Table S1 – Actin-profilin binding free energies computed from molecular dynamics simulations for the wild-type and mutant systems.

		Binding Free Energy		Binding Free Energy
Pb Pfn	GB	-46±13	*Pb* Pfn	-46±13 (n. d.)
	PB	-48±19		-48±19 (n. d.)
Pf Pfn	GB	-35±10	*Pf* Pfn	-35±10 (-62±9)
	PB	-35±13		-35±13 (-64±11)
Pb Pfn$^{Pf\text{loop}}$	GB	-15±11	*Pf* Pfn AAA	-17±7 (-34±11)
	PB	44±35		-26±10 (-46±8)
Pf Pfn$^{Pb\text{loop}}$	GB	-61±10	*Pf* Pfn QNQ	-54±14 (-44±13)
	PB	-61±14		-69±14 (-51±11)
Pf Pfn$^{Tg\text{loop}}$	GB	-56±14		
	PB	-51±22		

Average binding free energies (kcal/mol) and their standard deviations were calculated from the last 200 ns of the 500 ns long simulation using the MM-GBSA (GB) and MM-PBSA (PB) methods. Note that the (energetically unfavorable) translational, rotational and vibrational entropic contributions to binding were not computed. The values for the wild-type profilins are given followed by values for (left) acidic loop mutants and (right) arm motif mutants. The values obtained from the last 50 ns of the 150 ns long simulations previously reported in (Moreau et al., 2017) are given in brackets for comparison. Blue numbers denote values smaller in magnitude than those for the *P. berghei* wild type profiling, indicating weaker binding. Red numbers denote the weakest binding affinities.

Table S2

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Table S3

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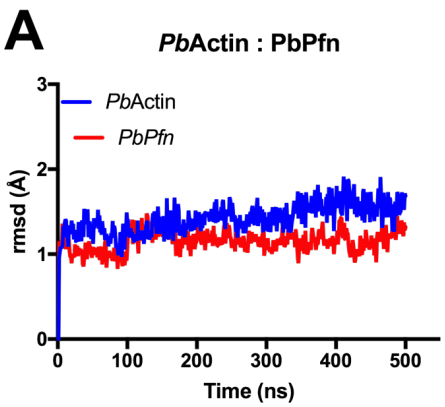
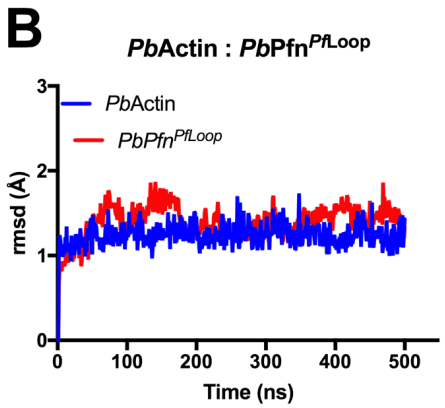
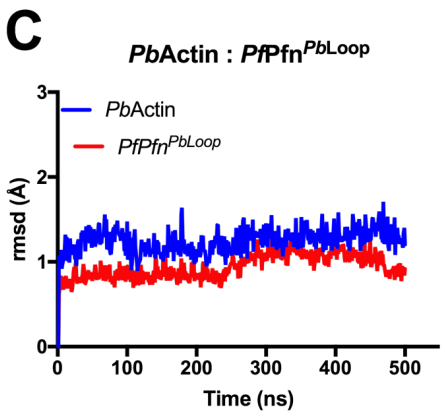
Table S4: Primers used in this study

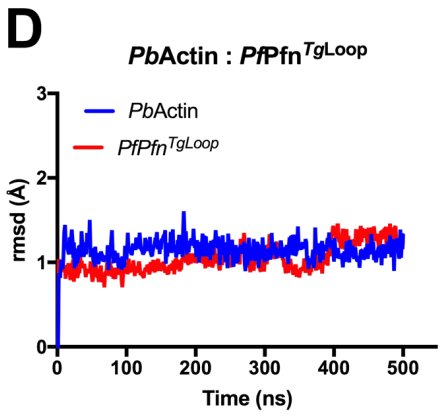
Primer	Sequence	Restriction site	Binding site
1 fw	GGTGCACACTCATTTGAATGTG	-	*Pb* Pfn 5' UTR, upstream of homologous recombination site
1a rv	GCtctagaTTATGCGGCACCTGTATCAG	XbaI	*Pb* Pfn end of CDS
1b rv	GCtctagaTTACTGTGAGCTTTCTGCCAG	XbaI	*Pf* Pfn end of CDS
2 fw	CTAGACAGCCATCTCCATCTGG	-	*Tg* DHFR end of CDS
2 rv	CAAGTTCTTTCCTCATGTGTTCATG	-	*Pb* Pfn 3'UTR, downstream of homologous recombination site
3 fw	ATTTgcggccgcATGGAAGAATATTCATGGG	NotI	*Pb* Pfn start of CDS
3 rv	GCtctagaTTATGCGGCACCTGTATCAG	XbaI	*Pb* Pfn end of CDS
4 fw	ATTTgcggccgcAAAATGGCAGAGGAGTATTCTTGG	NotI	*Pf* Pfn start of CDS
4 rv	GCtctagaTTACTGTGAGCTTTCTGCCAG	XbaI	*Pf* Pfn end of CDS
5 fw	TCCccgcggGAGATATTACACATTGCTAC	SacII	*Pb* Pfn 5' UTR
5 rv	TAAAgcggccgcCTTTATTATCTTAAAAATTATTTATATAATATGATG	NotI	*Pb* Pfn 5' UTR
6 fw	CCatcgatAATAAAGAAAATATTATAAAAATGTG	ClaI	*Pb* Pfn 3' UTR
6 rv	GGggtaccCACACATTGGCATTATATAGAAATTGAG	KpnI	*Pb* Pfn 3' UTR
7a	CAAAATTTGGGTCACTCTCTTCACCCTG TGCTACGCATTCATATAC	-	*Pb* Pfn with *Pf* loop A rv
7b	CACAGGGTGAAGAGAGTGACCCA AATTTTGATAAATGGTCTCTTTTTTATAAAGAAGA	-	*Pb* Pfn with *Pf* loop B fw
8a	TCAAAGTCTGGATTATTTTCATCGGGGGTAGCTACACAAGCATAGA	-	*Pf* Pfn with *Pb* loop A rv
8b	AGCTACCCCCGATGAAAATAATCCAGAC TTTGATAAATGGTCACTTTTTTATAAAGAAGATT	-	*Pf* Pfn with *Pb* loop B fw
9a	CAGCTTGGACCATCCGTCATCATCATCAGCCGCCGCGGCGAA GACAACTCCATCTTCTTCCGAAGCTAATC	-	*Pf* Pfn with *Tg* loop A rv
9b	TTCGCCGCGGCGGCTGATGATGATGACGGA TGGTCCAAGCTGTATAAAGAAGATTATGATAAGTTGAAGATGAAAATGGTAC	-	*Pf* Pfn with *Tg* loop B fw

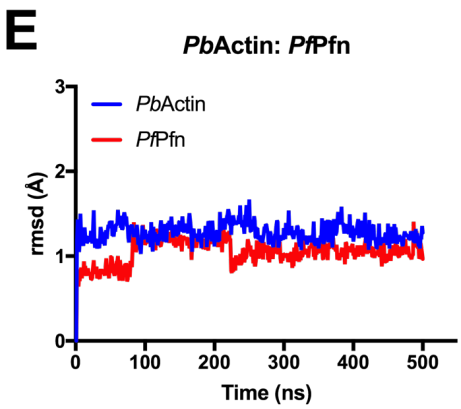
restriction sites in lower case, start codons indicated in **green**, stop codons indicated in **red**,
Pf Pfn loop in **blue**, *Pb* Pfn loop in **orange** and *Tg* Pfn loop in **purple**

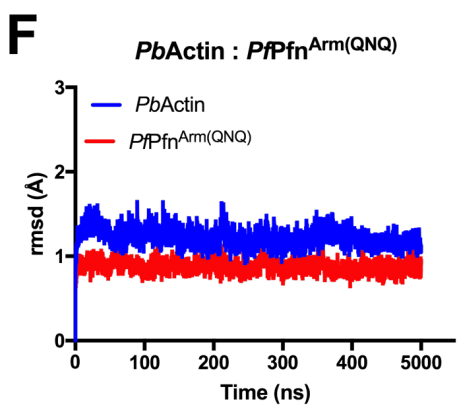












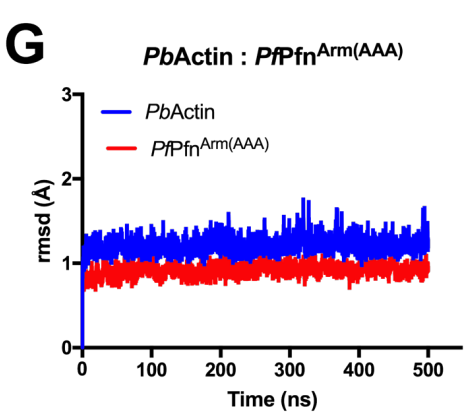


Figure S1: RMSDs of the backbone atoms of the different systems, showing that the individual protein structures are stable during the MD simulations. Plots of RMSD for each protein in the complex of *Pb* Actin with (A) *Pb* Pfn, (B) *Pb* Pfn $^{Pf\text{Loop}}$, (C) *Pf* Pfn $^{Pb\text{Loop}}$, (D) *Pf* Pfn $^{Tg\text{Loop}}$, (E) *Pf* Pfn, (F) *Pf*Pfn$^{\text{Arm(QNQ)}}$ and (G) *Pf*Pfn$^{\text{Arm(AAA)}}$ for 500 ns of simulation. Each trajectory is aligned to its respective first frame. The flexible regions, *i.e.* the D2 loop region in actin and the terminal and arm regions in profilin (M1-L10, E42-F84, T169-A174), were excluded while calculating RMSD values.

