

Supplementary Materials

MD Simulation Reveals Regulation of Mechanical Force and Extracellular Domain 2 on Binding of DNAM-1 to CD155

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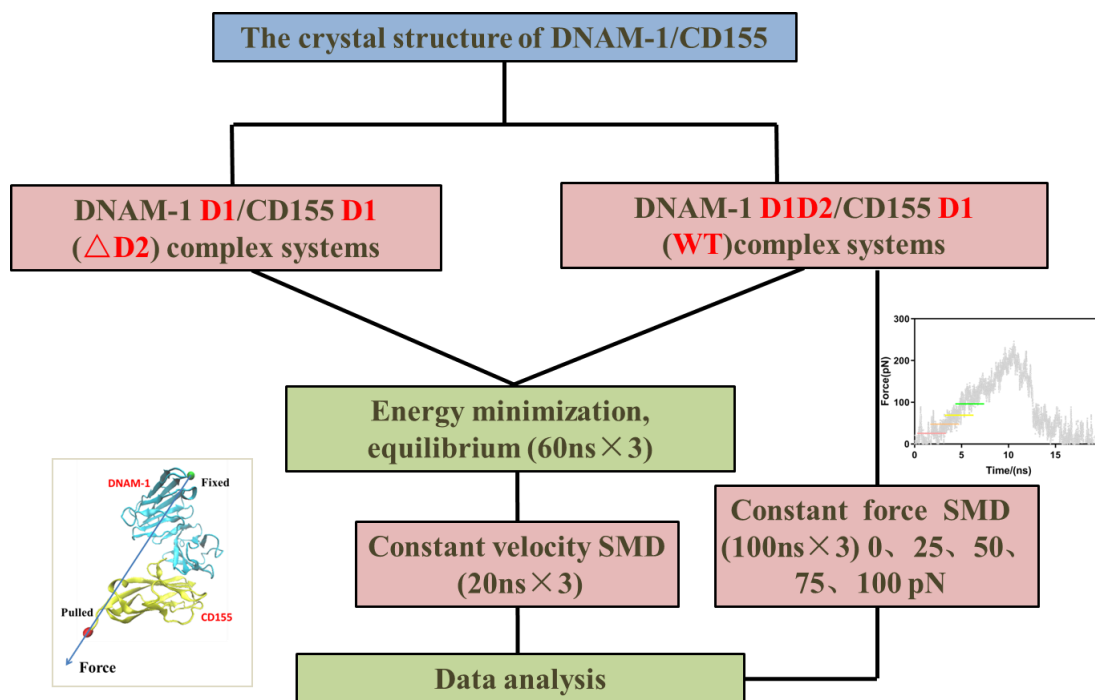


Figure S1. The ensemble workflow of computational procedure.

