Electronic Supplementary Material (ESI) for RSC Advances.

The Dimerization and Ligand Binding in TyrosylProtein Sulfotransferase - 2 are influenced by Molecular Motions

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Table S1: The MD setup for the wild type TPST-2

S.No	MD-setup	Occurrence	Ions	Timescale (ns)
1	W113A	α2	Na+ (10)	100
2	Apo-enzyme	Protomer A and B	Cl – (10)	100
3	Enzyme-substrate		Na+ (12)	100
4	Enzyme-cofactor		Cl- (2)	100
5	Protomer A		Cl- (5)	100
6	Protomer B		Cl- (5)	100
7	Cofactor			100
8	Substrate		Na+ (6)	100

Table S2: The cluster analysis of most populated clusters of the W133A and wild type TPST-2

Cluster Analysis					Initial crystal structure with hydrogen
	Wild type TPST-2		W133A mutant		Wild type TPST-2
Residue	Cluster 1 (A)	Cluster 2 (A)	Cluster 1 (A)	Cluster 2 (A)	Protomer (A)
W113 (sc) – R105 (sc)	3.83	3.89	9.24	6.49	4.89
W113 (sc) - R110 (sc)	3.63	4.66	5.71	6.26	4.31
W113(sc) - M109 (sc)	3.92	3.32	6.21	6.53	3.95
W113(sc) - I102(sc)	4.27	4.13	3.56	4.36	3.72
W113(sc) - L133(sc)	3.65	3.31	4.41	4.54	3.90

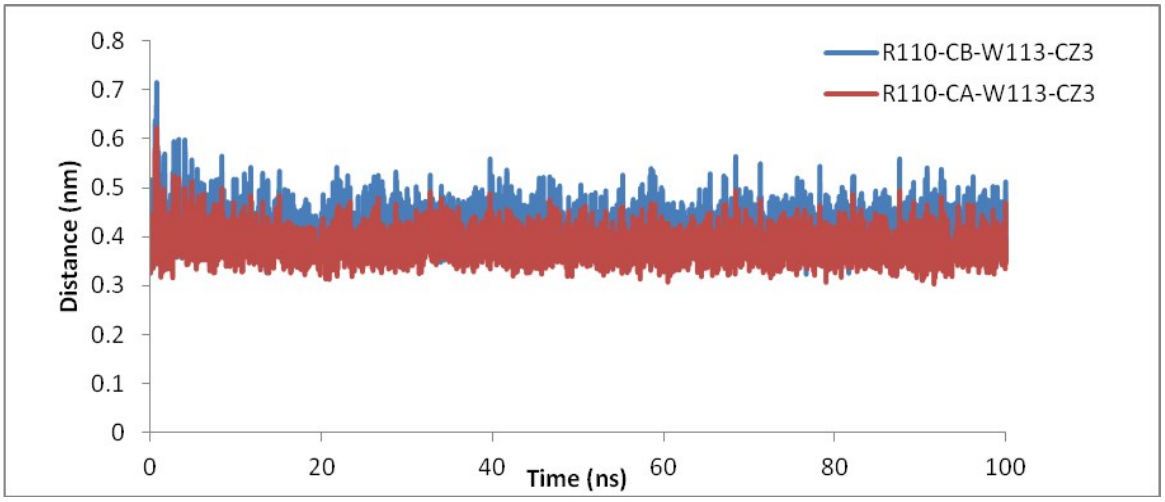
Table S3 The average properties of the multiple runs of W113A and important distances for 100ns

Name	Mean (Å)	S.D (Å)	S.E.M (Å)	A99(sc) – Y1006(sc0	A99(sc) – K158 (sc)	Substrate angle
Run 1	2.42	0.25	0.006	9.5	4.3	103.5°
Run 2	2.99	0.30	0.006	8.2	4.0	98.9°
Averaged all	2.7	0.27	0.006	8.8	4.1	101.2°

Table S4: The radius of gyration and solvent accessible surface area of different setups of TPST-2

	Radius of gyration in (Å)	SASA (Å)

	Mean	sd	Mean	sd
WT	28.73	0.19	2700.14	34.97
Apoenzyme	29.36	0.26	2638.35	44.57
Enzyme + Substrate	28.80	0.20	2663.38	52.21
Enzyme + cofactor	30.23	0.22	2694.05	34.83
Protomer A	18.61	0.21	1385.39	36.37
Protomer B	18.59	0.24	1426.67	31.77
Substrate	6.42	1.13	127.92	9.98



