

ESI_results_per_complex: Results per complex of each property's performance in ranking P:P complexes

Data 1. Ranking performance for the B:B set. The ranking performance of each property was assessed by the iRMSD of the first ranked pose; the percentages of high-quality poses (%HQ), high- or medium-quality poses (%HQ/MQ), and of incorrect poses (%IP_{top}) in the top-*N* predictions; and, finally, the percentage of incorrect poses at the bottom-*M* predictions (%IP_{bottom}). The top-*N* and bottom-*M* predictions were defined by the total number of high-quality poses, and the total number of incorrect poses per complex, respectively.

Part 1. Average results

property	iRMSd 1 st / Å		%HQ		%IP _{top}		%HQ/MQ		%IP _{bottom}	
	av.	SEM	av.	SEM	av.	SEM	av.	SEM	av.	SEM
TP	1.0	0.4	75	7	8	4	85	7	46	6
$\Delta\Delta G_{\text{bind}}^{\text{sum, TP}}$	1.0	0.4	79	6	2	2	88	6	54	6
$\Delta G_{\text{bind}}^{\text{P:P}}$	0.3	0.1	89	3	4	2	96	2	53	6
iA	3.1	1.0	72	8	11	5	84	6	40	6

Part 2. Detailed results

property	complex	iRMSd 1 st / Å	%HQ	%IP _{top}	%HQ/MQ	%IP _{bottom}
TP	1BRS	0.5	100	0	100	100
	1Z7X	0.7	67	33	67	40
	1CHO	0.8	100	0	100	40
	3HFM	0.0	67	17	83	40
	1VFB	0.9	88	0	100	33
	1JTG	0.6	83	0	100	60
	1TM1	0.6	83	0	83	60
	1DQJ	0.0	83	0	100	60
	1KTZ	0.5	100	0	100	60
	1F47	0.6	67	17	67	80
	3SGB	3.0	50	0	50	20
	1FCC	1.0	83	0	100	20
	1H9D	0.9	100	0	100	50
	1AK4	6.7	0	67	0	0
	2GOX	0.9	33	0	100	60
	1EMV	0.0	67	0	100	20
	1SMF	0.0	100	0	100	40
$\Delta\Delta G_{\text{bind}}^{\text{sum, TP}}$	1BRS	0.5	83	0	100	80
	1Z7X	0.7	100	0	100	60
	1CHO	0.5	100	0	100	80
	3HFM	0.0	100	0	100	40
	1VFB	0.0	75	0	100	33
	1JTG	0.6	83	0	100	60
	1TM1	0.6	83	0	83	40

$\Delta G_{\text{bind}}^{\text{P:P}}$	1DQJ	0.0	83	0	100	80
	1KTZ	0.5	100	0	100	100
	1F47	0.6	50	0	50	60
	3SGB	3.0	50	0	50	40
	1FCC	0.8	83	0	100	40
	1H9D	0.6	83	0	100	50
	1AK4	6.7	17	33	17	0
	2GOX	1.5	50	0	100	80
	1EMV	0.5	100	0	100	40
	1SMF	0.0	100	0	100	40
	1BRS	0.5	100	0	100	80
	1Z7X	0.7	67	0	100	100
	1CHO	0.0	100	0	100	60
	3HFM	0.7	100	0	100	20
	1VFB	0.0	75	13	88	33
	1JTG	0.0	83	0	100	40
	1TM1	0.4	100	0	100	40
	1DQJ	0.0	67	17	83	40
	1KTZ	0.5	100	0	100	80
	1F47	0.6	83	17	83	20
	3SGB	0.0	83	0	100	80
iA	1FCC	1.0	83	0	100	60
	1H9D	0.0	100	0	100	50
	1AK4	0.6	83	17	83	40
	2GOX	0.0	83	0	100	80
	1EMV	0.0	100	0	100	20
	1SMF	0.0	100	0	100	60
	1BRS	0.5	83	0	100	60
	1Z7X	0.7	100	0	100	40
	1CHO	0.8	100	0	100	100
	3HFM	0.7	83	17	83	40
	1VFB	0.9	75	0	100	33
	1JTG	0.6	83	0	100	60
	1TM1	0.4	100	0	100	60
	1DQJ	14.9	67	17	83	40
	1KTZ	9.0	67	33	67	40
	1F47	6.6	67	33	67	20
	3SGB	7.9	0	17	50	40
	1FCC	1.0	83	0	100	40
	1H9D	0.9	100	0	100	33
	1AK4	6.7	0	67	0	0
	2GOX	0.9	33	0	100	20
	1EMV	0.6	100	0	100	0
	1SMF	0.0	86	0	86	60

