ELECTRONIC SUPPLEMENTARY INFORMATION (ESI)

Comprehensive *in silico* modeling of plant PRR Xa21 and its interaction with RaxX21-sY and OsSERK2

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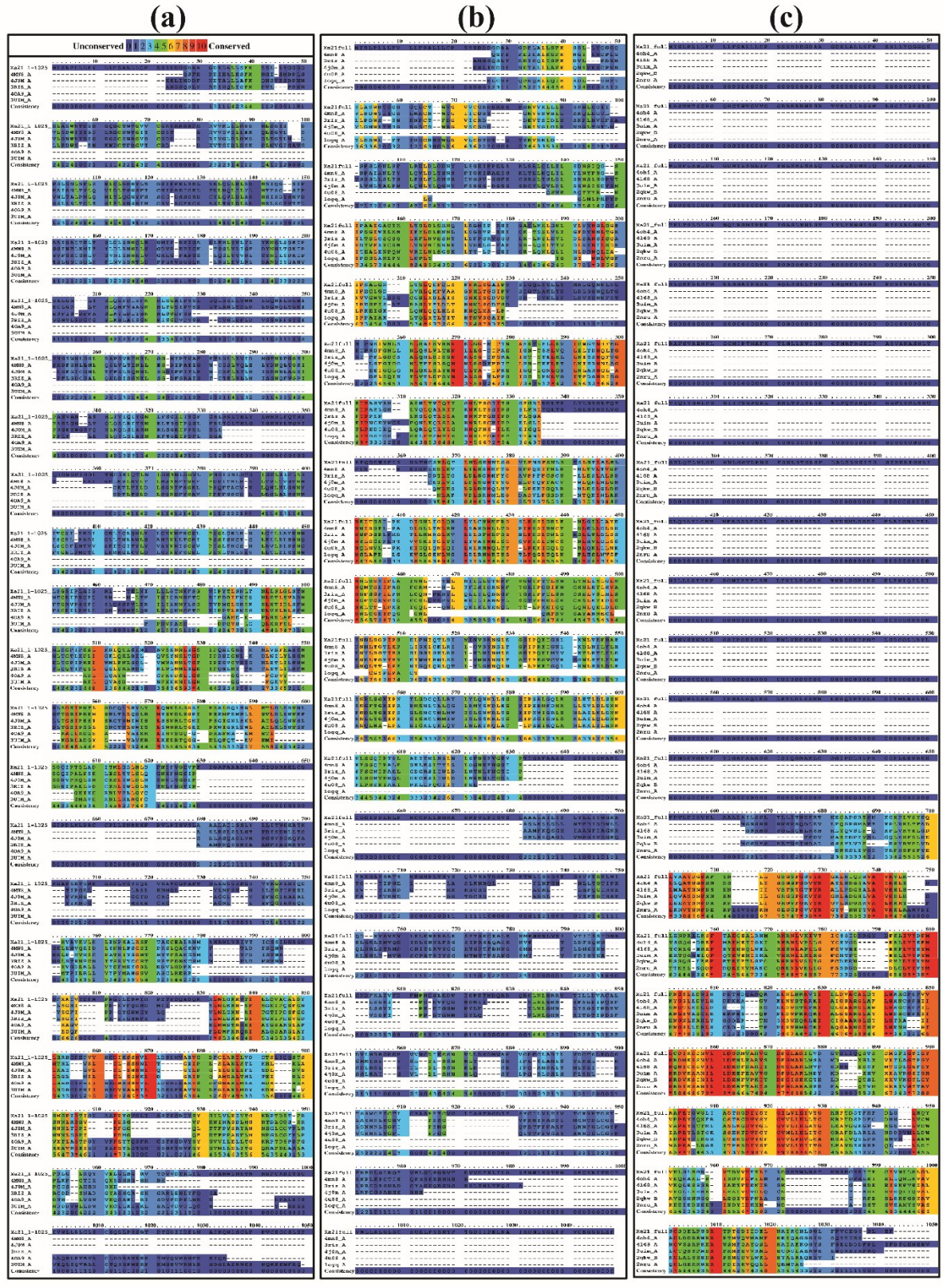

Fig. S1 Multiple sequence alignment (MSA) of Xa21 protein sequence and top five BLASTP results for (a) Full sequence 1-1025 (b) LRR templates (c) JM and Kinase templates

Fig. S2 Secondary structure of Xa21 protein predicted by PSIPRED

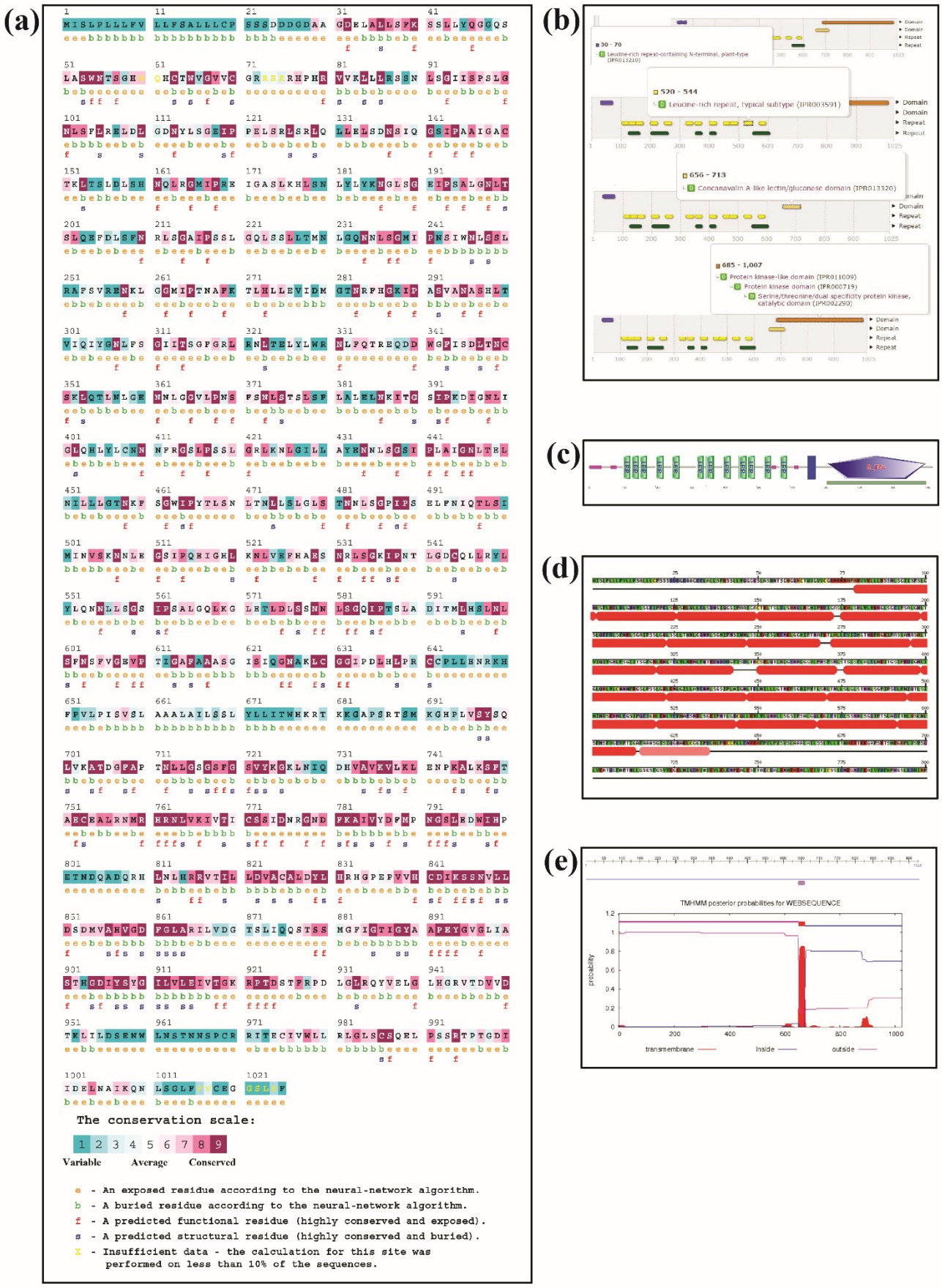

Fig. S3 (a) Conserved region prediction of Xa21 by the ConSurf tool. (b) Domain boundary prediction of Xa21 using InterPro. (c) Domain boundary prediction of Xa21 by the SMART tool. (d) Repeated Xa21 LRR region prediction by the HHrepID tool. (e) Transmembrane region prediction of Xa21 protein by the TMHMM tool.

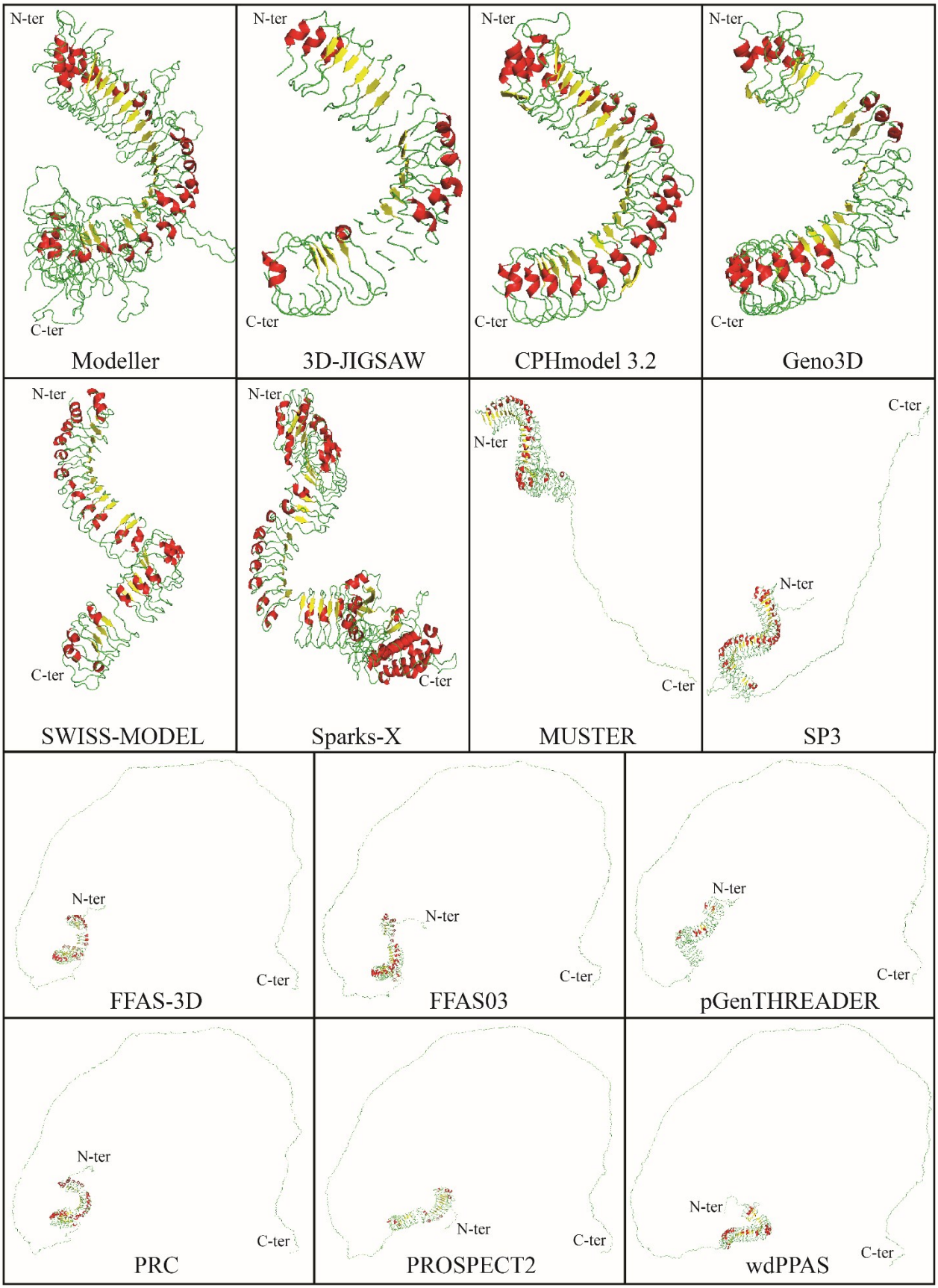

Fig. S4 Cartoon representations of the Xa21 proteins modeled using single template modeling approaches. Red colored regions indicate alpha helixes, yellow colored regions indicate beta sheets and green colored regions indicate coiled regions.

