

Supporting information for CryoEM Structure Refinement by Integrating NMR Chemical Shifts
with Molecular Dynamics Simulations

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Table S1. Chemical shifts of CA NL4-3 A92E

Res.	C δ	C α	C β	C δ	C δ 1	C δ 2	C ϵ	C γ	C γ 1	C γ 2	N
P1		62.45	33.20	50.41				24.80			
I2	174.95	61.95	38.36						28.24	17.41	121.32
V3		59.03	36.12						21.43	18.68	122.17
Q4	179.20	54.39	29.90								122.32
N5	176.03	51.11	38.68								125.02
L6		57.65	41.76								
Q7	178.17	59.99	28.04					33.60			117.39
G8	176.10	47.24									110.39
Q9											121.27
M10											
V11	180.03	59.41	35.97						21.66	19.24	119.36
H12	175.86	60.04	32.53								121.67
Q13		54.07	32.29					33.18			125.76
A14	175.41	51.76	18.77								125.08
I15	175.35	62.21	38.90		14.91				28.43	17.40	122.70
S16	174.44	56.49	63.47								123.84
P17	178.14	65.56	31.96	50.46				28.02			137.23
R18	179.56	59.63	30.18	43.59				27.74			116.25
T19	175.59	66.94	68.14							23.42	120.05
L20	178.22	58.02	41.06		25.14			26.57			121.93
N21	178.29	56.09	38.54								115.49
A22	180.20	54.98	18.47								122.11
W23	175.46	58.42	29.98			127.67		111.88			119.92
V24	175.93	66.01	31.20						24.01	22.33	118.12
K25	178.17	60.16	32.18	29.47			41.90	25.12			117.94
V26	177.60	65.97	31.01						23.94	22.17	119.47
V27	178.17	65.63	30.70						22.21		120.12

E28	176.64	59.09	29.48	183.36				37.27			119.77
E29	177.50	58.32	30.97	183.28				36.91			116.09
K30	176.38	55.80	33.18	27.15			42.01				115.60
A31	177.76	52.71	17.35								123.29
F32	175.81	58.34	38.21								114.13
S33	176.81	57.96	63.29								117.23
P34	178.35	66.41	31.68	50.85				28.16			
E35	178.67	58.53	29.92	183.04				36.56			115.21
V36	178.73	66.70	31.84						22.71	21.85	116.81
I37	176.23	67.79	34.95		13.88				30.54	18.84	118.71
P38		65.10	30.61	49.06				28.24			
M39	178.68	58.21	32.74								115.88
F40	179.64	61.76	38.07								120.42
S41	175.99	62.53	62.50								114.92
A42	180.86	54.22	19.20								122.18
L43	175.98	55.78	41.98		22.58			27.17			116.52
S44	174.84	57.46	63.81								109.89
E45	178.40	58.32	28.91					34.90			125.54
G46	174.67	45.54									115.94
A47	178.92	53.10	20.47								119.89
T48	174.54	60.16	69.73							22.34	108.88
P49		67.26	30.20	49.82							133.80
Q50	178.65	60.41	29.55					34.35			116.03
D51	177.84	57.75	41.21								119.38
L52	176.66	57.87	41.50		27.02						120.21
N53	178.44	56.98	38.42								118.17
T54	176.21	67.48	68.41							23.63	119.66
M55	179.47	60.44	32.98								119.79
L56	180.34	58.78	41.58					26.99			121.35
N57	175.89	55.77	37.66								116.89

