	mol	receptor	rseq	mseq	S	rmsd_ref...
1	1VTQ	4h0n	1	1	-87.8625	0.5222
2	1VTQ	4h0n	1	1	-75.9420	2.0390
3	1VTQ	4h0n	1	1	-75.5832	0.2884
4	1VTQ	4h0n	1	1	-74.7914	1.3314
5	1VTQ	4h0n	1	1	-74.6173	1.1551
6	1VTQ	4h0n	1	1	-73.9910	0.6383
7	1VTQ	4h0n	1	1	-73.7956	1.6819
8	1VTQ	4h0n	1	1	-73.7493	0.4833
9	1VTQ	4h0n	1	1	-73.4184	0.3081
10	1VTQ	4h0n	1	1	-73.2138	1.0089
11	1VTQ	4h0n	1	1	-73.0380	1.6771
12	1VTQ	4h0n	1	1	-72.9095	1.0685
13	1VTQ	4h0n	1	1	-72.6834	0.8488
14	1VTQ	4h0n	1	1	-72.6032	0.5162
15	1VTQ	4h0n	1	1	-71.1639	0.3915
16	1VTQ	4h0n	1	1	-70.9681	0.9135
17	1VTQ	4h0n	1	1	-70.9222	0.3617
18	1VTQ	4h0n	1	1	-70.0883	3.2524
19	1VTQ	4h0n	1	1	-69.7286	1.1266
20	1VTQ	4h0n	1	1	-69.5725	1.6652
21	1VTQ	4h0n	1	1	-69.1353	1.7794
22	1VTQ	4h0n	1	1	-69.0833	0.8989
23	1VTQ	4h0n	1	1	-68.1281	1.4993
24	1VTQ	4h0n	1	1	-67.8989	1.8373
25	1VTQ	4h0n	1	1	-67.8796	1.5526
26	1VTQ	4h0n	1	1	-67.3740	2.0780
27	1VTQ	4h0n	1	1	-67.2843	0.6037
28	1VTQ	4h0n	1	1	-66.8938	1.7008
29	1VTQ	4h0n	1	1	-66.6584	0.8654
30	1VTQ	4h0n	1	1	-66.1424	1.9466
31	1VTQ	4h0n	1	1	-65.9541	1.2023
32	1VTQ	4h0n	1	1	-65.8081	0.7394
33	1VTQ	4h0n	1	1	-65.7373	1.3273
34	1VTQ	4h0n	1	1	-65.6059	0.9015
35	1VTQ	4h0n	1	1	-65.3731	0.7609
36	1VTQ	4h0n	1	1	-65.0045	0.5758
37	1VTQ	4h0n	1	1	-64.8022	1.0714
38	1VTQ	4h0n	1	1	-64.7345	3.7752
39	1VTQ	4h0n	1	1	-64.4756	1.9534
40	1VTQ	4h0n	1	1	-64.0837	0.8213
41	1VTQ	4h0n	1	1	-64.0165	1.4607
42	1VTQ	4h0n	1	1	-63.9024	0.7254
43	1VTQ	4h0n	1	1	-63.8660	0.8512
44	1VTQ	4h0n	1	1	-63.7168	1.1788
45	1VTQ	4h0n	1	1	-63.6571	1.2854

	E_conf	E_place	E_refine	PLIF_raw	FP:PLIF	PLIF_ligidx
1	-13525.772	-35.0837	-87.8625	[[0,0,0,0,0,0,0	1 2 3 4 5	[0,0,0,0,0,0,0,
2	-13526.640	-24.0801	-75.9420	[[0,0,0,0,0,0,0	26 27 28 2	[0,0,0,0,0,0,0,
3	-13539.415	-27.6260	-75.5832	[[0,0,0,0,0,0,0	42 43 44 4	[0,0,0,0,0,0,0,
4	-13498.327	-24.8671	-74.7914	[[0,0,0,0,0,0,0	60 61 26 6	[0,0,0,0,0,0,0,
5	-13501.517	-24.9451	-74.6173	[[0,0,0,0,0,0,0	71 44 72 4	[0,0,0,0,0,0,0,
6	-13539.177	-25.3456	-73.9910	[[0,0,0,0,0,0,0	79 80 81 8	[0,0,0,0,0,0,0,
7	-13517.377	-24.0454	-73.7956	[[0,0,0,0,0,0,0	89 79 90 2	[0,0,0,0,0,0,0,
8	-13473.600	-27.8123	-73.7493	[[0,0,0,0,0,0,0	95 42 96 9	[0,0,0,0,0,0,0,
9	-13537.921	-26.0042	-73.4184	[[0,0,0,0,0,0,0	96 108 44	[0,0,0,0,0,0,0,
10	-13526.208	-23.1744	-73.2138	[[0,0,0,0,0,0,0	112 113 98	[0,0,0,0,0,0,0,
11	-13532.105	-23.1691	-73.0380	[[0,0,0,0,0,0,0	79 80 124	[0,0,0,0,0,0,0,
12	-13538.277	-24.4241	-72.9095	[[0,0,0,0,0,0,0	135 136 13	[0,0,0,0,0,0,0,
13	-13528.851	-25.0453	-72.6834	[[0,0,0,0,0,0,0	79 80 124	[0,0,0,0,0,0,0,
14	-13531.739	-26.2236	-72.6032	[[0,0,0,0,0,0,0	96 108 102	[0,0,0,0,0,0,0,
