Electronic Supplementary Material (ESI) for Molecular BioSystems.

Table A Range of variation in all parameters of rotamers for χ_1 amino acids within 400 triplets. Ranking for each amino acid is based on its number of low frequencies.

	Conf. type	Range of Frequency	Low Freq.	RFs' range	Range of variation in χ_1 angle averages	Range of variations in SDs
CYS	***g-***	10 – 167	22	0.29 - 0.84	-72.8 - -57.1	3.93 - 17.35
	t	10 – 92	75	0.1 - 0.57	-167.9 - 175.2	5.13 - 17.04
	g+	10 - 102	132	0.08 - 0.43	52.5 - 72.7	1.94 - 20.25
SER	***g+***	11 - 792	1	0.27 - 0.64	61.5 - 70	5.14 - 13.83
	g-	12 - 480	2	0.14 - 0.48	-69 - -57.4	5.41 - 16.85
	t	10 - 384	5	0.11 - 0.49	-169.8 - 173.4	6.06 - 18.14
THR	***g+***	10 - 865	1	0.25 - 0.77	55.8 - 64.9	5.06 - 16.94
	g-	13 - 820	2	0.16 - 0.71	-64.7 - -55.1	3.91 - 13.92
	t	10 - 137	61	0.03 - 0.25	-164.7 - 174.1	3.76 - 24.6
VAL	***t***	16 - 1369	0	0.52 - 0.9	172.6 - 179.8	4.69 - 10.1
	g-	10 - 405	9	0.07 - 0.37	-65.4 - -57.2	3.65 - 21.08
	g+	10 - 153	44	0.03 - 0.25	52.6 - 70.5	3.42 - 25.68
PRO	***g+***	10 - 560	2	0.23 - 0.8	22.8 - 30.4	3.98 - 11.44
	g-	10 - 739	3	0.29 - 0.77	-28.3 - -21.3	4.77 - 9.79
	t	0 – 0	400	0 - 0	0 - 0	0 - 0

Table B Range of variation in all parameters of rotamers for χ_{1+2} amino acids within 400 triplets; numbers have been rounded with two decimal then a 0.00 could be a 0.004. Rows has been ranked based on the number of low frequency rotamers.

	Conf. type	Range of Freq.	Low Freq.	RFs' Range	Range of variation in χ angle averages(χ°)		Range of variations in SDs	
					χ_1	χ_2	χ_1	χ_2
LEU	***g-t***	17 - 1582	0	0.41 - 0.79	-71.86 - -60.49	171.05 - 179.28	6 - 13	6.3 - 13.5
	tg+	14 - 827	1	0.14 - 0.45	-171.01 - 172.97	58.94 - 68.36	6.4 - 14.5	5.5 - 15.6
	g-g+	10 - 97	73	0.02 - 0.13	-99.3 - -65.87	33.48 - 77.68	6.4 - 20.8	9.1 - 34
	tt	10 - 96	120	0.01 - 0.09	-176.98 - -150.68	-170.28 - 153.24	5.5 - 30.6	4.3 - 36
	g-g-	10 - 31	318	0.01 - 0.03	-92.79 - -74.26	-69.91 - -41.74	3.7 - 20.4	4.5 - 31.8
	g+g+	10 - 32	333	0.01 - 0.03	53.85 - 71.85	70.95 - 89.75	5.6 - 18.2	4.4 - 23.8
	tg-	10 - 20	377	0.00(4) - 0.02	-178.21 - -159.96	-80.27 - -64.01	5.2 - 21.7	9.2 - 28.8
	g+t	10 - 14	382	0.01 - 0.03	62.7 - 79.1	153.36 - 177.25	4.1 - 21	5.8 - 20.5
ILE	***g-t***	16 - 1065	1	0.34 - 0.77	-67.16 - -59.1	165.81 - 172.94	3.6 - 10	5.9 - 11.9
	g-g-	10 - 205	15	0.08 - 0.25	-66.34 - -53.73	-67.03 - -53.8	4 - 13.3	3.5 - 17.1
	g+t	10 - 235	40	0.04 - 0.35	49.03 - 67.91	165.13 - 177.27	3.2 - 16	4.1 - 16.5
	tt	10 - 107	91	0.02 - 0.24	-161.83 - 175.81	156.21 - 176.01	3.1 - 21.3	3.7 - 17.2
	tg+	10 - 59	209	0.01 - 0.11	-174.49 - -157.93	60.23 - 75.28	4.7 - 23.1	2.8 - 18.8
	g-g+	10 - 32	291	0.01 - 0.05	-78.98 - -57.72	65.05 - 95.33	5.8 - 24.7	6.8 - 33.7
	g+g+	10 - 18	390	0.01 - 0.03	52.48 - 65.34	77.53 - 96.89	5.9 - 15	10.4 - 16.7
PHE	***tg+***	10 - 490	11	0.13 - 0.57	-167.33 - 175.15	57.78 - 84.03	6 - 15.5	8.9 - 26.9
	g-g-	11 - 327	11	0.13 - 0.55	-72.2 - -58.07	-87.23 - -57.28	5.8 - 19.2	13.2 - 32
	g-g+	10 - 174	27	0.07 - 0.36	-77.07 - -60.4	63.24 - 95.23	5.9 - 17.5	6.4 - 36.9
	g+g+	10 - 100	123	0.03 - 0.25	48.37 - 71.86	80.85 - 94.6	3.8 - 17	3.3 - 18.4
	tg-	10 - 68	167	0.02 - 0.18	-161.77 - 171.3	-100.79 - -62.98	4.9 - 20.5	4.8 - 37
	g+g-	10 - 48	214	0.01 - 0.19	51.93 - 73.86	-92.87 - -74.36	4.5 - 18.2	3.7 - 22.6
	g-t	10 - 24	300	0.01 - 0.07	-76.46 - -58.6	-176.64 - 130.62	5.1 - 18.4	8 - 39.7
	tt	11 - 15	397	0.01 - 0.03	-179.62 - -168.94	-174.01 - -149	10.4 - 15.1	21.4 - 38
TRP	***g-g+***	10 - 117	62	0.16 - 0.69	-76.1 - -59.28	64.01 - 105.21	5.3 - 16.2	8.5 - 45
	tg+	10 - 158	146	0.07 - 0.55	-169 - 171.83	44.25 - 88.29	2.6 - 20.9	3.7 - 36.4
	tg-	10 - 56	156	0.06 - 0.41	-164.15 - 176.23	-109.06 - -68.19	4 - 18.7	5.6 - 45.3
	g-g-	10 - 76	178	0.06 - 0.42	-77.33 - -58.01	-78.85 - -10.95	3.1 - 17.9	6.8 - 44.8
	g+g-	10 - 55	224	0.05 - 0.46	47.51 - 73.15	-99.09 - -70.45	2.3 - 19.3	3.2 - 36.6
	g+g+	10 - 29	336	0.04 - 0.26	44.61 - 72.17	62.91 - 94.68	2.3 - 15.7	3.6 - 34

Table B. (Continued)

