Indian Journal of Biochemistry & Biophysics
Vol. 63, October 2026, pp. 1158-1168
DOI: 10.56042/ijbb.v63i10.24642

In silico study on assembly of Dengue virus capsid protein with core histone proteins

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Received 08 October 2025; *revised 05 July 2026*

Supplementary data

Suppl. Table 1 — Residue wise Binding energy decomposition of capsid protein in complex with Histone H2A

Capsid-H2A	Average Binding free energy (Kcal/mol)
H2A-B-TYR-57	-5.95333
H2A-B-TYR-50	-5.72333
H2A-B-VAL-54	-5.29333
H2A-B-ALA-60	-5.00333
Capsid-A-PHE-53	-4.36
Capsid-A-LEU-95	-3.96
Capsid-A-LEU-50	-3.86667
Capsid-A-LEU-81	-3.85
Capsid-A-LEU-54	-3.57
H2A-B-PHE-25	-3.41667
Capsid-A-PRO-12	-3.29333
H2A-B-GLU-61	-3.27
Capsid-A-LEU-92	-3.23
H2A-B-VAL-30	-3.13667
H2A-B-GLU-64	-2.93333
Capsid-A-PHE-13	-2.8
Capsid-A-ILE-78	-2.76667
H2A-B-GLU-56	-2.76667
Capsid-A-ILE-88	-2.61667
Capsid-A-ASN-96	-2.45
H2A-B-PRO-117	-2.43667
H2A-B-ALA-47	-2.37
Capsid-A-PHE-47	-2.31667
H2A-B-ILE-87	-2.31667
Capsid-A-LEU-46	-2.19667
Capsid-A-ASP-3	-2.18667
H2A-B-VAL-27	-2.14333
Capsid-A-PHE-56	-2.09
Capsid-A-PRO-43	-1.96333
H2A-B-LEU-63	-1.88333
Capsid-A-ILE-59	-1.87667
Capsid-A-ASN-10	-1.85333
H2A-B-LEU-55	-1.83
H2A-B-HIS-82	-1.79333
H2A-B-ARG-42	-1.74333
H2A-B-GLU-41	-1.7

Capsid-A-ARG-99	-1.67
H2A-B-ASP-90	-1.66333
H2A-B-ILE-79	-1.65333
Capsid-A-PRO-61	-1.64
H2A-B-ALA-53	-1.63333
H2A-B-LEU-51	-1.57333
Capsid-A-VAL-51	-1.57
H2A-B-VAL-43	-1.55667
H2A-B-SER-40	-1.50667
H2A-B-ILE-78	-1.49
Capsid-A-LEU-57	-1.47333
H2A-B-LEU-83	-1.42333
H2A-B-TYR-39	-1.39667
Capsid-A-ARG-97	-1.35667
Capsid-A-LEU-16	-1.35
Capsid-A-THR-58	-1.32
H2A-B-ILE-62	-1.29333
Capsid-A-ARG-18	-1.23
H2A-B-GLU-91	-1.18
Capsid-A-PHE-84	-1.16333
H2A-B-ASN-89	-1.12
H2A-B-VAL-49	-1.10333
Capsid-A-GLU-19	-1.09
Capsid-A-GLN-39	-1.07667
H2A-B-ILE-102	-1.06667
Capsid-A-LYS-74	-1.06
H2A-B-ARG-32	-1.02
Capsid-A-ARG-98	-0.98333
H2A-B-ARG-20	-0.98
H2A-B-PRO-26	-0.97333
Capsid-A-ARG-100	-0.95667
Capsid-A-LEU-35	-0.94667
H2A-B-GLY-46	-0.93
H2A-B-LEU-65	-0.92667
H2A-B-PRO-109	-0.90333
H2A-B-LEU-115	-0.89
H2A-B-LEU-58	-0.89
H2A-B-ALA-21	-0.88
H2A-B-LYS-118	-0.82667
Capsid-A-ALA-77	-0.78
H2A-B-LEU-33	-0.74
H2A-B-GLY-98	-0.67667
H2A-B-ARG-77	-0.66333
Capsid-A-ALA-49	-0.65
Capsid-A-THR-71	-0.62667
H2A-B-ARG-71	-0.62
H2A-B-ARG-88	-0.62
H2A-B-GLY-44	-0.60333
Capsid-A-LEU-44	-0.6
Capsid-A-LEU-38	-0.59667
H2A-B-THR-101	-0.57
Capsid-A-GLN-28	-0.56667
H2A-B-GLU-92	-0.55667
Capsid-A-PRO-60	-0.54667
Capsid-A-VAL-23	-0.54333
H2A-B-PRO-48	-0.53667

