Table 1: Crystal data and structure refinement details.

Empirical formula	$C_{30}H_{28}Br_2NO_5$	
Formula weight	642.35	
Temperature	296(2) K	
Wavelength	1.54178 Å	
θ range for above	3.50° to 64.52°	
Crystal system	Triclinic	
Space group	$P-1$	
Cell dimensions		
$a = 9.9779(11)$ Å	$b = 11.5105(12)$ Å	$c = 13.4027(14)$ Å
$\alpha = 91.472(6)°$	$\beta = 107.929(6)°$	$\gamma = 109.296(6)°$
Volume	1368.3(3) Å^3	
Z	2	
Density(calculated)	1.559 Mg m^{-3}	
Absorption coefficient	4.094 mm^{-1}	
F_{000}	650	
Crystal size	0.25 × 0.25 × 0.25 mm	
θ range for data collection	3.50° to 64.52°	
Index ranges	$-11 \leq h \leq 11$	
	$-13 \leq k \leq 13$	
	$-15 \leq l \leq 14$	
Reflections collected	13269	
Independent reflections	4454 [$R_{\text{int}} = 0.0522$]	
Refinement method	Full matrix least-squares on F^2	
Data / restraints / parameters	4454 / 0 / 346	
Goodness-of-fit on F^2	1.041	
Final [$I > 2\sigma(I)$]	$R1 = 0.0609$, $wR2 = 0.1680$	
R indices (all data)	$R1 = 0.0758$, $wR2 = 0.1850$	
Largest diff. peak and hole	0.591 and −0.556 e Å^{-3}	

Table 2: Atomic coordinates and equivalent thermal parameters of the non-hydrogen atoms.

Atom	x	y	z	U_{eq}
Br1	0.81469(9)	0.24281(7)	0.25466(4)	0.0768(3)
C2	0.9232(6)	0.2883(5)	0.4022(4)	0.0523(12)
C3	1.0708(7)	0.2946(5)	0.4393(4)	0.0634(14)
C4	1.1500(6)	0.3276(6)	0.5467(4)	0.0648(15)
C5	1.0816(6)	0.3531(5)	0.6163(4)	0.0530(12)
O6	1.1715(4)	0.3848(4)	0.7209(3)	0.0685(11)
C7	1.1134(5)	0.4155(5)	0.7999(4)	0.0550(12)
C8	0.9463(5)	0.3471(4)	0.7668(3)	0.0411(10)
C9	0.8620(5)	0.3793(4)	0.8337(3)	0.0395(9)
C10	0.7043(5)	0.3737(4)	0.7478(3)	0.0363(9)
C11	0.5649(5)	0.2959(4)	0.7720(3)	0.0384(9)
C12	0.5438(5)	0.3310(4)	0.8646(3)	0.0436(10)
C13	0.4155(6)	0.2724(5)	0.8871(4)	0.0493(11)
C14	0.2980(6)	0.1749(5)	0.8144(4)	0.0523(12)
C15	0.3190(6)	0.1352(5)	0.7238(4)	0.0528(12)
C16	0.4533(5)	0.1946(4)	0.7024(3)	0.0432(10)
C17	0.4746(5)	0.1495(4)	0.6037(4)	0.0485(11)
C18	0.6410(5)	0.1900(4)	0.6187(3)	0.0415(10)
N19	0.7070(4)	0.3276(3)	0.6431(2)	0.0347(7)
C20	0.8702(5)	0.3800(4)	0.6594(3)	0.0373(9)
C21	0.9318(5)	0.3465(4)	0.5785(3)	0.0405(10)
C22	0.8540(5)	0.3154(4)	0.4701(3)	0.0454(10)
C23	0.6951(5)	0.5039(4)	0.7387(3)	0.0342(9)
C24	0.7783(5)	0.6081(4)	0.8140(3)	0.0444(10)
C25	0.7552(6)	0.7196(4)	0.8024(4)	0.0519(12)
C26	0.6462(5)	0.7287(4)	0.7135(3)	0.0433(10)
C27	0.5602(6)	0.6269(4)	0.6373(3)	0.0491(11)
C28	0.5855(6)	0.5161(4)	0.6496(3)	0.0455(10)
Br29	0.60863(7)	0.87909(5)	0.69793(4)	0.0650(3)
C30	0.8472(5)	0.3015(4)	0.9213(3)	0.0441(10)
O31	0.8673(4)	0.3421(3)	1.0093(2)	0.0598(9)
O32	0.8152(5)	0.1812(3)	0.8903(3)	0.0694(11)
C33	0.8062(10)	0.0976(7)	0.9713(5)	0.090(2)
C34	0.6577(12)	0.0543(8)	0.9739(6)	0.112(3)
O35	0.1704(4)	0.1259(4)	0.8383(3)	0.0742(12)
C36	0.0430(7)	0.0430(6)	0.7606(6)	0.086(2)
O37	0.3898(4)	0.3019(4)	0.9775(3)	0.0642(10)
C38	0.5202(7)	0.3633(7)	1.0677(4)	0.0798(19)