Pb Actin-*Pb* Pfn (Time interval in ns)

# Res.	200-220	220-240	240-260	260-280	280-300	300-320	320-340	340-360	360-380	380-400	400-420	420-440	440-460	460-480	480-500
Y4	177	186	164	498	160	319	576	460	330	238	485	259	132	326	197
S5	65.9	52.2	40.4	136	52.5	95.9	207	158	121	63.5	149	96.1	39.4	89	62.6
W6	33.1	20.2	28.2	46	19.7	29.7	41	37.9	20.2	21.2	43.6	29.6	26.3	25.5	22
E7	27.6	18.6	22.2	39.4	15	21.4	31.5	35.8	22	19.3	26.8	27.9	26.7	23.6	20.4
N8	24.5	18.9	29.2	40	15.2	26.9	35.8	34.8	27	22.3	36.1	39.5	28	30.4	25.5
F9	22.4	15.1	26.9	32.2	16.8	24.6	33.1	28.3	20.4	22.8	28.3	29.6	20.3	25.6	19.8
L10	19.2	12	14.8	21.4	12.5	18.8	23	24.6	13.5	14.3	18.2	16.4	14.8	19.1	11.1
N11	21.7	14.2	20	29	18.2	22	24.4	26.1	20	20	23.1	26.2	18.6	27.7	18.5
D12	30.5	19	24.4	33	23.8	31.8	32	28.1	24.9	25.3	27.6	37.2	25.8	31	22.5
K13	29.9	16.9	19.9	24	21	24.7	26.2	26.7	19.9	21.6	21.1	28.1	18.8	27.1	19.8
L14	23.3	12.9	13.4	17.9	11.1	15.6	21.6	14.5	12.5	16.2	13.1	17.8	13.4	17.5	13
L15	23	13.6	16.5	17.9	11.9	16.9	18.2	17.2	14.6	17.2	16.8	18.6	18.6	19.8	15
A16	42.6	20.7	21.1	24.4	19.5	31.7	31.4	25.2	21.7	31.6	26	24.3	25.6	32	22.3
T17	46.7	16.6	22.7	22.5	15.7	27.5	29.8	24.1	19.3	30.8	26	24.8	28.7	24	23
N18	42.8	17.4	24.8	23.9	17.1	33.7	37	20.5	18.1	25.1	25.6	31.6	20.8	22.2	21.3
Q19	33.7	13.2	13.9	16.8	14.6	20.2	20.1	17	11.1	15.7	17.8	26.2	15.8	16.8	17.8
V20	17.1	8.2	9.54	11.2	10.9	13.1	11.3	11.2	7.97	11.9	11	15.4	12.5	12.8	11.2
S21	17.8	8.56	10.8	15.1	11	14	10.8	10.2	9.85	15.6	15	21.1	13.2	14.9	11.6
A22	13.4	8.01	9.54	12.7	9.24	9.79	9.49	7.62	7.27	9.44	12	14.6	10.7	11.1	8.74
A23	8.92	7.58	9.03	11.1	6.84	8.97	11.1	7.19	5.77	8.93	10.7	10.1	7.13	6.92	7.83
G24	10.2	10.1	9.81	12.7	10.7	11	13	9.83	8.3	9.61	12.2	9.99	10.8	9.43	10.2
L25	8.39	8.14	10.3	14.6	7.44	8.49	14.1	11	8.36	8.72	14.4	10.3	10.1	8.34	10.8
A26	13.9	10.6	18.8	16.5	8.48	11	14.3	15.1	9.98	13.8	19.8	18.1	14	12.3	14
S27	34.7	17.6	45	24.6	15	20.7	21.1	32.4	16.8	25.4	32.8	40.9	32.5	25.5	28.7
E28	48.1	20.1	29.6	34.6	17.2	31.6	24.7	40.1	17.9	38.9	39.3	67.6	31.5	31.2	30.2
E29	57.6	22.5	31.7	45.1	27.9	42.5	29.5	51.4	22.7	46.7	44.2	94	35.8	48.5	24.5
D30	35.2	14.5	28	33	29.3	29.9	21	39.3	18.7	26.1	39.3	65.1	23	33.2	20
G31	18.3	9.51	16.1	19.2	19.9	13.4	14.8	18.2	11.9	18.2	31.5	33.8	14.1	18.2	11.6
V32	16.8	11.5	15.5	18.8	18.6	17.2	12.8	25.9	15	17.9	33.3	27.4	15.9	15.4	18.2
V33	15.1	8.07	13.8	16.5	11.6	13.6	11.7	14.5	8.47	8.89	19.6	18.4	12.2	10.2	15.2
Y34	21.2	10.7	18.8	28.9	16.8	20.1	15.8	20.1	16.9	11.7	26.7	26	16	12.3	19.3
E35	13.2	10.2	14.3	26.8	15.1	16.8	19.5	17.2	11.5	12.9	24	17.5	13.5	11.6	16.1
C36	10.9	10	11.5	19.2	12.8	12.7	16.3	13.2	9.11	12.9	18.3	16.6	11.3	10.8	12.9
V37	15.8	12.3	14.2	19.7	13.5	14.2	17.3	16.4	12.8	14.9	21.1	22.9	13.7	14.1	14.4
A38	23.4	13.1	14	21.4	14	15.9	20.7	15.8	12.2	13.3	19.1	23.8	18.3	20.2	16.1
T39	47.1	16.1	17.6	28.3	24	27.7	35.6	26	23.1	23.4	27.5	30.5	39.5	40.1	22.5
P40	53	25.2	29.6	38.9	58.7	77.3	67.5	149	77.4	58.4	62.2	95.7	249	102	36.5
D41	70.6	59.3	57.5	66.6	183	125	127	180	101	72.7	62.2	119	313	163	49.3
E42	115	102	89	101	240	160	212	189	150	108	69.2	180	252	223	43.1
N43	80.4	101	98	99.7	213	175	182	173	200	192	242	246	279	485	55.6
N44	140	174	109	88.4	144	135	276	182	177	253	189	168	245	364	155
P45	122	92.8	107	100	153	206	302	246	230	360	201	218	273	292	317
D46	81.5	127	95.3	102	82.6	140	283	204	159	322	125	223	291	254	349
F47	56.1	41.4	52.3	62.4	46.5	42	70	84.6	85.8	109	70.7	104	108	84.5	117
D48	33.3	20	26.4	47.2	28.2	35.5	35.6	40.8	45.5	45.6	36.1	70.8	33.3	37.4	33.8
K49	23.5	15.8	17.9	35.9	19.4	25.2	25.9	24.7	21.5	22.5	26.8	57.9	17.3	17.4	33.9
W50	22.3	14.8	16	32.9	19.7	17	20.6	21.5	18.8	19.7	23.3	40.1	15.1	11.2	23.9
S51	27.5	16.8	21.6	39.2	26.2	18.1	21.7	22.4	22.4	22.1	18.5	46.2	18.2	17.4	30.7
L52	17.4	10.8	14.3	19.5	15.7	12.3	15.6	12.5	14	14.3	13.4	31.2	13.1	13.4	21.4
F53	13.9	9.78	9.03	16.4	12	7.85	9.28	7.42	10.7	12.5	11.7	19.5	8.54	9.08	13
Y54	23.4	13.4	12.6	26.5	21.1	14.3	10.4	9.8	17.2	17.5	18.2	25.9	12.1	11.5	17.3
K55	36	25.1	18.4	35.4	26.9	25	19.9	14.6	28.3	17	29.8	42.9	19	17.3	25
E56	71.1	44.8	38.7	72.9	44.5	40.8	21.1	18	32	32.2	55.8	67	30.2	28	35.3
D57	63.1	50.7	46.3	92.5	36.6	38.2	18	15.7	31.7	32.9	60.4	61.8	23.8	25.4	35
Y58	53.5	35.1	32.1	50.3	26	31.8	17.8	22.7	48.3	60.8	86.3	89.2	31.6	32	57.9
D59	47.8	40.6	33.2	44.1	29.6	29.6	24.9	15.2	40.8	71.9	136	90.1	43.9	33.8	66.1
I60	30.5	41.9	29.7	58.2	28.5	43.3	21.6	19	43.5	188	207	76.2	43.3	27.5	77.8
E61	32.9	42.1	36.5	71.7	40.4	40.2	24.3	21.1	48.2	364	371	86.8	79.5	32.6	97.7
I62	20.7	31.8	31.7	69.3	49.1	26.5	16.3	24.1	41.2	383	426	56.8	102	31.3	82.7
E63	19.4	28.9	24.5	49.2	39	23.8	18.3	23.2	53.7	581	736	77.8	265	40.1	115
D64	13.3	22.2	15.3	35.9	26.5	15.7	14.8	20.5	65.7	637	741	184	401	78.9	82.7
E65	13.9	19.6	12.4	33.8	22.8	11.3	10.9	16.5	86.2	845	1128	324	809	212	182
N66	19.9	31.3	15.4	44.9	29.8	23.4	20.7	22.5	123	1117	1387	362	665	181	167
G67	27.5	44.5	27.6	42.1	45.6	35.8	26.3	32.9	113	1162	1493	239	591	199	215
S68	37.8	54.3	41.1	58.9	62.5	57.7	35.9	41.9	105	959	1155	263	320	109	177
K69	37.5	55	40.2	68.7	62.3	54.4	30.5	37.9	74.7	738	853	213	205	69	165
T70	42.9	59.4	44.9	62.6	54	57.7	34.4	30.1	63.6	540	542	162	129	58.1	116
T71	45.6	55.1	52.2	55	38.7	42.3	27.8	16.5	52.8	329	298	98.5	83.7	42.4	98.5
K72	42.4	45.8	45.3	52.6	42	32.3	22.8	22.4	46.4	138	130	79.8	69	39.3	65.7
T73	45.7	37.8	38	48	34.9	39.8	27.4	19.6	42.8	42.4	81.2	63.7	50.4	44	46.9
I74	28.6	19.2	15.7	39	23.2	38.7	20	20.6	36.5	24.6	55.6	49.2	24.4	28	19.9
T75	26	14.8	13.8	33	29.6	27.5	17.4	14.4	23.8	18.6	41.2	37.9	14.5	21	15.2
E76	12.9	7.89	8.03	16.5	14.7	15.5	9.83	10.5	13.6	13.7	30.9	23.9	10.4	13.4	10.8
G77	13.1	11.9	9.91	19.6	16.4	16.9	21	11.7	13.3	16.2	37.4	33.1	15.7	18.3	12.9
Q78	18.5	12.3	11.8	23.4	18.2	21.1	28.3	16.5	13.5	21.8	44.5	37.1	16.6	21.1	13.9
S79	13.9	9.82	8.83	14.1	15	12.7	17.2	10.3	13.9	13.9	36.8	21.4	14.4	17.2	11.7
I80	11.3	9.79	7.2	14.2	11.9	9.89	18	9.77	10.9	11.2	33.9	18.1	17	13.9	9.15
L81	18.5	11.7	11.1	19.3	15.2	19.5	23.3	18	9.91	18	43.4	30.5	18	19	15.6
T82	20.5	14.7	14.1	21.2	22.6	22.7	26.9	22.7	15.9	23.1	38.2	35.4	16.9	21.7	16.5
M83	15.5	12.1	12.4	17	14.5	16.3	22.6	16.6	9.86	15.3	30.9	23.7	20.9	20.7	16
F84	20.6	16.5	15.1	31.5	18.8	17	35	20.9	18.4	15.6	44.5	38.5	25.5	25.8	23.1
N85	29.8	20	21.9	54.6	29.7	28.8	46.7	39.3	34.2	27.7	60.9	53.9	26.6	33.7	36.5
E86	32.6	24	32.3	43.3	25.6	36.5	40	37.9	25.8	30.1	51.4	45.6	29.6	27.4	41.8
G87	30.5	20.1	31.2	36.5	20.4	29.5	41.4	31.1	16.9	19.2	50.7	49.3	41.2	26	32.4
Y88	21.8	11.2	21.7	24.4	13	28.1	27.3	24.2	10.6	17.4	39	31.8	31.6	15.1	25.1