Capsid-A-MET-15	-0.52667
Capsid-A-ASN-21	-0.52333
H2A-B-LEU-97	-0.52
H2A-B-LEU-96	-0.51667
Capsid-A-PHE-33	-0.49333
H2A-B-LEU-23	-0.48
Capsid-A-GLY-40	-0.47667
H2A-B-ASP-72	-0.42667
Capsid-A-GLU-87	-0.42333
Capsid-A-GLY-70	-0.41667
H2A-B-VAL-114	-0.36667
H2A-B-LYS-95	-0.35667
Capsid-A-MET-91	-0.35333
Capsid-A-ALA-63	-0.33333
Capsid-A-ARG-41	-0.33
H2A-B-GLY-106	-0.32667
Capsid-A-THR-11	-0.32333
Capsid-A-TRP-69	-0.25
H2A-B-ALA-66	-0.24667
Capsid-A-ALA-52	-0.24
H2A-B-GLY-105	-0.23
Capsid-A-VAL-80	-0.23
Capsid-A-ILE-94	-0.21
Capsid-A-ARG-85	-0.20667
H2A-B-PRO-80	-0.18667
Capsid-A-THR-30	-0.17333
Capsid-A-SER-34	-0.17
H2A-B-GLN-84	-0.15667
H2A-B-GLY-67	-0.15667
Capsid-A-GLN-4	-0.15333
H2A-B-GLY-28	-0.14667
Capsid-A-ARG-9	-0.13
H2A-B-GLN-24	-0.13
Capsid-A-GLY-64	-0.12667
Capsid-A-SER-75	-0.11667
Capsid-A-ILE-72	-0.10333
H2A-B-ALA-69	-0.10333
H2A-B-ASN-38	-0.09667
Capsid-A-LYS-7	-0.08333
Capsid-A-MET-48	-0.08333
Capsid-A-GLY-89	-0.06
H2A-B-GLY-22	-0.05333
Capsid-A-LEU-29	-0.04667
H2A-B-LEU-85	-0.04
Capsid-A-VAL-26	-0.03667
Capsid-A-ASN-2	-0.03
Capsid-A-LEU-66	-0.02667
H2A-B-LEU-108	-0.02333
Capsid-A-ARG-20	-0.01
H2A-B-ILE-111	-0.00333
Capsid-A-ILE-65	0.006667
Capsid-A-GLY-83	0.013333
H2A-B-ALA-52	0.016667
Capsid-A-ALA-8	0.023333
H2A-B-VAL-100	0.026667
H2A-B-THR-59	0.026667

H2A-B-ALA-103	0.03
H2A-B-GLN-112	0.03
Capsid-A-ASN-79	0.03
Capsid-A-GLY-36	0.033333
Capsid-A-SER-24	0.036667
H2A-B-VAL-107	0.04
H2A-B-ASN-94	0.05
H2A-B-ALA-45	0.056667
H2A-B-ASN-68	0.06
H2A-B-ALA-113	0.063333
Capsid-A-MET-37	0.066667
Capsid-A-THR-25	0.073333
H2A-B-SER-18	0.09
H2A-B-GLN-104	0.1
Capsid-A-GLN-27	0.103333
H2A-B-THR-16	0.106667
H2A-B-ASN-110	0.113333
H2A-B-GLY-37	0.12
H2A-B-SER-19	0.143333
H2A-B-LEU-116	0.176667
Capsid-A-ASN-93	0.183333
Capsid-A-ASN-14	0.25
Capsid-A-THR-62	0.266667
Capsid-A-GLY-42	0.276667
H2A-B-ARG-29	0.336667
H2A-B-ARG-99	0.353333
Capsid-A-ARG-82	0.426667
Capsid-A-LYS-31	0.526667
Capsid-A-ARG-5	0.54
Capsid-A-LYS-73	0.573333
Capsid-A-LYS-67	0.583333
Capsid-A-LYS-86	0.603333
Capsid-A-ARG-32	0.606667
H2A-B-LYS-75	0.626667
Capsid-A-LYS-76	0.636667
H2A-B-ARG-17	0.64
H2A-B-THR-76	0.64
Capsid-A-ARG-68	0.656667
Capsid-A-ARG-22	0.706667
H2A-B-LYS-36	0.753333
Capsid-A-ARG-90	0.766667
Capsid-A-MET-1	0.826667
Capsid-A-LYS-45	0.89
H2A-B-LEU-93	0.923333
H2A-B-ALA-86	0.983333
H2A-B-ALA-70	1.023333
Capsid-A-ARG-55	1.036667
H2A-B-LEU-34	1.04
H2A-B-ASN-73	1.32
Capsid-A-LYS-17	1.323333
Capsid-A-LYS-6	1.456667
H2A-B-LYS-74	1.936667
H2A-B-ARG-81	2.046667
H2A-B-ARG-35	2.113333
H2A-B-HIS-31	2.203333
H2A-B-LYS-15	3.16

Suppl. Table 2 — Residue wise Binding energy decomposition of capsid protein in complex with Histone H2B

Capsid-H2B	Average Binding free energy (Kcal/mol)
H2B-B-ASP-68	-7.92333
H2B-B-GLU-71	-6.66333
H2B-B-PHE-65	-6.51667
Capsid-A-MET-37	-6.43333
H2B-B-ILE-73	-5.86667
H2B-B-ILE-69	-4.51
Capsid-A-PHE-33	-4.44333
Capsid-A-ARG-98	-4.31667
Capsid-A-MET-48	-4.24
H2B-B-GLU-93	-4.17333
H2B-B-TYR-37	-4.09333
Capsid-A-VAL-51	-4.09
Capsid-A-ARG-9	-3.85667
H2B-B-ILE-61	-3.81667
Capsid-A-ARG-20	-3.79
Capsid-A-ARG-99	-3.78
Capsid-A-LEU-95	-3.63667
H2B-B-ASP-51	-3.63333
Capsid-A-LEU-44	-3.56
H2B-B-ALA-81	-3.47667
H2B-B-ILE-39	-3.41333
H2B-B-MET-62	-3.31667
Capsid-A-LEU-54	-3.29333
Capsid-A-PHE-47	-3.27
Capsid-A-ARG-32	-3.07
H2B-B-LEU-101	-3.01667
Capsid-A-ARG-41	-2.88333
H2B-B-VAL-48	-2.71333
H2B-B-ALA-77	-2.70333
Capsid-A-VAL-26	-2.62
H2B-B-THR-96	-2.62
Capsid-A-ARG-55	-2.57
H2B-B-GLU-76	-2.57
H2B-B-LEU-80	-2.49333
Capsid-A-PRO-12	-2.4
H2B-B-PHE-70	-2.31333
H2B-B-ILE-94	-2.31
Capsid-A-PRO-61	-2.30333
Capsid-A-GLN-27	-2.28333
H2B-B-GLU-35	-2.19
Capsid-A-LEU-29	-2.14
Capsid-A-MET-15	-2.08
H2B-B-ALA-124	-2.06333
Capsid-A-LEU-92	-2.05
H2B-B-GLU-113	-2.02667
Capsid-A-ILE-88	-2.02
H2B-B-LEU-45	-1.99667
H2B-B-ALA-74	-1.93333

