

## List of descriptors and labels for carbohydrate binding site clustering

### General information on protein and carbohydrate:

pdb\_id

Model

Carbohydrate\_name

Carbohydrate\_label

Carbohydrate\_type: 1 = free ligand; 2 = glycosylation head; 3 = glycosylation body

### Different properties of the binding site:

Polar\_sasa

Apolar\_sasa

Total\_sasa

Residues\_in\_helices

Residues\_in\_strands

Residues\_in\_turns

Residues\_in\_bends

Residues\_in\_loops

### Different functional groups present in ligands:

Function\_lipid

Function\_acid

Function\_amide

Function\_charged

Function\_aromatic

Function\_selenium

Function\_halogen

Function\_phosphorus

function\_sulfurfunction\_amino\_acid

### Carbohydrate binding site composition:

count_A	count_C	count_D	count_E	count_F	count_G
count_H	count_I	count_K	count_L	count_M	count_N
count_P	count_Q	count_R	count_S	count_T	count_V
count_W	count_Y				