

Table I

Protein-ligand complexes analyzed. The 19 complexes in which the holo conformation of the protein was used for docking and SiteInterlock analysis are listed first, followed by the 11 complexes in which the apo conformation of the protein was used. The binding site RMSD is based on main-chain superposition of the apo onto the holo structure, and defining the binding site atoms in the two structures as those within 9 Å of the ligand.

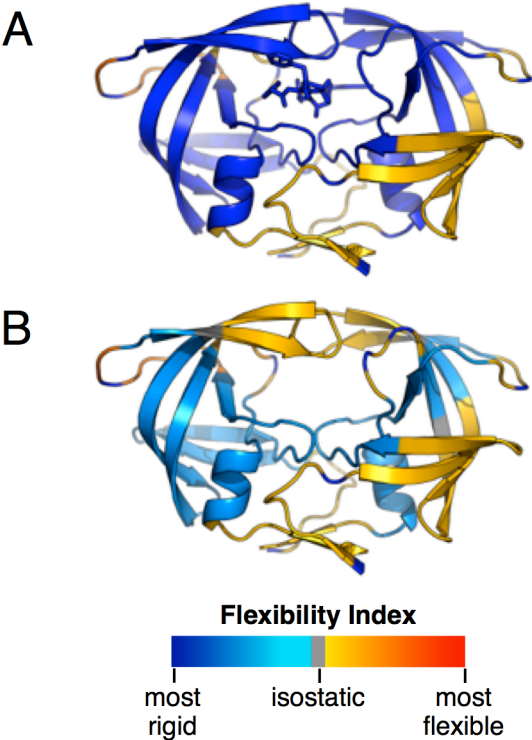
PDB entry (holo/apo)	Protein	Ligand	Resolution (Ångstrom)	Holo-apo binding site RMSD (Å)
1a9x ³¹ / -	carbamoyl phosphate synthetase	L-ornithine	1.80	-
1amu ³² / -	gramidicin synthetase 1	L-phenylalanine	1.90	-
1b5e ³³ / -	deoxycytidylate hydroxymethylase	deoxycytidylic acid	1.60	-
1bgv ³⁴ / -	glutamate dehydrogenase	L-glutamate	1.90	-
1bx4 ³⁵ / -	adenosine kinase	adenosine	1.50	-
1c96 ³⁶ / -	mitochondrial aconitase	citrate anion-iron/sulfur cluster	1.81	-
1cbs ³⁷ / -	retinoic acid binding protein	retinoic acid	1.80	-
1cbx ³⁸ / -	carboxypeptidase A	L-benzylsuccinic acid	2.00	-
1ccw ³⁹ / -	glutamate mutase	D-tartaric acid	1.60	-
1chm ⁴⁰ / -	creatine amidinohydrolase	carbamoyl sarcosine	1.90	-
1com ⁴¹ / -	chorismate mutase	prephenic acid	2.20	-
1coy ⁴² / -	cholesterol oxidase	dehydroepiandrosterone	1.80	-
1cps ⁴³ / -	carboxypeptidase A	sulfodiimine	2.25	-
1did ⁴⁴ / -	D-xylose isomerase	2,5-dideoxy-2,5-imino-D-glucitol	2.50	-
1hwr ⁴⁵ / -	HIV-1 protease	Xk216	1.80	-
1rxl ⁴⁶ / -	dihydrofolate reductase	NADP+	2.00	-
3ks9 ⁴⁷ / -	metabotropic glutamate receptor	Z99	1.90	-
3odu ⁴⁸ / -	G-protein-coupled chemokine receptor	IT1t	2.50	-
7tim ⁴⁹ / -	triosephosphate isomerase	phosphoglycolohydroxamic	1.90	-
10gs ⁵⁰ / 16gs ⁵¹	glutathione S-transferase	L-cysteine amide	2.20 / 1.90	0.27
1ahb ⁵² / 1ahc ⁵²	alpha-momorcharin	formycin-5'-monophosphate	1.90 / 2.00	0.75
1aj2 ⁵³ / 1ajz ⁵³	dihydropteroate synthase	pterin diphosphate	2.20 / 2.00	0.64
1gmr ⁵⁴ / 1gmq ⁵⁴	ribonuclease	guanosine-2'-monophosphate	1.77 / 1.80	0.46
1kel ⁵⁵ / 1kem ⁵⁵	sulfide oxidase antibody	methylphosphonic acid	1.90 / 2.20	0.68
1nsc ⁵⁶ / 1nsb ⁵⁷	influenza B neuraminidase	O-sialic acid	1.70 / 2.20	0.32
1swd ⁵⁸ / 1swa ⁵⁸	streptavidin	biotin	1.90 / 1.90	0.52
3tmn ⁵⁹ / 1tli ⁶⁰	thermolysin	tryptophan	1.70 / 2.05	0.69
1tmt ⁶¹ / 1vr1 ⁶²	alpha-thrombin	D-phenylalanine	2.20 / 1.90	0.66
1ydb ⁶³ / 1ydc ⁶³	carbonic anhydrase II	acetazolamide	1.90 / 1.95	0.30
5sga ⁶⁴ / 2sga ⁶⁵	proteinase A	acetyl group	1.80 / 1.50	0.19

