

Table S1. The 18 diverse complexes considered in this work. The number of Hot Spots (HS) by complex is also given. U:U stands for unbound-unbound, U:B stands for unbound-bound and B:B stands for bound-bound. The HS are residues whose mutation for Ala increases the binding free energy of the complex by ⁱ > 4 kcal/mol, ⁱⁱ >2 kcal/mol, ⁱⁱⁱ >1.5 kcal/mol.

case no.	docking type	complex	n. ^o of HS		
			> 4 ⁱ	> 2 ⁱⁱ	> 1.5 ⁱⁱⁱ
1	U:U	1BRS	6	9	10
2	U:B	1DVF	5	8	16
3	U:B	2EKS	3	5	6
4	U:U	1VFB	1	4	5
5	U:U	1DFJ	1	4	5
6	U:B	1FCC	1	4	5
7	U:B	1FQ9	1	4	4
8	U:U	1FLT	0	4	5
9	U:B	1A22	0	3	5
10	U:B	1F47	0	3	4
11	U:B	1IAR	0	2	3
12	B:B	1BRS	6	9	10
13	B:B	1EMV	2	6	7
14	B:B	1DFJ	1	4	5
15	B:B	1FCC	1	4	5
16	B:B	1FQ9	1	4	4
17	B:B	1VFB	1	3	6
18	B:B	1F47	0	3	4

Table S2. Value of the descriptors used in this work according to the three definitions of Hot Spot considered (i.e. residues whose mutation for Ala increases the binding free energy of the complex by (i) > 4 kcal/mol, (ii) >2 kcal/mol, and (iii) >1.5 kcal/mol. i-RMSD corresponds to the root mean square deviation for the interface residues, in relation to the X-ray structure, and is given in Å. U:U stands for unbound-unbound, U:B stands for unbound-bound and B:B stands for bound-bound. The names of the poses (first column of each table are the same as in the software used to generate them (HADDOCK)). *fnat* is the fraction of native contact present in each pose. The definition of the descriptors TP, FP, TN, FN, P, R, F1, Accuracy, and Specificity is given in Supplementary Information.

1BRS U:U MODEL	fnat	i-RMSD	DEFINITION (i)							DEFINITION (ii)							DEFINITION (iii)												
			TP	FP	TN	FN	P	R	F1	Accuracy	Specificity	TP	FP	TN	FN	P	R	F1	Accuracy	Specificity	TP	FP	TN	FN	P	R	F1	Accuracy	Specificity
X-Ray	1.00	0.00	6	0	2	0	1.00	1.00	1.00	1.00	1.00	7	1	2	2	0.88	0.78	0.82	0.75	0.67	8	1	1	2	0.89	0.80	0.84	0.75	0.50
complexfit_8	0.70	1.80	3	0	3	0	1.00	1.00	1.00	1.00	1.00	7	0	3	2	1.00	0.78	0.88	0.83	1.00	8	0	1	2	1.00	0.80	0.89	0.82	1.00
complexfit_5	0.72	1.80	6	1	2	0	0.86	1.00	0.92	0.89	0.67	7	1	2	2	0.88	0.78	0.82	0.75	0.67	7	1	1	3	0.88	0.70	0.78	0.67	0.50
complexfit_52	0.63	1.93	4	0	2	0	1.00	1.00	1.00	1.00	1.00	7	1	2	2	0.88	0.78	0.82	0.75	0.67	8	1	1	2	0.89	0.80	0.84	0.75	0.50
complexfit_7	0.54	2.26	3	0	3	0	1.00	1.00	1.00	1.00	1.00	7	0	3	2	1.00	0.78	0.88	0.83	1.00	7	0	1	2	1.00	0.78	0.88	0.80	1.00
complexfit_11	0.46	2.27	4	0	3	1	1.00	0.80	0.89	0.88	1.00	6	0	3	3	1.00	0.67	0.80	0.75	1.00	6	0	1	2	1.00	0.75	0.86	0.78	1.00
complexfit_4	0.61	2.34	3	0	2	1	1.00	0.75	0.86	0.83	1.00	6	1	2	3	0.86	0.67	0.75	0.67	0.67	7	1	1	2	0.88	0.78	0.82	0.73	0.50
complexfit_10	0.57	2.37	1	0	3	1	1.00	0.50	0.67	0.80	1.00	6	0	3	3	1.00	0.67	0.80	0.75	1.00	6	0	1	3	1.00	0.67	0.80	0.70	1.00
complexfit_3	0.50	2.56	4	1	2	1	0.80	0.80	0.80	0.75	0.67	6	1	2	3	0.86	0.67	0.75	0.67	0.67	7	1	1	2	0.88	0.78	0.82	0.73	0.50
complexfit_6	0.43	2.58	4	0	3	1	1.00	0.80	0.89	0.88	1.00	6	0	3	3	1.00	0.67	0.80	0.75	1.00	6	0	1	3	1.00	0.67	0.80	0.70	1.00
complexfit_37	0.35	3.06	3	0	3	1	1.00	0.75	0.86	0.86	1.00	6	0	3	3	1.00	0.67	0.80	0.75	1.00	6	0	2	3	1.00	0.67	0.80	0.73	1.00
complexfit_12	0.41	3.15	3	0	2	1	1.00	0.75	0.86	0.83	1.00	6	1	2	3	0.86	0.67	0.75	0.67	0.67	7	1	1	2	0.88	0.78	0.82	0.73	0.50
complexfit_69	0.15	3.24	0	0	3	1	0.00	0.00	0.00	0.75	1.00	5	0	3	4	1.00	0.56	0.71	0.67	1.00	7	0	2	2	1.00	0.78	0.88	0.82	1.00
complexfit_68	0.17	3.43	2	0	3	3	1.00	0.40	0.57	0.63	1.00	4	0	3	5	1.00	0.44	0.62	0.58	1.00	6	0	1	2	1.00	0.75	0.86	0.78	1.00
complexfit_94	0.22	3.67	1	0	3	3	1.00	0.25	0.40	0.57	1.00	4	0	3	5	1.00	0.44	0.62	0.58	1.00	6	0	2	3	1.00	0.67	0.80	0.73	1.00
complexfit_36	0.13	3.93	1	0	3	1	1.00	0.50	0.67	0.80	1.00	6	0	3	3	1.00	0.67	0.80	0.75	1.00	6	0	2	3	1.00	0.67	0.80	0.73	1.00
complexfit_1	0.11	7.43	2	1	1	1	0.67	0.67	0.67	0.60	0.50	6	2	1	3	0.75	0.67	0.71	0.58	0.33	8	1	1	2	0.89	0.80	0.84	0.75	0.50
complexfit_9	0.02	10.02	1	0	3	3	1.00	0.25	0.40	0.57	1.00	4	0	3	5	1.00	0.44	0.62	0.58	1.00	6	0	1	3	1.00	0.67	0.80	0.70	1.00
complexfit_2	0.00	10.75	0	0	2	5	0.00	0.00	0.00	0.29	1.00	2	1	2	7	0.67	0.22	0.33	0.33	0.67	3	1	1	5	0.75	0.38	0.50	0.40	0.50
complexfit_17	0.00	10.78	2	0	3	2	1.00	0.50	0.67	0.71	1.00	5	0	3	4	1.00	0.56	0.71	0.67	1.00	6	0	2	2	1.00	0.75	0.86	0.80	1.00
complexfit_14	0.00	10.79	1	0	3	4	1.00	0.20	0.33	0.50	1.00	3	0	3	6	1.00	0.33	0.50	0.50	1.00	5	0	2	3	1.00	0.63	0.77	0.70	1.00

1DVF U:B MODEL	fnat	i-RMSD	DEFINITION (i)							DEFINITION (ii)							DEFINITION (iii)												
			TP	FP	TN	FN	P	R	F1	Accuracy	Specificity	TP	FP	TN	FN	P	R	F1	Accuracy	Specificity	TP	FP	TN	FN	P	R	F1	Accuracy	Specificity
X-Ray	1.00	0.00	4	1	11	0	0.80	1.00	0.89	0.94	0.92	8	3	11	0	0.73	1.00	0.84	0.86	0.79	13	0	1	1	1.00	0.93	0.96	0.93	1.00
complexfit_18	0.71	0.91	4	3	6	0	0.57	1.00	0.73	0.77	0.67	8	8	6	0	0.50	1.00	0.67	0.64	0.43	14	1	0	0	0.93	1.00	0.97	0.93	0.00
complexfit_11	0.84	0.95	4	3	8	1	0.57	0.80	0.67	0.75	0.73	6	6	8	2	0.50	0.75	0.60	0.64	0.57	13	1	0	1	0.93	0.93	0.93	0.87	0.00
complexfit_5	0.84	0.97	4	2	8	1	0.67	0.80	0.73	0.80	0.80	6	6	8	2	0.50	0.75	0.60	0.64	0.57	14	0	1	0	1.00	1.00	1.00	1.00	1.00
complexfit_19	0.78	0.98	4	2	8	1	0.67	0.80	0.73	0.80	0.80	6	6	8	2	0.50	0.75	0.60	0.64	0.57	13	0	1	0	1.00	1.00	1.00	1.00	1.00
complexfit_1	0.78	1.04	4	1	12	0	0.80	1.00	0.89	0.94	0.92	6	2	12	2	0.75	0.75	0.75	0.82	0.86	9	0	1	2	1.00	0.82	0.90	0.83	1.00
complexfit_3	0.82	1.10	4	4	8	0	0.50	1.00	0.67	0.75	0.67	6	6	8	2	0.50	0.75	0.60	0.64	0.57	12	0	1	2	1.00	0.86	0.92	0.87	1.00
complexfit_2	0.80	1.13	5	4	7	0	0.56	1.00	0.71	0.75	0.64	6	7	7	2	0.46	0.75	0.57	0.59	0.50	14	0	1	0	1.00	1.00	1.00	1.00	1.00
complexfit_4	0.73	1.20	4	3	5	1	0.57	0.80	0.67	0.69	0.63	5	9	5	3	0.36	0.63	0.45	0.45	0.36	15	0	0	0	1.00	1.00	1.00	1.00	1.00
complexfit_120	0.55	2.07	1	2	12	3	0.33	0.25	0.29	0.72	0.86	4	2	12	4	0.67	0.50	0.57	0.73	0.86	7	0	1	4	1.00	0.64	0.78	0.67	1.00
complexfit_56	0.43	2.64	4	0	9	0	1.00	1.00	1.00	1.00	1.00	6	5	9	2	0.55	0.75	0.63	0.68	0.64	13	1	0	0	0.93	1.00	0.96	0.93	0.00
complexfit_126	0.43	2.73	3	0	12	0	1.00	1.00	1.00	1.00	1.00	7	2	12	1	0.78	0.88	0.82	0.86	0.86	12	0	1	3	1.00	0.80	0.89	0.81	1.00
complexfit_55	0.43	2.99	2	0	9	2	1.00	0.50	0.67	0.85	1.00	3	5	9	5	0.38	0.38	0.38	0.55	0.64	7	1	0	5	0.88	0.58	0.70	0.54	0.00
complexfit_112	0.29	3.18	0	0	11	3	0.00	0.00	0.00	0.79	1.00	3	3	11	5	0.50	0.38	0.43	0.64	0.79	6	1	0	3	0.86	0.67	0.75	0.60	0.00
complexfit_64	0.24	3.63	1	0	12	3	1.00	0.25	0.40	0.81	1.00	2	2	12	6	0.50	0.25	0.33	0.64	0.86	6	0	0	8	1.00	0.43	0.60	0.43	0.00
complexfit_98	0.18	3.79	1	0	9	2	1.00	0.33	0.50	0.83	1.00	3	5	9	5	0.38	0.38	0.38	0.55	0.64	8	1	0	2	0.89	0.80	0.84	0.73	0.00
complexfit_122	0.20	3.82	3	1	7	0	0.75	1.00	0.86	0.91	0.88	7	7	7	1	0.50	0.88	0.64	0.64	0.50	14	1	0	0	0.93	1.00	0.97	0.93	0.00
complexfit_59	0.10	12.89	1	1	7	3	0.50	0.25	0.33	0.67	0.88	2	7	7	6	0.22	0.25	0.24	0.41	0.50	7	1	0	4	0.88	0.64	0.74	0.58	0.00
complexfit_57	0.04	12.96	0	0	12	4	0.00	0.00	0.00	0.75	1.00	1	2	12	7	0.33	0.13	0.18	0.59	0.86	4	1	0	8	0.80	0.33	0.47	0.31	0.00
complexfit_35	0.16	13.02	1	1	6	2	0.50	0.33	0.40	0.70	0.86	4	8	6	4	0.33	0.50	0.40	0.45	0.43	11	1	0	1	0.92	0.92	0.92	0.85	0.00
complexfit_39	0.00	13.78	2	1	11	1	0.67	0.67	0.67	0.87	0.92	5	3	11	3	0.63	0.63	0.63	0.73	0.79	7	1	0	2	0.88	0.78	0.82	0.70	0.00

