

SUPPLEMENTARY MATERIAL

Reduced atomic coordinates for the mixed 1/1 α/β lactose.

	First molecule			Second molecule		
	x	y	z	x	y	z
Ci1	0.5276 (12)	0.0439 (5)	0.743 (3)	0.5146 (12)	0.5588 (5)	0.563 (3)
Ci2	0.7042 (11)	0.0766 (5)	0.781 (3)	0.3304 (11)	0.5882 (5)	0.637 (3)
Ci3	0.7147 (12)	0.1294 (6)	1.020 (3)	0.3207 (11)	0.6665 (5)	0.637 (3)
Ci4	0.5416 (11)	0.1821 (5)	0.992 (3)	0.4896 (12)	0.6942 (9)	0.825 (2)
Ci5	0.3692 (12)	0.1488 (5)	0.890 (3)	0.6633 (12)	0.6591 (5)	0.742 (3)
Ci6	0.2116 (15)	0.1994 (5)	0.750 (5)	0.8376 (15)	0.6874 (6)	0.909 (5)
Oi1	0.5	0.0	0.5	0.5446 (32)	0.4849 (5)	0.525 (4)
Oi2	0.8647 (20)	0.0296 (9)	0.856 (5)	0.1652 (20)	0.5729 (12)	0.444 (5)
Oi3	0.8698 (20)	0.1617 (10)	1.055 (5)	0.1590 (21)	0.6957 (12)	0.710 (5)
Oi4	0.5374 (30)	0.2325 (9)	0.814 (4)	0.5016 (32)	0.6858 (11)	1.108 (2)
Oi5	0.3837 (24)	0.0989 (8)	0.671 (3)	0.6701 (24)	0.5854 (5)	0.758 (4)
Oi6	0.0727 (25)	0.1562 (12)	0.628 (5)	0.9733 (24)	0.6328 (9)	1.017 (5)
Hi1	0.5226 (12)	0.0211 (5)	0.908 (3)	0.5062 (12)	0.5763 (5)	0.381 (3)
Hi2	0.6995 (11)	0.0999 (5)	0.612 (3)	0.3338 (11)	0.5749 (5)	0.824 (3)
Hi3	0.7276 (12)	0.1047 (6)	1.190 (3)	0.3071 (11)	0.6792 (5)	0.445 (3)
Hi4	0.5416 (11)	0.2063 (5)	1.176 (3)	0.4786 (12)	0.7446 (9)	0.799 (2)
Hi5	0.3396 (12)	0.1285 (5)	1.044 (3)	0.6483 (12)	0.6685 (5)	0.547 (3)
Hi6a	0.2474 (15)	0.2265 (5)	0.620 (5)	0.8110 (15)	0.7204 (6)	1.061 (5)
Hi6b	0.1664 (15)	0.2334 (5)	0.886 (5)	0.8880 (15)	0.7135 (6)	0.792 (5)
HOi2	0.9342 (20)	0.0403 (9)	1.045 (5)	0.1354 (20)	0.5307 (12)	0.503 (5)
HOi3	0.8910 (20)	0.1665 (10)	0.874 (5)	0.1015 (21)	0.6564 (12)	0.739 (5)
HOi4	0.6506 (30)	0.2526 (9)	0.887 (4)	0.4206 (32)	0.7258 (11)	1.160 (2)
HOi6	0.1268 (25)	0.1108 (12)	0.566 (5)	0.9712 (24)	0.6222 (9)	1.202 (5)
Ci1'	0.1795 (14)	-0.1628 (7)	0.202 (2)	0.8152 (12)	0.3286 (6)	0.156 (3)
Ci2'	0.0767 (13)	-0.0948 (4)	0.285 (3)	0.9214 (11)	0.3901 (6)	0.268 (3)
Ci3'	0.1876 (11)	-0.0342 (4)	0.298 (3)	0.8280 (11)	0.4363 (7)	0.462 (3)
Ci4'	0.3860 (11)	-0.0527 (5)	0.465 (3)	0.6268 (12)	0.4588 (7)	0.307 (2)
Ci5'	0.4650 (12)	-0.1142 (5)	0.310 (3)	0.5272 (11)	0.3980 (7)	0.142 (3)
Ci6'	0.6648 (18)	-0.1348 (22)	0.427 (3)	0.3302 (21)	0.4074 (6)	-0.037 (6)
Oi1'	0.1492 (35)	-0.1560 (17)	-0.082 (2)	0.9045 (29)	0.2855 (9)	-0.029 (4)
Oi2'	-0.0863 (23)	-0.0870 (10)	0.065 (4)	1.1121 (14)	0.3737 (13)	0.391 (4)
Oi3'	0.0994 (41)	0.0274 (12)	0.402 (8)	0.9401 (31)	0.4892 (10)	0.591 (6)
Oi5'	0.3732 (15)	-0.1710 (9)	0.333 (6)	0.6338 (18)	0.3530 (13)	-0.007 (3)
Oi6'	0.7278 (36)	-0.1650 (11)	0.193 (4)	0.2635 (30)	0.3418 (7)	-0.123 (4)

