Electronic Supplementary Material (ESI) for RSC Advances.

Pepsin-like aspartic proteases (PAPs) as model systems for combining biomolecular simulation with biophysical experiments

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Supporting Information Available

Input files for molecular dynamics, metadynamics simulations and order parameters (*plumed* input files) can be accessed at **Github**: https://github.com/sbhakat/PAP-review-inputs. Feature indexes corresponds to Figure 15 and 18 are mentioned as follows:

Index	Angle	Transformation	Res seq	Res name
0	chi1	sin	76	GLU
1	chi1	sin	77	MET
2	chi1	sin	78	ASN
3	chi1	sin	79	TYR
4	chi1	sin	80	VAL
5	chi1	sin	81	SER
6	chi1	sin	83	THR
7	chi1	sin	84	VAL
8	chi1	sin	85	SER
9	chi1	cos	76	GLU
10	chi1	cos	77	MET
11	chi1	cos	78	ASN
12	chi1	cos	79	TYR
13	chi1	cos	80	VAL
14	chi1	cos	81	SER
15	chi1	cos	83	THR
16	chi1	cos	84	VAL
17	chi1	cos	85	SER
18	chi2	sin	76	GLU
19	chi2	sin	77	MET
20	chi2	sin	78	ASN
21	chi2	sin	79	TYR
22	chi2	cos	76	GLU
23	chi2	cos	77	MET
24	chi2	cos	78	ASN
25	chi2	cos	79	TYR

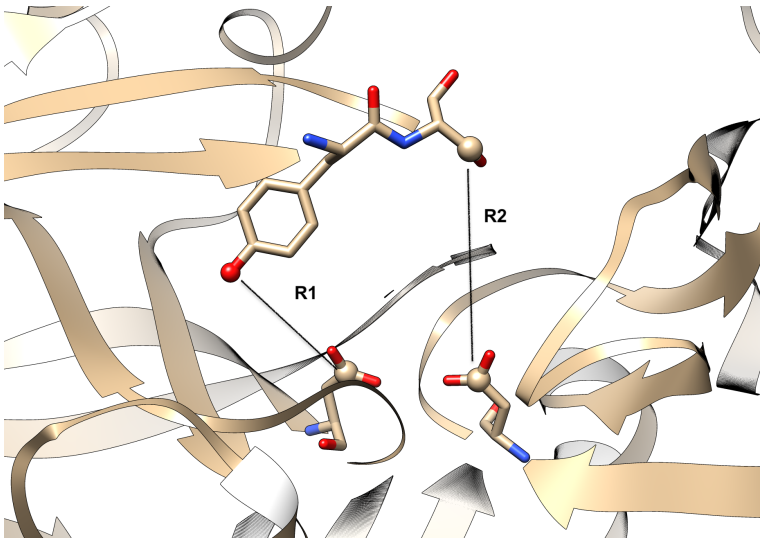

Fig. 27: Distance parameters proposed by *Shen and co-workers*. R1: distance between $Tyr-83-OH$ and $Asp-38-CG$ and R2: $Ser-84-CB$ and $Asp-38-CG$. The figure was created using $PDB:2REN$.