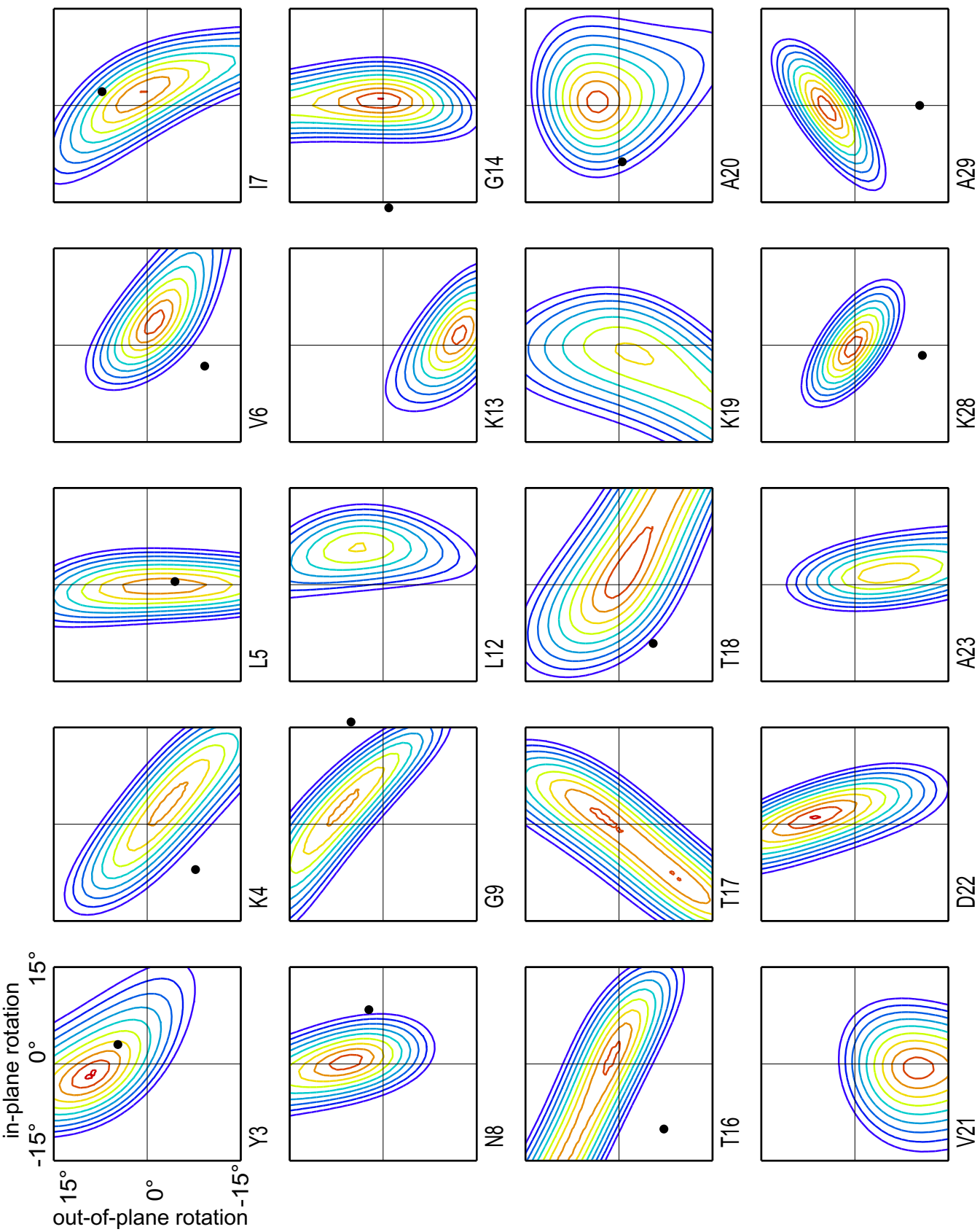
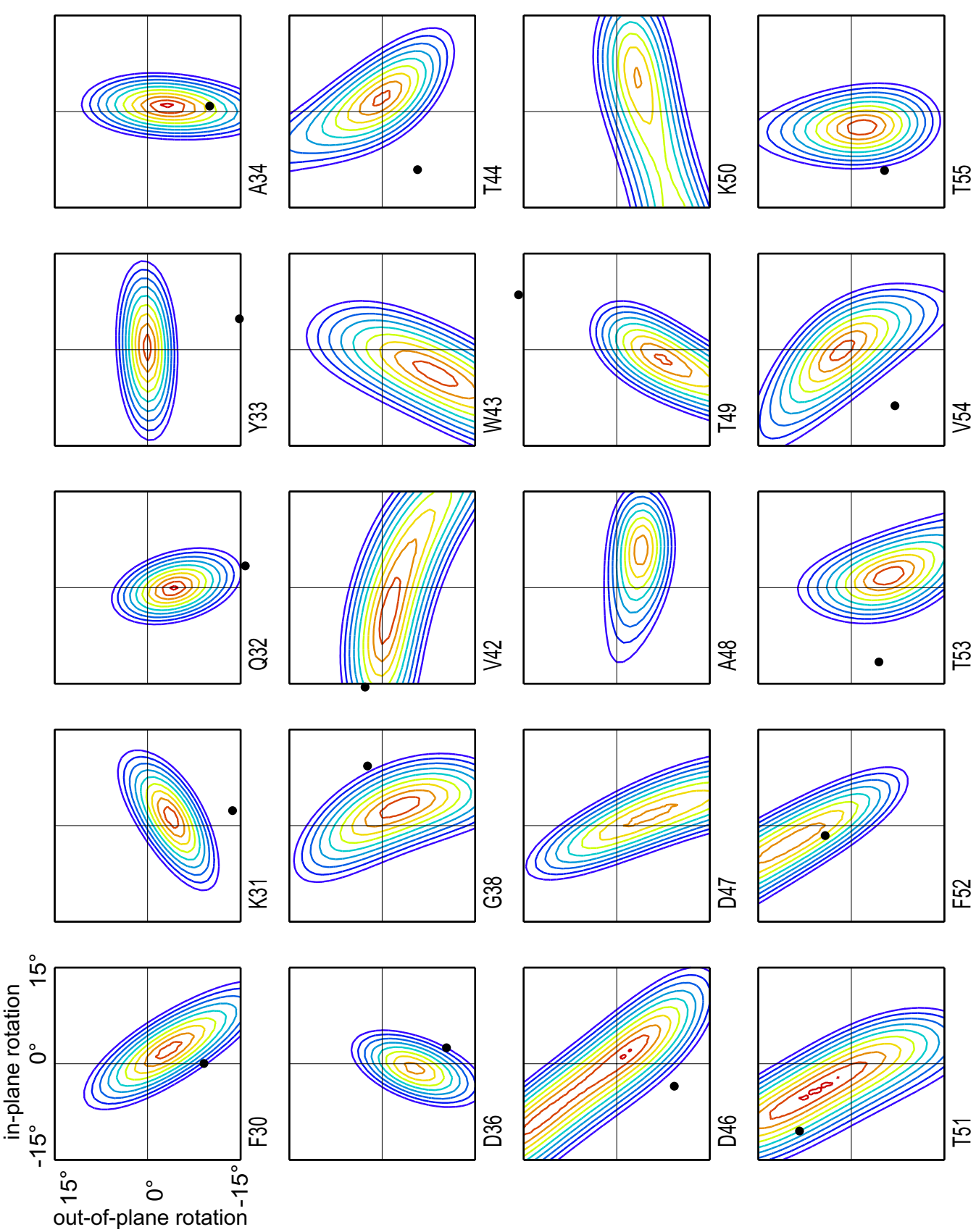
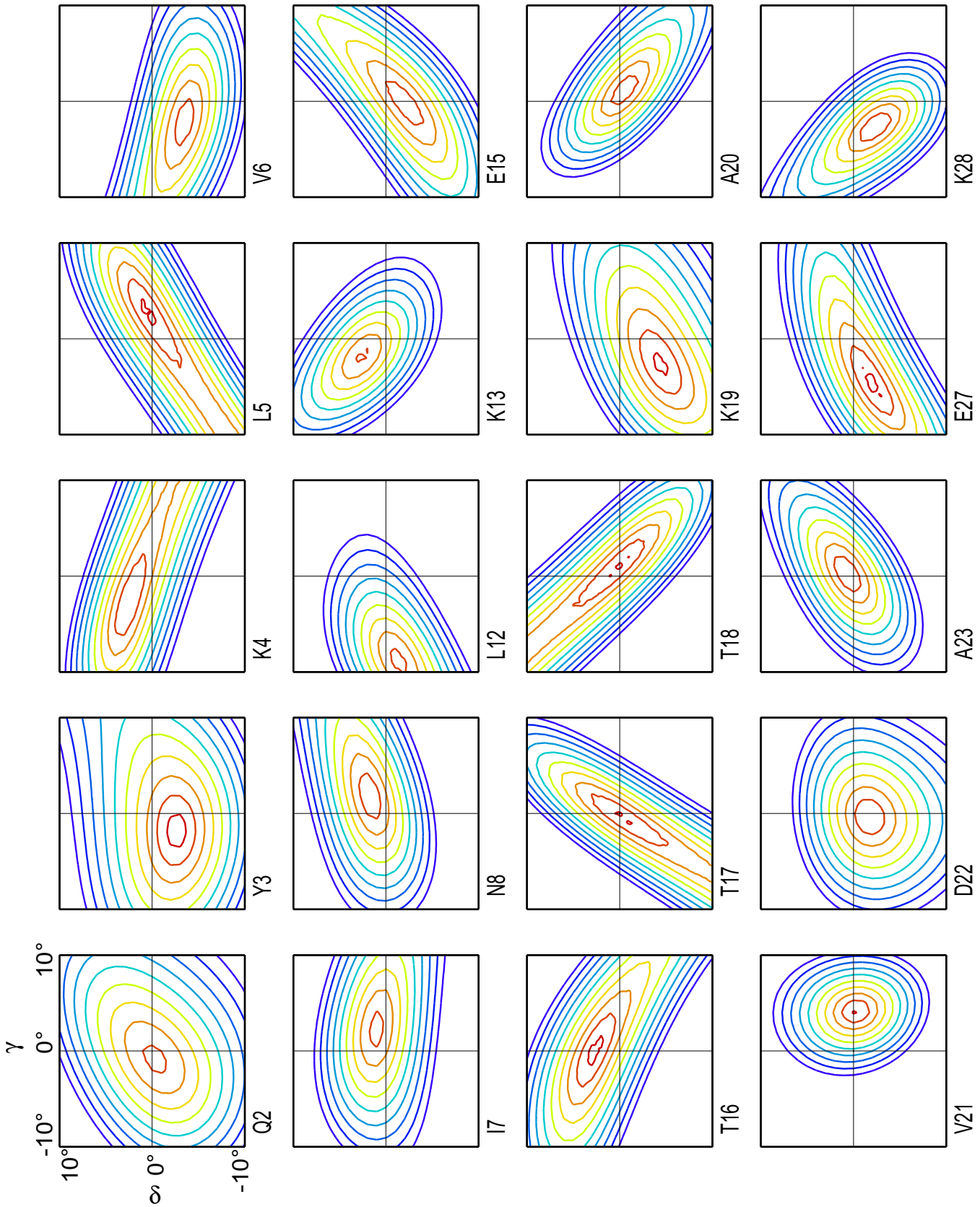


