 (13)	0.0003 (12)
C14	0.0620 (16)	0.0494 (15)	0.0474 (15)	0.0041 (12)	0.0339 (13)	0.0062 (12)
C14′	0.0560 (15)	0.0445 (14)	0.0360 (13)	0.0004 (11)	0.0207 (12)	0.0047 (11)
C15	0.0584 (15)	0.0487 (14)	0.0355 (13)	0.0021 (12)	0.0258 (12)	−0.0036 (11)
C15′	0.0538 (14)	0.0385 (12)	0.0380 (13)	−0.0012 (11)	0.0259 (11)	−0.0037 (10)
C16′	0.0606 (16)	0.0537 (15)	0.0434 (15)	−0.0075 (13)	0.0230 (13)	−0.0055 (12)
C16	0.0640 (17)	0.0696 (18)	0.0552 (17)	0.0114 (14)	0.0367 (14)	−0.0009 (14)
C17′	0.0456 (13)	0.0399 (13)	0.0355 (13)	0.0007 (10)	0.0205 (11)	0.0026 (10)
C17	0.0396 (12)	0.0455 (13)	0.0333 (12)	−0.0037 (10)	0.0167 (10)	−0.0020 (10)
C18	0.0412 (13)	0.0437 (13)	0.0364 (13)	−0.0032 (10)	0.0195 (11)	−0.0016 (10)
C18′	0.0525 (14)	0.0392 (13)	0.0398 (13)	0.0025 (11)	0.0247 (12)	0.0012 (10)
C19′	0.0600 (16)	0.0475 (14)	0.0420 (14)	0.0072 (12)	0.0299 (12)	0.0033 (11)
C19	0.0459 (13)	0.0476 (14)	0.0392 (13)	−0.0038 (11)	0.0232 (11)	−0.0045 (11)
C20′	0.0616 (16)	0.0439 (14)	0.0475 (15)	0.0042 (12)	0.0321 (13)	0.0085 (12)
C20	0.0468 (14)	0.0467 (14)	0.0409 (14)	−0.0042 (11)	0.0229 (11)	0.0002 (11)
C21	0.0617 (16)	0.0410 (13)	0.0529 (16)	0.0004 (12)	0.0322 (13)	0.0004 (12)
C21′	0.0699 (17)	0.0403 (13)	0.0469 (15)	−0.0032 (12)	0.0280 (13)	0.0034 (12)
C22′	0.0670 (17)	0.0431 (14)	0.0395 (14)	−0.0042 (12)	0.0254 (13)	−0.0023 (11)
C22	0.0652 (17)	0.0435 (14)	0.0465 (15)	0.0009 (12)	0.0337 (13)	−0.0037 (11)
C23	0.0518 (15)	0.0529 (15)	0.0426 (15)	−0.0041 (12)	0.0240 (12)	0.0011 (12)
C23′	0.083 (2)	0.0518 (16)	0.0539 (17)	0.0097 (14)	0.0444 (16)	0.0102 (13)
C24	0.0516 (14)	0.0518 (14)	0.0412 (14)	−0.0001 (12)	0.0277 (12)	0.0052 (11)
C24′	0.0702 (17)	0.0468 (14)	0.0389 (14)	0.0049 (12)	0.0302 (13)	0.0082 (11)
C25′	0.0715 (18)	0.0642 (18)	0.0509 (16)	0.0060 (14)	0.0388 (15)	0.0097 (13)
C25	0.0492 (15)	0.0634 (17)	0.0417 (14)	−0.0003 (12)	0.0216 (12)	0.0038 (12)
C26	0.0560 (16)	0.0609 (17)	0.0502 (16)	0.0134 (13)	0.0295 (14)	0.0183 (13)
C26′	0.086 (2)	0.0677 (19)	0.0566 (18)	−0.0169 (16)	0.0428 (17)	0.0033 (15)