2EKS U:B MODEL	fnat	i-RMSD	DEFINITION (i)							DEFINITION (ii)							DEFINITION (iii)												
			TP	FP	TN	FN	P	R	F1	Accuracy	Specificity	TP	FP	TN	FN	P	R	F1	Accuracy	Specificity	TP	FP	TN	FN	P	R	F1	Accuracy	Specificity
X-Ray	1.00	0.00	3	1	4	0	0.75	1.00	0.86	0.88	0.80	4	7	4	1	0.36	0.80	0.50	0.50	0.36	6	3	1	0	0.67	1.00	0.80	0.70	0.25
complexfit_51	0.23	3.93	0	0	11	3	0.00	0.00	0.00	0.79	1.00	0	0	11	5	0.00	0.00	0.00	0.69	1.00	2	1	3	0	0.67	1.00	0.80	0.83	0.75
complexfit_13	0.03	5.95	0	0	9	3	0.00	0.00	0.00	0.75	1.00	1	2	9	4	0.33	0.20	0.25	0.63	0.82	1	2	5	1	0.33	0.50	0.40	0.67	0.71
complexfit_12	0.00	5.96	0	0	9	2	0.00	0.00	0.00	0.82	1.00	1	2	9	4	0.33	0.20	0.25	0.63	0.82	3	2	3	3	0.60	0.50	0.55	0.55	0.60
complexfit_3	0.05	6.11	1	0	10	0	1.00	1.00	1.00	1.00	1.00	4	1	10	1	0.80	0.80	0.80	0.88										

1FCC U:B MODEL	fnat	i-RMSD	DEFINITION (i)								DEFINITION (ii)								DEFINITION (iii)										
			TP	FP	TN	FN	P	R	F1	Accuracy	Specificity	TP	FP	TN	FN	P	R	F1	Accuracy	Specificity	TP	FP	TN	FN	P	R	F1	Accuracy	Specificity
X-Ray	1.00	0.00	1	1	3	0	0.50	1.00	0.67	0.80	0.75	3	1	3	1	0.75	0.75	0.75	0.75	0.75	3	0	1	1	1.00	0.75	0.86	0.80	1.00
complexfit_7	0.90	0.66	1	1	3	0	0.50	1.00	0.67	0.80	0.75	2	1	3	2	0.67	0.50	0.57	0.63	0.75	2	0	1	2	1.00	0.50	0.67	0.60	1.00
complexfit_3	0.83	0.83	1	0	3	0	1.00	1.00	1.00	1.00	1.00	2	1	3	2	0.67	0.50	0.57	0.63	0.75	2	0	2	1	1.00	0.67	0.80	0.80	1.00
complexfit_4	0.85	0.88	1	1	3	0	0.50	1.00	0.67	0.80	0.75	3	1	3	1	0.75	0.75	0.75	0.75	0.75	3	0	2	1	1.00	0.75	0.86	0.83	1.00
complexfit_8	0.88	0.89	1	1	3	0	0.50	1.00	0.67	0.80	0.75	2	1	3	2	0.67	0.50	0.57	0.63	0.75	2	0	3	1	1.00	0.67	0.80	0.83	1.00
complexfit_2	0.88	0.91	1	1	2	0	0.50	1.00	0.67	0.75	0.67	2	2	2	2	0.50	0.50	0.50	0.50	0.50	2	2	1	1	0.50	0.67	0.57	0.50	0.33
complexfit_5	0.78	1.00	1	0	3	0	1.00	1.00	1.00	1.00	1.00	2	1	3	2	0.67	0.50	0.57	0.63	0.75	3	0	3	1	1.00	0.75	0.86	0.86	1.00
complexfit_20	0.80	1.06	1	0	3	0	1.00	1.00	1.00	1.00	1.00	3	1	3	1	0.75	0.75	0.75	0.75	0.75	3	0	2	1	1.00	0.75	0.86	0.83	1.00
complexfit_6	0.78	1.09	1	1	3	0	0.50	1.00	0.67	0.80	0.75	2	1	3	2	0.67	0.50	0.57	0.63	0.75	3	0	2	0	1.00	1.00	1.00	1.00	1.00
complexfit_15	0.78	1.13	1	0	3	0	1.00	1.00	1.00	1.00	1.00	2	1	3	2	0.67	0.50	0.57	0.63	0.75	2	0	3	2	1.00	0.50	0.67	0.71	1.00
complexfit_1	0.80	1.21	1	0	4	0	1.00	1.00	1.00	1.00	1.00	3	0	4	1	1.00	0.75	0.86	0.88	1.00	3	0	2	0	1.00	1.00	1.00	1.00	1.00
complexfit_101	0.50	2.06	1	1	3	0	0.50	1.00	0.67	0.80	0.75	2	1	3	2	0.67	0.50	0.57	0.63	0.75	2	0	2	2	1.00	0.50	0.67	0.67	1.00
complexfit_197	0.43	2.15	1	0	4	0	1.00	1.00	1.00	1.00	1.00	1	0	4	3	1.00	0.25	0.40	0.63	1.00	2	0	2	1	1.00	0.67	0.80	0.80	1.00
complexfit_188	0.43	2.20	1	0	3	0	1.00	1.00	1.00	1.00	1.00	2	1	3	2	0.67	0.50	0.57	0.63	0.75	2	0	2	0	1.00	1.00	1.00	1.00	1.00
complexfit_96	0.65	2.24	1	0	3	0	1.00	1.00	1.00	1.00	1.00	3	1	3	1	0.75	0.75	0.75	0.75	0.75	3	0	2	0	1.00	1.00	1.00	1.00	1.00
complexfit_193	0.33	2.50	1	0	4	0	1.00	1.00	1.00	1.00	1.00	2	0	4	2	1.00	0.50	0.67	0.75	1.00	4	0	3	0	1.00	1.00	1.00	1.00	1.00
complexfit_136	0.18	6.96	1	1	2	0	0.50	1.00	0.67	0.75	0.67	3	2	2	1	0.60	0.75	0.67	0.63	0.50	3	1	1	0	0.75	1.00	0.86	0.80	0.50
complexfit_192	0.08	9.72	0	0	4	1	0.00	0.00	0.00	0.80	1.00	0	0	4	4	0.00	0.00	0.00	0.50	1.00	0	0	3	4	0.00	0.00	0.00	0.43	1.00
complexfit_194	0.08	9.83	0	0	4	1	0.00	0.00	0.00	0.80	1.00	0	0	4	4	0.00	0.00	0.00	0.50	1.00	0	0	3	4	0.00	0.00	0.00	0.43	1.00
complexfit_196	0.05	10.00	0	0	3	1	0.00	0.00	0.00	0.75	1.00	0	1	3	4	0.00	0.00	0.00	0.38	0.75	0	1	2	3	0.00	0.00	0.00	0.33	0.67
complexfit_102	0.00	15.48	0	0	4	1	0.00	0.00	0.00	0.80	1.00	0	0	4	4	0.00	0.00	0.00	0.50	1.00	0	0	2	4	0.00	0.00	0.00	0.33	1.00

1FQ9 U:B MODEL	fnat	i-RMSD	DEFINITION (i)								DEFINITION (ii)								DEFINITION (iii)										
			TP	FP	TN	FN	P	R	F1	Accuracy	Specificity	TP	FP	TN	FN	P	R	F1	Accuracy	Specificity	TP	FP	TN	FN	P	R	F1	Accuracy	Specificity
X-Ray	1.00	0.00	1	0	12	0	1.00	1.00	1.00	1.00	1.00	4	2	12	0	0.67	1.00	0.80	0.89	0.86	4	0	8	0	1.00	1.00	1.00	1.00	1.00
complexfit_2	0.81	0.92	1	0	11	0	1.00	1.00	1.00	1.00	1.00	4	3	11	0	0.57	1.00	0.73	0.83	0.79	4	1	4	0	0.80	1.00	0.89	0.89	0.80
complexfit_10	0.78	0.93	1	1	12	0	0.50	1.00	0.67	0.93	0.92	4	2	12	0	0.67	1.00	0.80	0.89	0.86	4	0	5	0	1.00	1.00	1.00	1.00	1.00
complexfit_3	0.85	0.95	1	1	12	0	0.50	1.00	0.67	0.93	0.92	4	2	12	0	0.67	1.00	0.80	0.89	0.86	4	0	7	0	1.00	1.00	1.00	1.00	1.00
complexfit_4	0.79	1.00	0	0	13	0	0.00	0.00	0.00	1.00	1.00	4	1	13	0	0.80	1.00	0.89	0.94	0.93	4	0	6	0	1.00	1.00	1.00	1.00	1.00
complexfit_5	0.73	1.08	0	0	12	0	0.00	0.00	0.00	1.00	1.00	4	2	12	0	0.67	1.00	0.80	0.89	0.86	4	0	8	0	1.00	1.00	1.00	1.00	1.00
complexfit_1	0.85	1.11	0	0	12	0	0.00	0.00	0.00	1.00	1.00	4	2	12	0	0.67	1.00	0.80	0.89	0.86	4	0	7	0	1.00	1.00	1.00	1.00	1.00
complexfit_7	0.82	1.15	1	0	12	0	1.00	1.00	1.00	1.00	1.00	4	2	12	0	0.67	1.00	0.80	0.89	0.86	4	0	7	0	1.00	1.00	1.00	1.00	1.00
complexfit_6	0.79	1.20	0	1	13	0	0.00	0.00	0.00	0.93	0.93	3	1	13	1	0.75	0.75	0.75	0.89	0.93	4	0	8	0	1.00	1.00	1.00	1.00	1.00
complexfit_9	0.51	2.05	0	0	13	0	0.00	0.00	0.00	1.00	1.00	4	1	13	0	0.80	1.00	0.89	0.94	0.93	4	0	8	0	1.00	1.00	1.00	1.00	1.00
complexfit_53	0.33	2.24	0	0	14	1	0.00	0.00	0.00	0.93	1.00	0	0	14	4	0.00	0.00	0.00	0.78	1.00	0	0	8	3	0.00	0.00	0.00	0.73	1.00
complexfit_13	0.46	2.36	1	0	13	0	1.00	1.00	1.00	1.00	1.00	3	1	13	1	0.75	0.75	0.75	0.89	0.93	3	0	6	0	1.00	1.00	1.00	1.00	1.00
complexfit_67	0.27	2.91	0	0	12	1	0.00	0.00	0.00	0.92	1.00	2	2	12	2	0.50	0.50	0.50	0.78	0.86	4	0	6	0	1.00	1.00	1.00	1.00	1.00
complexfit_59	0.33	3.19	0	0	12	0	0.00	0.00	0.00	1.00	1.00	3	2	12	1	0.60	0.75	0.67	0.83	0.86	3	2	5	0	0.60	1.00	0.75	0.80	0.71
complexfit_94	0.19	3.65	0	0	13	1	0.00	0.00	0.00	0.93	1.00	2	1	13	2	0.67	0.50	0.57	0.83	0.93	2	0	6	1	1.00	0.67	0.80	0.89	1.00
complexfit_80	0.13	3.82	0	1	13	1	0.00	0.00	0.00	0.87	0.93	0	1	13	4	0.00	0.00	0.00	0.72	0.93	1	2	4	0	0.33	1.00	0.50	0.71	0.67
complexfit_89	0.12	3.93	0	1	12	0	0.00	0.00	0.00	0.92	0.92	1	2	12	3	0.33	0.25	0.29	0.72	0.86	1	1	6	2	0.50	0.33	0.40	0.70	0.86
complexfit_48	0.08	4.70	0	0	14	1	0.00	0.00	0.00	0.93	1.00	2	0	14	2	1.00	0.50	0.67	0.89	1.00	3	0	8	1	1.00	0.75	0.86	0.92	1.00
complexfit_43	0.04	7.02	0	0	12	1	0.00	0.00	0.00	0.92	1.00	0	2	12	4	0.00	0.00	0.00	0.67	0.86	0	3	4	1	0.00	0.00	0.00	0.50	0.57
complexfit_27	0.01	11.19	0	0	14	1	0.00	0.00	0.00	0.93	1.00	1	0	14	3	1.00	0.25	0.40	0.83	1.00	1	0	8	0	1.00	1.00	1.00	1.00	1.00
complexfit_38	0.04	12.37	0	0	14	1	0.00	0.00	0.00	0.93	1.00	0	0	14	4	0.00	0.00	0.00	0.78	1.00	1	0	7	2	1.00	0.33	0.50	0.80	1.00