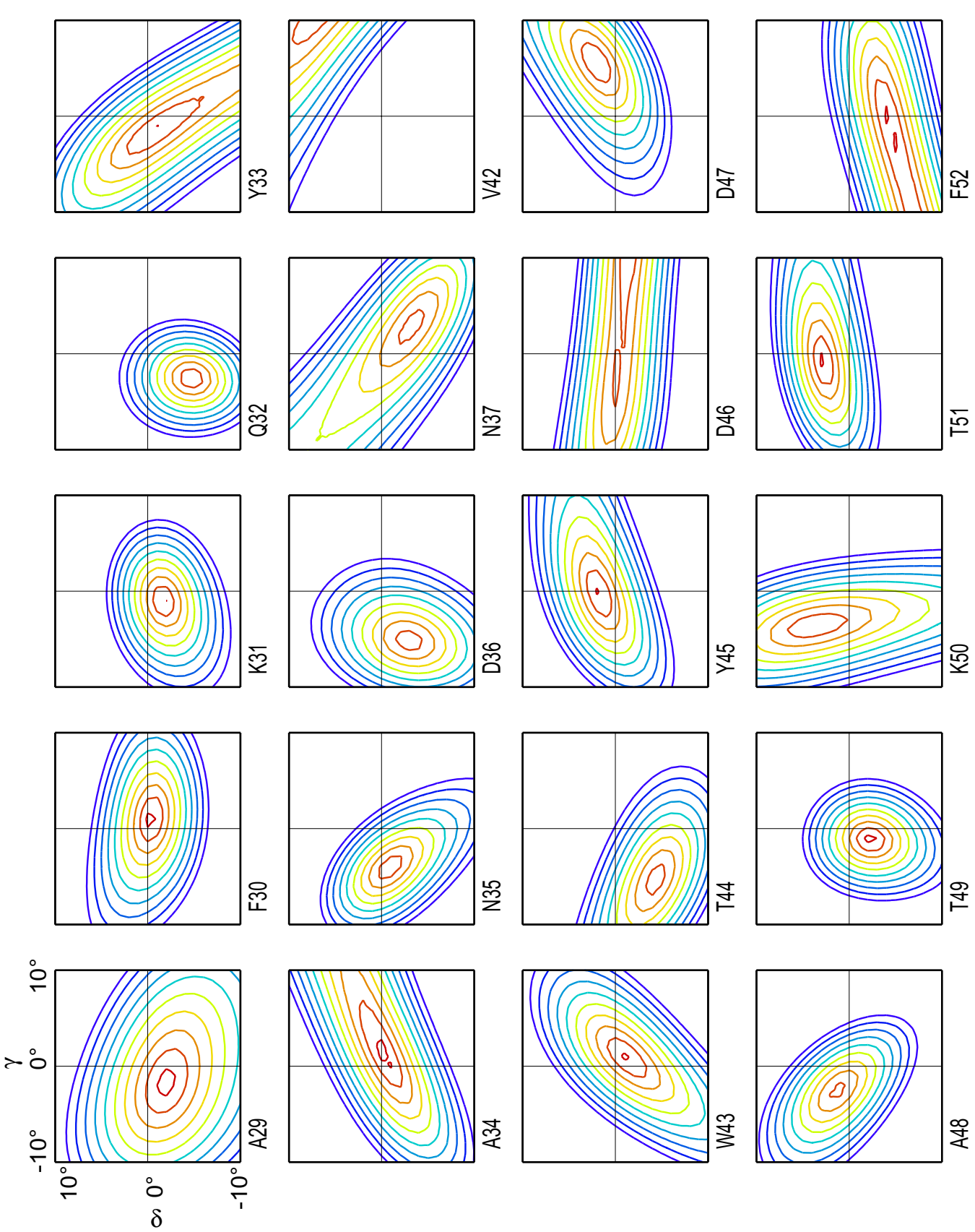
Supporting Information Figure 1. Contour plots of the rmsd between experimental and predicted N-H couplings as a function of N-H vector orientation. See Figure 4, main text, for further explanations.



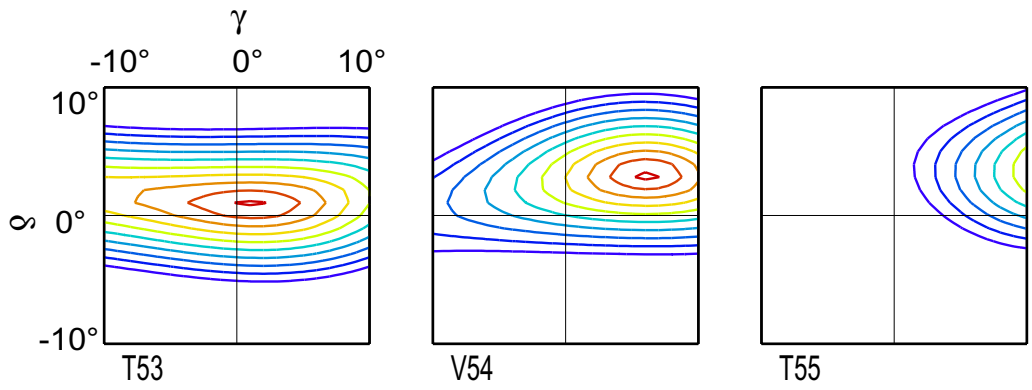
Supporting Information Figure 1 continued.



Supporting Information Figure 2. Contour plots of the rmsd between experimental and predicted C-H couplings as a function of C-H vector orientation. See Figure 7 for further explanations.



Supporting Information Figure 2 continued.



Supporting Information Figure 2 continued.

Supporting Information Table 1. Force constants used during simulated annealing.[a]

Force constant	Initialization/ High (500 K)	Cooling start, 500 K	Cooling end, 0 K	Final Energies [kcal mol^{-1}][d]	Rmsd to target[d]
Bond [kcal $mol^{-1}A^{-2}$]	1000	1000	1000	6.513	0.003 Å
Improper[b] [kcal mol^{-1} rad^{-2}]	25	25	180	48.364	2.013°
Angle[c] [kcal mol^{-1} rad^{-2}]	25	25	180	141.207	1.212°
NOE (H-bond) [kcal mol^{-1} A^{-2}]	2	2	30	0.153	0.012 Å
Van der Waals[e] [kcal mol^{-1} A^{-2}]	0	0.004	0.4	26.790	0.012 Å
AC [kcal mol^{-1} A^{-2}][f]	10	10	24	137.867	0.067 Å
DC [kcal mol^{-1} Hz^{-2}][g]	0	0.1	0.85	39.570	0.896 Hz

[a] The force constants were optimized such as to yield minimal Q factors (see footnote to Table 3) for the agreement between observed N-H and C-H dipolar couplings and values predicted for these couplings, when not included in the calculation of the refined structure.

[b] The H^N-N, C′-C^α improper force constant was reduced tenfold relative to the other improper terms. The H^α-N, C'-C^β force constant was increased fourfold relative to the improper terms. Improper rms deviations comparable to what is found in the 1IGD GB3 crystal structure were maintained.

[c] The force constants for H^α-C^α-C^β and N-C^α-C^β bond angles were increased fourfold relative to the other angular terms. Angular rms deviations comparable to what is found in the GB3 crystal structure were maintained.

[d] For the refined-II structure (see Table 3).

[e] The van der Waals radii were scaled by 0.9 at the start of cooling, ramped down to 0.81 at the end of cooling.

[f] Atomic coordinate restraints were derived from the 1IGD crystal coordinates of GB3 (see main text).

[g] Dipolar coupling force constant for $^1D_{NH}$. Values for other types of couplings are scaled as indicated in the Experimental Section to account for the different intrinsic magnitude of these couplings and their measurement error.

Supporting Information Table 2. GB3 alignment tensor parameters obtained in media A-E.[a]

Medium	Da [Hz][b]	R[b]	Psi [deg]	Theta [deg]	Phi [deg]
A[c]	-15.87	0.23	45.9	-5.2	-81.3
B	-8.83	0.20	69.8	-3.3	262.1
C	13.51	0.10	80.6	-30.7	-76.3
D	11.19	0.43	-79.9	231.2	53.3
E	-10.23	0.66	43.4	-15.9	-59.7

[a] Dipolar couplings for residues 10-11, 24-26, 39-41 and the N- and C-terminal residues are excluded. The refined-II GB3 structure (Table 2, main text) is used as input coordinates.

[b] The tensor magnitude, D_a, is given relative to N-H couplings. R denotes the tensor rhombicity.

[c] A, bicelle; B, PEG; C, Pf1 phage; D and E, negatively and positively charged polyacrylamide gels, respectively

Supporting Information Table 3. Comparison of Q factors for the crystal and refined GB3 structures in aligning media A-E as well as average Q and RMSD values.

Coupling[a]	Structure[b]	Q_A[c]	Q_B	Q_C	Q_D	Q_E	Q_{avrg}	DC $rmsd_{avrg}$[Hz][d]	backbone rmsd [Å][e]
C^{α}-C'	crystal	16.1	17.3	12.9	12.4	14.3	14.6	0.29 ± 0.15	0
	regularized	16.0	16.7	11.8	12.4	14.8	14.3	0.28 ± 0.13	0.049
	refined-I	9.1	9.2	7.9	7.6	8.5	8.5	0.18 ± 0.07	0.305
	refined-II	9.3	9.5	8.0	6.7	8.3	8.4	0.17 ± 0.07	0.315
	refined-III	9.2	9.5	8.0	6.6	8.2	8.3	0.17 ± 0.07	0.310
	refined-IV	9.4	9.3	7.9	7.4	8.6	8.5	0.18 ± 0.06	0.306
C′-N	crystal	24.8	21.2	20.3	14.2	30.3	22.2	0.21 ± 0.18	
	regularized	27.1	24.2	21.3	14.8	31.8	23.8	0.22 ± 0.19	
	refined-I	9.6	12.9	11.0	9.2	13.5	11.2	0.13 ± 0.07	
	refined-II	9.3	12.9	10.4	8.6	13.7	11.0	0.12 ± 0.07	
	refined-III	9.4	13.0	10.7	9.0	13.8	11.2	0.12 ± 0.07	
	refined-IV	9.2	12.7	10.5	8.7	13.3	10.9	0.13 ± 0.06	
C^{α}-H^{α}	crystal	12.1	9.3	12.0	16.3	11.0	12.1	1.99 ± 1.21	
	regularized	11.6	9.9	11.4	16.0	10.3	11.8	1.96 ± 0.20	
	refined-I	11.0	8.6	10.8	14.3	10.3	11.0	1.83 ± 1.11	
	refined-II	2.2	2.1	2.5	2.2	2.1	2.2	0.40 ± 0.19	
	refined-III	2.2	2.1	2.4	1.9	2.2	2.2	0.40 ± 0.19	
	refined-IV	10.9	8.7	10.6	14.0	10.5	10.9	1.79 ± 1.15	
N-H	crystal	12.9	12.5	17.2	19.5	14.5	15.3	1.35 ± 0.79	
	regularized	14.9	14.4	18.4	18.8	16.4	16.6	1.42 ± 0.83	
	refined-I	11.7	10.5	13.4	12.3	13.6	12.3	1.06 ± 0.66	
	refined-II	2.5	5.3	4.5	3.4	3.9	3.9	0.36 ± 0.19	
	refined-III	10.8	10.4	12.6	11.6	13.0	11.7	1.00 ± 0.62	
	refined-IV	2.3	5.2	4.6	3.4	3.9	3.9	0.45 ± 0.23	

[a] Dipolar couplings originating on residues 1, 10-11, 24-26, 39-41 and 56 are excluded.

