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Crystal structure of 12-benzylsulfanyl-2,9-dibromo-6*H*-dibenzo[*b*,*g*][1,8]-naphthyridin-11-one

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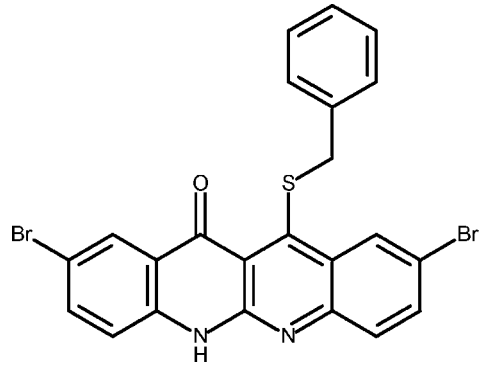
The heterotetracene skeleton of the title molecule, $C_{23}H_{14}Br_2N_2OS$, is defined by linear annulation of four six-membered rings, including two N heteroatoms. This moiety is nearly planar (r.m.s. deviation = 0.055 Å), with a slight twist of 4.1 (2)° between the two halves of the aromatic system. The dihedral angle between the least-squares plane of the skeleton and the benzyl group is 24.5 (3)°; the C—S—C angle involving the benzylsulfanyl group is 99.2 (4)°. In the crystal, molecules are π-stacked in an antiparallel fashion along [110], with a distance between the aromatic planes of 3.47 (2) Å. Intermolecular N—H···O hydrogen bonds form chains extending parallel to [001] and bridge the antiparallel interdigitated stacks of molecules.

Keywords: crystal structure; 1,8-naphthyridine; heterotetracene.

CCDC reference: 1416554

1. Related literature

The title compound was prepared as part of a study towards sulfur-containing 1,8-naphthyridine derivatives (Resch *et al.*, 2015) in which the structure of a dibenzo[*b*,*g*][1,2]dithiolo-[3,4,5-*d*,*e*][1,8]naphthyridine derivative is reported. For the structure of tetracene, see: Holmes *et al.* (1999).



2. Experimental

2.1. Crystal data

$C_{23}H_{14}Br_2N_2OS$
M_r = 526.24
Monoclinic, $P2_1/c$
a = 15.4915 (10) Å
b = 9.3953 (4) Å
c = 13.6501 (9) Å
β = 101.251 (5)°
V = 1948.6 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.29 mm^{-1}
T = 193 K
0.27 × 0.12 × 0.04 mm

2.2. Data collection

Stoe IPDS 2T diffractometer
Absorption correction: integration
X-RED (Stoe & Cie, 1995)
T_{min} = 0.363, T_{max} = 0.811
10437 measured reflections
4807 independent reflections
2850 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.222
S = 1.05
4807 reflections
262 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.29 e Å^{-3}
$\Delta\rho_{min}$ = −1.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5···O1^{i}	0.88	2.28	3.001 (7)	140

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

Data collection: *X-AREA* (Stoe & Cie, 1995); cell refinement: *X-AREA*; data reduction: *X-RED* (Stoe & Cie, 1995); program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: WM5191).

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supporting information

Acta Cryst. (2015). E**71**, o675–o676 [https://doi.org/10.1107/S2056989015014541]

Crystal structure of 12-benzylsulfanyl-2,9-dibromo-6*H*-dibenzo[*b*,*g*][1,8]naphthyridin-11-one