	Conf. type	Range of Freq.	Low Freq.	RFs' Range	Range of variation in χ angle averages (χ°)		Range of variations in SDs	
					χ_1		χ_2	
TRP	***g-t***	10 - 16	393	0.03 - 0.14	-76.54 - -56.75	125.67 - 165.81	8.7 - 20	4.2 - 47.8
	tt	11 - 12	397	0.04 - 0.06	-178.52 - -171.95	-127.94 - -124.25	9.4 - 16.4	2.7 - 5.4
TYR	***tg+***	10 - 384	6	0.09 - 0.73	-168.41 - 173.98	64.44 - 85.22	4.6 - 16	8.6 - 24.9
	g-g-	10 - 330	10	0.16 - 0.6	-72.03 - -58.81	-88.64 - -53.29	5 - 15.5	9 - 36.1
	g-g+	10 - 142	25	0.08 - 0.31	-76.44 - -58.81	71.86 - 96.01	3.9 - 17.9	6.6 - 36.1
	g+g+	10 - 73	119	0.02 - 0.31	48.36 - 70.83	72 - 98.02	5 - 18.8	4.7 - 26.9
	tg-	10 - 53	174	0.03 - 0.14	-164.93 - 176.46	-99.87 - -68.63	3.8 - 20.9	5.4 - 34.1
	g+g-	10 - 39	223	0.02 - 0.11	51.29 - 75.05	-92.9 - -71.29	3.9 - 18.5	3 - 23.5
	g-t	10 - 25	335	0.02 - 0.08	-78.19 - -60.01	136.36 - 171.67	4.1 - 19.4	10.4 - 40.4
ASN	***g-g-***	10 - 440	5	0.14 - 0.58	-75.72 - -61.46	-63.81 - -28.77	5.5 - 13.8	13.8 - 29.5
	tg+	10 - 195	31	0.06 - 0.31	-177.9 - -159.51	19.77 - 59.88	6 - 18.6	9.3 - 37.5
	tg-	10 - 186	58	0.04 - 0.51	-179.16 - -161.66	-74.95 - -28.7	5.5 - 21.6	19.5 - 47.3
	g-t	10 - 93	98	0.03 - 0.19	-80.58 - -59.69	131.92 - 170.1	2.9 - 19.3	9.3 - 36.2
	g-g+	10 - 77	104	0.03 - 0.19	-79.6 - -47.25	29.39 - 105.78	6.2 - 24.4	10.6 - 48.7
	g+g+	10 - 94	105	0.02 - 0.24	55.64 - 68.97	20.29 - 67.44	3.2 - 16.9	12.6 - 37.3
	g+g-	10 - 79	143	0.02 - 0.19	56.53 - 73.36	-63.61 - -12.99	3.9 - 19.7	8.3 - 37.9
	tt	10 - 41	260	0.01 - 0.08	-177.14 - -156.75	-139.79 - 167.35	5.3 - 22	12.5 - 42.9
	g+t	10 - 14	389	0.01 - 0.04	59.27 - 68.76	-163.05 - 162.23	4.7 - 21.6	13.8 - 38.4
HIS	***g-g-***	10 - 218	20	0.16 - 0.54	-72.79 - -52.86	-94.12 - -56.83	5.5 - 19.4	8.6 - 29.6
	tg+	10 - 139	66	0.07 - 0.37	-167.68 - 172.42	58.07 - 94.53	3.8 - 18.2	7.5 - 31.5
	g-g+	10 - 116	83	0.07 - 0.32	-74.7 - -56.67	68.88 - 105.29	3.8 - 17.4	9.4 - 34.1
	g-t	10 - 78	120	0.04 - 0.23	-75.51 - -59.46	-155.64 - 142.88	4.3 - 15.3	7.8 - 39.5
	tg-	10 - 127	125	0.04 - 0.42	-165.28 - 177.79	-99.08 - -72.49	3.4 - 21.7	8.2 - 34.3
	g+g-	10 - 72	211	0.03 - 0.34	57.39 - 76.99	-99.44 - -66.51	4.9 - 18.5	4.6 - 26.2
	tt	10 - 47	266	0.03 - 0.22	-157.41 - 179.48	-136.35 - 160.77	3.9 - 18.4	15.2 - 41.1
	g+g+	10 - 54	291	0.03 - 0.22	54.27 - 78.88	70.5 - 96.48	3.8 - 18.2	6.8 - 23.6
ASP	***g-g-***	10 - 784	0	0.07 - 0.62	-73.98 - -63.69	-43.63 - -18.11	4.7 - 14	10.7 - 28.1
	tg+	10 - 387	13	0.07 - 0.33	-179.41 - -165.28	21.63 - 62.35	5.9 - 16.3	12.9 - 37.2
	tg-	10 - 364	26	0.03 - 0.5	-178.83 - -149.9	-58.07 - -12.86	5.4 - 22.5	9.2 - 42.5
	g+g-	10 - 227	74	0.02 - 0.22	54.16 - 76.57	-66.09 - -11.73	4.3 - 19	9.7 - 47
	g+g+	10 - 257	83	0.02 - 0.27	50.14 - 71.6	10.8 - 47.04	3.1 - 23	6.6 - 40.4
	g-g+	10 - 84	105	0.02 - 0.13	-83.64 - -60.16	5.26 - 75.82	5 - 21.4	4.5 - 48.7
	g-t	10 - 84	144	0.01 - 0.2	-80.6 - -63.16	147.97 - 178.54	3.6 - 18.6	7.9 - 31.9
	tt	10 - 58	225	0.01 - 0.1	-178.56 - -154.78	-156.15 - 161.56	5 - 20.7	14.3 - 39.6
	g+t	10 - 49	297	0.01 - 0.08	53.02 - 71.36	-162.88 - 157.2	2.5 - 19.9	8.7 - 39.9

Table C Range of variation in all parameters of rotamers for χ_{1+2+3} amino acids within 400 triplets; Rows has been ranked based on the number of low frequency rotamers.