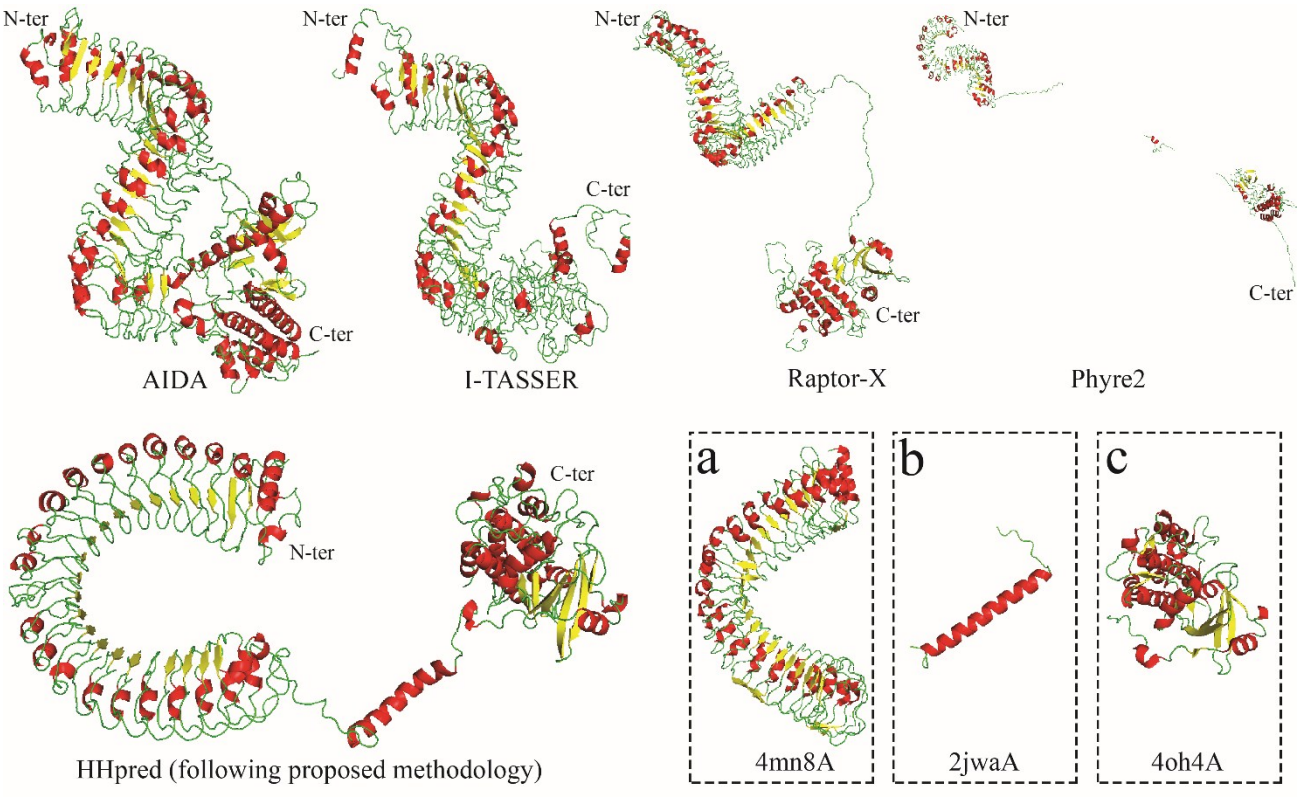

Fig. S5. Cartoon representations of the Xa21 protein modeled using multiple template modeling approaches. The boxed proteins are 3D structures of the best template from the PDB - (a) LRR domain, (b) TM domain, (c) Kinase domain, of Xa21. Red colored regions indicate alpha helixes, yellow colored regions indicate beta sheets and green colored regions indicate coil regions.

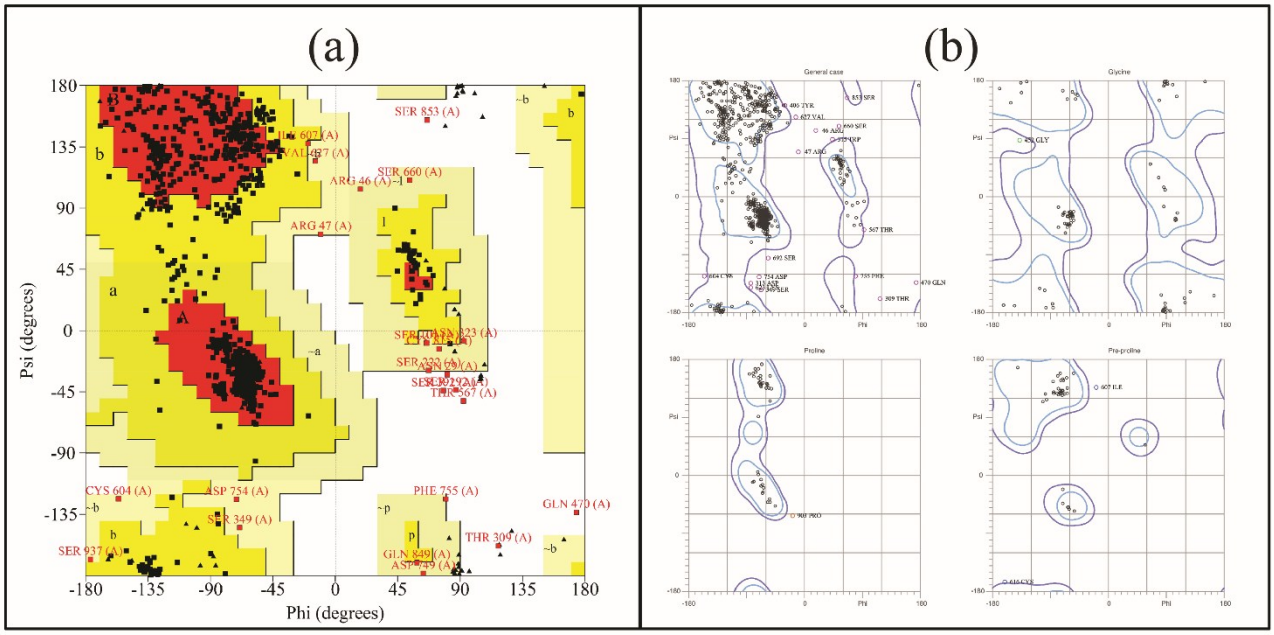

Fig. S6. Ramachandran plot summery for Xa21 protein modeled by the HHpred server is on the right-hand side and the left-hand side figure indicates the MolProbity for the Ramachandran plot.

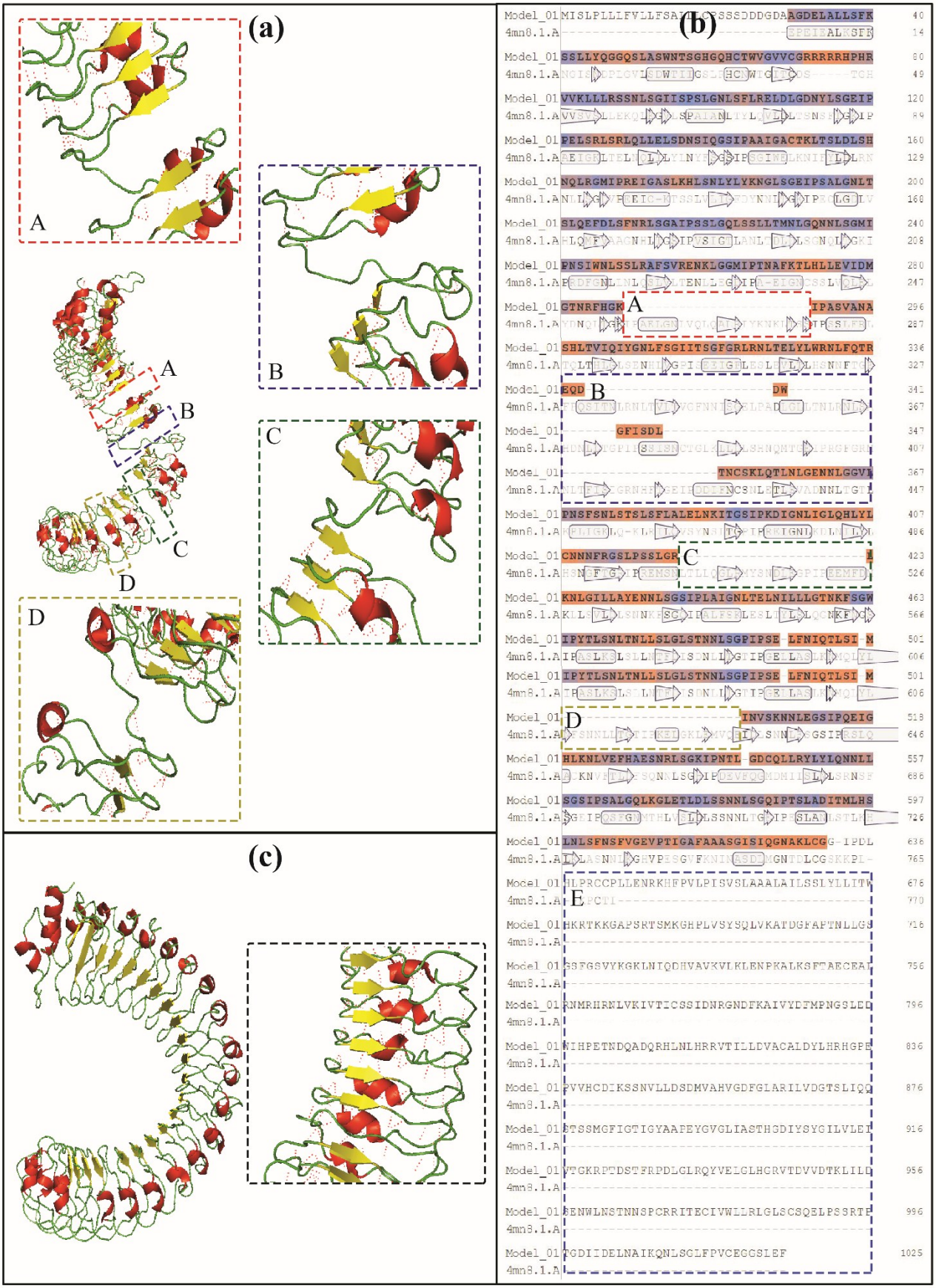

Fig. S7. (a) Cartoon representation of the Xa21 protein modeled by the Swiss-model tool showing the different gaps in the structure. (b) Alignment of the modeled protein sequence and the template sequence by Swiss-model. (c) Cartoon representation of LRR domain modeled by the HHpred server. Red colored regions indicate alpha helix, yellow colored regions indicate beta sheet and green colored regions indicate coil region.

Table S1A. Modeling methodology of the Xa21 Protein using Single Template Modeling approach

Tool	Modeling Method	Template
Modeller 9.15	Homology	4mn8A
3D-JIGSAW	Homology	4mn8A
CPHmodel 3.2	Homology	4mn8A
Geno3D	Homology	4mn8A
Swissmodel	Homology	4mn8A
PRC	Threading	4mn8A
pGenTHREADER	Threading	4mn8A
Prospect2	Threading	4mn8A
FFAS-3D	Threading	4mn8A
FFAS03	Threading	4mn8A
SP3	Threading	4mn8A
Sparks-X	Threading	4mn8A
Musterm	Threading	4mn8A
WdPPAS	Threading	4j0mA

Table S1B. Modeling methodology of the Xa21 Protein using Multiple Template Modeling Approach

R/P ID	R/P Name	AA boundary	Tool	Modeling Method	Template(s)
Xa21lrr_1	N-term+LRR	27-634	HHpred	Homology	4mn8A
Xa21lrr_2	N-term+LRR	27-634	HHpred	Homology	4mn8A+4j0mA
Xa21lrr_3	N-term+LRR	27-634	HHpred	Homology	4mn8A+3rgzA
Xa21lrr_4	N-term+LRR	27-634	HHpred	Homology	4mn8A+1ogqA
Xa21lrr_5	N-term+LRR	27-634	HHpred	Homology	4mn8A+4j0mA+1ogqA
Xa21lrr_6	N-term+LRR	27-634	HHpred	Homology	4mn8A+1ogqA+3rgzA
Xa21lrr_7	N-term+LRR	27-634	HHpred	Homology	4mn8A+3rgzA+4j0mA
Xa21lrr_8	N-term+LRR	27-634	HHpred	Homology	4mn8A+1ogqA+4j0mA+3rgzA
Xa21lrr_9	N-term+LRR	27-634	HHpred	Homology	4mn8A+4u08A
Xa21lrr_10	N-term+LRR	27-634	HHpred	Homology	4mn8A+4u08A+3rgzA
Xa21lrr_11	N-term+LRR	27-634	HHpred	Homology	4mn8A+4u08A+4j0mA
Xa21lrr_12	N-term+LRR	27-634	HHpred	Homology	4mn8A+4u08A+1ogqA
Xa21lrr_13	N-term+LRR	27-634	HHpred	Homology	4mn8A+4u08A+3rgzA+4j0mA
Xa21lrr_14	N-term+LRR	27-634	HHpred	Homology	4mn8A+4u08A+4j0mA+1ogqA
Xa21lrr_15	N-term+LRR	27-634	HHpred	Homology	4mn8A+4u08A+4j0mA+3rgzA+1ogqA
Xa21lrr_16	N-term+LRR	27-634	HHpred	Homology	4u08A+3rgzA
Xa21lrr_17	N-term+LRR	27-634	HHpred	Homology	4u08A+4j0mA
Xa21lrr_18	N-term+LRR	27-634	HHpred	Homology	4u08A+1ogqA
Xa21lrr_19	N-term+LRR	27-634	HHpred	Homology	3rgzA+4j0mA
Xa21lrr_20	N-term+LRR	27-634	HHpred	Homology	3rgzA+1ogqA
Xa21lrr_21	N-term+LRR	27-634	HHpred	Homology	4j0mA+1ogqA
Xa21lrr_22	N-term+LRR	27-634	HHpred	Homology	4u08A+3rgzA+4j0mA
Xa21lrr_23	N-term+LRR	27-634	HHpred	Homology	4u08A+3rgzA+1ogqA
Xa21lrr_24	N-term+LRR	27-634	HHpred	Homology	4u08A+4j0mA+1ogqA
Xa21lrr_25	N-term+LRR	27-634	HHpred	Homology	3rgzA+4j0mA+1ogqA

