

	mol	receptor	rseq	mseq	S	rmsd	rmsd_re...
1	1VTQ	AF-Q54JH6-F1_1	1	1	-71.2893	87.1059	0.8568
2	1VTQ	AF-Q54JH6-F1_1	1	1	-65.9735	66.3944	0.8853
3	1VTQ	AF-Q54JH6-F1_1	1	1	-64.1479	103.5457	3.5573
4	1VTQ	AF-Q54JH6-F1_1	1	1	-63.8903	71.4851	1.2760
5	1VTQ	AF-Q54JH6-F1_1	1	1	-61.6054	72.3237	2.9233
6	1VTQ	AF-Q54JH6-F1_1	1	1	-60.9558	46.6210	5.3129
7	1VTQ	AF-Q54JH6-F1_1	1	1	-60.4905	88.1418	0.7024
8	1VTQ	AF-Q54JH6-F1_1	1	1	-60.4181	97.7613	1.6245
9	1VTQ	AF-Q54JH6-F1_1	1	1	-60.2808	61.3540	2.2485
10	1VTQ	AF-Q54JH6-F1_1	1	1	-59.2338	84.8754	0.7216
11	1VTQ	AF-Q54JH6-F1_1	1	1	-59.0063	95.3885	1.1192
12	1VTQ	AF-Q54JH6-F1_1	1	1	-58.2370	91.2699	2.3248
13	1VTQ	AF-Q54JH6-F1_1	1	1	-57.6776	46.5913	4.1582
14	1VTQ	AF-Q54JH6-F1_1	1	1	-57.5612	92.8545	0.4035
15	1VTQ	AF-Q54JH6-F1_1	1	1	-57.3070	96.5270	0.5376
16	1VTQ	AF-Q54JH6-F1_1	1	1	-56.9261	54.7859	2.7286
17	1VTQ	AF-Q54JH6-F1_1	1	1	-56.4389	64.4119	9.6811
18	1VTQ	AF-Q54JH6-F1_1	1	1	-55.7509	84.6583	0.6957
19	1VTQ	AF-Q54JH6-F1_1	1	1	-55.1740	101.3849	0.5869
20	1VTQ	AF-Q54JH6-F1_1	1	1	-55.0178	84.3792	0.5847
21	1VTQ	AF-Q54JH6-F1_1	1	1	-54.4996	91.5540	1.5782
22	1VTQ	AF-Q54JH6-F1_1	1	1	-53.9997	51.8498	1.9667
23	1VTQ	AF-Q54JH6-F1_1	1	1	-53.5786	70.7811	3.0866
24	1VTQ	AF-Q54JH6-F1_1	1	1	-53.4886	67.4642	0.6131
25	1VTQ	AF-Q54JH6-F1_1	1	1	-53.4628	95.1668	2.4974
26	1VTQ	AF-Q54JH6-F1_1	1	1	-53.2353	91.3903	1.4446
27	1VTQ	AF-Q54JH6-F1_1	1	1	-52.3911	84.2622	1.1860
28	1VTQ	AF-Q54JH6-F1_1	1	1	-52.0576	92.4553	3.7621
29	1VTQ	AF-Q54JH6-F1_1	1	1	-52.0277	101.3061	1.4036
30	1VTQ	AF-Q54JH6-F1_1	1	1	-51.8988	53.7664	1.2399
31	1VTQ	AF-Q54JH6-F1_1	1	1	-51.8232	77.4552	0.8881
32	1VTQ	AF-Q54JH6-F1_1	1	1	-51.4980	97.7577	3.3226
33	1VTQ	AF-Q54JH6-F1_1	1	1	-51.4401	49.3357	2.7927
34	1VTQ	AF-Q54JH6-F1_1	1	1	-51.4276	93.4792	0.7176
35	1VTQ	AF-Q54JH6-F1_1	1	1	-50.8095	90.7894	2.2216
36	1VTQ	AF-Q54JH6-F1_1	1	1	-50.7633	98.2682	0.7803
37	1VTQ	AF-Q54JH6-F1_1	1	1	-50.1982	96.6755	0.6624
38	1VTQ	AF-Q54JH6-F1_1	1	1	-50.1919	62.7390	4.5980
39	1VTQ	AF-Q54JH6-F1_1	1	1	-50.0088	92.4974	1.9765
40	1VTQ	AF-Q54JH6-F1_1	1	1	-49.8499	76.6511	1.5375
