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Supporting Material

Driving Forces for Transmembrane α−helix Oligomerization

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	ALA	ARG	ASN	ASP	CYS
ALA	95.7	9	27.5	18.3	17.5
ARG	9	1.5	1	3.7	1
ASN	27.5	1	5	5.5	4
ASP	18.3	3.7	5.5	0	0
CYS	17.5	1	4	0	0
GLU	14.5	3	6.5	2.5	2
GLN	16	3	3	1	6
GLY	201.7	6.7	17	12	15.3
HIS	10	2	1	3	1
ILE	131.3	5	23.2	13.5	17.2
LEU	233	14.5	15.5	10.5	18.8
LYS	3	0	3	1	0
MET	55.2	8	1.5	4.5	11
PHE	95.7	8.3	14	8	9.5
PRO	32.2	3	10	6	4
SER	83.2	3	15	9	8
THR	100.8	7	15	12	6.2
TRP	36.7	1	5	3	4
TYR	41	8.3	6.5	2	4
VAL	175.1	7	13.7	10	15.3
LIP	1000.8	28.2	108	52.7	110.2
SURFACE	803.3	281.3	203.5	109.2	73.5

	GLU	GLN	GLY	HIS	ILE
ALA	14.5	16	201.7	10	131.3
ARG	3	3	6.7	2	5
ASN	6.5	3	17	1	23.2
ASP	2.5	1	12	3	13.5
CYS	2	6	15.3	1	17.2
GLU	1	2	11	1	13
GLN	2	2	22.5	1	7
GLY	11	22.5	86	11.3	106.8
HIS	1	1	11.3	2	8
ILE	13	7	106.8	8	64.7
LEU	17.7	11	154.7	4	103.7
LYS	3	0	4.5	1	5.4
MET	3	5.5	31.2	3	27.7
PHE	6	7	90.8	8	70.4
PRO	3.5	3	48	0	23.2
SER	6.3	12.5	96	3	64.5
THR	9	4	61.7	6.5	68.2
TRP	2	2	31	1.5	14.5
TYR	3	4	29.7	4	14.7
VAL	10.5	10	137.4	8	109.2
LIP	52.7	83.8	691.6	50.5	1148.7
SURFACE	114	160.3	676.8	33.2	917.9

	LEU	LYS	MET	PHE	PRO
ALA	233	3	55.2	95.7	32.2
ARG	14.5	0	8	8.3	3
ASN	15.5	3	1.5	14	10
ASP	10.5	1	4.5	8	6
CYS	18.8	0	11	9.5	4
GLU	17.7	3	3	6	3.5
GLN	11	0	5.5	7	3
GLY	154.7	4.5	31.2	90.8	48
HIS	4	1	3	8	0
ILE	103.7	5.4	27.7	70.4	23.2
LEU	114.5	6.2	54.3	114.5	28
LYS	6.2	0	1.5	1	3.7
MET	54.3	1.5	8.5	35	7.5
PHE	114.5	1	35	20	16.2
PRO	28	3.7	7.5	16.2	4.3
SER	59	3.5	21.3	38	15.5
THR	80.5	2	28.5	43.2	20.3
TRP	33.7	0	8	11.5	9
TYR	35.7	1	15.7	14	10
VAL	153.9	8.7	41.2	46.8	25.6
LIP	1936.8	51.5	325.6	847.5	182.8
SURFACE	1340.4	181.8	330	732	251.4

	SER	THR	TRP	TYR	VAL
ALA	83.2	100.8	36.7	41	175.1
ARG	3	7	1	8.3	7
ASN	15	15	5	6.5	13.7
ASP	9	12	3	2	10
CYS	8	6.2	4	4	15.3
GLU	6.3	9	2	3	10.5
GLN	12.5	4	2	4	10
GLY	96	61.7	31	29.7	137.4
HIS	3	6.5	1.5	4	8
ILE	64.5	68.2	14.5	14.7	109.2
LEU	59	80.5	33.7	35.7	153.9
LYS	3.5	2	0	1	8.7
MET	21.3	28.5	8	15.7	41.2
PHE	38	43.2	11.5	14	46.8
PRO	15.5	20.3	9	10	25.6
SER	18.5	40.2	10	19	67.8
THR	40.2	9.5	14	17.7	67
TRP	10	14	2	7.3	17
TYR	19	17.7	7.3	5	35.2
VAL	67.8	67	17	35.2	57
LIP	318	449.6	273.2	249.2	1094.2
SURFACE	393.5	385	355.7	450.8	865.2

Table S1: The native contact distribution for the 20 amino acids, lipid, and surface contacts.

	ALA	ARG	ASN	ASP	CYS
ALA	92.6	10.2	26.2	12.4	14.2
ARG	10.2	1.5	1.9	1.4	0.8
ASN	26.2	1.9	3.7	2.8	2.6
ASP	12.4	1.4	2.8	0.1	1.9
CYS	14.2	0.8	2.6	1.9	0.7
GLU	11.1	1.7	2.5	1.4	1.3
GLN	16.3	1	3.6	0.9	2
GLY	158.3	11.3	20	9.6	15
HIS	10.2	1.1	0.8	0.5	0.8
ILE	136.9	8.1	21.6	9.7	14
LEU	239.2	16.2	27.8	15.5	15.4
LYS	6.5	1.4	1.9	0.8	0.5
MET	48.2	3.2	6	4.5	5
PHE	99.9	6.6	13.7	8	9.4
PRO	38.3	2.5	4.9	2.8	4.2
SER	68	3.5	11.3	5.7	8.3
THR	76.3	4.9	10.8	8	6.1
TRP	36.6	2.6	4	2.1	3.1
TYR	40.9	4.9	4.8	3.6	2.8
VAL	150.7	8.2	19.7	11.4	14.9
LIP	1078.7	47.4	121.2	82.2	127.7
SURFACE	846.5	263.9	202	100	79.3

	GLU	GLN	GLY	HIS	ILE
ALA	11.1	16.3	158.3	10.2	136.9
ARG	1.7	1	11.3	1.1	8.1
ASN	2.5	3.6	20	0.8	21.6
ASP	1.4	0.9	9.6	0.5	9.7
CYS	1.3	2	15	0.8	14
GLU	0.5	1.4	10.9	0.8	11.1
GLN	1.4	1.4	12.4	0.2	11.8
GLY	10.9	12.4	69.5	9	110.7
HIS	0.8	0.2	9	0.6	5.5
ILE	11.1	11.8	110.7	5.5	64.3
LEU	14.9	18.3	199	8.4	165.3
LYS	1.7	0.7	5.5	0.4	6.8
MET	3.7	5.2	43.6	1.6	41.8
PHE	6.5	7.9	82.8	4.5	88.9
PRO	2.6	3.9	30.9	1.5	31.8
SER	4.9	8.3	61.2	2.8	58.6
THR	5.2	6.8	66	3.5	59.7
TRP	2.6	2.6	26.9	2.6	29.1
TYR	3.5	4.2	31.2	2.9	32.4
VAL	10.2	10.8	125	7.8	122.6
LIP	79.3	100.1	774.9	65.5	1038.8
SURFACE	111.5	146.1	690.2	35.6	908.2

