Appendix

X-ray Cxrystallography.

1. *X-ray crystallography of tert-butyl 3-((5-nitro-1H-indol-3-yl) thio) azetidine-1-carboxylate 2.41.*

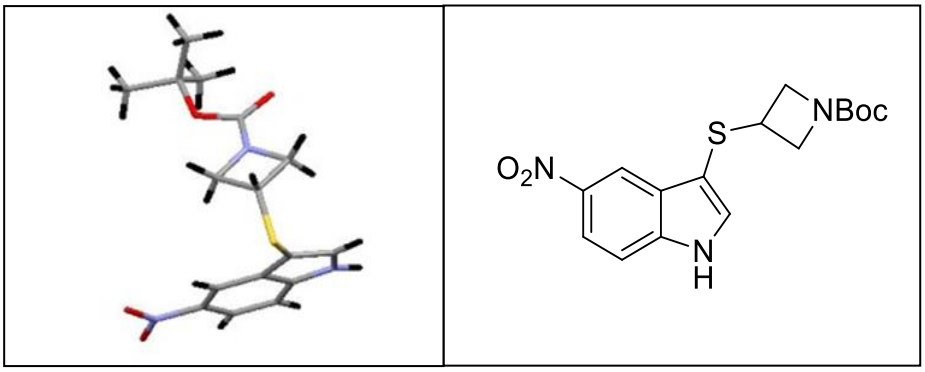

Table 1. Crystal data and structure refinement for 2.41.

Identification code	OHJ358p-1
Empirical formula	C16 H19 N3 O4 S
Formula weight	349.40
Temperature	100(2) K
Wavelength	1.54178 ¦
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 9.4629(11) ¦a= 71.509(10)°.
	b = 9.5127(13) ¦ b= 85.053(9)°.
	c = 9.9555(14) ¦ g = 86.298(9)°.
Volume	846.1(2) ^{3}¦
Z	2
Density (calculated)	1.371 Mg/m^3
Absorption coefficient	1.928 mm^{-1}
F(000)	368
Crystal size	0.300 x 0.020 x 0.010 mm^3
Theta range for data collection	4.694 to 66.945°.
Index ranges	-11<=h<=11, -10<=k<=11, -11<=l<=10
Reflections collected	7715
Independent reflections	2899 [R(int) = 0.2893]
Completeness to theta = 66.945°	96.2 %
Absorption correction	None

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2899 / 0 / 220
Goodness-of-fit on F^2	0.976
Final R indices [I>2sigma(I)]	R1 = 0.0980, wR2 = 0.2084
R indices (all data)	R1 = 0.2336, wR2 = 0.2786
Extinction coefficient	n/a
Largest diff. peak and hole	0.371 and -0.609 $e.^{3-}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (^{2}x 10^3) for 2.41.

U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	2117(2)	1061(3)	8469(3)	39(1)
O(1)	343(6)	7056(7)	5920(6)	38(2)
O(2)	2739(5)	7007(7)	5317(6)	35(2)
O(3)	7710(6)	3517(9)	11276(7)	61(2)
O(4)	7510(6)	2797(8)	9441(7)	49(2)
N(1)	1184(7)	2737(8)	11582(8)	41(2)
N(2)	1656(7)	4930(9)	6409(8)	44(2)
N(3)	6999(7)	3116(9)	10506(8)	42(2)
C(1)	2615(8)	2925(10)	11470(9)	35(2)
C(2)	3449(9)	3460(11)	12272(10)	42(2)
C(3)	4872(9)	3515(10)	11951(9)	38(2)
C(4)	5443(8)	2999(10)	10831(9)	37(2)
C(5)	4679(8)	2456(10)	10033(9)	40(2)
C(6)	3211(8)	2406(10)	10358(9)	33(2)
C(7)	2059(8)	1900(10)	9790(9)	33(2)
C(8)	854(9)	2100(10)	10609(9)	39(2)
C(9)	1799(8)	2627(10)	6934(9)	36(2)
C(10)	2876(8)	3910(10)	6444(10)	36(2)
C(11)	597(9)	3810(10)	7016(10)	43(2)
C(12)	1496(9)	6367(11)	5894(9)	36(2)
C(13)	2755(8)	8588(10)	4449(10)	34(2)
C(14)	1855(9)	8895(12)	3189(10)	49(3)
C(15)	2314(9)	9563(11)	5388(10)	44(3)
C(16)	4342(8)	8742(11)	3954(10)	47(3)

Table 3. Bond lengths [Å] and angles [°] for 2.41.

S(1)-C(7)	1.737(8)
S(1)-C(9)	1.795(9)
O(1)-C(12)	1.239(10)
O(2)-C(12)	1.356(9)
O(2)-C(13)	1.478(10)
O(3)-N(3)	1.222(9)
O(4)-N(3)	1.244(9)
N(1)-C(8)	1.360(11)
N(1)-C(1)	1.368(10)
N(1)-H(1)	0.8800
N(2)-C(12)	1.302(11)
N(2)-C(10)	1.454(11)
N(2)-C(11)	1.460(10)
N(3)-C(4)	1.484(10)
C(1)-C(2)	1.392(12)
C(1)-C(6)	1.411(11)
C(2)-C(3)	1.357(11)
C(2)-H(2)	0.9500
C(3)-C(4)	1.409(11)
C(3)-H(3)	0.9500
C(4)-C(5)	1.353(12)
C(5)-C(6)	1.399(10)
C(5)-H(5)	0.9500
C(6)-C(7)	1.444(11)
C(7)-C(8)	1.383(10)
C(8)-H(8)	0.9500
C(9)-C(11)	1.564(12)
C(9)-C(10)	1.570(11)
C(9)-H(9)	1.0000
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900

C(13)-C(14)	1.517(13)
C(13)-C(15)	1.530(11)
C(13)-C(16)	1.541(10)
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(7)-S(1)-C(9)	101.4(4)
C(12)-O(2)-C(13)	120.5(7)
C(8)-N(1)-C(1)	109.5(6)
C(8)-N(1)-H(1)	125.2
C(1)-N(1)-H(1)	125.2
C(12)-N(2)-C(10)	132.8(7)
C(12)-N(2)-C(11)	129.9(8)
C(10)-N(2)-C(11)	97.0(7)
O(3)-N(3)-O(4)	123.4(7)
O(3)-N(3)-C(4)	119.5(7)
O(4)-N(3)-C(4)	117.1(7)
N(1)-C(1)-C(2)	130.5(7)
N(1)-C(1)-C(6)	107.6(7)
C(2)-C(1)-C(6)	121.9(7)
C(3)-C(2)-C(1)	118.9(8)
C(3)-C(2)-H(2)	120.5
C(1)-C(2)-H(2)	120.5
C(2)-C(3)-C(4)	118.2(8)
C(2)-C(3)-H(3)	120.9
C(4)-C(3)-H(3)	120.9
C(5)-C(4)-C(3)	125.0(8)
C(5)-C(4)-N(3)	119.1(7)
C(3)-C(4)-N(3)	115.9(8)
C(4)-C(5)-C(6)	116.9(8)
C(4)-C(5)-H(5)	121.6
C(6)-C(5)-H(5)	121.6

C(5)-C(6)-C(1)	119.1(8)
C(5)-C(6)-C(7)	133.7(8)
C(1)-C(6)-C(7)	107.2(7)
C(8)-C(7)-C(6)	105.5(7)
C(8)-C(7)-S(1)	125.1(7)
C(6)-C(7)-S(1)	129.3(6)
N(1)-C(8)-C(7)	110.3(7)
N(1)-C(8)-H(8)	124.9
C(7)-C(8)-H(8)	124.9
C(11)-C(9)-C(10)	88.3(6)
C(11)-C(9)-S(1)	120.0(6)
C(10)-C(9)-S(1)	119.5(6)
C(11)-C(9)-H(9)	109.1
C(10)-C(9)-H(9)	109.1
S(1)-C(9)-H(9)	109.1
N(2)-C(10)-C(9)	87.0(6)
N(2)-C(10)-H(10A)	114.2
C(9)-C(10)-H(10A)	114.2
N(2)-C(10)-H(10B)	114.2
C(9)-C(10)-H(10B)	114.2
H(10A)-C(10)-H(10B)	111.3
N(2)-C(11)-C(9)	87.1(6)
N(2)-C(11)-H(11A)	114.1
C(9)-C(11)-H(11A)	114.1
N(2)-C(11)-H(11B)	114.1
C(9)-C(11)-H(11B)	114.1
H(11A)-C(11)-H(11B)	111.3
O(1)-C(12)-N(2)	123.8(8)
O(1)-C(12)-O(2)	124.4(9)
N(2)-C(12)-O(2)	111.8(8)
O(2)-C(13)-C(14)	111.2(7)
O(2)-C(13)-C(15)	109.7(7)
C(14)-C(13)-C(15)	113.1(8)
O(2)-C(13)-C(16)	100.8(7)
C(14)-C(13)-C(16)	110.8(7)
C(15)-C(13)-C(16)	110.5(7)
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5

H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(13)-C(15)-H(15A)	109.5
C(13)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(13)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(13)-C(16)-H(16A)	109.5
C(13)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(13)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (^{2}Å x 10^{3}) for 2.41.

