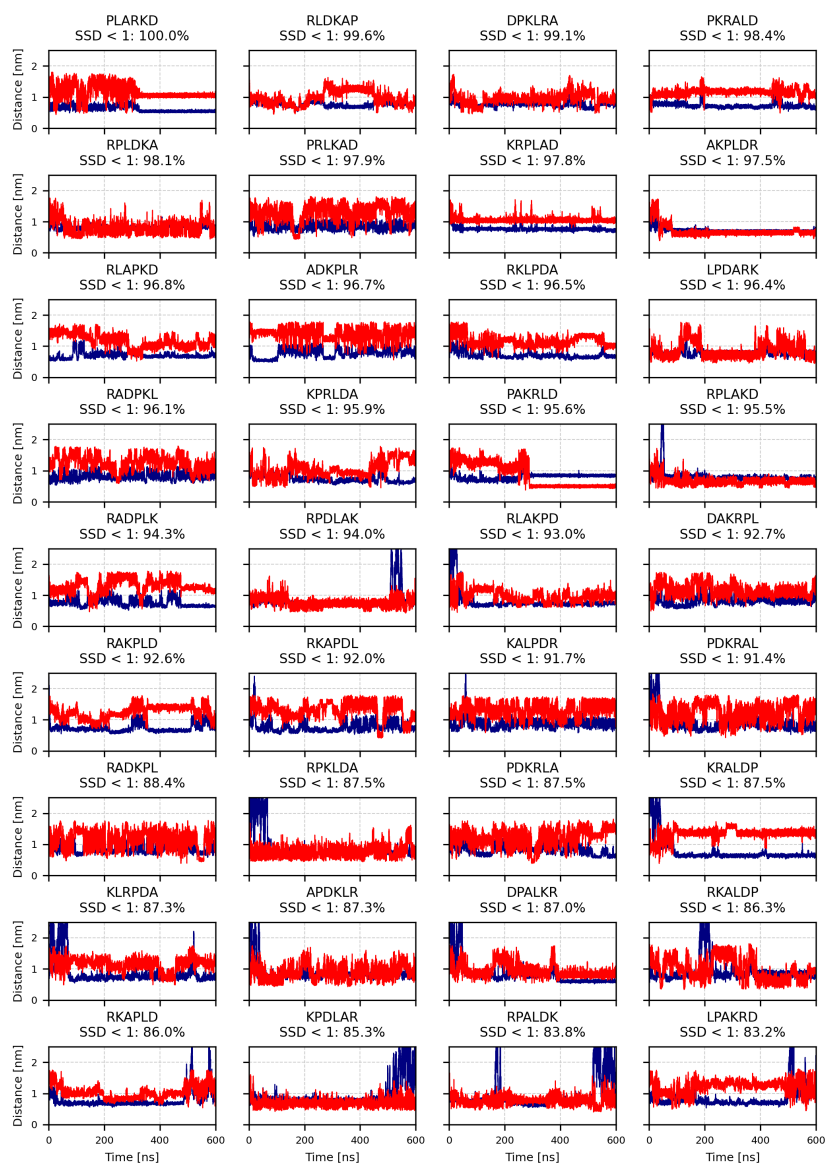


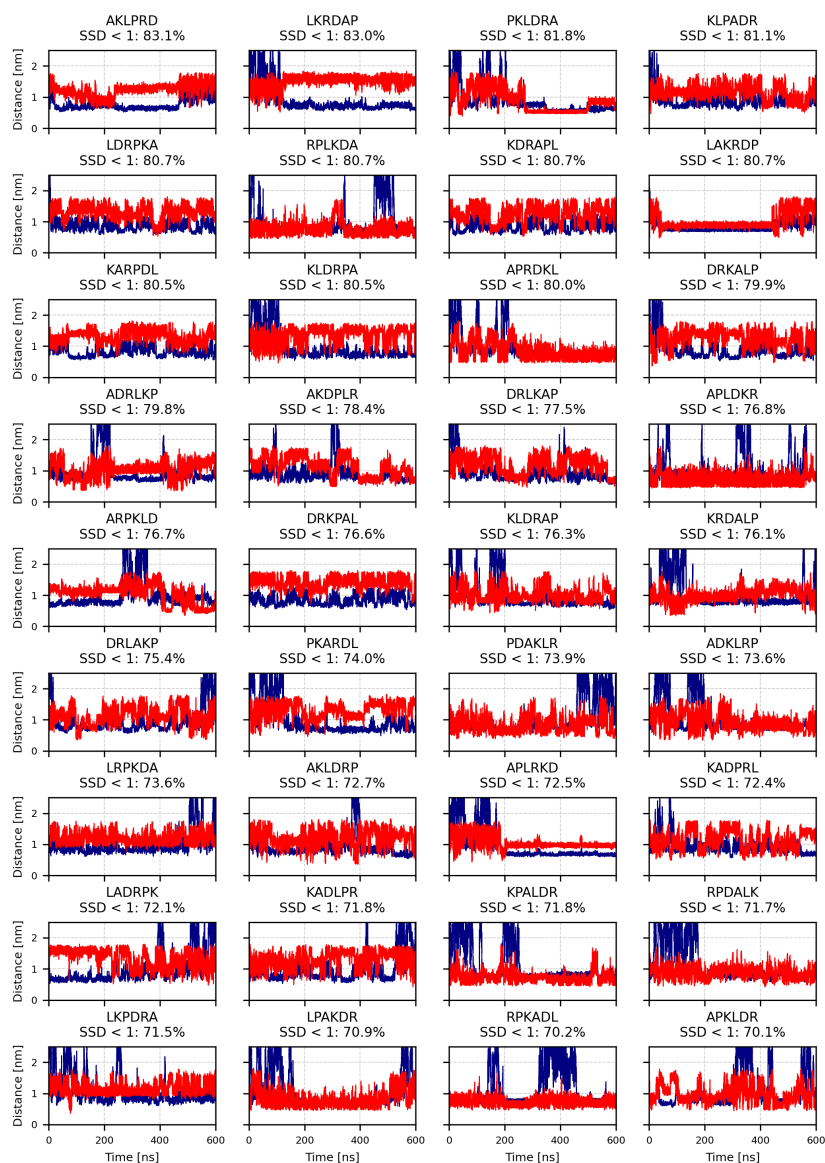
Supporting Information for: Uncovering Sequence Effects in Titanium Binding peptides adsorption on TiO₂: A Molecular Dynamics Study

