

SUPPORTING INFORMATION [Tables of Van der Waals (VDW), electrostatics (ELEC), solvation (SOLV), bonded free energy (BOND), and side chain entropic conformational free energy (CONF)]

Table S1a. Average INTE per residue for the GCN4-p1 sequence during four 0.6 ns (300 frames) Nosé-Hoover MD simulations. All entries are in units of kcal/mol•helix.

RESIDUE	I	II	III	IV	V
ACE	-4.04	-3.31	-4.58	-4.60	-4.58
ARG2g	4.04	2.87	4.00	4.78	4.03
MET3a	-1.97	-2.52	-2.67	-1.93	-3.13
LYS4b	0.86	1.30	0.63	0.57	0.80
GLN5c	-8.50	-8.58	-8.47	-8.45	-8.56
LEU6d	-4.21	-7.16	-6.24	-5.59	-6.32
GLU7e	-3.49	-4.58	-4.74	-4.80	-5.82
ASP8f	-10.47	-10.82	-10.69	-10.27	-10.91
LYS9g	-1.17	-1.33	-1.67	-2.27	-2.32
VAL10a	-2.53	-4.74	-4.93	-4.46	-4.64
GLU11b	-4.15	-4.85	-4.64	-4.63	-4.88
GLU12c	-4.45	-4.95	-4.61	-4.18	-4.72
LEU13d	-4.68	-8.01	-6.65	-7.31	-7.65
LEU14e	-5.78	-6.19	-6.26	-6.84	-5.94
SER15f	-8.21	-7.96	-7.75	-8.32	-7.86
LYS16g	0.14	-0.21	-0.85	-1.66	-1.48
ASN17a	-11.57	-11.88	-12.89	-11.37	-11.45
TYR18b	-1.42	-1.54	-1.40	-0.61	-0.77
HIS19c	-3.32	-3.25	-3.35	-3.71	-4.11
LEU20d	-4.52	-7.10	-6.86	-6.75	-6.21
GLU21e	-4.19	-4.51	-4.49	-4.82	-3.92
ASN22f	-11.63	-11.35	-11.55	-11.23	-11.43
GLU23g	-3.97	-4.30	-5.00	-4.78	-4.78
VAL24a	-2.61	-3.91	-4.59	-4.18	-4.71
ALA25b	-5.51	-6.39	-6.21	-5.93	-6.14
ARG26c	1.24	1.72	1.78	1.21	1.28
LEU27d	-4.03	-7.37	-6.84	-6.68	-7.16
LYS28e	1.30	0.22	-0.01	-0.19	-0.40
LYS29f	1.75	1.73	1.69	1.78	2.12
LEU30g	-1.78	-1.77	-1.77	-2.53	-3.26
VAL31a	2.20	2.12	1.00	1.20	0.20
CBX	-1.41	-1.39	-1.44	-1.62	-1.97
Σ [INTE]	-108.08	-130.04	-132.03	-130.16	-136.69

Table S1b. Average VDW per residue for the GCN4-p1 sequence during four 0.6 ns (300 frames) Nosé-Hoover MD simulations. All entries are in units of kcal/mol•helix.

RESIDUE	I	II	III	IV	V
ACE	-1.07	-1.38	-1.53	-1.51	-1.68
ARG2g	-3.68	-4.60	-5.44	-5.85	-6.86
MET3a	-3.73	-5.48	-5.76	-5.35	-5.75
LYS4b	-5.53	-5.51	-5.91	-5.56	-6.21
GLN5c	-6.62	-6.81	-6.88	-7.82	-8.39
LEU6d	-6.02	-9.96	-8.97	-9.00	-8.98
GLU7e	-7.16	-8.32	-9.33	-10.59	-11.71
ASP8f	-7.39	-7.60	-7.70	-7.54	-8.40
LYS9g	-7.17	-8.40	-8.65	-10.48	-11.26
VAL10a	-4.33	-6.70	-6.34	-6.77	-7.20
GLU11b	-7.48	-7.50	-7.80	-8.19	-8.62
GLU12c	-8.06	-8.30	-8.33	-9.05	-9.70
LEU13d	-6.23	-9.84	-9.35	-9.99	-9.93
LEU14e	-6.55	-7.74	-7.93	-9.34	-8.14
SER15f	-5.37	-5.20	-5.38	-5.57	-5.51
LYS16g	-6.45	-7.72	-9.44	-10.47	-11.10
ASN17a	-7.17	-10.64	-10.63	-10.25	-9.79
TYR18b	-9.19	-9.26	-9.79	-9.65	-9.07
HIS19c	-7.75	-7.98	-7.99	-8.98	-9.78
LEU20d	-6.49	-10.09	-10.07	-10.17	-9.66
GLU21e	-7.55	-8.54	-9.39	-10.60	-10.64
ASN22f	-6.58	-6.39	-6.57	-6.64	-7.78
GLU23g	-7.73	-9.14	-9.93	-11.30	-12.10
VAL24a	-4.88	-5.92	-6.51	-6.98	-6.75
ALA25b	-4.40	-4.48	-4.53	-4.93	-5.43
ARG26c	-7.39	-7.72	-7.62	-8.31	-8.44
LEU27d	-5.77	-9.44	-9.18	-9.22	-8.72
LYS28e	-5.34	-6.29	-6.95	-8.07	-8.83
LYS29f	-5.51	-5.18	-5.43	-5.44	-5.88
LEU30g	-4.74	-5.44	-5.15	-6.29	-6.99
VAL31a	-2.23	-3.61	-3.52	-4.03	-4.29
CBX	-1.22	-1.07	-1.27	-1.40	-1.65
Σ [VDW]	-186.76	-222.26	-229.26	-245.32	-255.25

Table S1c. Average ELEC per residue for the GCN4-p1 sequence during four 0.6 ns (300 frames) Nosé-Hoover MD simulations. All entries are in units of kcal/mol•helix.

RESIDUE	I	II	III	IV	V
ACE	-6.63	-5.26	-7.27	-7.35	-7.36
ARG2g	-15.06	-15.47	-14.99	-14.32	-14.84
MET3a	-12.93	-12.58	-12.53	-12.17	-13.05
LYS4b	-12.70	-12.04	-13.11	-13.28	-12.65
GLN5c	-21.28	-21.12	-21.59	-21.21	-20.82
LEU6d	-14.61	-13.79	-14.67	-13.56	-13.91
GLU7e	-15.53	-15.56	-16.33	-15.71	-16.82
ASP8f	-21.28	-21.87	-21.50	-21.43	-21.69
LYS9g	-15.20	-14.83	-15.36	-15.22	-15.30
VAL10a	-14.76	-14.22	-14.73	-14.09	-13.65
GLU11b	-15.86	-16.00	-16.06	-16.30	-16.36
GLU12c	-15.30	-15.89	-15.57	-15.34	-15.67
LEU13d	-14.68	-15.25	-14.68	-14.66	-15.28
LEU14e	-15.78	-15.40	-15.74	-15.17	-15.31
SER15f	-17.01	-16.57	-16.51	-16.85	-16.47
LYS16g	-13.48	-13.88	-14.24	-14.32	-14.14
ASN17a	-23.52	-23.84	-24.40	-23.23	-23.40
TYR18b	-14.22	-14.28	-14.25	-13.71	-14.25
HIS19c	-16.76	-16.40	-16.63	-16.63	-16.77
LEU20d	-14.68	-14.54	-14.67	-14.13	-14.18
GLU21e	-15.16	-15.40	-15.59	-15.26	-15.52
ASN22f	-24.02	-24.17	-24.26	-23.89	-23.67
GLU23g	-15.74	-15.45	-15.85	-15.41	-15.97
VAL24a	-13.94	-14.47	-14.31	-13.93	-14.34
ALA25b	-12.36	-13.43	-13.44	-13.18	-13.16
ARG26c	-17.01	-16.15	-16.68	-17.00	-16.71
LEU27d	-14.36	-14.25	-14.30	-13.60	-14.43
LYS28e	-12.19	-13.77	-13.92	-13.86	-14.33
LYS29f	-11.15	-11.40	-11.56	-11.38	-10.98
LEU30g	-11.20	-10.64	-11.17	-10.96	-10.77
VAL31a	-8.54	-8.20	-8.56	-8.02	-8.20
CBX	-3.55	-3.74	-3.82	-3.78	-4.01
Σ [ELEC]	-470.48	-469.86	-478.32	-468.91	-474.01

Table S1d. Average SOLV per residue for the GCN4-p1 sequence during four 0.6 ns (300 frames) Nosé-Hoover MD simulations. All entries are in units of kcal/mol•helix.