H2B-B-ALA-58	-1.91
H2B-B-SER-78	-1.89333
Capsid-A-VAL-23	-1.88667
H2B-B-TYR-121	-1.87
H2B-B-GLY-53	-1.72667
Capsid-A-ARG-68	-1.67333
H2B-B-LEU-102	-1.64
Capsid-A-ARG-97	-1.52333
H2B-B-TYR-42	-1.52
H2B-B-GLU-105	-1.40333
Capsid-A-LEU-38	-1.39
H2B-B-ILE-54	-1.38667
H2B-B-LEU-100	-1.38
H2B-B-SER-64	-1.37333
Capsid-A-GLY-36	-1.36667
H2B-B-GLN-95	-1.33
H2B-B-MET-59	-1.27
Capsid-A-ARG-18	-1.26
Capsid-A-ILE-59	-1.23333
Capsid-A-PHE-13	-1.23
H2B-B-VAL-118	-1.19333
H2B-B-GLY-114	-1.17667
Capsid-A-ALA-8	-1.10667
H2B-B-SER-56	-1.1
Capsid-A-LEU-50	-1.08667
H2B-B-SER-36	-1.08
Capsid-A-LYS-7	-1.07
H2B-B-ALA-117	-1.05333
H2B-B-LEU-106	-0.98333
Capsid-A-SER-24	-0.98
Capsid-A-LEU-35	-0.91667
H2B-B-ILE-89	-0.88
Capsid-A-GLN-28	-0.85333
Capsid-A-THR-11	-0.85
Capsid-A-THR-30	-0.84667
H2B-B-VAL-98	-0.83667
Capsid-A-ALA-63	-0.82667
Capsid-A-GLY-40	-0.82
Capsid-A-LEU-81	-0.8
Capsid-A-GLY-42	-0.79667
H2B-B-VAL-111	-0.77667
Capsid-A-LEU-16	-0.77333
Capsid-A-LEU-57	-0.74667
H2B-B-VAL-41	-0.73333
H2B-B-ALA-97	-0.73
Capsid-A-PHE-56	-0.71667
Capsid-A-MET-91	-0.71
H2B-B-GLY-75	-0.68667
Capsid-A-ARG-5	-0.68
Capsid-A-LEU-66	-0.65667
Capsid-A-GLN-4	-0.64

H2B-B-THR-52	-0.62
H2B-B-VAL-66	-0.58333
Capsid-A-GLU-19	-0.56333
Capsid-A-ASN-10	-0.45333
Capsid-A-ALA-49	-0.41
Capsid-A-THR-62	-0.41
Capsid-A-ALA-52	-0.39333
Capsid-A-GLU-87	-0.38
H2B-B-ARG-72	-0.37667
H2B-B-LYS-108	-0.37333
Capsid-A-SER-34	-0.37
Capsid-A-PHE-84	-0.35667
H2B-B-PRO-103	-0.3
Capsid-A-PRO-60	-0.29667
Capsid-A-ILE-94	-0.28
Capsid-A-THR-58	-0.27667
H2B-B-GLY-104	-0.26667
H2B-B-ALA-107	-0.22667
Capsid-A-PRO-43	-0.22
Capsid-A-TRP-69	-0.17
Capsid-A-LYS-45	-0.16667
Capsid-A-ILE-65	-0.14667
H2B-B-TYR-40	-0.10667
H2B-B-VAL-44	-0.10333
Capsid-A-LEU-46	-0.09667
H2B-B-GLY-60	-0.09
Capsid-A-PHE-53	-0.07333
Capsid-A-GLN-39	-0.07
Capsid-A-ASP-3	-0.06
Capsid-A-THR-25	-0.05
Capsid-A-GLY-64	-0.04667
Capsid-A-ILE-78	-0.04
H2B-B-THR-115	-0.03667
Capsid-A-ILE-72	-0.02667
Capsid-A-GLY-89	-0.02
Capsid-A-ASN-96	-0.01
Capsid-A-SER-75	0.003333
Capsid-A-ALA-77	0.006667
H2B-B-ASN-84	0.01
H2B-B-THR-119	0.01
Capsid-A-ASN-79	0.023333
Capsid-A-GLY-83	0.023333
Capsid-A-THR-71	0.03
Capsid-A-VAL-80	0.033333
Capsid-A-GLY-70	0.043333
H2B-B-SER-123	0.043333
H2B-B-ASN-67	0.05
H2B-B-SER-91	0.056667
H2B-B-SER-87	0.056667
H2B-B-SER-38	0.063333
H2B-B-SER-112	0.066667