	LEU	LYS	MET	PHE	PRO
ALA	239.2	6.5	48.2	99.9	38.3
ARG	16.2	1.4	3.2	6.6	2.5
ASN	27.8	1.9	6	13.7	4.9
ASP	15.5	0.8	4.5	8	2.8
CYS	15.4	0.5	5	9.4	4.2
GLU	14.9	1.7	3.7	6.5	2.6
GLN	18.3	0.7	5.2	7.9	3.9
GLY	199	5.5	43.6	82.8	30.9
HIS	8.4	0.4	1.6	4.5	1.5
ILE	165.3	6.8	41.8	88.9	31.8
LEU	160.7	11.5	62.6	123.8	42.9
LYS	11.5	0.4	2.4	5.4	2.1
MET	62.6	2.4	7.8	31.4	9
PHE	123.8	5.4	31.4	29.8	18.7
PRO	42.9	2.1	9	18.7	3.3
SER	75.2	3	19.6	43.6	15.6
THR	89.5	4.6	23.3	44	18.1
TRP	48	1.4	12.5	22	10.3
TYR	49.6	2.4	10.7	22.7	8.6
VAL	199.7	7	39.7	82.7	28.5
LIP	1616.1	51.3	326.5	778.7	172.8
SURFACE	1348.2	164.7	325.8	716.8	261.9

	SER	THR	TRP	TYR	VAL
ALA	68	76.3	36.6	40.9	150.7
ARG	3.5	4.9	2.6	4.9	8.2
ASN	11.3	10.8	4	4.8	19.7
ASP	5.7	8	2.1	3.6	11.4
CYS	8.3	6.1	3.1	2.8	14.9
GLU	4.9	5.2	2.6	3.5	10.2
GLN	8.3	6.8	2.6	4.2	10.8
GLY	61.2	66	26.9	31.2	125
HIS	2.8	3.5	2.6	2.9	7.8
ILE	58.6	59.7	29.1	32.4	122.6
LEU	75.2	89.5	48	49.6	199.7
LYS	3	4.6	1.4	2.4	7
MET	19.6	23.3	12.5	10.7	39.7
PHE	43.6	44	22	22.7	82.7
PRO	15.6	18.1	10.3	8.6	28.5
SER	13.9	27.9	15.4	17.1	61.9
THR	27.9	15.7	17.8	18.2	66.5
TRP	15.4	17.8	5.5	8.9	31.6
TYR	17.1	18.2	8.9	7.9	30.8
VAL	61.9	66.5	31.6	30.8	64
LIP	392.7	458.6	254.9	267.7	1020.4
SURFACE	390.2	418.9	302.8	404.7	869.1

Table S2: The neutral contact distribution for the 20 amino acids, lipid, and surface contacts.

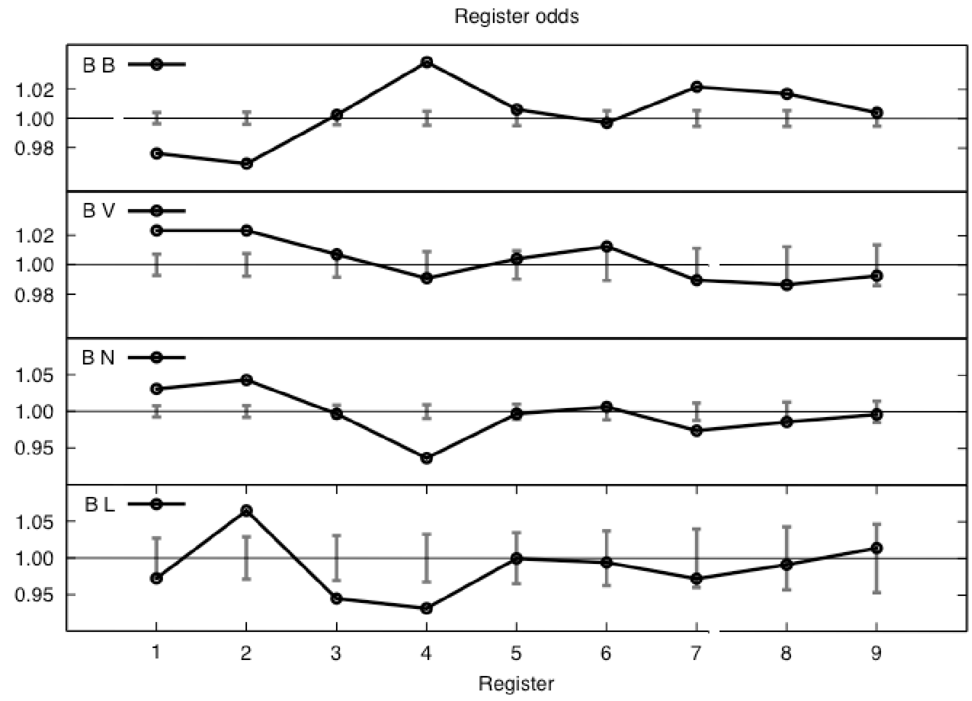

Figure S1. Register odds of the B/V/N/L breakdown, part 1. Ile/Val/Gly are included. Error bars show 95% confidence intervals.

