Table 3-1 Crystal parameters and refinement statistics of the FXYN/sugar complexes.

Sugar	X1	X2	X3	Glucose	Galactose	Lactose
Cell parameter ($P2_12_12_1$)						
a (Å)	74.8	75.0	75.4	75.2	79.4	79.5
b (Å)	93.9	94.2	94.5	94.5	95.1	95.3
c (Å)	137.9	138.0	138.3	138.3	141.8	141.8
Temperature (K)	100	100	100	100	293	293
Resolution (Å)	30-2.0	30-2.1	30-2.1	30-2.1	30-2.0	30-2.0
	(2.07-2.0)	(2.18-2.1)	(2.18-2.1)	(2.18-2.1)	(2.07-2.0)	(2.07-2.0)
No. of reflections	65,703	50,751	51,446	54,773	73,250	72,309
	(6,500)	(4,447)	(4,525)	(5,254)	(7,236)	(7,126)
Completeness (%)	99 .2	87.9	88.2	93.9	99.8	98.4
	(99.5)	(87.9)	(88.2)	(93.9)	(93.8)	(98.4)
R-factor (%)	18.8	19.6	19.1	19.3	17.9	19.1
	(28.4)	(24.4)	(24.0)	(21.0)	(30.5)	(26.4)
R_{free}-factor (%)	22.9	24.4	24.0	23.3	20.7	22.4
	(27.5)	(29.1)	(28.2)	(26.2)	(32.6)	(28.1)
Average B-factor (Å^2)	24.4	28.2	26.8	19.9	28.2	26.8
Rmsd Bond (Å)	0.005	0.005	0.005	0.005	0.005	0.005
Rmsd Angle (°)	1.26	1.24	1.26	1.29	1.26	1.26

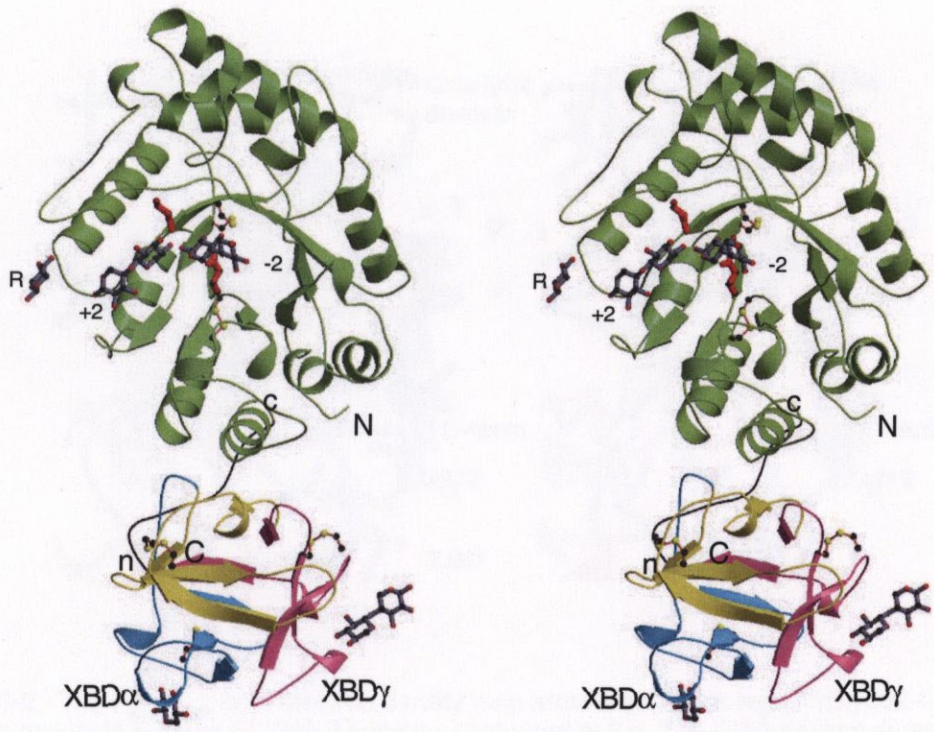

Fig. 3-1 Stereo view of the ribbon model of FXYN/X2 complex. The catalytic domain, linker, and subdomains α, β, γ of XBD are drawn in green, black, blue, yellow and pink, respectively. Two catalytic residues are displayed in red. Soaked xylose units and disulfide bonds are indicated by ball-and-stick drawings. The figure was drawn with the program Raster3d (Kraulis, 1991; Merritt & Murphy, 1994).

