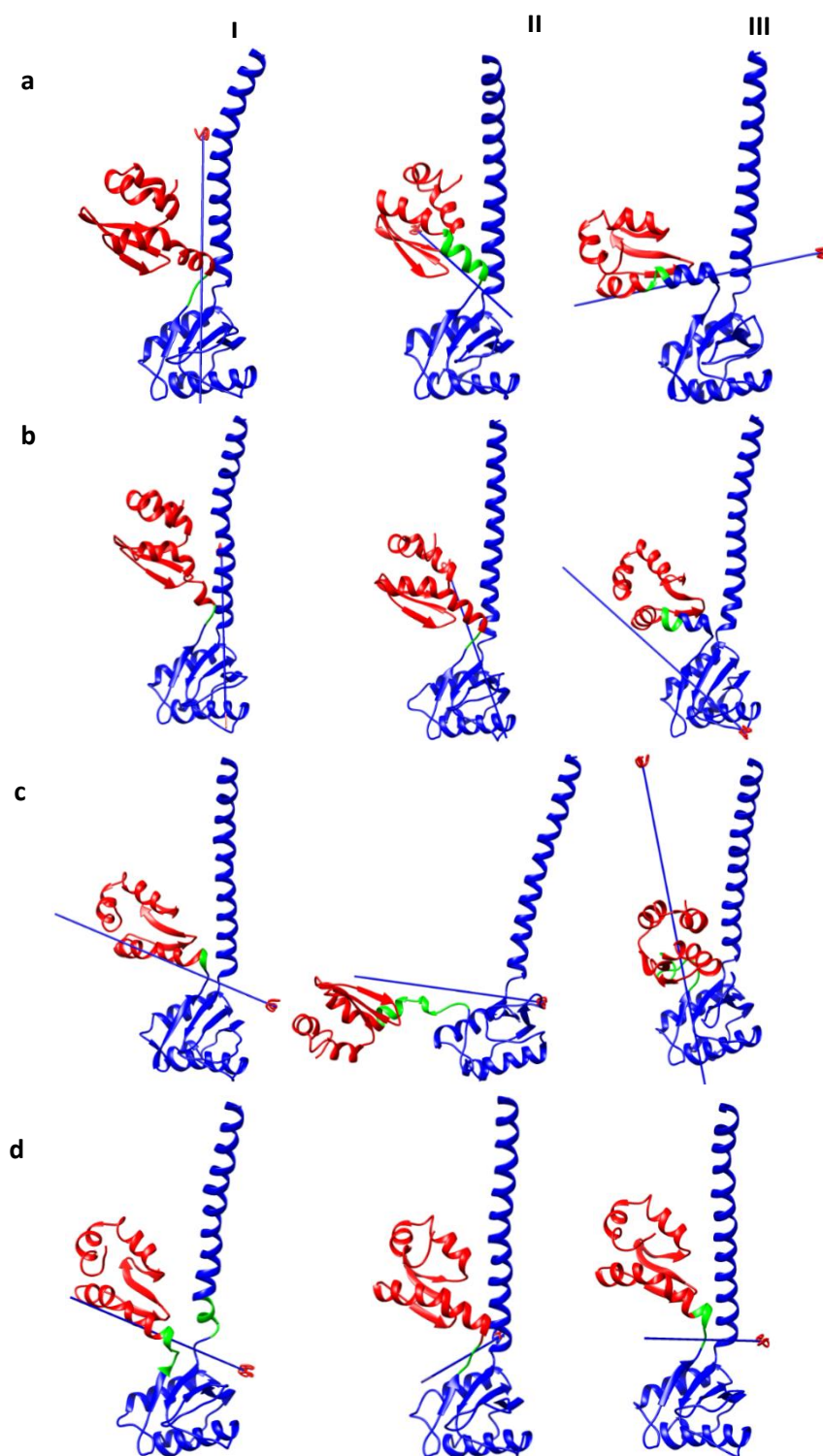
