Supplemental Table 1. Interactions between the tetrasaccharide and the two molecules of PPA with which it interacts..

Glucose and atom		distance (Å)	contacting atom		distance (Å)	contacting atom	
Possible direct hydrogen bonding interactions <3.5 Å							
602	O3	3.08	Thr52	O			
602	O2	2.87	Lys261 (2_1)	NZ			
603	O3	2.98	Thr52	OG1			
603	O2	2.78	Glu272 (2_1)	OE2			
603	O6	3.02	Asn279 (2_1)	ND2			
Water-mediated interactions (distances < 3.5 Å)							
601	O3	2.94	wat439	O	2.82	Asn53	OD1
601	O2	2.56	wat440	O	2.85	Ser55	N
601	O2	2.56	wat440	O	3.19	Ser55	OG
602	O3	3.35	wat440	O	2.85	Ser55	N
602	O3	3.35	wat440	O	3.19	Ser55	OG
604	O1	2.74	wat570	O	2.56	Gly106	O
Other contacts < 4Å							
601	C1	3.63	Asn53	OD1			
601	O2	2.97	Pro54	CB			
601	O2	3.95	Trp357	CZ2			
601	O6	3.82	Gly285 (2_1)	CA			
602	C3	3.77	Thr52	O			
602	C4	3.04	Asn53	OD1			
602	O4	3.41	Asn53	CG			
602	C2	3.99	Lys261 (2_1)	NZ			
602	C6	3.99	Gly283 (2_1)	O			
602	C2	3.51	Trp284 (2_1)	O			
602	C6	3.60	Gly285 (2_1)	N			
602	C2	3.80	Lys261 (2_1)	CE			
602	O2	3.10	Lys261 (2_1)	CE			
602	O5	3.21	Trp284 (2_1)	C			
603	C3	3.61	Thr52	OG1			
603	O3	3.64	Thr52	CB			
603	O4	3.68	Asn53	CB			
603	C2	3.41	Glu272 (2_1)	OE2			
603	C1	3.81	Tyr276 (2_1)	CD2			
603	C6	3.73	Trp284 (2_1)	NE1			
603	C2	3.32	Glu272 (2_1)	OE1			
603	C6	3.89	Asn279 (2_1)	ND2			
603	O2	3.28	Glu272 (2_1)	CD			
603	O2	3.81	Tyr276 (2_1)	CD2			
603	O6	3.73	Asn279 (2_1)	CG			
603	C6	3.89	Trp284 (2_1)	CD1			
603	O2	3.33	Glu272 (2_1)	CD			
603	O6	3.70	Asn279 (2_1)	CG			
604	O4	3.93	Ala108	CB			

Supplementary Table 2. Interactions between 2_1-screw related PPA molecules across the bridged interface.

Residue and atom		distance (Å)	contacting atom		distance (Å)	contacting atom	
Possible direct hydrogen bonding interactions <3.5 Å							
Thr52	O	3.21	Lys261	NZ			
Thr52	OG1	3.22	Glu272	OE2			
Trp344	O	3.19	Asn152	ND2			
Ala345	N	3.15	Asn152	ND2			
Asn364	ND2	3.22	Gly306	O			
Asn364	OD1	2.72	Gly308	N			
Asn364	ND2	3.49	Gly309	N			
Asp381	OD1	2.73	Ser150	OG			
Asp381	OD2	3.19	Asn152	ND2			
Water-mediated interactions (distances < 3.5 Å)							
Ala345	N	2.96	wat79	O	2.94	Gly239	O
Ala345	N	2.96	wat79	O	3.09	Asn152	OD1
Asn380	N	2.95	wat213	O	2.72	Glu149	O
Asp381	OD2	2.89	wat262	O	2.99	Tyr151	N
Ala109	O	3.01	wat362	O	3.03	Gly271	O
Asn355	ND2	3.08	wat464	O	2.63	Glu240	O
Ser55	OG	3.10	wat542	O	2.85	Leu237	O
Ser55	OG	3.10	wat542	O	2.58	Lys261	NZ
Thr52	O	3.01	wat547	O	3.08	Lys261	NZ
ASp381	N	3.07	wat303	O	2.92	Glu149	O
Asn364	O	3.37	wat387	O	3.00	Gly308	O
Asn364	O	3.37	wat387	O	3.34	Ser311	OG
Thr52	O	3.38	wat574	O	2.57	Lys261	NZ
Ser55	OG	2.80	wat574	O	2.75	Lys261	NZ
Other contacts < 4Å							
Thr52	CG2	3.92	Ser270	O			
Thr52	CB	3.54	Glu272	OE2			
Ala108	CB	3.82	Tyr276	OH			
Gly112	CA	3.85	Ser270	C			
Gly112	CA	3.85	Gly271	CA			
Gly112	CA	3.65	Gly271	N			
Trp316	CH2	3.80	Asn152	OD1			
Arg343	CG	3.82	Asn152	CG			
Arg343	CG	3.25	Asn152	OD1			
Arg343	C	3.88	Asn152	ND2			
Trp344	O	3.81	Asn152	CG			
Trp344	C	3.17	Asn152	ND2			
Trp344	CA	3.89	Asn152	ND2			
Ala345	CB	3.78	Ala241	CA			
Ala345	CB	3.66	Ala241	N			
Ala345	CA	3.28	Asn152	ND2			
Ala345	CA	3.90	Asn152	OD1			
Ala345	CB	3.59	Glu240	C			
Ala345	CB	3.54	Glu240	O			
Ile358	CD1	3.53	Gly239	CA			
Asn364	OD1	3.83	Leu237	CD1			
Asn364	OD1	3.80	Ala307	C			
Asn364	OD1	3.28	Gly308	CA			
Asn364	ND2	3.61	Gly309	CA			
Asn364	CG	3.81	Gly306	O			
Asn364	CG	3.60	Gly308	N			
Asn364	CG	3.45	Gly309	N			
Asp381	OD1	3.21	Ser150	CB			
Asp381	OD2	3.94	Asn152	CG			
Asp381	CG	3.53	Ser150	OG			
Asp381	CG	3.82	Asn152	ND2			

