Supporting information

for

D-Idose-based Monoaza-15-crown-5 Lariat Ethers: Synthesis of an Elusive D-Hexose and Application of Derived Macrocycles in Enantioselective Syntheses

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Crystal data of 6: $C_{14}H_{18}O_6$, *Fwt.*: 282.28, colourless, block, size: 0.50 x 0.50 x 0.30 mm, orthorhombic, space group $P\,2_1\,2_1\,2_1$, $a = 11.1137(5)$Å, $b = 11.2985(5)$Å, $c = 22.2672(11)$Å, $\alpha = 90°$, $\beta = 90°$, $\gamma = 90°$, $V = 2796.1(2)$Å^3, $T = 298(2)$K, $Z = 8$, Z'=2, $F(000) = 1200$, $D_x = 1.341$ Mg/m^3, μ 0.885mm^{-1}.

A crystal of compound **6** was mounted on a loop. Cell parameters were determined by least-squares using 18503 ($3.915 \le \theta \le 67.97°$) reflections. Intensity data were collected on a(n) Rigaku RAXIS-RAPID II diffractometer (monochromator; Cu-$K\alpha$ radiation, $\lambda = 1.54187$Å) at 298(2) K in the range $3.971 \le \theta \le 68.036$. A total of 23337 reflections were collected of which 4948 were unique [R(int) = 0.0401, $R(\sigma)$ = 0.0391]; intensities of 3307 reflections were greater than $2\sigma(I)$. Completeness to θ = 0.986.

A numerical absorption correction was applied to the data (the minimum and maximum transmission factors were 0.924071 and 0.969107). The structure was solved by constr methods (and subsequent difference syntheses).

Anisotropic full-matrix least-squares refinement on F^2 for all non-hydrogen atoms yielded $R_1 = 0.0498$ and $wR^2 = 0.1001$ for 1332 [$I > 2\sigma(I)$] and $R_1 = 0.0815$ and $wR^2 = 0.1131$ for all (4948) intensity data, (number of parameters = 367, goodness-of-fit = 1.009, the maximum and mean shift/esd is 0.000 and 0.000). The absolute structure parameter is 0.06(7). (Friedel coverage: 0.736, Friedel fraction max.: 0.950, Friedel fraction full: 0.954).

The maximum and minimum residual electron density in the final difference map was 0.16 and -0.20e.Å^{-3}.

The weighting scheme applied was $w = 1/[\sigma^2(F_o^2)+(0.04490.3834P)^2+0.3834P]$ where $P = (F_o^2+2F_c^2)/3$.

Hydrogen atomic positions were calculated from assumed geometries. Hydrogen atoms were included in structure factor calculations, but they were not refined. The isotropic displacement parameters of the hydrogen atoms were approximated from the U(eq) value of the atom they were bonded to.

The crystallographic information files (CIFs), which are deposited at Cambridge Crystallographic Data Centre (CCDC No. 2276749).
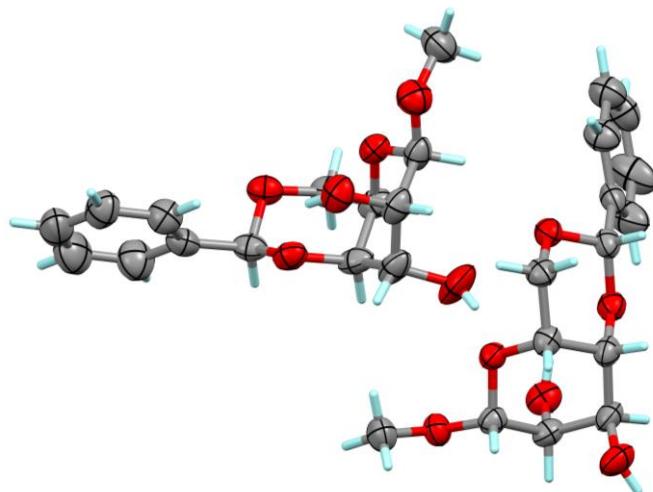

