Supplementary Material:

3-(4-Bromophenyl)-4-{[3-hydroxy-6-(hydroxymethyl)-4-oxo-4*H*-pyran-2-yl](*m*-tolyl)methyl}isoxazol-5(2*H*)-one

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XRD data

Table S1. Crystal data and structure refinement for **4**.

Identification code	**4**	
Empirical formula	$C_{23}H_{18}BrNO_6$	
Formula weight	484.29	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 9.4765(3) Å	α = 90 °.
	b = 9.2067(3) Å	β = 92.1209(7) °.
	c = 24.1253(7) Å	γ = 90 °.
Volume	2103.42(11) $Å^3$	
Z	4	
Density (calculated)	1.529 g/cm^3	
Absorption coefficient	1.995 mm^{-1}	
F(000)	984	
Crystal size	0.280 x 0.110 x 0.065 mm^3	
Theta range for data collection	2.340 to 31.510 °.	
Index ranges	-13<=h<=13, -13<=k<=13, -35<=l<=35	
Reflections collected	82080	
Independent reflections	7000 [R(int) = 0.0565]	
Observed reflections	5348	
Completeness to theta = 25.242 °	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.1033 and 0.0611	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7000 / 2 / 293	
Goodness-of-fit on F2	1.046	
Final R indices [I>2sigma(I)]	R1 = 0.0400, wR2 = 0.0893	
R indices (all data)	R1 = 0.0604, wR2 = 0.1023	
Largest diff. peak and hole	1.835 and -1.456 e.$Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(1)	-1188(1)	2444(1)	5035(1)	34(1)
C(1)	6383(2)	10349(2)	2506(1)	28(1)
O(1)	5192(1)	8685(2)	3052(1)	22(1)
O(2)	7045(2)	11722(2)	2540(1)	33(1)
C(2)	5899(2)	9949(2)	3068(1)	22(1)
O(3)	5576(2)	10939(2)	4490(1)	22(1)
C(3)	6096(2)	10729(2)	3538(1)	22(1)
O(4)	4131(2)	8340(2)	4456(1)	22(1)
C(4)	5496(2)	10246(2)	4040(1)	20(1)
O(5)	7173(1)	6296(2)	3513(1)	23(1)
C(5)	4745(2)	8887(2)	4004(1)	19(1)
O(6)	6793(1)	4416(2)	4082(1)	22(1)
C(6)	4631(2)	8150(2)	3520(1)	20(1)
N(1)	5620(2)	3870(2)	4352(1)	21(1)
C(7)	3913(2)	6686(2)	3455(1)	19(1)
C(8)	4803(2)	5561(2)	3754(1)	19(1)
C(9)	6310(2)	5532(2)	3741(1)	20(1)
C(10)	4435(2)	4511(2)	4127(1)	19(1)
C(11)	3067(2)	4051(2)	4336(1)	20(1)
C(12)	1809(2)	4201(2)	4019(1)	23(1)
C(13)	537(2)	3739(2)	4225(1)	26(1)
C(14)	535(2)	3107(2)	4748(1)	25(1)
C(15)	1765(2)	2947(2)	5070(1)	26(1)
C(16)	3027(2)	3418(2)	4862(1)	23(1)
C(17)	3556(2)	6366(2)	2844(1)	21(1)
C(18)	4413(2)	5530(2)	2520(1)	24(1)
C(19)	4134(2)	5372(3)	1948(1)	28(1)
C(20)	2955(2)	6063(3)	1712(1)	32(1)
C(21)	2084(3)	6894(3)	2035(1)	34(1)
C(22)	2375(2)	7041(2)	2599(1)	28(1)
C(23)	5100(3)	4496(3)	1594(1)	41(1)

Table S3. Bond lengths [Å] and angles [°] for **4**.

Br(1)-C(14)	1.8973(19)
C(1)-O(2)	1.412(3)
C(1)-C(2)	1.494(3)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
O(1)-C(2)	1.342(2)
O(1)-C(6)	1.358(2)
O(2)-H(2)	0.828(18)
C(2)-C(3)	1.349(3)
O(3)-C(4)	1.259(2)
C(3)-C(4)	1.428(3)
C(3)-H(3)	0.9500
O(4)-C(5)	1.352(2)
O(4)-H(4)	0.825(17)
C(4)-C(5)	1.441(3)
O(5)-C(9)	1.224(2)
C(5)-C(6)	1.351(3)
O(6)-C(9)	1.385(2)
O(6)-N(1)	1.402(2)
C(6)-C(7)	1.515(3)
N(1)-C(10)	1.363(2)
N(1)-H(1)	0.87(3)
C(7)-C(8)	1.504(3)
C(7)-C(17)	1.529(3)
C(7)-H(7)	1.0000
C(8)-C(10)	1.374(3)
C(8)-C(9)	1.430(2)
C(10)-C(11)	1.471(2)
C(11)-C(16)	1.398(3)
C(11)-C(12)	1.399(3)
C(12)-C(13)	1.388(3)
C(12)-H(12)	0.9500
C(13)-C(14)	1.388(3)
C(13)-H(13)	0.9500

