Supplementary materials

Molecular dynamics simulation of the interactions between EHD1 EH domain and multiple peptides

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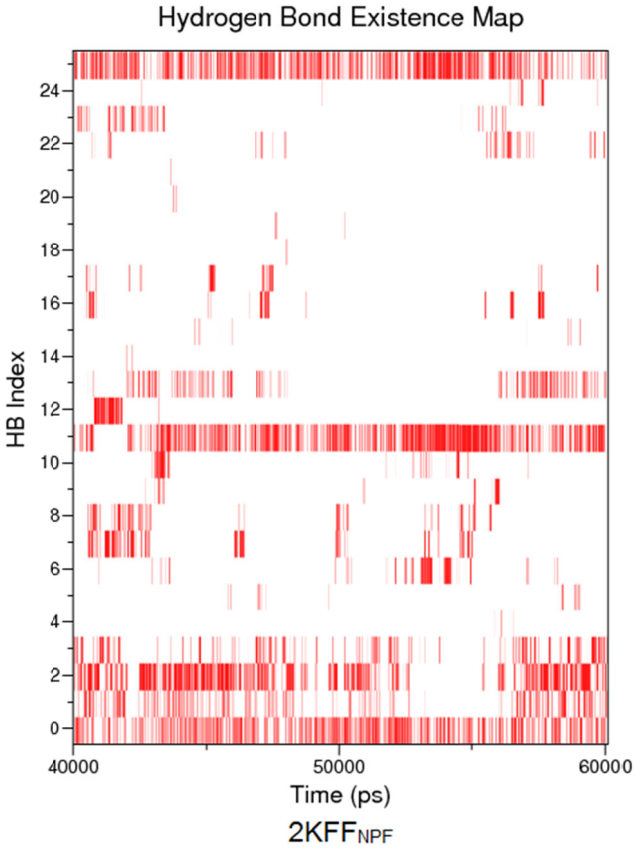
Table S1 Per-residue energy decomposition of the peptide residues in detail

Peptide Residue	2KFF$_{NPF}$				
	ΔE_{van} (kcal/mol)	ΔE_{ele} (kcal/mol)	ΔG_{polar} (kcal/mol)	$\Delta G_{nonpolar}$ (kcal/mol)	$\Delta G_{binding}$ (kcal/mol)
Phe143	−0.91	−11.90	12.94	−0.14	−0.02
Asn144	−0.15	0.36	−0.03	−0.0007	0.18
Tyr145	−2.11	−1.66	2.63	−0.39	−1.54
Glu146	−0.50	−9.43	10.19	−0.13	0.14
Ser147	−0.24	−0.30	0.83	−0.001	0.30
Thr148	−2.97	−0.18	2.24	−0.48	−1.39
Asn149	−3.74	−1.38	3.41	−0.45	−2.17
Pro150	−4.21	−8.75	8.53	−0.62	−5.06
Phe151	−8.49	−2.60	3.36	−1.36	−9.09
Thr152	−0.84	−0.55	1.03	−0.06	−0.43
Ala153	−0.47	−5.04	4.69	−0.05	−0.87
Lys154	−0.86	−20.95	21.25	−0.28	−0.84