C27	0.0564 (16)	0.0488 (15)	0.0601 (17)	0.0075 (12)	0.0379 (14)	0.0069 (13)
C27′	0.108 (2)	0.0478 (16)	0.0523 (17)	−0.0060 (16)	0.0468 (18)	0.0013 (13)
C28	0.0565 (16)	0.0512 (15)	0.0492 (15)	−0.0026 (12)	0.0282 (13)	−0.0003 (12)
C28′	0.087 (2)	0.0513 (16)	0.0550 (17)	0.0092 (15)	0.0401 (16)	0.0055 (13)
C29′	0.0697 (18)	0.0497 (15)	0.0509 (16)	0.0023 (13)	0.0364 (14)	0.0071 (12)

C29	0.0551 (15)	0.0517 (15)	0.0387 (14)	−0.0014 (12)	0.0198 (12)	0.0047 (12)
C30′	0.217 (5)	0.0494 (19)	0.135 (4)	−0.016 (2)	0.122 (4)	0.001 (2)
C30	0.079 (2)	0.0518 (16)	0.086 (2)	0.0113 (15)	0.0465 (18)	0.0132 (16)
N1	0.0509 (12)	0.0458 (11)	0.0340 (10)	0.0022 (9)	0.0245 (9)	−0.0029 (9)
N1′	0.0550 (12)	0.0367 (10)	0.0346 (10)	−0.0029 (9)	0.0237 (9)	−0.0027 (8)
O1′	0.0857 (14)	0.0470 (10)	0.0426 (11)	−0.0146 (9)	0.0203 (10)	−0.0037 (8)
O1	0.1114 (17)	0.0571 (12)	0.0918 (16)	0.0258 (11)	0.0768 (14)	0.0178 (11)
O2′	0.176 (3)	0.0556 (12)	0.0946 (17)	0.0102 (14)	0.1040 (19)	0.0063 (12)
O2	0.1067 (16)	0.0586 (12)	0.0480 (11)	−0.0054 (11)	0.0413 (11)	−0.0031 (9)
S1	0.0664 (4)	0.0486 (4)	0.0524 (4)	0.0089 (3)	0.0415 (3)	0.0042 (3)
S1′	0.1021 (6)	0.0439 (4)	0.0387 (4)	−0.0068 (4)	0.0353 (4)	−0.0031 (3)

Geometric parameters (Å, º)

C1′—C2′	1.507 (3)	C15′—H15D	0.9700
C1′—H1′1	0.9600	C16′—H16A	0.9600
C1′—H1′2	0.9600	C16′—H16B	0.9600
C1′—H1′3	0.9600	C16′—H16C	0.9600
C1—C2	1.504 (4)	C16—H16D	0.9600
C1—H1A	0.9600	C16—H16E	0.9600
C1—H1B	0.9600	C16—H16F	0.9600
C1—H1C	0.9600	C17′—C22′	1.393 (3)
C2—C3	1.379 (4)	C17′—N1′	1.401 (3)
C2—C7	1.391 (4)	C17′—C18′	1.413 (3)
C2′—C3′	1.381 (3)	C17—C22	1.398 (3)
C2′—C7′	1.388 (3)	C17—N1	1.402 (3)
C3′—C4′	1.377 (3)	C17—C18	1.409 (3)
C3′—H3′	0.9300	C18—C19	1.375 (3)
C3—C4	1.374 (3)	C18—S1	1.755 (2)
C3—H3	0.9300	C18′—C19′	1.373 (3)
C4′—C5′	1.390 (3)	C18′—S1′	1.749 (2)
C4′—H4′	0.9300	C19′—C20′	1.391 (3)
C4—C5	1.393 (3)	C19′—H19′	0.9300
C4—H4	0.9300	C19—C20	1.392 (3)
C5—C6	1.387 (3)	C19—H19	0.9300
C5—C8	1.495 (3)	C20′—C21′	1.382 (3)
C5′—C6′	1.396 (3)	C20′—C23′	1.485 (3)
C5′—C8′	1.489 (3)	C20—C21	1.387 (3)