C(14)-C(15)	1.385(3)
C(15)-C(16)	1.384(3)
C(15)-H(15)	0.9500
C(16)-H(16)	0.9500
C(17)-C(18)	1.383(3)
C(17)-C(22)	1.391(3)
C(18)-C(19)	1.402(3)
C(18)-H(18)	0.9500
C(19)-C(20)	1.389(3)
C(19)-C(23)	1.509(3)
C(20)-C(21)	1.385(4)
C(20)-H(20)	0.9500
C(21)-C(22)	1.386(3)
C(21)-H(21)	0.9500
C(22)-H(22)	0.9500
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
O(2)-C(1)-C(2)	108.53(17)
O(2)-C(1)-H(1A)	110.0
C(2)-C(1)-H(1A)	110.0
O(2)-C(1)-H(1B)	110.0
C(2)-C(1)-H(1B)	110.0
H(1A)-C(1)-H(1B)	108.4
C(2)-O(1)-C(6)	120.04(15)
C(1)-O(2)-H(2)	100(3)
O(1)-C(2)-C(3)	122.67(17)
O(1)-C(2)-C(1)	110.88(17)
C(3)-C(2)-C(1)	126.44(18)
C(2)-C(3)-C(4)	119.98(18)
C(2)-C(3)-H(3)	120.0
C(4)-C(3)-H(3)	120.0
C(5)-O(4)-H(4)	110(2)
O(3)-C(4)-C(3)	124.10(18)
O(3)-C(4)-C(5)	120.43(17)
C(3)-C(4)-C(5)	115.45(17)

C(6)-C(5)-O(4) 119.12(17)
C(6)-C(5)-C(4) 120.83(17)
O(4)-C(5)-C(4) 120.05(16)
C(9)-O(6)-N(1) 106.97(13)
C(5)-C(6)-O(1) 120.97(17)
C(5)-C(6)-C(7) 123.84(16)
O(1)-C(6)-C(7) 115.18(16)
C(10)-N(1)-O(6) 108.43(15)
C(10)-N(1)-H(1) 122.2(19)
O(6)-N(1)-H(1) 111.5(19)
C(8)-C(7)-C(6) 108.73(15)
C(8)-C(7)-C(17) 115.51(16)
C(6)-C(7)-C(17) 110.68(15)
C(8)-C(7)-H(7) 107.2
C(6)-C(7)-H(7) 107.2
C(17)-C(7)-H(7) 107.2
C(10)-C(8)-C(9) 106.25(16)
C(10)-C(8)-C(7) 130.36(16)
C(9)-C(8)-C(7) 123.00(16)
O(5)-C(9)-O(6) 118.79(16)
O(5)-C(9)-C(8) 133.20(18)
O(6)-C(9)-C(8) 107.95(15)
N(1)-C(10)-C(8) 109.86(16)
N(1)-C(10)-C(11) 117.57(16)
C(8)-C(10)-C(11) 132.46(17)
C(16)-C(11)-C(12) 119.08(17)
C(16)-C(11)-C(10) 119.01(17)
C(12)-C(11)-C(10) 121.89(17)
C(13)-C(12)-C(11) 120.49(18)
C(13)-C(12)-H(12) 119.8
C(11)-C(12)-H(12) 119.8
C(14)-C(13)-C(12) 118.97(18)
C(14)-C(13)-H(13) 120.5
C(12)-C(13)-H(13) 120.5
C(15)-C(14)-C(13) 121.70(18)
C(15)-C(14)-Br(1) 118.55(15)

