

Packing Protein Side-chain by Parallel Ant Colonies

Supplementary Information

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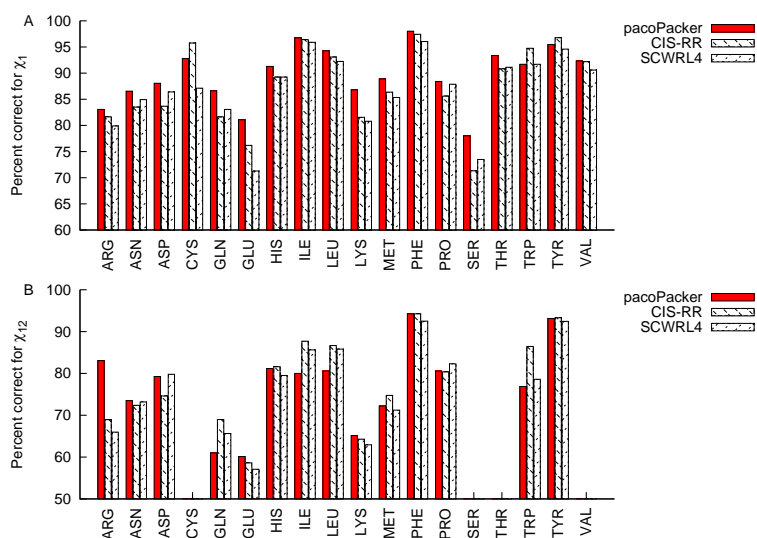


Fig. 1. Analysis of the performance of pacoPacker, CIS-RR and scwrl4 on different amino acids. (A) Percent correct within 40° for the χ_1 angle. (B) Percent correct within 40° for the χ_{12} angle. The test data used the 65 proteins set. Red, Green back slash and blue forward slash recolumns indicate the test results of pacoPacker, CIS-RR and SCWRL4, respectively.

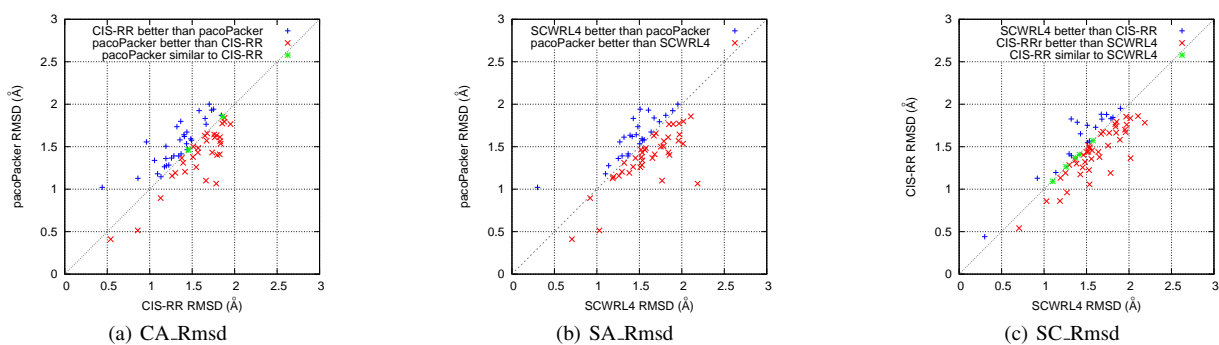


Fig. 2. RMSD comparison on benchmark of CIS-RR

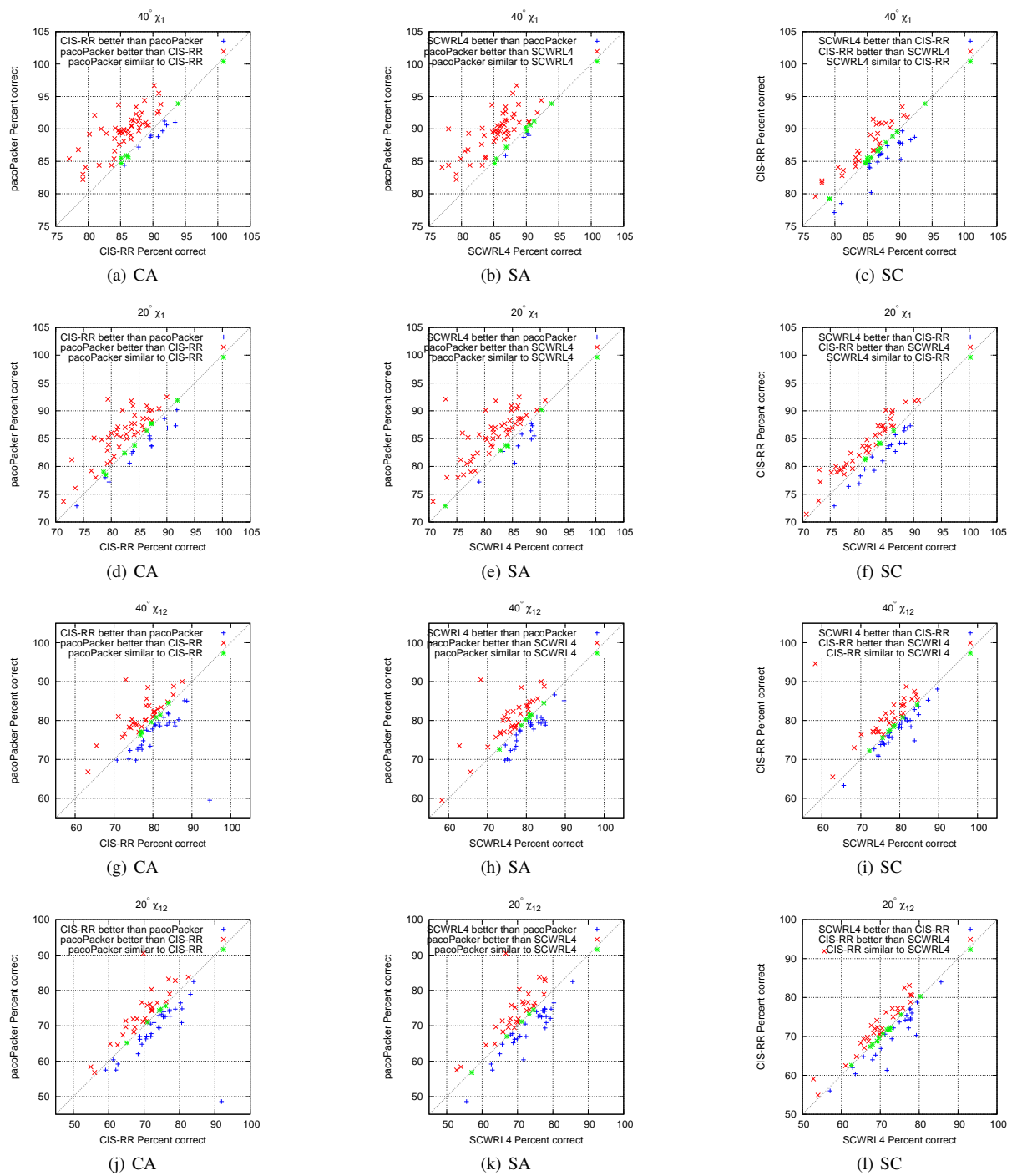


Fig. 3. Target comparison on benchmark of CIS-RR

Table 1. Comparison of pacoPacker, CIS-RR and scwrl4 on a 65-protein test set

PDB	NO. of Residues	$\chi_1(40^\circ/20^\circ)$			$\chi_{12}(40^\circ/20^\circ)$			RMSD(Å)		
		SCWRL4	CIS-RR	pacoPacker	SCWRL4	CIS-RR	pacoPacker	SCWRL4	CIS-RR	pacoPacker
153L	185	86.6 / 83.9	89.3 / 85.9	90.6 / 86.6	80.5 / 74.5	83.9 / 77.2	81.9 / 74.5	1.50	1.51	1.75
1A7S	263	86.6 / 84.4	84.9 / 81	89.4 / 86.6	80.4 / 74.9	78.2 / 73.7	83.8 / 76.5	1.26	1.55	1.51
1A8Q	132	90.2 / 86.7	85.3 / 82.7	89.3 / 85.8	82.7 / 76.4	80 / 74.2	80.9 / 72.9	1.63	1.79	1.39
1AGY	170	90.4 / 88.4	89.7 / 87	89 / 84.9	84.9 / 79.5	83.6 / 78.8	78.8 / 74.7	1.83	1.65	1.43
1AKO	121	86.8 / 83.8	85.9 / 84.2	85.9 / 83.8	76.9 / 69.2	76.1 / 68.8	72.6 / 66.2	1.92	1.58	1.89
1AMM	61	86.1 / 81.6	86.7 / 84.8	90.5 / 86.1	76.6 / 67.7	80.4 / 72.8	82.3 / 70.9	1.37	1.38	1.65
1ARB	237	90.6 / 86.1	92.1 / 89.6	90.6 / 88.6	84.2 / 77.7	86.6 / 80.7	80.2 / 74.8	1.56	0.96	1.27
1B9O	635	86.6 / 81.2	86.6 / 79.5	88.4 / 83.9	75.9 / 68.8	74.1 / 65.2	72.3 / 65.2	1.39	1.34	1.37
1BD8	169	81 / 80.2	78.5 / 76.9	86.8 / 85.1	74.4 / 70.2	71.1 / 66.9	81 / 71.9	1.57	1.83	1.79
1BJ7	122	85.9 / 81.5	86.7 / 83.7	90.4 / 86.7	73.3 / 67.4	77 / 67.4	77 / 69.6	1.53	1.43	1.50
1BYI	155	85.3 / 81.9	84.7 / 82.5	89.8 / 87	77.4 / 71.2	76.8 / 70.6	76.3 / 71.2	1.62	1.41	1.42
1C5E	221	90.1 / 88.3	87.8 / 86.4	89.7 / 86.4	84.5 / 80.3	84 / 80.3	84.5 / 76.5	0.89	1.13	0.92
1C9O	123	79.2 / 78.3	79.2 / 76.4	83 / 79.2	74.5 / 71.7	70.8 / 61.3	69.8 / 60.4	1.61	1.83	1.32
1CBN	46	61.1 / 58.3	97.3 / 94.6	64.9 / 56.8	58.3 / 55.6	94.6 / 91.9	59.5 / 48.6	1.02	0.44	0.30
1CC7	89	87.9 / 84.8	90.9 / 86.4	95.5 / 90.9	77.3 / 69.7	75.8 / 69.7	78.8 / 71.2	1.19	1.30	1.38
1CEM	136	86.3 / 83.6	88.4 / 87.3	90.8 / 87.7	80.5 / 72.6	81.2 / 72.3	82.9 / 74.3	1.43	1.57	1.53
1CEX	321	90.4 / 88.4	87.7 / 84.2	91.1 / 87.7	84.9 / 78.1	81.5 / 76	79.5 / 72.6	1.84	1.88	1.67
1CHD	113	85.1 / 77.9	85.1 / 80.5	89.6 / 81.8	73.4 / 63.6	72.7 / 60.4	76.6 / 64.9	1.61	1.76	1.84
1CKU	240	91.7 / 87.5	88.3 / 84.2	92.5 / 89.2	80.8 / 73.3	80.8 / 75	80.8 / 73.3	1.28	1.20	1.14
1CTJ	207	88.5 / 82	90.2 / 83.6	96.7 / 91.8	78.7 / 70.5	78.7 / 72.1	88.5 / 80.3	0.51	0.86	1.03
1CZ9	243	85.6 / 82.9	80.2 / 79.3	89.2 / 82.9	83.8 / 79.3	74.8 / 70.3	79.3 / 72.1	1.94	1.75	1.51
1CZB	129	84.7 / 80.2	84.7 / 82	93.7 / 90.1	82.9 / 73	82.9 / 69.4	85.6 / 76.6	1.79	1.88	1.74
1CZP	274	90.4 / 88.6	93.4 / 91.6	91 / 87.3	83.1 / 77.7	85.5 / 77.1	79.5 / 74.1	1.18	1.09	1.10
1D4T	156	93.9 / 90.9	93.9 / 91.9	93.9 / 91.9	80.8 / 77.8	83.8 / 78.8	84.8 / 82.8	1.15	1.13	1.19
1DHN	72	84.8 / 79	84.8 / 81	89.5 / 85.7	77.1 / 65.7	74.3 / 64.8	78.1 / 71.4	1.41	1.82	1.68
1ECA	139	87 / 78.7	86.1 / 82.4	89.8 / 82.4	78.7 / 65.7	80.6 / 69.4	78.7 / 64.8	1.37	1.26	1.45
1EDG	380	86.9 / 83.3	87.8 / 83.9	87.2 / 82.7	77.5 / 69.9	77.5 / 70.5	74.8 / 66.3	1.59	1.48	1.53
1GCI	172	91.2 / 90.2	91.8 / 91.8	91.2 / 90.2	89.7 / 85.6	88.1 / 84	85.1 / 82.5	2.00	1.70	1.95
1HCL	150	79.2 / 70.7	79.2 / 71.4	82.2 / 73.7	65.6 / 57.1	63.3 / 56	66.8 / 56.8	1.87	1.85	1.81
1IC6	198	85.9 / 85	91.5 / 90.1	89.7 / 86.9	81.7 / 77.5	88.7 / 83.1	85 / 78.9	1.80	1.37	2.02
1IFC	131	77 / 69.9	79.6 / 73.5	84.1 / 76.1	62.8 / 54	65.5 / 54.9	73.5 / 58.4	1.57	1.67	1.96
1IGD	164	78 / 76	82 / 80	90 / 86	74 / 68	78 / 68	80 / 72	1.07	1.78	2.19
1IXH	166	85.3 / 82.5	84.1 / 81.7	88.5 / 85.3	79.8 / 73.4	78.2 / 72.2	80.2 / 74.6	1.77	1.95	1.90
1KOE	197	85.4 / 85.4	84 / 83.3	85.4 / 80.6	81.9 / 77.8	79.9 / 74.3	77.8 / 69.4	1.93	1.73	1.61
1MLA	150	85 / 81.5	85.5 / 82.8	88.1 / 85	77.1 / 68.3	77.1 / 70.9	78.4 / 75.8	1.38	1.51	1.53
1MML	363	83.7 / 72.9	85.1 / 73.8	85.5 / 72.9	75.1 / 62.9	73.8 / 62	70.1 / 57.5	1.48	1.57	1.58
1NAR	141	85.1 / 77.5	85.1 / 78.6	84.7 / 79	75.6 / 62.6	75.6 / 62.6	69.8 / 59.2	1.64	1.40	1.46
1NLS	269	83.7 / 80.8	86.2 / 83.7	85.7 / 82.3	77.3 / 72.4	79.3 / 71.9	73.4 / 67	1.47	1.44	1.52
1NOA	305	88.8 / 86.2	91.2 / 90	93.8 / 92.5	83.8 / 76.2	85.5 / 82.5	90 / 83.8	1.13	0.86	1.19
1NPK	99	81.1 / 77	82.8 / 79.5	89.3 / 85.2	75.4 / 63.9	74.6 / 64.8	80.3 / 69.7	1.40	1.79	1.85
1PLC	245	80.5 / 76.8	84.1 / 79.3	86.6 / 80.5	78 / 65.9	75.6 / 67.1	79.3 / 68.3	1.16	1.26	1.26
1QJ4	108	86.8 / 85.8	90.9 / 88.6	92.7 / 90.4	78.5 / 73.1	84 / 77.2	81.7 / 79	1.34	1.06	1.54
1QL0	137	88.9 / 86.4	88.9 / 87.2	91 / 87.7	80.9 / 74.6	81.9 / 76.1	81.4 / 75.6	1.39	1.28	1.30
1QLW	58	87.2 / 84.1	86.2 / 84.1	89.3 / 85.7	81.4 / 75.4	80.6 / 75.6	78.9 / 74	1.58	1.49	1.54
1QNJ	268	87.2 / 84.2	90.8 / 87.2	88.8 / 83.7	81.1 / 78.1	85.7 / 80.6	78.6 / 70.9	1.58	1.36	1.56
1QQ4	224	88.1 / 86	87.4 / 83.9	92.3 / 90.9	84.6 / 77.6	85.3 / 76.9	88.8 / 83.2	1.28	1.22	1.53
1QTN	197	85.5 / 84.5	89.1 / 87.3	90.5 / 88.2	76.4 / 69.1	81.8 / 74.1	78.6 / 69.5	1.46	1.46	1.56
1QTW	196	88.1 / 85.5	85.5 / 83.7	89.9 / 87.7	78.4 / 72.2	78.4 / 71.8	77.5 / 70.5	1.43	1.74	1.84
1QU9	294	89.9 / 88.9	87.9 / 86.9	90.2 / 85.5	83.8 / 77.8	82.8 / 74.7	80.8 / 74.7	1.26	1.17	1.43
1RCF	251	92.3 / 89.4	88.7 / 87.3	94.4 / 90.1	87.3 / 76.8	85.2 / 75.4	86.6 / 72.5	1.21	1.42	1.30
1THV	256	83.2 / 79	85.6 / 79.6	84.4 / 77.2	78.4 / 70.7	79 / 70.7	77.2 / 67.1	1.76	1.66	1.85
1THX	285	85.6 / 81.4	85.6 / 81.4	89.7 / 83.5	81.4 / 77.3	80.4 / 72.2	81.4 / 74.2	1.50	1.19	1.78
1VFX	67	73 / 73	81 / 79.4	92.1 / 92.1	68.3 / 66.7	73 / 69.8	90.5 / 90.5	1.10	1.66	1.77
1VJS	273	81.3 / 76.2	83.6 / 79	84.4 / 78.5	73.1 / 65	77.2 / 68.3	72.6 / 62.1	1.63	1.65	1.67
1WHI	124	83.2 / 81.2	84.2 / 81.2	90.1 / 87.1	75.2 / 69.3	80.2 / 72.3	82.2 / 75.2	1.54	1.83	2.02
2BAA	174	83.1 / 77.5	84.8 / 79.8	87.6 / 80.9	75.8 / 68	76.4 / 64	77 / 67.4	1.74	1.32	1.48
2CPL	285	87.9 / 86.4	87.9 / 86.4	91.7 / 88.6	81.1 / 75.8	84.1 / 77.3	79.5 / 72.7	1.67	1.44	1.64
2END	198	86.4 / 83.1	90.7 / 85.6	92.4 / 87.3	74.6 / 68.6	77.1 / 72	73.7 / 67.8	1.64	1.76	1.97
2HVM	115	89.6 / 86	89.6 / 87.3	88.7 / 83.7	80.5 / 70.1	79.6 / 71	79.6 / 71	1.36	1.19	1.25
2PTH	279	86.8 / 84.8	87.4 / 86.8	93.4 / 90.1	78.1 / 71.5	82.1 / 76.2	83.4 / 76.8	1.31	1.39	1.32
2RN2	289	83.5 / 73.2	86.6 / 77.2	89 / 78	70.1 / 52.8	76.4 / 59.1	73.2 / 57.5	1.86	1.86	2.11
3LZT	482	86.7 / 86.7	86.7 / 85.7	91.4 / 88.6	80 / 77.1	79 / 74.3	83.8 / 74.3	1.42	1.37	1.37
5P21	378	79.9 / 75.7	77.1 / 72.9	85.4 / 81.2	72.2 / 61.1	72.2 / 62.5	75.7 / 64.6	1.77	1.85	1.97
5PTI	469	87 / 80.4	87 / 78.3	91.3 / 84.8	76.1 / 71.7	73.9 / 71.7	78.3 / 76.1	0.41	0.54	0.71
7RSA	193	78 / 75.2	81.7 / 78.9	84.4 / 78	74.3 / 67	77.1 / 68.8	77.1 / 67	1.66	1.68	1.69

