

Electronic Supplementary Information for
Correlated vibrations in ion-pair dynamics in mechanoactivation identifies functional domains of force-dependent titin kinase

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Here the same analysis as the main text on more realizations with the same and different pulling speeds are summarized.

I. SUMMARY OF THE SECOND REALIZATION WITH PULLING SPEED $v = 0.005$ Å/PS

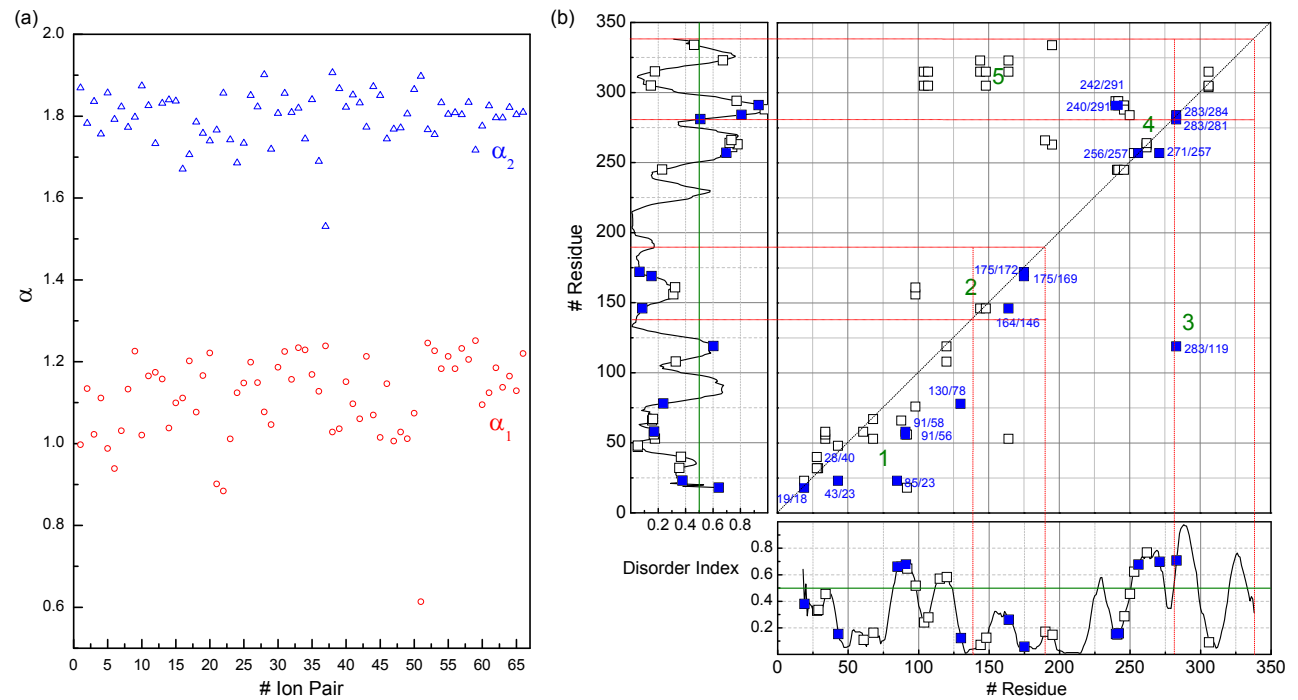


FIG. 1 (a) Distribution of the scaling index α of the 66 ion-pair time series. $\langle \alpha_1 \rangle = 1.11$ and $\langle \alpha_2 \rangle = 1.80$. (b) Diagonal map of all ion pairs ($\square$) and those with regular oscillatory behaviors in their time series ($\blacksquare$).

TABLE I Classification of ion pairs. Groups 1, 2, ... 5 are classified by topological locations in linear sequence and their subgroups (I, I*, ...) are classified by the existence of explicit oscillation. Salt-bridges in unstretched protein are underlined. Salt-bridges formed during stretch are without underline. The ion-pair time series having explicit oscillatory behaviors are further highlighted by bold fonts.