C(13)-C(14)-Br(1)	119.75(15)
C(16)-C(15)-C(14)	118.87(19)
C(16)-C(15)-H(15)	120.6
C(14)-C(15)-H(15)	120.6
C(15)-C(16)-C(11)	120.88(18)
C(15)-C(16)-H(16)	119.6
C(11)-C(16)-H(16)	119.6
C(18)-C(17)-C(22)	119.30(18)
C(18)-C(17)-C(7)	122.59(17)
C(22)-C(17)-C(7)	117.93(18)
C(17)-C(18)-C(19)	121.35(19)
C(17)-C(18)-H(18)	119.3
C(19)-C(18)-H(18)	119.3
C(20)-C(19)-C(18)	118.3(2)
C(20)-C(19)-C(23)	120.6(2)
C(18)-C(19)-C(23)	121.0(2)
C(21)-C(20)-C(19)	120.7(2)
C(21)-C(20)-H(20)	119.7
C(19)-C(20)-H(20)	119.7
C(20)-C(21)-C(22)	120.3(2)
C(20)-C(21)-H(21)	119.9
C(22)-C(21)-H(21)	119.9
C(21)-C(22)-C(17)	120.0(2)
C(21)-C(22)-H(22)	120.0
C(17)-C(22)-H(22)	120.0
C(19)-C(23)-H(23A)	109.5
C(19)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(19)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U11	U22	U33	U23	U13	U12
Br(1)	18(1)	47(1)	37(1)	14(1)	4(1)	-5(1)
C(1)	37(1)	25(1)	21(1)	-1(1)	10(1)	-6(1)
O(1)	24(1)	22(1)	19(1)	0(1)	5(1)	-4(1)
O(2)	48(1)	26(1)	26(1)	-2(1)	16(1)	-10(1)
C(2)	23(1)	21(1)	22(1)	1(1)	6(1)	-2(1)
O(3)	26(1)	22(1)	19(1)	-1(1)	3(1)	-3(1)
C(3)	23(1)	21(1)	21(1)	0(1)	5(1)	-3(1)
O(4)	24(1)	24(1)	17(1)	1(1)	5(1)	-5(1)
C(4)	18(1)	21(1)	19(1)	1(1)	2(1)	0(1)
O(5)	20(1)	29(1)	22(1)	2(1)	5(1)	-3(1)
C(5)	18(1)	20(1)	19(1)	2(1)	2(1)	0(1)
O(6)	17(1)	25(1)	23(1)	3(1)	4(1)	-1(1)
C(6)	19(1)	22(1)	19(1)	2(1)	3(1)	-1(1)
N(1)	17(1)	22(1)	25(1)	5(1)	3(1)	-2(1)
C(7)	18(1)	20(1)	19(1)	1(1)	2(1)	-1(1)
C(8)	18(1)	21(1)	17(1)	-1(1)	2(1)	-1(1)
C(9)	20(1)	22(1)	17(1)	-1(1)	2(1)	-1(1)
C(10)	19(1)	21(1)	17(1)	-1(1)	1(1)	-1(1)
C(11)	18(1)	21(1)	21(1)	0(1)	2(1)	-2(1)
C(12)	20(1)	26(1)	22(1)	2(1)	0(1)	-2(1)
C(13)	19(1)	32(1)	26(1)	4(1)	-2(1)	-2(1)
C(14)	18(1)	30(1)	28(1)	4(1)	4(1)	-3(1)
C(15)	21(1)	34(1)	24(1)	6(1)	2(1)	-2(1)
C(16)	18(1)	28(1)	22(1)	2(1)	0(1)	-1(1)
C(17)	21(1)	22(1)	20(1)	3(1)	-1(1)	-4(1)
C(18)	23(1)	28(1)	22(1)	1(1)	-1(1)	-3(1)
C(19)	30(1)	34(1)	21(1)	-2(1)	2(1)	-11(1)
C(20)	38(1)	36(1)	21(1)	3(1)	-7(1)	-11(1)
C(21)	34(1)	32(1)	34(1)	6(1)	-12(1)	-4(1)
C(22)	26(1)	27(1)	31(1)	1(1)	-5(1)	1(1)
C(23)	38(1)	60(2)	25(1)	-10(1)	5(1)	-7(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **4**.

	x	y	z	U(eq)
H(1A)	7057	9612	2376	33
H(1B)	5567	10386	2238	33
H(2)	7390(40)	11760(40)	2231(9)	64(11)
H(3)	6633	11600	3535	26
H(4)	4290(30)	8880(30)	4723(10)	47(9)
H(1)	5680(30)	2930(30)	4401(12)	33(7)
H(7)	2999	6747	3648	23
H(12)	1826	4622	3660	27
H(13)	-319	3854	4012	31
H(15)	1742	2521	5429	32
H(16)	3877	3310	5079	27
H(18)	5208	5052	2688	29
H(20)	2743	5965	1326	38
H(21)	1283	7365	1868	40
H(22)	1769	7603	2819	34
H(23A)	4542	4006	1300	61
H(23B)	5599	3769	1825	61
H(23C)	5789	5143	1428	61

Table S6. Torsion angles [°] for **4**.