15	-13515.186	-29.4278	-71.1639	[[0,0,0,0,0,0,0	42 96 160	[0,0,0,0,0,0,0,
16	-13536.005	-23.9020	-70.9681	[[0,0,0,0,0,0,0	79 90 164	[0,0,0,0,0,0,0,
17	-13514.648	-23.4702	-70.9222	[[0,0,0,0,0,0,0	71 118 119	[0,0,0,0,0,0,0,
18	-13533.035	-24.0892	-70.0883	[[0,0,0,0,0,0,0	108 98 46	[0,0,0,0,0,0,0,
19	-13537.897	-25.8425	-69.7286	[[0,0,0,0,0,0,0	79 90 1 14	[0,0,0,0,0,0,0,
20	-13517.993	-24.8313	-69.5725	[[0,0,0,0,0,0,0	114 191 11	[0,0,0,0,0,0,0,
21	-13530.535	-23.7336	-69.1353	[[0,0,0,0,0,0,0	79 124 26	[0,0,0,0,0,0,0,
22	-13518.534	-25.0596	-69.0833	[[0,0,0,0,0,0,0	95 207 208	[0,0,0,0,0,0,0,
23	-13508.549	-23.3331	-68.1281	[[0,0,0,0,0,0,0	90 64 65 2	[0,0,0,0,0,0,0,
24	-13531.224	-24.4015	-67.8989	[[0,0,0,0,0,0,0	136 213 13	[0,0,0,0,0,0,0,
25	-13512.019	-25.1225	-67.8796	[[0,0,0,0,0,0,0	44 72 45 1	[0,0,0,0,0,0,0,
26	-13542.267	-24.6546	-67.3740	[[0,0,0,0,0,0,0	44 72 45 1	[0,0,0,0,0,0,0,
27	-13527.104	-27.0208	-67.2843	[[0,0,0,0,0,0,0	95 42 108	[0,0,0,0,0,0,0,
28	-13537.185	-23.4726	-66.8938	[[0,0,0,0,0,0,0	124 30 187	[0,0,0,0,0,0,0,
29	-13515.741	-23.0603	-66.6584	[[0,0,0,0,0,0,0	136 213 22	[0,0,0,0,0,0,0,
30	-13536.264	-23.5134	-66.1424	[[0,0,0,0,0,0,0	95 42 96 1	[0,0,0,0,0,0,0,
31	-13545.748	-26.1943	-65.9541	[[0,0,0,0,0,0,0	228 82 83	[0,0,0,0,0,0,0,
32	-13555.429	-23.1524	-65.8081	[[0,0,0,0,0,0,0	232 233 23	[0,0,0,0,0,0,0,
33	-13504.652	-23.8245	-65.7373	[[0,0,0,0,0,0,0	79 80 124	[0,0,0,0,0,0,0,
34	-13536.619	-23.4652	-65.6059	[[0,0,0,0,0,0,0	35 241 37	[0,0,0,0,0,0,0,
35	-13518.045	-25.6575	-65.3731	[[0,0,0,0,0,0,0	114 116 71	[0,0,0,0,0,0,0,
36	-13548.729	-27.7333	-65.0045	[[0,0,0,0,0,0,0	124 60 61	[0,0,0,0,0,0,0,
37	-13508.499	-25.8999	-64.8022	[[0,0,0,0,0,0,0	135 252 82	[0,0,0,0,0,0,0,
38	-13470.161	-26.1487	-64.7345	[[0,0,0,0,0,0,0	95 42 96 1	[0,0,0,0,0,0,0,
39	-13548.392	-27.2860	-64.4756	[[0,0,0,0,0,0,0	108 45 104	[0,0,0,0,0,0,0,
40	-13523.174	-23.4118	-64.0837	[[0,0,0,0,0,0,0	102 257 10	[0,0,0,0,0,0,0,
41	-13541.372	-23.1828	-64.0165	[[0,0,0,0,0,0,0	260 261 79	[0,0,0,0,0,0,0,
42	-13524.456	-24.4361	-63.9024	[[0,0,0,0,0,0,0	99 100 46	[0,0,0,0,0,0,0,
43	-13549.185	-23.3048	-63.8660	[[0,0,0,0,0,0,0	265 266 26	[0,0,0,0,0,0,0,
44	-13514.612	-26.4949	-63.7168	[[0,0,0,0,0,0,0	95 42 43 9	[0,0,0,0,0,0,0,
45	-13483.529	-24.7510	-63.6571	[[0,0,0,0,0,0,0	108 112 98	[0,0,0,0,0,0,0,

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11	0
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17	0
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32	0
33	0
34	0
35	0
36	0
37	0
38	2
39	0
40	0
41	0
42	0
43	0
44	0
45	0

	mol	receptor	rseq	mseq	S	rmsd_ref...