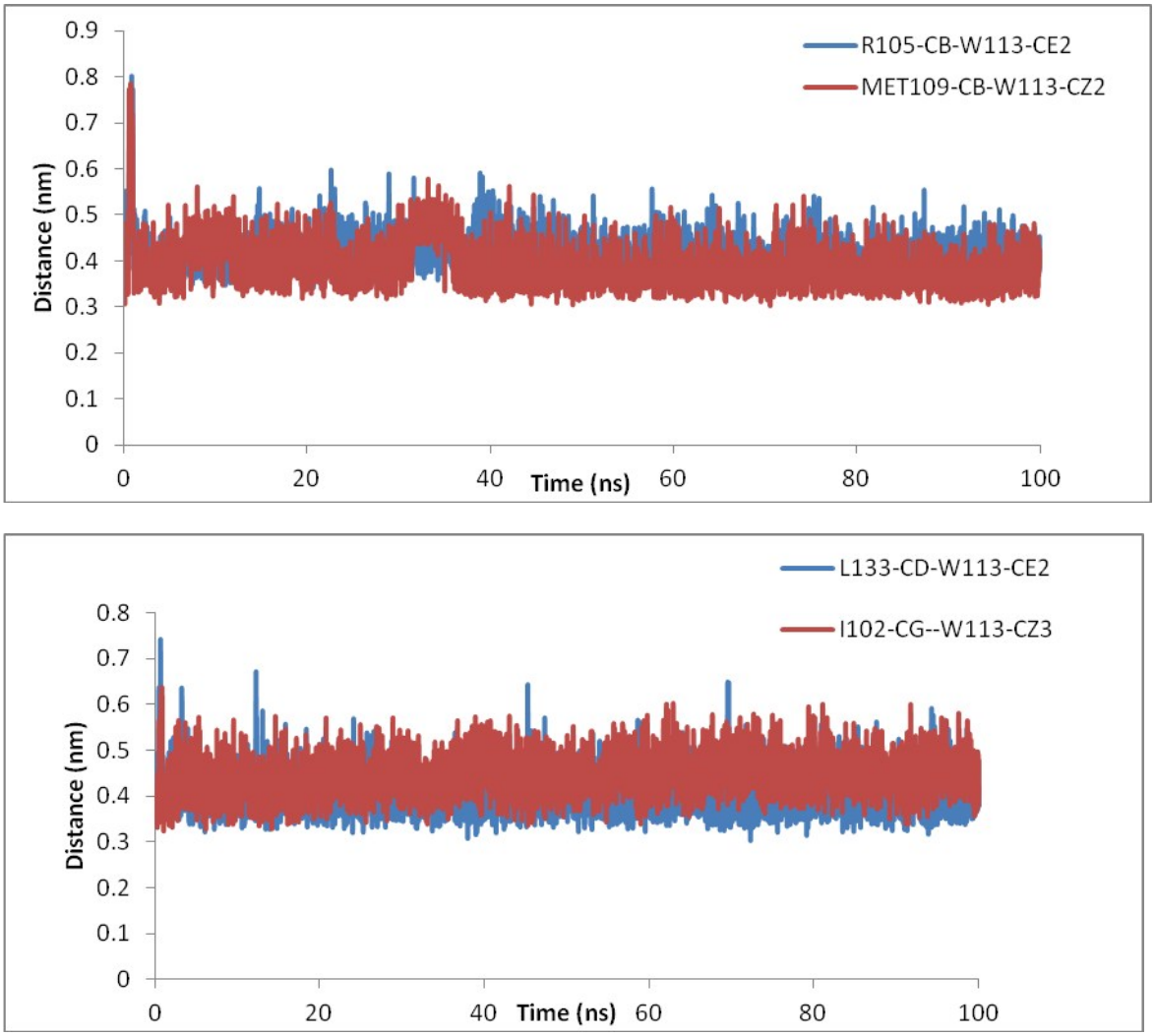


Figure S1 The Hydrophobic interactions of residues of wild type TPST-2 with W113 residue for 100 ns trajectory.

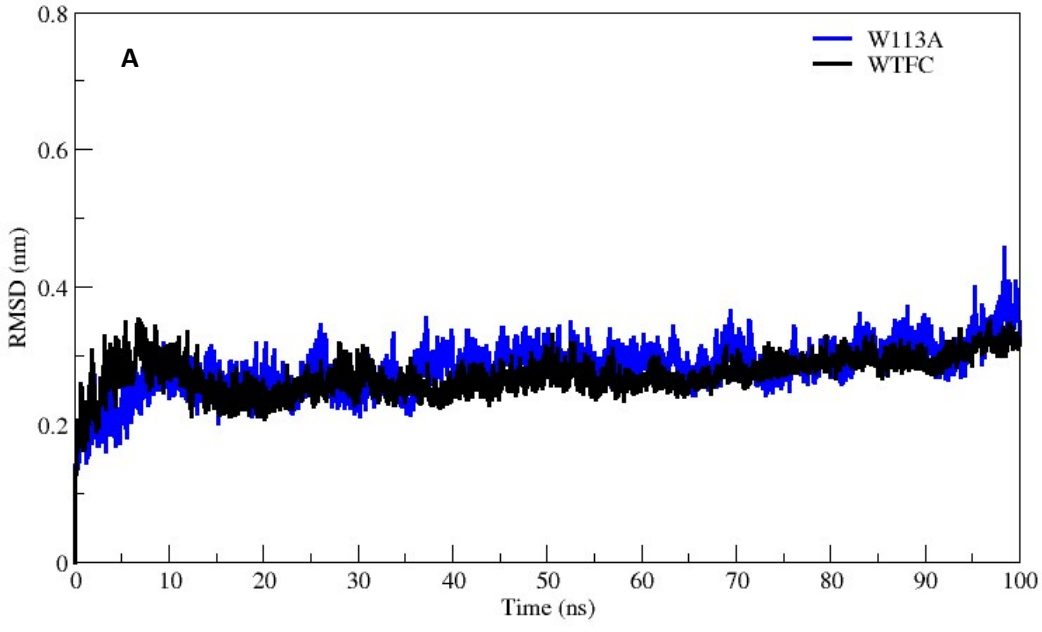


Figure S2 The Root Mean Square Deviation (RMSD) of wild type TPST-2 and W113A mutant using C α atoms. (A) The RMSD of WTFC and W113A. (B) The replica runs of the W113A mutant along with average run (100 ns) from two trajectories.