Supplementary Table 3. Glucose puckering parameters q_2, q_3, φ_2 after Cremer and Pople[a] with spherical polar equivalents Q, θ, and φ_2 for all glucose residues. Also listed are the aveage B and the occupancy of each glucose.

Residue	<B>	Occ.	q_2	q_3	φ_2	Q	θ	conformation
				tetrasaccharide				
601	98	0.50	0.67	0.08	146.00	0.67	166.39	$^4C_1$ (twisted)
602	56	0.80	0.08	0.54	174.74	0.55	16.85	$^4C_1$
603	42	0.80	0.05	0.51	73.72	0.51	11.20	$^4C_1$
604	64	0.70	0.05	0.47	249.34	0.47	12.15	$^4C_1$
				limit dextrin				
701	13	0.60	0.52	0.36	150.25	0.63	110.61	$^4C_1$
702	70	0.60	0.17	0.62	123.90	0.64	30.67	$^4C_1$
703	53	0.80	0.41	0.43	165.88	0.59	87.27	E_3
704	40	0.90	0.06	0.57	337.60	0.57	12.02	$^4C_1$
705	47	0.90	0.13	0.48	280.50	0.50	30.31	$^4C_1$
706	64	0.60	0.30	0.48	242.36	0.57	64.01	^4E
				glucose on Trp203				
801	31	0.50	0.09	0.58	22.84	0.59	17.64	$^4C_1$
				α-cyclodextrin I				
601	20	1.00	0.08	0.53	50.48	0.54	17.17	$^4C_1$
602	27	1.00	0.16	0.51	93.09	0.53	34.84	$^4C_1$
603	36	1.00	0.11	0.57	54.47	0.58	21.85	$^4C_1$
604	34	1.00	0.07	0.58	345.98	0.58	13.76	$^4C_1$
605	30	1.00	0.06	0.61	11.16	0.61	11.24	$^4C_1$
606	23	1.00	0.08	0.57	28.62	0.58	15.98	$^4C_1$
				α-cyclodextrin II				
701	88	1.00	0.04	0.52	92.94	0.52	8.80	$^4C_1$
702	94	1.00	0.27	0.46	60.79	0.53	60.82	$^4C_1$
703	102	1.00	0.13	0.54	72.47	0.56	27.07	$^4C_1$
704	101	1.00	0.14	0.56	25.42	0.58	28.07	$^4C_1$
705	106	1.00	0.18	0.48	78.78	0.51	41.11	$^4C_1$
706	101	1.00	0.23	0.49	75.74	0.54	50.29	$^4C_1$
				α-cyclodextrin III				
801	118	1.00	0.19	0.48	33.64	0.52	43.19	$^4C_1$
802	113	1.00	0.16	0.50	47.06	0.52	35.49	$^4C_1$
803	120	1.00	0.73	0.03	134.21	0.73	175.30	$^{2,5}B$
804	113	1.00	0.16	0.54	66.90	0.56	33.01	$^4C_1$
805	105	1.00	0.15	0.52	79.50	0.54	32.18	$^4C_1$
806	114	1.00	0.19	0.48	62.35	0.52	43.19	$^4C_1$

Supplementary Table 4. Glycosidic linkage torsion angles φ and ψ, inter-oxygen distances between linkages, O2'···O3 inter-residue distances, and ring twist torsion angles.