The anisotropic displacement factor exponent takes the form: $-2p^{2}[h^{2} a^{*2}U^{11} + ... + 2 h k a^{*} b^{*} U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
(1)	45(2)	41(2)	-19(1)	4(1)	-2(1)	
O(1)	29(3)	50(4)	39(4)	-22(3)	7(3)	-1(3)
O(2)	24(3)	35(4)	44(4)	-10(3)	5(3)	-2(3)
O(3)	31(3)	103(7)	61(5)	-43(5)	2(3)	-9(4)
O(4)	24(3)	82(6)	45(4)	-27(4)	1(3)	4(3)
N(1)	31(4)	49(5)	42(5)	-19(4)	11(3)	6(4)
N(2)	34(4)	29(5)	60(6)	-4(4)	22(4)	-12(4)
N(3)	33(4)	54(6)	38(5)	-13(4)	3(4)	4(4)
C(1)	29(4)	44(6)	25(5)	-5(4)	10(4)	-5(4)
C(2)	35(5)	55(7)	37(6)	-17(5)	6(4)	-3(4)
C(3)	38(5)	50(7)	31(5)	-20(5)	0(4)	-6(4)
C(4)	24(4)	45(6)	38(6)	-10(5)	4(4)	-1(4)
C(5)	25(4)	54(7)	38(6)	-14(5)	4(4)	2(4)
C(6)	30(4)	32(5)	35(5)	-9(4)	6(4)	-4(4)

C(7)	28(4)	35(6)	39(5)	-15(4)	1(4)	-3(4)
C(8)	26(4)	51(7)	37(6)	-12(5)	7(4)	-2(4)
C(9)	25(4)	49(6)	38(6)	-20(5)	7(4)	-1(4)
C(10)	26(4)	38(6)	40(5)	-11(4)	5(4)	3(4)
C(11)	27(4)	53(7)	53(6)	-24(5)	3(4)	-8(4)
C(12)	36(5)	46(7)	26(5)	-14(5)	17(4)	-10(5)
C(13)	28(4)	33(6)	41(5)	-13(4)	4(4)	2(4)
C(14)	31(5)	65(8)	52(7)	-22(6)	6(4)	-9(5)
C(15)	35(5)	51(7)	52(6)	-24(5)	10(4)	-7(5)
C(16)	27(5)	60(7)	52(6)	-18(5)	5(4)	2(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 2.41.

	x	y	z	U(eq)
H(1)	571	2989	12191	49
H(2)	3029	3782	13031	51
H(3)	5467	3891	12468	46
H(5)	5118	2123	9287	47
H(8)	-71	1832	10507	47
H(9)	1663	2266	6115	43
H(10A)	3546	3887	7162	43
H(10B)	3380	4023	5505	43
H(11A)	-185	3869	6399	51
H(11B)	228	3744	7995	51
H(14A)	2098	8155	2702	74
H(14B)	2038	9888	2531	74
H(14C)	849	8841	3522	74
H(15A)	1288	9518	5626	67
H(15B)	2558	10590	4878	67
H(15C)	2815	9205	6262	67
H(16A)	4913	8380	4781	70
H(16B)	4529	9788	3458	70
H(16C)	4594	8158	3310	70

Table 6. Hydrogen bonds for 2.41 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1)...O(1)#1	0.88	1.99	2.822(8)	157.2
C(8)-H(8)...O(4)#2	0.95	2.60	3.418(10)	145.0
C(14)-H(14A)...O(4)#3	0.98	2.56	3.476(11)	155.6
C(14)-H(14B)...N(1)#4	0.98	2.67	3.534(13)	147.5
C(14)-H(14C)...O(1)	0.98	2.48	3.022(11)	114.6
C(15)-H(15A)...O(1)	0.98	2.48	3.008(10)	113.4

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y+1,-z+2 #2 x-1,y,z #3 -x+1,-y+1,-z+1
#4 x,y+1,z-1

2. *X-ray crystallography of tert-butyl 3-((2-phenyl-1H-indol-3-yl) thio) azetidine-1-carboxylate 2.44.*

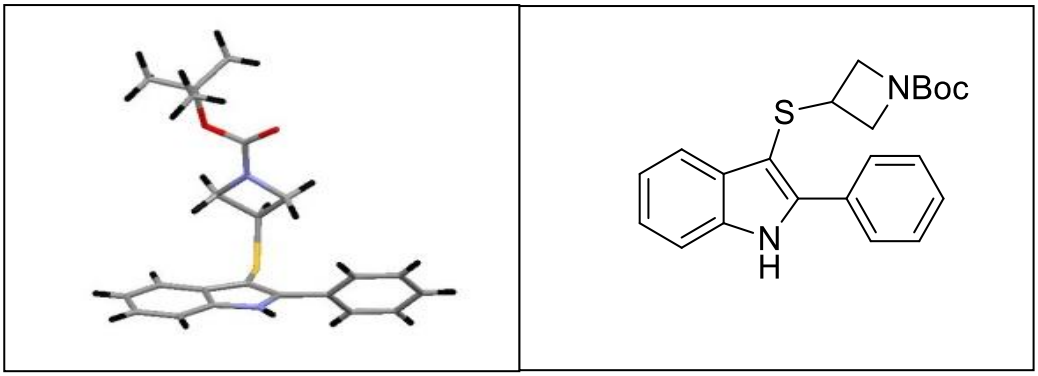

Table 7. Crystal data and structure refinement for 2.44.

Identification code	ohj356p-1	
Empirical formula	C22 H24 N2 O2 S	
Formula weight	380.49	
Temperature	100(2) K	
Wavelength	1.54178 ¦	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.7844(3) ¦	a= 64.2392(7)°.
	b = 10.1924(3) ¦	b=87.2909(11)°.
	c = 11.7207(4) ¦	g=71.0303(7)°.
Volume	989.44(6) ^{3}¦	

Z	2
Density (calculated)	1.277 Mg/m^3
Absorption coefficient	1.600 mm^{-1}
F(000)	404
Crystal size	0.300 x 0.200 x 0.200 mm^3
Theta range for data collection	4.808 to 66.995°.
Index ranges	-11<=h<=11, -12<=k<=12, -13<=l<=13
Reflections collected	24912
Independent reflections	3473 [R(int) = 0.0224]
Completeness to theta = 66.995°	98.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7528 and 0.6429
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3473 / 0 / 247
Goodness-of-fit on F^2	1.059
Final R indices [I>2sigma(I)]	R1 = 0.0315, wR2 = 0.0771
R indices (all data)	R1 = 0.0331, wR2 = 0.0782
Extinction coefficient	n/a
Largest diff. peak and hole	0.309 and -0.343 $e.^{3-}$

Table 8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (^{2} x 10^3) for 2.44.

U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	1557(1)	2946(1)	11224(1)	17(1)
N(1)	5649(1)	1850(1)	10514(1)	15(1)
N(2)	1062(1)	1744(1)	8823(1)	23(1)
O(1)	1518(1)	-130(1)	8181(1)	19(1)
O(2)	211(1)	2407(1)	6871(1)	21(1)
C(1)	5145(2)	3338(2)	9545(1)	15(1)
C(2)	5906(2)	4187(2)	8664(1)	20(1)
C(3)	5124(2)	5690(2)	7811(1)	22(1)
C(4)	3622(2)	6326(2)	7820(1)	22(1)
C(5)	2868(2)	5476(2)	8687(1)	19(1)
C(6)	3640(2)	3956(2)	9580(1)	15(1)
C(7)	3258(1)	2779(2)	10645(1)	14(1)

C(8)	4524(1)	1525(2)	11191(1)	14(1)
C(9)	4777(1)	2(2)	12293(1)	14(1)
C(10)	4319(2)	-106(2)	13467(1)	18(1)
C(11)	4552(2)	-1546(2)	14489(1)	21(1)
C(12)	5228(2)	-2889(2)	14357(1)	22(1)
C(13)	5690(2)	-2797(2)	13194(1)	21(1)
C(14)	5469(2)	-1356(2)	12168(1)	17(1)
C(15)	655(2)	2343(2)	10329(1)	18(1)
C(16)	1494(2)	846(2)	10201(1)	18(1)
C(17)	398(2)	3241(2)	8851(1)	20(1)
C(18)	971(1)	1238(2)	7962(1)	16(1)
C(19)	-4(2)	2121(2)	5763(1)	22(1)
C(20)	-1032(2)	3684(2)	4820(2)	40(1)
C(21)	-743(2)	914(2)	6134(2)	28(1)
C(22)	1444(2)	1678(2)	5268(2)	31(1)

Table 9. Bond lengths [Å] and angles [°] for 2.44.

S(1)-C(7)	1.7516(13)
S(1)-C(15)	1.8042(14)
N(1)-C(8)	1.3702(17)
N(1)-C(1)	1.3794(17)
N(1)-H(1)	0.8800
N(2)-C(18)	1.3343(18)
N(2)-C(17)	1.4661(18)
N(2)-C(16)	1.4677(18)
O(1)-C(18)	1.2298(17)
O(2)-C(18)	1.3409(16)
O(2)-C(19)	1.4870(16)
C(1)-C(2)	1.392(2)
C(1)-C(6)	1.4077(19)
C(2)-C(3)	1.382(2)
C(2)-H(2)	0.9500
C(3)-C(4)	1.402(2)
C(3)-H(3)	0.9500
C(4)-C(5)	1.381(2)
C(4)-H(4)	0.9500

C(5)-C(6)	1.4041(19)
C(5)-H(5)	0.9500
C(6)-C(7)	1.4429(18)
C(7)-C(8)	1.3831(19)
C(8)-C(9)	1.4759(18)
C(9)-C(10)	1.3950(19)
C(9)-C(14)	1.3975(19)
C(10)-C(11)	1.386(2)
C(10)-H(10)	0.9500
C(11)-C(12)	1.387(2)
C(11)-H(11)	0.9500
C(12)-C(13)	1.388(2)
C(12)-H(12)	0.9500
C(13)-C(14)	1.391(2)
C(13)-H(13)	0.9500
C(14)-H(14)	0.9500
C(15)-C(16)	1.5491(19)
C(15)-C(17)	1.554(2)
C(15)-H(15)	1.0000
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(19)-C(22)	1.511(2)
C(19)-C(20)	1.518(2)
C(19)-C(21)	1.519(2)
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800

C(7)-S(1)-C(15)	103.38(6)
C(8)-N(1)-C(1)	109.25(11)