A89	18	8.86	17.3	22.7	12.5	22	19.7	18.9	12.9	16	41.4	21.2	20.3	27	26.6
S90	29.2	15.8	26.1	25.4	17.8	23.6	28.6	24	19	22.2	66.6	34.5	44.5	28	34.2
D91	18.9	12.1	16.5	17.3	12.4	16.5	18.9	13.8	19.2	19.9	78.5	28.5	53.1	20.4	25.8
G92	14.2	8.23	9.21	12	10.8	15	10.4	10.3	11.7	15.5	39.5	17.8	23.9	14.7	22.4
I93	9.4	5.98	7.02	8.3	8.4	9.29	7.74	9.43	9.82	11.4	22.7	9.82	15.3	10.4	11
W94	9.76	5.97	7.8	9.18	8.87	9.1	8.89	8.85	11.7	10.4	17.8	13.9	13.3	10	9.89
L95	8.27	6.86	7.56	9.73	9.48	9.6	7.61	8.48	12	13.2	14.1	15.3	10.2	9.93	10.2
G96	13.8	11.2	12	16	13.3	11.7	11.9	12.7	19.9	19	16.7	23.9	11.7	11.4	13.9
G97	21.8	12.4	10.8	18.8	15.7	16.8	19.2	23.4	20.8	22.9	29.9	36	21.3	17.4	26.7
T98	23.9	9.51	10.9	15.5	11.5	11.1	15.8	16.1	17.4	12.6	21.8	26.1	21.5	14.5	21.3
K99	12.2	6.7	8.73	10.6	8.25	9.22	11	11.9	11.4	9.93	13	13.7	11.6	10.8	17.1
Y100	10	5.63	7.77	8.52	6.52	10.1	7.79	8.96	7.85	9.57	10.3	12.9	10.7	8.43	12.8
Q101	15.3	6.27	9.34	8.36	7.06	13	7.85	13.4	9.25	13	13	14.7	10.6	11.2	13
F102	15.4	5.31	7.8	8.71	7.98	11.1	9.4	12.4	8.72	13	13.3	14.4	9.21	10.7	13.7
I103	25.3	7.11	10	9.71	8	12.6	12.2	17.4	9.48	15.6	12.8	19	9.99	13.7	19.9
N104	29.8	7.45	11.6	11.1	11.3	13.2	15.2	20.2	10.6	16.6	10.7	21.3	11.5	13.9	22.9
M105	33.4	8.91	11.8	12.1	14	14.4	14.6	20.4	10.8	16.1	9.99	25.5	13.4	11.3	27.8
D106	58.9	11.3	16.7	21.3	26.9	18.7	25.5	26	19.6	23.1	15	37.6	24.3	17.1	52.7
K107	65.8	18.1	25.2	28.9	29.7	22.6	33.5	35.7	26.6	27.8	13.6	53.1	28.6	16.9	54.7
G108	75.7	23.5	31.3	32.5	27.3	25.6	41.2	40.3	32.1	26.2	20.8	67.7	33	21.3	53.9
L109	62.3	20.2	25	34.3	25.5	20.5	39.6	34.7	30.4	25.3	17.1	56.5	26.7	21	45.3
E110	55.8	21.2	32.3	49.2	31.8	30.9	33.3	47.7	29.5	22.6	19.5	60.3	33.8	23.4	51.8
Y111	45.1	16.5	33.4	42.9	25.7	22	24.3	30.9	26.8	17.8	15.6	49.7	26.6	21	41.7
E112	54.4	25.3	44.7	71.4	37.5	25.6	22.9	38.4	39.8	27.6	24.3	53	35.9	34.2	57.2
G113	58.9	36.3	51	69.5	46.8	47.6	36.2	61.5	51.5	45.1	35.6	58.8	42.7	41	68.3
H114	48.4	20.1	35.7	42.2	36.8	30.1	26.1	52	26.3	29.7	24.2	49.7	29.6	21.6	49.4
S115	49	22.8	28.9	34	32.4	23.8	24.7	48.5	23	26	18.1	46.3	24	20.6	41.6
F116	38.2	14.1	19.7	23.9	18.6	15.5	21.1	27.3	18.8	19.3	13.6	38.9	17.4	10.4	32.2
D117	37.3	12.3	17.6	17.2	17.9	15.7	21.1	23.6	16.2	18.3	11.4	33.9	15.7	10.7	30.8
V118	28	7.78	10.1	10.2	12.2	9.64	12.4	16	9.61	12.4	9.58	19.7	10.5	9.05	18.8
A119	14.9	7.02	7.42	7.63	8.38	8.35	10	12.8	6.1	10.5	6.85	13.1	8.12	8.28	11.9
T120	14.5	4.85	5.15	5.23	6.26	7.11	6.48	9.94	5.73	7.86	4.98	12	5.11	8.93	11.4
C121	13.3	4.01	6.37	6.48	6.06	5.73	5.07	8.49	5.94	8.24	5.2	11.1	6.05	9.38	11.9
A122	15.6	6.18	7.7	7.68	6.4	9.93	6.19	9.69	6.18	9.9	7.82	14.5	7.72	9.35	11.5
K123	18.4	10.6	12.6	11.7	9.99	13.2	9.62	12.2	10.1	13.3	8.65	17.1	9.55	12.1	16.5
S124	26.2	16.7	14.3	21.9	15.4	19	12.5	19.8	13.1	18	12.8	19.6	12.9	12.2	19.9
K125	26.1	21.1	17.4	28.3	23.9	16.4	15.1	23.8	14.3	27.7	24.4	23.8	15.9	13.6	26.1
G126	25.8	19.2	13.1	14.6	10.1	13	14.6	14.3	9.08	15.9	12.8	24.3	11.9	9.62	17.7
G127	12.1	9.7	7.29	7.43	7.33	9.26	6.21	9.44	5.84	9.29	9.2	15.5	10.7	9.64	9.92
M128	10.4	5.43	5.78	6.52	6.94	6.33	6.21	7.08	7.1	5.78	7.73	10.9	7.27	8.03	6.49
H129	9.76	4.49	4.84	4.64	4.75	6.11	6.49	6.07	8.24	6.12	3.97	7.72	6.02	6.72	6.66
I130	8.43	6.05	4.59	5.31	4.75	5.19	6.82	7.29	7.4	7.23	6.33	7.77	6.29	5.36	7.21
I131	14.9	8.37	8.41	9.11	7.21	8.89	9.04	12.4	7.83	9.92	6.53	14.3	7.48	6.71	10.3
K132	28.6	14.8	17.6	13.5	14.8	14.1	15.9	19.9	14.6	21	10.2	24.8	12.8	8.23	21.4
V133	46.5	22.9	24.3	32.7	17.2	21.9	19	25.8	20.9	23.9	24.6	34.1	15.2	19	24.1
G134	83.2	46.5	47.7	47.5	26.1	34.2	48.8	58.6	79.3	44.5	51.7	55.7	28	32.6	56
G135	86.6	88.5	97.9	104	60.8	51.5	71.5	127	83.1	65.4	81.2	91.2	69.3	57.9	75.7
G136	68	58.3	41.5	67.3	96.8	47	46.7	72.1	57.8	48.3	83.9	77	56.1	64	64.2
H137	35.9	24.4	24.1	38.7	39.8	23.6	22.4	36.2	28.9	25.6	28.4	31.9	24	20	32.7
I138	13.4	9.18	12.7	15.4	12	12.1	13.9	12.9	10.9	9.44	13	15.1	9.86	9.15	12.2
L139	8.17	7.36	9.25	13.1	8.57	7.32	9.83	7.89	6.64	7.47	11.1	8.47	8.28	6.82	7.46
I140	6.34	6.99	5.8	7.12	5.53	5.56	7.42	6.07	6.84	7.04	7.67	6.32	7.24	6.1	5.81
V141	9.64	6.29	5.23	5.76	5.42	6.34	6.54	6.32	9.14	7.41	6.64	6.36	7.36	6.89	6.49
L142	11.1	6.16	6.15	6.75	5.81	7.76	5.88	4.84	7.34	8.21	8.04	10.1	9.67	8.48	7.05
Y143	18.4	11.3	10.5	10.2	7.89	10.6	7.28	7.4	7.94	13.4	10.5	13.9	10.3	10.8	11.3
D144	23.2	14.6	14.2	17	10.5	13.8	10.4	11.1	9.13	19	18.9	20.7	12.3	10.5	16.2
E145	48.6	19.9	19.6	31.1	21.6	31.1	21.4	22.2	14.9	24.9	24.1	32.1	18.1	16.3	22.8
E146	55.4	29.6	24.5	43.2	33	50.9	41.9	32.9	22.1	32.3	34.1	61.1	39.2	23.8	30.9
K147	44.4	22.7	21.1	31.7	25.9	42.3	42	31.2	16.1	28	32.8	55.8	32.9	24.2	32.2
E148	45	20.5	21.2	38.2	27.9	42.4	38.8	34.5	16.5	25.1	31	46.4	29.1	22	37.4
Q149	35.1	12	11.7	20.6	17.4	16.5	15	16.4	9.94	14.6	19.4	28.2	13.6	14.6	24.5
D150	42	12.8	11.2	22.6	18.6	14.1	12.9	16.7	21.7	14.2	25.2	23	14.6	22.8	23.4
R151	22.6	8.43	7.45	11.3	11.6	8.45	9.86	14.7	10.5	10.2	10.1	14.3	10.6	15	11.9
G152	27.6	9.62	12	14.9	16.5	11.3	13.1	12.5	9.98	10.6	14.9	21.4	13.7	14.9	19.2
N153	35.4	10.8	13	13	12.7	10.5	16.6	10.5	9.53	11.1	13.9	29.6	15	15.3	20.9
S154	23.8	7.83	8.71	8.34	11.8	7.87	14	9.86	7.07	6.9	9.06	16.2	9.86	9.83	12.9
K155	20.3	9.27	9.1	9.74	12.7	6.68	14	11.8	8.45	6.71	9.29	16	9.52	9.19	11.7
N156	26.9	9.77	11.5	13	12.5	9.24	12.7	11.6	10.3	7.84	10.4	25.1	9.7	13.3	14.8
A157	21	9	12.7	11	11	11.8	15.5	12.7	9.28	9.47	12.2	20.9	8.61	12.6	12
A158	13.7	9.84	10	8.58	7.92	9.65	12.4	13.2	8.88	9.85	10	15.5	9.4	9.29	9.93
L159	20.4	10.3	9.96	14.6	10.7	9.25	12.8	16.9	12.7	10.8	8.97	18.8	9.09	9.52	11.9
A160	20.7	13.2	13.8	19.9	12.5	14.7	16	17	14.2	12.4	12.1	23.3	13.3	16.4	15.1
F161	17.2	14.8	13.5	16	11.2	16.4	15.4	16.6	14	13.7	10.7	16.9	12.5	13.7	13.3
S162	17.6	13.8	12	16	14.4	16.2	16.3	22	15.2	16.5	11.9	16.8	12.5	10.9	15.2
K163	28.1	19.4	17.4	21.6	20.6	20.3	19.2	30.6	19.8	23.8	18.7	31.3	21.8	17.1	22.8
E164	31.8	28.2	22.9	27.7	24.6	23.6	22.5	30.5	23.2	32	21.6	31	24.5	22.2	24.2
L165	27.5	29.3	18.2	21.9	29.1	24.9	24.9	39.2	27.1	28.9	25.6	28.6	21.8	22.9	26.4
I166	39.7	47.1	22.4	27.1	42	26.1	30.9	57.8	38.9	45.4	45	47.1	38.3	29.4	38.2
E167	67.5	68	39.4	72.9	66.3	32.8	40.6	72.4	60.6	64	58.4	52.5	68.1	40.5	65.4
S168	93.4	68.1	51.9	103	114	38.6	54.4	96.7	70.2	60.4	73.4	78.7	72.2	51.2	77.9
T169	146	154	42.4	138	161	71.1	76.1	133	79.9	105	157	129	86.5	62.3	88.8
D170	306	297	105	395	373	90.8	121	202	191	244	372	235	190	90.6	196
T171	644	555	230	759	605	211	272	397	391	526	670	375	309	209	474
G172	1284	901	318	1401	1143	367	470	439	633	1108	906	671	884	642	1175
A173	2425	1657	661	2343	1778	657	970	1075	1284	1529	1119	856	1675	1246	2059

