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Crystal structure of (9*S*,10*S*)-10-ethoxy-9-hydroxy-6,6,9-trimethyl-3-pentyl-7,8,9,10-tetrahydro-6*H*-benzo[*c*]-chromen-1-yl 4-methylbenzenesulfonate

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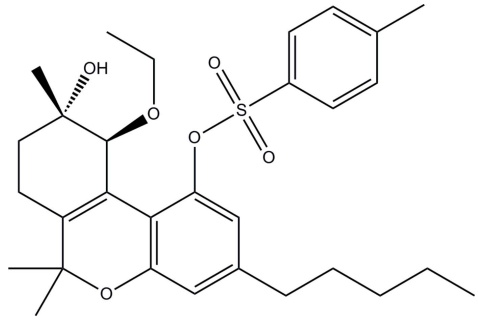
In the structure of the title compound, $C_{30}H_{40}O_6S$, the cyclohexene and heterocyclic rings are linked by a double bond. The cyclohexene ring has a half-chair conformation (the methylene group adjacent to the hydroxy substituent lies above the remaining atoms) and the hydroxy and ethoxy groups have equatorial and bisectional dispositions, respectively. The heterocyclic ring has an envelope conformation (with the CMe_2 C atom being the flap). The dihedral angle between the aromatic rings is 53.88 (10)°. A long intramolecular C—H···S interaction is noted. In the molecular packing, hydroxy-O—H···O(sulfonate) hydrogen bonds lead to a helical chain along [010]. Connections between chains are of the type methyl-C—H···O(sulfonate) and lead to supramolecular layers that lie parallel to (001). The studied crystal was an inversion twin.

Keywords: crystal structure; hydrogen bonding; Δ^9–THC tosylate; photooxygenation.

CCDC reference: 1442416

1. Related literature

For Δ^9–THC tosylate, see: Ducker (2004); Gul *et al.* (2008). For a related process of photooxygenation, see: Motoyoshiya *et al.* (1999); Griesbeck *et al.* (2014). For unusually long sulfur hydrogen bonding, see: Huang *et al.* (2009).



2. Experimental

2.1. Crystal data

$C_{30}H_{40}O_6S$
M_r = 528.68
Monoclinic, $P2_1$
a = 9.909 (1) Å
b = 10.2373 (10) Å
c = 13.8402 (10) Å
β = 101.00 (1)°
V = 1378.2 (2) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 1.38 mm^{-1}
T = 173 K
0.23 × 0.20 × 0.19 mm

2.2. Data collection

Bruker SMART CCD area-detector diffractometer
21062 measured reflections
4984 independent reflections
4834 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.066
S = 1.02
4984 reflections
342 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9···S1	0.98	2.94	3.687 (2)	134
C10—H10B···O5^{i}	0.96	2.57	3.459 (2)	154
O2—H2···O6^{ii}	0.82	2.22	3.014 (2)	165

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

Data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014*/7 (Sheldrick, 2015); molecular graphics: *Mercury* (Macrae *et al.*, 2008), *ORTEP-3 for Windows* (Farrugia, 2012), *POV-RAY* (Cason, 2003); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004), *publCIF* (Westrip, 2010).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: TK5416).

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supporting information

Acta Cryst. (2015). E**71**, o1082–o1083 [https://doi.org/10.1107/S2056989015024044]

Crystal structure of (9*S*,10*S*)-10-ethoxy-9-hydroxy-6,6,9-trimethyl-3-pentyl-7,8,9,10-tetrahydro-6*H*-benzo[*c*]chromen-1-yl 4-methylbenzenesulfonate

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S1. Experimental

Δ^9–THC tosylate was submitted to photooxygenation in dichloromethane/ethanol for 11 h and 30 min using *meso*-tetraphenylporphine in the presence of oxygen and light generated by a regular, incandescent light bulb, yielding the title compound, which was crystallized from ethyl acetate : hexanes 1:9, producing needle-like crystals

S1.1. Refinement

All H atoms were located in difference maps but were included in the model in the riding model approximation with O—H = 0.82 Å and C—H = 0.93–0.98 Å, and with *U*iso = 1.5*U*eq (O) for OH and *U*iso=1.2–1.5*U*eq(C).

