Table 1. Crystal data and structure refinement for **122c**

Identification code	**122c**	
Empirical formula	$C_{22}H_{27}NO_3S$	
Formula weight	385.51	
Temperature	100(2) K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	*P* 2_1/c	
Unit cell dimensions	a = 9.675(6) Å	α= 90°.
	b = 27.658(16) Å	β= 107.333(9)°.
	c = 7.812(4) Å	γ = 90°.
Volume	1996(2) $Å^3$	
Z	4	
Density (calculated)	1.283 Mg/m^3	
Absorption coefficient	0.184 mm^{-1}	
F(000)	824	
Crystal size	0.08 x 0.06 x 0.04 mm^3	
Theta range for data collection	2.95 to 27.48°.	
Index ranges	-12<=h<=12, -35<=k<=31, -9<=l<=10	
Reflections collected	11646	
Independent reflections	4563 [R(int) = 0.0559]	
Completeness to theta = 27.48°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.845	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4563 / 0 / 247	
Goodness-of-fit on F^2	1.087	
Final R indices [I>2sigma(I)]	R1 = 0.0610, wR2 = 0.1234	
R indices (all data)	R1 = 0.0799, wR2 = 0.1328	
Largest diff. peak and hole	0.299 and -0.351 e.$Å^{-3}$	

Notes:

The structure indicated the relative stereochemistry of the chiral centres. However, as the structure is in a centrosymmetric space group both enantiomers are present. This means that in two of the molecules in the unit cell C(2) and C(3) are *R* while C(4) is *S* and in the other two molecules C(2) and C(3) are *S* while C(4) is *R*.

The hydrogen atoms have been fixed as riding models.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **122c**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(2)	4562(2)	1440(1)	1067(3)	19(1)
C(3)	4398(2)	1565(1)	2918(3)	20(1)
C(4)	5634(2)	1902(1)	3998(3)	21(1)
C(5)	7115(2)	1710(1)	4067(3)	24(1)
C(6)	7215(2)	1629(1)	2189(3)	22(1)
C(10)	7779(2)	573(1)	748(3)	20(1)
C(11)	7420(3)	132(1)	1344(3)	26(1)
C(12)	8531(3)	-179(1)	2242(3)	31(1)
C(13)	9977(3)	-56(1)	2573(3)	28(1)
C(14)	10313(3)	388(1)	1939(3)	28(1)
C(15)	9217(3)	702(1)	1027(3)	24(1)
C(16)	11171(3)	-394(1)	3576(4)	42(1)
C(17)	4095(2)	1858(1)	-300(3)	22(1)
C(18)	2509(2)	1979(1)	-649(3)	20(1)
C(19)	1441(3)	1641(1)	-1434(3)	24(1)
C(20)	-12(3)	1746(1)	-1691(3)	28(1)
C(21)	-417(3)	2189(1)	-1191(3)	30(1)
C(22)	635(3)	2530(1)	-432(4)	32(1)
C(23)	2089(3)	2424(1)	-152(3)	26(1)
C(24)	4160(2)	1128(1)	3966(3)	23(1)
C(25)	4919(3)	700(1)	4059(4)	34(1)
C(26)	3062(3)	1174(1)	4862(3)	30(1)
N(1)	6076(2)	1281(1)	1270(2)	20(1)
O(8)	5083(2)	694(1)	-1170(2)	25(1)
O(9)	6918(2)	1276(1)	-1514(2)	23(1)
O(27)	5543(2)	2003(1)	5754(2)	25(1)
S(7)	6368(1)	971(1)	-369(1)	20(1)

Table 3. Bond lengths [Å] and angles [°] for **122c**.

C(2)-N(1)	1.492(3)	C(16)-H(16A)	0.9800
C(2)-C(3)	1.540(3)	C(16)-H(16B)	0.9800
C(2)-C(17)	1.547(3)	C(16)-H(16C)	0.9800
C(2)-H(2)	1.0000	C(17)-C(18)	1.514(3)
C(3)-C(24)	1.516(3)	C(17)-H(17A)	0.9900
C(3)-C(4)	1.553(3)	C(17)-H(17B)	0.9900
C(3)-H(3)	1.0000	C(18)-C(23)	1.387(3)
C(4)-O(27)	1.428(3)	C(18)-C(19)	1.393(3)
C(4)-C(5)	1.514(3)	C(19)-C(20)	1.390(3)
C(4)-H(4)	1.0000	C(19)-H(19)	0.9500
C(5)-C(6)	1.515(3)	C(20)-C(21)	1.379(4)
C(5)-H(5A)	0.9900	C(20)-H(20)	0.9500
C(5)-H(5B)	0.9900	C(21)-C(22)	1.385(4)
C(6)-N(1)	1.478(3)	C(21)-H(21)	0.9500
C(6)-H(6A)	0.9900	C(22)-C(23)	1.390(3)
C(6)-H(6B)	0.9900	C(22)-H(22)	0.9500
C(10)-C(11)	1.386(3)	C(23)-H(23)	0.9500
C(10)-C(15)	1.389(3)	C(24)-C(25)	1.383(3)
C(10)-S(7)	1.768(2)	C(24)-C(26)	1.442(3)
C(11)-C(12)	1.392(3)	C(25)-H(25A)	0.9500
C(11)-H(11)	0.9500	C(25)-H(25B)	0.9500
C(12)-C(13)	1.388(4)	C(26)-H(26A)	0.9800
C(12)-H(12)	0.9500	C(26)-H(26B)	0.9800
C(13)-C(14)	1.398(4)	C(26)-H(26C)	0.9800
C(13)-C(16)	1.511(3)	N(1)-S(7)	1.635(2)
C(14)-C(15)	1.392(3)	O(8)-S(7)	1.4359(17)
C(14)-H(14)	0.9500	O(9)-S(7)	1.4424(17)
C(15)-H(15)	0.9500	O(27)-H(27)	0.8400

N(1)-C(2)-C(3)	109.82(17)	C(17)-C(2)-H(2)	107.4
N(1)-C(2)-C(17)	111.67(18)	C(24)-C(3)-C(2)	113.73(19)
C(3)-C(2)-C(17)	112.94(19)	C(24)-C(3)-C(4)	113.71(18)
N(1)-C(2)-H(2)	107.4	C(2)-C(3)-C(4)	111.49(18)
C(3)-C(2)-H(2)	107.4	C(24)-C(3)-H(3)	105.7

C(2)-C(3)-H(3)	105.7	C(10)-C(15)-H(15)	120.2
C(4)-C(3)-H(3)	105.7	C(14)-C(15)-H(15)	120.2
O(27)-C(4)-C(5)	111.27(18)	C(13)-C(16)-H(16A)	109.5
O(27)-C(4)-C(3)	112.42(19)	C(13)-C(16)-H(16B)	109.5
C(5)-C(4)-C(3)	112.04(19)	H(16A)-C(16)-H(16B)	109.5
O(27)-C(4)-H(4)	106.9	C(13)-C(16)-H(16C)	109.5
C(5)-C(4)-H(4)	106.9	H(16A)-C(16)-H(16C)	109.5
C(3)-C(4)-H(4)	106.9	H(16B)-C(16)-H(16C)	109.5
C(4)-C(5)-C(6)	110.47(18)	C(18)-C(17)-C(2)	111.19(18)
C(4)-C(5)-H(5A)	109.6	C(18)-C(17)-H(17A)	109.4
C(6)-C(5)-H(5A)	109.6	C(2)-C(17)-H(17A)	109.4
C(4)-C(5)-H(5B)	109.6	C(18)-C(17)-H(17B)	109.4
C(6)-C(5)-H(5B)	109.6	C(2)-C(17)-H(17B)	109.4
H(5A)-C(5)-H(5B)	108.1	H(17A)-C(17)-H(17B)	108.0
N(1)-C(6)-C(5)	108.18(19)	C(23)-C(18)-C(19)	118.6(2)
N(1)-C(6)-H(6A)	110.1	C(23)-C(18)-C(17)	120.7(2)
C(5)-C(6)-H(6A)	110.1	C(19)-C(18)-C(17)	120.6(2)
N(1)-C(6)-H(6B)	110.1	C(20)-C(19)-C(18)	120.6(2)
C(5)-C(6)-H(6B)	110.1	C(20)-C(19)-H(19)	119.7
H(6A)-C(6)-H(6B)	108.4	C(18)-C(19)-H(19)	119.7
C(11)-C(10)-C(15)	120.8(2)	C(21)-C(20)-C(19)	120.3(2)
C(11)-C(10)-S(7)	118.62(18)	C(21)-C(20)-H(20)	119.8
C(15)-C(10)-S(7)	120.53(18)	C(19)-C(20)-H(20)	119.8
C(10)-C(11)-C(12)	118.7(2)	C(20)-C(21)-C(22)	119.6(2)
C(10)-C(11)-H(11)	120.7	C(20)-C(21)-H(21)	120.2
C(12)-C(11)-H(11)	120.7	C(22)-C(21)-H(21)	120.2
C(13)-C(12)-C(11)	121.8(2)	C(21)-C(22)-C(23)	120.2(2)
C(13)-C(12)-H(12)	119.1	C(21)-C(22)-H(22)	119.9
C(11)-C(12)-H(12)	119.1	C(23)-C(22)-H(22)	119.9
C(12)-C(13)-C(14)	118.5(2)	C(18)-C(23)-C(22)	120.7(2)
C(12)-C(13)-C(16)	121.2(3)	C(18)-C(23)-H(23)	119.6
C(14)-C(13)-C(16)	120.3(3)	C(22)-C(23)-H(23)	119.6
C(15)-C(14)-C(13)	120.5(2)	C(25)-C(24)-C(26)	120.5(2)
C(15)-C(14)-H(14)	119.7	C(25)-C(24)-C(3)	123.2(2)
C(13)-C(14)-H(14)	119.7	C(26)-C(24)-C(3)	116.3(2)
C(10)-C(15)-C(14)	119.6(2)	C(24)-C(25)-H(25A)	120.0