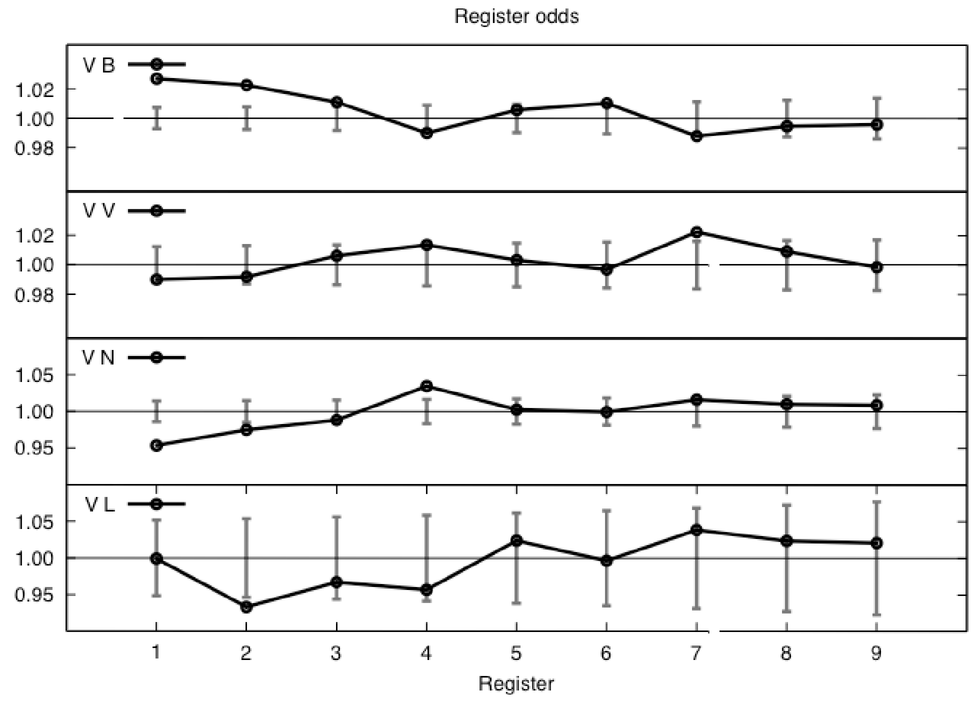

Figure S2. Register odds of the B/V/N/L breakdown, part 2. Ile/Val/Gly are included. Error bars show 95% confidence intervals.

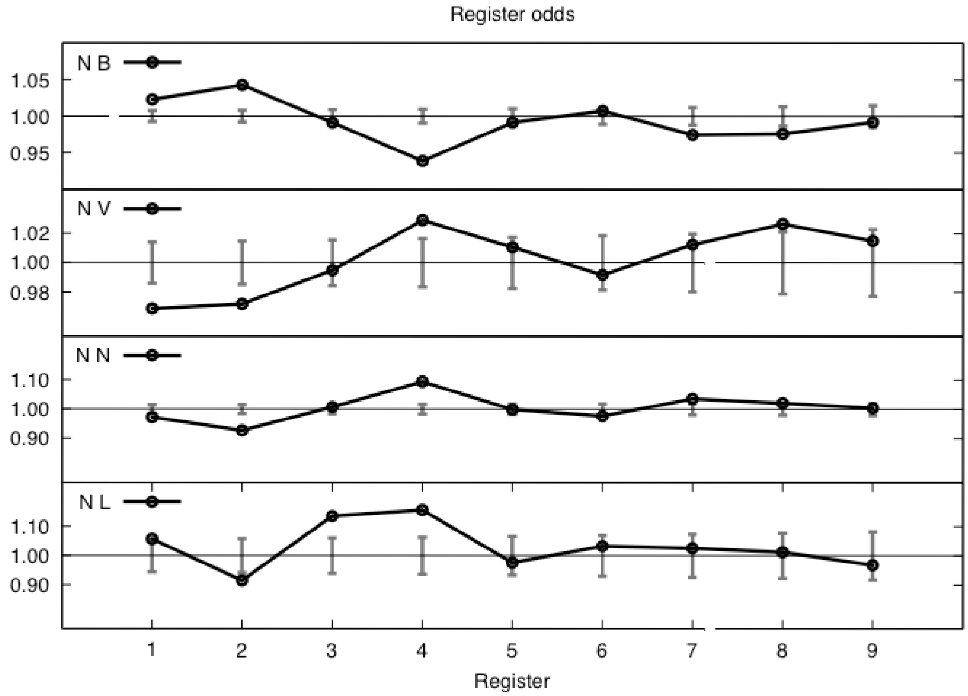

Figure S3. Register odds of the B/V/N/L breakdown, part 3. Ile/Val/Gly are included. Error bars show 95% confidence intervals.

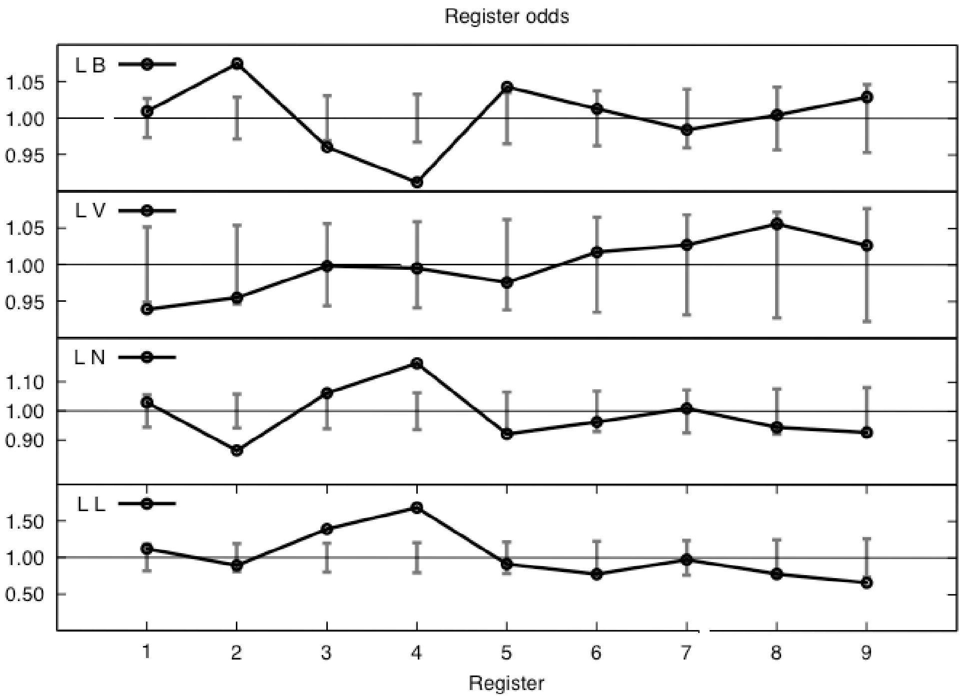

Figure S4. Register odds of the B/V/N/L breakdown, part 4. Ile/Val/Gly are included. Error bars show 95% confidence intervals.