Residues	∠O5'-C1'··C4-O4 φ (°)	∠C5-C4··O4-C1' ψ (°)	d(O4'···O4) (Å)	d(O2'···O3) (Å)	∠O1-C1··C4-O4 ring twist (°)
		tetrasaccharide			
601			4.68		-18.7
601 - 602	69.2	-111.2	4.88	4.18	-10.9
602 - 603	126.2	-109.6	4.53	2.82	-4.4
603 - 604	127.6	-113.9	4.78	2.51	-0.1
		limit dextrin			
701			4.56		-10.2
701 - 702	77.9	-136.6	4.20	3.55	-8.4
702 -703	104.8	-127.4	4.72	2.73	-16.2
703 - 704	115.8	-100.4	4.44	2.88	0.9
704 - 705	122.2	-123.6	5.46	2.51	3.8
		α-cyclodextrin I			
601 - 602	117.9	-114.4	4.13	2.64	0.8
602 - 603	108.5	-118.9	4.15	3.09	-4.5
603 - 604	101.8	-107.5	4.22	3.22	-0.4
604 - 605	105.2	-120.5	4.30	2.91	7.1
605 - 606	107.5	-111.4	4.15	2.96	0.3
606 - 601	105.7	-102.1	4.27	3.17	0.9
		α-cyclodextrin II			
701 - 702	131.9	-132.8	4.52	2.27	-6.9
702 - 703	104.4	-117.2	3.83	3.22	-3.3
703 - 704	145.2	-131.5	4.27	2.08	-4.4
704 - 705	107.1	-107.1	4.22	3.25	-0.5
705 - 706	137.8	-115.8	4.21	2.39	-1.4
706 - 701	139.5	-127.9	4.06	2.23	-5.3
		α-cyclodextrin III			
801 - 802	157.2	-104.2	4.15	2.59	1.8
802 - 803	134.3	-138.6	4.17	2.48	1.1
803 - 804	116.5	-108.5	4.28	2.82	-34.0
804 - 805	136.2	-128.9	4.04	2.33	-5.3
805 - 806	109.8	-80.6	4.15	3.92	-7.8
806 - 801	123.1	-151.6	4.12	2.57	-0.7

Supplementary Table 5. Interactions between the limit dextrin and PPA.

Glucose and atom		distance (Å)	contacting atom		distance (Å)	contacting atom	
Possible direct hydrogen bonding interactions <3.5 Å							
703	O6	2.97	Gln63	NE2			
704	O6	2.88	Trp59	O			
704	O6	2.84	Gln63	NE2			
704	O2	3.30	Asp300	OD1			
705	O6	3.47	His101	NE2			
705	O6	2.80	Asp197	OD2			
705	O1	2.83	Glu233	OE2			
705	O3	2.61	Asp300	OD2			
706	O6	3.01	Gly106	O			
Water-mediated interactions (distances < 3.5 Å)							
701	O3	2.68	wat34	O	2.77	Ser145	OG
701	O4	2.75	wat550	O	3.35	Ser105	OG
701	O4	2.75	wat550	O	2.94	Gln161	OE1
701	O3	2.95	wat576	O	2.93	Ile148	N
701	O3	2.95	wat576	O	2.69	Gln161	O
704	O2	3.02	wat428	O	2.83	Asp300	OD1
704	O2	2.71	wat584	O	2.44	Asp300	OD2
705	O5	3.31	wat402	O	3.21	Arg195	NH2
705	O5	3.31	wat402	O	2.67	Asp197	OD1
705	O1	2.43	wat552	O	3.43	His201	NE2
706	O3	3.23	wat549	O	2.32	Asn53	O
Other contacts < 4Å							
701	C3	3.97	Gly164	N			
701	O3	3.15	Gly147	CA			
702	C5	3.83	Val163	O			
702	O4	3.80	Val163	C			
703	C1	3.71	Trp59	CE3			
703	C5	3.62	Val163	O			
703	O6	3.85	Gln63	CD			
704	C2	3.59	Trp58	CH2			
704	C4	3.73	Trp59	CB			
704	C6	3.61	Gln63	NE2			
704	C6	3.78	Leu165	CD1			
704	O2	3.55	Trp58	CH2			
704	O6	3.43	Trp59	CE3			
704	O5	3.68	Tyr62	CB			
704	O6	3.46	Gln63	CG			
704	O4	4.00	Val163	CG2			
704	C6	3.78	Leu165	CD1			
705	O3	3.19	Asp300	CG			
705	O3	3.74	Asp300	CG			
705	O2	3.59	Ile235	CD1			
705	C6	3.97	Tyr62	CB			
705	C6	3.69	His101	CE1			
705	C5	3.75	Leu162	CD2			
705	C1	3.53	Glu233	OE2			
705	C2	3.32	Asp300	OD2			
705	O6	3.46	Tyr62	CB			
705	O6	3.32	His101	CE1			
705	O6	3.53	Asp197	CG			
705	O2	3.31	Ala198	CA			
705	O1	3.59	Glu233	CD			
706	C1	3.48	Gln63	NE2			
706	C6	3.59	Gly104	CA			
706	C6	3.36	Gly106	N			
706	C6	3.41	Ala107	N			
706	O2	3.53	Trp59	CH2			

706	O6	3.53	Gly104	CA
706	O6	3.47	Gly106	CA

Supplementary Table 6. Accessible surface areas of aromatic residues and the percentage of the surface area an isolated residue of the same type.