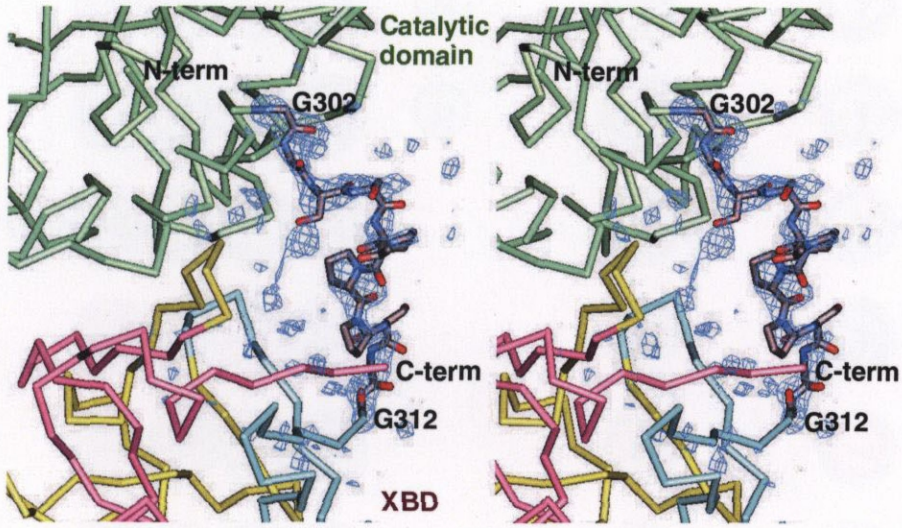

Fig. 3-2 The F_{obs}-F_{calc} omit electron density map around the linker region (Gly302-Gly312) of the molecule B in the FXYN/X2 complex contoured at 2 σ. The catalytic domain and XBD are shown in the Cα model.