Hi1'	0.1235 (14)	-0.2036 (7)	0.228 (2)	0.8081 (12)	0.3025 (6)	0.312 (3)
Hi2'	0.0464 (13)	-0.0997 (4)	0.462 (3)	0.9068 (11)	0.4171 (6)	0.104 (3)
Hi3'	0.1878 (11)	-0.0247 (4)	0.107 (3)	0.8252 (11)	0.4072 (7)	0.612 (3)
Hi4'	0.3875 (11)	-0.0679 (5)	0.648 (3)	0.6188 (12)	0.4959 (7)	0.181 (2)
Hi5'	0.4406 (12)	-0.1035 (5)	0.113 (3)	0.5184 (11)	0.3695 (7)	0.290 (3)
Hi6a'	0.6900 (18)	-0.1673 (22)	0.577 (3)	0.3267 (21)	0.4337 (6)	-0.198 (6)
Hi6b'	0.7265 (18)	-0.0935 (22)	0.508 (3)	0.2467 (21)	0.4358 (6)	0.067 (6)
HOi1'	0.2661 (35)	-0.1771 (17)	-0.117 (2)	0.8365 (29)	0.2973 (9)	-0.217 (4)
HOi2'	-0.0528 (23)	-0.0807 (10)	-0.103 (4)	1.1594 (14)	0.3368 (13)	0.271 (4)
HOi3'	-0.0224 (41)	0.0193 (12)	0.414 (8)	0.8869 (31)	0.5190 (10)	0.725 (6)
HOi6'	0.7165 (36)	-0.1287 (11)	0.066 (4)	0.1387 (30)	0.3513 (7)	-0.239 (4)

Bond lengths (Å) of the for the mixed 1/1 α/β lactose.