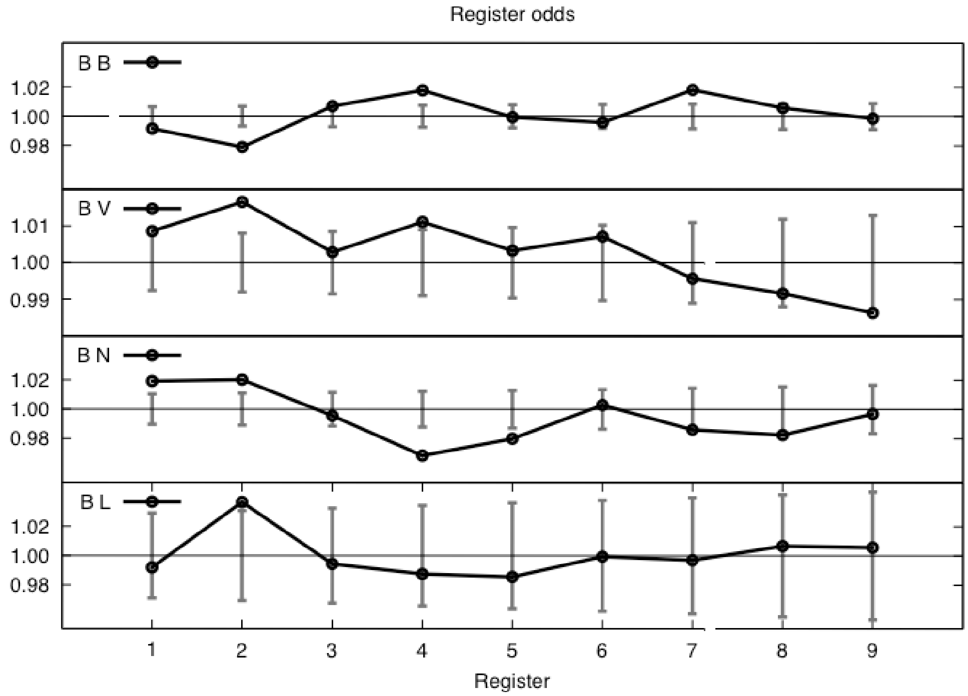

Figure S5. Register odds of the B/V/N/L breakdown, part 1. Ile/Val/Gly are not included. Error bars show 95% confidence intervals.

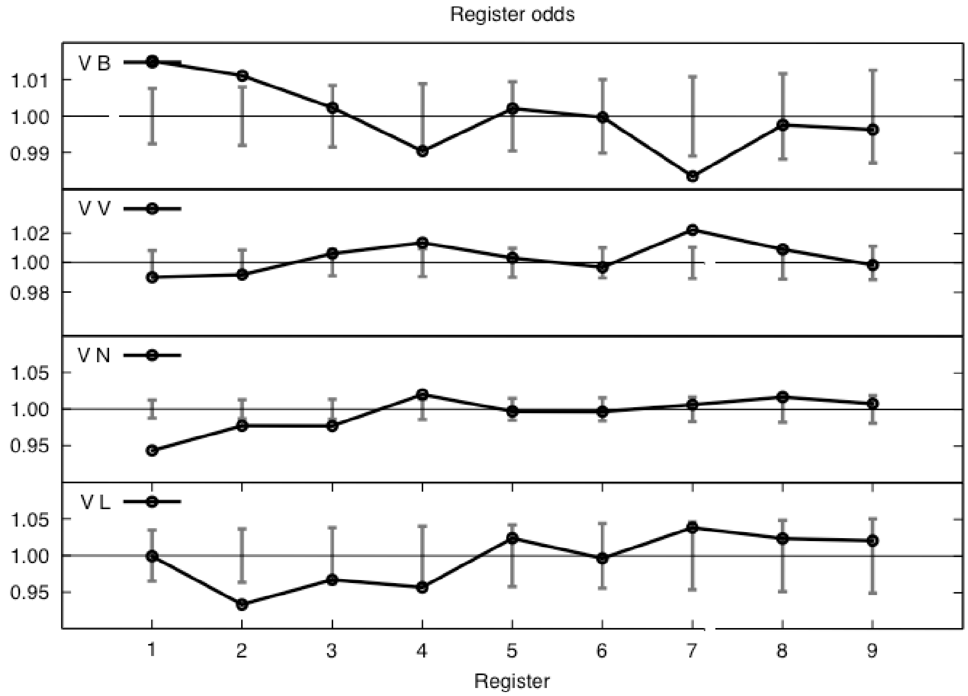

Figure S6. Register odds of the B/V/N/L breakdown, part 2. Ile/Val/Gly are not included. Error bars show 95% confidence intervals.

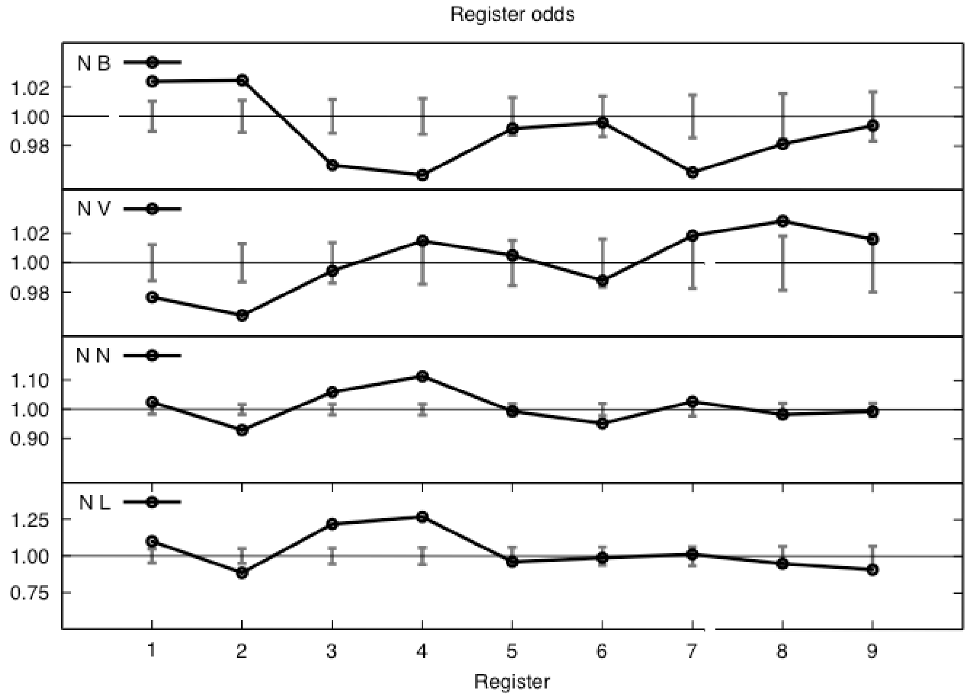

Figure S7. Register odds of the B/V/N/L breakdown, part 3. Ile/Val/Gly are not included. Error bars show 95% confidence intervals.