C6′—C7′	1.375 (3)	C20—C23	1.482 (3)
C6′—H6′	0.9300	C21—C22	1.380 (3)
C6—C7	1.375 (4)	C21—H21	0.9300
C6—H6	0.9300	C21′—C22′	1.384 (3)
C7—H7	0.9300	C21′—H21′	0.9300
C7′—H7′	0.9300	C22′—H22′	0.9300
C8—O1	1.220 (3)	C22—H22	0.9300
C8—C9	1.489 (3)	C23—O2	1.224 (3)
C8′—O1′	1.223 (3)	C23—C24	1.492 (3)
C8′—C9′	1.483 (3)	C23′—O2′	1.223 (3)

C9—C14	1.386 (3)	C23′—C24′	1.490 (4)
C9—C10	1.394 (3)	C24—C29	1.383 (3)
C9′—C14′	1.379 (3)	C24—C25	1.390 (3)
C9′—C10′	1.392 (3)	C24′—C25′	1.380 (4)
C10′—C11′	1.379 (3)	C24′—C29′	1.384 (4)
C10′—H10′	0.9300	C25′—C26′	1.378 (4)
C10—C11	1.376 (3)	C25′—H25′	0.9300
C10—H10	0.9300	C25—C26	1.377 (4)
C11—C12	1.408 (3)	C25—H25	0.9300
C11—S1	1.755 (2)	C26—C27	1.382 (4)
C11′—C12′	1.407 (3)	C26—H26	0.9300
C11′—S1′	1.758 (2)	C26′—C27′	1.382 (4)
C12′—C13′	1.399 (3)	C26′—H26′	0.9300
C12′—N1′	1.405 (3)	C27—C28	1.386 (4)
C12—C13	1.397 (3)	C27—C30	1.505 (3)
C12—N1	1.409 (3)	C27′—C28′	1.372 (4)
C13′—C14′	1.380 (3)	C27′—C30′	1.508 (4)
C13′—H13′	0.9300	C28—C29	1.378 (3)
C13—C14	1.382 (3)	C28—H28	0.9300
C13—H13	0.9300	C28′—C29′	1.378 (4)
C14—H14	0.9300	C28′—H28′	0.9300
C14′—H14′	0.9300	C29′—H29′	0.9300
C15—N1	1.479 (3)	C29—H29	0.9300
C15—C16	1.516 (3)	C30′—H30A	0.9600
C15—H15A	0.9700	C30′—H30B	0.9600
C15—H15B	0.9700	C30′—H30C	0.9600
C15′—N1′	1.475 (3)	C30—H30D	0.9600
C15′—C16′	1.514 (3)	C30—H30E	0.9600
C15′—H15C	0.9700	C30—H30F	0.9600
C2′—C1′—H1′1	109.5	H16A—C16′—H16C	109.5
C2′—C1′—H1′2	109.5	H16B—C16′—H16C	109.5
H1′1—C1′—H1′2	109.5	C15—C16—H16D	109.5
C2′—C1′—H1′3	109.5	C15—C16—H16E	109.5
H1′1—C1′—H1′3	109.5	H16D—C16—H16E	109.5
H1′2—C1′—H1′3	109.5	C15—C16—H16F	109.5
C2—C1—H1A	109.5	H16D—C16—H16F	109.5
C2—C1—H1B	109.5	H16E—C16—H16F	109.5
H1A—C1—H1B	109.5	C22′—C17′—N1′	121.4 (2)
C2—C1—H1C	109.5	C22′—C17′—C18′	116.4 (2)
H1A—C1—H1C	109.5	N1′—C17′—C18′	122.2 (2)
H1B—C1—H1C	109.5	C22—C17—N1	121.7 (2)
C3—C2—C7	117.5 (2)	C22—C17—C18	116.6 (2)
C3—C2—C1	120.9 (2)	N1—C17—C18	121.7 (2)
C7—C2—C1	121.5 (2)	C19—C18—C17	120.6 (2)
C3′—C2′—C7′	118.2 (2)	C19—C18—S1	116.76 (18)
C3′—C2′—C1′	120.9 (2)	C17—C18—S1	122.50 (18)