Xa21lrr_26	N-term+LRR	27-634	HHpred	Homology	4u08A+3rgzA+4j0mA+1ogqA
Xa21lrr_27	N-term+LRR	27-634	HHpred	Homology	3rgzA
Xa21lrr_28	N-term+LRR	27-634	HHpred	Homology	4j0mA
Xa21lrr_29	N-term+LRR	27-634	HHpred	Homology	1ogqA
Xa21lrr_30	N-term+LRR	27-634	HHpred	Homology	4u08A
Xa21lrr_31	N-term+LRR	27-634	HHpred	Homology	4mn8A+4u08A+3rgzA+1ogqA
Xa21c12tm_1	TM+c1+c2	651-707	HHpred	Homology	2jwaA
Xa21c12tm_2	TM+c1+c2	651-707	HHpred	Homology	2ks1B
Xa21c12tm_3	TM+c1+c2	651-707	HHpred	Homology	2jwaA+2ks1B
Xa21k_1	JM+K+C-term	708-1004	HHpred	Homology	4oh4A
Xa21k_2	JM+K+C-term	708-1004	HHpred	Homology	3uimA
Xa21k_3	JM+K+C-term	708-1004	HHpred	Homology	4l68A
Xa21k_4	JM+K+C-term	708-1004	HHpred	Homology	2nruA
Xa21k_5	JM+K+C-term	708-1004	HHpred	Homology	2qkwB
Xa21k_6	JM+K+C-term	708-1004	HHpred	Homology	4oh4A+3uimA
Xa21k_7	JM+K+C-term	708-1004	HHpred	Homology	4oh4A+4l68A
Xa21k_8	JM+K+C-term	708-1004	HHpred	Homology	4oh4A+2nruA
Xa21k_9	JM+K+C-term	708-1004	HHpred	Homology	4oh4A+2qkwB
Xa21k_10	JM+K+C-term	708-1004	HHpred	Homology	3uimA+4l68A
Xa21k_11	JM+K+C-term	708-1004	HHpred	Homology	3uimA+2nruA
Xa21k_12	JM+K+C-term	708-1004	HHpred	Homology	3uimA+2qkwB
Xa21k_13	JM+K+C-term	708-1004	HHpred	Homology	4l68A+2nruA
Xa21k_14	JM+K+C-term	708-1004	HHpred	Homology	4l68A+2qkwB
Xa21k_15	JM+K+C-term	708-1004	HHpred	Homology	2nruA+2qkwB
Xa21k_16	JM+K+C-term	708-1004	HHpred	Homology	40h4A+3uimA+4l68A
Xa21k_17	JM+K+C-term	708-1004	HHpred	Homology	4oh4A+3uimA+2nruA
Xa21k_18	JM+K+C-term	708-1004	HHpred	Homology	4oh4A+3uimA+2qkwB
Xa21k_19	JM+K+C-	708-1004	HHpred	Homology	3uimA+4l68A+2nruA

	term				
Xa21k_20	JM+K+C-term	708-1004	HHpred	Homology	3uimA+4l68A+2qkwB
Xa21k_21	JM+K+C-term	708-1004	HHpred	Homology	4l68A+2nruA+2qkwB
Xa21k_22	JM+K+C-term	708-1004	HHpred	Homology	40h4A+2nruA+2qkwB
Xa21k_23	JM+K+C-term	708-1004	HHpred	Homology	3uimA+4l68A+2qkwB
Xa21k_24	JM+K+C-term	708-1004	HHpred	Homology	3uimA+2nruA+2qkwB
Xa21k_25	JM+K+C-term	708-1004	HHpred	Homology	4oh4A+4l68A+2qkwB
Xa21k_26	JM+K+C-term	708-1004	HHpred	Homology	4oh4A+4l68A+2nruA+2qkwB
Xa21k_27	JM+K+C-term	708-1004	HHpred	Homology	4oh4A+3uimA+4l68A+2nruA
Xa21k_28	JM+K+C-term	708-1004	HHpred	Homology	3uimA+4l68A+2nruA+2qkwB
Xa21k_29	JM+K+C-term	708-1004	HHpred	Homology	4oh4A+4l68A+2nruA+2qkwB
Xa21k_30	JM+K+C-term	708-1004	HHpred	Homology	4oh4A+3uimA+4l68A+2nruA+2qkwB
Xa21k_31	JM+K+C-term	708-1004	HHpred	Homology	4oh4A+3uimA+2nruA+2qkwB
Xa21_Final	Xa21	27-1009	HHpred	Homology	Xa21lrr_15+Xa21c12tm_3+Xa21k_1
Xa21_AIDA	Xa21	27-1009	AIDA	Homology	4mnA+2jwA+4l68A
Xa21_I-Tas	Xa21	1-1025	I-Tasser	*Ab initio*& Threading	4mn8A(7)+4oa2A+4j0mA
Xa21_PhyI	Xa21	1-1025	Phyre2 Intensive	Homology&*Ab initio*	4mn8A(2)+4y93A+2j0kB+1oplA+4xi2A+1y57A+2fo0A
Xa21_RapX	Xa21	1-1025	Raptor-X	Threading	4mn8A+3tl8A+4oa2A+4oa6A

R/P ID, Region or Protein ID; R/P Name, Region or protein Name; AA, Amino Acid; LRR, Leucine rich repeat; TM+C1+C2, Transmembrane and Charged 1 and Charged 2 region; JM+K+C-term, Juxtamembrane and Kinase and C terminal region.

Table S2A. NCBI BLASP analysis of different domain regions of Xa21

Region	AA Boundary	PDB ID	Max. Score	E-value	Q C (%)	Idn. (%)	Template Short Identity
Xa21 full	**1-1025**	4mn8_A	311	4.00E-91	58	33	Chain A, Crystal Structure Of Flg22 In Complex With The Fls2 And Bak1 Ectodomains
		4j0m_A	206	3.00E-55	54	33	Chain A, Crystal Structure Of Brl1 (lrr) In Complex With Brassinolide
		3riz_A	201	2.00E-53	54	33	Chain A, Crystal Structure Of The Plant Steroid Receptor Bri1 Ectodomain
		4oa9_A	169	1.00E-45	25	38	Chain A, Crystal Structure Of The Bri1 Kinase Domain (865-1160) In Complex With Amppnp And Mn From Arabidopsis Thaliana
		3uim_A	129	8.00E-32	22	36	Chain A, Structural Basis For The Impact Of Phosphorylation On Plant Receptor- Like Kinase Bak1 Activation
Xa21	**27-1009**	4mn8_A	312	1.00E-91	61	33	Chain A, Crystal Structure Of Flg22 In Complex With The Fls2 And Bak1 Ectodomains
		4j0m_A	206	1.00E-55	57	33	Chain A, Crystal Structure Of Brl1 (lrr) In Complex With Brassinolide
		3riz_A	201	9.00E-54	57	33	Chain A, Crystal Structure Of The Plant Steroid Receptor Bri1 Ectodomain
		4oa9_A	169	8.00E-46	26	38	Chain A, Crystal Structure Of The Bri1 Kinase Domain (865-1160) In Complex With Amppnp And Mn From Arabidopsis Thaliana
		3uim_A	129	7.00E-32	23	36	Chain A, Structural Basis For The Impact Of Phosphorylation On Plant Receptor- Like Kinase Bak1 Activation
N-term+LRR	**27-634**	4mn8_A	312	4.00E-95	98	33	Chain A, Crystal Structure Of Flg22 In Complex With The Fls2 And Bak1 Ectodomains
		3riz_A	212	7.00E-59	91	32	Chain A, Crystal Structure Of The

							Plant Steroid Receptor Bri1 Ectodomain
		4j0m_A	207	3.00E-57	92	33	Chain A, Crystal Structure Of Brl1 (lrr) In Complex With Brassinolide
		1ogq_A	105	2.00E-24	98	32	Chain A, The Crystal Structure Of Pgip (Polygalacturonase Inhibiting Protein), A Leucine Rich Repeat Protein Involved In Plant Defense
		4u08_A	103	2.00E-23	67	29	Chain A, Structure Of LeptospiraInterrogansLrr Protein Lic11098
C1+TM+C2+JM+K	**635-1009**	4oh4_A	166	7.00E-47	69	38	Chain A, Crystal Structure Of Bri1 In Complex With Bki1
		3uim_A	130	7.00E-34	60	36	Chain A, Structural Basis For The Impact Of Phosphorylation On Plant Receptor- Like Kinase Bak1 Activation
		4l68_A	108	2.00E-26	88	28	Chain A, Structure Of The Psedudokinase Domain Of Bir2, An Immune Regulator Of The Rlk/pelle Family
		2nru_A	107	5.00E-26	63	34	Chain A, Crystal Structure Of Irak-4
		2qkw_B	99.4	3.00E-23	69	31	Chain B, Structural Basis For Activation Of Plant Immunity By Bacterial Effector Protein Avrpto
JM+K+C-term	**683-1009**	4oh4_A	166	2.00E-47	79	38	Chain A, Crystal Structure Of Bri1 In Complex With Bki1
		3uim_A	130	3.00E-34	69	35	Chain A, Structural Basis For The Impact Of Phosphorylation On Plant Receptor- Like Kinase Bak1 Activation
		4l68_A	108	2.00E-26	99	28	Chain A, Structure Of The Psedudokinase Domain Of Bir2, An Immune Regulator Of The Rlk/pelle Family
		2nru_A	107	2.00E-26	72	34	Chain A, Crystal Structure Of Irak-4
		2qkw_B	99.4	1.00E-23	79	31	Chain B, Structural Basis For

							Activation Of Plant Immunity By Bacterial Effector Protein Avrpto

AA, Amino Acid; Max. Score, Maximum Score; Q C, Query Coverage; Idn., Identity; N-term, N terminal region; LRR, Leucine Rich Repeat; C1, Charged1; TM, Transmembrane; C2, Charged2; JM, Juxtamembrane; K, Kinase; C-term, C terminal.

Table S2B. HHpred analysis of Charged1, Transmembrane and Charged2 regions of the Xa21 protein

Region	**AA Boundary**	**PDB ID**	**Score**	**E-value**	**P-value**	**Probability (%)**	**Template Short Identity**
C1+TM+C2	**635-682**	2jwa_A	30.7	0.0024	6.70E-08	96.1	Receptor tyrosine-protein kinase ERBB-2
		2ks1_B	27.8	0.016	4.30E-07	95.1	Epidermal growth factor receptor

AA, Amino Acid; C1, Charged1 region; TM, Transmembrane region; C2, Charged 2 region.

Table S3. Predictions of the Leucine rich repeat (LRR) domain and domain boundary using different tools

Domain Name	Song *et al* 1996		HHrepID		lrrfinder.com		SMART	
	Start AA	End AA	Start AA	End AA	Start AA	End AA	Start AA	End AA
LRR1	81	98	79	101	104	127	102	125
LRR2	99	122	102	125	128	151	126	150
LRR3	123	146	126	149	152	176	151	174
LRR4	147	170	150	172	177	200	199	223
LRR5	172	195	175	198	201	224	247	271
LRR6	196	219	199	222	225	248	320	343
LRR7	220	243	223	246	249*	273*	350	373
LRR8	244	267	247	268	274	321	399	423
LRR9	269	292	272	295	322	351	447	470
LRR10	293	316	296	319	352	376	471	495
LRR11	317	340	320	342	377	400	520	544
LRR12	347	370	350	373	401	448	568	591
LRR13	372	395	376	398	449*	472*		
LRR14	396	419	399	422	473*	545*		
LRR15	420	443	423	446	546	569		
LRR16	444	467	447	470	570	593		
LRR17	468	491	471	494	594**	1025**		
LRR18	492	516	495	519				
LRR19	517	540	520	543				
LRR20	541	564	544	567				
LRR21	565	588	568	591				
LRR22	589	611	592	613				
LRR23	612	634	615	635				

AA, Amino Acid.

*Insignificant hit.

** Potential Leucine Rich Repeat at C terminal.

Table S4. Model validation of different regions of the Xa21 Protein Modeled using the HHpred toolkit

R/P ID	Errat	Verify 3D (%)	Ramachandran Plot Summary from Procheck (%)			
			MFR	AAR	GAR	DR
Xa21lrr_1	67.5	93.91	77.6	19.9	1.3	1.1
Xa21lrr_2	61.333	97.7	72.5	25.2	1.7	0.6
Xa21lrr_3	55	93.59	72.1	24.9	1.1	1.9
Xa21lrr_4	74.167	96.71	76.5	21.8	1.3	0.4
Xa21lrr_5	64.167	96.71	74.6	23.1	1.5	0.8
Xa21lrr_6	61	93.03	71.3	25.8	0.8	2.1
Xa21lrr_7	58.794	96.71	70.6	27.2	1.3	1
Xa21lrr_8	58.667	99.84	71.9	26.4	1	0.8
Xa21lrr_9	71	93.91	75.7	21.2	1.7	1.3
Xa21lrr_10	51.5	95.07	70.7	25.8	1.7	1.7
Xa21lrr_11	61.833	99.67	72.5	1.1	1.1	
Xa21lrr_12	67.667	91.94	75	22.8	1.3	1
Xa21lrr_13	65.5	96.05	71.3	27	0.6	1.1
Xa21lrr_14	59.167	94.9	73.6	24.1	1	1.3
Xa21lrr_15	63.167	100	70.6	26.8	1	1.7
Xa21lrr_16	46.667	91.61	71.5	26.8	1.5	0.2
Xa21lrr_17	61.333	91.78	72.8	25.4	0.8	1
Xa21lrr_18	43.937	84.7	74.8	22.4	2.5	0.4
Xa21lrr_19	59.365	92.93	70.9	27.3	0.8	1
Xa21lrr_20	56.167	95.07	73.6	25.8	1.1	0
Xa21lrr_21	66	96.88	70.7	28.3	0.4	0.6
Xa21lrr_22	61	92.27	71.5	26.8	1	0.8
Xa21lrr_23	58.167	94.41	72.1	26.2	1.5	0.2
Xa21lrr_24	69.5	97.2	75	24.1	0.8	0.2
Xa21lrr_25	60.667	97.86	70.2	27.9	1	1
Xa21lrr_26	62.167	99.34	72.5	26.6	0.8	0.2
Xa21lrr_27	45.74	90.46	69.2	28.3	1.7	0.8
Xa21lrr_28	51.33	93.75	70	27.5	1.5	1