H2B-B-THR-122	0.066667
H2B-B-THR-88	0.083333
Capsid-A-ARG-22	0.103333
Capsid-A-ASN-93	0.11
H2B-B-GLN-47	0.156667
H2B-B-ASN-63	0.16
Capsid-A-ASN-2	0.176667
H2B-B-SER-55	0.176667
H2B-B-THR-90	0.193333
Capsid-A-LYS-6	0.196667
Capsid-A-ASN-14	0.21
Capsid-A-LYS-67	0.216667
Capsid-A-ASN-21	0.246667
Capsid-A-LYS-73	0.306667
Capsid-A-ARG-85	0.313333
Capsid-A-LYS-76	0.336667
Capsid-A-LYS-74	0.346667
Capsid-A-ARG-82	0.36
Capsid-A-LYS-86	0.383333
Capsid-A-ARG-90	0.523333
Capsid-A-LYS-31	0.556667
Capsid-A-ARG-100	0.58
Capsid-A-LYS-17	0.813333
Capsid-A-MET-1	1.03
H2B-B-LYS-120	1.193333
H2B-B-ARG-92	1.39
H2B-B-ARG-86	1.496667
H2B-B-LYS-116	1.653333
H2B-B-LYS-85	1.663333
H2B-B-LYS-43	1.77
H2B-B-ARG-99	1.986667
H2B-B-LYS-34	2.133333
H2B-B-LYS-57	2.263333
H2B-B-ARG-79	2.34
H2B-B-ALA-110	2.74
H2B-B-PRO-50	3.06
H2B-B-TYR-83	3.16
H2B-B-LYS-46	3.46
H2B-B-ARG-33	3.756667

Suppl. Table 3 — Residue wise Binding energy decomposition of capsid protein in complex with Histone H3

Capsid-H3	Average Binding free energy (Kcal/mol)
H3-B-TYR-98	-7.39333
H3-B-GLU-96	-6.05
Capsid-A-ARG-55	-5.58667
Capsid-A-ARG-82	-5.54
Capsid-A-ARG-22	-5.20667
H3-B-GLU-72	-4.82
H3-B-ILE-73	-4.73333
H3-B-ASP-76	-4.30667
Capsid-A-LEU-54	-4.06667

Capsid-A-ARG-100	-3.93667
H3-B-LEU-102	-3.75
H3-B-PHE-77	-3.62333
H3-B-GLU-49	-3.58
H3-B-GLU-93	-3.54667
H3-B-LEU-69	-3.47333
H3-B-LEU-99	-3.42667
Capsid-A-ILE-78	-3.41667
Capsid-A-PRO-60	-3.39333
Capsid-A-THR-62	-3.34
Capsid-A-PHE-56	-3.27333
Capsid-A-LEU-29	-3.22667
Capsid-A-VAL-51	-3.15333
Capsid-A-LEU-92	-3.05333
Capsid-A-LEU-16	-3.04
H3-B-PHE-83	-2.99
H3-B-LEU-81	-2.98667
H3-B-ASP-105	-2.98667
H3-B-ILE-50	-2.98
H3-B-ALA-97	-2.97333
Capsid-A-PRO-61	-2.80333
H3-B-GLU-58	-2.74667
H3-B-ASP-80	-2.71667
H3-B-LEU-91	-2.71
Capsid-A-MET-15	-2.68667
H3-B-ALA-94	-2.66333
H3-B-PRO-65	-2.65667
Capsid-A-ASN-2	-2.62
Capsid-A-GLY-64	-2.51
H3-B-SER-95	-2.46333
Capsid-A-ASN-10	-2.46
Capsid-A-ILE-65	-2.45333
Capsid-A-ASN-14	-2.27333
Capsid-A-LEU-57	-2.26333
Capsid-A-MET-48	-2.01667
H3-B-GLU-132	-1.99667
Capsid-A-ILE-88	-1.99333
Capsid-A-VAL-26	-1.97
Capsid-A-LEU-66	-1.91333
Capsid-A-PHE-33	-1.89
H3-B-GLN-84	-1.88
H3-B-ASP-122	-1.77667
H3-B-VAL-100	-1.76667
Capsid-A-TRP-69	-1.75333
H3-B-THR-79	-1.72667
H3-B-GLU-104	-1.69
H3-B-ILE-123	-1.66333
Capsid-A-ARG-99	-1.65667
Capsid-A-MET-37	-1.56667
Capsid-A-ARG-98	-1.55667
Capsid-A-ARG-32	-1.55333

