

Name	#	%	alpha	beta	other	χ^1 comm. ^a	χ^2 comm.	χ^3 comm.	χ^4 comm.	χ^1 1/2	χ^2 Width	χ^3 at	χ^4 1/2 Heig
Arginine													
ptp85° ^b	3	<1% ^c	0%	1%	<1%	62	180	65	85				
ptp180°	11	1%	0%	2%	2%	62	180	65	-175	14	17	10	13
ptt85°	16	2%	1%	2%	2%	62	180	180	85	13	14	13	17
ptt180°	16	2%	1%	2%	2%	62	180	180	180	15	13	15	19
ptt-85°	15	2%	1%	2%	2%	62	180	180	-85	15	14	12	14
ptm180°	6	1%	0%	1%	1%	62	180	-65	175				
ptm-85°	5	1%	0%	0%	1%	62	180	-65	-85				
tpp85°	11	1%	3%	1%	<1%	-177	65	65	85	13	13	12	15
tpp180°	8	1%	1%	0%	1%	-177	65	65	-175				
tpt85°	20	2%	3%	2%	2%	-177	65	180	85	14	13	15	14
tpt180°	15	2%	3%	1%	1%	-177	65	180	180	13	17	14	17
ttp85°	33	4%	5%	3%	3%	-177	180	65	85	14	17	13	15
ttp180°	25	3%	5%	3%	1%	-177	180	65	-175	14	16	14	26
ttp-105°	9	1%	1%	1%	1%	-177	180	65	-105				
ttt85°	19	2%	2%	2%	2%	-177	180	180	85	14	14	13	14
ttt180°	33	4%	3%	7%	3%	-177	180	180	180	15	13	12	27
ttt-85°	26	3%	3%	3%	2%	-177	180	180	-85	15	14	14	15
ttm105°	10	1%	2%	1%	<1%	-177	180	-65	105	15	16	15	15
ttm180°	13	1%	<1%	4%	1%	-177	180	-65	175	15	12	11	15
ttm-85°	28	3%	3%	3%	3%	-177	180	-65	-85	14	16	15	14
mtp85°	22	2%	2%	3%	2%	-67	180	65	85	13	17	13	13
mtp180°	45	5%	4%	3%	6%	-67	180	65	-175	12	19	13	19
mtp-105°	7	1%	0%	2%	1%	-67	180	65	-105	11	15	13	15
mtt85°	34	4%	4%	4%	3%	-67	180	180	85	12	19	13	19
mtt180°	89	9%	9%	5%	12%	-67	180	180	180	14	13	13	21
mtt-85°	53	6%	4%	7%	6%	-67	180	180	-85	13	13	13	13
mtm105°	15	2%	1%	1%	2%	-67	180	-65	105	12	13	13	15
mtm180°	48	5%	1%	4%	8%	-67	180	-65	175	14	17	13	30
mtm-85°	54	6%	13%	2%	3%	-67	-167	-65	-85	14	13	13	13
mmt85°	7	1%	1%	1%	1%	-62	-68	180	85				
mmt180°	18	2%	1%	3%	2%	-62	-68	180	180	13	13	10	29
mmt-85°	22	2%	<1%	4%	3%	-62	-68	180	-85	14	13	15	13
mmm180°	11	1%	<1%	2%	2%	-62	-68	-65	175	14	15	10	13
mmm-85°	22	2%	2%	3%	3%	-62	-68	-65	-85	14	13	15	13
		82%	79%	81%	84%								
	769/938 ^d		234	146	389								
Lysine													
ptpt	7	1%	0%	2%	<1%	62	180	68	180				
pttp	13	1%	0%	1%	2%	62	180	180	65	13	14	14	11
pttt	29	2%	0%	4%	3%	62	180	180	180	13	13	13	10
pttm	8	1%	0%	1%	1%	62	180	180	-65				
ptmt	5	<1%	0%	1%	<1%	62	180	-68	180				
tptp	11	1%	1%	1%	1%	-177	68	180	65	13	12	10	11
tppt	32	3%	5%	1%	2%	-177	68	180	180	10	10	13	14
tptm	7	1%	1%	1%	<1%	-177	68	180	-65	14	9	12	10
ttpp	12	1%	1%	<1%	1%	-177	180	68	65				
ttpt	25	2%	2%	5%	1%	-177	180	68	180	14	12	14	14
tttp	49	4%	5%	5%	3%	-177	180	180	65	14	13	12	12
tttt	162	13%	17%	19%	10%	-177	180	180	180	13	13	15	13
tttm	37	3%	4%	2%	3%	-177	180	180	-65	12	13	15	13
ttmt	20	2%	2%	4%	1%	-177	180	-68	180	14	14	10	15
ttmm	5	<1%	1%	0%	<1%	-177	180	-68	-65				
mppt	4	<1%	0%	0%	1%	-90	68	180	180	10	9	10	13
mtpp	12	1%	1%	1%	1%	-67	180	68	65	12	13	11	9
mtpt	38	3%	4%	2%	3%	-67	180	68	180	13	13	14	14
mttp	42	3%	2%	4%	4%	-67	180	180	65				
mttt	244	20%	23%	14%	21%	-67	180	180	180	14	13	12	14
mttm	56	5%	3%	5%	6%	-67	180	180	-65	13	12	13	14
mtmt	40	3%	6%	2%	3%	-67	180	-68	180	12	13	14	13
mtmm	12	1%	0%	1%	1%	-67	180	-68	-65	12	12	12	11
mmtp	9	1%	<1%	0%	1%	-62	-68	180	65				
mmtt	77	6%	3%	5%	8%	-62	-68	180	180	12	13	13	13
mmtm	18	1%	1%	1%	2%	-62	-68	180	-65	14	12	10	15
mmmt	10	1%	<1%	1%	1%	-62	-68	-68	180	12	13	10	15
		81%	82%	80%	82%								
	984/1209		261	194	529								