Xa21lrr_29	E	46.05	87	12	0.4	0.6
Xa21lrr_30	56.494	62.17	80.1	17	1.9	1
Xa21lrr_31	72.194	90.95	81.8	16.6	0.6	1
Xa21c12tm_1	67.5	0	95.2	4.8	0	0
Xa21c12tm_2	60.526	0	88.1	11.9	0	0
Xa21c12tm_3	81.579	0	92.9	7.1	0	0
Xa21k_1	80.189	84.71	90.6	7.7	1.4	0.3
Xa21k_2	67.192	74.92	89.2	8	1.7	1
Xa21k_3	50.159	76.45	85	12.9	0.3	1.7
Xa21k_4	64.353	67.89	86	9.4	2.8	1.7
Xa21k_5	67.192	70.03	81.8	15	2.8	0.3
Xa21k_6	70.219	90.52	88.8	7.3	1.4	2.4
Xa21k_7	69.231	82.26	88.8	9.1	1.4	0.7
Xa21k_8	65.696	88.38	87.1	10.5	2.1	0.3
Xa21k_9	69.206	85.93	85.7	10.5	2.1	1.7
Xa21k_10	76.025	80.43	87.8	9.4	2.1	0.7
Xa21k_11	59.873	81.65	88.1	8.7	2.4	0.7
Xa21k_12	59.973	76.15	85	11.9	2.8	0.3
Xa21k_13	73.27	63.91	85.3	12.2	2.1	0.3
Xa21k_14	75.159	82.87	82.5	15	1.7	0.7
Xa21k_15	53.312	66.97	86.4	9.4	2.8	1.4
Xa21k_16	78.797	78.9	87.8	10.8	0.7	0.7
Xa21k_17	74.922	88.07	88.8	9.1	1	1
Xa21k_18	69.401	87.16	88.8	8	2.4	0.7
Xa21k_19	60.568	81.96	87.1	9.8	2.4	0.7
Xa21k_20	67.628	79.51	85	11.2	2.1	1.7
Xa21k_21	66.139	69.72	81.5	15	2.8	0.7
Xa21k_22	77.987	92.97	87.4	10.8	1	0.7
Xa21k_23	67.628	79.51	85	11.2	2.1	1.7
Xa21k_24	62.3	88.38	82.2	16.8	0.3	0.7
Xa21k_25	75.786	85.93	86.4	10.5	1.4	1.7

Xa21k_26	68.671	77.06	88.8	7	3.1	1
Xa21k_27	69.811	86.85	85.7	10.1	2.4	1.7
Xa21k_28	68.889	79.2	82.9	14.7	1.7	0.7
Xa21k_29	74.051	87.16	87.1	10.1	1.4	1.4
Xa21k_30	67.089	89.6	88.8	9.8	0.7	0.7
Xa21k_31	60.417	74.41	87.3	10.4	1.2	1.2

R/P ID, Region or Protein ID; MFR, Most Favoured Regions; AAR, Additionally Allowed Regions; GAR, Generously Allowed Regions; DR, Disallowed Regions; E, Error.

Table S5A. Binding free energy contribution of the key binding-site residues calculated from the binding energy decomposition for Xa21 ($kJmol^{-1}$) of complex 1a and complex 3.

Residues	MM Energy	Polar Energy	Apolar Energy	Total Energy
GLY-1	-5.9687 ± 0.0086	0.0015 ± 0.0001	0.0000 ± 0.0000	-5.9673 ± 0.0088
GLY-1	-6.6173 ± 0.0110	0.0013 ± 0.0000	0.0000 ± 0.0000	-6.6161 ± 0.0111
LYS-14	-7.0653 ± 0.0099	0.0063 ± 0.0001	0.0000 ± 0.0000	-7.0595 ± 0.0100
LYS-14	-8.1081 ± 0.0149	0.0017 ± 0.0001	0.0000 ± 0.0000	-8.1064 ± 0.0151
ARG-46	-6.0954 ± 0.0079	0.0009 ± 0.0000	0.0000 ± 0.0000	-6.0944 ± 0.0081
ARG-46	-6.3763 ± 0.0124	0.0003 ± 0.0000	0.0000 ± 0.0000	-6.3765 ± 0.0119
ARG-47	-6.9610 ± 0.0162	-0.0007 ± 0.0000	0.0000 ± 0.0000	-6.9616 ± 0.0169
ARG-47	-7.7415 ± 0.0134	0.0016 ± 0.0001	0.0000 ± 0.0000	-7.7399 ± 0.0131
ARG-48	-6.8459 ± 0.0124	0.0002 ± 0.0001	0.0000 ± 0.0000	-6.8457 ± 0.0121
ARG-48	-6.8279 ± 0.0127	-6.8279 ± 0.0127	0.0000 ± 0.0000	-6.8281 ± 0.0130
ARG-49	-5.9652 ± 0.0092	-0.0003 ± 0.0000	0.0000 ± 0.0000	-5.9652 ± 0.0089
ARG-49	-6.0932 ± 0.0099	-0.0000 ± 0.0000	0.0000 ± 0.0000	-6.0934 ± 0.0097
ARG-50	-5.5553 ± 0.0070	-0.0000 ± 0.0000	0.0000 ± 0.0000	-5.5555 ± 0.0071
ARG-50	-5.7137 ± 0.0080	-0.0000 ± 0.0000	0.0000 ± 0.0000	-5.7136 ± 0.0082
ARG-54	-6.4122 ± 0.0072	0.0038 ± 0.0001	0.0000 ± 0.0000	-6.4084 ± 0.0071
ARG-54	-6.8861 ± 0.0103	0.0038 ± 0.0001	0.0000 ± 0.0000	-6.8820 ± 0.0101
LYS-57	-9.0314 ± 0.0137	0.0055 ± 0.0002	0.0000 ± 0.0000	-9.0257 ± 0.0133
LYS-57	-8.7035 ± 0.0188	-8.7035 ± 0.0188	0.0000 ± 0.0000	-8.6975 ± 0.0188
ARG-61	-11.7671 ± 0.0208	0.0299 ± 0.0009	0.0000 ± 0.0000	-11.7368 ± 0.0211
ARG-61	-12.0987 ± 0.0289	0.0007 ± 0.0011	0.0000 ± 0.0000	-12.0966 ± 0.0287
ARG-80	-8.1822 ± 0.0129	0.0088 ± 0.0002	0.0000 ± 0.0000	-8.1740 ± 0.0131
ARG-80	-7.7939 ± 0.0131	0.0094 ± 0.0003	0.0000 ± 0.0000	-7.7846 ± 0.0129
ARG-99	-7.0884 ± 0.0101	0.0123 ± 0.0002	0.0000 ± 0.0000	-7.0757 ± 0.0102
ARG-99	-8.1815 ± 0.0156	0.0061 ± 0.0002	0.0000 ± 0.0000	-8.1758 ± 0.0151
ARG-102	-6.9704 ± 0.0080	0.0082 ± 0.0001	0.0000 ± 0.0000	-6.9622 ± 0.0080
ARG-102	-7.3174 ± 0.0110	0.0070 ± 0.0002	0.0000 ± 0.0000	-7.3110 ± 0.0108
LYS-126	-7.7376 ± 0.0109	0.0153 ± 0.0002	0.0000 ± 0.0000	-7.7225 ± 0.0108
LYS-126	-7.7596 ± 0.0126	0.0143 ± 0.0004	0.0000 ± 0.0000	-7.7452 ± 0.0123
ARG-138	-12.7486 ± 0.0406	0.1348 ± 0.0030	0.0000 ± 0.0000	-12.6158 ± 0.0420
ARG-138	-15.9961 ± 0.0589	0.0159 ± 0.0031	0.0000 ± 0.0000	-15.9806 ± 0.0598
ARG-143	-9.4608 ± 0.0172	0.0433 ± 0.0010	0.0000 ± 0.0000	-9.4171 ± 0.0167
ARG-143	-10.4853 ± 0.0255	0.0920 ± 0.0027	0.0000 ± 0.0000	-10.3915 ± 0.0251
LYS-150	-8.6361 ± 0.0148	0.0563 ± 0.0009	0.0000 ± 0.0000	-8.5801 ± 0.0149
LYS-150	-8.1667 ± 0.0139	0.0326 ± 0.0007	0.0000 ± 0.0000	-8.1342 ± 0.0140
LYS-159	-20.3711 ± 0.0853	0.4720 ± 0.0136	0.0000 ± 0.0000	-19.8979 ± 0.0771
LYS-159	-24.6602 ± 0.1174	0.2545 ± 0.0190	0.0000 ± 0.0000	-24.4097 ± 0.1063

PHE-183	-0.8145 ± 0.0065	0.3040 ± 0.0067	0.0000 ± 0.0000	-0.5109 ± 0.0066
PHE-183	-0.7919 ± 0.0085	0.1788 ± 0.0062	-0.0028 ± 0.0005	-0.6157 ± 0.0064
ARG-185	-16.1800 ± 0.1050	0.0717 ± 0.0202	-0.0009 ± 0.0003	-16.1082 ± 0.1047
ARG-185	-20.2474 ± 0.1126	0.2793 ± 0.0210	-0.0003 ± 0.0003	-19.9701 ± 0.1071
ARG-225	-14.1212 ± 0.0362	0.2711 ± 0.0035	0.0000 ± 0.0000	-13.8508 ± 0.0342
ARG-225	-12.4740 ± 0.0454	0.1394 ± 0.0040	0.0000 ± 0.0000	-12.3361 ± 0.0452
ARG-230	-51.2735 ± 0.3173	30.8192 ± 0.4278	-0.4258 ± 0.0074	-20.8768 ± 0.1632
ARG-230	-45.8491 ± 0.4546	26.7476 ± 0.4994	-0.3229 ± 0.0068	-19.4217 ± 0.1459
LYS-233	-25.3704 ± 0.2250	3.8871 ± 0.2018	-0.0159 ± 0.0016	-21.5039 ± 0.1351
LYS-233	-19.5911 ± 0.1327	0.9838 ± 0.0358	0.0000 ± 0.0000	-18.6022 ± 0.1167
LYS-244	-10.8173 ± 0.0210	0.2516 ± 0.0029	0.0000 ± 0.0000	-10.5651 ± 0.0190
LYS-244	-8.7742 ± 0.0230	0.0442 ± 0.0031	0.0000 ± 0.0000	-8.7304 ± 0.0217
ARG-258	-23.3446 ± 0.1447	1.6989 ± 0.0749	-0.0021 ± 0.0006	-21.6513 ± 0.1107
ARG-258	-16.7439 ± 0.0917	0.5922 ± 0.0170	0.0000 ± 0.0000	-16.1503 ± 0.0838
LYS-262	-13.2970 ± 0.0336	0.3120 ± 0.0065	0.0000 ± 0.0000	-12.9841 ± 0.0292
LYS-262	-9.8426 ± 0.0371	-0.2366 ± 0.0064	0.0000 ± 0.0000	-10.0802 ± 0.0359
ARG-293	-11.5673 ± 0.0262	0.5609 ± 0.0067	0.0000 ± 0.0000	-11.0069 ± 0.0210
ARG-293	-8.8897 ± 0.0250	-0.0087 ± 0.0041	0.0000 ± 0.0000	-8.8993 ± 0.0246
ARG-295	-11.8382 ± 0.0256	0.5212 ± 0.0068	0.0000 ± 0.0000	-11.3179 ± 0.0217
ARG-295	-10.0747 ± 0.0287	0.0856 ± 0.0045	0.0000 ± 0.0000	-9.9901 ± 0.0278
TRP-303	-35.7820 ± 0.0836	24.4156 ± 0.0511	-1.9451 ± 0.0072	-1.9451 ± 0.0072
TRP-303	-29.0365 ± 0.1575	17.9697 ± 0.1082	-1.3214 ± 0.0084	-12.3897 ± 0.0892
ARG-304	-44.8842 ± 0.3680	18.6848 ± 0.4557	-0.6127 ± 0.0094	-26.8115 ± 0.1772
ARG-304	-30.1770 ± 0.3256	11.2788 ± 0.4504	-0.4571 ± 0.0105	-19.3743 ± 0.2091
ARG-310	-11.7278 ± 0.0279	0.2678 ± 0.0051	0.0000 ± 0.0000	-11.4595 ± 0.0236
ARG-310	-8.2929 ± 0.0343	-0.1811 ± 0.0035	0.0000 ± 0.0000	-8.4730 ± 0.0338
LYS-326	-14.6779 ± 0.0411	0.7315 ± 0.0092	0.0000 ± 0.0000	-13.9471 ± 0.0348
LYS-326	-13.1947 ± 0.0415	0.1141 ± 0.0054	0.0000 ± 0.0000	-13.0792 ± 0.0404
LYS-368	-9.2696 ± 0.0292	0.2457 ± 0.0062	0.0000 ± 0.0000	-9.0227 ± 0.0245
LYS-368	-8.4412 ± 0.0274	0.0376 ± 0.0032	0.0000 ± 0.0000	-8.4036 ± 0.0249
TYR-380	-17.6920 ± 0.1470	12.4566 ± 0.1215	-1.4746 ± 0.0082	-6.7080 ± 0.0751
TYR-380	-17.5009 ± 0.1034	13.7472 ± 0.0899	-1.3689 ± 0.0075	-5.1200 ± 0.0786
ARG-387	-10.6875 ± 0.0620	0.3596 ± 0.0126	0.0000 ± 0.0000	-10.3284 ± 0.0500
ARG-387	-7.1987 ± 0.0565	-0.2713 ± 0.0124	0.0000 ± 0.0000	-7.4707 ± 0.0460
ARG-396	-10.3049 ± 0.0263	0.5441 ± 0.0081	0.0000 ± 0.0000	-9.7604 ± 0.0214
ARG-396	-11.6806 ± 0.0288	0.5808 ± 0.0069	0.0000 ± 0.0000	-11.0986 ± 0.0258
LYS-398	-15.4063 ± 0.0680	1.0771 ± 0.0189	0.0000 ± 0.0000	-14.3305 ± 0.0528
LYS-398	-15.6341 ± 0.0597	1.2213 ± 0.0166	0.0000 ± 0.0000	-14.4128 ± 0.0544

LEU-404	-5.9956 ± 0.0290	0.0654 ± 0.0063	-0.5861 ± 0.0045	-6.5164 ± 0.0286
LEU-404	-7.3450 ± 0.0381	0.1033 ± 0.0064	-0.6953 ± 0.0047	-7.9384 ± 0.0405
LYS-433	-8.4102 ± 0.0782	-0.1268 ± 0.0177	0.0000 ± 0.0000	-8.5422 ± 0.0622
LYS-433	-5.4489 ± 0.0675	-0.5965 ± 0.0161	0.0000 ± 0.0000	-6.0441 ± 0.0551
ARG-522	-5.7350 ± 0.1159	-2.1403 ± 0.0406	-0.0091 ± 0.0014	-7.8838 ± 0.1036
ARG-522	-15.9112 ± 0.0918	-0.1566 ± 0.0236	-0.0008 ± 0.0004	-16.0673 ± 0.0839
PRO-608	6.1284 ± 0.0213	0.0269 ± 0.0005	0.0000 ± 0.0000	6.1555 ± 0.0216
PRO-608	6.9141 ± 0.0275	0.0034 ± 0.0003	0.0000 ± 0.0000	6.9174 ± 0.0278

Green markings represent residues showing higher interaction values; Yellow markings represent residues showing average interaction values.