Data 2. Ranking performance for the B:U set. The ranking performance of each property was assessed by the iRMSD of the first ranked pose; the percentages of high-quality poses (%HQ), high- or medium-quality poses (%HQ/MQ), and of incorrect poses (%IP_{top}) in the top-*N* predictions; and, finally, the percentage of incorrect poses at the bottom-*M* predictions (%IP_{bottom}). The top-*N* and bottom-*M* predictions were defined by the total number of high-quality poses, and the total number of incorrect poses per complex, respectively.

Part 1. Average results

property	iRMSd 1 st / Å		%HQ		%IP _{top}		%HQ/MQ		%IP _{bottom}	
	av.	SEM	av.	SEM	av.	SEM	av.	SEM	av.	SEM
TP	0.4	0.2	67	15	2	2	98	2	47	7
$\Delta\Delta G_{\text{bind}}^{\text{sum, TP}}$	0.8	0.4	52	15	5	5	83	11	51	8
$\Delta G_{\text{bind}}^{\text{P:P}}$	0.3	0.2	87	10	0	0	97	2	39	7
iA	1.1	0.4	57	16	0	0	87	10	37	8

Part 2. Detailed results

property	complex	iRMSd 1 st / Å	%HQ	%IP _{top}	%HQ/MQ	%IP _{bottom}
TP	1BRS	1.2	0	0	100	40
	1VFB	0.0	100	0	100	20
	1CHO	0.0	100	0	100	40
	1F47	1.3	0	0	100	80
	3SGB	1.2	0	0	100	67
	1FFW	0.0	100	0	100	40
	1DVF	0.0	83	0	100	83
	1A4Y	0.0	100	0	100	40
	2JEL	0.7	83	17	83	20
	1JTG	0.0	100	0	100	40
$\Delta\Delta G_{\text{bind}}^{\text{sum, TP}}$	1BRS	1.3	0	0	100	40
	1VFB	0.0	100	0	100	20
	1CHO	1.1	0	0	100	80
	1F47	3.5	0	0	0	60
	3SGB	1.4	0	0	100	67
	1FFW	0.0	100	0	100	40
	1DVF	0.7	83	0	100	83
	1A4Y	0.0	100	0	100	60
	2JEL	0.0	33	50	33	0
	1JTG	0.0	100	0	100	60
$\Delta G_{\text{bind}}^{\text{P:P}}$	1BRS	0.0	100	0	100	20
	1VFB	0.0	100	0	100	20
	1CHO	0.0	100	0	100	40
	1F47	0.0	100	0	100	60
	3SGB	1.4	0	0	100	50
	1FFW	0.0	100	0	100	20
	1DVF	0.7	83	0	83	83
	1A4Y	0.0	100	0	100	60

	2JEL	0.7	83	0	83	20
	1JTG	0.0	100	0	100	20
<i>iA</i>	1BRS	1.2	0	0	100	40
	1VFB	0.0	100	0	100	0
	1CHO	1.1	0	0	100	40
	1F47	1.3	0	0	100	40
	3SGB	3.0	0	0	0	67
	1FFW	0.0	100	0	100	40
	1DVF	0.7	83	0	83	67
	1A4Y	0.0	100	0	100	60
	2JEL	3.2	83	0	83	0
	1JTG	0.0	100	0	100	20