41	1VTQ	AF-Q54JH6-F1_1	1	1	-49.7927	56.5257	1.1482
42	1VTQ	AF-Q54JH6-F1_1	1	1	-49.7392	108.4553	0.9049
43	1VTQ	AF-Q54JH6-F1_1	1	1	-49.6278	117.6349	1.1252
44	1VTQ	AF-Q54JH6-F1_1	1	1	-49.5096	94.6214	1.4467
45	1VTQ	AF-Q54JH6-F1_1	1	1	-49.1393	84.8212	1.0273
46	1VTQ	AF-Q54JH6-F1_1	1	1	-48.7774	45.7180	1.2041
47	1VTQ	AF-Q54JH6-F1_1	1	1	-48.3495	99.4902	1.3544
48	1VTQ	AF-Q54JH6-F1_1	1	1	-48.2996	97.2849	2.2843
49	1VTQ	AF-Q54JH6-F1_1	1	1	-47.7883	86.6654	3.2248

	E_conf	E_place	E_refine	PLIF_raw	FP:PLIF	PLIF_ligidx	class
1	-12421.827	-3.9400	-71.2893	[[0,0,0,0,0,0,0	1 2 3 4 5	[0,0,0,0,0,0,0,	3
2	-12421.827	-4.4722	-65.9735	[[0,0,0,0,0,0,0	12 13 14 1	[0,0,0,0,0,0,0,	4
3	-12421.827	0.6185	-64.1479	[[0,0,0,0,0,0,0	1 2 25 26	[0,0,0,0,0,0,0,	0
4	-12421.827	0.0262	-63.8903	[[0,0,0,0,0,0,0	35 22 36 3	[0,0,0,0,0,0,0,	0
5	-12421.827	-0.1799	-61.6054	[[0,0,0,0,0,0,0	13 44 45 4	[0,0,0,0,0,0,0,	0
6	-12421.827	0.4126	-60.9558	[[0,0,0,0,0,0,0	55 56 57 5	[0,0,0,0,0,0,0,	5
7	-12421.827	-0.8411	-60.4905	[[0,0,0,0,0,0,0	66 67 68 1	[0,0,0,0,0,0,0,	0
8	-12421.827	1.5098	-60.4181	[[0,0,0,0,0,0,0	70 71 72 7	[0,0,0,0,0,0,0,	0
9	-12421.827	-2.5093	-60.2808	[[0,0,0,0,0,0,0	12 79 80 8	[0,0,0,0,0,0,0,	0
10	-12421.827	-5.8751	-59.2338	[[0,0,0,0,0,0,0	1 2 83 73	[0,0,0,0,0,0,0]	0
11	-12421.827	1.1139	-59.0063	[[0,0,0,0,0,0,0	85 86 87 8	[0,0,0,0,0,0,0,	0
12	-12421.827	1.3168	-58.2370	[[0,0,0,0,0,0,0	66 3 5 69	[0,0,0,0,0,0,0,	1
13	-12421.827	0.8103	-57.6776	[[0,0,0,0,0,0,0	55 56 57 5	[0,0,0,0,0,0,0,	5
14	-12421.827	-6.6238	-57.5612	[[0,0,0,0,0,0,0	66 98 99 3	[0,0,0,0,0,0,0,	0
15	-12421.827	-0.0480	-57.3070	[[0,0,0,0,0,0,0	2 25 103 1	[0,0,0,0,0,0,0,	0
16	-12421.827	-3.4084	-56.9261	[[0,0,0,0,0,0,0	110 111 11	[0,0,0,0,0,0,0,	0
17	-12421.827	1.6917	-56.4389	[[0,0,0,0,0,0,0	13 44 15 1	[0,0,0,0,0,0,0,	0
18	-12421.827	1.3062	-55.7509	[[0,0,0,0,0,0,0	83 122 123	[0,0,0,0,0,0,0,	0
19	-12421.827	-0.0195	-55.1740	[[0,0,0,0,0,0,0	132 133 13	[0,0,0,0,0,0,0,	0
20	-12421.827	-2.9375	-55.0178	[[0,0,0,0,0,0,0	2 25 140 1	[0,0,0,0,0,0,0,	2
21	-12421.827	-4.7277	-54.4996	[[0,0,0,0,0,0,0	3 4 5 24 6	[0,0,0,0,0,0,0,	1