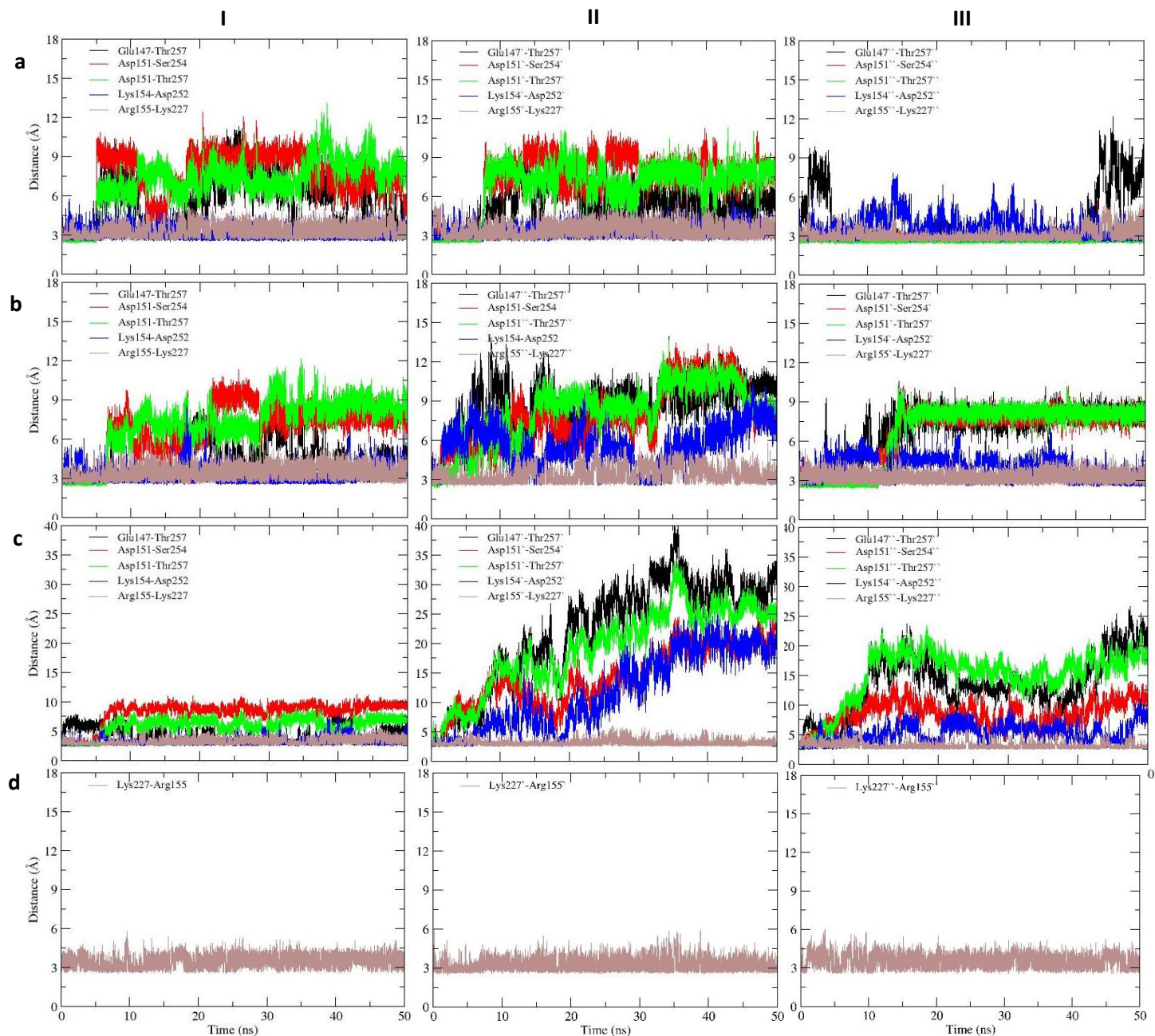


