Supplemental Information

Fig S1

Composition of G&R, loops and turns at each position within each cluster. Hatched bars indicate statistically significant differences between OMBBs and G&R based on permutation tests (see Methods); statistically significant values cannot be shown when the proportion is 0. Groups are colored as for the sequence logos of Fig 2,4 and 5.

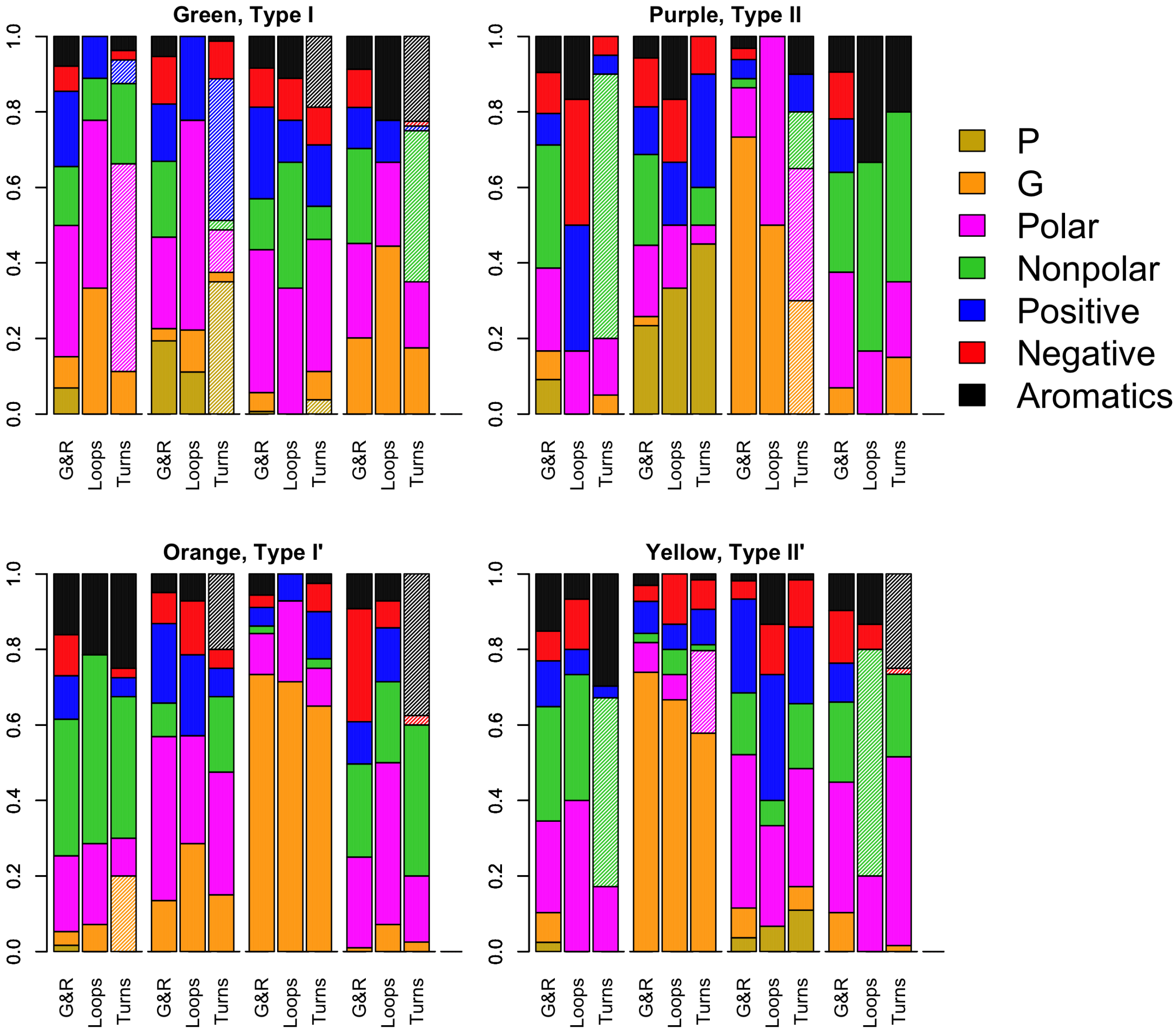

Fig S2

The proportion of backbone:backbone hydrogen bonding at each pair of positions. The carbonyl partner is shown along the x-axis; the identity of the other backbone partner is shown along the y-axis. “Other” indicates hydrogen bonding to a backbone partner outside the loop. The radius of the circles is equivalent to the proportion of structures at that position involved in bonding. Circles are colored to match the clusters marked on the Ramachandran plots in Figs 2, 4 and 5. A large circle at both i:i+3 and i+3:i, for example, would indicate the likelihood of a double hydrogen bond, while a circle in just one position indicates a single hydrogen bond.