C(24)-C(25)-H(25B)	120.0	C(6)-N(1)-S(7)	116.44(16)
H(25A)-C(25)-H(25B)	120.0	C(2)-N(1)-S(7)	117.68(14)
C(24)-C(26)-H(26A)	109.5	C(4)-O(27)-H(27)	109.5
C(24)-C(26)-H(26B)	109.5	O(8)-S(7)-O(9)	118.26(10)
H(26A)-C(26)-H(26B)	109.5	O(8)-S(7)-N(1)	107.04(10)
C(24)-C(26)-H(26C)	109.5	O(9)-S(7)-N(1)	111.11(10)
H(26A)-C(26)-H(26C)	109.5	O(8)-S(7)-C(10)	108.93(11)
H(26B)-C(26)-H(26C)	109.5	O(9)-S(7)-C(10)	107.25(11)
C(6)-N(1)-C(2)	115.21(18)	N(1)-S(7)-C(10)	103.21(11)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **122c**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(2)	14(1)	23(1)	20(1)	1(1)	4(1)	0(1)
C(3)	16(1)	24(1)	20(1)	1(1)	6(1)	3(1)
C(4)	21(1)	23(1)	20(1)	1(1)	7(1)	1(1)
C(5)	21(1)	25(1)	24(1)	-3(1)	2(1)	-1(1)
C(6)	16(1)	24(1)	26(1)	-3(1)	5(1)	-3(1)
C(10)	20(1)	22(1)	19(1)	-1(1)	5(1)	1(1)
C(11)	30(1)	23(1)	27(1)	-3(1)	12(1)	-1(1)
C(12)	48(2)	21(1)	26(1)	3(1)	16(1)	7(1)
C(13)	36(1)	29(1)	19(1)	-3(1)	7(1)	14(1)
C(14)	22(1)	34(1)	25(1)	-8(1)	4(1)	7(1)
C(15)	25(1)	23(1)	22(1)	1(1)	6(1)	2(1)
C(16)	51(2)	42(2)	30(2)	3(1)	8(1)	25(1)
C(17)	17(1)	25(1)	23(1)	4(1)	6(1)	-1(1)
C(18)	17(1)	25(1)	17(1)	5(1)	4(1)	0(1)
C(19)	26(1)	22(1)	22(1)	2(1)	5(1)	0(1)
C(20)	20(1)	32(1)	26(1)	5(1)	-1(1)	-6(1)
C(21)	18(1)	43(2)	31(1)	1(1)	8(1)	4(1)
C(22)	24(1)	34(1)	37(2)	-8(1)	8(1)	6(1)
C(23)	23(1)	26(1)	25(1)	-3(1)	4(1)	0(1)
C(24)	18(1)	29(1)	19(1)	2(1)	3(1)	-3(1)
C(25)	38(2)	28(1)	41(2)	12(1)	20(1)	4(1)
C(26)	30(1)	33(1)	28(1)	-1(1)	10(1)	-8(1)
N(1)	15(1)	23(1)	21(1)	-3(1)	5(1)	-1(1)
O(8)	20(1)	29(1)	24(1)	-3(1)	5(1)	-4(1)
O(9)	20(1)	27(1)	23(1)	6(1)	8(1)	2(1)
O(27)	28(1)	27(1)	21(1)	0(1)	7(1)	4(1)
S(7)	16(1)	23(1)	20(1)	1(1)	5(1)	0(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **122c**.

	x	y	z	U(eq)
H(2)	3912	1159	585	23
H(3)	3490	1761	2670	24
H(4)	5513	2217	3341	25
H(5A)	7290	1400	4736	29
H(5B)	7868	1943	4708	29
H(6A)	7075	1939	1525	27
H(6B)	8181	1500	2244	27
H(11)	6435	44	1144	31
H(12)	8292	-484	2639	37
H(14)	11297	475	2132	33
H(15)	9451	1003	597	28
H(16A)	10877	-562	4516	63
H(16B)	12055	-208	4122	63
H(16C)	11357	-632	2741	63
H(17A)	4688	2148	168	26
H(17B)	4270	1764	-1440	26
H(19)	1709	1336	-1798	29
H(20)	-729	1510	-2213	33
H(21)	-1410	2260	-1365	36
H(22)	360	2838	-103	38
H(23)	2804	2659	385	31
H(25A)	4719	434	4717	41
H(25B)	5642	672	3465	41
H(26A)	3010	875	5510	46
H(26B)	2123	1236	3973	46
H(26C)	3306	1444	5712	46
H(27)	5798	1758	6406	38

Table 6. Torsion angles [°] for **122c**

N(1)-C(2)-C(3)-C(24)	-81.5(2)
C(17)-C(2)-C(3)-C(24)	153.12(19)
N(1)-C(2)-C(3)-C(4)	48.7(2)
C(17)-C(2)-C(3)-C(4)	-76.7(2)
C(24)-C(3)-C(4)-O(27)	-46.9(3)
C(2)-C(3)-C(4)-O(27)	-177.07(17)
C(24)-C(3)-C(4)-C(5)	79.3(2)
C(2)-C(3)-C(4)-C(5)	-50.9(2)
O(27)-C(4)-C(5)-C(6)	-177.04(18)
C(3)-C(4)-C(5)-C(6)	56.1(2)
C(4)-C(5)-C(6)-N(1)	-59.1(2)
C(15)-C(10)-C(11)-C(12)	0.5(4)
S(7)-C(10)-C(11)-C(12)	-179.27(18)
C(10)-C(11)-C(12)-C(13)	0.9(4)
C(11)-C(12)-C(13)-C(14)	-1.7(4)
C(11)-C(12)-C(13)-C(16)	179.0(2)
C(12)-C(13)-C(14)-C(15)	1.2(4)
C(16)-C(13)-C(14)-C(15)	-179.5(2)
C(11)-C(10)-C(15)-C(14)	-1.0(4)
S(7)-C(10)-C(15)-C(14)	178.80(18)
C(13)-C(14)-C(15)-C(10)	0.1(4)
N(1)-C(2)-C(17)-C(18)	173.73(18)
C(3)-C(2)-C(17)-C(18)	-61.9(2)
C(2)-C(17)-C(18)-C(23)	114.7(2)
C(2)-C(17)-C(18)-C(19)	-63.7(3)
C(23)-C(18)-C(19)-C(20)	-0.9(3)
C(17)-C(18)-C(19)-C(20)	177.5(2)
C(18)-C(19)-C(20)-C(21)	0.8(4)
C(19)-C(20)-C(21)-C(22)	0.1(4)
C(20)-C(21)-C(22)-C(23)	-1.0(4)
C(19)-C(18)-C(23)-C(22)	0.0(4)
C(17)-C(18)-C(23)-C(22)	-178.4(2)
C(21)-C(22)-C(23)-C(18)	0.9(4)
C(2)-C(3)-C(24)-C(25)	42.5(3)