Group	Subgroup	Ion pairs
1	I*	E019-K018, E043-K023, E085-K023, E091-K058, E130-R078
	I	<u>D029-R032</u> , <u>E088-K066</u> , E019-K023, E028-R032, E028-R040, E034-K053, E034-K056, E034-K058, E043-K048, D061-K058, E068-K053, E068-K067, E091-K056, E092-K018, E092-K056, E098-R076, E120-R108, E120-R119, E164-K053
2	II*	E164-R146, D175-R169, D175-K172
	II	<u>E098-K161</u> , E098-R156, D144-R146, E148-R146
3	III*	E283-R119
4	IV*	D240-R291, E242-R291, D256-R257, E271-R257, E283-K281, E283-R284
	IV	E190-R266, D195-R263, D240-K294, E241-K245, E242-K245, E242-K294, E246-K245, E246-K288, E246-R291, E250-R284, D253-R257, E262-K261, E262-R263, E262-K264, D306-K304, D306-K305, D306-R315
5	V	D104-K305, D104-R315, E107-K305, E107-R315, D144-R315, D144-R323, E148-K305, E148-R315, E164-R315, E164-R323, D195-K334

II. SUMMARY OF THE FIRST REALIZATION WITH PULLING SPEED $v = 0.01 \text{ \AA/PS}$

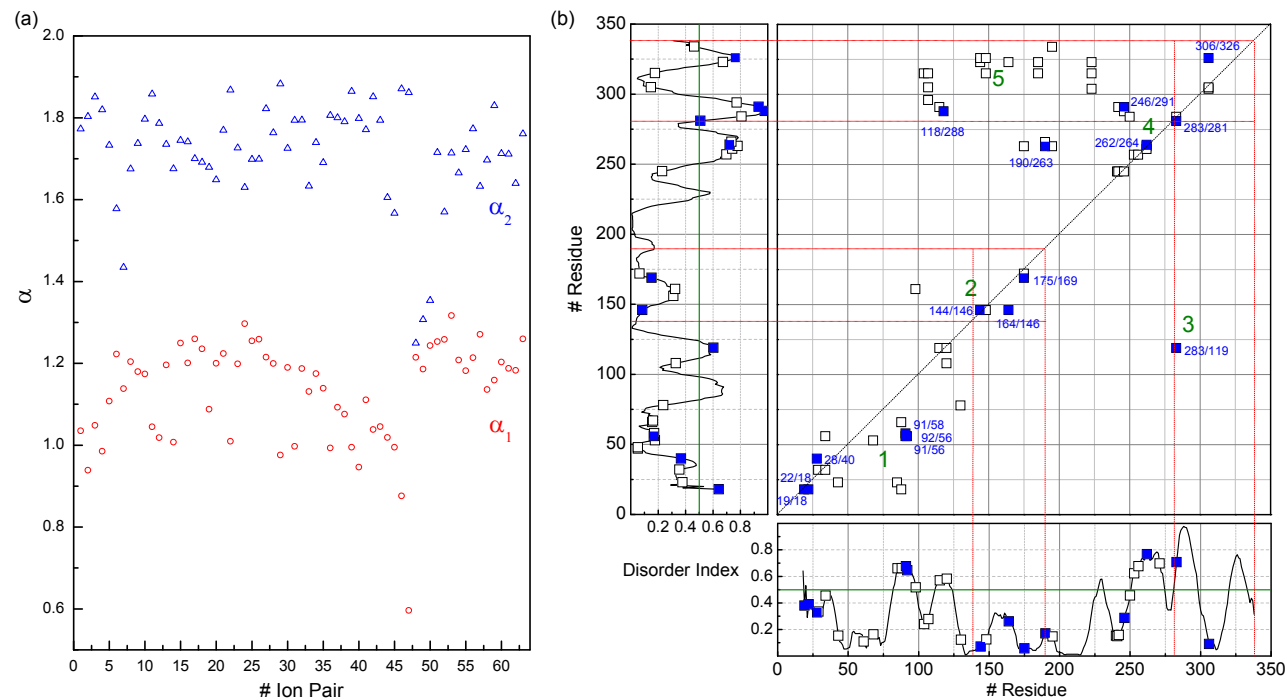


FIG. 2 (a) Distribution of the scaling index α of the 63 ion-pair time series. $\langle\alpha_1\rangle = 1.13$ and $\langle\alpha_2\rangle = 1.72$. (b) Diagonal map of all ion pairs ($\square$) and those with regular oscillatory behaviors in their time series ($\blacksquare$).