Pb Actin-*Pb* Pfn$^{Pf\ Loop}$ (Time interval in ns)

Acidic loop (rows Q39–N46)

# Res.	200-220	220-240	240-260	260-280	280-300	300-320	320-340	340-360	360-380	380-400	400-420	420-440	440-460	460-480	480-500
Y4	141	172	318	334	382	121	76.1	46.8	26.4	32	37.4	41.4	49.3	51.1	47.2
S5	42.3	42.9	107	104	54.7	133	35.7	21.7	15.7	25.2	26.2	28	32.3	30.5	36.1
W6	25.3	27.4	24.9	29	19.6	30.8	23.8	15.8	13	11.4	14.5	13.8	15.5	13.2	17.6
E7	19.6	24.3	22.7	23.6	18.6	25	23.2	16.2	13.2	11	14.4	14.3	13.6	15.6	17.3
N8	17.8	23	17.8	20.8	21.7	22.6	24.1	20	18.3	13.5	20.3	16	15.2	15.8	26
F9	17.2	21.1	16.9	17.8	22.1	24.2	20.8	15.8	15.3	11.9	19	12.8	14.4	12.2	23.8
L10	11.4	16.3	9.33	12.8	15.1	12.4	11.4	9.32	10.3	7.58	11	8.39	9.04	9.73	12.3
N11	15.1	18.9	12.2	15.6	18.3	16.4	13.7	10.8	12.2	9.92	15.5	12.3	12.6	13.1	20.8
D12	20.6	23.8	18.5	17.9	24.5	16.7	17.2	13.1	14.3	14.9	22.3	17.6	13.9	15	26.7
K13	19.6	18.9	14.5	16.4	18.6	19.3	12.7	11.4	10.4	12.7	20.2	13.7	12.2	13.3	21.1
L14	9.02	13.6	8.43	11.1	13.6	9.29	10.7	7.7	5.03	9.15	10.3	9.66	7.14	9.37	13.5
L15	9.03	15.3	11.3	12.8	13.4	12.7	11.6	7.88	7.12	8.42	10.8	10.5	8.49	8.72	14
A16	16.3	26.2	16.9	15.5	19.8	19.3	24.1	13.4	13	12.9	17.6	19.5	12.1	15.2	22
T17	15.1	21.4	11.2	17.2	19.2	18.3	19.7	11.8	11.4	11	18.9	18.2	12.5	15.5	21.3
N18	15.1	21.3	16.7	20	21.5	24.6	18.9	11.4	17.7	14.8	21.7	14.9	16.5	20.3	20.7
Q19	9.71	14.1	11.8	10.4	11.4	13.9	13.3	6.69	8.79	6.93	14.1	9.05	9.62	12.8	11.9
V20	6.45	9.17	6.97	8.53	8.76	12.3	5.72	4.22	4.27	6.03	7.73	6.48	5.59	6.96	7.14
S21	8.31	11.4	7.5	10.1	9.46	12	8.15	4.63	5.81	8.66	8.61	9.38	3.73	6.78	6.34
A22	7.12	9.83	7.01	7.68	8.12	9.32	7.05	4.96	4.07	5.7	7.24	4.99	4.17	5.41	5.8
A23	6.37	10.5	5.98	6.63	8.13	7.34	6.4	5.35	4.44	5.33	6.61	4.25	4.38	5.15	4.17
G24	11.9	13	7.28	7.99	9.21	10.6	9.57	9.42	4.81	10.3	9.59	3.91	5.8	5.11	6.13
L25	11	14.3	6.24	8.33	7.39	6.66	9.46	7.38	4.03	8.76	8.6	6.28	5.79	6.31	5.81
A26	14.6	19.8	10.8	9.76	8.82	8.27	9.92	11.1	6.9	10.2	11.6	9.62	7.77	9.2	6.53
S27	22.8	28	17.2	15.6	13.6	22.6	13.4	13.8	8.92	10.2	18.6	18.1	21.2	12	18.8
E28	24.7	27.7	18.1	17.9	19.8	30.9	16.1	19.4	12.2	11.8	21.5	23.1	23.3	16	24.4
E29	26.4	43.3	32.5	21	30	33	18.7	23.7	13.9	15	28.5	31.8	23.8	20.3	27.4
D30	20.1	33.4	24.7	16.2	21.6	21.1	14.4	15.3	13.4	12.5	23	18	17.8	19.4	18.9
G31	14.5	24	16	11.1	13.8	12.1	9.83	9.46	9	9.24	17.2	10.9	13.9	13.1	10.7
V32	15.2	25.3	19.2	10.2	16.6	14.7	13.1	11.5	11.4	10.1	17.5	15.6	13.2	14.9	14.1
V33	12.9	19.2	9.78	8.65	12.4	11	10.2	10	8.48	8.69	12.7	11.1	9.76	11.1	6.54
Y34	16.5	23.2	12.5	10.1	13.8	14.8	12.4	9.99	8.23	11	12.9	13.9	13.8	11.4	7.23
E35	18.3	19.6	8.7	14.6	11.6	13.7	11.5	10	7.27	8.85	11.2	10.1	11.2	8.25	6.56
C36	11.7	15.5	8.23	9.58	8.95	12	9.16	8.57	5.98	7.17	9.25	7.54	6.98	6.33	6.56
V37	8.06	15.2	9.65	12	9.85	13.2	10.3	9.5	7.32	7.88	8.71	9.15	7.36	7.96	7.89
A38	9.46	14.8	9.92	10.5	10.3	14.6	11.5	10.2	7.37	8.17	9.06	10.6	8.33	7.77	8.03
Q39	15.1	23.8	17.7	15	15.4	19.5	18.8	13.3	8.96	11	9.98	18.6	9.58	9.69	10.8
G40	39.9	40.7	40.7	24	27.4	45.1	39.8	24	20.1	29.4	22	35.9	26.8	17.8	24.8
E41	49.8	39.6	46.9	29	34	55.8	55.2	30.7	24.8	35.4	23.5	43.6	29.7	18.8	30.9
E42	37	33.4	38.2	24.3	30.2	34.9	45.1	27.1	25.9	34.4	28.4	38.5	24.1	20.7	27.3
S43	46.3	45.2	44.1	34.8	48.1	40.2	52.3	27.9	29.3	58.9	49.2	51.7	34.4	34.9	38.7
D44	77	70.3	77.3	65.3	83.2	70.3	79.1	47.7	47.8	85.5	80.9	81.6	52.4	69.7	62.5
P45	76.6	89.4	71.6	71.2	94.7	84.2	77.9	56.6	57.7	114	93.6	95.7	61	72.3	68.8
N46	69	64.5	67.4	46.8	78.4	72.5	53.9	57.1	57.9	83.1	62.3	59.8	61.3	43.6	53.1
F47	38.4	29.4	35.9	22.8	37.6	40.8	36.7	23.6	22.7	35.7	23.4	30.6	33.7	20	29.6
D48	31	26.7	23.7	18.1	25.1	25.5	24.3	18.5	14.2	24	19	16.3	18.4	13.9	20.8
K49	19.5	19.6	13.4	14.3	19.6	19	16.4	14.7	12.4	15.1	13.3	11.4	11.5	11.2	11.3
W50	20.4	20.2	11.1	16.4	16.3	14.6	13.2	12.6	9.58	13.4	14.7	12.5	11.7	12	10.4
S51	25.4	21.5	16	19.8	21.2	15.1	19.2	13.2	10.4	13.7	16.8	14.4	13.1	14.7	12.6
L52	14.3	14.1	9.46	12	14.2	13.2	13.7	11.9	7.3	8.5	12.2	8.57	8.7	10.5	8.58
F53	12	15.3	10.3	12.2	16.1	9.49	9.77	7.66	4.55	8.96	12.9	8.99	10.4	9.72	8.29
Y54	17.4	21.4	18.6	15.7	18.5	11.5	17.2	10.4	6.44	9.23	15.3	10.8	13.4	15.9	16.4
K55	26.5	31.3	31.5	26	23.8	15.5	23.4	15.1	10.7	11.8	17.1	14.5	18.2	27.5	26
E56	58.6	45.6	54.2	50.8	38.5	33.1	37	23.2	25.5	16.6	20.9	27.4	44.5	50.3	64.3
D57	92.3	64.1	96.2	70.2	61.4	48.7	50.7	43.2	46.2	19.1	32.2	59.9	118	68.4	79
Y58	72.5	59.4	77.2	50.4	34.9	30	30.2	22.2	24.8	13.9	21.5	57.4	116	50.3	72