C7′—C2′—C1′	120.8 (2)	C19′—C18′—C17′	120.9 (2)

C4′—C3′—C2′	121.2 (2)	C19′—C18′—S1′	116.20 (18)
C4′—C3′—H3′	119.4	C17′—C18′—S1′	122.74 (18)
C2′—C3′—H3′	119.4	C18′—C19′—C20′	122.1 (2)
C4—C3—C2	122.0 (2)	C18′—C19′—H19′	119.0
C4—C3—H3	119.0	C20′—C19′—H19′	119.0
C2—C3—H3	119.0	C18—C19—C20	122.2 (2)
C3′—C4′—C5′	120.7 (2)	C18—C19—H19	118.9
C3′—C4′—H4′	119.7	C20—C19—H19	118.9
C5′—C4′—H4′	119.7	C21′—C20′—C19′	117.4 (2)
C3—C4—C5	120.2 (2)	C21′—C20′—C23′	124.8 (2)
C3—C4—H4	119.9	C19′—C20′—C23′	117.7 (2)
C5—C4—H4	119.9	C21—C20—C19	117.4 (2)
C6—C5—C4	118.1 (2)	C21—C20—C23	124.4 (2)
C6—C5—C8	123.8 (2)	C19—C20—C23	118.1 (2)
C4—C5—C8	118.1 (2)	C22—C21—C20	120.9 (2)
C4′—C5′—C6′	118.3 (2)	C22—C21—H21	119.5
C4′—C5′—C8′	118.9 (2)	C20—C21—H21	119.5
C6′—C5′—C8′	122.7 (2)	C20′—C21′—C22′	121.2 (2)
C7′—C6′—C5′	120.4 (2)	C20′—C21′—H21′	119.4
C7′—C6′—H6′	119.8	C22′—C21′—H21′	119.4
C5′—C6′—H6′	119.8	C21′—C22′—C17′	122.0 (2)
C7—C6—C5	121.0 (2)	C21′—C22′—H22′	119.0
C7—C6—H6	119.5	C17′—C22′—H22′	119.0
C5—C6—H6	119.5	C21—C22—C17	122.1 (2)
C6—C7—C2	121.1 (2)	C21—C22—H22	118.9
C6—C7—H7	119.5	C17—C22—H22	118.9
C2—C7—H7	119.5	O2—C23—C20	120.2 (2)
C6′—C7′—C2′	121.2 (2)	O2—C23—C24	118.8 (2)
C6′—C7′—H7′	119.4	C20—C23—C24	120.9 (2)
C2′—C7′—H7′	119.4	O2′—C23′—C20′	120.3 (2)
O1—C8—C9	119.9 (2)	O2′—C23′—C24′	119.2 (2)
O1—C8—C5	120.0 (2)	C20′—C23′—C24′	120.4 (2)
C9—C8—C5	120.1 (2)	C29—C24—C25	118.4 (2)
O1′—C8′—C9′	120.3 (2)	C29—C24—C23	122.0 (2)
O1′—C8′—C5′	119.5 (2)	C25—C24—C23	119.3 (2)
C9′—C8′—C5′	120.2 (2)	C25′—C24′—C29′	118.5 (2)
C14—C9—C10	117.1 (2)	C25′—C24′—C23′	119.7 (2)
C14—C9—C8	123.2 (2)	C29′—C24′—C23′	121.7 (2)
C10—C9—C8	119.3 (2)	C26′—C25′—C24′	120.6 (3)
C14′—C9′—C10′	117.3 (2)	C26′—C25′—H25′	119.7
C14′—C9′—C8′	124.0 (2)	C24′—C25′—H25′	119.7
C10′—C9′—C8′	118.5 (2)	C26—C25—C24	120.4 (3)
C11′—C10′—C9′	122.0 (2)	C26—C25—H25	119.8
C11′—C10′—H10′	119.0	C24—C25—H25	119.8
C9′—C10′—H10′	119.0	C25—C26—C27	121.5 (2)
C11—C10—C9	122.1 (2)	C25—C26—H26	119.2
C11—C10—H10	118.9	C27—C26—H26	119.2
C9—C10—H10	118.9	C25′—C26′—C27′	121.1 (3)

