

- 1 **Table S1. Molecular docking results of leucine and photo-leucine ligands docked to wt and A494T**
- 2 **variant of *BsLeuS*. Models marked with # are depicted in Figure 8. Ex, exhaustiveness.**

Ex.	WT ColabFold model	leucine RMSD [Å]	photo- leucine RMSD [Å]	Ex.	A494T ColabFold model	leucine RMSD [Å]	photo- leucine RMSD [Å]
8	relaxed_rank1	1.442	3.538	8	relaxed_rank1	3.247	2.061
8	relaxed_rank2	0.743	7.918	8	relaxed_rank2	0.717	1.773
8	relaxed_rank3	7.622	2.986	8	relaxed_rank3	2.285	6.598
8	relaxed_rank4	3.839	3.522	8	relaxed_rank4	5.978	3.587
8	relaxed_rank5	2.687	1.635	8	not-relaxed_rank1	0.978	7.593
8	not-relaxed_rank2	0.7	7.633	8	not-relaxed_rank2	0.72	1.789
8	not-relaxed_rank3	1.22	7.763	8	not-relaxed_rank3	6.33	7.002
16	relaxed_rank1	3.597	3.842	16	relaxed_rank1	3.25	6.16
16	relaxed_rank3	3.43	3.618	16	relaxed_rank2	0.725	1.78
16	relaxed_rank4	3.789	3.516	16	relaxed_rank3	2.986	2.956
16	relaxed_rank5	2.385	2.478	16	relaxed_rank5	3.33	3.597
16	not-relaxed_rank1	1.392	3.246	16	not-relaxed_rank1	3.207	7.093
16	not-relaxed_rank2	0.715	7.719	16	not-relaxed_rank2	0.729	1.782
16	not-relaxed_rank3	7.831	7.812	16	not-relaxed_rank3	5.773	7.242
16	not-relaxed_rank4	1.048	7.701	16	not-relaxed_rank4	2.98	4.657
16	not-relaxed_rank5	1.307	2.539	16	not-relaxed_rank5	0.573	0.894
32	relaxed_rank1	3.59	3.788	32	relaxed_rank1	3.251	6.452
32	relaxed_rank3	5.939	8.139	32	relaxed_rank2	0.714	1.785
32	relaxed_rank4	3.812	3.516	32	relaxed_rank3	2.17	1.72
32	relaxed_rank5	2.37	2.455	32	relaxed_rank4	2.9	3.113
32	not-relaxed_rank1	2.352	2.409	32	not-relaxed_rank1	0.941	1.691
32	not-relaxed_rank2	0.727	7.142	32	not-relaxed_rank3	1.475	1.707
32	not-relaxed_rank3	7.341	7.998	32	not-relaxed_rank5	3.506	0.879
32	not-relaxed_rank4	3.774	3.539	64	relaxed_rank1	3.256	6.188
64	relaxed_rank1	3.614	3.785	64	relaxed_rank2	0.719	1.775
64	relaxed_rank3	3.718	6.518	64	relaxed_rank3	1.537	7.436
64	relaxed_rank4	3.793	3.523	64	relaxed_rank4	5.98	8.142
64	relaxed_rank5	2.422	2.468	64	relaxed_rank5	3.202	6.326
64	not-relaxed_rank1	1.394	2.98	64	not-relaxed_rank2	0.724	1.034
64	not-relaxed_rank2	0.732	7.17	64	not-relaxed_rank4	2.966	8.896
64	not-relaxed_rank3	6.051	8.4	8	#relaxed_rank5	0.6	7.078

64	not-relaxed_rank4	3.241	7.717	8	not-relaxed_rank1	0.978	7.593
8	not-relaxed_rank1	1.399	1.945	8	not-relaxed_rank4	1.457	7.816
8	not-relaxed_rank4	1.163	1.776	16	relaxed_rank4	1.166	7.965
8	not-relaxed_rank5	1.298	1.625	32	#relaxed_rank5	1.009	7.781
16	#relaxed_rank2	0.758	1.804	32	not-relaxed_rank2	0.715	7.71
32	#relaxed_rank2	0.739	1.763	32	not-relaxed_rank4	1.062	8.795
32	not-relaxed_rank5	1.304	1.331	64	not-relaxed_rank1	0.919	7.218
64	#relaxed_rank2	0.755	1.806	64	not-relaxed_rank3	1.455	6.686
64	not-relaxed_rank5	1.086	1.33	64	not-relaxed_rank5	0.579	7.264

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