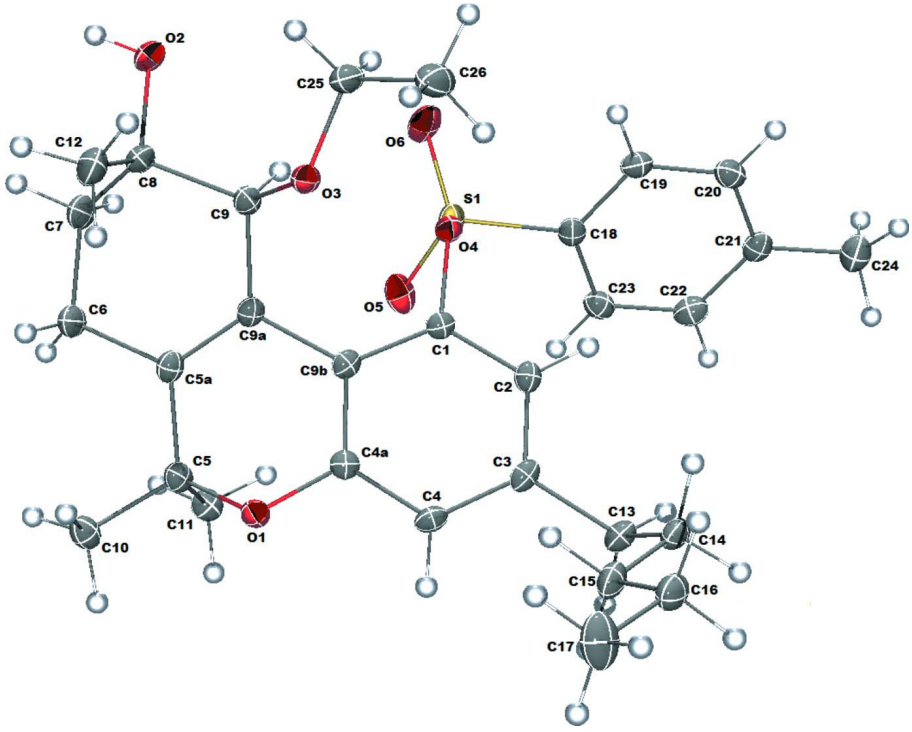

Figure 1

Plot of the molecular structure of the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

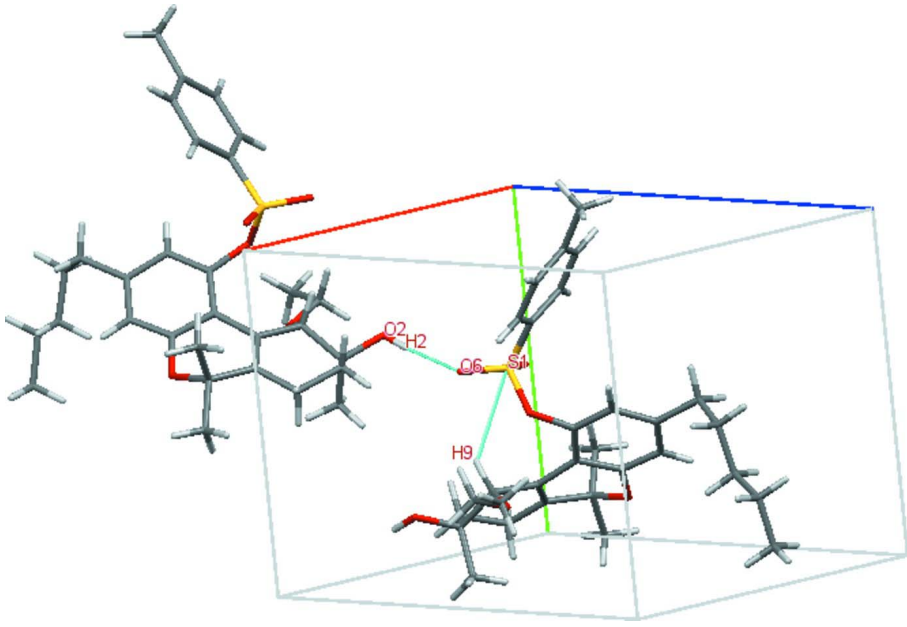

Figure 2

Partial plot of the unit cell contents of the title compound, showing an O6—H2···O2 intermolecular hydrogens bond and one long, intramolecular C9—H9···S1 hydrogen bond, both represented by light blue lines.

