

**Table S1.** Number of surface residues in bound and unbound proteins.

Amino acid	Interface U <sup>a</sup> /B <sup>b</sup>	Non-interface U/B
Ser	333/429	2409/2934
Val	175/259	1003/1116
Thr	321/406	2021/2375
Cys	40/58	183/190
Pro	250/295	1727/2029
Ile	136/202	560/638
Leu	245/348	1095/1258
Asn	291/350	1902/2074
Asp	329/433	2448/2856
His	126/174	682/741
Phe	108/176	457/487
Tyr	202/296	636/718
Trp	63/100	187/220
Gln	268/357	1687/1888
Glu	416/545	2933/3303
Met	73/119	311/329
Lys	427/555	2965/3387
Arg	325/474	1791/2014

<sup>a</sup> Unbound

<sup>b</sup> Bound

**Table S2.** Redundant rotamer libraries.**FULL SURFACE LIBRARY****CYS**

rotamer	$X_1$		rotamer occupancy		rotamer share, <sup>c</sup> %	
	U <sup>a</sup>	B <sup>b</sup>	U	B	U	B
1	-65.6	-61.0	129	129	57.8	52.0
2	-175.3	-177.3	53	55	23.8	22.2
3	65.3	63.4	41	57	18.4	23.0

**SER**

rotamer	$X_1$		rotamer occupancy		rotamer share, %	
	U	B	U	B	U	B
1	61.8	62.9	1366	1683	49.8	50.0
2	-63.6	-62.0	825	1000	30.1	29.7
3	177.6	-179.5	551	680	20.1	20.2

**THR**

rotamer	$X_1$		rotamer occupancy		rotamer share, %	
	U	B	U	B	U	B
1	61.0	61.3	1197	1376	51.1	49.5
2	-59.7	-59.4	953	1199	40.7	43.1
3	-174.7	-178.3	192	206	8.2	7.4

**VAL**

rotamer	$X_1$		rotamer occupancy		rotamer share, %	
	U	B	U	B	U	B
1	177.7	177.4	802	949	68.1	69.0
2	-62.9	-62.1	254	293	21.6	21.3
3	61.7	67.9	117	129	9.9	9.4

<sup>a</sup> Unbound.<sup>b</sup> Bound.

<sup>c</sup> Share of rotamer  $i$  is  $\frac{N_i}{\sum_i N_i + N_{non}}$  100%, where  $N_i$  is rotamer occupancy,  $N_{non}$  is the number of non-rotamer conformations, the sum runs over all rotamers.

## ASP

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-72.0	-14.7	-70.4	-16.2	1152	1325	41.6	40.3
2	-174.4	8.2	-173.8	1.8	512	585	18.5	17.8
3	63.6	1.6	61.3	2.2	365	362	13.2	11.0
4	-173.1	-19.6	-171.1	-20.9	293	347	10.6	10.6
5	-66.2	-76.3	-56.9	-68.3	263	383	9.5	11.6
6	64.7	-52.2	60.0	-55.1	187	284	6.7	8.6

## PHE

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-62.1	99.1	-62.3	102.8	250	312	44.2	47.1
2	179.8	75.8	-180.0	75.3	210	224	37.2	33.8
3	61.4	87.5	65.4	90.7	58	80	10.3	12.1
4	-63.9	-19.2	-68.0	-23.1	44	43	7.8	6.5

## HIS

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-62.6	-67.6	-60.6	-70.9	207	258	25.6	28.2
2	-66.5	88.5	-65.9	87.3	161	159	19.9	17.4
3	179.8	66.9	-178.2	83.1	106	128	13.1	14.0
4	-175.1	-82.1	-176.0	-75.3	93	80	11.5	8.7
5	76.1	-89.5	72.0	-93.2	82	84	10.1	9.2
6	-68.6	170.0	-67.2	168.7	64	72	7.9	7.9
7	67.5	95.7	72.4	91.8	32	41	4.0	4.5
8	-167.6	-160.3	-179.3	-157.7	29	40	3.6	4.4
9	-70.5	-1.0	-76.1	46.2	25	41	3.1	4.5

## ILE

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-63.1	172.2	-63.9	175.7	341	415	49.0	49.4
2	-61.0	-60.1	-58.4	-59.1	125	146	18.0	17.4
3	65.2	174.6	62.5	173.8	93	109	13.4	13.0
4	-168.6	172.6	-180.0	171.0	46	45	6.6	5.4
5	-65.1	73.9	-59.9	79.7	36	50	5.2	6.0
6	50.9	66.5	78.8	94.5	20	20	2.9	2.4
7	-170.7	61.0	-171.7	70.4	19	39	2.7	4.6

## LEU

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-63.4	175.1	-65.1	175.2	780	914	58.2	56.9
2	-178.3	60.3	-176.6	63.6	295	331	22.0	20.6
3	-94.9	31.9	-82.6	58.0	90	137	6.7	8.5
4	-144.1	148.8	-145.0	-146.8	47	68	3.5	4.2
5	-70.0	-57.2	-63.5	-48.9	37	58	2.8	3.6
6	-167.7	-82.2	-168.3	-86.2	22	29	1.6	1.8
7	-50.3	104.7	-59.6	74.4	14	27	1.0	1.7
8	53.9	74.5	20.5	78.7	20	12	1.5	0.7
9	-173.8	166.6			18		1.3	
10	68.0	140.6	58.8	174.7	12	24	0.9	1.5

## ASN

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-64.7	-47.4	-61.3	-47.2	863	958	39.4	39.5
2	-173.3	58.0	-168.8	49.6	357	420	16.3	17.3
3	-68.4	166.3	-67.0	166.0	386	478	17.6	19.7
4	59.6	13.8	55.2	50.1	236	262	10.8	10.8
5	-173.3	-49.1	-172.8	-83.3	265	225	12.1	9.3

## PRO

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-29.0	38.6	-29.1	40.4	1076	1269	54.4	54.6
2	30.8	-38.7	30.5	-39.8	901	1055	45.6	45.4

## TRP

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-61.9	87.5	-68.1	86.2	98	132	39.2	41.3
2	-177.9	-110.7	-179.2	-108.5	28	40	11.2	12.5
3	-65.8	-8.6	-76.2	0.0	26	26	10.4	8.1
4	177.6	74.3	-177.5	82.8	26	45	10.4	14.1
5	61.5	-92.2	61.4	-96.4	21	28	8.4	8.8
6	-54.4	-59.9	-61.8	-95.6	23	20	9.2	6.3
7	60.9	92.9	64.4	82.4	16	20	6.4	6.3

## TYR

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-62.6	93.9	-66.3	96.0	410	469	48.9	46.3
2	178.1	74.8	-179.7	74.8	270	360	32.2	35.5
3	61.1	93.5	60.4	89.8	102	115	12.2	11.3
4	-68.4	-1.2	-65.2	-29.1	52	62	6.2	6.1

## GLU

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	rotamer occupancy		rotamer share, %	
	U			B			U	B	U	B
1	-67.6	176.4	-10.0	-59.6	-177.0	-54.5	709	746	21.2	19.4
2	-66.9	-179.0	57.4	-73.7	179.2	53.0	417	539	12.5	14.0
3	-176.6	179.2	-6.6	-177.3	179.3	-7.5	447	529	13.3	13.7
4	-68.7	-58.0	-59.1	-68.4	-66.7	-60.0	383	463	11.4	12.0
5	173.4	174.0	50.5	-174.7	-176.4	-55.3	282	358	8.4	9.3
6	-178.1	62.2	24.6	-177.9	58.8	48.5	231	245	6.9	6.4
7	59.8	177.5	30.8	60.9	179.9	-4.0	150	85	4.5	2.2
8	-67.5	80.2	10.4	-72.5	62.8	54.2	139	141	4.2	3.7
9	68.8	176.1	-50.6	68.5	173.7	-56.0	110	166	3.3	4.3
10	-64.6	-82.2	38.2	-69.6	-51.1	74.2	82	119	2.4	3.1
11	65.7	-90.1	35.5	59.3	-75.8	-2.6	62	63	1.9	1.6
12	-63.6	97.0	-39.7	-72.0	85.5	-6.9	75	106	2.2	2.8
13	-170.9	63.3	-65.8	-175.9	70.4	5.4	44	104	1.3	2.7
14	-177.1	-77.9	-33.5	-173.5	-91.0	-20.5	51	37	1.5	1.0
15	61.9	-103.7	73.2	63.5	-93.8	25.3	47	38	1.4	1.0

## GLN

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	rotamer occupancy		rotamer share, %	
	U			B			U	B	U	B
1	-62.4	-170.7	-50.7	-61.2	-179.3	-55.0	323	386	16.5	17.2
2	-63.7	176.7	58.7	-70.3	-177.8	50.4	297	261	15.2	11.6
3	-60.6	-60.0	-57.7	-62.9	-58.0	-57.4	229	220	11.7	9.8
4	175.6	-174.6	60.5	177.6	177.6	53.0	137	145	7.0	6.5
5	-65.4	174.2	-180.0	-67.1	-179.0	171.8	144	149	7.4	6.6
6	-167.7	59.8	49.5	-174.1	54.8	60.3	114	151	5.8	6.7
7	-174.1	-178.2	-49.7	-174.4	-175.5	-55.5	112	173	5.7	7.7
8	-65.3	-56.8	120.2	-60.5	-58.6	134.4	105	135	5.4	6.0
9	-176.3	179.1	134.4	175.6	178.0	172.9	76	73	3.9	3.3
10	69.5	-177.7	-57.4	56.0	178.7	-65.5	49	52	2.5	2.3
11	179.2	71.0	-171.6	-157.0	66.5	-114.0	47	76	2.4	3.4
12	-71.6	79.6	7.0	-81.6	67.8	48.6	45	50	2.3	2.2
13	-175.2	43.2	-88.0	-64.2	101.8	-58.1	31	43	1.6	1.9

14	73.0	-176.7	73.2	51.8	-177.2	54.2	26	55	1.3	2.4
15	55.8	-95.5	30.8	71.3	-91.5	35.9	19	27	1.0	1.2
16	41.5	-172.4	179.1	78.2	-172.9	-158.3	18	25	0.9	1.1
17	-172.6	-87.1	-31.1	-128.9	-84.4	-70.0	13	22	0.7	1.1

### MET

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	rotamer occupancy		rotamer share, %	
	U			B			U	B	U	B
1	-61.0	-60.7	-71.0	-57.8	-54.4	-70.0	71	84	18.5	18.8
2	-65.6	178.2	-54.5	-59.7	-173.9	-74.1	50	47	13.0	10.5
3	-63.5	173.3	68.7	-67.9	175.4	66.6	42	69	10.9	15.4
4	171.9	161.0	65.1	-174.6	-176.9	76.2	25	23	6.5	5.1
5	-58.1	-61.9	106.4	-78.7	-59.4	104.5	25	31	6.5	6.9
6	-177.2	-174.8	-70.0	-175.1	172.3	-67.7	20	42	5.2	9.4
7	-65.5	176.1	-170.9	-69.6	170.4	164.1	19	17	4.9	3.8
8	-168.4	69.2	80.4	-177.5	55.7	75.6	16	29	4.2	6.5
9	170.6	75.0	-85.7				12		3.1	
9				64.3	168.6	73.7		9		2.0
10	76.0	-178.9	-68.1	59.2	-175.9	-70.8	9	16	2.3	3.6

### ARG

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>4</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>4</sub>	rotamer occupancy		rotamer share, %	
	U				B				U	B	U	B
1	-59.2	177.1	179.8	179.9	-59.9	-175.4	-179.8	-177.2	204	221	9.6	8.9
2	-72.8	169.3	179.1	-77.1	-73.6	174.5	178.3	-64.1	111	124	5.2	5.0
3	-172.9	177.3	-179.7	180.0	-179.6	177.7	180.0	-178.3	101	127	4.8	5.1
4	-169.5	179.0	-60.5	144.4	-178.1	-168.2	-55.5	165.3	110	109	5.2	4.4
5	-64.6	-172.5	-176.3	62.7	-60.1	-157.2	-171.3	86.0	104	101	4.9	4.1
6	-62.4	165.0	80.2	167.9	-69.0	-177.9	58.8	-173.2	110	120	5.2	4.8
7	-68.6	-165.7	-67.0	-82.5	-70.0	-163.1	-61.0	-85.9	94	103	4.4	4.1
8	-67.8	179.0	-65.6	102.0	-68.9	-175.0	-70.1	-178.8	124	127	5.9	5.1
9	-62.4	-63.4	178.2	-176.1	-67.1	-62.0	178.7	173.3	74	60	3.5	2.4
10	-171.7	171.8	106.6	-129.7	-172.4	174.8	61.5	-171.2	83	102	3.9	4.1
11	-177.0	-179.3	-68.4	-92.6	179.6	166.5	-61.2	-84.1	62	63	2.9	2.5
12	175.8	179.0	60.9	70.1	174.8	172.1	66.6	86.4	48	73	2.3	2.9
13	177.4	178.2	173.6	75.8	176.3	-173.7	179.4	65.4	40	47	1.9	1.9
14	169.4	175.7	176.3	-80.2	-168.1	173.3	177.2	-68.6	39	56	1.8	2.3
15	60.2	-178.3	174.5	71.5	58.7	-176.4	176.4	97.8	39	42	1.8	1.7
16	-61.0	-172.5	72.0	80.2	-65.5	-179.0	59.2	76.4	37	49	1.7	2.0
17	68.7	-177.1	-169.9	-176.7	69.4	178.9	-174.1	-71.6	31	37	1.5	1.5
18	87.1	-168.4	-54.6	173.6	49.4	-177.4	-71.4	-171.5	31	43	1.5	1.7
19	-179.7	51.5	-179.6	168.3	176.5	69.0	-169.7	-177.7	30	28	1.4	1.1
20	61.7	174.0	64.7	-152.9	67.3	-173.3	58.9	-158.4	27	33	1.3	1.3