Figure S1. Ortep-style representation of the asymmetric unit. The ellipsoids are drawn with 30% probability level. Two independent molecules are observed within the asymmetric unit. The configuration is the same, but the conformation of the phenyl rings is the difference within the molecules.
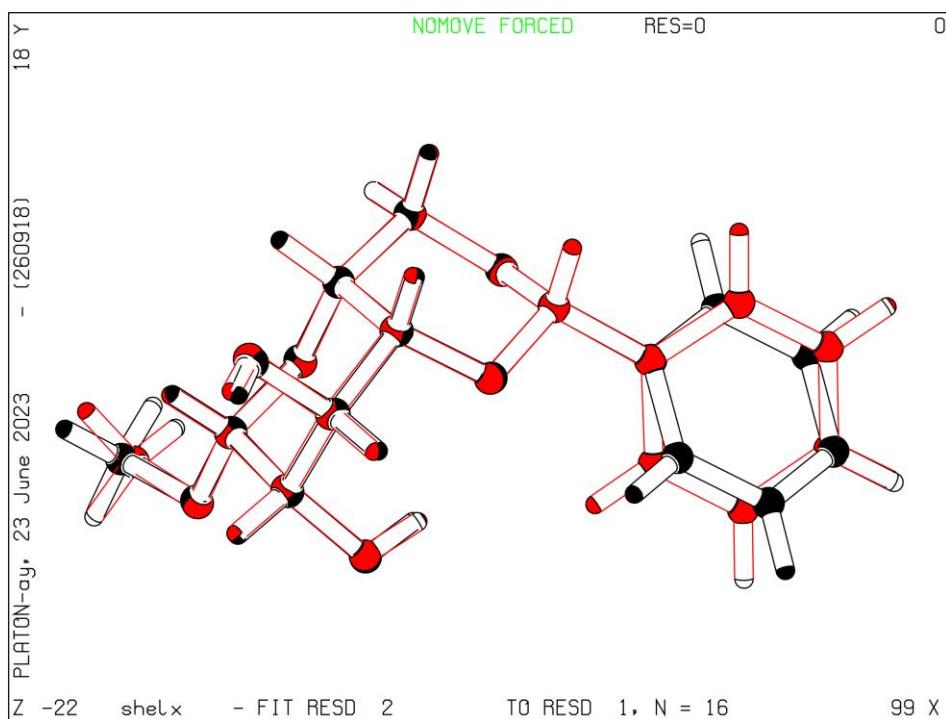
**Figure S2.** The conformation differences of the molecules.
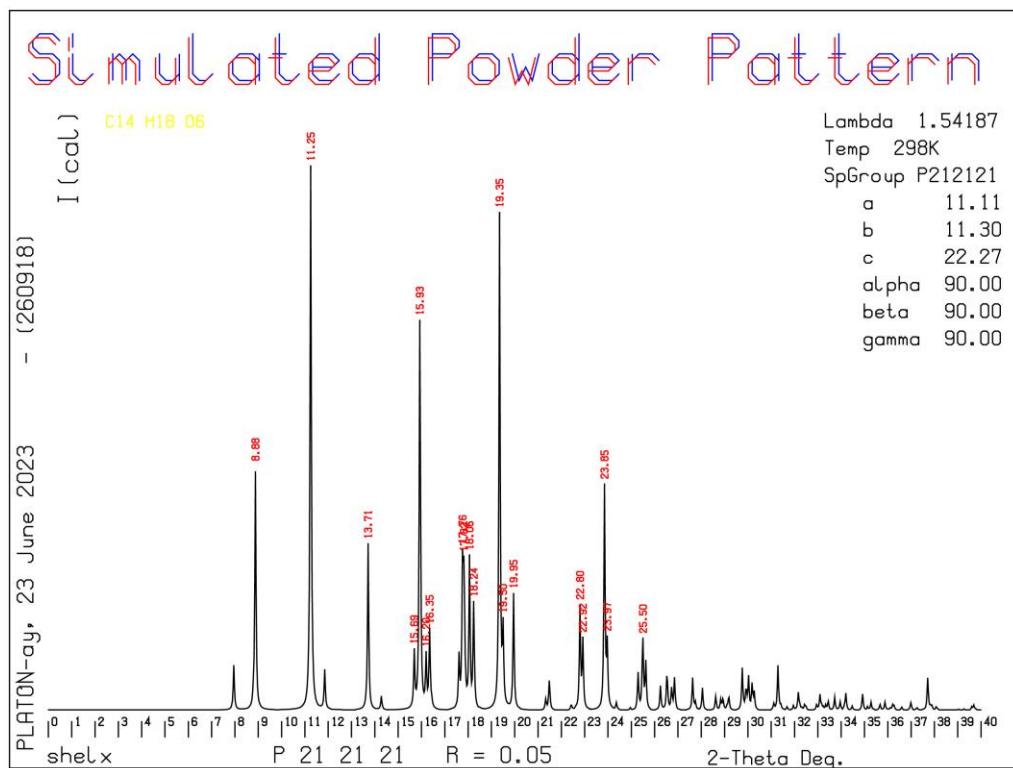
Figure S3. The simulated powder diffractogram of the measured single crystal.

Table S1. Summary of crystallographic data, data collections, structure determination and refinement for methyl-4,6-*O*-benzylidene-β-D-idopyranoside (**6**)

number	**6**
CCDC number	2276749
Empirical formula	$C_{14} H_{18} O_6$
Formula weight	282.28
Temperature	298(2)
Radiation and wavelength	Cu-Kα, $\lambda = 1.54187$Å
Crystal system	orthorhombic
Space group	$P\ 2_1\ 2_1\ 2_1$
Unit cell dimensions	$a = 11.1137(5)$Å
	$b = 11.2985(5)$Å
	$c = 22.2672(11)$Å
	$\alpha = 90°$
	$\beta = 90°$
	$\gamma = 90°$
Volume	$2796(1)$Å³
Z, Z'	8, 2
Density (calculated)	1.341 Mg/m³
Absorption coefficient, μ	0.885 mm⁻¹
F(000)	1200
Crystal colour and description	colourless, block
Crystal size	0.50 x 0.50 x 0.30 mm
Absorption correction	numerical
Max. and min. transmission	0.924071 and 0.969107
θ–range for data collection	$3.971 \leq \theta \leq 68.036°$
Index ranges	$-13 \leq h \leq 13$;
	$-13 \leq k \leq 11$;
	$-26 \leq l \leq 26$

