SUPPLEMENTARY MATERIAL

Reduced atomic coordinates for the hygroscopic phase of α-lactose.

	x	y	z
C1	0.3236 (10)	0.0424 (5)	0.7632 (26)
C2	0.4658 (11)	0.0969 (5)	0.8318 (24)
C3	0.3978 (11)	0.1444 (5)	1.0249 (25)
C4	0.2173 (12)	0.1728 (5)	0.8801 (8)
C5	0.0932 (12)	0.1124 (5)	0.7882 (24)
C6	-0.0800 (16)	0.1293 (7)	0.5857 (42)
O1	0.4001 (16)	0	0.5874 (26)
O2	0.6248 (14)	0.0728 (8)	1.0014 (28)
O3	0.5085 (17)	0.1997 (6)	1.1397 (27)
O4	0.2244 (17)	0.2102 (8)	0.6374 (24)
O5	0.1546 (13)	0.0670 (6)	0.6082 (21)
O6	-0.1938 (16)	0.0721 (6)	0.5593 (30)
H1	0.3141	0.0177	0.9379
H2	0.4829	0.1209	0.6591
H3	0.3815	0.1167	1.1870
H4	0.1710	0.2020	1.0152
H5	0.0708	0.0878	0.95510
H6a	-0.0579	0.1410	0.3968
H6b	-0.1357	0.16960	0.6502
HO2	0.7072	0.0655	0.8733
HO3	0.4471	0.2244	1.2644
HO4	0.1738	0.2553	0.6692
HO6	-0.2784	0.0742	0.3705
C1’	0.3292 (11)	-0.2011 (8)	0.3302 (17)
C2’	0.1633 (10)	-0.1684 (4)	0.3874 (32)
C3’	0.1862 (10)	-0.0912 (4)	0.3964 (28)
C4’	0.3554 (11)	-0.0699 (4)	0.6122 (28)
C5’	0.5109 (10)	-0.1105 (5)	0.5516 (31)
C6’	0.6886 (12)	-0.0982 (9)	0.7556 (35)
O1’	0.3408 (16)	-0.1899 (8)	0.0497 (20)
O2’	-0.0033 (11)	-0.1876 (7)	0.2153 (27)
O3’	0.0365 (15)	-0.0597 (7)	0.4610 (32)
O5’	0.4887 (13)	-0.1833 (4)	0.5318 (24)
O6’	0.8254 (14)	-0.1380 (6)	0.6860 (31)

H1'	0.3149	-0.2517	0.3508
H2'	0.1601	-0.1817	0.5816
H3'	0.1943	-0.0752	0.2035
H4'	0.3421	-0.0796	0.8031
H5'	0.5245	-0.0957	0.3623
H6a'	0.6820	-0.1070	0.9492
H6b'	0.7226	-0.0485	0.7447
HO1'	0.4277	-0.2254	0.0257
HO2'	0.0015	-0.1671	0.0188
HO3'	0.0407	-0.0098	0.4244
HO6'	0.8644	-0.1141	0.5273

Bond lengths (Å) of the hygroscopic phase of α-lactose.

C1–C2	1.522 (12)	O1–C4’	1.432 (9)
C1–O1	1.427 (16)	C1’–C2’	1.527 (14)
C1–O5	1.439 (13)	C1’–O1’	1.418 (14)
C1–H1	1.003	C1’–O5’	1.435 (12)
C2–C3	1.513 (14)	C1'–H1'	1.010
C2–O2	1.400 (14)	C2’–C3’	1.529 (12)
C2–H2	1.006	C2’–O2’	1.421 (13)
C3–C4	1.522 (12)	C2'–H2'	0.994
C3–O3	1.419 (15)	C3’–C4’	1.539 (13)
C3–H3	0.997	C3’–O3’	1.421 (17)
C4–C5	1.531 (11)	C3'–H3'	1.014
C4–O4	1.412 (15)	C4’–C5’	1.537 (14)
C4–H4	1.006	C4'–H4'	0.985
C5–C6	1.509 (15)	C5’–C6’	1.522 (14)
C5–O5	1.417 (13)	C5’–O5’	1.445 (12)
C5–H5	1.002	C5'–H5'	1.002
C6–O6	1.420 (17)	C6’–O6’	1.427 (19)
C6–H6a	1.009	C6'–H6a'	0.978
C6–H6b	0.991	C6'–H6b'	1.019
O2–HO2	1.009	O1'–HO1'	0.999
O3–HO3	0.989	O2'–HO2'	1.054
O4–HO4	0.998	O3'–HO3'	1.000
O6–HO6	1.002	O6'–HO6'	1.016

Bond angles (°) of the hygroscopic phase of α-lactose.