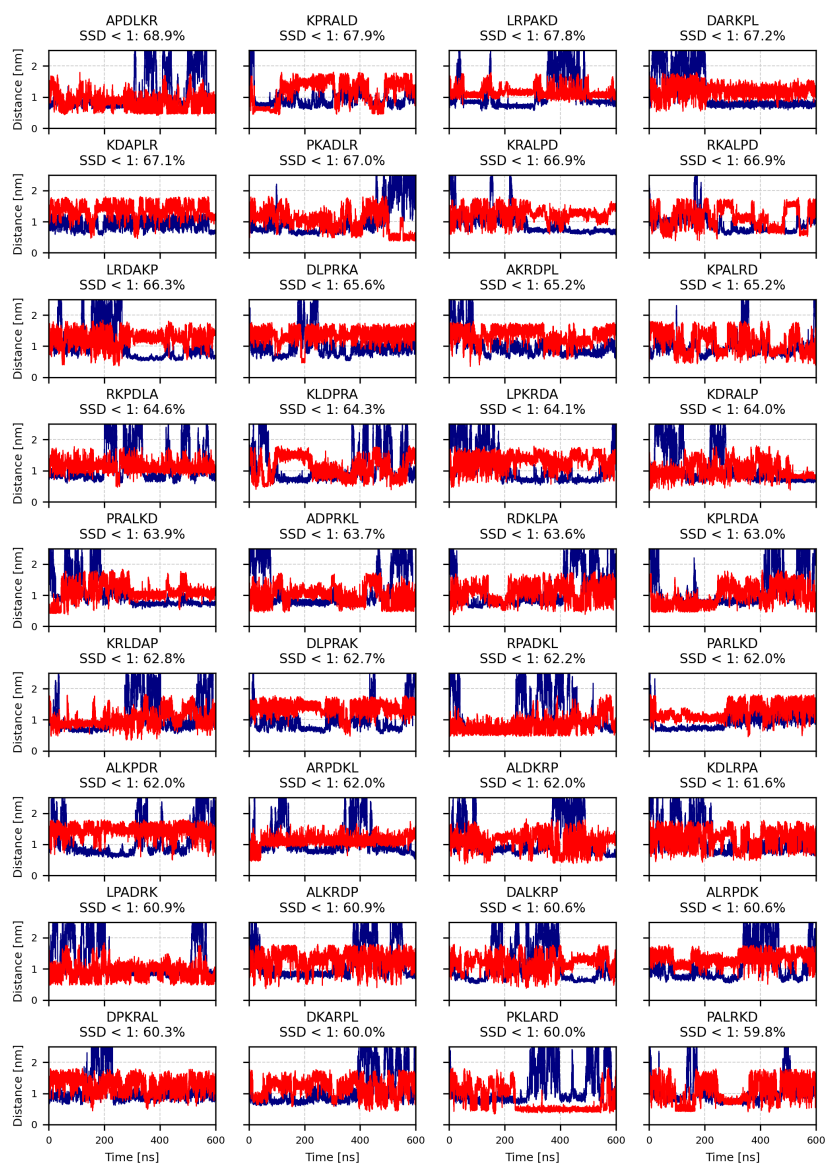
Roja Rahmani¹ and Alexander P. Lyubartsev^{2*}

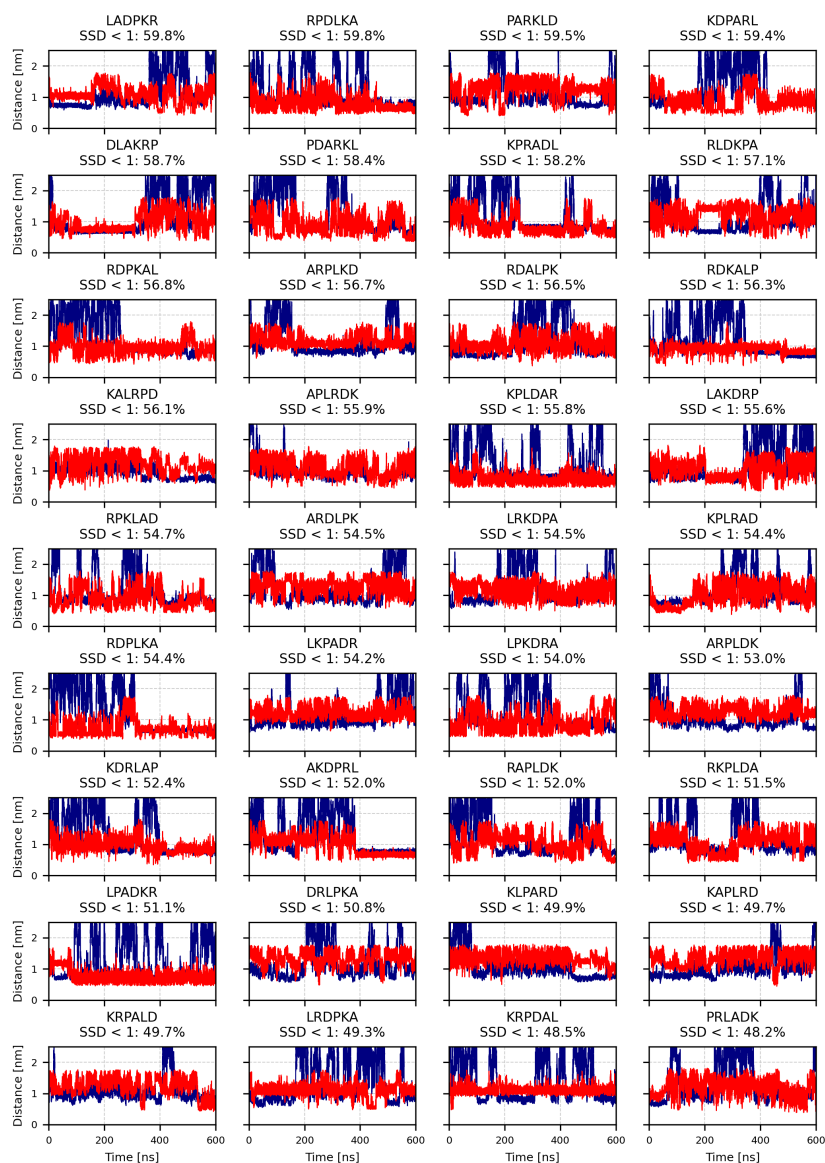
^{1,2}Department of Chemistry, Stockholm University, Svante Arrhenius väg 16C, Stockholm, 10691, Sweden.