C(8)-N(1)-H(1)	125.4
C(1)-N(1)-H(1)	125.4
C(18)-N(2)-C(17)	133.36(12)
C(18)-N(2)-C(16)	128.80(12)
C(17)-N(2)-C(16)	95.46(10)
C(18)-O(2)-C(19)	120.34(10)
N(1)-C(1)-C(2)	129.57(13)
N(1)-C(1)-C(6)	108.05(12)
C(2)-C(1)-C(6)	122.37(12)
C(3)-C(2)-C(1)	117.34(13)
C(3)-C(2)-H(2)	121.3
C(1)-C(2)-H(2)	121.3
C(2)-C(3)-C(4)	121.30(13)
C(2)-C(3)-H(3)	119.3
C(4)-C(3)-H(3)	119.3
C(5)-C(4)-C(3)	121.24(13)
C(5)-C(4)-H(4)	119.4
C(3)-C(4)-H(4)	119.4
C(4)-C(5)-C(6)	118.64(13)
C(4)-C(5)-H(5)	120.7
C(6)-C(5)-H(5)	120.7
C(5)-C(6)-C(1)	119.09(13)
C(5)-C(6)-C(7)	134.35(13)
C(1)-C(6)-C(7)	106.52(11)
C(8)-C(7)-C(6)	106.75(12)
C(8)-C(7)-S(1)	126.04(10)
C(6)-C(7)-S(1)	127.03(10)
N(1)-C(8)-C(7)	109.39(11)
N(1)-C(8)-C(9)	120.18(11)
C(7)-C(8)-C(9)	130.41(12)
C(10)-C(9)-C(14)	119.13(12)
C(10)-C(9)-C(8)	120.75(12)
C(14)-C(9)-C(8)	120.11(12)
C(11)-C(10)-C(9)	120.03(13)
C(11)-C(10)-H(10)	120.0
C(9)-C(10)-H(10)	120.0
C(10)-C(11)-C(12)	120.65(13)
C(10)-C(11)-H(11)	119.7

C(12)-C(11)-H(11)	119.7
C(11)-C(12)-C(13)	119.87(13)
C(11)-C(12)-H(12)	120.1
C(13)-C(12)-H(12)	120.1
C(12)-C(13)-C(14)	119.74(13)
C(12)-C(13)-H(13)	120.1
C(14)-C(13)-H(13)	120.1
C(13)-C(14)-C(9)	120.58(13)
C(13)-C(14)-H(14)	119.7
C(9)-C(14)-H(14)	119.7
C(16)-C(15)-C(17)	88.79(10)
C(16)-C(15)-S(1)	118.79(9)
C(17)-C(15)-S(1)	119.81(10)
C(16)-C(15)-H(15)	109.3
C(17)-C(15)-H(15)	109.3
S(1)-C(15)-H(15)	109.3
N(2)-C(16)-C(15)	87.61(10)
N(2)-C(16)-H(16A)	114.1
C(15)-C(16)-H(16A)	114.1
N(2)-C(16)-H(16B)	114.1
C(15)-C(16)-H(16B)	114.1
H(16A)-C(16)-H(16B)	111.2
N(2)-C(17)-C(15)	87.48(10)
N(2)-C(17)-H(17A)	114.1
C(15)-C(17)-H(17A)	114.1
N(2)-C(17)-H(17B)	114.1
C(15)-C(17)-H(17B)	114.1
H(17A)-C(17)-H(17B)	111.3
O(1)-C(18)-N(2)	122.84(12)
O(1)-C(18)-O(2)	126.29(12)
N(2)-C(18)-O(2)	110.87(12)
O(2)-C(19)-C(22)	108.96(11)
O(2)-C(19)-C(20)	102.33(11)
C(22)-C(19)-C(20)	111.83(14)
O(2)-C(19)-C(21)	110.12(12)
C(22)-C(19)-C(21)	113.33(13)
C(20)-C(19)-C(21)	109.71(13)
C(19)-C(20)-H(20A)	109.5

C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(19)-C(22)-H(22A)	109.5
C(19)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(19)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 10. Anisotropic displacement parameters ($Å^2$x 10^3) for 2.44.

The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	15(1)	21(1)	17(1)	-12(1)	2(1)	-3(1)
N(1)	13(1)	13(1)	15(1)	-5(1)	0(1)	-3(1)
N(2)	29(1)	16(1)	17(1)	-8(1)	-5(1)	-1(1)
O(1)	17(1)	16(1)	22(1)	-9(1)	-2(1)	-2(1)
O(2)	24(1)	18(1)	19(1)	-10(1)	-8(1)	-1(1)
C(1)	20(1)	15(1)	13(1)	-6(1)	-2(1)	-6(1)
C(2)	22(1)	23(1)	16(1)	-7(1)	1(1)	-11(1)
C(3)	35(1)	22(1)	13(1)	-5(1)	1(1)	-16(1)
C(4)	34(1)	14(1)	14(1)	-3(1)	-4(1)	-6(1)
C(5)	24(1)	16(1)	17(1)	-8(1)	-3(1)	-2(1)
C(6)	20(1)	15(1)	13(1)	-8(1)	-1(1)	-5(1)

C(7)	16(1)	15(1)	13(1)	-8(1)	0(1)	-4(1)
C(8)	16(1)	15(1)	13(1)	-8(1)	1(1)	-6(1)
C(9)	12(1)	15(1)	15(1)	-5(1)	-2(1)	-5(1)
C(10)	17(1)	18(1)	17(1)	-8(1)	1(1)	-5(1)
C(11)	21(1)	25(1)	14(1)	-6(1)	2(1)	-8(1)
C(12)	25(1)	17(1)	18(1)	-1(1)	-4(1)	-9(1)
C(13)	24(1)	15(1)	23(1)	-8(1)	-4(1)	-5(1)
C(14)	19(1)	17(1)	15(1)	-7(1)	0(1)	-6(1)
C(15)	13(1)	22(1)	21(1)	-12(1)	2(1)	-5(1)
C(16)	19(1)	20(1)	16(1)	-8(1)	1(1)	-6(1)
C(17)	18(1)	18(1)	23(1)	-12(1)	-3(1)	-1(1)
C(18)	12(1)	19(1)	18(1)	-8(1)	0(1)	-5(1)
C(19)	26(1)	23(1)	19(1)	-11(1)	-6(1)	-7(1)
C(20)	54(1)	30(1)	30(1)	-11(1)	-22(1)	-4(1)
C(21)	28(1)	37(1)	28(1)	-17(1)	-1(1)	-16(1)
C(22)	34(1)	44(1)	26(1)	-20(1)	7(1)	-21(1)

Table 11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (^{2} x 10^3) for 2.44.

	x	y	z	U(eq)
H(1)	6551	1210	10672	18
H(2)	6921	3751	8650	23
H(3)	5615	6304	7206	27
H(4)	3113	7360	7218	27
H(5)	1848	5911	8679	23
H(10)	3848	808	13565	21
H(11)	4245	-1612	15287	25
H(12)	5376	-3871	15061	26
H(13)	6154	-3715	13100	25
H(14)	5792	-1293	11375	21
H(15)	-288	2274	10672	22
H(16A)	2556	463	10445	21
H(16B)	1080	5	10621	21
H(17A)	-640	3764	8504	24

H(17B)	958	3954	8478	24
H(20A)	-1920	3977	5205	61
H(20B)	-1279	3621	4049	61
H(20C)	-559	4464	4596	61
H(21A)	-46	-111	6675	43
H(21B)	-1094	916	5364	43
H(21C)	-1566	1159	6604	43
H(22A)	1908	2448	5125	47
H(22B)	1293	1640	4464	47
H(22C)	2071	658	5895	47

Table 12. Hydrogen bonds for 2.44 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1)...O(1)#1	0.88	2.05	2.8297(14)	147.6
C(15)-H(15)...O(1)#2	1.00	2.65	3.4646(17)	138.4
C(21)-H(21A)...O(1)	0.98	2.38	2.9212(18)	114.2
C(22)-H(22C)...O(1)	0.98	2.53	3.0858(19)	116.0

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z+2 #2 -x,-y,-z+2

3. X-ray crystallography of tert-butyl 3-(imidazo[1,2-a]pyridin-3-ylthio)azetidine-1-carboxylate 2.48.

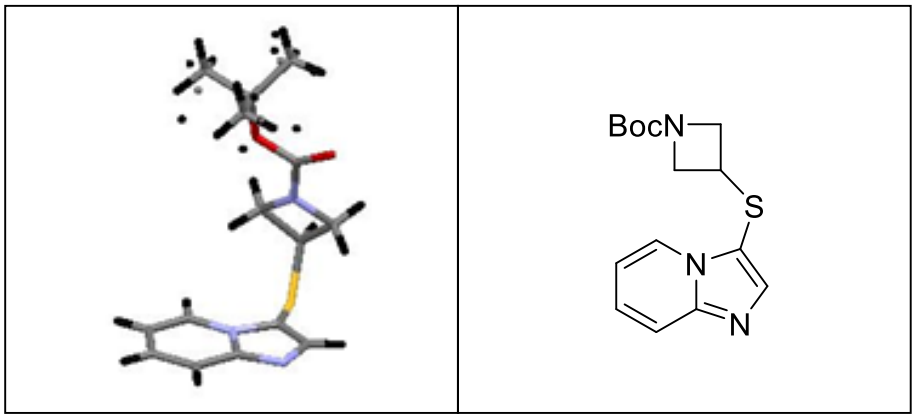

Table 13. Crystal data and structure refinement for 2.48.

Identification code	ojh362v_0m	
Empirical formula	C15 H19 N3 O2 S	
Formula weight	305.39	
Temperature	99.99 K	
Wavelength	1.54178 ¦	
Crystal system	Monoclinic	
Space group	C 1 2/c 1	
Unit cell dimensions	a = 26.0678(8) ¦	α= 90°.
	b = 6.5548(2) ¦	β= 119.764(2)°.
	c = 20.9279(6) ¦	γ = 90°.
Volume	3104.19(17) ^{3}¦	
Z	8	
Density (calculated)	1.307 Mg/m^3	
Absorption coefficient	1.922 mm^{-1}	
F(000)	1296	
Crystal size	0.1 x 0.07 x 0.03 mm^3	
Theta range for data collection	3.907 to 66.576°.	
Index ranges	-30<=h<=30, -7<=k<=7, -24<=l<=22	
Reflections collected	12598	
Independent reflections	2728 [R(int) = 0.0656]	
Completeness to theta = 66.576°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7528 and 0.6486	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2728 / 0 / 224	
Goodness-of-fit on F^2	1.036	
Final R indices [I>2sigma(I)]	R1 = 0.0429, wR2 = 0.0837	
R indices (all data)	R1 = 0.0698, wR2 = 0.0929	

Extinction coefficient	n/a
Largest diff. peak and hole	0.261 and -0.259 e.$^{3-}$¦

Table 14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (^{2}¦x 10^3) for 2.48.