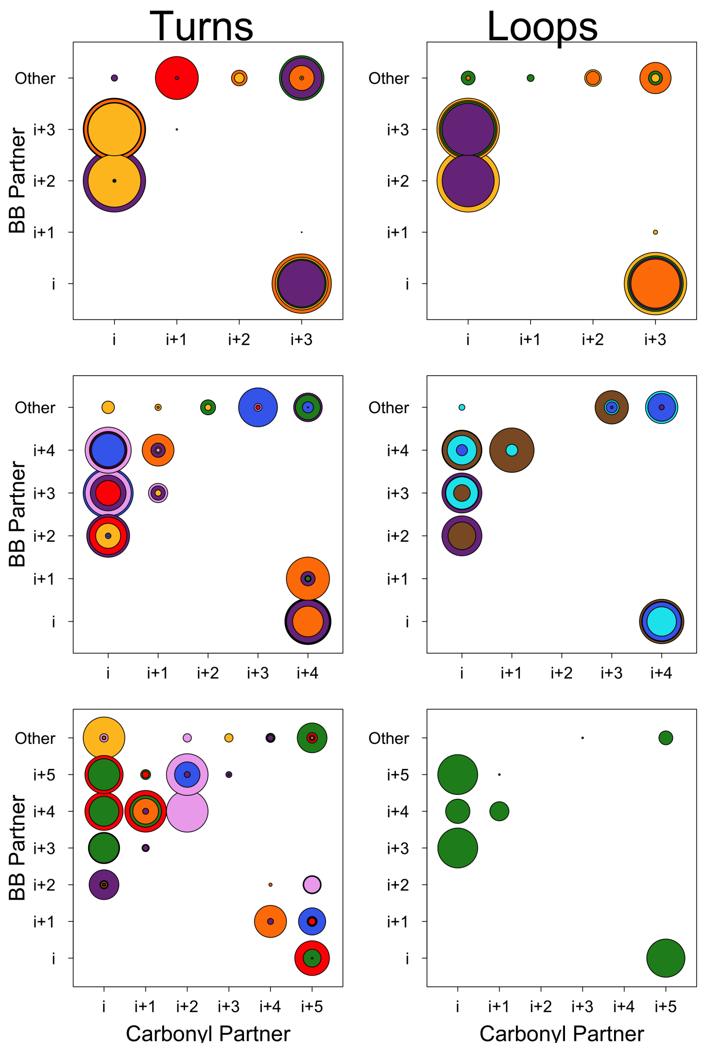

Fig S3

Proportion of sidechain:backbone hydrogen bonding of all positions and strand connector lengths. The x-axis shows the average van der Waals volume of all residues at that position, regardless of polarity.

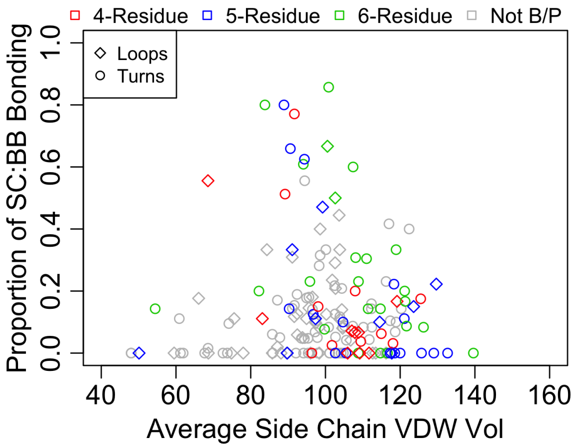

Table S1

For each length, the cluster assignments were permuted 10,000 times and the sum of the absolute differences between each pair of groups was calculated. Approximate p-values reported below are the proportion of permutations for which the sum differences was greater than or equal to the observed sum difference. P-values are red when stastically significant after Holm-Bonferonni adjustment for familywise error rates. 6-residues loops are not shown because there is only one cluster identified.

