Supporting Information

Figure SI1. From left to right, Root Mean Square Deviation (RMSD) of FABP (top) and S100 (bottom) simulations, over the protein Calpha. In both cases, the first 5 ns (green) were discarded in order to minimize convergence artifacts. The second panels report the results of clustering over the MD Simulation trajectories. The total number of clusters is displayed on Y axis, and the interconversions between the different conformational clusters are displayed in the simulation timeframe. The last panel represents the representative structure of the most populated structural cluster (orange) superimposed on the first conformer of the NMR bundle (blu). The difference between the PDB and central cluster structures is expressed as average RSMD.

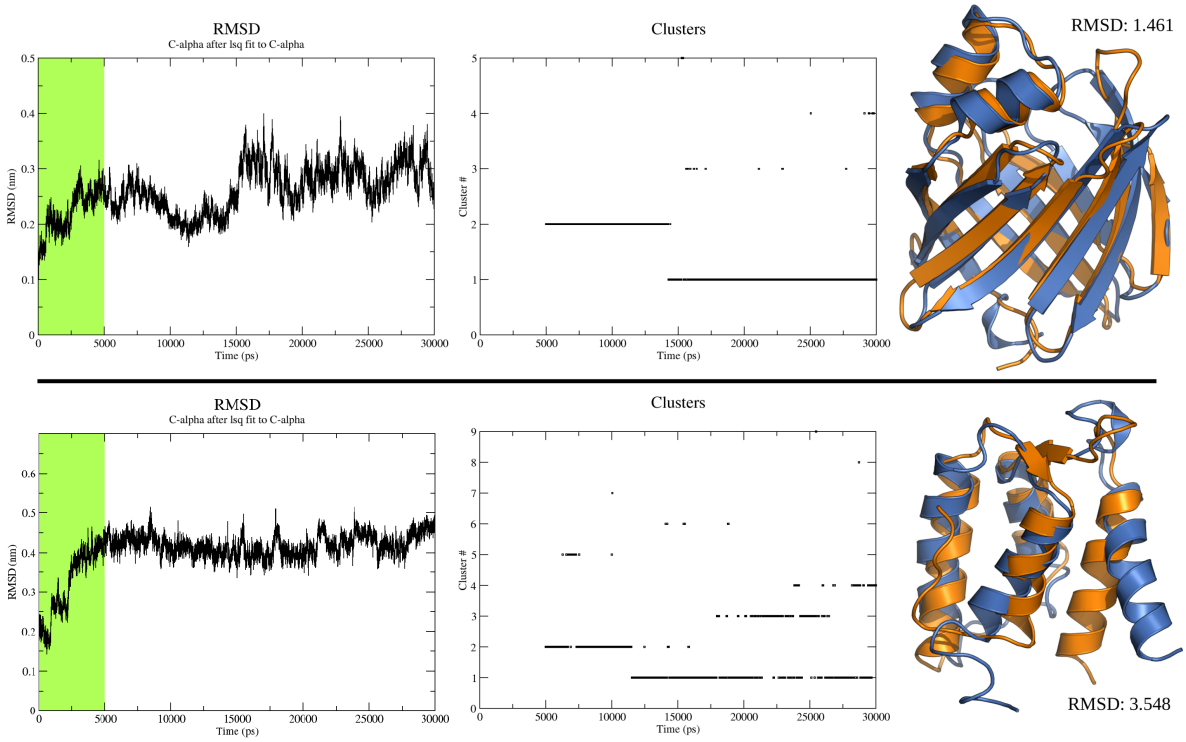

Table SI1. MLCE predictions calculated over the representative structures of FABP and S100 after considering the clustering of the protein trajectories. The different epitopes are represented in different colors with the same code as Figure SI1 and expressed as residue numbers (according to the UniProt annotation), one and three-letter code. The presence of two shades of the main color (red, blue, yellow) indicates the presence of chain gaps in the epitope predictions.

MLCE PREDICTIONS					
FABP			S100B		
f-ep1			**s-ep1**		
THR	T	74	ASP	D	12
ALA	A	75	VAL	V	13
ASP	D	76	PHE	F	14
ASP	D	77	HIS	H	15
ARG	R	78	GLN	Q	16
LYS	K	79	TYR	Y	17
TRP	W	97	SER	S	18
ASP	D	98	GLY	G	19
GLY	G	99	ARG	R	20
GLN	Q	100	GLU	E	21
GLU	E	101	GLY	G	22
f-ep2			ASP	D	23
MET	M	20	LYS	K	24
LYS	K	21	HIS	H	25
SER	S	22	LYS	K	26
LEU	L	23	GLU	E	67
GLY	G	24	**s-ep2**		
VAL	V	25	HIS	H	86
GLY	G	26	GLU	E	87
PHE	F	27	PHE	F	88
AL A	A	28	PHE	F	89
THR	T	29	GLU	E	90
ARG	R	30	HIS	H	91
GLN	Q	31	GLU	E	92
VAL	V	32			
ALA	A	33			
SER	S	34			
MET	M	35			
THR	T	36			
THR	T	118			
HIS	H	119			
GLY	G	120			
THR	T	121			
ALA	A	122			