(9*S*,10*S*)-10-Ethoxy-9-hydroxy-6,6,9-trimethyl-3-pentyl-7,8,9,10-tetrahydro-6*H*-benzo[*c*]chromen-1-yl 4-methylbenzenesulfonate

Crystal data

$C_{30}H_{40}O_6S$
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Monoclinic, $P2_1$
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$b = 10.2373$ (10) Å
$c = 13.8402$ (10) Å
$\beta = 101.00$ (1)°
$V = 1378.2$ (2) Å^3
$Z = 2$
$F(000) = 568$
$D_x = 1.274$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 9903 reflections
$\theta = 4.6$–$68.1°$
$\mu = 1.38$ mm^{-1}
$T = 173$ K
Needle, colourless
0.23 × 0.20 × 0.19 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: X-ray
φ and ω scans
21062 measured reflections
4984 independent reflections
4834 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 68.2°$, $\theta_{min} = 3.3°$
$h = -11 \rightarrow 11$
$k = -12 \rightarrow 12$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.066$
$S = 1.02$
4984 reflections
342 parameters
1 restraint
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0429P)^2 + 0.1558P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}
Absolute structure: Twinning involves inversion, so Flack parameter cannot be determined

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. Refined as a 2-component inversion twin.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.33896 (5)	0.44735 (5)	0.19766 (3)	0.01720 (12)
O1	0.01053 (14)	0.87882 (14)	0.24328 (10)	0.0163 (3)
O2	0.54967 (16)	0.84850 (17)	0.05710 (11)	0.0269 (4)
H2	0.5600	0.8838	0.0058	0.040*
O3	0.47179 (14)	0.82165 (14)	0.25792 (10)	0.0174 (3)
O4	0.37762 (14)	0.56548 (14)	0.27376 (10)	0.0158 (3)
O5	0.20422 (16)	0.46627 (15)	0.14151 (10)	0.0247 (3)
O6	0.45457 (17)	0.44066 (17)	0.15025 (11)	0.0269 (3)
C1	0.2680 (2)	0.6273 (2)	0.30887 (14)	0.0144 (4)
C2	0.2306 (2)	0.5743 (2)	0.39227 (14)	0.0156 (4)
H2A	0.2785	0.5035	0.4240	0.019*
C3	0.1205 (2)	0.6281 (2)	0.42811 (14)	0.0163 (4)
C4	0.0496 (2)	0.7316 (2)	0.37639 (14)	0.0164 (4)
H4	−0.0246	0.7688	0.3986	0.020*
C4A	0.0882 (2)	0.78021 (19)	0.29185 (14)	0.0147 (4)
C5	0.0027 (2)	0.8815 (2)	0.13601 (14)	0.0169 (4)
C5A	0.1471 (2)	0.8735 (2)	0.11459 (14)	0.0170 (4)
C6	0.1735 (2)	0.9385 (3)	0.02247 (14)	0.0228 (4)
H6A	0.1767	1.0324	0.0319	0.027*
H6B	0.0984	0.9190	−0.0316	0.027*
C7	0.3085 (2)	0.8924 (3)	−0.00372 (15)	0.0255 (5)
H7A	0.2977	0.8036	−0.0284	0.031*
H7B	0.3309	0.9474	−0.0555	0.031*
C8	0.4260 (2)	0.8973 (2)	0.08512 (15)	0.0203 (4)
C9	0.3933 (2)	0.7990 (2)	0.16179 (14)	0.0164 (4)
H9	0.4138	0.7108	0.1410	0.020*
C9A	0.2436 (2)	0.80314 (19)	0.17329 (14)	0.0150 (4)
C9B	0.2036 (2)	0.7346 (2)	0.25771 (14)	0.0148 (4)
C10	−0.0683 (2)	1.0112 (2)	0.10561 (15)	0.0201 (4)
H10A	−0.1549	1.0139	0.1269	0.030*
H10B	−0.0834	1.0196	0.0353	0.030*
H10C	−0.0112	1.0816	0.1354	0.030*
C11	−0.0845 (2)	0.7666 (2)	0.08950 (15)	0.0205 (4)
H11A	−0.0413	0.6862	0.1141	0.031*