TRP - Accessible surface area - stand alone enzyme

	<----- whole residue ---->			<------- Side chain ------>		
Res #	Area	Free Area	% free	Area	Free area	% free
19	1.7	355.1	0.	1.1	267.2	0.
21	2.0	355.1	1.	2.0	267.2	1.
58	26.4	355.1	7.	26.0	267.2	10.
59	82.3	355.1	23.	80.9	267.2	30.
134	215.2	355.1	61.	198.5	267.2	74.
203	72.8	355.1	20.	72.8	267.2	27.
221	59.8	355.1	17.	38.3	267.2	14.
269	113.2	355.1	32.	109.8	267.2	41.
280	13.0	355.1	4.	0.0	267.2	0.
284	50.4	355.1	14.	28.7	267.2	11.
316	81.0	355.1	23.	52.1	267.2	19.
344	17.1	355.1	5.	1.5	267.2	1.
357	72.4	355.1	20.	72.4	267.2	27.
382	6.0	355.1	2.	0.9	267.2	0.
388	52.2	355.1	15.	46.0	267.2	17.
396	68.5	355.1	19.	68.2	267.2	26.
409	42.4	355.1	12.	13.1	267.2	5.
410	69.5	355.1	20.	65.4	267.2	24.
434	137.5	355.1	39.	134.0	267.2	50.
134	0.0	355.1	0.	0.0	267.2	0.
396	0.0	355.1	0.	0.0	267.2	0.

TYR - Accessible surface area - stand alone enzyme

	<----- whole residue ---->			<------- Side chain ------>		
Res #	Area	Free Area	% free	Area	Free area	% free
2	59.5	323.3	18.	58.8	238.2	25.
31	10.7	323.3	3.	10.7	238.2	4.
62	24.1	323.3	7.	24.1	238.2	10.
67	28.2	323.3	9.	17.3	238.2	7.
94	0.0	323.3	0.	0.0	238.2	0.
118	103.5	323.3	32.	98.2	238.2	41.
131	2.9	323.3	1.	0.0	238.2	0.
151	83.1	323.3	26.	77.7	238.2	33.
155	141.5	323.3	44.	140.5	238.2	59.
174	98.7	323.3	31.	89.9	238.2	38.
182	9.0	323.3	3.	2.9	238.2	1.
247	0.5	323.3	0.	0.0	238.2	0.
258	0.0	323.3	0.	0.0	238.2	0.
276	111.0	323.3	34.	104.0	238.2	44.
321	4.1	323.3	1.	4.1	238.2	2.
333	9.1	323.3	3.	6.1	238.2	3.
342	0.5	323.3	0.	0.3	238.2	0.
449	2.4	323.3	1.	2.4	238.2	1.
468	153.7	323.3	48.	140.5	238.2	59.

PHE - Accessible surface area - stand alone enzyme

	<----- whole residue ---->			<------- Side chain ------>		
Res #	Area	Free Area	% free	Area	Free area	% free
17	2.2	311.0	1.	2.1	229.7	1.
37	0.2	311.0	0.	0.1	229.7	0.
79	0.1	311.0	0.	0.1	229.7	0.
126	0.1	311.0	0.	0.0	229.7	0.
136	13.9	311.0	4.	0.0	229.7	0.
194	0.1	311.0	0.	0.1	229.7	0.
222	9.5	311.0	3.	2.8	229.7	1.
229	0.0	311.0	0.	0.0	229.7	0.
231	0.1	311.0	0.	0.1	229.7	0.

248	46.9	311.0	15.	45.5	229.7	20.
256	7.2	311.0	2.	4.3	229.7	2.
286	12.7	311.0	4.	0.0	229.7	0.
295	2.6	311.0	1.	2.5	229.7	1.
315	7.5	311.0	2.	0.9	229.7	0.
327	0.0	311.0	0.	0.0	229.7	0.
335	19.5	311.0	6.	19.0	229.7	8.
348	121.6	311.0	39.	93.5	229.7	41.
397	0.5	311.0	0.	0.5	229.7	0.
406	69.1	311.0	22.	50.3	229.7	22.
419	0.4	311.0	0.	0.3	229.7	0.
426	0.8	311.0	0.	0.4	229.7	0.
429	0.7	311.0	0.	0.7	229.7	0.
477	2.2	311.0	1.	0.8	229.7	0.
487	2.4	311.0	1.	0.7	229.7	0.