Supplementary Figure 1. Functional dynamics of chains A (I), B (II) and C (III) in ORF_{wt} (a), ORF₂₆₁ (b), ORF₂₈₂ (c), and ORF_{tri} (d). The fixed and moving domains are colored in blue and red, respectively, whereas the bending residues are colored in green. Arrows indicate the hinge axis for the dynamics of CTD



Supplementary Figure 2. Variation in the H-bond distance for hinge 2- CC interactions such as Glu147-Thr257 (black), Asp151-Ser254 (red), Asp151-Thr257 (green) and Lys154-Asp252 (blue) along with the CC-RRM interaction Arg227-Lys155 (brown). The variations in chains A (I), B (II) and C (III) of ORF_{wt} (a), ORF₂₆₁ (b), and ORF₂₈₂ (c) are shown



Supplementary Table 1. List of inter-chain H-bonds observed from 50 ns simulations of ORF1p structures

Acceptor	Donor	Life time (%)	Average Distance (Å)	Average Angle (Å)
ORF1p_{wt}				
ORF_{wt} AC interface				
TYR152	ASN157 ^{``}	9	3.172	148.646
GLU148	ARG206 ^{``}	21	2.913	154.897
GLU225	GLY171 ^{``}	27	2.996	155.564
THR222	GLN198 ^{``}	13	2.968	159.141
GLN205 ^{``}	ARG155	9	2.868	153.372
GLU199 ^{``}	VAL224	48	3.003	162.16
GLU199 ^{``}	GLU225	12	2.924	158.019
GLU256 ^{``}	ARG141	12	2.927	158.743
ORF_{wt} AB interface				
TYR152 [`]	ASN157	47	3.136	155.056
THR222 [`]	GLN198	30	2.93	158.613
GLU199	ARG155 [`]	69	2.894	156.75
GLU256	ARG141 [`]	77	2.852	158.38
GLN259	ARG141 [`]	44	2.863	157.54
GLU256	SER145 [`]	14	2.727	164.427
ASP305 [`]	ARG206	10	2.867	155.174
ORF_{wt} BC interface				
TYR152 ^{``}	ASN157 [`]	90	3.001	157.521
GLU225 ^{``}	ASN170 [`]	7	2.845	158.281
GLU225 ^{``}	GLY171 [`]	7	3.13	143.984
GLU225 ^{``}	THR172 [`]	34	2.705	163.874
LEU286 ^{``}	ARG206 [`]	28	2.822	157.898
GLU256 [`]	ARG141 ^{``}	65	2.978	157.893
GLU199 [`]	ARG155 ^{``}	9	3.001	150.087
GLN201 [`]	ARG155 ^{``}	6	2.958	148.798
GLN205 [`]	ARG155 ^{``}	7	2.916	157.075
GLU175 [`]	LYS223 ^{``}	24	2.878	155.416
GLN198 [`]	VAL224 ^{``}	87	3.036	155.396
SER287 ^{``}	ARG206 [`]	20	2.916	150.378
PHE297 ^{``}	ARG206 [`]	30	2.859	157.195

ORF_{tri}				
ORF_{tri} AC interface				
TYR152	ASN157 ^{^^}	87.37	2.9957	154.7292
ASP252	TYR152 ^{^^}	13.32	2.7112	161.6443
GLN198	VAL224 ^{^^}	8.38	3.19	157.8041
GLU199	ARG155 ^{^^}	70.64	2.9087	156.0697
SER198	ILE294 ^{^^}	64.06	2.9713	161.473
GLU225	THR172 ^{^^}	21.27	2.7144	163.1247
GLN198	GLN198 ^{^^}	9.16	2.9884	151.4924
THR222	GLN198 ^{^^}	21.01	2.9309	158.4734
LEU286	ARG206 ^{^^}	8.01	2.8679	149.0658
SER287	ARG206 ^{^^}	6.17	2.9982	151.8094
PHE297	ARG206 ^{^^}	14.31	2.8715	161.5167
GLU293	ARG210 ^{^^}	20.8	2.8708	156.1755
GLU199 ^{^^}	ARG155	65.6	2.9477	151.6269
GLN201 ^{^^}	ARG155	6.79	2.8698	151.0475
GLU175 ^{^^}	LYS223	22.54	2.8623	156.5854
GLN198 ^{^^}	VAL224	71.31	3.1354	156.878
GLU256 ^{^^}	SER145	86.05	2.6351	166.2183
ORF_{tri} AB interface				
TYR152 [`]	ASN157	38.12	3.0672	153.6789
GLN198 [`]	GLN198	9.18	3.0539	152.1559
THR222 [`]	GLN198	16.16	2.9018	159.3357
GLU256	ARG141 [`]	31.5	2.839	152.318
GLU256	SER145 [`]	37.41	2.6904	164.5952
GLY292 [`]	TYR207	42.88	2.7833	159.6418
GLU293 [`]	SER209	15.62	2.681	163.8816
ORF₂₆₁ BC interface				
TYR152 [`]	ASN157 ^{^^}	75.8	3.0701	154.8027
GLU225 ^{^^}	THR172 [`]	31.57	2.7406	161.6628
GLN196 ^{^^}	GLN196 [`]	7.06	2.9636	157.8271
GLN198 ^{^^}	GLN198 [`]	8.8	3.0325	147.7331
THR222 ^{^^}	GLN198 [`]	51.78	2.9034	160.8635
GLU293 ^{^^}	TYR207 [`]	12.98	2.739	162.4219
TYR296 ^{^^}	TYR207 [`]	18.43	2.8302	157.2753
GLU293 ^{^^}	ARG210 [`]	12.48	2.8652	156.7362
GLU199 [`]	ARG155 ^{^^}	62.08	2.8783	157.0242
GLN201 [`]	ARG155 ^{^^}	9.05	2.9185	149.9969
GLN198 [`]	GLN198 ^{^^}	20.09	2.9854	158.438