22	-12421.827	0.2003	-53.9997	[[0,0,0,0,0,0,0	143 3 20 5	[0,0,0,0,0,0,0,	0
23	-12421.827	-0.6059	-53.5786	[[0,0,0,0,0,0,0	147 12 80	[0,0,0,0,0,0,0]	0
24	-12421.827	-6.8305	-53.4886	[[0,0,0,0,0,0,0	147 12 79	[0,0,0,0,0,0,0,	0
25	-12421.827	1.8795	-53.4628	[[0,0,0,0,0,0,0	66 67 148	[0,0,0,0,0,0,0]	0
26	-12421.827	1.5542	-53.2353	[[0,0,0,0,0,0,0	67 3 4 5 6	[0,0,0,0,0,0,0,	1
27	-12421.827	-2.0705	-52.3911	[[0,0,0,0,0,0,0	150 20 151	[0,0,0,0,0,0,0,	2
28	-12421.827	-6.6838	-52.0576	[[0,0,0,0,0,0,0	153 3 4 5	[0,0,0,0,0,0,0,	1
29	-12421.827	-0.3030	-52.0277	[[0,0,0,0,0,0,0	152 155 15	[0,0,0,0,0,0]	0
30	-12421.827	-2.4671	-51.8988	[[0,0,0,0,0,0,0	158 159 16	[0,0,0,0,0,0,0]	0
31	-12421.827	-1.2013	-51.8232	[[0,0,0,0,0,0,0	67 68 12 1	[0,0,0,0,0,0,0,	0
32	-12421.827	-1.8682	-51.4980	[[0,0,0,0,0,0,0	5 40 41 16	[0,0,0,0,0,0,0,	0
33	-12421.827	-2.4428	-51.4401	[[0,0,0,0,0,0,0	56 3 4 57	[0,0,0,0,0,0,0,	0
34	-12421.827	0.4308	-51.4276	[[0,0,0,0,0,0,0	3 4 20 140	[0,0,0,0,0,0,0,	0
35	-12421.827	-1.4272	-50.8095	[[0,0,0,0,0,0,0	66 67 5 6	[0,0,0,0,0,0,0,	0
36	-12421.827	1.8349	-50.7633	[[0,0,0,0,0,0,0	1 2 28 29	[0,0,0,0,0,0]	0
37	-12421.827	-0.0953	-50.1982	[[0,0,0,0,0,0,0	96 75 76 7	[0,0,0,0,0,0,0,	0
38	-12421.827	1.9482	-50.1919	[[0,0,0,0,0,0,0	147 15 18	[0,0,0,0,0,0,0,	0
39	-12421.827	-7.1358	-50.0088	[[0,0,0,0,0,0,0	66 99 3 5	[0,0,0,0,0,0,0,	0
40	-12421.827	-1.5917	-49.8499	[[0,0,0,0,0,0,0	179 180 18	[0,0,0,0,0,0,0,	0
41	-12421.827	-2.1462	-49.7927	[[0,0,0,0,0,0,0	190 191 19	[0,0,0,0,0,0,0,	0
42	-12421.827	1.7227	-49.7392	[[0,0,0,0,0,0,0	1 150 196	[0,0,0,0,0,0,0,	0
43	-12421.827	0.1843	-49.6278	[[0,0,0,0,0,0,0	85 87 199	[0,0,0,0,0,0,0,	0
44	-12421.827	-1.0571	-49.5096	[[0,0,0,0,0,0,0	66 67 203	[0,0,0,0,0,0,0,	0
45	-12421.827	0.5911	-49.1393	[[0,0,0,0,0,0,0	208 209 11	[0,0,0,0,0,0,0]	0
46	-12421.827	-2.1389	-48.7774	[[0,0,0,0,0,0,0	63 64 211	[0,0,0,0]	0
47	-12421.827	1.3257	-48.3495	[[0,0,0,0,0,0,0	3 4 5 212	[0,0,0,0,0,0,0]	0
48	-12421.827	-0.0862	-48.2996	[[0,0,0,0,0,0,0	1 2 25 85	[0,0,0,0,0,0,0,	0
49	-12421.827	2.2465	-47.7883	[[0,0,0,0,0,0,0	1 2 25 83	[0,0,0,0,0,0,0,	0

	mol	receptor	rseq	mseq	S	rmsd	rmsd_re...