H11B	−0.0926	0.7697	0.0193	0.031*
H11C	−0.1742	0.7718	0.1058	0.031*
C12	0.4513 (3)	1.0345 (2)	0.12656 (18)	0.0277 (5)
H12A	0.5337	1.0353	0.1760	0.042*
H12B	0.3749	1.0612	0.1553	0.042*
H12C	0.4612	1.0937	0.0746	0.042*
C13	0.0733 (2)	0.5677 (2)	0.51606 (15)	0.0195 (4)
H13A	0.0891	0.4743	0.5152	0.023*
H13B	−0.0250	0.5813	0.5089	0.023*
C14	0.1441 (2)	0.6214 (2)	0.61665 (15)	0.0197 (4)
H14A	0.1119	0.5729	0.6680	0.024*
H14B	0.2424	0.6073	0.6246	0.024*
C15	0.1177 (2)	0.7662 (2)	0.62955 (15)	0.0215 (4)
H15A	0.0193	0.7816	0.6137	0.026*
H15B	0.1594	0.8151	0.5829	0.026*
C16	0.1730 (2)	0.8183 (2)	0.73286 (15)	0.0223 (5)
H16A	0.2713	0.8030	0.7495	0.027*
H16B	0.1302	0.7714	0.7799	0.027*
C17	0.1449 (3)	0.9644 (3)	0.74043 (16)	0.0333 (6)
H17A	0.1857	1.0110	0.6931	0.050*
H17B	0.1838	0.9946	0.8055	0.050*
H17C	0.0474	0.9793	0.7275	0.050*
C18	0.3399 (2)	0.31006 (19)	0.27416 (15)	0.0159 (4)
C19	0.4624 (2)	0.2741 (2)	0.33485 (15)	0.0185 (4)
H19	0.5419	0.3228	0.3360	0.022*
C20	0.4641 (2)	0.1648 (2)	0.39354 (15)	0.0202 (4)
H20	0.5454	0.1408	0.4353	0.024*
C21	0.3458 (2)	0.0896 (2)	0.39119 (15)	0.0186 (4)
C22	0.2245 (2)	0.1286 (2)	0.32967 (16)	0.0214 (5)
H22	0.1449	0.0797	0.3275	0.026*
C23	0.2205 (2)	0.2395 (2)	0.27151 (15)	0.0193 (4)
H23	0.1388	0.2659	0.2314	0.023*
C24	0.3507 (2)	−0.0315 (2)	0.45314 (16)	0.0265 (5)
H24A	0.3732	−0.1053	0.4165	0.040*
H24B	0.2625	−0.0452	0.4707	0.040*
H24C	0.4193	−0.0213	0.5118	0.040*
C25	0.6098 (2)	0.7735 (2)	0.27438 (16)	0.0229 (5)
H25A	0.6684	0.8324	0.2461	0.027*
H25B	0.6129	0.6880	0.2447	0.027*
C26	0.6567 (2)	0.7654 (3)	0.38428 (17)	0.0305 (5)
H26A	0.6577	0.8513	0.4122	0.046*
H26B	0.7476	0.7289	0.3991	0.046*
H26C	0.5948	0.7107	0.4116	0.046*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0244 (3)	0.0168 (2)	0.0111 (2)	0.0027 (2)	0.00518 (17)	−0.00065 (18)