[b] PDB entry 1IGD was used for the GB3 crystal structure. For the regularized structure only the "standard" force-field and atomic coordinate (AC) energy terms were operative (see Table 1); no dipolar coupling restraints were operative. For the refined-I structure only C^{α}-C' and C'-N dipolar couplings were included; hydrogen atoms were placed at their standard positions (see text). For

the refined-II structure all dipolar couplings (C^{α}-C′, C′-N, C^{α}-H^{α} and N-H) were used. For the refined-III structure C^{α}-C′, C′-N and C^{α}-H^{α} dipolar couplings were included, while H^{N} was placed at its standard position. For the refined-IV structure C^{α}-C′, C′-N and N-H dipolar couplings were included, while H^{α} was placed at its standard position.

[c] Q-factors reflect the agreement between structure and dipolar couplings: $Q = \mathrm{rms}(D^{calc} - D^{obs})/(\{D_a^2[4 + 3R^2]/5\}^{1/2})$, where D_a and the rhombicity, R refer to the magnitude and rhombicity of the alignment tensor, and D^{calc} and D^{obs} are the calculated and observed dipolar couplings. Subscripts A-E refer to the alignment medium used: A, bicelle; B, PEG; C, Pf1; phage; D and E, negatively and positively charged polyacrylamide gels, respectively. Q_{avrg} refers to the average value over all five media.

[d] Root-mean-square deviation (rmsd) per residue between observed and predicted dipolar. Values are normalized to a D_a^{N-H} of 10 Hz. A single tensor was used to fit all types of couplings obtained in one medium.

[e] Minimal rmsd between the C^{α}, C' and N coordinates in the 1IGD crystal structure and the structure indicated in the first column.

Supporting Information Table 4. Comparison between the minimal rmsd between all five N-H dipolar couplings for couplings not-scaled and scaled with the inverse of the general order parameter, 1/***S***, determined from ^{15}N relaxation analysis.[a]

Residue[b]	not scaled, minimal rmsd [Hz]	1/***S*** scaled, minimal rmsd [Hz]	scaling factor, $1/S_{\text{axially-symmetric}}$
3	0.168	0.159	1.10
4	0.591	0.574	1.08
5	0.497	0.38	1.07
6	0.282	0.397	1.07
7	0.427	0.486	1.10
8	0.279	0.333	1.08
9	0.601	0.86	1.10
10	0.373	0.391	1.11
11	0.439	0.47	1.14
12	0.864	0.65	1.23
13	0.32	0.193	1.14
14	0.203	0.48	1.17
16	0.376	0.4	1.10
17	0.402	0.519	1.12
18	0.233	0.292	1.09
19	0.847	0.613	1.14
20	0.323	0.253	1.15
21	0.307	0.125	1.09
22	0.174	0.174	1.08
23	0.722	0.485	1.05
24	0.511	0.419	1.11
26	0.203	0.256	1.05
28	0.213	0.242	1.06
29	0.222	0.127	1.06
30	0.305	0.16	1.06
31	0.258	0.314	1.05
32	0.133	0.204	1.06
33	0.297	0.058	1.05

34	0.12	0.383	1.05
36	0.562	0.432	1.06
38	0.259	0.216	1.13
39	0.137	0.13	1.09
40	0.477	0.363	1.17
41	1.596	0.376	1.41
42	0.253	0.325	1.10
43	0.303	0.253	1.08
44	0.356	0.284	1.08
46	0.177	0.191	1.08
47	0.597	0.896	1.11
48	0.497	0.176	1.15
49	0.388	0.246	1.10
50	0.631	0.782	1.06
51	0.156	0.157	1.08
52	0.512	0.544	1.07
53	0.211	0.232	1.09
54	0.313	0.213	1.06
55	0.211	0.208	1.10
average	0.390 ± 0.256	0.349 ± 0.193	1.10 ± 0.06

[a] The alignment tensors for the non-scaled and 1/***S***-scaled case have been determined by SVD fits of the C^{α}-C′, C′-N and C^{α}-H^{α} couplings to the refined-III structure. In the scaled case, the C^{α}-C′, C′-N and C^{α}-H^{α} couplings were first scaled identically to the N-H couplings. For the alignment tensor determination, dipolar couplings originating on residues 1, 10-11, 24-26, 39-41 and 56 excluded. ***S*** values are taken from the values reported by Hall, J.B. and Fushman, D. *J. Biomol. NMR*, in press, for the axially symmetric diffusion tensor model.

[b] Due to spectral overlap, less than five N-H couplings could be obtained for residues T2, E15, T25, E27, N35, N37, and Y45 and these residues are excluded.

[c] All couplings were normalized to D_a^{NH} = 10 Hz for each medium.

Supporting Information Table 5. C^{α}-H^{α} vector orientations, expressed as rotations from their standard orientations, at the point of minimal rmsd between all five experimental and predicted C^{α}-H^{α} dipolar couplings.[a]

Residue[b]	minimal rmsd [Hz][c]	δ [deg][d]	γ [deg]
2	0.769	-0.5 ± 1.5	-1 ± 2
3	0.094	-2.5 ± 2	-2 ± 1.5
4	0.366	2.5 ± 1	-2.5 ± 1.5
5	0.268	0.5 ± 2	3 ± 2.5
6	0.594	-3.5 ± 1	-2 ± 1.5
7	0.699	1 ± 1	2 ± 1.5
8	0.536	1.5 ± 1	1.5 ± 2
12	0.729	-1.5 ± 1.5	-9 ± 2
13	0.806	2.5 ± 1.5	-2 ± 1
15	0.579	-2 ± 1.5	0 ± 1.5
16	0.22	3 ± 1	-0.5 ± 1
17	0.332	-0.5 ± 2	-0.5 ± 1.5
18	0.34	0 ± 4	1 ± 3.5
19	0.313	-4.5 ± 1.5	-3 ± 1.5
20	0.538	-0.5 ± 1	1 ± 1
21	0.39	0 ± 1	4 ± 1
22	0.488	-1.5 ± 1	-0.5 ± 1
23	0.426	0.5 ± 1	0 ± 1
27	0.227	-2 ± 1	-4.5 ± 1.5
28	0.413	-2.5 ± 1	-2.5 ± 1
29	0.239	-2 ± 1	-1.5 ± 1.5
30	0.189	-0.5 ± 1	1 ± 1
31	0.407	-1.5 ± 0.5	-1 ± 1
32	0.484	-4.5 ± 1	-2.5 ± 0.5
33	0.411	-1 ± 2	-1.5 ± 1
34	0.227	0 ± 1	1.5 ± 1.5
35	0.553	-1 ± 1	-4 ± 1
36	0.632	-3 ± 1.5	-5 ± 0.5
37	0.693	-3.5 ± 1.5	3 ± 1.5
42	0.563	6 ± 2.5	11.5 ± 2.5
43	0.347	-1 ± 1	1 ± 1

44	0.65	-4.5 ± 1	-5 ± 1
45	0.385	1.5 ± 1	-0.5 ± 1.5
46	0.415	-1.5 ± 1	12 ± 6
47	0.417	2 ± 1	5.5 ± 1.5
48	0.748	1 ± 1.5	-2.5 ± 1
49	0.244	-2.5 ± 1	-1 ± 0.5
50	0.487	3.5 ± 2	-3.5 ± 1
51	0.36	3 ± 0.5	-0.5 ± 1
52	0.328	-4.5 ± 2	-1 ± 6
53	0.375	1 ± 0.5	1 ± 2
54	0.341	3 ± 1	6 ± 1.5
55	0.545	4.5 ± 0.5	>15

[a] The standard H^{α} positions (see text) were calculated using the GB3 crystal structure (PDB entry 1IGD) refined with C^{α}-C′, C′-N and N-H dipolar couplings (Model Refined-III). Rotations are performed in steps of 0.5°.

[b] Dipolar couplings originating on residues 10-11, 24-26 and 39-41 are, besides the N- and C-terminal residues, excluded. Residue 9, 14 and 38 are Gly.

[c] All couplings were normalized to D_a^{NH} = 10 Hz or D_a^{CH} = 20.6 Hz for each medium.

[d] 500 Monte Carlo simulations using Gaussian-distributed noise with standard deviation of 0.58 Hz were performed to estimate the uncertainties.

Supporting Information Table 6. GB3 dipolar couplings measured in bicelle, PEG, Pf1 phage and negatively and positively charged polyacrylamide gel media.