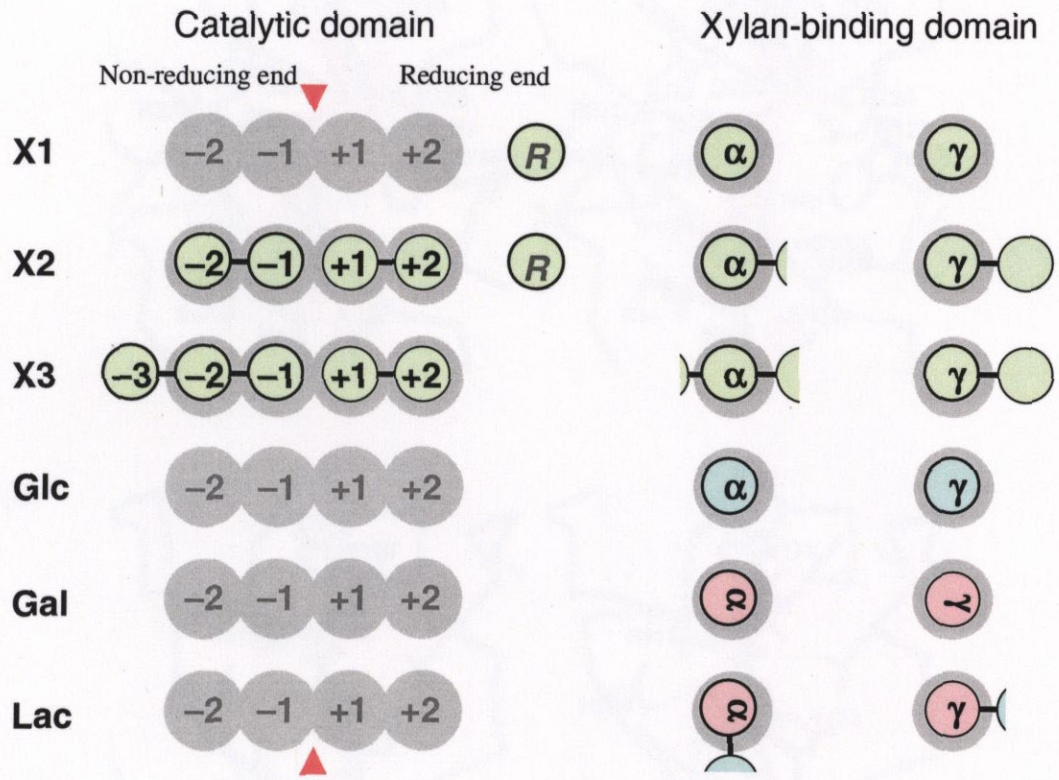

Fig. 3-3 Sugar binding diagram at the sugar binding sites of molecule A of FXYN in the sugar complex structures. Red triangle indicates the cleavage site and gray solid circle indicates the possible sugar binding sites with the subsite or subdomain names. Bound sugars are shown in green, blue and pink circles corresponding to xylose, glucose and galactose units, respectively. Incomplete circle indicates the sugar whose electron density was partly observed. Rotated letter in FXYN/Gal or FXYN/Lac complex indicates that orientation of the bound galactose in XBD is different from that of bound xylose in FXYN/X1~X3 complexes.