RESIDUE	I	II	III	IV	V
ACE	1.67	1.41	2.17	2.19	2.31
ARG2g	8.18	8.68	9.72	9.79	10.27
MET3a	6.69	7.21	7.53	7.17	7.76
LYS4b	8.35	8.28	8.92	8.68	8.98
GLN5c	9.60	9.67	10.10	10.67	10.92
LEU6d	8.49	9.26	9.08	8.38	8.51
GLU7e	10.59	11.11	12.41	13.09	14.39
ASP8f	11.07	11.44	11.28	11.38	12.03
LYS9g	10.35	10.86	11.36	12.62	13.43
VAL10a	8.76	9.17	8.70	8.94	8.81
GLU11b	10.45	10.50	10.86	11.38	11.83
GLU12c	10.88	11.15	11.18	11.73	12.30
LEU13d	8.28	9.46	8.70	8.85	9.11
LEU14e	8.57	8.70	9.12	9.55	9.95
SER15f	8.21	7.99	8.17	8.33	8.33
LYS16g	9.27	10.53	11.87	12.66	13.05
ASN17a	10.08	12.88	12.72	12.11	11.85
TYR18b	9.66	9.65	10.12	10.16	10.25
HIS19c	9.49	9.47	9.68	10.35	10.90
LEU20d	8.71	9.96	9.81	9.34	9.35
GLU21e	10.39	11.07	12.14	12.80	13.54
ASN22f	10.08	10.04	10.30	10.34	10.86
GLU23g	10.85	11.69	12.49	13.48	14.37
VAL24a	8.57	9.13	8.98	9.06	8.99
ALA25b	6.55	6.85	7.11	7.21	7.59
ARG26c	11.38	11.41	11.73	12.54	12.38
LEU27d	7.92	8.67	8.41	8.02	8.06
LYS28e	7.95	9.05	9.95	10.65	11.50
LYS29f	7.66	7.59	7.94	7.92	8.25
LEU30g	6.09	6.20	6.31	6.55	6.85
VAL31a	5.61	5.94	5.66	5.66	5.69
CBX	1.84	1.85	2.03	1.96	2.17
Σ [SOLV]	272.25	286.86	296.54	303.55	314.59

Table S1e. Average BOND per residue for the GCN4-p1 sequence during four 0.6 ns (300 frames) Nosé-Hoover MD simulations. All entries are in units of kcal/mol•helix..

RESIDUE	I	II	III	IV	V
ACE	2.00	1.92	2.06	2.08	2.15
ARG2g	14.59	14.27	14.72	15.16	15.45
MET3a	8.00	8.32	8.09	8.43	7.91
LYS4b	10.74	10.58	10.73	10.73	10.68
GLN5c	9.80	9.67	9.89	9.92	9.74
LEU6d	7.93	7.33	8.31	8.59	8.06
GLU7e	8.62	8.20	8.51	8.41	8.32
ASP8f	7.12	7.21	7.23	7.33	7.14
LYS9g	10.84	11.05	10.98	10.82	10.81
VAL10a	7.80	7.01	7.43	7.46	7.40
GLU11b	8.73	8.15	8.35	8.47	8.27
GLU12c	8.04	8.09	8.11	8.48	8.35
LEU13d	7.94	7.61	8.69	8.49	8.45
LEU14e	7.98	8.26	8.30	8.12	7.55
SER15f	5.96	5.82	5.98	5.77	5.79
LYS16g	10.81	10.86	10.96	10.47	10.71
ASN17a	9.03	9.72	9.42	9.99	9.89
TYR18b	12.33	12.35	12.52	12.59	12.30
HIS19c	11.71	11.66	11.60	11.55	11.55
LEU20d	7.94	7.57	8.08	8.21	8.29
GLU21e	8.13	8.37	8.34	8.24	8.70
ASN22f	8.90	9.16	8.99	8.96	9.16
GLU23g	8.65	8.59	8.30	8.44	8.92
VAL24a	7.64	7.35	7.24	7.67	7.40
ALA25b	4.69	4.67	4.65	4.96	4.85
ARG26c	14.25	14.18	14.34	13.98	14.05
LEU27d	8.18	7.65	8.23	8.11	7.93
LYS28e	10.88	11.24	10.91	11.09	11.27
LYS29f	10.74	10.71	10.75	10.68	10.72
LEU30g	8.06	8.10	8.24	8.17	7.64
VAL31a	7.36	8.00	7.43	7.58	7.00
CBX	1.52	1.57	1.63	1.59	1.52
Σ [BOND]	276.92	275.22	279.01	280.53	277.98

Table S1f. Average CONF per residue for the GCN4-p1 sequence during four 0.6 ns (300 frames) Nosé-Hoover MD simulations. All entries are in units of kcal/mol•helix.

RESIDUE	I	II	III	IV	V
ACE	0	0.00	0.00	0.00	0.00
ARG2g	0	0.52	2.28	2.15	1.31
MET3a	0	0.91	1.49	1.18	1.19
LYS4b	0	-0.04	0.42	0.30	0.08
GLN5c	0	-0.03	-0.02	0.17	0.29
LEU6d	0	0.24	0.34	0.10	0.32
GLU7e	0	0.05	0.62	1.14	1.15
ASP8f	0	-0.02	0.05	-0.06	0.09
LYS9g	0	0.34	1.01	1.71	1.98
VAL10a	0	0.11	0.11	0.16	0.17
GLU11b	0	0.06	0.19	0.66	0.45
GLU12c	0	0.09	0.17	0.13	0.32
LEU13d	0	0.31	0.56	0.53	0.47
LEU14e	0	0.38	0.39	0.39	0.54
SER15f	0	0.00	-0.07	-0.09	-0.12
LYS16g	0	0.92	2.37	2.70	2.99
ASN17a	0	0.69	0.67	0.57	0.77
TYR18b	0	-0.03	0.22	0.10	-0.06
HIS19c	0	-0.02	-0.06	0.01	-0.03
LEU20d	0	0.50	0.54	0.26	0.29
GLU21e	0	-0.13	0.13	0.22	0.24
ASN22f	0	0.00	0.06	0.08	0.31
GLU23g	0	0.56	0.84	0.74	0.79
VAL24a	0	0.23	0.14	0.31	0.31
ALA25b	0	0.00	0.00	0.00	0.00
ARG26c	0	0.15	0.18	0.55	0.86
LEU27d	0	0.56	0.39	0.33	0.46
LYS28e	0	0.37	1.11	1.52	1.73
LYS29f	0	-0.12	0.16	-0.13	0.59
LEU30g	0	0.07	0.07	0.13	0.40
VAL31a	0	0.05	0.08	0.12	0.11
CBX	0	0.00	0.00	0.00	0.00
Σ [CONF]	0	6.72	14.46	16.00	18.00

Table S2a. Average INTE per residue for the H38-p1 sequence during four 0.6 ns (300 frames) Nosé-Hoover MD simulations. All entries are in units of kcal/mol•helix.