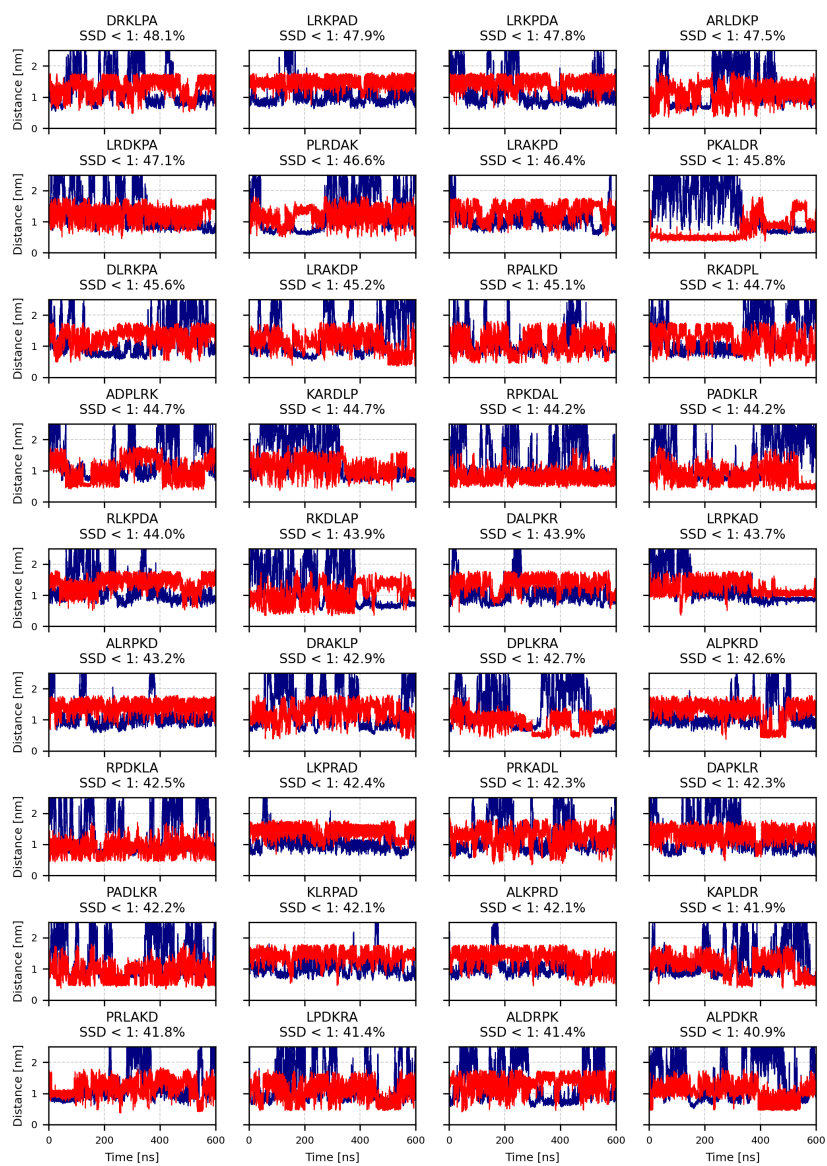
*Corresponding author(s). E-mail(s): alexander.lyubartsev@su.se;
Contributing authors: roja.rahmani@su.se;