	1 st molec.	2 nd molec.		1 st molec.	2 nd molec.
Ci1–Ci2	1.540 (14)	1.559 (15)	Oi1–Ci4'	1.423 (10)	1.424 (25)
Ci1–Oi1	1.418 (11)	1.438 (14)	Ci1'–Ci2'	1.521 (15)	1.537 (16)
Ci1–Oi5	1.413 (17)	1.455 (19)	Ci1'–Oi1'	1.409 (16)	1.438 (24)
Ci1–Hi1	1.000	1.000	Ci1'–Oi5'	1.440 (15)	1.445 (15)
Ci2–Ci3	1.508 (18)	1.529 (13)	Ci1'–Hi1'	1.000	1.000
Ci2–Oi2	1.401 (17)	1.429 (19)	Ci2'–Ci3'	1.551 (14)	1.516 (19)
Ci2–Hi2	1.000	1.000	Ci2'–Oi2'	1.428 (19)	1.421 (13)
Ci3–Ci4	1.529 (13)	1.524 (14)	Ci2'–Hi2'	1.000	1.000
Ci3–Oi3	1.392 (21)	1.401 (22)	Ci3'–Ci4'	1.530 (13)	1.543 (12)
Ci3–Hi3	1.000	1.000	Ci3'–Oi3'	1.415 (30)	1.445 (24)
Ci4–Ci5	1.505 (13)	1.535 (15)	Ci3'–Hi3'	1.000	1.000
Ci4–Oi4	1.396 (25)	1.439 (16)	Ci4'–Ci5'	1.508 (16)	1.565 (18)
Ci4–Hi4	1.000	1.000	Ci4'–Hi4'	1.000	1.000
Ci5–Ci6	1.498 (13)	1.526 (15)	Ci5'–Ci6'	1.486 (16)	1.528 (19)
Ci5–Oi5	1.420 (18)	1.450 (14)	Ci5'–Oi5'	1.435 (22)	1.409 (22)
Ci5–Hi5	1.000	1.000	Ci5'–Hi5'	1.000	1.001
Ci6–Oi6	1.433 (23)	1.412 (21)	Ci6'–Oi6'	1.430 (28)	1.449 (20)
Ci6–Hi6a	1.000	1.000	Ci6'–Hi6a'	1.000	0.999
Ci6–Hi6b	1.000	1.000	Ci6'–Hi6b'	0.999	0.999
Oi2–HOi2	0.983	0.986	Oi1'–HOi1'	0.976	0.983
Oi3–HOi3	0.988	0.988	Oi2'–HOi2'	0.977	0.986
Oi4–HOi4	0.972	0.980	Oi3'–HOi3'	0.985	0.979
Oi6–HOi6	0.982	0.981	Oi6'–HOi6'	0.984	0.978

Bond angles ($^{\circ}$) of the for the mixed 1/1 α/β lactose.

	1 st molecule	2 nd molecule
Ci2–Ci1–Oi1	109.7 (8)	114.4 (9)
Ci2–Ci1–Oi5	104.5 (10)	111.4 (10)
Oi1–Ci1–Oi5	102.2 (9)	111.9 (10)
Ci2–Ci1–Hi1	113.6	106.3
Oi1–Ci1–Hi1	113.4	105.2
Oi5–Ci1–Hi1	112.5	107.0
Ci1–Ci2–Ci3	107.6 (9)	104.5 (8)
Ci1–Ci2–Oi2	113.3 (10)	116.9 (10)
Ci3–Ci2–Oi2	105.0 (10)	104.3 (12)
Ci1–Ci2–Hi2	110.0	110.0
Ci3–Ci2–Hi2	109.4	110.0
Oi2–Ci2–Hi2	111.3	110.6
Ci2–Ci3–Ci4	113.4 (9)	113.2 (9)
Ci2–Ci3–Oi3	109.1 (12)	106.8 (12)
Ci4–Ci3–Oi3	111.2 (10)	112.1 (11)
Ci2–Ci3–Hi3	108.1	108.8
Ci4–Ci3–Hi3	106.3	108.9
Oi3–Ci3–Hi3	108.5	106.9
Ci3–Ci4–Ci5	112.0 (8)	110.1 (8)
Ci3–Ci4–Oi4	111.3 (12)	111.2 (10)
Ci5–Ci4–Oi4	108.5 (12)	111.6 (10)
Ci3–Ci4–Hi4	109.1	108.3
Ci5–Ci4–Hi4	108.6	107.3
Oi4–Ci4–Hi4	107.2	108.2
Ci4–Ci5–Ci6	111.0 (9)	113.4 (9)
Ci4–Ci5–Oi5	111.1 (11)	107.1 (10)
Ci6–Ci5–Oi5	101.3 (10)	113.8 (9)
Ci4–Ci5–Hi5	110.6	107.5
Ci6–Ci5–Hi5	110.9	106.7
Oi5–Ci5–Hi5	111.7	108.2
Ci5–Ci6–Oi6	102.5 (12)	110.1 (13)
Ci5–Ci6–Hi6a	111.6	110.5
Ci5–Ci6–Hi6b	111.5	111.2
Oi6–Ci6–Hi6a	115.8	109.8
Oi6–Ci6–Hi6b	108.5	108.3
Hi6a–Ci6–Hi6b	107.0	107.0
Ci1–Oi1–Ci4'	120.2 (6)	115.3 (11)
Ci2–Oi2–HOi2	111.0	106.2
Ci3–Oi3–HOi3	109.6	105.7
Ci4–Oi4–HOi4	105.9	103.7