C10—C11—C12	120.9 (2)	C25′—C26′—H26′	119.5
C10—C11—S1	116.79 (18)	C27′—C26′—H26′	119.5
C12—C11—S1	122.12 (18)	C26—C27—C28	117.6 (2)
C10′—C11′—C12′	120.7 (2)	C26—C27—C30	121.9 (3)
C10′—C11′—S1′	116.28 (18)	C28—C27—C30	120.5 (3)
C12′—C11′—S1′	122.64 (18)	C28′—C27′—C26′	118.0 (3)
C13′—C12′—N1′	121.0 (2)	C28′—C27′—C30′	121.1 (3)
C13′—C12′—C11′	116.7 (2)	C26′—C27′—C30′	120.9 (3)
N1′—C12′—C11′	122.3 (2)	C29—C28—C27	121.5 (2)
C13—C12—C11	116.5 (2)	C29—C28—H28	119.3
C13—C12—N1	121.2 (2)	C27—C28—H28	119.3
C11—C12—N1	122.2 (2)	C27′—C28′—C29′	121.5 (3)
C14′—C13′—C12′	121.6 (2)	C27′—C28′—H28′	119.2
C14′—C13′—H13′	119.2	C29′—C28′—H28′	119.2
C12′—C13′—H13′	119.2	C28′—C29′—C24′	120.3 (3)
C14—C13—C12	121.9 (2)	C28′—C29′—H29′	119.8
C14—C13—H13	119.0	C24′—C29′—H29′	119.8
C12—C13—H13	119.0	C28—C29—C24	120.5 (2)
C13—C14—C9	121.3 (2)	C28—C29—H29	119.8
C13—C14—H14	119.4	C24—C29—H29	119.8
C9—C14—H14	119.4	C27′—C30′—H30A	109.5
C9′—C14′—C13′	121.6 (2)	C27′—C30′—H30B	109.5
C9′—C14′—H14′	119.2	H30A—C30′—H30B	109.5
C13′—C14′—H14′	119.2	C27′—C30′—H30C	109.5
N1—C15—C16	113.7 (2)	H30A—C30′—H30C	109.5
N1—C15—H15A	108.8	H30B—C30′—H30C	109.5
C16—C15—H15A	108.8	C27—C30—H30D	109.5
N1—C15—H15B	108.8	C27—C30—H30E	109.5
C16—C15—H15B	108.8	H30D—C30—H30E	109.5
H15A—C15—H15B	107.7	C27—C30—H30F	109.5
N1′—C15′—C16′	113.1 (2)	H30D—C30—H30F	109.5
N1′—C15′—H15C	109.0	H30E—C30—H30F	109.5
C16′—C15′—H15C	109.0	C17—N1—C12	122.98 (18)
N1′—C15′—H15D	109.0	C17—N1—C15	117.77 (19)
C16′—C15′—H15D	109.0	C12—N1—C15	117.40 (19)
H15C—C15′—H15D	107.8	C17′—N1′—C12′	123.24 (19)
C15′—C16′—H16A	109.5	C17′—N1′—C15′	117.77 (18)
C15′—C16′—H16B	109.5	C12′—N1′—C15′	117.68 (18)
H16A—C16′—H16B	109.5	C11—S1—C18	100.62 (11)
C15′—C16′—H16C	109.5	C18′—S1′—C11′	100.88 (11)

C7′—C2′—C3′—C4′	−0.8 (4)	C18—C19—C20—C21	−1.2 (4)
C1′—C2′—C3′—C4′	177.3 (2)	C18—C19—C20—C23	−178.3 (2)
C7—C2—C3—C4	2.1 (4)	C19—C20—C21—C22	−1.8 (4)
C1—C2—C3—C4	−175.8 (2)	C23—C20—C21—C22	175.0 (2)
C2′—C3′—C4′—C5′	−1.0 (4)	C19′—C20′—C21′—C22′	0.5 (4)
C2—C3—C4—C5	0.4 (4)	C23′—C20′—C21′—C22′	−175.1 (3)