The test data used the 65 proteins set.

Table 2. Analysis of the performance of pacoPacker, CIS-RR and scwrl4 on individual residues

PDB	χ_1			χ_{1+2}		
	SCWRL4	CIS-RR	pacoPacker	SCWRL4	CIS-RR	pacoPacker
ARG	79.89	81.66	83.07	65.96	68.96	83.07
ASN	84.95	83.51	86.54	73.20	72.37	73.50
ASP	86.40	83.68	88.07	79.79	74.61	79.25
CYS	87.12	95.76	92.80	0.00	0.00	0.00
GLN	83.05	81.62	86.60	65.63	68.97	61.00
GLU	71.28	76.18	81.08	57.09	58.61	60.14
HIS	89.24	89.24	91.29	79.51	81.60	81.18
ILE	95.90	96.41	96.75	85.64	87.69	80.00
LEU	92.24	93.09	94.29	85.82	86.67	80.56
LYS	80.79	81.54	86.82	62.93	64.30	65.15
MET	85.35	86.36	88.89	71.21	74.75	72.22
PHE	96.05	97.43	98.02	92.49	94.27	94.27
PRO	87.87	85.62	88.40	82.30	80.39	80.56
SER	73.50	71.32	78.02	0.00	0.00	0.00
THR	91.13	90.85	93.36	0.00	0.00	0.00
TRP	91.70	94.76	91.70	78.60	86.46	76.86
TYR	94.60	96.77	95.47	92.44	93.32	93.10
VAL	90.60	92.19	92.32	0.00	0.00	0.00

The test data used the 65 proteins set.

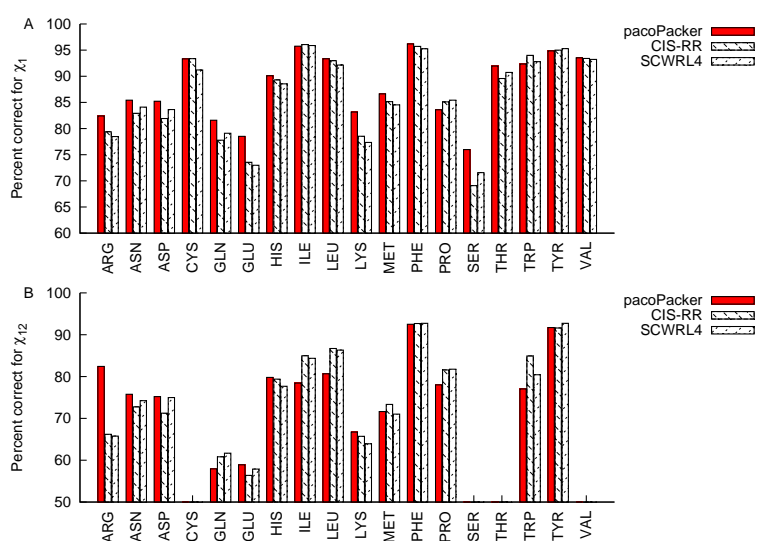


Fig. 4. Analysis of the performance of pacoPacker, CIS-RR and scwrl4 on different amino acids. (A) Percent correct within 40° for the χ_1 angle. (B) Percent correct within 40° for the χ_{12} angle. The test data used the 65 proteins set. Red, Green back slash and blue forward slash indicate the test results of pacoPacker, CIS-RR and SCWRL4, respectively. Note: Because 2QOL can't be predicted by CIS-RR and 1G8Q miss mainchain atomsand, we exclude them from the testing sets of 379 proteins used by the original paper of SCWRL4.

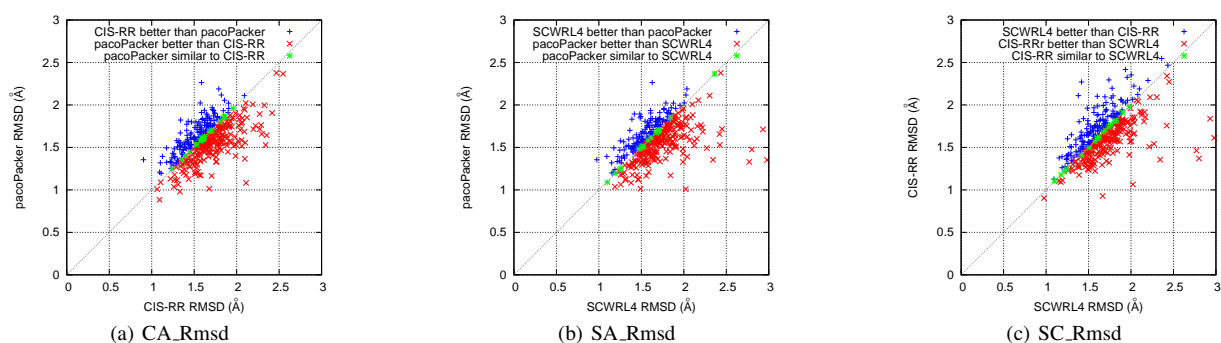


Fig. 5. RMSD comparison on benchmark of SCWRL4

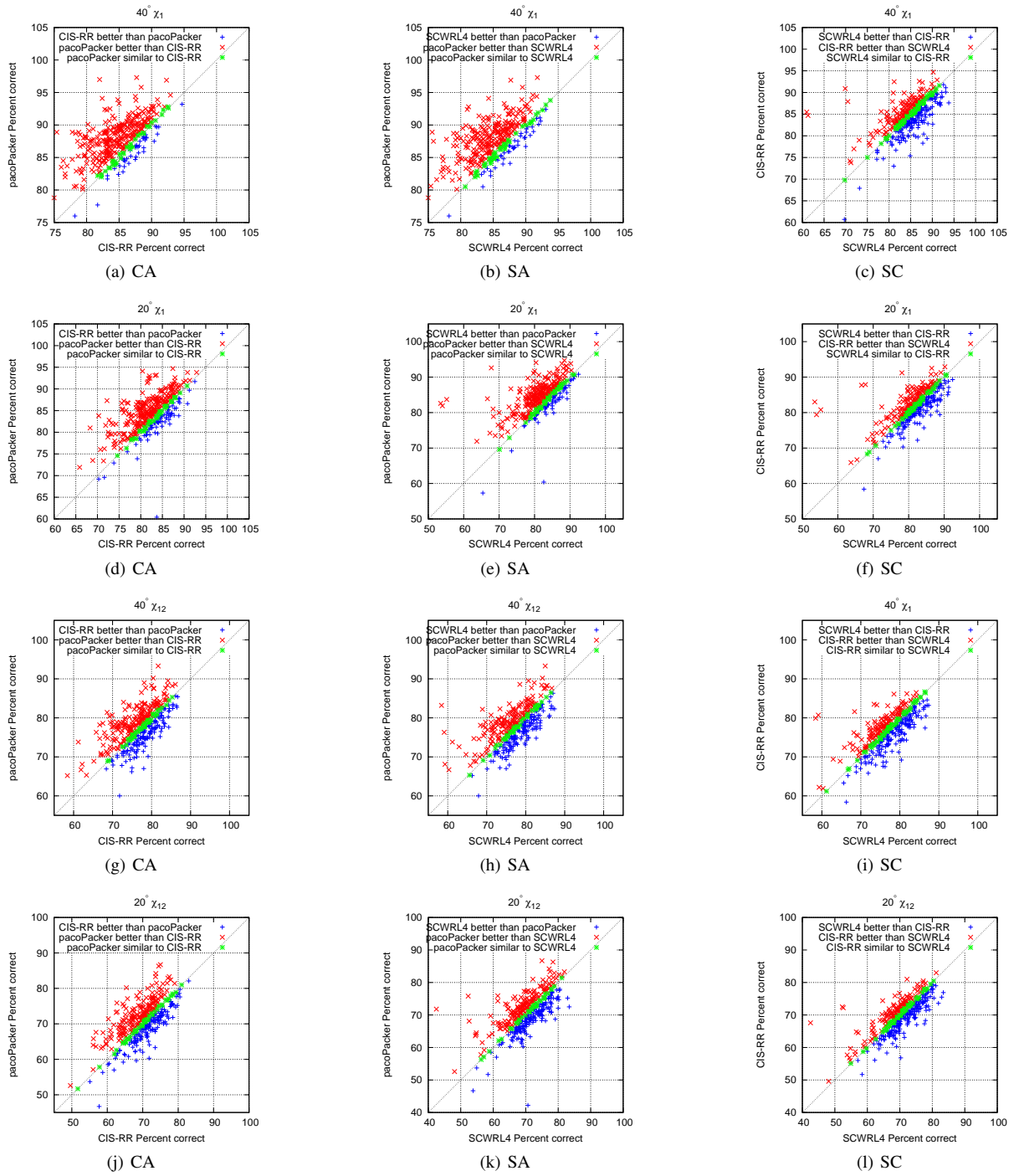


Fig. 6. Target comparison on benchmark of SCWRL4

Table 3. Part 1: Comparison of pacoPacker, CIS-RR and scwrl4 on a 377-protein test set