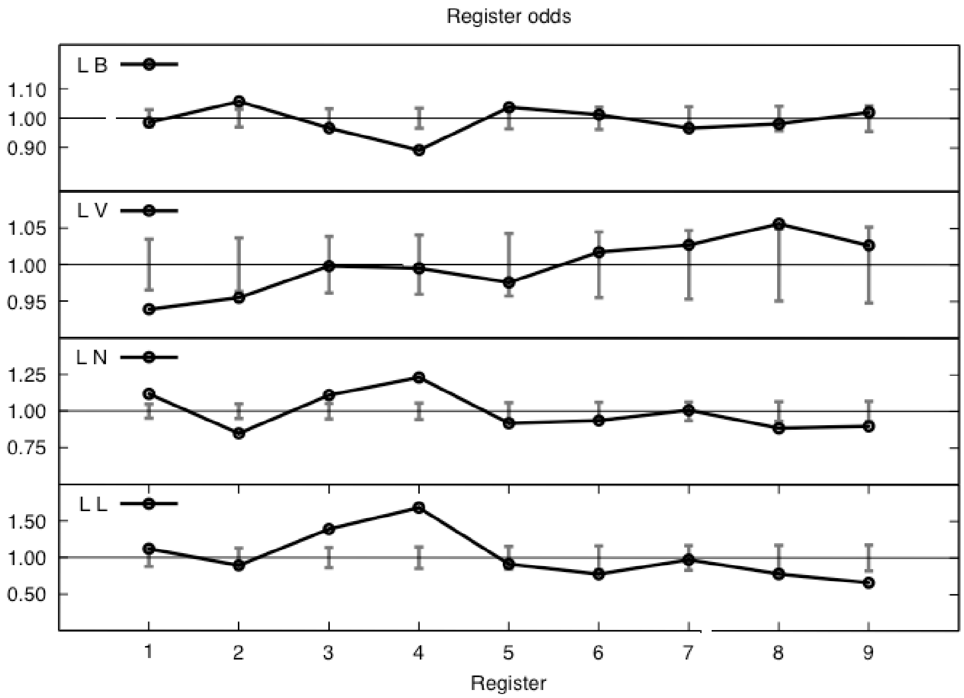

Figure S8. Register odds of the B/V/N/L breakdown, part 4. Ile/Val/Gly are not included. Error bars show 95% confidence intervals.

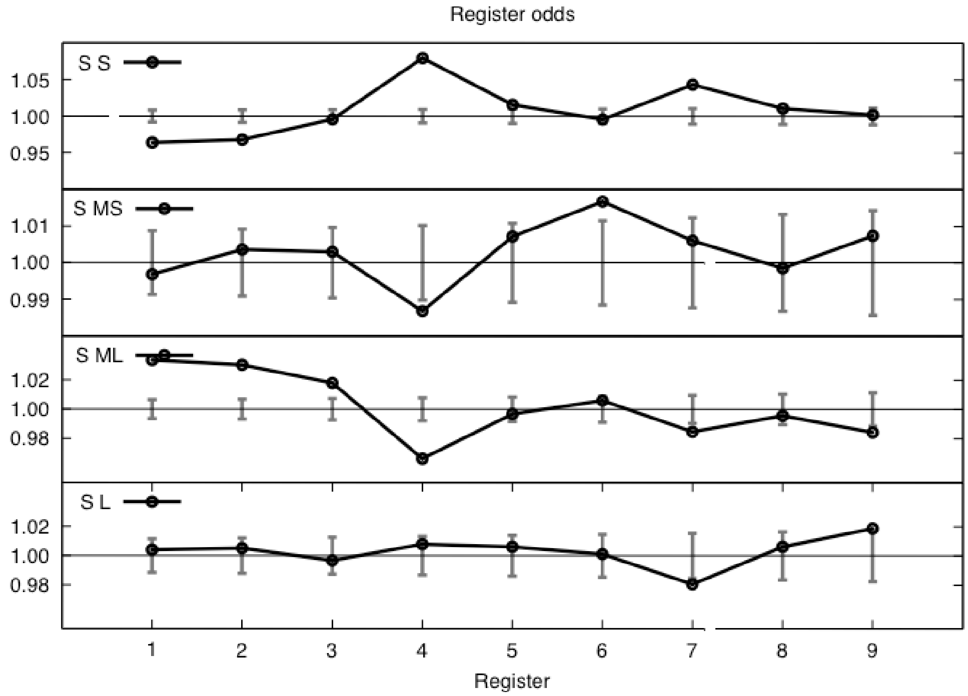

Figure S9. Register odds of the S/MS/ML/L breakdown, part 1. Ile/Val/Gly are included. Error bars show 95% confidence intervals.

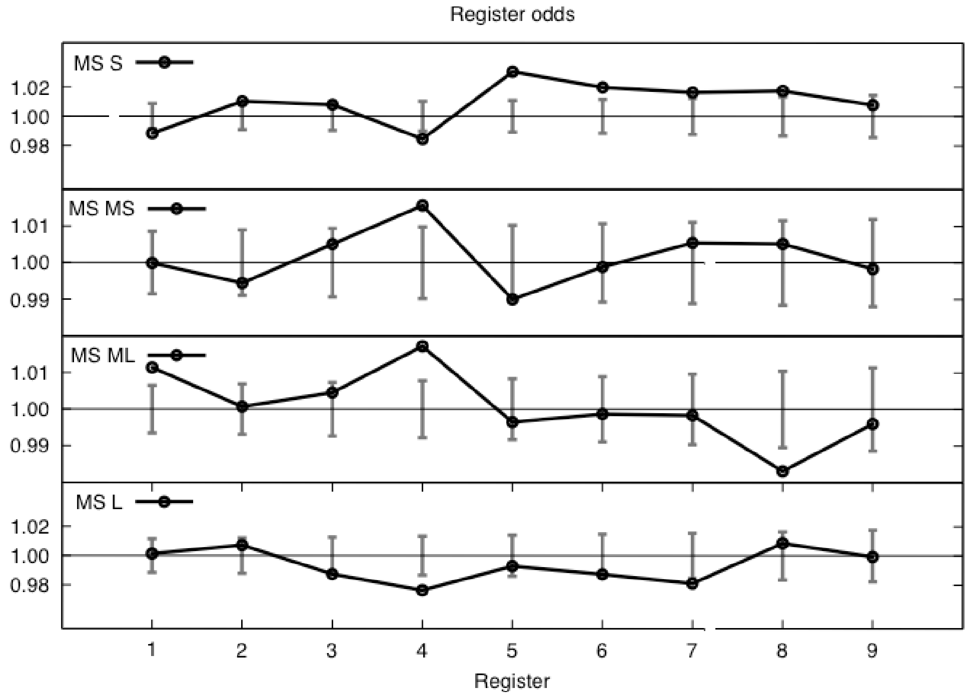

Figure S10. Register odds of the S/MS/ML/L breakdown, part 2. Ile/Val/Gly are included. Error bars show 95% confidence intervals.