Table S5B. Binding free energy contribution of the key binding-site residues calculated from the binding energy decomposition for Xa21 (kJmol^{-1}) of complex 1b and complex 2.

Residues	MM Energy	Polar Energy	Apolar Energy	Total Energy
GLY-1	-9.7687 ± 0.0477	0.0551 ± 0.0374	0.0004 ± 0.0011	-9.7131 ± 0.0613
GLY-1	-7.5079 ± 0.0301	0.1413 ± 0.0351	-0.0025 ± 0.0020	-7.3705 ± 0.0457
LYS-14	-13.2228 ± 0.0361	0.1253 ± 0.0151	0.0040 ± 0.0023	-13.0940 ± 0.0397
LYS-14	-12.7693 ± 0.0555	1.1321 ± 0.0321	0.0015 ± 0.0027	-11.6347 ± 0.0530
ARG-46	-8.7174 ± 0.0210	0.0420 ± 0.0153	-0.0010 ± 0.0034	-8.6771 ± 0.0268
ARG-46	-7.9087 ± 0.0231	0.0626 ± 0.0178	-0.0027 ± 0.0026	-7.8475 ± 0.0293
ARG-47	-10.6854 ± 0.0529	0.0389 ± 0.0182	0.0016 ± 0.0025	-10.6396 ± 0.0568
ARG-47	-9.7357 ± 0.0387	0.1075 ± 0.0182	-0.0010 ± 0.0034	-9.6296 ± 0.0430
ARG-48	-10.6700 ± 0.0354	0.0453 ± 0.0183	0.0035 ± 0.0029	-10.6213 ± 0.0391
ARG-48	-7.3358 ± 0.0293	0.0272 ± 0.0192	0.0024 ± 0.0025	-7.3062 ± 0.0351
ARG-49	-8.1130 ± 0.0235	0.0321 ± 0.0192	0.0003 ± 0.0021	-8.0799 ± 0.0299
ARG-49	-6.1361 ± 0.0236	0.0446 ± 0.0203	0.0001 ± 0.0017	-6.0928 ± 0.0305
ARG-50	-7.2799 ± 0.0188	0.0055 ± 0.0177	-0.0016 ± 0.0017	-7.2757 ± 0.0258
ARG-50	-6.1409 ± 0.0224	0.0311 ± 0.0196	0.0030 ± 0.0020	-6.1063 ± 0.0287
ARG-54	-9.7234 ± 0.0181	0.0734 ± 0.0167	-0.0057 ± 0.0025	-9.6553 ± 0.0247
ARG-54	-8.4683 ± 0.0269	0.1564 ± 0.0186	-0.0045 ± 0.0032	-8.3167 ± 0.0317
LYS-57	-15.9923 ± 0.0486	0.1749 ± 0.0320	0.0013 ± 0.0028	-15.8120 ± 0.0575
LYS-57	-15.8912 ± 0.0428	0.7352 ± 0.0342	-0.0093 ± 0.0031	-15.1653 ± 0.0514
ARG-61	-27.2170 ± 0.0696	1.1002 ± 0.0183	0.0005 ± 0.0032	-26.1161 ± 0.0670
ARG-61	-23.5408 ± 0.0673	1.8516 ± 0.0280	-0.0004 ± 0.0021	-21.6908 ± 0.0631
ARG-80	-13.1232 ± 0.0303	0.1285 ± 0.0147	-0.0006 ± 0.0023	-12.9947 ± 0.0328
ARG-80	-10.9371 ± 0.0295	0.3749 ± 0.0153	-0.0028 ± 0.0026	-10.5658 ± 0.0311
ARG-99	-12.8909 ± 0.0278	0.1415 ± 0.0157	0.0030 ± 0.0022	-12.7473 ± 0.0316
ARG-99	-8.8306 ± 0.0444	0.1862 ± 0.0175	0.0012 ± 0.0028	-8.6446 ± 0.0450
ARG-102	-10.9864 ± 0.0197	0.1216 ± 0.0162	-0.0030 ± 0.0022	-10.8691 ± 0.0253
ARG-102	-10.7391 ± 0.0396	0.3819 ± 0.0176	-0.0023 ± 0.0027	-10.3588 ± 0.0387

LYS-126	-12.0785 ± 0.0219	0.1093 ± 0.0350	-0.0044 ± 0.0026	-11.9721 ± 0.0409
LYS-126	-10.7144 ± 0.0278	0.2339 ± 0.0350	-0.0017 ± 0.0027	-10.4822 ± 0.0420
ARG-138	-60.8613 ± 0.3245	12.7899 ± 0.3309	-0.4855 ± 0.0125	-48.5570 ± 0.1529
ARG-138	-49.5846 ± 0.5068	22.8854 ± 0.4595	-0.9228 ± 0.0164	-27.6154 ± 0.2646
ARG-143	-16.7600 ± 0.0606	0.0757 ± 0.0182	0.0025 ± 0.0019	-16.6808 ± 0.0643
ARG-143	-13.3313 ± 0.0719	0.4140 ± 0.0186	-0.0012 ± 0.0029	-12.9194 ± 0.0750
LYS-150	-13.0782 ± 0.0282	0.1741 ± 0.0336	-0.0002 ± 0.0025	-12.9043 ± 0.0425
LYS-150	-9.8829 ± 0.0297	0.2478 ± 0.0338	-0.0023 ± 0.0023	-9.6369 ± 0.0439
LYS-159	-73.7898 ± 0.3612	54.5355 ± 0.6430	-1.1879 ± 0.0091	-20.4579 ± 0.3622
LYS-159	-91.6969 ± 0.3070	75.9152 ± 0.6604	-1.7192 ± 0.0106	-17.4810 ± 0.4501
PHE-183	-13.6334 ± 0.0724	4.4258 ± 0.0718	-2.2752 ± 0.0075	-11.4786 ± 0.0552
PHE-183	-15.3290 ± 0.0619	8.0958 ± 0.0418	-2.0325 ± 0.0088	-9.2657 ± 0.0619
ARG-185	-113.5355 ± 0.5004	88.6535 ± 0.4657	-2.6790 ± 0.0145	-27.5459 ± 0.2336
ARG-185	-74.7709 ± 0.4661	58.1120 ± 0.6605	-1.8893 ± 0.0163	-18.5529 ± 0.2538
ARG-225	-17.6968 ± 0.0623	-0.0072 ± 0.0153	-0.0004 ± 0.0023	-17.7024 ± 0.0654
ARG-225	-17.9356 ± 0.0651	0.1791 ± 0.0164	0.0061 ± 0.0034	-17.7503 ± 0.0659
ARG-230	-37.4765 ± 0.2447	4.4832 ± 0.2574	-0.1962 ± 0.0080	-33.1992 ± 0.1140
ARG-230	-39.5601 ± 0.1824	9.1658 ± 0.1995	-0.1078 ± 0.0049	-30.5009 ± 0.1469
LYS-233	-31.9923 ± 0.2901	2.9629 ± 0.2473	-0.0813 ± 0.0046	-29.1132 ± 0.1918
LYS-233	-19.4239 ± 0.1366	0.3268 ± 0.0549	-0.0026 ± 0.0021	-19.0988 ± 0.1230
LYS-244	-9.1315 ± 0.0192	0.0687 ± 0.0366	-0.0037 ± 0.0027	-9.0665 ± 0.0431
LYS-244	-7.7724 ± 0.0322	0.0699 ± 0.0368	-0.0010 ± 0.0031	-7.7030 ± 0.0477
ARG-258	-17.3387 ± 0.1255	-0.3142 ± 0.0374	-0.0019 ± 0.0027	-17.6526 ± 0.1205
ARG-258	-16.1880 ± 0.1022	0.3972 ± 0.0434	-0.0033 ± 0.0024	-15.7961 ± 0.0937
LYS-262	-8.0191 ± 0.0282	0.0078 ± 0.0362	-0.0031 ± 0.0029	-8.0134 ± 0.0471
LYS-262	-6.8243 ± 0.0348	0.0015 ± 0.0369	-0.0012 ± 0.0038	-6.8230 ± 0.0501
ARG-293	-8.1288 ± 0.0219	0.0178 ± 0.0148	-0.0036 ± 0.0028	-8.1146 ± 0.0271
ARG-293	-7.4879 ± 0.0309	-0.0379 ± 0.0152	0.0026 ± 0.0038	-7.5227 ± 0.0319
ARG-295	-9.0904 ± 0.0235	0.0002 ± 0.0156	0.0001 ± 0.0023	-9.0921 ± 0.0280
ARG-295	-9.5394 ± 0.0308	0.0043 ± 0.0176	0.0037 ± 0.0029	-9.5315 ± 0.0350
TRP-303	-0.8300 ± 0.0061	-0.0050 ± 0.0070	-0.0006 ± 0.0024	-0.8357 ± 0.0100
TRP-303	0.2776 ± 0.0173	-0.2211 ± 0.0131	0.0018 ± 0.0024	0.0580 ± 0.0133
ARG-304	-6.4413 ± 0.1145	-0.5703 ± 0.0485	-0.0017 ± 0.0020	-7.0067 ± 0.1053
ARG-304	-9.9707 ± 0.0927	-0.3307 ± 0.0196	0.0001 ± 0.0024	-10.2977 ± 0.0899
ARG-310	-6.3695 ± 0.0226	0.0136 ± 0.0165	-0.0007 ± 0.0027	-6.3562 ± 0.0276
ARG-310	-6.0378 ± 0.0236	0.0127 ± 0.0155	0.0068 ± 0.0029	-6.0196 ± 0.0280
LYS-326	-12.4760 ± 0.0391	0.0166 ± 0.0333	-0.0036 ± 0.0026	-12.4629 ± 0.0522
LYS-326	-14.4390 ± 0.0570	-0.0933 ± 0.0350	-0.0013 ± 0.0029	-14.5316 ± 0.0653

LYS-368	-4.9048 ± 0.0218	0.0424 ± 0.0357	0.0012 ± 0.0020	-4.8615 ± 0.0419
LYS-368	-5.6806 ± 0.0319	0.0640 ± 0.0339	-0.0016 ± 0.0026	-5.6164 ± 0.0459
TYR-380	-0.0417 ± 0.0044	0.0071 ± 0.0093	0.0010 ± 0.0025	-0.0333 ± 0.0109
TYR-380	-1.1177 ± 0.0377	0.6878 ± 0.0470	-0.0535 ± 0.0035	-0.4825 ± 0.0217
ARG-387	-3.6936 ± 0.0291	0.0355 ± 0.0161	0.0004 ± 0.0022	-3.6592 ± 0.0338
ARG-387	-4.2876 ± 0.0465	-0.0777 ± 0.0161	0.0009 ± 0.0021	-4.3656 ± 0.0470
ARG-396	-7.1893 ± 0.0237	0.0282 ± 0.0166	0.0009 ± 0.0026	-7.1616 ± 0.0294
ARG-396	-7.7624 ± 0.0312	-0.0491 ± 0.0173	0.0049 ± 0.0028	-7.8072 ± 0.0351
LYS-398	-11.9927 ± 0.0495	0.0646 ± 0.0333	-0.0044 ± 0.0024	-11.9305 ± 0.0580
LYS-398	-9.1156 ± 0.0365	-9.1156 ± 0.0365	0.0052 ± 0.0025	-9.1836 ± 0.0489
LEU-404	-0.1325 ± 0.0014	-0.0008 ± 0.0024	0.0015 ± 0.0024	-0.1319 ± 0.0037
LEU-404	-0.5346 ± 0.0064	0.0512 ± 0.0027	-0.0045 ± 0.0027	-0.4880 ± 0.0061
LYS-433	-2.7775 ± 0.0368	0.0212 ± 0.0322	0.0031 ± 0.0026	-2.7561 ± 0.0494
LYS-433	-3.7705 ± 0.0586	0.0964 ± 0.0254	-0.0013 ± 0.0017	-3.6767 ± 0.0637
ARG-522	-26.6830 ± 0.3555	16.4826 ± 0.4122	-0.6542 ± 0.0112	-10.8558 ± 0.1752
ARG-522	-72.0310 ± 0.5148	73.5158 ± 0.5014	-1.9091 ± 0.0136	-0.4415 ± 0.3213
PRO-608	-22.3819 ± 0.4220	4.0357 ± 0.2917	-0.0727 ± 0.0058	-18.4335 ± 0.2748
PRO-608	-4.4437 ± 0.1578	0.2507 ± 0.0439	0.0002 ± 0.0024	-4.1905 ± 0.1637

Green markings represent residues showing higher interaction values; Yellow markings represent residues showing average interaction values.