Table 3: Anisotropic thermal parameters of the non-hydrogen atoms.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Br1	0.1042(6)	0.0965(5)	0.0485(4)	0.0537(4)	0.0316(4)	0.0129(3)
C2	0.071(4)	0.054(3)	0.052(3)	0.034(3)	0.035(3)	0.020(2)
C3	0.075(4)	0.073(3)	0.068(3)	0.038(3)	0.045(3)	0.022(3)
C4	0.045(3)	0.093(4)	0.074(3)	0.037(3)	0.031(3)	0.022(3)
C5	0.047(3)	0.061(3)	0.059(3)	0.024(2)	0.021(2)	0.020(2)
O6	0.039(2)	0.111(3)	0.060(2)	0.034(2)	0.0135(17)	0.014(2)
C7	0.035(3)	0.072(3)	0.051(3)	0.018(2)	0.008(2)	0.002(2)
C8	0.042(3)	0.041(2)	0.041(2)	0.0184(19)	0.011(2)	0.0079(17)
C9	0.039(2)	0.037(2)	0.039(2)	0.0138(18)	0.0100(19)	0.0051(17)
C10	0.038(2)	0.038(2)	0.0328(19)	0.0143(18)	0.0104(18)	0.0040(16)
C11	0.038(2)	0.033(2)	0.044(2)	0.0133(18)	0.0138(19)	0.0105(17)
C12	0.043(3)	0.043(2)	0.048(2)	0.016(2)	0.017(2)	0.0091(18)
C13	0.049(3)	0.058(3)	0.052(3)	0.023(2)	0.025(2)	0.017(2)
C14	0.045(3)	0.048(3)	0.071(3)	0.013(2)	0.031(3)	0.016(2)
C15	0.038(3)	0.045(2)	0.066(3)	0.004(2)	0.017(2)	0.004(2)
C16	0.040(3)	0.038(2)	0.053(2)	0.0134(19)	0.018(2)	0.0077(18)
C17	0.047(3)	0.041(2)	0.050(2)	0.008(2)	0.015(2)	−0.0030(19)
C18	0.043(3)	0.035(2)	0.046(2)	0.0115(18)	0.016(2)	−0.0005(17)
N19	0.0347(19)	0.0312(16)	0.0377(17)	0.0108(14)	0.0124(15)	0.0030(13)
C20	0.032(2)	0.038(2)	0.042(2)	0.0120(17)	0.0118(19)	0.0073(16)
C21	0.036(2)	0.043(2)	0.049(2)	0.0183(19)	0.018(2)	0.0132(18)
C22	0.046(3)	0.051(2)	0.047(2)	0.024(2)	0.019(2)	0.0135(19)
C23	0.035(2)	0.034(2)	0.0357(19)	0.0113(17)	0.0150(18)	0.0051(15)
C24	0.043(3)	0.040(2)	0.043(2)	0.0184(19)	0.001(2)	0.0016(18)
C25	0.048(3)	0.038(2)	0.056(3)	0.010(2)	0.005(2)	−0.0086(19)
C26	0.046(3)	0.040(2)	0.050(2)	0.019(2)	0.020(2)	0.0073(18)
C27	0.051(3)	0.049(3)	0.044(2)	0.024(2)	0.005(2)	0.0047(19)
C28	0.047(3)	0.044(2)	0.042(2)	0.019(2)	0.007(2)	−0.0032(18)
Br29	0.0777(5)	0.0432(3)	0.0732(4)	0.0313(3)	0.0134(3)	0.0066(2)
C30	0.048(3)	0.049(2)	0.037(2)	0.020(2)	0.013(2)	0.0077(18)
O31	0.071(2)	0.064(2)	0.0369(17)	0.0229(19)	0.0096(16)	0.0032(15)
O32	0.121(3)	0.0490(19)	0.0499(18)	0.035(2)	0.039(2)	0.0185(15)
C33	0.138(7)	0.071(4)	0.075(4)	0.034(4)	0.056(4)	0.030(3)
C34	0.142(8)	0.100(6)	0.092(5)	0.034(5)	0.043(5)	0.039(5)
O35	0.050(2)	0.077(3)	0.094(3)	0.006(2)	0.041(2)	0.012(2)
C36	0.058(4)	0.062(4)	0.142(6)	0.009(3)	0.051(4)	0.006(4)
O37	0.054(2)	0.089(3)	0.058(2)	0.0251(19)	0.0317(18)	0.0117(18)
C38	0.077(4)	0.120(6)	0.052(3)	0.038(4)	0.031(3)	0.012(3)

Table 4: Bond lengths (Å).