Medium A (bicelle)

2	GLN	C	2	GLN	CA	-1.579
3	TYR	C	3	TYR	CA	-3.240
4	LYS	C	4	LYS	CA	-0.906
5	LEU	C	5	LEU	CA	-3.766
6	VAL	C	6	VAL	CA	-0.942
7	ILE	C	7	ILE	CA	-5.069
8	ASN	C	8	ASN	CA	-0.653
9	GLY	C	9	GLY	CA	-5.592
12	LEU	C	12	LEU	CA	2.284
13	LYS	C	13	LYS	CA	-2.267
14	GLY	C	14	GLY	CA	-3.154
15	GLU	C	15	GLU	CA	-1.073
16	THR	C	16	THR	CA	-2.778
17	THR	C	17	THR	CA	-1.404
19	LYS	C	19	LYS	CA	1.123
21	VAL	C	21	VAL	CA	3.047
22	ASP	C	22	ASP	CA	-6.355
23	ALA	C	23	ALA	CA	1.469
27	GLU	C	27	GLU	CA	2.827
28	LYS	C	28	LYS	CA	3.352
29	ALA	C	29	ALA	CA	-5.988
30	PHE	C	30	PHE	CA	-1.041
31	LYS	C	31	LYS	CA	3.967
32	GLN	C	32	GLN	CA	-0.380
33	TYR	C	33	TYR	CA	-6.058
34	ALA	C	34	ALA	CA	1.194
35	ASN	C	35	ASN	CA	3.851
36	ASP	C	36	ASP	CA	-3.454
37	ASN	C	37	ASN	CA	-3.213
38	GLY	C	38	GLY	CA	3.026
42	VAL	C	42	VAL	CA	-1.931
43	TRP	C	43	TRP	CA	3.132
44	THR	C	44	THR	CA	-2.915
45	TYR	C	45	TYR	CA	2.879
47	ASP	C	47	ASP	CA	2.031
48	ALA	C	48	ALA	CA	4.071
49	THR	C	49	THR	CA	2.542
50	LYS	C	50	LYS	CA	-1.149
51	THR	C	51	THR	CA	1.065
52	PHE	C	52	PHE	CA	-4.706
53	THR	C	53	THR	CA	1.505
54	VAL	C	54	VAL	CA	-5.869
55	THR	C	55	THR	CA	-0.263
2	GLN	C	3	TYR	N	-0.320
3	TYR	C	4	LYS	N	-1.906
4	LYS	C	5	LEU	N	-0.024
5	LEU	C	6	VAL	N	-0.476
6	VAL	C	7	ILE	N	0.578
7	ILE	C	8	ASN	N	0.944
8	ASN	C	9	GLY	N	2.356

9	GLY	C	10	LYS	N	-0.564
12	LEU	C	13	LYS	N	1.016
13	LYS	C	14	GLY	N	-1.894
14	GLY	C	15	GLU	N	-1.914
15	GLU	C	16	THR	N	-1.834
17	THR	C	18	THR	N	-1.150
18	THR	C	19	LYS	N	-2.606
19	LYS	C	20	ALA	N	1.722
20	ALA	C	21	VAL	N	-1.028
21	VAL	C	22	ASP	N	-1.952
22	ASP	C	23	ALA	N	0.950
23	ALA	C	24	GLU	N	-0.274
27	GLU	C	28	LYS	N	-1.928
28	LYS	C	29	ALA	N	0.528
30	PHE	C	31	LYS	N	1.348
31	LYS	C	32	GLN	N	-1.522
32	GLN	C	33	TYR	N	1.216
33	TYR	C	34	ALA	N	1.898
34	ALA	C	35	ASN	N	-0.472
35	ASN	C	36	ASP	N	-0.618
36	ASP	C	37	ASN	N	1.366
37	ASN	C	38	GLY	N	1.742
38	GLY	C	39	VAL	N	-0.444
42	VAL	C	43	TRP	N	-2.984
43	TRP	C	44	THR	N	0.968
44	THR	C	45	TYR	N	-0.594
45	TYR	C	46	ASP	N	0.940
46	ASP	C	47	ASP	N	-0.402
47	ASP	C	48	ALA	N	-0.194
48	ALA	C	49	THR	N	-0.868
49	THR	C	50	LYS	N	0.326
50	LYS	C	51	THR	N	-2.602
51	THR	C	52	PHE	N	1.666
52	PHE	C	53	THR	N	-1.054
53	THR	C	54	VAL	N	0.352
54	VAL	C	55	THR	N	0.076
55	THR	C	56	GLU	N	-0.386

2	GLN	CA	2	GLN	HA	29.248
3	TYR	CA	3	TYR	HA	36.404
4	LYS	CA	4	LYS	HA	41.096
5	LEU	CA	5	LEU	HA	42.639
6	VAL	CA	6	VAL	HA	37.904
7	ILE	CA	7	ILE	HA	26.974
8	ASN	CA	8	ASN	HA	23.801
9	GLY	CA	9	GLY	HA#	54.500
12	LEU	CA	12	LEU	HA	30.329
13	LYS	CA	13	LYS	HA	26.588
14	GLY	CA	14	GLY	HA#	54.760
15	GLU	CA	15	GLU	HA	34.267
16	THR	CA	16	THR	HA	33.305
17	THR	CA	17	THR	HA	39.254
18	THR	CA	18	THR	HA	41.240
19	LYS	CA	19	LYS	HA	31.762
20	ALA	CA	20	ALA	HA	10.636
21	VAL	CA	21	VAL	HA	9.944
22	ASP	CA	22	ASP	HA	27.710

23	ALA	CA	23	ALA	HA	19.491
27	GLU	CA	27	GLU	HA	-34.244
28	LYS	CA	28	LYS	HA	-20.276
29	ALA	CA	29	ALA	HA	32.192
30	PHE	CA	30	PHE	HA	33.187
31	LYS	CA	31	LYS	HA	-51.346
32	GLN	CA	32	GLN	HA	4.506
33	TYR	CA	33	TYR	HA	42.230
34	ALA	CA	34	ALA	HA	-3.207
35	ASN	CA	35	ASN	HA	-41.750
36	ASP	CA	36	ASP	HA	24.039
37	ASN	CA	37	ASN	HA	37.686
38	GLY	CA	38	GLY	HA#	-1.692
42	VAL	CA	42	VAL	HA	6.185
43	TRP	CA	43	TRP	HA	27.419
44	THR	CA	44	THR	HA	23.599
45	TYR	CA	45	TYR	HA	37.344
46	ASP	CA	46	ASP	HA	40.329
47	ASP	CA	47	ASP	HA	30.267
48	ALA	CA	48	ALA	HA	-56.646
49	THR	CA	49	THR	HA	-3.485
50	LYS	CA	50	LYS	HA	23.735
51	THR	CA	51	THR	HA	34.829
52	PHE	CA	52	PHE	HA	43.214
53	THR	CA	53	THR	HA	39.814
54	VAL	CA	54	VAL	HA	36.424
55	THR	CA	55	THR	HA	29.428
3	TYR	HN	3	TYR	N	17.168
4	LYS	HN	4	LYS	N	21.874
5	LEU	HN	5	LEU	N	20.181
6	VAL	HN	6	VAL	N	17.237
7	ILE	HN	7	ILE	N	16.428
8	ASN	HN	8	ASN	N	5.470
9	GLY	HN	9	GLY	N	12.408
12	LEU	HN	12	LEU	N	16.178
13	LYS	HN	13	LYS	N	15.896
14	GLY	HN	14	GLY	N	19.671
15	GLU	HN	15	GLU	N	19.811
16	THR	HN	16	THR	N	21.622
17	THR	HN	17	THR	N	21.296
18	THR	HN	18	THR	N	19.770
19	LYS	HN	19	LYS	N	19.137
20	ALA	HN	20	ALA	N	12.772
21	VAL	HN	21	VAL	N	14.060
22	ASP	HN	22	ASP	N	7.346
23	ALA	HN	23	ALA	N	10.892
28	LYS	HN	28	LYS	N	-20.215
29	ALA	HN	29	ALA	N	-2.426
30	PHE	HN	30	PHE	N	0.908
31	LYS	HN	31	LYS	N	-18.406
32	GLN	HN	32	GLN	N	-20.754
33	TYR	HN	33	TYR	N	-6.338
34	ALA	HN	34	ALA	N	-5.420
35	ASN	HN	35	ASN	N	-23.762
36	ASP	HN	36	ASP	N	-15.885
38	GLY	HN	38	GLY	N	-20.376

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   42    VAL     HN    42    VAL      N   -11.010
   43    TRP     HN    43    TRP      N    12.075
   44    THR     HN    44    THR      N    18.342
   45    TYR     HN    45    TYR      N    19.799
   46    ASP     HN    46    ASP      N    20.868
   47    ASP     HN    47    ASP      N    15.362
   48    ALA     HN    48    ALA      N   -10.992
   49    THR     HN    49    THR      N    -2.067
   50    LYS     HN    50    LYS      N    19.409
   51    THR     HN    51    THR      N    21.409
   52    PHE     HN    52    PHE      N    18.507
   53    THR     HN    53    THR      N    16.459
   54    VAL     HN    54    VAL      N    15.767
   55    THR     HN    55    THR      N     9.279

excluded couplings
#   10    LYS      C    10    LYS     CA     3.795
#   11    THR      C    11    THR     CA    -2.830
#   24    GLU      C    24    GLU     CA     3.502
#   25    THR      C    25    THR     CA    -2.526
#   26    ALA      C    26    ALA     CA    -2.976
#   39    VAL      C    39    VAL     CA     1.869
#   40    ASP      C    40    ASP     CA     1.813
#   41    GLY      C    41    GLY     CA     0.338

#   10    LYS      C    11    THR      N    -0.012
#   11    THR      C    12    LEU      N    -1.896
#   24    GLU      C    25    THR      N    -1.320
#   25    THR      C    26    ALA      N     1.084
#   26    ALA      C    27    GLU      N     1.820
#   39    VAL      C    40    ASP      N    -0.262
#   40    ASP      C    41    GLY      N     0.222
#   41    GLY      C    42    VAL      N     1.784

#   10    LYS     CA    10    LYS     HA    18.139
#   11    THR     CA    11    THR     HA   -23.085
#   24    GLU     CA    24    GLU     HA   -52.233
#   25    THR     CA    25    THR     HA    25.500
#   26    ALA     CA    26    ALA     HA    41.889
#   39    VAL     CA    39    VAL     HA   -59.692
#   40    ASP     CA    40    ASP     HA   -56.871
#   41    GLY     CA    41    GLY     HA#  -22.020

#   10    LYS     HN    10    LYS      N     5.028
#   11    THR     HN    11    THR      N    -7.451
#   24    GLU     HN    24    GLU      N   -13.218
#   26    ALA     HN    26    ALA      N     7.253
#   39    VAL     HN    39    VAL      N   -26.871
#   40    ASP     HN    40    ASP      N   -25.108
#   41    GLY     HN    41    GLY      N   -22.136
#   56    GLU     HN    56    GLU      N    13.482
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Medium B (PEG)

2	GLN	C	2	GLN	CA	-0.668
3	TYR	C	3	TYR	CA	-1.119
4	LYS	C	4	LYS	CA	-2.096
5	LEU	C	5	LEU	CA	-0.356
6	VAL	C	6	VAL	CA	-2.366
7	ILE	C	7	ILE	CA	-1.245
8	ASN	C	8	ASN	CA	-2.399
9	GLY	C	9	GLY	CA	-1.891
12	LEU	C	12	LEU	CA	0.003
13	LYS	C	13	LYS	CA	-1.538
14	GLY	C	14	GLY	CA	-1.414
15	GLU	C	15	GLU	CA	0.218
16	THR	C	16	THR	CA	-1.506
17	THR	C	17	THR	CA	0.815
18	THR	C	18	THR	CA	-2.669
19	LYS	C	19	LYS	CA	1.710
20	ALA	C	20	ALA	CA	-0.999
21	VAL	C	21	VAL	CA	2.162
22	ASP	C	22	ASP	CA	-3.228
23	ALA	C	23	ALA	CA	-0.822
27	GLU	C	27	GLU	CA	0.415
28	LYS	C	28	LYS	CA	2.127
29	ALA	C	29	ALA	CA	-1.752
30	PHE	C	30	PHE	CA	-2.436
31	LYS	C	31	LYS	CA	1.240
32	GLN	C	32	GLN	CA	1.045
33	TYR	C	33	TYR	CA	-2.868
34	ALA	C	34	ALA	CA	-1.379
35	ASN	C	35	ASN	CA	2.113
36	ASP	C	36	ASP	CA	-0.038
37	ASN	C	37	ASN	CA	-1.703
38	GLY	C	38	GLY	CA	1.854
42	VAL	C	42	VAL	CA	-2.529
43	TRP	C	43	TRP	CA	0.578
44	THR	C	44	THR	CA	-2.334
45	TYR	C	45	TYR	CA	0.307
46	ASP	C	46	ASP	CA	-2.944
47	ASP	C	47	ASP	CA	-0.043
48	ALA	C	48	ALA	CA	2.287
49	THR	C	49	THR	CA	1.483
50	LYS	C	50	LYS	CA	-1.928
51	THR	C	51	THR	CA	-0.942
52	PHE	C	52	PHE	CA	-1.691
53	THR	C	53	THR	CA	-1.022
54	VAL	C	54	VAL	CA	-2.068
55	THR	C	55	THR	CA	-2.146

