

TABLE S1: Stepwise docking simulations for DDX3X-CRM-1 interaction.

Rank	Solution Number	Global Energy	Attractive VdW	Repulsive VdW	ACE	HB
1	229	-31.28	-24.22	14.37	-7.00	-1.17
2	323	-21.85	-21.60	9.28	2.67	-1.91
3	184	-18.37	-33.72	21.57	7.11	-4.35
4	167	-18.10	-24.15	18.39	8.21	-1.99
5	11	-17.38	-31.82	17.22	2.49	-2.30
6	341	-15.02	-19.40	8.74	2.72	-2.76
7	436	-13.50	-37.59	26.99	5.95	-3.19
8	437	-13.34	-25.59	9.26	6.68	-1.78
9	260	-12.86	-34.94	13.11	18.57	-7.06
10	152	-12.10	-31.24	18.96	11.94	-3.27
11	334	-12.08	-17.80	4.47	2.97	-3.61

Solution No	Score	Area	ACE	Transformation
1	17206	2686.00	288.52	-1.20 1.09 2.56 4.98 160.55 -6.24
2	16856	4283.80	126.91	-2.55 -1.19 1.07 -10.85 73.54 44.37
3	16300	2770.70	359.85	0.03 -0.93 -0.15 -77.93 132.05 57.65
4	16014	3230.80	144.98	-0.51 -1.10 -2.09 26.21 101.09 47.46
5	15726	2386.20	309.05	-0.63 0.18 1.50 39.91 121.60 5.27
6	15422	2923.00	440.90	1.46 0.10 0.08 -25.47 103.53 57.70
7	15130	2334.90	-22.58	2.53 -0.43 -1.07 -30.91 61.84 60.60
8	15024	2002.10	425.51	-0.82 -0.59 3.06 13.61 77.95 -15.96
9	14698	1949.60	268.94	-2.24 -1.11 1.52 53.64 134.97 49.15
10	14532	2193.80	309.15	1.15 0.10 -1.72 81.04 133.72 51.83
11	14492	2248.90	-75.41	1.35 1.36 0.72 -78.72 78.75 23.03
12	14484	2359.10	324.60	-1.40 -0.54 -0.92 -81.06 108.52 8.79
13	14146	2283.50	321.81	-1.18 0.94 2.52 12.18 156.16 -12.06
14	14054	2283.50	424.53	-2.25 0.37 -1.95 -58.88 86.76 72.92
15	13970	2108.90	300.93	0.71 0.78 -3.07 6.03 121.69 17.81

Rank	Solution No.	Global Energy	Attractive VdW	Repulsive VdW	ACE	HB
1	1	-33.37	-38.36	29.92	8.45	-4.14
2	2	-30.18	-26.82	13.16	-6.33	-1.70
3	11	-24.54	-44.20	19.02	16.76	-5.68
4	4	-21.12	-43.69	26.38	7.49	-1.67
5	5	-18.91	-34.77	14.91	12.51	-3.30