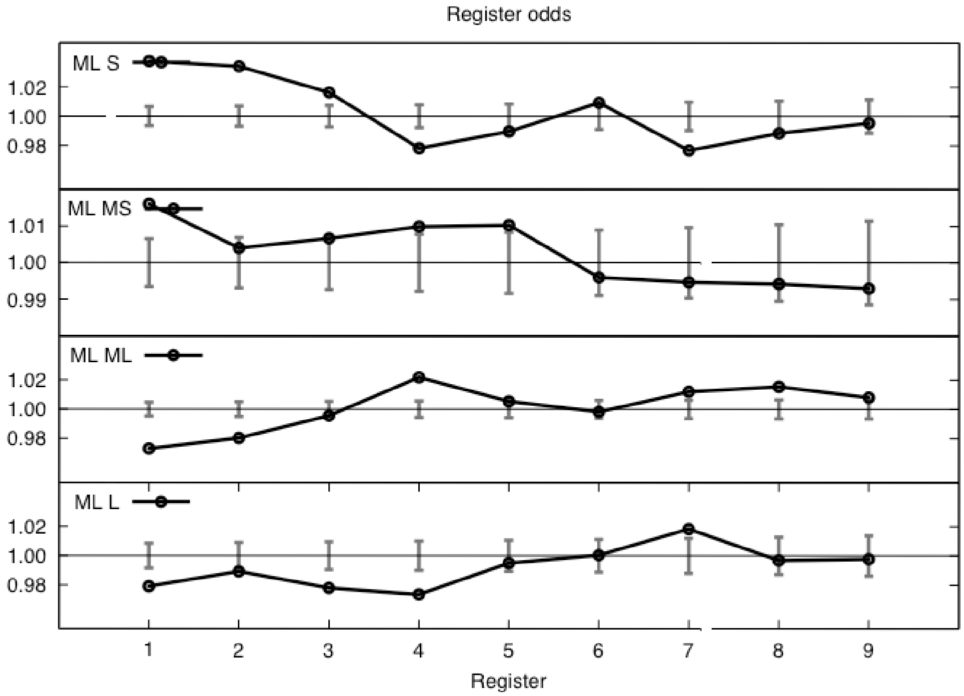

Figure S11. Register odds of the S/MS/ML/L breakdown, part 3. Ile/Val/Gly are included. Error bars show 95% confidence intervals.

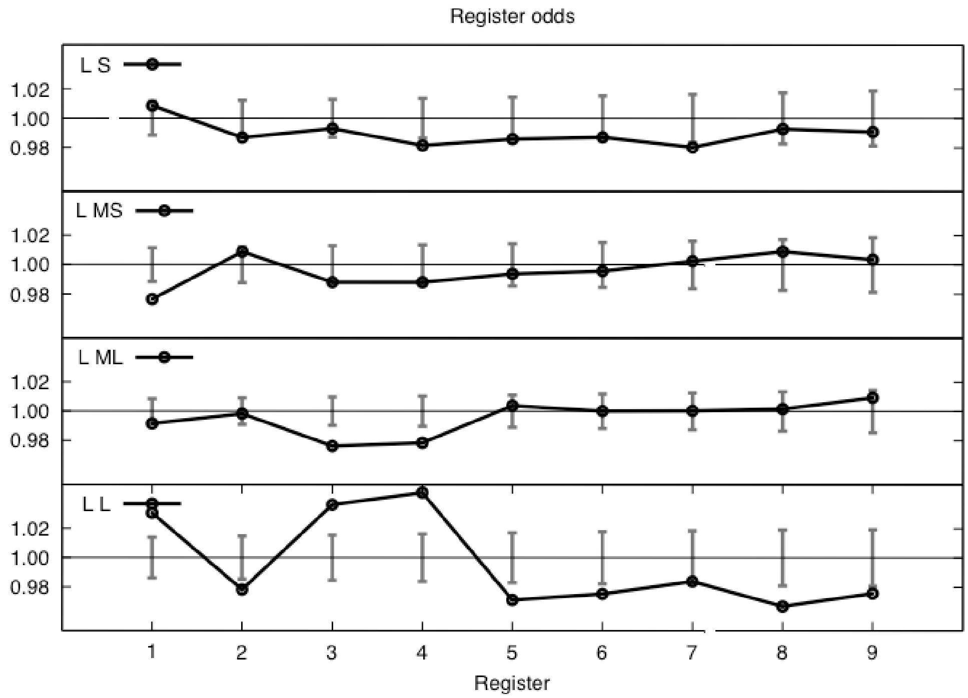

Figure S12. Register odds of the S/MS/ML/L breakdown, part 4. Ile/Val/Gly are included. Error bars show 95% confidence intervals.