Data 3. Ranking performance for the U:U set. The ranking performance of each property was assessed by the iRMSD of the first ranked pose; the percentages of high-quality poses (%HQ), high- or medium-quality poses (%HQ/MQ), and of incorrect poses (%IP_{top}) in the top-*N* predictions; and, finally, the percentage of incorrect poses at the bottom-*M* predictions (%IP_{bottom}). The top-*N* and bottom-*M* predictions were defined by the total number of high-quality poses, and the total number of incorrect poses per complex, respectively.

Part 1. Average results

property	iRMSd 1 st / Å		%HQ		%IP _{top}		%HQ/MQ		%IP _{bottom}	
	av.	SEM	av.	SEM	av.	SEM	av.	SEM	av.	SEM
TP	0.5	0.3	70	15	0	0	90	10	58	4
$\Delta\Delta G_{\text{bind}}^{\text{sum, TP}}$	1.0	0.7	78	13	10	10	90	10	54	5
$\Delta G_{\text{bind}}^{\text{P:P}}$	0.9	0.8	90	10	10	10	90	10	49	6
<i>iA</i>	1.9	0.8	58	16	23	13	58	16	48	7

Part 2. Detailed results

property	complex	iRMSd 1 st / Å	%HQ	%IP _{top}	%HQ/MQ	%IP _{bottom}
TP	1BRS	0.0	100	0	100	60
	1VFB	0.0	100	0	100	67
	1CHO	0.0	100	0	100	67
	3SGB	1.9	0	0	100	60
	1CBW	0.0	100	0	100	62
	1FFW	2.1	0	0	0	38
	1R0R	1.2	0	0	100	40
	1PPF	0.0	100	0	100	40
	2GUG	0.0	100	0	100	70
	1EAW	0.0	100	0	100	75
$\Delta\Delta G_{\text{bind}}^{\text{sum, TP}}$	1BRS	0.0	100	0	100	60
	1VFB	0.0	100	0	100	56
	1CHO	1.3	75	0	100	67
	3SGB	1.9	0	0	100	60

	1CBW	0.0	100	0	100	54
	1FFW	0.0	100	0	100	25
	1R0R	0.0	100	0	100	80
	1PPF	0.0	100	0	100	60
	2GUG	0.0	100	0	100	40
	1EAW	6.6	0	100	0	38
$\Delta G_{\text{bind}}^{\text{P:P}}$	1BRS	0.0	100	0	100	50
	1VFB	7.7	0	100	0	33
	1CHO	0.9	100	0	100	83
	3SGB	0.0	100	0	100	40
	1CBW	0.0	100	0	100	77
	1FFW	0.0	100	0	100	25
	1R0R	0.0	100	0	100	40
	1PPF	0.0	100	0	100	50
	2GUG	0.0	100	0	100	40
	1EAW	0.0	100	0	100	50
iA	1BRS	0.0	100	0	100	40
	1VFB	0.0	100	0	100	56
	1CHO	1.0	75	25	75	50
	3SGB	3.0	0	0	0	80
	1CBW	5.5	0	100	0	54
	1FFW	2.1	0	0	0	25
	1R0R	0.0	100	0	100	20
	1PPF	7.1	0	100	0	20
	2GUG	0.0	100	0	100	70
	1EAW	0.0	100	0	100	63

Data 4. Ranking performance for the B:B set and for the cASM protocol independent of experimental information. The ranking performance of each property was assessed by the iRMSD of the first ranked pose; the percentages of high-quality poses (%HQ), high- or medium-quality poses (%HQ/MQ), and of incorrect poses (%IP_{top}) in the top-*N* predictions; and, finally, the percentage of incorrect poses at the bottom-*M* predictions (%IP_{bottom}). The top-*N* and bottom-*M* predictions were defined by the total number of high-quality poses, and the total number of incorrect poses per complex, respectively.