GLU175`	LYS223``	21.55	2.8777	154.4872
ILE197`	LYS223``	7.01	2.8519	154.3053
GLN198`	VAL224``	79.48	3.1416	161.0206
GLU256`	ARG141``	18.58	2.8929	156.1003
ORF₂₆₁				
ORF₂₆₁ AC interface				
TYR152	ASN44``	61.38	3.0716	154.3233
GLU225	ASN57``	5.22	2.9261	151.1627
GLU225	THR59``	33.77	2.7137	163.4698
THR222	GLN85``	12.3	2.9349	160.152
GLU199``	ARG155	50.15	2.8774	156.6312
GLN201``	ARG155	11.08	2.9267	153.3994
GLU175``	LYS223	21.35	2.8449	154.6409
GLN198``	VAL224	78.91	3.041	161.6119
ORF₂₆₁ AB interface				
TYR152`	ASN157	14.93	3.1676	158.6455
GLU225`	ASN170	10.44	2.9418	161.4796
GLN198`	GLN198	9.96	3.0038	150.4739
THR222`	GLN198	42.91	2.942	158.7919
GLU263	ARG138`	16.8	2.822	157.9955
GLU256	ARG141`	83.72	2.8811	157.7379
GLU256	SER145`	57.47	2.6856	164.3026
GLU199	ARG42`	70.93	2.8934	156.0516
GLU175	LYS110`	12.29	2.8735	155.0878
ILE197	LYS110`	5.13	2.8549	152.9967
GLN198	VAL111`	22.41	3.2019	158.306
ORF₂₆₁ BC interface				
TYR152``	ASN157`	10.7	3.1226	152.6239
GLU225``	THR172`	11.82	2.7165	163.4789
THR222``	GLN198`	15.94	2.9144	159.5295
GLU225``	GLN201`	7.54	2.8799	161.1271
THR222``	ARG220`	7.96	2.8674	156.6893
LEU286``	ARG206`	6.94	2.915	156.3234
SER287``	ARG206`	5.58	2.9613	151.6471
GLU293``	ARG206`	20.15	2.8663	156.1891
GLU293``	TYR207`	12.07	2.748	161.1985
GLN198`	VAL224``	30.17	3.1168	159.8224
GLU199`	VAL224``	9.62	3.0209	161.6244

GLU263`	ARG138``	19.94	2.9118	153.5112
GLU256`	ARG141``	53.92	2.8796	155.3166
GLU256`	SER145``	31.85	2.6767	165.2409
SER145``	TRP150`	25.1	3.1184	148.9828
SER145``	TRP150`	23.71	3.1995	152.3336
ORF₂₈₂				
ORF₂₈₂ AC interface				
TYR152	ASN157``	42.85	3.0583	154.7124
GLU148	ARG206``	34.82	2.9162	155.2563
SER281	ARG206``	7.98	2.9377	157.978
ALA284	ARG206``	15.09	2.8257	151.8396
ILE294	SER208``	24.03	2.7218	161.7479
TYR296	SER208``	6.22	2.8812	156.0161
ILE294	SER209``	10.57	3.0497	156.7861
GLU291	ARG210``	5.88	2.88	152.0622
GLU293	ARG210``	22.32	2.8468	157.906
GLU199``	TYR152	17.36	2.6875	164.4942
GLU199``	ARG155	46.07	2.8474	156.0604
GLN201``	ARG155	17.62	2.9359	152.7932
GLU175``	LYS223	24.39	2.8647	154.0996
GLN198``	VAL224	76.58	3.0636	159.7656
ASP167``	ARG279	37.09	2.8678	157.6842
GLN205``	LYS285	10.4	2.8502	152.4792
SER209``	ILE294	10.62	2.958	161.3802
GLU256``	ARG141	5.27	2.8711	158.7432
GLU263``	ARG141	9.44	2.9176	155.5516
GLU273``	LYS295	9.71	2.8542	156.2675
GLU273``	TYR296	8.22	2.9613	160.2838
ORF₂₈₂ AB interface				
TYR152`	ASN157	83.73	3.046	156.0275
THR222`	GLN198	41.48	2.9421	158.333
GLU256`	ARG206	15.54	2.8992	155.4612
GLU256	ARG141`	30.75	2.9184	153.8248
ORF₂₈₂ BC interface				
TYR152``	ASN157`	72.38	3.0681	155.7883
GLU199`	ARG155``	62.73	2.9922	153.2048
GLN201`	ARG155``	14.29	2.9136	150.4711
GLU175`	LYS223``	22.94	2.8825	153.3362
GLN198`	VAL224``	78.14	3.1084	160.6324

GLN196`	LYS223``	5.7	2.8611	156.3588
GLU225``	THR172`	5.94	2.743	161.8091
THR222``	GLN198`	56.82	2.9092	160.6052