Sebastian Resch, Thomas Quell, Dieter Schollmeyer and Siegfried R. Waldvogel

S1. Synthesis and crystallization

In argon atmosphere, 50 mg (2.0 mmol, 3 eq) NaH and 340 mg (2.7 mmol, 4 eq) benzyl thiol were given to 40 ml of anhydrous dioxane and stirred at room temperature for 30 min. 300 mg (0.68 mmol, 1 eq) of 6*H*-12-chloro-2,9-dibromo-dibenzo[*b,g*]-1,8-naphthyridin-11-one were added and the mixture stirred at room temperature for additional 5 h. After completion of the reaction, the solvent was removed under reduced pressure and the residue purified by column chromatography on silica gel using a mixture of dichloromethane and acetic acid (97:3). The solvent was removed under reduced pressure and the residue alkalized using 1*M* ammonium hydroxide solution. Yield: 276 mg (0.52 mmol, 77%) of an orange solid with mp. = > 513 K (decomposition). Suitable single crystals were obtained by slowly diluting a saturated solution of the title compound in dichloromethane/methanol (5:1) by cyclohexane (diffusion method).

S2. Refinement

Hydrogen atoms attached to carbon atoms were placed at calculated positions with C—H = 0.95 Å (aromatic) or 0.99 Å (methylene C atom). The H atom bonded to the N atom was placed at calculated positions with N—H = 0.88 Å. All H atoms were refined in the riding-model approximation with isotropic displacement parameters (set at 1.2–1.5U_{eq} of the parent atom).

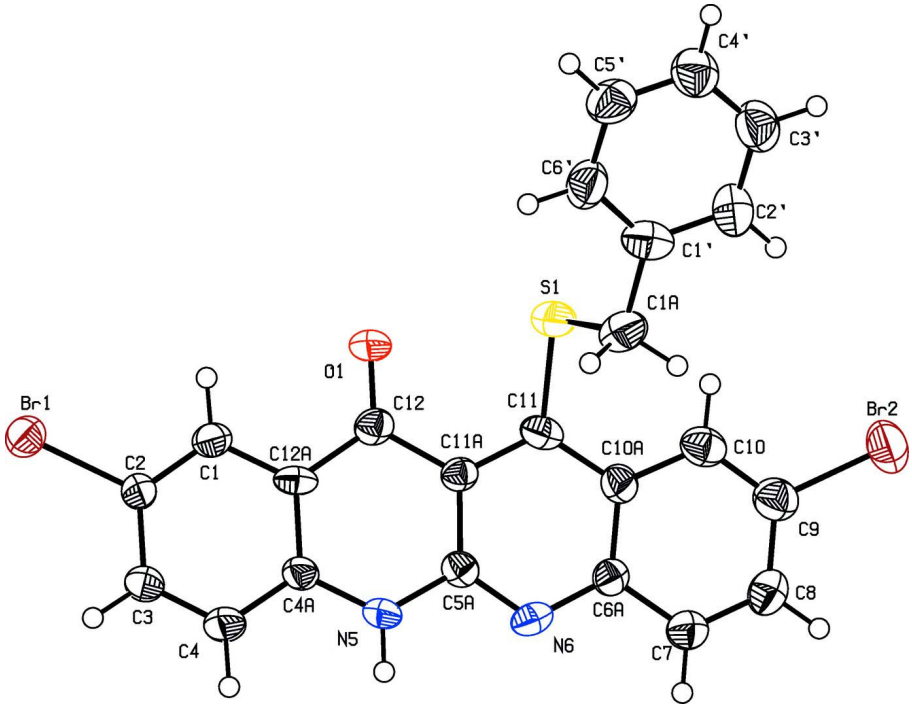

Figure 1

The molecular structure of the title compound with labeling and displacement ellipsoids drawn at the 50% probability level.