Part 1. Average results

property	iRMSd 1 st / Å		%HQ		%IP _{top}		%HQ/MQ		%IP _{bottom}	
	av.	SEM	av.	SEM	av.	SEM	av.	SEM	av.	SEM
cHS	0.9	0.4	76	5	9	3	88	4	43	6
$\Delta\Delta G_{\text{bind}}^{\text{sum, cHS}}$	1.3	0.6	81	5	8	3	89	4	50	6

Part 2. Detailed results

property	complex	iRMSd 1 st / Å	%HQ	%IP _{top}	%HQ/MQ	%IP _{bottom}
cHS	1BRS	0.0	100	0	100	80
	1JTG	0.5	83	0	100	60
	1VFB	0.0	75	13	88	33
	1Z7X	0.7	83	0	100	60
	1CHO	0.5	67	0	67	40
	3HFM	0.7	67	33	67	20
	1TM1	0.4	100	0	100	20
	1DQJ	0.0	67	17	83	40
	1KTZ	0.5	83	0	100	40
	1F47	0.6	83	0	100	20
	1FCC	1.0	100	0	100	80
	2GOX	0.9	50	0	100	60
	3SGB	1.2	17	33	50	40
	1H9D	0.6	83	17	83	17
	1AK4	6.7	67	17	67	20
	1EMV	0.6	67	17	83	20
	1SMF	0.0	100	0	100	80
$\Delta\Delta G_{\text{bind}}^{\text{sum, cHS}}$	1BRS	0.5	100	0	100	80
	1JTG	0.6	83	0	100	60
	1VFB	0.9	63	13	88	33
	1Z7X	0.7	67	0	100	60
	1CHO	0.0	83	0	83	40
	3HFM	0.0	83	17	83	20
	1TM1	0.4	100	0	100	60
	1DQJ	0.0	83	17	83	40
	1KTZ	0.5	100	0	100	40
	1F47	0.6	83	17	83	40
	1FCC	0.8	83	0	100	60
	2GOX	1.0	50	0	100	80
	3SGB	7.9	33	33	33	60
	1H9D	0.6	100	0	100	17
	1AK4	6.7	67	33	67	20
	1EMV	0.5	100	0	100	40
	1SMF	0.0	100	0	100	100

Data 5. Ranking performance for the B:U set and for the cASM protocol independent of experimental information. The ranking performance of each property was assessed by the iRMSD of the first ranked pose; the percentages of high-quality poses (%HQ), high- or medium-quality poses (%HQ/MQ), and of incorrect poses (%IP_{top}) in the top-*N* predictions; and, finally, the percentage of incorrect poses at the bottom-*M* predictions (%IP_{bottom}). The top-*N* and bottom-*M* predictions were defined by the total number of high-quality poses, and the total number of incorrect poses per complex, respectively.

Part 1. Average results

property	iRMSd 1 st / Å		%HQ		%IP _{top}		%HQ/MQ		%IP _{bottom}	
	av.	SEM	av.	SEM	av.	SEM	av.	SEM	av.	SEM
cHS	0.4	0.2	62	14	2	2	92	6	46	7
$\Delta\Delta G_{\text{bind}}^{\text{sum, cHS}}$	0.4	0.2	73	13	2	2	95	4	44	6

Part 2. Detailed results

property	complex	iRMSd 1 st / Å	%HQ	%IP _{top}	%HQ/MQ	%IP _{bottom}
cHS	3SGB	1.4	0	0	100	80
	1F47	0.0	100	0	100	60
	1FFW	0.0	100	0	100	40
	1DVF	0.7	50	0	50	80
	1A4Y	0.0	100	0	100	40
	1JTG	0.0	100	0	100	40
	2JEL	0.0	67	17	67	20
	1VFB	0.0	100	0	100	40
	1CHO	1.1	0	0	100	20
	1BRS	1.2	0	0	100	40
$\Delta\Delta G_{\text{bind}}^{\text{sum, cHS}}$	3SGB	1.4	0	0	100	40
	1F47	0.0	100	0	100	80
	1FFW	0.0	100	0	100	20
	1DVF	0.7	67	0	83	60
	1A4Y	0.0	100	0	100	40
	1JTG	0.0	100	0	100	60
	2JEL	0.7	67	17	67	20
	1VFB	0.0	100	0	100	40
	1CHO	0.0	100	0	100	40
	1BRS	1.2	0	0	100	40