PDB	NO. of Residues	$\chi_1(40^\circ/20^\circ)$			$\chi_{12}(40^\circ/20^\circ)$			RMSD(Å)		
		SCWRL4	CIS-RR	pacoPacker	SCWRL4	CIS-RR	pacoPacker	SCWRL4	CIS-RR	pacoPacker
1AHO	64	84.3/80.4	82.4/80.4	94.1/94.1	84.3/78.4	80.4/74.5	90.2/86.3	2.42	2.34	1.53
1ATZ	373	86/84.4	85.7/83.7	86.3/83.7	78.5/70.7	79.8/72	76.5/70	1.55	1.46	1.53
1B2P	238	87.9/84.5	89.3/85.4	89.8/86.4	81.6/75.7	81.6/73.3	84/77.2	1.19	1.11	1.19
1B8Z	134	73.2/71.4	67.9/67	55/47.7	68.8/65.2	66.1/62.5	40.5/35.1	1.86	1.90	3.34
1B9W	91	78.2/65.4	78.2/66.7	76/57.3	67.9/53.8	71.8/57.7	60/46.7	1.63	1.59	2.26
1BGF	124	84.8/79.5	81.2/77.7	85.7/79.5	81.2/72.3	75.9/67	80.4/72.3	1.60	1.80	1.74
1BYI	224	85.3/81.9	84.7/82.5	89.3/85.9	77.4/71.2	76.8/70.6	78.5/73.4	1.42	1.41	1.49
1CO2	332	84.4/77.5	80.1/73.8	84.8/77.2	74.8/65.2	71.2/62.3	69.9/60.3	1.45	1.64	1.60
1C48	345	92.3/91.3	89/87.1	90.6/90.3	87.4/82.9	83.2/75.5	82.3/75.2	1.25	1.37	1.47
1CEI	85	80/70.7	80/70.7	88/76	66.7/54.7	66.7/56	74.7/64	1.83	1.90	1.77
1DPT	351	84.2/79.3	84.6/80.7	87.4/82.1	75.1/68.4	76.5/69.5	71.9/65.6	1.68	1.70	1.75
1DQ0	237	83.3/78.8	85.7/80.8	88.7/85.2	78.3/70.4	80.8/73.4	82.8/73.4	1.66	1.46	1.35
1DV7	212	79.4/78.8	80/78.2	84.1/82.4	70/68.2	69.4/65.3	71.8/67.6	2.02	2.07	1.84
1DYS	690	89.5/83.1	88.9/82.5	89.8/84.4	83.8/74.5	81.8/71.1	82.7/73.3	1.38	1.27	1.48
1E5M	411	87/85.7	87.9/86	88.9/86.7	81.3/72.7	81/73.3	80.3/72.7	1.51	1.36	1.30
1E6F	260	86.6/80.6	84.3/78.7	87.5/81.5	77.8/68.1	74.5/67.1	77.8/71.8	1.35	1.45	1.27
1EDQ	540	87.7/86.3	87.4/85.8	90/87	82.6/77	82.1/74	82.1/75.1	1.44	1.37	1.54
1ELK	306	82.5/79.9	84.7/82.1	88/84.7	75.9/70.1	79.2/74.8	78.8/72.3	1.72	1.44	1.54
1ERZ	606	89.8/88.4	89.4/87.3	91.2/89.6	83.7/77.7	83.1/75.5	78.7/72.5	1.45	1.34	1.56
1ES5	260	90.5/88.6	89.1/87.1	92.5/90.5	85.1/76.1	83.6/74.6	87.6/80.1	1.10	1.11	1.09
1ES9	212	83.6/79.8	83.6/79.8	46.9/37.3	74.3/68.3	77/69.9	31.1/23.7	1.77	1.71	1.95
1F41	231	85.5/81.3	85.5/82.4	90.2/85	80.3/72	81.3/71.5	85/75.1	1.22	1.22	1.33
1F60	530	86.1/84.8	88.3/86.3	88.6/85.7	78/72.2	81.2/75.8	77.6/72.6	1.69	1.60	1.57
1F94	63	84.2/84.2	87.7/87.7	91.2/91.2	80.7/77.2	84.2/73.7	89.5/84.2	2.43	2.47	2.38
1FCQ	314	86.6/82.6	87/83.7	67/60.4	77.2/70.7	77.5/71	50.7/42.2	1.91	1.81	1.50
1FO9	331	89.9/87.1	89.2/86.7	88.1/84.3	80.4/74.8	79/73.1	79.4/71	1.55	1.56	1.53
1FPO	499	80.7/78.8	78.1/75.8	80.5/78.4	71.1/65.6	68.7/63.5	68.9/62.4	1.71	1.94	1.75
1FTR	1184	90.1/88.1	88.5/86	89.4/86.1	82.2/75	80.9/72.8	80.5/72.5	1.39	1.46	1.49
1FVK	376	87.5/81.9	85.9/80.9	86.8/81.2	77/68.1	73/63.8	74.7/67.4	1.40	1.49	1.61
1G61	450	84.8/83.2	83.2/82.7	87.4/84.3	82.5/78.1	79.6/76.5	81.7/76.8	1.45	1.56	1.18
1G8A	227	82.3/80.3	83.3/81.3	85.4/84.8	77.3/73.2	77.3/70.2	77.3/72.7	1.67	1.82	1.84
1GMU	554	84.6/83.7	88.1/87	86.8/84.2	75.7/71.1	77.9/71.4	71.4/67.2	1.54	1.43	1.81
1GO3	564	87/85.6	85.8/84.5	87/84.7	80.7/75.1	78.9/74.2	74.8/69	1.58	1.65	1.76
1GPP	217	21.3/13.8	83/80.9	88.8/84	8.5/2.1	75/68.6	75.5/69.7	8.08	1.76	1.66
1GQN	252	88/82.3	87.6/82.3	90/85.6	78.9/68.4	77.5/68.4	81.3/69.4	1.63	1.64	1.57
1GS9	144	82.1/74.8	79.7/74	85.4/78	69.1/59.3	69.1/60.2	69.1/58.5	2.02	1.82	2.12
1GSO	419	31.5/23.8	86.7/84	86.1/82.4	13.9/5.6	77.2/70.7	76.2/71.9	18.59	1.37	1.48
1GVP	87	78.9/68.4	80.3/72.4	86.8/78.9	69.7/59.2	71.1/61.8	78.9/69.7	1.79	1.68	1.45
1GXN	323	85.7/83.8	86.9/83.8	88.8/86.5	81.1/75.7	81.5/71.8	81.9/75.3	1.35	1.33	1.52
1H03	250	81.6/78.3	81.6/76.9	84.9/82.1	75.5/67.5	75.5/65.1	77.8/72.6	1.69	1.58	1.57
1H4A	173	85/79.7	87.6/86.3	91.5/88.9	74.5/66.7	77.1/71.9	79.7/70.6	1.79	1.43	1.37
1H4Y	230	82.5/78.4	78.4/75.3	82.9/77.7	75.8/68.6	70.1/62.9	67.9/61.7	1.95	2.33	2.00
1HCL	294	79.2/70.7	79.2/71.4	82.6/73.4	65.6/57.1	63.3/56	65.3/57.1	1.81	1.85	1.74
1HM5	1112	87.3/84.1	89/86.8	87.7/83.6	79/71.1	82.2/73.5	75.2/67.8	1.53	1.34	1.67
1HZ6	193	70.5/67.8	87.9/87.9	92.6/92.6	58.4/52.3	79.9/72.5	83.2/75.8	2.34	1.36	1.35
1HZ9	132	81.6/78.6	76.7/72.8	82.5/79.6	69.9/66	67/58.3	70.9/63.1	1.49	1.96	1.85
1I4J	220	77.3/73.9	76.1/73.3	83.5/79.5	67/59.7	67/59.7	70.5/64.2	2.08	2.12	1.85
1IGQ	227	78.2/72.4	85.6/81.6	82.8/78.2	73/65.5	74.7/66.7	74.7/69	1.67	1.42	1.64
1IJQ	613	86.6/84	88.1/86.4	89/83.9	79.6/73.2	81.3/76.3	78.9/70.6	1.51	1.42	1.60
1IJY	244	83.2/82.3	85.9/85	88.2/87.3	74.1/69.1	77.7/71.4	78.6/72.3	1.81	1.59	1.56
1ILK	151	71.9/63.7	77/65.9	83.7/71.9	59.3/48.1	62.2/49.6	68.1/52.6	2.45	2.27	1.72
1IU8	412	84.9/82.4	83.8/82.4	84.9/81.8	77/71.6	75/70.7	74.7/68.8	1.73	1.86	1.77
1J23	131	86.8/84.2	82.5/80.7	87.7/86	78.9/74.6	75.4/70.2	78.1/71.1	1.64	1.83	1.65
1J2A	166	87.8/85.6	88.5/87.1	89.9/87.1	79.9/76.3	82/77	82.7/73.4	1.54	1.57	1.34
1J7G	144	81.8/77.7	85.1/79.3	89.3/85.1	70.2/64.5	74.4/70.2	76.9/71.9	1.84	1.59	1.51
1JB3	127	87.8/84.3	78.3/75.7	88.7/85.2	76.5/67.8	68.7/63.5	74.8/68.7	1.78	2.20	1.72
1JCD	152	69.7/67.4	60.7/58.4	76.4/74.2	66.3/58.4	58.4/51.7	65.2/51.7	1.79	2.11	2.02
1JKS	280	87.6/86.3	85.9/84.3	90/88	79.1/73.5	77.1/70.3	78.3/72.7	1.52	1.68	1.52
1JY2	278	83/81.4	82.6/81	84.6/83.8	75.9/72.3	75.5/70	76.3/74.7	1.86	1.69	1.78
1K33	62	79.6/79.6	83.7/83.7	85.7/83.7	77.6/71.4	77.6/73.5	73.5/63.3	1.51	1.50	1.61
1KMT	276	85.8/82.1	82.9/80.4	90.4/86.2	80.4/72.5	76.2/68.8	82.9/77.1	1.50	1.34	1.32
1KMZ	125	83.8/77.8	78.8/72.7	88.9/82.8	74.7/63.6	70.7/59.6	74.7/65.7	1.89	1.81	1.81
1KN3	180	87.3/85.4	85.4/82.3	89.2/84.2	79.7/72.2	77.8/70.9	77.8/67.7	1.64	1.72	1.66
1KOE	172	85.4/85.4	84/83.3	84.7/79.9	81.9/77.8	79.9/74.3	78.5/70.8	1.61	1.73	1.93
1KPT	210	90/87.1	90/88.2	92.9/90	85.3/78.8	85.3/77.1	88.2/82.9	1.39	1.18	1.32
1KU8	596	91.2/89.2	89.6/87.6	90.8/89	82.8/78	82.6/77.4	83.2/77	1.15	1.10	1.32
1KVA	155	84.1/77	82.5/75.4	85.7/76.2	73/56.3	76.2/58.7	71.4/56.3	2.01	1.57	2.02
1KVE	280	87.4/81.3	88.9/84.8	90.4/87.9	76.3/67.7	80.3/70.7	80.8/69.7	1.58	1.22	1.33
1KYF	252	86.2/81.8	83.6/79.1	87.6/81.3	76.4/67.6	75.6/67.6	75.1/68.9	1.88	1.80	1.71
1KZQ	506	85.7/83.6	85.7/84.1	84.6/82.2	79.4/74.1	78/73.6	76.4/71.3	1.50	1.52	1.50
1L3K	163	84.3/82.9	87.1/85.7	90.7/90	80/71.4	80.7/74.3	84.3/77.1	1.90	1.80	1.67
1LBV	504	79.4/70.1	79.4/71.6	80.1/69.6	70.1/54.9	68.4/55.1	66.9/53.7	1.82	1.84	1.93
1LM5	382	82.1/79.2	82.4/78.9	84.3/79.6	72.8/67.4	73.5/67.7	70.9/64.5	1.86	1.85	1.84
1LTU	284	83.3/80.3	82/77.8	84.5/78.2	77/69	74.5/66.5	74.5/68.2	1.60	1.61	1.59
1M5T	123	91.6/90.7	91.6/90.7	91.6/90.7	84.1/79.4	81.3/75.7	84.1/81.3	1.63	1.65	1.84
1M6J	520	89.7/87.2	89.4/87.2	90.9/87.2	80/75.9	79.3/75.4	78.8/73.4	1.40	1.62	1.45

There are 76 proteins in part one.