RESIDUE	I	II	III	IV	V
ACE	-4.67	-3.46	-4.91	-4.80	-4.65
ARG2g	3.79	2.59	3.83	4.80	3.27
ILE3a	-0.20	-1.27	-1.66	-0.50	-1.11
LYS4b	0.58	1.29	0.46	0.45	0.47
GLN5c	-8.16	-8.74	-8.41	-8.28	-8.91
GLN6d	-9.33	-10.84	-11.68	-11.18	-11.02
GLU7e	-4.03	-4.14	-4.95	-4.66	-5.60
ASP8f	-10.62	-10.91	-10.61	-10.44	-10.99
LYS9g	-2.35	-1.87	-2.92	-3.76	-3.62
LEU10a	-4.30	-4.49	-6.55	-6.65	-6.53
GLU11b	-4.81	-4.91	-4.82	-4.62	-5.20
GLU12c	-4.95	-5.50	-4.92	-4.88	-5.34
THR13d	-4.85	-5.05	-5.29	-5.60	-5.34
LEU14e	-5.24	-5.43	-5.72	-5.47	-4.58
SER15f	-8.11	-7.87	-7.75	-8.13	-8.03
LYS16g	0.03	-0.23	-1.18	-1.44	-1.59
ILE17a	-3.11	-3.58	-5.16	-4.52	-4.22
TYR18b	-1.30	-1.14	-1.48	-0.47	-0.74
HIS19c	-3.51	-3.40	-3.48	-3.82	-4.16
LEU20d	-4.76	-7.82	-7.47	-7.61	-7.05
GLU21e	-3.56	-3.61	-4.03	-5.28	-3.90
ASN22f	-11.28	-11.46	-11.48	-11.19	-11.10
GLU23g	-4.10	-4.38	-4.87	-5.07	-4.61
ILE24a	-1.89	-1.83	-4.16	-3.75	-3.83
ALA25b	-5.61	-6.16	-6.13	-6.01	-6.09
ARG26c	1.22	1.95	1.27	1.19	0.99
VAL27d	-2.71	-3.64	-4.77	-4.76	-4.35
LYS28e	1.36	0.40	-0.38	-0.32	-0.18
LYS29f	1.96	2.08	1.95	1.92	2.04
LEU30g	-1.92	-1.90	-2.07	-3.22	-3.46
LEU31a	1.21	1.68	-0.53	-1.78	-1.75
CBX	-1.39	-1.26	-1.56	-1.66	-1.91
Σ [INTE]	-106.62	-114.89	-131.44	-131.50	-133.11

Table S2b. Average VDW per residue for the H38-p1 sequence during four 0.6 ns (300 frames) Nosé-Hoover MD simulations. All entries are in units of kcal/mol•helix.

RESIDUE	I	II	III	IV	V
ACE	-1.30	-1.32	-1.54	-1.49	-1.82
ARG2g	-4.08	-5.04	-6.10	-5.85	-7.28
ILE3a	-3.57	-5.28	-6.14	-5.40	-5.61
LYS4b	-5.61	-5.40	-5.98	-5.79	-6.59
GLN5c	-6.54	-7.13	-6.82	-7.81	-8.62
GLN6d	-6.85	-11.31	-11.34	-11.13	-10.93
GLU7e	-7.48	-8.59	-10.18	-10.68	-11.91
ASP8f	-7.49	-7.79	-7.51	-7.71	-8.54
LYS9g	-7.05	-8.41	-8.13	-10.60	-11.17
LEU10a	-5.93	-8.29	-9.20	-9.85	-9.68
GLU11b	-7.43	-7.55	-7.87	-8.00	-8.64
GLU12c	-8.10	-8.28	-8.23	-9.17	-9.70
THR13d	-4.67	-7.47	-6.36	-6.61	-6.50
LEU14e	-6.88	-7.76	-8.47	-9.17	-7.77
SER15f	-5.36	-5.22	-5.35	-5.50	-5.48
LYS16g	-6.35	-7.46	-8.93	-9.90	-10.68
ILE17a	-5.31	-6.44	-7.57	-7.88	-6.87
TYR18b	-8.87	-8.65	-9.72	-9.64	-9.01
HIS19c	-7.80	-8.20	-8.05	-9.20	-9.87
LEU20d	-6.50	-10.43	-9.82	-10.28	-9.81
GLU21e	-7.16	-7.82	-8.72	-10.90	-10.49
ASN22f	-6.58	-6.36	-6.60	-6.48	-7.69
GLU23g	-7.67	-9.32	-9.88	-11.70	-12.02
ILE24a	-4.99	-6.44	-7.14	-7.06	-7.07
ALA25b	-4.46	-4.45	-4.46	-4.87	-5.43
ARG26c	-7.61	-7.63	-7.78	-8.31	-8.59
VAL27d	-4.20	-6.41	-6.40	-6.76	-6.37
LYS28e	-5.38	-6.65	-7.11	-7.99	-8.65
LYS29f	-5.52	-5.09	-5.40	-5.53	-5.98
LEU30g	-4.74	-5.41	-5.28	-6.58	-7.00
LEU31a	-3.26	-4.78	-5.75	-6.85	-6.56
CBX	-1.11	-1.06	-1.29	-1.31	-1.62
Σ [VDW]	-185.87	-217.48	-229.11	-246.01	-253.92

Table S2c. Average ELEC per residue for the H38-p1 sequence during four 0.6 ns (300 frames) Nosé-Hoover MD simulations. All entries are in units of kcal/mol•helix.

RESIDUE	I	II	III	IV	V
ACE	-7.55	-5.44	-7.79	-7.69	-7.33
ARG2g	-16.12	-15.88	-14.77	-14.10	-15.39
ILE3a	-12.85	-13.26	-12.22	-12.27	-12.85
LYS4b	-12.94	-12.31	-13.05	-13.31	-12.82
GLN5c	-20.85	-21.59	-21.20	-20.97	-21.13
GLN6d	-22.35	-21.64	-23.68	-22.58	-22.30
GLU7e	-15.67	-15.66	-16.46	-15.54	-16.61
ASP8f	-21.44	-22.02	-21.49	-21.57	-21.87
LYS9g	-16.80	-15.72	-17.29	-16.88	-17.07
LEU10a	-15.05	-13.50	-14.92	-14.32	-13.97
GLU11b	-16.11	-16.10	-16.28	-16.31	-16.49
GLU12c	-15.86	-16.63	-16.06	-15.93	-16.21
THR13d	-16.70	-16.38	-16.57	-16.26	-16.27
LEU14e	-14.83	-14.47	-14.78	-14.17	-14.38
SER15f	-16.76	-16.42	-16.52	-16.53	-16.57
LYS16g	-13.50	-13.55	-14.39	-14.10	-14.23
ILE17a	-15.00	-15.46	-15.09	-14.37	-14.55
TYR18b	-14.21	-14.08	-14.23	-13.58	-14.29
HIS19c	-16.81	-16.43	-16.70	-16.74	-16.82
LEU20d	-14.84	-14.44	-14.82	-14.19	-14.31
GLU21e	-14.92	-15.09	-15.61	-15.57	-15.71
ASN22f	-23.85	-24.17	-24.16	-23.90	-23.38
GLU23g	-15.98	-15.54	-15.85	-15.37	-16.23
ILE24a	-13.99	-14.26	-14.53	-14.30	-14.42
ALA25b	-12.49	-13.22	-13.44	-13.30	-13.16
ARG26c	-17.13	-16.01	-16.93	-17.09	-16.95
VAL27d	-14.41	-13.87	-14.23	-13.75	-14.48
LYS28e	-12.10	-13.48	-14.17	-14.13	-14.08
LYS29f	-11.37	-11.39	-11.47	-11.28	-11.03
LEU30g	-11.22	-10.69	-11.24	-11.07	-10.88
LEU31a	-8.70	-8.24	-8.57	-8.17	-8.41
CBX	-3.58	-3.50	-3.88	-3.83	-3.94
Σ [ELEC]	-475.99	-470.43	-482.38	-473.17	-478.14

Table S2d. Average SOLV per residue for the H38-p1 sequence during four 0.6 ns (300 frames) Nosé-Hoover MD simulations. All entries are in units of kcal/mol•helix.