C(4)-C(3)-C(24)-C(25)	-86.5(3)
C(2)-C(3)-C(24)-C(26)	-136.4(2)
C(4)-C(3)-C(24)-C(26)	94.5(2)
C(5)-C(6)-N(1)-C(2)	61.0(2)
C(5)-C(6)-N(1)-S(7)	-155.16(15)
C(3)-C(2)-N(1)-C(6)	-56.0(2)
C(17)-C(2)-N(1)-C(6)	70.1(2)
C(3)-C(2)-N(1)-S(7)	160.60(15)
C(17)-C(2)-N(1)-S(7)	-73.3(2)
C(6)-N(1)-S(7)-O(8)	-174.61(15)
C(2)-N(1)-S(7)-O(8)	-31.67(18)
C(6)-N(1)-S(7)-O(9)	-44.13(18)
C(2)-N(1)-S(7)-O(9)	98.82(17)
C(6)-N(1)-S(7)-C(10)	70.52(18)
C(2)-N(1)-S(7)-C(10)	-146.53(16)
C(11)-C(10)-S(7)-O(8)	-25.4(2)
C(15)-C(10)-S(7)-O(8)	154.81(19)
C(11)-C(10)-S(7)-O(9)	-154.53(18)
C(15)-C(10)-S(7)-O(9)	25.7(2)
C(11)-C(10)-S(7)-N(1)	88.1(2)
C(15)-C(10)-S(7)-N(1)	-91.7(2)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for **122c** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(27)-H(27)...O(9)#1	0.84	2.13	2.947(2)	163.3

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z+1

Table 1. Crystal data and structure refinement for **126**

Identification code	**126**	
Empirical formula	$C_{22}H_{27}NO_3S$	
Formula weight	385.51	
Temperature	100(2) K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	*P* 2_1/c	
Unit cell dimensions	a = 20.061(7) Å	α= 90°.
	b = 6.637(2) Å	β= 104.124(7)°.
	c = 14.843(6) Å	γ = 90°.
Volume	1916.6(12) $Å^3$	
Z	4	
Density (calculated)	1.336 Mg/m^3	
Absorption coefficient	0.192 mm^{-1}	
F(000)	824	
Crystal size	0.12 x 0.09 x 0.01 mm^3	
Theta range for data collection	3.08 to 27.48°.	
Index ranges	-25<=h<=26, -8<=k<=8, -14<=l<=19	
Reflections collected	10755	
Independent reflections	4376 [R(int) = 0.0294]	
Completeness to theta = 27.48°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.886	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4376 / 0 / 248	
Goodness-of-fit on F^2	1.093	
Final R indices [I>2sigma(I)]	R1 = 0.0466, wR2 = 0.1077	
R indices (all data)	R1 = 0.0549, wR2 = 0.1125	
Largest diff. peak and hole	0.650 and -0.388 e.$Å^{-3}$	

Notes:

The structure indicated the relative stereochemistry of the chiral centres. However, as the structure is in a centrosymmetric space group both enantiomers are present. This means that in two of the molecules in the unit cell C(2) and C(3) are *R* while C(4) is *S* and in the other two molecules C(2) and C(3) are *S* while C(4) is *R*.

The hydrogen atoms have been fixed as riding models.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **126**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(2)	2285(1)	4104(2)	8165(1)	17(1)
C(3)	1967(1)	2941(2)	7274(1)	17(1)
C(4)	2520(1)	1535(3)	7069(1)	19(1)
C(5)	2644(1)	-161(3)	7790(1)	22(1)
C(6)	2567(1)	555(2)	8742(1)	20(1)
C(10)	4114(1)	3260(3)	9165(1)	18(1)
C(11)	4433(1)	4920(3)	8897(1)	21(1)
C(12)	5032(1)	4649(3)	8595(1)	23(1)
C(13)	5310(1)	2735(3)	8558(1)	22(1)
C(14)	4975(1)	1087(3)	8821(1)	23(1)
C(15)	4379(1)	1334(3)	9130(1)	22(1)
C(16)	5975(1)	2482(3)	8268(1)	31(1)
C(17)	1719(1)	5071(3)	8538(1)	21(1)
C(18)	1240(1)	6299(3)	7805(1)	19(1)
C(19)	856(1)	7819(3)	8093(1)	24(1)
C(20)	390(1)	8979(3)	7464(1)	27(1)
C(21)	307(1)	8620(3)	6519(1)	27(1)
C(22)	696(1)	7155(3)	6223(1)	25(1)
C(23)	1170(1)	5960(3)	6854(1)	20(1)
C(24)	1596(1)	4378(3)	6478(1)	20(1)
C(25)	1111(1)	3090(3)	5731(1)	29(1)
C(26)	2102(1)	5489(3)	6019(1)	24(1)
N(1)	2701(1)	2731(2)	8874(1)	17(1)
O(8)	3272(1)	5713(2)	9676(1)	24(1)
O(9)	3484(1)	2328(2)	10414(1)	25(1)
O(27)	3148(1)	2623(2)	7149(1)	22(1)
S(7)	3377(1)	3588(1)	9599(1)	18(1)

Table 3. Bond lengths [Å] and angles [°] for **126**.

C(2)-N(1)	1.485(2)	C(16)-H(16B)	0.9800
C(2)-C(17)	1.520(2)	C(16)-H(16C)	0.9800
C(2)-C(3)	1.530(2)	C(17)-C(18)	1.503(2)
C(2)-H(2)	1.0000	C(17)-H(17A)	0.9900
C(3)-C(4)	1.537(2)	C(17)-H(17B)	0.9900
C(3)-C(24)	1.558(2)	C(18)-C(19)	1.399(2)
C(3)-H(3)	1.0000	C(18)-C(23)	1.403(2)
C(4)-O(27)	1.4312(19)	C(19)-C(20)	1.383(3)
C(4)-C(5)	1.531(2)	C(19)-H(19)	0.9500
C(4)-H(4)	1.0000	C(20)-C(21)	1.392(3)
C(5)-C(6)	1.534(2)	C(20)-H(20)	0.9500
C(5)-H(5A)	0.9900	C(21)-C(22)	1.384(3)
C(5)-H(5B)	0.9900	C(21)-H(21)	0.9500
C(6)-N(1)	1.473(2)	C(22)-C(23)	1.405(2)
C(6)-H(6A)	0.9900	C(22)-H(22)	0.9500
C(6)-H(6B)	0.9900	C(23)-C(24)	1.542(2)
C(10)-C(11)	1.381(2)	C(24)-C(26)	1.542(2)
C(10)-C(15)	1.390(2)	C(24)-C(25)	1.543(2)
C(10)-S(7)	1.7635(17)	C(25)-H(25A)	0.9800
C(11)-C(12)	1.392(2)	C(25)-H(25B)	0.9800
C(11)-H(11)	0.9500	C(25)-H(25C)	0.9800
C(12)-C(13)	1.394(3)	C(26)-H(26A)	0.9800
C(12)-H(12)	0.9500	C(26)-H(26B)	0.9800
C(13)-C(14)	1.388(3)	C(26)-H(26C)	0.9800
C(13)-C(16)	1.508(2)	N(1)-S(7)	1.6157(14)
C(14)-C(15)	1.391(2)	O(8)-S(7)	1.4351(14)
C(14)-H(14)	0.9500	O(9)-S(7)	1.4426(13)
C(15)-H(15)	0.9500	O(27)-H(27)	0.8400
C(16)-H(16A)	0.9800		

N(1)-C(2)-C(17)	109.97(13)	C(17)-C(2)-H(2)	109.0
N(1)-C(2)-C(3)	110.28(13)	C(3)-C(2)-H(2)	109.0
C(17)-C(2)-C(3)	109.70(13)	C(2)-C(3)-C(4)	107.98(13)
N(1)-C(2)-H(2)	109.0	C(2)-C(3)-C(24)	111.56(14)