O1	0.0180 (7)	0.0179 (7)	0.0134 (6)	0.0035 (6)	0.0041 (5)	−0.0009 (5)
O2	0.0259 (8)	0.0394 (9)	0.0193 (7)	0.0076 (7)	0.0136 (6)	0.0107 (7)
O3	0.0158 (7)	0.0233 (7)	0.0133 (7)	0.0012 (6)	0.0030 (5)	0.0015 (5)
O4	0.0170 (7)	0.0160 (7)	0.0154 (7)	0.0019 (6)	0.0056 (6)	0.0006 (5)
O5	0.0327 (8)	0.0238 (8)	0.0150 (6)	0.0034 (7)	−0.0024 (6)	−0.0019 (6)
O6	0.0393 (9)	0.0238 (7)	0.0222 (7)	0.0036 (7)	0.0177 (7)	−0.0009 (7)
C1	0.0149 (10)	0.0162 (9)	0.0121 (9)	−0.0014 (8)	0.0023 (8)	−0.0030 (7)
C2	0.0178 (10)	0.0152 (9)	0.0128 (9)	−0.0019 (8)	0.0007 (8)	−0.0005 (7)
C3	0.0196 (10)	0.0183 (9)	0.0110 (9)	−0.0065 (8)	0.0032 (8)	−0.0029 (7)
C4	0.0162 (10)	0.0197 (10)	0.0148 (9)	−0.0015 (8)	0.0065 (8)	−0.0037 (8)
C4A	0.0150 (9)	0.0149 (9)	0.0134 (9)	−0.0020 (8)	0.0009 (7)	−0.0034 (7)
C5	0.0186 (10)	0.0206 (9)	0.0111 (9)	0.0027 (8)	0.0017 (8)	−0.0006 (8)
C5A	0.0212 (11)	0.0168 (10)	0.0134 (9)	−0.0007 (8)	0.0040 (8)	−0.0003 (8)
C6	0.0218 (10)	0.0306 (11)	0.0163 (9)	0.0048 (10)	0.0042 (8)	0.0081 (9)
C7	0.0275 (12)	0.0356 (12)	0.0147 (9)	0.0060 (10)	0.0075 (9)	0.0089 (9)
C8	0.0195 (11)	0.0252 (11)	0.0183 (10)	0.0024 (9)	0.0090 (8)	0.0051 (8)
C9	0.0188 (10)	0.0187 (10)	0.0124 (9)	0.0026 (8)	0.0045 (8)	0.0005 (7)
C9A	0.0197 (10)	0.0149 (9)	0.0111 (9)	0.0005 (8)	0.0047 (8)	−0.0024 (7)
C9B	0.0163 (10)	0.0170 (9)	0.0109 (9)	−0.0025 (8)	0.0022 (7)	−0.0025 (7)
C10	0.0226 (11)	0.0206 (10)	0.0164 (9)	0.0045 (9)	0.0019 (8)	−0.0005 (8)
C11	0.0213 (11)	0.0214 (11)	0.0180 (9)	0.0004 (9)	0.0017 (8)	−0.0022 (8)
C12	0.0308 (13)	0.0252 (12)	0.0296 (12)	0.0010 (10)	0.0121 (10)	0.0091 (10)
C13	0.0213 (11)	0.0215 (10)	0.0172 (10)	−0.0026 (9)	0.0076 (8)	0.0008 (8)
C14	0.0194 (11)	0.0264 (11)	0.0143 (9)	−0.0011 (9)	0.0057 (8)	0.0035 (8)
C15	0.0240 (11)	0.0263 (11)	0.0143 (9)	−0.0029 (9)	0.0041 (8)	0.0044 (8)
C16	0.0226 (11)	0.0291 (12)	0.0152 (10)	−0.0007 (9)	0.0038 (8)	0.0025 (8)
C17	0.0470 (14)	0.0297 (13)	0.0193 (10)	−0.0033 (12)	−0.0036 (10)	−0.0003 (10)
C18	0.0205 (10)	0.0143 (9)	0.0139 (9)	0.0028 (8)	0.0055 (8)	−0.0023 (7)
C19	0.0154 (10)	0.0229 (11)	0.0178 (9)	−0.0017 (8)	0.0046 (8)	−0.0023 (8)
C20	0.0186 (10)	0.0247 (11)	0.0169 (9)	0.0033 (9)	0.0024 (8)	−0.0015 (8)
C21	0.0236 (11)	0.0180 (10)	0.0159 (9)	0.0007 (8)	0.0077 (8)	−0.0032 (8)
C22	0.0211 (11)	0.0194 (10)	0.0247 (11)	−0.0049 (8)	0.0071 (9)	−0.0048 (8)
C23	0.0179 (10)	0.0219 (11)	0.0177 (9)	0.0029 (9)	0.0021 (8)	−0.0025 (8)
C24	0.0340 (12)	0.0235 (12)	0.0231 (10)	−0.0001 (10)	0.0080 (9)	0.0020 (9)
C25	0.0169 (10)	0.0309 (12)	0.0220 (11)	0.0009 (9)	0.0064 (9)	0.0040 (9)
C26	0.0192 (11)	0.0478 (15)	0.0237 (11)	0.0032 (11)	0.0020 (9)	0.0053 (11)

Geometric parameters (Å, º)