C3—C4—C5—C6	−2.1 (4)	C20′—C21′—C22′—C17′	−0.1 (4)

C3—C4—C5—C8	179.8 (2)	N1′—C17′—C22′—C21′	179.1 (2)
C3′—C4′—C5′—C6′	1.5 (4)	C18′—C17′—C22′—C21′	−1.2 (4)
C3′—C4′—C5′—C8′	178.5 (2)	C20—C21—C22—C17	2.3 (4)
C4′—C5′—C6′—C7′	−0.3 (4)	N1—C17—C22—C21	−178.5 (2)
C8′—C5′—C6′—C7′	−177.2 (2)	C18—C17—C22—C21	0.3 (4)
C4—C5—C6—C7	1.3 (4)	C21—C20—C23—O2	−161.9 (3)
C8—C5—C6—C7	179.2 (2)	C19—C20—C23—O2	15.0 (4)
C5—C6—C7—C2	1.3 (4)	C21—C20—C23—C24	18.8 (4)
C3—C2—C7—C6	−2.9 (4)	C19—C20—C23—C24	−164.4 (2)
C1—C2—C7—C6	174.9 (3)	C21′—C20′—C23′—O2′	167.4 (3)
C5′—C6′—C7′—C2′	−1.4 (4)	C19′—C20′—C23′—O2′	−8.2 (4)
C3′—C2′—C7′—C6′	2.0 (4)	C21′—C20′—C23′—C24′	−11.1 (4)
C1′—C2′—C7′—C6′	−176.1 (3)	C19′—C20′—C23′—C24′	173.3 (2)
C6—C5—C8—O1	−141.5 (3)	O2—C23—C24—C29	−135.8 (3)
C4—C5—C8—O1	36.5 (4)	C20—C23—C24—C29	43.5 (4)
C6—C5—C8—C9	40.9 (4)	O2—C23—C24—C25	38.8 (4)
C4—C5—C8—C9	−141.2 (2)	C20—C23—C24—C25	−141.8 (2)
C4′—C5′—C8′—O1′	−33.8 (3)	O2′—C23′—C24′—C25′	−42.2 (4)
C6′—C5′—C8′—O1′	143.0 (3)	C20′—C23′—C24′—C25′	136.3 (3)
C4′—C5′—C8′—C9′	145.3 (2)	O2′—C23′—C24′—C29′	133.6 (3)
C6′—C5′—C8′—C9′	−37.8 (3)	C20′—C23′—C24′—C29′	−47.9 (4)
O1—C8—C9—C14	−156.1 (3)	C29′—C24′—C25′—C26′	0.2 (4)
C5—C8—C9—C14	21.6 (4)	C23′—C24′—C25′—C26′	176.2 (3)
O1—C8—C9—C10	17.4 (4)	C29—C24—C25—C26	1.1 (4)
C5—C8—C9—C10	−165.0 (2)	C23—C24—C25—C26	−173.8 (2)
O1′—C8′—C9′—C14′	155.5 (2)	C24—C25—C26—C27	2.1 (4)
C5′—C8′—C9′—C14′	−23.7 (4)	C24′—C25′—C26′—C27′	−1.4 (5)
O1′—C8′—C9′—C10′	−18.4 (4)	C25—C26—C27—C28	−3.0 (4)
C5′—C8′—C9′—C10′	162.5 (2)	C25—C26—C27—C30	174.7 (2)
C14′—C9′—C10′—C11′	−2.3 (4)	C25′—C26′—C27′—C28′	1.1 (5)
C8′—C9′—C10′—C11′	171.9 (2)	C25′—C26′—C27′—C30′	−179.0 (3)
C14—C9—C10—C11	1.8 (4)	C26—C27—C28—C29	1.0 (4)
C8—C9—C10—C11	−172.1 (2)	C30—C27—C28—C29	−176.8 (2)
C9—C10—C11—C12	−2.0 (4)	C26′—C27′—C28′—C29′	0.3 (5)
C9—C10—C11—S1	173.12 (19)	C30′—C27′—C28′—C29′	−179.5 (3)
C9′—C10′—C11′—C12′	2.4 (4)	C27′—C28′—C29′—C24′	−1.5 (4)
C9′—C10′—C11′—S1′	−170.67 (19)	C25′—C24′—C29′—C28′	1.2 (4)
C10′—C11′—C12′—C13′	−0.1 (3)	C23′—C24′—C29′—C28′	−174.7 (3)