Ci1–Oi5–Ci5	114.2 (12)	111.8 (10)
Ci6–Oi6–HOi6	111.0	113.2
Ci2’–Ci1’–Oi1’	100.6 (12)	109.0 (11)
Ci2’–Ci1’–Oi5’	113.5 (11)	109.7 (10)
Oi1’–Ci1’–Oi5’	110.2 (14)	105.6 (12)
Ci2’–Ci1’–Hi1’	112.5	109.9
Oi1’–Ci1’–Hi1’	108.6	111.5
Oi5’–Ci1’–Hi1’	110.9	111.0
Ci1’–Ci2’–Ci3’	111.1 (8)	109.6 (10)
Ci1’–Ci2’–Oi2’	102.8 (11)	116.2 (10)
Ci3’–Ci2’–Oi2’	109.9 (11)	110.5 (10)
Ci1’–Ci2’–Hi2’	108.7	105.0
Ci3’–Ci2’–Hi2’	113.2	106.7
Oi2’–Ci2’–Hi2’	110.7	108.3
Ci2’–Ci3’–Ci4’	110.3 (8)	108.3 (9)
Ci2’–Ci3’–Oi3’	110.4 (12)	109.3 (13)
Ci4’–Ci3’–Oi3’	112.5 (14)	118.3 (13)
Ci2’–Ci3’–Hi3’	109.4	106.9
Ci4’–Ci3’–Hi3’	109.0	107.1
Oi3’–Ci3’–Hi3’	105.0	106.3
Oi1–Ci4’–Ci3’	115.5 (8)	102.2 (11)
Oi1–Ci4’–Ci5’	108.5 (7)	109.4 (10)
Ci3’–Ci4’–Ci5’	105.6 (8)	113.7 (9)
Oi1–Ci4’–Hi4’	109.6	110.6
Ci3’–Ci4’–Hi4’	109.9	110.9
Ci5’–Ci4’–Hi4’	107.3	109.7
Ci4’–Ci5’–Ci6’	113.1 (11)	123.7 (11)
Ci4’–Ci5’–Oi5’	106.8 (10)	113.7 (13)
Ci6’–Ci5’–Oi5’	107.3 (11)	107.2 (11)
Ci4’–Ci5’–Hi5’	108.8	103.1
Ci6’–Ci5’–Hi5’	110.3	102.6
Oi5’–Ci5’–Hi5’	110.4	103.9
Ci5’–Ci6’–Oi6’	103.3 (15)	111.4 (15)
Ci5’–Ci6’–Hi6a’	112.4	108.4
Ci5’–Ci6’–Hi6b’	110.6	110.2
Oi6’–Ci6’–Hi6a’	112.9	111.5
Oi6’–Ci6’–Hi6b’	110.7	108.2
Hi6a’–Ci6’–Hi6b’	107.0	107.1
Ci1’–Oi1’–HOi1’	102.6	107.2
Ci2’–Oi2’–HOi2’	108.8	106.4
Ci3’–Oi3’–HOi3’	108.8	111.7
Ci1’–Oi5’–Ci5’	114.8 (12)	113.4 (13)
Ci6’–Oi6’–HOi6’	108.9	107.3

Torsion angles ($^{\circ}$) of the for the mixed 1/1 α/β lactose after Rietveld refinements.