Capsid-A-ILE-72	-1.49667
H3-B-GLN-124	-1.47333
Capsid-A-THR-71	-1.46
Capsid-A-VAL-80	-1.45333
H3-B-ILE-111	-1.42333
Capsid-A-ARG-68	-1.41333
H3-B-ARG-133	-1.41333
Capsid-A-PHE-13	-1.41
Capsid-A-ALA-63	-1.39333
Capsid-A-GLN-4	-1.34667
H3-B-SER-85	-1.29667
H3-B-THR-44	-1.25
H3-B-LEU-47	-1.24667
Capsid-A-ASP-3	-1.22667
Capsid-A-GLY-36	-1.22
Capsid-A-LEU-95	-1.19667
H3-B-LEU-125	-1.16333
H3-B-PHE-66	-1.15667
H3-B-ALA-46	-1.14
Capsid-A-ARG-90	-1.11667
H3-B-ALA-90	-1.11333
Capsid-A-LYS-73	-1.05667
Capsid-A-GLU-87	-1.05
H3-B-ILE-129	-1.05
H3-B-ILE-118	-1.04667
H3-B-VAL-45	-1.00333
H3-B-ARG-52	-0.99667
Capsid-A-LEU-50	-0.98333
Capsid-A-THR-25	-0.94333
H3-B-GLY-131	-0.93333
Capsid-A-LYS-17	-0.92667
Capsid-A-ASN-96	-0.92
Capsid-A-PHE-53	-0.90667
Capsid-A-ALA-52	-0.86333
H3-B-PRO-42	-0.86
Capsid-A-MET-91	-0.85667
Capsid-A-SER-75	-0.84
H3-B-GLN-75	-0.84
H3-B-TYR-53	-0.83333
Capsid-A-PHE-47	-0.82
Capsid-A-LYS-7	-0.81667
H3-B-LEU-59	-0.81333
Capsid-A-ALA-77	-0.78667
H3-B-GLY-101	-0.76667
H3-B-LEU-60	-0.74667
H3-B-LEU-103	-0.71667
H3-B-LEU-64	-0.71333
Capsid-A-ASN-93	-0.65
H3-B-ALA-74	-0.62
H3-B-ILE-61	-0.61
H3-B-GLY-43	-0.6

H3-B-ALA-126	-0.57667
H3-B-LEU-108	-0.56667
H3-B-GLN-92	-0.56333
H3-B-VAL-70	-0.50667
H3-B-VAL-88	-0.47667
Capsid-A-GLY-70	-0.44667
Capsid-A-ARG-97	-0.43
Capsid-A-ARG-5	-0.41
Capsid-A-ALA-49	-0.37667
Capsid-A-LEU-44	-0.36
Capsid-A-GLY-89	-0.32333
H3-B-TYR-40	-0.32333
Capsid-A-PRO-43	-0.31667
Capsid-A-THR-58	-0.31
H3-B-ALA-87	-0.29
Capsid-A-THR-11	-0.28
Capsid-A-ILE-59	-0.25
Capsid-A-ILE-94	-0.24667
Capsid-A-LEU-38	-0.22
Capsid-A-PHE-84	-0.19667
Capsid-A-LEU-81	-0.17333
Capsid-A-GLY-83	-0.15667
Capsid-A-GLU-19	-0.15333
Capsid-A-VAL-23	-0.12333
Capsid-A-ASN-21	-0.09333
Capsid-A-ASN-79	-0.09
Capsid-A-PRO-12	-0.07
H3-B-ALA-86	-0.06667
Capsid-A-LEU-35	-0.06333
Capsid-A-THR-30	-0.04
H3-B-PRO-120	-0.01667
Capsid-A-ALA-8	-0.01667
H3-B-GLY-89	-0.01333
H3-B-ALA-110	0.006667
Capsid-A-SER-34	0.013333
H3-B-ASN-78	0.013333
H3-B-MET-119	0.026667
H3-B-ARG-48	0.036667
H3-B-THR-117	0.04
Capsid-A-SER-24	0.046667
H3-B-CYS-109	0.046667
H3-B-VAL-116	0.046667
Capsid-A-LEU-46	0.063333
Capsid-A-GLY-40	0.066667
H3-B-SER-56	0.086667
Capsid-A-GLN-27	0.096667
Capsid-A-GLY-42	0.103333
Capsid-A-GLN-39	0.106667
H3-B-THR-57	0.123333
H3-B-THR-106	0.133333
Capsid-A-GLN-28	0.136667

H3-B-GLN-54	0.183333
H3-B-GLN-67	0.213333
H3-B-ARG-128	0.24
H3-B-ARG-71	0.286667
H3-B-ASN-107	0.3
Capsid-A-ARG-85	0.32
Capsid-A-LYS-45	0.37
H3-B-ARG-82	0.38
Capsid-A-LYS-76	0.4
Capsid-A-ARG-20	0.41
Capsid-A-ARG-18	0.436667
Capsid-A-LYS-67	0.443333
Capsid-A-LYS-31	0.453333
H3-B-ARG-127	0.456667
Capsid-A-ARG-41	0.456667
H3-B-ARG-51	0.483333
Capsid-A-LYS-74	0.496667
H3-B-LYS-121	0.546667
Capsid-A-LYS-86	0.596667
Capsid-A-ARG-9	0.613333
Capsid-A-LYS-6	0.8
H3-B-ARG-130	0.836667
H3-B-ARG-41	0.95
H3-B-ARG-68	1.146667
H3-B-ARG-62	1.333333
Capsid-A-MET-1	1.423333
H3-B-LYS-55	1.496667
H3-B-ARG-115	1.723333
H3-B-ALA-113	1.8
H3-B-LYS-114	1.833333
H3-B-LYS-63	2.3
H3-B-ARG-39	4.706667

Suppl. Table 4 — Residue wise Binding energy decomposition of capsid protein in complex with Histone H4