1FLT U:U MODEL	fnat	i-RMSD	DEFINITION (i)								DEFINITION (ii)								DEFINITION (iii)										
			TP	FP	TN	FN	P	R	F1	Accuracy	Specificity	TP	FP	TN	FN	P	R	F1	Accuracy	Specificity	TP	FP	TN	FN	P	R	F1	Accuracy	Specificity
X-Ray	1.00	0.00	0	0	14	0	0.00	0.00	0.00	1.00	1.00	3	2	14	1	0.60	0.75	0.67	0.85	0.88	4	4	2	0	0.50	1.00	0.67	0.60	0.33
complexfit_1	0.64	1.65	0	1	13	0	0.00	0.00	0.00	0.93	0.93	2	3	13	2	0.40	0.50	0.44	0.75	0.81	3	3	1	1	0.50	0.75	0.60	0.50	0.25
complexfit_10	0.50	1.76	0	0	14	0	0.00	0.00	0.00	1.00	1.00	1	2	14	3	0.33	0.25	0.29	0.75	0.88	4	1	4	0	0.80	1.00	0.89	0.89	0.80
complexfit_14	0.48	1.85	0	2	14	0	0.00	0.00	0.00	0.88	0.88	4	2	14	0	0.67	1.00	0.80	0.90	0.88	5	3	2	0	0.63	1.00	0.77	0.70	0.40
complexfit_7	0.56	1.85	0	0	13	0	0.00	0.00	0.00	1.00	1.00	1	3	13	3	0.25	0.25	0.25	0.70	0.81	4	1	2	0	0.80	1.00	0.89	0.86	0.67
complexfit_15	0.56	1.88	0	0	13	0	0.00	0.00	0.00	1.00	1.00	2	3	13	2	0.40	0.												

1IAR U-B MODEL	fnat	i-RMSD	DEFINITION (i)							DEFINITION (ii)							DEFINITION (iii)												
			TP	FP	TN	FN	P	R	F1	Accuracy	Specificity	TP	FP	TN	FN	P	R	F1	Accuracy	Specificity	TP	FP	TN	FN	P	R	F1	Accuracy	Specificity
X-Ray	1.00	0.00	0	2	12	0	0.00	0.00	0.00	0.86	0.86	2	4	12	0	0.33	1.00	0.50	0.78	0.75	3	4	5	0	0.43	1.00	0.60	0.67	0.56
complexfit_62	0.23	2.80	0	1	15	0	0.00	0.00	0.00	0.94	0.94	1	1	15	1	0.50	0.50	0.50	0.89	0.94	1	0	8	1	1.00	0.50	0.67	0.90	1.00
complexfit_91	0.21	2.91	0	0	14	0	0.00	0.00	0.00	1.00	1.00	2	2	14	0	0.50	1.00	0.67	0.89	0.88	3	2	6	0	0.60	1.00	0.75	0.82	0.75
complexfit_2	0.28	3.20	0	0	15	0	0.00	0.00	0.00	1.00	1.00	2	1	15	0	0.67	1.00	0.80	0.94	0.94	2	1	5	0	0.67	1.00	0.80	0.88	0.83
complexfit_14	0.23	3.36	0	0	14	0	0.00	0.00	0.00	1.00	1.00	1	2	14	1	0.33	0.50	0.40	0.83	0.88	1	1	6	0	0.50	1.00	0.67	0.88	0.86
complexfit_10	0.30	3.45	0	0	16	0	0.00	0.00	0.00	1.00	1.00	2	0	16	0	1.00	1.00	1.00	1.00	1.00	2	0	9	0	1.00	1.00	1.00	1.00	1.00
complexfit_12	0.26	3.50	0	0	15	0	0.00	0.00	0.00	1.00	1.00	1	1	15	1	0.50	0.50	0.50	0.89	0.94	1	3	4	2	0.25	0.33	0.29	0.50	0.57
complexfit_4	0.28	3.53	0	0	13	0	0.00	0.00	0.00	1.00	1.00	1	3	13	1	0.25	0.50	0.33	0.78	0.81	2	2	5	0	0.50	1.00	0.67	0.78	0.71
complexfit_7	0.33	3.64	0	0	15	0	0.00	0.00	0.00	1.00	1.00	2	1	15	0	0.67	1.00	0.80	0.94	0.94	2	1	6	1	0.67	0.67	0.67	0.80	0.86
complexfit_15	0.35	3.76	0	0	14	0	0.00	0.00	0.00	1.00	1.00	2	2	14	0	0.50	1.00	0.67	0.89	0.88	2	3	4	0	0.40	1.00	0.57	0.67	0.57
complexfit_1	0.30	3.97	0	0	16	0	0.00	0.00	0.00	1.00	1.00	1	0	16	1	1.00	0.50	0.67	0.94	1.00	2	0	8	1	1.00	0.67	0.80	0.91	1.00
complexfit_11	0.30	3.98	0	0	14	0	0.00	0.00	0.00	1.00	1.00	2	2	14	0	0.50	1.00	0.67	0.89	0.88	3	2	4	0	0.60	1.00	0.75	0.78	0.67
complexfit_8	0.28	4.02	0	0	16	0	0.00	0.00	0.00	1.00	1.00	1	0	16	1	1.00	0.50	0.67	0.94	1.00	1	1	11	2	0.50	0.33	0.40	0.80	0.92
complexfit_16	0.28	4.05	0	0	14	0	0.00	0.00	0.00	1.00	1.00	2	2	14	0	0.50	1.00	0.67	0.89	0.88	2	1	8	1	0.67	0.67	0.67	0.83	0.89
complexfit_9	0.28	4.17	0	0	16	0	0.00	0.00	0.00	1.00	1.00	1	0	16	1	1.00	0.50	0.67	0.94	1.00	1	1	10	1	0.50	0.50	0.50	0.85	0.91
complexfit_6	0.28	4.27	0	0	14	0	0.00	0.00	0.00	1.00	1.00	2	2	14	0	0.50	1.00	0.67	0.89	0.88	2	3	5	1	0.40	0.67	0.50	0.64	0.63
complexfit_5	0.19	5.15	0	0	14	0	0.00	0.00	0.00	1.00	1.00	2	2	14	0	0.50	1.00	0.67	0.89	0.88	2	3	7	0	0.40	1.00	0.57	0.75	0.70
complexfit_17	0.19	5.24	0	0	14	0	0.00	0.00	0.00	1.00	1.00	1	2	14	1	0.33	0.50	0.40	0.83	0.88	1	2	7	0	0.33	1.00	0.50	0.80	0.78
complexfit_3	0.16	6.52	0	2	12	0	0.00	0.00	0.00	0.86	0.86	1	4	12	1	0.20	0.50	0.29	0.72	0.75	1	4	4	1	0.20	0.50	0.29	0.50	0.50
complexfit_13	0.07	7.76	0	0	12	0	0.00	0.00	0.00	1.00	1.00	1	4	12	1	0.20	0.50	0.29	0.72	0.75	1	4	5	1	0.20	0.50	0.29	0.55	0.56
complexfit_19	0.12	10.18	0	1	13	0	0.00	0.00	0.00	0.93	0.93	0	3	13	2	0.00	0.00	0.00	0.72	0.81	0	3	7	2	0.00	0.00	0.00	0.58	0.70