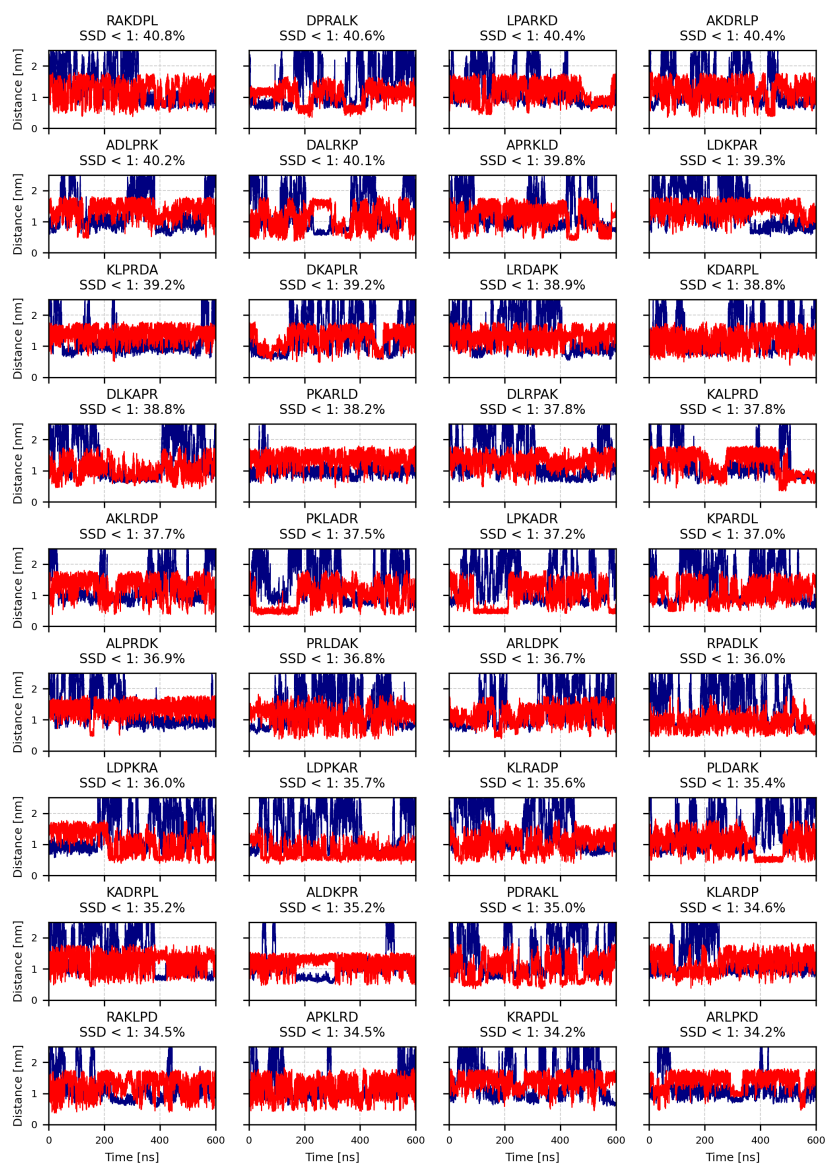


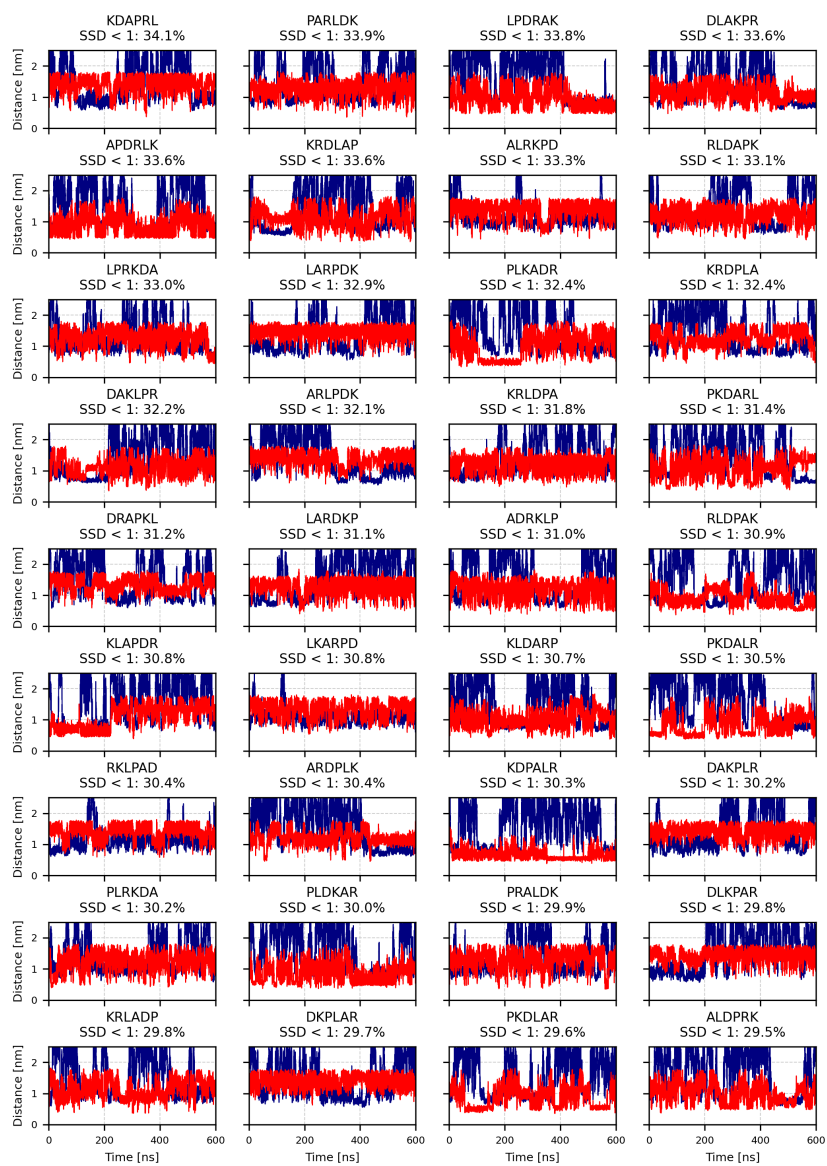


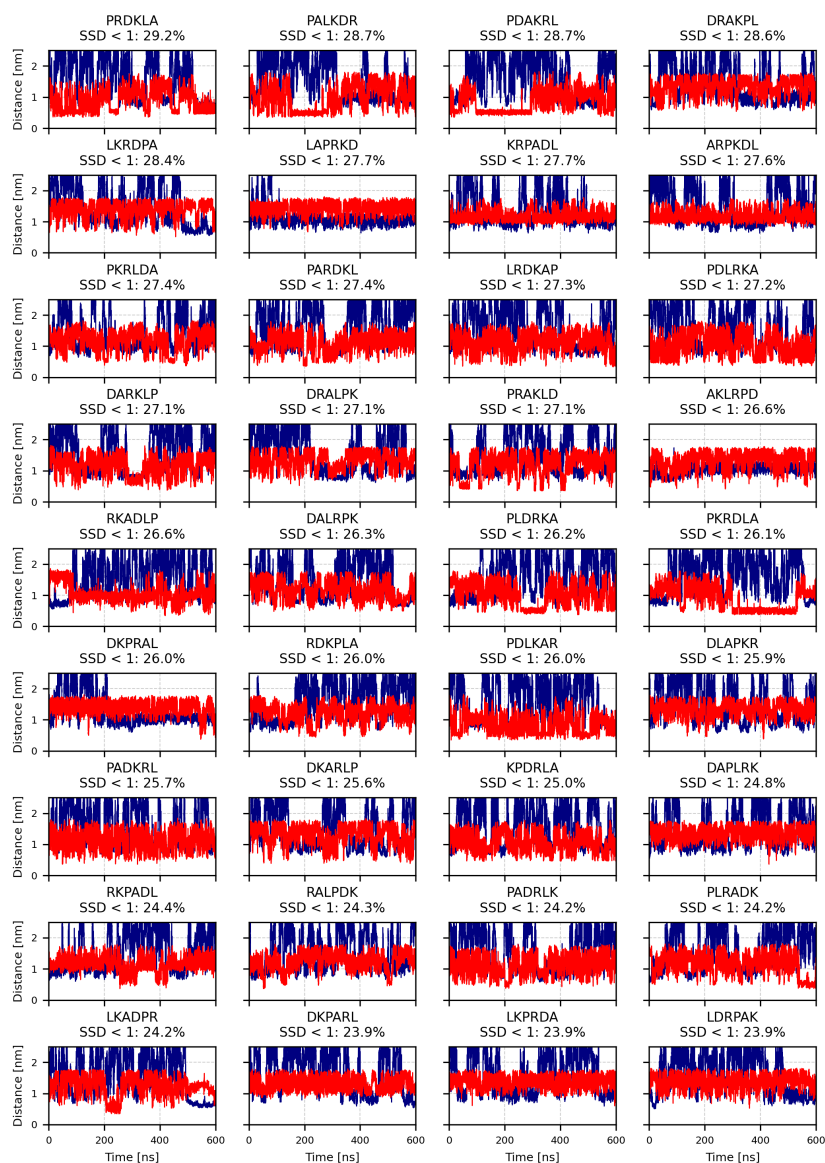