U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	6811(1)	7288(1)	5099(1)	20(1)
O(1)	6961(1)	5860(3)	7811(1)	34(1)
O(2)	6370(1)	8663(3)	7413(1)	25(1)
N(1)	5665(1)	5897(3)	4570(1)	17(1)
N(2)	5768(1)	2483(3)	4713(1)	22(1)
N(3)	6758(1)	7433(3)	6759(1)	20(1)
C(1)	6272(1)	5480(4)	4932(1)	18(1)
C(2)	6307(1)	3401(4)	5002(1)	22(1)
C(3)	5382(1)	4023(4)	4452(1)	19(1)
C(4)	4757(1)	4014(4)	4090(1)	21(1)
C(5)	4458(1)	5805(4)	3873(1)	24(1)
C(6)	4766(1)	7675(4)	4010(1)	22(1)
C(7)	5367(1)	7715(4)	4357(1)	20(1)
C(8)	7069(1)	8124(4)	6031(1)	18(1)
C(9)	6630(1)	9120(4)	6240(1)	22(1)
C(10)	7205(1)	6490(4)	6628(1)	20(1)
C(11)	6718(1)	7231(4)	7374(1)	18(1)
C(12)	6228(1)	8606(5)	8021(1)	29(1)
C(13A)	6813(9)	8630(30)	8800(11)	19(3)
C(13B)	6733(11)	9010(40)	8693(13)	37(6)
C(14A)	5986(4)	10889(13)	7986(4)	33(2)
C(14B)	5711(4)	9987(15)	7741(5)	28(2)
C(15A)	5836(4)	7101(16)	7944(6)	29(2)
C(15B)	5953(5)	6278(16)	8001(7)	26(2)

Table 15. Bond lengths [¦] and angles [°] for 2.48.

S(1)-C(1)	1.736(2)

S(1)-C(8)	1.804(2)
O(1)-C(11)	1.212(3)
O(2)-C(11)	1.337(3)
O(2)-C(12)	1.491(3)
N(1)-C(1)	1.400(3)
N(1)-C(3)	1.391(3)
N(1)-C(7)	1.370(3)
N(2)-C(2)	1.363(3)
N(2)-C(3)	1.336(3)
N(3)-C(9)	1.467(3)
N(3)-C(10)	1.459(3)
N(3)-C(11)	1.348(3)
C(1)-C(2)	1.368(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.415(3)
C(4)-H(4)	0.9500
C(4)-C(5)	1.358(3)
C(5)-H(5)	0.9500
C(5)-C(6)	1.415(3)
C(6)-H(6)	0.9500
C(6)-C(7)	1.361(3)
C(7)-H(7)	0.9500
C(8)-H(8)	1.0000
C(8)-C(9)	1.558(3)
C(8)-C(10)	1.547(3)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(12)-C(13A)	1.585(19)
C(12)-C(13B)	1.39(2)
C(12)-C(14A)	1.612(7)
C(12)-C(14B)	1.482(6)
C(12)-C(15A)	1.371(10)
C(12)-C(15B)	1.678(12)
C(13A)-H(13A)	0.9800
C(13A)-H(13B)	0.9800
C(13A)-H(13C)	0.9800

C(13B)-H(13D)	0.9800
C(13B)-H(13E)	0.9800
C(13B)-H(13F)	0.9800
C(14A)-H(14A)	0.9800
C(14A)-H(14B)	0.9800
C(14A)-H(14C)	0.9800
C(14B)-H(14D)	0.9800
C(14B)-H(14E)	0.9800
C(14B)-H(14F)	0.9800
C(15A)-H(15A)	0.9800
C(15A)-H(15B)	0.9800
C(15A)-H(15C)	0.9800
C(15B)-H(15D)	0.9800
C(15B)-H(15E)	0.9800
C(15B)-H(15F)	0.9800
C(1)-S(1)-C(8)	104.78(11)
C(11)-O(2)-C(12)	119.85(19)
C(3)-N(1)-C(1)	106.28(19)
C(7)-N(1)-C(1)	130.7(2)
C(7)-N(1)-C(3)	123.02(19)
C(3)-N(2)-C(2)	104.4(2)
C(10)-N(3)-C(9)	95.22(17)
C(11)-N(3)-C(9)	133.1(2)
C(11)-N(3)-C(10)	125.73(19)
N(1)-C(1)-S(1)	124.01(18)
C(2)-C(1)-S(1)	130.79(19)
C(2)-C(1)-N(1)	104.5(2)
N(2)-C(2)-C(1)	113.1(2)
N(2)-C(2)-H(2)	123.5
C(1)-C(2)-H(2)	123.5
N(1)-C(3)-C(4)	117.8(2)
N(2)-C(3)-N(1)	111.7(2)
N(2)-C(3)-C(4)	130.5(2)
C(3)-C(4)-H(4)	120.2
C(5)-C(4)-C(3)	119.6(2)
C(5)-C(4)-H(4)	120.2
C(4)-C(5)-H(5)	119.8
C(4)-C(5)-C(6)	120.4(2)

C(6)-C(5)-H(5)	119.8
C(5)-C(6)-H(6)	119.6
C(7)-C(6)-C(5)	120.8(2)
C(7)-C(6)-H(6)	119.6
N(1)-C(7)-H(7)	120.9
C(6)-C(7)-N(1)	118.3(2)
C(6)-C(7)-H(7)	120.9
S(1)-C(8)-H(8)	109.5
C(9)-C(8)-S(1)	119.96(16)
C(9)-C(8)-H(8)	109.5
C(10)-C(8)-S(1)	118.41(17)
C(10)-C(8)-H(8)	109.5
C(10)-C(8)-C(9)	88.19(17)
N(3)-C(9)-C(8)	87.84(17)
N(3)-C(9)-H(9A)	114.0
N(3)-C(9)-H(9B)	114.0
C(8)-C(9)-H(9A)	114.0
C(8)-C(9)-H(9B)	114.0
H(9A)-C(9)-H(9B)	111.2
N(3)-C(10)-C(8)	88.53(17)
N(3)-C(10)-H(10A)	113.9
N(3)-C(10)-H(10B)	113.9
C(8)-C(10)-H(10A)	113.9
C(8)-C(10)-H(10B)	113.9
H(10A)-C(10)-H(10B)	111.1
O(1)-C(11)-O(2)	126.1(2)
O(1)-C(11)-N(3)	122.4(2)
O(2)-C(11)-N(3)	111.4(2)
O(2)-C(12)-C(13A)	111.0(9)
O(2)-C(12)-C(14A)	101.3(3)
O(2)-C(12)-C(15B)	106.6(5)
C(13A)-C(12)-C(14A)	101.0(8)
C(13B)-C(12)-O(2)	110.4(12)
C(13B)-C(12)-C(14B)	120.1(12)
C(13B)-C(12)-C(15B)	112.0(12)
C(14B)-C(12)-O(2)	102.0(3)
C(14B)-C(12)-C(15B)	104.6(5)
C(15A)-C(12)-O(2)	113.8(5)

C(15A)-C(12)-C(13A)	114.1(9)
C(15A)-C(12)-C(14A)	114.2(4)
C(12)-C(13A)-H(13A)	109.5
C(12)-C(13A)-H(13B)	109.5
C(12)-C(13A)-H(13C)	109.5
H(13A)-C(13A)-H(13B)	109.5
H(13A)-C(13A)-H(13C)	109.5
H(13B)-C(13A)-H(13C)	109.5
C(12)-C(13B)-H(13D)	109.5
C(12)-C(13B)-H(13E)	109.5
C(12)-C(13B)-H(13F)	109.5
H(13D)-C(13B)-H(13E)	109.5
H(13D)-C(13B)-H(13F)	109.5
H(13E)-C(13B)-H(13F)	109.5
C(12)-C(14A)-H(14A)	109.5
C(12)-C(14A)-H(14B)	109.5
C(12)-C(14A)-H(14C)	109.5
H(14A)-C(14A)-H(14B)	109.5
H(14A)-C(14A)-H(14C)	109.5
H(14B)-C(14A)-H(14C)	109.5
C(12)-C(14B)-H(14D)	109.5
C(12)-C(14B)-H(14E)	109.5
C(12)-C(14B)-H(14F)	109.5
H(14D)-C(14B)-H(14E)	109.5
H(14D)-C(14B)-H(14F)	109.5
H(14E)-C(14B)-H(14F)	109.5
C(12)-C(15A)-H(15A)	109.5
C(12)-C(15A)-H(15B)	109.5
C(12)-C(15A)-H(15C)	109.5
H(15A)-C(15A)-H(15B)	109.5
H(15A)-C(15A)-H(15C)	109.5
H(15B)-C(15A)-H(15C)	109.5
C(12)-C(15B)-H(15D)	109.5
C(12)-C(15B)-H(15E)	109.5
C(12)-C(15B)-H(15F)	109.5
H(15D)-C(15B)-H(15E)	109.5
H(15D)-C(15B)-H(15F)	109.5
H(15E)-C(15B)-H(15F)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 16. Anisotropic displacement parameters ($Å^2$ x 10^3) for 2.48.