1BRS B-B MODEL	fnat	i-RMSD	DEFINITION (i)							DEFINITION (ii)							DEFINITION (iii)												
			TP	FP	TN	FN	P	R	F1	Accuracy	Specificity	TP	FP	TN	FN	P	R	F1	Accuracy	Specificity	TP	FP	TN	FN	P	R	F1	Accuracy	Specificity
X-Ray	1.00	0.00	5	0	4	1	1.00	0.83	0.91	0.90	1.00	6	1	4	3	0.86	0.67	0.75	0.71	0.80	6	1	1	2	0.86	0.75	0.80	0.70	0.50
complexfit_5	0.89	0.70	6	0	4	0	1.00	1.00	1.00	1.00	1.00	7	1	4	2	0.88	0.78	0.82	0.79	0.80	7	1	1	2	0.88	0.78	0.82	0.73	0.50
complexfit_4	0.96	0.73	6	0	3	0	1.00	1.00	1.00	1.00	1.00	7	2	3	2	0.78	0.78	0.78	0.71	0.60	8	1	1	2	0.89	0.80	0.84	0.75	0.50
complexfit_2	0.91	0.74	6	0	2	0	1.00	1.00	1.00	1.00	1.00	7	3	2	2	0.70	0.78	0.74	0.64	0.40	8	1	1	0	0.89	1.00	0.94	0.90	0.50
complexfit_3	0.91	0.80	6	0	4	0	1.00	1.00	1.00	1.00	1.00	7	1	4	2	0.88	0.78	0.82	0.79	0.80	8	1	1	2	0.89	0.80	0.84	0.75	0.50
complexfit_1	0.87	1.01	6	0	2	0	1.00	1.00	1.00	1.00	1.00	8	3	2	1	0.73	0.89	0.80	0.71	0.40	9	1	1	1	0.90	0.90	0.90	0.83	0.50
complexfit_13	0.78	1.02	6	0	3	0	1.00	1.00	1.00	1.00	1.00	7	2	3	2	0.78	0.78	0.78	0.71	0.60	8	1	1	2	0.89	0.80	0.84	0.75	0.50
complexfit_9	0.85	1.03	5	0	1	1	1.00	0.83	0.91	0.86	1.00	6	4	1	3	0.60	0.67	0.63	0.50	0.20	8	1	1	2	0.89	0.80	0.84	0.75	0.50
complexfit_17	0.76	1.07	6	0	2	0	1.00	1.00	1.00	1.00	1.00	7	3	2	2	0.70	0.78	0.74	0.64	0.40	8	1	1	2	0.89	0.80	0.84	0.75	0.50
complexfit_52	0.39	2.06	4	0	5	1	1.00	0.80	0.89	0.90	1.00	6	0	5	3	1.00	0.67	0.80	0.79	1.00	7	0	2	2	1.00	0.78	0.88	0.82	1.00
complexfit_57	0.39	2.12	1	0	5	1	1.00	0.50	0.67	0.86	1.00	6	0	5	3	1.00	0.67	0.80	0.79	1.00	6	0	2	4	1.00	0.60	0.75	0.67	1.00
complexfit_59	0.52	2.41	3	0	3	2	1.00	0.60	0.75	0.75	1.00	4	2	3	5	0.67	0.44	0.53	0.50	0.60	4	0	2	4	1.00	0.50	0.67	0.60	1.00
complexfit_67	0.33	2.57	1	0	5	2	1.00	0.33	0.50	0.75	1.00	5	0	5	4	1.00	0.56	0.71	0.71	1.00	5	0	2	2	1.00	0.71	0.83	0.78	1.00
complexfit_87	0.24	3.64	2	0	5	1	1.00	0.67	0.80	0.88	1.00	6	0	5	3	1.00	0.67	0.80	0.79	1.00	6	0	2	1	1.00	0.86	0.92	0.89	1.00
complexfit_88	0.22	3.71	2	0	5	3	1.00	0.40	0.57	0.70	1.00	4	0	5	5	1.00	0.44	0.62	0.64	1.00	4	0	2	2	1.00	0.67	0.80	0.75	1.00
complexfit_80	0.33	3.77	2	0	5	2	1.00	0.50	0.67	0.78	1.00	5	0	5	4	1.00	0.56	0.71	0.71	1.00	6	0	2	3	1.00	0.67	0.80	0.73	1.00
complexfit_62	0.26	3.91	3	0	4	2	1.00	0.60	0.75	0.78	1.00	5	0	4	4	0.83	0.56	0.67	0.64	0.80	5	0	2	3	1.00	0.63	0.77	0.70	1.00
complexfit_37	0.09	8.05	3	0	5	0	1.00	1.00	1.00	1.00	1.00	7	0	5	2	1.00	0.78	0.88	0.86	1.00	7	0	1	1	1.00	0.88	0.93	0.89	1.00
complexfit_55	0.04	8.11	1	0	4	1	1.00	0.50	0.67	0.83	1.00	6	1	4	3	0.86	0.67	0.75	0.71	0.80	7	0	1	1	1.00	0.88	0.93	0.89	1.00
complexfit_47	0.02	9.34	4	0	4	1	1.00	0.80	0.89	0.89	1.00	6	1	4	3	0.86	0.67	0.75	0.71	0.80	7	1	0	1	0.88	0.88	0.88	0.78	0.00
complexfit_43	0.04	9.45	3	0	4	2	1.00	0.60	0.75	0.78	1.00	6	1	4	3	0.86	0.67	0.75	0.71	0.80	6	1	1	1	0.86	0.86	0.86	0.78	0.50

1EMV B-B MODEL	fnat	i-RMSD	DEFINITION (i)							DEFINITION (ii)							DEFINITION (iii)												
			TP	FP	TN	FN	P	R	F1	Accuracy	Specificity	TP	FP	TN	FN	P	R	F1	Accuracy	Specificity	TP	FP	TN	FN	P	R	F1	Accuracy	Specificity
X-Ray	1.00	0.00	1	2	17	0	0.33	1.00	0.50	0.90	0.89	4	2	17	2	0.67	0.67	0.67	0.84	0.89	5	2	4	2	0.71	0.71	0.71	0.69	0.67
complexfit_6	0.85	0.63	2	1	18	0	0.67	1.00	0.80	0.95	0.95	3	1	18	3	0.75	0.50	0.60	0.84	0.95	4	0	6	0	1.00	1.00	1.00	1.00	1.00
complexfit_8	0.93	0.68	2	1	17	0	0.67	1.00	0.80	0.95	0.94	3	2	17	3	0.60	0.50	0.55	0.80	0.89	5	2	3	1	0.71	0.83	0.77	0.73	0.60
complexfit_2	0.96	0.70	2	2	16	0	0.50	1.00	0.67	0.90	0.89	4	3	16	2	0.57	0.67	0.62	0.80	0.84	6	2	4	1	0.75	0.86	0.80	0.77	0.67
complexfit_7	0.87	0.76	1	1	16	0	0.50	1.00	0.67	0.94	0.94	6	3	16	0	0.67	1.00	0.80	0.88	0.84	7	1	3	0					

1FQ9 B:B		DEFINITION (i)										DEFINITION (ii)						DEFINITION (iii)											
MODEL	fnat	i-RMSD	TP	FP	TN	FN	P	R	F1	Accuracy	Specificity	TP	FP	TN	FN	P	R	F1	Accuracy	Specificity	TP	FP	TN	FN	P	R	F1	Accuracy	Specificity
X-Ray	1.00	0.00	1	0	12	0	1.00	1.00	1.00	1.00	1.00	4	2	12	0	0.67	1.00	0.80	0.89	0.86	4	0	4	0	1.00	1.00	1.00	1.00	1.00
complexfit_35	0.35	2.73	0	0	13	0	0.00	0.00	0.00	1.00	1.00	1	1	13	3	0.50	0.25	0.33	0.78	0.93	1	1	7	3	0.50	0.25	0.33	0.67	0.88
complexfit_118	0.12	3.32	0	0	12	1	0.00	0.00	0.00	0.92	1.00	2	2	12	2	0.50	0.50	0.50	0.78	0.86	2	0	4	1	1.00	0.67	0.80	0.86	1.00
complexfit_30	0.19	3.32	0	0	14	1	0.00	0.00	0.00	0.93	1.00	1	0	14	3	1.00	0.25	0.40	0.83	1.00	1	0	8	2	1.00	0.33	0.50	0.82	1.00
complexfit_124	0.35	3.34	0	0	14	1	0.00	0.00	0.00	0.93	1.00	1	0	14	3	1.00	0.25	0.40	0.83	1.00	2	0	5	1	1.00	0.67	0.80	0.88	1.00
complexfit_42	0.35	3.47	0	0	11	0	0.00	0.00	0.00	1.00	1.00	2	3	11	2	0.40	0.50	0.44	0.72	0.79	3	2	6	1	0.60	0.75	0.67	0.75	0.75
complexfit_40	0.26	3.55	0	0	14	1	0.00	0.00	0.00	0.93	1.00	0	0	14	4	0.00	0.00	0.00	0.78	1.00	0	0	8	1	0.00	0.00	0.00	0.89	1.00
complexfit_22	0.27	3.65	0	0	14	1	0.00	0.00	0.00	0.93	1.00	0	0	14	4	0.00	0.00	0.00	0.78	1.00	0	0	7	2	0.00	0.00	0.00	0.78	1.00
complexfit_79	0.23	3.66	0	0	14	1	0.00	0.00	0.00	0.93	1.00	0	0	14	4	0.00	0.00	0.00	0.78	1.00	1	0	8	1	1.00	0.50	0.67	0.90	1.00
complexfit_51	0.09	3.84	0	0	14	1	0.00	0.00	0.00	0.93	1.00	2	0	14	2	1.00	0.50	0.67	0.89	1.00	3	0	8	0	1.00	1.00	1.00	1.00	1.00
complexfit_69	0.06	3.89	0	0	14	1	0.00	0.00	0.00	0.93	1.00	2	0	14	2	1.00	0.50	0.67	0.89	1.00	3	0	6	0	1.00	1.00	1.00	1.00	1.00
complexfit_75	0.27	3.89	0	0	13	1	0.00	0.00	0.00	0.93	1.00	0	1	13	4	0.00	0.00	0.00	0.72	0.93	2	1	7	1	0.67	0.67	0.67	0.82	0.88
complexfit_7	0.09	4.00	0	0	14	0	0.00	0.00	0.00	1.00	1.00	2	0	14	2	1.00	0.50	0.67	0.89	1.00	3	0	8	0	1.00	1.00	1.00	1.00	1.00
complexfit_9	0.18	4.33	0	0	13	1	0.00	0.00	0.00	0.93	1.00	0	1	13	4	0.00	0.00	0.00	0.72	0.93	1	0	7	1	1.00	0.50	0.67	0.89	1.00
complexfit_4	0.08	7.23	0	0	13	0	0.00	0.00	0.00	1.00	1.00	2	1	13	2	0.67	0.50	0.57	0.83	0.93	3	0	7	0	1.00	1.00	1.00	1.00	1.00
complexfit_6	0.09	8.08	0	0	13	1	0.00	0.00	0.00	0.93	1.00	0	1	13	4	0.00	0.00	0.00	0.72	0.93	1	1	7	3	0.50	0.25	0.33	0.67	0.88
complexfit_5	0.09	10.27	0	0	14	1	0.00	0.00	0.00	0.93	1.00	0	0	14	4	0.00	0.00	0.00	0.78	1.00	1	1	7	3	0.50	0.25	0.33	0.67	0.88
complexfit_2	0.06	11.93	0	1	12	1	0.00	0.00	0.00	0.86	0.92	1	2	12	3	0.33	0.25	0.29	0.72	0.86	1	1	5	1	0.50	0.50	0.50	0.75	0.83
complexfit_1	0.05	13.98	0	0	13	1	0.00	0.00	0.00	0.93	1.00	1	1	13	3	0.50	0.25	0.33	0.78	0.93	1	0	8	0	1.00	1.00	1.00	1.00	1.00
complexfit_3	0.05	14.16	0	0	14	1	0.00	0.00	0.00	0.93	1.00	2	0	14	2	1.00	0.50	0.67	0.89	1.00	2	0	7	1	1.00	0.67	0.80	0.90	1.00
complexfit_8	0.03	14.46	0	0	14	1	0.00	0.00	0.00	0.93	1.00	0	0	14	4	0.00	0.00	0.00	0.78	1.00	1	0	8	2	1.00	0.33	0.50	0.82	1.00