T58	174.31	64.71	69.61							21.44	111.47
V59	176.57	62.33	33.09						21.47		121.28
G60	177.19	45.32									116.08
G61	174.93	47.20									106.27
H62	177.50	55.77	28.86								121.43
Q63	179.60	60.09	28.81					32.94			118.05
A64	178.44	54.50	18.13								121.83
A65	180.15	54.69	18.84								120.93
M66	178.58	56.23	28.95					31.79			112.98
Q67	178.78	58.29	27.32	181.52				32.67			120.41
M68	178.10	58.27	32.71				17.95				119.52
L69	179.53	58.90	41.85					27.21			122.71
K70	178.63	60.03	31.89	29.08			42.12	25.36			119.05
E71	178.22	59.97	29.70	182.95				36.81			118.69
T72	176.73	67.33	68.24							21.86	117.86
I73	176.92	66.10	38.01		14.77				29.76	18.32	122.42
N74	178.55	55.93	37.41					175.84			116.93
E75	179.60	59.28	29.37	183.52				35.94			122.09
E76	177.40	58.86	29.15	184.29				37.36			120.40
A77	179.32	54.65	17.81								123.91
A78	181.49	54.44	17.97								119.19
E79	178.27	58.57	28.58	183.86				34.84			121.34
W80	180.03	61.64	28.02		126.64			110.36			121.08
D81	178.49	57.28	39.99								119.84
R82	178.59	59.37	30.97	43.07				28.22			120.26
L83		55.34	42.77					25.48			116.76
H84	170.84	53.03	27.16			119.01		130.60			116.91
P85		63.01	32.12	50.42				27.49			137.03
V86	176.51	62.56	32.86						21.31		120.84
H87	175.75	55.64	29.19								124.52

A88	177.93	52.23	19.20								127.79
G89	171.61	44.41									109.42
P90	176.73	62.69	32.29	49.58				27.10			133.03
I91	175.15	60.19	38.41		15.31				28.45	18.03	122.45
E92		54.61	29.42								128.20
P93	177.10	64.31	31.79	50.60				27.60			
G94	174.35	45.48									112.45
Q95	175.24	54.42	30.19					33.85			119.64
M96	176.35	54.79	34.76					30.49			120.66
R97	174.76	55.46	30.04	43.66				26.93			123.60
E98		54.20	29.53	183.45				36.72			122.63
P99		62.71	30.38	49.08				26.39			
R100	178.64	52.75	30.82					26.06			121.48
G101	176.24	48.32									117.10
S102	176.97	60.85	61.95								114.78
D103	175.94	56.95	41.43					179.58			122.89
I104	172.67	65.73	36.85		11.02				30.62	17.09	125.88
A105	177.22	50.44	18.81								112.11
G106	173.84	45.33									102.08
T107	177.23	63.96	68.88							22.76	112.65
T108	173.18	61.01	69.29							20.34	106.05
S109	173.89	54.11	66.85								112.37
T110	175.80	59.48	71.23							22.04	112.40
L111	178.12	58.01	40.98		22.56	25.15		26.64			122.83
Q112	178.47	59.73	28.05	179.55				34.88			116.29
E113	178.42	58.88	29.00	184.14				37.35			120.73
Q114	177.90	60.37	28.24	179.62				32.92			117.71
I115	179.62	65.62	38.39		14.22				29.23	17.24	117.57
G116	176.08	47.35									111.60
W117	178.79	62.11	28.47		125.22						121.52

M118	177.54	59.60	34.91				14.86	33.09			116.02
T119	173.54	61.12	70.05							21.92	104.64
H120		57.25	28.36								122.93
N121		48.90	39.58					177.59			120.11
P122											
P123	177.83	63.53	31.99	50.73				28.09			
I124	176.10	59.25	38.86		14.72				27.37	17.17	122.57
P125	176.74	63.07	29.13	51.22				27.50			
V126	176.88	65.81	31.02						23.76	19.54	115.52
G127	174.83	47.19									106.97
E128	180.00	58.43	29.54					36.04			121.81
I129	176.20	65.27	38.29		15.06				28.47	18.27	121.53
Y130	176.06	56.26	36.44								117.18
K131	177.71	60.67	32.23	29.74			41.24	25.62			116.73
R132	178.26	60.15	29.89	44.21				28.44			117.71
W133	178.79	58.47	29.51					110.67			121.73
I134	178.28	65.13	38.03		14.87				29.85	17.83	119.23
I135	178.06	66.51	37.89		13.69				31.47	17.55	121.34
L136	181.69	58.91	41.61					27.23			121.56
G137	176.09	47.55									106.90
L138	178.64	58.15	42.25		24.98	22.72		26.33			123.23
N139	178.04	57.02	38.78								119.00
K140	178.63	60.17	32.11	29.81			42.03	25.21			118.33
I141	178.33	65.12	38.03		14.98				29.88	17.97	119.06
V142	177.40	65.62	32.29						21.87		119.21
R143											
M144	177.61	57.88	32.80					30.24			119.09
Y145	177.88	59.69	38.03								117.45
S146	178.09	56.98	64.27								118.61
P147		63.34	32.65	51.83				28.71			