D59	116	87.8	122	83.8	49.3	29.7	28.1	28.9	26.5	18.8	18.4	61.7	118	39.8	123
I60	193	88.6	97	43.6	32	32.7	24.9	19.5	16.6	21.5	16.9	40.7	59.9	42.3	69.4
E61	298	210	57.1	29.1	33.9	36.6	41.2	16.8	15.5	23.6	20.5	26.3	80.8	73.6	102
I62	267	373	30.4	23.7	27.7	51.2	47.7	16.9	12.4	24.2	17	16.6	83.8	105	124
E63	393	572	25.3	16.4	14.9	49.1	33.4	16.4	11.2	28.9	21.4	21	156	201	182
D64	460	741	34	19	15.1	68.7	36.6	25.3	20.8	70.8	26.1	39.2	252	327	337
E65	578	1152	53.3	19.4	17.9	120	63.5	41.5	25.8	90.1	29.5	54.6	408	606	500
N66	698	1339	54	26.6	24.4	142	83	74.9	48.9	118	74.3	117	430	494	517
G67	692	1104	46.1	18.4	21.2	114	85.5	66.3	43.7	78.3	80.1	104	412	392	347
S68	649	855	46.4	22.5	23.6	65.8	42.5	42.5	34.6	75.9	63	91.3	285	243	268
K69	456	525	36	20.2	31.9	38.4	38.3	22.8	25.6	34.5	36.2	56.6	196	155	235
T70	381	311	69.8	27	51.5	35.6	50.9	21.2	23.7	21.7	36.4	43	124	104	150
T71	280	194	121	32.3	41.2	36.7	45.5	23.2	19.1	22.1	31	30.6	91.5	68.2	88.1
K72	161	191	65.2	44.7	40.4	35.7	50	26.8	18.8	22.7	29	46	58.5	56.2	52.3
T73	90.8	214	80.7	75.1	54.2	29.9	50.1	38.5	19.3	28.7	35.1	55.1	90.8	68	70.3
I74	67.5	207	54.9	45.5	26.7	20.9	30.4	19	14.5	14	24.9	31.2	42.1	35.3	44.4
T75	40.5	49	34.1	23.9	19.8	17.7	17.5	14.7	10.8	9.41	17.1	16.8	22.7	18.6	25.8
E76	15.4	42.8	29.1	14.6	13.6	16.7	12.6	13.2	9.51	8.3	10.5	12.9	19.2	12.8	15.1
G77	16	26.5	19.3	12.9	14.1	15.6	9.81	10.9	10.1	9.32	11.8	11.9	13.4	13.1	12.8
Q78	22.1	20.6	12.5	13.2	17.2	14.8	11.9	12.5	11.5	10.2	16.3	11.5	17.5	14.3	16.2
S79	16.4	21.4	12.3	14.1	14.6	12.9	9.72	9.12	8.75	6.68	11.7	9.8	13.6	13.3	14.1
I80	12.3	16	11.1	10.6	10.2	13.5	7.55	8.8	6.8	7.52	10.1	9.38	11.1	13.2	11.6
L81	19.3	18.8	12.9	16.7	17	16.6	12.9	13.3	10.1	9.98	12.7	10.5	15.5	16.6	15.2
T82	19.6	23.7	13.4	20.2	22.8	19.1	14.1	13.8	13.9	11	14.1	9.97	15.4	15.1	19.5
M83	15.6	18.5	16.8	16.4	14.8	18.5	10.7	12.5	13.3	11.2	12.3	14.1	12.4	11.7	17.3
F84	26.7	23	17.3	20.1	16.5	24.7	30.8	16.3	14.5	12.2	15.9	21.2	17.4	16.7	20.5
N85	45.5	29.1	25.1	22.8	23.5	28.8	52	19.3	19.6	20.2	17.6	22.7	20.9	18.1	30.6
E86	34.9	32.6	30.7	18.2	20.5	31	38.3	18.8	20.2	25.5	18.6	21	20.1	21.6	28
G87	27.2	33.9	32.3	20.9	18.8	30.8	30.8	17.8	25	22.6	20.8	21.6	24.5	23.3	19.9
Y88	19.1	24.8	32.2	15.7	10	21.9	17.1	18.5	20.7	19.3	19.8	15.1	20.8	17.9	16.3
A89	15.1	17.8	25.9	12.7	8.52	16.2	18.2	15.9	15.4	14.2	20.4	14.3	24.6	17.3	13.6
S90	23.6	36.1	32.6	12	10.7	35.7	60.2	17.5	33	24.6	48.8	21.7	41.7	28.6	41.5
D91	14.3	18.5	15.6	8.54	6.99	13.2	16.5	8.6	15.5	12.2	18.4	11.6	15.6	18.3	18.2
G92	13.8	15.1	19.8	8.74	6.6	13.1	13.8	10.2	9.51	5.39	12.2	12.1	14.1	12.4	16.6
I93	10.6	13.2	18.1	6.42	8.19	9.09	10.9	10.2	8.44	4.14	10.8	8.96	11.4	10.4	9.86
W94	11.1	19.1	23.8	6.44	10.9	13.4	14.1	8.19	9.11	7.21	10.8	9.52	13.5	7.75	11.5
L95	9.63	13.3	9	8.22	10.3	10.9	15.3	10.4	10.7	8.5	13.7	9.07	10.7	6.2	8.83
G96	12.2	22.7	10.9	14.8	19.9	16.6	17.3	15.2	12.8	12.1	19.2	11.6	17.3	9.17	12.8
G97	18.1	35.3	22.3	14.9	17.5	22.2	14.1	15.6	16.6	14	19.5	12.4	16.9	16	19.7
T98	14.7	18.7	19	8.59	14.1	15.9	8.78	10.2	15.8	15	15.2	10.9	12.7	16.4	20.7
K99	12.2	14.6	29.2	7.1	10.5	15.1	12.7	13.3	11.3	10.7	12	12.3	14.8	11.7	13
Y100	9.17	9.92	12.1	6.88	6.65	8.3	8.1	11.1	8.12	7.82	6.38	6.79	7.9	8.01	10.7
Q101	9.73	8.89	9.7	6.75	4.82	10.1	8.71	8.83	8.01	6.66	7.89	7.08	6.75	7.32	11.3
F102	11.3	9.83	11.4	7.96	5.85	12.1	9.38	8.41	6.69	7.41	10.2	8.87	7.18	8.19	12.5
I103	16.3	10.2	10.8	6.29	7.36	13.2	12.1	8.34	6.94	7.6	9.81	10.7	9.02	9.39	14.8
N104	18.8	12.7	11.6	8.14	6.92	13.8	16.9	9.5	10.2	7.54	12.3	8.04	7.22	12.2	14.2
M105	21.6	12.7	14.6	9.41	8.75	15	20.4	10.2	10.8	8.05	14.9	7.86	8.86	11.4	15.9
D106	33.4	16.5	15	14.6	15.8	28.4	34.8	15.7	11.9	8.45	15.9	9.11	7.08	11.8	18.6
K107	33.4	19	14.2	22.5	21	23.2	38.7	26.3	12.7	11.9	16	13	8.4	17.5	22
G108	34.4	23.6	19.6	30.2	25.4	30.2	40.8	40.8	14.2	14.4	17.4	19.5	12.6	30.8	33.7
L109	13.5	19.8	11.3	19.6	19.4	22.1	24.7	36.3	10.8	11.7	12.3	12.1	7.57	20.3	20.8
E110	23.7	34.4	14.3	16.3	27.9	28.9	28.5	46	7.78	18.9	19.2	13.9	13.7	28.5	31.3
Y111	19.4	48.1	11.9	9.38	28.3	27	23.3	51.6	9.03	18.2	21.3	14	21.6	32.9	38.4
E112	25	84.2	18.9	13	41.5	39.2	34.8	86.8	18.4	30.2	31	20.2	41.7	57.5	69.2
G113	47.1	84.2	30.1	15.2	51.4	50.3	42.5	85.1	23.8	30.6	32.2	21.9	38	71.4	90
H114	19	29.8	23.5	10.8	22.1	28.7	30.5	32.2	14.9	14.6	20.1	14.3	18.6	37.3	36.4
S115	16.8	20.3	20.7	19	17.7	21.9	27.9	20.5	14.4	12.3	14.3	13.4	12.7	21.2	20.5
F116	15.6	14.6	11.4	10.9	10.7	13.9	20.5	13.1	11.3	8.14	10.6	9.25	8.49	10.8	15.8