C(4)-C(3)-C(24)	117.13(13)	C(15)-C(14)-H(14)	119.6
C(2)-C(3)-H(3)	106.5	C(10)-C(15)-C(14)	119.22(16)
C(4)-C(3)-H(3)	106.5	C(10)-C(15)-H(15)	120.4
C(24)-C(3)-H(3)	106.5	C(14)-C(15)-H(15)	120.4
O(27)-C(4)-C(5)	108.90(13)	C(13)-C(16)-H(16A)	109.5
O(27)-C(4)-C(3)	109.91(14)	C(13)-C(16)-H(16B)	109.5
C(5)-C(4)-C(3)	108.04(13)	H(16A)-C(16)-H(16B)	109.5
O(27)-C(4)-H(4)	110.0	C(13)-C(16)-H(16C)	109.5
C(5)-C(4)-H(4)	110.0	H(16A)-C(16)-H(16C)	109.5
C(3)-C(4)-H(4)	110.0	H(16B)-C(16)-H(16C)	109.5
C(4)-C(5)-C(6)	112.37(14)	C(18)-C(17)-C(2)	111.55(14)
C(4)-C(5)-H(5A)	109.1	C(18)-C(17)-H(17A)	109.3
C(6)-C(5)-H(5A)	109.1	C(2)-C(17)-H(17A)	109.3
C(4)-C(5)-H(5B)	109.1	C(18)-C(17)-H(17B)	109.3
C(6)-C(5)-H(5B)	109.1	C(2)-C(17)-H(17B)	109.3
H(5A)-C(5)-H(5B)	107.9	H(17A)-C(17)-H(17B)	108.0
N(1)-C(6)-C(5)	111.71(13)	C(19)-C(18)-C(23)	119.71(16)
N(1)-C(6)-H(6A)	109.3	C(19)-C(18)-C(17)	118.22(15)
C(5)-C(6)-H(6A)	109.3	C(23)-C(18)-C(17)	122.07(15)
N(1)-C(6)-H(6B)	109.3	C(20)-C(19)-C(18)	121.81(17)
C(5)-C(6)-H(6B)	109.3	C(20)-C(19)-H(19)	119.1
H(6A)-C(6)-H(6B)	107.9	C(18)-C(19)-H(19)	119.1
C(11)-C(10)-C(15)	120.98(15)	C(19)-C(20)-C(21)	118.70(17)
C(11)-C(10)-S(7)	119.68(13)	C(19)-C(20)-H(20)	120.6
C(15)-C(10)-S(7)	119.30(13)	C(21)-C(20)-H(20)	120.6
C(10)-C(11)-C(12)	119.11(16)	C(22)-C(21)-C(20)	120.14(17)
C(10)-C(11)-H(11)	120.4	C(22)-C(21)-H(21)	119.9
C(12)-C(11)-H(11)	120.4	C(20)-C(21)-H(21)	119.9
C(11)-C(12)-C(13)	121.00(16)	C(21)-C(22)-C(23)	121.79(18)
C(11)-C(12)-H(12)	119.5	C(21)-C(22)-H(22)	119.1
C(13)-C(12)-H(12)	119.5	C(23)-C(22)-H(22)	119.1
C(14)-C(13)-C(12)	118.81(15)	C(18)-C(23)-C(22)	117.81(16)
C(14)-C(13)-C(16)	120.98(17)	C(18)-C(23)-C(24)	123.00(15)
C(12)-C(13)-C(16)	120.17(17)	C(22)-C(23)-C(24)	119.19(16)
C(13)-C(14)-C(15)	120.88(17)	C(26)-C(24)-C(23)	108.54(14)
C(13)-C(14)-H(14)	119.6	C(26)-C(24)-C(25)	108.38(14)

C(23)-C(24)-C(25)	109.18(14)	C(24)-C(26)-H(26C)	109.5
C(26)-C(24)-C(3)	112.58(14)	H(26A)-C(26)-H(26C)	109.5
C(23)-C(24)-C(3)	110.29(13)	H(26B)-C(26)-H(26C)	109.5
C(25)-C(24)-C(3)	107.81(14)	C(6)-N(1)-C(2)	117.05(13)
C(24)-C(25)-H(25A)	109.5	C(6)-N(1)-S(7)	121.99(11)
C(24)-C(25)-H(25B)	109.5	C(2)-N(1)-S(7)	119.43(11)
H(25A)-C(25)-H(25B)	109.5	C(4)-O(27)-H(27)	109.5
C(24)-C(25)-H(25C)	109.5	O(8)-S(7)-O(9)	119.80(8)
H(25A)-C(25)-H(25C)	109.5	O(8)-S(7)-N(1)	106.48(7)
H(25B)-C(25)-H(25C)	109.5	O(9)-S(7)-N(1)	106.43(8)
C(24)-C(26)-H(26A)	109.5	O(8)-S(7)-C(10)	107.63(8)
C(24)-C(26)-H(26B)	109.5	O(9)-S(7)-C(10)	105.59(8)
H(26A)-C(26)-H(26B)	109.5	N(1)-S(7)-C(10)	110.84(8)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **126**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(2)	15(1)	19(1)	17(1)	0(1)	5(1)	0(1)
C(3)	15(1)	20(1)	18(1)	-2(1)	5(1)	-3(1)
C(4)	18(1)	23(1)	18(1)	-4(1)	5(1)	-2(1)
C(5)	22(1)	18(1)	26(1)	-2(1)	8(1)	0(1)
C(6)	19(1)	19(1)	23(1)	2(1)	7(1)	-2(1)
C(10)	16(1)	25(1)	14(1)	-1(1)	3(1)	2(1)
C(11)	21(1)	22(1)	19(1)	1(1)	3(1)	1(1)
C(12)	22(1)	29(1)	20(1)	2(1)	5(1)	-5(1)
C(13)	16(1)	35(1)	14(1)	-3(1)	3(1)	-1(1)
C(14)	19(1)	27(1)	24(1)	-1(1)	5(1)	4(1)
C(15)	20(1)	24(1)	22(1)	2(1)	6(1)	-1(1)
C(16)	19(1)	48(1)	28(1)	-10(1)	9(1)	-5(1)
C(17)	17(1)	26(1)	19(1)	-3(1)	5(1)	2(1)
C(18)	13(1)	20(1)	26(1)	-1(1)	5(1)	-2(1)
C(19)	15(1)	25(1)	32(1)	-5(1)	9(1)	-1(1)
C(20)	18(1)	21(1)	44(1)	1(1)	11(1)	2(1)
C(21)	18(1)	25(1)	38(1)	9(1)	5(1)	3(1)
C(22)	18(1)	29(1)	28(1)	5(1)	5(1)	-1(1)
C(23)	14(1)	21(1)	25(1)	1(1)	6(1)	-2(1)
C(24)	17(1)	23(1)	18(1)	-1(1)	3(1)	0(1)
C(25)	28(1)	30(1)	24(1)	-2(1)	-3(1)	-3(1)
C(26)	25(1)	27(1)	21(1)	3(1)	10(1)	1(1)
N(1)	15(1)	20(1)	17(1)	0(1)	4(1)	0(1)
O(8)	21(1)	25(1)	26(1)	-9(1)	3(1)	2(1)
O(9)	21(1)	39(1)	16(1)	4(1)	7(1)	1(1)
O(27)	17(1)	31(1)	20(1)	-2(1)	10(1)	-4(1)
S(7)	15(1)	25(1)	16(1)	-2(1)	4(1)	1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **126**.

	x	y	z	U(eq)
H(2)	2589	5186	8021	20
H(3)	1603	2054	7417	21
H(4)	2362	959	6430	23
H(5A)	3112	-708	7857	26
H(5B)	2312	-1263	7566	26
H(6A)	2095	260	8799	24
H(6B)	2892	-197	9237	24
H(11)	4247	6230	8919	25
H(12)	5254	5786	8411	28
H(14)	5156	-227	8790	28
H(15)	4156	200	9315	26
H(16A)	6362	2746	8800	47
H(16B)	5987	3435	7768	47
H(16C)	6006	1103	8047	47
H(17A)	1454	4005	8763	25
H(17B)	1928	5948	9071	25
H(19)	916	8060	8739	28
H(20)	132	10002	7672	33
H(21)	-17	9383	6077	33
H(22)	642	6951	5576	30
H(25A)	921	3922	5183	43
H(25B)	735	2567	5980	43
H(25C)	1368	1962	5556	43
H(26A)	1852	6489	5578	35
H(26B)	2323	4515	5688	35
H(26C)	2454	6167	6498	35
H(27)	3258	2595	6638	33

Table 6. Torsion angles [°] for **126**.