50	1VTQ	AF-Q54JH6-F1_1	1	1	-47.7868	45.8078	1.4828
51	1VTQ	AF-Q54JH6-F1_1	1	1	-47.7154	94.6060	0.6010
52	1VTQ	AF-Q54JH6-F1_1	1	1	-47.5090	75.4096	1.0231
53	1VTQ	AF-Q54JH6-F1_1	1	1	-47.3437	106.5861	1.5396
54	1VTQ	AF-Q54JH6-F1_1	1	1	-47.1227	45.3158	3.6663
55	1VTQ	AF-Q54JH6-F1_1	1	1	-46.8608	84.4735	1.5714
56	1VTQ	AF-Q54JH6-F1_1	1	1	-46.6887	97.6769	0.3681
57	1VTQ	AF-Q54JH6-F1_1	1	1	-46.6884	100.8392	2.3479
58	1VTQ	AF-Q54JH6-F1_1	1	1	-46.4994	100.7173	4.3204
59	1VTQ	AF-Q54JH6-F1_1	1	1	-46.4558	92.8437	1.1438
60	1VTQ	AF-Q54JH6-F1_1	1	1	-46.2777	93.5494	2.0625
61	1VTQ	AF-Q54JH6-F1_1	1	1	-46.0695	48.9722	2.4229
62	1VTQ	AF-Q54JH6-F1_1	1	1	-46.0405	46.4737	2.9541
63	1VTQ	AF-Q54JH6-F1_1	1	1	-46.0200	45.6973	0.9234
64	1VTQ	AF-Q54JH6-F1_1	1	1	-45.1809	96.7176	0.8302
65	1VTQ	AF-Q54JH6-F1_1	1	1	-44.8554	104.8173	3.2836
66	1VTQ	AF-Q54JH6-F1_1	1	1	-44.5548	83.6056	0.7482
67	1VTQ	AF-Q54JH6-F1_1	1	1	-44.3385	101.8685	6.4095
68	1VTQ	AF-Q54JH6-F1_1	1	1	-43.8484	105.1598	0.9232
69	1VTQ	AF-Q54JH6-F1_1	1	1	-43.7499	55.1902	1.3697
70	1VTQ	AF-Q54JH6-F1_1	1	1	-43.4939	46.8281	0.6566
71	1VTQ	AF-Q54JH6-F1_1	1	1	-42.8378	88.0187	1.7273
72	1VTQ	AF-Q54JH6-F1_1	1	1	-42.8340	94.3039	3.5289
73	1VTQ	AF-Q54JH6-F1_1	1	1	-42.3289	104.9549	3.5417
74	1VTQ	AF-Q54JH6-F1_1	1	1	-42.2002	75.5735	3.5772
75	1VTQ	AF-Q54JH6-F1_1	1	1	-42.1034	76.2880	1.6175
76	1VTQ	AF-Q54JH6-F1_1	1	1	-42.0551	90.5403	1.6487
77	1VTQ	AF-Q54JH6-F1_1	1	1	-41.9653	58.5020	2.8736
78	1VTQ	AF-Q54JH6-F1_1	1	1	-41.9410	51.8813	1.8384
79	1VTQ	AF-Q54JH6-F1_1	1	1	-41.9014	105.3147	2.7145
80	1VTQ	AF-Q54JH6-F1_1	1	1	-41.8072	103.9904	2.5178
81	1VTQ	AF-Q54JH6-F1_1	1	1	-41.0264	82.7928	2.8747
82	1VTQ	AF-Q54JH6-F1_1	1	1	-40.8116	99.3215	1.1612
83	1VTQ	AF-Q54JH6-F1_1	1	1	-40.7063	101.5207	2.0323
84	1VTQ	AF-Q54JH6-F1_1	1	1	-39.5664	66.1459	1.1030
85	1VTQ	AF-Q54JH6-F1_1	1	1	-39.5052	101.1218	1.0773
86	1VTQ	AF-Q54JH6-F1_1	1	1	-39.4389	105.1640	3.1455
87	1VTQ	AF-Q54JH6-F1_1	1	1	-39.3083	46.1358	27.1136
88	1VTQ	AF-Q54JH6-F1_1	1	1	-39.0104	105.3770	0.9918
89	1VTQ	AF-Q54JH6-F1_1	1	1	-38.0171	82.0365	0.6940
90	1VTQ	AF-Q54JH6-F1_1	1	1	-37.7498	101.4249	0.7306
91	1VTQ	AF-Q54JH6-F1_1	1	1	-37.5242	49.3671	2.8414
92	1VTQ	AF-Q54JH6-F1_1	1	1	-36.7165	98.4069	1.1351
93	1VTQ	AF-Q54JH6-F1_1	1	1	-36.0720	97.4223	1.8017