21	-46.2	-43.9	-66.2	160.2	-67.7	-74.6	-66.5	176.3	27	49	1.3	2.0
22	-79.4	-64.8	-178.4	-82.1	-64.3	-61.0	-176.1	-89.2	27	42	1.3	1.7
23	70.7	-172.8	177.4	-77.5					23		1.1	
24	173.1	78.5	171.3	80.9	-160.7	91.4	168.8	-56.0	21	25	1.0	1.0
25	-64.3	-62.2	-55.0	-84.2					21		1.0	
25					177.9	111.2	69.0	173.0		23		0.9
26	-46.7	-64.8	-164.6	73.7	-60.2	-60.5	160.4	65.1	21	27	1.0	1.1

LYS

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>4</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>4</sub>	rotamer occupancy		rotamer share, %	
	U				B				U	B	U	B
1	-65.5	-178.1	179.5	-179.8	-66.1	-178.3	178.0	179.2	702	756	20.7	19.2
2	-178.3	-177.7	178.1	-179.0	-177.8	-179.5	179.2	-178.8	360	433	10.6	11.0
3	-65.9	-62.9	-178.5	-177.4	-67.3	-65.7	-177.7	177.5	202	247	6.0	6.3
4	-60.3	178.9	179.5	62.0	-63.4	-177.7	-174.7	59.7	154	185	4.5	4.7
5	-60.1	-179.7	-174.9	-61.4	-62.7	-179.5	-178.3	-60.0	146	164	4.3	4.2
6	-71.9	-167.2	-69.2	-175.8	-73.5	-172.6	-68.9	-172.6	113	132	3.3	3.3
7	-178.7	176.4	-178.7	-64.6	-178.1	176.2	-175.5	-68.0	106	124	3.1	3.1
8	64.9	179.2	176.9	-177.6	63.3	-179.9	-174.0	-179.9	100	106	2.9	2.7
9	-61.3	-179.1	64.6	-179.8	-66.4	-178.9	64.2	-179.5	99	133	2.9	3.4
10	-174.7	174.6	179.4	56.9	178.8	175.0	173.8	58.4	95	120	2.8	3.0
11	-178.2	173.5	67.7	172.6	-171.4	177.0	64.7	-179.7	87	104	2.6	2.6
12	179.4	67.1	174.1	178.8	-175.7	60.3	-178.4	-179.9	92	125	2.7	3.2
13	-57.5	-60.4	-169.9	-62.3	-55.2	-59.7	-176.1	-60.3	68	70	2.0	1.8
14	-178.8	-168.1	-63.6	179.3	178.2	178.6	-65.2	-174.6	67	85	2.0	2.2
15	-68.7	-69.0	-172.6	62.9	-56.8	-69.6	-174.4	53.7	61	82	1.8	2.1
16	-60.7	-67.0	-57.4	-178.2	-54.7	-62.8	-67.3	180.0	37	38	1.1	1.0
17	67.0	-179.1	-169.6	-54.0					36		1.1	
					-175.8	72.4	176.5	-66.4		39		1.0
18	-169.4	176.3	-21.3	-63.5					35		1.0	
					52.5	176.3	-71.6	-171.5		36		0.9
19	61.1	171.8	67.3	176.7					33		1.0	
					-65.8	-175.4	-65.3	-65.0		38		1.0
20	174.7	60.8	164.9	59.0	-179.6	61.1	-178.5	57.4	36	40	1.1	1.0
21	179.3	-178.3	71.6	66.4					30		0.9	

## NON-INTERFACE SURFACE LIBRARY

### CYS

rotamer	$X_1$		rotamer occupancy		rotamer share, %	
	U	B	U	B	U	B
1	-65.6	-62.1	109	103	59.6	54.2
2	-173.9	-173.4	42	38	23.0	20.0
3	65.1	61.3	32	46	17.5	24.2

### SER

rotamer	$X_1$		rotamer occupancy		rotamer share, %	
	U	B	U	B	U	B
1	61.8	61.0	1218	1487	50.6	50.7
2	-62.8	-62.0	721	858	29.9	29.2
3	177.5	179.3	470	589	19.5	20.1

### THR

rotamer	$X_1$		rotamer occupancy		rotamer share, %	
	U	B	U	B	U	B
1	61.0	61.3	1026	1166	50.8	49.1
2	-61.4	-59.4	830	1035	41.1	43.6
3	-174.7	-176.3	162	174	8.0	7.3

### VAL

rotamer	$X_1$		rotamer occupancy		rotamer share, %	
	U	B	U	B	U	B
1	177.7	177.4	692	783	69.0	70.2
2	-60.5	-62.1	212	229	21.1	20.5
3	61.7	67.6	95	91	9.5	8.2

### ASP

rotamer	$X_1$	$X_2$	$X_1$	$X_2$	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-72.0	-14.7	-70.4	-16.2	1037	1162	42.4	40.7
2	-174.4	8.2	-172.3	56.2	468	463	19.1	16.2
3	63.6	1.6	60.8	-6.3	340	305	13.9	10.7
4	-173.1	-19.6	-173.3	-10.9	235	340	9.6	11.9
5	-66.2	-76.3	-78.2	11.8	210	323	8.6	11.3
6	62.0	-69.0	60.0	-55.1	157	257	6.4	9.0



## PHE

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-62.1	99.1	-62.3	102.8	204	224	44.6	46.0
2	-177.6	76.3	-180.0	75.3	169	167	37.0	34.3
3	61.4	87.5	66.6	94.0	45	53	9.8	10.9
4	-68.1	-11.9	-68.0	-23.1	38	41	8.3	8.4

## HIS

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-62.6	-67.6	-56.0	-62.2	184	202	27.0	27.3
2	-66.5	88.5	-63.1	92.4	133	128	19.5	17.3
3	176.7	68.9	176.0	75.2	90	113	13.2	15.2
4	-175.1	-82.1	178.1	-81.2	85	70	12.5	9.4
5	-72.4	172.5	-74.2	171.7	54	68	7.9	9.2
6	66.5	-70.8	61.4	-65.7	56	57	8.2	7.7
7	56.7	89.0	72.4	91.8	29	31	4.3	4.2
8	-168.1	-168.9	-164.8	-174.0	25	26	3.7	3.5
9	-70.0	-5.8	-71.4	-35.2	21	35	3.1	4.7

## ILE

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-63.1	172.2	-63.9	175.7	278	306	49.6	48.0
2	-61.4	-61.8	-54.6	-58.1	100	110	17.9	17.2
3	65.2	174.6	62.5	173.8	74	90	13.2	14.1
4	-177.5	176.6	-176.2	171.9	35	34	6.3	5.3
5	-55.8	75.0	-59.9	79.7	31	45	5.5	7.1
6	50.9	66.5	82.5	101.3	14	13	2.5	2.0
7	-177.2	62.0	-179.8	65.4	14	28	2.5	4.4

## LEU

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-61.9	175.9	-65.1	175.2	625	703	57.1	55.9
2	-178.3	60.3	-179.6	65.3	247	267	22.6	21.2
3	-78.0	48.0	-80.7	51.6	79	105	7.2	8.3
4	-144.1	-148.8	-172.0	164.7	45	54	4.1	4.3
5	-70.0	-57.2	-72.0	-44.1	28	44	2.6	3.5

6	-167.7	-82.2	-174.8	-94.0	18	24	1.6	1.9
7	60.1	71.3	58.8	174.7	14	21	1.3	1.7
8	166.4	124.7	26.3	84.7	12	8	1.1	0.6
9	-42.6	109.7	-59.6	74.4	10	28	0.9	2.2
10	100.7	121.9			12		1.1	

### ASN

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-64.7	-47.4	-61.3	-47.2	739	801	38.9	38.6
2	-72.8	164.6	-69.1	171.6	353	407	18.6	19.6
3	-173.3	58.0	-168.8	49.6	298	372	15.7	17.9
4	59.7	26.3	55.2	50.1	217	232	11.4	11.2
5	-175.1	-46.3	-172.8	-83.3	225	192	11.8	9.3

### PRO

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-28.2	38.4	-29.1	40.4	941	1117	54.5	55.1
2	30.8	-38.7	32.1	-39.2	786	912	45.5	44.9

### TRP

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-61.9	87.5	-68.1	86.2	76	91	40.6	41.4
2	-177.0	81.2	-177.5	82.8	22	36	11.8	16.4
3	62.5	-82.4	61.4	-96.4	18	14	9.6	6.4
4	-65.8	-8.6	-76.2	0.0	18	18	9.6	8.2
5	-177.9	-110.7	-174.2	-107.1	17	26	9.1	11.8
6	-70.5	-88.4	-61.8	-95.6	16	12	8.6	5.5
7	62.2	84.7	61.4	81.9	14	16	7.5	7.3

### TYR

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-62.6	93.9	-66.3	96.0	322	332	50.6	46.2
2	178.1	74.9	178.8	77.3	201	268	31.6	37.3
3	56.2	96.6	60.4	89.8	73	78	11.5	10.9
4	-68.4	-1.2	-63.7	-27.0	36	36	5.7	5.0

## GLU

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	rotamer occupancy		rotamer share, %	
	U			B			U	B	U	B
1	-69.1	177.7	-7.2	-59.6	-177.0	-54.5	633	633	21.6	19.2
2	-67.2	176.4	51.1	-73.7	179.2	53.0	355	470	12.1	14.2
3	-176.6	179.2	-6.6	-178.4	173.3	-4.3	363	455	12.4	13.8
4	-68.7	-58.0	-59.1	-68.4	-66.7	-60.0	339	387	11.6	11.7
5	176.5	170.1	42.8	-176.3	-178.8	-55.1	260	303	8.9	9.2
6	-178.5	61.2	21.6	-176.1	57.0	51.3	205	219	7.0	6.6
7	-67.5	80.2	10.4	-66.3	84.6	-2.8	112	88	3.8	2.7
8	57.0	-177.6	54.5	63.5	-93.8	25.3	120	74	4.1	2.2
9	68.8	176.1	-50.6	68.5	173.7	-56.0	107	142	3.6	4.3
10	-64.6	-82.2	38.2	-69.6	-51.1	74.2	71	102	2.4	3.1
11	65.7	-90.1	35.5	64.5	-174.6	0.9	57	78	1.9	2.4
12	-63.9	91.6	-41.5	-72.5	62.8	54.2	72	120	2.5	3.6
13	-177.1	-77.9	-33.5	-120.4	-55.9	-43.1	47	39	1.6	1.2
14	-168.2	69.2	-62.1	176.8	72.8	3.8	32	93	1.1	2.8
15	61.9	-103.7	73.2				37		1.3	

## GLN

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	rotamer occupancy		rotamer share, %	
	U			B			U	B	U	B
1	-61.0	-171.3	-46.5	-58.0	-176.8	-46.3	280	327	16.6	17.3
2	-73.5	174.1	50.0	-68.0	178.0	53.2	256	223	15.2	11.8
3	-60.6	-60.0	-57.7	-59.6	-55.5	-55.9	190	186	11.3	9.9
4	175.6	-174.6	60.5	177.6	177.6	53.0	128	116	7.6	6.1
5	-65.4	174.2	-180.0	-67.1	-179.0	171.8	132	128	7.8	6.8
6	-167.7	59.8	49.5	-179.3	58.2	63.0	100	131	5.9	6.9
7	-175.9	178.9	-58.9	-174.4	-175.5	-55.5	95	143	5.6	7.6
8	-65.3	-56.8	120.2	-59.2	-54.2	131.0	88	109	5.2	5.8
9	162.3	-151.7	139.7	175.6	178.0	172.9	63	61	3.7	3.2
10	69.5	-177.7	-57.4	63.1	-179.4	-55.7	41	44	2.4	2.3
11	179.3	71.0	-171.6	-173.0	67.3	-66.6	37	68	2.2	3.6
12	-58.9	82.7	37.5	-81.6	67.8	48.6	37	40	2.2	2.1
13	-158.4	72.6	-52.4				29		1.7	
14	56.9	-174.4	59.3	48.6	179.0	53.3	21	42	1.2	2.2
15	66.8	-91.3	29.1	81.8	-77.7	25.8	16	24	0.9	1.3
16	41.5	-172.4	179.1				13		0.8	
17	-73.6	71.6	-164.9	-64.8	102.9	-50.4	15	33	0.9	1.7