Table S5C. Binding free energy contribution of the key binding-site residues calculated from the binding energy decomposition for RaxX21-sY (kJmol^{-1}) of complex 1a and complex 3.

Residues	MM Energy	Polar Energy	Apolar Energy	Total Energy
VAL-2	-24.6045 ± 0.1332	12.6492 ± 0.1220	-1.5783 ± 0.0093	-13.5344 ± 0.0765
VAL-2	-13.0105 ± 0.1020	7.0837 ± 0.0886	-0.5546 ± 0.0079	-6.4884 ± 0.0514
GLY-3	-13.6600 ± 0.1274	8.9606 ± 0.1514	-1.4675 ± 0.0076	-6.1731 ± 0.0591
GLY-3	-16.0877 ± 0.1713	12.1984 ± 0.1730	-1.0387 ± 0.0132	-4.9325 ± 0.0554
PRO-14	-13.3340 ± 0.0830	5.3404 ± 0.0618	-1.2992 ± 0.0104	-9.2938 ± 0.0723
PRO-14	-18.7857 ± 0.1110	7.9902 ± 0.0944	-1.8124 ± 0.0082	-12.6051 ± 0.0563
LYS-15	-88.6216 ± 0.4083	81.5238 ± 0.7059	-2.6593 ± 0.0128	-9.7518 ± 0.4931
LYS-15	-65.9948 ± 0.3908	53.6579 ± 0.7919	-2.0346 ± 0.0109	-14.3603 ± 0.5324

Green markings represent residues showing higher interaction values; Yellow markings represent residues showing average interaction values.

Table S5D. Binding free energy contribution of the key binding-site residues calculated from the binding energy decomposition for OsSERK2 ($kJmol^{-1}$) of complex 1b and complex 2.

Residues	MM Energy	Polar Energy	Apolar Energy	Total Energy
LYS-46	20.2439 ± 0.2959	-0.6592 ± 0.1510	-0.0167 ± 0.0039	19.5717 ± 0.2614
LYS-46	-15.7543 ± 0.3780	3.4063 ± 0.2380	-0.1518 ± 0.0063	-12.4987 ± 0.2876
ASP-47	-47.8659 ± 0.2763	22.9919 ± 0.2677	-0.0552 ± 0.0039	-24.9359 ± 0.1862
ASP-47	-16.3727 ± 0.2586	0.0132 ± 0.1916	-0.0054 ± 0.0031	-16.3583 ± 0.1525
LEU-59	-8.3827 ± 0.0711	0.0982 ± 0.0334	-1.2386 ± 0.0090	-9.5206 ± 0.0585
LEU-59	-4.8219 ± 0.0675	0.1678 ± 0.0182	-0.5323 ± 0.0122	-5.1878 ± 0.0849
ASP-80	-23.5021 ± 0.2628	5.3938 ± 0.1197	0.0047 ± 0.0045	-18.1082 ± 0.1873
ASP-80	-40.5096 ± 0.2140	10.5007 ± 0.1642	-0.0024 ± 0.0043	-30.0019 ± 0.1448
PHE-137	-13.6270 ± 0.0961	4.9343 ± 0.0622	-1.6782 ± 0.0128	-10.3732 ± 0.0657
PHE-137	-24.0051 ± 0.2385	14.2520 ± 0.1632	-1.4993 ± 0.0222	-11.2639 ± 0.1178
LYS-164	-85.3566 ± 0.6218	63.6532 ± 0.9761	-0.6962 ± 0.0122	-22.4333 ± 0.4886
LYS-164	-53.8833 ± 0.6652	28.6518 ± 0.7936	-0.6757 ± 0.0153	-25.9628 ± 0.3910
LYS-183	-56.9942 ± 0.4190	6.9810 ± 0.2642	-0.0728 ± 0.0063	-50.0972 ± 0.2914
LYS-183	-42.8270 ± 0.4131	10.7269 ± 0.4008	-0.1961 ± 0.0093	-32.3350 ± 0.2338
ARG-192	-18.2370 ± 0.1072	0.9081 ± 0.0294	-0.0042 ± 0.0049	-17.3383 ± 0.1031
ARG-192	-18.2371 ± 0.2376	1.3801 ± 0.0571	-0.0050 ± 0.0048	-16.8526 ± 0.2047
ARG-212	-51.5250 ± 0.4645	8.0290 ± 0.3351	-0.2861 ± 0.0124	-43.7914 ± 0.2648
ARG-212	-34.6025 ± 0.3026	2.0019 ± 0.0980	-0.0222 ± 0.0051	-32.6356 ± 0.2480
ARG-218	-14.9573 ± 0.1097	0.5054 ± 0.0249	-0.0056 ± 0.0045	-14.4520 ± 0.1065
ARG-218	-15.4568 ± 0.1678	0.6392 ± 0.0271	-0.0000 ± 0.0050	-14.8206 ± 0.1576
LYS-222	-8.8753 ± 0.0885	0.3428 ± 0.0542	0.0018 ± 0.0043	-8.5338 ± 0.1009
LYS-222	-7.5329 ± 0.1065	0.5910 ± 0.0484	0.0029 ± 0.0041	-6.9419 ± 0.1145
LYS-232	-6.4713 ± 0.0955	0.2985 ± 0.0473	-0.0015 ± 0.0053	-6.1758 ± 0.1048
LYS-232	-0.0178 ± 0.0810	0.5993 ± 0.0478	0.0012 ± 0.0059	0.5819 ± 0.0915
LYS-238	-11.9570 ± 0.1207	0.1138 ± 0.0472	-0.0023 ± 0.0047	-11.8461 ± 0.1287
LYS-238	-6.7402 ± 0.1094	0.3987 ± 0.0503	0.0018 ± 0.0052	-6.3363 ± 0.1185

Green markings represent residues showing higher interaction values; Yellow markings represent residues showing average interaction values.

Table S6A: Protein-Protein Main Chain-Side Chain Hydrogen Bonds of complex 1.

Before Simulation								
Protein-Protein Main Chain-Side Chain Hydrogen Bonds								
DONOR				ACCEPTOR				
POS	CHAIN	RES	ATOM	POS	CHAIN	RES	ATOM	Dd-a
62	A	SER	OG	72	C	PRO	O	3.18
86	A	ASP	OD2	71	C	ASN	O	3.46
86	A	ASP	OD2	71	C	ASN	O	3.46
110	A	ASP	OD2	63	C	CYS	O	2.78
110	A	ASP	OD2	63	C	CYS	O	2.78
134	A	HIS	NE2	63	C	CYS	O	3.19
134	A	HIS	ND1	64	C	THR	O	3.17
134	A	HIS	ND1	65	C	TRP	O	2.68
134	A	HIS	NE2	65	C	TRP	O	2.05
134	A	HIS	NE2	68	C	VAL	O	3.08
159	A	LYS	NZ	65	C	TRP	O	3.4
159	A	LYS	NZ	66	C	PHE	O	3.37
207	A	GLN	OE1	53	C	GLN	O	2.01
207	A	GLN	OE1	53	C	GLN	O	2.01
331	**A**	**ASN**	**ND2**	1	B	HIS	O	2.33
331	**A**	**ASN**	**ND2**	1	B	HIS	O	2.33
567	**A**	**THR**	**N**	**140**	**C**	**GLU**	**OE1**	3.34
567	**A**	**THR**	**N**	**140**	**C**	**GLU**	**OE2**	1.63
568	**A**	**MET**	**N**	**140**	**C**	**GLU**	**OE2**	3
4	B	GLY	N	301	A	TYR	OH	3.4
11	B	GLY	N	93	C	GLN	NE2	2.59
16	B	HIS	NE2	43	C	GLN	O	2.5
21	B	ARG	N	39	C	TYR	OH	3.03
21	B	ARG	N	43	C	GLN	OE1	2.25
21	B	ARG	N	43	C	GLN	NE2	2.89
36	C	ASP	OD1	8	B	PRO	O	3.26
36	C	ASP	OD1	8	B	PRO	O	3.26
39	C	TYR	OH	6	B	ASP	O	1.86
40	C	SER	OG	10	B	PRO	O	2.06
42	C	ARG	NE	21	B	ARG	O	2.91
43	C	GLN	NE2	6	B	ASP	O	3.34
43	C	GLN	NE2	6	B	ASP	O	3.34

43	C	GLN	OE1	21	B	ARG	O	3.09
43	C	GLN	OE1	21	B	ARG	O	3.09
43	C	GLN	OE1	21	B	ARG	OXT	3.19
43	C	GLN	OE1	21	B	ARG	OXT	3.19
65	C	TRP	N	134	A	HIS	NE2	2.92
66	C	PHE	N	134	A	HIS	ND1	3.36
116	C	ASN	ND2	544	A	GLY	O	2.47
116	C	ASN	ND2	544	A	GLY	O	2.47
140	C	GLU	OE1	565	A	ASP	O	3.12
140	C	GLU	OE1	565	A	ASP	O	3.12
140	C	GLU	OE2	565	A	ASP	O	3.5
140	C	GLU	OE2	565	A	ASP	O	3.5

After Simulation

Protein-Protein Main Chain-Side Chain Hydrogen Bonds

	DONOR				**ACCEPTOR**			
POS	**CHAIN**	**RES**	**ATOM**	**POS**	**CHAIN**	**RES**	**ATOM**	**Dd-a**
185	A	ARG	NH2	52	C	LEU	O	3.36
185	A	ARG	NH2	52	C	LEU	O	3.36
303	A	TRP	NE1	1	B	HIS	O	3.06
303	A	TRP	NE1	4	B	GLY	O	3.00
331	**A**	**ASN**	**ND2**	2	B	VAL	O	2.97
331	**A**	**ASN**	**ND2**	2	B	VAL	O	2.97
382	A	CYS	SG	15	B	LYS	O	3.90
544	A	GLY	N	116	C	ASN	ND2	3.43
567	**A**	**THR**	**N**	**140**	**C**	**GLU**	**OE1**	3.10
567	**A**	**THR**	**N**	**140**	**C**	**GLU**	**OE2**	2.91
568	**A**	**MET**	**N**	**140**	**C**	**GLU**	**OE1**	2.94
1	B	HIS	N	334	A	GLU	OE1	3.06
1	B	HIS	N	334	A	GLU	OE2	3.38
1	B	HIS	N	358	A	GLU	OE2	2.94
2	B	VAL	N	358	A	GLU	OE2	3.43
6	B	ASP	N	279	A	TYR	OH	2.73
53	C	GLN	NE2	183	A	PHE	O	2.84
53	C	GLN	NE2	183	A	PHE	O	2.84
53	C	GLN	OE1	184	A	ASN	O	3.07
53	C	GLN	OE1	184	A	ASN	O	3.07

Pos, Position; Res, Residue; Dd-a, Distance between donor atom and acceptor atom; Red colored residues are hot residues; Green color indicates sustained bonds after simulation; Bold residues are sustained residues after simulation.

Table S 6b: Protein-Protein Side Chain-Side Chain Hydrogen Bonds from complex 1

Before Simulation								
Protein-Protein Side Chain-Side Chain Hydrogen Bonds								
DONOR				ACCEPTOR				
POS	CHAIN	RES	ATOM	POS	CHAIN	RES	ATOM	Dd-a
207	A	GLN	OE1	53	C	GLN	NE2	2.83
207	A	GLN	OE1	53	C	GLN	NE2	2.83
230	A	ARG	NH2	56	C	ASP	OD2	2.5
230	A	ARG	NH2	56	C	ASP	OD2	2.5
231	A	GLU	OE1	53	C	GLN	OE1	3.09
231	A	GLU	OE1	53	C	GLN	OE1	3.09
231	A	GLU	OE1	53	C	GLN	NE2	2.7
231	A	GLU	OE1	53	C	GLN	NE2	2.7
231	A	GLU	OE2	53	C	GLN	OE1	1.69
231	A	GLU	OE2	53	C	GLN	OE1	1.69
231	A	GLU	OE2	53	C	GLN	NE2	2.24
231	A	GLU	OE2	53	C	GLN	NE2	2.24
279	A	TYR	OH	6	B	ASP	OD1	3.34
279	A	TYR	OH	6	B	ASP	OD2	3.15
358	A	GLU	OE1	1	B	HIS	ND1	3.06
358	A	GLU	OE1	1	B	HIS	ND1	3.06
522	A	ARG	NH1	117	C	GLU	OE1	2.98
522	A	ARG	NH1	117	C	GLU	OE1	2.98
546	A	GLU	OE2	116	C	ASN	ND2	3.28
546	A	GLU	OE2	116	C	ASN	ND2	3.28
567	A	THR	OG1	140	C	GLU	OE1	2.36
567	A	THR	OG1	140	C	GLU	OE2	2.27
1	B	HIS	ND1	358	A	GLU	OE1	3.06
15	B	LYS	NZ	383	A	ASN	OD1	2.99
15	B	LYS	NZ	383	A	ASN	ND2	2.63
21	B	ARG	NH2	231	A	GLU	OE1	2.1
21	B	ARG	NH2	231	A	GLU	OE1	2.1
21	B	ARG	NH1	279	A	TYR	OH	3.38
21	B	ARG	NH1	279	A	TYR	OH	3.38
53	C	GLN	NE2	207	A	GLN	OE1	2.83
53	C	GLN	NE2	207	A	GLN	OE1	2.83
53	C	GLN	OE1	231	A	GLU	OE1	3.09
53	C	GLN	OE1	231	A	GLU	OE1	3.09