2	GLN	C	3	TYR	N	-1.216
3	TYR	C	4	LYS	N	-0.526
4	LYS	C	5	LEU	N	-0.690
5	LEU	C	6	VAL	N	-0.088
6	VAL	C	7	ILE	N	0.050
7	ILE	C	8	ASN	N	0.600
8	ASN	C	9	GLY	N	1.006

9	GLY	C	10	LYS	N	-1.232
12	LEU	C	13	LYS	N	0.032
13	LYS	C	14	GLY	N	-1.096
14	GLY	C	15	GLU	N	-1.266
15	GLU	C	16	THR	N	-0.114
16	THR	C	17	THR	N	-0.838
17	THR	C	18	THR	N	-0.286
18	THR	C	19	LYS	N	-0.556
19	LYS	C	20	ALA	N	0.938
20	ALA	C	21	VAL	N	0.600
21	VAL	C	22	ASP	N	-1.600
22	ASP	C	23	ALA	N	0.840
23	ALA	C	24	GLU	N	0.754
27	GLU	C	28	LYS	N	0.146
28	LYS	C	29	ALA	N	-0.318
30	PHE	C	31	LYS	N	1.102
31	LYS	C	32	GLN	N	-0.228
32	GLN	C	33	TYR	N	0.200
33	TYR	C	34	ALA	N	1.160
34	ALA	C	35	ASN	N	0.622
35	ASN	C	36	ASP	N	-0.586
36	ASP	C	37	ASN	N	0.978
37	ASN	C	38	GLY	N	1.126
38	GLY	C	39	VAL	N	-1.030
42	VAL	C	43	TRP	N	-1.152
43	TRP	C	44	THR	N	-0.168
44	THR	C	45	TYR	N	-0.788
45	TYR	C	46	ASP	N	0.224
46	ASP	C	47	ASP	N	0.050
47	ASP	C	48	ALA	N	0.670
48	ALA	C	49	THR	N	-1.290
49	THR	C	50	LYS	N	0.984
50	LYS	C	51	THR	N	-1.112
51	THR	C	52	PHE	N	0.208
52	PHE	C	53	THR	N	-0.974
53	THR	C	54	VAL	N	-0.314
54	VAL	C	55	THR	N	-0.102
55	THR	C	56	GLU	N	-0.264

2	GLN	CA	2	GLN	HA	12.017
3	TYR	CA	3	TYR	HA	14.734
4	LYS	CA	4	LYS	HA	22.676
5	LEU	CA	5	LEU	HA	23.759
6	VAL	CA	6	VAL	HA	22.100
7	ILE	CA	7	ILE	HA	19.873
8	ASN	CA	8	ASN	HA	19.539
9	GLY	CA	9	GLY	HA#	36.970
12	LEU	CA	12	LEU	HA	21.038
13	LYS	CA	13	LYS	HA	19.835
14	GLY	CA	14	GLY	HA#	32.850
15	GLU	CA	15	GLU	HA	19.452
16	THR	CA	16	THR	HA	17.231
17	THR	CA	17	THR	HA	21.852
18	THR	CA	18	THR	HA	22.756
19	LYS	CA	19	LYS	HA	15.474
20	ALA	CA	20	ALA	HA	13.703
21	VAL	CA	21	VAL	HA	-8.593

22	ASP	CA	22	ASP	HA	4.420
23	ALA	CA	23	ALA	HA	18.319
27	GLU	CA	27	GLU	HA	0.694
28	LYS	CA	28	LYS	HA	-23.575
29	ALA	CA	29	ALA	HA	11.731
30	PHE	CA	30	PHE	HA	22.091
31	LYS	CA	31	LYS	HA	-11.487
32	GLN	CA	32	GLN	HA	-15.368
33	TYR	CA	33	TYR	HA	20.755
34	ALA	CA	34	ALA	HA	12.615
35	ASN	CA	35	ASN	HA	-21.200
36	ASP	CA	36	ASP	HA	-0.657
37	ASN	CA	37	ASN	HA	16.711
38	GLY	CA	38	GLY	HA#	2.392
42	VAL	CA	42	VAL	HA	14.010
43	TRP	CA	43	TRP	HA	20.295
44	THR	CA	44	THR	HA	20.218
45	TYR	CA	45	TYR	HA	23.196
46	ASP	CA	46	ASP	HA	23.105
47	ASP	CA	47	ASP	HA	18.431
48	ALA	CA	48	ALA	HA	-31.788
49	THR	CA	49	THR	HA	-18.012
50	LYS	CA	50	LYS	HA	18.733
51	THR	CA	51	THR	HA	20.671
52	PHE	CA	52	PHE	HA	23.543
53	THR	CA	53	THR	HA	23.197
54	VAL	CA	54	VAL	HA	22.685
55	THR	CA	55	THR	HA	20.791
3	TYR	HN	3	TYR	N	8.878
4	LYS	HN	4	LYS	N	10.584
5	LEU	HN	5	LEU	N	11.162
6	VAL	HN	6	VAL	N	10.768
7	ILE	HN	7	ILE	N	8.784
8	ASN	HN	8	ASN	N	7.791
9	GLY	HN	9	GLY	N	5.210
12	LEU	HN	12	LEU	N	8.599
13	LYS	HN	13	LYS	N	9.598
14	GLY	HN	14	GLY	N	11.174
15	GLU	HN	15	GLU	N	11.160
16	THR	HN	16	THR	N	11.281
17	THR	HN	17	THR	N	10.417
18	THR	HN	18	THR	N	7.495
19	LYS	HN	19	LYS	N	6.883
20	ALA	HN	20	ALA	N	3.734
21	VAL	HN	21	VAL	N	5.021
22	ASP	HN	22	ASP	N	-1.665
23	ALA	HN	23	ALA	N	1.174
28	LYS	HN	28	LYS	N	-13.783
29	ALA	HN	29	ALA	N	-9.107
30	PHE	HN	30	PHE	N	-3.803
31	LYS	HN	31	LYS	N	-9.141
32	GLN	HN	32	GLN	N	-15.848
33	TYR	HN	33	TYR	N	-9.585
34	ALA	HN	34	ALA	N	-4.899
35	ASN	HN	35	ASN	N	-11.417
36	ASP	HN	36	ASP	N	-14.628

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   38    GLY     HN    38    GLY      N    -1.726
   42    VAL     HN    42    VAL      N     2.720
   43    TRP     HN    43    TRP      N     7.463
   44    THR     HN    44    THR      N    11.237
   45    TYR     HN    45    TYR      N    11.335
   46    ASP     HN    46    ASP      N    11.217
   47    ASP     HN    47    ASP      N     7.896
   48    ALA     HN    48    ALA      N    -6.654
   49    THR     HN    49    THR      N    -6.331
   50    LYS     HN    50    LYS      N    10.328
   51    THR     HN    51    THR      N    10.868
   52    PHE     HN    52    PHE      N    10.165
   53    THR     HN    53    THR      N    10.967
   54    VAL     HN    54    VAL      N     9.879
   55    THR     HN    55    THR      N     9.152

excluded couplings
#    1    MET      C     1    MET     CA    -1.825
#   10    LYS      C    10    LYS     CA     2.207
#   11    THR      C    11    THR     CA    -2.325
#   24    GLU      C    24    GLU     CA     1.293
#   25    THR      C    25    THR     CA     0.103
#   26    ALA      C    26    ALA     CA    -2.514
#   39    VAL      C    39    VAL     CA     1.772
#   40    ASP      C    40    ASP     CA     1.321
#   41    GLY      C    41    GLY     CA    -0.109

#    1    MET      C     2    GLN      N     0.568
#   10    LYS      C    11    THR      N     0.600
#   11    THR      C    12    LEU      N    -0.774
#   24    GLU      C    25    THR      N    -1.230
#   25    THR      C    26    ALA      N     0.686
#   26    ALA      C    27    GLU      N     0.898
#   39    VAL      C    40    ASP      N    -0.050
#   40    ASP      C    41    GLY      N    -0.596
#   41    GLY      C    42    VAL      N     0.910

#   1     MET     CA     1    MET     HA    -4.807
#   10    LYS     CA    10    LYS     HA    13.756
#   11    THR     CA    11    THR     HA     2.450
#   24    GLU     CA    24    GLU     HA   -26.790
#   25    THR     CA    25    THR     HA    -1.300
#   26    ALA     CA    26    ALA     HA    22.898
#   39    VAL     CA    39    VAL     HA   -23.490
#   40    ASP     CA    40    ASP     HA   -25.074
#   41    GLY     CA    41    GLY     HA#  -12.140

#   10    LYS     HN    10    LYS      N     6.090
#   11    THR     HN    11    THR      N     3.032
#   24    GLU     HN    24    GLU      N    -9.867
#   26    ALA     HN    26    ALA      N    -2.407
#   39    VAL     HN    39    VAL      N   -10.420
#   40    ASP     HN    40    ASP      N    -6.234
#   41    GLY     HN    41    GLY      N    -6.378
#   56    GLU     HN    56    GLU      N     8.291
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Medium C (Pf1 phage)