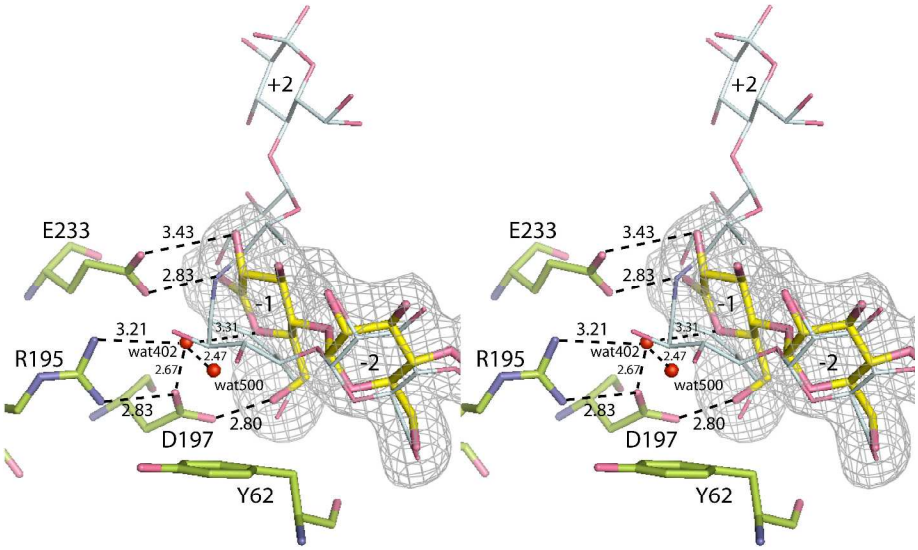
Supplementary Table 7. Closest contacts between aromatic residues that have at least one interatomic contact less than 4 Å.

Residue 1		Residue 2		closest nonbonded atoms			closest sidechain atoms		
				Res 1		Res 2	Res 1		Res 2
TYR	2	PHE	229	O	3.33	CE2	CB	5.65	CE2
		PHE	248	OH	2.77	O	OH	5.51	CB
PHE	17	TRP	19	C	3.16	N	CB	5.56	CD1
		TRP	58	CZ	3.87	CB	CZ	3.87	CB
		TYR	342	CE2	3.53	CE1	CE2	3.53	CE1
		TRP	382	O	3.67	CZ3	CB	6.35	CZ3
TRP	19	PHE	17	N	3.16	C	CD1	5.56	CB
		TRP	21	O	3.79	CZ3	CB	6.15	CE3
		TRP	382	NE1	3.54	CE3	NE1	3.54	CE3
TRP	21	TRP	19	CZ3	3.79	O	CE3	6.15	CB
		PHE	79	CD1	3.62	N	CE2	3.70	CD1
TYR	31	PHE	37	CE2	3.76	CE2	CE2	3.76	CE2
PHE	37	TYR	31	CE2	3.76	CE2	CE2	3.76	CE2
TRP	58	PHE	17	CB	3.87	CZ	CB	3.87	CZ
		TRP	59	N	2.73	N	CE2	3.76	CD1
		TYR	342	CB	3.58	OH	CB	3.58	OH
		TRP	357	N	3.24	O	NE1	5.34	CB
TRP	59	TRP	58	N	2.73	N	CD1	3.76	CE2
		TYR	62	O	3.13	N	CB	4.93	CD1
		TRP	357	NE1	3.70	CB	NE1	3.70	CB
TYR	62	TRP	59	N	3.13	O	CD1	4.93	CB
TYR	67	TYR	131	OH	3.01	OH	OH	3.01	OH
		TYR	182	CB	3.66	CD1	CB	3.66	CD1
PHE	79	TRP	21	N	3.62	CD1	CD1	3.70	CE2
TYR	94	PHE	229	CE2	3.68	CD1	CE2	3.68	CD1
TYR	118								
PHE	126	TYR	131	O	2.97	N	CB	4.16	CB
		PHE	136	CE1	3.72	CZ	CE1	3.72	CZ
TYR	131	TYR	67	OH	3.01	OH	OH	3.01	OH
		PHE	126	N	2.97	O	CB	4.16	CB
TRP	134	PHE	136	C	3.32	N			
		TRP	134	C	0.05	C	CB	0.55	CB
PHE	136	PHE	126	CZ	3.72	CE1	CZ	3.72	CE1
		TRP	134	N	3.32	C			
		TRP	134	N	3.36	C			
TYR	151								
TYR	155	TRP	203	CD2	3.69	CZ2	CD2	3.69	CZ2
TYR	174								
TYR	182	TYR	67	CD1	3.66	CB	CD1	3.66	CB
PHE	194	PHE	229	N	2.84	O			
		PHE	231	O	3.07	N	CB	6.41	CE1
TRP	203	TYR	155	CZ2	3.69	CD2	CZ2	3.69	CD2
TRP	221	PHE	222	O	2.74	CA	CB	3.93	CD1
PHE	222	TRP	221	CA	2.74	O	CD1	3.93	CB
PHE	229	TYR	2	CE2	3.33	O	CE2	5.65	CB
		TYR	94	CD1	3.68	CE2	CD1	3.68	CE2
		PHE	194	O	2.84	N			
		PHE	231	CE1	3.47	CD1	CE1	3.47	CD1
PHE	231	PHE	194	N	3.07	O	CE1	6.41	CB
		PHE	229	CD1	3.47	CE1	CD1	3.47	CE1
TYR	247	PHE	248	O	2.75	CA	CB	5.42	CD1
PHE	248	TYR	2	O	2.77	OH	CB	5.51	OH
		TYR	247	CA	2.75	O	CD1	5.42	CB
PHE	256	TYR	258	C	3.08	N	CB	6.92	CB
		PHE	295	CE1	3.63	CZ	CE1	3.63	CZ
TYR	258	PHE	256	N	3.08	C	CB	6.92	CB
		TRP	280	CE2	3.16	NE1	CE2	3.16	NE1
		PHE	286	CD2	3.88	CE1	CD2	3.88	CE1
		PHE	295	CD1	3.79	O	CD1	6.45	CB