H4	Average Binding free energy (Kcal/mol)
Capsid-A-ARG-82	-6.92667
H4-B-PHE-61	-6.22
H4-B-GLU-53	-4.74333
H4-B-LEU-58	-4.36333
H4-B-TYR-72	-3.92667
H4-B-ILE-50	-3.84333
H4-B-VAL-57	-3.68667
H4-B-ASP-85	-3.44333
H4-B-THR-54	-3.19
Capsid-A-LEU-46	-3.07667
Capsid-A-PHE-47	-3.07333
H4-B-GLU-74	-3.02333
Capsid-A-LEU-95	-2.92
Capsid-A-MET-91	-2.79
Capsid-A-PHE-56	-2.76333
H4-B-PHE-100	-2.76

H4-B-GLY-102	-2.61333
H4-B-GLU-52	-2.41667
H4-B-LEU-62	-2.38333
Capsid-A-LEU-38	-1.98333
Capsid-A-LEU-35	-1.97667
Capsid-A-MET-48	-1.95
Capsid-A-ARG-100	-1.89333
H4-B-VAL-65	-1.84333
Capsid-A-PHE-33	-1.82
Capsid-A-ARG-85	-1.74333
H4-B-GLU-63	-1.74333
Capsid-A-ILE-94	-1.73667
H4-B-ASP-68	-1.57667
H4-B-TYR-51	-1.50333
Capsid-A-ARG-32	-1.42667
Capsid-A-VAL-51	-1.39333
Capsid-A-LEU-81	-1.24667
H4-B-VAL-60	-1.12
H4-B-LEU-90	-1.11667
Capsid-A-VAL-80	-1.08667
H4-B-MET-84	-1.04667
Capsid-A-MET-37	-1.04
Capsid-A-GLU-87	-1.03333
Capsid-A-ARG-98	-0.98
H4-B-ALA-89	-0.97
Capsid-A-PHE-53	-0.94333
H4-B-GLY-101	-0.86667
Capsid-A-ARG-97	-0.83667
H4-B-LEU-37	-0.83333
Capsid-A-ALA-77	-0.81667
H4-B-LEU-49	-0.79667
Capsid-A-LEU-50	-0.79
H4-B-GLY-94	-0.79
H4-B-ILE-66	-0.7
H4-B-LEU-97	-0.69
Capsid-A-LEU-44	-0.65333
H4-B-ILE-46	-0.64667
Capsid-A-ALA-52	-0.62667
H4-B-ALA-69	-0.62333
Capsid-A-MET-15	-0.62
Capsid-A-SER-75	-0.61
Capsid-A-LYS-6	-0.6
H4-B-ASN-64	-0.59333
Capsid-A-ILE-88	-0.58
Capsid-A-LEU-29	-0.54333
Capsid-A-ILE-78	-0.52333
H4-B-GLY-99	-0.49333
Capsid-A-GLY-83	-0.49
Capsid-A-PHE-84	-0.47
Capsid-A-GLU-19	-0.46667
H4-B-TYR-88	-0.46333

Capsid-A-GLY-36	-0.44
Capsid-A-ASN-14	-0.42333
Capsid-A-LYS-76	-0.40667
Capsid-A-LEU-54	-0.39
H4-B-GLN-93	-0.38
Capsid-A-ASP-3	-0.35333
Capsid-A-LEU-92	-0.31
Capsid-A-PRO-12	-0.29
Capsid-A-ALA-49	-0.26667
Capsid-A-ILE-59	-0.26333
H4-B-VAL-86	-0.26
Capsid-A-LYS-45	-0.24333
H4-B-ASN-25	-0.24
Capsid-A-GLN-39	-0.20667
H4-B-THR-71	-0.20333
Capsid-A-ALA-63	-0.19667
H4-B-THR-96	-0.19
H4-B-ILE-26	-0.18667
Capsid-A-ASN-79	-0.15333
H4-B-GLY-56	-0.10333
H4-B-VAL-70	-0.09667
H4-B-TYR-98	-0.06333
Capsid-A-LEU-57	-0.06
H4-B-SER-47	-0.05
H4-B-ILE-34	-0.04667
Capsid-A-PRO-43	-0.04
Capsid-A-PRO-61	-0.03
Capsid-A-THR-62	-0.02333
H4-B-VAL-87	-0.02333
Capsid-A-LEU-16	-0.01667
Capsid-A-VAL-23	-0.01
Capsid-A-PRO-60	-0.01
H4-B-PRO-32	-0.01
Capsid-A-ILE-65	-0.00333
Capsid-A-LEU-66	0
Capsid-A-TRP-69	0
Capsid-A-ILE-72	0
Capsid-A-VAL-26	0.003333
Capsid-A-GLY-64	0.006667
Capsid-A-GLN-4	0.01
Capsid-A-ALA-8	0.01
Capsid-A-GLY-70	0.01
Capsid-A-GLY-89	0.01
H4-B-ILE-29	0.01
Capsid-A-SER-24	0.016667
H4-B-GLY-41	0.023333
Capsid-A-PHE-13	0.023333
Capsid-A-THR-58	0.023333
Capsid-A-THR-71	0.023333
H4-B-THR-30	0.023333
Capsid-A-ASN-21	0.03