Table 4. Part 2: Comparison of pacoPacker, CIS-RR and scwrl4 on a 377-protein test set

PDB	NO. of Residues	$\chi_1(40^\circ/20^\circ)$			$\chi_{12}(40^\circ/20^\circ)$			RMSD(\AA)		
		SCWRL4	CIS-RR	pacoPacker	SCWRL4	CIS-RR	pacoPacker	SCWRL4	CIS-RR	pacoPacker
1MD6	154	79.2/75.4	80.8/77.7	87.7/83.8	69.2/61.5	75.4/66.9	75.4/67.7	1.79	1.59	1.73
1MF7	194	86.2/81.6	87.4/83.9	89.1/85.1	79.9/71.8	80.5/72.4	81/71.8	1.84	1.46	1.60
1MG7	703	82.2/80.7	82.3/80.6	82/80.3	76.1/70.2	76.3/71	72.8/67	1.61	1.55	1.62
1MIX	206	82/79.8	83.1/79.8	89.1/85.2	75.4/66.7	76/67.2	75.4/67.2	1.84	1.90	1.45
1MKK	187	82.6/82	83.1/83.1	85.5/84.3	75/70.9	75.6/72.7	75.6/70.9	1.38	1.29	1.27
1MML	251	83.7/72.9	85.1/73.8	83.7/72.9	75.1/62.9	73.8/62	71.5/61.5	1.58	1.57	1.58
1MOL	188	86.1/81.9	84.9/82.5	86.7/83.1	79.5/70.5	76.5/69.9	76.5/69.3	1.76	1.77	1.83
1NIJ	165	83.6/82.9	82.9/81.5	87/84.9	75.3/69.9	71.9/67.1	78.8/74	1.70	1.93	1.65
1N93	335	83.9/82.4	84.6/82.4	85.7/83.5	76.3/72.4	77.8/71.3	75.3/69.5	1.74	1.74	1.64
1NAR	289	85.1/77.5	85.1/78.6	85.5/78.6	75.6/62.6	75.6/62.6	71.4/61.1	1.46	1.40	1.57
1NM8	591	86.6/83.9	86.2/83.1	84.8/82.1	80/73.7	79.7/73.1	76.6/70.6	1.50	1.46	1.67
1NWA	168	27.5/19	81/76.1	89.4/84.5	14.1/9.2	74.6/64.1	77.5/69	13.75	1.92	1.75
1NXM	388	89.2/85.8	86.1/84.3	88.3/85.5	83.7/75	78.3/72	78/71.4	1.30	1.65	1.47
1OAI	68	88.1/83.1	83.1/81.4	86.4/84.7	79.7/71.2	71.2/64.4	78/71.2	1.72	1.76	1.33
1OAG	230	84/82.9	83.4/82.4	86.6/85	79.1/74.3	78.6/73.3	80.2/74.3	1.39	1.40	1.50
1OGM	572	90.3/88.4	91.1/89	89.7/86.8	86.6/80	86.4/78.1	83.1/75.6	1.17	1.09	1.21
1OK7	739	82.4/79	82.3/79.7	82.4/78.6	75/69	74.5/67.9	69.3/62.3	1.90	1.91	1.96
1PIX	501	85.9/83.8	87.9/86.9	91.3/89.7	81.8/76.4	86.2/78.5	85.6/78.5	1.48	1.45	1.48
1P6Z	200	57/55.2	82/80.8	85.5/83.7	43/38.4	69.8/66.9	69.2/65.1	31.85	2.09	1.94
1P9H	179	83.5/82.6	86.8/86	89.3/88.4	74.4/69.4	76/69.4	79.3/74.4	1.31	1.30	1.12
1PCF	528	86.7/83.1	79.7/76.9	87.1/81.8	76.3/67.8	71.2/61.2	72.2/62.9	1.48	1.72	1.63
1PDO	129	88.5/81.7	86.5/79.8	91.3/85.6	81.7/69.2	80.8/69.2	83.7/73.1	1.50	1.24	1.33
1PE9	722	89.2/88	89.5/88.2	92.1/90.9	81.6/76	81.4/74.5	80.9/75	1.26	1.23	1.25
1PGV	167	76.3/73.7	79.6/78.3	81.6/78.9	65.8/57.2	72.4/64.5	67.8/59.2	2.30	2.09	2.11
1PM4	351	80.2/74.3	81.5/75.9	84.8/79.5	74.9/64.7	76.9/64.7	77.2/68	1.52	1.30	1.35
1PXZ	692	84.6/81	83.2/78.9	82.2/77.2	79.8/69.7	75.6/65.1	73.5/64.5	1.61	1.57	1.68
1QAH	264	84.3/81.4	83.3/80.4	88.2/85.3	76/66.2	75/67.2	78.4/71.1	1.68	1.78	1.46
1QKD	124	77.2/72.8	74.6/71.9	85.1/81.6	71.9/62.3	65.8/56.1	76.3/65.8	1.58	1.76	1.45
1R12	502	84.5/83	85.7/84.5	85.7/83.2	77.3/71.1	78/69.3	78.2/72	1.56	1.63	1.66
1R29	122	83/82.1	83/81.2	87.5/83	72.3/67.9	76.8/69.6	78.6/69.6	1.72	1.69	1.59
1R77	202	82.6/81.5	84.8/83.7	88.8/87.1	75.3/72.5	79.8/73	79.2/75.8	1.52	1.55	1.51
1R8N	185	82.2/79	79/75.8	88.5/85.4	71.3/64.3	68.2/63.7	75.2/66.9	1.91	1.78	1.51
1RFY	177	87.4/85.3	88.1/87.4	91.6/90.9	78.3/72.7	76.2/72.7	83.2/77.6	1.68	1.67	1.44
1RGX	272	82.6/77.2	81.7/76.7	82.2/76.3	71.7/62.6	69.9/63.5	68.9/62.6	1.72	1.59	1.91
1RL0	255	83.3/81	87.5/85.6	84.7/82.4	76.9/70.4	80.1/71.8	77.3/69.4	1.62	1.45	1.66
1RWZ	244	84.4/82.9	86.3/83.9	89.6/87.7	78.7/73	78.2/71.1	83.4/73	1.50	1.57	1.42
1RYL	306	83.6/79.9	82.1/78.7	82.8/79.5	72.8/66.4	72.4/67.2	70.9/63.4	1.61	1.70	1.82
1RZ2	214	85.2/79.6	84.7/79.6	87.2/82.1	75.5/66.8	74/63.3	75.5/65.3	1.32	1.34	1.51
1S7I	124	79.4/72.2	84.5/77.3	88.7/78.4	72.2/61.9	75.3/66	73.2/60.8	1.96	1.80	1.62
1S7K	158	90.2/86.5	94.7/92.5	93.2/91.7	84.2/69.9	86.5/76.7	82.7/69.9	1.66	1.29	1.58
1SAU	114	83.2/83.2	83.2/83.2	87.1/84.2	77.2/69.3	73.3/67.3	78.2/71.3	1.74	1.76	1.52
1SH8	302	61/53.5	85.5/83	86.7/82.6	45.2/39.4	79.7/74.7	75.9/70.1	2.10	1.92	1.88
1SMX	168	78.9/75.9	82/78.9	88.7/85.7	72.2/63.9	77.4/68.4	77.4/66.9	1.98	1.67	1.73
1SNT	352	86.7/84.4	85/83.7	86.7/84.7	79.9/73.8	76.9/70.7	73.1/70.1	1.60	1.62	1.79
1SQE	207	85.3/80.1	85.3/80.6	89.5/86.4	73.8/67	75.4/67.5	76.4/64.9	1.58	1.53	1.41
1SRV	145	73.1/69.7	79/73.9	83.2/76.5	64.7/58.8	68.9/60.5	70.6/58.8	2.00	1.96	1.96
1SUU	293	86.7/83.5	86.7/81.9	86.7/82.3	80.3/69.1	76.3/67.9	75.5/65.9	1.27	1.24	1.38
1SWH	459	83.4/73.5	79.4/70.3	80.5/69.2	75.6/61	72.7/61.9	70.3/57	1.39	1.80	1.83
1TIJ	244	52.2/47.8	83.6/80.1	87.6/83.6	41.8/38.3	74.6/70.1	77.1/72.1	2.93	1.84	1.71
1TJE	224	85.2/81.5	83.1/79.9	88.9/85.7	75.1/69.8	70.4/65.1	74.1/68.8	1.77	1.88	1.55
1TKS	392	90/86.1	89.7/86.7	48.3/35.9	77.3/69.4	76.4/69.1	26.1/18.5	1.51	1.56	4.48
1TP6	126	80.8/79.8	87.9/85.9	89.9/86.9	73.7/65.7	78.8/70.7	78.8/70.7	2.12	1.92	1.57
1TUA	189	79.9/79.9	83/82.4	84.9/84.9	73.6/67.9	74.2/67.9	74.2/65.4	2.17	1.86	2.06
1TUO	437	82.2/79.6	83.1/81.4	85.5/82.5	74.3/68	76/68.9	71/67.2	1.80	1.81	1.77
1TY0	626	85.3/82.9	81.9/79.7	83.4/80.2	75.9/68.6	75.2/64.5	71.9/64.7	1.53	1.45	1.50
1TZV	141	81.2/78.9	85.9/83.6	84.4/81.2	73.4/70.3	75/71.9	67.2/64.1	1.48	1.64	1.89
1U07	178	83.2/79.2	87.9/83.9	86.6/83.2	77.2/69.8	77.9/69.1	75.2/71.8	1.79	1.67	1.59
1U2H	96	80.3/80.3	84.2/84.2	89.5/85.5	69.7/68.4	71.1/71.1	77.6/72.4	1.98	1.62	1.94
1U5X	130	82.9/78.1	79/74.3	86.7/81.9	79/66.7	73.3/63.8	80/69.5	1.64	1.41	1.36
1UEB	362	86.5/85.5	88.8/87.5	88.1/86.8	79.9/77.6	82.5/77.9	80.5/76.2	1.77	1.59	1.69
1UEK	268	87.3/80.7	85.8/78.7	88.8/80.2	74.1/66.5	72.6/64.5	72.6/64.5	1.88	1.90	2.02
1UJN	674	85.1/83	86.8/84.9	85.2/81.4	75.7/71.5	77.8/72	75/69.1	1.75	1.55	1.80
1UKF	188	81.9/80.5	85.2/85.2	87.9/87.2	77.2/69.1	79.2/69.8	79.2/71.8	1.90	1.83	1.60
1ULN	82	88.1/88.1	83.6/82.1	92.5/92.5	83.6/79.1	77.6/71.6	80.6/68.7	1.61	1.69	1.69
1ULR	87	89.4/86.4	84.8/81.8	93.9/92.4	80.3/78.8	74.2/72.7	83.3/78.8	1.56	1.97	1.52
1UNP	119	82.6/78.9	79.8/76.1	88.1/87.2	74.3/67	71.6/64.2	78/70.6	1.79	2.02	1.58
1USM	77	87.7/87.7	92.3/90.8	96.9/93.8	76.9/76.9	83.1/75.4	80/72.3	1.85	1.71	1.97
1UXZ	262	90.9/90.4	90.9/90.4	93.9/91.9	83.3/79.8	83.8/78.8	83.3/75.3	0.98	0.90	1.35
1UZ3	199	77.3/74.4	80.8/78.5	83.1/79.7	70.3/65.7	71.5/68	72.1/66.9	1.92	1.72	1.76
1V05	96	27.2/21	84/81.5	91.4/91.4	16/9.9	72.8/65.4	84/80.2	10.66	1.61	1.35
1V0S	495	91.2/87.2	87.5/83.2	89/85.5	83.2/74.9	78.9/73.2	80.7/71.7	1.42	1.57	1.52
1V6T	249	85.9/83.5	86.9/85.4	90.3/86.9	78.2/71.8	76.2/69.9	79.6/71.8	1.86	1.83	1.56
1V7Q	169	82.7/80.5	82.7/80.5	88.7/84.2	75.2/70.7	74.4/71.4	75.9/72.2	2.09	2.04	1.70
1V8E	217	85.8/82.2	88.8/86.4	88.8/85.2	79.3/73.4	81.1/75.1	77.5/71	1.82	1.78	1.63
1V8H	212	86.5/84.1	88.2/84.7	89.4/87.6	79.4/75.9	78.8/73.5	81.2/77.6	1.60	1.60	1.46
1V8I	150	84.7/82.3	88.7/87.1	87.9/87.9	76.6/72.6	80.6/72.6	79/74.2	1.85	1.66	1.88

There are 76 proteins in part two.