2	GLN	C	2	GLN	CA	4.257
3	TYR	C	3	TYR	CA	-1.986
4	LYS	C	4	LYS	CA	5.443
5	LEU	C	5	LEU	CA	-1.664
6	VAL	C	6	VAL	CA	3.479
7	ILE	C	7	ILE	CA	0.067
8	ASN	C	8	ASN	CA	2.472
9	GLY	C	9	GLY	CA	0.227
12	LEU	C	12	LEU	CA	-2.137
13	LYS	C	13	LYS	CA	5.354
14	GLY	C	14	GLY	CA	-1.435
15	GLU	C	15	GLU	CA	0.814
16	THR	C	16	THR	CA	-1.437
17	THR	C	17	THR	CA	-2.215
18	THR	C	18	THR	CA	-0.076
19	LYS	C	19	LYS	CA	-1.695
20	ALA	C	20	ALA	CA	-1.508
21	VAL	C	21	VAL	CA	0.389
22	ASP	C	22	ASP	CA	2.703
23	ALA	C	23	ALA	CA	0.426
27	GLU	C	27	GLU	CA	-2.558
28	LYS	C	28	LYS	CA	-2.154
29	ALA	C	29	ALA	CA	0.348
30	PHE	C	30	PHE	CA	4.765
31	LYS	C	31	LYS	CA	-3.308
32	GLN	C	32	GLN	CA	-2.472
33	TYR	C	33	TYR	CA	3.782
34	ALA	C	34	ALA	CA	0.238
35	ASN	C	35	ASN	CA	-2.560
36	ASP	C	36	ASP	CA	-1.487
37	ASN	C	37	ASN	CA	4.592
38	GLY	C	38	GLY	CA	-1.976
42	VAL	C	42	VAL	CA	5.090
43	TRP	C	43	TRP	CA	-2.883
44	THR	C	44	THR	CA	5.853
45	TYR	C	45	TYR	CA	-2.561
46	ASP	C	46	ASP	CA	4.740
47	ASP	C	47	ASP	CA	1.580
48	ALA	C	48	ALA	CA	-1.084
49	THR	C	49	THR	CA	-2.953
50	LYS	C	50	LYS	CA	-1.010
51	THR	C	51	THR	CA	4.045
52	PHE	C	52	PHE	CA	-0.720
53	THR	C	53	THR	CA	2.402
54	VAL	C	54	VAL	CA	-0.041
55	THR	C	55	THR	CA	3.011
2	GLN	C	3	TYR	N	1.084
3	TYR	C	4	LYS	N	1.268
4	LYS	C	5	LEU	N	-0.954
5	LEU	C	6	VAL	N	1.106
6	VAL	C	7	ILE	N	-1.562
7	ILE	C	8	ASN	N	1.758
8	ASN	C	9	GLY	N	-1.514

9	GLY	C	10	LYS	N	1.506
12	LEU	C	13	LYS	N	0.896
13	LYS	C	14	GLY	N	-0.416
14	GLY	C	15	GLU	N	2.704
15	GLU	C	16	THR	N	-0.978
16	THR	C	17	THR	N	1.720
17	THR	C	18	THR	N	-1.286
18	THR	C	19	LYS	N	0.858
19	LYS	C	20	ALA	N	-1.568
20	ALA	C	21	VAL	N	-1.566
21	VAL	C	22	ASP	N	2.992
22	ASP	C	23	ALA	N	0.618
23	ALA	C	24	GLU	N	-1.200
27	GLU	C	28	LYS	N	-0.594
28	LYS	C	29	ALA	N	2.416
30	PHE	C	31	LYS	N	-0.522
31	LYS	C	32	GLN	N	1.640
32	GLN	C	33	TYR	N	0.370
33	TYR	C	34	ALA	N	-0.146
34	ALA	C	35	ASN	N	-1.280
35	ASN	C	36	ASP	N	2.896
36	ASP	C	37	ASN	N	-1.340
37	ASN	C	38	GLY	N	0.664
38	GLY	C	39	VAL	N	-0.212
42	VAL	C	43	TRP	N	-0.660
43	TRP	C	44	THR	N	1.136
44	THR	C	45	TYR	N	-0.844
45	TYR	C	46	ASP	N	1.404
46	ASP	C	47	ASP	N	-1.384
47	ASP	C	48	ALA	N	-1.210
48	ALA	C	49	THR	N	-0.274
49	THR	C	50	LYS	N	-0.994
50	LYS	C	51	THR	N	2.212
51	THR	C	52	PHE	N	-1.346
52	PHE	C	53	THR	N	2.714
53	THR	C	54	VAL	N	-1.484
54	VAL	C	55	THR	N	2.454
55	THR	C	56	GLU	N	-1.560

2	GLN	CA	2	GLN	HA	-30.753
3	TYR	CA	3	TYR	HA	-30.549
4	LYS	CA	4	LYS	HA	-14.304
5	LEU	CA	5	LEU	HA	-9.886
6	VAL	CA	6	VAL	HA	-3.219
7	ILE	CA	7	ILE	HA	-7.028
8	ASN	CA	8	ASN	HA	-11.673
9	GLY	CA	9	GLY	HA#	-14.710
12	LEU	CA	12	LEU	HA	-10.696
13	LYS	CA	13	LYS	HA	-16.938
14	GLY	CA	14	GLY	HA#	-32.380
15	GLU	CA	15	GLU	HA	6.533
16	THR	CA	16	THR	HA	12.711
17	THR	CA	17	THR	HA	-1.616
18	THR	CA	18	THR	HA	-7.219
19	LYS	CA	19	LYS	HA	-29.553
20	ALA	CA	20	ALA	HA	-18.181
21	VAL	CA	21	VAL	HA	27.473

22	ASP	CA	22	ASP	HA	-19.749
23	ALA	CA	23	ALA	HA	-20.083
27	GLU	CA	27	GLU	HA	-18.974
28	LYS	CA	28	LYS	HA	55.162
29	ALA	CA	29	ALA	HA	-29.428
30	PHE	CA	30	PHE	HA	-16.442
31	LYS	CA	31	LYS	HA	7.185
32	GLN	CA	32	GLN	HA	30.856
33	TYR	CA	33	TYR	HA	-22.753
34	ALA	CA	34	ALA	HA	-22.876
35	ASN	CA	35	ASN	HA	44.819
36	ASP	CA	36	ASP	HA	-9.526
37	ASN	CA	37	ASN	HA	-27.666
38	GLY	CA	38	GLY	HA#	-26.938
42	VAL	CA	42	VAL	HA	-18.492
43	TRP	CA	43	TRP	HA	-9.169
44	THR	CA	44	THR	HA	-14.323
45	TYR	CA	45	TYR	HA	-13.291
46	ASP	CA	46	ASP	HA	-3.639
47	ASP	CA	47	ASP	HA	-22.235
48	ALA	CA	48	ALA	HA	14.762
49	THR	CA	49	THR	HA	43.515
50	LYS	CA	50	LYS	HA	-7.877
51	THR	CA	51	THR	HA	-9.700
52	PHE	CA	52	PHE	HA	-9.535
53	THR	CA	53	THR	HA	-3.820
54	VAL	CA	54	VAL	HA	-9.270
55	THR	CA	55	THR	HA	-8.267
3	TYR	HN	3	TYR	N	-12.720
4	LYS	HN	4	LYS	N	-10.641
5	LEU	HN	5	LEU	N	1.384
6	VAL	HN	6	VAL	N	-6.942
7	ILE	HN	7	ILE	N	4.445
8	ASN	HN	8	ASN	N	-9.344
9	GLY	HN	9	GLY	N	15.914
12	LEU	HN	12	LEU	N	-1.390
13	LYS	HN	13	LYS	N	-9.651
14	GLY	HN	14	GLY	N	-4.878
15	GLU	HN	15	GLU	N	-5.053
16	THR	HN	16	THR	N	-7.263
17	THR	HN	17	THR	N	-12.536
18	THR	HN	18	THR	N	-15.558
19	LYS	HN	19	LYS	N	-13.134
20	ALA	HN	20	ALA	N	-11.090
21	VAL	HN	21	VAL	N	-12.548
22	ASP	HN	22	ASP	N	-11.591
23	ALA	HN	23	ALA	N	-15.371
28	LYS	HN	28	LYS	N	2.314
29	ALA	HN	29	ALA	N	-3.031
30	PHE	HN	30	PHE	N	-10.815
31	LYS	HN	31	LYS	N	-4.414
32	GLN	HN	32	GLN	N	7.091
33	TYR	HN	33	TYR	N	-4.535
34	ALA	HN	34	ALA	N	-9.864
35	ASN	HN	35	ASN	N	-0.132
36	ASP	HN	36	ASP	N	2.161

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   38    GLY     HN    38    GLY      N    -6.736
   42    VAL     HN    42    VAL      N   -11.635
   43    TRP     HN    43    TRP      N    -1.462
   44    THR     HN    44    THR      N    -6.081
   45    TYR     HN    45    TYR      N     0.637
   46    ASP     HN    46    ASP      N    -8.182
   47    ASP     HN    47    ASP      N    11.084
   48    ALA     HN    48    ALA      N    22.294
   49    THR     HN    49    THR      N    24.224
   50    LYS     HN    50    LYS      N    -7.604
   51    THR     HN    51    THR      N   -10.406
   52    PHE     HN    52    PHE      N     2.713
   53    THR     HN    53    THR      N    -5.031
   54    VAL     HN    54    VAL      N    -1.318
   55    THR     HN    55    THR      N    -9.796

excluded couplings
#   10    LYS      C    10    LYS     CA    -1.624
#   11    THR      C    11    THR     CA     5.840
#   24    GLU      C    24    GLU     CA    -3.326
#   25    THR      C    25    THR     CA    -2.260
#   26    ALA      C    26    ALA     CA     5.963
#   39    VAL      C    39    VAL     CA    -1.464
#   40    ASP      C    40    ASP     CA    -1.453
#   41    GLY      C    41    GLY     CA    -2.599

#   10    LYS      C    11    THR      N    -0.200
#   11    THR      C    12    LEU      N    -0.772
#   24    GLU      C    25    THR      N     2.694
#   25    THR      C    26    ALA      N    -1.338
#   26    ALA      C    27    GLU      N     0.172
#   39    VAL      C    40    ASP      N     1.462
#   40    ASP      C    41    GLY      N    -1.408
#   41    GLY      C    42    VAL      N    -1.544

#   10    LYS     CA    10    LYS     HA   -22.415
#   11    THR     CA    11    THR     HA   -19.399
#   24    GLU     CA    24    GLU     HA    42.271
#   25    THR     CA    25    THR     HA     0.500
#   26    ALA     CA    26    ALA     HA   -10.082
#   39    VAL     CA    39    VAL     HA    18.405
#   40    ASP     CA    40    ASP     HA    14.973
#   41    GLY     CA    41    GLY     HA#   42.270

#   10    LYS     HN    10    LYS      N    -9.728
#   11    THR     HN    11    THR      N   -11.940
#   24    GLU     HN    24    GLU      N    -2.619
#   26    ALA     HN    26    ALA      N   -10.897
#   39    VAL     HN    39    VAL      N    15.549
#   40    ASP     HN    40    ASP      N    -2.658
#   41    GLY     HN    41    GLY      N     5.299
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Medium D (negatively charged polyacrylamide gel)