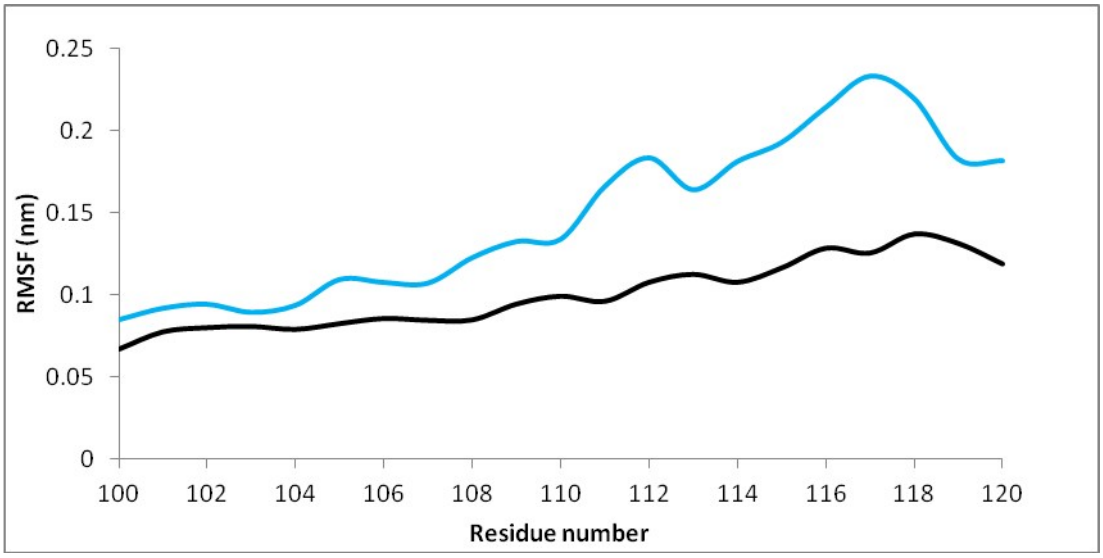
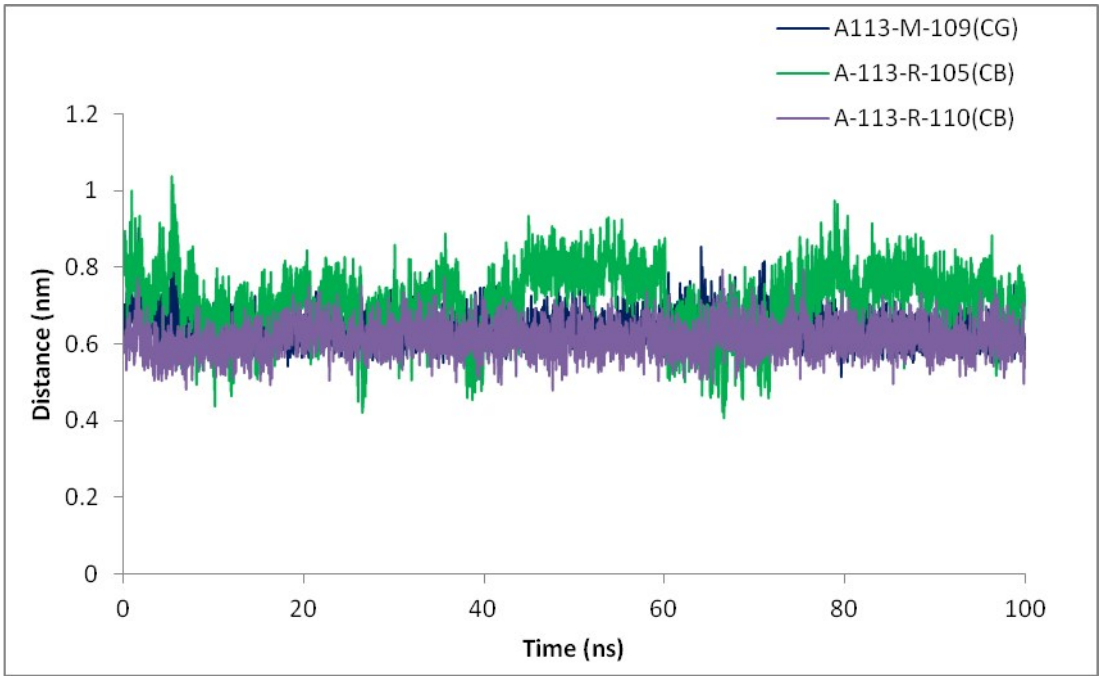


Figure S3 RMSF plot of residues in vicinity of W113 residue in wild type TPST-2 (WTFC, black colour) and the mutant W113A (cyan colour) for 100 ns trajectory.



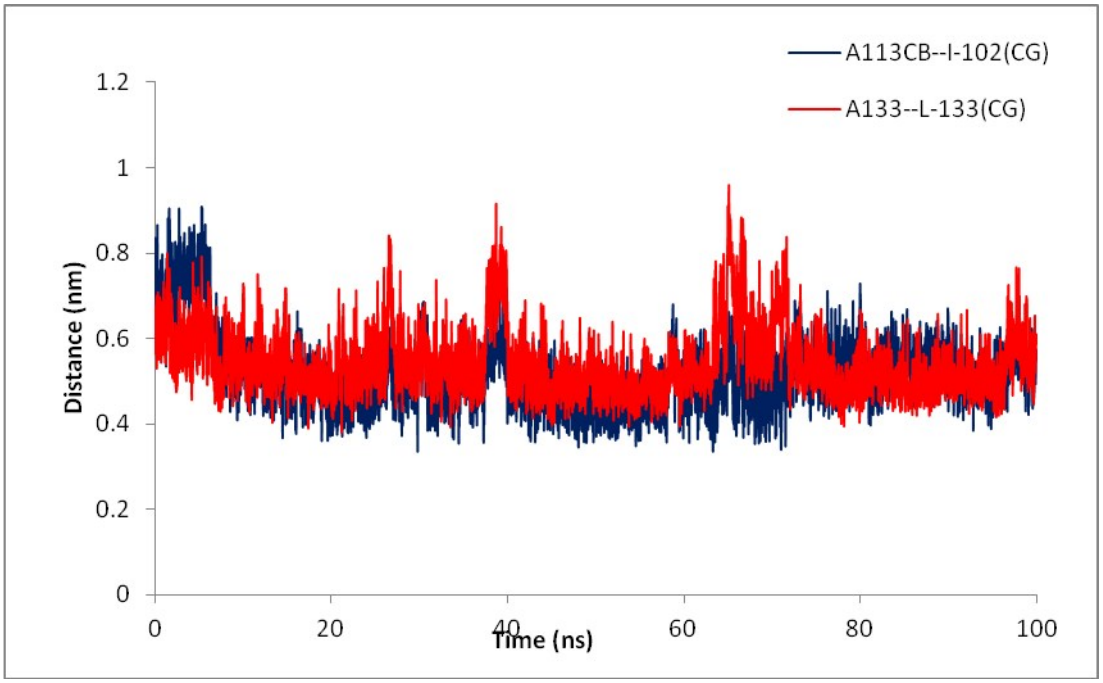
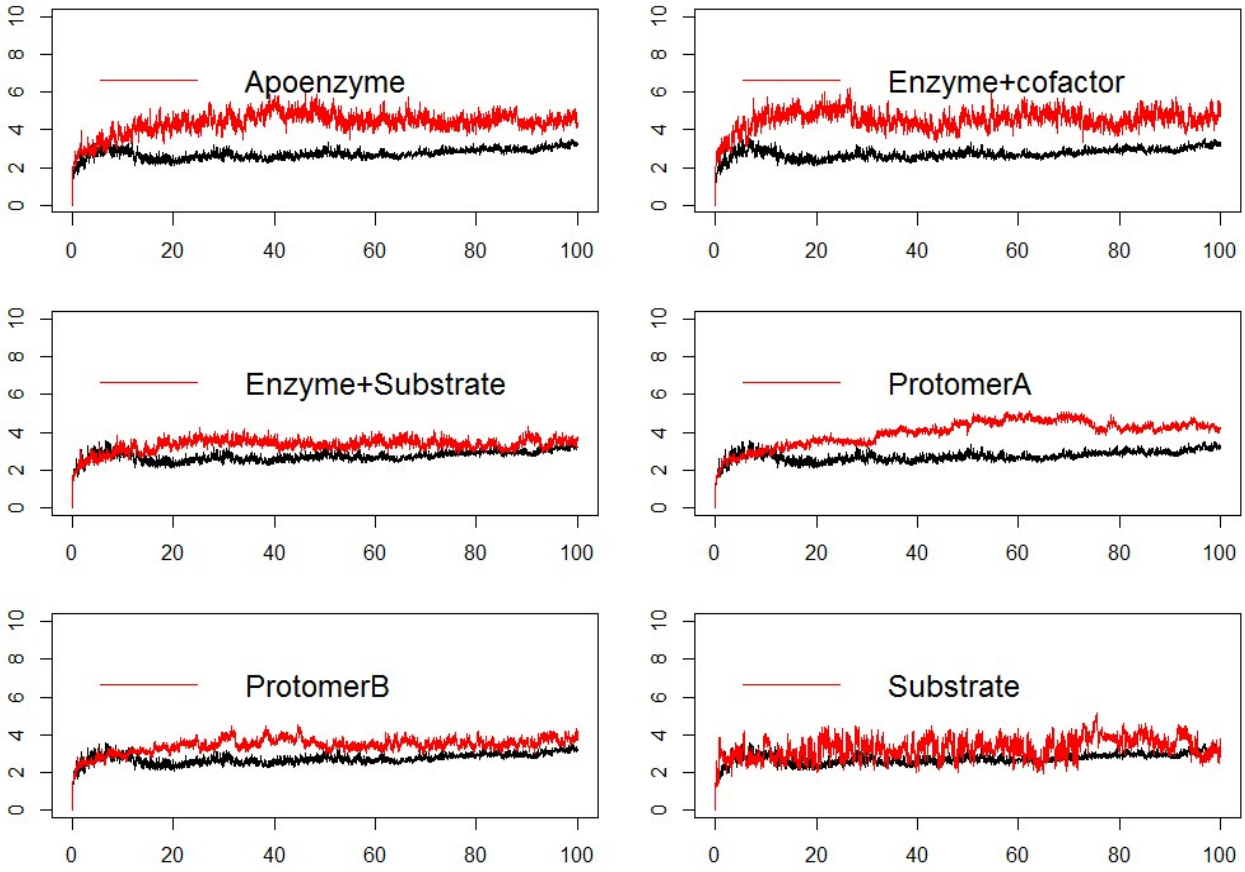