Name	#	%	alpha	beta	other	χ^1	χ^2	χ^3	χ^3	χ^1	χ^2	χ^3
<u>Methionine</u>						comm.	comm.	comm.	range ^e	1/2	Width at	1/2 Heig
ptp	12	2%	1%	3%	3%	62	180	75		11	17	12
ptm	17	3%	1%	6%	4%	62	180	-75		9	10	9
tpp	30	5%	8%	2%	5%	-177	65	75		10	15	15
tpt	9	2%	1%	4%	1%	-177	65	180		9	8	9
ttp	28	5%	7%	7%	2%	-177	180	75		10	11	11
ttt	17	3%	5%	2%	2%	-177	180	180		9	9	19
ttm	36	7%	3%	10%	8%	-177	180	-75		10	10	13
mtp	92	17%	22%	10%	17%	-67	180	75		10	12	14
mtt	43	8%	9%	8%	7%	-67	180	180		10	13	15
mtm	58	11%	12%	11%	9%	-67	180	-75		12	11	16
mmp	15	3%	3%	1%	4%	-65	-65	103		9	10	10
mmt	10	2%	0%	2%	3%	-65	-65	180		12	14	19
mmm	105	19%	21%	16%	19%	-65	-65	-70		11	13	16
		86%	91%	84%	83%							
	472/550		175	112	185							
<u>Glutamate</u>												
Spt-60°						62	180	-60				
pt-20°	80	5%	1%	9%	7%	62	180	-20	-90 to 90	14	13	23
Spt60°						62	180	60				
pm0°	32	2%	0%	0%	4%	70	-80	0	-50 to 50	14	13	17
tp10°	91	6%	10%	2%	6%	-177	65	10	-10 to 90	14	13	17
Stt-60°						-177	180	-60				
tt 0°	350	24%	25%	42%	18%	-177	180	0	-90 to 90	14	14	30
Stt60°						-177	180	60				
tm-20°	17	1%	1%	1%	1%	-177	-80	-25	-50 to 10	13	13	15
mp0°	88	6%	<1%	2%	10%	-65	85	0	-60 to 60	14	13	25
Smt-60°						-67	180	-60				
mt-10°	484	33%	36%	29%	32%	-67	180	-10	-90 to 90	13	16	25
Smt60°						-67	180	60				
mm-40°	197	13%	19%	7%	12%	-65	-65	-40	-90 to 30	14	14	25
Smm0°						-65	-75	0				
		91%	92%	92%	90%							
	1339/1470		394	225	720							
<u>Glutamine</u>												
Spt-60°						62	180	-60				
pt 20°	37	4%	1%	5%	6%	62	180	20	-90 to 90	13	14	16
Spt60°						62	180	60				
pm0°	15	2%	0%	1%	3%	70	-75	0	-60 to 60			
tp-100°	14	2%	4%	2%	<1%	-177	65	-100	-150 to 0			
tp60°	78	9%	13%	9%	7%	-177	65	60	0 to 90	14	15	24
Stt-60°						-177	180	-60				
tt 0°	140	16%	16%	29%	12%	-177	180	0	-90 to 90	14	13	40
Stt60°						-177	180	60				
mp0°	24	3%	<1%	1%	5%	-65	85	0	-60 to 60			
Smt-60°						-67	180	-60				
mt -30°	304	35%	40%	26%	36%	-67	180	-25	-90 to 90	16	15	37
Smt60°						-67	180	60				
mm-40°	127	15%	12%	13%	17%	-65	-65	-40	-95 to 0	16	18	26
mm100°	22	3%	4%	1%	2%	-65	-65	100	0 to 150			
		88%	89%	86%	88%							
	761/863		229	137	395				χ^2			
<u>Aspartate</u>												
Sp-50°						62	-50					
p-10°	203	10%	1%	2%	13%	62	-10		-90 to 0	9	19	
p30°	194	9%	1%	5%	12%	62	30		0 to 90	8	14	
St-30°						-170	-30					
t0°	438	21%	8%	44%	20%	-177	0		-50 to 50	12	30	
t70°	118	6%	11%	7%	4%	-177	65		50 to 90	12	18	
m -20°	1088	51%	77%	38%	47%	-70	-15		-90 to 20	10	16	
Sm-60°						-65	-60					
		96%	97%	95%	96%							
	2041/2124		365	232	1444							

