

2θ range / °	2.74 – 28.00
Crystal size / mm	0.52 × 0.39 × 0.22
Crystal habit	orange, prism
F(000)	320
Index ranges	-10<=h<=10, -12<=k<=12, -14<=l<=14
Reflections collected	32733
Independent reflections	3575 [R(int) = 0.0288]
Number of ref. parameters	183
R_1 / wR_2 [$I > 2\sigma(I)$]	0.0359 / 0.0975
R_1 / wR_2 (all data)	0.0436 / 0.1043
Goodness-of-fit on F^2	1.032
Completeness [%]	99.6
Largest diff. peak and hole / e·Å ⁻³	0.269/ -0.216
Weight scheme	$w=1/[\sigma^2(F_o^2)+(0.0550P)^2+0.2155P]$ where $P=(F_o^2+2F_c^2)/3$

Table 6. Selected bond lengths, bond angles and torsion angles for compound 7 b

Bond	<i>l</i> , Å	Angle	ϕ , °	Torsion angle	θ , °
S2-C11	1.6992(19)	C11-S2-C8	91.75(8)	O1-C2-C3-C4	-10.7(2)
S1-C16	1.7008(19)	O1-C2-C3	121.53(14)	O1-C2-C3-S1	166.78(12)
O2-C9	1.205(2)	C3-C2-C1	118.42(13)	C16-S1-C3-C4	0.51(11)
C1-C2	1.508(2)	C4-C3-S1	111.28(11)	C2-C3-C4-C15	177.15(13)
C2-C3	1.471(2)	C3-C4-C15	111.92(12)	C2-C3-C4-C5	-1.1(2)
C4-C15	1.432(2)	C15-C4-C5	122.23(12)	C3-C4-C5-C6	102.30(16)
C5-C6	1.554(2)	C8-C7-C6	125.53(13)	C4-C5-C6-C7	108.69(14)
C7-C8	1.388(2)	C7-C8-C9	129.56(13)	C5-C6-C7-C12	-72.05(18)
C8-C9	1.478(2)	C9-C8-S2	119.12(12)	C6-C7-C8-C9	-0.7(2)
C12-C13	1.508(2)	O2-C9-C10	119.75(16)	C6-C7-C8-S2	-178.75(11)
C13-C14	1.548(2)	C11-C12-C7	111.64(14)	C11-S2-C8-C9	-177.93(12)
C15-C16	1.370(2)	C7-C12-C13	126.16(13)	S2-C8-C9-O2	-175.09(15)
S2-C8	1.7318(17)	C12-C13-C14	115.02(14)	S2-C8-C9-C10	5.4(2)
S1-C3	1.7315(15)	C15-C14-C13	114.11(13)	C6-C7-C12-C11	178.67(13)
O1-C2	1.2160(19)	C16-C15-C4	112.04(13)	C6-C7-C12-C13	-0.8(2)

C3-C4	1.388(2)	C4-C15-C14	125.03(13)	C13-C12-C11-S2	179.42(11)
C4-C5	1.5060(19)	C16-S1-C3	91.79(8)	C11-C12-C13-C14	-108.48(17)
C6-C7	1.504(2)	O1-C2-C1	120.04(14)	C12-C13-C14-C15	-100.91(17)
C7-C12	1.436(2)	C4-C3-C2	129.05(13)	C5-C4-C15-C16	178.56(13)
C9-C10	1.503(2)	C2-C3-S1	119.63(11)	C5-C4-C15-C14	0.3(2)
C12-C11	1.373(2)	C3-C4-C5	125.83(12)	C13-C14-C15-C4	72.44(19)
C14-C15	1.507(2)	C4-C5-C6	112.31(12)	C14-C15-C16-S1	178.53(11)
		C7-C6-C5	113.03(12)	C1-C2-C3-C4	170.66(15)
		C8-C7-C12	112.07(12)	C1-C2-C3-S1	-11.87(19)
		C12-C7-C6	122.38(13)	C16-S1-C3-C2	-177.38(12)
		C7-C8-S2	111.29(11)	S1-C3-C4-C15	-0.49(15)
		O2-C9-C8	122.22(15)	S1-C3-C4-C5	-178.78(10)
		C8-C9-C10	118.03(15)	C15-C4-C5-C6	-75.82(16)
		C11-C12-C13	122.20(14)	C5-C6-C7-C8	106.06(16)
		C12-C11-S2	113.25(12)	C12-C7-C8-C9	177.61(14)
		C16-C15-C14	122.91(13)	C12-C7-C8-S2	-0.47(15)
		C15-C16-S1	112.96(12)	C11-S2-C8-C7	0.38(12)
				C7-C8-C9-O2	7.0(3)

C7-C8-C9-C10	-172.57(16)
C8-C7-C12-C11	0.33(18)
C8-C7-C12-C13	-179.10(13)
C7-C12-C11-S2	-0.04(17)
C8-S2-C11-C12	-0.19(13)
C7-C12-C13-C14	70.90(19)
C3-C4-C15-C16	0.20(18)
C3-C4-C15-C14	-178.09(13)
C13-C14-C15-C16	-105.67(17)
C4-C15-C16-S1	0.19(17)
C3-S1-C16-C15	-0.40(13)