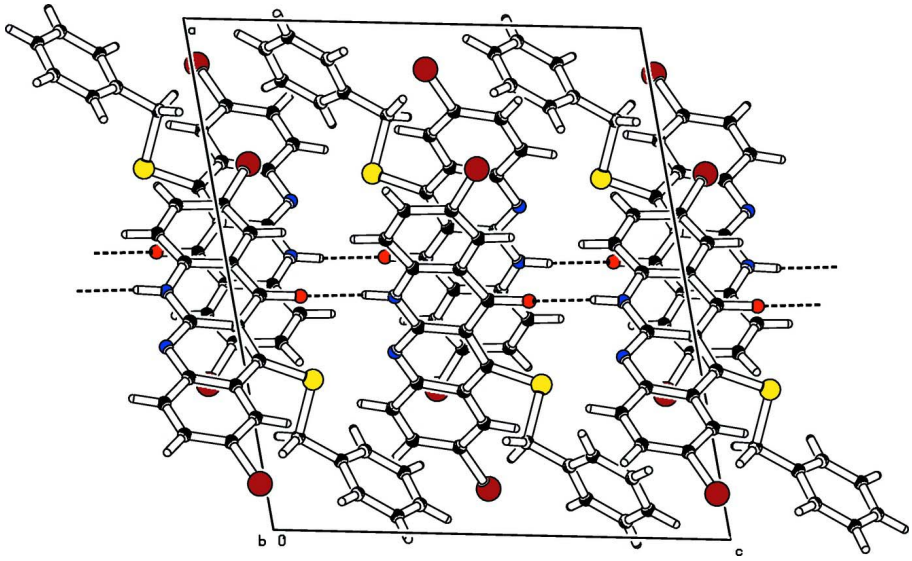

Figure 2

The crystal structure of the title compound in a view along [010]. N—H···O hydrogen bonds are shown as dashed lines.

12-Benzylsulfanyl-2,9-dibromo-6,11-dihydro-5-azatetracen-11-one

Crystal data

$C_{23}H_{14}Br_2N_2OS$
$M_r = 526.24$
Monoclinic, $P2_1/c$
$a = 15.4915$ (10) Å
$b = 9.3953$ (4) Å
$c = 13.6501$ (9) Å
$\beta = 101.251$ (5)°
$V = 1948.6$ (2) Å^3
$Z = 4$
$F(000) = 1040$
$D_x = 1.794$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7178 reflections
$\theta = 2.6$–$28.2°$
$\mu = 4.29$ mm^{-1}
$T = 193$ K
Plate, orange
0.27 × 0.12 × 0.04 mm

Data collection

Stoe IPDS 2T diffractometer
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus
Detector resolution: 6.67 pixels mm^{-1}
rotation method scans
Absorption correction: integration *X-RED* (Stoe & Cie, 1995)
$T_{min} = 0.363$, $T_{max} = 0.811$
10437 measured reflections
4807 independent reflections
2850 reflections with $I > 2\sigma(I)$
$R_{int} = 0.058$
$\theta_{max} = 28.3°$, $\theta_{min} = 2.6°$
$h = -20 \rightarrow 20$
$k = -10 \rightarrow 12$
$l = -18 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.068$
$wR(F^2) = 0.222$
$S = 1.05$
4807 reflections
262 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1106P)^2 + 4.6375P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 2.29$ e Å^{-3}
$\Delta\rho_{min} = -1.21$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.71684 (5)	1.08811 (8)	0.58620 (5)	0.0411 (2)
Br2	0.08972 (7)	0.12934 (12)	0.48824 (9)	0.0689 (3)
S1	0.29644 (15)	0.5906 (3)	0.64477 (16)	0.0589 (6)
O1	0.4597 (3)	0.7273 (6)	0.6495 (3)	0.0438 (12)
C1	0.5809 (5)	0.8812 (7)	0.5634 (5)	0.0348 (14)
H1	0.5838	0.8954	0.6329	0.042*
C2	0.6354 (4)	0.9552 (7)	0.5144 (5)	0.0328 (13)
C3	0.6323 (5)	0.9381 (8)	0.4114 (5)	0.0377 (15)
H3	0.6694	0.9933	0.3785	0.045*