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}
S(1)	19(1)	26(1)	16(1)	0(1)	10(1)	-5(1)
O(1)	52(1)	32(1)	23(1)	11(1)	22(1)	21(1)
O(2)	26(1)	34(1)	21(1)	10(1)	17(1)	12(1)
N(1)	18(1)	17(1)	14(1)	1(1)	7(1)	-4(1)
N(2)	28(1)	16(1)	21(1)	-2(1)	13(1)	-2(1)
N(3)	22(1)	22(1)	18(1)	7(1)	10(1)	7(1)
C(1)	19(1)	21(1)	14(1)	-1(1)	9(1)	-4(1)
C(2)	22(1)	24(1)	18(1)	-1(1)	9(1)	0(1)
C(3)	24(1)	19(1)	14(1)	-3(1)	10(1)	-6(1)
C(4)	24(1)	22(1)	19(1)	-2(1)	11(1)	-8(1)
C(5)	19(1)	31(2)	20(1)	-4(1)	8(1)	-6(1)
C(6)	22(1)	21(1)	21(1)	3(1)	8(1)	1(1)
C(7)	24(1)	17(1)	16(1)	4(1)	9(1)	-3(1)
C(8)	15(1)	21(1)	18(1)	-2(1)	8(1)	-2(1)
C(9)	23(1)	23(1)	20(1)	4(1)	12(1)	4(1)
C(10)	21(1)	23(1)	16(1)	-2(1)	8(1)	4(1)
C(11)	16(1)	18(1)	16(1)	-3(1)	6(1)	-3(1)
C(12)	26(1)	47(2)	23(2)	11(1)	18(1)	12(1)
C(13A)	18(4)	24(5)	11(4)	-10(4)	3(3)	-8(4)
C(13B)	43(10)	49(11)	34(10)	-4(7)	30(9)	-8(8)
C(14A)	40(4)	37(4)	28(4)	3(3)	22(4)	12(3)
C(14B)	31(4)	30(5)	33(4)	-1(3)	23(4)	4(3)
C(15A)	29(4)	39(6)	25(3)	-4(4)	17(3)	-9(4)
C(15B)	34(5)	23(6)	23(4)	-3(4)	17(4)	-7(4)

Table 17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 2.48.

	x	y	z	U(eq)
H(2)	6670	2673	5229	26
H(4)	4549	2762	4000	26
H(5)	4038	5803	3628	29
H(6)	4551	8918	3857	27
H(7)	5574	8970	4449	23
H(8)	7421	9031	6194	22
H(9A)	6757	10473	6478	26
H(9B)	6215	9156	5832	26
H(10A)	7107	5082	6434	24
H(10B)	7611	6568	7054	24
H(13A)	7004	7291	8897	29
H(13B)	6714	8953	9183	29
H(13C)	7084	9671	8800	29
H(13D)	7024	7925	8802	55
H(13E)	6628	9057	9082	55
H(13F)	6900	10322	8667	55
H(14A)	6292	11874	8052	49
H(14B)	5888	11069	8378	49
H(14C)	5632	11111	7507	49
H(14D)	5819	11332	7639	42
H(14E)	5588	10123	8112	42
H(14F)	5385	9421	7287	42
H(15A)	5481	7212	7459	44
H(15B)	5727	7254	8327	44
H(15C)	6020	5764	7992	44
H(15D)	5634	5981	7501	38
H(15E)	5798	6237	8342	38
H(15F)	6266	5257	8148	38

Table 6. Hydrogen bonds for ojh362v_0m [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(7)-H(7)...N(2)#1	0.95	2.36	3.263(3)	157.7

C(8)-H(8)...O(1)#2	1.00	2.24	3.065(3)	138.4
C(13A)-H(13A)...O(1)	0.98	2.41	2.92(2)	111.8
C(13B)-H(13D)...O(1)	0.98	2.41	3.02(3)	119.4
C(15B)-H(15F)...O(1)	0.98	2.28	2.859(12)	116.8

Symmetry transformations used to generate equivalent atoms:
#1 x,y+1,z #2 -x+3/2,y+1/2,-z+3/2

4. *X-ray crystallography of 3,3'-sulfonyl bis(6-bromo 1H-indole) 3.20*

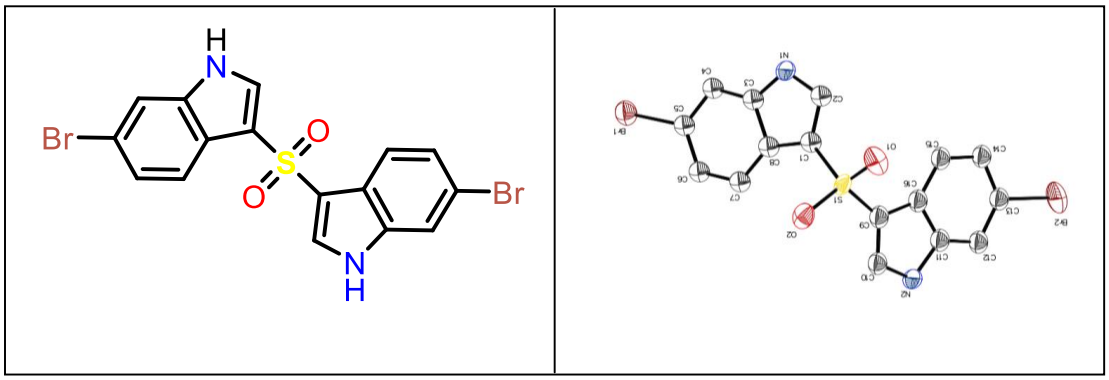

Table 1 Crystal data and structure refinement for 3,3'-sulfonyl bis(6-bromo 1H-indole)

Identification code	2017ncs0415s
Empirical formula	$C_{16}H_{11}Br_2N_2O_{2.5}S$
Formula weight	463.15
Temperature/K	100.00(10)
Crystal system	Triclinic
Space group	P-1
a/Å	8.8847(4)
b/Å	12.6224(5)
c/Å	15.4429(7)
α/°	98.300(4)
β/°	90.384(4)
γ/°	108.869(4)

Volume/Å^3	1618.99(13)
Z	4
ρ_{calc}g/cm^3	1.900
μ/mm^{-1}	5.150
F(000)	908.0
Crystal size/mm^3	0.08 × 0.02 × 0.005
Radiation	MoKα (λ = 0.71075)
2Θ range for data collection/°	3.452 to 54.97
Index ranges	-11 ≤ h ≤ 11, -16 ≤ k ≤ 16, -20 ≤ l ≤ 19
Reflections collected	36651
Independent reflections	7406 [R_{int} = 0.0702, R_{sigma} = 0.0649]
Data/restraints/parameters	7406/0/448
Goodness-of-fit on F^2	1.040
Final R indexes [I>=2σ (I)]	R_1 = 0.0481, wR_2 = 0.0856
Final R indexes [all data]	R_1 = 0.0835, wR_2 = 0.0966
Largest diff. peak/hole / e Å^{-3}	0.82/-0.92

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 2017ncs0415s. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Br1A	-3239.8(6)	-1506.6(5)	5755.3(4)	38.93(15)
Br2A	8375.1(5)	5638.0(4)	3583.9(3)	28.66(13)
S1A	-51.9(13)	2103.4(9)	2367.7(8)	20.2(2)
O1A	-1582(4)	2284(2)	2435(2)	22.7(7)

O2A	613(4)	2064(3)	1514(2)	25.6(7)
N1A	-26(5)	-825(3)	2862(3)	28.2(10)
N2A	2174(5)	4698(3)	4098(3)	24.3(9)
C1A	-226(5)	857(4)	2753(3)	20.2(10)
C2A	356(5)	31(4)	2377(3)	24.9(10)
C3A	-855(5)	-558(4)	3570(3)	22.9(10)
C4A	-1521(5)	-1191(4)	4224(3)	26.3(11)
C5A	-2310(6)	-698(4)	4833(3)	28.5(11)
C6A	-2435(6)	381(4)	4836(3)	26.8(11)
C7A	-1771(5)	995(4)	4175(3)	24(1)
C8A	-985(5)	517(4)	3532(3)	21.5(10)
C9A	1270(5)	3172(4)	3082(3)	21.7(10)
C10A	845(5)	3895(4)	3698(3)	22.5(10)
C11A	3502(5)	4515(4)	3736(3)	20.6(10)
C12A	5114(5)	5157(4)	3909(3)	23.4(10)
C13A	6177(5)	4753(4)	3450(3)	22.7(10)
C14A	5727(5)	3748(4)	2848(3)	22.3(10)
C15A	4118(5)	3134(4)	2662(3)	22(1)

C16A	2986(5)	3536(3)	3103(3)	17.5(9)
Br1B	2781.9(6)	11221.4(4)	-539.9(3)	31.09(13)
Br2B	7842.8(7)	4137.1(5)	517.3(4)	39.43(15)
S1B	2920.3(14)	7431.4(9)	2748.7(8)	23.9(3)
O1B	1242(4)	7308(3)	2777(2)	31.0(8)
O2B	3797(4)	7567(3)	3574(2)	31.0(8)
N1B	5556(5)	10331(4)	2212(3)	23.0(9)
N2B	2212(5)	4515(4)	1317(3)	23.0(9)
C1B	3867(5)	8615(4)	2275(3)	21.2(10)
C2B	5195(5)	9446(4)	2663(3)	21.7(10)
C3B	4457(5)	10092(4)	1520(3)	20.6(10)
C4B	4319(5)	10768(4)	901(3)	21.2(10)
C5B	3056(6)	10317(4)	295(3)	24.6(10)
C6B	1946(6)	9227(4)	267(3)	25(1)
C7B	2106(5)	8567(4)	887(3)	23.9(10)
C8B	3348(5)	8996(4)	1528(3)	20.9(10)
C9B	3030(5)	6253(4)	2067(3)	21.6(10)
C10B	1729(6)	5319(4)	1796(3)	22.9(10)
C11B	3847(5)	4892(4)	1279(3)	22.3(10)

C12B	4835(6)	4331(4)	880(3)	25.5(11)
C13B	6445(6)	4911(4)	989(3)	27.1(11)
C14B	7075(6)	6006(4)	1448(3)	28.9(11)
C15B	6083(5)	6560(4)	1833(3)	24.8(11)
C16B	4434(5)	5999(4)	1753(3)	22.3(10)
O1S	2812(4)	6779(3)	5172(3)	32.0(8)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 2017ncs0415s. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Br1A	32.1(3)	43.3(3)	37.6(3)	23.8(3)	-2.1(2)	-0.1(2)
Br2A	17.4(2)	26.6(3)	42.9(3)	10.7(2)	1.7(2)	6.22(19)
S1A	17.3(6)	18.6(5)	24.9(6)	6.1(5)	0.9(4)	4.9(4)
O1A	20.1(17)	19.2(16)	31.7(19)	8.9(14)	-0.2(14)	8.1(13)
O2A	27.9(18)	25.9(17)	20.4(17)	4.1(14)	3.0(14)	5.1(14)
N1A	26(2)	22(2)	41(3)	5(2)	1.8(19)	13.1(18)
N2A	21(2)	23(2)	28(2)	-2.3(18)	2.0(17)	8.8(17)
C1A	14(2)	20(2)	26(3)	5.7(19)	0.4(18)	4.1(18)
C2A	18(2)	27(3)	31(3)	4(2)	0(2)	9(2)
C3A	18(2)	21(2)	32(3)	4(2)	-1(2)	8.5(19)
C4A	22(3)	19(2)	37(3)	8(2)	-4(2)	5.5(19)
C5A	21(3)	32(3)	31(3)	18(2)	-5(2)	1(2)
C6A	24(3)	31(3)	24(3)	5(2)	0(2)	7(2)
C7A	21(2)	22(2)	32(3)	7(2)	0(2)	9.3(19)