Reflections collected	23337
Completeness to 2θ	0.987
Absolute structure parameter	
Flack	0.06(7)
Hooft	0.07(6)
Parsonz	0.08(7)
Friedel coverage	0.736
Friedel fraction max.	0.950
Friedel fraction full	0.954
Independent reflections	4948 [R(int) =0.0401]
Reflections $I>2\sigma(I)$	3307
Data / restraints / parameters	4948 /0 /367
Goodness-of-fit on $F2$	1.009
Final R indices [$I>2\sigma(I)$]	R_1 =0.0498, wR^2 =0.1001
R indices (all data)	R_1 =0.0815, wR^2 =0.1131
Max. and mean shift/esd	0.000;0.000
Largest diff. peak and hole	0.16 and -0.20 e.Å^{-3}

However, two independent molecules are observed within the asymmetric unit. These two molecules exhibit slight conformational differences within the phenyl rings (Figure S2). The differences between the two molecules are also evident in the short contacts with neighboring molecules. A useful program for analyzing the spatial arrangement and contacts surrounding the molecules is the Crystal Explorer Hirshfeld Surface Analysis program. The Hirshfeld surface analysis provides a visualization of the molecular interactions, often referred to as a "fingerprint." These fingerprint shapes illustrate the variations between the molecules. The interactions can be categorized into different element types, with the most notable difference observed between carbon and oxygen atoms. The dissimilarity in carbon atoms can arise from the rotation of the phenyl groups, while the disparity in oxygen atoms is particularly noticeable in