C4	0.5755 (5)	0.8415 (8)	0.3590 (5)	0.0390 (16)
H4	0.5736	0.8280	0.2897	0.047*
C4A	0.5201 (4)	0.7624 (8)	0.4081 (5)	0.0322 (14)
N5	0.4632 (4)	0.6622 (6)	0.3565 (4)	0.0355 (12)
H5	0.4652	0.6476	0.2933	0.043*
C5A	0.4042 (4)	0.5846 (7)	0.3968 (5)	0.0301 (13)
N6	0.3543 (4)	0.4954 (6)	0.3354 (4)	0.0347 (12)
C6A	0.2948 (4)	0.4160 (7)	0.3729 (5)	0.0315 (13)
C7	0.2433 (5)	0.3168 (8)	0.3085 (5)	0.0409 (16)
H7	0.2516	0.3067	0.2417	0.049*
C8	0.1822 (5)	0.2364 (8)	0.3411 (6)	0.0451 (17)
H8	0.1472	0.1713	0.2970	0.054*
C9	0.1706 (5)	0.2493 (9)	0.4408 (6)	0.0477 (18)
C10	0.2184 (5)	0.3449 (8)	0.5041 (6)	0.0425 (16)
H10	0.2094	0.3526	0.5708	0.051*
C10A	0.2809 (4)	0.4321 (7)	0.4720 (5)	0.0353 (14)
C11	0.3307 (4)	0.5375 (8)	0.5332 (5)	0.0361 (14)
C11A	0.3987 (4)	0.6075 (7)	0.4993 (5)	0.0293 (13)
C12	0.4597 (4)	0.7092 (7)	0.5603 (5)	0.0335 (14)
C12A	0.5203 (4)	0.7839 (7)	0.5102 (4)	0.0319 (14)
C1A	0.1824 (6)	0.6501 (11)	0.5902 (6)	0.057 (2)
H1AA	0.1841	0.7334	0.5462	0.068*
H1AB	0.1497	0.5726	0.5500	0.068*
C1′	0.1381 (6)	0.6890 (10)	0.6749 (6)	0.0500 (19)
C2′	0.0739 (6)	0.6017 (10)	0.6987 (7)	0.055 (2)
H2′	0.0582	0.5173	0.6612	0.066*
C3′	0.0318 (6)	0.6350 (11)	0.7769 (7)	0.058 (2)
H3′	−0.0128	0.5746	0.7925	0.070*
C4′	0.0557 (6)	0.7568 (10)	0.8311 (7)	0.055 (2)
H4′	0.0282	0.7796	0.8855	0.066*
C5′	0.1175 (6)	0.8441 (10)	0.8082 (7)	0.054 (2)
H5′	0.1328	0.9281	0.8464	0.065*
C6′	0.1586 (6)	0.8136 (9)	0.7307 (7)	0.052 (2)
H6′	0.2014	0.8774	0.7146	0.062*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0434 (4)	0.0406 (4)	0.0375 (4)	−0.0045 (3)	0.0034 (3)	−0.0001 (3)
Br2	0.0683 (6)	0.0662 (6)	0.0812 (7)	−0.0265 (5)	0.0367 (5)	−0.0144 (5)
S1	0.0482 (11)	0.0958 (18)	0.0361 (10)	−0.0175 (11)	0.0165 (8)	−0.0164 (10)
O1	0.048 (3)	0.062 (3)	0.022 (2)	−0.011 (3)	0.008 (2)	−0.002 (2)
C1	0.034 (3)	0.041 (4)	0.028 (3)	0.001 (3)	0.005 (3)	−0.004 (3)
C2	0.032 (3)	0.037 (3)	0.029 (3)	−0.005 (3)	0.005 (3)	0.001 (3)
C3	0.043 (4)	0.043 (4)	0.027 (3)	−0.006 (3)	0.006 (3)	0.006 (3)
C4	0.042 (4)	0.049 (4)	0.025 (3)	−0.002 (3)	0.004 (3)	0.003 (3)
C4A	0.028 (3)	0.044 (4)	0.024 (3)	−0.002 (3)	0.004 (2)	0.003 (3)
N5	0.039 (3)	0.047 (3)	0.022 (3)	−0.005 (3)	0.010 (2)	0.001 (2)