C8A	14(2)	24(2)	26(3)	6(2)	-2.0(19)	4.3(18)
C9A	18(2)	23(2)	27(3)	7(2)	2.7(19)	8.1(19)
C10A	15(2)	23(2)	31(3)	8(2)	4.2(19)	6.6(19)
C11A	19(2)	23(2)	22(2)	6(2)	2.1(19)	9.2(19)
C12A	22(2)	21(2)	29(3)	7(2)	3(2)	8.1(19)
C13A	15(2)	23(2)	32(3)	11(2)	-2(2)	6.9(19)
C14A	19(2)	24(2)	29(3)	9(2)	8(2)	12.0(19)
C15A	27(3)	22(2)	22(2)	8(2)	7(2)	13(2)
C16A	16(2)	16(2)	22(2)	7.7(18)	2.2(18)	5.6(17)
Br1B	36.9(3)	35.9(3)	27.1(3)	10.0(2)	3.6(2)	18.8(2)
Br2B	42.0(3)	59.3(4)	32.4(3)	9.9(3)	7.5(2)	36.4(3)
S1B	23.7(6)	18.8(6)	31.5(7)	8.6(5)	8.9(5)	7.8(5)
O1B	24.3(18)	21.8(17)	50(2)	11.6(16)	13.8(16)	8.9(14)
O2B	41(2)	30.9(19)	22.4(18)	6.6(15)	3.1(15)	12.7(16)
N1B	17(2)	17(2)	32(2)	4.7(18)	-0.1(18)	1.8(18)
N2B	18(2)	20(2)	30(2)	7.5(18)	1.6(17)	3.1(17)
C1B	17(2)	18(2)	30(3)	8(2)	6.0(19)	6.3(18)
C2B	21(2)	25(2)	23(2)	8(2)	2.5(19)	12.0(19)
C3B	19(2)	19(2)	24(2)	1.9(19)	4.6(19)	7.2(18)
C4B	19(2)	21(2)	26(3)	8(2)	5.7(19)	7.3(19)
C5B	30(3)	28(3)	22(2)	8(2)	9(2)	15(2)
C6B	22(3)	29(3)	24(3)	-3(2)	4(2)	11(2)
C7B	20(2)	19(2)	33(3)	5(2)	5(2)	6.3(19)
C8B	18(2)	21(2)	25(3)	0.2(19)	5.5(19)	9.6(19)
C9B	17(2)	22(2)	29(3)	11(2)	4.5(19)	7.2(19)
C10B	23(3)	22(2)	26(3)	11(2)	8(2)	9(2)
C11B	27(3)	20(2)	24(3)	8(2)	-1(2)	10.3(19)
C12B	31(3)	30(3)	21(3)	6(2)	2(2)	18(2)
C13B	33(3)	36(3)	22(3)	11(2)	9(2)	22(2)

C14B	22(3)	39(3)	29(3)	15(2)	5(2)	10(2)
C15B	22(3)	26(2)	28(3)	13(2)	2(2)	6(2)
C16B	23(2)	24(2)	24(3)	10(2)	5.7(19)	10(2)
O1S	34(2)	29(2)	35(2)	6.0(17)	5.1(18)	12.8(16)

Table 4 Bond Lengths for 3,3'-sulfonyl bis(6-bromo 1H-indole).

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br1A	C5A	1.909(5)	Br1B	C5B	1.904(5)
Br2A	C13A	1.903(4)	Br2B	C13B	1.902(5)
S1A	O1A	1.451(3)	S1B	O1B	1.450(3)
S1A	O2A	1.449(3)	S1B	O2B	1.449(4)
S1A	C1A	1.723(4)	S1B	C1B	1.728(4)
S1A	C9A	1.716(5)	S1B	C9B	1.725(5)
N1A	C2A	1.358(6)	N1B	C2B	1.354(6)
N1A	C3A	1.384(6)	N1B	C3B	1.374(6)
N2A	C10A	1.356(6)	N2B	C10B	1.352(6)
N2A	C11A	1.380(6)	N2B	C11B	1.379(6)
C1A	C2A	1.367(6)	C1B	C2B	1.364(6)
C1A	C8A	1.434(6)	C1B	C8B	1.438(6)
C3A	C4A	1.393(6)	C3B	C4B	1.399(6)
C3A	C8A	1.408(6)	C3B	C8B	1.418(6)
C4A	C5A	1.373(7)	C4B	C5B	1.370(7)
C5A	C6A	1.401(7)	C5B	C6B	1.404(6)
C6A	C7A	1.389(6)	C6B	C7B	1.391(6)
C7A	C8A	1.396(6)	C7B	C8B	1.391(6)
C9A	C10A	1.363(6)	C9B	C10B	1.367(6)
C9A	C16A	1.441(6)	C9B	C16B	1.454(6)
C11A	C12A	1.401(6)	C11B	C12B	1.392(6)

C11A	C16A	1.404(6)	C11B	C16B	1.410(6)
C12A	C13A	1.368(6)	C12B	C13B	1.377(7)
C13A	C14A	1.400(7)	C13B	C14B	1.393(7)
C14A	C15A	1.393(6)	C14B	C15B	1.380(7)
C15A	C16A	1.405(6)	C15B	C16B	1.401(6)

Table 5 Bond Angles for 3,3'-sulfonyl bis(6-bromo 1H-indole).

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
O1A	S1A	C1A	107.60(19)	O1B	S1B	C1B	108.4(2)
O1A	S1A	C9A	106.7(2)	O1B	S1B	C9B	106.2(2)
O2A	S1A	O1A	117.95(19)	O2B	S1B	O1B	117.5(2)
O2A	S1A	C1A	108.7(2)	O2B	S1B	C1B	106.3(2)
O2A	S1A	C9A	108.7(2)	O2B	S1B	C9B	109.8(2)
C9A	S1A	C1A	106.7(2)	C9B	S1B	C1B	108.3(2)
C2A	N1A	C3A	109.4(4)	C2B	N1B	C3B	109.4(4)
C10A	N2A	C11A	109.2(4)	C10B	N2B	C11B	110.2(4)
C2A	C1A	S1A	125.9(4)	C2B	C1B	S1B	122.0(4)
C2A	C1A	C8A	108.3(4)	C2B	C1B	C8B	108.2(4)
C8A	C1A	S1A	125.8(3)	C8B	C1B	S1B	129.1(3)
N1A	C2A	C1A	108.9(4)	N1B	C2B	C1B	109.3(4)
N1A	C3A	C4A	129.7(4)	N1B	C3B	C4B	129.6(4)
N1A	C3A	C8A	108.0(4)	N1B	C3B	C8B	108.3(4)
C4A	C3A	C8A	122.3(4)	C4B	C3B	C8B	122.1(4)
C5A	C4A	C3A	115.8(4)	C5B	C4B	C3B	116.8(4)
C4A	C5A	Br1A	118.3(4)	C4B	C5B	Br1B	118.3(3)
C4A	C5A	C6A	124.0(4)	C4B	C5B	C6B	123.2(4)
C6A	C5A	Br1A	117.7(4)	C6B	C5B	Br1B	118.6(4)
C7A	C6A	C5A	119.3(5)	C7B	C6B	C5B	119.2(4)

C6A	C7A	C8A	118.7(4)	C8B	C7B	C6B	119.8(4)
C3A	C8A	C1A	105.4(4)	C3B	C8B	C1B	104.7(4)
C7A	C8A	C1A	134.7(4)	C7B	C8B	C1B	136.4(4)
C7A	C8A	C3A	119.9(4)	C7B	C8B	C3B	118.9(4)
C10A	C9A	S1A	124.3(4)	C10B	C9B	S1B	123.0(4)
C10A	C9A	C16A	107.7(4)	C10B	C9B	C16B	107.8(4)
C16A	C9A	S1A	127.8(4)	C16B	C9B	S1B	128.9(4)
N2A	C10A	C9A	109.4(4)	N2B	C10B	C9B	109.0(4)
N2A	C11A	C12A	129.4(4)	N2B	C11B	C12B	129.3(4)
N2A	C11A	C16A	108.1(4)	N2B	C11B	C16B	107.9(4)
C12A	C11A	C16A	122.4(4)	C12B	C11B	C16B	122.8(4)
C13A	C12A	C11A	116.2(4)	C13B	C12B	C11B	116.0(4)
C12A	C13A	Br2A	118.6(4)	C12B	C13B	Br2B	117.3(4)
C12A	C13A	C14A	123.4(4)	C12B	C13B	C14B	123.0(4)
C14A	C13A	Br2A	117.9(3)	C14B	C13B	Br2B	119.6(4)
C15A	C14A	C13A	119.8(4)	C15B	C14B	C13B	120.5(5)
C14A	C15A	C16A	118.5(4)	C14B	C15B	C16B	118.8(5)
C11A	C16A	C9A	105.5(4)	C11B	C16B	C9B	105.1(4)
C11A	C16A	C15A	119.4(4)	C15B	C16B	C9B	136.0(4)
C15A	C16A	C9A	135.1(4)	C15B	C16B	C11B	118.9(4)

Table 6 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 3,3'-sulfonyl bis(6-bromo 1H-indole).