the hydrogen bonding pattern (Figure S3). The hydrogen bonding motifs differ between the two molecules. molecule #1 has more acceptor positions than molecule #2 (Figure S4). Additionally, the distances between the hydrogen bond atoms also vary (Table S2).
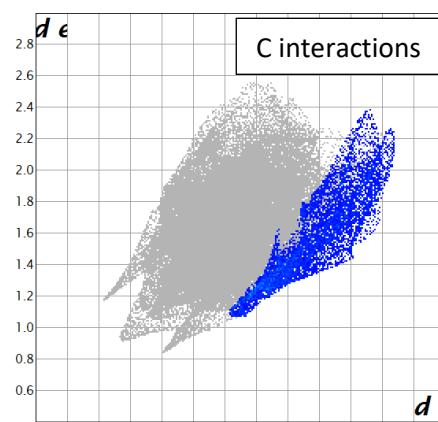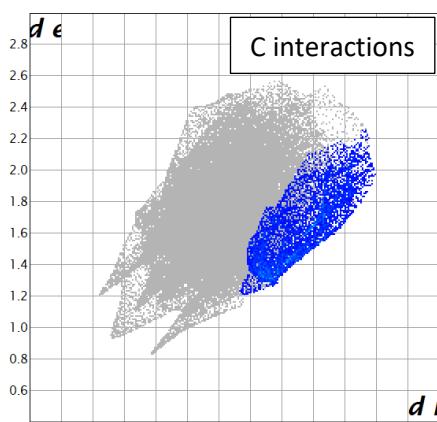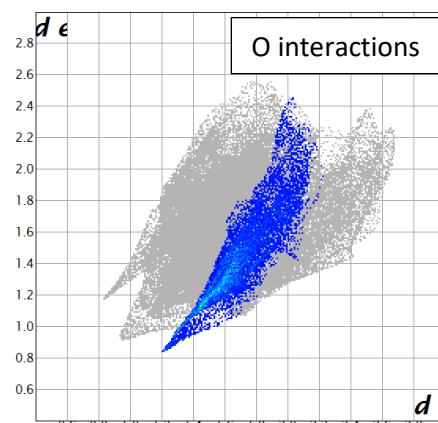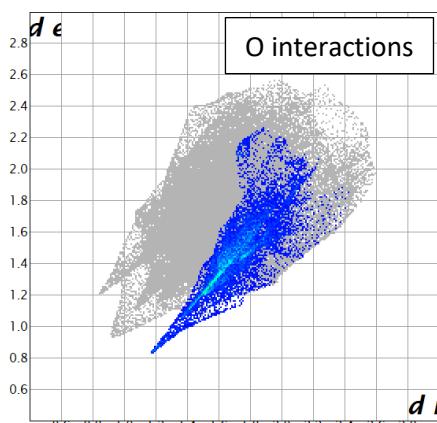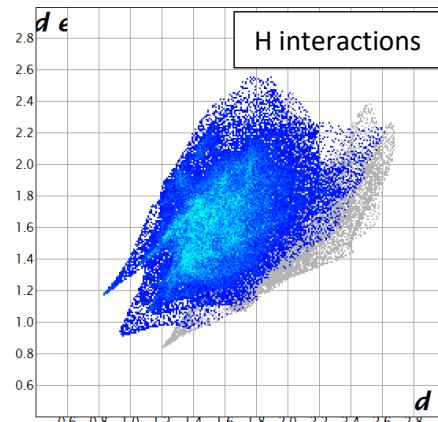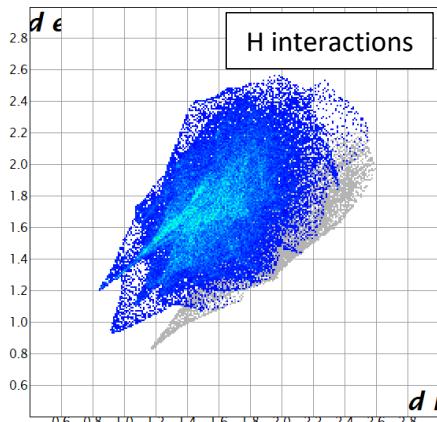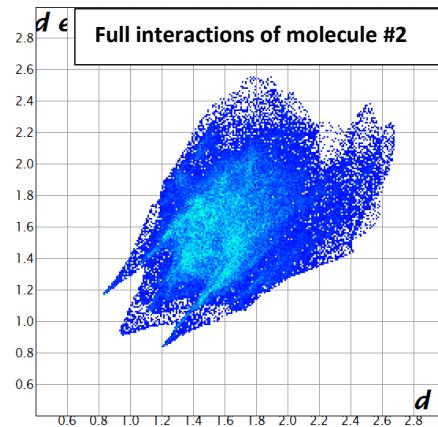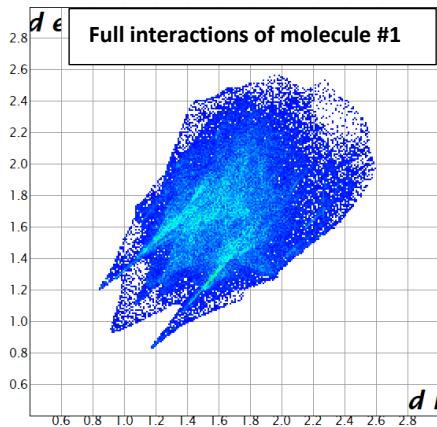
Figure S3. The Hirshfeld surface analysis of the two molecules in the asymmetric unit. First column is the named molecule #1 a.), and the second column is the named molecule #2 b.).
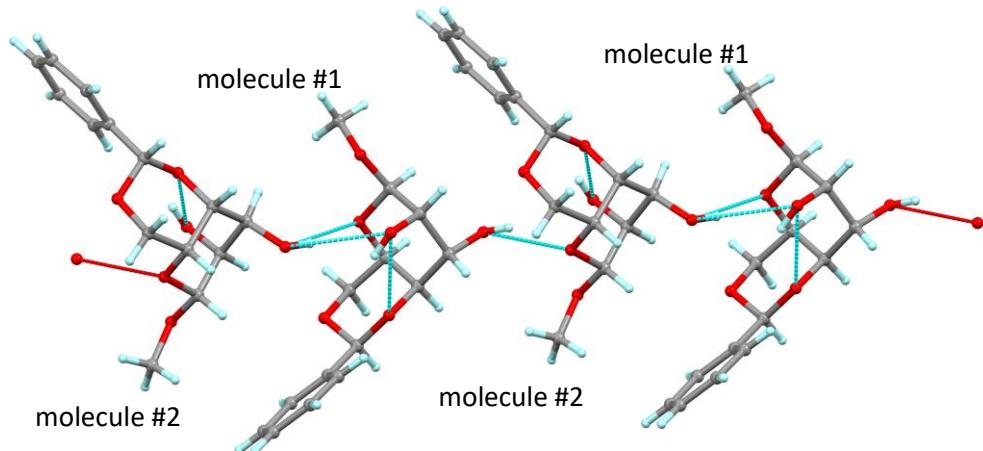
Figure S4. The Hydrogen-bond motifs within the molecules.

Table S2. The hydrogen bond Donor (D), hydrogen (H) and Acceptor (A) distances and angles

D _flag_hbond_publ	H	A	d(D-H) (Å)	d(H...A) (Å)	d(D...A) (Å)	<(D-H...A) (°)
O18_1	H18_1	O1_1	0.82	2.21	2.844(4)	134
O18_1	H18_1	O35_2	0.82	2.52	3.030(5)	121
O19_1	H19_1	O32_2[$1]	0.82	2.16	2.924(4)	154
O34_2	H34_2	O21_2	0.82	2.13	2.819(4)	142
O35_2	H35_2	O13_1	0.82	2.22	3.008(4)	162
O35_2	H35_2	O18_1	0.82	2.54	3.030(5)	120
C22_2	H22_2	O18_1	0.98	2.32	3.274(5)	163
C23_2	H23B_2	O17_1	0.97	2.6	3.496(5)	153
C33_2	H33_2	O3_1	0.98	2.64	3.499(6)	146
C2_1	H2_1	O34_2[$2]	0.98	2.63	3.540(5)	155
C15_1	H15_1	O23_2[$1]	0.98	2.52	3.405(5)	150