C5A	0.031 (3)	0.030 (3)	0.028 (3)	0.003 (3)	0.004 (2)	0.007 (2)
N6	0.038 (3)	0.038 (3)	0.027 (3)	0.004 (2)	0.003 (2)	−0.008 (2)
C6A	0.025 (3)	0.035 (3)	0.033 (3)	0.003 (3)	0.004 (2)	−0.002 (3)
C7	0.044 (4)	0.043 (4)	0.035 (4)	−0.002 (3)	0.007 (3)	0.000 (3)
C8	0.044 (4)	0.039 (4)	0.050 (4)	−0.004 (3)	0.005 (3)	−0.007 (3)
C9	0.048 (4)	0.050 (5)	0.047 (4)	0.001 (3)	0.015 (4)	−0.002 (3)
C10	0.040 (4)	0.049 (4)	0.040 (4)	0.008 (3)	0.012 (3)	0.002 (3)
C10A	0.031 (3)	0.038 (4)	0.038 (4)	−0.001 (3)	0.009 (3)	−0.001 (3)
C11	0.035 (3)	0.046 (4)	0.029 (3)	0.006 (3)	0.011 (3)	0.003 (3)
C11A	0.028 (3)	0.033 (3)	0.026 (3)	0.003 (2)	0.003 (2)	0.000 (2)
C12	0.032 (3)	0.038 (4)	0.028 (3)	0.003 (3)	0.000 (3)	0.003 (3)
C12A	0.038 (3)	0.039 (4)	0.019 (3)	0.009 (3)	0.007 (2)	0.003 (2)
C1A	0.055 (5)	0.075 (6)	0.039 (4)	−0.007 (4)	0.004 (4)	−0.011 (4)
C1′	0.056 (5)	0.059 (5)	0.037 (4)	0.010 (4)	0.013 (3)	0.004 (3)
C2′	0.047 (5)	0.053 (5)	0.067 (6)	−0.010 (4)	0.013 (4)	0.000 (4)
C3′	0.042 (4)	0.069 (6)	0.063 (6)	−0.005 (4)	0.012 (4)	0.004 (5)
C4′	0.044 (4)	0.064 (6)	0.058 (5)	0.003 (4)	0.011 (4)	0.001 (4)
C5′	0.053 (5)	0.057 (5)	0.054 (5)	0.006 (4)	0.013 (4)	−0.016 (4)
C6′	0.052 (5)	0.045 (4)	0.058 (5)	−0.010 (4)	0.008 (4)	−0.008 (4)

Geometric parameters (Å, º)

Br1—C2	1.905 (7)	C8—C9	1.413 (11)
Br2—C9	1.890 (9)	C8—H8	0.9500
S1—C11	1.779 (7)	C9—C10	1.362 (11)
S1—C1A	1.864 (9)	C10—C10A	1.402 (10)
O1—C12	1.229 (8)	C10—H10	0.9500
C1—C2	1.366 (10)	C10A—C11	1.422 (10)
C1—C12A	1.406 (10)	C11—C11A	1.395 (10)
C1—H1	0.9500	C11A—C12	1.481 (9)
C2—C3	1.407 (9)	C12—C12A	1.447 (10)
C3—C4	1.365 (10)	C1A—C1′	1.501 (12)
C3—H3	0.9500	C1A—H1AA	0.9900
C4—C4A	1.400 (10)	C1A—H1AB	0.9900
C4—H4	0.9500	C1′—C2′	1.376 (12)
C4A—N5	1.385 (9)	C1′—C6′	1.398 (12)
C4A—C12A	1.408 (9)	C2′—C3′	1.391 (13)
N5—C5A	1.366 (8)	C2′—H2′	0.9500
N5—H5	0.8800	C3′—C4′	1.374 (13)
C5A—N6	1.323 (8)	C3′—H3′	0.9500
C5A—C11A	1.435 (9)	C4′—C5′	1.342 (13)
N6—C6A	1.360 (9)	C4′—H4′	0.9500
C6A—C7	1.416 (10)	C5′—C6′	1.368 (12)
C6A—C10A	1.420 (10)	C5′—H5′	0.9500
C7—C8	1.352 (11)	C6′—H6′	0.9500
C7—H7	0.9500		
C11—S1—C1A	99.2 (4)	C10—C10A—C11	123.5 (7)