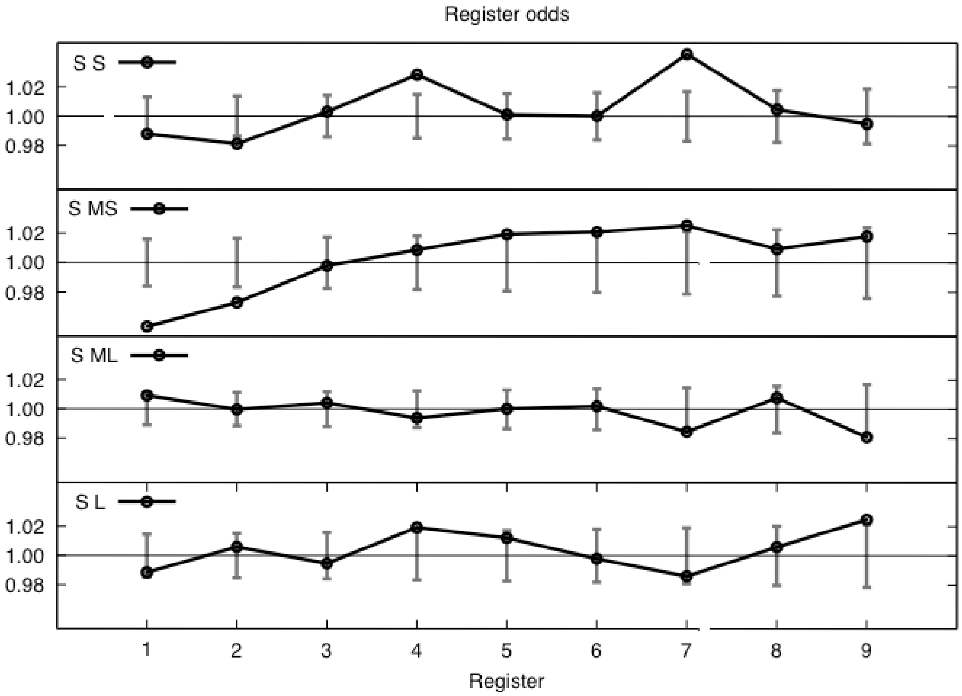

Figure S13. Register odds of the S/MS/ML/L breakdown, part 1. Ile/Val/Gly are not included. Error bars show 95% confidence intervals.

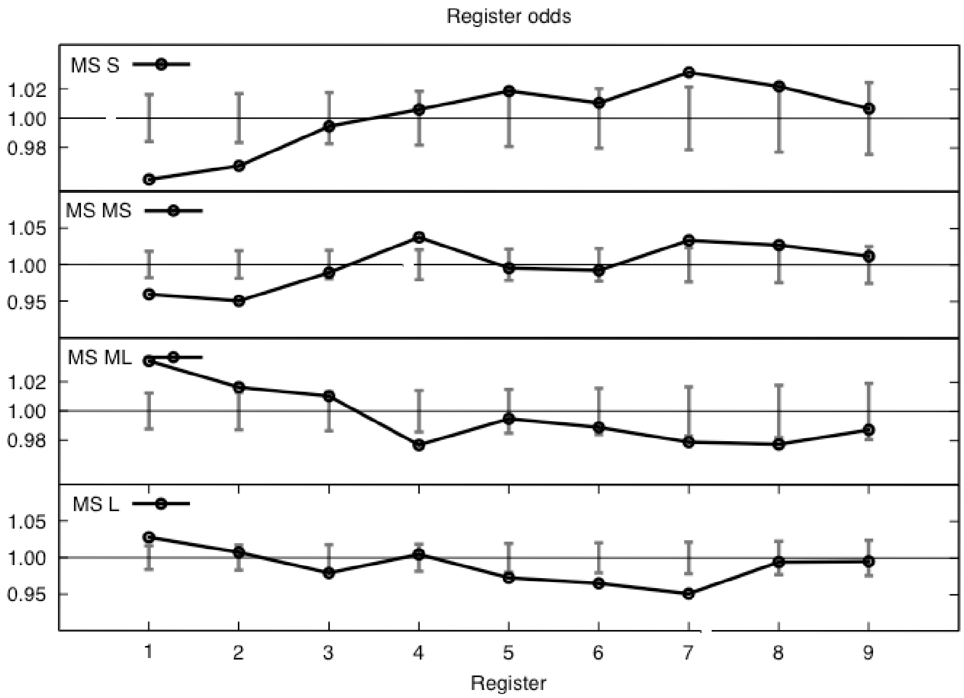

Figure S14. Register odds of the S/MS/ML/L breakdown, part 2. Ile/Val/Gly are not included. Error bars show 95% confidence intervals.

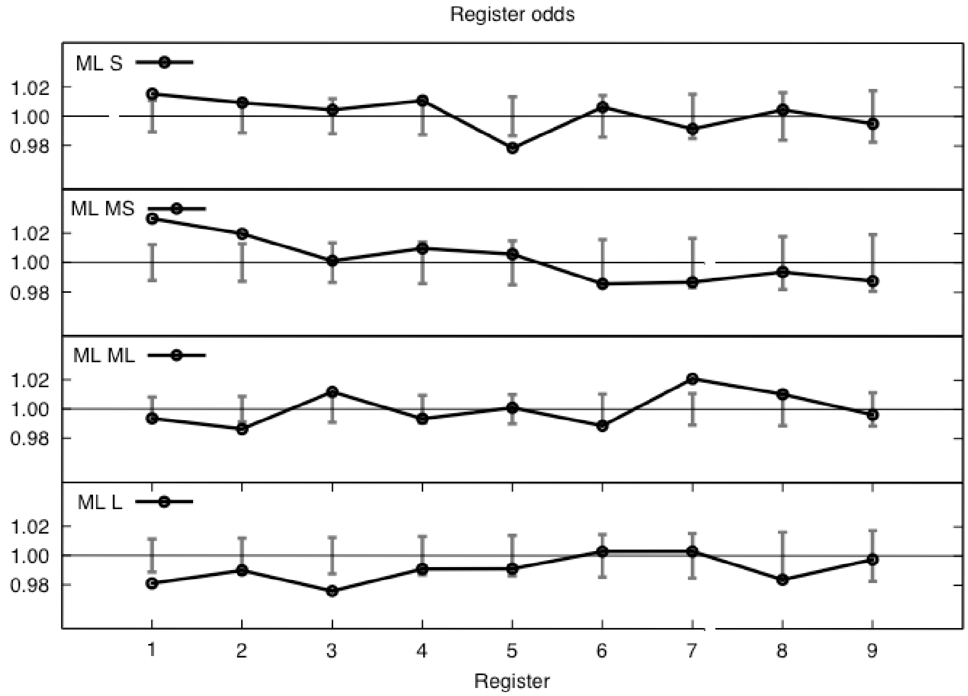

Figure S15. Register odds of the S/MS/ML/L breakdown, part 3. Ile/Val/Gly are not included. Error bars show 95% confidence intervals.