Data 6. Ranking performance for the U:U set and for the cASM protocol independent of experimental information. The ranking performance of each property was assessed by the iRMSD of the first ranked pose; the percentages of high-quality poses (%HQ), high- or medium-quality poses (%HQ/MQ), and of incorrect poses (%IP_{top}) in the top-*N* predictions; and, finally, the percentage of incorrect poses at the bottom-*M* predictions (%IP_{bottom}). The top-*N* and bottom-*M* predictions were defined by the total number of high-quality poses, and the total number of incorrect poses per complex, respectively.

Part 1. Average results

property	iRMSd 1 st / Å		%HQ		%IP _{top}		%HQ/MQ		%IP _{bottom}	
	av.	SEM	av.	SEM	av.	SEM	av.	SEM	av.	SEM
cHS	1.3	0.8	65	15	10	10	80	13	53	5
$\Delta\Delta G_{\text{bind}}^{\text{sum, cHS}}$	1.0	0.8	78	13	10	10	90	10	55	6

Part 2. Detailed results

property	complex	iRMSd 1 st / Å	%HQ	%IP _{top}	%HQ/MQ	%IP _{bottom}
cHS	1BRS	0.0	100	0	100	50
	1VFB	7.7	0	100	0	44
	1CHO	1.3	50	0	100	67
	3SGB	1.8	0	0	100	80
	1CBW	0.0	100	0	100	54
	1FFW	0.0	100	0	100	25
	1R0R	0.0	100	0	100	40
	1PPF	2.6	0	0	0	60
	2GUG	0.0	100	0	100	60
	1EAW	0.0	100	0	100	50
$\Delta\Delta G_{\text{bind}}^{\text{sum, cHS}}$	1BRS	0.0	100	0	100	60
	1VFB	7.7	0	100	0	44
	1CHO	0.9	75	0	100	67
	3SGB	1.8	0	0	100	60
	1CBW	0.0	100	0	100	54
	1FFW	0.0	100	0	100	13
	1R0R	0.0	100	0	100	80
	1PPF	0.0	100	0	100	60
	2GUG	0.0	100	0	100	50
	1EAW	0.0	100	0	100	63

Data 7. Ranking performance considering MD generated poses. The ranking performance of each property was assessed by the iRMSD of the first ranked pose; the percentages of high-quality poses (%HQ), high- or medium-quality poses (%HQ/MQ), and of incorrect poses (%IP_{top}) in the top-*N* predictions; and, finally, the percentage of incorrect poses at the bottom-*M* predictions (%IP_{bottom}). The top-*N* and bottom-*M* predictions were defined by the total number of high-quality poses, and the total number of incorrect poses per complex, respectively.

property		complex	iRMSD 1 st / Å	%HQ	%IP _{top}	%HQ/MQ	%IP _{bottom}
TP	HADDOCK	1BRS	0.0	100	0	100	60
		1R0R	1.2	0	0	100	40
	HADDOCK+MD	1BRS	0.0	100	0	100	60
		1R0R	1.2	33	17	50	40
$\Delta\Delta G_{\text{bind}}^{\text{sum, TP}}$	HADDOCK	1BRS	0.0	100	0	100	60
		1R0R	0.0	100	0	100	80
	HADDOCK+MD	1BRS	0.0	100	0	100	60
		1R0R	0.9	83	0	100	80
$\Delta G_{\text{bind}}^{\text{P:P}}$	HADDOCK	1BRS	0.0	100	0	100	50
		1R0R	0.0	100	0	100	40
	HADDOCK+MD	1BRS	0.0	100	0	100	50
		1R0R	0.9	100	0	100	40
iA	HADDOCK	1BRS	0.0	100	0	100	40
		1R0R	0.0	100	0	100	20
	HADDOCK+MD	1BRS	1.0	100	0	100	40
		1R0R	0.8	100	0	100	20