94	1VTQ	AF-Q54JH6-F1_1	1	1	-35.0253	99.9318	2.5476
95	1VTQ	AF-Q54JH6-F1_1	1	1	-34.9735	107.2877	1.3012
96	1VTQ	AF-Q54JH6-F1_1	1	1	-33.2775	85.1950	4.5743
97	1VTQ	AF-Q54JH6-F1_1	1	1	-31.5360	97.9318	23.3261
98	1VTQ	AF-Q54JH6-F1_1	1	1	-22.8754	78.2525	6.5297

	E_conf	E_place	E_refine	PLIF_raw	FP:PLIF	PLIF_ligidx	class
50	-12421.827	-4.4735	-47.7868	[[0,0,0,0,0,0,0,0	59 149 60	[0,0,0,0,0,0,0,0,	0
51	-12421.827	-1.5111	-47.7154	[[0,0,0,0,0,0,0,0	94 95 109	[0,0,0,0,0,0,0,0,	0
52	-12421.827	-0.7384	-47.5090	[[0,0,0,0,0,0,0,0	3 220 221	[0,0,0,0,0,0,0,0,	0
53	-12421.827	-1.4736	-47.3437	[[0,0,0,0,0,0,0,0	92 30 157	[0,0,0,0,0]	0
54	-12421.827	2.1407	-47.1227	[[0,0,0,0,0,0,0,0	226 3 59 1	[0,0,0,0,0,0,0]	0
55	-12421.827	-4.4080	-46.8608	[[0,0,0,0,0,0,0,0	5 122 227	[0,0,0,0,0,0]	0
56	-12421.827	-3.1444	-46.6887	[[0,0,0,0,0,0,0,0	87 72 202	[0,0,0,0,0,0]	0
57	-12421.827	1.4909	-46.6884	[[0,0,0,0,0,0,0,0	229 155 15	[0,0,0,0,0,0,0,0,	0
58	-12421.827	0.8935	-46.4994	[[0,0,0,0,0,0,0,0	2 232 83 1	[0,0,0,0,0,0,0,0,	0
59	-12421.827	-0.9157	-46.4558	[[0,0,0,0,0,0,0,0	66 99 233	[0,0,0,0,0,0,0,0,	0
60	-12421.827	2.1925	-46.2777	[[0,0,0,0,0,0,0,0	235 135 23	[0,0,0,0,0,0]	0
61	-12421.827	-0.6805	-46.0695	[[0,0,0,0,0,0,0,0	3 59 144 2	[0,0,0,0,0,0,0,0]	0
62	-12421.827	-2.1232	-46.0405	[[0,0,0,0,0,0,0,0	60 61 65 5	[0,0,0,0,0]	0
63	-12421.827	-0.6854	-46.0200	[[0,0,0,0,0,0,0,0	64 211	[0,0]	0
64	-12421.827	0.3845	-45.1809	[[0,0,0,0,0,0,0,0	107 240 75	[0,0,0,0,0,0,0,0]	0
65	-12421.827	0.7220	-44.8554	[[0,0,0,0,0,0,0,0	241 242 24	[0,0,0,0,0,0]	0
66	-12421.827	0.5376	-44.5548	[[0,0,0,0,0,0,0,0	1 245 2 25	[0,0,0,0,0,0,0,0,	2
67	-12421.827	1.6955	-44.3385	[[0,0,0,0,0,0,0,0	1 2 25 3 2	[0,0,0,0,0,0,0,0,	0
68	-12421.827	1.8636	-43.8484	[[0,0,0,0,0,0,0,0	3 247 248	[0,0,0,0,0,0,0,0,	0
69	-12421.827	1.9741	-43.7499	[[0,0,0,0,0,0,0,0	147 172 22	[0,0,0,0,0,0]	0
70	-12421.827	2.0151	-43.4939	[[0,0,0,0,0,0,0,0	169 170 57	[0,0,0,0,0,0,0,0,	0
71	-12421.827	-2.5424	-42.8378	[[0,0,0,0,0,0,0,0	67 204 147	[0,0,0,0,0,0,0,0,	0
72	-12421.827	1.2569	-42.8340	[[0,0,0,0,0,0,0,0	203 204 20	[0,0,0,0,0,0,0,0]	0
73	-12421.827	1.7706	-42.3289	[[0,0,0,0,0,0,0,0	174 256 27	[0,0,0,0]	0
74	-12421.827	1.1899	-42.2002	[[0,0,0,0,0,0,0,0	67 3 4 5 6	[0,0,0,0,0,0,0,0,	1