	Conf. type	Range of Freq.	Low Freq.	RFs' range	Range of variation in chi angle averages($\chi°$)			Range of variations in SDs		
					χ_1	χ_2	χ_3	χ_1	χ_2	χ_3
MET	***g-tg+***	10 - 92	103	0.07 - 0.41	-72 - -58	-175 - 168	58 - 82	3 - 17	6 - 19	4 - 27
	g-g-g-	10 - 92	105	0.06 - 0.44	-77 - -55	-70 - -53	-77 - -58	4 - 15	3 - 18	5 - 19
	g-tg-	10 - 61	165	0.06 - 0.27	-79 - -55	-168 - 173	-84 - -60	4 - 19	4 - 22	6 - 27
	g-tt	10 - 40	224	0.05 - 0.15	-74 - -60	-161 - 172	-166 - 170	3 - 20	5 - 22	8 - 28
	ttg+	10 - 46	253	0.04 - 0.29	-167 - 175	-154 - 170	61 - 83	4 - 20	4 - 23	3 - 24
	ttg-	10 - 38	262	0.03 - 0.19	-166 - 175	-173 - 171	-80 - -57	5 - 20	4 - 20	7 - 27
	tg+g+	10 - 38	276	0.04 - 0.23	-165 - 179	54 - 72	57 - 83	4 - 18	3 - 16	6 - 23
	g-g-g+	10 - 29	350	0.03 - 0.14	-70 - -58	-76 - -56	91 - 105	3 - 19	5 - 23	5 - 28
	g-g-t	10 - 23	351	0.03 - 0.11	-72 - -57	-72 - -54	-165 - 154	5 - 15	4 - 17	12 - 33
	ttt	10 - 19	357	0.03 - 0.15	-165 - 176	-169 - 168	-169 - 160	3 - 22	4 - 24	12 - 31
	g+tg+	10 - 18	387	0.03 - 0.1	62 - 70	-170 - 177	63 - 80	6 - 17	6 - 17	11 - 22
	tg-g-	10 - 24	389	0.03 - 0.13	-164 - 173	-91 - -82	-82 - -66	3 - 21	2 - 9	5 - 19
	g+tg-	10 - 12	392	0.03 - 0.13	61 - 82	-172 - 174	-75 - -58	5 - 17	5 - 12	5 - 20
	tg+t	10 - 12	396	0.03 - 0.04	-173 - -167	63 - 71	-168 - 176	9 - 16	7 - 14	18 - 34
	g+tt	10 - 12	398	0.04 - 0.05	65 - 71	-176 - 177	-175 - 174	10 - 11	5 - 12	18 - 21
	tg+g-	10 - 10	399	0.04 - 0.04	-168 - -168	66 - 66	-102 - -102	8 - 8	4 - 4	5 - 5
GLU	***g-tg-***	10 - 386	12	0.07 - 0.34	-72 - -59	-170 - 170	-59 - -20	4 - 20	7 - 21	14 - 37
	g-tg+	10 - 270	19	0.07 - 0.24	-74 - -60	-173 - 171	20 - 67	5 - 16	7 - 22	14 - 38
	g-g-g-	10 - 203	24	0.06 - 0.32	-76 - -58	-71 - -54	-52 - -23	4 - 18	4 - 22	12 - 33
	ttg+	10 - 218	39	0.04 - 0.2	-169 - 177	-175 - 167	16 - 63	4 - 22	5 - 24	13 - 38
	ttg-	10 - 198	40	0.04 - 0.18	-168 - 176	-172 - 170	-57 - -16	5 - 21	5 - 21	8 - 40
	tg+g+	10 - 152	94	0.03 - 0.15	-166 - 170	58 - 72	15 - 53	5 - 22	5 - 21	11 - 34
	g-tt	10 - 91	125	0.02 - 0.14	-76 - -57	-166 - 169	-162 - 165	4 - 18	6 - 27	8 - 38
	ttt	10 - 68	183	0.01 - 0.07	-168 - 174	-173 - 169	-161 - 162	4 - 25	6 - 26	9 - 37
	g-g+g+	10 - 138	184	0.01 - 0.18	-80 - -56	64 - 86	16 - 53	4 - 29	4 - 25	9 - 34
	g-g-g+	10 - 50	208	0.01 - 0.06	-74 - -56	-85 - -61	19 - 86	5 - 25	5 - 27	15 - 47
	g+tg-	10 - 46	208	0.01 - 0.12	54 - 74	-165 - 174	-72 - -17	5 - 24	5 - 25	13 - 41
	g+tg+	10 - 52	210	0.01 - 0.07	53 - 75	-165 - 169	18 - 73	6 - 22	5 - 25	16 - 38
	g-g+g-	10 - 88	231	0.01 - 0.08	-77 - -55	77 - 95	-56 - -13	3 - 23	2 - 28	10 - 44
	g-g-t	10 - 41	261	0.01 - 0.05	-80 - -56	-77 - -59	134 - 178	4 - 27	5 - 21	9 - 35
	tg-g-	10 - 45	317	0.01 - 0.05	-156 - 180	-92 - -75	-52 - -21	5 - 25	3 - 22	11 - 28
	tg+g-	10 - 36	319	0.01 - 0.08	-163 - 170	64 - 85	-73 - -19	6 - 28	6 - 24	17 - 44

Table C. (Continued)

	Conf. type	Range of Freq.	Low Freq.	RFs' range	Range of variation in chi angle averages(χ°)			Range of variations in SDs		
					χ_1	χ_2	χ_3	χ_1	χ_2	χ_3
GLU	***g+g-g+***	10 - 117	329	0.01 - 0.13	58 - 75	-97 - -77	14 - 45	5 - 24	4 - 18	10 - 39
	tg+t	10 - 34	335	0.01 - 0.03	-162 - 176	61 - 82	-179 - -148	6 - 23	6 - 18	11 - 36
	g+tt	10 - 22	360	0.01 - 0.04	57 - 74	-168 - 170	-158 - 159	7 - 21	7 - 27	19 - 37
	g+g-g-	10 - 31	375	0.01 - 0.05	42 - 72	-83 - -62	-62 - -18	7 - 26	6 - 17	13 - 35
	g-g+t	10 - 30	376	0.01 - 0.04	-78 - -58	73 - 85	-157 - 172	6 - 23	6 - 15	11 - 33
	g+g-t	11 - 19	392	0.02 - 0.02	52 - 70	-90 - -78	-164 - 174	10 - 19	6 - 12	12 - 32
	tg-t	10 - 11	398	0.01 - 0.01	-170 - -167	-85 - -85	156 - 171	13 - 21	10 - 16	19 - 22
GLN	***g-tg-***	10 - 260	26	0.06 - 0.36	-72 - -60	-168 - 170	-67 - -22	4 - 17	6 - 24	12 - 43
	g-tg+	10 - 182	45	0.05 - 0.29	-72 - -60	-172 - 168	25 - 70	3 - 18	7 - 21	10 - 40
	g-g-g-	10 - 161	58	0.07 - 0.32	-72 - -56	-75 - -56	-64 - -31	5 - 19	5 - 23	9 - 27
	ttg+	10 - 107	99	0.03 - 0.17	-168 - 168	-171 - 166	28 - 63	4 - 24	6 - 22	7 - 44
	ttg-	10 - 83	105	0.04 - 0.17	-166 - 177	-171 - 167	-72 - -18	4 - 20	5 - 28	9 - 43
	tg+g+	10 - 126	122	0.03 - 0.2	-165 - 175	53 - 75	29 - 67	4 - 22	4 - 18	9 - 28
	g-tt	10 - 51	188	0.02 - 0.18	-75 - -58	-168 - 171	-152 - 152	3 - 19	6 - 23	14 - 44
	g-g-g+	10 - 40	222	0.02 - 0.11	-77 - -54	-83 - -59	48 - 103	4 - 22	6 - 23	15 - 49
	g-g-t	10 - 30	309	0.01 - 0.06	-72 - -55	-74 - -54	133 - 164	5 - 21	5 - 20	9 - 41
	ttt	10 - 38	311	0.01 - 0.08	-157 - 175	-170 - 165	-159 - 154	3 - 20	6 - 25	17 - 43
	g+tg-	10 - 24	318	0.01 - 0.09	48 - 74	-168 - 169	-81 - -28	3 - 21	3 - 23	13 - 41
	g+tg+	10 - 44	327	0.01 - 0.08	55 - 76	-168 - 170	29 - 76	5 - 21	5 - 22	18 - 38
	g-g+g+	10 - 44	332	0.01 - 0.14	-79 - -60	69 - 83	26 - 60	4 - 21	3 - 23	11 - 28
	tg+g-	10 - 25	354	0.01 - 0.08	-163 - 174	52 - 85	-100 - -47	6 - 21	3 - 22	4 - 49
	tg+t	10 - 19	374	0.01 - 0.03	-165 - 177	60 - 73	-163 - -139	5 - 20	4 - 21	13 - 42
	g-g+g-	10 - 29	377	0.01 - 0.09	-73 - -56	72 - 95	-71 - -26	4 - 21	3 - 25	9 - 43
	tg-g-	10 - 19	384	0.01 - 0.03	-165 - 178	-91 - -75	-43 - -26	5 - 18	5 - 24	12 - 25
	g+g-g+	10 - 21	385	0.02 - 0.08	62 - 78	-93 - -84	28 - 50	4 - 11	3 - 10	9 - 27
	g+g+g+	11 - 11	399	0.05 - 0.05	59 - 59	80 - 80	48 - 48	9 - 9	7 - 7	19 - 19
	g+g-g-	12 - 12	399	0.03 - 0.03	76 - 76	-69 - -69	-19 - -19	6 - 6	4 - 4	15 - 15
	g+tt	10 - 10	399	0.01 - 0.01	60 - 60	-179 - -179	150 - 150	22 - 22	20 - 20	24 - 24

