

Table. Molecular Dynamics Simulation parameters values.

Parameters		Wild_MCL	R215G	V216G	L235Q	R263S	G271D
RMSD (nm)	H. RMSD (nm)	0.6015724	0.6213057	0.5524397	0.5984163	0.5316835	0.5643897
	L. RMSD (nm)	0.0000005	0.0000005	0.0000005	0.0000003	0.0000004	0.0000004
	A. RMSD (nm)	0.4811997	0.5040285	0.4204425	0.4753986	0.4403705	0.4611233
	Mean±SD	0.4812±0.067	0.504±0.0851	0.4204±0.0679	0.4753±0.0728	0.4403±0.0463	0.4611±0.0691
RMSF (nm)	H. RMSF (nm)	0.8498	1.4655	0.6799	0.9835	1.0324	1.0775
	L. RMSF (nm)	0.1369	0.235	0.1178	0.151	0.0961	0.128
	A. RMSF (nm)	0.3867361	0.567102	0.2806144	0.3730328	0.3435052	0.3503708
	Mean±SD	0.3867±0.1382	0.5671±0.198	0.2806±0.1045	0.373±0.1361	0.3435±0.1344	0.3503±0.1173
Radius of Gyration (nm)	H. Rg (nm)	2.20955	2.19632	2.11899	2.14709	2.18381	2.17394
	L. Rg (nm)	2.09468	2.04686	1.99409	2.04162	2.02638	2.04347
	A. Rg(nm)	2.14304022	2.127679481	2.063388902	2.094207305	2.076657126	2.107527964
	Mean±SD	2.143±0.0214	2.1276±0.029	2.0633±0.0207	2.0942±0.0184	2.0766±0.0194	2.1075±0.0207
Number of Hydrogen bonds	H. H bond (numbers)	237	209	252	239	250	240
	L. H bond (numbers)	131	120	135	134	135	135
	A. H bond (numbers)	156.3866	145.3736	158.9250	161.6403	166.0609	158.1388
	Mean±SD	156.39±9.23	145.37±9.44	158.93±10.41	161.64±12.55	166.06±9.57	158.14±9.70

H. Highest, L. Lowest, and A. Average