Data 8. Area under the ROC curve (AUC-ROC) and enrichment factor at 10% for each P:P complex.

COMPLEX	AUC-ROC			EF10%		
	$\Delta G_{\text{bind}}^{\text{P:P}}$	iA	$\Delta\Delta G_{\text{bind}}^{\text{sum, cHS}}$	$\Delta G_{\text{bind}}^{\text{P:P}}$	iA	$\Delta\Delta G_{\text{bind}}^{\text{sum, cHS}}$
2A1A	0.98	0.97	0.98	4.86	4.32	5.14
3A4S	0.94	0.90	0.92	3.66	2.68	3.41
3FN1	0.95	0.97	0.98	8.00	8.67	9.33
3H11	0.99	0.99	1.00	9.73	8.92	9.46
3K75	0.90	0.94	0.89	5.00	6.00	4.00
3PC8	0.98	0.97	0.98	7.14	6.67	7.62
3VLB	0.99	0.96	0.98	9.23	7.69	8.46
4IZ7	0.96	0.92	0.93	8.18	4.55	6.36
2VXT	0.99	0.99	0.98	4.65	4.42	4.42
2W9E	0.94	0.99	0.97	5.50	8.00	7.00
3EOA	0.97	0.97	0.97	4.05	4.05	4.05
3L5W	0.94	0.88	0.97	3.81	2.50	4.29
4DN4	0.97	0.98	0.98	7.07	6.83	7.56
4G6M	0.99	0.99	0.99	7.73	8.18	8.18
1M27	0.94	0.75	0.93	7.46	0.62	7.46
3H2V	0.90	0.83	0.83	5.71	1.43	4.29
1BRS	1.00	1.00	1.00	3.28	3.28	3.28
1AK4	0.93	0.30	0.69	6.00	0.00	0.00
1F47	1.00	0.93	0.99	2.90	2.17	2.90
1CHO	1.00	1.00	0.95	3.17	3.17	2.86
1KTZ	1.00	0.94	0.99	5.13	3.59	4.87
1FCC	0.98	0.93	0.98	2.32	2.20	2.32
3SGB	0.91	0.62	0.77	1.74	0.64	1.19
1VFB	0.87	0.94	0.88	2.14	2.71	2.43
1TM1	1.00	1.00	1.00	4.44	4.44	4.44
1EMV	1.00	1.00	1.00	2.90	2.90	2.90
1SMF	1.00	0.99	1.00	6.90	6.21	6.90
1H9D	1.00	1.00	1.00	2.82	2.82	2.82
2GOX	0.91	0.77	0.89	5.00	2.00	4.00
3HFM	0.97	0.97	0.97	5.86	5.52	5.17
1DQJ	0.89	0.95	0.90	3.26	3.26	3.02
1JTG	1.00	1.00	1.00	3.57	3.57	3.57
1Z7X	0.97	1.00	0.95	3.45	3.45	3.28
2X9A	0.99	1.00	0.99	9.44	10.00	8.89
3BX7	0.83	0.89	0.89	3.51	3.78	3.78
3S9D	0.94	0.96	0.95	5.38	5.77	5.77
4M76	0.74	0.86	0.68	1.56	2.34	0.78
3AAD	0.88	0.90	0.91	4.29	4.29	4.86
3F1P	0.89	0.94	0.94	6.11	6.11	6.67
av.	0.95	0.92	0.94	-	-	-