## MET

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	rotamer occupancy		rotamer share, %	
	U			B			U	B	U	B
1	-61.0	-60.7	-71.0	-59.4	-54.3	-72.4	61	60	19.6	18.2
2	-68.3	179.8	-87.4	-59.1	-171.9	-78.3	41	35	13.2	10.6
3	-62.1	176.7	83.3	-67.9	175.4	66.6	36	45	11.6	13.7
4	171.9	161.1	65.2	-174.6	-176.9	76.2	18	13	5.8	4.0
5	-58.1	-61.9	106.4	-69.3	-62.7	108.7	23	23	7.4	7.0
6	-65.5	176.1	-170.9	-83.0	172.7	171.5	18	13	5.8	4.0
7	-177.2	-174.8	-70.0	-175.1	172.3	-67.7	17	32	5.5	9.7
8	-169.9	60.8	79.2	-174.0	60.3	72.5	14	24	4.5	7.3
9	-164.1	87.8	-118.5				11		3.5	
9				64.3	168.6	73.7		8		2.4
10	76.0	-178.9	-68.1	59.2	-175.9	-70.8	8	13	2.6	4.0

## ARG

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>4</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>4</sub>	rotamer occupancy		rotamer share, %	
	U				B				U	B	U	B
1	-59.2	177.1	179.8	179.9	-59.9	-175.4	-179.8	-177.2	182	167	10.2	8.3
2	-72.8	169.3	179.1	-77.1	-61.8	-179.7	-170.6	-73.8	93	105	5.2	5.2
3	-172.9	177.3	-179.7	180.0	-178.6	-175.8	179.4	-177.3	85	108	4.7	5.4
4	-62.4	165.0	80.2	167.9	-49.5	-169.4	75.8	-170.7	96	102	5.4	5.1
5	-169.5	179.0	-60.5	144.4	-176.1	-152.3	-63.8	143.1	93	91	5.2	4.5
6	-67.9	179.0	-65.6	101.9	-67.6	179.2	-67.6	175.7	102	98	5.7	4.9
7	-70.5	-170.1	-65.9	-89.4	-75.1	-162.5	-68.9	-77.6	81	90	4.5	4.5
8	-67.3	-171.9	177.4	99.1	-64.6	178.3	175.1	63.8	71	84	4.0	4.2
9	-62.4	-63.4	178.2	-176.1	-67.1	-62.0	178.7	173.3	60	52	3.4	2.6
10	178.3	-169.5	56.4	-162.1	-175.6	162.8	51.8	-175.3	78	86	4.4	4.3
11	-173.1	178.3	-62.1	-79.4	179.6	166.5	-61.2	-84.1	56	50	3.1	2.5
12	175.8	179.0	60.9	70.1	-179.2	178.2	56.5	76.2	48	62	2.7	3.1
13	177.4	178.2	173.6	75.7	176.3	-173.7	179.4	65.4	33	34	1.8	1.7
14	-61.0	-172.5	72.0	80.2	-65.5	-179.0	59.2	76.4	32	33	1.8	1.6
15	60.2	-178.3	174.5	71.5	66.2	-174.3	173.6	93.9	34	30	1.9	1.5
16	173.9	175.1	173.3	-78.3	-168.5	165.4	172.1	-72.8	31	44	1.7	2.2
17	56.0	177.7	68.6	-170.3	54.5	154.8	61.2	149.3	26	28	1.5	1.4
18	87.1	-168.5	-54.6	173.6	49.4	-177.4	-71.4	-171.5	27	32	1.5	1.6
19	-179.7	51.5	-179.6	168.3	179.8	71.9	-168.0	-177.2	24	19	1.3	0.9
20	-64.0	-78.7	-74.8	-176.6	-71.1	-79.5	-72.0	176.7	22	44	1.2	2.2
21	70.7	-172.8	177.4	-77.5	54.8	177.9	-171.8	-75.8	21	21	1.2	1.0
22	-59.1	-70.6	-173.2	-75.4	-69.6	-64.3	-179.7	-92.2	23	30	1.3	1.5
23	70.4	-170.0	-179.5	-180.0	69.8	165.0	-173.7	172.9	19	30	1.1	1.5
24	-179.7	70.2	-171.1	85.1	159.8	71.7	-176.6	-76.6	17	19	0.9	0.9

25	-64.3	-62.3	-55.0	-84.2					16		0.9	
25					-60.2	-60.5	160.4	65.1		20		1.0
26					177.6	115.5	77.1	-163.6		19		0.9

LYS

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>4</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>4</sub>	rotamer occupancy		rotamer share, %	
	U				B				U	B	U	B
1	-65.1	-177.8	-178.7	-179.5	-64.8	-177.1	-179.4	-178.6	611	648	20.6	19.1
2	-178.3	-177.7	178.1	-179.0	-177.8	-179.5	179.2	-178.8	325	373	11.0	11.0
3	-65.9	-62.9	-178.5	-177.4	-67.3	-65.7	-177.7	177.5	176	193	5.9	5.7
4	-60.3	178.9	179.5	62.0	-63.4	-177.7	-174.7	59.7	141	163	4.8	4.8
5	-64.8	175.3	-179.3	-65.3	-62.7	-179.5	-178.3	-60.0	123	140	4.1	4.1
6	-178.7	176.4	-178.7	-64.6	-178.1	176.2	-175.5	-68.0	97	111	3.3	3.3
7	-68.7	-176.1	-69.0	-178.2	-73.5	-172.6	-68.9	-172.6	95	113	3.2	3.3
8	-59.7	175.4	66.6	177.6	-66.4	-178.9	64.2	-179.5	89	117	3.0	3.5
9	-179.3	178.4	176.0	58.3	-171.9	174.1	-177.7	59.4	85	100	2.9	3.0
10	64.9	179.2	176.9	-177.6	63.3	-179.9	-174.0	-179.9	82	89	2.8	2.6
11	179.4	67.1	174.1	178.8	-175.7	60.3	-178.4	-179.9	81	114	2.7	3.4
12	-178.2	173.5	67.7	172.6	-171.4	177.0	64.7	-179.7	75	92	2.5	2.7
13	-51.7	-55.8	-174.3	-65.4	-64.6	-55.4	171.7	-61.3	55	54	1.9	1.6
14	-178.8	-168.1	-63.6	179.3	178.2	178.6	-65.2	-174.6	60	65	2.0	1.9
15	-68.7	-69.0	-172.6	62.9	-56.8	-69.6	-174.4	53.7	54	70	1.8	2.1
16	-60.8	-66.9	-57.5	-178.2	-54.7	-62.8	-67.3	180.0	37	32	1.2	0.9
17	68.0	-176.2	-171.5	-55.9					33		1.1	
					-65.8	-175.4	-65.3	-65.0		34		1.0
18	61.1	171.8	67.3	176.7					28		0.9	
					-173.7	72.7	174.5	-61.6		33		1.0
19	179.5	-177.4	-58.1	-59.2					27		0.9	
20	174.7	60.8	164.9	59.0	-179.6	61.1	-178.5	57.4	34	38	1.1	1.1
21	53.3	-170.5	-61.3	176.8	69.0	174.5	-64.1	-177.4	26	29	0.9	0.9

## INTERFACE SURFACE LIBRARY

### CYS

rotamer	$X_1$		rotamer occupancy		rotamer share, %	
	U	B	U	B	U	B
1	-69.8	-66.2	20	29	50.0	50.0
2	-179.0	178.8	11	17	27.5	29.3
3	74.9	62.1	9	11	22.5	19.0

### SER

rotamer	$X_1$		rotamer occupancy		rotamer share, %	
	U	B	U	B	U	B
1	58.1	62.7	146	192	43.8	44.8
2	-61.7	-58.2	102	141	30.6	32.9
3	179.3	177.0	79	91	23.7	21.2

### THR

rotamer	$X_1$		rotamer occupancy		rotamer share, %	
	U	B	U	B	U	B
1	62.5	55.1	171	205	53.3	50.5
2	-59.3	-61.1	121	163	37.7	40.1
3	-174.3	-174.0	21	31	6.5	7.6

### VAL

rotamer	$X_1$		rotamer occupancy		rotamer share, %	
	U	B	U	B	U	B
1	173.7	177.3	110	166	62.9	64.1
2	-61.5	-62.2	40	64	22.9	24.7
3	70.4	67.9	22	23	12.6	8.9

### ASP

rotamer	$X_1$	$X_2$	$X_1$	$X_2$	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-70.5	-26.3	-62.3	-33.9	140	192	42.6	44.3
2	-166.4	14.5	-174.7	11.6	61	80	18.5	18.5
3	61.2	0.9	63.3	10.3	45	63	13.7	14.5
4	-176.4	59.9	-175.5	76.0	42	42	12.8	9.7

5	-53.6	71.8	-53.4	-82.2	27	33	8.2	7.6
6	44.3	44.6	56.6	87.0	14	22	4.3	5.1

### PHE

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-58.8	105.0	-61.3	86.3	52	86	48.1	48.9
2	177.6	76.4	177.0	77.4	41	57	38.0	32.4
3	51.6	76.8	60.4	81.8	13	27	12.0	15.3
4			-66.3	-18.6		5		2.8

### HIS

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-71.1	85.6	-63.3	91.1	26	36	20.6	20.7
2	78.4	-101.0	72.0	-93.2	26	28	20.6	16.1
3	-61.6	-76.7	-54.8	-79.6	24	43	19.0	24.7
4	-174.6	80.9	-174.5	91.6	16	15	12.7	8.6
5	-62.2	137.4	-74.3	-167.9	12	17	9.5	9.8
6	-147.8	-44.5	-167.4	-83.0	9	14	7.1	8.0
7	-167.9	-154.1	176.5	-154.0	4	7	3.2	4.0
8	65.3	96.2	78.0	111.7	5	11	4.0	6.3
9	-65.2	6.6			3		2.4	

### ILE

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-63.1	171.4	-62.3	174.9	64	111	47.1	55.0
2	-60.5	-57.8	-57.6	-62.2	25	36	18.4	17.8
3	64.2	169.7	57.8	169.8	19	21	14.0	10.4
4	-168.1	167.8	179.6	169.7	11	12	8.1	5.9
5	-170.7	61.0	-171.7	70.4	5	11	3.7	5.4
6	-106.0	71.5	-34.9	84.9	4	6	2.9	3.0
7	28.7	104.7	60.6	70.3	6	5	4.4	2.5

## LEU

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-63.4	175.9	-67.7	174.3	161	203	65.7	58.3
2	179.8	57.6	-179.5	61.8	47	70	19.2	20.1
3	-99.6	28.1	-98.1	30.0	13	28	5.3	8.0
4	-83.1	-71.6	-72.5	-51.6	8	10	3.3	2.9
5	-133.1	-65.3	-159.8	-65.8	5	4	2.0	1.1
6	100.6	121.9	-145.0	-146.8	5	15	2.0	4.3
7	-148.3	-140.5			5		2.0	
7			-84.1	109.5		9		2.6
8			45.2	86.1		4		1.1
9			32.3	176.6		3		0.9

## ASN

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-66.5	-50.2	-68.9	-37.3	124	141	42.6	40.3
2	-177.5	66.9	-178.8	42.8	52	53	17.9	15.1
3	-72.7	152.3	-71.3	173.0	40	62	13.7	17.7
4	-166.6	-51.5	-178.3	-79.2	34	45	11.7	12.9
5	61.5	21.8	64.0	24.6	16	30	5.5	8.6

## PRO

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-29.5	38.1	-28.5	40.6	127	151	50.8	51.2
2	32.3	-39.5	30.2	-40.8	123	144	49.2	48.8

## TRP

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-63.2	93.5	-71.3	85.4	21	43	33.3	43.0
2	175.1	-107.1	177.0	-108.0	11	13	17.5	13.0
3	-68.2	-25.0	-51.3	-22.7	9	11	14.3	11.0
4	-75.8	-96.4	-61.7	-84.8	7	4	11.1	4.0
5	61.4	94.2	62.4	85.2	4	4	6.3	4.0
6	-176.2	69.2	-177.7	69.5	4	9	6.3	9.0
7	54.6	-93.0	55.7	-93.3	3	14	4.8	14.0



TYR

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-65.0	88.8	-69.2	88.2	86	143	42.6	48.3
2	-174.3	70.8	-179.7	74.8	69	93	34.2	31.4
3	61.2	93.5	61.5	94.7	28	37	13.9	12.5
4	-64.8	146.4	-70.9	-21.1	18	20	8.9	6.8