TABLE II Classification of ion pairs. Groups 1, 2, ... 5 are classified by topological locations in linear sequence and their subgroups (I, I*, ...) are classified by the existence of explicit oscillation. Salt-bridges in unstretched protein are underlined. Salt-bridges formed during stretch are without underline. The ion-pair time series having explicit oscillatory behaviors are further highlighted by bold fonts.

Group	Subgroup	Ion pairs
1	I*	<u>E022-K018</u>, <u>E091-K058</u>, <u>E019-K018</u>, <u>E028-R040</u>, <u>E091-K056</u>, <u>E092-K056</u>
	I	D029-R032, E034-R032, E034-K056, E043-K023, E068-K053, E085-K023, E088-K018, E088-K066, E115-R119, E120-R108, E120-R119, E130-R078
2	II*	<u>D144-R146</u>, <u>E164-R146</u>, <u>D175-R169</u>
	II	<u>E098-K161</u> , E148-R146, D175-K172
3	III*	<u>E283-R119</u>
4	IV*	<u>E190-R263</u>, <u>E246-R291</u>, <u>E262-K264</u>, <u>E283-K281</u>, <u>D306-K326</u>
	IV	<u>E246-K288</u> , D175-R263, E190-R266, D195-R263, E223-K304, E223-R315, E223-R323, E241-K245, E242-K245, E242-R291, E246-K245, E250-R284, D253-R257, D256-R257, E262-K261, E262-R263, E283-R284, D306-K304, D306-K305
5	V*	<u>E118-K288</u>
5	V	<u>E107-K305</u> , D104-R315, E107-R296, E107-R315, E115-R291, D144-R323, D144-K326, E148-R315, E148-K326, E164-R323, E185-R315, E185-R323, D195-K334