53	C	GLN	OE1	231	A	GLU	OE2	1.69
53	C	GLN	OE1	231	A	GLU	OE2	1.69
53	C	GLN	NE2	231	A	GLU	OE1	2.7
53	C	GLN	NE2	231	A	GLU	OE1	2.7
53	C	GLN	NE2	231	A	GLU	OE2	2.24
53	C	GLN	NE2	231	A	GLU	OE2	2.24
113	C	THR	OG1	546	A	GLU	OE1	3.48
116	C	ASN	ND2	546	A	GLU	OE2	3.28
116	C	ASN	ND2	546	A	GLU	OE2	3.28
116	C	ASN	OD1	568	A	MET	SD	1.15
116	C	ASN	OD1	568	A	MET	SD	1.15
116	C	ASN	ND2	568	A	MET	SD	2.66
116	C	ASN	ND2	568	A	MET	SD	2.66
After Simulation								
Protein-Protein Side Chain-Side Chain Hydrogen Bonds								
DONOR				**ACCEPTOR**				
POS	**CHAIN**	**RES**	**ATOM**	**POS**	**CHAIN**	**RES**	**ATOM**	**Dd-a**
209	A	ASN	ND2	50	C	ASN	OD1	2.83
209	A	ASN	ND2	50	C	ASN	OD1	2.83
230	**A**	**ARG**	**NH2**	6	B	ASP	OD1	3.44
230	A	ARG	NH2	6	B	ASP	OD1	3.44
406	A	TYR	OH	16	B	HIS	NE2	2.78
543	A	LYS	NZ	117	C	GLU	OE1	3.17
543	A	LYS	NZ	117	C	GLU	OE2	3.37
567	**A**	**THR**	**OG1**	**140**	**C**	**GLU**	**OE2**	2.85
16	B	HIS	NE2	406	A	TYR	OH	2.78
50	C	ASN	OD1	209	A	ASN	ND2	2.83
50	C	ASN	OD1	209	A	ASN	ND2	2.83

Pos, Position; Res, Residue; Dd-a, Distance between donor atom and acceptor atom; Red colored residues are hot residues; Green color indicates sustained bonds after simulation; Bold residues are sustained residues after simulation.

Table S6C: Protein-Protein Hydrophobic Interactions from complex 1

Before Simulation					
Protein-Protein Hydrophobic Interactions					
Position	**Residue**	**Chain**	**Position**	**Residue**	**Chain**
8	PRO	B	39	TYR	C
9	PRO	B	31	LEU	C
88	TYR	A	77	ILE	C
183	**PHE**	**A**	**59**	**LEU**	**C**

183	PHE	A	65	TRP	C
183	PHE	A	66	PHE	C
301	TYR	A	2	VAL	B
303	**TRP**	**A**	**19**	**PRO**	**B**
354	PHE	A	2	VAL	B
380	TYR	A	2	VAL	B
404	LEU	A	14	PRO	B
426	ILE	A	14	PRO	B
428	**LEU**	**A**	**14**	**PRO**	**B**
568	**MET**	**A**	**139**	**PRO**	**C**
569	LEU	A	137	PHE	C
588	ALA	A	137	PHE	C
591	ALA	A	137	PHE	C
After Simulation					
Protein-Protein Hydrophobic Interactions					
Position	**Residue**	**Chain**	**Position**	**Residue**	**Chain**
183	**PHE**	**A**	**59**	**LEU**	**C**
303	**TRP**	**A**	**19**	**PRO**	**B**
356	ALA	A	2	VAL	B
380	TYR	A	14	PRO	B
380	TYR	A	2	VAL	B
402	ILE	A	14	PRO	B
428	**LEU**	**A**	**14**	**PRO**	**B**
568	**MET**	**A**	**139**	**PRO**	**C**

Red colored residues are hot residues; Green color indicates sustain bond after simulation.

Table S6D: Protein-Protein Ionic Interactions from complex 1

Before Simulation					
Protein-Protein Ionic Interactions					
Position	**Residue**	**Chain**	**Position**	**Residue**	**Chain**
230	ARG	A	56	ASP	C
230	**ARG**	**A**	**6**	**ASP**	**B**
231	**GLU**	**A**	**21**	**ARG**	**B**
231	GLU	A	42	ARG	C
253	ASP	A	21	ARG	B
304	ARG	A	6	ASP	B
334	**GLU**	**A**	**1**	**HIS**	**B**
358	GLU	A	1	HIS	B
358	GLU	A	15	LYS	B

407	GLU	A	15	LYS	B
522	ARG	A	117	GLU	C
543	**LYS**	**A**	140	GLU	C
565	**ASP**	**A**	**164**	**LYS**	**C**
After Simulation					
Protein-Protein Ionic Interactions					
Position	**Residue**	**Chain**	**Position**	**Residue**	**Chain**
21	ARG	B	46	LYS	C
185	ARG	A	47	ASP	C
230	**ARG**	**A**	**6**	**ASP**	**B**
231	**GLU**	**A**	**21**	**ARG**	**B**
304	ARG	A	17	ASP	B
334	**GLU**	**A**	**1**	**HIS**	**B**
334	GLU	A	16	HIS	B
543	**LYS**	**A**	117	GLU	C
565	**ASP**	**A**	**164**	**LYS**	**C**

Red colored residues are hot residues; Green color indicates sustained bonds after simulation; Bold residues are sustained residues after simulation.

Table S6E: Cation-Pi Interactions within 6 Angstroms from complex 1.

Before Simulation							
Cation-Pi Interactions within 6 Angstroms							
Position	**Residue**	**Chain**	**Position**	**Residue**	**Chain**	**D (cation-pi)**	**Angle**
66	**PHE**	**C**	159	LYS	A	4.06	121.59
279	TYR	A	21	ARG	B	5.75	75.47
After Simulation							
Cation-Pi Interactions within 6 Angstroms							
Position	**Residue**	**Chain**	**Position**	**Residue**	**Chain**	**D (cation-pi)**	**Angle**
66	**PHE**	**C**	138	ARG	A	4.21	17.57
406	TYR	A	15	LYS	B	5.96	148.06

D (cation-pi**)**, Distance between two chains; Red colored residues are hot residues; Bold residues are sustained residues after simulation.

Table S6F: Protein-Protein Aromatic-Sulphur Interactions from complex 1

Before Simulation							
Protein-Protein Aromatic-Sulphur Interactions							
NO PROTEIN-PROTEIN AROMATIC-SULPHUR INTERACTIONS FOUND							
After Simulation							
Protein-Protein Aromatic-Sulphur Interactions							
Position	**Residue**	**Chain**	**Position**	**Residue**	**Chain**	**D(Centroid-Sulphur)**	**Angle**
137	PHE	C	568	MET	A	5.10	52.38

D(Centroid-Sulphur), Distance between two chains

Table S6G: Protein-Protein Main Chain-Main Chain Hydrogen Bonds from complex 2

Before Simulation								
Protein-Protein Main Chain-Main Chain Hydrogen Bonds								
No Protein-Protein Main Chain-Main Chain Hydrogen Bonds								
After Simulation								
Protein-Protein Main Chain-Main Chain Hydrogen Bonds								
DONOR				**ACCEPTOR**				
POS	**CHAIN**	**RES**	**ATOM**	**POS**	**CHAIN**	**RES**	**ATOM**	**Dd-a**
164	C	LYS	N	567	A	THR	O	3.11

Pos, Position; Res, Residue; Dd-a, Distance between donor atom and acceptor atom; Red colored residues are hot residues.

Table S6H: Protein-Protein Main Chain-Side Chain Hydrogen Bonds from complex 2

Before Simulation								
Protein-Protein Main Chain-Side Chain Hydrogen Bonds								
DONOR				**ACCEPTOR**				
POS	**CHAIN**	**RES**	**ATOM**	**POS**	**CHAIN**	**RES**	**ATOM**	**Dd-a**
62	A	SER	OG	72	C	PRO	O	3.18
86	A	ASP	OD2	71	C	ASN	O	3.46
86	A	ASP	OD2	71	C	ASN	O	3.46
110	A	ASP	OD2	63	C	CYS	O	2.78
110	A	ASP	OD2	63	C	CYS	O	2.78
134	A	HIS	NE2	63	C	CYS	O	3.19
134	A	HIS	ND1	64	C	THR	O	3.17
134	A	HIS	ND1	65	C	TRP	O	2.68
134	A	HIS	NE2	65	C	TRP	O	2.05
134	A	HIS	NE2	68	C	VAL	O	3.08
159	A	LYS	NZ	65	C	TRP	O	3.4

159	A	LYS	NZ	66	C	PHE	O	3.37
207	A	GLN	OE1	53	C	GLN	O	2.01
207	A	GLN	OE1	53	C	GLN	O	2.01
567	A	THR	N	140	C	GLU	OE1	3.34
567	A	THR	N	140	C	GLU	OE2	1.63
568	A	MET	N	140	C	GLU	OE2	3
65	C	TRP	N	134	A	HIS	NE2	2.92
66	C	PHE	N	134	A	HIS	ND1	3.36
116	C	ASN	ND2	544	A	GLY	O	2.47
116	C	ASN	ND2	544	A	GLY	O	2.47
140	C	GLU	OE1	565	A	ASP	O	3.12
140	C	GLU	OE1	565	A	ASP	O	3.12
140	C	GLU	OE2	565	A	ASP	O	3.5
140	C	GLU	OE2	565	A	ASP	O	3.5
After Simulation								
Protein-Protein Main Chain-Side Chain Hydrogen Bonds								
	DONOR				**ACCEPTOR**			
POS	**CHAIN**	**RES**	**ATOM**	**POS**	**CHAIN**	**RES**	**ATOM**	**Dd-a**
522	A	ARG	NE	114	C	ILE	O	3.4
522	A	ARG	NH2	115	C	PRO	O	3.02
522	A	ARG	NH2	115	C	PRO	O	3.02
522	A	ARG	NH1	135	C	THR	O	3
522	A	ARG	NH1	135	C	THR	O	3
522	A	ARG	NH1	137	C	PHE	O	3.04
522	A	ARG	NH1	137	C	PHE	O	3.04
522	A	ARG	NH2	137	C	PHE	O	3.44
522	A	ARG	NH2	137	C	PHE	O	3.44
50	C	ASN	N	231	A	GLU	OE2	2.94
137	C	PHE	N	546	A	GLU	OE2	2.91
161	C	SER	OG	569	A	LEU	O	3.47
161	C	SER	N	570	A	HIS	ND1	3.06

Pos, Position; Res, Residue; Dd-a, Distance between donor atom and acceptor atom; Red colored residues are hot residues.

Table S6I: Protein-Protein Side Chain-Side Chain Hydrogen Bonds from complex 2

Before Simulation								
Protein-Protein Side Chain-Side Chain Hydrogen Bonds								
	DONOR				**ACCEPTOR**			
POS	**CHAIN**	**RES**	**ATOM**	**POS**	**CHAIN**	**RES**	**ATOM**	**Dd-a**

207	A	GLN	OE1	53	C	GLN	NE2	2.83
207	A	GLN	OE1	53	C	GLN	NE2	2.83
230	A	ARG	NH2	56	C	ASP	OD2	2.5
230	A	ARG	NH2	56	C	ASP	OD2	2.5
231	**A**	**GLU**	**OE1**	53	C	GLN	OE1	3.09
231	**A**	**GLU**	**OE1**	53	C	GLN	OE1	3.09
231	**A**	**GLU**	**OE1**	53	C	GLN	NE2	2.7
231	**A**	**GLU**	**OE1**	53	C	GLN	NE2	2.7
231	A	GLU	OE2	53	C	GLN	OE1	1.69
231	A	GLU	OE2	53	C	GLN	OE1	1.69
231	A	GLU	OE2	53	C	GLN	NE2	2.24
231	A	GLU	OE2	53	C	GLN	NE2	2.24
522	**A**	**ARG**	**NH1**	117	C	GLU	OE1	2.98
522	**A**	**ARG**	**NH1**	117	C	GLU	OE1	2.98
546	A	GLU	OE2	116	C	ASN	ND2	3.28
546	A	GLU	OE2	116	C	ASN	ND2	3.28
567	A	THR	OG1	140	C	GLU	OE1	2.36
567	**A**	**THR**	**OG1**	**140**	**C**	**GLU**	**OE2**	2.27
53	C	GLN	NE2	207	A	GLN	OE1	2.83
53	C	GLN	NE2	207	A	GLN	OE1	2.83
53	C	GLN	OE1	231	A	GLU	OE1	3.09
53	C	GLN	OE1	231	A	GLU	OE1	3.09
53	C	GLN	OE1	231	A	GLU	OE2	1.69
53	C	GLN	OE1	231	A	GLU	OE2	1.69
53	C	GLN	NE2	231	A	GLU	OE1	2.7
53	C	GLN	NE2	231	A	GLU	OE1	2.7
53	C	GLN	NE2	231	A	GLU	OE2	2.24
53	C	GLN	NE2	231	A	GLU	OE2	2.24
113	C	THR	OG1	546	A	GLU	OE1	3.48
116	C	ASN	ND2	546	A	GLU	OE2	3.28
116	C	ASN	ND2	546	A	GLU	OE2	3.28
116	**C**	**ASN**	**OD1**	**568**	**A**	**MET**	**SD**	1.15
116	**C**	**ASN**	**OD1**	**568**	**A**	**MET**	**SD**	1.15
116	**C**	**ASN**	**ND2**	**568**	**A**	**MET**	**SD**	2.66
116	**C**	**ASN**	**ND2**	**568**	**A**	**MET**	**SD**	2.66