D117	16.3	15.2	10.2	11.2	9.66	13.3	24.3	15.3	10.2	9.05	10.4	7.84	6.64	10.7	14.8
V118	9.87	11.9	7.55	8.11	5.62	10.6	13.2	6.71	8.13	7.87	7.37	4.76	5.1	8.26	11.5
A119	9.63	9.6	7.3	6.14	6.43	12.3	9.62	5.46	7.27	6.69	7.18	6.2	4.48	6.31	10.9
T120	8.59	8.65	5.94	4.99	4.72	10.4	7.38	5.34	6.05	5.93	5.97	7.32	4.37	6.05	7.52
C121	7.86	7.19	6.66	4.54	6.27	7.64	6.44	5.86	4.72	5.13	6.99	5.52	5.01	6.31	7.95
A122	9.35	8.87	9.09	5.86	7.34	10.7	8.65	8.71	8.31	7.05	7.93	9.78	6.77	6.69	9.36
K123	13.4	8.85	18.8	14.8	12.3	21.9	12.1	14.8	10.9	11.8	13	22	10.8	9.03	12.8
S124	16.3	20.8	22.2	24.4	23.2	37.2	20.3	20.5	15.5	23.7	17.5	30.6	14	10.4	18.4
K125	20.4	30.2	18.3	17.3	33.4	35.2	21.5	18.8	24.3	32.1	22.9	27.3	15.4	15.6	16.8
G126	12.5	10.9	9.87	12.1	13.8	16.3	13.4	14	21.4	25.9	19.4	13.3	12	9.49	14.4
G127	8.5	8.43	7.65	4.98	6.92	11	8	5.66	7.62	6.86	7.52	8.36	7.27	6.21	6.87
M128	7.24	7.45	4.21	4.13	5.22	7.37	7.01	3.73	3.56	5.2	5.79	6.12	4.25	3.65	5.43
H129	7.01	8.87	4.34	4.94	2.65	6.72	5.82	2.89	2.9	4.15	4.13	4.65	2.94	4.29	5.29
I130	8.65	7.22	5.63	5.34	3.48	6.47	6.08	3.55	3.42	3.59	5.07	3.95	3.71	4.04	7.12
I131	10.8	8.05	6.1	6.17	4.21	8.15	8.17	6.01	4.57	4.67	6.68	4.64	5.17	6.03	9.34
K132	21.8	14.6	10.7	11.5	10.2	14.2	16.3	12.9	5.43	8.45	10.8	7.45	7.01	8.87	16.3
V133	28.7	15.2	13.3	12.3	10.4	19	15.8	17	8.03	10.6	12.4	10.2	7.15	10.5	18
G134	31.2	28.7	27.2	22.1	21.2	32.3	21.2	23.4	10.6	16.5	24.5	19.9	15.9	20.9	24.6
G135	84.3	47.4	46	24.6	32.4	61.2	113	35.6	11.6	20.7	25.7	33.1	36	35.8	36.8
G136	33	43.2	23.5	19.5	24.3	40.5	33	25.7	12.9	18.5	25.6	38.4	28.3	28.9	29.4
H137	25.8	29.5	20.1	16.3	10.6	20.8	20.3	18.6	10.4	13.5	13.8	15.3	16.4	17.8	16.8
I138	18.8	13.7	8.11	8.5	5.85	8.28	11.6	11.9	5.71	6.73	10.2	8.36	6.95	8.1	11
L139	13.2	9.85	6.74	5.79	5.32	5.59	6.29	9.02	3.79	4.87	7.62	4.48	4.47	4.91	7.96
I140	10.3	7.4	5.46	4.85	5.19	4.17	5.57	5.16	2.68	4.2	5.79	4.06	2.7	5.62	5.4
V141	7.24	7.67	4.54	6.14	4.87	4.88	5.41	4.23	2.97	4.57	3.97	4.55	3.24	6.51	6.49
L142	7.23	8.65	4.68	5.39	5.45	7.96	7.8	4.28	3.74	4.55	4.82	4.24	3.8	6.91	4.46
Y143	7.94	7.95	4.97	7.37	10	13.5	8.94	4.51	6.25	6.53	6.31	6.93	5.99	5.98	5.73
D144	9.38	10.3	11	9.56	9.56	18.6	13.6	5.62	9.03	11.4	10	13.1	7.19	7.1	8.22
E145	15.1	11.5	17.7	18.6	18.9	34.1	25.8	14.8	17.8	21	17	17	13.6	11.5	12.9
E146	19.3	24.9	35.4	29.6	27.3	46.9	39	22.7	28.1	37.1	28.2	28.7	20.2	18.2	17.7
K147	18	20	23.7	17.7	21.6	33	20.9	13	20.5	28.2	21.9	24	19.3	16.3	18
E148	21.4	15.3	13.9	13	24.7	31.7	17.1	11.8	16	19.3	18.7	16.6	18.2	17.6	15.6
Q149	9.92	7.3	8.07	6.76	10.2	14.8	9.12	5.92	6	8.98	9.64	8.48	11.5	8.33	10.6
D150	10.9	6.41	5.55	5.3	10.7	14.6	16	7.36	7.61	12.6	9.31	9.47	12.3	12.6	10.3
R151	7.78	6.69	5.09	5.41	5.34	8.32	11.9	6.44	7.07	7.06	8.13	6.18	9.57	10.6	8.13
G152	6.86	7.44	5.46	4.85	6.19	8.67	8.16	5.07	5.22	7.31	8.68	4.27	5.03	9.53	6.73
N153	6.74	6.37	4.89	4.22	5.96	9.77	6.9	4.99	4.43	6.58	7.91	5.29	6.12	9.83	6.22
S154	4.93	5.63	4.51	3.35	4.77	7	6.1	4.46	3.75	6.32	6.23	4.56	6.43	7.59	6.91
K155	4.72	6.06	4.48	4	4.39	6.52	6.1	4.11	4.71	5.65	6.37	4.13	6.72	6.68	7.09
N156	5.09	6.24	6.85	5.04	4.76	6.56	6.21	5.39	5.88	5.91	7.9	4.17	7.46	7.44	7.26
A157	5.97	5.81	8.48	4.82	5.23	6.07	5.62	5.51	6.74	7.38	7.91	6.5	7.76	7.15	8.97
A158	5.68	5.79	6.26	4.66	4.42	5.69	7.76	5.3	5.64	7.06	5.68	6.69	6.3	6.19	7.9
L159	6.5	7.83	7.24	5.15	5.39	7.38	9.19	5.48	5.54	7.94	7.35	6.08	7.3	7.87	11
A160	8.75	9.01	10.1	7.16	9.09	9.46	9.72	6.89	7.89	10.6	9.1	7.22	12.3	13.2	13.1
F161	9.48	11.7	8.59	6.03	6.87	10.3	9.11	8.33	6.28	7.89	7.96	6.06	8.5	9.72	11.2
S162	10.5	11	9.05	5.67	7.18	11	13.6	9.77	7.03	8.49	7.97	6.7	7.29	10.8	10.3
K163	13.2	13.1	14	7.82	9.22	12.8	15.4	13.1	8.52	9.78	12.9	7.82	8.89	15.6	16.3
E164	17.9	17.3	16.3	11.9	13.3	19.1	17.1	14.1	9.47	10.9	13.1	11.3	13.8	15.9	17.5
L165	24.2	22.6	14.8	13.7	14.6	21.2	19.6	18.2	8.25	10.5	12.2	9.49	13.9	15.9	15.3
I166	39.5	66.1	23.5	22.6	14.7	27.7	33.9	29.5	11.1	15	19.3	9.85	20.7	20.6	20.2
E167	66.6	117	31	28.9	19.4	38.7	49.1	34.9	19.1	20.9	22.1	20	31.2	26.1	33.8
S168	65.7	84.5	34	28.8	24.1	40.4	45.8	39.9	16.9	15.4	20.7	23.9	33.7	32.6	34.8
T169	113	183	44.9	44	32.4	48.3	63.3	55.8	27.4	23	26.2	26.7	48	49.2	40.3
D170	169	352	69.1	63.1	54.1	67.3	119	81	45.8	48.7	47.4	45.2	112	103	76.4
T171	316	477	101	107	74.3	87.7	169	106	59.5	59.1	61.3	70.1	230	275	131
G172	427	536	203	211	241	197	261	224	163	180	107	109	545	476	156
A173	930	883	521	636	640	653	499	716	599	549	530	285	1100	998	601