C2—C1—C12A	119.5 (6)	C6A—C10A—C11	117.9 (6)
C2—C1—H1	120.3	C11A—C11—C10A	119.5 (6)
C12A—C1—H1	120.3	C11A—C11—S1	121.5 (5)
C1—C2—C3	121.8 (6)	C10A—C11—S1	118.6 (5)
C1—C2—Br1	119.5 (5)	C11—C11A—C5A	116.4 (6)
C3—C2—Br1	118.7 (5)	C11—C11A—C12	123.9 (6)
C4—C3—C2	119.5 (6)	C5A—C11A—C12	119.5 (6)
C4—C3—H3	120.2	O1—C12—C12A	121.8 (6)
C2—C3—H3	120.2	O1—C12—C11A	121.5 (6)
C3—C4—C4A	119.7 (6)	C12A—C12—C11A	116.7 (6)
C3—C4—H4	120.2	C1—C12A—C4A	118.5 (6)
C4A—C4—H4	120.2	C1—C12A—C12	120.0 (6)
N5—C4A—C4	120.4 (6)	C4A—C12A—C12	121.5 (6)
N5—C4A—C12A	118.6 (6)	C1′—C1A—S1	107.8 (6)
C4—C4A—C12A	120.9 (6)	C1′—C1A—H1AA	110.1
C5A—N5—C4A	124.6 (6)	S1—C1A—H1AA	110.1
C5A—N5—H5	117.7	C1′—C1A—H1AB	110.1
C4A—N5—H5	117.7	S1—C1A—H1AB	110.1
N6—C5A—N5	116.0 (6)	H1AA—C1A—H1AB	108.5
N6—C5A—C11A	125.1 (6)	C2′—C1′—C6′	117.9 (8)
N5—C5A—C11A	119.0 (6)	C2′—C1′—C1A	119.8 (8)
C5A—N6—C6A	117.7 (6)	C6′—C1′—C1A	122.3 (8)
N6—C6A—C7	117.9 (6)	C1′—C2′—C3′	121.1 (9)
N6—C6A—C10A	122.7 (6)	C1′—C2′—H2′	119.5
C7—C6A—C10A	119.3 (6)	C3′—C2′—H2′	119.5
C8—C7—C6A	120.6 (7)	C4′—C3′—C2′	118.8 (9)
C8—C7—H7	119.7	C4′—C3′—H3′	120.6
C6A—C7—H7	119.7	C2′—C3′—H3′	120.6
C7—C8—C9	119.9 (7)	C5′—C4′—C3′	120.9 (9)
C7—C8—H8	120.0	C5′—C4′—H4′	119.5
C9—C8—H8	120.0	C3′—C4′—H4′	119.5
C10—C9—C8	120.8 (8)	C4′—C5′—C6′	120.8 (9)
C10—C9—Br2	119.4 (6)	C4′—C5′—H5′	119.6
C8—C9—Br2	119.8 (6)	C6′—C5′—H5′	119.6
C9—C10—C10A	120.7 (7)	C5′—C6′—C1′	120.4 (8)
C9—C10—H10	119.6	C5′—C6′—H6′	119.8
C10A—C10—H10	119.6	C1′—C6′—H6′	119.8
C10—C10A—C6A	118.5 (6)		