Table 5. Part 3: Comparison of pacoPacker, CIS-RR and scwrl4 on a 377-protein test set

PDB	NO. of Residues	$\chi_1(40^\circ/20^\circ)$			$\chi_{12}(40^\circ/20^\circ)$			RMSD(Å)		
		SCWRL4	CIS-RR	pacoPacker	SCWRL4	CIS-RR	pacoPacker	SCWRL4	CIS-RR	pacoPacker
1VDK	915	88.6 / 87.5	86.8 / 85.7	89.8 / 87.8	79.1 / 77.4	79.1 / 71.6	78.5 / 71.2	1.69	1.74	1.59
1VE2	442	83 / 80.6	85.8 / 82.1	83.6 / 79.4	76.4 / 71.8	78.5 / 74.5	74.8 / 71.2	1.84	1.75	1.90
1VGT	424	84.2 / 81.1	85.7 / 82.3	86.6 / 82.6	75.2 / 69.3	77.6 / 71.4	73.6 / 66.5	1.50	1.47	1.54
1VH5	276	87.3 / 85.5	90.8 / 87.7	91.7 / 88.6	81.6 / 75.4	83.8 / 79.4	84.6 / 78.9	1.94	1.66	1.79
1VJS	469	81.3 / 76.2	83.6 / 79	83.4 / 78.5	73.1 / 64.7	77.2 / 68.3	74.9 / 63.9	1.68	1.65	1.74
1VPI	122	84.2 / 78.2	85.1 / 81.2	87.1 / 84.2	77.2 / 61.4	74.3 / 65.3	80.2 / 74.3	1.63	1.76	1.39
1W5R	546	87.5 / 83.9	87.5 / 83.9	86.8 / 82.3	79.5 / 72.5	80.2 / 70.9	77.3 / 69.3	1.63	1.54	1.57
1W7B	319	85.7 / 84.6	85.4 / 83.9	90 / 86.4	77.9 / 73.6	78.2 / 72.1	78.6 / 75	1.65	1.64	1.46
1WBA	171	89 / 86.2	82.8 / 79.3	92.4 / 86.9	85.5 / 77.9	80 / 68.3	88.3 / 77.9	1.19	1.26	1.04
1WD7	509	83.4 / 78.4	83.1 / 78.4	85.2 / 80	74.3 / 66.8	73.8 / 66.2	71.7 / 64.2	1.80	1.90	1.91
1WKA	143	79.5 / 77.8	85.5 / 84.6	88 / 83.8	71.8 / 66.7	78.6 / 70.9	77.8 / 68.4	1.88	1.69	1.84
1WKO	330	83.8 / 79.5	84.5 / 79.8	89.2 / 84.5	77.1 / 69	77.4 / 68.4	81.1 / 72.7	1.56	1.71	1.17
1WLG	586	81.9 / 78.5	82.1 / 79.1	83.8 / 79.8	75.1 / 70.2	74.7 / 69.6	75.3 / 68.7	1.48	1.43	1.38
1WLZ	335	90 / 89.2	86.7 / 84.9	86.7 / 83.9	83.2 / 79.6	82.1 / 77.8	79.9 / 74.9	1.61	1.89	1.84
1WM3	72	87.7 / 86.2	83.1 / 81.5	92.3 / 87.7	81.5 / 78.5	78.5 / 76.9	87.7 / 81.5	1.66	1.72	1.41
1WMH	165	86.9 / 86.2	84.1 / 82.8	89.7 / 88.3	80 / 75.2	77.9 / 72.4	82.1 / 73.1	1.42	1.51	1.33
1WQJ	142	86.2 / 81.7	79.8 / 77.1	85.3 / 82.6	81.7 / 75.2	74.3 / 67	77.1 / 69.7	1.49	1.81	1.46
1WTJ	669	85.3 / 83.5	85.1 / 84.1	86.9 / 85.1	80.4 / 74	78.8 / 72	80.2 / 75.2	1.87	1.73	1.82
1WU9	126	80.9 / 77.4	81.7 / 76.5	87 / 81.7	74.8 / 68.7	73 / 62.6	73.9 / 62.6	1.63	1.82	1.55
1WVH	132	83 / 80.4	83 / 81.2	54.2 / 45.8	75 / 69.6	75 / 67	33.6 / 28	1.71	1.79	3.02
1WYC	384	89.3 / 87.4	88.7 / 88.7	88.7 / 87.1	83.8 / 78	82.8 / 76.4	79.3 / 73.5	1.47	1.50	1.62
1WZ3	168	82.5 / 80.3	83.9 / 81.8	86.1 / 83.9	78.1 / 68.6	81 / 70.8	81 / 70.8	1.56	1.29	1.31
1X1E	239	85.4 / 82	87.1 / 83.7	89.9 / 85.4	78.1 / 71.9	78.1 / 70.2	80.3 / 76.4	1.88	2.06	1.80
1X2I	136	91.1 / 90.2	92.9 / 92.9	94.6 / 93.8	83.9 / 81.2	83.9 / 83	85.7 / 82.1	1.64	1.53	1.41
1X6I	176	88.1 / 85.5	86.2 / 84.3	90.6 / 87.4	81.8 / 73	79.2 / 73	83 / 76.1	1.67	1.74	1.67
1XDZ	238	83.4 / 80.6	86.7 / 83.9	86.3 / 83.4	73.5 / 67.3	79.1 / 69.2	70.1 / 62.6	1.64	1.53	1.71
1XFK	324	84.6 / 81.1	83 / 80.7	84.9 / 80.3	78 / 68.7	76.1 / 68	76.8 / 68	1.76	1.74	1.68
1XS0	384	78.7 / 74.4	74.7 / 71.6	81.5 / 76.2	73.1 / 64.8	71 / 63.6	74.4 / 67	1.55	1.73	1.56
1XXO	286	81.9 / 79	83.2 / 80.3	85.7 / 83.2	73.5 / 66.8	73.5 / 64.7	73.1 / 68.9	1.68	1.81	1.80
1Y2T	284	90.9 / 89.7	88.8 / 86.8	90.5 / 87.6	84.3 / 78.5	85.5 / 78.1	83.5 / 75.2	1.60	1.54	1.68
1Y7Y	135	93.8 / 91.2	87.6 / 85.8	93.8 / 90.3	86.7 / 80.5	80.5 / 75.2	87.6 / 77.9	1.61	1.99	1.40
1YAC	408	84.3 / 80.5	84.3 / 80.5	85.8 / 82	76.9 / 70.1	75.1 / 68	76.6 / 68	1.78	1.67	1.60
1YHH	229	82.8 / 77.8	81.3 / 79.3	83.8 / 82.3	77.8 / 66.2	76.8 / 69.7	78.8 / 71.2	1.48	1.65	1.53
1YN3	196	83.9 / 79.4	87.2 / 82.8	88.3 / 84.4	76.7 / 68.3	77.8 / 68.9	79.4 / 70.6	1.39	1.27	1.18
1YO3	255	20.7 / 17.6	82.9 / 82	88.7 / 86.9	9 / 5	79.3 / 71.2	79.3 / 73.9	8.43	1.67	1.39
1YPF	590	86.2 / 81.9	85.5 / 81.7	86.2 / 81.7	77.4 / 69.5	76.6 / 68.6	75.4 / 65.2	1.51	1.66	1.56
1YT4	263	86.1 / 81.9	86.1 / 82.4	88 / 84.7	76.4 / 70.4	77.3 / 73.1	77.3 / 72.2	1.58	1.63	1.62
1YTL	631	85.2 / 79.9	83.7 / 78	85.4 / 78.4	76.7 / 68.8	74.6 / 65	71.6 / 61.2	1.57	1.60	1.59
1YU5	67	83.1 / 83.1	84.7 / 84.7	89.8 / 89.8	76.3 / 74.6	79.7 / 78	81.4 / 76.3	1.60	2.10	1.56
1YW5	177	81.6 / 79.7	81 / 81	84.2 / 81.6	71.5 / 67.1	72.8 / 67.7	74.1 / 67.7	1.96	2.06	1.78
1YXY	460	88.5 / 87.4	84.3 / 83.5	88.7 / 87.6	81.6 / 78.6	78.3 / 75.3	81.9 / 79.7	1.50	1.64	1.56
1YZM	46	81.1 / 78.4	73 / 70.3	86.5 / 83.8	75.7 / 70.3	67.6 / 56.8	73 / 67.6	1.42	2.27	1.89
1Z0C	200	83.5 / 79.3	85.4 / 80.5	87.8 / 83.5	73.8 / 61.6	77.4 / 64.6	78.7 / 67.1	1.75	1.60	1.52
1Z0P	73	79.7 / 75	84.4 / 79.7	84.4 / 81.2	67.2 / 56.2	73.4 / 57.8	68.8 / 57.8	1.82	1.82	1.72
1ZKR	291	84.6 / 80.4	85.8 / 80.8	84.6 / 79.2	75.8 / 70.8	77.7 / 71.2	76.9 / 70	1.48	1.36	1.42
1ZO2	248	81.1 / 77.5	82.9 / 80.2	87.4 / 83.8	72.5 / 65.3	76.1 / 68.5	73 / 65.8	1.71	1.59	1.66
1ZRS	588	88.8 / 86.6	90.4 / 88.8	87.5 / 83.8	82.9 / 74.8	84.4 / 75.9	77.6 / 70	1.80	1.63	1.82
1ZUH	151	75 / 68.9	75 / 68.9	78.8 / 73.5	66.7 / 54.5	65.2 / 56.8	68.9 / 63.6	1.90	2.04	1.88
1ZV1	118	84 / 83	82 / 80	87 / 84	75 / 66	78 / 70	67 / 62	2.04	1.79	2.19
1ZVA	75	71 / 71	74.2 / 74.2	82.3 / 77.4	62.9 / 54.8	69.4 / 59.7	72.6 / 64.5	1.86	1.79	1.73
1ZVT	491	88.3 / 84.9	87.1 / 83.6	86.6 / 82.6	82.9 / 76.2	79.4 / 72	78.7 / 73.9	1.55	1.58	1.71
1ZXT	276	84.7 / 77.4	83.1 / 76.2	85.9 / 78.2	77 / 65.3	75.4 / 65.3	75.4 / 66.5	2.22	2.09	1.69
2A35	416	84.6 / 82.4	87.1 / 85.6	88.4 / 85.9	78.1 / 71.2	78.1 / 71.2	77.7 / 73.4	1.73	1.72	1.60
2A6W	435	81.6 / 76.2	81.9 / 76.2	84.5 / 79.5	75.1 / 67.1	74.6 / 64.5	76.2 / 67.4	1.67	1.68	1.57
2A8F	196	86.1 / 85.5	86.1 / 86.1	86.7 / 84.3	83.7 / 79.5	83.1 / 79.5	82.5 / 77.7	1.26	1.31	1.06
2AHF	754	87.3 / 85	88.8 / 86.7	85.9 / 81.9	77.1 / 70.2	78.9 / 69.4	74.7 / 66.4	1.89	1.73	1.87
2AHN	222	92.2 / 87.8	90 / 87.2	91.1 / 84.4	83.9 / 77.2	84.4 / 78.3	83.3 / 75.6	1.18	1.18	1.49
2B0A	186	87.4 / 82.6	86.2 / 80.8	90.4 / 86.8	82 / 72.5	77.8 / 68.9	79.6 / 71.9	1.44	1.53	1.26
2B0J	344	78 / 70.8	83.4 / 76.9	83.4 / 75.5	68.2 / 61.7	76.2 / 67.9	70 / 62.1	1.76	1.50	1.61
2B2F	391	86.5 / 83.7	88.2 / 86.1	87.5 / 84.7	77.8 / 71.9	79.2 / 72.9	78.5 / 74	1.57	1.52	1.80
2BAY	340	81.2 / 78.1	92.5 / 91.2	92.8 / 89.7	68.4 / 64.7	81.6 / 74.4	78.1 / 71.9	1.49	1.25	1.43
2BK8	97	79.5 / 75.9	79.5 / 77.1	88 / 86.7	71.1 / 61.4	69.9 / 62.7	80.7 / 75.9	1.67	1.99	1.53
2BPD	256	85.8 / 83.2	83.2 / 79.3	87.1 / 81.9	79.7 / 74.6	74.1 / 69	78 / 70.3	1.55	1.70	1.44
2BVP	382	85.2 / 83	83 / 80.3	84.8 / 81.5	79.7 / 74.2	77 / 70	77 / 69.7	1.61	1.74	1.90
2CG7	90	82.4 / 79.7	83.8 / 83.8	87.8 / 82.4	73 / 67.6	75.7 / 67.6	79.7 / 74.3	1.84	1.58	1.17
2CGH	480	86 / 83.4	86.8 / 84.6	87.1 / 84.3	80.9 / 75.6	80.9 / 75	78.9 / 73	1.42	1.64	1.51
2CHC	489	69.9 / 66.7	90.9 / 87.7	88.6 / 83.9	59.1 / 52.6	80.7 / 72.2	76.3 / 68.1	2.22	1.51	1.73
2CI3	274	86.8 / 85.5	86.8 / 85.5	90.2 / 88.9	77.4 / 71.4	79.1 / 71.4	80.3 / 73.9	1.54	1.56	1.40
2CIU	123	77.3 / 75.5	76.4 / 73.6	84.5 / 81.8	70.9 / 63.6	70 / 60.9	74.5 / 68.2	1.79	1.93	1.80
2COV	534	88.8 / 84.8	85.9 / 82.3	49.9 / 40	82.3 / 70.3	78.1 / 69.2	37.6 / 26.6	1.49	1.68	1.01
2CWC	284	81.8 / 79.8	83.7 / 79.8	89.2 / 85.2	71.4 / 66	72.4 / 66.5	76.8 / 70	1.96	1.79	1.73
2CWK	305	80.8 / 78.5	83.5 / 83.1	86.6 / 85.4	73.9 / 68.6	77 / 72	80.1 / 75.5	1.89	1.77	1.55
2CWL	597	88.3 / 87.6	88.5 / 87.8	89.3 / 88.1	83.4 / 77.6	81.1 / 76.1	82.2 / 74	1.35	1.33	1.52
2CWR	97	83.5 / 81	89.9 / 87.3	91.1 / 88.6	78.5 / 72.2	86.1 / 81	88.6 / 81	2.02	1.06	1.01
2CYG	312	88.8 / 86.7	89.2 / 88	90.4 / 88	83.5 / 77.1	85.5 / 79.9	83.1 / 78.3	1.43	1.49	1.35
2D4P	130	93.1 / 90.1	91.1 / 89.1	93.1 / 89.1	86.1 / 77.2	82.2 / 76.2	84.2 / 78.2	1.86	1.79	1.55

There are 76 proteins in part three.