GLU

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	rotamer occupancy		rotamer share, %	
	U			B			U	B	U	B
1	-62.1	-178.4	-14.1	-62.9	177.9	3.5	89	104	21.4	19.1
2	-177.8	177.1	-7.9	178.2	174.7	-13.8	66	83	15.9	15.2
3	-70.1	-176.8	60.1	-67.5	176.3	55.3	47	69	11.3	12.7
4	179.9	177.2	56.5	-176.4	-169.4	-49.3	36	41	8.7	7.5
5	-58.9	-69.2	-46.8	-70.2	-64.9	-76.7	32	60	7.7	11.0
6	-175.5	56.6	45.9	-177.9	55.6	30.1	26	26	6.3	4.8
7	70.7	-174.0	18.6	65.7	-177.7	18.6	24	18	5.8	3.3
8	-58.4	48.0	62.2	-72.5	76.1	23.5	19	25	4.6	4.6
9	-68.1	-64.2	20.2	-87.3	-74.5	77.0	15	14	3.6	2.6
10	43.7	175.3	-65.0	66.5	179.8	-63.0	9	17	2.2	3.1
11	145.6	106.7	-71.9	-158.3	51.5	-81.4	10	13	2.4	2.4
12	68.7	-94.0	28.0	70.2	-85.2	39.1	6	14	1.4	2.6
13	28.1	-72.1	0.6				3		0.7	
				29.4	68.8	27.1		4		0.7

GLN

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	rotamer occupancy		rotamer share, %	
	U			B			U	B	U	B
1	-62.4	-175.8	57.7	-60.4	-169.9	-56.6	42	53	15.7	14.8
2	-65.1	-52.3	-49.2	-59.5	-58.3	-40.2	38	35	14.2	9.8
3	-61.8	179.8	-55.4	-65.4	-174.4	53.8	36	40	13.4	11.2
4	-174.0	-177.2	-47.9	-179.1	-152.6	-63.0	19	23	7.1	6.4
5	-158.3	58.8	68.6	-161.4	57.6	53.0	15	17	5.6	4.8
6	-80.3	-155.9	173.8	-72.9	-172.5	-142.8	13	27	4.9	7.6
7	-176.3	179.1	134.5	-169.0	-174.8	57.9	12	29	4.5	8.1
8	179.3	71.0	-171.5	-179.0	49.9	-87.8	11	7	4.1	2.0
9	-59.3	-95.7	101.8	-63.5	-63.6	153.9	8	20	3.0	5.6
10	75.9	176.7	75.6	53.9	-164.5	50.9	6	7	2.2	2.0
11	-76.1	77.8	7.9	-83.4	79.5	23.0	6	13	2.2	3.6
12	46.3	-172.0	-95.8	44.8	169.2	-68.6	6	10	2.2	2.8
13	-173.7	-109.5	55.0	-173.6	174.4	-173.7	4	11	1.5	3.1

14	-68.6	74.6	-170.3	-64.5	91.1	136.7	3	5	1.1	1.4
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### MET

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	rotamer occupancy		rotamer share, %	
	U			B			U	B	U	B
1	-79.8	-52.6	-97.0	-52.7	-69.5	-92.0	10	23	13.7	19.3
2	-71.4	172.1	-55.2	-121.3	-174.6	-56.0	7	11	9.6	9.2
3	-64.5	172.5	66.1	-67.0	179.7	79.5	7	21	9.6	17.6
4	-161.5	165.1	87.7				5		6.8	
4				-63.8	-177.9	-71.8		10		8.4
5	177.7	177.8	174.8				4		5.5	
5				-69.1	168.3	162.9		8		6.7
6	53.8	-148.2	17.0				4		5.5	
6				-78.7	-59.4	104.5		6		5.0

### ARG

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>4</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>4</sub>	rotamer occupancy		rotamer share, %	
	U				B				U	B	U	B
1	-72.0	178.5	177.0	-176.7	-69.9	167.0	171.6	-173.0	31	47	9.5	9.9
2	-72.1	140.9	-174.1	86.7	-61.6	-158.9	179.6	84.2	24	21	7.4	4.4
3	-163.8	-144.6	-37.4	162.7	158.3	166.9	-30.3	171.8	17	17	5.2	3.6
4	-174.7	161.7	-165.9	173.1	-174.4	174.4	-178.6	177.3	15	23	4.6	4.9
5	-54.0	175.5	-174.2	-78.6	-72.6	170.9	171.0	-74.0	15	17	4.6	3.6
6	-56.9	-164.2	-58.3	-81.6	-60.4	-166.7	-61.5	174.9	14	28	4.3	5.9
7	-86.2	174.2	-91.7	154.1	-66.8	-164.6	-69.0	-88.8	14	13	4.3	2.7
8	-62.4	-57.9	-172.6	-174.5	-60.2	-69.4	-168.0	-174.7	13	8	4.0	1.7
9	-72.2	-162.5	64.3	-168.9	-67.8	-168.9	65.7	-173.8	11	22	3.4	4.6
10	-171.7	171.8	106.6	-129.7	-172.5	169.6	60.6	-159.6	10	13	3.1	2.7
11	102.8	172.9	171.4	-153.4	179.7	100.9	175.5	162.7	9	9	2.8	1.9
12	-69.5	170.0	91.7	-106.8	-65.8	172.2	58.1	92.4	8	14	2.5	3.0
13	-46.8	-64.8	-164.5	73.7	-58.8	-71.2	176.1	55.4	7	7	2.2	1.5
14	-177.2	174.3	165.6	75.6	177.0	178.1	175.5	-67.3	7	14	2.2	3.0
15	176.8	73.5	-168.3	-175.0					6		1.8	
16	-164.7	172.3	-169.0	-99.3					7		2.2	
16					71.1	176.7	177.8	-75.7		10		2.1
17	-171.0	-173.3	-57.2	-81.9	178.3	176.6	-70.2	-79.0	5	14	1.5	3.0
18	55.0	-173.0	175.6	98.1	81.8	167.6	164.9	80.0	5	9	1.5	1.9
19	173.1	78.5	171.3	80.9					4		1.2	
20	173.1	65.4	64.2	82.2					4		1.2	
21	55.7	157.6	-74.9	178.3	64.1	-176.5	-69.5	156.0	4	8	1.2	1.7
22	178.2	-170.1	68.4	67.4	179.3	168.2	61.1	83.4	3	8	0.9	1.7
23	-31.2	-164.8	69.6	64.2					3		0.9	
24	-97.7	-60.2	-172.1	-61.0	-71.3	-68.8	-176.3	-76.5	3	12	0.9	2.5

25	-64.2	-62.3	-54.9	-84.3					3		0.9	
26	-46.1	-43.9	-66.2	160.2	-44.4	-59.8	-106.7	152.7	3	5	0.9	1.1

### LYS

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>4</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>4</sub>	rotamer occupancy		rotamer share, %	
	U				B				U	B	U	B
1	-69.3	-179.7	179.2	-180.0	-66.5	178.8	179.6	177.2	91	106	21.3	19.1
2	-173.2	179.9	179.7	-176.8	-175.5	-179.1	175.5	-174.4	42	58	9.8	10.5
3	-62.3	-64.5	175.8	174.5	-60.0	-59.1	-179.7	179.9	26	45	6.1	8.1
4	-62.6	-177.7	179.8	-58.1	-71.2	-166.9	-159.0	-60.5	23	20	5.4	3.6
5	66.8	-179.2	180.0	173.3	63.2	-179.6	-179.3	177.1	16	17	3.7	3.1
6	-72.0	-167.1	-69.2	-175.9	-67.0	-170.9	-63.1	-176.9	15	20	3.5	3.6
7	-53.2	-154.3	179.3	61.0	-68.7	-170.5	-177.8	64.9	15	25	3.5	4.5
8	-179.0	171.5	62.8	171.9	-136.6	173.9	77.4	146.2	12	10	2.8	1.8
9	-177.0	-178.1	-178.1	67.6	177.6	175.4	165.3	52.9	11	16	2.6	2.9
10	-102.5	-158.3	62.4	-177.4	-65.3	176.5	53.6	-175.9	10	17	2.3	3.1
11	175.6	-179.0	-177.0	-70.0	177.4	-159.1	-176.1	-48.0	9	13	2.1	2.3
12	-169.4	176.3	-21.4	-63.5	-109.3	-173.6	-87.4	-46.6	8	6	1.9	1.1
13	-86.3	-69.7	-177.6	-52.6					8		1.9	
14	-178.7	58.2	-175.3	173.2	174.6	74.2	175.2	-66.5	8	8	1.9	1.4
15	174.6	60.8	164.9	59.0	-159.4	75.8	179.0	177.7	8	14	1.9	2.5
16	-168.2	-171.7	-72.1	177.7	-164.0	170.5	-64.0	169.9	7	18	1.6	3.2
17	-74.9	-177.1	102.1	46.4	175.5	-154.1	-105.2	78.6	7	5	1.6	0.9
18	-67.8	-63.7	166.9	63.6	-67.5	-54.0	169.5	69.2	6	7	1.4	1.3
19	-168.9	-174.2	63.8	61.4					6		1.4	
19					-62.2	-101.8	-158.7	-69.9		13		2.3
20	61.1	171.8	67.3	176.7	71.1	167.7	61.5	-178.3	5	7	1.2	1.3
21	-88.7	-58.4	-61.6	168.9	-52.5	-66.7	-72.6	-173.1	4	6	0.9	1.1
22	78.3	-172.7	158.0	62.8					4		0.9	
22					67.0	-169.7	-65.9	-175.1		5		0.9
23	-141.3	95.2	60.2	-167.5	-159.0	53.6	57.6	-175.9	4	5	0.9	0.9

**Table S3.** Non-redundant rotamer libraries**FULL SURFACE LIBRARY****CYS**

rotamer	$X_1$		rotamer occupancy		rotamer share, <sup>c</sup> %	
	U <sup>a</sup>	B <sup>b</sup>	U	B	U	B
1	-65.6	-61.0	129	129	57.8	52.0
2	-175.3	-177.3	53	55	23.8	22.2
3	65.3	63.4	41	57	18.4	23.0

**SER**

rotamer	$X_1$		rotamer occupancy		rotamer share, %	
	U	B	U	B	U	B
1	61.8	62.9	1366	1683	49.8	50.0
2	-63.6	-62.0	825	1000	30.1	29.7
3	177.6	-179.5	551	680	20.1	20.2

**THR**

rotamer	$X_1$		rotamer occupancy		rotamer share, %	
	U	B	U	B	U	B
1	61.0	61.3	1197	1376	51.1	49.5
2	-59.7	-59.4	953	1199	40.7	43.1
3	-174.7	-178.3	192	206	8.2	7.4

**VAL**

rotamer	$X_1$		rotamer occupancy		rotamer share, %	
	U	B	U	B	U	B
1	177.7	177.4	802	949	68.1	69.0
2	-62.9	-62.1	254	293	21.6	21.3
3	61.7	67.9	117	129	9.9	9.4

<sup>a</sup> Unbound.<sup>b</sup> Bound.

<sup>c</sup> Share of rotamer  $i$  is  $\frac{N_i}{\sum_i N_i + N_{non}}$  100%, where  $N_i$  is rotamer occupancy,  $N_{non}$  is the number of non-rotamer conformations, the sum runs over all rotamers.

PRO

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-29.0	38.6	-29.1	40.4	1076	1269	54.4	54.6
2	30.8	-38.7	30.5	-39.8	901	1055	45.6	45.4

TRP

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-61.9	87.5	-68.1	86.2	98	132	39.2	41.3
2	-177.9	-110.7	-179.2	-108.5	28	40	11.2	12.5
3	-65.8	-8.6	-76.2	0.0	26	26	10.4	8.1
4	177.6	74.3	-177.5	82.8	26	45	10.4	14.1
5	61.5	-92.2	61.4	-96.4	21	28	8.4	8.8
6	-54.4	-59.9	-61.8	-95.6	23	20	9.2	6.3
7	60.9	92.9	64.4	82.4	16	20	6.4	6.3

ASP

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-72.0	-14.7	-70.4	-16.2	1415	1708	51.0	51.9
2	-174.4	8.2	-173.8	1.8	805	932	29.0	28.3
3	63.6	1.6	61.3	2.2	552	646	19.9	19.6

PHE

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-62.1	99.1	-62.3	102.8	294	355	52.0	53.5
2	179.8	75.8	-180.0	75.3	210	224	37.2	33.8
3	61.4	87.5	65.4	90.7	58	80	10.3	12.1

HIS

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-62.6	-67.6	-60.6	-70.9	457	530	56.6	57.9
2	179.8	66.9	-178.2	83.1	228	248	28.2	27.1
3	76.1	-89.5	72.0	-93.2	114	125	14.1	13.7

ILE

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-63.1	172.2	-63.9	175.7	502	611	72.1	72.7
2	65.2	174.6	62.5	173.8	113	129	16.2	15.4
3	-168.6	172.6	-180.0	171.0	65	84	9.3	10.0

LEU

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-63.4	175.1	-65.1	175.2	921	1136	68.8	70.7
2	-178.3	60.3	-176.6	63.6	382	428	28.5	26.6
3	53.9	74.5	58.8	174.7	32	36	2.4	2.2

ASN

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-64.7	-47.4	-61.3	-47.2	1249	1436	57.0	59.2
2	-173.3	58.0	-168.8	49.6	622	645	28.4	26.6
3	59.6	13.8	55.2	50.1	236	262	10.8	10.8

TYR

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-62.6	93.9	-66.3	96.0	462	531	55.1	52.4
2	178.1	74.8	-179.7	74.8	270	360	32.2	35.5
3	61.1	93.5	60.4	89.8	102	115	12.2	11.3