Table II

Ligand RMSD values of the best predicted docking poses

PDB entry	Holo/apo	Best sampled	SiteInterlock Score	PoseScore	AutoDock		DOCK6	
					Vina	DSX	Amber Score	X- Score
1a9x	holo	0.66	0.66	3.65	0.66	1.88	3.65	3.00
1amu	holo	0.40	2.37	0.40	0.40	0.40	0.40	2.37
1b5e	holo	1.12	1.93	1.93	2.28	1.12	1.12	1.12
1bgv	holo	0.56	3.87	2.03	2.43	2.43	3.00	2.43
1bx4	holo	0.10	0.32	0.10	0.10	0.10	2.21	0.10
1c96	holo	1.04	1.04	2.88	2.88	2.88	1.04	2.88
1cbs	holo	1.00	2.25	1.27	1.00	2.47	1.50	1.75
1cbx	holo	0.78	0.97	0.97	0.97	2.26	1.52	0.97
1ccw	holo	0.83	1.97	2.63	0.83	0.83	2.09	0.83
1chm	holo	1.04	1.04	1.97	1.97	1.97	1.90	1.97
1com	holo	0.36	0.36	1.51	0.36	0.36	1.00	0.36
1coy	holo	0.24	1.96	0.24	0.24	0.51	3.19	0.51
1cps	holo	0.97	2.26	1.53	1.53	1.73	0.97	1.53
1did	holo	0.97	2.78	0.97	1.80	1.80	2.52	1.80
1hwr	holo	0.77	1.56	0.77	0.77	0.83	0.83	1.17
1rx1	holo	0.22	0.22	0.22	0.22	0.22	0.22	0.22
3ks9	holo	1.21	1.21	2.00	2.74	1.21	2.74	1.21
3odu	holo	0.99	2.50	0.99	0.99	2.16	2.16	2.16
7tim	holo	0.66	1.25	0.66	1.50	1.50	1.25	0.77
16gs	apo	0.78	1.75	0.78	1.05	1.05	0.78	0.78
1ahc	apo	0.84	1.25	1.50	1.50	1.25	3.00	1.25
1ajz	apo	1.35	2.85	6.44	2.85	6.44	9.33	3.02
1gmq	apo	1.23	1.23	1.23	1.23	1.23	2.07	1.23
1kem	apo	0.44	0.99	0.44	0.44	0.44	2.01	0.73
1nsb	apo	0.50	1.50	0.70	0.70	0.70	0.70	1.50
1swa	apo	0.50	2.13	0.50	0.50	0.50	1.70	1.70
1tli	apo	0.65	0.65	0.65	1.01	5.84	0.83	5.84
1vr1	apo	0.83	0.96	1.65	0.96	0.96	0.83	0.96
1ydc	apo	1.37	2.18	2.18	2.18	5.35	2.18	2.18
2sga	apo	0.40	0.73	0.40	0.40	0.40	1.03	0.81