Figure S4 The interactions of A113 of W113A mutant for 100 ns trajectory.

Figure S5 The RMSD different setups of wild type TPST-2 using C α atoms.



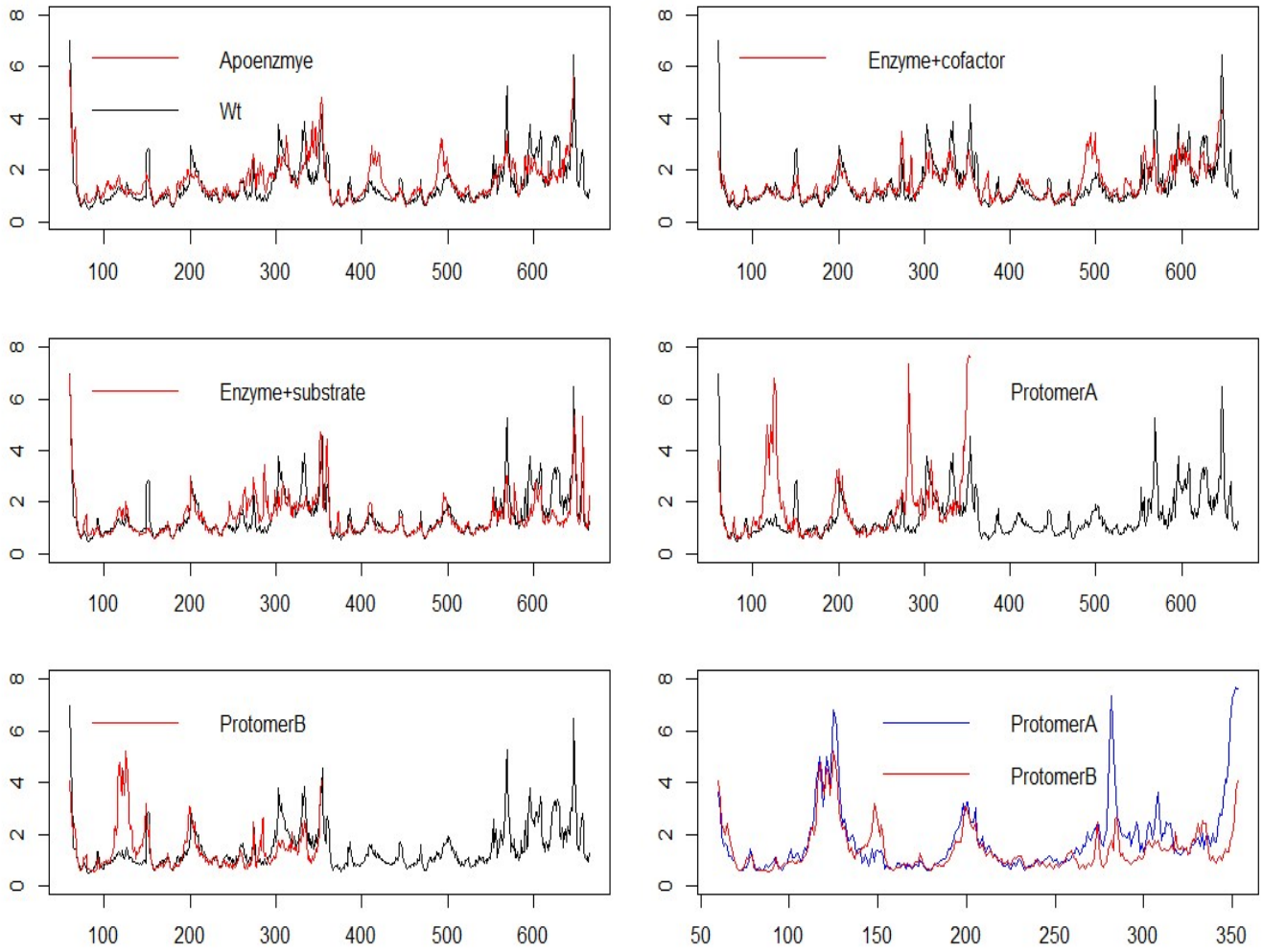


Figure S6 The RMSF of the different TPST-2 setups for 100 ns trajectory

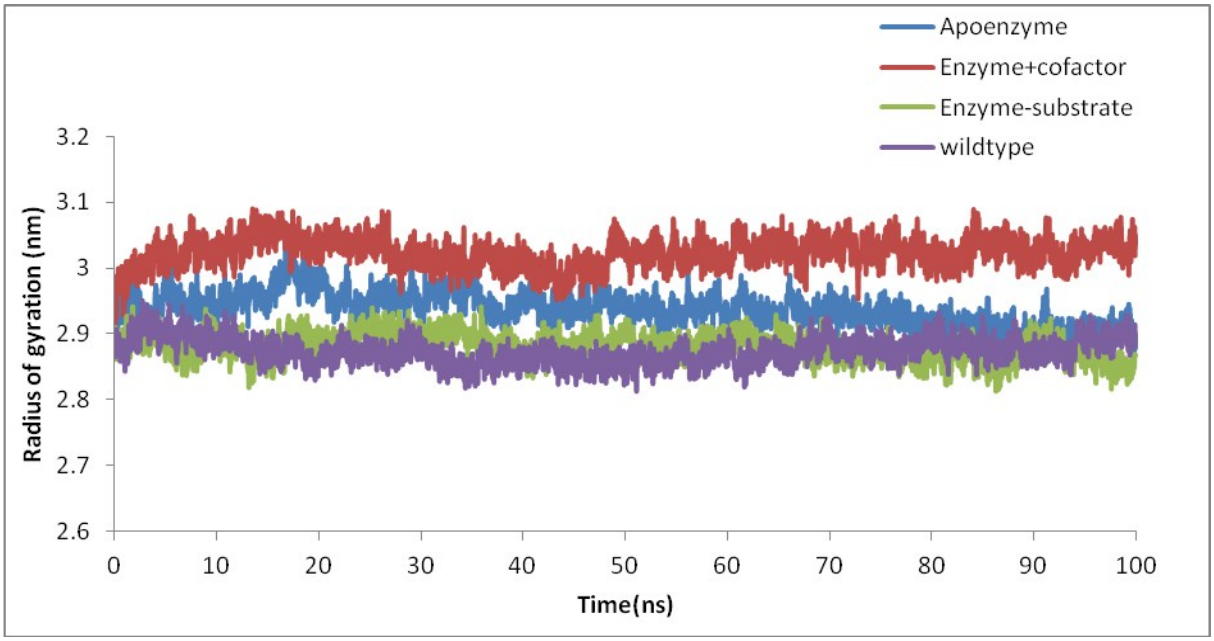


Figure S7 The radius of gyration of WTFC, APO, EC and ES for 100 ns trajectory

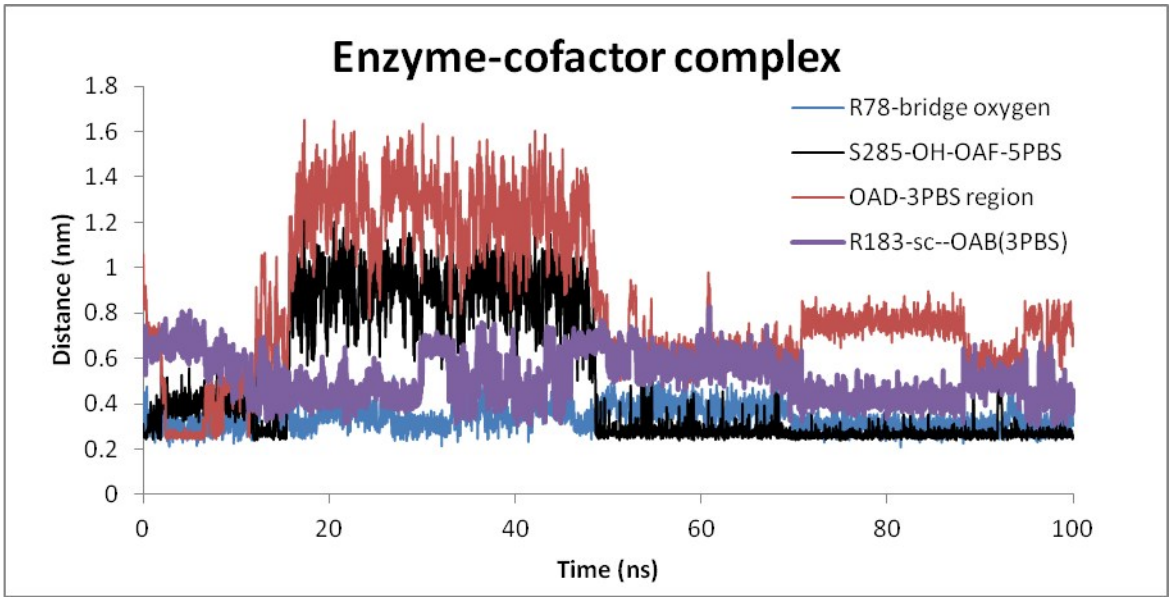


Figure S8 The enzyme cofactor setup (EC) and important distances between the protein and cofactor for 100 ns trajectory