RESIDUE	I	II	III	IV	V
ACE	2.10	1.37	2.30	2.26	2.40
ARG2g	8.87	9.12	9.90	9.43	10.73
ILE3a	7.73	8.17	8.33	8.45	8.66
LYS4b	8.50	8.39	8.91	8.85	9.35
GLN5c	9.51	10.14	9.91	10.62	11.10
GLN6d	10.11	12.52	13.63	12.74	12.32
GLU7e	10.71	11.60	13.14	13.23	14.55
ASP8f	11.10	11.67	11.18	11.53	12.21
LYS9g	10.69	11.34	11.59	12.95	13.77
LEU10a	8.63	9.58	9.39	9.22	8.97
GLU11b	10.44	10.66	11.00	11.23	11.84
GLU12c	10.96	11.33	11.20	11.86	12.37
THR13d	9.30	11.25	10.00	9.90	9.97
LEU14e	8.58	8.70	9.47	9.79	10.02
SER15f	8.11	7.92	8.14	8.19	8.28
LYS16g	9.25	9.86	11.21	12.00	12.58
ILE17a	8.89	9.81	9.19	9.03	8.67
TYR18b	9.46	9.42	10.13	10.15	10.32
HIS19c	9.51	9.56	9.70	10.48	10.99
LEU20d	8.57	9.52	9.26	8.99	8.82
GLU21e	10.10	10.73	11.78	12.95	13.52
ASN22f	10.08	10.08	10.34	10.23	10.77
GLU23g	11.03	11.85	12.54	13.78	14.51
ILE24a	8.59	9.50	9.07	9.09	8.84
ALA25b	6.63	6.85	7.09	7.23	7.61
ARG26c	11.61	11.32	11.92	12.53	12.55
VAL27d	8.29	8.73	8.39	8.30	8.69
LYS28e	8.12	9.28	9.92	10.79	11.34
LYS29f	7.86	7.62	7.96	7.95	8.31
LEU30g	6.10	6.17	6.29	6.55	6.84
LEU31a	5.02	5.73	5.34	5.12	5.29
CBX	1.75	1.73	2.01	1.89	2.09
Σ [SOLV]	276.22	291.51	300.23	307.29	318.29

Table S2e. Average BOND per residue for the H38-p1 sequence during four 0.6 ns (300 frames) Nosé-Hoover MD simulations. All entries are in units of kcal/mol•helix.

RESIDUE	I	II	III	IV	V
ACE	2.09	1.94	2.12	2.12	2.10
ARG2g	15.12	14.40	14.79	15.31	15.21
ILE3a	8.49	9.11	8.37	8.72	8.68
LYS4b	10.63	10.60	10.57	10.70	10.53
GLN5c	9.72	9.85	9.70	9.89	9.74
GLN6d	9.76	9.58	9.71	9.79	9.90
GLU7e	8.41	8.50	8.55	8.34	8.37
ASP8f	7.22	7.23	7.20	7.31	7.20
LYS9g	10.81	10.92	10.91	10.77	10.85
LEU10a	8.05	7.72	8.17	8.30	8.15
GLU11b	8.29	8.08	8.33	8.46	8.10
GLU12c	8.04	8.09	8.17	8.36	8.19
THR13d	7.22	7.55	7.63	7.36	7.46
LEU14e	7.88	8.10	8.06	8.07	7.55
SER15f	5.90	5.86	5.98	5.71	5.74
LYS16g	10.64	10.92	10.93	10.56	10.75
ILE17a	8.32	8.51	8.31	8.70	8.53
TYR18b	12.31	12.17	12.34	12.60	12.25
HIS19c	11.59	11.67	11.57	11.64	11.53
LEU20d	8.01	7.52	7.90	7.87	8.24
GLU21e	8.41	8.57	8.51	8.25	8.78
ASN22f	9.08	8.99	8.95	8.96	9.19
GLU23g	8.52	8.64	8.33	8.23	9.12
ILE24a	8.51	9.37	8.44	8.53	8.82
ALA25b	4.70	4.66	4.68	4.93	4.89
ARG26c	14.35	14.28	14.06	14.07	13.98
VAL27d	7.60	7.90	7.47	7.45	7.81
LYS28e	10.72	11.25	10.99	11.02	11.22
LYS29f	10.99	10.94	10.87	10.78	10.73
LEU30g	7.95	8.03	8.16	7.88	7.58
LEU31a	8.16	8.97	8.45	8.11	7.93
CBX	1.54	1.58	1.60	1.58	1.55
Σ [BOND]	279.02	281.51	279.81	280.39	280.67

Table S2f. Average CONF per residue for the H38-p1 sequence during four 0.6 ns (300 frames) Nosé-Hoover MD simulations. All entries are in units of kcal/mol•helix.

RESIDUE	I	II	III	IV	V
ACE	0	0.00	0.00	0.00	0.00
ARG2g	0	-0.50	-0.11	-1.01	0.45
ILE3a	0	0.29	0.34	0.43	0.32
LYS4b	0	0.06	0.35	0.58	0.43
GLN5c	0	0.54	-0.01	0.49	0.50
GLN6d	0	0.47	0.82	0.35	0.57
GLU7e	0	0.20	0.85	0.86	1.17
ASP8f	0	0.04	-0.01	0.00	0.12
LYS9g	0	0.66	0.47	1.30	1.93
LEU10a	0	0.27	0.31	0.38	0.32
GLU11b	0	-0.01	0.08	0.40	0.30
GLU12c	0	0.03	-0.21	0.05	0.36
THR13d	0	-0.11	-0.06	-0.04	0.02
LEU14e	0	0.19	0.19	0.42	0.58
SER15f	0	0.11	-0.04	0.00	-0.06
LYS16g	0	0.88	2.35	2.67	2.81
ILE17a	0	0.46	0.51	0.49	0.51
TYR18b	0	-0.04	0.27	0.24	0.03
HIS19c	0	-0.28	0.04	0.14	0.11
LEU20d	0	0.45	0.54	0.53	0.52
GLU21e	0	0.35	0.54	1.09	0.93
ASN22f	0	0.03	0.08	0.04	0.23
GLU23g	0	0.59	0.57	0.05	0.52
ILE24a	0	0.26	0.40	0.52	0.37
ALA25b	0	0.00	0.00	0.00	0.00
ARG26c	0	0.00	-0.09	0.03	0.41
VAL27d	0	0.18	0.03	0.13	0.08
LYS28e	0	0.33	1.45	1.63	1.77
LYS29f	0	-0.14	-0.07	-0.07	-0.04
LEU30g	0	-0.04	0.02	0.07	0.37
LEU31a	0	0.26	0.50	0.54	0.34
CBX	0	0.00	0.00	0.00	0.00
Σ [CONF]	0	5.54	10.08	12.33	15.98

Table S3a. Average INTE per residue for the GCN4-LI sequence during four 0.6 ns (300 frames) Nosé-Hoover MD simulations. All entries are in units of kcal/mol•helix.