Figure 1



Review

Figure 2

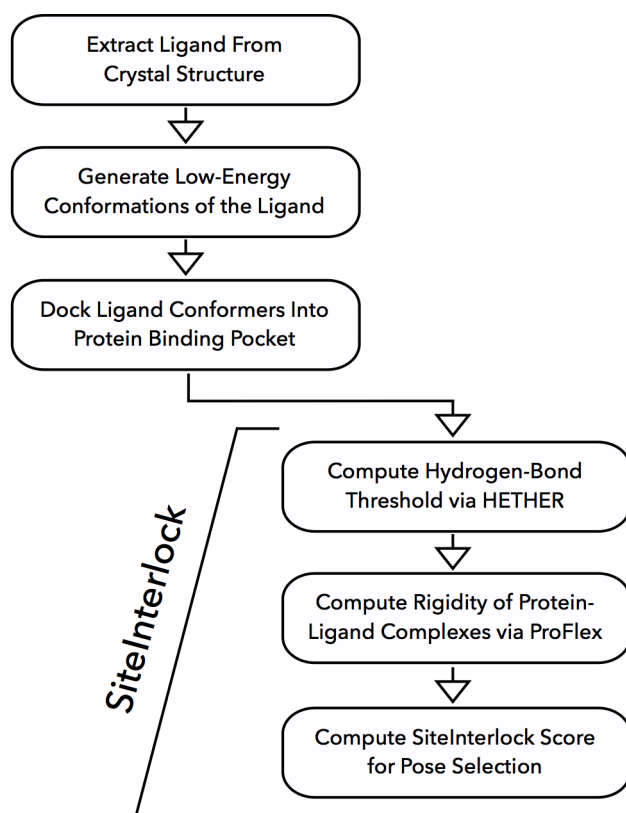


Figure 3