75	-12421.827	-4.4509	-42.1034	[[0,0,0,0,0,0,0,0	110 258 25	[0,0,0,0,0,0,0,0]	0
76	-12421.827	0.0499	-42.0551	[[0,0,0,0,0,0,0,0	67 3 36 15	[0,0,0,0,0,0,0,0]	0
77	-12421.827	-1.0999	-41.9653	[[0,0,0,0,0,0,0,0	15 3 5 57	[0,0,0,0,0,0,0,0]	0
78	-12421.827	0.2395	-41.9410	[[0,0,0,0,0,0,0,0	262 263 26	[0,0,0,0,0,0,0,0,	0
79	-12421.827	1.9606	-41.9014	[[0,0,0,0,0,0,0,0	18 269 270	[0,0,0,0,0,0,0,0,	0
80	-12421.827	-0.9122	-41.8072	[[0,0,0,0,0,0,0,0	272 273 27	[0,0,0,0,0,0,0,0]	0
81	-12421.827	1.4899	-41.0264	[[0,0,0,0,0,0,0,0	7 275 212	[0,0,0,0,0,0,0,0,	2
82	-12421.827	1.4501	-40.8116	[[0,0,0,0,0,0,0,0	40 144 268	[0,0,0,0,0,0]	0
83	-12421.827	2.2301	-40.7063	[[0,0,0,0,0,0,0,0	1 2 25 229	[0,0,0,0,0,0,0,0,	0
84	-12421.827	-0.7306	-39.5664	[[0,0,0,0,0,0,0,0	3 4 20 140	[0,0,0,0,0,0,0,0]	0
85	-12421.827	-1.7851	-39.5052	[[0,0,0,0,0,0,0,0	1 2 25 155	[0,0,0,0,0,0,0,0,	0
86	-12421.827	1.2697	-39.4389	[[0,0,0,0,0,0,0,0	241 135	[0,0]	0
87	-12421.827	1.0559	-39.3083	[[0,0,0,0,0,0,0,0	282 37 283	[0,0,0,0,0,0,0,0,	0
88	-12421.827	1.7249	-39.0104	[[0,0,0,0,0,0,0,0	288 242 24	[0,0,0,0,0,0,0,0]	0
89	-12421.827	-2.6270	-38.0171	[[0,0,0,0,0,0,0,0	24 69 97 8	[0,0,0,0,0,0,0,0]	0
90	-12421.827	0.9587	-37.7498	[[0,0,0,0,0,0,0,0	2 272 291	[0,0,0,0,0,0,0,0,	0
91	-12421.827	1.1790	-37.5242	[[0,0,0,0,0,0,0,0	3 4 20 266	[0,0,0,0,0,0,0,0]	0
92	-12421.827	1.7919	-36.7165	[[0,0,0,0,0,0,0,0	20 21 298	[0,0,0,0,0,0,0,0,	0
93	-12421.827	-0.6901	-36.0720	[[0,0,0,0,0,0,0,0	2 25 75 76	[0,0,0,0,0,0,0,0]	0
94	-12421.827	-1.3640	-35.0253	[[0,0,0,0,0,0,0,0	1 2 229 15	[0,0,0,0,0,0,0,0,	0
95	-12421.827	1.9593	-34.9735	[[0,0,0,0,0,0,0,0	300 301 28	[0,0,0,0,0]	0
96	-12421.827	-3.9925	-33.2775	[[0,0,0,0,0,0,0,0	2 272 291	[0,0,0,0,0,0,0,0,	0
97	-12421.827	0.4325	-31.5360	[[0,0,0,0,0,0,0,0	140 152 15	[0,0,0,0,0,0,0,0]	0
98	-12421.827	-0.4488	-22.8754	[[0,0,0,0,0,0,0,0	2 25 3 4 2	[0,0,0,0,0,0,0,0,	0

	mol	receptor	rseq	mseq	S	rmsd	rmsd_re...
99	1VTQ	AF-Q54JH6-F1_1	1	1	-21.6469	91.1044	12.1818
100	1VTQ	AF-Q54JH6-F1_1	1	1	-17.0752	98.2891	5.2014

	E_conf	E_place	E_refine	PLIF_raw	FP:PLIF	PLIF_ligidx	class
99	-12421.827	0.2881	-21.6469	[[0,0,0,0,0,0,0,0]	155 303 24	[0,0,0,0,0,0]	0
100	-12421.827	-0.6785	-17.0752	[[0,0,0,0,0,0,0,0]	229 155 15	[0,0,0,0,0,0]	0