Table D Range of variations within the $\chi_{1+2+3+4}$ amino acids, numbers were have been rounded for two decimal.

	Conf. type	Range of Freq.	Low Freq.	RFs' range	Range of variation in χ angle averages				Range of variations in SDs			
					χ_1	χ_2	χ_3	χ_4	χ_1	χ_2	χ_3	χ_4
ARG	***g-ttt***	10 - 169	52	0.05 - 0.27	-77 - -55	-167 - 173	-167 - 172	-166 - 159	4 - 18	6 - 26	6 - 22	9 - 33
	g-ttg-	10 - 106	110	0.03 - 0.14	-76 - -58	-169 - 167	-166 - 174	-95 - -74	4 - 17	4 - 19	5 - 25	4 - 24
	g-tg+t	10 - 121	111	0.03 - 0.13	-74 - -58	-161 - 168	57 - 78	-158 - 168	3 - 21	7 - 28	6 - 23	6 - 31
	g-tg-t	10 - 106	125	0.02 - 0.16	-80 - -59	-165 - 167	-81 - -58	-151 - 154	4 - 24	6 - 26	6 - 26	6 - 36
	tttt	10 - 83	127	0.02 - 0.24	-168 - 169	-173 - 167	-170 - 170	-164 - 163	4 - 20	4 - 25	5 - 26	11 - 35
	g-tg-g-	10 - 132	129	0.02 - 0.13	-78 - -58	-161 - 174	-81 - -56	-97 - -79	4 - 21	4 - 22	4 - 24	3 - 20
	g-ttg+	10 - 85	136	0.02 - 0.14	-75 - -60	-170 - 166	-162 - 168	76 - 98	4 - 16	7 - 26	5 - 25	5 - 29
	g-tg+g+	10 - 57	165	0.02 - 0.08	-75 - -57	-169 - 167	53 - 76	74 - 97	5 - 19	6 - 25	3 - 23	4 - 24
	ttg-t	10 - 69	203	0.02 - 0.08	-167 - 175	-169 - 156	-80 - -54	-173 - 142	5 - 21	6 - 33	7 - 27	11 - 38
	ttg+t	10 - 168	214	0.02 - 0.18	-160 - 178	-167 - 163	57 - 77	-151 - 171	5 - 20	8 - 26	6 - 28	12 - 36
	ttg+g+	10 - 88	216	0.02 - 0.12	-168 - 176	-168 - 168	50 - 74	67 - 92	5 - 19	7 - 27	3 - 22	6 - 29
	tttg-	10 - 45	224	0.01 - 0.08	-166 - 174	-168 - 163	-165 - 171	-104 - -69	4 - 19	5 - 28	4 - 23	6 - 27
	g-g-tt	10 - 54	229	0.02 - 0.08	-73 - -49	-82 - -56	-164 - 170	-159 - 162	4 - 19	4 - 26	5 - 27	10 - 37
	ttg-g-	10 - 64	230	0.02 - 0.07	-166 - 172	-169 - 169	-76 - -54	-94 - -77	5 - 20	4 - 20	5 - 22	4 - 28
	tttg+	10 - 48	245	0.02 - 0.09	-167 - 177	-173 - 167	-172 - 169	68 - 97	5 - 19	4 - 25	4 - 24	3 - 28
	g-g-tg-	10 - 38	257	0.01 - 0.11	-68 - -59	-81 - -62	-163 - 177	-98 - -80	3 - 19	4 - 20	3 - 23	6 - 24
	g-g-g-g-	10 - 43	298	0.01 - 0.06	-70 - -55	-77 - -60	-72 - -51	-95 - -74	5 - 19	7 - 21	4 - 20	5 - 23
	g-g-g-t	10 - 38	302	0.01 - 0.05	-71 - -56	-83 - -51	-77 - -56	-176 - 151	4 - 22	7 - 28	7 - 24	9 - 36
	g+ttt	10 - 23	322	0.01 - 0.09	54 - 72	-169 - 167	-171 - 171	-163 - 164	5 - 21	3 - 22	5 - 29	8 - 31
	tg+tt	10 - 47	326	0.01 - 0.05	-168 - 172	59 - 80	-170 - 165	-172 - 158	4 - 22	4 - 20	4 - 23	10 - 32
	g+ttg+	10 - 32	330	0.01 - 0.07	55 - 74	-172 - 169	-175 - 167	75 - 102	3 - 17	6 - 19	2 - 21	4 - 26
	ttg-g+	10 - 37	336	0.01 - 0.05	-165 - 176	-171 - 172	-74 - -53	95 - 112	5 - 18	5 - 20	5 - 24	5 - 28
	g-tg-g+	10 - 37	337	0.01 - 0.07	-82 - -62	-167 - 177	-82 - -61	94 - 110	5 - 16	6 - 17	8 - 27	5 - 17
	ttg+g-	10 - 40	340	0.01 - 0.06	-169 - 179	-174 - 166	49 - 78	-111 - -92	4 - 18	3 - 23	8 - 30	5 - 31
	g+ttg-	10 - 26	341	0.01 - 0.15	55 - 72	-165 - 172	-168 - 173	-92 - -77	2 - 20	5 - 22	4 - 28	6 - 17
	g-g-tg+	10 - 26	344	0.01 - 0.06	-68 - -52	-79 - -60	-168 - 170	76 - 97	5 - 18	3 - 22	4 - 29	7 - 27
	tg+tg+	10 - 28	361	0.01 - 0.04	-176 - 170	59 - 73	-174 - 164	79 - 93	4 - 18	3 - 16	2 - 20	5 - 25
	tg+g+t	10 - 21	370	0.01 - 0.03	-173 - 176	58 - 79	58 - 76	-164 - 155	5 - 19	7 - 24	3 - 22	9 - 32
	g+tg+t	10 - 21	378	0.01 - 0.04	60 - 73	-165 - 167	61 - 75	-159 - 178	4 - 19	8 - 23	10 - 17	9 - 31
	g-tg+g-	10 - 21	381	0.01 - 0.03	-73 - -61	-170 - 172	49 - 79	-108 - -97	4 - 14	5 - 22	6 - 29	6 - 27
	tg+tg-	10 - 28	383	0.01 - 0.02	-173 - 172	61 - 75	-174 - 170	-97 - -78	5 - 15	7 - 14	6 - 26	8 - 27
	g+tg-t	10 - 19	385	0.01 - 0.04	57 - 70	-161 - 175	-78 - -62	-168 - 148	5 - 20	5 - 26	5 - 21	7 - 31
	tg+g+g+	10 - 19	386	0.01 - 0.02	-167 - 179	60 - 79	53 - 67	81 - 90	5 - 16	8 - 21	6 - 19	4 - 15
	g-g-g+t	10 - 18	397	0.01 - 0.02	-67 - -64	-75 - -70	80 - 83	-166 - -161	6 - 9	13 - 16	10 - 14	13 - 20
	g-g+tt	10 - 11	397	0.01 - 0.02	-93 - -73	64 - 76	-176 - 178	-174 - 176	9 - 14	11 - 27	13 - 16	7 - 16
	tg-tt	11 - 11	397	0.01 - 0.02	-172 - 179	-102 - -85	-163 - 168	-168 - 161	6 - 18	8 - 10	7 - 20	5 - 23
	tg+g-t	10 - 14	398	0.01 - 0.01	178 - 179	71 - 73	-84 - -80	169 - 178	7 - 11	5 - 7	11 - 12	9 - 19
	tg-g-g-	11 - 16	398	0.02 - 0.02	-175 - -174	-87 - -84	-50 - -48	-78 - -78	5 - 5	6 - 8	8 - 9	7 - 9