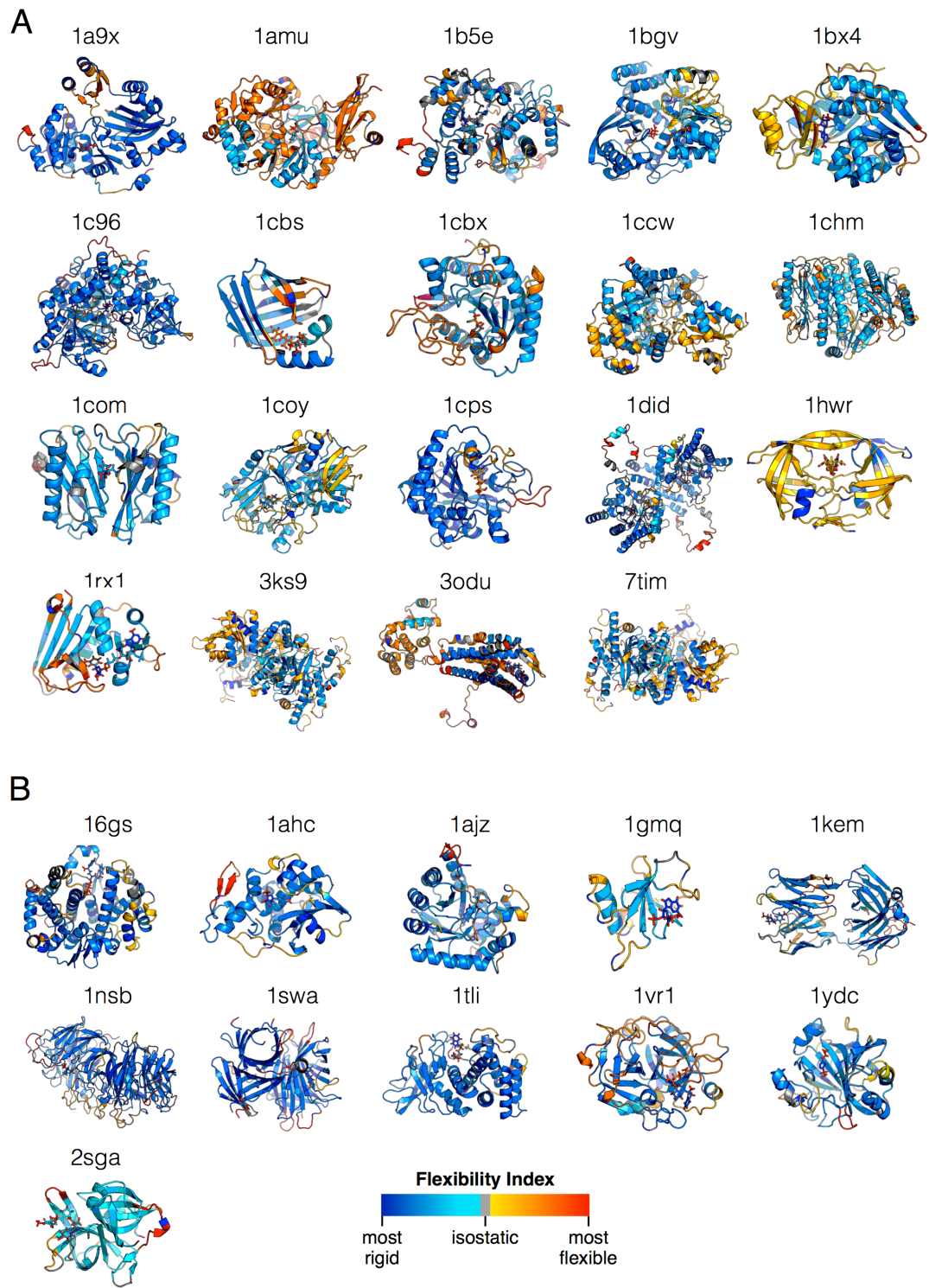


Figure 4

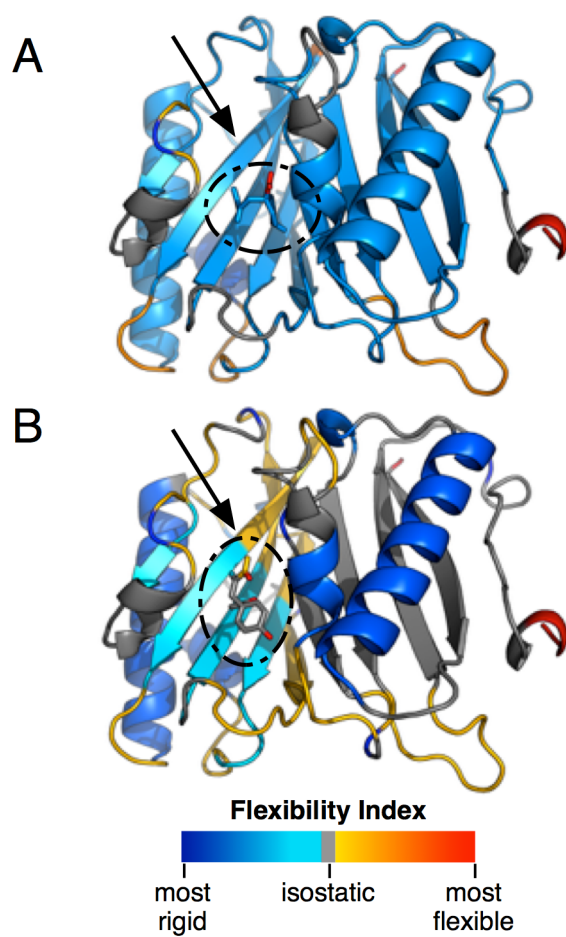


Figure 5