Symmetry codes to generate equivalent atoms:

$1. [1_545] x,y-*,z

$2. [3_556] x+1/2,-y+1/2,-z+1

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O1_1	3768(2)	184(2)	3847(1)	70(1)
O3_1	3796(2)	1723(2)	4542(1)	69(1)
O13_1	1442(2)	723(2)	4401(1)	64(1)
O17_1	-274(2)	635(3)	3853(1)	76(1)
O18_1	1648(3)	69(3)	3133(1)	86(1)
O19_1	1891(4)	-2287(3)	4244(2)	98(1)
C2_1	4503(4)	992(4)	4165(2)	67(1)
C4_1	3185(4)	1030(4)	4983(2)	71(1)
C5_1	2406(4)	106(4)	4691(2)	67(1)
C6_1	3128(4)	-596(4)	4241(2)	69(1)
C7_1	5154(4)	1780(4)	3729(2)	73(1)
C8_1	5803(4)	2721(5)	3940(2)	93(2)
C9_1	6426(5)	3452(5)	3554(3)	102(2)
C10_1	6402(5)	3274(6)	2959(3)	105(2)
C11_1	5760(5)	2347(7)	2741(2)	132(2)
C12_1	5139(5)	1588(6)	3124(2)	115(2)
C14_1	629(4)	-56(4)	4095(2)	65(1)
C15_1	1267(4)	-704(4)	3594(2)	71(1)
C16_1	2334(4)	-1379(4)	3862(2)	75(1)
C20_1	-1126(4)	1075(4)	4279(2)	95(2)
O21_2	-151(3)	5151(3)	3580(1)	79(1)
O23_2	335(3)	6724(3)	2947(1)	79(1)
O32_2	2408(3)	5656(2)	3490(1)	69(1)
O33_2	3613(3)	5497(3)	4310(1)	99(1)
O34_2	1302(3)	4942(3)	4612(1)	93(1)
O35_2	1861(5)	2647(3)	3491(2)	126(1)
C22_2	-605(4)	5991(4)	3160(2)	77(1)
C23_2	1215(4)	6041(4)	2630(2)	85(1)

C24_2	1724(4)	5085(4)	3029(2)	78(1)
C25_2	721(5)	4368(4)	3313(2)	83(1)
C26_2	-1497(4)	6781(4)	3460(2)	78(1)
C27_2	-1436(5)	7093(5)	4057(2)	93(2)
C28_2	-2238(6)	7876(5)	4309(3)	108(2)
C29_2	-3111(6)	8374(6)	3961(4)	121(2)
C30_2	-3190(7)	8080(7)	3370(4)	138(2)
C31_2	-2394(6)	7291(6)	3120(3)	122(2)
C32_2	1189(5)	3545(4)	3802(2)	90(2)
C33_2	1988(5)	4188(4)	4239(2)	85(1)
C34_2	2956(4)	4840(4)	3908(2)	79(1)
C38_2	4640(5)	6053(5)	4071(3)	118(2)

Table S4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3).

	x	y	z	U(iso)
H18_1	2197	487	3258	129
H19_1	1801	-2897	4049	147
H2_1	5089	555	4407	81
H4A_1	2690	1541	5231	85
H4B_1	3771	647	5241	85
H5_1	2080	-426	4998	80
H6_1	3709	-1091	4457	83
H8_1	5824	2869	4350	111
H9_1	6869	4080	3709	123
H10_1	6818	3775	2701	127
H11_1	5735	2216	2329	159
H12_1	4713	950	2968	138
H14_1	287	-626	4379	78
H15_1	707	-1280	3420	85
H16_1	2811	-1732	3538	90
H20A_1	-1770	1465	4070	143
H20B_1	-738	1627	4543	143
H20C_1	-1444	428	4509	143
H34_2	779	5268	4412	139
H35_2	1832	2027	3682	189
H22_2	-986	5579	2822	93
H23A_2	1860	6555	2496	102
H23B_2	848	5683	2279	102
H24_2	2248	4563	2794	93
H25_2	326	3895	3001	100
H27_2	-836	6766	4296	112
H28_2	-2185	8066	4715	130
H29_2	-3650	8911	4126	145
H30_2	-3788	8417	3133	165

H31_2	-2461	7099	2715	146
H32_2	512	3184	4016	108
H33_2	2376	3595	4495	101
H34A_2	3479	4282	3695	95
H38A_2	5020	5534	3787	178
H38B_2	5193	6231	4390	178
H38C_2	4408	6773	3874	178

