MX1516

Total number of crystals (including replicates): 150
Total number of crystals with complete data sets: 33

The purpose of this experiment was the following:

1. Norovirus P domain in complex with their receptors
We are investigating the interaction of the norovirus capsid P domain in complex with the receptor (histo-blood group antigens – HBGAs). We are looking at different norovirus strains and their interactions with HBGA. To this end, we plan to analyze the panel of available HBGAs with the antigentically diverse norovirus genotypes (GII.1, GII.2,…GII.12), including the clinically important GII.4 variant noroviruses (saga, UNSW, and Farmington Hills). The following data sets were successful. We are now analyzing the binding interactions.

Saga P domain (GII.4)

HBGA	Resolution approx. (Å)	Interaction
LeA (tri)	1.5	bound
LeB (tetra)	1.14	unbound

SMV P domain (GII.2)

HBGA	Resolution approx. (Å)	Interaction
Apo	1.93	
Apo	2.3	
A (tri)	1.85	No
A (tri) soak	1.84	No
A (tetra)	1.85	No
LeB (tetra)	1.88	No
LeB(tetra)	1.9	No
LeX (tri)	2.29	No
D fuc	1.94	No
H2 (tri) soak	1.97	
LeX (tri) soak	2.2	
LeA (tri) soak	2.18	
LeB (tetra) soak	1.94	
LeY (tetra)	2.01	

UNSW P domain (GII.4)

HBGA	Resolution approx. (Å)	Interaction
D fuc	1.74	No
A soak	1.15	Yes
H2 soak	1.34	No
LeX	1.45	No
LeA	1.48	No
A	1.35	Yes
GNA	1.64	No
A soak	1.33	

LeY	1.43	
LeB	1.43	
A (tetra)	1.27	
H2	1.29	
LeB (tetra)	1.19	
LeA	1.22	

2. **Farmington Hills P domain.**
We collected data for a new norovirus P domain, Farmington Hills virus. This strain caused epidemic outbreaks of gastroenteritis worldwide, and represents an important virus to better understanding norovirus capsid evolution. We were unable previously to crystallize this protein, but now we have finally found a condition to produce nice crystals and the resolution was at 1.63 Å. We will continue to analyze this P domain in complex with the panel of HBGAs.

3. **Norovirus P domains with drug compounds**
We are investigating the norovirus P domain with libraries of drug compounds. We collected four data sets with different compounds bound to the norovirus GII.10 P domain (026 strain). These drugs might prove to be important for reducing norovirus infections.

026 P domain (GII.10)

Drug	**Resolution approx. (Å)**	**Interaction**
Com-34	1.5	no
Com-37	1.69	no
Com-24	1.65	yes
Com-88	1.48	yes