GLU

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	rotamer occupancy		rotamer share, %	
	U			B			U	B	U	B
1	-67.6	176.4	-10.0	-59.6	-177.0	-54.5	1126	1285	33.6	33.4
2	-176.6	179.2	-6.6	-177.3	179.3	-7.5	729	887	21.8	23.1
3	-68.7	-58.0	-59.1	-68.4	-66.7	-60.0	465	686	13.9	17.8
4	-178.1	62.2	24.6	-177.9	58.8	48.5	275	245	8.2	6.4
5	59.8	177.5	30.8	68.5	173.7	-56.0	260	251	7.8	6.5
6	-67.5	80.2	10.4	-72.5	62.8	54.2	214	247	6.4	6.4
7	65.7	-90.1	35.5	59.3	-75.8	-2.6	109	101	3.3	2.6
8	-177.1	-77.9	-33.5	-173.5	-91.0	-20.5	51	37	1.5	1.0

## GLN

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	rotamer occupancy		rotamer share, %	
	U			B			U	B	U	B
1	-62.4	-170.7	-50.7	-61.2	-179.3	-55.0	764	796	39.1	35.5
2	-60.6	-60.0	-57.7	-62.9	-58.0	-57.4	334	431	17.1	19.2
3	175.6	-174.6	60.5	-174.4	-175.5	-55.5	325	391	16.6	17.4
4	-167.7	59.8	49.5	-174.1	54.8	60.3	192	173	9.8	7.7
5	69.5	-177.7	-57.4	51.8	-177.2	54.2	93	132	4.8	5.9
6	-71.6	79.6	7.0	-81.6	67.8	48.6	45	93	2.3	4.1
7	55.8	-95.5	30.8	71.3	-91.5	35.9	19	27	1.0	1.2
8	-172.6	-87.1	-31.1				13		0.7	

## MET

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	rotamer occupancy		rotamer share, %	
	U			B			U	B	U	B
1	-61.0	-60.7	-71.0	-57.8	-54.4	-70.0	112	115	29.2	25.7
2	-65.6	178.2	-54.5	-67.9	175.4	66.6	111	175	28.9	39.1
3	171.9	161.0	65.1	-174.6	-176.9	76.2	45	23	11.8	5.1
4	170.6	75.0	-85.7	-177.5	55.7	75.6	12	29	3.1	6.5
5	76.0	-178.9	-68.1	59.2	-175.9	-70.8	9	25	2.3	5.6

## ARG

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>4</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>4</sub>	rotamer occupancy		rotamer share, %	
	U				B				U	B	U	B
1	-59.2	177.1	179.8	179.9	-59.9	-175.4	-179.8	-177.2	660	702	31.1	28.3
2	-172.9	177.3	-179.7	180.0	-179.6	177.7	180.0	-178.3	141	174	6.7	7.0
3	-68.6	-165.7	-67.0	-82.5	-70.0	-163.1	-61.0	-85.9	218	230	10.3	9.2
4	-62.4	-63.4	178.2	-176.1	-67.1	-62.0	178.7	173.3	155	184	7.4	7.4
5	-171.7	171.8	106.6	-129.7	-172.4	174.8	61.5	-171.2	201	274	9.5	11
6	-177.0	-179.3	-68.4	-92.6	179.6	166.5	-61.2	-84.1	99	112	4.6	4.5
7	60.2	-178.3	174.5	71.5	58.7	-176.4	176.4	97.8	93	79	4.4	3.2
8	-179.7	51.5	-179.6	168.3	176.5	69.0	-169.7	-177.7	51	53	2.4	2.1
9	-64.3	-62.2	-55.0	-84.2					21		1.0	
9					177.9	111.2	69.0	173.0		23		0.9

LYS

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>4</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>4</sub>	rotamer occupancy		rotamer share, %	
	U				B				U	B	U	B
1	-65.5	-178.1	179.5	-179.8	-66.1	-178.3	178.0	179.2	1275	1490	37.6	37.8
2	-178.3	-177.7	178.1	-179.0	-177.8	-179.5	179.2	-178.8	780	905	23.0	23.0
3	-65.9	-62.9	-178.5	-177.4	-67.3	-65.7	-177.7	177.5	307	355	9.1	9.0
4	64.9	179.2	176.9	-177.6	63.3	-179.9	-174.0	-179.9	169	142	5.0	3.6
5	179.4	67.1	174.1	178.8	-175.7	60.3	-178.4	-179.9	128	165	3.8	4.2



## NON-INTERFACE SURFACE LIBRARY

### CYS

rotamer	$X_1$		rotamer occupancy		rotamer share, %	
	U	B	U	B	U	B
1	-65.6	-62.1	109	103	59.6	54.2
2	-173.9	-173.4	42	38	23.0	20.0
3	65.1	61.3	32	46	17.5	24.2

### SER

rotamer	$X_1$		rotamer occupancy		rotamer share, %	
	U	B	U	B	U	B
1	61.8	61.0	1218	1487	50.6	50.7
2	-62.8	-62.0	721	858	29.9	29.2
3	177.5	179.3	470	589	19.5	20.1

### THR

rotamer	$X_1$		rotamer occupancy		rotamer share, %	
	U	B	U	B	U	B
1	61.0	61.3	1026	1166	50.8	49.1
2	-61.4	-59.4	830	1035	41.1	43.6
3	-174.7	-176.3	162	174	8.0	7.3

### VAL

rotamer	$X_1$		rotamer occupancy		rotamer share, %	
	U	B	U	B	U	B
1	177.7	177.4	692	783	69.0	70.2
2	-60.5	-62.1	212	229	21.1	20.5
3	61.7	67.6	95	91	9.5	8.2

### PRO

rotamer	$X_1$	$X_2$	$X_1$	$X_2$	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-28.2	38.4	-29.1	40.4	941	1117	54.5	55.1
2	30.8	-38.7	32.1	-39.2	786	912	45.5	44.9

## TRP

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-61.9	87.5	-68.1	86.2	76	91	40.6	41.4
2	-177.0	81.2	-177.5	82.8	22	36	11.8	16.4
3	62.5	-82.4	61.4	-96.4	18	14	9.6	6.4
4	-65.8	-8.6	-76.2	0.0	18	18	9.6	8.2
5	-177.9	-110.7	-174.2	-107.1	17	26	9.1	11.8
6	-70.5	-88.4	-61.8	-95.6	16	12	8.6	5.5
7	62.2	84.7	61.4	81.9	14	16	7.5	7.3

## ASP

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-72.0	-14.7	-70.4	-16.2	1247	1485	50.9	52.0
2	-174.4	8.2	-172.3	56.2	703	803	28.7	28.1
3	63.6	1.6	60.8	-6.3	497	562	20.3	19.7

## PHE

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-62.1	99.1	-62.3	102.8	242	265	53.0	54.4
2	-177.6	76.3	-180.0	75.3	169	167	37.0	34.3
3	61.4	87.5	66.6	94.0	45	53	9.8	10.9

## HIS

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-62.6	-67.6	-56.0	-62.2	392	433	57.5	58.4
2	176.7	68.9	176.0	75.2	200	209	29.3	28.2
3	66.5	-70.8	61.4	-65.7	85	88	12.5	11.9

## ILE

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-63.1	172.2	-63.9	175.7	409	461	73.0	72.3
2	65.2	174.6	62.5	173.8	88	103	15.7	16.1
3	-177.5	176.6	-176.2	171.9	49	62	8.8	9.7

## LEU

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-61.9	175.9	-65.1	175.2	742	880	67.8	70.0
2	-178.3	60.3	-179.6	65.3	322	345	29.5	27.4
3	60.1	71.3	58.8	174.7	26	29	2.4	2.3

## ASN

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-64.7	-47.4	-61.3	-47.2	1092	1208	57.4	58.2
2	-173.3	58.0	-168.8	49.6	523	564	27.5	27.2
3	59.7	26.3	55.2	50.1	217	232	11.4	11.2

## TYR

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-62.6	93.9	-66.3	96.0	358	368	56.3	51.3
2	178.1	74.9	178.8	77.3	201	268	31.6	37.3
3	56.2	96.6	60.4	89.8	73	78	11.5	10.9

## GLU

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	rotamer occupancy		rotamer share, %	
	U			B			U	B	U	B
1	-69.1	177.7	-7.2	-59.6	-177.0	-54.5	988	1103	33.7	33.4
2	-176.6	179.2	-6.6	-178.4	173.3	-4.3	623	758	21.2	22.9
3	-68.7	-58.0	-59.1	-68.4	-66.7	-60.0	442	489	15.1	14.8
4	-178.5	61.2	21.6	-176.1	57.0	51.3	205	351	7.0	10.6
5	-67.5	80.2	10.4	-72.5	62.8	54.2	184	208	6.3	6.3
6	57.0	-177.6	54.5	68.5	173.7	-56.0	227	220	7.7	6.7
7	65.7	-90.1	35.5	63.5	-93.8	25.3	94	74	3.2	2.2
8	-177.1	-77.9	-33.5				47		1.6	

## GLN

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	rotamer occupancy		rotamer share, %	
	U			B			U	B	U	B
1	-61.0	-171.3	-46.5	-58.0	-176.8	-46.3	668	678	39.6	35.9
2	-60.6	-60.0	-57.7	-59.6	-55.5	-55.9	278	295	16.5	15.6

3	175.6	-174.6	60.5	-174.4	-175.5	-55.5	286	320	17.0	16.9
4	-167.7	59.8	49.5	-179.3	58.2	63.0	166	199	9.8	10.5
5	69.5	-177.7	-57.4	48.6	179.0	53.3	75	86	4.4	4.6
6	-58.9	82.7	37.5	-81.6	67.8	48.6	52	73	3.1	3.9
7	66.8	-91.3	29.1	81.8	-77.7	25.8	16	24	0.9	1.3

### MET

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	rotamer occupancy		rotamer share, %	
	U			B			U	B	U	B
1	-61.0	-60.7	-71.0	-59.4	-54.3	-72.4	84	107	27.1	32.5
2	-68.3	179.8	-87.4	-67.9	175.4	66.6	95	125	30.5	38.0
3	171.9	161.1	65.2	-174.6	-176.9	76.2	35	13	11.2	4.0
4	-169.9	60.8	79.2	-174.0	60.3	72.5	25	24	8.0	7.3
5	76.0	-178.9	-68.1	59.2	-175.9	-70.8	8	21	2.6	6.4

### ARG

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>4</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>4</sub>	rotamer occupancy		rotamer share, %	
	U				B				U	B	U	B
1	-59.2	177.1	179.8	179.9	-59.9	-175.4	-179.8	-177.2	561	577	31.5	28.7
2	-172.9	177.3	-179.7	180.0	-178.6	-175.8	179.4	-177.3	149	186	8.2	9.3
3	-67.9	179.0	-65.6	101.9	-67.6	179.2	-67.6	175.7	261	274	14.6	13.7
4	-62.4	-63.4	178.2	-176.1	-67.1	-62.0	178.7	173.3	83	82	4.7	4.1
5	-173.1	178.3	-62.1	-79.4	179.6	166.5	-61.2	-84.1	56	50	3.1	2.5
6	175.8	179.0	60.9	70.1	-179.2	178.2	56.5	76.2	48	62	2.7	3.1
7	-61.0	-172.5	72.0	80.2	-65.5	-179.0	59.2	76.4	32	33	1.8	1.6
8	60.2	-178.3	174.5	71.5	66.2	-174.3	173.6	93.9	74	81	4.2	4
9	87.1	-168.5	-54.6	173.6	49.4	-177.4	-71.4	-171.5	27	32	1.5	1.6
10	-179.7	51.5	-179.6	168.3	179.8	71.9	-168.0	-177.2	41	38	2.2	1.8
11	-64.0	-78.7	-74.8	-176.6	-71.1	-79.5	-72.0	176.7	38	44	2.1	2.2
12					-60.2	-60.5	160.4	65.1		20		1.0
13					177.6	115.5	77.1	-163.6		19		0.9

### LYS

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>4</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>4</sub>	rotamer occupancy		rotamer share, %	
	U				B				U	B	U	B
1	-65.1	-177.8	-178.7	-179.5	-64.8	-177.1	-179.4	-178.6	1113	1285	37.5	37.9
2	-178.3	-177.7	178.1	-179.0	-177.8	-179.5	179.2	-178.8	669	741	22.6	21.9
3	-65.9	-62.9	-178.5	-177.4	-67.3	-65.7	-177.7	177.5	268	279	9.0	8.2
4	64.9	179.2	176.9	-177.6	63.3	-179.9	-174.0	-179.9	169	118	5.7	3.5
5	179.4	67.1	174.1	178.8	-175.7	60.3	-178.4	-179.9	115	185	3.9	5.5

## INTERFACE SURFACE LIBRARY

### CYS

rotamer	$X_1$		rotamer occupancy		rotamer share, %	
	U	B	U	B	U	B
1	-69.8	-66.2	20	29	50.0	50.0
2	-179.0	178.8	11	17	27.5	29.3
3	74.9	62.1	9	11	22.5	19.0