Asparagine

Sp-50°						62	-50			
p-10°	103	7%	0%	1%	10%	62	-10	-90 to 0	8	9
p30°	132	9%	<1%	7%	12%	62	30	0 to 90	6	7
St-80°						-174	-80			
t-20°	177	12%	5%	21%	12%	-174	-20	-120 to 0	5	21
t30°	228	15%	13%	18%	15%	-177	30	0 to 80	14	22
m-20°	580	39%	65%	28%	33%	-65	-20	-60 to 10	10	20
m-80°	118	8%	8%	9%	8%	-65	-75	-100 to -60	9	9
m120°	58	4%	3%	3%	4%	-65	120	60 to 160	9	18

94% 95% 88% 95%
1396/1490 293 179 924

Name	#	%	alpha	beta	other	χ^1	χ^2	χ^2	χ^1	χ^2
Isoleucine						comm.	comm.	range	1/2 Width	at 1/2 Heig
pp	10	1%	<1%	1%	<1%	62	100			
pt	216	13%	4%	13%	22%	62	170		10	10
tp	36	2%	2%	1%	4%	-177	66		13	11
tt	127	8%	1%	8%	14%	-177	165		13	11
mp	19	1%	0%	2%	1%	-65	100			
mt	993	60%	81%	58%	41%	-65	170		10	10
mm	242	15%	10%	16%	17%	-57	-60		10	10
		99%	99%	98%	99%					
	1643/1667		496	629	518					

Leucine

pp	21	1%	<1%	2%	1%	62	80			
tp	750	29%	30%	36%	23%	-177	65		10	10
tt	49	2%	1%	3%	1%	-172	145	120 to 180	9	9
mp	63	2%	1%	5%	2%	-85	65	45 to 105	11	14
mt	1548	59%	62%	46%	66%	-65	175		11	11
		93%	95%	93%	93%					
	2431/2602		836	644	951					

Histidine

p-80°	51	9%	0%	6%	13%	62	-75	-120 to -50	10	12
p80°	26	4%	0%	4%	6%	62	80	50 to 120	13	10
t-160°	31	5%	5%	14%	1%	-177	-165	150 to -120	12	20
t-80°	64	11%	17%	9%	9%	-177	-80	-120 to -50	10	22
t60°	94	16%	24%	17%	12%	-177	60	50 to 120	13	19
m-70°	174	29%	26%	30%	30%	-65	-70	-120 to -30	11	23
m170°	44	7%	9%	3%	9%	-65	165	120 to -160	10	16
m80°	78	13%	14%	10%	14%	-65	80	50 to 120	11	18
		94%	94%	92%	95%					
	562/598		124	143	295					

Tryptophan

p-90°	67	11%	2%	13%	14%	62	-90	-130 to -60	12	10
p90°	34	6%	1%	9%	6%	62	90	60 to 130	12	8
t-105°	100	16%	27%	10%	14%	-177	-105	-130 to -60	16	14
t90°	109	18%	28%	14%	15%	-177	90	0 to 100	10	11
m-90°	31	5%	0%	7%	7%	-65	-90	-130 to -60	9	12
m0°	48	8%	15%	2%	8%	-65	-5	-40 to 20	9	20
m95°	195	32%	22%	43%	29%	-65	95	60 to 130	11	19
		94%	95%	98%	92%					
	584/618		140	175	269					

