

**Supplementary tables with data obtained from models 1-10 clustering as cluster 1-3**

Supplementary Table S1. Selected models of the His6: A $\beta$  peptide complex forming the Cluster 1

Cluster 1	Receptor (A $\beta$ peptide)	Ligand (His6)	H-bond	Salt bridges	Binding Energy $\Delta^iG$ kcal/mol
Model 1	HIS13, LYS16, LEU17, PHE20, ALA21, VAL24, GLY25, LYS28, ILE31, LEU34, MET35, GLY38, VAL39, ALA42	HIS1, HIS3, HIS4, HIS5, HIS6	GLY38:HIS6 ALA42:HIS6	ALA42: HIS6	-6.6
Model 4	LYS16, LEU17, VAL18, PHE20, ALA21, GLU22, VAL24, GLY25, SER26, LYS28, ILE31, LEU34, MET35	HIS1, HIS2, HIS3, HIS4, HIS5, HIS6	LEU17:HIS4 ALA21:HIS3	GLU22: HIS1	-4.3
Model 7	LYS16, LEU17, VAL18, PHE20, ALA21, GLU22, ASP23, VAL24, GLY25, LYS28, ALA30, ILE31, GLY33, LEU34, MET35	HIS1, HIS2, HIS3, HIS4, HIS5, HIS6	ALA21:HIS3		-6.8
Model 8	HIS13, LYS16, LEU17, VAL18, PHE20, ALA21, VAL24, GLY25, LYS28, ILE31, LEU34, MET35, GLY38, VAL39, ALA42	HIS1, HIS2, HIS3, HIS4, HIS5, HIS6	GLY38:HIS3		-6.6
Selected amino acids constituting the interacting interface	LYS16, LEU1, PHE20, ALA21, VAL24, GLY25, LYS2, ILE31, LEU34, MET35,	HIS1, HIS3, HIS4, HIS5, HIS6			-6.8

Supplementary Table S2. Selected models of the His6: A $\beta$  peptide complex forming the Cluster 2

Cluster 2	Receptor (A $\beta$ peptide)	Ligand (His6)	H-bond	Salt bridges	Binding Energy $\Delta^iG$ kcal/mol
Model 2	ASP1, ALA2, <b>GLU3, HIS6,</b> <b>ASP7,</b> <b>TYR10,</b> <b>HIS14</b>	<b>HIS1,</b> <b>HIS2,</b> HIS3, HIS4, HIS5, <b>HIS6</b>			-1.4
Model 5	ALA2, <b>GLU3,</b> <b>HIS6, ASP7,</b> <b>TYR10,</b> <b>HIS14,</b> LEU17	<b>HIS1,</b> <b>HIS2,</b> HIS3, HIS5, <b>HIS6</b>	HIS6: HIS5 HIS6:HIS6 GLY9:HIS1 GLY9:HIS1 TYR10:HIS1		-4.1
Model 9	<b>GLU3,</b> PHE4, <b>HIS6, ASP7,</b> <b>TYR10,</b> <b>HIS14,</b> GLN15, LEU17, VAL18	<b>HIS1,</b> <b>HIS2,</b> HIS5, <b>HIS6</b>	GLU3:HIS5 HIS6:HIS5 ASP7:HIS6	GLU3:HIS6 GLU11:HIS2	<b>-4.8</b>
Model 10	ALA2, <b>GLU3,</b> <b>HIS6, ASP7,</b> <b>TYR10,</b> <b>HIS14</b>	<b>HIS1,</b> <b>HIS2,</b> HIS3, HIS4, <b>HIS6</b>	ALA2:HIS3 GLU3:HIS2 GLU3:HIS1 ASP7:HIS2 GLY9:HIS6	GLU3:HIS1 ASP7:HIS2	-3.3

Selected  
amino acids  
constituting  
the  
interacting  
interface

**GLU3, HIS6,**  
**ASP7,**  
**TYR10,**  
**HIS14**

**HIS1,**  
**HIS2,**  
**HIS6**

**-4.8**

Supplementary Table S3. Selected models of the His6: A $\beta$  peptide complex forming the Cluster 3

Cluster 3	Receptor (A $\beta$ peptide)	Ligand (His6)	Binding Energy $\Delta^iG$ kcal/mol		
Model 3	GLY9, TYR10, VAL12, HIS13, HIS14, LEU17, VAL18	HIS1, HIS2, HIS3, HIS4, HIS5, HIS6	TYR10: HIS6 HIS14:HIS4		-2.6
Model 6	ASP7, SER8, GLY9, GLU11, VAL12, GLN15, LYS16, PHE19	HIS1, HIS2, HIS6	GLN15:HIS3 ASP7:HIS2 GLN15:HIS2	ASP7:HIS2 ASP7:HIS2 GLU11:HIS2 GLU11:HIS2	-1.7
Selected amino acids constituting the interacting interface	GLY9, VAL18	HIS1, HIS2, HIS6			-2.6