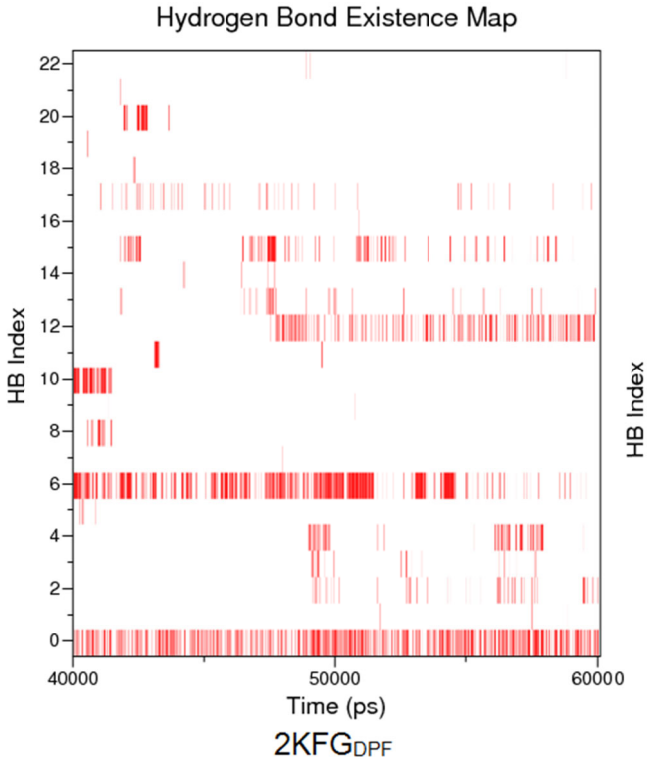
Peptide Residue	2KFG$_{DPF}$				
	ΔE_{van} (kcal/mol)	ΔE_{ele} (kcal/mol)	ΔG_{polar} (kcal/mol)	$\Delta G_{nonpolar}$ (kcal/mol)	$\Delta G_{binding}$ (kcal/mol)
Phe143	−0.60	−13.91	14.96	−0.15	0.30
Asn144	−0.09	−0.18	0.38	−0.008	0.11
Tyr145	−0.70	−0.65	1.08	−0.14	−0.41
Glu146	−0.21	−3.60	4.37	−0.02	0.54
Ser147	−0.50	1.83	−1.66	−0.08	−0.42
Thr148	−2.73	−0.37	2.67	−0.53	−0.96
Asp149	−3.72	−13.01	15.02	−0.34	−2.05
Pro150	−4.12	−8.42	8.20	−0.64	−4.98
Phe151	−8.56	−3.60	3.91	−1.37	−9.62
Thr152	−1.25	−0.60	1.18	−0.15	−0.82
Ala153	−0.28	−2.86	2.95	−0.04	−0.23
Lys154	−0.20	−8.40	9.07	−0.04	0.42

Peptide Residue	2KFH$_{GPF}$				
	ΔE_{van} (kcal/mol)	ΔE_{ele} (kcal/mol)	ΔG_{polar} (kcal/mol)	$\Delta G_{nonpolar}$ (kcal/mol)	$\Delta G_{binding}$ (kcal/mol)
Phe143	−0.27	4.88	−4.13	−0.05	0.42
Asn144	−0.09	−0.38	0.59	−0.006	0.12
Tyr145	−0.92	0.96	−0.48	−0.17	−0.61
Glu146	−0.19	−6.83	7.27	−0.02	0.22
Ser147	−0.13	−0.65	1.04	−0.004	0.26
Thr148	−0.19	−0.61	1.05	−0.01	0.23
Gly149	−0.35	−1.95	2.74	−0.03	0.41
Pro150	−3.30	−7.43	7.36	−0.69	−4.06
Phe151	−8.42	−1.63	2.57	−1.26	−8.73
Thr152	−2.76	−2.97	4.79	−0.43	−1.37
Ala153	−1.38	1.06	−0.49	−0.24	−1.05
Lys154	−0.61	−13.56	14.51	−0.22	0.12

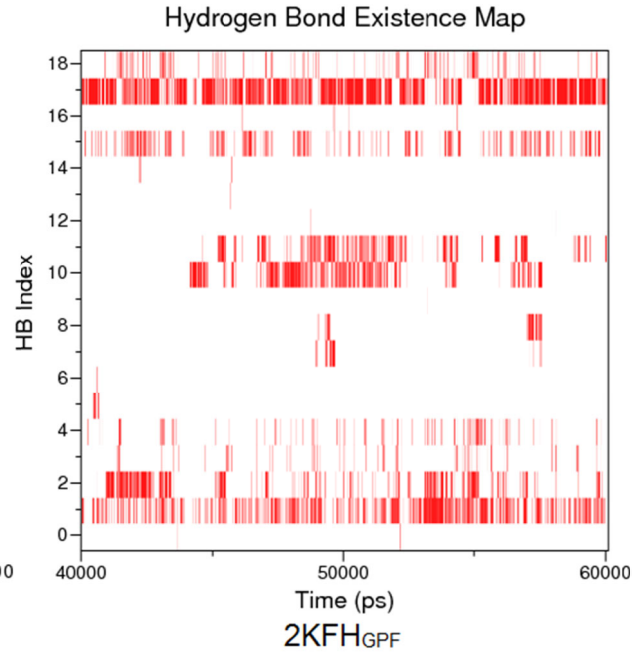
kcal/mol is the unit of energy adopted in AMBER (1 kcal=4.184 kJ)