III. SUMMARY OF THE SECOND REALIZATION WITH PULLING SPEED $v = 0.01 \text{ Å/PS}$

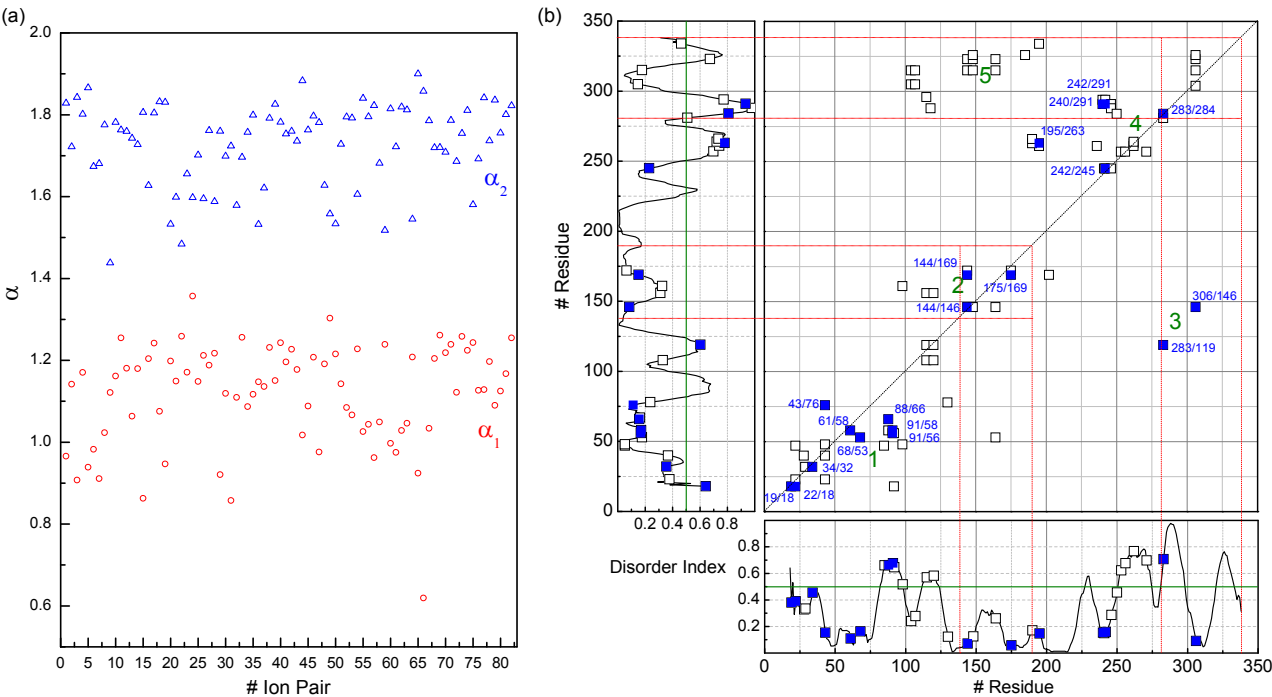


FIG. 3 (a) Distribution of the scaling index α of the 63 ion-pair time series. $\langle\alpha_1\rangle = 1.12$ and $\langle\alpha_2\rangle = 1.73$. (b) Diagonal map of all ion pairs ($\square$) and those with regular oscillatory behaviors in their time series ($\blacksquare$).

TABLE III Classification of ion pairs. Groups 1, 2, ... 5 are classified by topological locations in linear sequence and their subgroups (I, I*, ...) are classified by the existence of explicit oscillation. Salt-bridges in unstretched protein are underlined. Salt-bridges formed during stretch are without underline. The ion-pair time series having explicit oscillatory behaviors are further highlighted by bold fonts.

Group	Subgroup	Ion pairs
1	I*	E019-K018, E022-K018, E034-R032, E043-R076, D061-K058, E068-K053, E088-K066, E091-K056, E091-K058
	I	E022-K023, E022-K047, E028-R040, D029-R032, E043-K023, E043-R040, E043-K048, E085-K047, E088-K058, E092-K018, E092-K056, E098-K048, E115-R108, E115-R119, E120-R108, E120-R119, E130-R078, E164-K053
2	II*	D144-R146, D144-R169, D175-R169
	II	<u>E098-K161</u> , E115-R156, E120-R156, D144-K172, E148-R146, E164-R146, D175-K172
3	III*	E283-R119, D306-R146
4	IV*	D195-R263, D240-R291, E242-R291, E242-K245, E283-R284
	IV	<u>E283-K281</u> , E190-R263, E190-R266, D195-K261, D195-K334, D202-R169, E236-K261, D240-K294, E241-K245, E242-K294, E246-K245, E246-K288, E246-R291, E250-R284, D253-R257, D256-R257, E262-K261, E262-R263, E262-K264, E271-R257, D306-K304, D306-R315, D306-R323, D306-K326
5	V	D104-K305, D104-R315, E107-K305, E107-R315, E115-R296, E118-K288, D144-R315, D144-R323, E148-R315, E148-R323, E148-K326, E164-R315, E164-R323, E185-K326