46	1VTQ	4h0n	1	1	-63.0391	0.7980
47	1VTQ	4h0n	1	1	-62.9725	0.4938
48	1VTQ	4h0n	1	1	-62.9589	1.9296
49	1VTQ	4h0n	1	1	-62.9295	0.6824
50	1VTQ	4h0n	1	1	-62.8507	1.1637
51	1VTQ	4h0n	1	1	-62.7397	0.4384
52	1VTQ	4h0n	1	1	-62.5634	0.6436
53	1VTQ	4h0n	1	1	-62.5581	0.9629
54	1VTQ	4h0n	1	1	-62.4781	2.0486
55	1VTQ	4h0n	1	1	-62.4079	1.1679
56	1VTQ	4h0n	1	1	-61.9103	0.6984
57	1VTQ	4h0n	1	1	-61.4557	2.0865
58	1VTQ	4h0n	1	1	-60.9113	0.7826
59	1VTQ	4h0n	1	1	-60.9053	0.8720
60	1VTQ	4h0n	1	1	-60.7450	1.1945
61	1VTQ	4h0n	1	1	-60.5661	0.8128
62	1VTQ	4h0n	1	1	-60.5529	0.6673
63	1VTQ	4h0n	1	1	-60.1786	1.1928
64	1VTQ	4h0n	1	1	-59.8862	0.5306
65	1VTQ	4h0n	1	1	-59.5776	2.9858
66	1VTQ	4h0n	1	1	-59.4045	0.9189
67	1VTQ	4h0n	1	1	-59.0276	3.8513
68	1VTQ	4h0n	1	1	-58.9951	2.4293
69	1VTQ	4h0n	1	1	-58.8778	1.2344
70	1VTQ	4h0n	1	1	-58.0222	2.0866
71	1VTQ	4h0n	1	1	-57.9200	1.1335
72	1VTQ	4h0n	1	1	-57.8534	0.7287
73	1VTQ	4h0n	1	1	-57.5051	0.8218
74	1VTQ	4h0n	1	1	-56.6276	0.4656
75	1VTQ	4h0n	1	1	-55.8074	2.4489
76	1VTQ	4h0n	1	1	-54.8214	0.5740
77	1VTQ	4h0n	1	1	-54.7330	1.9569
78	1VTQ	4h0n	1	1	-54.6895	0.5227
79	1VTQ	4h0n	1	1	-54.5963	0.4249
80	1VTQ	4h0n	1	1	-54.4028	0.9099
81	1VTQ	4h0n	1	1	-53.5286	1.0615
82	1VTQ	4h0n	1	1	-53.4366	2.6192
83	1VTQ	4h0n	1	1	-52.9887	1.6167
84	1VTQ	4h0n	1	1	-52.6031	1.7221
85	1VTQ	4h0n	1	1	-52.4890	1.3243
86	1VTQ	4h0n	1	1	-52.0039	2.2365
87	1VTQ	4h0n	1	1	-51.3550	0.8063
88	1VTQ	4h0n	1	1	-51.2149	0.5322
89	1VTQ	4h0n	1	1	-51.0679	0.9447
90	1VTQ	4h0n	1	1	-50.3745	1.0123

	E_conf	E_place	E_refine	PLIF_raw	FP:PLIF	PLIF_ligidx
46	-13508.035	-24.4233	-63.0391	[[0,0,0,0,0,0,0	95 208 96	[0,0,0,0,0,0,0,
47	-13529.258	-24.8740	-62.9725	[[0,0,0,0,0,0,0	79 90 1 14	[0,0,0,0,0,0,0,
48	-13488.017	-24.2809	-62.9589	[[0,0,0,0,0,0,0	104 105 1	[0,0,0,0,0,0,0,
49	-13497.801	-24.5298	-62.9295	[[0,0,0,0,0,0,0	96 160 253	[0,0,0,0,0,0,0,
50	-13502.694	-28.5779	-62.8507	[[0,0,0,0,0,0,0	95 42 43 9	[0,0,0,0,0,0,0,
51	-13468.188	-26.4575	-62.7397	[[0,0,0,0,0,0,0	42 44 278	[0,0,0,0,0,0,0,
52	-13527.150	-25.6341	-62.5634	[[0,0,0,0,0,0,0	108 227 13	[0,0,0,0,0,0,0,