Atoms	Length	Atoms	Length
Br1-C2	1.900(5)	C14-C15	1.385(7)
C2-C3	1.377(8)	C15-C16	1.409(7)
C2-C22	1.384(6)	C16-C17	1.508(6)
C3-C4	1.384(8)	C17-C18	1.514(6)
C4-C5	1.389(7)	C18-N19	1.483(5)
C5-O6	1.373(6)	N19-C20	1.480(5)
C5-C21	1.398(7)	C20-C21	1.498(6)
O6-C7	1.441(6)	C21-C22	1.392(6)
C7-C8	1.502(7)	C23-C24	1.382(6)
C8-C9	1.517(6)	C23-C28	1.396(6)
C8-C20	1.530(6)	C24-C25	1.381(7)
C9-C30	1.510(6)	C25-C26	1.377(7)
C9-C10	1.618(6)	C26-C27	1.374(6)
C10-N19	1.499(5)	C26-Br29	1.892(4)
C10-C11	1.520(6)	C27-C28	1.384(7)
C10-C23	1.538(6)	C30-O31	1.189(5)
C11-C16	1.385(6)	C30-O32	1.338(6)
C11-C12	1.393(6)	O32-C33	1.473(6)
C12-C13	1.365(6)	C33-C34	1.411(13)
C13-O37	1.369(6)	O35-C36	1.395(7)
C13-C14	1.398(7)	O37-C38	1.426(7)
C14-O35	1.352(6)		

Table 5: Bond angles (°).

Atoms	Angle	Atoms	Angle
C3-C2-C22	121.2(5)	C11-C16-C15	119.5(4)
C3-C2-Br1	118.9(4)	C11-C16-C17	120.1(4)
C22-C2-Br1	119.9(4)	C15-C16-C17	120.4(4)
C2-C3-C4	119.0(5)	C16-C17-C18	109.9(4)
C3-C4-C5	120.7(5)	N19-C18-C17	108.4(4)
O6-C5-C4	115.3(5)	C20-N19-C18	114.0(3)
O6-C5-C21	124.3(4)	C20-N19-C10	101.0(3)
C4-C5-C21	120.3(5)	C18-N19-C10	112.1(3)
C5-O6-C7	120.2(4)	N19-C20-C21	120.9(4)
O6-C7-C8	110.3(4)	N19-C20-C8	104.9(3)
C7-C8-C9	117.9(4)	C21-C20-C8	110.1(4)
C7-C8-C20	109.0(4)	C22-C21-C5	118.6(4)
C9-C8-C20	101.7(3)	C22-C21-C20	125.2(4)
C30-C9-C8	115.0(4)	C5-C21-C20	116.2(4)
C30-C9-C10	115.1(3)	C2-C22-C21	120.3(5)
C8-C9-C10	104.0(3)	C24-C23-C28	116.9(4)
N19-C10-C11	112.8(3)	C24-C23-C10	126.0(4)
N19-C10-C23	106.2(3)	C28-C23-C10	117.0(4)
C11-C10-C23	106.2(3)	C25-C24-C23	122.1(4)
N19-C10-C9	105.4(3)	C26-C25-C24	119.7(4)
C11-C10-C9	114.4(3)	C27-C26-C25	120.0(4)
C23-C10-C9	111.6(3)	C27-C26-Br29	119.5(4)
C16-C11-C12	118.3(4)	C25-C26-Br29	120.4(3)
C16-C11-C10	122.4(4)	C26-C27-C28	119.6(4)
C12-C11-C10	119.2(4)	C27-C28-C23	121.7(4)
C13-C12-C11	122.6(4)	O31-C30-O32	123.3(4)
C12-C13-O37	125.0(5)	O31-C30-C9	124.4(4)
C12-C13-C14	119.6(4)	O32-C30-C9	112.3(3)
O37-C13-C14	115.4(4)	C30-O32-C33	116.8(4)
O35-C14-C15	124.6(5)	C34-C33-O32	109.0(7)
O35-C14-C13	116.7(4)	C14-O35-C36	118.3(5)
C15-C14-C13	118.7(4)	C13-O37-C38	116.2(4)
C14-C15-C16	121.1(5)		