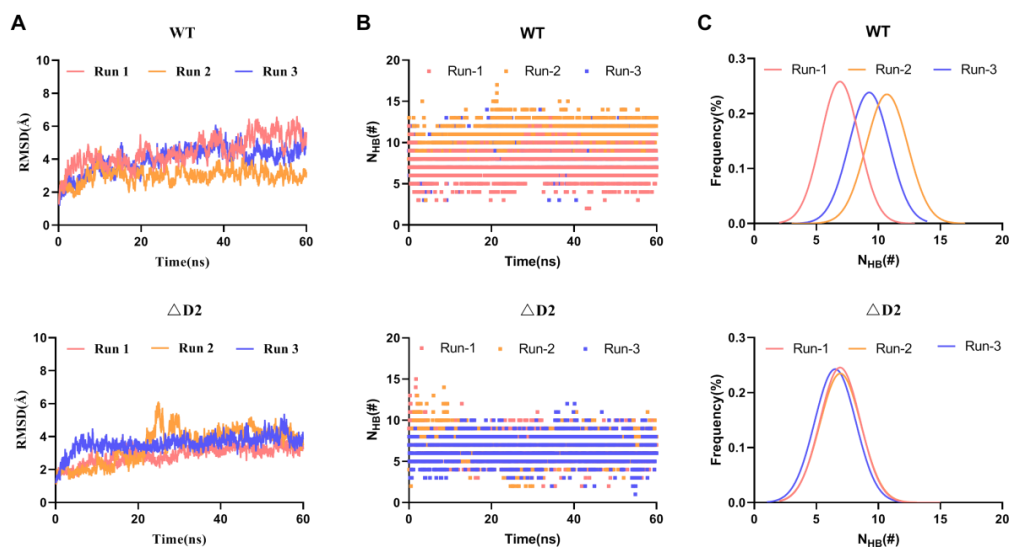


Figure S2. The time courses of root mean square deviation (RMSD) of heavy atoms and the number of H-bonds (NHB) between the interfaces, and the distributions of H-bonding events within 60 ns at binding site of the two complexes (WT and $\Delta D2$) for thrice 60 ns equilibriums. (A) The time courses of RMSD, (B) the time courses of NHB, and (C) the Gaussian frequencies of NHB for three runs with the two complex.

Table S1. Residue interaction on binding site of DNAM-1/CD155 complex.

No	Residue name		Force(pN)				
	DNAM-1	CD155	0pN	25pN	50pN	75pN	100pN
1	T46	Q63	0.85±0.02	0.87±0.04	0.89±0.02	0.87±0.01	0.83±0.06
2	Q47	T127	0.80±0.01	0.77±0.01	0.74±0.04	0.76±0.05	0.76±0.05
3	E49	S132	0.86±0.04	0.78±0.09	0.80±0.09	0.80±0.05	0.77±0.09
4	Q115	S74	0.65±0.05	0.60±0.09	0.58±0.06	0.58±0.04	0.63±0.04
5	Q47	S62	0.80±0.05	0.73±0.03	0.69±0.2	0.78±0.04	0.72±0.15
6	R72	E57	0.54±0.03	0.68±0.17	0.68±0.22	0.54±0.23	0.20±0.24
7	S59	R133	0.22±0.09	0.17±0.02	0.18±0.02	0.25±0.11	0.06±0.06
8	Y113	G83	0.52±0.06	0.48±0.12	0.40±0.09	0.36±0.16	0.41±0.03
9	T112	Q63	0.44±0.07	0.51±0.08	0.53±0.12	0.49±0.04	0.49±0.07
10	K190	E71	0.39±0.06	0.38±0.15	0.29±0.28	0.38±0.13	0.34±0.18
11	Y111	S132	0.10±0.01	0.15±0.14	0.10±0.18	0.25±0.02	0.15±0.17
12	Q119	E71	0.33±0.10	0.40±0.20	0.33±0.28	0.40±0.10	0.39±0.18
13	R72	P129	0.29±0.09	0.19±0.16	0.13±0.22	0.23±0.13	0.32±0.20
14	R72	Q130	0.11±0.06	0.15±0.14	0.11±0.19	0.18±0.09	0.31±0.13

Table S2. Residue interaction on interface of DNAM-1 D1 and D2.

No	Residue name		Force(pN)				
	D1	D2	0pN	25pN	50pN	75pN	100pN
1	S26	I173	0.97±0.01	0.95±0.04	0.96±0.04	0.98±0.00	0.98±0.01
2	T25	D174	0.56±0.11	0.57±0.08	0.57±0.08	0.54±0.04	0.62±0.01
3	D128	R221	0.05±0.09	0.83±0.20	0.64±0.20	0.91±0.01	0.82±0.14
4	E36	R171	0.45±0.27	0.65±0.15	0.60±0.15	0.58±0.13	0.79±0.02
5	Q119	K190	0.17±0.15	0.25±0.26	0.25±0.26	0.19±0.13	0.31±0.07
6	H24	L175	0.45±0.39	0.54±0.23	0.51±0.23	0.67±0.01	0.50±0.15
7	H24	K190	0.15±0.13	0.07±0.17	0.18±0.17	0.17±0.09	0.15±0.12
8	E19	R185	0.28±0.24	0.12±0.07	0.20±0.07	0.33±0.06	0.18±0.17
9	K120	D174	0.21±0.20	0.22±0.24	0.25±0.24	0.04±0.04	0.25±0.07
10	E36	Q172	0.35±0.29	0.44±0.24	0.55±0.24	0.31±0.05	0.33±0.09
11	E20	R185	0.27±0.17	0.19±0.43	0.30±0.43	0.22±0.18	0.16±0.14