Atom	***x***	***y***	***z***	**U(eq)**
H2AA	921	53	1872	30
H4A	-1437	-1902	4246	32
H6A	-2956	683	5276	32
H7A	-1850	1709	4162	29

H10A	-196	3845	3824	27
H12A	5443	5820	4314	28
H14A	6499	3492	2572	27
H15A	3801	2472	2256	26
H2BA	5763	9410	3160	26
H4B	5049	11487	900	25
H6B	1114	8950	-160	30
H7B	1384	7841	873	29
H10B	682	5248	1921	27
H12B	4431	3607	558	31
H14B	8172	6367	1496	35
H15B	6500	7292	2139	30
H1SA	3270(80)	7250(60)	4790(50)	80(20)
H1SB	3660(90)	6940(60)	5610(50)	80(30)
H2A	2250(60)	5300(40)	4520(30)	34(15)
H2B	1670(70)	3880(50)	1150(40)	49(19)
H1A	210(60)	-1450(50)	2730(30)	37(16)
H1B	6180(70)	10830(50)	2300(40)	32(18)

Crystal structure determination of 3,3'-sulfonyl bis(6-bromo 1H-indole)

Crystal Data for $C_{16}H_{11}Br_2N_2O_{2.5}S$ (M =463.15 g/mol): triclinic, space group P-1 (no. 2), a = 8.8847(4) Å, b = 12.6224(5) Å, c = 15.4429(7) Å, α = 98.300(4)°, β = 90.384(4)°, γ = 108.869(4)°, V = 1618.99(13) Å^3, Z = 4, T = 100.00(10) K, μ(MoKα) = 5.150 mm^{-1}, *Dcalc* = 1.900 g/cm^3, 36651 reflections measured (3.452° ≤ 2Θ ≤ 54.97°), 7406 unique (R_{int} = 0.0702, R_{sigma} = 0.0649) which were used in all calculations. The final R_1 was 0.0481 (I > 2σ(I)) and wR_2 was 0.0966 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

1. Fixed Uiso

   At 1.2 times of:

   All C(H) groups

2. a Aromatic/amide H refined with riding coordinates:

   C2A(H2AA), C4A(H4A), C6A(H6A), C7A(H7A), C10A(H10A), C12A(H12A), C14A(H14A),

C15A(H15A), C2B(H2BA), C4B(H4B), C6B(H6B), C7B(H7B), C10B(H10B), C12B(H12B), C14B(H14B), C15B(H15B)

5. X-ray crystal structures and data of compound 4.58.

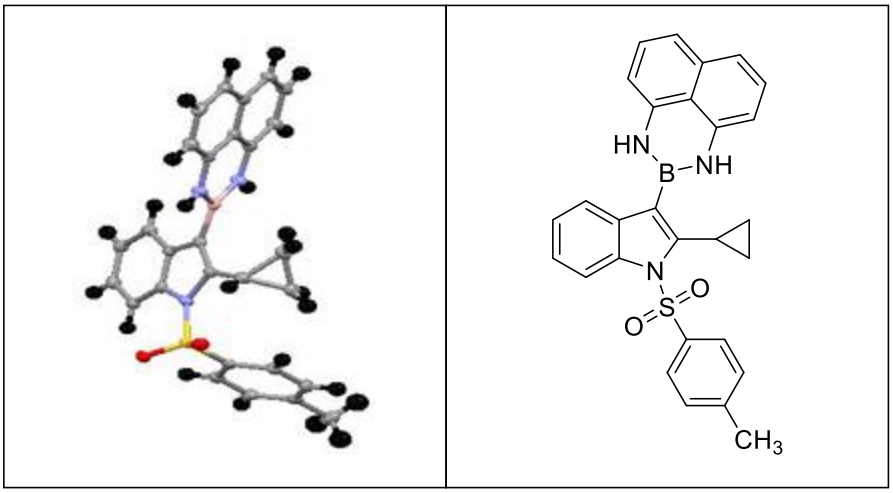

Table 7. Crystal data and structure refinement for OHJ326_0m_a.

Identification code	OHJ326_0m_a	
Empirical formula	C28 H24 B N3 O2 S	
Formula weight	477.37	
Temperature	100(2) K	
Wavelength	1.54178 ¦	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 15.5122(8) ¦	α= 90°.
	b = 8.5781(5) ¦	β= 102.953(3)°.
	c = 17.9625(10) ¦	γ = 90°.
Volume	2329.4(2) ^{3}¦	
Z	4	
Density (calculated)	1.361 Mg/m^3	
Absorption coefficient	1.489 mm^{-1}	
F(000)	1000	
Crystal size	0.410 x 0.040 x 0.040 mm^3	
Theta range for data collection	3.408 to 66.796°.	
Index ranges	-12<=h<=18, -9<=k<=10, -21<=l<=21	
Reflections collected	18135	
Independent reflections	4108 [R(int) = 0.0528]	
Completeness to theta = 66.796°	99.3 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.91 and 0.48
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4108 / 0 / 317
Goodness-of-fit on F^2	1.060
Final R indices [I>2sigma(I)]	R1 = 0.0437, wR2 = 0.0980
R indices (all data)	R1 = 0.0661, wR2 = 0.1077
Extinction coefficient	n/a
Largest diff. peak and hole	0.221 and -0.496 $e.^{3-}$¦

Table 8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (^{2}¦x 10^3) for OHJ326_0m_a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	8835(1)	2514(1)	6338(1)	19(1)
B(1)	5544(2)	3052(3)	6742(1)	21(1)
O(1)	9487(1)	1716(2)	6900(1)	24(1)
O(2)	8501(1)	1804(2)	5614(1)	23(1)
N(1)	7984(1)	2805(2)	6743(1)	20(1)
N(2)	5030(1)	4277(2)	6941(1)	22(1)
N(3)	5071(1)	1709(2)	6412(1)	22(1)
C(1)	8053(1)	3010(3)	7538(1)	19(1)
C(2)	8779(1)	3035(3)	8154(1)	21(1)
C(3)	8616(1)	3260(3)	8872(1)	24(1)
C(4)	7763(1)	3451(3)	8985(1)	26(1)
C(5)	7046(1)	3417(3)	8370(1)	24(1)
C(6)	7184(1)	3197(3)	7637(1)	20(1)
C(7)	6579(1)	3096(3)	6897(1)	20(1)
C(8)	7066(1)	2901(3)	6367(1)	19(1)
C(9)	6770(1)	2867(3)	5525(1)	23(1)
C(10)	6818(1)	4352(3)	5080(1)	28(1)
C(11)	5938(1)	3741(3)	5159(1)	27(1)
C(12)	4108(1)	4224(3)	6822(1)	21(1)
C(13)	3625(1)	5445(3)	7018(1)	23(1)
C(14)	2701(1)	5319(3)	6908(1)	27(1)
C(15)	2266(1)	3998(3)	6612(1)	25(1)
C(16)	2736(1)	2711(3)	6409(1)	22(1)

C(17)	2323(1)	1290(3)	6136(1)	24(1)
C(18)	2802(1)	54(3)	5974(1)	27(1)
C(19)	3724(1)	170(3)	6055(1)	24(1)
C(20)	4156(1)	1539(3)	6313(1)	20(1)
C(21)	3671(1)	2835(3)	6502(1)	20(1)
C(22)	9266(1)	4348(3)	6200(1)	20(1)
C(23)	9898(1)	5005(3)	6788(1)	24(1)
C(24)	10261(1)	6434(3)	6673(1)	24(1)
C(25)	10004(1)	7227(3)	5988(1)	23(1)
C(26)	9377(1)	6532(3)	5404(1)	28(1)
C(27)	9008(1)	5102(3)	5500(1)	24(1)
C(28)	10396(2)	8786(3)	5881(1)	32(1)

Table 9. Bond lengths [Å] and angles [°] for OHJ326_0m_a.

S(1)-O(2)	1.4233(15)
S(1)-O(1)	1.4334(15)
S(1)-N(1)	1.6628(18)
S(1)-C(22)	1.747(2)
B(1)-N(2)	1.412(3)
B(1)-N(3)	1.422(3)
B(1)-C(7)	1.567(3)
N(1)-C(1)	1.419(3)
N(1)-C(8)	1.435(2)
N(2)-C(12)	1.398(3)
N(2)-H(2)	0.8800
N(3)-C(20)	1.398(3)
N(3)-H(3)	0.8800
C(1)-C(2)	1.392(3)
C(1)-C(6)	1.407(3)
C(2)-C(3)	1.382(3)
C(2)-H(2A)	0.9500
C(3)-C(4)	1.392(3)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.381(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.393(3)

C(5)-H(5)	0.9500
C(6)-C(7)	1.449(3)
C(7)-C(8)	1.351(3)
C(8)-C(9)	1.480(3)
C(9)-C(11)	1.510(3)
C(9)-C(10)	1.514(3)
C(9)-H(9)	1.0000
C(10)-C(11)	1.499(3)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.378(3)
C(12)-C(21)	1.427(3)
C(13)-C(14)	1.407(3)
C(13)-H(13)	0.9500
C(14)-C(15)	1.364(3)
C(14)-H(14)	0.9500
C(15)-C(16)	1.415(3)
C(15)-H(15)	0.9500
C(16)-C(17)	1.413(3)
C(16)-C(21)	1.426(3)
C(17)-C(18)	1.364(3)
C(17)-H(17)	0.9500
C(18)-C(19)	1.408(3)
C(18)-H(18)	0.9500
C(19)-C(20)	1.379(3)
C(19)-H(19)	0.9500
C(20)-C(21)	1.425(3)
C(22)-C(23)	1.390(3)
C(22)-C(27)	1.391(3)
C(23)-C(24)	1.383(3)
C(23)-H(23)	0.9500
C(24)-C(25)	1.384(3)
C(24)-H(24)	0.9500
C(25)-C(26)	1.394(3)
C(25)-C(28)	1.500(3)
C(26)-C(27)	1.380(3)

C(26)-H(26)	0.9500
C(27)-H(27)	0.9500
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800