IV. SUMMARY OF THE REALIZATION WITH PULLING SPEED $v = 0.05 \text{ Å/PS}$

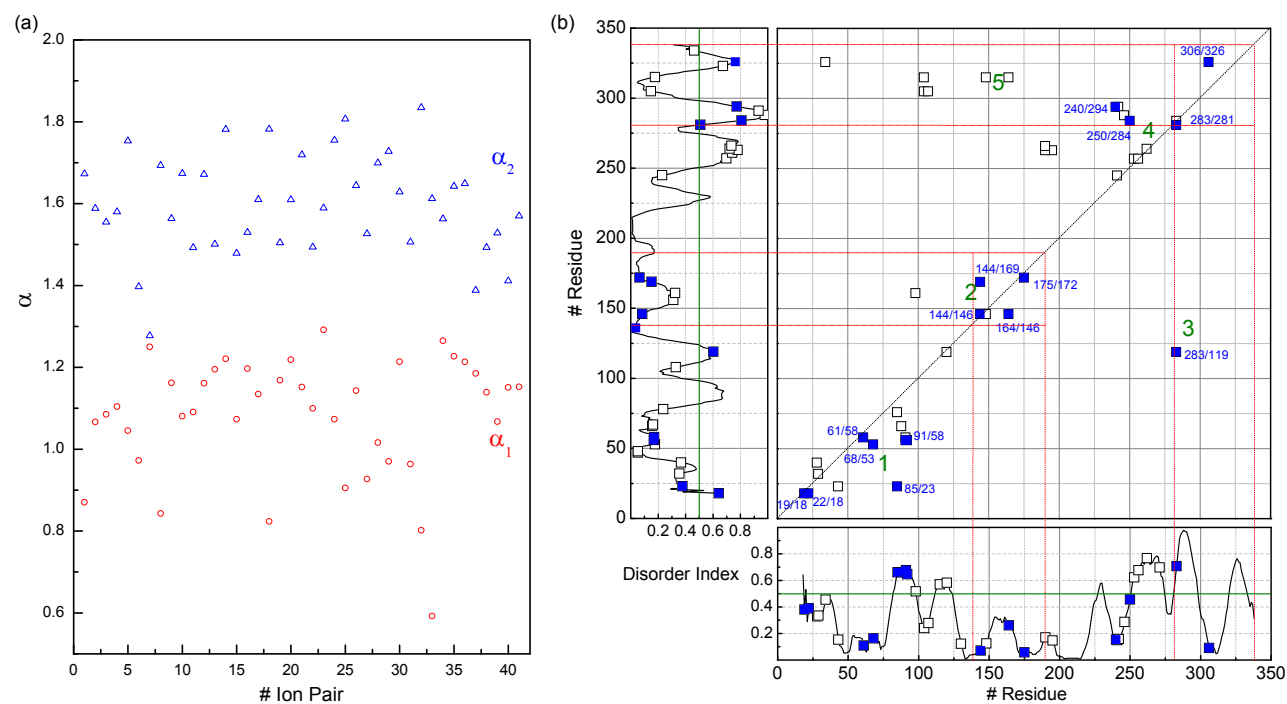


FIG. 4 (a) Distribution of the scaling index α of the 63 ion-pair time series. $\langle \alpha_1 \rangle = 1.08$ and $\langle \alpha_2 \rangle = 1.60$. (b) Diagonal map of all ion pairs ($\square$) and those with regular oscillatory behaviors in their time series ($\blacksquare$).

TABLE IV Classification of ion pairs. Groups 1, 2, ... 5 are classified by topological locations in linear sequence and their subgroups (I, I*, ...) are classified by the existence of explicit oscillation. Salt-bridges in unstretched protein are underlined. Salt-bridges formed during stretch are without underline. The ion-pair time series having explicit oscillatory behaviors are further highlighted by bold fonts.

Group	Subgroup	Ion pairs
1	I*	<u>E022-K018</u>, <u>E091-K058</u>, <u>E019-K018</u>, <u>D061-K058</u>, <u>E068-K053</u>, <u>E085-K023</u>, <u>E091-K056</u>, <u>E092-K056</u>
	I	E028-R040, D029-R032, E043-K023, E085-R076, E088-K066, E120-R119
2	II*	<u>D144-R146</u>, <u>D144-R169</u>, <u>E164-R146</u>, <u>D175-K172</u>
	II	<u>E098-K161</u> , E148-R146
3	III*	<u>E283-R119</u>
4	IV*	<u>D240-K294</u>, <u>E250-R284</u>, <u>E283-K281</u>, <u>D306-K326</u>
	IV	E190-R263, E190-R266, D195-R263, E241-K245, E242-K294, E246-K288, D253-R257, D256-R257, E262-K264, E283-R284
5	V	<u>E107-K305</u> , E034-K326, D104-K305, D104-R315, E148-R315, E164-R315