RESIDUE	I	II	III	IV	V
ACE	-4.78	-3.39	-4.45	-4.56	-4.30
ARG2g	5.27	2.95	4.06	5.50	3.39
MET3a	-2.12	-2.06	-2.65	-2.35	-2.86
LYS4b	0.02	1.80	0.56	0.44	0.69
GLN5c	-9.21	-9.09	-8.73	-8.73	-8.96
ILE6d	-1.68	-3.68	-4.37	-4.56	-4.29
GLU7e	-4.07	-4.20	-4.59	-4.57	-5.20
ASP8f	-10.19	-10.73	-10.52	-10.13	-10.52
LYS9g	-1.40	-1.39	-1.52	-2.59	-2.21
LEU10a	-4.17	-5.37	-6.32	-8.06	-8.03
GLU11b	-4.73	-4.73	-5.08	-4.85	-5.31
GLU12c	-4.32	-4.92	-4.59	-4.31	-4.88
ILE13d	-2.21	-3.75	-4.92	-5.85	-5.20
LEU14e	-5.72	-6.39	-6.59	-6.94	-6.09
SER15f	-8.06	-7.96	-7.70	-7.99	-7.84
LYS16g	-0.14	-0.67	-1.01	-1.89	-2.20
LEU17a	-5.56	-6.89	-7.59	-8.41	-8.14
TYR18b	-1.36	-1.30	-1.45	-0.72	-0.97
HIS19c	-3.53	-3.38	-3.38	-3.93	-4.64
ILE20d	-2.40	-3.04	-4.66	-5.45	-5.17
GLU21e	-3.38	-4.18	-4.20	-5.15	-4.38
ASN22f	-11.30	-11.57	-11.57	-11.14	-11.18
GLU23g	-3.82	-4.46	-4.70	-5.44	-4.97
LEU24a	-4.15	-4.96	-6.19	-7.98	-8.28
ALA25b	-5.71	-6.29	-6.31	-6.23	-6.39
ARG26c	0.89	1.40	1.45	1.12	1.00
ILE27d	-1.61	-3.32	-4.68	-4.93	-4.85
LYS28e	1.60	0.52	-0.63	-0.28	-0.40
LYS29f	1.80	2.16	1.66	2.05	2.03
LEU30g	-2.09	-2.09	-2.00	-3.20	-3.54
LEU31a	0.77	1.86	-0.51	-1.99	-1.75
CBX	-1.35	-1.20	-1.58	-1.68	-1.94
Σ [INTE]	-98.70	-110.32	-124.75	-134.81	-137.41

Table S3b. Average VDW per residue for the GCN4-LI sequence during four 0.6 ns (300 frames) Nosé-Hoover MD simulations. All entries are in units of kcal/mol•helix.

RESIDUE	I	II	III	IV	V
ACE	-1.38	-1.30	-1.48	-1.34	-1.61
ARG2g	-3.43	-4.49	-5.17	-5.52	-7.04
MET3a	-3.95	-5.09	-5.73	-5.13	-5.67
LYS4b	-5.65	-5.23	-5.75	-5.56	-6.31
GLN5c	-6.69	-7.03	-6.88	-7.79	-8.80
ILE6d	-4.73	-8.41	-6.97	-7.55	-7.85
GLU7e	-7.58	-8.63	-9.30	-10.64	-11.35
ASP8f	-7.20	-7.68	-7.65	-7.61	-8.49
LYS9g	-7.00	-8.40	-8.47	-10.49	-11.22
LEU10a	-5.93	-8.22	-9.22	-9.97	-9.97
GLU11b	-7.37	-7.36	-7.97	-8.15	-8.82
GLU12c	-8.00	-8.47	-8.41	-9.19	-9.78
ILE13d	-4.62	-7.33	-7.19	-7.65	-7.86
LEU14e	-6.87	-8.05	-7.78	-9.43	-8.32
SER15f	-5.28	-5.20	-5.32	-5.51	-5.44
LYS16g	-6.50	-7.71	-8.67	-9.98	-10.86
LEU17a	-7.09	-9.28	-10.04	-9.96	-9.66
TYR18b	-8.72	-8.80	-9.66	-9.61	-9.17
HIS19c	-7.82	-8.21	-8.06	-9.13	-9.88
ILE20d	-4.85	-8.03	-7.05	-8.02	-8.48
GLU21e	-7.13	-8.60	-9.11	-10.92	-11.01
ASN22f	-6.65	-6.41	-6.72	-6.61	-7.72
GLU23g	-7.32	-9.51	-9.73	-11.85	-12.32
LEU24a	-5.80	-8.04	-9.22	-9.91	-9.95
ALA25b	-4.30	-4.42	-4.49	-4.95	-5.54
ARG26c	-7.50	-7.90	-7.87	-8.24	-8.49
ILE27d	-4.40	-7.21	-7.33	-7.59	-7.54
LYS28e	-5.41	-6.83	-7.13	-8.01	-8.75
LYS29f	-5.44	-5.02	-5.50	-5.49	-5.94
LEU30g	-4.82	-5.56	-5.31	-6.60	-7.04
LEU31a	-3.44	-4.82	-5.85	-6.91	-6.63
CBX	-1.12	-1.10	-1.30	-1.32	-1.62
Σ [VDW]	-184.00	-218.37	-226.34	-246.62	-259.14

Table S3c. Average ELEC per residue for the GCN4-LI sequence during four 0.6 ns (300 frames) Nosé-Hoover MD simulations. All entries are in units of kcal/mol•helix.

RESIDUE	I	II	III	IV	V
ACE	-7.75	-5.43	-7.11	-7.47	-6.98
ARG2g	-14.58	-15.54	-15.57	-13.93	-15.69
MET3a	-13.08	-12.66	-12.81	-12.37	-12.72
LYS4b	-13.26	-11.90	-12.97	-13.37	-12.63
GLN5c	-21.52	-21.56	-21.72	-21.80	-21.37
ILE6d	-14.45	-13.55	-14.65	-13.78	-14.09
GLU7e	-15.58	-15.32	-16.15	-15.44	-16.35
ASP8f	-21.16	-21.84	-21.40	-21.35	-21.59
LYS9g	-15.38	-14.75	-15.66	-15.76	-15.90
LEU10a	-14.83	-14.15	-14.68	-14.23	-13.82
GLU11b	-16.11	-15.99	-16.22	-16.35	-16.46
GLU12c	-15.31	-15.80	-15.47	-15.27	-15.62
ILE13d	-14.85	-14.17	-14.94	-14.60	-14.32
LEU14e	-15.58	-14.99	-15.35	-14.91	-15.01
SER15f	-16.89	-16.65	-16.45	-16.61	-16.47
LYS16g	-13.89	-13.42	-14.53	-14.64	-14.78
LEU17a	-15.07	-15.18	-15.06	-14.49	-14.53
TYR18b	-14.26	-14.02	-14.26	-13.64	-14.27
HIS19c	-16.83	-16.37	-16.60	-16.70	-17.16
ILE20d	-14.88	-14.01	-14.97	-14.57	-14.27
GLU21e	-14.95	-15.02	-15.48	-15.55	-15.61
ASN22f	-23.97	-24.20	-24.19	-23.88	-23.60
GLU23g	-15.69	-15.31	-15.96	-15.63	-16.57
LEU24a	-14.18	-14.14	-14.36	-14.30	-14.32
ALA25b	-12.55	-13.32	-13.55	-13.28	-13.15
ARG26c	-17.19	-16.17	-16.90	-17.03	-17.03
ILE27d	-14.49	-13.74	-14.27	-13.85	-14.48
LYS28e	-12.04	-13.26	-14.05	-13.92	-14.02
LYS29f	-11.34	-11.46	-11.51	-11.31	-11.01
LEU30g	-11.25	-10.73	-11.24	-11.06	-10.88
LEU31a	-8.73	-8.29	-8.59	-8.18	-8.40
CBX	-3.58	-3.43	-3.86	-3.82	-3.94
Σ [ELEC]	-465.21	-456.36	-470.52	-463.08	-467.02

Table S3d. Average SOLV per residue for the GCN4-LI sequence during four 0.6 ns (300 frames) Nosé-Hoover MD simulations. All entries are in units of kcal/mol•helix.