Table S5. Anisotropic displacement parameters (Å^2 x 10^3). The anisotropic displacement factor exponent takes the form: $-2\pi^2(h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12})$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1_1	70(2)	72(2)	69(2)	-11(2)	-1(1)	4(2)
O3_1	66(2)	72(2)	70(2)	-12(2)	3(1)	2(2)
O13_1	67(2)	55(2)	68(2)	-4(1)	-5(1)	3(2)
O17_1	67(2)	81(2)	82(2)	3(2)	-7(2)	11(2)
O18_1	105(2)	87(2)	66(2)	-2(2)	-2(2)	-3(2)
O19_1	126(3)	54(2)	113(2)	-2(2)	-19(2)	2(2)
C2_1	57(2)	75(3)	70(2)	-12(2)	-9(2)	11(2)
C4_1	73(3)	77(3)	63(2)	-12(2)	-4(2)	-3(3)
C5_1	78(3)	64(3)	59(2)	0(2)	-7(2)	7(3)
C6_1	73(3)	62(3)	73(3)	-6(2)	-10(2)	14(2)
C7_1	49(2)	93(4)	76(3)	-10(3)	1(2)	12(3)
C8_1	90(3)	108(4)	80(3)	-5(3)	-7(3)	-10(3)
C9_1	90(4)	110(4)	107(4)	1(4)	4(3)	-12(4)
C10_1	83(4)	136(5)	98(4)	16(4)	19(3)	1(4)
C11_1	109(4)	215(7)	73(3)	-5(4)	23(3)	-40(5)
C12_1	97(4)	158(6)	88(4)	-33(4)	19(3)	-31(4)
C14_1	71(3)	56(3)	67(2)	3(2)	-6(2)	1(2)
C15_1	85(3)	56(3)	70(3)	-7(2)	-4(2)	-5(3)
C16_1	91(3)	50(2)	84(3)	-12(2)	-4(3)	8(3)
C20_1	77(3)	93(4)	115(4)	-4(3)	13(3)	11(3)
O21_2	91(2)	68(2)	78(2)	0(2)	14(2)	-16(2)
O23_2	86(2)	85(2)	67(2)	8(2)	1(2)	-16(2)
O32_2	83(2)	60(2)	63(2)	-1(1)	4(2)	0(2)
O33_2	98(2)	107(3)	94(2)	2(2)	-13(2)	1(2)
O34_2	112(3)	92(2)	74(2)	0(2)	23(2)	8(2)
O35_2	186(4)	55(2)	137(3)	-11(2)	58(3)	3(3)
C22_2	78(3)	87(4)	66(3)	-8(3)	-7(2)	-19(3)
C23_2	91(3)	103(4)	60(2)	-7(3)	8(3)	-20(3)
C24_2	102(3)	68(3)	64(3)	-8(2)	11(2)	-7(3)

C25_2	100(3)	71(3)	79(3)	-21(3)	12(3)	-24(3)
C26_2	71(3)	82(3)	82(3)	6(3)	-3(3)	-16(3)
C27_2	100(4)	97(4)	83(3)	2(3)	-5(3)	2(3)
C28_2	118(5)	96(4)	110(4)	-4(4)	26(4)	5(4)
C29_2	99(4)	101(5)	163(6)	10(5)	22(5)	9(4)
C30_2	117(5)	142(7)	154(7)	20(5)	-23(5)	19(5)
C31_2	115(5)	135(6)	116(5)	-1(4)	-16(4)	13(5)
C32_2	123(4)	53(3)	95(3)	4(3)	39(3)	-3(3)
C33_2	110(4)	64(3)	80(3)	8(3)	11(3)	12(3)
C34_2	91(3)	58(3)	87(3)	11(3)	17(3)	12(3)
C38_2	77(3)	134(5)	144(5)	4(4)	-2(3)	-4(4)

Table S6. Bond lengths (Å) and angles (°) to be deposited

O1_1-C2_1	1.415(4)	O1_1-C6_1	1.433(5)
O3_1-C2_1	1.417(4)	O3_1-C4_1	1.428(5)
O13_1-C5_1	1.431(5)	O13_1-C14_1	1.434(4)
O17_1-C14_1	1.380(4)	O17_1-C20_1	1.429(5)
O18_1-C15_1	1.412(5)	O19_1-C16_1	1.420(5)
C2_1-C7_1	1.503(6)	C4_1-C5_1	1.504(6)
C5_1-C6_1	1.509(5)	C6_1-C16_1	1.509(5)
C7_1-C12_1	1.363(6)	C7_1-C8_1	1.368(6)
C8_1-C9_1	1.378(7)	C9_1-C10_1	1.341(7)
C10_1-C11_1	1.357(7)	C11_1-C12_1	1.393(7)
C14_1-C15_1	1.511(5)	C15_1-C16_1	1.531(6)
O21_2-C22_2	1.426(5)	O21_2-C25_2	1.441(5)
O23_2-C22_2	1.415(5)	O23_2-C23_2	1.431(5)
O32_2-C24_2	1.430(5)	O32_2-C34_2	1.446(5)
O33_2-C34_2	1.373(5)	O33_2-C38_2	1.408(6)
O34_2-C33_2	1.413(5)	O35_2-C32_2	1.437(5)
C22_2-C26_2	1.492(6)	C23_2-C24_2	1.509(6)
C24_2-C25_2	1.516(6)	C25_2-C32_2	1.524(6)
C26_2-C27_2	1.377(6)	C26_2-C31_2	1.379(7)
C27_2-C28_2	1.376(7)	C28_2-C29_2	1.363(8)
C29_2-C30_2	1.359(8)	C30_2-C31_2	1.374(8)
C32_2-C33_2	1.505(6)	C33_2-C34_2	1.497(6)