	4-residue Turns				
	Green, Type I	Orange, Type I'	Purple, Type II	Yellow, Type II'	Red, Unk
Green, Type I		**<1e-04**	0.1243	**<1e-04**	**<1e-04**
Orange, Type I'	NA	NA	**<1e-04**	**<1e-04**	**<1e-04**
Purple, Type II				**<1e-04**	**<1e-04**
Yellow, Type II'	NA	NA	NA	NA	**<1e-04**
Red, Unk					

	4-residue Loops			
	Green, Type I	Orange, Type I'	Purple, Type II	Yellow, Type II'
Green, Type I		**0.0059**	**0.0014**	**5e-04**
Orange, Type I'	NA	NA	0.192	0.0325
Purple, Type II				0.0683
Yellow, Type II'	NA	NA	NA	NA

	5-residue Turns						
	Orange	Pink	Red	Green	Blue	Yellow	Purple
Orange		0.0119	0.0242	**<1e-04**	0.1394	**<1e-04**	0.1946
Pink	NA	NA	0.1213	**0.0024**	0.1792	**<1e-04**	0.258
Red				**<1e-04**	0.0525	**<1e-04**	0.0917
Green	NA	NA	NA	NA	0.0397	**<1e-04**	0.0085
Blue						**1e-04**	0.029
Yellow	NA	NA	NA	NA	NA	NA	0.0555
Purple							

	5-residue Loops			
	Purple	Bright Green	Brown	Blue
Purple		**<1e-04**	**0.0015**	**<1e-04**
Bright Green	NA	NA	**2e-04**	0.0173
Brown				0.244
Blue	NA	NA	NA	NA

	6-residue Turns						
	Blue	Green	Orange	Red	Purple	Yellow	Pink
Blue		**<1e-04**	**<1e-04**	**<1e-04**	**<1e-04**	**5e-04**	0.0736
Green	NA	NA	0.0046	**2e-04**	**<1e-04**	0.0084	0.0586
Orange				**<1e-04**	0.0063	0.0296	0.0061
Red	NA	NA	NA	NA	**<1e-04**	**0.0025**	0.0095
Purple						0.0146	0.0146
Yellow	NA	NA	NA	NA	NA	NA	0.1821
Pink							

Table S2

Representative examples of 4-residue strand connectors and the average angles for each cluster.

Cluster Name	Number Observed	PDB	Loop/Turn ID	Sequence	Avg Phi (i)	Avg Psi (i)	Avg Phi (i+1)	Avg Psi (i+1)	Avg Phi (i+2)	Avg Psi (i+2)	Avg Phi (i+3)	Avg Psi (i+3)
Green, Type I	9	3BS0	L5	SQLG	-152.21	176.00	-68.63	-22.83	-99.41	-5.66	-173.29	143.52
Green, Type I	80	2WJR	T3	TKDL	-144.65	173.92	-59.30	-24.63	-107.51	1.20	-153.71	135.53
Orange, Type I'	14	2GR7	L1	YQGQ	-127.43	124.92	54.28	39.01	82.14	-1.42	-105.81	150.29
Orange, Type I'	40	3KVN	T2	ENRW	-170.05	130.43	54.03	43.67	82.31	-6.14	-100.68	143.76
Purple, Type II	6	4D5B	L2	EPGY	-146.58	171.46	-54.67	124.65	79.13	2.99	-150.34	143.56
Purple, Type II	20	3PRN	T7	AEGV	-144.74	170.91	-59.22	133.05	74.26	4.08	-147.94	138.41
Red, Unk	48	5IVA	T4	RGDT	-90.07	-1.91	-137.92	-175.06	-67.85	-23.66	-108.28	-16.16
Yellow, Type II'	15	4RDR	L4	AGDA	-109.34	105.15	61.06	-117.56	-97.48	3.44	-108.57	143.66
Yellow, Type II'	64	2GSK	T5	VGDF	-133.55	108.73	60.24	-119.81	-94.35	5.21	-106.87	138.51

Table S3

Representative examples of 5-residue strand connectors and the average angles for each cluster.