1VFB B:B		DEFINITION (i)										DEFINITION (ii)						DEFINITION (iii)											
MODEL	fnat	i-RMSD	TP	FP	TN	FN	P	R	F1	Accuracy	Specificity	TP	FP	TN	FN	P	R	F1	Accuracy	Specificity	TP	FP	TN	FN	P	R	F1	Accuracy	Specificity
X-Ray	1.00	0.00	1	4	13	0	0.20	1.00	0.33	0.78	0.76	3	11	13	0	0.21	1.00	0.35	0.59	0.54	5	2	5	0	0.71	1.00	0.83	0.83	0.71
complexfit_2	0.90	0.53	1	3	11	0	0.25	1.00	0.40	0.80	0.79	3	14	11	0	0.18	1.00	0.30	0.50	0.44	6	3	5	0	0.67	1.00	0.80	0.79	0.63
complexfit_8	0.87	0.54	1	1	16	0	0.50	1.00	0.67	0.94	0.94	3	9	16	0	0.25	1.00	0.40	0.68	0.64	6	4	4	0	0.60	1.00	0.75	0.71	0.50
complexfit_13	0.85	0.54	1	3	13	0	0.25	1.00	0.40	0.82	0.81	3	12	13	0	0.20	1.00	0.33	0.57	0.52	6	3	4	0	0.67	1.00	0.80	0.77	0.57
complexfit_17	0.79	0.61	1	2	13	0	0.33	1.00	0.50	0.88	0.87	3	12	13	0	0.20	1.00	0.33	0.57	0.52	6	4	0	0	0.60	1.00	0.75	0.60	0.00
complexfit_3	0.90	0.73	1	2	17	0	0.33	1.00	0.50	0.90	0.89	3	8	17	0	0.27	1.00	0.43	0.71	0.68	6	2	5	0	0.75	1.00	0.86	0.85	0.71
complexfit_15	0.74	0.81	1	0	15	0	1.00	1.00	1.00	1.00	1.00	3	10	15	0	0.23	1.00	0.38	0.64	0.60	5	4	3	1	0.56	0.83	0.67	0.62	0.43
complexfit_1	0.92	0.88	1	2	11	0	0.33	1.00	0.50	0.86	0.85	3	14	11	0	0.18	1.00	0.30	0.50	0.44	6	4	2	0	0.60	1.00	0.75	0.67	0.33
complexfit_127	0.33	3.08	0	0	20	0	0.00	0.00	0.00	1.00	1.00	2	5	20	1	0.29	0.67	0.40	0.79	0.80	6	1	5	0	0.86	1.00	0.92	0.92	0.83
complexfit_70	0.15	3.62	1	2	20	0	0.33	1.00	0.50	0.91	0.91	3	5	20	0	0.38	1.00	0.55	0.82	0.80	4	1	2	0	0.80	1.00	0.89	0.86	0.67
complexfit_98	0.21	3.65	1	2	22	0	0.33	1.00	0.50	0.92	0.92	3	3	22	0	0.50	1.00	0.67	0.89	0.88	5	1	4	1	0.83	0.83	0.83	0.82	0.80
complexfit_53	0.15	3.71	0	4	16	0	0.00	0.00	0.00	0.80	0.80	3	9	16	0	0.25	1.00	0.40	0.68	0.64	6	4	1	0	0.60	1.00	0.75	0.64	0.20
complexfit_121	0.15	3.78	0	1	21	0	0.00	0.00	0.00	0.95	0.95	3	3	21	0	0.50	1.00	0.67	0.89	0.88	5	0	5	0	1.00	1.00	1.00	1.00	1.00
complexfit_148	0.13	3.91	1	2	18	0	0.33	1.00	0.50	0.90	0.90	3	7	18	0	0.30	1.00	0.46	0.75	0.72	5	3	5	1	0.63	0.83	0.71	0.71	0.63
complexfit_44	0.13	3.99	0	2	21	1	0.00	0.00	0.00	0.88	0.91	2	4	21	1	0.33	0.67	0.44	0.82	0.84	4	3	5	1	0.57	0.80	0.67	0.69	0.63
complexfit_10	0.18	5.29	0	1	21	0	0.00	0.00	0.00	0.95	0.95	3	4	21	0	0.43	1.00	0.60	0.86	0.84	5	0	4	1	1.00	0.83	0.91	0.90	1.00
complexfit_6	0.00	7.10	0	2	18	0	0.00	0.00	0.00	0.90	0.90	1	7	18	2	0.13	0.33	0.18	0.68	0.72	4	2	6	1	0.67	0.80	0.73	0.77	0.75
complexfit_5	0.08	9.54	1	1	15	0	0.50	1.00	0.67	0.94	0.94	3	10	15	0	0.23	1.00	0.38	0.64	0.60	6	4	2	0	0.60	1.00	0.75	0.67	0.33
complexfit_7	0.10	9.55	0	1	19	0	0.00	0.00	0.00	0.95	0.95	3	6	19	0	0.33	1.00	0.50	0.79	0.76	5	0	7	0	1.00	1.00	1.00	1.00	1.00
complexfit_4	0.08	10.93	1	2	19	0	0.33	1.00	0.50	0.91	0.90	3	6	19	0	0.33	1.00	0.50	0.79	0.76	6	5	3	0	0.55	1.00	0.71	0.64	0.38
complexfit_9	0.00	11.20	0	1	21	0	0.00	0.00	0.00	0.95	0.95	2	4	21	1	0.33	0.67	0.44	0.82	0.84	4	0	8	1	1.00	0.80	0.89	0.92	1.00

1F47 B:B		DEFINITION (i)										DEFINITION (ii)						DEFINITION (iii)											
MODEL	fnat	i-RMSD	TP	FP	TN	FN	P	R	F1	Accuracy	Specificity	TP	FP	TN	FN	P	R	F1	Accuracy	Specificity	TP	FP	TN	FN	P	R	F1	Accuracy	Specificity
X-Ray	1.00	0.00	0	0	5	0	0.00	0.00	0.00	1.00	1.00	3	1	5	0	0.75	1.00	0.86	0.89	0.83	3	0	0	1	1.00	0.75	0.86	0.75	0.00
complexfit_10	0.74	1.75	0	2	4	0	0.00	0.00	0.00	0.67	0.67	3	2	4	0	0.60	1.00	0.75	0.78	0.67	3	1	0	1	0.75	0.75	0.75	0.60	0.00
complexfit_12	0.77	1.78	0	1	4	0	0.00	0.00	0.00	0.80	0.80	3	2	4	0	0.60	1.00	0.75	0.78	0.67	3	1	0	1	0.75	0.75	0.75	0.60	0.00
complexfit_4	0.79	1.83	0	0	4	0	0.00	0.00	0.00	1.00	1.00	3	2	4	0	0.60	1.00	0.75	0.78	0.67	3	1	0	1	0.75	0.75	0.75	0.60	0.00
complexfit_6	0.82	1.90	0	1	4	0	0.00	0.00	0.00	0.80	0.80	3	2	4	0	0.60	1.00	0.75	0.78	0.67	3	0	0	1	1.00	0.75	0.86	0.75	0.00
complexfit_15	0.79	1.92	0																										

Table S3. Ranking of the 21 poses for each of the 18 complexes considered in this study. The root mean square deviation for the interfacial residues (i-RMSD) of the pose ranked first is shown in bold face and colored red. The X-ray solution is colored green. The left columns show the ranking obtained with the SF_{ASM} scoring function and the columns on the left show the ranking obtained with the SF_{ASM:iA} scoring function. TP correspond to the hot spot residues correctly detected, and defined according to three definitions (residues whose mutation for Ala increases the binding free energy of the complex by (i) > 4 kcal/mol, (ii) >2 kcal/mol, and (iii) >1.5 kcal/mol. The total number of experimental hot spots (no. HS) is also shown. The score of the SFASM:iA scoring function is calculated as the average ranking position of the poses if they are ordered by the ASM results of by the iA results, as explained in the main text.

Docking poses ranked by the SF_{ASM} scoring function

1BRS U:U	n. ^o HS	6	9	10	
	i-RMSD	TP ⁱ	TP ⁱⁱ	TP ⁱⁱⁱ	iA
X-Ray	0.00	1.00	0.78	0.80	1589
complexfit_5	1.80	0.50	0.78	0.80	1453
complexfit_52	1.93	1.00	0.78	0.70	1245
complexfit_3	2.56	0.67	0.78	0.80	1198
complexfit_11	2.27	0.67	0.67	0.60	1210
complexfit_6	2.58	0.50	0.78	0.70	1106
complexfit_8	1.80	0.50	0.67	0.70	1390
complexfit_7	2.26	0.17	0.67	0.60	1249
complexfit_4	2.34	0.67	0.67	0.70	1272
complexfit_12	3.15	0.67	0.67	0.60	1078
complexfit_37	3.06	0.50	0.67	0.60	899
complexfit_1	7.43	0.50	0.67	0.70	1314
complexfit_17	10.78	0.00	0.56	0.70	1119
complexfit_68	3.43	0.33	0.44	0.60	1081
complexfit_10	2.37	0.17	0.44	0.60	1162
complexfit_36	3.93	0.17	0.67	0.60	1024
complexfit_9	10.02	0.33	0.67	0.80	1316
complexfit_94	3.67	0.17	0.44	0.60	956
complexfit_14	10.79	0.00	0.22	0.30	1319
complexfit_69	3.24	0.33	0.56	0.60	623
complexfit_2	10.75	0.17	0.33	0.50	1477

Docking poses ranked by the SF_{ASM:iA} scoring function

1BRS U:U	i-RMSD	Score
X-Ray	0.00	1.0
complexfit_5	1.80	2.5
complexfit_8	1.80	5.5
complexfit_52	1.93	6.5
complexfit_11	2.27	8.0
complexfit_3	2.56	8.0
complexfit_7	2.26	8.5
complexfit_4	2.34	8.5
complexfit_1	7.43	9.5
complexfit_6	2.58	10.0
complexfit_9	10.02	11.5
complexfit_2	10.75	11.5
complexfit_14	10.79	12.0
complexfit_12	3.15	13.0
complexfit_17	10.78	13.5
complexfit_10	2.37	14.0
complexfit_68	3.43	15.0
complexfit_37	3.06	15.5
complexfit_36	3.93	16.5
complexfit_94	3.67	18.0
complexfit_69	3.24	20.5

1DVF U:B	n. ^o HS	5	8	16	
	i-RMSD	TP ⁱ	TP ⁱⁱ	TP ⁱⁱⁱ	iA
complexfit_2	1.13	0.80	1.00	0.81	1611
complexfit_18	0.91	0.80	1.00	0.88	1464
X-ray	0.00	0.80	0.75	0.81	1774
complexfit_5	0.97	0.80	0.75	0.88	1596
complexfit_11	0.95	0.80	0.75	0.81	1705
complexfit_19	0.98	0.80	0.75	0.56	1629
complexfit_56	2.64	0.80	0.75	0.75	1162
complexfit_3	1.10	1.00	0.75	0.88	1579
complexfit_1	1.04	0.80	0.63	0.94	1653
complexfit_4	1.20	0.20	0.50	0.44	1712
complexfit_122	3.82	0.80	0.75	0.81	1429
complexfit_126	2.73	0.60	0.88	0.75	1209
complexfit_39	13.78	0.40	0.38	0.44	1421
complexfit_55	2.99	0.00	0.38	0.38	1502
complexfit_35	13.02	0.20	0.25	0.38	1577
complexfit_120	2.07	0.20	0.38	0.50	1187
complexfit_98	3.79	0.60	0.88	0.88	1281
complexfit_59	12.89	0.20	0.25	0.44	1287
complexfit_64	3.63	0.00	0.13	0.25	1198
complexfit_112	3.18	0.20	0.50	0.69	1013
complexfit_57	12.96	0.40	0.63	0.44	1177

1DVF U:B	i-RMSD	position
X-ray	0.00	2.0
complexfit_2	1.13	3.5
complexfit_11	0.95	4.0
complexfit_19	0.98	5.0
complexfit_5	0.97	5.5
complexfit_4	1.20	6.0
complexfit_18	0.91	6.5
complexfit_1	1.04	6.5
complexfit_3	1.10	8.0
complexfit_122	3.82	11.5
complexfit_55	2.99	12.0
complexfit_35	13.02	12.0
complexfit_56	2.64	12.5
complexfit_39	13.78	13.0
complexfit_126	2.73	14.0
complexfit_98	3.79	16.0
complexfit_59	12.89	16.0
complexfit_120	2.07	17.0
complexfit_64	3.63	18.0
complexfit_57	12.96	20.0
complexfit_112	3.18	20.5

2EKS U:B	n.° HS	3	5	6	
	i-RMSD	TP ^I	TP ^{II}	TP ^{III}	iA
X-Ray	0.00	1.00	0.80	1.00	1865
complexfit_17	7.42	0.00	0.00	0.33	1007
complexfit_3	6.11	0.00	0.20	0.17	1284
complexfit_4	7.80	0.00	0.20	0.50	1261
complexfit_19	7.64	0.33	0.80	0.67	918
complexfit_10	8.60	0.33	0.80	0.83	1259
complexfit_6	8.45	0.00	0.60	0.67	1261
complexfit_1	12.13	0.00	0.40	0.50	1118
complexfit_14	10.28	0.33	0.80	0.67	1177
complexfit_7	13.69	0.33	0.80	0.67	918
complexfit_18	13.36	0.33	0.60	0.67	1007
complexfit_8	7.57	0.33	0.60	0.50	870
complexfit_9	9.53	0.00	0.40	0.50	1284
complexfit_2	12.71	0.00	0.20	0.17	1154
complexfit_11	9.74	0.00	0.60	0.50	1069
complexfit_5	9.53	0.00	0.40	0.67	1372
complexfit_16	7.44	0.33	0.40	0.33	1255
complexfit_12	5.96	0.33	0.60	0.50	853
complexfit_15	9.17	0.00	0.60	0.67	1165
complexfit_13	5.95	0.00	0.60	0.50	993
complexfit_51	3.93	0.00	1.00	0.83	1018