Table D. (Continued)

	Conf. type	Range of Freq.	Low Freq.	RFs' range	Range of variation in χ angle averages				Range of variations in SDs			
					χ_1	χ_2	χ_3	χ_4	χ_1	χ_2	χ_3	χ_4
ARG	***g+tg-g-***	10 - 11	398	0.01 - 0.02	60 - 62	-175 - 166	-66 - -62	-89 - -88	6 - 16	3 - 21	8 - 18	9 - 12
	g-g-g+g+	10 - 10	399	0.01 - 0.01	-66 - -66	-73 - -73	75 - 75	74 - 74	8 - 8	15 - 15	10 - 10	11 - 11
	g+tg+g+	13 - 13	399	0.02 - 0.02	60 - 60	176 - 176	62 - 62	85 - 85	9 - 9	11 - 11	12 - 12	9 - 9
	tg-g-t	12 - 12	399	0.01 - 0.01	-171 - -171	-91 - -91	-70 - -70	165 - 165	15 - 15	17 - 17	14 - 14	17 - 17
LYS	***g-ttt***	10 - 405	13	0.12 - 0.41	-74 - -60	-170 - 171	-171 - 174	-173 - 163	5 - 14	5 - 22	5 - 22	5 - 20
	tttt	10 - 253	34	0.06 - 0.29	-169 - 177	-171 - 170	-171 - 172	-170 - 173	4 - 18	6 - 22	4 - 19	7 - 23
	g-g-tt	10 - 157	95	0.03 - 0.19	-70 - -54	-76 - -59	-168 - 175	-170 - 174	4 - 18	5 - 21	5 - 22	5 - 22
	g-ttg-	10 - 111	116	0.03 - 0.11	-78 - -61	-170 - 174	-166 - 173	-78 - -56	3 - 20	6 - 21	5 - 23	7 - 27
	g-ttg+	10 - 91	133	0.02 - 0.12	-76 - -59	-168 - 171	-170 - 166	53 - 79	4 - 18	5 - 23	6 - 29	8 - 28
	g-tg+t	10 - 87	167	0.02 - 0.09	-78 - -61	-173 - 166	62 - 82	-170 - 167	5 - 22	5 - 25	7 - 23	6 - 25
	tttg+	10 - 81	168	0.02 - 0.1	-171 - 173	-175 - 168	-172 - 162	56 - 75	4 - 19	4 - 21	6 - 24	7 - 27
	g-tg-t	10 - 86	174	0.02 - 0.09	-76 - -61	-163 - 171	-83 - -56	-162 - 174	4 - 17	6 - 22	5 - 29	6 - 24
	tttg-	10 - 93	180	0.02 - 0.12	-166 - 171	-173 - 167	-161 - 172	-79 - -56	4 - 19	6 - 29	6 - 26	7 - 29
	g+ttt	10 - 65	185	0.01 - 0.11	54 - 73	-167 - 173	-169 - 168	-170 - 172	4 - 18	6 - 20	4 - 27	3 - 27
	tg+tt	10 - 70	225	0.01 - 0.13	-159 - 173	62 - 79	-168 - 164	-175 - 168	4 - 25	4 - 24	5 - 22	6 - 25
	ttg+t	10 - 58	240	0.01 - 0.07	-166 - 174	-171 - 161	62 - 86	-173 - 166	5 - 21	7 - 25	7 - 25	7 - 26
	g-g-tg-	10 - 41	247	0.01 - 0.06	-73 - -54	-83 - -56	-159 - 176	-80 - -56	5 - 22	5 - 21	7 - 28	6 - 29
	ttg-t	10 - 58	248	0.01 - 0.07	-164 - 177	-169 - 167	-81 - -59	-165 - 174	4 - 22	7 - 26	7 - 26	6 - 27
	g-g-tg+	10 - 40	277	0.01 - 0.06	-72 - -55	-80 - -57	-167 - 167	52 - 79	4 - 22	8 - 24	5 - 26	7 - 27
	g-g-g-t	10 - 31	320	0.01 - 0.04	-73 - -57	-76 - -50	-80 - -63	-168 - 173	3 - 19	8 - 23	6 - 23	6 - 25
	g-tg+g+	10 - 27	330	0.01 - 0.05	-79 - -60	-176 - 163	58 - 83	56 - 80	6 - 18	6 - 25	7 - 27	6 - 20
	g-tg-g-	10 - 111	350	0.01 - 0.11	-76 - -58	-165 - 175	-83 - -58	-77 - -57	4 - 18	3 - 27	7 - 25	5 - 23
	tg+tg+	10 - 29	360	0.01 - 0.03	-171 - 177	64 - 77	-176 - 161	56 - 73	6 - 22	5 - 23	6 - 23	6 - 25
	ttg+g+	10 - 24	374	0.01 - 0.04	-170 - 170	-172 - 165	64 - 83	58 - 82	6 - 24	8 - 22	7 - 27	6 - 25
	g+ttg+	10 - 37	374	0.01 - 0.07	60 - 71	-176 - 167	-174 - 160	55 - 73	4 - 15	7 - 20	7 - 20	6 - 24
	g+ttg-	10 - 24	379	0.01 - 0.07	57 - 69	-173 - 173	-163 - 174	-77 - -56	6 - 19	6 - 20	5 - 27	6 - 26
	tg+tg-	10 - 22	380	0.01 - 0.03	-168 - 178	64 - 78	-176 - 175	-80 - -50	6 - 18	4 - 25	9 - 23	6 - 27
	ttg-g-	10 - 20	381	0.01 - 0.02	-163 - 174	-168 - 172	-90 - -63	-83 - -63	7 - 21	7 - 25	13 - 23	7 - 25
	tg+g+t	10 - 21	384	0.01 - 0.02	-180 - -169	60 - 74	62 - 81	170 - 180	5 - 21	5 - 20	4 - 18	5 - 19
	g+tg-t	10 - 13	392	0.01 - 0.05	58 - 72	-167 - 174	-80 - -60	-171 - 167	4 - 16	9 - 16	6 - 21	10 - 24
	g-g+tt	10 - 15	392	0.01 - 0.02	-95 - -72	55 - 76	-172 - 171	-174 - 177	11 - 18	7 - 26	7 - 24	7 - 26
	g+tg+t	10 - 13	396	0.01 - 0.02	60 - 63	-178 - 167	68 - 74	-178 - 167	10 - 14	10 - 18	12 - 21	10 - 15
	g-g-g-g-	10 - 11	398	0.01 - 0.01	-65 - -64	-70 - -68	-69 - -67	-69 - -62	7 - 8	5 - 15	5 - 12	4 - 21
	tg-tt	10 - 10	399	0.01 - 0.01	-173 - -173	-85 - -85	-171 - -171	-177 - -177	14 - 14	10 - 10	14 - 14	16 - 16