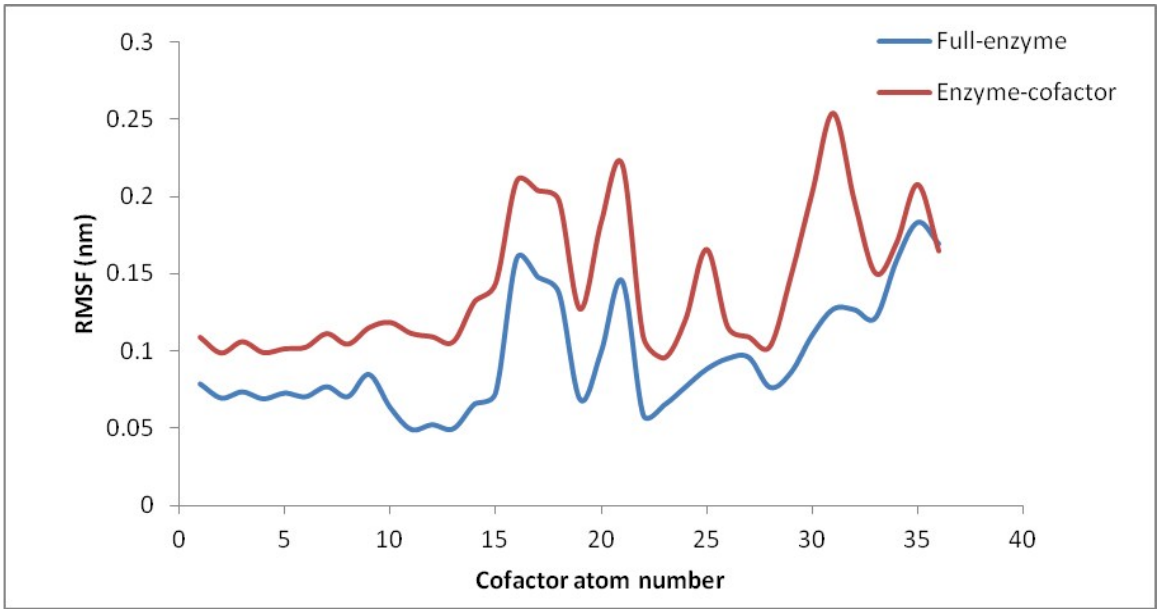


Figure S9 The cofactor RMSF in wild type full complex (WT FC) and enzyme-cofactor complex (EC) for 100 ns trajectory

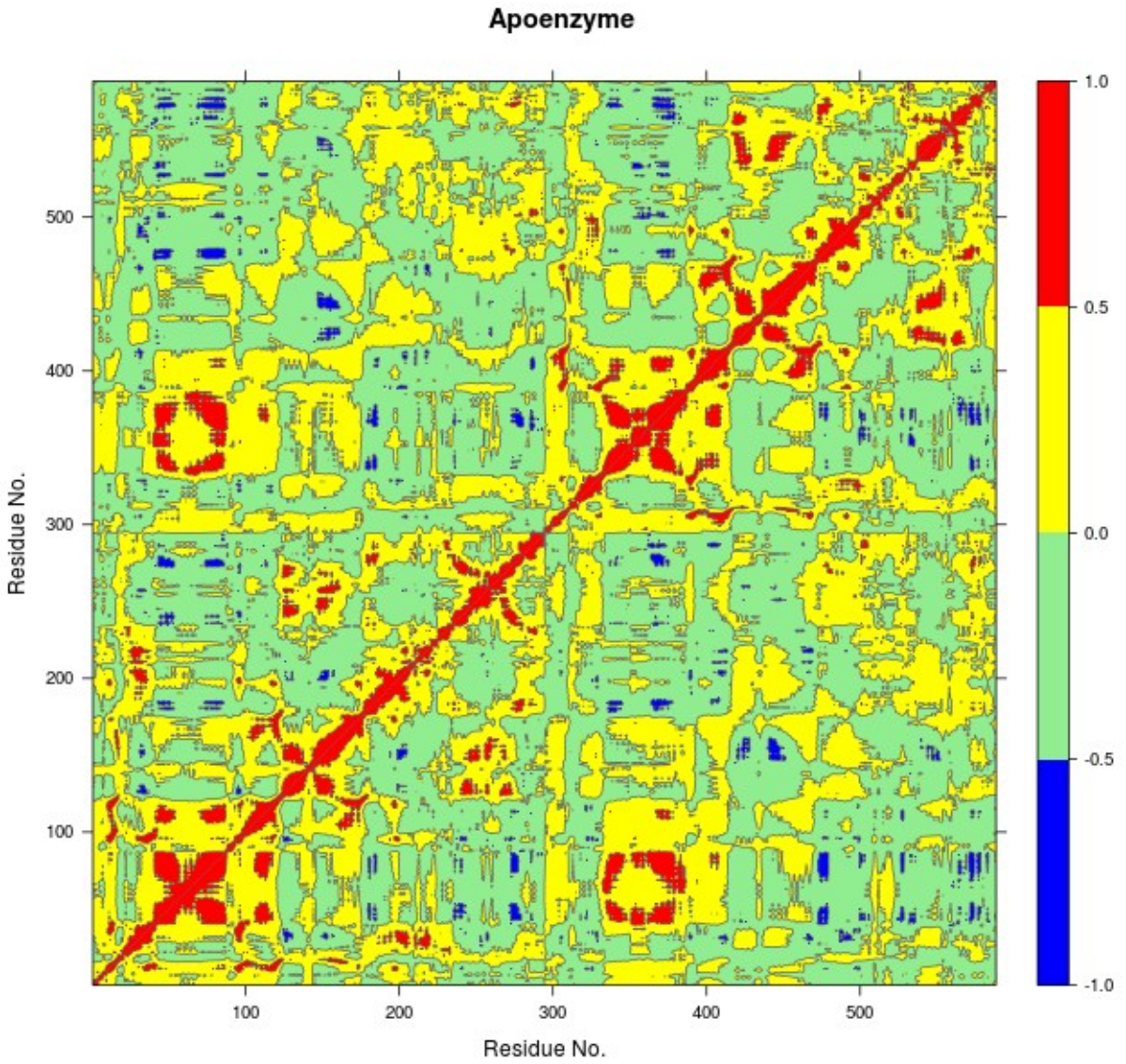


Figure S10 Dynamic Cross Correlation Analysis of Apoenzyme (Apo) for 100 ns trajectory