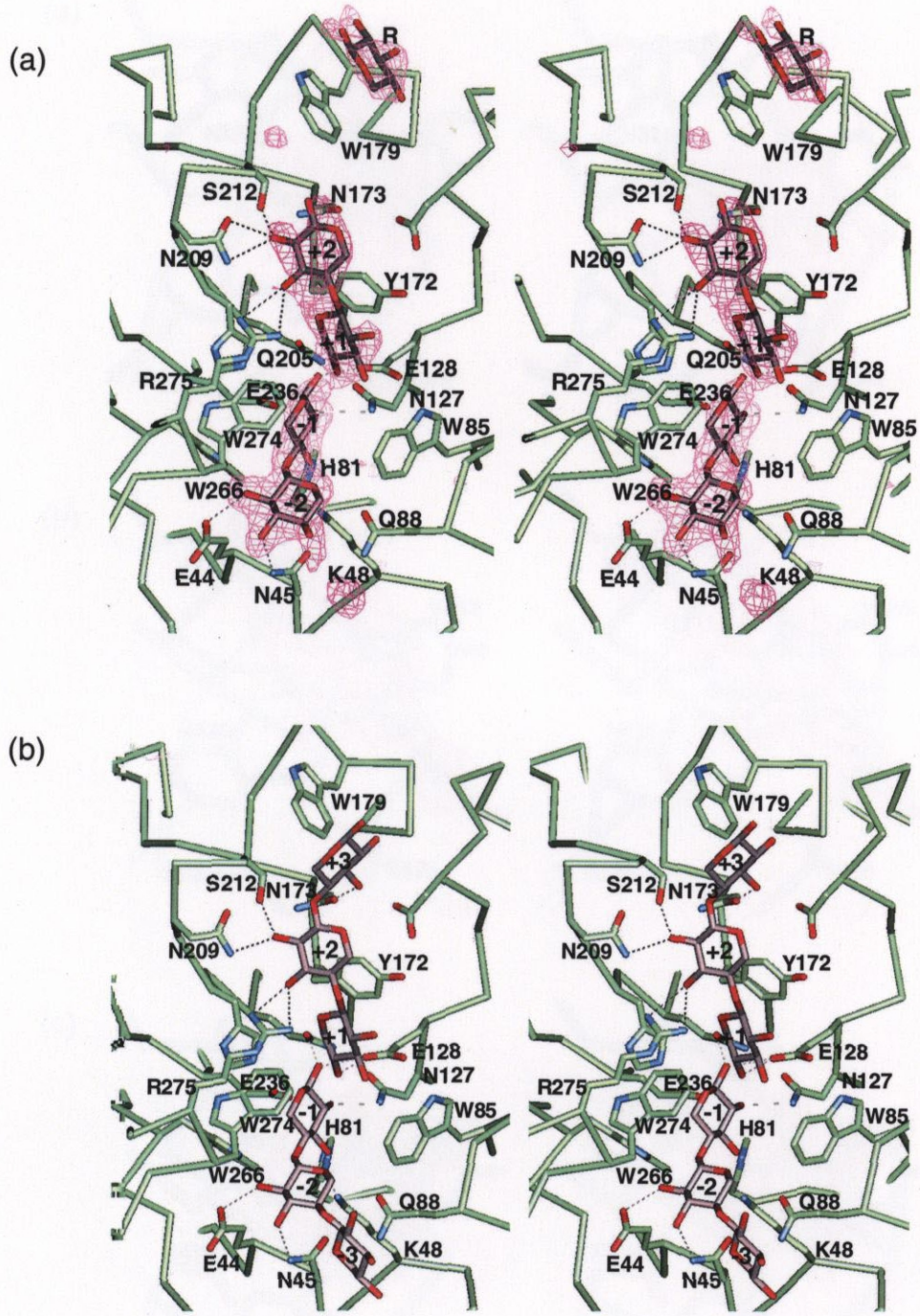

Fig. 3-4 Stereo view of the bound xylooligosaccharides in the catalytic cleft. (a) In the molecule A of the FXYN/X2 complex with the F_{obs}-F_{calc} omit electron density map contoured at 3 σ. (b) In the molecule B of the FXYN/X3 complex. Hydrogen bonding interaction between the enzyme and sugars are indicated by broken lines.