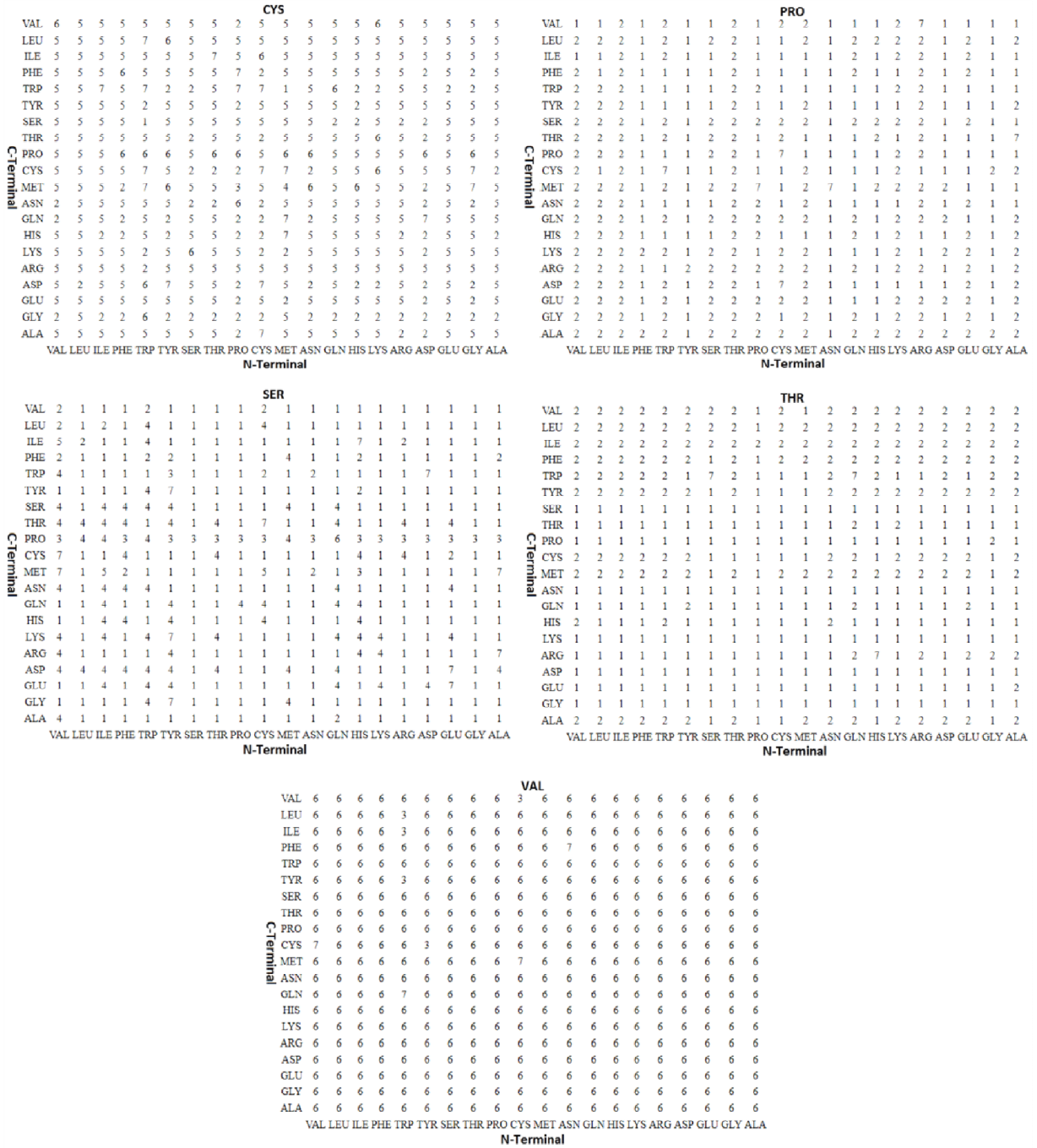

Fig. A BPO patterns of 400 triplets for the five χ1 amino acids. Description of each pattern number has been mentioned in Methods section.