Table 6. Part 4: Comparison of pacoPacker, CIS-RR and scwrl4 on a 377-protein test set

PDB	NO. of Residues	$\chi_1(40^\circ/20^\circ)$			$\chi_{12}(40^\circ/20^\circ)$			RMSD(Å)		
		SCWRL4	CIS-RR	pacoPacker	SCWRL4	CIS-RR	pacoPacker	SCWRL4	CIS-RR	pacoPacker
2D68	152	85.8 / 82.7	83.5 / 81.1	86.6 / 82.7	82.7 / 78	80.3 / 72.4	74.8 / 70.9	1.49	1.77	1.86
2D8E	88	71.2 / 70	73.8 / 72.5	83.8 / 80	61.2 / 60	61.2 / 58.8	73.8 / 67.5	2.36	2.55	2.37
2DPO	310	82.1 / 81.3	81 / 81	84.7 / 83.6	77.6 / 73.1	74.3 / 70.1	73.5 / 68.3	1.67	1.89	1.81
2DQW	497	84.1 / 83	84.3 / 82.5	83.3 / 81	77 / 71.1	77.2 / 69.4	74.7 / 68.4	1.94	1.82	1.84
2DYU	644	86.8 / 82.5	87.7 / 85.4	86.9 / 84	75.4 / 67.5	78.2 / 70.3	76.3 / 70.5	1.67	1.47	1.80
2E01	445	29.6 / 19.5	81.7 / 79.2	77.7 / 73.9	14.3 / 6.3	74.9 / 68.2	66.2 / 59.6	9.21	1.63	1.69
2E10	439	84.6 / 80.5	86.5 / 83.9	84.1 / 79.7	76.8 / 71.6	78.4 / 73.7	72.7 / 68.5	1.71	1.60	1.84
2E3Z	919	89.8 / 87.2	89.2 / 87.8	88 / 85.5	83.7 / 77.3	82.6 / 78.5	77.3 / 71.8	1.47	1.30	1.51
2E64	461	83.2 / 80.5	84 / 82.2	84.5 / 81	76 / 71.5	77.2 / 72	74.8 / 70.8	1.82	1.67	1.72
2E7A	435	81.6 / 78.6	79.2 / 76.2	82.7 / 79.7	72.7 / 64.1	68.4 / 60.8	71.4 / 66.2	1.70	1.73	1.76
2E8F	132	83.2 / 83.2	84.9 / 82.4	82.4 / 81.5	74.8 / 71.4	74.8 / 68.9	72.3 / 68.9	1.63	1.62	1.76
2E8G	480	83.6 / 77.2	84.3 / 77.9	83.8 / 78.7	72.1 / 65.4	73 / 65.2	71.3 / 64.7	1.84	1.77	1.85
2E9Y	625	82.7 / 80.4	81.5 / 78.8	87.1 / 83.9	76.6 / 70	73.2 / 67.5	78 / 73.4	1.81	1.76	1.67
2EBB	96	84.5 / 82.1	79.8 / 79.8	88.1 / 86.9	73.8 / 71.4	67.9 / 63.1	76.2 / 69	1.93	2.42	1.91
2EBE	212	80.7 / 80.1	77.8 / 77.8	84.7 / 83	71.6 / 68.8	72.2 / 70.5	76.1 / 73.3	1.90	1.83	1.64
2ECR	298	90.7 / 86.7	90.3 / 86.7	92 / 88.5	80.5 / 76.5	77 / 72.1	81 / 77.4	1.67	1.72	1.62
2EGJ	252	86 / 83.3	85.5 / 82	89.9 / 87.7	79.4 / 71.1	78.1 / 70.2	79.8 / 74.6	1.84	1.70	1.71
2EHG	149	82.8 / 81.2	87.5 / 86.7	91.4 / 90.6	75.8 / 70.3	78.1 / 72.7	83.6 / 77.3	1.99	1.76	1.33
2EPI	388	83.8 / 82.9	82.9 / 82.1	84.1 / 82.4	77.9 / 72.9	76.8 / 71.2	73.2 / 69.1	1.68	1.66	1.76
2ETX	389	86.9 / 85.4	86.9 / 86.3	90.6 / 87.8	80.5 / 76.9	82.1 / 76.9	81.2 / 76.6	1.63	1.53	1.46
2EX0	782	88 / 85.1	87.6 / 85.9	86.6 / 83.3	82.1 / 73.9	81 / 74.5	77.2 / 71	1.53	1.39	1.50
2F23	308	82.3 / 81.5	81.9 / 81.2	82.7 / 80.8	70.8 / 66.9	71.2 / 66.5	70.4 / 65.8	1.90	1.94	1.84
2F5G	260	80.8 / 76.9	79.5 / 76.9	83.3 / 78.6	68.8 / 62	67.5 / 61.1	70.5 / 65.8	1.83	1.87	1.86
2F6L	330	85.9 / 83.9	83.5 / 82	87.8 / 83.9	79.6 / 71	78 / 70.6	76.9 / 71	1.70	1.61	1.69
2FBN	304	85.3 / 83.9	89.4 / 88.6	90.1 / 89.4	77.3 / 67.8	77.7 / 67.8	81.7 / 72.2	1.55	1.51	1.38
2FBQ	213	77.3 / 75	76.7 / 75	82 / 79.7	72.1 / 67.4	68.6 / 64.5	70.9 / 65.1	2.10	2.19	2.01
2FD5	180	83.7 / 80.7	84.4 / 82.2	86.7 / 81.5	77 / 70.4	77.8 / 71.9	76.3 / 69.6	1.71	1.65	1.76
2FHZ	199	87.1 / 87.1	85.3 / 84.7	89.4 / 89.4	82.4 / 78.2	77.6 / 72.9	82.9 / 77.1	1.49	1.54	1.57
2FJZ	59	87 / 83.3	92.6 / 87	92.6 / 87	74.1 / 68.5	83.3 / 75.9	77.8 / 70.4	1.74	1.32	1.58
2FL4	147	84.9 / 82.5	75.4 / 72.2	88.9 / 87.3	76.2 / 69.9	67.5 / 60.3	78.6 / 71.4	1.74	2.30	1.66
2FLU	301	28.2 / 20.2	90.3 / 89.9	92.9 / 91.6	11.3 / 6.3	84.5 / 80.3	84.5 / 78.6	18.76	1.09	0.88
2FRG	106	89.8 / 85.2	88.6 / 83	90.9 / 86.4	80.7 / 76.1	79.5 / 72.7	75 / 68.2	1.56	1.91	1.74
2FVH	297	84.3 / 81.3	83 / 79.6	86 / 81.3	74.9 / 67.7	74 / 66.4	74.5 / 66.4	1.81	1.99	1.90
2FW7	320	86.9 / 85.6	85.2 / 82.6	89.4 / 87.7	76.7 / 73.3	75.8 / 72.9	76.3 / 73.7	1.69	1.78	1.75
2G2U	430	86.1 / 83.1	86.9 / 83.7	88.4 / 84.6	79.5 / 75.4	79.5 / 75.4	76 / 73.3	1.69	1.59	1.83
2G30	252	86.3 / 81.7	83.1 / 79.5	87.7 / 83.6	77.2 / 68.9	74.4 / 64.8	74.4 / 66.7	1.25	1.60	1.58
2G40	164	87 / 86.2	90.2 / 88.6	92.7 / 90.2	80.5 / 77.2	83.7 / 80.5	84.6 / 79.7	1.74	1.70	1.58
2G69	99	90.1 / 84	82.7 / 79	88.9 / 86.4	80.2 / 72.8	74.1 / 67.9	76.5 / 71.6	1.60	1.75	1.56
2G71	124	86.7 / 84.8	81.9 / 80	87.6 / 86.7	81 / 78.1	74.3 / 71.4	82.9 / 80	1.56	1.65	1.54
2G70	68	69.8 / 68.3	69.8 / 68.3	84.1 / 81	60.3 / 58.7	61.9 / 58.7	66.7 / 63.5	1.71	2.03	1.83
2GAS	614	84.3 / 82.8	85.1 / 82.8	87 / 83.9	73.4 / 68	73.2 / 67.6	72.6 / 66.3	1.66	1.60	1.61
2GDQ	746	86.2 / 81.6	86.2 / 82.1	86.6 / 82.3	78.2 / 67.7	78.3 / 68	76.7 / 67.9	1.67	1.74	1.77
2GEC	277	85.3 / 83.1	81.8 / 79.6	45 / 34.6	74.7 / 69.8	72.9 / 64.4	25.6 / 19.4	1.70	1.79	4.83
2GGV	213	89 / 84.9	88.4 / 83.7	90.1 / 86.6	82 / 72.1	82.6 / 75.6	82.6 / 75	1.41	1.34	1.28
2GIY	357	86.2 / 83.8	85.2 / 84.2	89.6 / 87.2	81.1 / 77.8	80.5 / 75.1	83.5 / 78.8	1.59	1.54	1.21
2GKG	122	88.8 / 88.8	88.8 / 87.8	91.8 / 91.8	82.7 / 74.5	77.6 / 73.5	79.6 / 70.4	1.31	1.25	1.29
2GKV	287	28.1 / 17.5	88.6 / 87.3	92.1 / 89.9	16.2 / 7	83.3 / 76.8	86 / 79.4	32.85	1.45	1.27
2GOM	121	88.8 / 88.8	79.4 / 79.4	86.9 / 86.9	80.4 / 77.6	69.2 / 67.3	80.4 / 73.8	1.60	1.88	1.64
2GQV	59	75.6 / 73.3	77.8 / 75.6	88.9 / 86.7	68.9 / 66.7	75.6 / 64.4	82.2 / 75.6	1.98	1.41	1.77
2GXF	140	81.7 / 80.2	81.7 / 79.4	88.1 / 85.7	74.6 / 69.8	72.2 / 66.7	78.6 / 70.6	2.03	2.22	1.76
2H14	303	89.6 / 85	89.6 / 86.5	91.9 / 88.1	83.8 / 75.8	82.3 / 75.4	83.1 / 75.4	1.25	1.41	1.18
2H2R	269	86.6 / 82.8	86.2 / 84.1	89.2 / 84.1	76.7 / 68.1	79.7 / 72.8	76.3 / 68.5	1.58	1.51	1.32
2H2Z	306	85.9 / 83.3	85.6 / 84	89 / 86.7	79.5 / 72.6	79.8 / 73.8	80.6 / 73	1.57	1.52	1.47
2H7W	216	88.2 / 85.9	88.8 / 86.5	86.5 / 82.9	79.4 / 71.8	82.4 / 74.1	76.5 / 71.8	1.57	1.31	1.56
2H7Z	152	75.4 / 72.4	78.4 / 74.6	80.6 / 74.6	69.4 / 64.9	70.1 / 63.4	76.1 / 67.9	2.15	1.81	1.60
2H8E	120	83.2 / 79.2	80.2 / 77.2	86.1 / 84.2	71.3 / 65.3	71.3 / 65.3	77.2 / 70.3	2.20	2.29	1.76
2H8O	283	79.8 / 76.9	83.2 / 81.2	81.7 / 79.3	74 / 68.3	75.5 / 69.7	69.7 / 66.3	1.68	1.57	1.74
2HC8	113	85.4 / 80.9	88.8 / 82	89.9 / 84.3	75.3 / 70.8	79.8 / 75.3	80.9 / 77.5	1.46	1.31	1.34
2HLR	67	86.7 / 80	85 / 81.7	93.3 / 91.7	85 / 75	81.7 / 75	93.3 / 86.7	1.69	2.10	1.37
2HLY	205	86.5 / 83.3	84.6 / 81.4	84 / 79.5	81.4 / 72.4	79.5 / 70.5	78.8 / 70.5	1.52	1.57	1.69
2HOQ	237	82 / 81.6	83.5 / 82.5	87.9 / 85.9	72.8 / 67.5	75.2 / 70.9	75.7 / 67.5	1.77	1.61	1.64
2HPL	105	85.7 / 82.4	80.2 / 76.9	90.1 / 86.8	78 / 68.1	71.4 / 63.7	76.9 / 65.9	1.50	1.67	1.63
2HWW	461	80.9 / 79.2	82.1 / 79	42 / 29.1	72.7 / 65.9	71.5 / 65.7	25.2 / 14.6	1.79	1.86	3.79
2HY5	363	81.6 / 78.6	84.2 / 79.9	84.2 / 80.3	72.4 / 65.8	72.7 / 65.5	71.4 / 65.8	1.71	1.73	1.70
2HZF	219	29.6 / 20.1	84.1 / 81.5	86.8 / 84.1	13.2 / 6.3	77.2 / 72.5	79.4 / 73	8.72	1.46	1.33
2I3F	412	83.7 / 81.2	85.1 / 82.3	87.6 / 83.7	77.3 / 71.3	78.2 / 70.4	74.6 / 68.5	1.57	1.54	1.76
2I49	398	92 / 90.4	88.9 / 88.3	90.1 / 89.2	87 / 80.2	84.6 / 79.3	82.4 / 74.7	1.24	1.24	1.24
2I5D	195	84.4 / 80.6	85.6 / 81.9	85.6 / 80.6	75.6 / 66.9	76.2 / 71.2	73.8 / 66.2	1.71	1.34	1.82
2I6V	87	81 / 79.7	89.9 / 87.3	92.4 / 91.1	73.4 / 65.8	83.5 / 69.6	82.3 / 70.9	1.99	1.57	1.43
2IBL	108	88 / 88	80.4 / 80.4	89.1 / 89.1	82.6 / 77.2	78.3 / 73.9	83.7 / 81.5	1.43	1.57	1.46
2IC6	147	75.8 / 75.8	80.5 / 80.5	87.5 / 85.9	71.1 / 69.5	72.7 / 72.7	78.9 / 77.3	2.07	2.06	1.59
2IC7	555	90.6 / 86.9	88.5 / 86.3	90.2 / 87.1	86.5 / 80	83 / 76.9	82.4 / 72.1	1.53	1.75	1.58
2IIA	89	91 / 85.9	89.7 / 85.9	89.7 / 83.3	80.8 / 69.2	83.3 / 69.2	84.6 / 66.7	1.69	1.45	1.52
2IJK	115	83.3 / 81.2	83.3 / 81.2	89.6 / 86.5	72.9 / 66.7	72.9 / 63.5	78.1 / 69.8	1.81	1.85	1.86
2IP2	660	85.1 / 80.2	85.3 / 80	84.9 / 78.2	76.9 / 68.2	76.5 / 67.8	73.9 / 64.9	1.80	1.68	1.75
2IPR	251	90.8 / 89.1	90 / 88.2	90.4 / 85.6	86 / 83.4	84.3 / 76.9	80.3 / 72.5	1.49	1.46	1.45

There are 76 proteins in part four.