After Simulation

Protein-Protein Side Chain-Side Chain Hydrogen Bonds

DONOR				**ACCEPTOR**				

POS	CHAIN	RES	ATOM	POS	CHAIN	RES	ATOM	Dd-a
88	A	TYR	OH	73	C	ASP	OD1	2.8
136	A	GLN	OE1	61	C	ASN	ND2	3.13
136	A	GLN	OE1	61	C	ASN	ND2	3.13
136	A	GLN	NE2	61	C	ASN	ND2	3.27
136	A	GLN	NE2	61	C	ASN	ND2	3.27
138	A	ARG	NH1	71	C	ASN	OD1	3.04
138	A	ARG	NH1	71	C	ASN	OD1	3.04
185	A	ARG	NH2	50	C	ASN	OD1	3.37
185	A	ARG	NH2	50	C	ASN	OD1	3.37
185	A	ARG	NH2	67	C	HIS	ND1	2.83
185	A	ARG	NH2	67	C	HIS	ND1	2.83
231	**A**	**GLU**	**OE1**	49	C	ASN	ND2	3.01
231	**A**	**GLU**	**OE1**	49	C	ASN	ND2	3.01
231	**A**	**GLU**	**OE1**	50	C	ASN	ND2	2.99
231	**A**	**GLU**	**OE1**	50	C	ASN	ND2	2.99
495	A	LYS	NZ	93	C	GLN	OE1	2.85
496	A	ASN	ND2	93	C	GLN	OE1	2.94
496	A	ASN	ND2	93	C	GLN	OE1	2.94
522	**A**	**ARG**	**NE**	116	C	ASN	OD1	2.69
522	**A**	**ARG**	**NH2**	116	C	ASN	OD1	3.03
522	A	ARG	NH2	116	C	ASN	OD1	3.03
567	**A**	**THR**	**OG1**	**140**	**C**	**GLU**	**OE2**	2.73
570	A	HIS	ND1	161	C	SER	OG	3.44
49	C	ASN	ND2	231	A	GLU	OE1	3.01
49	C	ASN	ND2	231	A	GLU	OE1	3.01
50	C	ASN	ND2	231	A	GLU	OE1	2.99
50	C	ASN	ND2	231	A	GLU	OE1	2.99
61	C	ASN	ND2	136	A	GLN	OE1	3.13
61	C	ASN	ND2	136	A	GLN	OE1	3.13
61	C	ASN	ND2	136	A	GLN	NE2	3.27
61	C	ASN	ND2	136	A	GLN	NE2	3.27
93	C	GLN	OE1	496	A	ASN	ND2	2.94
93	C	GLN	OE1	496	A	ASN	ND2	2.94
116	**C**	**ASN**	**OD1**	**568**	**A**	**MET**	**SD**	3.68
116	**C**	**ASN**	**OD1**	**568**	**A**	**MET**	**SD**	3.68
116	**C**	**ASN**	**ND2**	**568**	**A**	**MET**	**SD**	3.32

116	**C**	**ASN**	**ND2**	**568**	**A**	**MET**	**SD**	3.32
161	C	SER	OG	570	A	HIS	ND1	3.44

Pos, Position; Res, Residue; Dd-a, Distance between donor atom and acceptor atom; Red colored residues are hot residues; Green color indicates sustained bonds after simulation; Bold residues are sustained residues after simulation.

Table S6J: Protein-Protein Hydrophobic Interactions from complex 2

Before Simulation					
Protein-Protein Hydrophobic Interactions					
Position	**Residue**	**Chain**	**Position**	**Residue**	**Chain**
88	TYR	A	77	ILE	C
183	PHE	A	59	LEU	C
183	PHE	A	65	TRP	C
183	PHE	A	66	PHE	C
568	**MET**	**A**	139	PRO	C
569	LEU	A	137	PHE	C
588	ALA	A	137	PHE	C
591	ALA	A	137	PHE	C
After Simulation					
Protein-Protein Hydrophobic Interactions					
Position	**Residue**	**Chain**	**Position**	**Residue**	**Chain**
183	PHE	A	66	PHE	C
474	ILE	A	91	VAL	C
520	LEU	A	115	PRO	C
568	**MET**	**A**	137	PHE	C
568	MET	A	163	PRO	C

Bold residues are sustained residues after simulation.

Table S6K: Protein-Protein Ionic Interactions from complex 2

Before Simulation					
Protein-Protein Ionic Interactions					
Position	**Residue**	**Chain**	**Position**	**Residue**	**Chain**
230	ARG	A	56	ASP	C
231	GLU	A	42	ARG	C
522	ARG	A	117	GLU	C
543	**LYS**	**A**	140	GLU	C
565	ASP	A	164	LYS	C
After Simulation					
Protein-Protein Ionic Interactions					
Position	**Residue**	**Chain**	**Position**	**Residue**	**Chain**
159	LYS	A	56	ASP	C
543	**LYS**	**A**	117	GLU	C

Red coloured residues are hot residues; Bold residues are sustained residues after simulation.

Table S6L: Protein-Protein Cation-Pi Interactions from complex 2

Before Simulation							
Protein-Protein Cation-Pi Interactions							
Position	**Residue**	**Chain**	**Position**	**Residue**	**Chain**	**D(cation-Pi)**	**Angle**
66	**PHE**	**C**	159	LYS	A	4.06	121.59
After Simulation							
Protein-Protein Cation-Pi Interactions							
Position	**Residue**	**Chain**	**Position**	**Residue**	**Chain**	**D(cation-Pi)**	**Angle**
66	**PHE**	**C**	185	ARG	A	3.89	39.7

D (cation-pi**)**, Distance between two chains; Red colored residues are hot residues; Bold residues are sustained residues after simulation.

Table S6M: Protein-Protein Aromatic-Aromatic Interactions from complex 2

Before Simulation							
Protein-Protein Aromatic-Aromatic Interactions							
NO PROTEIN-PROTEIN AROMATIC-AROMATIC INTERACTIONS FOUND							
After Simulation							
Protein-Protein Aromatic-Aromatic Interactions							
Position	**Residue**	**Chain**	**Position**	**Residue**	**Chain**	**D(cation-Pi)**	**Angle**
183	PHE	A	66	PHE	C	5.77	51.71

D(cation-pi**)**: Distance between two chains

Table S6N: Protein-Protein Main Chain-Side Chain Hydrogen Bonds from complex 3

Before Simulation								
Protein-Protein Main Chain-Side Chain Hydrogen Bonds								
DONOR				**ACCEPTOR**				
POS	**CHAIN**	**RES**	**ATOM**	**POS**	**CHAIN**	**RES**	**ATOM**	**Dd-a**
331	**A**	**ASN**	**ND2**	**1**	**B**	**HIS**	**O**	2.33
331	**A**	**ASN**	**ND2**	**1**	**B**	**HIS**	**O**	2.33
4	B	GLY	N	301	A	TYR	OH	3.4
After Simulation								
Protein-Protein Main Chain-Side Chain Hydrogen Bonds								
DONOR				**ACCEPTOR**				
POS	**CHAIN**	**RES**	**ATOM**	**POS**	**CHAIN**	**RES**	**ATOM**	**Dd-a**
303	A	TRP	NE1	1	B	HIS	O	3.27
331	**A**	**ASN**	**ND2**	**1**	**B**	**HIS**	**O**	3.47
331	**A**	**ASN**	**ND2**	**1**	**B**	**HIS**	**O**	3.47
331	A	ASN	ND2	2	B	VAL	O	3.08

331	A	ASN	ND2	2	B	VAL	O	3.08
382	A	CYS	SG	14	B	PRO	O	3.55
1	B	HIS	N	334	A	GLU	OE1	3.38
1	B	HIS	N	334	A	GLU	OE2	3.33
1	B	HIS	N	358	A	GLU	OE2	2.95
4	B	GLY	N	331	A	ASN	OD1	3.41
5	B	GLY	N	301	A	TYR	OH	2.72

Pos, Position; Res, Residue; Dd-a, Distance between donor atom and acceptor atom; Red colored residues are hot residues; Green color indicates sustained bonds after simulation; Bold residues are sustained residues after simulation.

Table S6O: Protein-Protein Side Chain-Side Chain Hydrogen Bonds from complex 3

Before Simulation								
Protein-Protein Side Chain-Side Chain Hydrogen Bonds								
DONOR				**ACCEPTOR**				
POS	**CHAIN**	**RES**	**ATOM**	**POS**	**CHAIN**	**RES**	**ATOM**	**Dd-a**
279	A	TYR	OH	6	B	ASP	OD1	3.34
279	A	TYR	OH	6	B	ASP	OD2	3.15
358	A	GLU	OE1	1	B	HIS	ND1	3.06
358	A	GLU	OE1	1	B	HIS	ND1	3.06
1	B	HIS	ND1	358	A	GLU	OE1	3.06
7	**B**	**X**	**OH**	380	A	TYR	OH	3.07
15	B	LYS	NZ	383	A	ASN	OD1	2.99
15	B	LYS	NZ	383	A	ASN	ND2	2.63
21	B	ARG	NH2	231	A	GLU	OE1	2.1
21	B	ARG	NH2	231	A	GLU	OE1	2.1
21	B	ARG	NH1	279	A	TYR	OH	3.38
21	B	ARG	NH1	279	A	TYR	OH	3.38
After Simulation								
Protein-Protein Side Chain-Side Chain Hydrogen Bonds								
DONOR				**ACCEPTOR**				
POS	**CHAIN**	**RES**	**ATOM**	**POS**	**CHAIN**	**RES**	**ATOM**	**Dd-a**
378	A	HIS	NE2	7	B	X	OH	2.83
7	**B**	**X**	**OH**	378	A	HIS	NE2	2.83

Pos, Position; Res, Residue; Dd-a, Distance between donor atom and acceptor atom; Red colored residues are hot residues; Green color indicates sustained bonds after simulation; Bold residues are sustained residues after simulation.

Table S6P: Protein-Protein Hydrophobic Interactions from complex 3

Before Simulation					
Protein-Protein Hydrophobic Interactions					
Position	**Residue**	**Chain**	**Position**	**Residue**	**Chain**
301	TYR	A	2	VAL	B
303	TRP	A	19	PRO	B

354	PHE	A	2	VAL	B
380	**TYR**	**A**	**2**	**VAL**	**B**
404	**LEU**	**A**	**14**	**PRO**	**B**
426	ILE	A	14	PRO	B
428	LEU	A	14	PRO	B
After Simulation					
Protein-Protein Hydrophobic Interactions					
Position	**Residue**	**Chain**	**Position**	**Residue**	**Chain**
380	TYR	A	14	PRO	B
380	**TYR**	**A**	**2**	**VAL**	**B**
402	ILE	A	12	ALA	B
404	**LEU**	**A**	**14**	**PRO**	**B**

Red colored residues are hot residues; Green color indicates sustain bond after simulation.

Table S6Q: Protein-Protein Ionic Interactions from complex 3

Before Simulation					
Protein-Protein Ionic Interactions					
Position	**Residue**	**Chain**	**Position**	**Residue**	**Chain**
230	**ARG**	**A**	**6**	**ASP**	**B**
231	GLU	A	21	ARG	B
253	**ASP**	**A**	21	ARG	B
304	**ARG**	**A**	6	ASP	B
334	**GLU**	**A**	**1**	**HIS**	**B**
358	GLU	A	1	HIS	B
358	GLU	A	15	LYS	B
407	**GLU**	**A**	15	LYS	B
After Simulation					
Protein-Protein Ionic Interactions					
Position	**Residue**	**Chain**	**Position**	**Residue**	**Chain**
230	**ARG**	**A**	**6**	**ASP**	**B**
304	**ARG**	**A**	17	ASP	B
334	**GLU**	**A**	**1**	**HIS**	**B**
407	**GLU**	**A**	16	HIS	B

Red colored residues are hot residues; Green color indicates sustained bonds after simulation; Bold residues are sustained residues after simulation.

Table S6R: Protein-Protein Cation-Pi Interactions from complex 3

Before Simulation							
Protein-Protein Cation-Pi Interactions							
Position	**Residue**	**Chain**	**Position**	**Residue**	**Chain**	**D(cation-Pi)**	**Angle**
279	TYR	A	21	ARG	B	5.75	75.47

After Simulation

Protein-Protein Cation-Pi Interactions

NO PROTEIN-PROTEIN CATION-PI INTERACTIONS FOUND

D (cation-pi**)**, Distance between two chain

Complex	**Inter. Bet.**	**H-Bond**		**Hydrophobic Interaction**		**Ionic Interaction**		**Cation - Pi Interaction**		**Aromatic - Aromatic Interaction**		**Aromatic - Sulphar Interaction**		**Total**	
		B. MD	*A. MD*	*B. MD*	*A. MD*	*B. MD*	*A. MD*	*B. MD*	*A. MD*	*B. MD*	*A. MD*	*B. MD*	*A. MD*	*B. MD*	*A. MD*
Xa21 +Raxsn +Os	*Xa21 +Raxsn*	15	14	7	6	8	5	1	1	0	0	0	0	31	26
	Xa21 +Os	60	17	8	2	5	3	1	1	0	0	0	1	74	24
	Raxsn +Os	16	0	2	0	0	1	0	0	0	0	0	0	18	1
Xa21 +Os	*Xa21 +Os*	60	52	8	5	5	2	1	1	0	1	0	0	74	79
Xa21 +Raxsn	*Xa21 +Raxsn*	15	13	7	4	8	4	1	0	0	0	0	0	31	21

Table S6S: Summary of interactions between Xa21, RaxX21-sY and OsSERK2

Inter. Bet., Interactions Between; H-Bond, Hydrogen Bond; B. MD, Before Molecular Dynamics simulation; A. MD, After Molecular Dynamics simulation