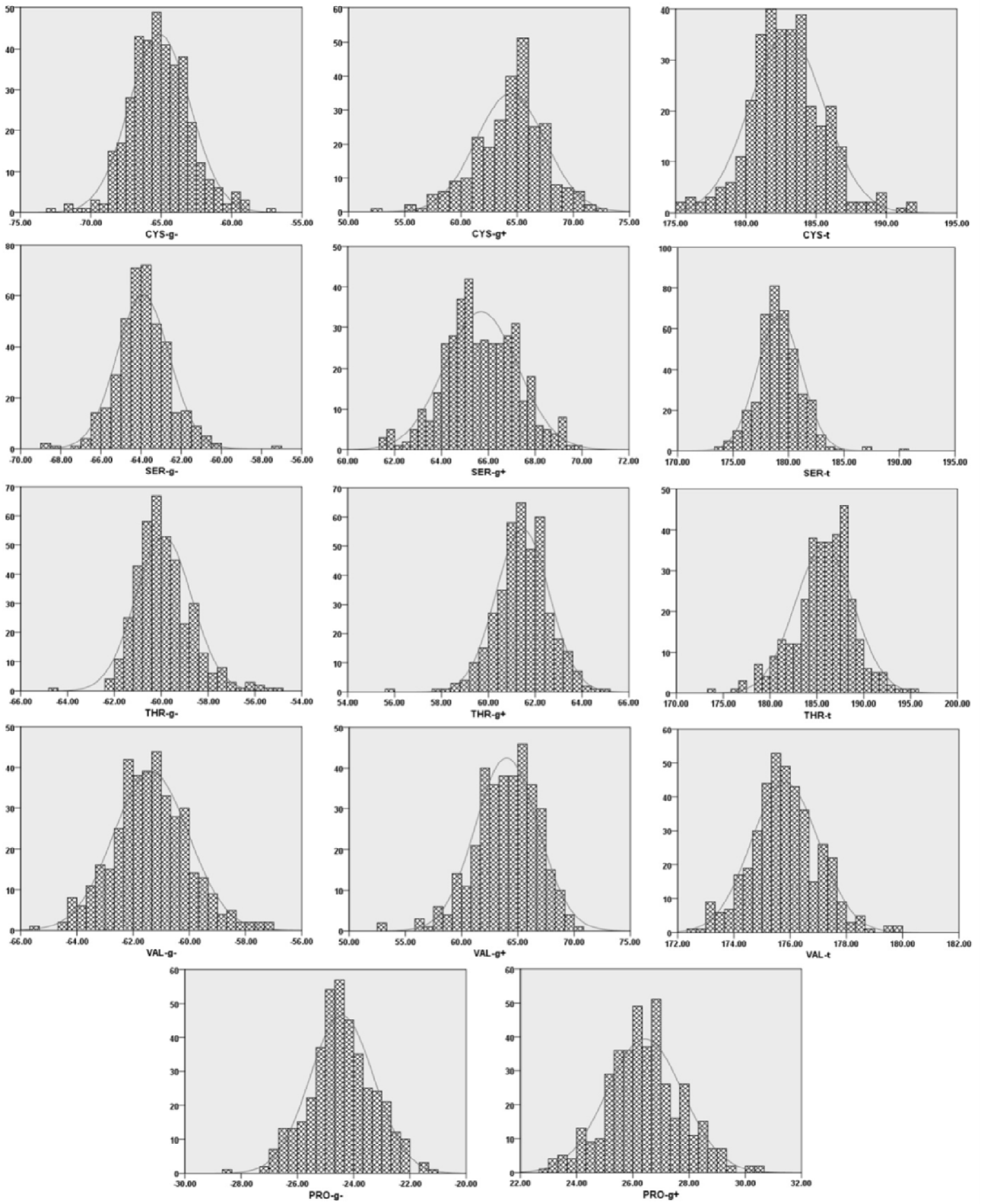

Fig. B Statistical distributions of χ_1 angle means for five χ_1 amino acids. Horizontal axis is χ_1 angle means for each 400 triplets and vertical axis is numbers of cases for each angle (i.e. AUC = 400).

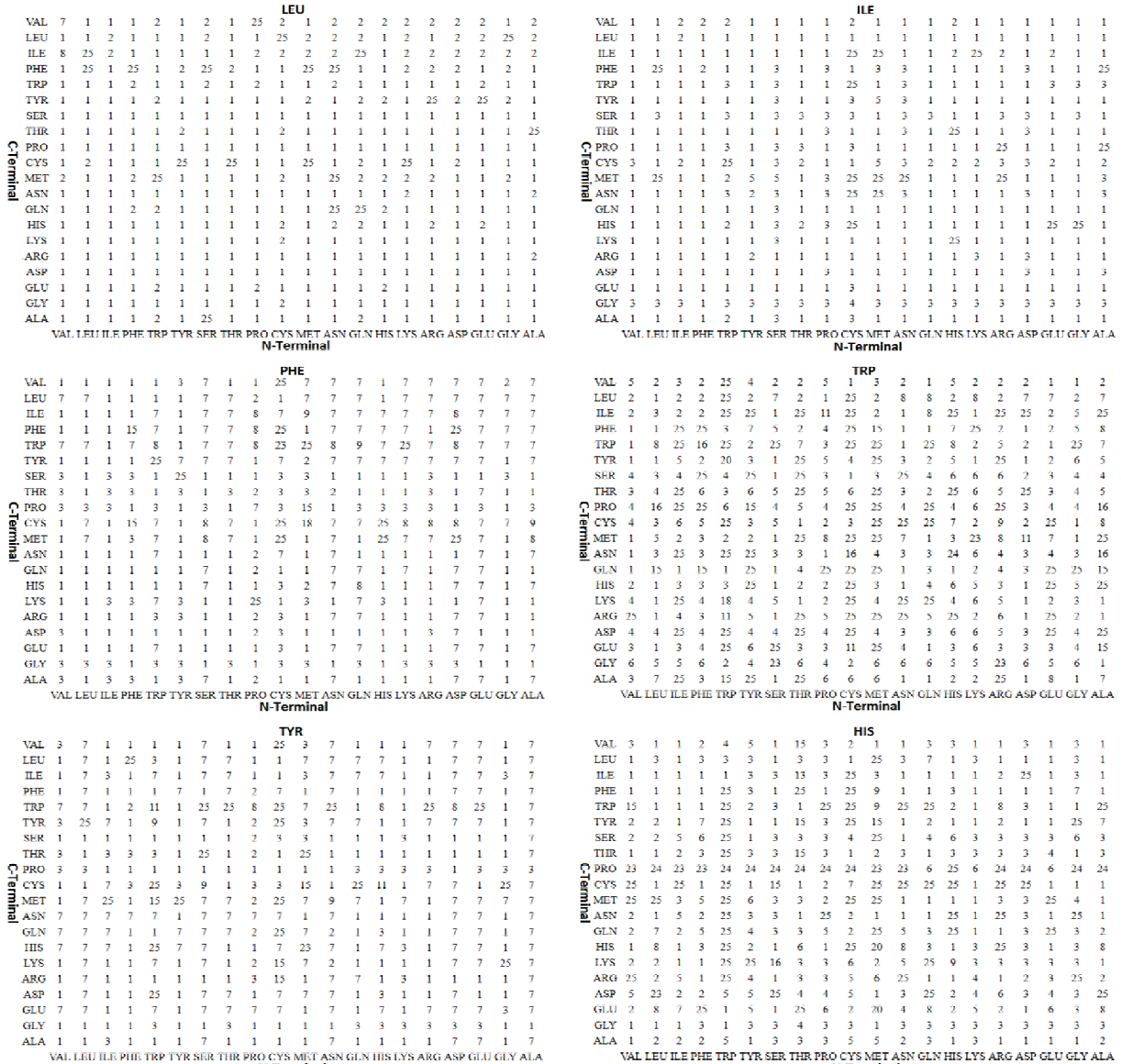

Fig. C The BPO patterns of 400 triplets for the χ_{1+2} amino acids. From 1 to 24, BPO numbers have fixed definitions. BPO number 25 was considered for all the cases with equalisation of two or more RFs in a triplet.

