

Table 1 Crystal data and structure refinement for 6b.

Identification code	6b
Empirical formula	C ₁₆ H ₁₄ O ₆
Formula weight	302.27
Temperature/K	170
Crystal system	monoclinic
Space group	P2 ₁ /n
a/Å	9.0938(5)
b/Å	8.2393(5)
c/Å	18.5309(13)
α /°	90
β /°	94.730(2)
γ /°	90
Volume/Å ³	1383.73(15)
Z	4
ρ_{calc} /cm ³	1.451
μ /mm ⁻¹	0.946
F(000)	632.0
Crystal size/mm ³	0.15 × 0.08 × 0.02
Radiation	CuK α (λ = 1.54178)
2 Θ range for data collection/°	10.512 to 145.354
Index ranges	-11 ≤ h ≤ 11, -10 ≤ k ≤ 9, -22 ≤ l ≤ 22
Reflections collected	12221
Independent reflections	2734 [R _{int} = 0.0638, R _{sigma} = 0.0489]
Data/restraints/parameters	2734/0/207
Goodness-of-fit on F ²	1.035
Final R indexes [$I \geq 2\sigma(I)$]	R ₁ = 0.0540, wR ₂ = 0.1515
Final R indexes [all data]	R ₁ = 0.0633, wR ₂ = 0.1635
Largest diff. peak/hole / e Å ⁻³	0.33/-0.32

Table 2 Bond Lengths for 6b.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O2	C11	1.378(2)	C8	C7	1.341(3)
O2	C8	1.394(2)	C8	C9	1.483(3)
O4	C12	1.359(2)	C7	C6	1.451(3)
O1	C5	1.366(2)	C5	C6	1.411(2)
O6	C16	1.416(3)	C5	C4	1.386(3)
O5	C13	1.350(2)	C6	C1	1.406(2)
O3	C9	1.236(2)	C4	C3	1.380(3)
C11	C10	1.387(3)	C13	C14	1.400(3)
C11	C12	1.382(2)	C1	C2	1.376(3)
C10	C9	1.446(2)	C15	C14	1.377(3)
C10	C15	1.398(3)	C2	C3	1.392(3)

Table 3 Bond Angles for 6b.

Atom Atom Atom	Angle/°	Atom Atom Atom	Angle/°
C11 O2 C8	106.14(14)	C10 C9 C8	104.42(15)
O2 C11 C10	113.33(15)	O1 C5 C6	117.09(16)
O2 C11 C12	123.60(16)	O1 C5 C4	121.77(17)
C12 C11 C10	123.07(17)	C4 C5 C6	121.13(17)
C11 C10 C9	106.63(16)	C5 C6 C7	118.25(16)
C11 C10 C15	120.34(17)	C1 C6 C7	124.25(17)
C15 C10 C9	133.03(17)	C1 C6 C5	117.50(17)
O4 C12 C11	126.47(17)	C3 C4 C5	119.88(18)
O4 C12 C13	117.77(16)	O5 C13 C12	120.26(17)
C11 C12 C13	115.76(16)	O5 C13 C14	117.67(17)
O2 C8 C9	109.46(15)	C12 C13 C14	122.07(17)
C7 C8 O2	124.28(17)	C2 C1 C6	121.14(18)
C7 C8 C9	126.26(17)	C14 C15 C10	117.96(18)
C8 C7 C6	131.07(17)	C15 C14 C13	120.76(18)
O3 C9 C10	128.58(18)	C1 C2 C3	120.18(18)
O3 C9 C8	127.00(17)	C4 C3 C2	120.17(18)