Table 7. Part 5: Comparison of pacoPacker, CIS-RR and scwrl4 on a 377-protein test set

PDB	NO. of Residues	$\chi_1(40^\circ/20^\circ)$			$\chi_{12}(40^\circ/20^\circ)$			RMSD(\AA)		
		SCWRL4	CIS-RR	pacoPacker	SCWRL4	CIS-RR	pacoPacker	SCWRL4	CIS-RR	pacoPacker
2IRU	568	85.3 / 81.6	82.3 / 79.2	85.8 / 81.2	78.8 / 69.8	75.9 / 68.3	74.6 / 67.4	1.72	1.68	1.84
2IUM	633	86.7 / 83.2	88 / 84.8	85.7 / 82.5	81.3 / 75.4	83.4 / 77.3	78.5 / 71.6	1.09	1.13	1.39
2IXM	300	87.8 / 86.3	90.8 / 90.8	89.7 / 86.6	82.8 / 77.9	84.4 / 79.8	81.7 / 75.2	1.61	1.39	1.54
2IY9	309	87.9 / 86.6	87.9 / 87.9	90.3 / 87.9	80.2 / 75.7	82.6 / 78.5	81.4 / 78.1	1.53	1.29	1.32
2IZ6	315	89.6 / 88.2	86.4 / 83.7	91 / 88.2	82.4 / 77.8	79.6 / 74.2	82.4 / 76	1.30	1.51	1.21
2J2J	1092	89.7 / 88.7	90.6 / 89	90.7 / 87.7	84.5 / 80.4	84.5 / 80.5	81.8 / 77.6	1.29	1.40	1.40
2J5Y	122	37 / 33	82 / 82	97 / 93	21 / 8	70 / 67	79 / 71	11.08	1.33	0.98
2J6B	109	87.5 / 86.5	86.5 / 84.4	91.7 / 89.6	76 / 69.8	76 / 69.8	78.1 / 75	1.51	1.53	1.53
2J71	102	84.3 / 80.9	84.3 / 79.8	91 / 85.4	77.5 / 69.7	77.5 / 66.3	80.9 / 73	1.69	1.51	1.60
2J8B	78	91.8 / 89	87.7 / 83.6	97.3 / 93.2	82.2 / 75.3	78.1 / 72.6	89 / 80.8	1.38	2.11	1.08
2J9W	200	84.9 / 81.2	82.3 / 79.6	84.9 / 80.6	76.3 / 69.4	72.6 / 66.1	72.6 / 65.6	1.65	1.63	1.67
2JCP	150	93.1 / 92.4	90.1 / 89.3	92.4 / 90.8	87 / 80.2	83.2 / 77.9	86.3 / 82.4	1.35	1.53	1.30
2NML	100	77.8 / 77.8	81.1 / 81.1	87.8 / 86.7	71.1 / 62.2	72.2 / 63.3	73.3 / 66.7	2.04	1.85	1.63
2NNU	221	83.2 / 80.7	84.2 / 80.7	87.6 / 86.6	77.2 / 70.3	78.2 / 69.8	77.7 / 69.3	1.60	1.42	1.55
2NPT	375	83.9 / 81.9	85.5 / 83.5	84.8 / 83.2	74.2 / 68.1	78.4 / 73.2	74.5 / 68.4	1.70	1.46	1.62
2NRR	139	84.6 / 82.9	82.9 / 81.3	82.9 / 82.9	77.2 / 72.4	74 / 68.3	73.2 / 68.3	1.77	2.08	1.96
2NV0	378	86.2 / 81.9	87.5 / 82.9	88.5 / 84.9	78.9 / 70.4	80.9 / 73.4	79.3 / 74	1.52	1.68	1.57
2O0Q	114	83.5 / 80	83.5 / 80	90.6 / 83.5	72.9 / 63.5	69.4 / 61.2	78.8 / 67.1	1.57	1.75	1.44
2O2K	665	87.6 / 85	84.6 / 82.6	84.1 / 81.1	80.3 / 74.9	76.5 / 69.2	74.3 / 68.3	1.70	1.70	1.71
2O37	81	79.4 / 79.4	80.9 / 80.9	86.8 / 86.8	69.1 / 66.2	72.1 / 64.7	77.9 / 75	1.46	1.43	1.13
2O6S	416	92.6 / 91.2	91.8 / 88.8	92.3 / 90.7	86.4 / 81.1	86.7 / 79	85.4 / 81.4	1.19	1.39	1.24
2O6X	306	86.8 / 84	86.4 / 84	88.3 / 85.2	82.5 / 75.1	79.4 / 71.2	77.8 / 71.2	1.35	1.59	1.60
2OEB	152	87.5 / 85.2	83.6 / 80.5	85.9 / 84.4	81.2 / 73.4	75.8 / 71.1	78.1 / 71.1	1.24	1.40	1.34
2OHW	256	85.7 / 83.9	85.2 / 83.5	89.1 / 85.7	76.5 / 71.7	76.5 / 68.7	76.5 / 70	1.76	1.87	1.72
2OIX	178	81.5 / 77.4	86.3 / 82.9	89.7 / 84.2	74 / 64.4	74 / 65.1	74.7 / 65.1	2.12	1.88	1.52
2OL7	496	87.4 / 85.7	86.4 / 84.3	87.4 / 84.8	82.7 / 76.4	80.6 / 74.8	77.1 / 72.2	1.22	1.27	1.39
2OSA	196	87.5 / 85.2	83.5 / 81.8	87.5 / 85.8	81.2 / 72.7	78.4 / 69.3	80.1 / 75	1.44	1.84	1.65
2OTU	976	84.7 / 80.9	82.8 / 81.2	84.5 / 82.4	77.8 / 70.3	77.7 / 69.8	74.9 / 67.7	1.33	1.39	1.41
2P1G	459	90.7 / 86.9	87.9 / 84.8	88.4 / 83.6	86.1 / 77	82.6 / 73.5	80.6 / 75	1.40	1.45	1.44
2P38	310	87.3 / 80.1	86.5 / 80.1	88.4 / 82.1	80.5 / 68.9	79.7 / 71.7	81.7 / 69.3	1.44	1.48	1.42
2P4H	310	88.3 / 86.8	85 / 83.8	87.6 / 86.5	80.1 / 74.1	79.3 / 73.3	77.8 / 72.6	1.41	1.68	1.55
2P52	196	85.5 / 85	86.1 / 84.4	87.3 / 85.5	79.2 / 73.4	77.5 / 73.4	79.8 / 76.3	1.36	1.41	1.70
2P5D	145	81.5 / 77.8	83 / 78.5	87.4 / 82.2	71.1 / 62.2	71.9 / 64.4	73.3 / 67.4	1.83	1.89	1.61
2P5K	63	80.4 / 75	78.6 / 73.2	87.5 / 82.1	76.8 / 64.3	73.2 / 62.5	82.1 / 73.2	1.89	2.06	1.51
2P65	185	82.2 / 81.5	82.9 / 82.9	89 / 87.7	77.4 / 74.7	77.4 / 74	82.2 / 78.8	1.81	1.64	1.70
2P84	133	77 / 73.8	81.1 / 78.7	82.8 / 80.3	68 / 56.6	73 / 64.8	74.6 / 61.5	2.03	1.66	1.86
2PBP	255	87.4 / 86.9	84.9 / 83.4	89.4 / 87.9	73.9 / 68.3	70.4 / 66.3	77.9 / 70.9	1.96	1.80	1.73
2PBQ	511	86.8 / 86.1	83.1 / 82.9	86.3 / 85.2	82.2 / 75.5	78.5 / 71.8	79.4 / 75	1.40	1.61	1.51
2PEF	366	87.2 / 85.2	87.6 / 85.6	89.3 / 87.2	81.5 / 74.5	79.9 / 71.8	79.5 / 74.5	1.30	1.35	1.37
2PET	231	87.2 / 84.1	87.7 / 84.6	90.3 / 86.2	82.1 / 73.3	81.5 / 73.8	83.6 / 76.4	1.56	1.51	1.60
2PGE	356	82.6 / 80.1	84 / 81.5	84 / 80.1	76 / 69.7	78 / 71.1	73.5 / 66.6	2.02	1.85	1.77
2PKF	665	30 / 22.4	88.8 / 87.3	88.2 / 86.1	13.1 / 8	80.8 / 75.3	77.6 / 74.1	17.26	1.61	1.52
2PMR	76	88.6 / 87.1	85.7 / 84.3	90 / 87.1	75.7 / 70	68.6 / 65.7	81.4 / 77.1	1.62	1.64	1.49
2PND	119	84.4 / 82.6	85.3 / 83.5	88.1 / 84.4	75.2 / 69.7	78.9 / 71.6	75.2 / 65.1	1.70	1.82	1.57
2PST	61	83.3 / 79.6	79.6 / 77.8	85.2 / 79.6	72.2 / 68.5	70.4 / 66.7	72.2 / 64.8	1.98	1.98	1.63
2PTV	96	83 / 78.4	80.7 / 77.3	87.5 / 84.1	79.5 / 65.9	79.5 / 68.2	76.1 / 64.8	1.59	1.61	1.61
2PV2	436	87.2 / 85.8	87.5 / 85.8	87.8 / 86	80.5 / 71.8	78.5 / 73.3	77.9 / 72.4	1.29	1.43	1.57
2PZ4	239	32.2 / 22	80.5 / 78	86.3 / 83.9	17.6 / 6.8	69.8 / 66.8	77.6 / 71.7	9.26	1.69	1.48
2Q8O	250	84.1 / 78.4	85 / 79.3	89.9 / 82.4	75.8 / 66.5	74.4 / 64.8	77.5 / 70.9	1.32	1.22	1.13
2QIY	317	61.3 / 54	84.7 / 79.4	87.5 / 81.9	48.4 / 42.5	73.2 / 67.6	77.4 / 71.8	4.68	1.69	1.54
2QPW	147	85.6 / 84	84 / 82.4	88.8 / 87.2	76.8 / 70.4	76.8 / 68.8	82.4 / 75.2	1.67	1.92	1.63
2QR3	121	79.6 / 76.9	78.7 / 74.1	85.2 / 79.6	73.1 / 67.6	73.1 / 67.6	79.6 / 72.2	1.87	1.57	1.63
2QT4	95	91.7 / 88.9	87.5 / 83.3	94.4 / 93.1	84.7 / 81.9	80.6 / 73.6	87.5 / 83.3	1.58	1.35	1.43
2R6U	510	44.2 / 38.5	90.6 / 88.8	89.8 / 87.8	32.3 / 27	85.4 / 78.4	82.4 / 75.7	4.57	1.26	1.38
2R77	190	89.8 / 88.6	89.8 / 86.8	90.4 / 88.6	82.6 / 75.4	80.8 / 74.9	83.2 / 71.9	1.28	1.51	1.19
2R99	164	89.9 / 89.1	92 / 91.3	92.8 / 92	84.1 / 77.5	84.1 / 77.5	88.4 / 83.3	1.46	1.27	1.12
2RCZ	160	82.4 / 77.9	80.9 / 77.1	85.5 / 78.6	77.1 / 70.2	73.3 / 67.2	78.6 / 67.9	1.71	1.94	1.56
2RFA	222	82 / 78.1	83.1 / 78.1	86.3 / 78.7	72.1 / 67.2	74.3 / 69.4	70.5 / 65.6	1.75	1.67	1.66
2RIK	283	22 / 16.3	86.9 / 84.9	87.8 / 84.9	8.2 / 5.3	79.6 / 71.8	79.2 / 72.2	9.01	1.54	1.49
2RJD	321	86.2 / 83.4	83.7 / 80.9	85.2 / 81.6	80.6 / 72.4	74.6 / 67.5	76.7 / 69.6	1.81	1.57	1.77
2RK5	86	84.6 / 83.3	83.3 / 83.3	85.9 / 82.1	74.4 / 69.2	75.6 / 71.8	73.1 / 60.3	1.55	1.33	1.48
2VC8	72	91.9 / 88.7	87.1 / 83.9	91.9 / 87.1	79 / 75.8	77.4 / 71	83.9 / 77.4	1.15	1.38	1.20
2YXF	99	80.9 / 79.8	79.8 / 76.6	88.3 / 85.1	71.3 / 63.8	70.2 / 62.8	77.7 / 73.4	2.00	2.35	1.64
2YYV	447	85.3 / 83.2	87.1 / 85.6	87.9 / 85.6	77.4 / 73.5	79.8 / 75.3	78.2 / 73	1.74	1.50	1.60
2YZ1	228	90 / 88	85 / 83.5	90 / 87	83 / 76	79.5 / 74	82.5 / 76.5	1.40	1.39	1.31
2Z14	116	88 / 86.1	88 / 87	91.7 / 90.7	80.6 / 72.2	81.5 / 74.1	83.3 / 74.1	1.62	1.52	1.55
2Z1E	298	84.4 / 80.9	82.7 / 80	87.6 / 84	72.4 / 69.3	75.1 / 70.2	79.1 / 73.3	1.73	1.61	1.59
2Z37	976	87.4 / 85.6	89.1 / 86.5	88.5 / 85.9	82.2 / 75.2	81.8 / 74.4	80.2 / 73.5	1.24	1.36	1.22
2ZFY	226	85.6 / 83.5	87.6 / 84.5	85.1 / 82.5	80.9 / 77.3	82 / 74.2	77.8 / 71.1	1.26	1.42	1.32
3BB7	314	87 / 83	87.7 / 84.2	88.5 / 83	79.8 / 72.7	81 / 75.1	79.1 / 71.9	1.51	1.26	1.42
3BN6	158	91.7 / 91	87.2 / 85	91 / 89.5	86.5 / 74.4	77.4 / 69.2	86.5 / 78.9	1.56	1.57	1.34
3C4S	112	89.5 / 88.4	88.4 / 87.4	95.8 / 94.7	85.3 / 77.9	85.3 / 77.9	85.3 / 77.9	1.58	1.50	1.29
6XIA	387	84.8 / 80.9	83.8 / 80.2	86.8 / 84.5	75.2 / 67.7	73.9 / 65.3	77.6 / 71.6	1.94	2.02	1.76

There are 73 proteins in part five.

