

S3 Table. The ranks of all cocrystallized proteins of Astex Diverse Set before and after score normalization in the reverse docking by DOCK, Glide and AutoDock Vina.

Docking software	Protein	Raw score	Rank before score normalization	Normalized score	Rank after score normalization
DOCK	1hnn	-43.16	11	-1.21	2
	1hp0	-39.22	3	-0.14	8
	1hq2	-34.80	3	0.68	16
	1j3j	-59.46	5	-1.91	9
	1jla	-54.47	1	-2.38	1
	1ke5	-40.62	8	-0.57	4
	1l7f	-45.34	5	-0.96	3
	1lpz	-69.99	2	-2.62	2
	1m2z	-56.44	1	-1.92	1
	1n1m	-41.96	11	-0.73	8
	1of1	-37.10	3	-0.03	5
	1of6	-34.26	16	-0.59	2
	1q41	-39.17	3	-0.06	5
	1s19	-35.67	13	-0.41	6
	1sqn	-40.77	1	-0.73	1
	1t40	-49.29	2	-2.00	1
	1u1c	-43.20	3	-0.75	4
	1unl	-49.19	1	-1.52	3
	1v48	-40.73	12	-0.72	8
	1vcj	-68.06	1	-3.02	1
	1w2g	-39.72	1	-0.15	5
	1xoq	-43.24	5	-0.27	10
	1y6b	-61.61	6	-3.26	2
	1yqy	-37.04	10	-0.01	12
	1yv3	-41.97	1	-0.54	2
	2bsm	-44.60	1	-0.84	1
Glide	1gkc	-6.93	3	-0.73	2
	1gpk	-8.48	2	-1.40	3
	1hnn	-7.67	13	-1.25	7
	1hp0	-7.25	24	-0.52	21
	1hq2	-11.81	1	-3.00	1
	1hwi	-10.20	2	-4.94	1
	1hww	-7.56	2	-1.85	1
	1ia1	-8.01	6	-1.08	1
	1ig3	-7.42	15	-1.11	2
	1j3j	-7.92	5	-0.83	2
	1jje	-7.39	20	-2.26	1
	1jla	-13.05	1	-2.52	1
	1k3u	-12.53	1	-3.20	1

1ke5	-10.42	2	-2.54	1
1l2s	-6.70	26	-0.87	5
1l7f	-6.74	9	-1.58	4
1lrh	-7.58	17	-1.68	1
1m2z	-11.94	1	-2.88	1
1mmv	-3.73	20	2.41	29
1n1m	-7.83	2	-2.13	1
1n2j	-5.37	7	0.84	14
1n46	-12.31	1	-2.64	1
1nav	-11.60	2	-2.18	2
1of1	-10.89	1	-2.81	1
1of6	-10.31	1	-2.09	1
1opk	-12.82	1	-3.21	1
1owe	-8.48	8	-2.24	1
1p62	-10.05	1	-2.89	1
1pmn	-11.00	1	-2.57	2
1q1g	-8.11	7	-0.65	15
1q41	-11.01	1	-2.78	1
1q4g	-10.96	1	-2.86	1
1r1h	-11.12	1	-3.41	2
1r55	-7.80	1	-2.31	1
1r9o	-7.89	13	-0.80	14
1s19	-13.25	1	-3.34	1
1s3v	-9.30	2	-1.76	1
1sj0	-12.33	1	-3.52	1
1sqn	-10.76	1	-2.37	1
1t46	-12.97	1	-4.48	1
1t9b	-6.93	14	-0.29	12
1tow	-8.62	4	-2.00	1
1tt1	-9.69	1	-2.33	1
1tz8	-8.73	6	-2.01	1
1u1c	-8.40	2	-1.99	1
1u4d	-10.08	1	-2.95	1
1uml	-8.49	20	-2.54	3
1unl	-9.22	4	-1.91	2
1uou	-10.13	1	-2.35	1
1v0p	-9.48	4	-2.51	2
1v48	-10.06	3	-3.01	1
1v4s	-12.16	1	-2.83	1
1vcj	-8.04	8	-2.76	1
1w1p	-5.84	50	-0.12	24
1w2g	-7.92	12	-1.48	6
1x8x	-7.52	6	-1.38	4
1xoq	-7.31	15	-0.55	6
1y6b	-10.96	1	-2.88	1

	1ygc	-7.97	7	-1.83	1
	1yv3	-10.69	1	-2.18	1
	1yvf	-8.19	5	-1.59	1
	1ywr	-11.35	2	-3.56	2
	1z95	-11.96	1	-2.71	1
	2br1	-7.68	6	-1.14	4
	2bsm	-7.97	9	-1.77	4
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	1gkc	-6.60	21	1.37	39
	1hnn	-8.90	1	-0.75	2
	1hp0	-8.40	2	0.09	18
	1hq2	-9.20	1	-3.38	1
	1hwi	-9.20	6	-1.88	1
	1ig3	-7.30	7	0.42	12
	1jla	-11.60	1	-2.19	1
	1k3u	-10.00	1	-1.43	2
	1ke5	-9.40	9	-1.32	4
	1l2s	-7.80	12	-0.20	9
	1lpz	-10.30	4	-2.11	2
	1lrh	-7.90	16	-2.14	2
	1m2z	-12.40	1	-1.94	1
	1n1m	-5.80	20	1.60	21
	1n46	-11.80	1	-1.41	3
	1nav	-10.30	2	-1.05	4
	1of1	-8.50	4	-1.12	1
	1opk	-11.90	1	-2.74	1
AutoDock	1oyt	-9.40	6	-1.38	4
Vina	1p62	-7.80	3	-1.28	1
	1q1g	-9.10	1	-1.15	1
	1q4g	-9.30	6	-1.29	1
	1r1h	-9.70	3	-1.99	1
	1r55	-6.60	35	0.11	13
	1r9o	-8.70	12	-0.19	23
	1sqn	-11.60	1	-1.29	3
	1t40	-11.00	1	-1.62	2
	1t46	-13.40	1	-3.91	1
	1tow	-8.00	16	-0.20	13
	1uml	-10.30	3	-1.51	6
	1unl	-8.50	11	-0.55	7
	1v48	-8.70	4	-2.22	1
	1vcj	-7.90	3	-0.79	1
	1w2g	-9.10	1	-0.80	1
	1x8x	-6.80	14	1.32	29
	1xm6	-8.80	1	-0.27	5
	1xoq	-9.50	2	-0.67	4
	1xoz	-12.50	1	-2.48	1

1y6b	-9.40	20	-1.49	12
1ygc	-9.60	3	-2.36	1
1yqy	-9.90	2	-1.67	1
1yvf	-9.00	14	-1.42	2
1ywr	-10.60	5	-1.99	3
1z95	-10.60	3	-1.90	3
2bsm	-9.30	2	-1.84	1