S1—O5	1.4240 (16)	C11—H11B	0.9600
S1—O6	1.4264 (15)	C11—H11C	0.9600
S1—O4	1.6014 (15)	C12—H12A	0.9600
S1—C18	1.759 (2)	C12—H12B	0.9600
O1—C4A	1.366 (3)	C12—H12C	0.9600
O1—C5	1.472 (2)	C13—C14	1.536 (3)
O2—C8	1.443 (2)	C13—H13A	0.9700
O2—H2	0.8200	C13—H13B	0.9700
O3—C9	1.426 (2)	C14—C15	1.521 (3)

O3—C25	1.431 (3)	C14—H14A	0.9700
O4—C1	1.421 (2)	C14—H14B	0.9700
C1—C2	1.388 (3)	C15—C16	1.527 (3)
C1—C9B	1.394 (3)	C15—H15A	0.9700
C2—C3	1.395 (3)	C15—H15B	0.9700
C2—H2A	0.9300	C16—C17	1.528 (3)
C3—C4	1.392 (3)	C16—H16A	0.9700
C3—C13	1.517 (3)	C16—H16B	0.9700
C4—C4A	1.391 (3)	C17—H17A	0.9600
C4—H4	0.9300	C17—H17B	0.9600
C4A—C9B	1.398 (3)	C17—H17C	0.9600
C5—C5A	1.518 (3)	C18—C23	1.380 (3)
C5—C10	1.523 (3)	C18—C19	1.387 (3)
C5—C11	1.526 (3)	C19—C20	1.381 (3)
C5A—C9A	1.340 (3)	C19—H19	0.9300
C5A—C6	1.505 (3)	C20—C21	1.397 (3)
C6—C7	1.526 (3)	C20—H20	0.9300
C6—H6A	0.9700	C21—C22	1.393 (3)
C6—H6B	0.9700	C21—C24	1.503 (3)
C7—C8	1.524 (3)	C22—C23	1.388 (3)
C7—H7A	0.9700	C22—H22	0.9300
C7—H7B	0.9700	C23—H23	0.9300
C8—C12	1.520 (3)	C24—H24A	0.9600
C8—C9	1.541 (3)	C24—H24B	0.9600
C9—C9A	1.523 (3)	C24—H24C	0.9600
C9—H9	0.9800	C25—C26	1.506 (3)
C9A—C9B	1.480 (3)	C25—H25A	0.9700
C10—H10A	0.9600	C25—H25B	0.9700
C10—H10B	0.9600	C26—H26A	0.9600
C10—H10C	0.9600	C26—H26B	0.9600
C11—H11A	0.9600	C26—H26C	0.9600

O5—S1—O6	120.48 (9)	H11A—C11—H11C	109.5
O5—S1—O4	109.74 (8)	H11B—C11—H11C	109.5
O6—S1—O4	103.09 (9)	C8—C12—H12A	109.5
O5—S1—C18	109.51 (10)	C8—C12—H12B	109.5
O6—S1—C18	109.04 (10)	H12A—C12—H12B	109.5
O4—S1—C18	103.56 (8)	C8—C12—H12C	109.5
C4A—O1—C5	115.24 (15)	H12A—C12—H12C	109.5
C8—O2—H2	109.5	H12B—C12—H12C	109.5
C9—O3—C25	115.27 (15)	C3—C13—C14	115.09 (17)
C1—O4—S1	117.32 (12)	C3—C13—H13A	108.5
C2—C1—C9B	124.13 (19)	C14—C13—H13A	108.5
C2—C1—O4	116.98 (18)	C3—C13—H13B	108.5
C9B—C1—O4	118.88 (17)	C14—C13—H13B	108.5
C1—C2—C3	119.5 (2)	H13A—C13—H13B	107.5
C1—C2—H2A	120.2	C15—C14—C13	113.32 (18)
C3—C2—H2A	120.2	C15—C14—H14A	108.9