	1 st molecule	2 nd molecule
Oi1–Ci1–Ci2–Ci3	173.0 (8)	-174.0 (12)
Oi1–Ci1–Ci2–Oi2	-71.4 (12)	-59.4 (18)
Oi5–Ci1–Ci2–Ci3	64.0 (12)	57.8 (14)
Oi5–Ci1–Ci2–Oi2	179.6 (12)	172.5 (14)
Ci2–Ci1–Oi1–Ci4'	159.1 (8)	141.0 (13)
Oi5–Ci1–Oi1–Ci4'	-90.4 (10)	-91.1(17)
Ci2–Ci1–Oi5–Ci5	-70.7 (14)	-66.1 (16)
Oi1–Ci1–Oi5–Ci5	175.0 (10)	164.5 (14)
Ci1–Ci2–Ci3–Ci4	-53.4 (13)	-54.7 (12)
Ci1–Ci2–Ci3–Oi3	-178.0 (12)	-178.5 (13)
Oi2–Ci2–Ci3–Ci4	-174.3 (11)	-177.9 (12)
Oi2–Ci2–Ci3–Oi3	61.1 (15)	58.2 (16)
Ci2–Ci3–Ci4–Ci5	43.2 (14)	57.4 (13)
Ci2–Ci3–Ci4–Oi4	-78.4 (15)	-66.8 (15)
Oi3–Ci3–Ci4–Ci5	166.6 (12)	178.2 (13)
Oi3–Ci3–Ci4–Oi4	45.0 (17)	54.0 (18)
Ci3–Ci4–Ci5–Ci6	-155.3 (10)	176.1 (11)
Ci3–Ci4–Ci5–Oi5	-43.4 (14)	-57.6 (14)
Oi4–Ci4–Ci5–Ci6	-32.1 (15)	-59.9 (16)
Oi4–Ci4–Ci5–Oi5	79.8 (15)	66.4 (16)
Ci4–Ci5–Ci6–Oi6	170.5 (13)	128.7 (15)
Oi5–Ci5–Ci6–Oi6	52.5 (14)	6.0 (19)
Ci4–Ci5–Oi5–Ci1	60.9 (15)	63.1 (15)
Ci6–Ci5–Oi5–Ci1	178.8 (11)	-170.9 (13)
Ci1–Oi1–Ci4'–Ci3'	96.6 (10)	102.1 (15)
Ci1–Oi1–Ci4'–Ci5'	-145.0 (8)	-137.1 (14)
Oi1'–Ci1'–Ci2'–Ci3'	-76.0 (15)	179.7 (12)
Oi1'–Ci1'–Ci2'–Oi2'	41.5 (16)	-54.1 (17)
Oi5'–Ci1'–Ci2'–Ci3'	41.7 (15)	64.4 (14)
Oi5'–Ci1'–Ci2'–Oi2'	159.2 (14)	-169.4 (14)
Ci2'–Ci1'–Oi5'–Ci5'	-51.2 (20)	-61.1 (17)
Oi1'–Ci1'–Oi5'–Ci5'	60.7 (21)	178.5 (14)
Ci1'–Ci2'–Ci3'–Ci4'	-49.0 (13)	-56.7 (12)
Ci1'–Ci2'–Ci3'–Oi3'	-174.0 (16)	173.1 (14)
Oi2'–Ci2'–Ci3'–Ci4'	-162.1 (12)	173.9 (12)
Oi2'–Ci2'–Ci3'–Oi3'	72.9 (19)	43.7 (18)
Ci2'–Ci3'–Ci4'–Oi1	177.7 (9)	164.9 (12)
Ci2'–Ci3'–Ci4'–Ci5'	62.4 (12)	47.1 (13)

Oi3'-Ci3'-Ci4'-Oi1'	-53.9 (19)	-70.1 (18)
Oi3'-Ci3'-Ci4'-Ci5'	-173.9 (17)	172.1 (15)
Oi1-Ci4'-Ci5'-Ci6'	49.3 (16)	69.0 (18)
Oi1-Ci4'-Ci5'-Oi5'	167.1 (12)	-158.1 (14)
Ci3'-Ci4'-Ci5'-Ci6'	173.7 (14)	-177.4 (14)
Ci3'-Ci4'-Ci5'-Oi5'	-68.5 (14)	-44.5 (16)
Ci4'-Ci5'-Ci6'-Oi6'	-151.0 (16)	-169.5 (14)
Oi5'-Ci5'-Ci6'-Oi6'	91.4 (21)	55.0 (20)
Ci4'-Ci5'-Oi5'-Ci1'	64.8 (18)	51.0 (18)
Ci6'-Ci5'-Oi5'-Ci1'	-173.7 (17)	-168.6 (14)