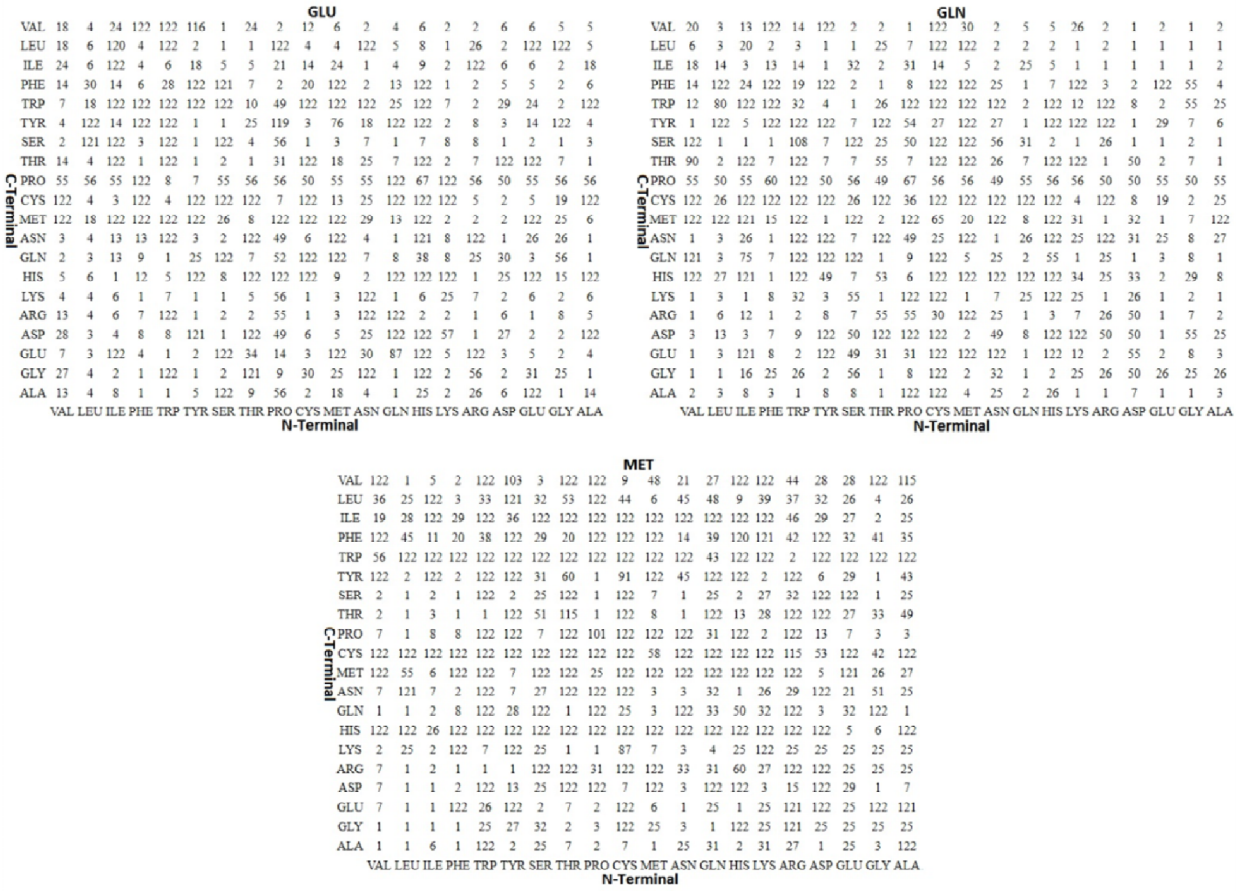

Fig. D The BPO patterns of 400 triplets for the χ_{1+2+3} amino acids. From 1 to 121, BPO numbers have fixed definitions. BPO number 122 was considered for all the cases with equalisation of two or more RFs in a triplet.

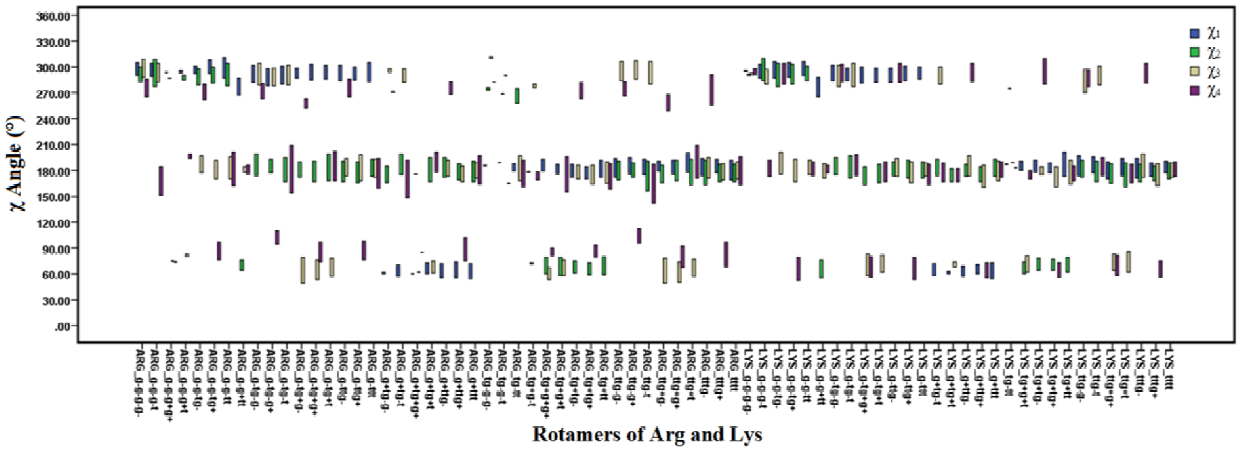

Fig. E Range of variation of χ angle averages within 400 triplets of $\chi_{1+2+3+4}$ residue types.

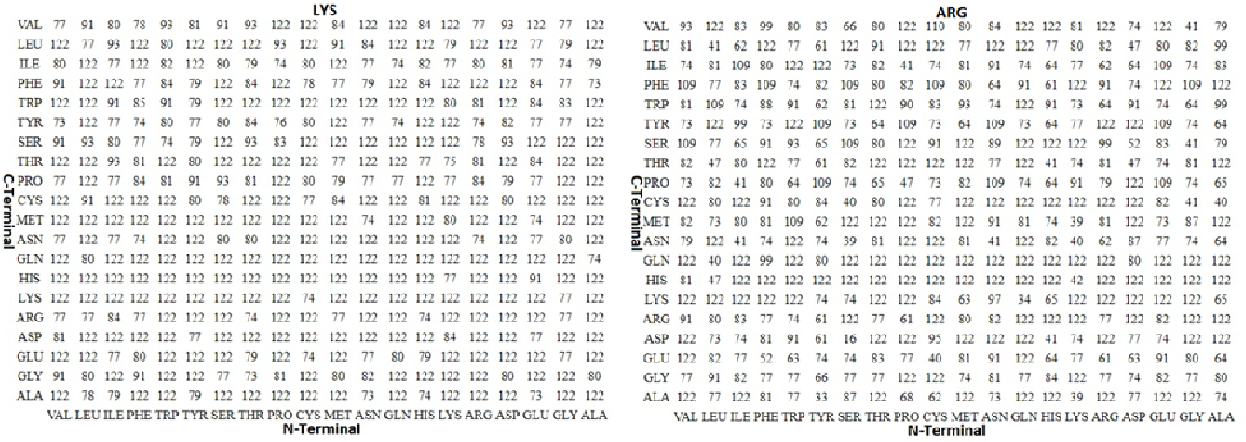

Fig. F The BPO patterns of 400 triplets for the $\chi_{1+2+3+4}$ amino acids. From 1 to 121, BPO numbers have fixed definitions. BPO number 122 was considered for all the cases with equalisations of two or more RFs in a triplet.