Cluster Name	Number Observed	PDB	Loop/Turn ID	Sequence	Avg Phi (i)	Avg Psi (i)	Avg Phi (i+1)	Avg Psi (i+1)	Avg Phi (i+2)	Avg Psi (i+2)	Avg Phi (i+3)	Avg Psi (i+3)	Avg Phi (i+4)	Avg Psi (i+4)
Blue (AAL)	9	4D5B	L1	GFNNT	-107.24	-164.86	-72.03	-22.19	-88.55	-0.50	74.09	31.79	-105.34	147.16
Blue (AAL)	9	5IVA	T8	EENGF	-116.74	150.64	-65.10	-21.26	-69.05	-6.76	92.30	5.86	-78.38	115.07
Brown (PLL)	9	5FP1	L1	GTDNY	-158.83	-174.88	-62.07	157.96	61.30	41.49	60.19	32.71	-79.59	119.89
Cyan (AAA)	17	4C00	L1	STDVG	-116.00	152.04	-65.31	-38.21	-80.31	-44.72	-89.83	-24.21	118.19	169.55
Green (ABA)	10	2FGR	T4	DNGPL	-92.76	114.48	-87.94	-31.33	-156.42	-150.37	-74.41	-17.73	-119.56	-19.39
Orange (BAD)	44	3BRY	T4	FNDQL	-98.55	10.43	-129.28	-177.87	-66.11	-23.64	-109.50	-17.99	-131.76	126.92
Pink (LLD)	13	4C00	T5	LYDRH	-117.55	120.44	58.23	36.81	62.02	-5.12	-118.53	-27.57	-111.18	130.34
Purple (PLD)	20	3SYS	L5	LEDVY	-98.90	111.09	-55.16	131.15	67.88	9.32	-125.52	-64.75	-166.37	165.64
Purple (PLD)	7	5FR8	T1	IKDVL	-125.46	86.85	-68.34	123.07	60.89	-18.79	-122.82	-23.38	-152.36	142.12
Red (GAD)	12	3OHN	T7	LGRTS	-109.97	94.09	67.59	-149.39	-95.58	-9.01	-105.37	-17.98	-142.39	151.24
Yellow (PGA)	8	4FSP	T1	TEGTL	-62.81	146.17	-81.04	148.50	117.68	177.20	-59.71	-29.80	-120.96	131.65

Table S4

Representative examples of 6-residue strand connectors and the average angles for each cluster.

Cluster Name	Number Observed	PDB	Loop/Turn ID	Sequence	Avg Phi (i)	Avg Psi (i)	Avg Phi (i+1)	Avg Psi (i+1)	Avg Phi (i+2)	Avg Psi (i+2)	Avg Phi (i+3)	Avg Psi (i+3)	Avg Phi (i+4)	Avg Psi (i+4)	Avg Phi (i+5)	Avg Psi (i+5)
Blue (ABAD)	23	1QJ8	T3	NPMENV	-97.46	114.53	-77.28	-14.58	-119.07	-179.75	-64.10	-17.48	-108.21	-11.94	-134.86	114.94
Green (AAAL)	24	4E1S	L3	DFSGDN	-105.54	108.34	-68.92	-29.98	-69.70	-37.92	-99.90	-1.99	58.84	37.94	-137.94	147.54
Green (AADL)	21	4D5B	T3	NNDYNM	-99.67	64.27	-66.04	1.88	-66.89	-24.14	-102.06	2.77	77.08	17.52	-117.14	103.46
Orange (BADB)	13	5IVA	T3	TGLDSR	-110.00	123.17	-125.94	152.46	-71.73	-35.08	-110.66	-6.54	-133.70	170.35	-123.34	109.49
Pink (ABPL)	5	3SYS	T3	RELPGL	-121.45	96.10	-86.34	-13.05	-100.81	129.70	-49.53	130.23	84.56	-2.43	-133.27	136.55
Purple (PGAB)	7	4FSO	T1	TEGALG	-72.45	146.59	-84.66	153.00	118.56	-177.65	-65.78	-36.44	-108.25	126.48	-106.80	134.14
Red (LLLA)	12	5FP1	T7	FLDNHL	-141.68	159.59	35.27	64.89	52.15	38.84	73.92	18.42	-95.64	-13.28	-136.35	130.90
Yellow (PABA)	5	2IAH	T5	FNVTDD	-104.71	120.47	-92.65	76.94	-68.04	-14.97	-136.93	166.52	-81.08	-35.99	-104.09	-18.23