2EKS U:B	i-RMSD	position
X-Ray	0.00	1.0
complexfit_19	7.64	5.0
complexfit_17	7.42	5.5
complexfit_4	7.80	5.5
complexfit_10	8.60	5.5
complexfit_6	8.45	5.5
complexfit_3	6.11	8.0
complexfit_9	9.53	8.0
complexfit_5	9.53	9.0
complexfit_14	10.28	9.5
complexfit_1	12.13	10.5
complexfit_16	7.44	11.0
complexfit_2	12.71	12.5
complexfit_18	13.36	14.0
complexfit_7	13.69	14.5
complexfit_11	9.74	15.0
complexfit_15	9.17	15.0
complexfit_8	7.57	15.5
complexfit_13	5.95	18.5
complexfit_51	3.93	18.5
complexfit_12	5.96	19.5

1VFB U:U	n.° HS	1	4	5	
	i-RMSD	TP ^I	TP ^{II}	TP ^{III}	iA
X-Ray	0.00	1.00	0.75	1.00	1420
complexfit_27	3.55	0.00	0.75	1.00	1034
complexfit_14	3.42	1.00	0.75	0.80	1149
complexfit_33	3.75	0.00	0.50	0.80	1057
complexfit_64	2.24	1.00	0.75	0.60	1044
complexfit_9	2.42	0.00	0.75	0.80	1213
complexfit_7	4.52	0.00	0.50	1.00	1254
complexfit_6	4.42	1.00	0.75	0.80	1104
complexfit_58	1.80	0.00	0.75	0.80	1032
complexfit_8	9.75	0.00	0.75	0.80	943
complexfit_11	7.39	1.00	0.75	1.00	939
complexfit_2	4.49	0.00	0.75	0.80	1263
complexfit_4	3.57	1.00	0.50	0.60	1262
complexfit_36	3.10	0.00	0.75	1.00	1053
complexfit_5	6.96	0.00	0.75	0.80	1021
complexfit_10	3.70	1.00	0.50	1.00	1009
complexfit_3	4.96	1.00	0.75	0.80	1000
complexfit_21	3.51	0.00	0.75	0.80	930
complexfit_12	9.03	0.00	0.75	0.80	865
complexfit_1	3.32	0.00	0.75	0.80	1134
complexfit_49	2.36	0.00	0.75	1.00	1053

1VFB U:U	i-RMSD	position
X-Ray	0.00	1.0
complexfit_14	3.42	4.5
complexfit_9	2.42	5.5
complexfit_7	4.52	5.5
complexfit_33	3.75	6.0
complexfit_27	3.55	7.0
complexfit_64	2.24	7.5
complexfit_2	4.49	7.0
complexfit_4	3.57	7.5
complexfit_6	4.42	8.0
complexfit_58	1.80	11.5
complexfit_36	3.10	11.5
complexfit_5	6.96	13.5
complexfit_1	3.32	13.5
complexfit_8	9.75	13.5
complexfit_11	7.39	14.0
complexfit_10	3.70	14.0
complexfit_3	4.96	14.5
complexfit_49	2.36	15.5
complexfit_21	3.51	16.0
complexfit_12	9.03	16.5

1DFJ U:U	n.° HS	1	4	5	
	i-RMSD	TP ^I	TP ^{II}	TP ^{III}	iA
X-Ray	0.00	1.00	1.00	0.80	2760
complexfit_7	4.10	0.00	1.00	0.80	1866
complexfit_13	4.33	1.00	0.75	0.80	1849
complexfit_49	3.90	1.00	0.75	0.60	1883
complexfit_17	3.90	0.00	0.75	0.60	2050
complexfit_6	4.52	0.00	0.50	0.60	1783
complexfit_8	3.97	0.00	1.00	1.00	1781
complexfit_1	4.49	0.00	0.75	0.80	1674
complexfit_12	4.48	1.00	0.75	0.60	1650
complexfit_67	3.96	0.00	0.75	0.60	1648
complexfit_18	3.84	0.00	0.50	0.60	1914
complexfit_2	16.88	1.00	1.00	0.80	1828
complexfit_5	4.36	1.00	1.00	0.80	2066
complexfit_63	3.93	0.00	0.75	0.80	1601
complexfit_4	3.97	1.00	0.50	0.40	1980
complexfit_61	3.96	1.00	0.75	0.60	1681
complexfit_9	3.93	0.00	0.50	0.40	1962
complexfit_3	6.11	1.00	0.75	0.60	1750
complexfit_10	4.16	0.00	0.50	0.40	1648
complexfit_11	5.64	0.00	0.50	0.60	1659
complexfit_14	4.66	0.00	1.00	0.80	1415

1DFJ U:U	i-RMSD	position
X-Ray	0.00	1.0
complexfit_17	3.90	4.0
complexfit_7	4.10	4.5
complexfit_13	4.33	5.0
complexfit_49	3.90	5.5
complexfit_5	4.36	7.5
complexfit_6	4.52	8.0
complexfit_8	3.97	8.5
complexfit_18	3.84	8.5
complexfit_4	3.97	9.5
complexfit_1	4.49	10.0
complexfit_2	16.88	10.5
complexfit_9	3.93	11.0
complexfit_12	4.48	13.0
complexfit_67	3.96	14.5
complexfit_61	3.96	14.5
complexfit_3	6.11	15.0
complexfit_63	3.93	16.5
complexfit_10	4.16	17.5
complexfit_11	5.64	18.0
complexfit_14	4.66	20.5

1FCC U:B	n.º HS	1	4	5	
	i-RMSD	TP ^I	TP ^{II}	TP ^{III}	iA
X-Ray	0.00	1.00	0.75	0.60	1436
complexfit_4	0.88	1.00	0.50	0.40	1325
complexfit_1	1.21	1.00	0.50	0.40	1313
complexfit_20	1.06	1.00	0.75	0.60	1251
complexfit_136	6.96	1.00	0.50	0.40	1181
complexfit_96	2.24	1.00	0.50	0.40	1049
complexfit_193	2.50	1.00	0.50	0.60	653
complexfit_6	1.09	1.00	0.50	0.60	1252
complexfit_5	1.00	1.00	0.75	0.60	1192
complexfit_2	0.91	1.00	0.50	0.40	1524
complexfit_8	0.89	1.00	0.25	0.40	1318
complexfit_7	0.66	1.00	0.50	0.40	1302
complexfit_15	1.13	1.00	0.50	0.40	1269
complexfit_3	0.83	1.00	0.75	0.60	1193
complexfit_101	2.06	1.00	0.75	0.60	1165
complexfit_188	2.20	1.00	0.50	0.80	806
complexfit_197	2.15	1.00	0.75	0.60	613
complexfit_102	15.48	0.00	0.00	0.00	1175
complexfit_194	9.83	0.00	0.00	0.00	684
complexfit_192	9.72	0.00	0.00	0.00	666
complexfit_196	10.00	0.00	0.00	0.00	502

1FCC U:B	i-RMSD	position
X-Ray	0.00	1.5
complexfit_4	0.88	2
complexfit_1	1.21	3
complexfit_20	1.06	5
complexfit_2	0.91	5.5
complexfit_136	6.96	6.5
complexfit_8	0.89	7
complexfit_96	2.24	8
complexfit_6	1.09	8
complexfit_7	0.66	8
complexfit_15	1.13	8.5
complexfit_5	1.00	9.5
complexfit_3	0.83	10
complexfit_101	2.06	12
complexfit_193	2.50	13
complexfit_188	2.20	13
complexfit_102	15.48	15.5
complexfit_194	9.83	17.5
complexfit_192	9.72	18
complexfit_197	2.15	18.5
complexfit_196	10.00	19.5

1FQ9 U:B	n.º HS	1	4	4	
	i-RMSD	TP ^I	TP ^{II}	TP ^{III}	iA
complexfit_2	0.92	1.00	1.00	1.00	2305
complexfit_7	1.15	1.00	1.00	1.00	2262
complexfit_3	0.95	1.00	1.00	1.00	2258
X-Ray	0.00	1.00	1.00	1.00	2222
complexfit_10	0.93	0.00	1.00	1.00	2081
complexfit_13	2.36	0.00	1.00	1.00	1767
complexfit_1	1.11	0.00	1.00	1.00	2379
complexfit_4	1.00	1.00	1.00	1.00	2217
complexfit_5	1.08	0.00	0.75	1.00	2028
complexfit_9	2.05	0.00	1.00	1.00	1897
complexfit_6	1.20	0.00	0.00	0.00	2226
complexfit_59	3.19	1.00	0.75	0.75	1466
complexfit_67	2.91	0.00	0.50	1.00	1397
complexfit_48	4.70	0.00	0.75	0.75	1416
complexfit_94	3.65	0.00	0.50	0.50	1296
complexfit_27	11.19	0.00	0.00	0.25	1643
complexfit_89	3.93	0.00	0.25	0.25	1295
complexfit_38	12.37	0.00	0.50	0.75	1513
complexfit_80	3.82	0.00	0.00	0.00	1338
complexfit_43	7.02	0.00	0.25	0.25	1732
complexfit_53	2.24	0.00	0.00	0.25	1485

1FQ9 U:B	i-RMSD	position
complexfit_2	0.92	1.5
complexfit_7	1.15	2.0
complexfit_3	0.95	2.5
X-Ray	0.00	3.5
complexfit_1	1.11	4.0
complexfit_10	0.93	4.5
complexfit_4	1.00	7.0
complexfit_5	1.08	8.0
complexfit_6	1.20	8.0
complexfit_13	2.36	8.5
complexfit_9	2.05	8.5
complexfit_59	3.19	14.0
complexfit_27	11.19	14.5
complexfit_67	2.91	15.5
complexfit_48	4.70	15.5
complexfit_38	12.37	16.0
complexfit_43	7.02	16.0
complexfit_94	3.65	17.5
complexfit_89	3.93	18.5
complexfit_80	3.82	18.5
complexfit_53	2.24	17.5

1FLT U:U	n.º HS	0	4	5	
	i-RMSD	TP ^I	TP ^{II}	TP ^{III}	iA
complexfit_14	1.85	NA	0.75	0.80	1475
complexfit_43	12.62	NA	0.50	0.60	1530
X-Ray	0.00	NA	0.25	0.80	1851
complexfit_3	2.82	NA	1.00	1.00	1573
complexfit_32	3.01	NA	0.25	0.80	1508
complexfit_53	12.41	NA	0.50	0.60	1494
complexfit_5	2.89	NA	0.75	0.80	1573
complexfit_54	12.55	NA	0.25	0.40	1439
complexfit_45	3.20	NA	0.50	0.80	1436
complexfit_1	1.65	NA	0.25	0.40	1664
complexfit_48	10.75	NA	0.50	0.60	1549
complexfit_15	1.88	NA	0.00	0.40	1540
complexfit_49	10.86	NA	0.50	0.60	1433
complexfit_41	3.09	NA	0.75	0.80	1389
complexfit_52	3.08	NA	0.50	0.80	1305
complexfit_7	1.85	NA	0.25	0.60	1642
complexfit_10	1.76	NA	0.50	0.60	1479
complexfit_36	3.63	NA	0.50	0.60	1485
complexfit_6	2.91	NA	0.50	0.80	1593
complexfit_4	2.92	NA	0.75	0.80	1493
complexfit_2	2.95	NA	0.75	1.00	1536