C2_1-O1_1-C6_1	112.1(3)	C2_1-O3_1-C4_1	110.6(3)
C5_1-O13_1-C14_1	112.8(3)	C14_1-O17_1-C20_1	114.9(3)
O1_1-C2_1-O3_1	110.7(3)	O1_1-C2_1-C7_1	109.7(3)
O3_1-C2_1-C7_1	107.8(3)	O3_1-C4_1-C5_1	110.9(3)
O13_1-C5_1-C4_1	106.8(3)	O13_1-C5_1-C6_1	110.8(3)
C4_1-C5_1-C6_1	110.2(4)	O1_1-C6_1-C5_1	110.3(3)
O1_1-C6_1-C16_1	107.9(3)	C5_1-C6_1-C16_1	111.6(4)

C12_1-C7_1-C8_1	118.0(5)	C12_1-C7_1-C2_1	122.5(5)
C8_1-C7_1-C2_1	119.5(4)	C7_1-C8_1-C9_1	121.1(5)
C10_1-C9_1-C8_1	121.0(5)	C9_1-C10_1-C11_1	118.7(5)
C10_1-C11_1-C12_1	121.1(5)	C7_1-C12_1-C11_1	120.0(6)
O17_1-C14_1-O13_1	107.2(3)	O17_1-C14_1-C15_1	109.1(3)
O13_1-C14_1-C15_1	110.7(3)	O18_1-C15_1-C14_1	112.1(3)
O18_1-C15_1-C16_1	111.0(4)	C14_1-C15_1-C16_1	108.5(3)
O19_1-C16_1-C6_1	106.9(4)	O19_1-C16_1-C15_1	109.0(4)
C6_1-C16_1-C15_1	112.3(3)	C22_2-O21_2-C25_2	112.0(3)
C22_2-O23_2-C23_2	110.7(3)	C24_2-O32_2-C34_2	113.5(3)
C34_2-O33_2-C38_2	115.2(4)	O23_2-C22_2-O21_2	110.4(3)
O23_2-C22_2-C26_2	106.9(4)	O21_2-C22_2-C26_2	109.8(4)
O23_2-C23_2-C24_2	110.6(3)	O32_2-C24_2-C23_2	107.3(4)
O32_2-C24_2-C25_2	109.5(3)	C23_2-C24_2-C25_2	110.6(4)
O21_2-C25_2-C24_2	109.8(4)	O21_2-C25_2-C32_2	108.0(3)
C24_2-C25_2-C32_2	111.9(4)	C27_2-C26_2-C31_2	117.3(5)
C27_2-C26_2-C22_2	123.6(5)	C31_2-C26_2-C22_2	118.9(5)
C28_2-C27_2-	121.8(5)	C29_2-C28_2-	119.6(6)

C26_2		C27_2	
C30_2-C29_2-C28_2	119.8(7)	C29_2-C30_2-C31_2	120.6(7)
C30_2-C31_2-C26_2	120.9(6)	O35_2-C32_2-C33_2	110.2(5)
O35_2-C32_2-C25_2	105.3(4)	C33_2-C32_2-C25_2	111.7(4)
O34_2-C33_2-C34_2	112.3(4)	O34_2-C33_2-C32_2	110.7(4)
C34_2-C33_2-C32_2	110.1(4)	O33_2-C34_2-O32_2	107.4(3)
O33_2-C34_2-C33_2	109.1(4)	O32_2-C34_2-C33_2	109.2(4)