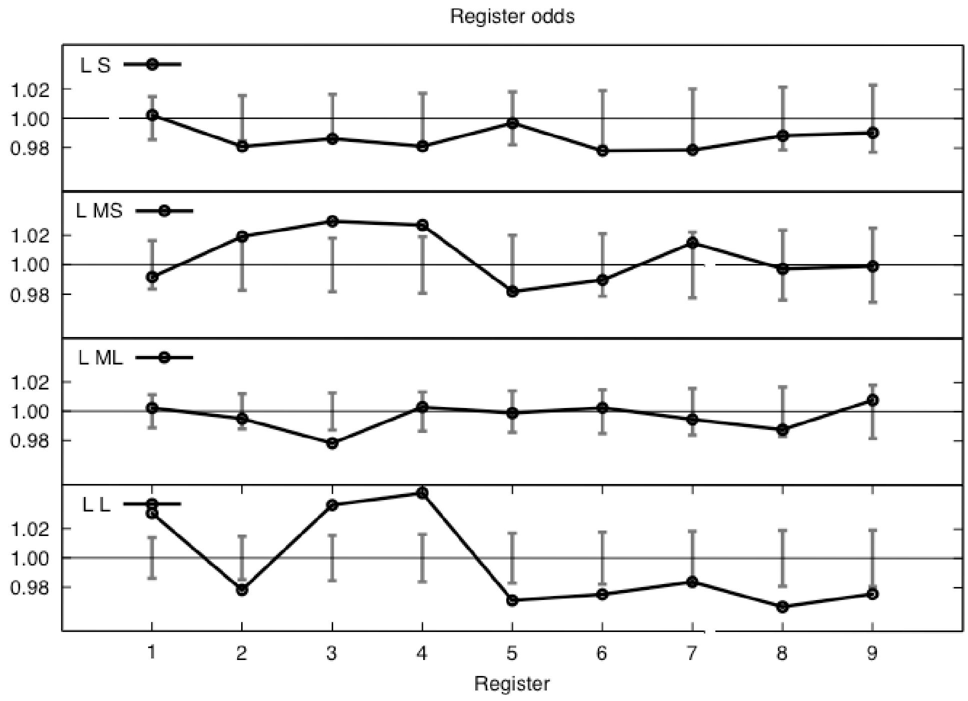

Figure S16. Register odds of the S/MS/ML/L breakdown, part 4. Ile/Val/Gly are not included. Error bars show 95% confidence intervals.

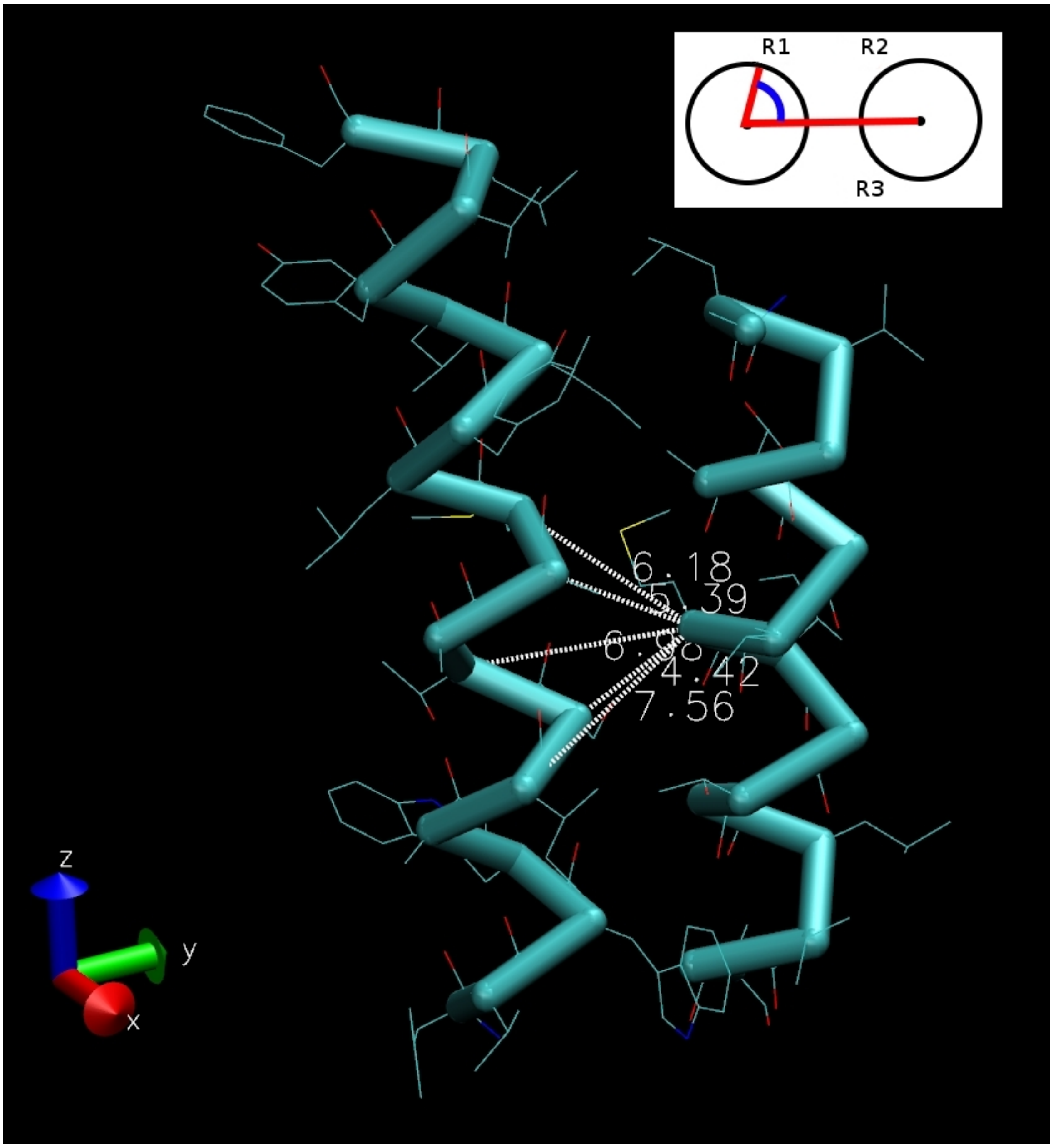

Figure S17. Shown above is an example of two interacting helices, with potential contacts within 7.75 Angstroms shown. Alpha carbons are shown in licorice and all-atoms are shown in lines. The contacts labeled 6.98 and 7.56 are discarded based on an angle criterion described in the main text. The contact labeled 6.98 has angles 112.4 and -19.5, while the contact labeled 7.56 has angles -19.5 and -86.5. An angle of 112.4 is outside the 100 degree per-angle cutoff, while -19.5 and -86.5 sum to be greater than 100 degrees. The illustration was created with VMD (Humphrey, W., Dalke, A. and

Schulten, K., "VMD - Visual Molecular Dynamics", *J. Molec. Graphics*, 1996, **14** 33-38). See inset for an example of the angle computation.

Inset:
Inset is an example of the angle computation (angle section shown in blue). The circles represent helices looking down the bilayer normal, with alpha-carbons on the circle. Residues R1 and R2 are contacts based on the angle cutoff (they have opposite signs) whereas R1/R3 would not be a contact (they have the same sign, and so add to be greater than 100 degrees).