1FLT U:U	i-RMSD	position
X-Ray	0.00	2
complexfit_3	2.82	4
complexfit_43	12.62	5.5
complexfit_1	1.65	6
complexfit_5	2.89	6.5
complexfit_32	3.01	7
complexfit_53	12.41	7.5
complexfit_14	1.85	8.5
complexfit_48	10.75	8.5
complexfit_15	1.88	9
complexfit_7	1.85	9.5
complexfit_6	2.91	11.5
complexfit_54	12.55	12
complexfit_45	3.20	12.5
complexfit_2	2.95	14
complexfit_49	10.86	14.5
complexfit_41	3.09	15
complexfit_52	3.08	15.5
complexfit_10	1.76	15.5
complexfit_36	3.63	16
complexfit_4	2.92	16

1A22 U:B	n.º HS	0	3	5	
	i-RMSD	TP ^I	TP ^{II}	TP ^{III}	iA
complexfit_76	3.94	NA	0.67	1.00	1440
X-Ray	0.00	NA	0.67	0.60	2691
complexfit_4	16.83	NA	0.67	0.60	1810
complexfit_5	13.98	NA	0.00	0.20	1531
complexfit_60	3.61	NA	0.33	0.60	1122
complexfit_43	3.62	NA	1.00	1.00	999
complexfit_2	12.74	NA	0.33	0.40	1847
complexfit_15	8.62	NA	0.33	0.40	1567
complexfit_12	16.11	NA	0.00	0.60	1364
complexfit_10	15.74	NA	0.33	0.60	1626
complexfit_14	8.66	NA	0.00	0.20	1583
complexfit_13	10.78	NA	0.00	0.80	1169
complexfit_11	15.40	NA	0.33	0.20	1744
complexfit_8	14.05	NA	0.67	0.60	1409
complexfit_7	12.74	NA	0.00	0.60	1178
complexfit_1	15.31	NA	0.33	0.20	1573
complexfit_3	8.76	NA	0.00	0.20	1457
complexfit_16	15.84	NA	0.33	0.40	1450
complexfit_9	15.52	NA	0.33	0.60	1644
complexfit_6	13.44	NA	0.00	0.40	1267
complexfit_63	3.81	NA	0.67	0.60	1092

1A22 U:B	i-RMSD	position
X-Ray	0.0	1.5
complexfit_4	16.8	3.0
complexfit_2	12.7	4.5
complexfit_5	14.0	6.5
complexfit_76	3.9	7.0
complexfit_60	3.6	11.0
complexfit_43	3.6	12.0
complexfit_15	8.6	8.0
complexfit_12	16.1	11.0
complexfit_10	15.7	8.0
complexfit_14	8.7	8.5
complexfit_11	15.4	8.5
complexfit_1	15.3	12.0
complexfit_9	15.5	12.0
complexfit_8	14.1	13.5
complexfit_3	8.8	13.5
complexfit_13	10.8	14.0
complexfit_16	15.8	15.0
complexfit_7	12.7	16.0
complexfit_6	13.4	17.5
complexfit_63	3.8	19.5

1F47 U:B	n.º HS	0	3	4	
	i-RMSD	TP ^I	TP ^{II}	TP ^{III}	iA
X-Ray	0.00	NA	1.00	0.75	1221
complexfit_2	2.35	NA	1.00	0.75	1217
complexfit_13	11.98	NA	1.00	0.75	916
complexfit_16	7.31	NA	0.67	0.75	873
complexfit_195	1.91	NA	0.67	0.75	795
complexfit_7	12.26	NA	0.67	0.50	757
complexfit_6	11.97	NA	1.00	0.75	659
complexfit_5	8.40	NA	0.33	0.25	1007
complexfit_17	8.71	NA	0.33	0.50	983
complexfit_15	13.32	NA	0.33	0.25	966
complexfit_18	11.70	NA	0.67	0.75	930
complexfit_53	2.83	NA	1.00	0.75	962
complexfit_9	12.03	NA	1.00	0.75	840
complexfit_4	11.63	NA	0.33	0.50	1056
complexfit_3	12.14	NA	0.67	0.50	917
complexfit_1	9.26	NA	1.00	0.75	849
complexfit_14	10.34	NA	0.67	0.75	645
complexfit_11	14.16	NA	0.00	0.25	859
complexfit_10	14.27	NA	0.00	0.00	918
complexfit_12	14.56	NA	0.00	0.00	898
complexfit_8	14.82	NA	0.00	0.00	792

1F47 U:B	i-RMSD	position
X-Ray	0.00	1.0
complexfit_2	2.35	1.5
complexfit_13	11.98	6.0
complexfit_5	8.40	6.0
complexfit_17	8.71	6.5
complexfit_16	7.31	7.0
complexfit_15	13.32	7.0
complexfit_18	11.70	8.0
complexfit_4	11.63	8.5
complexfit_195	1.91	9.0
complexfit_53	2.83	9.5
complexfit_7	12.26	10.0
complexfit_6	11.97	10.5
complexfit_3	12.14	12.0
complexfit_9	12.03	14.0
complexfit_10	14.27	14.0
complexfit_1	9.26	15.5
complexfit_12	14.56	15.5
complexfit_11	14.16	16.0
complexfit_14	10.34	18.5
complexfit_8	14.82	18.5

1IAR U:B	n.º HS	0	2	3	
	i-RMSD	TP ^I	TP ^{II}	TP ^{III}	iA
X-Ray	0.00	NA	1.00	1.00	1566
complexfit_11	3.98	NA	0.50	0.33	1135
complexfit_91	2.91	NA	1.00	1.00	1089
complexfit_16	4.05	NA	1.00	0.67	1145
complexfit_15	3.76	NA	1.00	0.67	1132
complexfit_7	3.64	NA	0.50	0.33	1126
complexfit_6	4.27	NA	1.00	0.67	1066
complexfit_5	5.15	NA	0.50	0.33	1042
complexfit_2	3.20	NA	1.00	0.67	1013
complexfit_10	3.45	NA	0.50	0.67	931
complexfit_1	3.97	NA	0.50	0.67	1194
complexfit_4	3.53	NA	1.00	1.00	1144
complexfit_3	6.52	NA	0.50	0.33	1294
complexfit_9	4.17	NA	0.50	0.33	1194
complexfit_12	3.50	NA	1.00	0.67	1148
complexfit_8	4.02	NA	1.00	0.67	1108
complexfit_13	7.76	NA	1.00	0.67	1049
complexfit_17	5.24	NA	0.50	0.33	990
complexfit_14	3.36	NA	0.50	0.33	977
complexfit_62	2.80	NA	0.50	0.33	946
complexfit_19	10.18	NA	0.00	0.00	1234

1IAR U:B	i-RMSD	position
X-Ray	0.00	1
complexfit_11	3.98	5
complexfit_16	4.05	5.5
complexfit_91	2.91	7
complexfit_15	3.76	7
complexfit_7	3.64	7.5
complexfit_3	6.52	7.5
complexfit_1	3.97	8
complexfit_9	4.17	8.5
complexfit_6	4.27	9
complexfit_4	3.53	9.5
complexfit_12	3.50	9.5
complexfit_5	5.15	10
complexfit_2	3.20	10.5
complexfit_19	10.18	12
complexfit_10	3.45	12.5
complexfit_8	4.02	12.5
complexfit_13	7.76	14
complexfit_17	5.24	15.5
complexfit_14	3.36	16
complexfit_62	2.80	16.5

1BRS B:B	n.º HS	6	9	10	
	i-RMSD	TP ⁱ	TP ⁱⁱ	TP ⁱⁱⁱ	iA
complexfit_1	1.01	0.83	0.67	0.60	1718
complexfit_4	0.73	1.00	0.78	0.80	1803
complexfit_3	0.80	1.00	0.78	0.80	1800
complexfit_2	0.74	1.00	0.78	0.70	1724
complexfit_17	1.07	1.00	0.89	0.90	1661
complexfit_13	1.02	1.00	0.78	0.80	1586
complexfit_5	0.70	1.00	0.78	0.80	1750
complexfit_9	1.03	0.83	0.67	0.80	1913
X-Ray	0.00	1.00	0.78	0.80	1647
complexfit_47	9.34	0.67	0.67	0.70	1480
complexfit_52	2.06	0.17	0.67	0.60	1241
complexfit_37	8.05	0.50	0.44	0.40	1520
complexfit_43	9.45	0.17	0.56	0.50	1512
complexfit_62	3.91	0.33	0.67	0.60	1346
complexfit_59	2.41	0.33	0.44	0.40	1459
complexfit_87	3.64	0.33	0.56	0.60	1160
complexfit_80	3.77	0.50	0.56	0.50	1286
complexfit_88	3.71	0.50	0.78	0.70	1273
complexfit_55	8.11	0.17	0.67	0.70	1263
complexfit_57	2.12	0.67	0.67	0.70	1284
complexfit_67	2.57	0.50	0.67	0.60	1480

1BRS B:B	i-RMSD	position
complexfit_4	0.73	2
complexfit_3	0.80	2.5
complexfit_1	1.01	3.5
complexfit_2	0.74	3.5
complexfit_17	1.07	4.5
complexfit_9	1.03	4.5
complexfit_13	1.02	5.5
complexfit_5	0.70	5.5
X-Ray	0.00	8.5
complexfit_47	9.34	11
complexfit_37	8.05	11
complexfit_43	9.45	12
complexfit_62	3.91	14.5
complexfit_59	2.41	14.5
complexfit_52	2.06	15
complexfit_80	3.77	16.5
complexfit_67	2.57	16.5
complexfit_88	3.71	18
complexfit_87	3.64	18.5
complexfit_57	2.12	18.5
complexfit_55	8.11	19

1EMV B:B	n.º HS	2	6	7	
	i-RMSD	TP ⁱ	TP ⁱⁱ	TP ⁱⁱⁱ	iA
complexfit_2	0.70	0.50	0.67	0.71	1775
complexfit_8	0.68	1.00	0.50	0.57	1622
complexfit_6	0.63	1.00	0.50	0.71	1636
complexfit_7	0.76	1.00	0.67	0.86	1685
complexfit_9	0.84	0.50	1.00	1.00	1740
complexfit_124	1.11	0.50	0.83	1.00	1539
complexfit_4	0.95	0.50	0.67	0.86	1776
complexfit_1	0.89	0.50	0.50	0.71	1883
complexfit_132	1.08	0.50	0.83	0.71	1725
X-Ray	0.00	0.50	0.33	0.57	1634
complexfit_108	1.17	0.50	0.33	0.43	1853
complexfit_3	0.90	0.50	0.33	0.29	1750
complexfit_110	1.24	0.00	0.50	0.57	1619
complexfit_5	0.93	0.50	0.67	0.71	1763
complexfit_199	2.86	0.50	0.83	0.86	896
complexfit_21	1.01	0.50	0.67	0.57	1839
complexfit_38	1.04	0.50	0.33	0.29	1786
complexfit_76	1.22	0.50	0.50	0.57	1613
complexfit_198	11.81	0.50	0.33	0.57	1066
complexfit_72	1.04	0.00	0.17	0.29	1703
complexfit_200	3.11	0.50	0.17	0.14	728