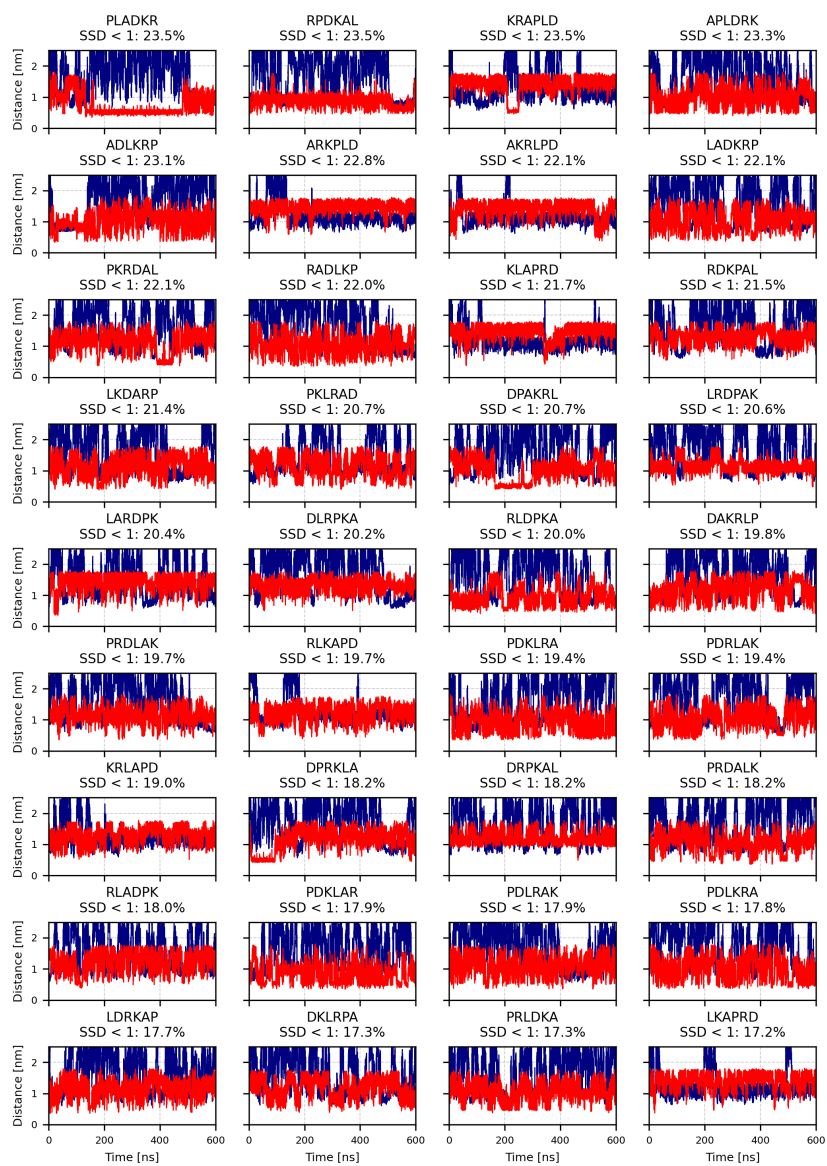












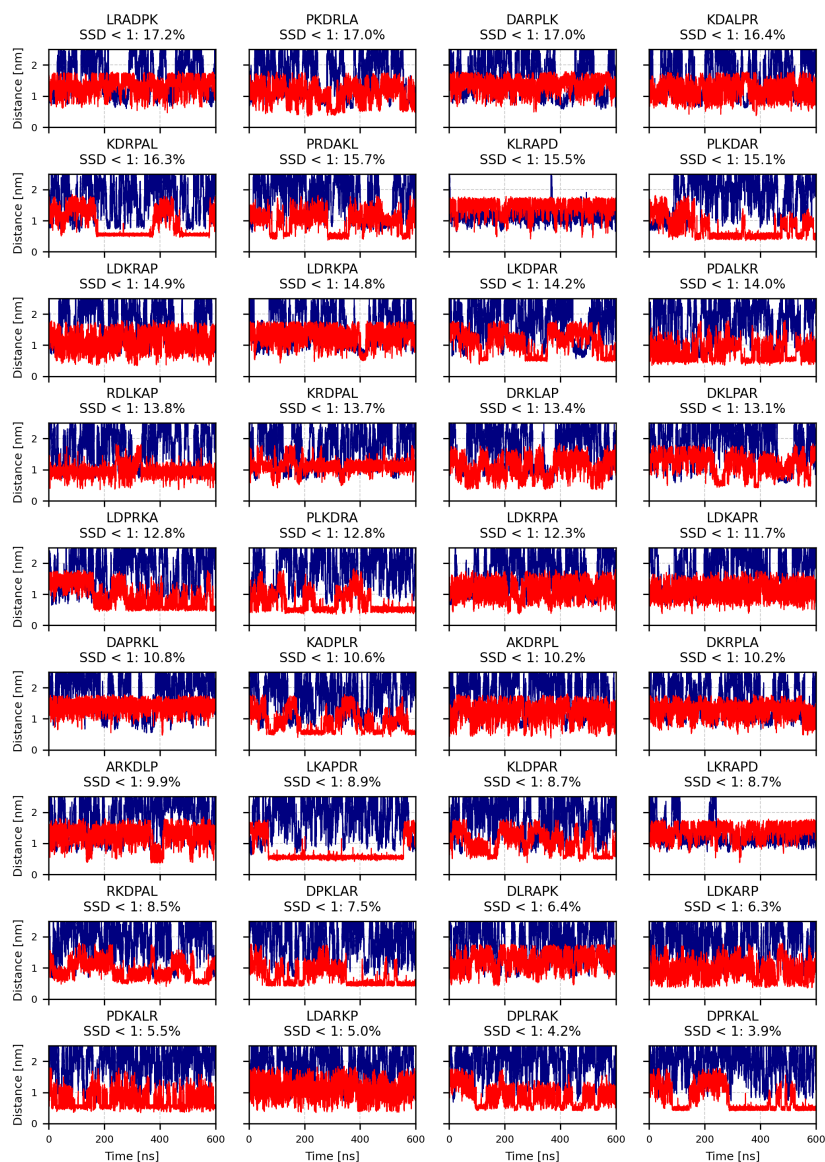


Fig. S1 SSD and EED for all 360 sequences in this study.