2KFF$_{NPF}$



2KFG$_{DPF}$



2KFH$_{GPF}$

	$2KFF_{NPF}$		$2KFG_{DPF}$		$2KFH_{GPF}$	
HB Index	Protein residue	Peptide residue	Protein residue	Peptide residue	Protein residue	Peptide residue
25	Gly87	Asn149				
24	Lys97	Thr148				
23	Lys97	Tyr145				
22	Asn83	Lys154	Gly99	Thr148		
21	Asp98	Phe143	Asp98	Tyr145		
20	Trp90	Thr148	Lys97	Tyr145		
19	Trp90	Thr148	Lys91	Asn144		
18	Lys91	Glu146	Asp98	Phe143	Asn83	Thr152
17	Lys91	Glu146	Trp90	Thr148	Asn83	Thr152
16	Lys91	Glu146	Lys91	Thr152	Asn83	Thr152
15	Asn83	Lys154	Lys91	Asp149	Asn83	Thr152
14	Asn83	Lys154	Lys91	Thr148	Lys88	Lys154
13	Asn83	Ala153	Lys91	Thr148	Lys88	Lys154
12	Asn83	Thr152	Lys91	Ser147	Lys88	Tyr145
11	Asn83	Phe151	Lys91	Glu146	Lys91	Lys154
10	Lys97	Thr148	Lys91	Tyr145	Lys91	Lys154
9	Lys97	Glu146	Lys91	Tyr145	Lys91	Thr148
8	Lys97	Glu146	Lys91	Asn144	Lys91	Glu146
7	Lys97	Glu146	Asn83	Ala153	Lys91	Glu146
6	Lys97	Tyr145	Asn83	Phe151	Lys91	Asn144
5	Lys97	Tyr145	Lys97	Tyr145	Lys91	Asn144
4	Asp98	Thr148	Lys73	Lys154	Asn83	Thr152
3	Lys73	Lys154	Lys73	Lys154	Asn83	Thr152
2	Lys73	Lys154	Lys73	Ala153	Asn83	Pro150
1	Lys73	Ala153	Lys73	Phe151	Lys73	Pro150
0	Lys73	Pro150	Lys73	Pro150	Lys73	Gly149

Fig. S1 Hydrogen bond interaction network at the interaction interface

Red, hydrogen bond is present; white, hydrogen bond is not present. Every HB Index represents a specific hydrogen bond that clearly shows in the table below. Table below shows the residue pairs forming the hydrogen bond corresponding to the HB Index marked in the three figures above

Formula S1 Calculation of ΔG by FoldX

$$\Delta G = W_1\Delta G_{\mathrm{van}} + W_2\Delta G_{\mathrm{solvH}} + W_3\Delta G_{\mathrm{solvP}} + \Delta G_{\mathrm{wb}} + \Delta G_{\mathrm{hbond}} +$$

$$\Delta G_{\mathrm{ele}} + \Delta G_{K\mathrm{on}} + W_4 T\Delta S_{\mathrm{mc}} + W_5 T\Delta S_{\mathrm{sc}},$$

where ΔG_{van} is van der Waals interaction energy; $\Delta G_{\mathrm{solvH}}$ and $\Delta G_{\mathrm{solvP}}$ are the solvation free energy for nonpolar and polar residues, respectively; ΔG_{wb} is the extra stabilizing free energy provided by water bridges; $\Delta G_{\mathrm{hbond}}$ is the contribution of hydrogen bond and ΔG_{ele} is the electrostatic interaction energy; $\Delta G_{K\mathrm{on}}$ reflects the effect of electrostatic interactions on the association constant K_{on}; ΔS_{mc} and ΔS_{sc} are the entropy cost of the main chain and the side chain, respectively. The terms W_1–W_5 correspond to the weighting factors, and they all equal to 1 except for W_1 which is 0.33.