Table 1: Crystal data and structure refinement details **4C**.

Empirical formula	$C_{30}H_{26}BrClN_2O_3$	
Formula weight	577.89	
Temperature	296(2) K	
Wavelength	1.54178 Å	
Reflns. for cell determination	4104	
θ range for above	6.72° to 64.51°	
Crystal system	Triclinic	
Space group	$P-1$	
Cell dimensions		
$a = 9.5848(7)$ Å	$b = 11.0031(8)$ Å	$c = 14.0353(11)$ Å
$\alpha = 87.764(2)°$	$\beta = 70.878(2)°$	$\gamma = 65.624(2)°$
Volume	1265.88(16) Å^3	
Z	2	
Density(calculated)	1.516 Mg m^{-3}	
Absorption coefficient	3.478 mm^{-1}	
F_{000}	592	
Crystal size	0.25 × 0.25 × 0.25 mm	
θ range for data collection	6.72° to 64.51°	
Index ranges	$-11 \leq h \leq 11$	
	$-12 \leq k \leq 12$	
	$-16 \leq l \leq 16$	
Reflections collected	14548	
Independent reflections	4174 [$R_{\text{int}} = 0.0313$]	
Absorption correction	multi-scan	
Refinement method	Full matrix least-squares on F^2	
Data / restraints / parameters	4174 / 0 / 335	
Goodness-of-fit on F^2	1.103	
Final [$I > 2\sigma(I)$]	$R1 = 0.0331$, $wR2 = 0.0959$	
R indices (all data)	$R1 = 0.0335$, $wR2 = 0.0965$	
Largest diff. peak and hole	0.376 and −0.584 e Å^{-3}	

Table 2: Bond lengths (Å).

Atoms	Length	Atoms	Length
Br1-C2	1.904(2)	C15-C16	1.406(3)
C2-C25	1.381(3)	C16-C17	1.384(3)
C2-C3	1.387(3)	C17-C18	1.402(3)
C3-C4	1.376(3)	C18-C19	1.435(3)
C4-C5	1.390(3)	C19-C20	1.495(3)
C5-O6	1.369(3)	C20-C21	1.532(3)
C5-C24	1.403(3)	C21-N22	1.484(2)
O6-C7	1.443(3)	N22-C23	1.478(3)
C7-C8	1.516(3)	C23-C24	1.499(3)
C8-C23	1.523(3)	C24-C25	1.395(3)
C8-C9	1.532(3)	C26-C31	1.387(3)
C9-C33	1.514(3)	C26-C27	1.397(3)
C9-C10	1.614(3)	C27-C28	1.386(3)
C10-N22	1.493(3)	C28-C29	1.387(3)
C10-C11	1.504(3)	C29-C30	1.381(3)
C10-C26	1.546(3)	C29-Cl32	1.741(2)
C11-C19	1.360(3)	C30-C31	1.395(3)
C11-N12	1.378(3)	C33-O34	1.209(3)
N12-C13	1.378(3)	C33-O35	1.334(2)
C13-C14	1.392(3)	O35-C36	1.456(2)
C13-C18	1.420(3)	C36-C37	1.506(3)
C14-C15	1.385(3)		

Table 3: Bond angles (°).

Atoms	Angle	Atoms	Angle
C25-C2-C3	121.0(2)	C17-C18-C13	118.72(19)
C25-C2-Br1	120.01(17)	C17-C18-C19	134.58(19)
C3-C2-Br1	118.95(17)	C13-C18-C19	106.68(17)
C4-C3-C2	119.3(2)	C11-C19-C18	106.57(18)
C3-C4-C5	120.7(2)	C11-C19-C20	121.23(18)
O6-C5-C4	115.67(19)	C18-C19-C20	132.19(18)
O6-C5-C24	124.4(2)	C19-C20-C21	108.48(16)
C4-C5-C24	119.9(2)	N22-C21-C20	109.64(16)
C5-O6-C7	118.03(16)	C23-N22-C21	115.14(15)
O6-C7-C8	108.07(17)	C23-N22-C10	100.67(14)
C7-C8-C23	109.03(16)	C21-N22-C10	114.62(15)
C7-C8-C9	120.24(17)	N22-C23-C24	120.64(17)
C23-C8-C9	101.80(16)	N22-C23-C8	104.31(15)
C33-C9-C8	111.98(16)	C24-C23-C8	110.13(16)
C33-C9-C10	114.35(15)	C25-C24-C5	118.84(19)
C8-C9-C10	102.51(15)	C25-C24-C23	123.36(19)
N22-C10-C11	109.88(16)	C5-C24-C23	117.67(18)
N22-C10-C26	107.57(15)	C2-C25-C24	120.1(2)
C11-C10-C26	105.35(15)	C31-C26-C27	118.56(18)
N22-C10-C9	106.39(15)	C31-C26-C10	123.30(17)
C11-C10-C9	115.43(15)	C27-C26-C10	117.75(17)
C26-C10-C9	112.01(15)	C28-C27-C26	121.25(19)
C19-C11-N12	110.83(17)	C27-C28-C29	119.01(19)
C19-C11-C10	125.37(18)	C30-C29-C28	120.90(18)
N12-C11-C10	123.40(17)	C30-C29-Cl32	120.10(16)
C11-N12-C13	108.13(16)	C28-C29-Cl32	118.99(16)
N12-C13-C14	129.87(19)	C29-C30-C31	119.46(19)
N12-C13-C18	107.78(17)	C26-C31-C30	120.78(19)
C14-C13-C18	122.35(19)	O34-C33-O35	123.99(18)
C15-C14-C13	117.6(2)	O34-C33-C9	124.55(18)
C14-C15-C16	121.1(2)	O35-C33-C9	111.45(16)
C17-C16-C15	121.2(2)	C33-O35-C36	118.01(15)
C16-C17-C18	119.00(19)	O35-C36-C37	110.88(16)