### SER

rotamer	$X_1$		rotamer occupancy		rotamer share, %	
	U	B	U	B	U	B
1	58.1	62.7	146	192	43.8	44.8
2	-61.7	-58.2	102	141	30.6	32.9
3	179.3	177.0	79	91	23.7	21.2

### THR

rotamer	$X_1$		rotamer occupancy		rotamer share, %	
	U	B	U	B	U	B
1	62.5	55.1	171	205	53.3	50.5
2	-59.3	-61.1	121	163	37.7	40.1
3	-174.3	-174.0	21	31	6.5	7.6

### VAL

rotamer	$X_1$		rotamer occupancy		rotamer share, %	
	U	B	U	B	U	B
1	173.7	177.3	110	166	62.9	64.1
2	-61.5	-62.2	40	64	22.9	24.7
3	70.4	67.9	22	23	12.6	8.9

### PRO

rotamer	$X_1$	$X_2$	$X_1$	$X_2$	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-29.5	38.1	-28.5	40.6	127	151	50.8	51.2
2	32.3	-39.5	30.2	-40.8	123	144	49.2	48.8

## TRP

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-63.2	93.5	-71.3	85.4	21	43	33.3	43.0
2	175.1	-107.1	177.0	-108.0	11	13	17.5	13.0
3	-68.2	-25.0	-51.3	-22.7	9	11	14.3	11.0
4	-75.8	-96.4	-61.7	-84.8	7	4	11.1	4.0
5	61.4	94.2	62.4	85.2	4	4	6.3	4.0
6	-176.2	69.2	-177.7	69.5	4	9	6.3	9.0
7	54.6	-93.0	55.7	-93.3	3	14	4.8	14.0

## ASP

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-70.5	-26.3	-62.3	-33.9	167	225	50.8	52.0
2	-166.4	14.5	-174.7	11.6	103	122	31.3	28.2
3	61.2	0.9	63.3	10.3	59	85	17.9	19.6

## PHE

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-58.8	105.0	-61.3	86.3	52	91	48.1	51.7
2	177.6	76.4	177.0	77.4	41	57	38.0	32.4
3	51.6	76.8	60.4	81.8	13	27	12.0	15.3

## HIS

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-71.1	85.6	-54.8	-79.6	65	96	51.6	55.2
2	78.4	-101.0	72.0	-93.2	31	39	24.6	22.4
3	-174.6	80.9	-174.5	91.6	29	36	23.0	20.7

## ILE

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-63.1	171.4	-62.3	174.9	93	153	68.4	75.7
2	64.2	169.7	57.8	169.8	25	26	18.4	12.9
3	-168.1	167.8	179.6	169.7	16	23	11.8	11.4

## LEU

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-63.4	175.9	-67.7	174.3	182	250	74.3	71.8
2	179.8	57.6	-179.5	61.8	57	89	23.2	25.6
3	100.6	121.9	45.2	86.1	5	7	2.0	2.0

## ASN

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-66.5	-50.2	-68.9	-37.3	164	203	56.4	58.0
2	-177.5	66.9	-178.8	42.8	86	98	29.6	28.0
3	61.5	21.8	64.0	24.6	16	30	5.5	8.6

## TYR

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>1</sub>	X <sub>2</sub>	rotamer occupancy		rotamer share, %	
	U		B		U	B	U	B
1	-65.0	88.8	-69.2	88.2	104	163	51.5	55.1
2	-174.3	70.8	-179.7	74.8	69	93	34.2	31.4
3	61.2	93.5	61.5	94.7	28	37	13.9	12.5

## GLU

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	rotamer occupancy		rotamer share, %	
	U			B			U	B	U	B
1	-62.1	-178.4	-14.1	-62.9	177.9	3.5	136	173	32.7	31.7
2	-177.8	177.1	-7.9	178.2	174.7	-13.8	112	124	26.9	22.8
3	-58.9	-69.2	-46.8	-70.2	-64.9	-76.7	47	87	11.3	16.0
4	-175.5	56.6	45.9	-177.9	55.6	30.1	26	26	6.3	4.8
5	70.7	-174.0	18.6	65.7	-177.7	18.6	33	35	7.9	6.4
6	-58.4	48.0	62.2	-72.5	76.1	23.5	22	25	5.3	4.6
7	68.7	-94.0	28.0	70.2	-85.2	39.1	6	18	1.4	3.3

## GLN

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	rotamer occupancy		rotamer share, %	
	U			B			U	B	U	B
1	-62.4	-175.8	57.7	-60.4	-169.9	-56.6	91	120	34.0	33.6
2	-65.1	-52.3	-49.2	-59.5	-58.3	-40.2	46	55	17.2	15.4
3	-174.0	-177.2	-47.9	-169.0	-174.8	57.9	35	63	13.1	17.6

4	-158.3	58.8	68.6	-161.4	57.6	53.0	26	24	9.7	6.7
5	75.9	176.7	75.6	44.8	169.2	-68.6	12	17	4.5	4.8
6	-76.1	77.8	7.9	-83.4	79.5	23.0	9	18	3.4	5.0

### MET

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	rotamer occupancy		rotamer share, %	
	U			B			U	B	U	B
1	-79.8	-52.6	-97.0	-52.7	-69.5	-92.0	10	29	13.7	24.3
2	-71.4	172.1	-55.2	-67.0	179.7	79.5	14	39	19.2	32.7
3	-161.5	165.1	87.7	-121.3	-174.6	-56.0	9	11	12.3	9.2
4	53.8	-148.2	17.0				4		5.5	

### ARG

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>4</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>4</sub>	rotamer occupancy		rotamer share, %	
	U				B				U	B	U	B
1	-72.0	178.5	177.0	-176.7	-69.9	167.0	171.6	-173.0	67	84	20.6	17.7
2	-72.1	140.9	-174.1	86.7	-61.6	-158.9	179.6	84.2	24	21	7.4	4.4
3	-163.8	-144.6	-37.4	162.7	158.3	166.9	-30.3	171.8	39	47	12.0	9.9
4	-174.7	161.7	-165.9	173.1	-174.4	174.4	-178.6	177.3	48	73	14.9	15.5
5	-56.9	-164.2	-58.3	-81.6	-60.4	-166.7	-61.5	174.9	14	28	4.3	5.9
6	-62.4	-57.9	-172.6	-174.5	-60.2	-69.4	-168.0	-174.7	19	25	5.8	6.3
7	176.8	73.5	-168.3	-175.0					10		3.0	
					71.1	176.7	177.8	-75.7		10		2.1
8	-171.0	-173.3	-57.2	-81.9	178.3	176.6	-70.2	-79.0	9	14	2.7	3.0
9	55.0	-173.0	175.6	98.1	81.8	167.6	164.9	80.0	5	9	1.5	1.9
10	55.7	157.6	-74.9	178.3	64.1	-176.5	-69.5	156.0	4	8	1.2	1.7
11	-31.2	-164.8	69.6	64.2					3		0.9	
12	-64.2	-62.3	-54.9	-84.3					3		0.9	

### LYS

rotamer	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>4</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>4</sub>	rotamer occupancy		rotamer share, %	
	U				B				U	B	U	B
1	-69.3	-179.7	179.2	-180.0	-66.5	178.8	179.6	177.2	155	225	36.3	40.5
2	-173.2	179.9	179.7	-176.8	-175.5	-179.1	175.5	-174.4	105	110	24.6	19.8
3	-62.3	-64.5	175.8	174.5	-60.0	-59.1	-179.7	179.9	40	63	9.4	11.4
4	66.8	-179.2	180.0	173.3	63.2	-179.6	-179.3	177.1	25	29	5.9	5.2
5	-178.7	58.2	-175.3	173.2	-159.4	75.8	179.0	177.7	20	14	4.7	2.5



**Table S4.** Number of rotamers in the libraries for different RMSD clustering radii for surface residues with more than one dihedral angle, excluding Pro.

radius, Å			0.5	1	1.5	2	2.5	3	3.5	4	4.5
Amino Acid	Library		Number of rotamers								
Asp	Bound	Full	5	3	3	3	3	2	1	1	1
		Non-interface	5	3	3	3	3	2	1	1	1
		Interface	6	4	3	3	3	3	1	1	1
	Unbound	Full	5	3	3	3	3	2	1	1	1
		Non-interface	5	4	3	3	3	2	1	1	1
		Interface	6	4	3	3	3	2	1	1	1
Glu	Bound	Full	15	9	8	8	6	3	2	1	1
		Non-interface	14	8	7	7	5	3	2	1	1
		Interface	10	8	7	7	3	3	2	1	1
	Unbound	Full	15	10	8	8	5	3	2	2	1
		Non-interface	15	11	8	8	5	3	2	2	1
		Interface	11	7	7	6	4	2	2	1	1
Phe	Bound	Full	4	3	3	3	3	3	3	3	3
		Non-interface	4	3	3	3	3	3	3	3	3
		Interface	4	4	3	3	3	3	3	3	3
	Unbound	Full	4	3	3	3	3	3	3	3	3
		Non-interface	4	4	3	3	3	3	3	3	3
		Interface	3	3	3	3	3	3	3	3	3
His	Bound	Full	9	8	6	3	3	3	3	3	3
		Non-interface	9	8	6	3	3	3	3	3	3
		Interface	8	8	6	3	3	3	3	3	3
	Unbound	Full	9	8	6	3	3	3	3	3	2
		Non-interface	9	8	6	3	3	3	3	3	3
		Interface	9	8	6	3	3	3	3	3	2
Ile	Bound	Full	7	7	3	3	3	2	1	1	1
		Non-interface	7	7	3	3	3	2	1	1	1
		Interface	7	7	4	3	3	2	1	1	1
	Unbound	Full	7	7	3	3	3	2	1	1	1
		Non-interface	7	7	3	3	3	2	1	1	1
		Interface	7	6	3	3	3	1	1	1	1
Lys	Bound	Full	20	19	10	6	5	4	3	2	2
		Non-interface	20	20	11	5	5	4	3	2	2
		Interface	22	17	10	5	5	4	4	2	1
	Unbound	Full	21	21	10	6	5	4	3	3	2
		Non-interface	21	21	12	6	5	4	3	3	2
		Interface	23	23	11	7	5	4	3	2	2
Leu	Bound	Full	9	8	7	5	3	2	1	1	1
		Non-interface	9	8	8	5	3	2	1	1	1
		Interface	9	9	6	5	3	2	1	1	1
	Unbound	Full	10	10	5	5	3	3	1	1	1
		Non-interface	10	10	6	5	3	3	2	1	1
		Interface	7	7	7	5	3	2	2	1	1
Met	Bound	Full	10	10	10	5	4	2	2	2	1
		Non-interface	10	10	9	4	3	2	2	2	1