53	-13459.738	-25.0543	-62.5581	[[0,0,0,0,0,0,0	116 117 44	[0,0,0,0,0,0,0,
54	-13530.874	-25.3726	-62.4781	[[0,0,0,0,0,0,0	83 64 65 6	[0,0,0,0,0,0,0,
55	-13420.999	-25.6097	-62.4079	[[0,0,0,0,0,0,0	208 96 160	[0,0,0,0,0,0,0,
56	-13545.249	-24.7550	-61.9103	[[0,0,0,0,0,0,0	108 227 11	[0,0,0,0,0,0,0,
57	-13499.680	-23.7022	-61.4557	[[0,0,0,0,0,0,0	96 112 113	[0,0,0,0,0,0]
58	-13531.862	-23.5522	-60.9113	[[0,0,0,0,0,0,0	112 44 99	[0,0,0,0,0,0,0]
59	-13532.290	-23.7254	-60.9053	[[0,0,0,0,0,0,0	26 199 63	[0,0,0,0,0,0,0,
60	-13477.284	-23.0191	-60.7450	[[0,0,0,0,0,0,0	79 124 125	[0,0,0,0,0,0,0,
61	-13511.244	-23.3536	-60.5661	[[0,0,0,0,0,0,0	102 257 1	[0,0,0,0,0,0,0,
62	-13542.707	-23.2732	-60.5529	[[0,0,0,0,0,0,0	221 212 35	[0,0,0,0,0,0,0,
63	-13500.787	-23.4213	-60.1786	[[0,0,0,0,0,0,0	99 46 101	[0,0,0,0,0,0,0,
64	-13552.335	-23.1574	-59.8862	[[0,0,0,0,0,0,0	96 97 44 4	[0,0,0,0,0,0,0,
65	-13490.648	-24.3029	-59.5776	[[0,0,0,0,0,0,0	112 135 25	[0,0,0,0,0,0,0,
66	-13525.785	-26.9362	-59.4045	[[0,0,0,0,0,0,0	79 90 28 6	[0,0,0,0,0,0,0,
67	-13534.248	-23.3172	-59.0276	[[0,0,0,0,0,0,0	30 187 273	[0,0,0,0,0,0,0,
68	-13549.366	-24.5329	-58.9951	[[0,0,0,0,0,0,0	114 191 11	[0,0,0,0,0,0,0,
69	-13518.105	-23.0251	-58.8778	[[0,0,0,0,0,0,0	260 261 30	[0,0,0,0,0,0,0,
70	9623.6504	-24.5311	-58.0222	[[0,0,0,0,0,0,0	1 149 186	[0,0,0,0,0,0,0,
71	-13518.831	-24.0830	-57.9200	[[0,0,0,0,0,0,0	309 90 250	[0,0,0,0,0,0,0,
72	-13536.161	-23.3595	-57.8534	[[0,0,0,0,0,0,0	96 108 227	[0,0,0,0,0,0,0,
73	-13537.757	-23.2945	-57.5051	[[0,0,0,0,0,0,0	3 232 233	[0,0,0,0,0,0,0,
74	-13531.405	-23.8523	-56.6276	[[0,0,0,0,0,0,0	47 1 2 149	[0,0,0,0,0,0,0,
75	-13516.000	-23.3571	-55.8074	[[0,0,0,0,0,0,0	114 115 11	[0,0,0,0,0,0,0,
76	-10259.508	-23.0266	-54.8214	[[0,0,0,0,0,0,0	315 44 72	[0,0,0,0,0,0,0,
77	-13536.910	-23.9131	-54.7330	[[0,0,0,0,0,0,0	116 71 320	[0,0,0,0,0,0,0,
78	-13519.930	-23.0938	-54.6895	[[0,0,0,0,0,0,0	96 321 322	[0,0,0,0,0,0]
79	-13533.846	-24.2536	-54.5963	[[0,0,0,0,0,0,0	323 267 44	[0,0,0,0,0,0,0,
80	-13545.612	-23.5559	-54.4028	[[0,0,0,0,0,0,0	102 151 47	[0,0,0,0,0,0,0,