RESIDUE	I	II	III	IV	V
ACE	2.24	1.42	2.10	2.15	2.19
ARG2g	8.05	8.69	9.89	9.47	10.84
MET3a	6.99	7.16	7.62	7.03	7.46
LYS4b	8.57	8.09	8.70	8.72	9.03
GLN5c	9.55	9.96	10.07	10.82	11.30
ILE6d	8.75	9.48	9.18	8.76	9.16
GLU7e	10.76	11.19	12.36	13.07	14.05
ASP8f	10.85	11.49	11.27	11.46	12.23
LYS9g	10.42	10.92	11.42	12.85	13.81
LEU10a	8.32	8.91	8.62	8.60	8.29
GLU11b	10.34	10.45	10.91	11.28	11.87
GLU12c	10.82	11.30	11.21	11.79	12.34
ILE13d	8.83	9.10	8.51	8.41	8.61
LEU14e	8.57	8.54	8.84	9.46	9.83
SER15f	8.12	8.01	8.15	8.25	8.30
LYS16g	9.40	9.82	11.11	12.17	12.78
LEU17a	8.49	9.35	8.79	8.53	8.18
TYR18b	9.39	9.42	9.87	10.07	10.32
HIS19c	9.54	9.56	9.66	10.45	11.05
ILE20d	9.04	9.57	9.17	9.16	9.29
GLU21e	10.12	10.99	11.80	13.03	13.66
ASN22f	10.09	10.07	10.36	10.27	10.85
GLU23g	10.71	11.77	12.43	13.81	14.76
LEU24a	8.07	8.92	8.79	8.76	8.38
ALA25b	6.48	6.76	7.04	7.12	7.52
ARG26c	11.44	11.42	11.95	12.38	12.48
ILE27d	8.28	8.78	8.52	8.26	8.70
LYS28e	8.06	9.24	9.80	10.60	11.32
LYS29f	7.77	7.64	7.93	7.88	8.25
LEU30g	6.07	6.20	6.26	6.53	6.84
LEU31a	5.02	5.68	5.33	5.09	5.31
CBX	1.74	1.74	2.00	1.89	2.10
Σ [SOLV]	270.85	281.65	289.68	298.15	311.11

Table S3e. Average BOND per residue for the GCN4-LI sequence during four 0.6 ns (300 frames) Nosé-Hoover MD simulations. All entries are in units of kcal/mol•helix.

RESIDUE	I	II	III	IV	V
ACE	2.11	1.92	2.04	2.09	2.09
ARG2g	15.24	14.29	14.92	15.47	15.28
MET3a	7.92	8.53	8.27	8.12	8.06
LYS4b	10.35	10.85	10.59	10.65	10.61
GLN5c	9.45	9.54	9.80	10.04	9.91
ILE6d	8.75	8.80	8.07	8.01	8.48
GLU7e	8.34	8.56	8.50	8.44	8.45
ASP8f	7.32	7.30	7.25	7.36	7.32
LYS9g	10.56	10.85	11.19	10.81	11.09
LEU10a	8.27	8.09	8.96	7.54	7.47
GLU11b	8.41	8.17	8.20	8.37	8.10
GLU12c	8.17	8.05	8.09	8.36	8.19
ILE13d	8.42	8.65	8.71	7.99	8.35
LEU14e	8.16	8.11	7.70	7.94	7.40
SER15f	5.99	5.87	5.91	5.88	5.78
LYS16g	10.85	10.64	11.08	10.56	10.67
LEU17a	8.12	8.22	8.71	7.51	7.86
TYR18b	12.23	12.10	12.59	12.45	12.16
HIS19c	11.58	11.64	11.61	11.44	11.34
ILE20d	8.29	9.43	8.18	7.99	8.29
GLU21e	8.57	8.45	8.60	8.29	8.58
ASN22f	9.22	8.96	8.97	9.08	9.28
GLU23g	8.48	8.59	8.56	8.22	9.16
LEU24a	7.76	8.30	8.60	7.48	7.61
ALA25b	4.67	4.69	4.69	4.87	4.77
ARG26c	14.15	14.04	14.27	14.01	14.04
ILE27d	9.00	8.85	8.40	8.24	8.46
LYS28e	10.99	11.37	10.75	11.05	11.05
LYS29f	10.81	11.02	10.74	10.98	10.73
LEU30g	7.91	8.01	8.29	7.93	7.55
LEU31a	7.93	9.29	8.60	8.01	7.97
CBX	1.62	1.60	1.59	1.57	1.52
Σ [BOND]	279.65	282.75	282.44	276.74	277.63

Table S3f. Average CONF per residue for the GCN4-LI sequence during four 0.6 ns (300 frames) Nosé-Hoover MD simulations. All entries are in units of kcal/mol•helix.

RESIDUE	I	II	III	IV	V
ACE	0	0.00	0.00	0.00	0.00
ARG2g	0	1.15	1.78	1.00	2.72
MET3a	0	0.83	2.10	1.13	1.21
LYS4b	0	-0.25	0.22	0.06	0.20
GLN5c	0	0.34	0.30	0.41	0.50
ILE6d	0	0.47	0.46	0.64	0.63
GLU7e	0	0.10	0.52	0.86	1.00
ASP8f	0	0.00	0.01	-0.01	0.14
LYS9g	0	-0.03	1.02	1.72	1.97
LEU10a	0	0.50	0.60	0.88	0.70
GLU11b	0	0.03	0.07	0.30	0.35
GLU12c	0	0.16	0.06	0.13	0.43
ILE13d	0	0.71	0.53	0.88	0.79
LEU14e	0	0.34	0.45	0.40	0.59
SER15f	0	0.03	-0.03	0.04	-0.09
LYS16g	0	0.36	2.40	2.55	2.63
LEU17a	0	0.40	0.50	0.70	0.58
TYR18b	0	-0.14	0.12	0.12	-0.04
HIS19c	0	-0.09	0.03	0.15	0.17
ILE20d	0	0.51	0.43	0.50	0.55
GLU21e	0	0.40	0.64	0.93	0.97
ASN22f	0	0.02	0.06	0.06	0.31
GLU23g	0	0.62	0.80	0.78	1.10
LEU24a	0	0.33	0.45	0.67	0.55
ALA25b	0	0.00	0.00	0.00	0.00
ARG26c	0	0.01	0.18	0.11	0.74
ILE27d	0	0.78	0.46	0.73	0.63
LYS28e	0	0.35	1.27	1.29	1.53
LYS29f	0	-0.10	-0.33	-0.23	-0.17
LEU30g	0	0.03	0.04	0.11	0.37
LEU31a	0	0.18	0.37	0.38	0.19
CBX	0	0.00	0.00	0.00	0.00
Σ [CONF]	0	8.05	15.53	17.29	21.26

Table S4a. Average INTE per residue for the COMP sequence during four 0.6 ns (300 frames) Nosé-Hoover MD simulations. All entries are in units of kcal/mol•helix.