O(2)-S(1)-O(1)	119.61(10)
O(2)-S(1)-N(1)	107.56(9)
O(1)-S(1)-N(1)	105.51(9)
O(2)-S(1)-C(22)	109.19(10)
O(1)-S(1)-C(22)	107.30(10)
N(1)-S(1)-C(22)	107.01(10)
N(2)-B(1)-N(3)	116.13(19)
N(2)-B(1)-C(7)	123.4(2)
N(3)-B(1)-C(7)	120.4(2)
C(1)-N(1)-C(8)	107.97(17)
C(1)-N(1)-S(1)	124.84(14)
C(8)-N(1)-S(1)	127.18(15)
C(12)-N(2)-B(1)	123.60(19)
C(12)-N(2)-H(2)	118.2
B(1)-N(2)-H(2)	118.2
C(20)-N(3)-B(1)	123.48(19)
C(20)-N(3)-H(3)	118.3
B(1)-N(3)-H(3)	118.3
C(2)-C(1)-C(6)	121.6(2)
C(2)-C(1)-N(1)	131.86(19)
C(6)-C(1)-N(1)	106.51(17)
C(3)-C(2)-C(1)	117.36(19)
C(3)-C(2)-H(2A)	121.3
C(1)-C(2)-H(2A)	121.3
C(2)-C(3)-C(4)	122.1(2)
C(2)-C(3)-H(3A)	119.0
C(4)-C(3)-H(3A)	119.0
C(5)-C(4)-C(3)	120.2(2)
C(5)-C(4)-H(4)	119.9
C(3)-C(4)-H(4)	119.9
C(4)-C(5)-C(6)	119.4(2)
C(4)-C(5)-H(5)	120.3

C(6)-C(5)-H(5)	120.3
C(5)-C(6)-C(1)	119.36(19)
C(5)-C(6)-C(7)	132.06(19)
C(1)-C(6)-C(7)	108.58(19)
C(8)-C(7)-C(6)	107.70(18)
C(8)-C(7)-B(1)	125.78(19)
C(6)-C(7)-B(1)	126.3(2)
C(7)-C(8)-N(1)	109.18(18)
C(7)-C(8)-C(9)	128.89(19)
N(1)-C(8)-C(9)	121.84(19)
C(8)-C(9)-C(11)	118.34(19)
C(8)-C(9)-C(10)	118.8(2)
C(11)-C(9)-C(10)	59.40(15)
C(8)-C(9)-H(9)	116.1
C(11)-C(9)-H(9)	116.1
C(10)-C(9)-H(9)	116.1
C(11)-C(10)-C(9)	60.16(15)
C(11)-C(10)-H(10A)	117.8
C(9)-C(10)-H(10A)	117.8
C(11)-C(10)-H(10B)	117.8
C(9)-C(10)-H(10B)	117.8
H(10A)-C(10)-H(10B)	114.9
C(10)-C(11)-C(9)	60.44(15)
C(10)-C(11)-H(11A)	117.7
C(9)-C(11)-H(11A)	117.7
C(10)-C(11)-H(11B)	117.7
C(9)-C(11)-H(11B)	117.7
H(11A)-C(11)-H(11B)	114.8
C(13)-C(12)-N(2)	122.2(2)
C(13)-C(12)-C(21)	120.04(19)
N(2)-C(12)-C(21)	117.75(19)
C(12)-C(13)-C(14)	120.1(2)
C(12)-C(13)-H(13)	120.0
C(14)-C(13)-H(13)	120.0
C(15)-C(14)-C(13)	121.2(2)
C(15)-C(14)-H(14)	119.4
C(13)-C(14)-H(14)	119.4
C(14)-C(15)-C(16)	120.7(2)

C(14)-C(15)-H(15)	119.6
C(16)-C(15)-H(15)	119.6
C(17)-C(16)-C(15)	122.83(19)
C(17)-C(16)-C(21)	118.4(2)
C(15)-C(16)-C(21)	118.7(2)
C(18)-C(17)-C(16)	121.2(2)
C(18)-C(17)-H(17)	119.4
C(16)-C(17)-H(17)	119.4
C(17)-C(18)-C(19)	120.8(2)
C(17)-C(18)-H(18)	119.6
C(19)-C(18)-H(18)	119.6
C(20)-C(19)-C(18)	120.0(2)
C(20)-C(19)-H(19)	120.0
C(18)-C(19)-H(19)	120.0
C(19)-C(20)-N(3)	122.3(2)
C(19)-C(20)-C(21)	120.10(19)
N(3)-C(20)-C(21)	117.6(2)
C(20)-C(21)-C(16)	119.4(2)
C(20)-C(21)-C(12)	121.27(19)
C(16)-C(21)-C(12)	119.2(2)
C(23)-C(22)-C(27)	120.6(2)
C(23)-C(22)-S(1)	119.05(17)
C(27)-C(22)-S(1)	120.32(17)
C(24)-C(23)-C(22)	119.2(2)
C(24)-C(23)-H(23)	120.4
C(22)-C(23)-H(23)	120.4
C(23)-C(24)-C(25)	121.4(2)
C(23)-C(24)-H(24)	119.3
C(25)-C(24)-H(24)	119.3
C(24)-C(25)-C(26)	118.2(2)
C(24)-C(25)-C(28)	120.5(2)
C(26)-C(25)-C(28)	121.3(2)
C(27)-C(26)-C(25)	121.6(2)
C(27)-C(26)-H(26)	119.2
C(25)-C(26)-H(26)	119.2
C(26)-C(27)-C(22)	118.9(2)
C(26)-C(27)-H(27)	120.5
C(22)-C(27)-H(27)	120.5

C(25)-C(28)-H(28A)	109.5
C(25)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(25)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 10. Anisotropic displacement parameters (^{2}¦x 10^3) for OHJ326_0m_a. 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}
S(1)	17(1)	22(1)	18(1)	-1(1)	3(1)	2(1)
B(1)	22(1)	26(2)	15(1)	1(1)	2(1)	1(1)
O(1)	19(1)	27(1)	24(1)	4(1)	2(1)	4(1)
O(2)	23(1)	27(1)	18(1)	-5(1)	5(1)	-1(1)
N(1)	15(1)	25(1)	17(1)	-2(1)	1(1)	1(1)
N(2)	17(1)	25(1)	22(1)	-4(1)	1(1)	-2(1)
N(3)	17(1)	27(1)	22(1)	-5(1)	4(1)	1(1)
C(1)	22(1)	18(1)	17(1)	2(1)	3(1)	0(1)
C(2)	18(1)	22(1)	22(1)	0(1)	3(1)	1(1)
C(3)	23(1)	28(1)	16(1)	2(1)	-3(1)	-2(1)
C(4)	30(1)	30(1)	18(1)	0(1)	5(1)	-2(1)
C(5)	21(1)	28(1)	23(1)	-1(1)	6(1)	-1(1)
C(6)	18(1)	20(1)	20(1)	1(1)	3(1)	-1(1)
C(7)	20(1)	19(1)	20(1)	-1(1)	1(1)	-1(1)
C(8)	15(1)	20(1)	21(1)	-1(1)	1(1)	1(1)
C(9)	19(1)	30(1)	19(1)	-2(1)	1(1)	2(1)
C(10)	26(1)	38(2)	20(1)	4(1)	0(1)	1(1)
C(11)	22(1)	34(2)	21(1)	0(1)	-2(1)	5(1)
C(12)	18(1)	29(1)	14(1)	-1(1)	2(1)	-1(1)
C(13)	21(1)	27(1)	20(1)	-4(1)	0(1)	1(1)
C(14)	24(1)	35(2)	21(1)	-2(1)	4(1)	8(1)
C(15)	16(1)	39(2)	21(1)	1(1)	3(1)	3(1)
C(16)	17(1)	33(1)	13(1)	2(1)	1(1)	0(1)
C(17)	19(1)	34(1)	18(1)	2(1)	1(1)	-4(1)

C(18)	27(1)	30(1)	20(1)	-1(1)	-1(1)	-9(1)
C(19)	24(1)	27(1)	20(1)	-4(1)	1(1)	-1(1)
C(20)	18(1)	27(1)	12(1)	1(1)	1(1)	1(1)
C(21)	20(1)	26(1)	12(1)	1(1)	1(1)	0(1)
C(22)	16(1)	24(1)	20(1)	0(1)	6(1)	2(1)
C(23)	21(1)	31(1)	19(1)	0(1)	3(1)	2(1)
C(24)	20(1)	30(1)	24(1)	-6(1)	5(1)	-4(1)
C(25)	20(1)	26(1)	26(1)	0(1)	11(1)	1(1)
C(26)	26(1)	32(2)	23(1)	6(1)	4(1)	3(1)
C(27)	19(1)	31(1)	19(1)	0(1)	1(1)	-1(1)
C(28)	38(1)	29(2)	31(1)	-4(1)	12(1)	-7(1)

Table 11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (^{2}x 10 ^{3}) for OHJ326_0m_a.

	x	y	z	U(eq)
H(2)	5305	5119	7151	26
H(3)	5370	944	6262	27
H(2A)	9364	2903	8084	25
H(3A)	9101	3285	9302	28
H(4)	7674	3605	9486	31
H(5)	6463	3542	8446	28
H(9)	6880	1875	5269	28
H(10A)	7048	5300	5373	34
H(10B)	6969	4260	4575	34
H(11A)	5547	3274	4701	32
H(11B)	5626	4313	5499	32
H(13)	3916	6372	7227	28
H(14)	2373	6168	7043	32
H(15)	1642	3941	6541	30
H(17)	1700	1194	6064	29
H(18)	2511	-898	5804	32
H(19)	4049	-694	5932	29
H(23)	10079	4480	7263	28
H(24)	10697	6880	7073	29

H(26)	9199	7056	4928	33
H(27)	8586	4641	5095	28
H(28A)	10795	9107	6359	48
H(28B)	9921	9556	5736	48
H(28C)	10727	8713	5477	48

Table 12. Hydrogen bonds for OHJ326_0m_a [¦ and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2)...O(1)#1	0.88	2.15	2.929(2)	146.4
C(2)-H(2A)...O(1)	0.95	2.40	2.945(3)	115.8
C(13)-H(13)...O(1)#1	0.95	2.63	3.315(2)	129.0

Symmetry transformations used to generate equivalent atoms:

#1 -x+3/2,y+1/2,-z+3/2