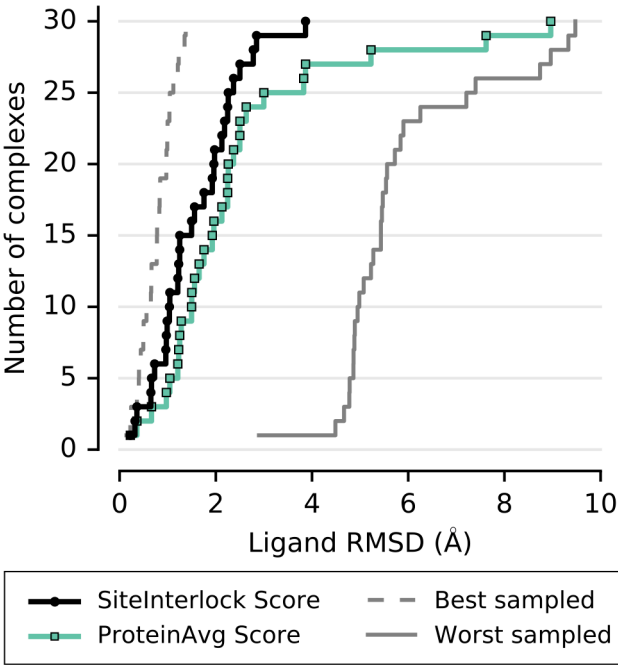


Figure 6

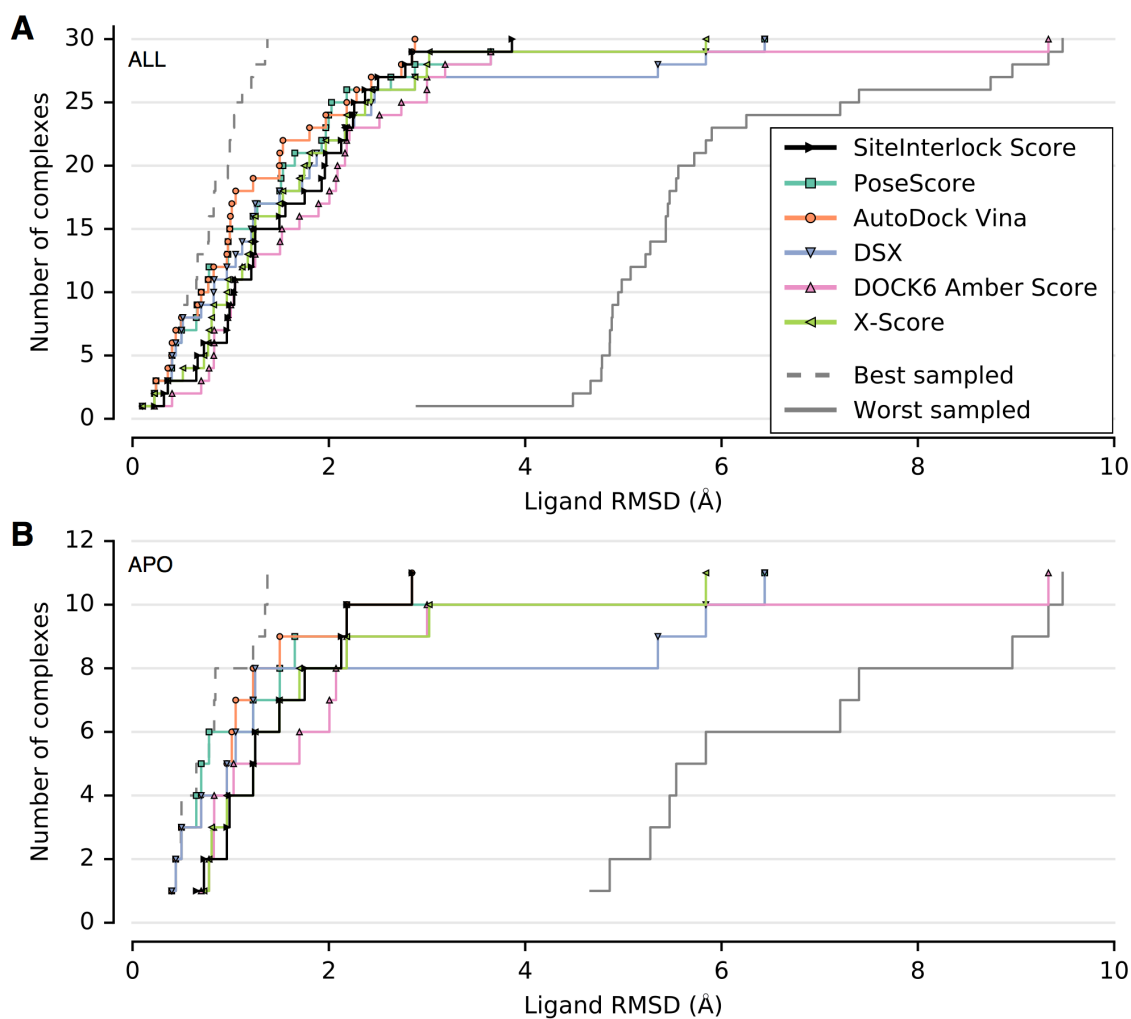


Figure 7