N(1)-C(2)-C(3)-C(4)	-43.42(17)
C(17)-C(2)-C(3)-C(4)	-164.68(14)
N(1)-C(2)-C(3)-C(24)	-173.49(12)
C(17)-C(2)-C(3)-C(24)	65.25(17)
C(2)-C(3)-C(4)-O(27)	-47.50(17)
C(24)-C(3)-C(4)-O(27)	79.40(17)
C(2)-C(3)-C(4)-C(5)	71.20(16)
C(24)-C(3)-C(4)-C(5)	-161.90(14)
O(27)-C(4)-C(5)-C(6)	85.28(16)
C(3)-C(4)-C(5)-C(6)	-34.06(18)
C(4)-C(5)-C(6)-N(1)	-25.50(19)
C(15)-C(10)-C(11)-C(12)	-0.4(2)
S(7)-C(10)-C(11)-C(12)	177.15(12)
C(10)-C(11)-C(12)-C(13)	0.1(3)
C(11)-C(12)-C(13)-C(14)	0.6(3)
C(11)-C(12)-C(13)-C(16)	-177.39(16)
C(12)-C(13)-C(14)-C(15)	-1.0(3)
C(16)-C(13)-C(14)-C(15)	176.99(16)
C(11)-C(10)-C(15)-C(14)	0.0(2)
S(7)-C(10)-C(15)-C(14)	-177.53(13)
C(13)-C(14)-C(15)-C(10)	0.7(3)
N(1)-C(2)-C(17)-C(18)	-173.91(13)
C(3)-C(2)-C(17)-C(18)	-52.47(19)
C(2)-C(17)-C(18)-C(19)	-157.70(15)
C(2)-C(17)-C(18)-C(23)	22.5(2)
C(23)-C(18)-C(19)-C(20)	1.6(3)
C(17)-C(18)-C(19)-C(20)	-178.21(16)
C(18)-C(19)-C(20)-C(21)	-0.2(3)
C(19)-C(20)-C(21)-C(22)	-1.3(3)
C(20)-C(21)-C(22)-C(23)	1.6(3)
C(19)-C(18)-C(23)-C(22)	-1.4(2)
C(17)-C(18)-C(23)-C(22)	178.44(15)
C(19)-C(18)-C(23)-C(24)	177.35(15)
C(17)-C(18)-C(23)-C(24)	-2.8(2)

C(21)-C(22)-C(23)-C(18)	-0.2(3)
C(21)-C(22)-C(23)-C(24)	-178.94(16)
C(18)-C(23)-C(24)-C(26)	-110.59(18)
C(22)-C(23)-C(24)-C(26)	68.10(19)
C(18)-C(23)-C(24)-C(25)	131.46(17)
C(22)-C(23)-C(24)-C(25)	-49.8(2)
C(18)-C(23)-C(24)-C(3)	13.2(2)
C(22)-C(23)-C(24)-C(3)	-168.13(15)
C(2)-C(3)-C(24)-C(26)	77.88(17)
C(4)-C(3)-C(24)-C(26)	-47.2(2)
C(2)-C(3)-C(24)-C(23)	-43.52(17)
C(4)-C(3)-C(24)-C(23)	-168.64(13)
C(2)-C(3)-C(24)-C(25)	-162.64(13)
C(4)-C(3)-C(24)-C(25)	72.24(18)
C(5)-C(6)-N(1)-C(2)	55.82(18)
C(5)-C(6)-N(1)-S(7)	-110.00(14)
C(17)-C(2)-N(1)-C(6)	102.31(16)
C(3)-C(2)-N(1)-C(6)	-18.80(18)
C(17)-C(2)-N(1)-S(7)	-91.50(15)
C(3)-C(2)-N(1)-S(7)	147.40(11)
C(6)-N(1)-S(7)-O(8)	-169.02(12)
C(2)-N(1)-S(7)-O(8)	25.49(13)
C(6)-N(1)-S(7)-O(9)	-40.15(14)
C(2)-N(1)-S(7)-O(9)	154.36(11)
C(6)-N(1)-S(7)-C(10)	74.19(14)
C(2)-N(1)-S(7)-C(10)	-91.30(13)
C(11)-C(10)-S(7)-O(8)	-5.42(16)
C(15)-C(10)-S(7)-O(8)	172.19(13)
C(11)-C(10)-S(7)-O(9)	-134.47(14)
C(15)-C(10)-S(7)-O(9)	43.14(15)
C(11)-C(10)-S(7)-N(1)	110.66(14)
C(15)-C(10)-S(7)-N(1)	-71.73(15)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for **126** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(27)-H(27)...O(9)#1	0.84	1.98	2.8172(18)	176.7

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+1/2,z-1/2

Data for **der-122d:**

Bond search complete.

4	Br	- C	bonds ... from	1.899	to	1.899 Å (mean	1.899 Å)
260	C	- C	bonds ... from	1.320	to	1.551 Å (mean	1.448 Å)
324	C	- H	bonds ... from	0.949	to	1.001 Å (mean	0.973 Å)
24	C	- O	bonds ... from	1.203	to	1.453 Å (mean	1.337 Å)
32	C	- N	bonds ... from	1.467	to	1.478 Å (mean	1.472 Å)
16	C	- S	bonds ... from	1.766	to	1.766 Å (mean	1.766 Å)
32	O	- S	bonds ... from	1.434	to	1.435 Å (mean	1.435 Å)

Total of 692 bonds generated in 0.0067 secs (103670 bonds/sec).

			Fractional Coordinates			Orthogonal Coordinates		
	Label	Elmt	x	y	z	xor[Å]	yor[Å]	zor[Å]
1.	Br1	Br	0.9783	0.2528	0.2942	-7.754	1.031	-1.298
2.	Br1	Br	0.0217	0.7472	0.7058	-0.478	9.336	-4.918
3.	C1	C	0.1392	0.3686	0.4236	-1.111	4.430	-3.215
4.	C1	C	0.8608	0.6314	0.5764	-7.121	5.937	-3.001
5.	C2	C	0.1624	0.4769	0.4151	-1.550	5.565	-2.543
6.	C2	C	0.8376	0.5231	0.5849	-6.681	4.802	-3.673
7.	C3	C	0.2846	0.5595	0.5078	-2.525	6.347	-3.138
8.	C3	C	0.7154	0.4405	0.4922	-5.707	4.020	-3.079
9.	C4	C	0.3833	0.5343	0.6070	-3.062	5.998	-4.380
10.	C4	C	0.6167	0.4657	0.3930	-5.170	4.370	-1.837
11.	C5	C	0.3545	0.4253	0.6140	-2.580	4.867	-5.042
12.	C5	C	0.6455	0.5747	0.3860	-5.652	5.501	-1.174
13.	C6	C	0.2311	0.3420	0.5224	-1.592	4.081	-4.465
14.	C6	C	0.7689	0.6580	0.4776	-6.640	6.286	-1.751
15.	C7	C	0.5152	0.6259	0.7029	-4.128	6.862	-4.958
16.	C7	C	0.4848	0.3741	0.2971	-4.104	3.505	-1.259
17.	C8	C	0.7333	0.6724	0.8914	-5.600	7.175	-6.810
18.	C8	C	0.2667	0.3276	0.1086	-2.632	3.192	0.594
19.	C9	C	0.6529	0.7449	0.9815	-4.951	8.303	-7.641
20.	C9	C	0.3471	0.2551	0.0185	-3.281	2.064	1.425
21.	C10	C	0.7950	0.8249	0.0926	-7.951	7.471	3.852
22.	C10	C	0.2050	0.1751	0.9074	-0.281	2.897	-10.068
23.	C11	C	0.0046	0.6890	0.0518	-1.462	7.705	2.820
24.	C11	C	0.9954	0.3110	0.9482	-6.770	2.663	-9.036
25.	C12	C	0.8665	0.6057	0.9452	-6.406	6.217	-7.663
26.	C12	C	0.1335	0.3943	0.0548	-1.826	4.150	1.446
27.	C13	C	0.5297	0.6735	0.0093	-5.671	6.268	3.831
28.	C13	C	0.4703	0.3265	0.9907	-2.561	4.099	-10.048
29.	C14	C	0.5733	0.6353	0.1020	-5.756	5.891	2.547
30.	C14	C	0.4267	0.3647	0.8980	-2.476	4.476	-8.763
31.	C15	C	0.3495	0.6496	0.9273	-2.438	7.855	-7.780
32.	C15	C	0.6505	0.3504	0.0727	-5.794	2.513	1.564
33.	C16	C	0.8718	0.9271	0.0691	-8.830	8.391	4.736
34.	C16	C	0.1282	0.0729	0.9309	0.599	1.976	-10.953
35.	C17	C	0.7444	0.0069	0.0427	-5.836	-1.554	0.312
36.	C17	C	0.2556	0.9931	0.9573	-2.396	11.921	-6.529
37.	C18	C	0.6905	0.0279	0.9416	-3.739	0.212	-10.703
38.	C18	C	0.3095	0.9721	0.0584	-4.492	10.155	4.487
39.	C19	C	0.2204	0.8727	0.3144	-3.078	9.659	0.742
40.	C19	C	0.7796	0.1273	0.6856	-5.154	0.709	-6.958
41.	C20	C	0.2273	0.9916	0.3530	-3.322	11.022	0.870
42.	C20	C	0.7727	0.0084	0.6470	-4.910	-0.654	-7.087
43.	C21	C	0.3767	0.0589	0.3743	-2.403	0.381	-3.905
44.	C21	C	0.6233	0.9411	0.6257	-5.829	9.986	-2.312
45.	C22	C	0.5205	0.0087	0.3591	-3.461	-0.527	-3.814
46.	C22	C	0.4795	0.9913	0.6409	-4.771	10.894	-2.403
47.	C23	C	0.5118	0.8897	0.3233	-5.409	9.197	1.032
48.	C23	C	0.4882	0.1103	0.6767	-2.823	1.171	-7.248
49.	C24	C	0.3628	0.8209	0.3004	-4.119	8.738	0.808