Figure S2: Atomic fluctuations (B-factor) of *Pb* Pfn (left) or *Pb* Pfn ^{PfLoop} (right) during MD simulations (each complexed with *Pb*Actin). Residue numbers are highlighted in yellow at the left corner of each panel. Each column represents B-factor values (units are $Å^2x(8/3)\pi^2$) for the Cα atoms for the interval of 20 ns during 200-500 ns of simulations. The acidic loop residues are bordered with bold lines and are highlighted with grey text (right corner). Color code: blue, white, red: low, intermediate and high B-factor values, respectively. Please note that this data is also available as separate Excel file.

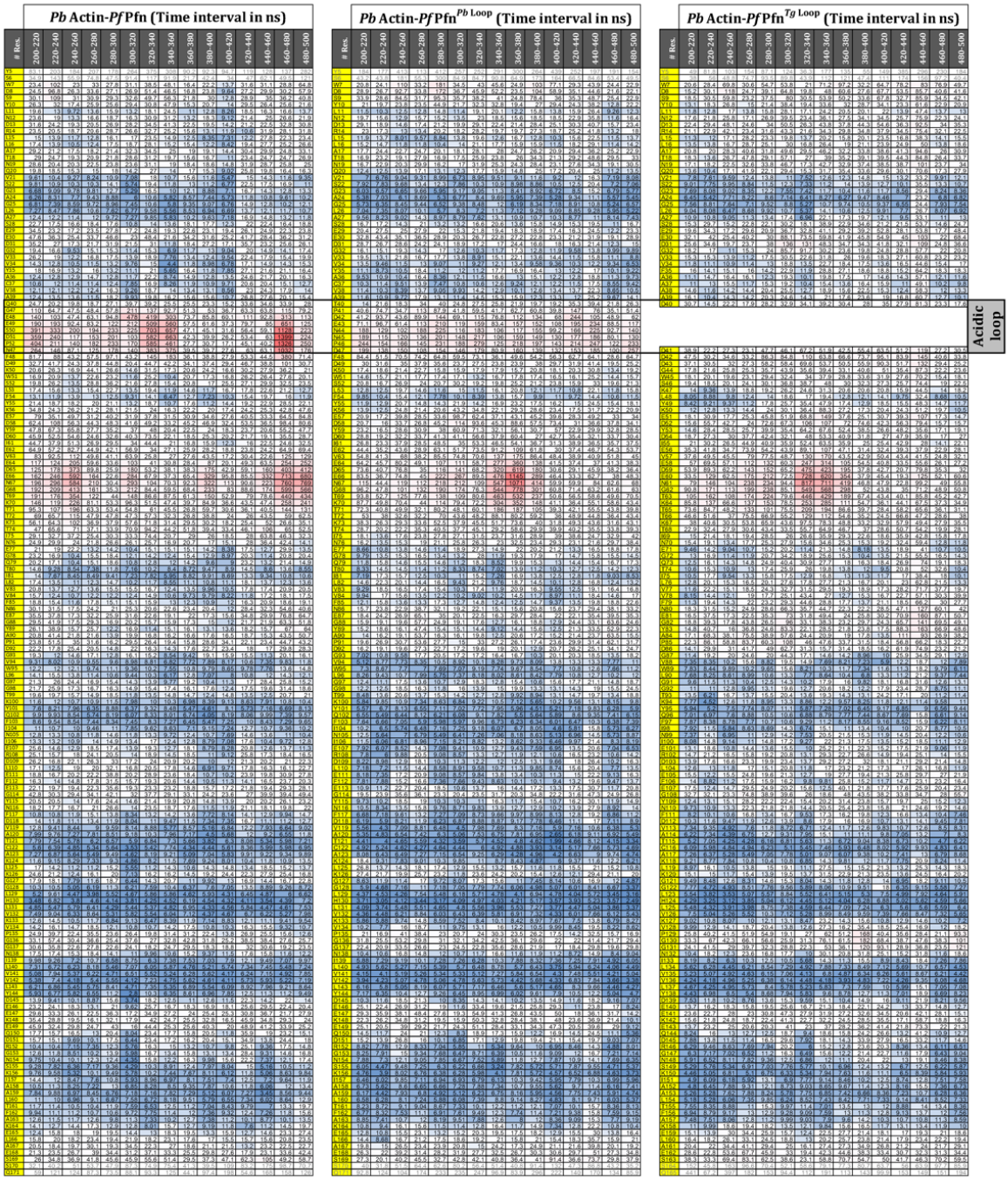


Figure S3: Atomic fluctuations (B-factor) of *Pf* Pfn (left), *Pf* Pfn $^{Pb\text{Loop}}$ (middle) and *Pf* Pfn $^{Tg\text{Loop}}$ (right) during MD simulations (each complexed with *Pb*Actin). Residue numbers are highlighted in yellow at the left corner of each panel. Each column represents B-factor values (units are $Å^2x(8/3)\pi^2$) for the Cα atoms for the interval of 20 ns during 200-500 ns of simulations. The acidic loop residues are bordered with bold lines and are highlighted with grey text (right corner). Blue, white, red: low, intermediate and high B-factor values, respectively. Please note that this data is also available as separate Excel file.

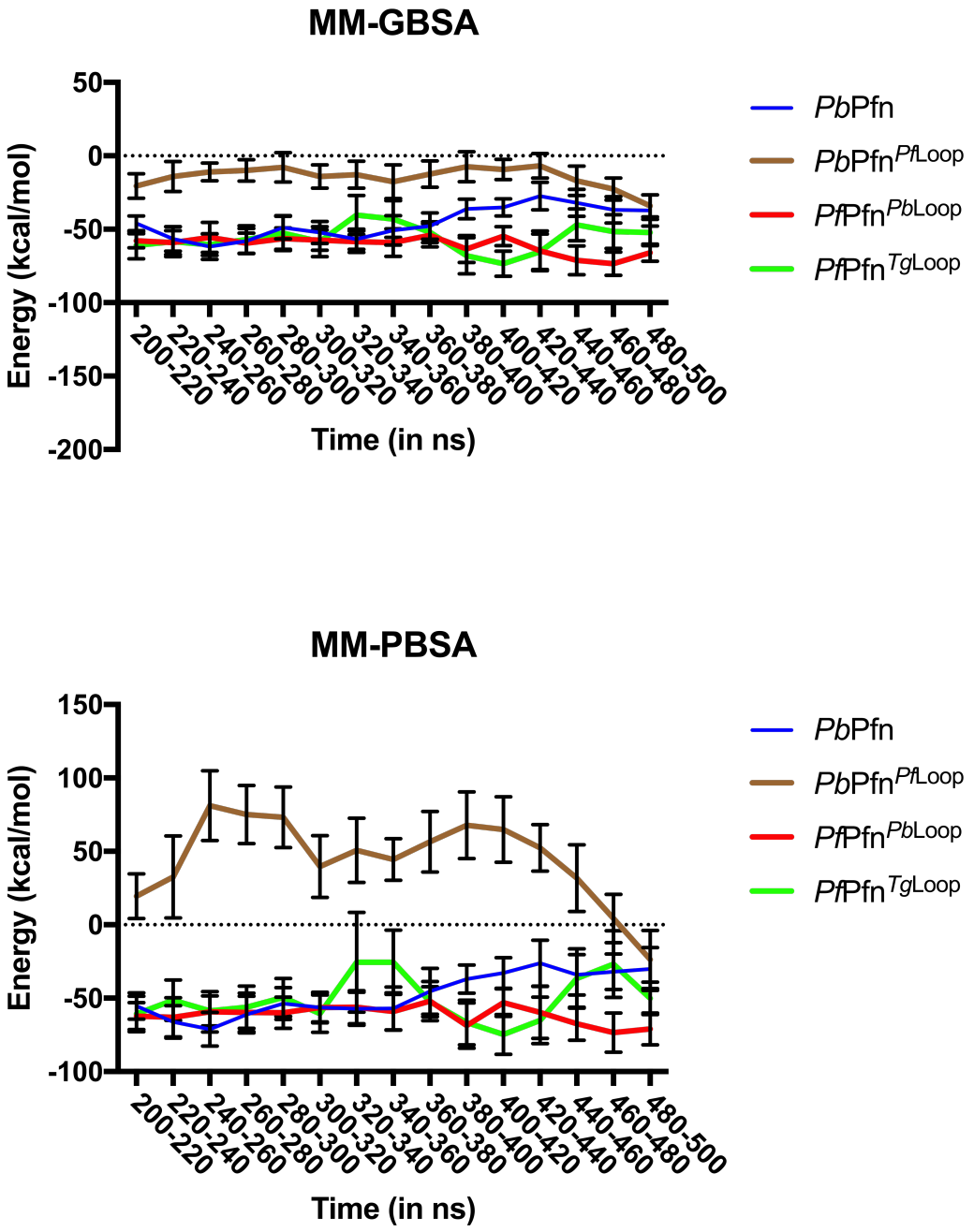


Figure S4: MM-PBSA and MM-GBSA estimated binding free energy of *Pb*Actin complexed with different profilin mutants. Average ± standard deviation binding free energies (kcal/mol) were calculated for intervals of 20 ns during 200-500 ns of simulations using the MM-GBSA and MM-PBSA methods. Note that the (energetically unfavorable) translational, rotational and vibrational entropic contributions to binding were not computed.