Table S7. Torsion angles (°) to be deposited

C6_1-O1_1-C2_1-O3_1	-61.5(4)	C6_1-O1_1-C2_1-C7_1	179.7(3)
C4_1-O3_1-C2_1-O1_1	62.2(4)	C4_1-O3_1-C2_1-C7_1	-177.9(3)
C2_1-O3_1-C4_1-C5_1	-57.7(4)	C14_1-O13_1-C5_1-C4_1	179.3(3)
C14_1-O13_1-C5_1-C6_1	59.3(4)	O3_1-C4_1-C5_1-O13_1	-68.7(4)
O3_1-C4_1-C5_1-C6_1	51.6(4)	C2_1-O1_1-C6_1-C5_1	55.3(4)
C2_1-O1_1-C6_1-C16_1	177.5(3)	O13_1-C5_1-C6_1-O1_1	68.1(4)
C4_1-C5_1-C6_1-O1_1	-49.9(4)	O13_1-C5_1-C6_1-C16_1	-52.0(5)
C4_1-C5_1-C6_1-C16_1	-169.9(4)	O1_1-C2_1-C7_1-C12_1	-8.7(6)
O3_1-C2_1-C7_1-C12_1	-129.2(5)	O1_1-C2_1-C7_1-C8_1	172.2(4)
O3_1-C2_1-C7_1-C8_1	51.6(5)	C12_1-C7_1-C8_1-C9_1	-0.1(7)
C2_1-C7_1-C8_1-C9_1	179.1(4)	C7_1-C8_1-C9_1-C10_1	0.9(8)
C8_1-C9_1-C10_1-C11_1	-0.7(9)	C9_1-C10_1-C11_1-C12_1	-0.3(9)
C8_1-C7_1-C12_1-C11_1	-0.7(8)	C2_1-C7_1-C12_1-C11_1	-179.9(5)
C10_1-C11_1-C12_1-C7_1	1.0(9)	C20_1-O17_1-C14_1-O13_1	-74.2(4)
C20_1-O17_1-C14_1-C15_1	165.9(4)	C5_1-O13_1-C14_1-O17_1	178.0(3)
C5_1-O13_1-C14_1-	-63.0(4)	O17_1-C14_1-C15_1-	52.1(4)

C15_1		O18_1	
O13_1-C14_1-C15_1-O18_1	-65.7(4)	O17_1-C14_1-C15_1-C16_1	175.1(3)
O13_1-C14_1-C15_1-C16_1	57.3(4)	O1_1-C6_1-C16_1-O19_1	168.9(3)
C5_1-C6_1-C16_1-O19_1	-69.7(4)	O1_1-C6_1-C16_1-C15_1	-71.6(4)
C5_1-C6_1-C16_1-C15_1	49.8(5)	O18_1-C15_1-C16_1-O19_1	-169.8(3)
C14_1-C15_1-C16_1-O19_1	66.5(4)	O18_1-C15_1-C16_1-C6_1	71.9(4)
C14_1-C15_1-C16_1-C6_1	-51.8(5)	C23_2-O23_2-C22_2-O21_2	62.8(4)
C23_2-O23_2-C22_2-C26_2	-177.8(3)	C25_2-O21_2-C22_2-O23_2	-62.1(4)
C25_2-O21_2-C22_2-C26_2	-179.7(3)	C22_2-O23_2-C23_2-C24_2	-58.0(4)
C34_2-O32_2-C24_2-C23_2	-179.9(3)	C34_2-O32_2-C24_2-C25_2	60.0(4)
O23_2-C23_2-C24_2-O32_2	-67.8(4)	O23_2-C23_2-C24_2-C25_2	51.6(5)
C22_2-O21_2-C25_2-C24_2	55.4(4)	C22_2-O21_2-C25_2-C32_2	177.6(4)
O32_2-C24_2-C25_2-O21_2	68.2(5)	C23_2-C24_2-C25_2-O21_2	-49.9(5)
O32_2-C24_2-C25_2-C32_2	-51.7(5)	C23_2-C24_2-C25_2-C32_2	-169.8(4)
O23_2-C22_2-C26_2-C27_2	-88.2(5)	O21_2-C22_2-C26_2-C27_2	31.5(6)
O23_2-C22_2-C26_2-C31_2	87.5(5)	O21_2-C22_2-C26_2-C31_2	-152.7(5)
C31_2-C26_2-C27_2-C28_2	0.4(7)	C22_2-C26_2-C27_2-C28_2	176.3(4)

C26_2-C27_2-C28_2-C29_2	-0.9(8)	C27_2-C28_2-C29_2-C30_2	0.8(9)
C28_2-C29_2-C30_2-C31_2	0(1)	C29_2-C30_2-C31_2-C26_2	0(1)
C27_2-C26_2-C31_2-C30_2	0.1(8)	C22_2-C26_2-C31_2-C30_2	-176.0(5)
O21_2-C25_2-C32_2-O35_2	168.9(4)	C24_2-C25_2-C32_2-O35_2	-70.1(5)
O21_2-C25_2-C32_2-C33_2	-71.5(5)	C24_2-C25_2-C32_2-C33_2	49.5(5)
O35_2-C32_2-C33_2-O34_2	-170.9(3)	C25_2-C32_2-C33_2-O34_2	72.5(5)
O35_2-C32_2-C33_2-C34_2	64.4(5)	C25_2-C32_2-C33_2-C34_2	-52.3(5)
C38_2-O33_2-C34_2-O32_2	-68.6(5)	C38_2-O33_2-C34_2-C33_2	173.1(4)
C24_2-O32_2-C34_2-O33_2	178.0(3)	C24_2-O32_2-C34_2-C33_2	-63.8(4)
O34_2-C33_2-C34_2-O33_2	51.3(5)	C32_2-C33_2-C34_2-O33_2	175.1(4)
O34_2-C33_2-C34_2-O32_2	-65.9(5)	C32_2-C33_2-C34_2-O32_2	57.9(5)