50.	C24	C	0.6372	0.1791	0.6996	-4.113	1.629	-7.024
51.	C25	C	0.6811	0.0821	0.3784	-4.859	-0.050	-3.511
52.	C25	C	0.3189	0.9179	0.6216	-3.372	10.417	-2.706
53.	H2	H	0.0959	0.4939	0.3473	-1.190	5.798	-1.696
54.	H2	H	0.9041	0.5061	0.6527	-7.042	4.569	-4.521
55.	H3	H	0.3015	0.6343	0.5038	-2.832	7.130	-2.696
56.	H3	H	0.6985	0.3657	0.4962	-5.400	3.237	-3.520
57.	H5	H	0.4200	0.4081	0.6819	-2.931	4.633	-5.894
58.	H5	H	0.5800	0.5919	0.3181	-5.301	5.734	-0.323
59.	H6	H	0.2102	0.2681	0.5274	-1.253	3.318	-4.920
60.	H6	H	0.7898	0.7319	0.4726	-6.979	7.049	-1.296
61.	H8	H	0.7875	0.7246	0.8617	-6.202	7.584	-6.124
62.	H8	H	0.2125	0.2754	0.1383	-2.030	2.783	-0.093
63.	H9	H	0.5841	0.7961	0.9430	-4.592	8.967	-6.985
64.	H9	H	0.4159	0.2039	0.0570	-3.640	1.400	0.769
65.	H10	H	0.7426	0.8575	0.1558	-7.487	8.051	3.181
66.	H10	H	0.2574	0.1425	0.8442	-0.745	2.316	-9.397
67.	H17	H	0.6990	0.0452	0.1032	-5.445	-0.931	-0.289
68.	H17	H	0.3010	0.9548	0.8968	-2.787	11.299	-5.927
69.	H20	H	0.1306	0.0264	0.3646	-0.398	0.567	-4.214
70.	H20	H	0.8694	0.9736	0.6354	-7.834	9.800	-2.003
71.	H21	H	0.3815	0.1402	0.3996	-2.572	1.310	-3.803
72.	H21	H	0.6185	0.8598	0.6004	-5.660	9.057	-2.413
73.	H23	H	0.6097	0.8548	0.3143	-6.125	8.573	1.074
74.	H23	H	0.3903	0.1452	0.6857	-2.107	1.794	-7.290
75.	H24	H	0.3580	0.7396	0.2755	-3.948	7.810	0.702
76.	H24	H	0.6420	0.2604	0.7245	-4.283	2.557	-6.918
77.	H11A	H	0.0896	0.6460	0.0900	-1.967	7.094	2.226
78.	H11A	H	0.9104	0.3540	0.9100	-6.264	3.273	-8.443
79.	H11B	H	0.0638	0.7412	0.0258	-2.096	8.107	3.466
80.	H11B	H	0.9362	0.2588	0.9742	-6.136	2.261	-9.682
81.	H12A	H	0.9171	0.5624	0.8854	-6.825	5.528	-7.088
82.	H12A	H	0.0829	0.4376	0.1146	-1.406	4.839	0.872
83.	H12B	H	0.8131	0.5500	0.9705	-5.811	5.762	-8.310
84.	H12B	H	0.1869	0.4500	0.0295	-2.421	4.606	2.094
85.	H14A	H	0.4896	0.5929	0.1158	-4.972	5.634	2.074
86.	H14A	H	0.5104	0.4071	0.8842	-3.260	4.733	-8.291
87.	H14B	H	0.6878	0.6506	0.1539	-6.598	5.881	2.108
88.	H14B	H	0.3122	0.3494	0.8461	-1.633	4.486	-8.325
89.	H15A	H	0.2793	0.6076	0.9553	-1.735	7.593	-8.410
90.	H15A	H	0.7207	0.3924	0.0447	-6.496	2.774	2.194
91.	H15B	H	0.3452	0.6032	0.8471	-2.455	7.225	-7.030
92.	H15B	H	0.6548	0.3968	0.1529	-5.777	3.143	0.813
93.	H15C	H	0.3061	0.7223	0.9259	-2.258	8.757	-7.445
94.	H15C	H	0.6939	0.2777	0.0741	-5.974	1.610	1.228
95.	H16A	H	0.9703	0.9702	0.1396	-9.572	8.755	4.191
96.	H16A	H	0.0297	0.0298	0.8604	1.340	1.612	-10.407
97.	H16B	H	0.9138	0.8970	0.0010	-9.227	7.855	5.469
98.	H16B	H	0.0862	0.1030	0.9990	0.995	2.512	-11.685
99.	H18A	H	0.7330	0.9912	0.8791	-6.326	10.689	-5.061
100.	H18A	H	0.2670	0.0088	0.1209	-1.906	-0.322	-1.156
101.	H18B	H	0.6092	0.0798	0.9314	-3.229	0.956	-10.405
102.	H18B	H	0.3908	0.9202	0.0686	-5.003	9.411	4.189
103.	H25A	H	0.7773	0.0376	0.3890	-5.504	-0.746	-3.760
104.	H25A	H	0.2227	0.9624	0.6110	-2.728	11.113	-2.456
105.	H25B	H	0.7027	0.1500	0.4496	-5.045	0.765	-4.023
106.	H25B	H	0.2973	0.8500	0.5504	-3.187	9.603	-2.193
107.	H25C	H	0.6678	0.1064	0.3093	-4.940	0.141	-2.553
108.	H25C	H	0.3322	0.8936	0.6907	-3.292	10.226	-3.664
109.	N1	N	0.9258	0.7560	0.1368	-8.751	6.478	3.104
110.	N1	N	0.0742	0.2440	0.8632	0.519	3.889	-9.320
111.	O1	O	0.5394	0.7224	0.7034	-4.532	7.877	-4.454
112.	O1	O	0.4606	0.2776	0.2966	-3.700	2.490	-1.762
113.	O2	O	0.6052	0.5882	0.7912	-4.589	6.378	-6.136
114.	O2	O	0.3948	0.4118	0.2088	-3.643	3.989	-0.080
115.	O3	O	0.9239	0.8482	0.3410	-8.550	7.825	1.052
116.	O3	O	0.0761	0.1518	0.6590	0.318	2.542	-7.268
117.	O4	O	0.0742	0.6775	0.2929	-1.528	7.796	-0.129
118.	O4	O	0.9258	0.3225	0.7071	-6.704	2.571	-6.087
119.	S1	S	0.0283	0.7844	0.2782	-1.428	9.062	0.538
120.	S1	S	0.9717	0.2156	0.7218	-6.804	1.305	-6.754

Table 1. Crystal data and structure refinement details.