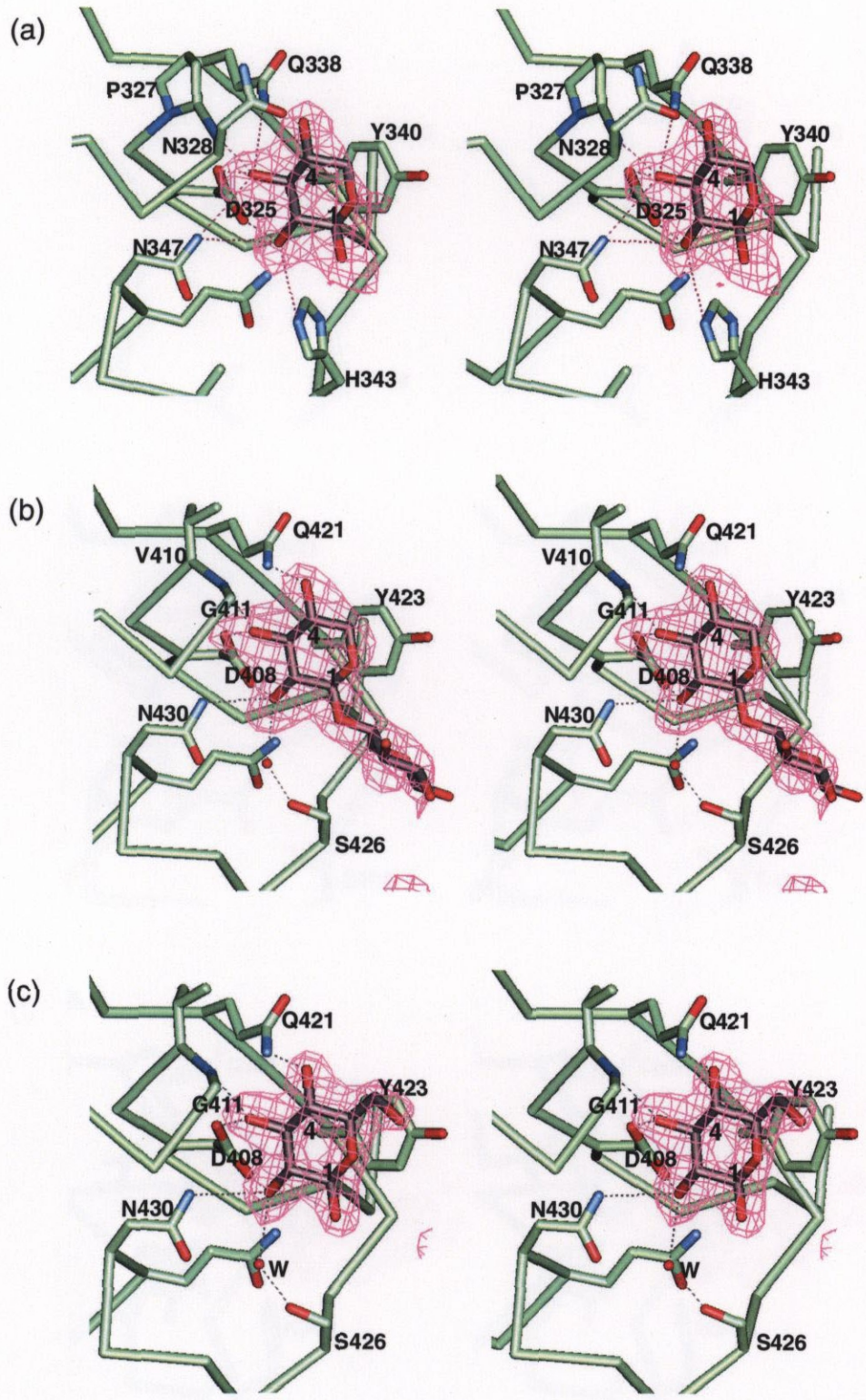

Fig. 3-5 Stereo views of the sugar binding structures in the XBD with the F_{obs}-F_{calc} omit electron density maps contoured at 3 σ. (a) In the subdomain a in the FXYN/X2 complex, (b) subdomain γ in the FXYN/X3 complex, (c) subdomain γ in the FXYN/Glc complex, (d) subdomain α in the FXYN/Gal complex, (e) subdomain γ in the FXYN/Lac complex, and (f) subdomain α in the FXYN/Lac complex from a different view point. Hydrogen bonding interaction between the enzyme and sugars are indicated by broken lines. Carbon numbers of bound xylose are indicated.