		TYR	333	CE2	3.73	CD1	CE2	3.73	CD1
TRP	269								
TYR	276	TRP	284	O	3.23	NE1	CB	3.79	CZ2
TRP	280	TYR	258	NE1	3.16	CE2	NE1	3.16	CE2
		TRP	284	CA	3.62	CD1	CE3	3.75	CD2
		PHE	286	CH2	3.66	CE1	CH2	3.66	CE1
		PHE	327	CD1	3.55	CE1	CD1	3.55	CE1
TRP	284	TYR	276	NE1	3.23	O	CZ2	3.79	CB
		TRP	280	CD1	3.62	CA	CD2	3.75	CE3
		PHE	286	C	3.43	N	CB	3.89	CE2
PHE	286	TYR	258	CE1	3.88	CD2	CE1	3.88	CD2
		TRP	280	CE1	3.66	CH2	CE1	3.66	CH2
		TRP	284	N	3.43	C	CE2	3.89	CB
		TYR	333	CB	3.24	OH	CB	3.24	OH
PHE	295	PHE	256	CZ	3.63	CE1	CZ	3.63	CE1
		TYR	258	O	3.79	CD1	CB	6.45	CD1
PHE	315	TRP	316	O	2.73	CA	CZ	3.35	NE1
		TYR	342	CZ	3.68	O	CZ	6.81	CB
		TRP	344	CZ	3.82	CZ3	CZ	3.82	CZ3
		TRP	388	CB	3.94	CH2	CB	3.94	CH2
TRP	316	PHE	315	CA	2.73	O	NE1	3.35	CZ
		TRP	344	CH2	3.36	O	NE1	3.39	CH2
TYR	321								
PHE	327	TRP	280	CE1	3.55	CD1	CE1	3.55	CD1
		PHE	419	CE2	3.60	CE1	CE2	3.60	CE1
		PHE	429	CA	3.66	CZ	CB	3.83	CZ
TYR	333	TYR	258	CD1	3.73	CE2	CD1	3.73	CE2
		PHE	286	OH	3.24	CB	OH	3.24	CB
PHE	335								
TYR	342	PHE	17	CE1	3.53	CE2	CE1	3.53	CE2
		TRP	58	OH	3.58	CB	OH	3.58	CB
		PHE	315	O	3.68	CZ	CB	6.81	CZ
		TRP	344	O	3.26	CE3	CE2	4.56	CB
		TRP	382	CB	3.87	CE3	CB	3.87	CE3
TRP	344	PHE	315	CZ3	3.82	CZ	CZ3	3.82	CZ
		TRP	316	O	3.36	CH2	CH2	3.39	NE1
		TYR	342	CE3	3.26	O	CB	4.56	CE2
PHE	348								
TRP	357	TRP	58	O	3.24	N	CB	5.34	NE1
		TRP	59	CB	3.70	NE1	CB	3.70	NE1
TRP	382	PHE	17	CZ3	3.67	O	CZ3	6.35	CB
		TRP	19	CE3	3.54	NE1	CE3	3.54	NE1
		TYR	342	CE3	3.87	CB	CE3	3.87	CB
TRP	388	PHE	315	CH2	3.94	CB	CH2	3.94	CB
TRP	396	PHE	397	O	2.79	CA	CB	5.46	CB
		TRP	396	N	0.02	N	CB	0.27	CB
PHE	397	TRP	396	CA	2.79	O	CB	5.46	CB
		PHE	426	CZ	3.79	N	CZ	5.96	CB
		TRP	396	N	2.82	N	CB	5.39	CB
PHE	406	TRP	409	CZ	3.54	CE3	CZ	3.54	CE3
		PHE	419	CE1	3.54	CG	CE1	3.54	CG
TRP	409	PHE	406	CE3	3.54	CZ	CE3	3.54	CZ
		TRP	410	O	2.80	CA	CD1	5.38	CB
		PHE	419	CZ3	3.84	CD1	CZ3	3.84	CD1
TRP	410	TRP	409	CA	2.80	O	CB	5.38	CD1
PHE	419	PHE	327	CE1	3.60	CE2	CE1	3.60	CE2
		PHE	406	CG	3.54	CE1	CG	3.54	CE1
		TRP	409	CD1	3.84	CZ3	CD1	3.84	CZ3
		PHE	426	O	3.30	CD1	CB	5.52	CE1
PHE	426	PHE	397	N	3.79	CZ	CB	5.96	CZ
		PHE	419	CD1	3.30	O	CE1	5.52	CB
		PHE	477	CE2	3.73	CE1	CE2	3.73	CE1
PHE	429	PHE	327	CZ	3.66	CA	CZ	3.83	CB