C12A—C1—C2—C3	0.7 (11)	C10A—C11—C11A—C5A	10.1 (9)
C12A—C1—C2—Br1	179.5 (5)	S1—C11—C11A—C5A	−162.6 (5)
C1—C2—C3—C4	−2.3 (11)	C10A—C11—C11A—C12	−174.3 (6)
Br1—C2—C3—C4	178.8 (6)	S1—C11—C11A—C12	13.0 (9)
C2—C3—C4—C4A	1.0 (11)	N6—C5A—C11A—C11	−5.1 (10)
C3—C4—C4A—N5	−178.9 (7)	N5—C5A—C11A—C11	172.9 (6)
C3—C4—C4A—C12A	1.9 (11)	N6—C5A—C11A—C12	179.0 (6)
C4—C4A—N5—C5A	−177.0 (6)	N5—C5A—C11A—C12	−2.9 (9)
C12A—C4A—N5—C5A	2.2 (10)	C11—C11A—C12—O1	7.7 (10)

C4A—N5—C5A—N6	179.0 (6)	C5A—C11A—C12—O1	−176.8 (6)
C4A—N5—C5A—C11A	0.8 (10)	C11—C11A—C12—C12A	−173.5 (6)
N5—C5A—N6—C6A	179.9 (6)	C5A—C11A—C12—C12A	2.0 (9)
C11A—C5A—N6—C6A	−2.0 (9)	C2—C1—C12A—C4A	2.2 (10)
C5A—N6—C6A—C7	−177.9 (6)	C2—C1—C12A—C12	−177.5 (6)
C5A—N6—C6A—C10A	4.1 (9)	N5—C4A—C12A—C1	177.3 (6)
N6—C6A—C7—C8	−179.0 (7)	C4—C4A—C12A—C1	−3.5 (10)
C10A—C6A—C7—C8	−1.0 (11)	N5—C4A—C12A—C12	−3.1 (10)
C6A—C7—C8—C9	−1.1 (12)	C4—C4A—C12A—C12	176.2 (6)
C7—C8—C9—C10	1.9 (12)	O1—C12—C12A—C1	−0.5 (10)
C7—C8—C9—Br2	−176.6 (6)	C11A—C12—C12A—C1	−179.4 (6)
C8—C9—C10—C10A	−0.5 (12)	O1—C12—C12A—C4A	179.8 (7)
Br2—C9—C10—C10A	178.0 (6)	C11A—C12—C12A—C4A	1.0 (9)
C9—C10—C10A—C6A	−1.7 (11)	C11—S1—C1A—C1′	175.4 (7)
C9—C10—C10A—C11	177.7 (7)	S1—C1A—C1′—C2′	−107.4 (8)
N6—C6A—C10A—C10	−179.7 (6)	S1—C1A—C1′—C6′	73.6 (10)
C7—C6A—C10A—C10	2.4 (10)	C6′—C1′—C2′—C3′	−1.0 (14)
N6—C6A—C10A—C11	0.9 (10)	C1A—C1′—C2′—C3′	179.9 (8)
C7—C6A—C10A—C11	−177.0 (6)	C1′—C2′—C3′—C4′	−0.5 (14)
C10—C10A—C11—C11A	172.4 (7)	C2′—C3′—C4′—C5′	1.3 (14)
C6A—C10A—C11—C11A	−8.3 (10)	C3′—C4′—C5′—C6′	−0.4 (14)
C10—C10A—C11—S1	−14.7 (10)	C4′—C5′—C6′—C1′	−1.2 (14)
C6A—C10A—C11—S1	164.7 (5)	C2′—C1′—C6′—C5′	1.9 (13)
C1A—S1—C11—C11A	115.4 (6)	C1A—C1′—C6′—C5′	−179.1 (8)
C1A—S1—C11—C10A	−57.4 (7)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5···O1^{i}	0.88	2.28	3.001 (7)	140

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