RESIDUE	I	II	III	IV	V
ACE	-3.16	-3.33	-3.75	-3.68	-3.71
LEU2g	-3.27	-2.90	-2.88	-2.45	-2.96
ALA3a	0.09	-0.41	-0.48	0.14	-0.93
PRO4b	5.56	5.48	5.25	4.84	4.98
GLN5c	-8.04	-8.22	-8.37	-8.60	-9.00
MET6d	-4.51	-5.30	-5.94	-5.50	-6.10
LEU7e	-5.05	-4.93	-5.55	-5.54	-5.77
ARG8f	1.46	1.39	1.61	1.44	0.74
GLU9g	-5.91	-6.08	-6.40	-6.61	-6.85
LEU10a	-4.57	-5.17	-6.62	-7.04	-7.07
GLN11b	-8.65	-8.54	-8.68	-8.81	-9.13
GLU12c	-5.20	-5.44	-5.06	-4.70	-5.56
THR13d	-4.57	-4.31	-6.19	-5.28	-5.34
ASN14e	-10.59	-10.77	-11.77	-10.56	-11.52
ALA15f	-6.72	-6.81	-6.68	-6.64	-6.18
ALA16g	-6.56	-7.12	-7.20	-7.42	-7.92
LEU17a	-4.15	-5.26	-5.61	-6.06	-5.99
GLN18b	-8.99	-9.25	-9.09	-8.76	-9.43
ASP19c	-10.33	-10.15	-11.04	-10.73	-9.98
VAL20d	-3.07	-4.14	-4.45	-5.38	-4.98
ARG21e	2.48	1.90	2.20	1.27	0.28
GLU22f	-4.44	-4.23	-4.10	-3.69	-4.18
LEU23g	-4.95	-5.25	-5.18	-6.41	-7.47
LEU24a	-4.40	-5.66	-7.02	-7.50	-7.26
ARG25b	2.95	2.17	2.95	2.11	2.32
GLN26c	-9.63	-8.73	-9.13	-9.26	-9.35
GLN27d	-8.00	-9.16	-10.94	-10.68	-11.93
VAL28e	-1.49	-2.35	-2.14	-3.09	-4.16
LYS29f	1.85	2.02	2.16	1.85	2.08
GLU30g	-1.38	-2.29	-1.66	-2.16	-1.58
ILE31a	3.57	3.45	1.83	1.73	1.26
CBX	-1.48	-1.29	-1.48	-1.58	-2.03
Σ [INTE]	-121.15	-130.69	-141.42	-144.79	-154.73

Table S4b. Average VDW per residue for the COMP sequence during four 0.6 ns (300 frames) Nosé-Hoover MD simulations. All entries are in units of kcal/mol•helix.

RESIDUE	I	II	III	IV	V
ACE	-0.91	-1.07	-1.42	-1.34	-1.33
LEU2g	-3.30	-3.63	-3.92	-3.94	-4.83
ALA3a	-1.45	-2.11	-2.33	-2.20	-2.45
PRO4b	-3.33	-3.17	-3.61	-3.52	-4.10
GLN5c	-6.78	-7.25	-7.22	-7.81	-8.41
MET6d	-5.47	-8.93	-8.90	-8.60	-8.70
LEU7e	-6.52	-6.92	-7.65	-8.69	-8.70
ARG8f	-7.88	-7.71	-7.79	-8.06	-9.05
GLU9g	-7.56	-8.89	-8.77	-11.34	-13.30
LEU10a	-5.80	-8.14	-9.02	-10.03	-9.88
GLN11b	-7.06	-7.11	-7.25	-7.67	-8.16
GLU12c	-7.57	-7.50	-7.37	-8.03	-9.62
THR13d	-4.38	-6.40	-6.33	-6.60	-6.80
ASN14e	-5.83	-6.33	-6.77	-7.32	-8.75
ALA15f	-4.25	-4.19	-4.29	-4.21	-4.27
ALA16g	-3.88	-4.51	-4.56	-4.80	-5.46
LEU17a	-6.40	-7.96	-8.82	-9.17	-8.97
GLN18b	-7.62	-7.70	-7.49	-7.77	-8.52
ASP19c	-6.64	-6.85	-7.55	-8.37	-9.17
VAL20d	-4.64	-7.31	-6.41	-6.96	-7.21
ARG21e	-7.47	-9.02	-9.29	-10.47	-11.93
GLU22f	-8.62	-8.59	-8.27	-8.46	-9.13
LEU23g	-6.89	-8.00	-8.43	-9.66	-10.55
LEU24a	-5.77	-7.64	-10.22	-9.85	-9.65
ARG25b	-7.81	-7.96	-7.57	-9.02	-9.70
GLN26c	-8.03	-7.93	-7.47	-7.96	-8.11
GLN27d	-6.68	-10.44	-11.54	-11.68	-11.13
VAL28e	-3.71	-4.23	-5.39	-6.15	-6.86
LYS29f	-6.30	-5.62	-5.78	-5.84	-6.20
GLU30g	-5.92	-7.33	-6.81	-8.66	-8.30
ILE31a	-2.21	-4.50	-4.68	-5.45	-5.17
CBX	-1.28	-1.07	-1.32	-1.48	-1.72
Σ [VDW]	-177.95	-206.01	-214.21	-231.13	-246.11

Table S4c. Average ELEC per residue for the COMP sequence during four 0.6 ns (300 frames) Nosé-Hoover MD simulations. All entries are in units of kcal/mol•helix.

RESIDUE	I	II	III	IV	V
ACE	-5.24	-5.24	-5.50	-5.45	-5.68
LEU2g	-13.60	-12.98	-12.84	-12.07	-11.71
ALA3a	-10.18	-10.48	-10.19	-9.84	-10.48
PRO4b	-9.82	-9.72	-9.89	-10.28	-9.75
GLN5c	-20.47	-20.16	-20.87	-20.47	-20.70
MET6d	-14.90	-13.66	-14.48	-13.59	-14.04
LEU7e	-14.55	-14.28	-14.34	-13.76	-14.45
ARG8f	-16.24	-16.65	-16.40	-16.72	-17.44
GLU9g	-18.02	-17.50	-18.13	-17.74	-17.99
LEU10a	-14.96	-14.14	-14.98	-14.40	-14.13
GLN11b	-20.59	-20.53	-20.88	-21.24	-21.43
GLU12c	-15.97	-16.54	-16.03	-15.89	-16.45
THR13d	-16.31	-15.94	-16.67	-15.89	-16.02
ASN14e	-23.42	-23.20	-24.19	-22.93	-23.56
ALA15f	-13.89	-13.84	-13.87	-13.71	-13.13
ALA16g	-14.28	-14.02	-14.53	-14.42	-14.47
LEU17a	-14.03	-14.25	-14.04	-13.45	-13.78
GLN18b	-21.70	-22.24	-21.68	-21.88	-22.34
ASP19c	-21.34	-20.87	-21.87	-21.52	-21.16
VAL20d	-14.81	-14.05	-14.82	-14.49	-14.22
ARG21e	-15.50	-15.81	-16.06	-15.95	-16.90
GLU22f	-15.81	-15.88	-15.58	-15.05	-15.49
LEU23g	-14.82	-14.20	-14.29	-14.15	-14.25
LEU24a	-14.51	-14.80	-14.89	-14.31	-14.41
ARG25b	-15.06	-15.56	-15.32	-15.84	-15.78
GLN26c	-22.37	-20.96	-21.53	-21.58	-21.02
GLN27d	-20.66	-21.61	-22.84	-22.47	-23.71
VAL28e	-12.93	-14.19	-13.68	-13.57	-14.18
LYS29f	-11.26	-11.50	-11.35	-11.60	-10.99
GLU30g	-12.55	-12.57	-12.77	-12.70	-12.30
ILE31a	-8.45	-8.10	-8.44	-8.31	-8.28
CBX	-3.63	-3.76	-3.87	-3.81	-4.15
Σ [ELEC]	-481.88	-479.25	-486.85	-479.08	-484.41

Table S4d. Average SOLV per residue for the COMP sequence during four 0.6 ns (300 frames) Nosé-Hoover MD simulations. All entries are in units of kcal/mol•helix.