		PHE	487	CD2	3.52	CB	CD2	3.52	CB
TRP	434								
TYR	449								
TYR	468								
PHE	477	PHE	426	CE1	3.73	CE2	CE1	3.73	CE2
PHE	487	PHE	429	CB	3.52	CD2	CB	3.52	CD2
TRP	134	TRP	134	C	0.05	C	CB	0.55	CB
		PHE	136	C	3.36	N			
TRP	396	TRP	396	N	0.02	N	CB	0.27	CB
		PHE	397	N	2.82	N	CB	5.39	CB

Supplemenary Figure 1. Stereoviews of the sites along the active site cleft with interactions between the limit dextrin and α-amylase identified. Superimposed as slendor sticks is the acarbose-derived inhibitor from 1HX0 (*27*). The overlayed map is a difference density map contoured at 2.0 σ. Residues from PPA are green; the limit dextrin is yellow; and, the inhibitor is pale cyan. (a) and (b) are two views that concentrate on the glucose interactions of sites –1 and –2. (c) and (d) are two views that focus on sites –2 and –3. (e) and (f) are two views that focus on sites –4, -4b and –5.


+2
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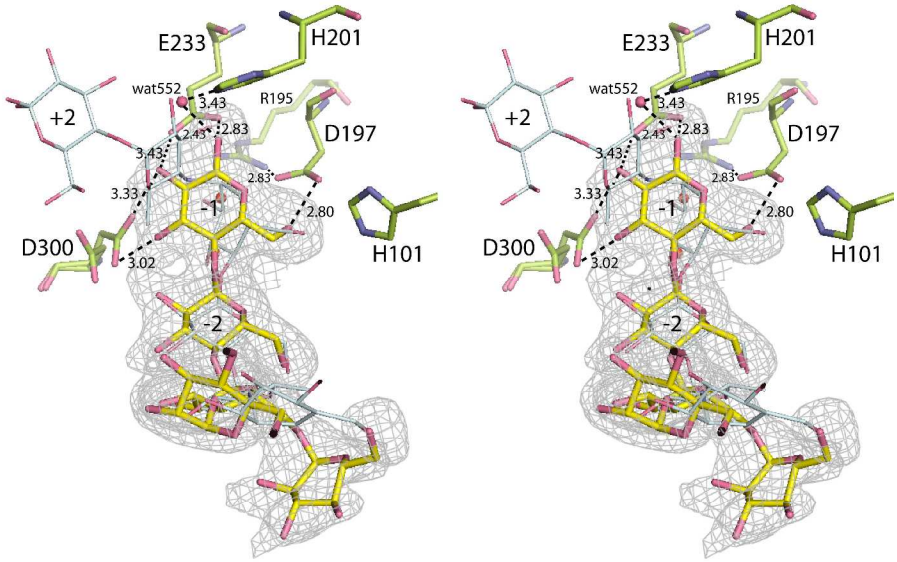
2.83
-1
3.21
3.31
R195
wat402
2.47
2.67
wat500
-2
2.83
2.80
D197
Y62
+2
E233
3.43
2.83
-1
3.21
3.31
R195
wat402
2.47
2.67
wat500
-2
2.83
2.80
D197
Y62

(a)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3.43
R195
+2
2.43
2.83
D197
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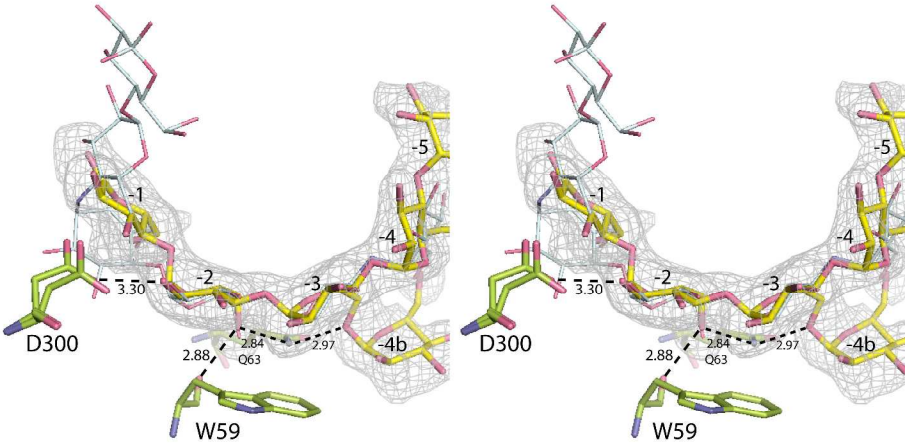
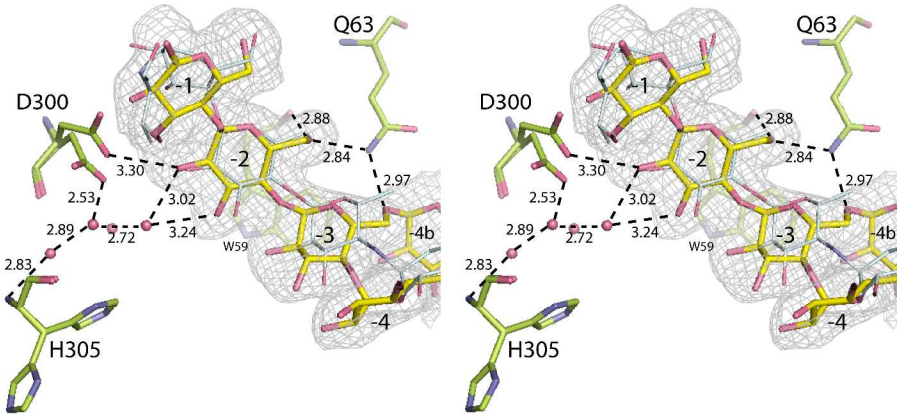
2.83
3.33
-1
2.80
D300
3.02
H101
-2
E233
H201
wat552
3.43
R195
+2
2.43
2.83
D197
3.43
2.83
3.33
-1
2.80
D300
3.02
H101
-2