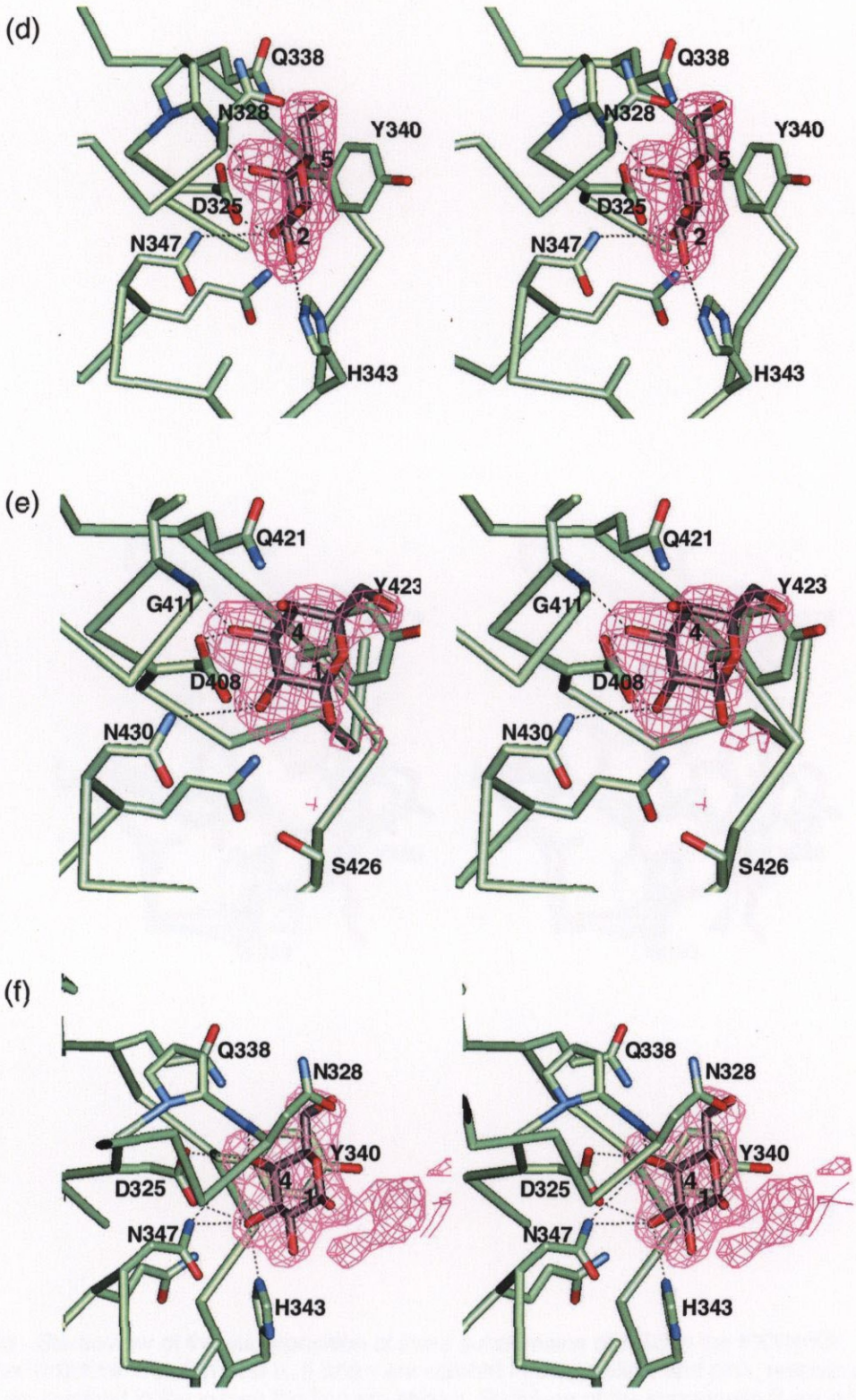

Fig. 3-5 continued.

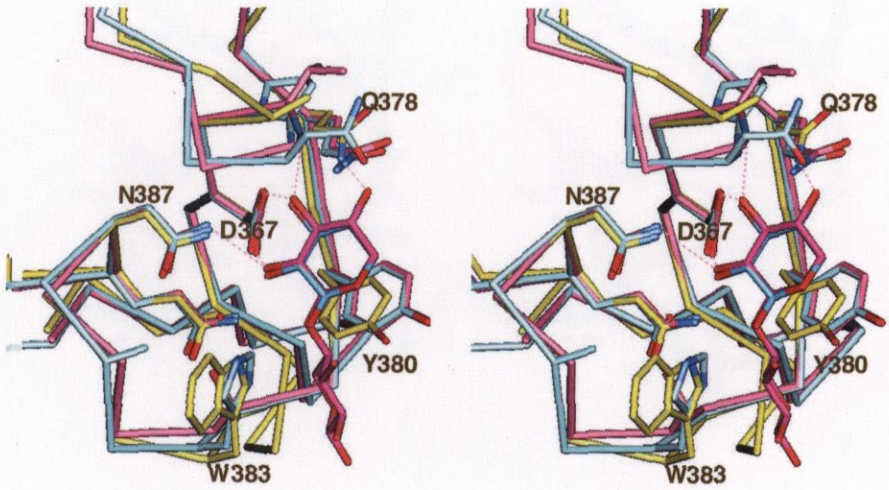

Fig. 3-6 Stereoview of the superposition of three subdomains of XBD in the FXYN/X2 complex structure. Subdomains α, β and γ are colored in blue, yellow and pink, respectively. Residues involved in the xylose binding are shown. Residues of the subdomain β are labeled.

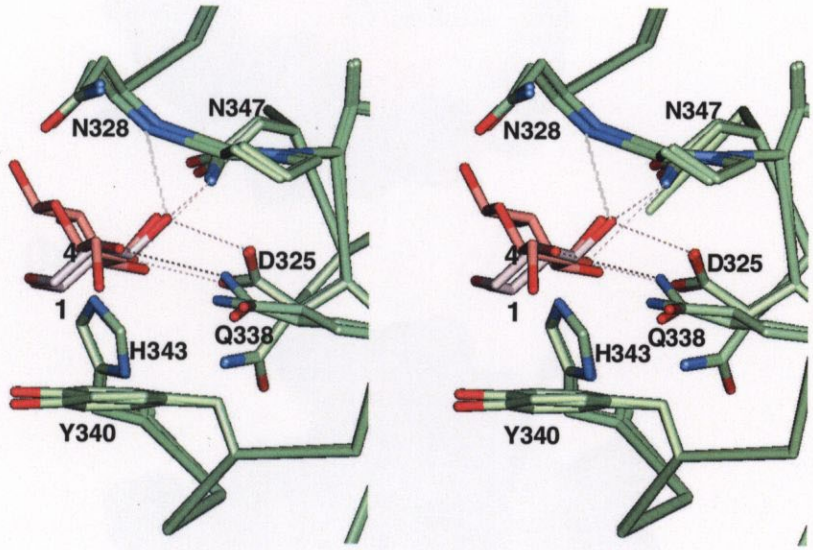

Fig. 3-7 Stereoview of the superposition xylose binding structure in the FXYN/X1 complex and galactose binding structure in the FXYN/Gal in the subdomain α. Bound xylose and galactose are shown in white and orange. C1 and C4 positions of bound xylose are indicated by numbers.

