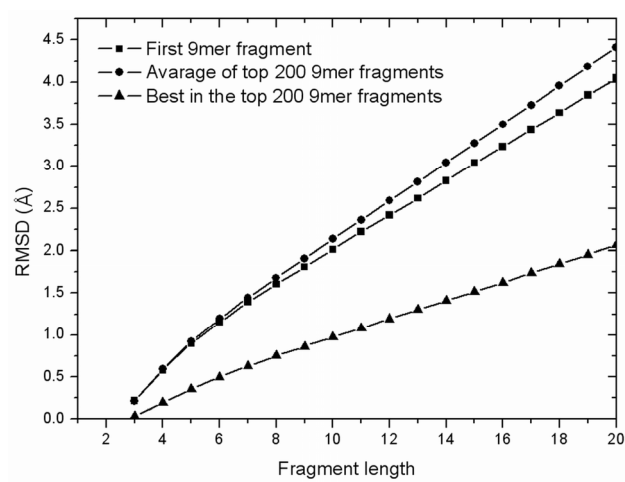


## Supporting Information

# Towards Optimal Fragment Generations for *Ab Initio* Protein Structure Assembly

Dong Xu and Yang Zhang

**Figure S1.** RMSD of fragments of different lengths retrieved by using 6 features.



**Table S1.** Accurately predicted distances ( $<1$  Å to the real value) which correspond to the maximum numbers in the distance profiles for the three CASP9 free-modeling targets.

T0553-D2				
#C $\alpha_i$	#C $\alpha_j$	Real (Å)	Predicted (Å)	Max. Num.
72	81	6.41	5.75	25
86	94	7.14	6.75	241
87	92	5.25	5.25	1369
87	93	6.23	5.75	662
106	115	6.13	6.75	103
Region [243, 288] of T0571-D2				
244	261	5.82	5.75	17
244	263	6.33	5.75	83
244	260	6.59	6.25	15
245	260	5.52	5.75	76
245	261	5.32	5.25	50
245	262	6.46	5.75	60
246	258	7.02	7.25	142
246	259	5.75	5.75	206
246	260	4.21	4.75	83
246	261	6.37	5.75	101
247	258	5.72	5.75	447
247	259	5.55	5.25	283
247	260	6.10	6.75	144
247	261	7.82	7.75	50
248	256	5.97	6.75	813
248	257	5.19	5.75	913
248	258	4.30	4.75	520
248	259	6.10	6.25	373
249	256	5.51	5.75	1758
249	257	5.32	5.25	1514
249	258	6.78	6.25	684
250	255	5.39	5.25	2094
250	256	4.66	4.25	1866
250	257	5.88	6.25	949
251	256	6.60	6.75	1552
251	257	6.75	6.75	700
265	270	5.83	5.75	2233
265	271	4.30	4.75	2310
265	272	6.75	6.25	1371
264	271	5.14	5.75	2503
264	272	5.37	5.25	2075
264	273	6.44	6.75	1073
264	270	8.38	8.25	2538
263	271	6.15	6.75	1109
263	272	5.91	5.75	1367

263	273	4.72	4.75	771
263	274	6.28	6.75	507
262	273	5.77	5.75	737
262	274	4.92	5.25	590
262	275	5.47	6.25	234
261	275	4.90	4.75	139
261	274	5.86	5.75	323
261	273	6.83	6.75	263
260	275	6.55	5.75	101
260	276	4.75	5.25	46
275	281	5.66	6.25	548
274	284	7.16	6.25	53
273	285	5.53	6.25	25
272	285	4.38	5.25	30
272	284	5.81	6.25	26
T0604-D1				
11	71	7.05	6.25	45
12	69	4.93	5.75	14
13	69	6.13	6.25	14
14	68	6.53	5.75	18
15	67	6.33	6.25	17
15	68	8.67	8.25	18
16	66	6.25	5.75	18
17	66	6.54	5.75	24
19	26	7.64	8.25	93
32	40	8.23	8.25	587
32	43	8.34	7.75	242
33	38	4.97	5.25	2298
33	39	5.65	5.75	1238
51	63	5.72	4.75	21
53	64	5.35	5.75	14
53	62	5.80	5.25	63
55	61	7.31	7.75	135
79	90	7.17	6.25	48