81	-13497.006	-23.0627	-53.5286	[[0,0,0,0,0,0,0	90 1 149 1	[0,0,0,0,0,0,0,
82	-13520.768	-23.9172	-53.4366	[[0,0,0,0,0,0,0	208 52 53	[0,0,0,0,0,0,0,
83	-13511.770	-23.9033	-52.9887	[[0,0,0,0,0,0,0	136 328 11	[0,0,0,0,0,0,0,
84	-13523.340	-24.0069	-52.6031	[[0,0,0,0,0,0,0	331 265 26	[0,0,0,0,0,0,0,
85	-13518.607	-23.8397	-52.4890	[[0,0,0,0,0,0,0	28 30 187	[0,0,0,0,0,0,0,
86	-13541.414	-23.5315	-52.0039	[[0,0,0,0,0,0,0	208 262 16	[0,0,0,0,0,0,0]
87	-13527.286	-25.4128	-51.3550	[[0,0,0,0,0,0,0	112 135 44	[0,0,0,0,0,0,0,
88	-13513.883	-23.5852	-51.2149	[[0,0,0,0,0,0,0	28 63 188	[0,0,0,0,0,0,0,
89	-13518.298	-23.4484	-51.0679	[[0,0,0,0,0,0,0	122 336 64	[0,0,0,0,0,0,0,
90	-13537.344	-23.3123	-50.3745	[[0,0,0,0,0,0,0	118 119 12	[0,0,0,0,0,0,0,

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77	0
78	0
79	0
80	0
81	0
82	0
83	0
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85	0
86	0
87	0
88	0
89	0
90	0

	mol	receptor	rseq	mseq	S	rmsd_ref...
91	1VTQ	4h0n	1	1	-49.9819	0.5607
92	1VTQ	4h0n	1	1	-48.5897	2.5864
93	1VTQ	4h0n	1	1	-48.2822	0.9641
94	1VTQ	4h0n	1	1	-47.7147	0.7629
95	1VTQ	4h0n	1	1	-47.5128	0.3969
96	1VTQ	4h0n	1	1	-46.2668	1.1397
97	1VTQ	4h0n	1	1	-44.7119	1.6039
98	1VTQ	4h0n	1	1	-32.9347	32.0998
99	1VTQ	4h0n	1	1	-14.0442	0.8825
100	1VTQ	4h0n	1	1	-0.0599	33.5198

	E_conf	E_place	E_refine	PLIF_raw	FP:PLIF	PLIF_ligidx
91	-13540.243	-23.6218	-49.9819	[[0,0,0,0,0,0,0	44 72 45 1	[0,0,0,0,0,0,0,
92	-13522.124	-23.6194	-48.5897	[[0,0,0,0,0,0,0	135 114 11	[0,0,0,0,0,0,0]
93	-13529.201	-24.5959	-48.2822	[[0,0,0,0,0,0,0	260 341 44	[0,0,0,0,0,0,0,
94	-13531.000	-23.8955	-47.7147	[[0,0,0,0,0,0,0	95 208 99	[0,0,0,0,0,0,0,
95	-13529.642	-23.1456	-47.5128	[[0,0,0,0,0,0,0	42 44 262	[0,0,0,0,0,0,0,
96	-13546.946	-25.4236	-46.2668	[[0,0,0,0,0,0,0	1 2 233 91	[0,0,0,0,0,0,0,
97	-13501.967	-24.2882	-44.7119	[[0,0,0,0,0,0,0	91 165 15	[0,0,0,0,0,0,0,
98	-13479.958	-23.3601	-32.9347	[[0,0,0,0,0,0,0	136 137 13	[0,0,0,0,0,0,0,
99	-13531.301	-24.3242	-14.0442	[[0,0,0,0,0,0,0	137 116 22	[0,0,0,0,0,0,0,
100	-13552.666	-23.0526	-0.0599			

	clus
91	0
92	0
93	0
94	0
95	0
96	0
97	0
98	0
99	0
100	0