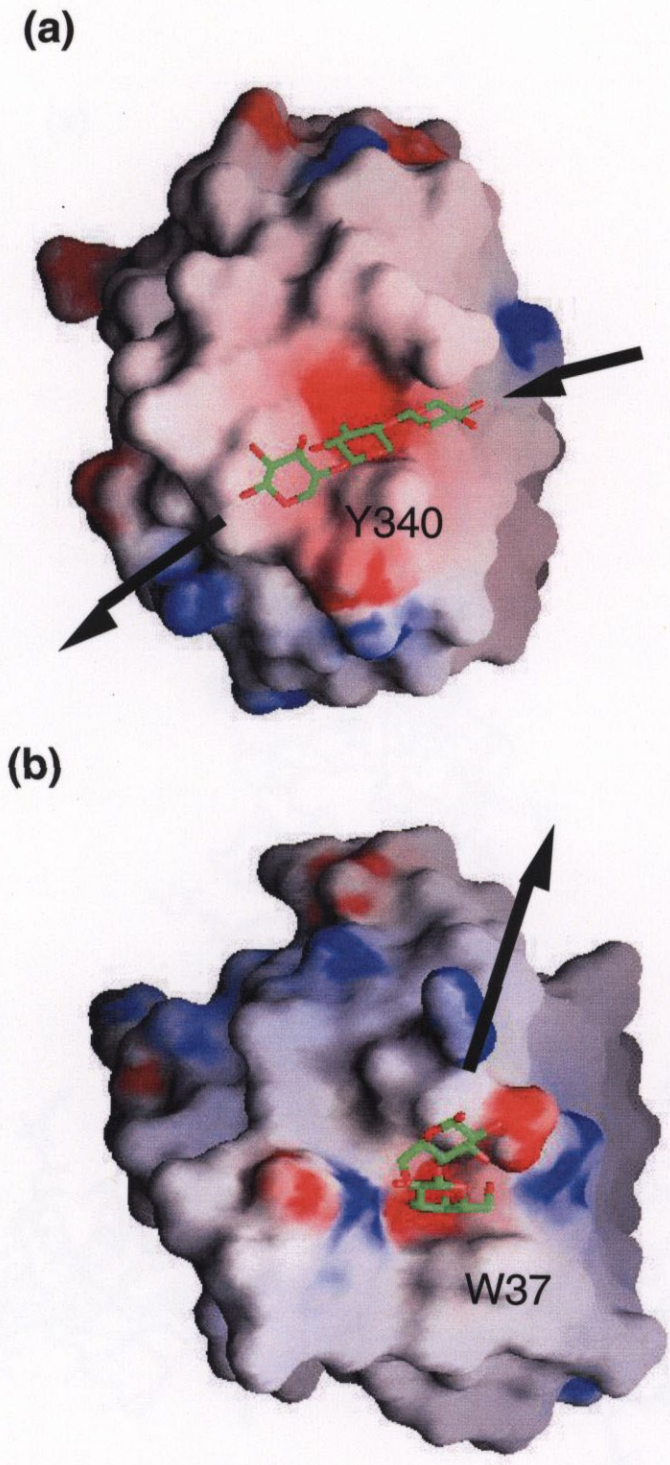

Fig. 3-8 Surface potential models of (a) XBDα/X3 and (b) RTB1α/Lac complexes. The model of XBDα/X3 was prepared based on the FXYN/X3 complex structure. The model of RTB1α/Lac complex structure was obtained from the RCSB protein data bank (accession code 1aai). Arrows indicate the direction of the extended sugar chain from the bound sugar. Surface models are drawn with the program GRASP (Nicholls, 1992).