C(6)-O(1)-C(2)-C(3)	0.6(3)
C(6)-O(1)-C(2)-C(1)	-178.29(17)
O(2)-C(1)-C(2)-O(1)	176.64(17)
O(2)-C(1)-C(2)-C(3)	-2.2(3)
O(1)-C(2)-C(3)-C(4)	-2.5(3)
C(1)-C(2)-C(3)-C(4)	176.30(19)
C(2)-C(3)-C(4)-O(3)	-176.77(19)
C(2)-C(3)-C(4)-C(5)	2.2(3)
O(3)-C(4)-C(5)-C(6)	178.74(18)
C(3)-C(4)-C(5)-C(6)	-0.2(3)
O(3)-C(4)-C(5)-O(4)	-0.6(3)
C(3)-C(4)-C(5)-O(4)	-179.62(17)
O(4)-C(5)-C(6)-O(1)	177.85(16)
C(4)-C(5)-C(6)-O(1)	-1.5(3)
O(4)-C(5)-C(6)-C(7)	-3.3(3)
C(4)-C(5)-C(6)-C(7)	177.32(17)
C(2)-O(1)-C(6)-C(5)	1.4(3)
C(2)-O(1)-C(6)-C(7)	-177.54(16)
C(9)-O(6)-N(1)-C(10)	7.5(2)
C(5)-C(6)-C(7)-C(8)	-69.7(2)
O(1)-C(6)-C(7)-C(8)	109.24(18)
C(5)-C(6)-C(7)-C(17)	162.44(18)
O(1)-C(6)-C(7)-C(17)	-18.6(2)
C(6)-C(7)-C(8)-C(10)	131.1(2)
C(17)-C(7)-C(8)-C(10)	-103.8(2)
C(6)-C(7)-C(8)-C(9)	-40.7(2)
C(17)-C(7)-C(8)-C(9)	84.4(2)
N(1)-O(6)-C(9)-O(5)	171.13(17)
N(1)-O(6)-C(9)-C(8)	-6.49(19)
C(10)-C(8)-C(9)-O(5)	-174.0(2)
C(7)-C(8)-C(9)-O(5)	-0.5(3)
C(10)-C(8)-C(9)-O(6)	3.2(2)
C(7)-C(8)-C(9)-O(6)	176.68(16)
O(6)-N(1)-C(10)-C(8)	-5.6(2)

O(6)-N(1)-C(10)-C(11)	177.77(15)
C(9)-C(8)-C(10)-N(1)	1.5(2)
C(7)-C(8)-C(10)-N(1)	-171.33(18)
C(9)-C(8)-C(10)-C(11)	177.46(19)
C(7)-C(8)-C(10)-C(11)	4.6(3)
N(1)-C(10)-C(11)-C(16)	22.5(3)
C(8)-C(10)-C(11)-C(16)	-153.2(2)
N(1)-C(10)-C(11)-C(12)	-156.14(19)
C(8)-C(10)-C(11)-C(12)	28.2(3)
C(16)-C(11)-C(12)-C(13)	0.6(3)
C(10)-C(11)-C(12)-C(13)	179.16(19)
C(11)-C(12)-C(13)-C(14)	-0.9(3)
C(12)-C(13)-C(14)-C(15)	1.0(3)
C(12)-C(13)-C(14)-Br(1)	-179.17(16)
C(13)-C(14)-C(15)-C(16)	-0.7(3)
Br(1)-C(14)-C(15)-C(16)	179.52(17)
C(14)-C(15)-C(16)-C(11)	0.2(3)
C(12)-C(11)-C(16)-C(15)	-0.2(3)
C(10)-C(11)-C(16)-C(15)	-178.84(19)
C(8)-C(7)-C(17)-C(18)	-27.4(3)
C(6)-C(7)-C(17)-C(18)	96.7(2)
C(8)-C(7)-C(17)-C(22)	157.61(18)
C(6)-C(7)-C(17)-C(22)	-78.3(2)
C(22)-C(17)-C(18)-C(19)	1.3(3)
C(7)-C(17)-C(18)-C(19)	-173.61(18)
C(17)-C(18)-C(19)-C(20)	-1.0(3)
C(17)-C(18)-C(19)-C(23)	178.1(2)
C(18)-C(19)-C(20)-C(21)	0.4(3)
C(23)-C(19)-C(20)-C(21)	-178.6(2)
C(19)-C(20)-C(21)-C(22)	-0.3(3)
C(20)-C(21)-C(22)-C(17)	0.7(3)
C(18)-C(17)-C(22)-C(21)	-1.2(3)
C(7)-C(17)-C(22)-C(21)	173.97(19)

Table S7. Hydrogen bonds for **4** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2)...O(5)#1	0.828(18)	1.90(2)	2.703(2)	162(4)
O(4)-H(4)...O(3)	0.825(17)	2.33(3)	2.757(2)	113(3)
O(4)-H(4)...O(3)#2	0.825(17)	1.90(2)	2.6333(19)	147(3)
N(1)-H(1)...O(3)#3	0.87(3)	1.85(3)	2.720(2)	173(3)

Symmetry transformations used to generate equivalent atoms:

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