H4-B-GLY-28	0.03
H4-B-VAL-43	0.03
H4-B-ALA-83	0.03
H4-B-GLY-42	0.03
Capsid-A-ASN-2	0.036667
H4-B-VAL-81	0.036667
H4-B-ALA-33	0.04
H4-B-THR-73	0.043333
Capsid-A-THR-30	0.046667
Capsid-A-GLN-27	0.05
Capsid-A-GLY-40	0.05
Capsid-A-SER-34	0.053333
Capsid-A-GLN-28	0.056667
H4-B-THR-80	0.06
Capsid-A-THR-11	0.063333
Capsid-A-ASN-10	0.073333
Capsid-A-THR-25	0.073333
H4-B-ALA-38	0.073333
H4-B-THR-82	0.113333
H4-B-GLN-27	0.123333
H4-B-GLY-48	0.123333
Capsid-A-ARG-99	0.136667
Capsid-A-ASN-96	0.136667
Capsid-A-GLY-42	0.143333
Capsid-A-ARG-18	0.15
Capsid-A-ASN-93	0.176667
Capsid-A-LYS-74	0.18
Capsid-A-ARG-90	0.193333
Capsid-A-LYS-7	0.35
H4-B-ARG-92	0.386667
Capsid-A-ARG-5	0.403333
Capsid-A-ARG-55	0.42
Capsid-A-LYS-67	0.42
Capsid-A-ARG-68	0.423333
Capsid-A-ARG-9	0.446667
Capsid-A-LYS-73	0.493333
Capsid-A-MET-1	0.513333
Capsid-A-ARG-20	0.55
Capsid-A-ARG-22	0.566667
Capsid-A-LYS-17	0.593333
H4-B-ARG-39	0.663333
H4-B-ASP-24	0.76
Capsid-A-LYS-86	0.87
Capsid-A-ARG-41	0.906667
Capsid-A-LYS-31	0.923333
H4-B-ARG-45	0.963333
H4-B-ARG-67	1.136667
H4-B-ARG-55	1.296667
H4-B-ARG-78	1.423333
H4-B-LYS-31	1.476667
H4-B-LYS-79	1.49

H4-B-ARG-95	1.613333
H4-B-ARG-40	1.64
H4-B-ARG-36	1.643333
H4-B-LYS-44	1.673333
H4-B-ARG-35	1.766667
H4-B-LYS-91	1.83
H4-B-LYS-59	1.866667
H4-B-LYS-77	1.993333
H4-B-ALA-76	2.116667

Suppl. Table 5 — Contact analysis of capsid-histone H2A complex

Capsid residue	Histone residue	Contact frequency
A:ARG:41	B:ARG:77	0.998
A:ARG:99	B:GLU:61	0.998
A:ARG:99	B:GLU:64	0.982
A:PHE:53	B:THR:59	0.94
A:PHE:53	B:VAL:30	0.88
A:GLN:39	B:ARG:77	0.858
A:PHE:56	B:ARG:29	0.834
A:ARG:85	B:TYR:50	0.828
A:ASN:96	B:GLU:61	0.766
A:LEU:54	B:ARG:29	0.756
A:PHE:33	B:ILE:111	0.719
A:PHE:53	B:LEU:33	0.711
A:LEU:81	B:LEU:51	0.705
A:ILE:88	B:VAL:54	0.695
A:LEU:92	B:LEU:58	0.683
A:LEU:54	B:VAL:27	0.677
A:LEU:54	B:PHE:25	0.645
A:ASN:96	B:LEU:65	0.639
A:PHE:33	B:ARG:77	0.635
A:LEU:54	B:VAL:30	0.621
A:LEU:95	B:LEU:65	0.619
A:ILE:88	B:LEU:55	0.581
A:PHE:84	B:LEU:51	0.581
A:ARG:55	B:VAL:27	0.577
A:LEU:92	B:TYR:57	0.569
A:THR:30	B:LEU:108	0.559
A:ASN:96	B:ASN:68	0.547
A:ARG:82	B:GLY:44	0.545
A:PHE:53	B:LEU:55	0.541
A:PHE:13	B:PRO:80	0.531
A:ASN:10	B:GLN:84	0.513

Suppl. Table 6 — Contact analysis of capsid-histone H2B complex

Capsid residue	Histone residue	Contact frequency
A:ARG:97	B:ASP:68	0.998
A:ARG:18	B:GLU:71	0.998
A:ARG:99	B:ASP:68	0.998
A:ARG:41	B:GLU:76	0.998
A:ARG:98	B:ASP:68	0.994

A:ARG:97	B:SER:64	0.984
A:SER:24	B:LEU:100	0.974
A:ASP:3	B:LYS:46	0.966
A:LYS:17	B:SER:78	0.964
A:ARG:32	B:ALA:77	0.948
A:ARG:55	B:ALA:124	0.908
A:MET:48	B:TYR:37	0.908
A:VAL:23	B:LEU:100	0.908
A:VAL:26	B:ARG:99	0.876
A:ARG:98	B:GLU:71	0.872
A:VAL:23	B:ARG:99	0.862
A:VAL:51	B:PHE:65	0.86
A:ARG:18	B:ALA:74	0.858
A:ARG:41	B:ARG:79	0.844
A:MET:37	B:TYR:37	0.822
A:ARG:20	B:ALA:97	0.81
A:ALA:63	B:VAL:44	0.808
A:PHE:47	B:ILE:69	0.804
A:ARG:41	B:ARG:72	0.739
A:ARG:32	B:ALA:81	0.727
A:MET:1	B:ASN:63	0.719
A:ARG:99	B:ASN:67	0.711
A:GLY:40	B:GLU:76	0.701
A:SER:24	B:ALA:110	0.699
A:LEU:35	B:LEU:80	0.697
A:MET:37	B:ILE:73	0.693
A:THR:62	B:ASP:51	0.683
A:ARG:55	B:VAL:41	0.665
A:ASP:3	B:LYS:43	0.649
A:GLN:39	B:LEU:80	0.649
A:VAL:51	B:VAL:41	0.643
A:PHE:33	B:ILE:73	0.605
A:MET:15	B:ARG:92	0.605
A:PRO:61	B:ASP:51	0.601
A:GLY:64	B:GLN:47	0.589
A:LYS:17	B:HSD:82	0.581
A:LYS:45	B:GLU:35	0.563
A:PHE:33	B:ALA:77	0.561
A:LEU:95	B:ILE:69	0.557
A:ARG:32	B:HSD:82	0.557
A:PHE:33	B:ILE:39	0.547
A:ARG:22	B:LEU:101	0.543
A:MET:15	B:HSD:82	0.537
A:LEU:92	B:SER:64	0.531
A:ILE:88	B:ILE:61	0.525
A:PRO:12	B:ILE:94	0.523
A:THR:25	B:GLY:114	0.523
A:MET:1	B:LYS:46	0.519
A:GLY:36	B:ALA:77	0.513
A:ASN:2	B:ASN:67	0.511
A:PRO:12	B:VAL:98	0.505