Tyrosine

p90°	182	13%	1%	21%	12%	62	90	60 to 90, -90 to -60	13	13
t80°	486	34%	55%	25%	30%	-177	80	20 to 90, -90 to -75	11	14
m-85°	618	43%	26%	50%	45%	-65	-85	50 to 90, -90 to -50	11	21
m-30°	124	9%	15%	4%	9%	-65	-30	-50 to 0, 0 to 50	11	18
Sm35°						-85	30			
		98%	97%	99%	97%					
	1410/1443		290	468	652					

Phenylalanine

p90°	202	13%	1%	24%	11%	62	90	60 to 90, -90 to -60	11	11
t80°	522	33%	57%	18%	29%	-177	80	20 to 90, -90 to -75	13	17
m-85°	697	44%	29%	51%	47%	-65	-85	50 to 90, -90 to -50	12	17
m-30°	149	9%	12%	5%	11%	-65	-30	-50 to 0, 0 to 50	9	20
Sm35°						-85	30			
		98%	97%	99%	98%					
	1570/1599		389	514	667					

Proline

Cy endo	379	44%	23%	54%	43%	30	15 to 60	7
Cy exo	372	43%	68%	28%	44%	-30	-60 to -15	6
cis, Cy endo	56	6%	0%	1%	7%	30	15 to 60	5
		93%	91%	84%	94%			
	807/928		20	57	730			

Name	#	%	alpha	beta	other	χ^1	χ^1
<u>Threonine</u>						com.	1/2 Width at 1/2 Heig
p	1200	49%	25%	31%	65%	62	10
t	169	7%	0%	13%	6%	-175	6
m	1062	43%	74%	55%	29%	-65	7
		99%	100%	99%	99%		
	2431/2447		395	672	1364		

Valine

p	169	6%	2%	8%	8%	63 ="177" ^{af}	8
t	1931	73%	90%	72%	63%	175 ="-65"	8
m	526	20%	7%	20%	28%	-60 ="60"	7
		99%	100%	99%	99%		
	2626/2649		622	1080	924		

Serine

p	1201	48%	33%	36%	55%	62	10
t	541	22%	22%	34%	18%	-177	11
m	714	29%	44%	29%	25%	-65	9
		98%	98%	100%	98%		
	2456/2498		350	485	1621		

Cysteine

p	64	23%	5%	23%	34%	62	14
t	74	26%	20%	45%	21%	-177	10
m	142	50%	75%	32%	43%	-65	11
		99%	100%	100%	98%		
	280/285		85	65	130		

Name	#	%	χ^2	χ^3	$\chi^{2'}$	χ^2	χ^3	$\chi^{2'}$
<u>Disulfide</u> ^g						range	range	range
mmm	70	36%	-61	-81	-75	-95 to -30	10 to -50	20 to -40
ppp	15	8%	63	85	85	30 to 90	55 to 115	60 to 115
mpp	33	17%	-65	100	85	00 to -35	70 to 130	50 to 115
pmm	6	3%	90	-91	-64	60 to 120	20 to -60	-95 to -35
mpm	11	6%	-86	102	-102	20 to -40	70 to 130	60 to -90
mmt	19	10%	-92	-90	-149	20 to -30	20 to -60	0 to -120
ppt	16	8%	52	82	180	30 to 95	50 to 110	0 to -120
mpt	5	3%	-68	96	147	00 to -40	65 to 125	15 to 175
tmt	6	3%	172	-83	-168	0 to -160	15 to -55	0 to -140
tpt	1	1%	122	87	163	95 to 150	55 to 115	0 to -170
		95%						
	182/198							

^a"mode" indicates the peak of the smoothed distribution, "comm." indicates the common-atom value (given in bold face)

^b mode and width at 1/2 height values are not given for minor rotamers.

^c <1% indicates a value between 1% and 0%. 0% indicates no observations.

^d Total number of rotameric side chains / Total number that pass all data filters.

^e Ranges used in determining frequencies are normally common-atom values $\pm 30^\circ$.

Exceptions (always in the terminal c value) are listed here.

^f Standard conventions result in c angles being named differently for Val than for Thr and Ile.

These figures indicate the equivalent angles.

^g Disulphides are ordered such that conformations with opposite handedness are grouped together.