Identification code	**der-123c**	
Empirical formula	$C_{29}H_{30}BrNO_4S$	
Formula weight	568.51	
Temperature	100(2) K	
Wavelength	0.71075 Å	
Crystal system	Triclinic	
Space group	*P*–1	
Unit cell dimensions	*a* = 8.0661(3) Å	α = 113.869(8)°
	b = 13.4521(6) Å	β = 100.322(7)°
	c = 13.5936(9) Å	γ = 94.839(7)°
Volume	1306.68(16) Å^3	
Z	2	
Density (calculated)	1.445 Mg / m^3	
Absorption coefficient	1.689 mm^{-1}	
F(000)	588	
Crystal	Block; Colourless	
Crystal size	0.12 × 0.06 × 0.03 mm^3	
θ range for data collection	3.05 – 27.48°	
Index ranges	$-10 \le h \le 8$, $-17 \le k \le 17$, $-17 \le l \le 17$	
Reflections collected	17527	
Independent reflections	5990 [R_{int} = 0.0358]	
Completeness to θ = 27.48°	99.8 %	
Absorption correction	Semi–empirical from equivalents	
Max. and min. transmission	0.9511 and 0.8230	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5990 / 0 / 327
Goodness-of-fit on F^2	1.060
Final R indices [$F^2 > 2\sigma(F^2)$]	$R1$ = 0.0340, $wR2$ = 0.0794
R indices (all data)	$R1$ = 0.0409, $wR2$ = 0.0821
Largest diff. peak and hole	0.708 and −0.766 e Å^{-3}

Diffractometer: Rigaku R-Axis Spider Diffractometer equipped with Rapid image plate detector (profile data from \w-**scans Cell determination:** CrystalClear-SM Expert 2.0 r7 (Rigaku, 2011) **Data collection:** CrystalClear-SM Expert 2.0 r7 (Rigaku, 2011) **Data reduction and cell refinement:** CrystalClear-SM Expert 2.0 r7 (Rigaku, 2011) **Absorption correction:** CrystalClear-SM Expert 2.0 r7 (Rigaku, 2011) **Structure solution:** SHELXS97 (Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.) **Structure refinement:** SHELXL97 (G Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.).

Special details:

The compound crystallises in triclinic centrosymmetric spacegroup P-1 which means that the unit cell contains 50/50 mixture of enantiomers.

Table 2. Atomic coordinates [$\times 10^4$], equivalent isotropic displacement parameters [$Å^2 \times 10^3$] and site occupancy factors. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
C1	7861(3)	6084(2)	1350(2)	19(1)	1
C2	9180(3)	6906(2)	1516(2)	20(1)	1
C3	10836(3)	6699(2)	1626(2)	20(1)	1
C4	11209(3)	5689(2)	1557(2)	26(1)	1
C5	9876(3)	4880(2)	1407(2)	24(1)	1
C6	8207(3)	5077(2)	1309(2)	17(1)	1
C7	6744(3)	4227(2)	1144(2)	18(1)	1
C8	5899(2)	2380(1)	864(2)	16(1)	1
C9	6615(3)	1326(1)	370(2)	16(1)	1
C10	7668(2)	1006(2)	1209(2)	16(1)	1
C11	6267(2)	2123(1)	2662(2)	14(1)	1
C12	5152(2)	2483(1)	1864(2)	15(1)	1
C13	3279(2)	1920(2)	1447(2)	16(1)	1
C14	2117(3)	2464(2)	905(2)	27(1)	1
C15	2666(3)	1038(2)	1557(2)	18(1)	1
C16	7923(2)	2961(1)	3360(2)	17(1)	1
C17	7631(2)	4014(2)	4244(2)	17(1)	1
C18	8002(3)	5015(2)	4197(2)	21(1)	1
C19	7811(3)	5991(2)	5041(2)	26(1)	1

C20	7248(3)	5967(2)	5932(2)	28(1)	1
C21	6865(3)	4974(2)	5987(2)	28(1)	1
C22	7056(3)	3998(2)	5146(2)	22(1)	1
C23	8774(2)	550(2)	3551(2)	16(1)	1
C24	8794(3)	1131(2)	4661(2)	19(1)	1
C25	10344(3)	1519(2)	5433(2)	23(1)	1
C26	11873(3)	1334(2)	5117(2)	23(1)	1
C27	11829(3)	728(2)	4002(2)	23(1)	1
C28	10282(3)	335(2)	3216(2)	19(1)	1
C29	13557(3)	1785(2)	5957(2)	35(1)	1
Br1	12657(1)	7832(1)	1897(1)	28(1)	1
N1	6661(2)	1018(1)	2012(1)	14(1)	1
O1	7269(2)	3305(1)	1162(1)	16(1)	1
O2	5272(2)	4342(1)	1010(1)	27(1)	1
O3	5475(2)	184(1)	3101(1)	21(1)	1
O4	6936(2)	−896(1)	1664(1)	22(1)	1
S1	6836(1)	130(1)	2545(1)	15(1)	1

Table 3. Bond lengths [Å] and angles [°].

C1–C2	1.385(3)
C1–C6	1.386(3)
C1–H1	0.9500
C2–C3	1.381(3)
C2–H2	0.9500
C3–C4	1.386(3)
C3–Br1	1.8943(19)
C4–C5	1.388(3)
C4–H4	0.9500
C5–C6	1.387(3)
C5–H5	0.9500
C6–C7	1.491(3)
C7–O2	1.201(2)
C7–O1	1.352(2)
C8–O1	1.460(2)
C8–C9	1.518(2)
C8–C12	1.544(3)
C8–H8	1.0000
C9–C10	1.522(3)
C9–H9A	0.9900
C9–H9B	0.9900
C10–N1	1.469(2)
C10–H10A	0.9900
C10–H10B	0.9900
C11–N1	1.486(2)
C11–C12	1.539(2)
C11–C16	1.543(2)

C11–H11	1.0000
C12–C13	1.527(3)
C12–H12	1.0000
C13–C15	1.321(3)
C13–C14	1.504(3)
C14–H14A	0.9800
C14–H14B	0.9800
C14–H14C	0.9800
C15–H15A	0.9500
C15–H15B	0.9500
C16–C17	1.513(2)
C16–H16A	0.9900
C16–H16B	0.9900
C17–C18	1.384(3)
C17–C22	1.394(3)
C18–C19	1.393(3)
C18–H18	0.9500
C19–C20	1.379(3)
C19–H19	0.9500
C20–C21	1.380(3)
C20–H20	0.9500
C21–C22	1.392(3)
C21–H21	0.9500
C22–H22	0.9500
C23–C28	1.386(3)
C23–C24	1.387(3)
C23–S1	1.7583(19)
C24–C25	1.383(3)

C24–H24	0.9500
C25–C26	1.386(3)
C25–H25	0.9500
C26–C27	1.392(3)
C26–C29	1.504(3)
C27–C28	1.390(3)
C27–H27	0.9500
C28–H28	0.9500
C29–H29A	0.9800
C29–H29B	0.9800
C29–H29C	0.9800
N1–S1	1.6319(15)
O3–S1	1.4319(15)
O4–S1	1.4356(13)

C2–C1–C6	120.30(19)
C2–C1–H1	119.9
C6–C1–H1	119.9
C3–C2–C1	118.87(18)
C3–C2–H2	120.6
C1–C2–H2	120.6
C2–C3–C4	121.91(19)
C2–C3–Br1	119.24(15)
C4–C3–Br1	118.85(16)
C3–C4–C5	118.5(2)
C3–C4–H4	120.8
C5–C4–H4	120.8
C6–C5–C4	120.44(18)