Suppl. Table 7 — Contact analysis of capsid-histone H3 complex

Capsid residue	Histone residue	Contact frequency
A:ARG:82	B:ASP:76	0.998
A:ARG:22	B:GLU:93	0.998
A:ARG:22	B:GLU:96	0.998
A:ARG:100	B:ARG:133	0.998
A:ASN:96	B:ARG:133	0.998
A:ARG:82	B:GLU:72	0.996
A:ARG:99	B:GLU:93	0.996
A:ARG:99	B:GLU:96	0.994
A:ALA:63	B:ARG:52	0.974
A:ARG:98	B:GLU:49	0.958
A:ARG:32	B:ARG:82	0.952
A:ALA:63	B:ARG:51	0.948
A:ARG:100	B:VAL:45	0.93
A:ILE:78	B:ARG:68	0.92
A:MET:48	B:TYR:98	0.91
A:THR:30	B:TYR:98	0.904
A:PHE:53	B:PHE:77	0.872
A:ARG:99	B:ARG:133	0.864
A:ASN:14	B:ARG:127	0.826
A:ARG:97	B:GLU:49	0.814
A:THR:25	B:ALA:90	0.808
A:ARG:85	B:PHE:77	0.802
A:VAL:51	B:TYR:98	0.782
A:ARG:5	B:ASP:105	0.778
A:VAL:26	B:TYR:98	0.776
A:THR:25	B:ALA:94	0.776
A:ARG:85	B:ASP:76	0.774
A:GLY:36	B:ASP:80	0.731
A:LEU:29	B:ALA:94	0.723
A:ARG:55	B:PHE:77	0.713
A:LEU:16	B:VAL:100	0.699
A:LEU:16	B:ARG:127	0.697
A:GLY:64	B:ARG:52	0.675
A:ARG:5	B:LEU:108	0.671
A:ILE:88	B:LEU:99	0.671
A:LEU:50	B:TYR:98	0.667
A:LEU:54	B:PHE:77	0.665
A:VAL:26	B:ALA:97	0.665
A:TRP:69	B:PRO:65	0.639
A:MET:15	B:ARG:127	0.637
A:ARG:32	B:LEU:81	0.629
A:ARG:100	B:GLY:43	0.627
A:LEU:29	B:PHE:83	0.625
A:PRO:60	B:ILE:61	0.619
A:ARG:100	B:THR:44	0.611
A:PHE:47	B:TYR:98	0.609
A:ARG:9	B:ASP:105	0.603
A:LEU:92	B:LEU:103	0.601
A:ARG:100	B:LEU:47	0.601

A:LEU:95	B:GLN:92	0.593
A:PRO:61	B:GLN:92	0.591
A:ILE:65	B:ILE:50	0.579
A:PHE:56	B:SER:95	0.573
A:ARG:100	B:ARG:51	0.569
A:VAL:80	B:LEU:69	0.563
A:ARG:97	B:LEU:47	0.563
A:VAL:51	B:LEU:99	0.559
A:VAL:80	B:GLU:72	0.555
A:LEU:95	B:GLU:96	0.549
A:ARG:100	B:ARG:39	0.537
A:GLY:64	B:ILE:50	0.521
A:MET:15	B:GLY:101	0.519
A:MET:48	B:LEU:102	0.517
A:ARG:100	B:ARG:48	0.513
A:LEU:54	B:LEU:81	0.511
A:GLY:89	B:LEU:103	0.503
A:PRO:61	B:LEU:60	0.501
A:ARG:99	B:GLN:92	0.501

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Suppl. Table 8 — Contact analysis of capsid-histone H4 complex

Capsid residue	Histone residue	Contact frequency
A:ARG:82	B:ASP:68	0.971
A:ARG:97	B:GLU:53	0.941
A:ARG:82	B:TYR:72	0.882
A:ARG:55	B:ASP:68	0.868
A:ALA:52	B:PHE:61	0.853
A:ARG:32	B:ILE:50	0.706
A:PHE:33	B:THR:54	0.691
A:PHE:56	B:PHE:61	0.662
A:GLY:36	B:THR:54	0.647
A:ARG:55	B:ASN:64	0.632
A:GLY:36	B:TYR:51	0.632
A:ARG:90	B:GLU:63	0.632
A:PHE:47	B:PHE:61	0.588
A:VAL:51	B:ASP:68	0.574
A:GLY:83	B:TYR:72	0.529