**Table S5.** Non-interface (NI) and Interface (I) transition maps.

Cys

NI	1	2	3	0.0
1	50.0	4.5	1.8	0.0
2	4.5	13.6	2.7	0.0
3	0.9	0.9	17.3	0.9
	0.0	1.8	0.9	0.0

I	1	2	3	0.0
1	50.0	5.9	2.9	0.0
2	2.9	20.6	2.9	0.0
3	0.0	0.0	14.7	0.0
	0.0	0.0	0.0	0.0

Ser

NI	1	2	3	0.0
1	39.0	7.0	5.9	0.0
2	7.7	17.0	4.3	0.0
3	5.2	4.1	9.9	0.0
	0.0	0.0	0.0	0.0

I	1	2	3	0.7
1	28.8	7.5	5.6	0.7
2	11.1	17.3	3.6	0.0
3	5.6	6.9	10.1	0.7
	0.7	0.7	1.0	0.0

Thr

NI	1	2	3	0.0
1	40.4	8.2	2.5	0.0
2	7.4	31.9	2.0	0.0
3	2.7	2.3	2.4	0.0
	0.0	0.0	0.0	0.0

I	1	2	3	0.7
1	39.5	8.8	2.4	0.3
2	9.5	25.9	1.4	0.7
3	2.4	2.0	3.7	0.0
	0.7	1.7	1.0	0.0

Val

NI	1	2	3	1.2
1	50.6	7.6	3.5	1.2
2	4.7	18.2	1.2	1.2
3	3.5	2.9	3.5	0.6
	1.2	0.0	0.0	0.0

I	1	2	3	0.6
1	59.5	6.3	2.7	0.6
2	5.5	13.4	1.6	0.4
3	3.3	1.8	4.7	0.1
	0.1	0.0	0.0	0.0

Pro

NI	1	2	0.0
1	40.0	15.7	0.0
2	14.9	29.4	0.0
	0.0	0.0	0.0

I	1	2	0.0
1	38.3	14.5	0.0
2	14.5	32.6	0.0
	0.0	0.0	0.0

Asp

NI	1	2	3	0.1
1	44.9	5.0	2.7	0.1
2	5.6	20.1	1.5	0.0
3	2.9	1.5	15.5	0.1
	0.0	0.0	0.0	0.0

I	1	2	3	0.3
1	43.6	5.5	2.8	0.3
2	7.1	19.3	2.1	0.0
3	3.7	1.5	14.1	0.0
	0.0	0.0	0.0	0.0

Phe

NI	1	2	3	
1	48.7	3.1	3.1	0.3
2	3.4	30.5	0.3	0.0
3	1.4	1.4	7.4	0.0
	0.3	0.0	0.0	0.0

I	1	2	3	
1	40.6	4.7	0.9	0.9
2	1.9	32.1	0.0	0.0
3	4.7	1.9	9.4	0.0
	0.9	1.9	0.0	0.0

His

NI	1	2	3	
1	48.6	6.8	2.4	0.2
2	6.6	19.9	1.0	0.8
3	2.7	1.7	8.6	0.0
	0.2	0.3	0.2	0.0

I	1	2	3	
1	46.5	3.9	7.0	0.8
2	3.1	14.7	0.8	0.0
3	3.9	3.9	14.7	0.0
	0.8	0.0	0.0	0.0

Ile

NI	1	2	3	
1	64.7	4.9	2.5	0.7
2	4.7	8.5	1.3	0.4
3	4.5	0.9	4.3	0.4
	0.9	0.4	0.4	0.4

I	1	2	3	
1	68.3	3.2	4.0	0.0
2	6.3	5.6	1.6	0.0
3	2.4	2.4	5.6	0.0
	0.0	0.8	0.0	0.0

Leu

NI	1	2	3	
1	60.3	5.5	1.2	0.1
2	8.3	21.6	0.2	0.1
3	0.9	0.4	1.1	0.0
	0.0	0.0	0.0	0.2

I	1	2	3	
1	59.6	7.7	0.9	0.4
2	10.6	16.6	0.4	0.0
3	1.7	0.4	0.9	0.0
	0.9	0.0	0.0	0.0

Asn

NI	1	2	3	
1	47.8	7.6	2.4	0.5
2	7.6	18.6	0.8	0.2
3	2.3	0.8	7.4	1.2
	0.9	0.3	1.1	0.5

I	1	2	3	
1	47.6	7.5	0.7	1.5
2	11.2	18.7	0.7	0.0
3	2.6	1.5	4.5	0.4
	1.1	0.4	0.7	0.7

Trp

NI	1	2	3	4	5	6	7
1	33.7	2.4	0.0	0.6	1.2	0.6	0.6
2	0.0	12.4	0.6	0.0	1.2	0.0	0.6
3	0.0	0.0	4.1	0.0	0.0	0.0	1.2
4	3.6	0.0	0.6	8.9	0.6	0.0	0.0
5	0.6	0.6	0.0	0.0	5.3	0.0	0.6
6	1.8	1.2	0.0	1.2	0.0	3.6	0.6
7	0.6	0.0	0.0	0.0	0.0	0.0	6.5
	0.0	0.0	0.0	0.0	1.2	0.0	1.8

I	1	2	3	4	5	6	7
1	31.9	1.4	2.9	0.0	1.4	0.0	1.4
2	1.4	10.1	0.0	0.0	0.0	0.0	0.0
3	4.3	0.0	5.8	0.0	0.0	0.0	2.9
4	4.3	1.4	1.4	2.9	0.0	0.0	0.0
5	0.0	0.0	0.0	1.4	2.9	0.0	1.4
6	0.0	0.0	0.0	0.0	0.0	7.2	0.0
7	0.0	0.0	0.0	0.0	0.0	0.0	8.7
	2.9	0.0	0.0	0.0	0.0	1.4	0.0

Tyr

NI	1	2	3	
1	51.4	2.3	0.8	0.0
2	2.1	31.6	0.2	0.6
3	1.1	0.4	9.2	0.0
	0.2	0.0	0.0	0.2

l	1	2	3	
1	49.5	3.3	1.1	1.1
2	6.0	27.7	2.2	0.0
3	1.1	0.5	7.6	0.0
	0.0	0.0	0.0	0.0

Met

NI	1	2	3	4	5	
1	20.3	1.9	1.4	1.4	1.9	5.8
2	3.9	21.7	0.0	0.0	1.9	5.3
3	1.9	3.4	1.4	1.0	0.5	1.9
4	0.0	1.9	0.5	2.4	0.0	1.0
5	0.0	0.0	0.0	0.0	1.0	1.0
	2.9	3.9	0.5	0.5	1.9	6.8

l	1	2	3	
1	10.8	2.7	1.4	1.4
2	2.7	12.2	2.7	4.1
3	1.4	1.4	1.4	5.4
4	1.4	1.4	0.0	4.1
	6.8	12.2	5.4	21.6

Glu

NI	1	2	3	4	5	6	7	
1	21.8	4.0	3.3	1.6	1.1	1.2	0.2	0.7
2	3.8	12.6	1.3	2.0	0.7	0.7	0.1	0.9
3	3.2	1.1	7.6	1.9	0.6	0.5	0.1	0.4
4	0.8	0.5	1.0	3.7	0.4	0.2	0.1	0.2
5	1.1	0.7	0.6	0.4	2.3	0.5	0.3	0.3
6	1.0	1.3	0.6	0.2	0.4	2.8	0.3	0.4
7	0.4	0.3	0.2	0.2	0.5	0.2	1.1	0.4
8	0.3	0.3	0.1	0.5	0.1	0.0	0.0	0.2
	1.0	0.9	0.8	0.5	0.2	0.2	0.2	0.3

l	1	2	3	4	5	6	7	
1	17.7	6.1	3.9	0.5	1.0	0.7	0.2	4.1
2	4.6	13.1	1.9	0.7	1.2	1.2	1.0	1.7
3	2.4	1.2	5.6	0.0	0.7	0.5	0.2	0.7
4	1.0	2.2	0.5	1.0	0.5	0.0	0.0	0.5
5	2.9	0.7	0.2	0.2	1.5	0.7	0.0	0.5
6	1.0	0.2	0.0	0.5	0.2	1.5	0.2	1.0
7	0.0	0.0	0.0	0.0	0.0	0.0	0.5	0.5
	2.9	1.5	1.5	1.2	0.5	0.7	0.2	2.4

Gln

NI	1	2	3	4	5	6	7	
1	25.7	3.6	2.8	1.6	0.7	1.1	0.0	3.2
2	3.8	8.1	0.9	1.5	0.5	0.3	0.3	1.7
3	3.3	1.0	8.8	1.0	0.5	0.3	0.0	2.0
4	1.3	1.3	0.9	5.0	0.0	0.2	0.1	1.4
5	1.1	0.2	0.7	0.0	1.1	0.1	0.1	0.7
6	0.3	0.8	0.1	0.4	0.1	0.7	0.1	0.3
7	0.1	0.3	0.0	0.0	0.1	0.1	0.2	0.2
	1.7	1.5	1.2	0.8	0.7	0.9	0.2	2.3

l	1	2	3	4	5	6	
1	19.3	5.4	1.2	1.5	1.2	0.4	4.2
2	3.9	7.7	1.9	1.2	0.8	0.4	0.4
3	1.5	0.0	9.3	0.4	0.0	0.0	1.9
4	1.5	1.2	0.8	2.3	0.0	0.4	1.5
5	0.8	0.8	0.4	0.0	0.8	0.0	1.2
6	2.3	0.0	0.0	0.4	0.0	1.5	1.2
	3.9	3.5	5.0	1.5	0.8	0.8	5.0

Lys

NI	1	2	3	4	5	
1	25.0	2.6	2.2	1.4	0.5	6.1
2	3.1	12.4	0.5	0.7	0.5	5.4
3	2.7	0.4	3.2	0.6	0.1	2.3
4	0.9	0.7	0.1	0.1	1.4	1.8
5	0.7	0.7	0.2	1.2	0.0	1.1
	6.3	4.0	2.0	1.2	0.8	6.9

l	1	2	3	4	5	
1	19.8	2.7	2.5	1.0	1.0	6.9
2	7.2	9.9	2.2	0.7	0.5	5.4
3	3.2	0.5	3.2	1.2	0.2	1.2
4	1.0	0.7	0.2	1.7	0.0	1.0
5	1.2	2.2	0.2	0.0	0.2	1.0
	6.2	4.2	2.2	0.7	0.7	6.7

Arg

NI	1	2	3	4	5	6	7	8	9	10	11	12	13	
1	15.1	1.2	3.3	1.0	1.0	0.3	0.4	0.2	0.2	0.3	0.3	0.1	0.0	7.0
2	1.1	4.0	1.0	0.0	0.2	0.3	0.3	0.1	0.0	0.0	0.4	0.1	0.0	1.4
3	3.0	0.5	6.4	0.3	0.5	0.5	0.4	0.2	0.1	0.1	0.3	0.1	0.0	2.7
4	0.8	0.1	0.3	1.6	0.1	0.0	0.0	0.0	0.1	0.1	0.0	0.0	0.0	1.2
5	1.1	0.4	0.6	0.0	1.2	0.2	0.0	0.1	0.0	0.1	0.1	0.1	0.0	0.7
6	0.5	0.1	0.4	0.0	0.1	0.8	0.1	0.0	0.1	0.0	0.0	0.0	0.0	0.6
7	0.4	0.1	0.6	0.1	0.1	0.1	1.4	0.0	0.0	0.1	0.1	0.0	0.0	1.2
8	0.1	0.1	0.0	0.0	0.0	0.0	0.2	0.4	0.0	0.1	0.0	0.0	0.0	0.5
9	0.3	0.1	0.1	0.0	0.1	0.0	0.1	0.0	0.0	0.0	0.5	0.1	0.0	0.6
10	0.6	0.0	0.0	0.2	0.2	0.0	0.0	0.0	0.0	0.5	0.0	0.1	0.0	0.6
11	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	6.2	2.2	1.9	1.1	0.8	0.5	0.8	0.4	0.3	1.0	0.5	0.5	0.0	8.6

l	1	2	3	4	5	6	7	8	9	10	
1	5.8	1.2	1.4	2.6	2.6	0.9	1.2	0.3	0.3	0.0	5.8
2	1.4	0.9	0.3	0.9	0.3	0.0	0.0	0.3	0.0	0.3	1.4
3	0.9	0.6	3.5	1.7	1.2	0.6	0.0	0.0	0.3	0.0	5.2
4	2.3	0.6	1.4	4.6	0.3	0.6	0.0	0.6	0.3	0.6	2.9
5	1.4	0.0	0.0	0.9	0.3	0.0	0.0	0.0	0.0	0.0	1.4
6	0.6	0.3	0.3	0.6	0.6	1.7	0.0	0.0	0.0	0.0	2.3
7	0.0	0.0	1.2	0.3	0.0	0.0	0.0	0.0	0.0	0.0	1.4
8	0.3	0.0	0.3	0.3	0.0	0.0	0.0	0.0	0.0	0.0	1.2
9	0.0	0.0	0.3	0.0	0.0	0.0	0.0	0.3	0.3	0.0	0.6
10	0.3	0.0	0.0	0.0	0.0	0.0	0.0	0.3	0.0	0.6	0.0
11	0.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.3
12	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.3
	4.0	0.6	2.6	2.6	0.9	2.3	0.9	1.2	0.3	0.3	9.8