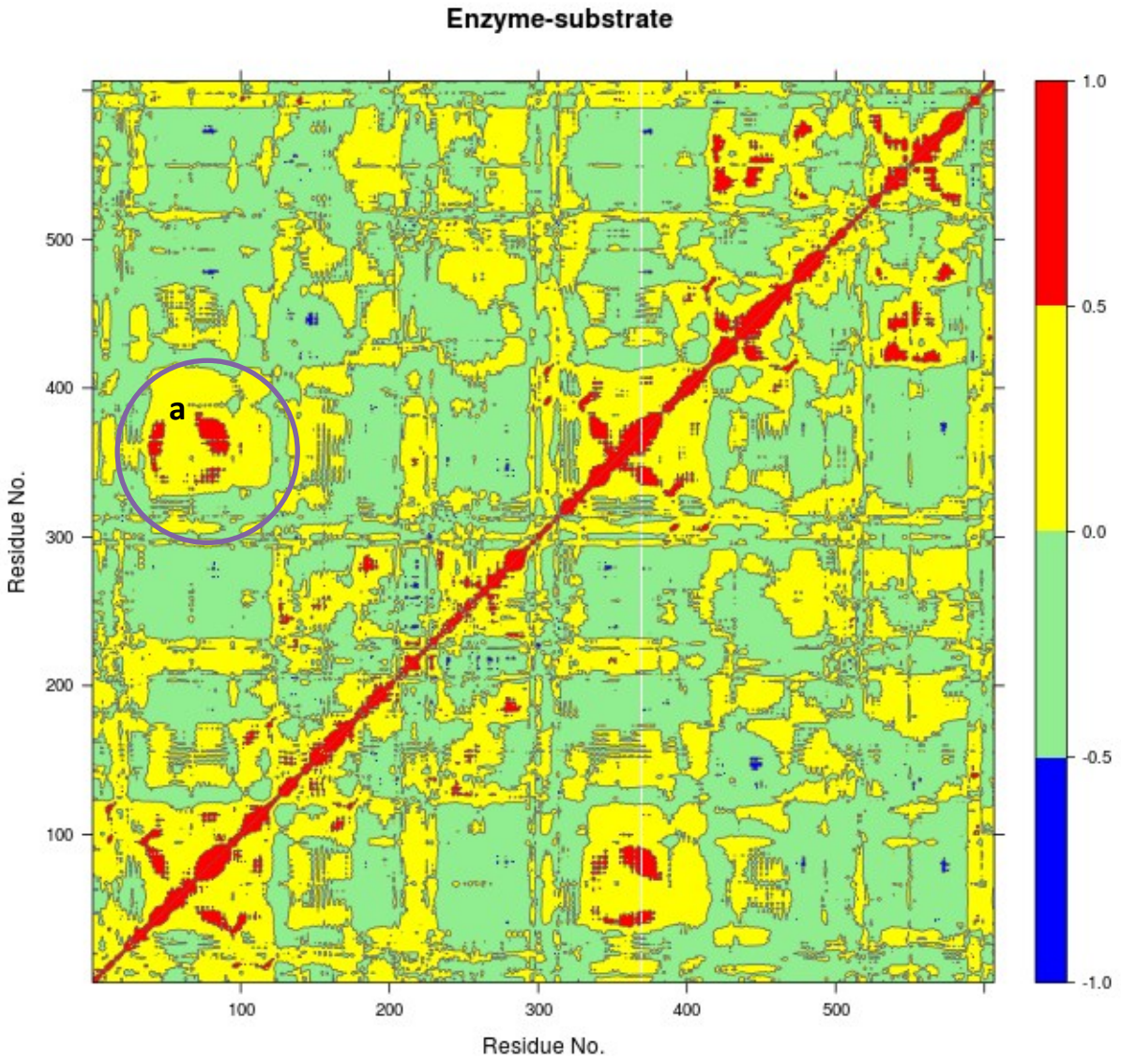


Figure S11 Dynamic Cross Correlation Analysis of Enzyme + substrate complex (ES) for 100 ns trajectory

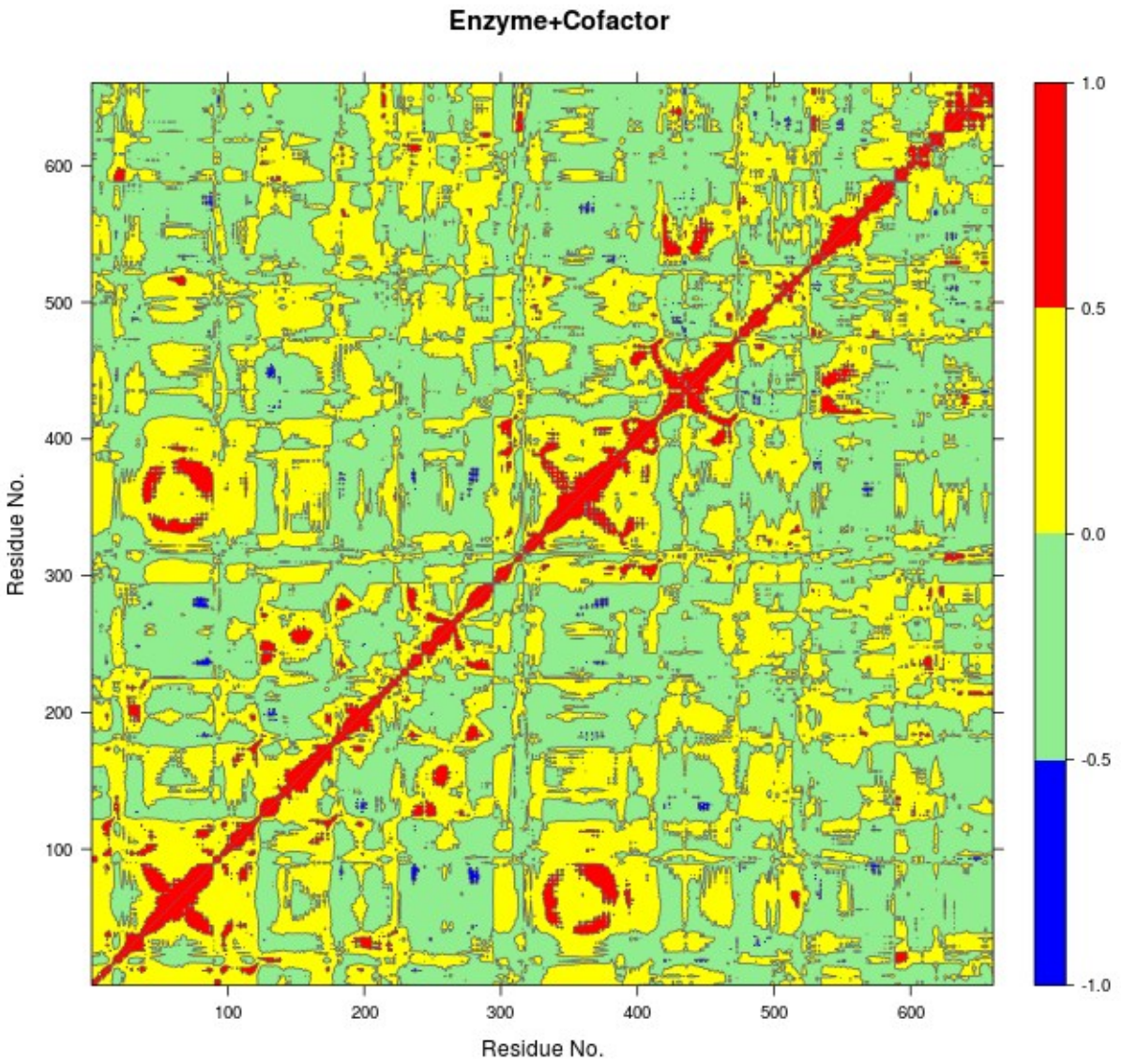


Figure S12 Dynamic Cross Correlation Analysis of Enzyme + cofactor (EC) for 100 ns trajectory