2	GLN	C	2	GLN	CA	3.557
3	TYR	C	3	TYR	CA	-3.761
4	LYS	C	4	LYS	CA	3.170
5	LEU	C	5	LEU	CA	-2.637
6	VAL	C	6	VAL	CA	1.092
7	ILE	C	7	ILE	CA	-1.567
8	ASN	C	8	ASN	CA	0.222
9	GLY	C	9	GLY	CA	-2.496
12	LEU	C	12	LEU	CA	-2.306
13	LYS	C	13	LYS	CA	3.188
14	GLY	C	14	GLY	CA	-3.692
15	GLU	C	15	GLU	CA	1.132
16	THR	C	16	THR	CA	-3.966
17	THR	C	17	THR	CA	-1.043
18	THR	C	18	THR	CA	-3.291
19	LYS	C	19	LYS	CA	0.419
20	ALA	C	20	ALA	CA	-3.543
21	VAL	C	21	VAL	CA	2.381
22	ASP	C	22	ASP	CA	-1.749
23	ALA	C	23	ALA	CA	0.098
27	GLU	C	27	GLU	CA	-1.802
28	LYS	C	28	LYS	CA	-0.165
29	ALA	C	29	ALA	CA	-2.287
30	PHE	C	30	PHE	CA	2.133
31	LYS	C	31	LYS	CA	-1.787
32	GLN	C	32	GLN	CA	-1.490
33	TYR	C	33	TYR	CA	0.204
34	ALA	C	34	ALA	CA	-0.762
35	ASN	C	35	ASN	CA	-0.379
36	ASP	C	36	ASP	CA	-2.552
37	ASN	C	37	ASN	CA	2.830
38	GLY	C	38	GLY	CA	0.104
42	VAL	C	42	VAL	CA	2.270
43	TRP	C	43	TRP	CA	-2.329
44	THR	C	44	THR	CA	3.125
45	TYR	C	45	TYR	CA	-1.725
46	ASP	C	46	ASP	CA	0.681
47	ASP	C	47	ASP	CA	2.284
48	ALA	C	48	ALA	CA	1.188
49	THR	C	49	THR	CA	-0.895
50	LYS	C	50	LYS	CA	-3.442
51	THR	C	51	THR	CA	3.662
52	PHE	C	52	PHE	CA	-3.241
53	THR	C	53	THR	CA	1.615
54	VAL	C	54	VAL	CA	-2.523
55	THR	C	55	THR	CA	0.824

2	GLN	C	3	TYR	N	-0.282
3	TYR	C	4	LYS	N	0.562
4	LYS	C	5	LEU	N	-1.986
5	LEU	C	6	VAL	N	1.236
6	VAL	C	7	ILE	N	-1.790
7	ILE	C	8	ASN	N	2.318
8	ASN	C	9	GLY	N	-0.594

9	GLY	C	10	LYS	N	0.348
12	LEU	C	13	LYS	N	1.370
13	LYS	C	14	GLY	N	-1.890
14	GLY	C	15	GLU	N	1.538
15	GLU	C	16	THR	N	-1.608
16	THR	C	17	THR	N	0.674
17	THR	C	18	THR	N	-1.918
18	THR	C	19	LYS	N	0.080
19	LYS	C	20	ALA	N	-0.828
20	ALA	C	21	VAL	N	-1.022
21	VAL	C	22	ASP	N	1.058
22	ASP	C	23	ALA	N	1.376
23	ALA	C	24	GLU	N	-0.516
27	GLU	C	28	LYS	N	-0.776
28	LYS	C	29	ALA	N	2.158
30	PHE	C	31	LYS	N	0.712
31	LYS	C	32	GLN	N	1.134
32	GLN	C	33	TYR	N	0.700
33	TYR	C	34	ALA	N	1.086
34	ALA	C	35	ASN	N	-0.542
35	ASN	C	36	ASP	N	2.254
36	ASP	C	37	ASN	N	-0.236
37	ASN	C	38	GLY	N	1.744
38	GLY	C	39	VAL	N	-1.642
42	VAL	C	43	TRP	N	-1.854
43	TRP	C	44	THR	N	1.324
44	THR	C	45	TYR	N	-1.994
45	TYR	C	46	ASP	N	1.738
46	ASP	C	47	ASP	N	-1.564
47	ASP	C	48	ALA	N	-0.490
49	THR	C	50	LYS	N	0.036
50	LYS	C	51	THR	N	0.922
51	THR	C	52	PHE	N	-1.054
52	PHE	C	53	THR	N	1.932
53	THR	C	54	VAL	N	-2.008
54	VAL	C	55	THR	N	2.410
55	THR	C	56	GLU	N	-2.142

2	GLN	CA	2	GLN	HA	-13.014
3	TYR	CA	3	TYR	HA	-12.086
4	LYS	CA	4	LYS	HA	11.765
5	LEU	CA	5	LEU	HA	16.081
6	VAL	CA	6	VAL	HA	21.995
7	ILE	CA	7	ILE	HA	17.504
8	ASN	CA	8	ASN	HA	11.796
9	GLY	CA	9	GLY	HA#	28.990
12	LEU	CA	12	LEU	HA	13.394
13	LYS	CA	13	LYS	HA	4.464
14	GLY	CA	14	GLY	HA#	9.803
15	GLU	CA	15	GLU	HA	31.001
16	THR	CA	16	THR	HA	35.424
17	THR	CA	17	THR	HA	23.698
18	THR	CA	18	THR	HA	18.721
19	LYS	CA	19	LYS	HA	-8.793
20	ALA	CA	20	ALA	HA	-0.009
21	VAL	CA	21	VAL	HA	23.351
22	ASP	CA	22	ASP	HA	-9.447

23	ALA	CA	23	ALA	HA	0.387
27	GLU	CA	27	GLU	HA	-21.934
28	LYS	CA	28	LYS	HA	30.026
29	ALA	CA	29	ALA	HA	-12.347
30	PHE	CA	30	PHE	HA	6.836
31	LYS	CA	31	LYS	HA	-9.116
32	GLN	CA	32	GLN	HA	18.209
33	TYR	CA	33	TYR	HA	1.079
34	ALA	CA	34	ALA	HA	-9.747
35	ASN	CA	35	ASN	HA	19.389
36	ASP	CA	36	ASP	HA	-5.320
37	ASN	CA	37	ASN	HA	-11.430
38	GLY	CA	38	GLY	HA#	-25.541
42	VAL	CA	42	VAL	HA	-0.258
43	TRP	CA	43	TRP	HA	14.742
44	THR	CA	44	THR	HA	8.327
45	TYR	CA	45	TYR	HA	12.458
46	ASP	CA	46	ASP	HA	22.070
47	ASP	CA	47	ASP	HA	-0.320
48	ALA	CA	48	ALA	HA	-25.743
49	THR	CA	49	THR	HA	26.771
50	LYS	CA	50	LYS	HA	16.038
51	THR	CA	51	THR	HA	13.743
52	PHE	CA	52	PHE	HA	16.933
53	THR	CA	53	THR	HA	22.748
54	VAL	CA	54	VAL	HA	16.989
55	THR	CA	55	THR	HA	16.716
3	TYR	HN	3	TYR	N	-2.449
4	LYS	HN	4	LYS	N	1.166
5	LEU	HN	5	LEU	N	14.249
6	VAL	HN	6	VAL	N	3.957
7	ILE	HN	7	ILE	N	16.308
8	ASN	HN	8	ASN	N	-1.247
9	GLY	HN	9	GLY	N	22.454
12	LEU	HN	12	LEU	N	10.887
13	LYS	HN	13	LYS	N	0.741
14	GLY	HN	14	GLY	N	7.872
16	THR	HN	16	THR	N	5.804
17	THR	HN	17	THR	N	0.284
18	THR	HN	18	THR	N	-6.629
19	LYS	HN	19	LYS	N	-4.832
20	ALA	HN	20	ALA	N	-4.900
21	VAL	HN	21	VAL	N	-4.989
22	ASP	HN	22	ASP	N	-14.821
23	ALA	HN	23	ALA	N	-15.514
28	LYS	HN	28	LYS	N	-16.343
29	ALA	HN	29	ALA	N	-14.487
30	PHE	HN	30	PHE	N	-17.627
31	LYS	HN	31	LYS	N	-18.509
32	GLN	HN	32	GLN	N	-13.004
33	TYR	HN	33	TYR	N	-16.955
34	ALA	HN	34	ALA	N	-17.732
36	ASP	HN	36	ASP	N	-15.581
37	ASN	HN	37	ASN	N	-13.956
38	GLY	HN	38	GLY	N	-10.461
42	VAL	HN	42	VAL	N	-8.638

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   43    TRP     HN    43    TRP      N     9.458
   44    THR     HN    44    THR      N     7.018
   46    ASP     HN    46    ASP      N     4.863
   47    ASP     HN    47    ASP      N    19.872
   48    ALA     HN    48    ALA      N    14.253
   49    THR     HN    49    THR      N    18.689
   50    LYS     HN    50    LYS      N     2.469
   51    THR     HN    51    THR      N     1.331
   52    PHE     HN    52    PHE      N    14.862
   53    THR     HN    53    THR      N     6.394
   54    VAL     HN    54    VAL      N    11.351
   55    THR     HN    55    THR      N     0.023

excluded couplings
#   10    LYS      C    10    LYS     CA     0.821
#   11    THR      C    11    THR     CA     2.649
#   24    GLU      C    24    GLU     CA    -1.004
#   25    THR      C    25    THR     CA    -2.694
#   26    ALA      C    26    ALA     CA     2.057
#   39    VAL      C    39    VAL     CA     0.261
#   40    ASP      C    40    ASP     CA     0.165
#   41    GLY      C    41    GLY     CA    -3.256

#   10    LYS      C    11    THR      N     0.458
#   11    THR      C    12    LEU      N    -1.822
#   24    GLU      C    25    THR      N     1.714
#   25    THR      C    26    ALA      N    -0.418
#   26    ALA      C    27    GLU      N     1.446
#   39    VAL      C    40    ASP      N     1.476
#   40    ASP      C    41    GLY      N    -1.784
#   41    GLY      C    42    VAL      N    -0.474

#    1    MET     CA     1    MET     HA    21.041
#   10    LYS     CA    10    LYS     HA    -4.172
#   11    THR     CA    11    THR     HA   -17.839
#   24    GLU     CA    24    GLU     HA     9.113
#   25    THR     CA    25    THR     HA     3.429
#   26    ALA     CA    26    ALA     HA    15.209
#   39    VAL     CA    39    VAL     HA   -12.620
#   40    ASP     CA    40    ASP     HA   -18.765
#   41    GLY     CA    41    GLY     HA#   30.559

#   10    LYS     HN    10    LYS      N    -0.844
#   11    THR     HN    11    THR      N    -8.303
#   24    GLU     HN    24    GLU      N   -17.036
#   26    ALA     HN    26    ALA      N   -15.210
#   39    VAL     HN    39    VAL      N     1.750
#   40    ASP     HN    40    ASP      N   -11.245
#   41    GLY     HN    41    GLY      N    -4.503
#   56    GLU     HN    56    GLU      N    13.341
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Medium E (positively charged polyacrylamide gel)