Table 8. Analysis of the performance of pacoPacker, CIS-RR and scwrl4 on individual residues

PDB	χ_1			χ_{1+2}		
	SCWRL4	CIS-RR	pacoPacker	SCWRL4	CIS-RR	pacoPacker
ARG	78.46	79.38	82.41	65.76	66.20	82.41
ASN	84.11	82.91	85.44	74.24	72.75	75.76
ASP	83.64	81.91	85.23	74.98	71.24	75.21
CYS	91.20	93.36	93.33	0.00	0.00	0.00
GLN	79.09	77.78	81.58	61.69	60.82	57.94
GLU	72.99	73.55	78.51	57.88	56.36	58.91
HIS	88.56	89.31	90.10	77.67	79.40	79.79
ILE	95.87	96.06	95.75	84.35	84.98	78.45
LEU	92.15	92.99	93.34	86.33	86.71	80.67
LYS	77.35	78.53	83.16	63.93	65.73	66.72
MET	84.53	85.14	86.63	71.03	73.34	71.62
PHE	95.26	95.70	96.18	92.74	92.67	92.51
PRO	85.42	85.11	83.59	81.76	81.58	78.02
SER	71.57	69.09	75.98	0.00	0.00	0.00
THR	90.73	89.58	91.96	0.00	0.00	0.00
TRP	92.79	94.01	92.34	80.43	84.92	77.03
TYR	95.29	94.99	94.85	92.74	91.61	91.70
VAL	93.23	93.41	93.52	0.00	0.00	0.00

The test data used the 377 proteins set.

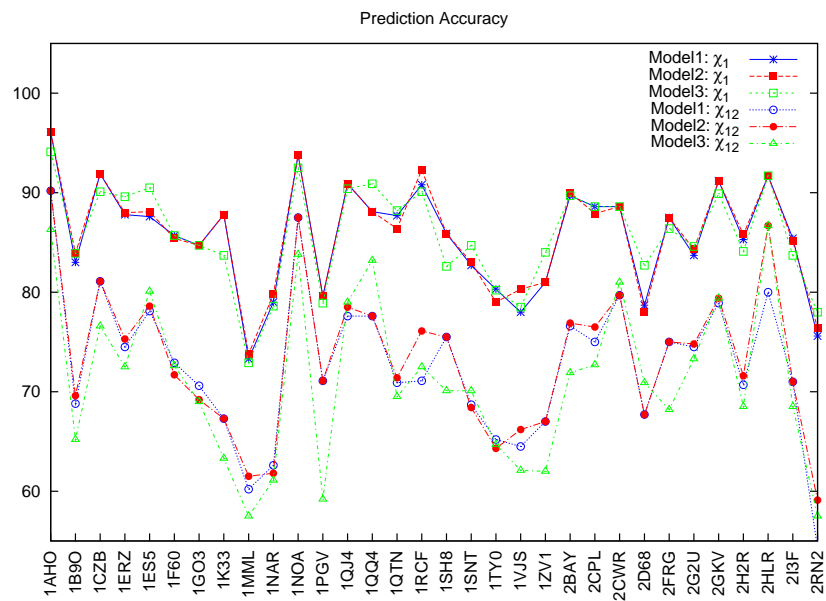


Fig. 7. Comparisons between model1, model2 and model3 for χ_1, χ_2

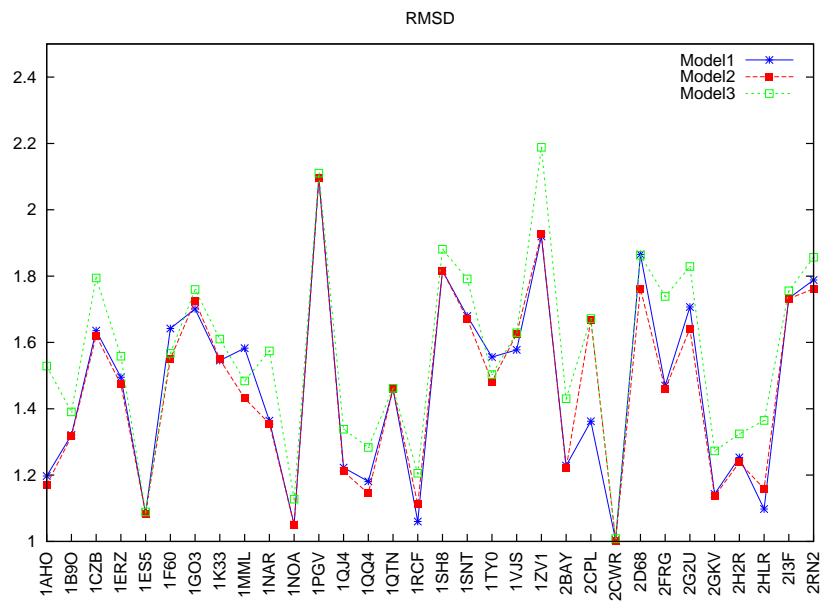


Fig. 8. Comparisons between model1, model2 and model3 for RMSD

Table 9. Part 5: Comparison of Model1 Model2 Model3 on a 50-protein test set selected from CIS-RR and SCWRL4

PDB	$\chi_1(40^\circ/20^\circ)$			$\chi_{12}(40^\circ/20^\circ)$			RMSD(Å)		
	Model1	Model2	Model3	Model1	Model2	Model3	Model1	Model2	Model3
1AHO	98/96.1	98/96.1	94.1/94.1	96.1/90.2	96.1/90.2	90.2/86.3	1.20	1.17	1.53
1AKO	85.9/82.9	85.9/82.5	85.9/83.8	73.2/67.9	73.9/69.2	72.6/66.2	1.99	1.98	1.92
1B9O	87.5/83	87.5/83.9	88.4/83.9	74.1/68.8	74.1/69.6	72.3/65.2	1.32	1.32	1.39
1CTJ	95.1/78.1	95.1/90.2	96.7/91.8	88.5/63	88.5/80.3	88.5/80.3	0.64	0.64	0.51
1CZB	94.6/91.9	94.6/91.9	93.7/90.1	89.2/81.1	89.2/81.1	85.6/76.6	1.64	1.62	1.79
1DPT	86/81.1	86/80.7	87.4/82.1	73.3/68.4	73.3/68.4	71.9/65.6	1.89	1.88	1.75
1ERZ	90.2/87.8	89.8/88	91.2/89.6	81.1/74.5	80.5/75.3	78.7/72.5	1.50	1.47	1.56
1ES5	92/87.6	92.5/88.1	92.5/90.5	85.6/78.1	86.6/78.6	87.6/80.1	1.08	1.08	1.09
1F60	87.7/85.7	87.9/85.4	88.6/85.7	77.4/72.9	78/71.7	77.6/72.6	1.64	1.55	1.57
1F94	94.7/93	94.7/93	91.2/91.2	87.7/78.9	87.7/78.9	89.5/84.2	2.40	2.39	2.38
1GO3	87/84.7	87/84.7	87/84.7	76.4/70.6	75.3/69.2	74.8/69	1.70	1.73	1.76
1K33	87.8/87.8	87.8/87.8	85.7/83.7	75.5/67.3	75.5/67.3	73.5/63.3	1.55	1.55	1.61
1KPT	91.2/90	91.2/90	92.9/90	88.2/84.7	88.2/84.7	88.2/82.9	1.44	1.44	1.32
1KVA	84.9/78.6	84.9/78.6	85.7/76.2	72.2/57.9	72.2/57.9	71.4/56.3	2.15	2.15	2.02
1MML	83.7/73.3	83.7/73.8	85.5/72.9	70.1/60.2	70.6/61.5	70.1/57.5	1.58	1.43	1.48
1NAR	85.5/79	85.1/79.8	85.5/78.6	72.1/62.6	71.8/61.8	71.4/61.1	1.36	1.36	1.57
1NOA	95/93.8	95/93.8	93.8/92.5	92.5/87.5	92.5/87.5	90/83.8	1.05	1.05	1.13
1OK7	82.3/77.8	82.3/78.5	82.4/78.6	70.3/64.1	70.6/64.6	69.3/62.3	2.00	1.99	1.96
1PGV	80.9/79.6	80.9/79.6	81.6/78.9	75.7/71.1	75.7/71.1	67.8/59.2	2.10	2.09	2.11
1QJ4	92.7/90.9	92.7/90.9	92.7/90.4	82.6/77.6	82.6/78.5	81.7/79	1.22	1.21	1.34
1QQ4	91.6/88.1	91.6/88.1	92.3/90.9	84.6/77.6	84.6/77.6	88.8/83.2	1.18	1.14	1.28
1QTN	90.9/87.7	90.9/86.4	90.5/88.2	79.1/70.9	80/71.4	78.6/69.5	1.46	1.46	1.46
1RCF	94.4/90.8	94.4/92.3	94.4/90.1	83.8/71.1	86.6/76.1	86.6/72.5	1.06	1.11	1.21
1SH8	88/85.9	88/85.9	86.7/82.6	78.8/75.5	78.8/75.5	75.9/70.1	1.82	1.82	1.88
1SNT	86.7/82.7	86.4/83	86.7/84.7	73.8/68.7	73.8/68.4	73.1/70.1	1.68	1.67	1.79
1TUO	85.5/82.2	85.8/82.2	85.5/82.5	73.4/69.5	73.4/70.1	71/67.2	1.80	1.80	1.77
1TYO	82.9/80.3	83.1/79	83.4/80.2	70/65.2	70.3/64.3	71.9/64.7	1.56	1.48	1.50
1Vfy	88.9/88.9	88.9/88.9	92.1/92.1	88.9/87.3	88.9/87.3	90.5/90.5	1.44	1.44	1.10
1VJS	83.6/78	83.6/80.3	84.4/78.5	74.2/64.5	74.2/66.2	72.6/62.1	1.58	1.63	1.63
1WBA	93.1/89	93.1/89.7	92.4/86.9	85.5/78.6	86.9/77.2	88.3/77.9	1.46	1.26	1.04
1WM3	90.8/86.2	89.2/84.6	92.3/87.7	78.5/69.2	83.1/78.5	87.7/81.5	1.59	1.60	1.41
1Y7Y	95.6/90.3	95.6/90.3	93.8/90.3	87.6/73.5	86.7/75.2	87.6/77.9	1.52	1.51	1.40
1YTL	84.5/78	84.3/77.7	85.4/78.4	71.6/63.1	72.9/65.5	71.6/61.2	1.64	1.67	1.59
1ZV1	85/81	85/81	87/84	73/67	74/67	67/62	1.92	1.93	2.19
2BAY	92.5/89.7	92.5/90	92.8/89.7	82.5/76.6	82.5/76.9	78.1/71.9	1.23	1.22	1.43
2CPL	90.2/88.6	90.2/87.9	91.7/88.6	80.3/75	81.8/76.5	79.5/72.7	1.36	1.67	1.67
2CWR	91.1/88.6	91.1/88.6	91.1/88.6	84.8/79.7	84.8/79.7	88.6/81	1.00	1.00	1.01
2D68	81.9/78.7	81.9/78	86.6/82.7	72.4/67.7	71.7/67.7	74.8/70.9	1.87	1.76	1.86
2END	92.4/87.3	92.4/87.3	92.4/87.3	79.7/72	79.7/72	73.7/67.8	1.79	1.79	1.64
2EPI	82.9/81.2	83.2/80.6	84.1/82.4	73.8/67.6	74.1/68.5	73.2/69.1	1.78	1.77	1.76
2FRG	93.2/87.5	93.2/87.5	90.9/86.4	83/75	83/75	75/68.2	1.47	1.46	1.74
2G2U	87.8/83.7	87.8/84.3	88.4/84.6	79.2/74.5	78.6/74.8	76/73.3	1.71	1.64	1.83
2GKV	92.5/91.2	92.5/91.2	92.1/89.9	86/78.9	86/79.4	86/79.4	1.14	1.14	1.27
2H2R	89.2/85.3	89.2/85.8	89.2/84.1	78.9/70.7	78.9/71.6	76.3/68.5	1.25	1.24	1.32
2HLR	95/91.7	95/91.7	93.3/91.7	86.7/80	91.7/86.7	93.3/86.7	1.10	1.16	1.37
2I3F	87.6/85.4	87.6/85.1	87.6/83.7	76.5/71	76.5/71	74.6/68.5	1.73	1.73	1.76
2IPR	89.5/85.2	89.5/85.2	90.4/85.6	80.3/71.6	80.3/72.1	80.3/72.5	1.46	1.46	1.45
2I8B	95.9/90.4	95.9/90.4	97.3/93.2	89/79.5	89/79.5	89/80.8	1.15	1.16	1.08
2JCP	92.4/90.8	92.4/90.8	92.4/90.8	86.3/84	86.3/83.2	86.3/82.4	1.35	1.34	1.30
2OL7	86.9/83.6	86.9/83.6	87.4/84.8	78.5/73.6	78.5/73.6	77.1/72.2	1.42	1.42	1.39