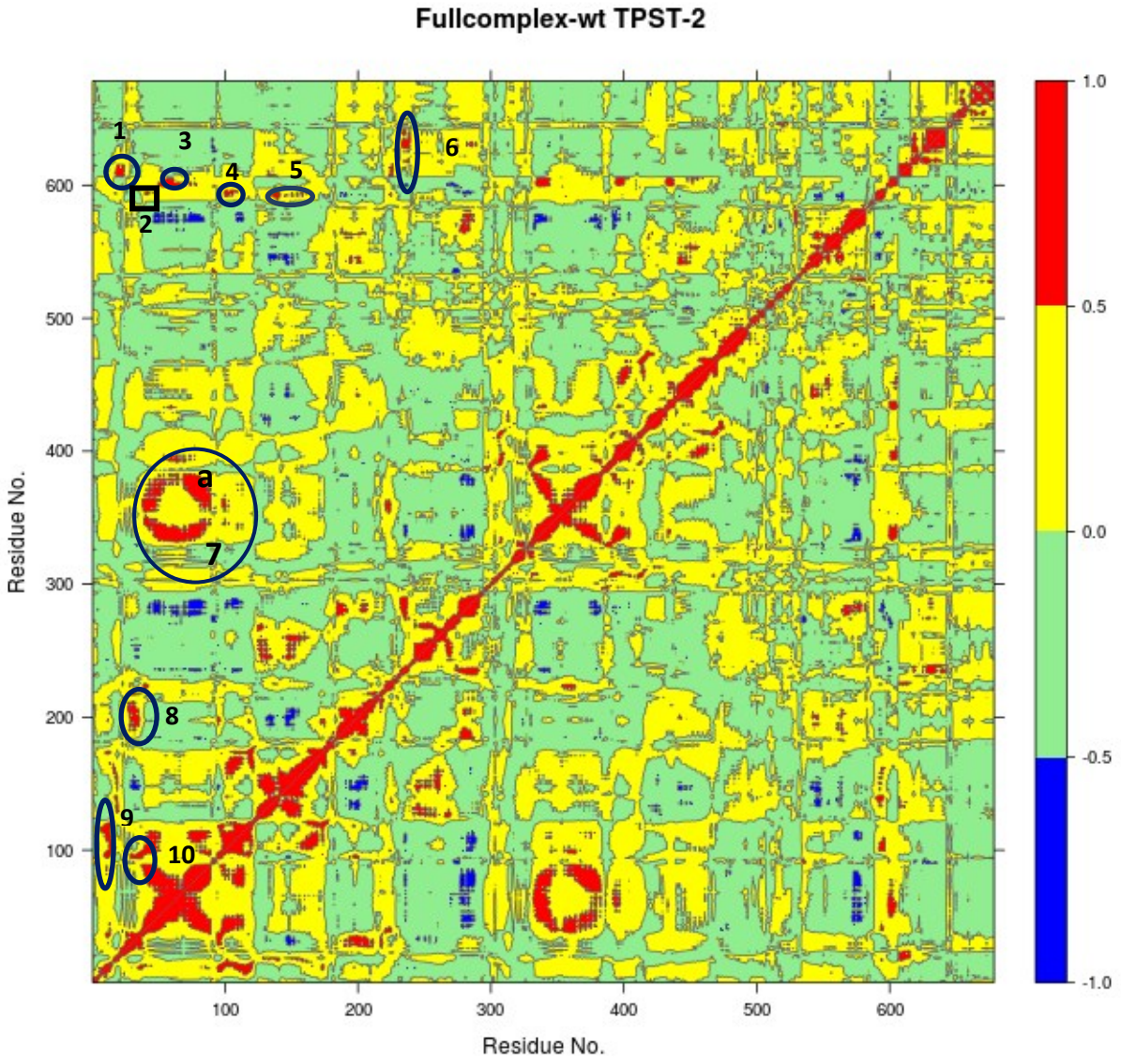


Figure S13 Dynamic Cross Correlation Analysis of wild type TPST-2 Full complex (WT FC) for 100ns trajectory

Strong positive (magnitude +1, colour red) correlation in wild type full complex

1. Residues (78-82) of protomer A, it is also the part of 5'PBS region in wild type TPST-2 correlates to 5 sulphate group of the PAPS cofactor.

2. Residues E99, R101,R105 show strong correlation against the substrate peptide residues (residue 1004,1005)

3. residue (60-80) α3-α4 (this is substrate binding area and contains residues which bind to substrate or stabilize the substrate) of protomer A show strong correlation to whole substrate peptide

4. Residue K158 also shows strong correlation to the substrate peptide (Y1006) however it shows weak correlation to the 5 sulphate group of the cofactor.

5. The residue of βe show strong correlation to the substrate peptide (1005,1006) residues
6. The residue 240-250 (loop between α13-α14) show correlation towards adnenosine ring atoms of PAPS
7. Residue of α2, α3 and α4 of protomer A interacts with α15, α16 of protomer A and 5'PBS binding region of protomer B
8. Residues 90-101 (α1, β4) protomer A show correlation against residues (250-270) α10, α11 and α12 of protomer A.
9. Residues 70-80 residues show correlation towards residues 160-180 residues (α5-α6 and β7).
10. Residues 99-110 show correlation against residue 160-170 residues

Weak positive correlation (magnitude 0-0.5, colour yellow) correlation in wild type TPST-2

Residues (75-85) of protomer A, it is 5'PBS region in wild type TPST-2 correlates to the 5 phosphate and sulphate group of PAPS.

The substrate binding region of TPST-2 shows correlation to the substrate peptide.