Sequence	% bound	RDF	Sequence	% bound	RDF	Sequence	% bound	RDF
PLARKD	100.00	K_OF_NZ	LRPKDA	73.60	L_OF_N	KALRPD	56.09	K_OF_N
RLDKAP	99.56	R_OF_N	AKLDRP	72.67	A_OF_N	APLRDK	55.88	A_OF_N
DPKLRA	99.14	A_OF_OC2	APLRKD	72.45	A_OF_N	KPLDAR	55.79	K_OF_NZ
PKRALD	98.36	P_OF_N	KADPRL	72.44	K_OF_N	LAKDRP	55.58	L_OF_N
RPLDKA	98.09	R_OF_N	LADRPK	72.07	L_OF_N	RPKLAD	54.70	K_OF_NZ
PRLKAD	97.90	D_OF_OC2	KADLPR	71.84	K_OF_N	ARDLPK	54.54	A_OF_N
KRPLAD	97.76	K_OF_N	KPALDR	71.77	K_OF_NZ	LRKDPA	54.49	K_OF_NZ
AKPLDR	97.52	A_OF_N	RPDALK	71.68	R_OF_N	KPLRAD	54.39	K_OF_N
RLAPKD	96.76	R_OF_N	LKPDRA	71.49	L_OF_N	RDPLKA	54.35	R_OF_N
ADKPLR	96.70	R_OF_OC2	LPAKDR	70.92	K_OF_NZ	LKPADR	54.23	L_OF_N
RKLPDA	96.51	R_OF_N	RPKADL	70.23	R_OF_N	LPKDRA	54.05	L_OF_N
LPDARK	96.41	L_OF_N	APKLDL	70.07	A_OF_N	ARPLDK	53.04	A_OF_N
RADPKL	96.10	L_OF_OC1	APDLKR	68.93	A_OF_N	KDRLAP	52.38	K_OF_N
KPRLDA	95.93	K_OF_N	KPRALD	67.92	K_OF_NZ	AKDPRL	52.03	A_OF_N
PAKRLD	95.63	P_OF_N	LRPAKD	67.82	L_OF_N	RAPLDK	52.03	R_OF_N
RPLAKD	95.55	R_OF_NH2	DARKPL	67.20	D_OF_N	RKPLDA	51.52	R_OF_N
RADPLK	94.34	R_OF_N	KDAPLR	67.09	K_OF_N	LPADKR	51.07	L_OF_N
RPDLAK	93.99	R_OF_N	PKADLR	67.03	P_OF_N	DRLPKA	50.80	D_OF_N
RLAKPD	93.02	R_OF_N	KRALPD	66.94	K_OF_N	KLPARD	49.92	K_OF_N
DAKRPL	92.74	D_OF_N	RKALPD	66.86	R_OF_N	KAPLRD	49.72	K_OF_N
RAKPLD	92.64	R_OF_N	LRDAKP	66.32	L_OF_N	KRPALD	49.69	D_OF_OC1
RKAPDL	91.96	R_OF_N	DLPRKA	65.59	D_OF_N	LRDPKA	49.29	L_OF_N
KALPDR	91.73	R_OF_NH2	AKRDPL	65.20	A_OF_N	KRPDAL	48.51	K_OF_N
PDKRAL	91.40	P_OF_N	KPALRD	65.15	K_OF_NZ	PRLADK	48.18	K_OF_NZ
RADKPL	88.43	R_OF_N	RKPDLA	64.58	R_OF_N	DRKLPA	48.11	D_OF_N
RPKLDA	87.53	R_OF_N	KLDPRA	64.35	K_OF_N	LRKPAD	47.85	K_OF_NZ
PDKRLA	87.53	P_OF_N	LPKRDA	64.08	L_OF_N	LRKPDA	47.84	K_OF_NZ
KRALDP	87.47	K_OF_N	KDRALP	63.99	K_OF_N	ARLDKP	47.54	A_OF_N
KLRPDA	87.30	K_OF_N	PRALKD	63.85	D_OF_OC1	LRDKPA	47.11	L_OF_N
APDKLR	87.26	A_OF_N	ADPRKL	63.66	A_OF_N	PLRDAK	46.56	P_OF_N
DPALKR	87.04	D_OF_N	RDKLPA	63.58	R_OF_N	LRAKPD	46.39	K_OF_NZ
RKALDP	86.32	K_OF_NZ	KPLRDA	63.05	D_OF_OD2	PKALDR	45.83	P_OF_N
RKAPLD	86.03	R_OF_N	KRLDAP	62.81	K_OF_N	DLRKPA	45.60	D_OF_N
KPDLAR	85.32	K_OF_NZ	DLPRAK	62.68	D_OF_N	LRAKDP	45.20	L_OF_N
RPALDK	83.82	R_OF_N	RPADKL	62.18	R_OF_N	RPALKD	45.14	D_OF_OD1
LPAKRD	83.22	L_OF_N	PARLKD	62.01	P_OF_N	RKADPL	44.71	R_OF_N
AKLPRD	83.08	A_OF_N	ALKPDR	61.99	A_OF_N	ADPLRK	44.70	K_OF_NZ
LKRDPAP	83.05	K_OF_NZ	ARPDKL	61.98	A_OF_N	KARDLP	44.69	K_OF_N
PKLDRA	81.84	P_OF_N	ALDKRP	61.96	A_OF_N	RPKDAL	44.20	K_OF_NZ
KLPADR	81.09	K_OF_N	KDLRPA	61.56	K_OF_N	PADKLR	44.16	K_OF_NZ
LDRPKA	80.73	L_OF_N	LPADRK	60.86	D_OF_OD1	RLKPDA	44.02	K_OF_NZ
RPLKDA	80.72	R_OF_N	ALKRDP	60.86	D_OF_OD1	RKDLAP	43.93	R_OF_N
KDRAPL	80.71	K_OF_N	DALKRP	60.65	D_OF_N	DALPKR	43.85	D_OF_N
LAKRDP	80.69	L_OF_N	ALRPDK	60.64	A_OF_N	LRPKAD	43.71	D_OF_OD1
KARPDL	80.49	K_OF_N	DPKRAL	60.29	D_OF_N	ALRPKD	43.20	D_OF_OD2
KLDRPA	80.47	K_OF_N	DKARPL	60.00	D_OF_N	DRAKLP	42.86	D_OF_N
APRDKL	79.95	K_OF_NZ	PKLARD	59.95	D_OF_OC1	DPLKRA	42.71	D_OF_N
DRKALP	79.90	D_OF_N	PALRKD	59.84	P_OF_N	ALPKRD	42.56	K_OF_NZ
ADRLKP	79.79	A_OF_N	LADPKR	59.82	L_OF_N	RPDKLA	42.45	R_OF_N
AKDPRL	78.40	A_OF_N	RPDLKA	59.75	K_OF_NZ	LKPRAD	42.39	D_OF_OD2
DRLKAP	77.49	D_OF_N	PARKLD	59.46	P_OF_N	PRKADL	42.34	P_OF_N
APLDKR	76.84	K_OF_NZ	KDPARL	59.42	K_OF_N	DAPKLR	42.30	D_OF_N
ARPKLD	76.70	A_OF_N	DLAKRP	58.66	D_OF_N	PADLKR	42.19	K_OF_NZ
DRKPAL	76.63	D_OF_N	PDARKL	58.41	P_OF_N	KLRPAD	42.15	K_OF_NZ
KLDRAP	76.26	K_OF_N	KPRADL	58.20	K_OF_NZ	ALKPRD	42.09	D_OF_OC2
KRDALP	76.14	K_OF_NZ	RLDKPA	57.10	R_OF_N	KAPLDR	41.94	R_OF_OC1
DRLAKP	75.37	D_OF_N	RDPKAL	56.75	R_OF_N	PRLAKD	41.79	D_OF_OC2
PKARDL	74.02	P_OF_N	ARPLKD	56.73	A_OF_N	LPDKRA	41.38	K_OF_NZ
PDAKLR	73.94	P_OF_N	RDALPK	56.55	R_OF_N	ALDRPK	41.38	A_OF_N
ADKLRP	73.64	A_OF_N	RDKALP	56.32	R_OF_N	ALPDKR	40.86	A_OF_N