T148	172.68	61.71	70.64							21.10	111.49
S149	174.31	56.71	63.51								122.33
I150	175.25	60.83	39.53		15.57				28.81	18.38	128.54
L151	178.35	56.83	41.53		23.87	25.95		28.02			118.87
D152	175.83	54.15	42.04								115.06
I153	173.61	59.01	33.87		9.75				26.84	16.97	122.25
R154	175.43	54.33	33.16	43.25				27.24			125.69
Q155	177.01	56.08	27.30					32.51			127.96
G156	173.50	44.77									116.75
P157	177.28	65.68	32.13	50.26				27.69			
K158	175.67	54.13	32.53				41.95	25.05			114.91
E159	174.56	53.60	32.36					35.03			125.88
P160	177.45	63.48	32.71	51.83							
F161	177.14	62.62	39.42								127.93
R162	179.33	59.72	30.27					27.76			115.49
D163	178.89	57.39	39.86								120.07
Y164	176.29	59.71	38.15								124.04
V165											117.03
D166											
R167											
F168	177.11	62.60	39.39								123.63
Y169	179.29	63.58	38.13								115.10
K170											
T171	176.21	66.63	68.89							21.49	115.93
L172	178.94	58.14	42.37					26.24			123.81
R173	179.57	59.33	30.29								116.15
A174	178.38	53.47	18.55								119.63
E175	179.07	57.38	29.88								120.09
Q176	179.14	54.46	27.40								124.81
A177	176.85	51.28	20.57								124.98

S178	177.76	57.46	64.92								116.45
Q179	177.79	58.56	28.61								121.64
E180	179.92	59.96	29.68								118.23
V181	178.02	66.67	31.04						23.95	20.59	121.41
K182	178.96	61.00	32.58	30.21							120.61
N183	175.78	57.02	37.87								117.67
W184	180.50	61.99	28.36								122.75
M185	178.77	59.59	31.00								120.21
T186	176.35	66.76	69.12							21.76	111.98
E187	178.98	60.19	29.52								118.90
T188	174.37	63.50	69.64							23.54	107.93
L189	178.63	58.32	42.29								120.99
L190	177.85	58.08	41.32								118.43
V191	177.13	65.58	32.04						21.74		115.63
Q192	177.18	58.47	28.41								115.37
N193	175.48	52.74	38.38								114.14
A194		51.60	18.96								124.86
N195	174.30	51.70	35.82								119.37
P196	178.55	66.83	32.52	50.12				28.46			
D197	178.64	57.30	40.36								116.16
C198	176.01	62.37	27.89								
K199	177.67	61.46	32.53	29.61							121.95
T200	176.19	66.54	68.82							21.77	112.17
I201	178.92	64.35	38.36		14.41				29.60	18.72	123.52
L202	178.48	57.19	41.79		25.73	23.22		27.54			119.06
K203	178.47	59.52	30.88								119.48
A204	178.98	53.30	18.49								120.10
L205		57.27	41.44					25.86			118.02
G206	172.77	44.54									104.48
P207		63.28	31.83	49.87				27.45			130.78

G208		45.59									110.07
A209	178.23	52.47	20.05								122.84
T210	175.24	60.24	70.64							22.23	113.91
L211		58.62	40.55					27.31			125.24
E212											
E213											
M214		59.31	32.77								
M215	178.33	59.06	32.42								117.53
T216	176.47	66.62	68.88							21.76	115.69
A217	178.28	55.53	18.70								123.81
C218	179.03	60.27	28.55								110.91
Q219											121.66
G220	46.99										
V221											
G222											
G223											
P224											
G225											
H226											
K227											
A228											
R229											
V230											
L231											