Table S1. Comparative analysis of the EROS (1, 2) and two Backrub ensembles (4)

								% of structures with p-value < 0.1			
			RMSD 0.5 Å	**RMSD 25Å**	δ value	**p-value median**	**p-value average**	**0.5 Å**	**1.5 Å**	**3.0 Å**	**5.0 Å**
EROS	without tail	bb	0.78 +/- 0.22	0.60 +/- 0.05	30 %	0.29	3.5667e-09	33,00%	53,00%	53,00%	37,00%
		sc	2.00 +/- 0.38	1.42 +/- 0.08	41 %	0.06	< 2.2e-16	61,00%	79,00%	74,00%	42,00%
	with tail	bb	1.41 +/- 0.79	0.79 +/- 0.17	78 %	0.04	< 2.2e-16	72,00%	74,00%	47,00%	53,00%
		sc	2.58 +/- 1.00	1.67 +/- 0.20	54 %	0.07	< 2.2e-16	63,00%	68,00%	68,00%	63,00%
BACKRUB 1.2	without tail	bb	0.76 +/- 0.23	0.67 +/- 0.07	13 %	0.52	0.42	28,00%	47,00%	37,00%	31,00%
		sc	2.01 +/- 0.38	1.56 +/- 0.12	29 %	0.18	4.1660e-10	28,00%	21,00%	21,00%	31,00%
	with tail	bb	1.98 +/- 2.12	0.85 +/- 0.26	133 %	0.18	< 2.2e-16	44,00%	58,00%	58,00%	37,00%
		sc	2.28 +/- 0.51	1.73 +/- 0.18	32 %	0.09	< 2.2e-16	53,00%	53,00%	53,00%	47,00%
BACKRUB 2.4	without tail	bb	0.65 +/- 0.29	0.57 +/- 0.09	14 %	0.29	0.03	27,00%	42,00%	37,00%	31,00%
		sc	2.02 +/- 0.45	1.51 +/- 0.12	34 %	0.10	8.2635e-10	50,00%	42,00%	37,00%	26,00%
	with tail	bb	1.88 +/- 2.14	0.75 +/- 0.27	151 %	0.17	< 2.2e-16	50,00%	58,00%	58,00%	47,00%
		sc	2.40 +/- 0.43	1.63 +/- 0.20	47 %	0.16	< 2.2e-16	47,00%	47,00%	47,00%	47,00%

Analysis was carried out for structures with and without the C-terminal tail and for backbone (bb) and side-chain atoms (sc), separately. The rmsd calculations are presented for the binding-site atoms (0.5 Å range) and the whole molecule (25 Å range). δ value is defined as $(rmsd_{0.5Å} - rmsd_{25Å})/rmsd_{25Å}) \times 100\%$. The median of the *p*-value distribution is presented for the binding site only (0.5 Å range). The average *p*-value (for pooled data) is given for the binding site only. The percentage of structures with *p*-value < 0.1 is given for four distance ranges from the binding site.