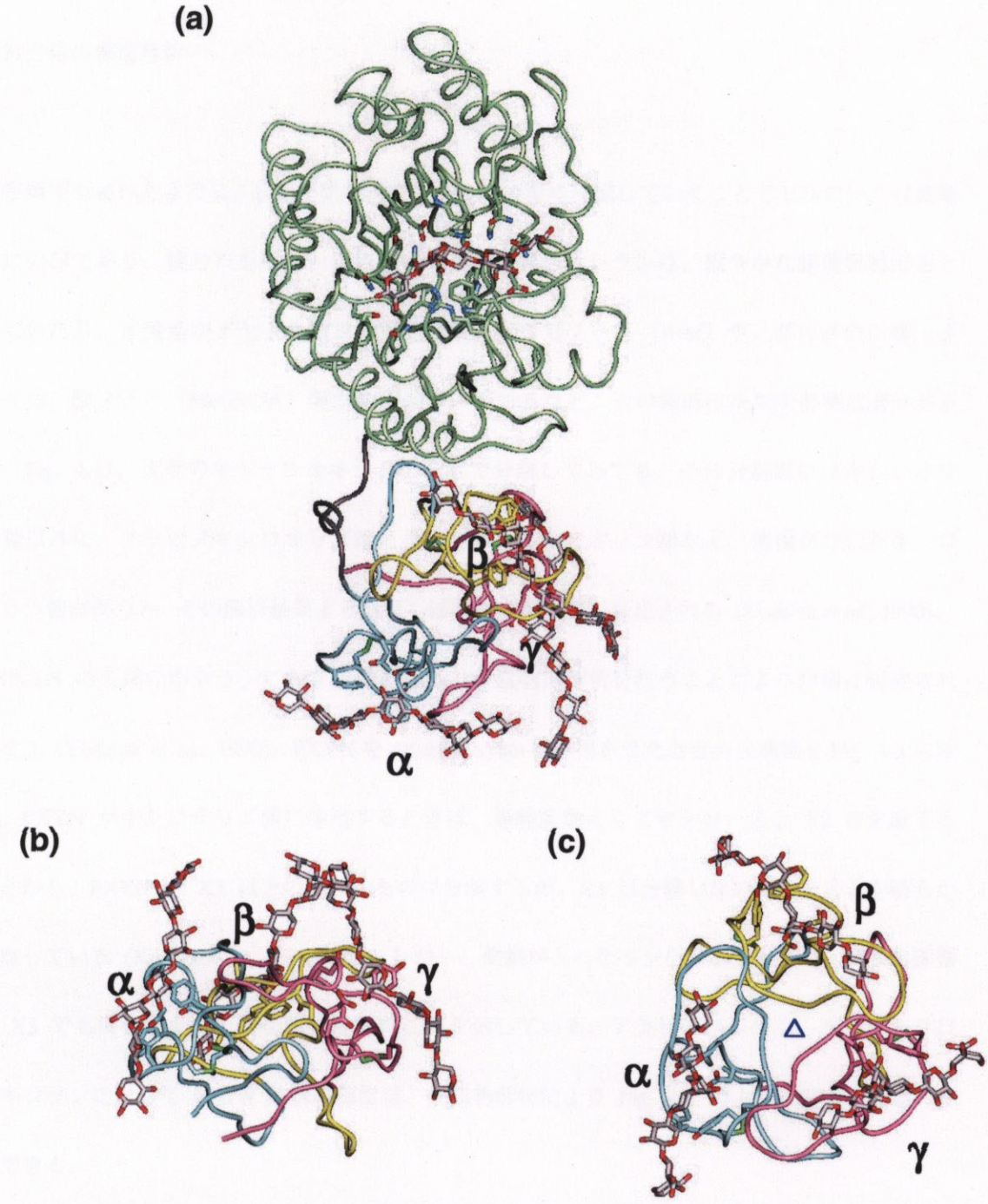

Fig. 3-9 Xyloheptaose docking models on (a) FXYN, (b) XBD from the side view, and (c) XBD from the top view. Central 4th xylose of the xyloheptaose molecule is superimposed on the bound xylose unit in the xylan binding sites α and γ in the FXYN/X3 complex. Xyloheptaose docking model in subdomain β is modeled similarly with respect to the subdomains α and γ.