S1′—C11′—C12′—C13′	172.56 (18)	C27—C28—C29—C24	2.1 (4)
C10′—C11′—C12′—N1′	−178.0 (2)	C25—C24—C29—C28	−3.1 (4)
S1′—C11′—C12′—N1′	−5.4 (3)	C23—C24—C29—C28	171.6 (2)
C10—C11—C12—C13	0.0 (3)	C22—C17—N1—C12	161.2 (2)
S1—C11—C12—C13	−174.90 (18)	C18—C17—N1—C12	−17.6 (3)
C10—C11—C12—N1	179.2 (2)	C22—C17—N1—C15	−2.9 (3)
S1—C11—C12—N1	4.3 (3)	C18—C17—N1—C15	178.3 (2)
N1′—C12′—C13′—C14′	175.7 (2)	C13—C12—N1—C17	−161.1 (2)
C11′—C12′—C13′—C14′	−2.3 (4)	C11—C12—N1—C17	19.7 (3)
C11—C12—C13—C14	2.3 (4)	C13—C12—N1—C15	3.0 (3)

N1—C12—C13—C14	−177.0 (2)	C11—C12—N1—C15	−176.1 (2)
C12—C13—C14—C9	−2.5 (4)	C16—C15—N1—C17	81.4 (3)
C10—C9—C14—C13	0.5 (4)	C16—C15—N1—C12	−83.6 (3)
C8—C9—C14—C13	174.1 (2)	C22′—C17′—N1′—C12′	−164.4 (2)
C10′—C9′—C14′—C13′	−0.1 (4)	C18′—C17′—N1′—C12′	15.9 (3)
C8′—C9′—C14′—C13′	−174.0 (2)	C22′—C17′—N1′—C15′	2.2 (3)
C12′—C13′—C14′—C9′	2.5 (4)	C18′—C17′—N1′—C15′	−177.5 (2)
C22—C17—C18—C19	−3.3 (3)	C13′—C12′—N1′—C17′	165.8 (2)
N1—C17—C18—C19	175.6 (2)	C11′—C12′—N1′—C17′	−16.3 (3)
C22—C17—C18—S1	173.00 (18)	C13′—C12′—N1′—C15′	−0.8 (3)
N1—C17—C18—S1	−8.1 (3)	C11′—C12′—N1′—C15′	177.1 (2)
C22′—C17′—C18′—C19′	2.1 (3)	C16′—C15′—N1′—C17′	−83.7 (3)
N1′—C17′—C18′—C19′	−178.2 (2)	C16′—C15′—N1′—C12′	83.7 (3)
C22′—C17′—C18′—S1′	−173.43 (19)	C10—C11—S1—C18	162.02 (19)
N1′—C17′—C18′—S1′	6.2 (3)	C12—C11—S1—C18	−22.9 (2)
C17′—C18′—C19′—C20′	−1.9 (4)	C19—C18—S1—C11	−158.69 (18)
S1′—C18′—C19′—C20′	174.0 (2)	C17—C18—S1—C11	24.9 (2)
C17—C18—C19—C20	3.9 (4)	C19′—C18′—S1′—C11′	162.75 (19)
S1—C18—C19—C20	−172.67 (18)	C17′—C18′—S1′—C11′	−21.5 (2)
C18′—C19′—C20′—C21′	0.5 (4)	C10′—C11′—S1′—C18′	−165.95 (19)
C18′—C19′—C20′—C23′	176.4 (2)	C12′—C11′—S1′—C18′	21.1 (2)

Hydrogen-bond geometry (Å, º)

Cg2 and Cg3 are the centroids of rings C2–C7 (molecule *A*) and C2′–C7′ (molecule *B*), respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4′—H4′···O1′^{i}	0.93	2.55	3.325 (3)	141
C30—H30*F*···*Cg*2^{ii}	0.96	2.98	3.716 (3)	134
C1—H1*A*···*Cg*3	0.96	2.91	3.667 (4)	137

Symmetry codes: (i) −*x*, −*y*, −*z*+1; (ii) *x*, −*y*+3/2, *z*−1/2.