Sequence	% bound	RDF	Sequence	% bound	RDF	Sequence	% bound	RDF
RAKDPL	40.77	R_OF_N	RKLPAD	30.45	D_OF_OD2	LKDARP	21.45	K_OF_NZ
DPRALK	40.60	D_OF_N	ARDPLK	30.44	A_OF_N	PKLRAD	20.74	D_OF_OC2
LPARKD	40.44	L_OF_N	KDPALR	30.27	K_OF_NZ	DPAKRL	20.69	K_OF_NZ
AKDRLP	40.35	A_OF_N	DAKPLR	30.18	D_OF_N	LRDPAK	20.63	K_OF_NZ
ADLPRK	40.22	A_OF_N	PLRKDA	30.16	D_OF_OD2	LARDPK	20.45	L_OF_N
DALRKP	40.14	D_OF_N	PLDKAR	30.04	R_OF_OC1	DLRPKA	20.25	D_OF_N
APRKLD	39.84	K_OF_NZ	PRALDK	29.86	K_OF_NZ	RLDPKA	19.97	K_OF_NZ
LDKPAR	39.34	L_OF_N	DLKPAR	29.82	D_OF_N	DAKRLP	19.82	K_OF_NZ
KLPRDA	39.22	K_OF_N	KRLADP	29.76	P_OF_OC1	PRDLAK	19.73	K_OF_NZ
DKAPLR	39.18	D_OF_N	DKPLAR	29.71	D_OF_N	RLKAPD	19.73	D_OF_OD1
LRDAPK	38.86	L_OF_N	PKDLAR	29.64	R_OF_OC1	PDKLRA	19.42	P_OF_N
KDARPL	38.81	K_OF_N	ALDPRK	29.49	A_OF_N	PDRLAK	19.36	P_OF_N
DLKAPR	38.79	D_OF_N	PRDKLA	29.16	K_OF_NZ	KRLAPD	19.03	D_OF_OD2
PKARLD	38.18	R_OF_NH1	PALKDR	28.66	R_OF_OC2	DPRKLA	18.23	D_OF_N
DLRPAK	37.79	D_OF_N	PDAKRL	28.66	P_OF_N	DRPKAL	18.23	K_OF_NZ
KALPRD	37.77	K_OF_NZ	DRAKPL	28.61	D_OF_N	PRDALK	18.22	K_OF_NZ
AKLRDP	37.66	A_OF_N	LKRDPK	28.45	L_OF_N	RLADPK	17.99	K_OF_NZ
PKLADR	37.48	P_OF_N	LAPRKD	27.72	D_OF_OD2	PDKLAR	17.95	K_OF_NZ
LPKADR	37.25	K_OF_NZ	KRPADL	27.68	L_OF_OC2	PDLRAK	17.88	P_OF_N
KPARDL	37.00	K_OF_NZ	ARPKDL	27.56	A_OF_N	PDLKRA	17.80	K_OF_NZ
ALPRDK	36.89	K_OF_NZ	PKRLDA	27.44	A_OF_OC2	LDRKAP	17.72	K_OF_NZ
PRLDAK	36.84	K_OF_NZ	PARDKL	27.40	K_OF_NZ	DKLRPA	17.32	K_OF_NZ
ARLDPK	36.66	A_OF_N	LRDKAP	27.27	K_OF_NZ	PRLDKA	17.29	K_OF_NZ
RPADLK	36.05	R_OF_N	PDLRKA	27.21	K_OF_NZ	LKAPRD	17.19	D_OF_OD
LDPKRA	35.98	L_OF_N	DARKLP	27.12	D_OF_N	LRADPK	17.18	K_OF_NZ
LDPKAR	35.72	K_OF_NZ	DRALPK	27.08	D_OF_N	PKDRLA	16.98	P_OF_N
KLRADP	35.59	K_OF_NZ	PRAKLD	27.05	K_OF_NZ	DARPLK	16.97	K_OF_NZ
PLDARK	35.39	K_OF_NZ	AKLRPD	26.62	D_OF_OD1	KDALPR	16.45	R_OF_OC
KADRPL	35.21	K_OF_N	RKADLP	26.55	K_OF_NZ	KDRPAL	16.30	K_OF_NZ
ALDKPR	35.16	A_OF_N	DALRPK	26.31	D_OF_N	PRDAKL	15.74	K_OF_NZ
PDRAKL	35.00	K_OF_NZ	PLDRKA	26.24	P_OF_N	KLRAPD	15.46	D_OF_OC
KLARDP	34.64	P_OF_OC2	PKRDLA	26.15	R_OF_NH2	PLKDAR	15.06	K_OF_NZ
RAKLDP	34.49	K_OF_NZ	DKPRAL	26.04	D_OF_N	LDKRAP	14.87	K_OF_NZ
APKLRD	34.47	D_OF_OC2	RDKPLA	26.02	R_OF_N	LDRKPA	14.84	L_OF_N
KRAPDL	34.25	K_OF_N	PDLKAR	25.96	K_OF_NZ	LKDPAR	14.20	L_OF_N
ARLPKD	34.24	D_OF_OC2	DLAPKR	25.90	K_OF_NZ	PDALKR	14.02	K_OF_NZ
KDAPRL	34.09	K_OF_N	PADKRL	25.74	P_OF_N	RDLKAP	13.83	K_OF_NZ
PARLDK	33.87	R_OF_NH1	DKARLP	25.61	D_OF_N	KRDPAL	13.68	K_OF_NZ
LPDRAK	33.83	K_OF_NZ	KPDRLA	25.04	K_OF_NZ	DRKLAP	13.41	K_OF_NZ
DLAKPR	33.61	D_OF_N	DAPLRK	24.76	D_OF_N	DKLPAR	13.05	D_OF_N
APDRLK	33.58	K_OF_NZ	RKPADL	24.37	K_OF_NZ	LDPRKA	12.81	A_OF_OC1
KRDLAP	33.57	K_OF_N	RALPDK	24.33	K_OF_NZ	PLKDRA	12.80	K_OF_NZ
ALRKPD	33.31	K_OF_NZ	PADRLK	24.19	K_OF_NZ	LDKRPA	12.30	A_OF_OC1
RLDAPK	33.15	R_OF_N	PLRADK	24.17	K_OF_NZ	LDKAPR	11.70	K_OF_NZ
LPRKDA	32.95	K_OF_NZ	LKADPR	24.17	L_OF_N	DAPRKL	10.84	D_OF_N
LARPDK	32.94	L_OF_N	DKPARL	23.90	K_OF_NZ	KADPLR	10.60	K_OF_NZ
PLKADR	32.43	R_OF_OC2	LKPRDA	23.90	K_OF_NZ	AKDRPL	10.25	L_OF_OC2
KRDPLA	32.39	K_OF_NZ	LDRPAK	23.86	L_OF_N	DKRPLA	10.24	K_OF_NZ
DAKLPR	32.22	D_OF_N	PLADKR	23.54	K_OF_NZ	ARKDLP	9.90	A_OF_N
ARLPDK	32.14	A_OF_N	RPDKAL	23.54	R_OF_NH2	LKAPDR	8.90	D_OF_OD1
KRLDPA	31.84	K_OF_N	KRAPLD	23.49	K_OF_NZ	KLDPAR	8.72	K_OF_NZ
PKDARL	31.45	P_OF_N	APLDRK	23.31	A_OF_N	LKRAPD	8.65	D_OF_OD2
DRAPKL	31.20	D_OF_N	ADLKRP	23.11	A_OF_N	RKDPAK	8.46	R_OF_N
LARDKP	31.05	L_OF_N	ARKPLD	22.82	D_OF_OD2	DPKLAR	7.53	K_OF_NZ
ADRKLP	30.99	A_OF_N	AKRLPD	22.13	D_OF_OC2	DLRAPK	6.42	K_OF_NZ
RLDPAK	30.90	R_OF_N	LADKRP	22.10	L_OF_N	LDKARP	6.26	K_OF_NZ
KLAPDR	30.81	K_OF_N	PKRDAL	22.05	P_OF_N	PDKALR	5.48	R_OF_OC2
LKARPDP	30.75	D_OF_OC2	RADLKP	21.98	R_OF_N	LDARKP	5.02	P_OF_OC2
KLDARP	30.73	K_OF_N	KLAPRD	21.72	D_OF_OC1	DPLRAK	4.25	K_OF_NZ
PKDALR	30.54	P_OF_N	RDKPAL	21.47	K_OF_NZ	DPRKAL	3.89	R_OF_NH1

Table S1 Peptides binding ranking according to the percentage of time to have SSD value less than 1 nm over simulation time, and notation for RDFs having highest maximum.