1EMV B:B	i-RMSD	position
complexfit_2	0.70	3.5
complexfit_1	0.89	4.5
complexfit_4	0.95	6
complexfit_108	1.17	6.5
complexfit_9	0.84	7
complexfit_6	0.63	8
complexfit_7	0.76	8
complexfit_8	0.68	8.5
complexfit_132	1.08	9.5
complexfit_21	1.01	9.5
complexfit_3	0.90	10
complexfit_5	0.93	10.5
complexfit_38	1.04	10.5
X-Ray	0.00	11.5
complexfit_124	1.11	12
complexfit_110	1.24	14.5
complexfit_72	1.04	15.5
complexfit_199	2.86	17
complexfit_76	1.22	17
complexfit_198	11.81	19
complexfit_200	3.11	21

1DFJ B:B	n.º HS	1	4	5	
	i-RMSD	TP ⁱ	TP ⁱⁱ	TP ⁱⁱⁱ	iA
complexfit_4	0.89	0.00	0.25	0.60	2899
complexfit_10	2.39	0.00	0.25	0.20	2493
complexfit_3	2.57	1.00	0.50	0.60	2133
complexfit_92	3.22	0.00	0.75	0.80	1960
complexfit_6	2.71	0.00	0.25	0.60	2581
complexfit_1	2.63	0.00	0.75	0.80	2317
complexfit_45	3.06	0.00	0.50	0.40	2046
X-Ray	0.00	0.00	0.00	0.20	2821
complexfit_5	2.61	0.00	0.50	0.40	2127
complexfit_75	3.61	0.00	0.25	0.20	1764
complexfit_8	2.91	0.00	0.25	0.20	2104
complexfit_105	3.36	0.00	0.50	0.40	1938
complexfit_87	3.04	0.00	0.25	0.40	1798
complexfit_99	3.12	0.00	0.25	0.40	1699
complexfit_9	2.72	0.00	0.00	0.00	2350
complexfit_11	2.36	0.00	0.00	0.00	2133
complexfit_7	2.77	0.00	0.25	0.40	2073
complexfit_100	3.51	0.00	0.50	0.60	1855
complexfit_2	2.66	0.00	0.25	0.40	2358
complexfit_114	3.14	0.00	0.25	0.60	1841
complexfit_57	3.15	0.00	0.00	0.40	1803

1DFJ B:B	i-RMSD	position
complexfit_4	0.89	1
complexfit_10	2.39	3
complexfit_6	2.71	4
complexfit_3	2.57	5
X-Ray	0.00	5
complexfit_1	2.63	6
complexfit_92	3.22	9
complexfit_45	3.06	9
complexfit_5	2.61	9
complexfit_9	2.72	10.5
complexfit_8	2.91	11
complexfit_11	2.36	11.5
complexfit_2	2.66	12
complexfit_105	3.36	13
complexfit_7	2.77	13.5
complexfit_75	3.61	14
complexfit_87	3.04	15
complexfit_99	3.12	16
complexfit_100	3.51	17
complexfit_114	3.14	18.5
complexfit_57	3.15	19

1FCC B:B	n.º HS	1	4	5	
	i-RMSD	TP ^I	TP ^{II}	TP ^{III}	iA
complexfit_4	1.44	1.00	0.75	0.80	1556
complexfit_2	0.88	1.00	0.50	0.40	1623
X-Ray	0.00	1.00	0.50	0.40	1441
complexfit_6	1.41	1.00	0.50	0.60	1584
complexfit_11	0.82	1.00	0.50	0.80	1575
complexfit_3	1.82	1.00	0.75	0.80	1742
complexfit_8	0.80	1.00	0.50	0.40	1268
complexfit_96	2.05	1.00	0.50	0.40	1161
complexfit_135	2.10	1.00	0.75	0.60	1119
complexfit_5	7.92	1.00	0.50	0.60	1746
complexfit_1	1.12	1.00	0.75	1.00	1542
complexfit_12	0.75	1.00	0.50	0.40	1457
complexfit_17	0.65	1.00	0.50	0.60	1457
complexfit_7	1.02	1.00	0.50	0.60	1422
complexfit_100	2.06	1.00	0.25	0.20	1193
complexfit_167	2.19	1.00	0.25	0.20	940
complexfit_176	2.85	0.00	0.50	0.40	860
complexfit_35	9.71	0.00	0.75	1.00	1631
complexfit_44	4.31	1.00	0.50	0.40	1397
complexfit_21	8.05	0.00	0.50	0.40	1507
complexfit_200	3.48	0.00	1.25	1.00	841

1FCC B:B	i-RMSD	position
complexfit_2	0.88	3
complexfit_4	1.44	4
complexfit_3	1.82	4
complexfit_6	1.41	4.5
complexfit_11	0.82	5.5
complexfit_5	7.92	5.5
X-Ray	0.00	7
complexfit_1	1.12	9
complexfit_12	0.75	10
complexfit_17	0.65	10
complexfit_8	0.80	10.5
complexfit_35	9.71	10.5
complexfit_96	2.05	11.5
complexfit_7	1.02	11.5
complexfit_135	2.10	12
complexfit_100	2.06	13
complexfit_21	8.05	14.5
complexfit_44	4.31	16.5
complexfit_167	2.19	17.5
complexfit_176	2.85	18
complexfit_200	3.48	20.5

1FQ9 B:B	n.º HS	1	4	4	
	i-RMSD	TP ^I	TP ^{II}	TP ^{III}	iA
X-Ray	0.00	1.00	1.00	1.00	2456
complexfit_42	3.47	0.00	0.25	0.25	1878
complexfit_4	7.23	0.00	0.25	0.25	1495
complexfit_7	4.00	0.00	0.50	0.50	1480
complexfit_51	3.84	0.00	0.25	0.50	1384
complexfit_69	3.89	0.00	0.50	0.75	1103
complexfit_3	14.16	0.00	0.00	0.00	1824
complexfit_118	3.32	0.00	0.00	0.00	1189
complexfit_124	3.34	0.00	0.00	0.25	1803
complexfit_1	13.98	0.00	0.50	0.75	1894
complexfit_35	2.73	0.00	0.50	0.75	1814
complexfit_2	11.93	0.00	0.50	0.75	1710
complexfit_30	3.32	0.00	0.00	0.50	1344
complexfit_75	3.89	0.00	0.00	0.25	1596
complexfit_9	4.33	0.00	0.25	0.25	1646
complexfit_5	10.27	0.00	0.50	0.75	1599
complexfit_8	14.46	0.00	0.00	0.25	1544
complexfit_79	3.66	0.00	0.25	0.25	1497
complexfit_6	8.08	0.00	0.00	0.25	1482
complexfit_22	3.65	0.00	0.50	0.50	1610
complexfit_40	3.55	0.00	0.00	0.25	1528

1FQ9 B:B	i-RMSD	position
X-Ray	0.00	1
complexfit_42	3.47	2.5
complexfit_3	14.16	5.5
complexfit_1	13.98	6
complexfit_124	3.34	7.5
complexfit_35	2.73	7.5
complexfit_4	7.23	8.5
complexfit_2	11.93	8.5
complexfit_7	4.00	9.5
complexfit_51	3.84	10
complexfit_69	3.89	11.5
complexfit_9	4.33	11.5
complexfit_75	3.89	12.5
complexfit_5	10.27	12.5
complexfit_118	3.32	13.5
complexfit_8	14.46	13.5
complexfit_30	3.32	14.5
complexfit_79	3.66	14.5
complexfit_22	3.65	14.5
complexfit_6	8.08	15.5
complexfit_40	3.55	16.5

1VFB B:B	n.º HS	1	3	6	
	i-RMSD	TP ^I	TP ^{II}	TP ^{III}	iA
complexfit_1	0.88	1.00	1.00	0.83	1627
complexfit_3	0.73	1.00	1.00	1.00	1478
complexfit_2	0.53	1.00	1.00	1.00	1449
complexfit_8	0.54	1.00	1.00	1.00	1392
complexfit_17	0.61	1.00	1.00	1.00	1377
complexfit_13	0.54	1.00	1.00	0.83	1366
complexfit_4	10.93	1.00	1.00	1.00	1296
complexfit_5	9.54	1.00	1.00	1.00	1032
X-Ray	0.00	0.00	1.00	1.00	1400
complexfit_15	0.81	0.00	0.67	1.00	1201
complexfit_98	3.65	1.00	1.00	0.67	1036
complexfit_148	3.91	1.00	1.00	0.83	876
complexfit_70	3.62	0.00	1.00	0.83	927
complexfit_53	3.71	1.00	1.00	0.83	1018
complexfit_10	5.29	0.00	1.00	0.83	1179
complexfit_7	9.55	0.00	0.67	0.67	1106
complexfit_121	3.78	0.00	0.33	0.67	1079
complexfit_127	3.08	1.00	1.00	1.00	650
complexfit_44	3.99	1.00	1.00	1.00	1006
complexfit_9	11.20	0.00	1.00	0.83	951
complexfit_6	7.10	0.00	0.67	0.67	1072

1VFB B:B	i-RMSD	position
complexfit_1	0.88	1
complexfit_3	0.73	1.5
complexfit_2	0.53	2
complexfit_8	0.54	3
complexfit_17	0.61	3.5
complexfit_13	0.54	4
complexfit_4	10.93	4.5
X-Ray	0.00	6.5
complexfit_5	9.54	8
complexfit_15	0.81	9
complexfit_98	3.65	11.5
complexfit_10	5.29	12.5
complexfit_7	9.55	13
complexfit_121	3.78	13.5
complexfit_148	3.91	14.5
complexfit_53	3.71	15
complexfit_70	3.62	16
complexfit_6	7.10	17
complexfit_44	3.99	18
complexfit_9	11.20	18.5
complexfit_127	3.08	19.5

1F47 B:B	n.º HS	0	3	4	
	i-RMSD	TP ⁱ	TP ⁱⁱ	TP ⁱⁱⁱ	iA
complexfit_2	2.11	NA	1.00	0.75	1313
X-Ray	0.00	NA	1.00	0.75	1227
complexfit_4	1.83	NA	1.00	0.75	1214
complexfit_15	1.92	NA	1.00	0.75	1213
complexfit_6	1.90	NA	1.00	0.75	1208
complexfit_25	2.01	NA	1.00	0.75	1196
complexfit_12	1.78	NA	1.00	0.75	1184
complexfit_10	1.75	NA	1.00	0.75	1175
complexfit_99	3.67	NA	0.33	0.75	1036
complexfit_3	7.87	NA	0.67	0.75	1289
complexfit_103	3.04	NA	0.67	0.75	1072
complexfit_83	3.98	NA	0.33	0.25	1055
complexfit_125	2.89	NA	0.33	0.25	995
complexfit_5	8.01	NA	1.00	0.75	1211
complexfit_58	2.61	NA	0.33	0.50	1017
complexfit_61	3.84	NA	0.67	0.75	1026
complexfit_1	5.63	NA	0.33	0.25	1331
complexfit_7	9.14	NA	0.67	0.75	1180
complexfit_78	3.57	NA	0.67	0.50	909
complexfit_168	2.97	NA	0.00	0.00	753
complexfit_8	9.14	NA	0.33	0.25	1002

1F47 B:B	i-RMSD	position
complexfit_2	2.11	1.5
X-Ray	0.00	2.5
complexfit_4	1.83	3
complexfit_15	1.92	3.5
complexfit_6	1.90	4.5
complexfit_25	2.01	5
complexfit_12	1.78	5.5
complexfit_10	1.75	6.5
complexfit_3	7.87	6.5
complexfit_99	3.67	8
complexfit_1	5.63	9
complexfit_5	8.01	10.5
complexfit_103	3.04	11.5
complexfit_83	3.98	12
complexfit_7	9.14	14
complexfit_125	2.89	14.5
complexfit_58	2.61	16
complexfit_61	3.84	16
complexfit_78	3.57	18.5
complexfit_168	2.97	19
complexfit_8	9.14	19.5