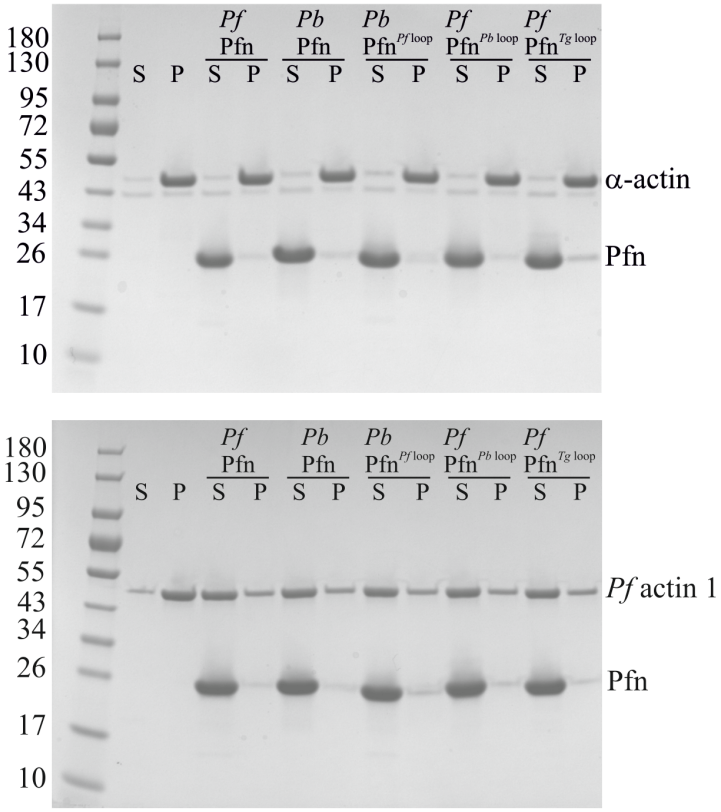
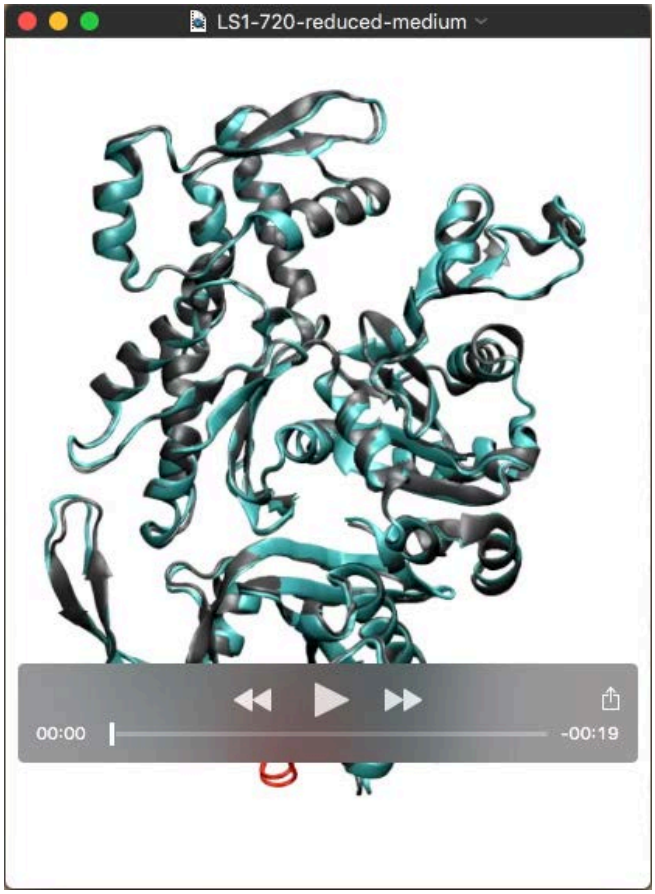


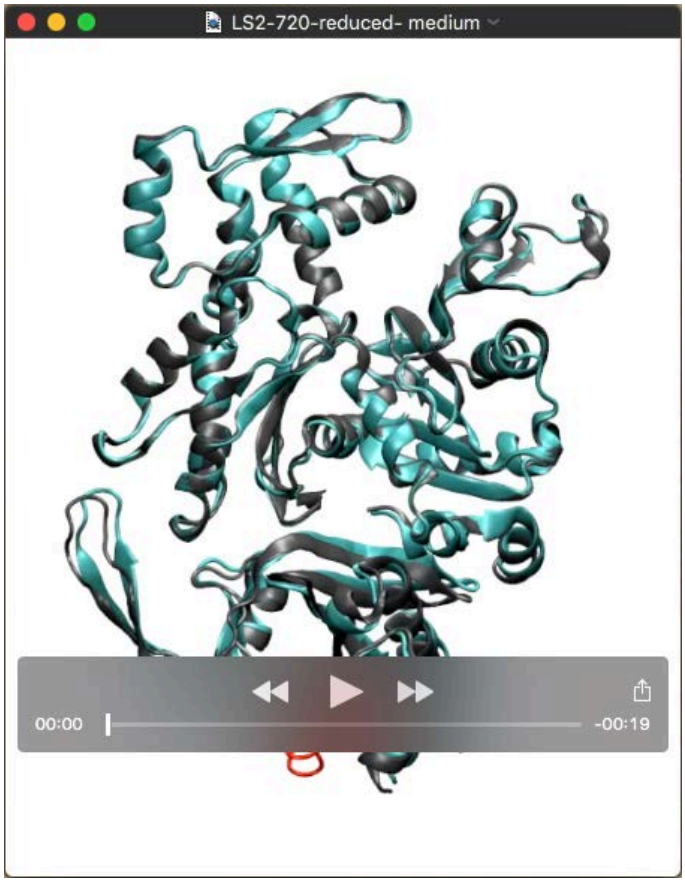
Figure S5: Co-sedimentation gels. Sedimentation of 4 µM *S. scrofa* (domestic pig) α-actin (top gel) or *P. falciparum* actin 1 (bottom gel) alone and in the presence of 16 µM *P. falciparum* and *P. berghei* profiling as well as profiling chimeras (*Pb* Pfn$^{Pf\ Loop}$, *Pf* Pfn$^{Pb\ Loop}$ and *Pf* Pfn$^{Tg\ Loop}$). Samples were analyzed on 4- 20% SDS-PAGE gels and protein bands were visualized with PageBlue stain (Thermo Scientific). S denotes supernatant and P pellet. Quantification from duplicate gels is presented in Fig. 3B.

Supplementary movies



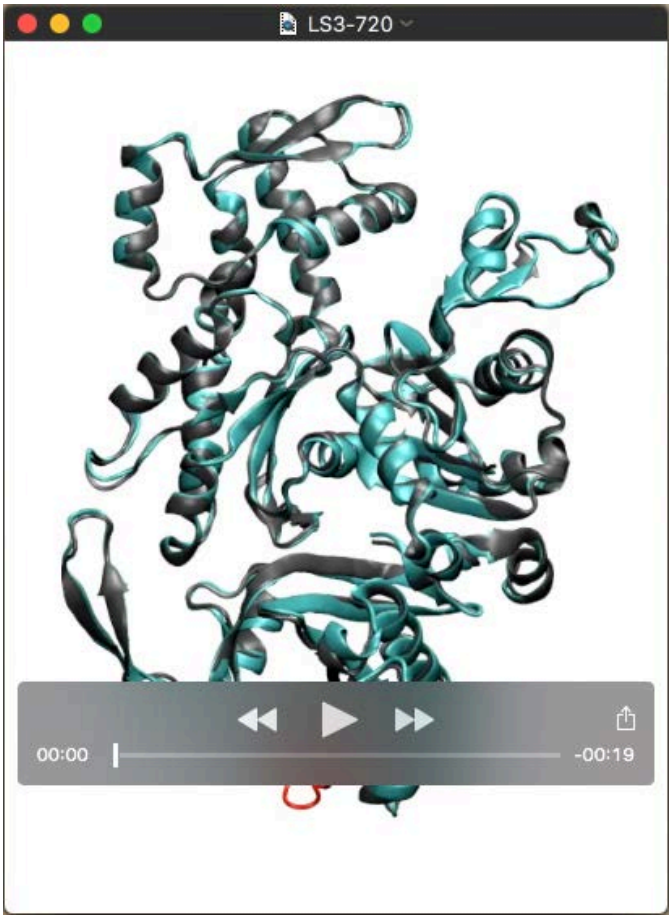
Movie 1

500 ns simulation of the chimeric mutant *Pb* Pfn$^{Pf\ Loop}$ in grey compared to *Plasmodium berghei* profilin-WT (cyan) using all atom molecular dynamics simulation. The profilin mutant (or WT) is bound to *Plasmodium berghei* actin. For comparison, see movies in Moreau et al., 2017 (ref 5), for 150 ns simulations for mutants of the profilin arm.



Movie 2

500 ns simulation of the chimeric mutant *Pf* Pfn$^{Pb\ Loop}$ in grey compared to *Plasmodium berghei* profilin-WT (cyan) using all atom molecular dynamics simulation. The profilin mutant (or WT) is bound to *Plasmodium berghei* actin.



Movie 3

500 ns simulation of the chimeric mutant *Pf* Pfn$^{Tg\ Loop}$ in grey compared to *Plasmodium berghei* profilin-WT (cyan) using all atom molecular dynamics simulation. The profilin mutant (or WT) is bound to *Plasmodium berghei* actin.