Sequence	EED _a	std _a	EED _d	std _d	Sequence	EED _a	std _a	EED _d	std _d	Sequence	EED _a	std _a	EED _d	std _d
PLARKD	1.16	0.22	1.15	-	APRDKL	0.79	0.23	1.09	0.32	KRLDAP	1.03	0.23	1.00	0.24
RLDKAP	0.98	0.21	1.30	0.25	DRKALP	1.26	0.23	1.30	0.29	DLPRAK	1.36	0.19	1.44	0.14
DPKLRRA	0.94	0.17	1.49	0.15	ADRLKP	1.01	0.24	1.19	0.23	RPADKL	0.81	0.24	0.82	0.22
PKRALD	1.15	0.11	1.32	0.18	AKDPLR	1.11	0.30	1.24	0.31	PARLKD	1.16	0.17	1.47	0.18
RPLDKA	0.79	0.20	1.20	0.21	DRLKAP	1.16	0.27	1.38	0.18	ALKPDR	1.46	0.16	1.40	0.17
PRLKAD	1.31	0.26	1.46	0.13	APLDKR	0.70	0.14	0.77	0.26	ARPDKL	1.12	0.18	1.10	0.12
KRPLAD	1.05	0.07	1.23	0.17	ARPKLD	1.01	0.28	1.18	0.28	ALDKRP	1.12	0.21	1.07	0.31
AKPLDR	0.68	0.15	1.46	0.13	DRKPAL	1.39	0.17	1.52	0.10	KDLRPA	1.15	0.26	1.25	0.26
RLAPKD	1.17	0.21	1.46	0.10	KLDRAP	0.99	0.18	1.16	0.26	LPADRK	0.89	0.18	0.92	0.28
ADKPLR	1.39	0.17	1.52	0.15	KRDALP	1.05	0.16	0.90	0.24	ALKRDP	1.30	0.26	1.30	0.26
RKLPPA	1.17	0.16	1.48	0.14	DRLAKP	1.11	0.26	1.21	0.29	DALKRP	1.20	0.20	1.19	0.29
LPDARK	0.84	0.23	1.34	0.16	PKARDL	1.30	0.23	1.34	0.22	ALRPDK	1.30	0.17	1.39	0.16
RADPKL	1.26	0.22	1.52	0.10	PDAKLR	0.82	0.23	0.95	0.29	DPKRAL	1.25	0.23	1.32	0.21
KPRLDA	1.04	0.26	1.33	0.15	ADKLRP	0.90	0.22	1.05	0.28	DKARPL	1.20	0.24	1.21	0.32
PAKRLD	0.84	0.39	1.35	0.20	LRPKDA	1.17	0.15	1.25	0.19	PKLARD	0.82	0.35	0.68	0.35
RPLAKD	0.66	0.10	0.92	0.27	AKLDRP	1.20	0.24	1.26	0.27	PALRKD	0.95	0.34	1.27	0.33
RADPLK	1.30	0.22	1.43	0.14	APLRKD	0.98	0.11	1.29	0.20	LADPKR	1.09	0.20	1.13	0.33
RPDLAK	0.76	0.13	0.82	0.15	KADPRL	1.14	0.30	1.20	0.28	RPDLKA	0.76	0.21	0.87	0.25
RLAKPD	0.96	0.17	1.16	0.30	LADRPK	1.38	0.27	1.29	0.23	PARKLD	1.26	0.32	1.32	0.34
DAKRPL	1.15	0.17	1.40	0.17	KADLPR	1.29	0.23	1.34	0.23	KDPAKL	0.86	0.20	0.94	0.35
RAKPLD	1.22	0.19	1.46	0.10	KPALDR	0.71	0.14	0.82	0.22	DLAKRP	0.90	0.25	1.14	0.29
RKAPDL	1.31	0.27	1.46	0.14	RPDALK	0.86	0.15	0.90	0.16	PDARKL	0.85	0.27	0.99	0.34
KALPDR	1.33	0.19	1.44	0.13	LKPDRA	1.14	0.17	1.19	0.21	KPRADL	0.78	0.21	1.05	0.33
PDKRAL	1.24	0.27	1.31	0.22	LPAKDR	0.77	0.21	0.98	0.31	RLDKPA	1.29	0.23	1.15	0.27
RADKPL	1.11	0.26	1.36	0.19	RPKADL	0.72	0.10	0.77	0.13	RDPKAL	0.96	0.18	0.98	0.28
RPKLDA	0.74	0.16	0.74	0.20	APKLDR	0.93	0.26	1.13	0.30	ARPLKD	1.12	0.14	1.27	0.20
PKRLA	1.21	0.25	1.39	0.15	APDLKR	0.83	0.22	0.84	0.28	RDALPK	1.07	0.20	1.17	0.25
KRALDP	1.37	0.10	1.09	0.22	KPRALD	1.12	0.40	1.35	0.29	RDKALP	0.87	0.12	0.92	0.11
KLRPDA	1.15	0.19	1.26	0.19	LRPAKD	1.13	0.12	1.22	0.19	KALRPD	1.09	0.22	1.39	0.23
APDKLR	0.87	0.21	1.07	0.23	DARKPL	1.20	0.12	1.25	0.25	APLRDK	1.02	0.25	1.27	0.18
DPALKR	0.92	0.18	1.21	0.23	KDAPLR	1.31	0.23	1.50	0.12	KPLDAR	0.72	0.15	0.76	0.17
RKALDP	0.96	0.36	1.14	0.32	PKADLR	1.09	0.25	0.94	0.43	LAKDRP	0.97	0.25	1.17	0.31
RKAPLD	1.00	0.16	1.34	0.21	KRALPD	1.22	0.16	1.33	0.24	RPKLAD	0.78	0.25	1.05	0.28
KPDLAR	0.69	0.11	0.73	0.15	RKALPD	1.07	0.32	1.30	0.29	ARDLPK	1.26	0.21	1.36	0.20
RPALDK	0.78	0.11	0.76	0.22	LRDAKP	1.28	0.16	1.23	0.26	LRKDPA	1.18	0.21	1.21	0.19
LPAKRD	1.21	0.19	1.24	0.24	DLPRKA	1.36	0.15	1.39	0.25	KPLRAD	0.86	0.28	1.18	0.26
AKLPRD	1.19	0.19	1.43	0.19	AKRDPL	1.29	0.21	1.46	0.18	RDPLKA	0.69	0.16	0.79	0.31
LKRDAP	1.56	0.10	1.32	0.17	KPALRD	1.02	0.30	1.32	0.29	LKPADR	1.18	0.17	1.32	0.18
PKLDRA	0.80	0.32	1.24	0.32	RKPDLA	1.12	0.16	1.14	0.17	LPKDRA	0.89	0.32	0.91	0.32
KLPADR	1.12	0.22	1.31	0.21	KLDPPA	1.15	0.33	1.06	0.33	ARPLDK	1.23	0.16	1.30	0.19
LDRPKA	1.30	0.21	1.46	0.13	LPKRDA	1.34	0.19	1.27	0.22	KDRLAP	0.94	0.17	1.04	0.22
RPLKDA	0.75	0.21	0.75	0.19	KDRALP	1.04	0.24	0.99	0.22	AKDPRL	0.81	0.25	1.16	0.25
KDRAPL	1.21	0.25	1.49	0.13	PRALKD	1.07	0.21	1.21	0.35	RAPLKD	1.00	0.26	1.13	0.30
LAKRDP	0.94	0.19	1.37	0.26	ADPRKL	1.01	0.24	1.01	0.32	RKPLDA	0.98	0.29	1.14	0.28
KARPD	1.31	0.19	1.38	0.15	RDKLPA	1.09	0.24	1.09	0.31	LPADKR	0.79	0.23	0.70	0.16
KLDRPA	1.39	0.20	1.20	0.22	KPLRDA	0.94	0.29	1.07	0.33	DRLPKA	1.29	0.22	1.39	0.22

Table S2 Peptides binding ranking according to the percentage of time to have SSD value less than 1 nm over simulation time.