**Table S6.** Non-interface (NI) and Interface (I) transition matrices.

Cys

NI	1	2	3	0.0
1	88.8	8.0	3.2	0.0
2	21.6	65.4	13.0	0.0
3	4.5	4.5	86.5	4.5
	0.0	66.7	33.3	0.0

I	1	2	3	0.0
1	85.0	10.0	4.9	0.0
2	11.0	78.0	11.0	0.0
3	0.0	0.0	100.0	0.0
	0.0	0.0	0.0	0.0

Ser

NI	1	2	3	0.0
1	75.1	13.5	11.4	0.0
2	26.6	58.6	14.8	0.0
3	27.1	21.4	51.6	0.0
	0.0	0.0	0.0	0.0

I	1	2	3	0.0
1	67.6	17.6	13.1	1.6
2	34.7	54.1	11.3	0.0
3	24.0	29.6	43.3	3.0
	29.2	29.2	41.7	0.0

Thr

NI	1	2	3	0.0
1	79.1	16.0	4.9	0.0
2	17.9	77.2	4.8	0.0
3	36.5	31.1	32.4	0.0
	0.0	0.0	0.0	0.0

I	1	2	3	0.0
1	77.4	17.3	4.7	0.6
2	25.3	69.1	3.7	1.9
3	29.6	24.7	45.7	0.0
	20.6	50.0	29.4	0.0

Val

NI	1	2	3	1.9
1	80.4	12.1	5.6	1.9
2	18.6	71.9	4.7	4.7
3	33.3	27.6	33.3	5.7
	100.0	0.0	0.0	0.0

I	1	2	3	0.0
1	86.1	9.1	3.9	0.9
2	26.3	64.1	7.7	1.9
3	33.3	18.2	47.5	1.0
	100.0	0.0	0.0	0.0

Pro

NI	1	2	0.0
1	71.8	28.2	0.0
2	33.6	66.4	0.0
	0.0	0.0	0.0

I	1	2	0.0
1	72.5	27.5	0.0
2	30.8	69.2	0.0
	0.0	0.0	0.0

Asp

NI	1	2	3	0.2
1	85.2	9.5	5.1	0.2
2	20.6	73.9	5.5	0.0
3	14.5	7.5	77.5	0.5
	0.0	0.0	0.0	0.0

I	1	2	3	0.0
1	83.5	10.5	5.4	0.6
2	24.9	67.7	7.4	0.0
3	19.2	7.8	73.1	0.0
	0.0	0.0	0.0	0.0

Phe

NI	1	2	3	
1	88.2	5.6	5.6	0.5
2	9.9	89.2	0.9	0.0
3	13.7	13.7	72.5	0.0
	100.0	0.0	0.0	0.0

I	1	2	3	
1	86.2	10.0	1.9	1.9
2	5.6	94.4	0.0	0.0
3	29.4	11.9	58.8	0.0
	32.1	67.9	0.0	0.0

His

NI	1	2	3	
1	83.8	11.7	4.1	0.3
2	23.3	70.3	3.5	2.8
3	20.8	13.1	66.2	0.0
	28.6	42.9	28.6	0.0

I	1	2	3	
1	79.9	6.7	12.0	1.4
2	16.7	79.0	4.3	0.0
3	17.3	17.3	65.3	0.0
	100.0	0.0	0.0	0.0

Ile

NI	1	2	3	
1	88.9	6.7	3.4	1.0
2	31.5	57.0	8.7	2.7
3	44.6	8.9	42.6	4.0
	42.9	19.0	19.0	19.0

I	1	2	3	
1	90.5	4.2	5.3	0.0
2	46.7	41.5	11.9	0.0
3	23.1	23.1	53.8	0.0
	0.0	100.0	0.0	0.0

Leu

NI	1	2	3	
1	89.9	8.2	1.8	0.1
2	27.5	71.5	0.7	0.3
3	37.5	16.7	45.8	0.0
	0.0	0.0	0.0	100.0

I	1	2	3	
1	86.9	11.2	1.3	0.6
2	38.4	60.1	1.4	0.0
3	56.7	13.3	30.0	0.0
	100.0	0.0	0.0	0.0

Asn

NI	1	2	3	
1	82.0	13.0	4.1	0.9
2	27.9	68.4	2.9	0.7
3	19.7	6.8	63.2	10.3
	32.1	10.7	39.3	17.9

I	1	2	3	
1	83.1	13.1	1.2	2.6
2	36.6	61.1	2.3	0.0
3	28.9	16.7	50.0	4.4
	37.9	13.8	24.1	24.1

Tyr

NI	1	2	3	
1	94.3	4.2	1.5	0.0
2	6.1	91.6	0.6	1.7
3	10.3	3.7	86.0	0.0
	50.0	0.0	0.0	50.0

I	1	2	3	
1	90.0	6.0	2.0	2.0
2	16.7	77.2	6.1	0.0
3	12.0	5.4	82.6	0.0
	0.0	0.0	0.0	0.0



Trp

NI	1	2	3	4	5	6	7
1	84.9	6.0	0.0	1.5	3.0	1.5	1.5
2	0.0	83.8	4.1	0.0	8.1	0.0	4.1
3	0.0	0.0	77.4	0.0	0.0	0.0	22.6
4	26.3	0.0	4.4	65.0	4.4	0.0	0.0
5	8.5	8.5	0.0	0.0	74.6	0.0	8.5
6	20.0	13.3	0.0	13.3	0.0	40.0	6.7
7	7.8	0.0	0.0	0.0	0.0	0.0	84.4
	0.0	0.0	0.0	0.0	40.0	0.0	0.0

l	1	2	3	4	5	6	7
1	81.8	3.6	7.4	0.0	3.6	0.0	3.6
2	12.2	87.8	0.0	0.0	0.0	0.0	0.0
3	33.1	0.0	44.6	0.0	0.0	0.0	22.3
4	43.0	14.0	14.0	29.0	0.0	0.0	0.0
5	0.0	0.0	0.0	24.6	50.9	0.0	24.6
6	0.0	0.0	0.0	0.0	0.0	100.0	0.0
7	0.0	0.0	0.0	0.0	0.0	0.0	100.0
	67.4	0.0	0.0	0.0	0.0	32.6	0.0

Met

NI	1	2	3	4	5
1	62.1	5.8	4.3	4.3	5.8
2	11.9	66.2	0.0	0.0	5.8
3	18.8	33.7	13.9	9.9	5.0
4	0.0	32.8	8.6	41.4	0.0
5	0.0	0.0	0.0	0.0	50.0
	17.6	23.6	3.0	3.0	11.5

l	1	2	3
1	66.3	16.6	8.6
2	12.4	56.2	12.4
3	14.6	14.6	14.6
4	20.3	20.3	0.0
	14.8	26.5	11.7

Glu

NI	1	2	3	4	5	6	7
1	64.3	11.8	9.7	4.7	3.2	3.5	0.6
2	17.2	57.0	5.9	9.0	3.2	3.2	0.5
3	20.8	7.1	49.4	12.3	3.9	3.2	0.6
4	11.6	7.2	14.5	53.6	5.8	2.9	1.4
5	17.7	11.3	9.7	6.5	37.1	8.1	4.8
6	14.3	18.6	8.6	2.9	5.7	40.0	4.3
7	12.1	9.1	6.1	6.1	15.2	6.1	33.3
8	20.0	20.0	6.7	33.3	6.7	0.0	0.0
	24.4	22.0	19.5	12.2	4.9	4.9	4.9

l	1	2	3	4	5	6	7
1	51.8	17.8	11.4	1.5	2.9	2.0	0.6
2	18.1	51.6	7.5	2.8	4.7	4.7	3.9
3	21.2	10.6	49.6	0.0	6.2	4.4	1.8
4	17.5	38.6	8.8	17.5	8.8	0.0	0.0
5	43.3	10.4	3.0	3.0	22.4	10.4	0.0
6	21.7	4.3	0.0	10.9	4.3	32.6	4.3
7	0.0	0.0	0.0	0.0	0.0	0.0	50.0
	26.6	13.8	13.8	11.0	4.6	6.4	1.8

Gln

NI	1	2	3	4	5	6	7
1	66.4	9.3	7.2	4.1	1.8	2.8	0.0
2	22.2	47.4	5.3	8.8	2.9	1.8	1.8
3	19.5	5.9	52.1	5.9	3.0	1.8	0.0
4	12.7	12.7	8.8	49.0	0.0	2.0	1.0
5	27.5	5.0	17.5	0.0	27.5	2.5	2.5
6	10.7	28.6	3.6	14.3	3.6	25.0	3.6
7	10.0	30.0	0.0	0.0	10.0	10.0	20.0
	18.3	16.1	12.9	8.6	7.5	9.7	2.2

l	1	2	3	4	5	6
1	58.1	16.3	3.6	4.5	3.6	1.2
2	23.9	47.2	11.7	7.4	4.9	2.5
3	11.5	0.0	71.0	3.1	0.0	0.0
4	19.5	15.6	10.4	29.9	0.0	5.2
5	20.0	20.0	10.0	0.0	20.0	0.0
6	42.6	0.0	0.0	7.4	0.0	27.8
	19.0	17.1	24.4	7.3	3.9	3.9

## Lys

NI	1	2	3	4	5	1	1	2	3	4	5		
1	66.1	6.9	5.8	3.7	1.3	16.1	1	58.4	8.0	7.4	2.9	2.9	20.4
2	13.7	54.9	2.2	3.1	2.2	23.9	2	27.8	38.2	8.5	2.7	1.9	20.8
3	29.0	4.3	34.4	6.5	1.1	24.7	3	33.7	5.3	33.7	12.6	2.1	12.6
4	18.0	14.0	2.0	2.0	28.0	36.0	4	21.7	15.2	4.3	37.0	0.0	21.7
5	17.9	17.9	5.1	30.8	0.0	28.2	5	25.0	45.8	4.2	0.0	4.2	20.8
	29.7	18.9	9.4	5.7	3.8	32.5		30.0	20.3	10.6	3.4	3.4	32.4

## Arg

NI	1	2	3	4	5	6	7	8	9	10	11	12	13	
1	49.7	3.9	10.9	3.3	3.3	1.0	1.3	0.7	0.7	1.0	1.0	0.3	0.0	23.0
2	12.4	44.9	11.2	0.0	2.2	3.4	3.4	1.1	0.0	0.0	4.5	1.1	0.0	15.7
3	19.9	3.3	42.4	2.0	3.3	3.3	2.6	1.3	0.7	0.7	2.0	0.7	0.0	17.9
4	18.6	2.3	7.0	37.2	2.3	0.0	0.0	0.0	2.3	2.3	0.0	0.0	0.0	27.9
5	23.9	8.7	13.0	0.0	26.1	4.3	0.0	2.2	0.0	2.2	2.2	2.2	0.0	15.2
6	18.5	3.7	14.8	0.0	3.7	29.6	3.7	0.0	3.7	0.0	0.0	0.0	0.0	22.2
7	9.5	2.4	14.3	2.4	2.4	2.4	33.3	0.0	0.0	2.4	2.4	0.0	0.0	28.6
8	7.1	7.1	0.0	0.0	0.0	0.0	14.3	28.6	0.0	7.1	0.0	0.0	0.0	35.7
9	15.8	5.3	5.3	0.0	5.3	0.0	5.3	0.0	0.0	0.0	26.3	5.3	0.0	31.6
10	27.3	0.0	0.0	9.1	9.1	0.0	0.0	0.0	0.0	22.7	0.0	4.5	0.0	27.3
11	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	25.0	8.9	7.7	4.4	3.2	2.0	3.2	1.6	1.2	4.0	2.0	2.0	0.0	34.7

l	1	2	3	4	5	6	7	8	9	10	
1	26.2	5.4	6.3	11.8	11.8	4.1	5.4	1.4	1.4	0.0	26.2
2	24.1	15.5	5.2	15.5	5.2	0.0	0.0	5.2	0.0	5.2	24.1
3	6.4	4.3	25.0	12.1	8.6	4.3	0.0	0.0	2.1	0.0	37.1
4	16.2	4.2	9.9	32.4	2.1	4.2	0.0	4.2	2.1	4.2	20.4
5	35.0	0.0	0.0	22.5	7.5	0.0	0.0	0.0	0.0	0.0	35.0
6	9.4	4.7	4.7	9.4	9.4	26.6	0.0	0.0	0.0	0.0	35.9
7	0.0	0.0	41.4	10.3	0.0	0.0	0.0	0.0	0.0	0.0	48.3
8	14.3	0.0	14.3	14.3	0.0	0.0	0.0	0.0	0.0	0.0	57.1
9	0.0	0.0	20.0	0.0	0.0	0.0	0.0	20.0	20.0	0.0	40.0
10	25.0	0.0	0.0	0.0	0.0	0.0	0.0	25.0	0.0	50.0	0.0
11	50.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	50.0
12	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0
	15.7	2.4	10.2	10.2	3.5	9.0	3.5	4.7	1.2	1.2	38.4

**Table S7.** Comparison of “Penultimate rotamer library”<sup>47</sup> (PL) and the redundant full unbound rotamer library.

Amino acid	Rotamer <sup>a</sup>								
	1	2	3	4	5	6	7	8	9
SER	-2 <sup>b</sup>	1	0						
	2 <sup>c</sup>	1	-2						
VAL	3	1	-1						
	-5	2	5						
THR	2	1	-4						
	2	-2	1						
CYS	-1	2	10						
	8	-2	-5						
PRO	0	0							
	11	-4							
ILE	4	4	6	8	26	35	5		
	-11	3	0	-1	4	2	1		
LEU	1	5	36					10	20
	-1	-7	5					1	-1
ASN	25	28	35	21	29				
	0.4	1	14	2	0				
ASP	1	7	8			48			
	-9	-3	4			-3			
HIS	3	6	5	2	22	8	19	15	
	-3	7	-3	1	1	1	0	-1	
PHE	3	5	3	0					
	0	4	-3	-1					
TYR	3	3	5	41					
	6	-2	-1	-3					
TRP	10	7	5	14	6	31	1		
	7	-5	2	-8	-3	4	0		

<sup>a</sup> Rotamer number is as in the redundant full unbound library

<sup>b</sup> RMSD in the dihedral angles space ( $\Delta\chi = \sqrt{\sum_i \Delta\chi_i^2}$ ) between closest rotamers in the two libraries

<sup>c</sup> Difference between rotamer shares in the two libraries

Amino acid	Rotamer																														
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26					
GLN	29		19	67		13		22				11	25	54	40																
	-19		-3	-9		-3		2				-1	0	-3	-1																
GLU	1		9	19		12		14	34		33			9																	
	-12		-11	-2		1		-2	-2		0			1																	
MET	6	22	7	19	7	12	7	11		15																					
	-1	2	-6	2	4	-2	-3	-1		-1																					
LYS	7	5	8	17	8	5	9	4	19	12	13	9	13	9	10	20	16		9	5	6										
	1	-2	0	2	-1	0	0	1	0	-1	1	0	1	0	1	0	0		0	0	0										
ARG	11	17	12	40	23	27	5	2	9		10	15	12	14	18	16	14	30	10	13	37	23	9	18	7	25					
	1	-1	1	4	1	0	-2	4	2		0	-2	0	-1	0	0	-1	1	-1	0	0	-1	-1	-1	-1	-1	0				