C6–C5–H5	119.8
C4–C5–H5	119.8
C1–C6–C5	119.98(18)
C1–C6–C7	118.12(18)
C5–C6–C7	121.90(17)
O2–C7–O1	123.77(18)
O2–C7–C6	124.34(17)
O1–C7–C6	111.90(16)
O1–C8–C9	107.45(15)
O1–C8–C12	111.48(14)
C9–C8–C12	113.46(15)
O1–C8–H8	108.1
C9–C8–H8	108.1
C12–C8–H8	108.1
C8–C9–C10	115.03(15)
C8–C9–H9A	108.5
C10–C9–H9A	108.5
C8–C9–H9B	108.5
C10–C9–H9B	108.5
H9A–C9–H9B	107.5
N1–C10–C9	108.25(15)
N1–C10–H10A	110.0
C9–C10–H10A	110.0
N1–C10–H10B	110.0
C9–C10–H10B	110.0
H10A–C10–H10B	108.4
N1–C11–C12	108.72(14)
N1–C11–C16	110.95(15)

C12–C11–C16	113.15(15)
N1–C11–H11	107.9
C12–C11–H11	107.9
C16–C11–H11	107.9
C13–C12–C11	115.33(15)
C13–C12–C8	109.05(15)
C11–C12–C8	113.11(15)
C13–C12–H12	106.2
C11–C12–H12	106.2
C8–C12–H12	106.2
C15–C13–C14	120.79(18)
C15–C13–C12	124.50(18)
C14–C13–C12	114.70(16)
C13–C14–H14A	109.5
C13–C14–H14B	109.5
H14A–C14–H14B	109.5
C13–C14–H14C	109.5
H14A–C14–H14C	109.5
H14B–C14–H14C	109.5
C13–C15–H15A	120.0
C13–C15–H15B	120.0
H15A–C15–H15B	120.0
C17–C16–C11	113.88(16)
C17–C16–H16A	108.8
C11–C16–H16A	108.8
C17–C16–H16B	108.8
C11–C16–H16B	108.8
H16A–C16–H16B	107.7

C18–C17–C22	118.93(17)
C18–C17–C16	120.64(18)
C22–C17–C16	120.37(17)
C17–C18–C19	120.5(2)
C17–C18–H18	119.8
C19–C18–H18	119.8
C20–C19–C18	120.2(2)
C20–C19–H19	119.9
C18–C19–H19	119.9
C19–C20–C21	119.97(19)
C19–C20–H20	120.0
C21–C20–H20	120.0
C20–C21–C22	120.0(2)
C20–C21–H21	120.0
C22–C21–H21	120.0
C21–C22–C17	120.44(19)
C21–C22–H22	119.8
C17–C22–H22	119.8
C28–C23–C24	120.66(18)
C28–C23–S1	119.19(14)
C24–C23–S1	120.09(15)
C25–C24–C23	119.23(19)
C25–C24–H24	120.4
C23–C24–H24	120.4
C24–C25–C26	121.22(19)
C24–C25–H25	119.4
C26–C25–H25	119.4
C25–C26–C27	118.88(19)

C25–C26–C29	120.9(2)
C27–C26–C29	120.2(2)
C28–C27–C26	120.6(2)
C28–C27–H27	119.7
C26–C27–H27	119.7
C23–C28–C27	119.38(18)
C23–C28–H28	120.3
C27–C28–H28	120.3
C26–C29–H29A	109.5
C26–C29–H29B	109.5
H29A–C29–H29B	109.5
C26–C29–H29C	109.5
H29A–C29–H29C	109.5
H29B–C29–H29C	109.5
C10–N1–C11	113.67(14)
C10–N1–S1	119.35(12)
C11–N1–S1	120.24(12)
C7–O1–C8	115.16(15)
O3–S1–O4	119.50(9)
O3–S1–N1	106.44(8)
O4–S1–N1	106.44(8)
O3–S1–C23	107.43(9)
O4–S1–C23	107.53(9)
N1–S1–C23	109.21(8)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \cdots + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C1	21(1)	16(1)	21(1)	9(1)	3(1)	3(1)
C2	27(1)	15(1)	19(1)	9(1)	2(1)	2(1)
C3	23(1)	19(1)	17(1)	10(1)	2(1)	−4(1)
C4	19(1)	26(1)	39(1)	19(1)	7(1)	4(1)
C5	23(1)	18(1)	38(1)	17(1)	8(1)	7(1)
C6	19(1)	16(1)	18(1)	9(1)	4(1)	1(1)
C7	19(1)	17(1)	21(1)	10(1)	3(1)	3(1)
C8	15(1)	13(1)	18(1)	7(1)	2(1)	−1(1)
C9	20(1)	14(1)	16(1)	7(1)	5(1)	3(1)
C10	17(1)	15(1)	18(1)	6(1)	7(1)	3(1)
C11	17(1)	10(1)	16(1)	5(1)	4(1)	4(1)
C12	16(1)	11(1)	16(1)	5(1)	4(1)	4(1)
C13	16(1)	16(1)	14(1)	5(1)	5(1)	6(1)
C14	20(1)	30(1)	37(1)	21(1)	5(1)	7(1)
C15	15(1)	19(1)	21(1)	8(1)	6(1)	4(1)
C16	15(1)	14(1)	18(1)	5(1)	2(1)	2(1)
C17	14(1)	15(1)	17(1)	4(1)	−1(1)	2(1)
C18	19(1)	19(1)	21(1)	7(1)	0(1)	1(1)
C19	24(1)	14(1)	32(1)	5(1)	0(1)	2(1)
C20	25(1)	20(1)	25(1)	−2(1)	1(1)	6(1)
C21	31(1)	30(1)	19(1)	5(1)	6(1)	5(1)
C22	27(1)	19(1)	19(1)	6(1)	4(1)	2(1)
C23	17(1)	16(1)	18(1)	10(1)	3(1)	4(1)
C24	23(1)	18(1)	21(1)	10(1)	8(1)	7(1)

C25	33(1)	19(1)	16(1)	8(1)	2(1)	3(1)
C26	23(1)	21(1)	26(1)	16(1)	−4(1)	−2(1)
C27	17(1)	28(1)	32(1)	20(1)	6(1)	5(1)
C28	20(1)	22(1)	20(1)	12(1)	7(1)	6(1)
C29	31(1)	33(1)	37(1)	20(1)	−9(1)	−5(1)
Br1	26(1)	26(1)	33(1)	18(1)	0(1)	−7(1)
N1	16(1)	11(1)	15(1)	6(1)	5(1)	4(1)
O1	17(1)	11(1)	23(1)	9(1)	4(1)	1(1)
O2	20(1)	21(1)	43(1)	19(1)	5(1)	5(1)
O3	16(1)	25(1)	30(1)	19(1)	7(1)	4(1)
O4	25(1)	13(1)	23(1)	6(1)	0(1)	5(1)
S1	15(1)	13(1)	19(1)	8(1)	3(1)	3(1)

Table 5. Hydrogen coordinates [$\times 10^4$] and isotropic displacement parameters [$Å^2 \times 10^3$].

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
H1	6714	6211	1265	23	1
H2	8950	7599	1552	24	1
H4	12352	5554	1612	31	1
H5	10108	4187	1370	29	1
H8	4961	2388	278	19	1
H9A	7341	1410	−116	20	1
H9B	5651	713	−100	20	1
H10A	7942	261	830	19	1
H10B	8756	1537	1593	19	1
H11	5581	2050	3180	17	1
H12	5151	3287	2292	18	1
H14A	2369	2349	191	40	1
H14B	2304	3258	1383	40	1
H14C	923	2142	788	40	1
H15A	1478	741	1292	22	1
H15B	3412	702	1901	22	1
H16A	8696	2607	3718	20	1
H16B	8507	3149	2861	20	1
H18	8389	5037	3585	25	1
H19	8069	6675	5002	31	1
H20	7124	6634	6508	33	1
H21	6471	4957	6599	34	1
H22	6794	3316	5187	27	1
H24	7755	1262	4889	23	1

H25	10362	1919	6194	28	1
H27	12866	583	3777	28	1
H28	10258	−77	2456	23	1
H29A	14327	1246	5763	53	1
H29B	13369	1928	6691	53	1
H29C	14071	2475	5963	53	1