2	GLN	C	2	GLN	CA	-2.088
3	TYR	C	3	TYR	CA	-0.699
4	LYS	C	4	LYS	CA	-1.676
5	LEU	C	5	LEU	CA	-2.524
6	VAL	C	6	VAL	CA	-0.591
7	ILE	C	7	ILE	CA	-3.685
8	ASN	C	8	ASN	CA	0.072
9	GLY	C	9	GLY	CA	-3.076
12	LEU	C	12	LEU	CA	3.499
13	LYS	C	13	LYS	CA	-2.713
14	GLY	C	14	GLY	CA	-0.078
15	GLU	C	15	GLU	CA	-1.805
16	THR	C	16	THR	CA	0.415
17	THR	C	17	THR	CA	-1.440
18	THR	C	18	THR	CA	0.178
19	LYS	C	19	LYS	CA	-0.361
20	ALA	C	20	ALA	CA	2.106
21	VAL	C	21	VAL	CA	1.172
22	ASP	C	22	ASP	CA	-3.042
23	ALA	C	23	ALA	CA	1.366
27	GLU	C	27	GLU	CA	3.243
28	LYS	C	28	LYS	CA	2.297
29	ALA	C	29	ALA	CA	-3.576
30	PHE	C	30	PHE	CA	-1.041
31	LYS	C	31	LYS	CA	3.893
32	GLN	C	32	GLN	CA	-0.343
33	TYR	C	33	TYR	CA	-4.089
34	ALA	C	34	ALA	CA	1.765
35	ASN	C	35	ASN	CA	3.473
36	ASP	C	36	ASP	CA	-2.071
37	ASN	C	37	ASN	CA	-3.170
38	GLY	C	38	GLY	CA	2.337
42	VAL	C	42	VAL	CA	-1.652
43	TRP	C	43	TRP	CA	4.246
44	THR	C	44	THR	CA	-2.653
45	TYR	C	45	TYR	CA	3.557
46	ASP	C	46	ASP	CA	-3.612
47	ASP	C	47	ASP	CA	0.420
48	ALA	C	48	ALA	CA	2.088
49	THR	C	49	THR	CA	2.097
50	LYS	C	50	LYS	CA	1.248
51	THR	C	51	THR	CA	-0.927
52	PHE	C	52	PHE	CA	-2.394
53	THR	C	53	THR	CA	0.443
54	VAL	C	54	VAL	CA	-3.452
55	THR	C	55	THR	CA	0.123
2	GLN	C	3	TYR	N	0.282
3	TYR	C	4	LYS	N	-1.846
4	LYS	C	5	LEU	N	1.178
5	LEU	C	6	VAL	N	-1.138
6	VAL	C	7	ILE	N	1.486
7	ILE	C	8	ASN	N	-0.256
8	ASN	C	9	GLY	N	2.272

9	GLY	C	10	LYS	N	-0.076
12	LEU	C	13	LYS	N	-0.184
13	LYS	C	14	GLY	N	-0.240
14	GLY	C	15	GLU	N	-1.916
15	GLU	C	16	THR	N	-0.900
16	THR	C	17	THR	N	-2.150
17	THR	C	18	THR	N	0.108
18	THR	C	19	LYS	N	-2.016
19	LYS	C	20	ALA	N	1.878
20	ALA	C	21	VAL	N	-0.998
21	VAL	C	22	ASP	N	-1.422
22	ASP	C	23	ALA	N	0.138
23	ALA	C	24	GLU	N	-0.556
27	GLU	C	28	LYS	N	-1.506
28	LYS	C	29	ALA	N	-0.408
30	PHE	C	31	LYS	N	0.022
31	LYS	C	32	GLN	N	-1.460
32	GLN	C	33	TYR	N	0.600
33	TYR	C	34	ALA	N	1.018
34	ALA	C	35	ASN	N	-0.700
35	ASN	C	36	ASP	N	-1.284
36	ASP	C	37	ASN	N	0.984
37	ASN	C	38	GLY	N	0.172
38	GLY	C	39	VAL	N	0.918
42	VAL	C	43	TRP	N	-1.432
43	TRP	C	44	THR	N	0.126
44	THR	C	45	TYR	N	0.960
45	TYR	C	46	ASP	N	-0.204
46	ASP	C	47	ASP	N	0.510
47	ASP	C	48	ALA	N	-0.342
48	ALA	C	49	THR	N	0.630
49	THR	C	50	LYS	N	-0.284
50	LYS	C	51	THR	N	-2.066
51	THR	C	52	PHE	N	2.038
52	PHE	C	53	THR	N	-1.590
53	THR	C	54	VAL	N	1.468
54	VAL	C	55	THR	N	-0.908
55	THR	C	56	GLU	N	1.338

2	GLN	CA	2	GLN	HA	27.943
3	TYR	CA	3	TYR	HA	35.052
4	LYS	CA	4	LYS	HA	28.758
5	LEU	CA	5	LEU	HA	24.381
6	VAL	CA	6	VAL	HA	15.878
7	ILE	CA	7	ILE	HA	7.264
8	ASN	CA	8	ASN	HA	6.016
9	GLY	CA	9	GLY	HA#	23.708
12	LEU	CA	12	LEU	HA	12.875
13	LYS	CA	13	LYS	HA	14.494
14	GLY	CA	14	GLY	HA#	29.293
15	GLU	CA	15	GLU	HA	9.201
16	THR	CA	16	THR	HA	5.095
17	THR	CA	17	THR	HA	21.154
18	THR	CA	18	THR	HA	23.391
19	LYS	CA	19	LYS	HA	29.109
20	ALA	CA	20	ALA	HA	6.991
21	VAL	CA	21	VAL	HA	-1.679

22	ASP	CA	22	ASP	HA	25.020
23	ALA	CA	23	ALA	HA	8.538
27	GLU	CA	27	GLU	HA	-24.919
28	LYS	CA	28	LYS	HA	-22.814
29	ALA	CA	29	ALA	HA	30.398
30	PHE	CA	30	PHE	HA	18.634
31	LYS	CA	31	LYS	HA	-36.756
32	GLN	CA	32	GLN	HA	-0.927
33	TYR	CA	33	TYR	HA	34.939
34	ALA	CA	34	ALA	HA	-8.558
35	ASN	CA	35	ASN	HA	-35.709
36	ASP	CA	36	ASP	HA	21.381
37	ASN	CA	37	ASN	HA	37.140
38	GLY	CA	38	GLY	HA#	2.507
42	VAL	CA	42	VAL	HA	-5.519
43	TRP	CA	43	TRP	HA	7.284
44	THR	CA	44	THR	HA	9.185
45	TYR	CA	45	TYR	HA	21.276
46	ASP	CA	46	ASP	HA	21.746
47	ASP	CA	47	ASP	HA	24.770
48	ALA	CA	48	ALA	HA	-26.343
49	THR	CA	49	THR	HA	-10.572
50	LYS	CA	50	LYS	HA	3.608
51	THR	CA	51	THR	HA	22.599
52	PHE	CA	52	PHE	HA	25.207
53	THR	CA	53	THR	HA	18.763
54	VAL	CA	54	VAL	HA	16.600
55	THR	CA	55	THR	HA	9.544
3	TYR	HN	3	TYR	N	15.140
4	LYS	HN	4	LYS	N	18.345
5	LEU	HN	5	LEU	N	8.644
6	VAL	HN	6	VAL	N	10.578
7	ILE	HN	7	ILE	N	1.981
8	ASN	HN	8	ASN	N	0.314
9	GLY	HN	9	GLY	N	-0.347
12	LEU	HN	12	LEU	N	5.219
13	LYS	HN	13	LYS	N	10.723
14	GLY	HN	14	GLY	N	10.128
16	THR	HN	16	THR	N	12.925
17	THR	HN	17	THR	N	16.826
18	THR	HN	18	THR	N	19.034
19	LYS	HN	19	LYS	N	18.853
20	ALA	HN	20	ALA	N	12.745
21	VAL	HN	21	VAL	N	13.011
22	ASP	HN	22	ASP	N	16.357
23	ALA	HN	23	ALA	N	17.196
28	LYS	HN	28	LYS	N	-4.470
29	ALA	HN	29	ALA	N	9.454
30	PHE	HN	30	PHE	N	12.013
31	LYS	HN	31	LYS	N	-3.259
32	GLN	HN	32	GLN	N	-5.652
33	TYR	HN	33	TYR	N	7.249
34	ALA	HN	34	ALA	N	6.827
36	ASP	HN	36	ASP	N	-1.878
37	ASN	HN	37	ASN	N	15.613
38	GLY	HN	38	GLY	N	-13.673

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   42    VAL     HN    42    VAL      N    -9.537
   43    TRP     HN    43    TRP      N     0.143
   44    THR     HN    44    THR      N     8.604
   45    TYR     HN    45    TYR      N     9.521
   46    ASP     HN    46    ASP      N    14.096
   47    ASP     HN    47    ASP      N     3.498
   48    ALA     HN    48    ALA      N   -13.468
   49    THR     HN    49    THR      N    -8.976
   50    LYS     HN    50    LYS      N    14.134
   51    THR     HN    51    THR      N    17.133
   52    PHE     HN    52    PHE      N     8.868
   53    THR     HN    53    THR      N     8.133
   54    VAL     HN    54    VAL      N     3.354
   55    THR     HN    55    THR      N     3.381

excluded couplings
#   10    LYS      C    10    LYS     CA     1.788
#   11    THR      C    11    THR     CA    -2.574
#   24    GLU      C    24    GLU     CA     2.713
#   25    THR      C    25    THR     CA    -1.328
#   26    ALA      C    26    ALA     CA    -1.819
#   39    VAL      C    39    VAL     CA     0.670
#   40    ASP      C    40    ASP     CA     1.390
#   41    GLY      C    41    GLY     CA     1.990

#   10    LYS      C    11    THR      N    -0.098
#   11    THR      C    12    LEU      N    -0.564
#   24    GLU      C    25    THR      N    -1.724
#   25    THR      C    26    ALA      N     0.626
#   26    ALA      C    27    GLU      N     0.402
#   39    VAL      C    40    ASP      N    -0.824
#   40    ASP      C    41    GLY      N    -0.158
#   41    GLY      C    42    VAL      N     1.396

#   10    LYS     CA    10    LYS     HA    13.896
#   11    THR     CA    11    THR     HA   -16.749
#   24    GLU     CA    24    GLU     HA   -39.239
#   25    THR     CA    25    THR     HA    15.789
#   26    ALA     CA    26    ALA     HA    26.731
#   39    VAL     CA    39    VAL     HA   -37.990
#   40    ASP     CA    40    ASP     HA   -32.065
#   41    GLY     CA    41    GLY     HA#  -33.644

#   10    LYS     HN    10    LYS      N    -1.895
#   11    THR     HN    11    THR      N    -7.125
#   24    GLU     HN    24    GLU      N     0.695
#   26    ALA     HN    26    ALA      N    15.966
#   39    VAL     HN    39    VAL      N   -20.068
#   40    ASP     HN    40    ASP      N   -15.864
#   41    GLY     HN    41    GLY      N   -14.876
#   56    GLU     HN    56    GLU      N     1.151
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