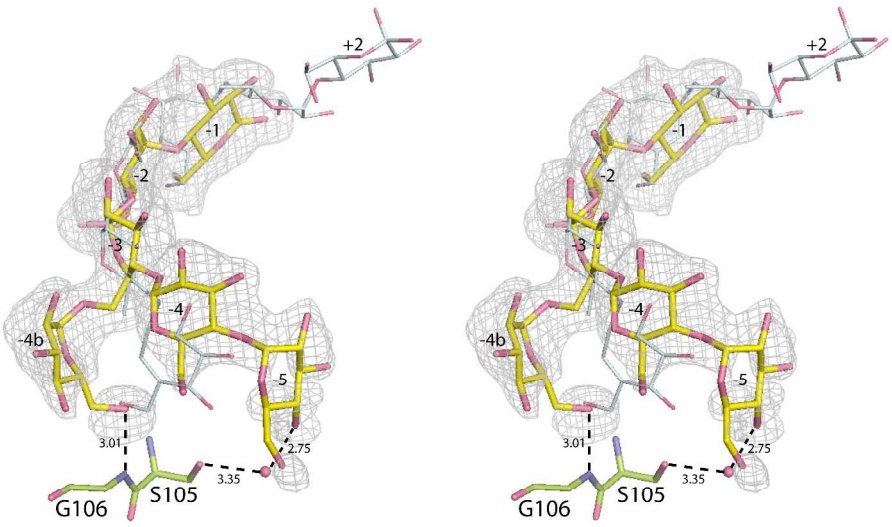
(b)


-5
-1
-4
3.30
-2
-3
D300
2.84
2.97
-4b
2.88
Q63
W59
-5
-1
-4
3.30
-2
-3
D300
2.84
2.97
-4b
2.88
Q63
W59

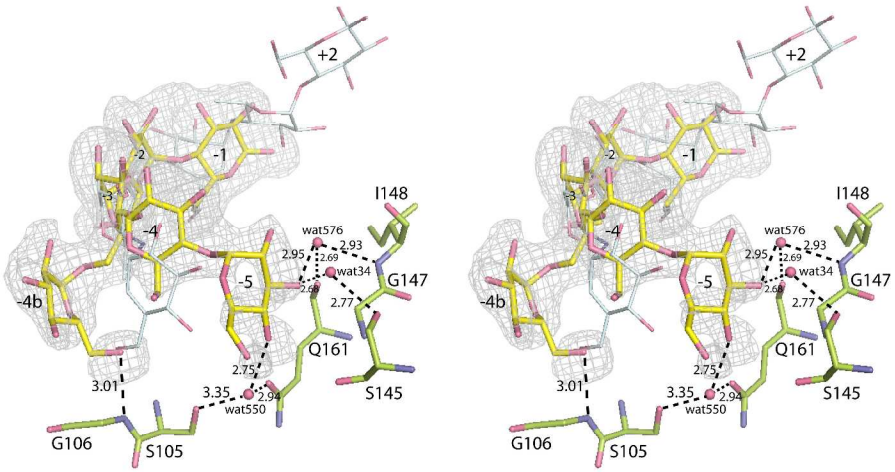
(c)


Q63
D300
-1
2.88
3.30
-2
2.84
2.97
2.53
3.02
2.89
2.72
3.24
-3
-4b
W59
2.83
-4
H305
Q63
D300
-1
2.88
3.30
-2
2.84
2.97
2.53
3.02
2.89
2.72
3.24
-3
-4b
W59
2.83
-4
H305

(d)



(e)



(f)

Supplementary Figure 1