C2–C1–O1	99.3 (7)	C2’–C1’–O1’	111.3 (9)
C2–C1–O5	113.8 (8)	C2’–C1’–O5’	113.7 (8)
O1–C1–O5	109.7 (7)	O1’–C1’–O5’	112.8 (8)
O1–C1–H1	111.0	O1'–C1'–H1'	106.5
O5–C1–H1	111.9	O5'–C1'–H1'	105.6
C2–C1–H1	110.5	C2'–C1'–H1'	106.3
C1–C2–C3	103.4 (8)	C1’–C2’–C3’	109.1 (8)
C1–C2–O2	112.7 (9)	C1’–C2’–O2’	118.0 (8)
C3–C2–O2	103.2 (8)	C3’–C2’–O2’	111.5 (9)
O2–C2–H2	112.6	O2'–C2'–H2'	105.8
C3–C2–H2	111.9	C1'–C2'–H2'	106.1
C1–C2–H2	112.3	C3'–C2'–H2'	105.3
C2–C3–C4	110.8 (7)	C2’–C3’–C4’	111.5 (7)

C2–C3–O3	116.9 (7)	C2’–C3’–O3’	110.1 (8)
C4–C3–O3	108.0 (9)	C4’–C3’–O3’	109.9 (8)
O3–C3–H3	106.4	O3'–C3'–H3'	107.9
C2–C3–H3	106.9	C2'–C3'–H3'	108.3
C4–C3–H3	107.2	C4'–C3'–H3'	109.0
C3–C4–C5	107.4 (5)	C3’–C4’–C5’	108.0 (7)
C3–C4–O4	111.7 (6)	C3’–C4’–O1	112.9 (7)
C5–C4–O4	107.7 (8)	C5’–C4’–O1	105.4 (6)
O4–C4–H4	110.5	O1–C4'–H4'	110.5
C3–C4–H4	109.7	C5'–C4'–H4'	110.3
C5–C4–H4	109.8	C3'–C4'–H4'	109.7
C4–C5–C6	115.2 (6)	C4’–C5’–C6’	115.1 (8)
C4–C5–O5	113.1 (5)	C4’–C5’–O5’	116.3 (8)
C6–C5–O5	96.2 (7)	C6’–C5’–O5’	106.1 (10)
O5–C5–H5	110.7	O5'–C5'–H5'	105.3
C6–C5–H5	110.1	C6'–C5'–H5'	106.5
C4–C5–H5	110.8	C4'–C5'–H5'	106.8
C5–C6–O6	109.0 (10)	C5’–C6’–O6’	111.6 (9)
O6–C6–H6a	109.6	O6'–C6'–H6a'	110.4
C5–C6–H6a	109.6	C5'–C6'–H6a'	111.2
O6–C6–H6b	110.7	O6'–C6'–H6b'	107.3
C5–C6–H6b	110.8	C5'–C6'–H6b'	109.0
H6a–C6–H6b	107.0	H6a'–C6'–H6b'	107.2
C1–O1–C4’	111.5 (5)	C1'–O1'–HO1'	101.9
C2–O2–HO2	106.3	C2'–O2'–HO2'	102.5
C3–O3–HO3	106.6	C3'–O3'–HO3'	109.0
C4–O4–HO4	103.7	C1’–O5’–C5’	111.0 (9)
C1–O5–C5	106.5 (8)	C6'–O6'–HO6'	107.7
C6–O6–HO6	108.1		

Torsion angles (°) of the hygroscopic phase of α-lactose after Rietveld refinements.

O1–C1–C2–C3	-178.9 (8)	C1–O1–C4'–C3'	91.5 (11)
O1–C1–C2–O2	-68.2 (11)	C1–O1–C4'–C5'	-150.9 (9)
O5–C1–C2–C3	64.5 (11)	O1'–C1'–C2'–C3'	-71.5 (12)
O5–C1–C2–O2	175.2 (10)	O1'–C1'–C2'–O2'	57.1 (14)
C2–C1–O1–C4'	148.1 (9)	O5'–C1'–C2'–C3'	57.1 (12)
O5–C1–O1–C4'	-92.3 (11)	O5'–C1'–C2'–O2'	-174.3 (10)
C2–C1–O5–C5	-65.5 (11)	C2'–C1'–O5'–C5'	-55.6 (12)
O1–C1–O5–C5	-175.7 (8)	O1'–C1'–O5'–C5'	72.2 (12)
C1–C2–C3–C4	-59.0 (9)	C1'–C2'–C3'–C4'	-55.3 (11)
C1–C2–C3–O3	176.6 (9)	C1'–C2'–C3'–O3'	-177.6 (10)
O2–C2–C3–C4	-176.6 (8)	O2'–C2'–C3'–C4'	172.6 (9)
O2–C2–C3–O3	59.0 (12)	O2'–C2'–C3'–O3'	50.3 (13)
C2–C3–C4–C5	57.3 (8)	C2'–C3'–C4'–O1	168.2 (9)
C2–C3–C4–O4	-60.6 (10)	C2'–C3'–C4'–C5'	52.1 (11)
O3–C3–C4–C5	-173.4 (8)	O3'–C3'–C4'–O1	-69.4 (12)
O3–C3–C4–O4	68.7 (11)	O3'–C3'–C4'–C5'	174.5 (10)
C3–C4–C5–C6	-167.1 (8)	O1–C4'–C5'–C6'	61.9 (12)
C3–C4–C5–O5	-57.8 (9)	O1–C4'–C5'–O5'	-173.1 (9)
O4–C4–C5–C6	-46.6 (11)	C3'–C4'–C5'–C6'	-177.2 (10)
O4–C4–C5–O5	62.7 (10)	C3'–C4'–C5'–O5'	-52.2(12)
C4–C5–C6–O6	-169.4 (9)	C4'–C5'–C6'–O6'	179.6 (11)
O5–C5–C6–O6	71.5 (12)	O5'–C5'–C6'–O6'	49.6 (14)
C4–C5–O5–C1	60.2 (10)	C4'–C5'–O5'–C1'	54.1 (12)
C6–C5–O5–C1	-179.0 (10)	C6'–C5'–O5'–C1'	-176.5 (10)