C4—C3—C2	118.04 (18)	C13—C14—H14A	108.9
C4—C3—C13	121.37 (19)	C15—C14—H14B	108.9
C2—C3—C13	120.41 (19)	C13—C14—H14B	108.9
C4A—C4—C3	120.78 (18)	H14A—C14—H14B	107.7
C4A—C4—H4	119.6	C14—C15—C16	114.31 (18)
C3—C4—H4	119.6	C14—C15—H15A	108.7
O1—C4A—C4	117.27 (18)	C16—C15—H15A	108.7
O1—C4A—C9B	120.06 (17)	C14—C15—H15B	108.7
C4—C4A—C9B	122.64 (19)	C16—C15—H15B	108.7
O1—C5—C5A	109.00 (16)	H15A—C15—H15B	107.6
O1—C5—C10	103.17 (15)	C15—C16—C17	111.65 (19)
C5A—C5—C10	113.29 (17)	C15—C16—H16A	109.3
O1—C5—C11	109.13 (16)	C17—C16—H16A	109.3
C5A—C5—C11	110.76 (17)	C15—C16—H16B	109.3
C10—C5—C11	111.16 (16)	C17—C16—H16B	109.3
C9A—C5A—C6	122.14 (18)	H16A—C16—H16B	108.0
C9A—C5A—C5	120.03 (17)	C16—C17—H17A	109.5
C6—C5A—C5	117.68 (17)	C16—C17—H17B	109.5
C5A—C6—C7	111.51 (18)	H17A—C17—H17B	109.5
C5A—C6—H6A	109.3	C16—C17—H17C	109.5
C7—C6—H6A	109.3	H17A—C17—H17C	109.5
C5A—C6—H6B	109.3	H17B—C17—H17C	109.5
C7—C6—H6B	109.3	C23—C18—C19	121.6 (2)
H6A—C6—H6B	108.0	C23—C18—S1	119.73 (16)
C8—C7—C6	111.56 (17)	C19—C18—S1	118.70 (16)
C8—C7—H7A	109.3	C20—C19—C18	118.86 (19)
C6—C7—H7A	109.3	C20—C19—H19	120.6
C8—C7—H7B	109.3	C18—C19—H19	120.6
C6—C7—H7B	109.3	C19—C20—C21	121.07 (19)
H7A—C7—H7B	108.0	C19—C20—H20	119.5
O2—C8—C12	109.50 (18)	C21—C20—H20	119.5
O2—C8—C7	109.20 (17)	C22—C21—C20	118.61 (19)
C12—C8—C7	112.3 (2)	C22—C21—C24	121.0 (2)
O2—C8—C9	105.08 (16)	C20—C21—C24	120.4 (2)
C12—C8—C9	112.64 (17)	C23—C22—C21	121.0 (2)
C7—C8—C9	107.81 (18)	C23—C22—H22	119.5
O3—C9—C9A	105.46 (15)	C21—C22—H22	119.5
O3—C9—C8	112.79 (17)	C18—C23—C22	118.9 (2)
C9A—C9—C8	113.00 (17)	C18—C23—H23	120.5
O3—C9—H9	108.5	C22—C23—H23	120.5
C9A—C9—H9	108.5	C21—C24—H24A	109.5
C8—C9—H9	108.5	C21—C24—H24B	109.5
C5A—C9A—C9B	117.76 (18)	H24A—C24—H24B	109.5
C5A—C9A—C9	123.25 (18)	C21—C24—H24C	109.5
C9B—C9A—C9	118.82 (17)	H24A—C24—H24C	109.5
C1—C9B—C4A	114.59 (18)	H24B—C24—H24C	109.5
C1—C9B—C9A	127.53 (18)	O3—C25—C26	106.32 (17)
C4A—C9B—C9A	117.88 (18)	O3—C25—H25A	110.5

C5—C10—H10A	109.5	C26—C25—H25A	110.5
C5—C10—H10B	109.5	O3—C25—H25B	110.5
H10A—C10—H10B	109.5	C26—C25—H25B	110.5
C5—C10—H10C	109.5	H25A—C25—H25B	108.7
H10A—C10—H10C	109.5	C25—C26—H26A	109.5
H10B—C10—H10C	109.5	C25—C26—H26B	109.5
C5—C11—H11A	109.5	H26A—C26—H26B	109.5
C5—C11—H11B	109.5	C25—C26—H26C	109.5
H11A—C11—H11B	109.5	H26A—C26—H26C	109.5
C5—C11—H11C	109.5	H26B—C26—H26C	109.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9···S1	0.98	2.94	3.687 (2)	134
C10—H10*B*···O5^{i}	0.96	2.57	3.459 (2)	154
O2—H2···O6^{ii}	0.82	2.22	3.014 (2)	165

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