RESIDUE	I	II	III	IV	V
ACE	1.09	1.07	1.28	1.21	1.38
LEU2g	5.51	5.44	5.55	5.20	5.32
ALA3a	4.88	5.12	5.35	5.01	5.38
PRO4b	4.66	4.61	4.79	4.78	4.82
GLN5c	9.39	9.47	9.82	9.84	10.23
MET6d	7.96	9.26	9.48	8.68	8.84
LEU7e	8.08	8.17	8.63	8.92	9.40
ARG8f	11.61	11.84	11.77	12.14	13.15
GLU9g	11.10	11.66	11.98	13.56	14.99
LEU10a	8.15	9.24	9.16	9.18	9.00
GLN11b	9.35	9.42	9.76	10.18	10.65
GLU12c	10.31	10.42	10.23	10.90	12.24
THR13d	8.89	10.06	9.54	9.80	10.11
ASN14e	9.68	9.80	10.32	10.62	12.00
ALA15f	6.61	6.54	6.70	6.58	6.54
ALA16g	6.67	6.69	7.03	7.04	7.34
LEU17a	8.52	9.19	8.78	8.32	8.28
GLN18b	10.35	10.77	10.22	10.83	11.39
ASP19c	10.46	10.44	11.10	11.65	12.37
VAL20d	8.92	9.21	9.22	8.75	8.84
ARG21e	11.70	12.63	13.42	13.81	15.16
GLU22f	11.31	11.37	11.19	11.25	11.72
LEU23g	8.97	9.00	9.25	9.46	9.97
LEU24a	8.10	8.72	9.53	9.01	8.85
ARG25b	11.84	11.93	11.93	12.77	13.32
GLN26c	10.71	10.31	10.09	10.42	10.11
GLN27d	9.43	12.06	13.57	13.09	12.82
VAL28e	7.60	8.52	8.96	9.25	9.49
LYS29f	8.68	8.20	8.39	8.50	8.57
GLU30g	8.27	9.19	9.11	10.35	10.12
ILE31a	5.64	6.67	6.15	6.55	6.29
CBX	1.88	1.87	2.09	2.07	2.33
Σ [SOLV]	266.33	278.87	284.40	289.71	301.00

Table S4e. Average BOND per residue for the COMP sequence during four 0.6 ns (300 frames) Nosé-Hoover MD simulations. All entries are in units of kcal/mol•helix.

RESIDUE	I	II	III	IV	V
ACE	1.90	1.91	1.89	1.90	1.92
LEU2g	8.12	8.28	8.32	8.36	8.26
ALA3a	6.84	7.06	6.68	7.17	6.62
PRO4b	14.05	13.76	13.95	13.86	14.02
GLN5c	9.82	9.72	9.91	9.84	9.89
MET6d	7.90	8.03	7.96	8.00	7.80
LEU7e	7.95	8.10	7.80	7.99	7.97
ARG8f	13.97	13.92	14.03	14.09	14.08
GLU9g	8.57	8.64	8.52	8.91	9.45
LEU10a	8.04	7.87	8.22	8.20	7.94
GLN11b	9.66	9.68	9.68	9.93	9.81
GLU12c	8.02	8.18	8.11	8.31	8.28
THR13d	7.23	7.98	7.27	7.41	7.36
ASN14e	8.98	8.97	8.86	9.08	8.79
ALA15f	4.80	4.68	4.79	4.70	4.68
ALA16g	4.93	4.73	4.85	4.75	4.66
LEU17a	7.76	7.76	8.48	8.23	8.48
GLN18b	9.98	9.92	9.86	10.06	10.04
ASP19c	7.19	7.13	7.27	7.51	7.98
VAL20d	7.45	8.01	7.56	7.33	7.61
ARG21e	13.75	14.10	14.13	13.87	13.95
GLU22f	8.68	8.87	8.56	8.57	8.71
LEU23g	7.79	7.95	8.28	7.94	7.36
LEU24a	7.78	8.06	8.55	7.65	7.96
ARG25b	13.98	13.77	13.92	14.20	14.48
GLN26c	10.07	9.84	9.77	9.87	9.67
GLN27d	9.90	10.83	9.88	10.38	10.09
VAL28e	7.55	7.55	7.98	7.39	7.39
LYS29f	10.73	10.94	10.91	10.79	10.69
GLU30g	8.82	8.42	8.82	8.84	8.89
ILE31a	8.60	9.39	8.80	8.94	8.42
CBX	1.55	1.68	1.62	1.64	1.51
Σ [BOND]	272.36	275.71	275.25	275.72	274.78

Table S4f. Average CONF per residue for the COMP sequence during four 0.6 ns (300 frames) Nosé-Hoover MD simulations. All entries are in units of kcal/mol•helix.

RESIDUE	I	II	III	IV	V
ACE	0.00	0.00	0.00	0.00	0.00
LEU2g	0.00	-0.01	0.18	0.03	0.22
ALA3a	0.00	0.00	0.00	0.00	0.00
PRO4b	0.00	0.00	0.00	0.00	0.00
GLN5c	0.00	-0.16	-0.09	0.14	0.35
MET6d	0.00	1.43	1.61	1.40	1.53
LEU7e	0.00	0.16	0.32	0.47	0.54
ARG8f	0.00	0.16	-0.17	0.77	1.10
GLU9g	0.00	0.04	0.03	0.34	1.20
LEU10a	0.00	0.25	0.33	0.33	0.31
GLN11b	0.00	0.10	0.08	0.32	0.19
GLU12c	0.00	0.03	-0.46	-0.24	0.13
THR13d	0.00	-0.09	0.13	0.05	0.00
ASN14e	0.00	-0.22	0.34	0.00	0.26
ALA15f	0.00	0.00	0.00	0.00	0.00
ALA16g	0.00	0.00	0.00	0.00	0.00
LEU17a	0.00	0.48	0.52	0.51	0.35
GLN18b	0.00	0.05	-0.06	0.26	0.48
ASP19c	0.00	-0.02	0.41	0.28	0.33
VAL20d	0.00	0.13	0.11	0.10	0.06
ARG21e	0.00	0.46	1.10	1.27	1.45
GLU22f	0.00	0.00	-0.33	-0.51	-0.13
LEU23g	0.00	-0.02	-0.02	0.15	0.41
LEU24a	0.00	0.29	0.56	0.64	0.38
ARG25b	0.00	0.06	-0.52	1.51	0.68
GLN26c	0.00	-0.01	-0.37	-0.75	0.10
GLN27d	0.00	1.54	1.27	1.38	1.69
VAL28e	0.00	0.08	0.04	0.11	0.15
LYS29f	0.00	-0.12	-0.27	-0.54	0.32
GLU30g	0.00	0.50	0.06	0.40	0.63
ILE31a	0.00	0.07	0.62	0.43	0.43
CBX	0.00	0.00	0.00	0.00	0.00
Σ [CONF]	0.00	5.17	5.43	8.84	13.15