Complex PDB (a)	Class (b)	Unbound PDB 1	Component 1	Unbound PDB 2	Component 2	iRMSD (Å) (c)	ΔASA (Å²) (d)	Kd (M)	ΔG (kcal/mol) (e)	Temp. (K)	pH	Method (f)	Ref. (g)
3H2V_A:E	OX	3MYI_A	Vinculin tail domain	1WI6_A(8)	Raver1 RRM1 domain	0.8	1263	2.21e-5	-6.31	296.0	8	ITC	1
3DAW_A:B	OX	1IJJ_A	Alpha actin	2HD7_A(5)	Twinfilin-1 C-terminal domain	1.49	2323	2e-5	-6.41			SA	2
4HX3_BD:A	EI	4HWX_AB	Neutral proteinase inhibitor ScNPI	1C7K_A	Zinc endoprotease	0.9	2086	6e-6	-7.41	310.0	7.4	SA	3
3HI6_XY:B	A	3HI5_HL	AL-57 Fab fragment	1MJN_A	Integrin alpha-L I domain	1.65	1871	4.7e-6	-7.27		7.4	SPR	4
2X9A_D:C	OR	1S62_A(8)	TolA C-terminal domain	2X9B_A	G3P TolA binding domain	1.33	1571	4.4e-6	-7.31	298.0	7	SA	5
3R9A_AC:B	OR	1H0C_AB	Alanine-glyoxylate aminotransferase	2C0M_A	PEX5P TPR repeat domain	1.91	1926	3.5e-6	-7.44	298.0	7.5	ITC	6
1M27_AB:C	OX	1D4T_AB	SAP-SLAM Complex	3UA6_A	Fyn kinase SH3 domain	1.22	799	3.45e-6	-7.45	298.0	8	ITC	7
3A4S_A:D	EI	1A3S_A	SUMO-conjugating enzyme UBC9	3A4R_A	NFATC2-interacting protein SLD2 ubiquitin-like domain	0.72	1116	2.81e-6	-7.57	298.0	7.5	ITC	8
3F1P_A:B	OX	1P97_A(9)	HIF2 alpha C-terminal PAS domain	1X0O_A(5)	ARNT C-terminal PAS domain	2.52	1919	1.4e-6	-7.85	293.0	7.5	ITC	9
4M76_A:B	OR	1C3D_A	C3D	1M1U_A	Integrin alpha-M CD11B A-domain	0.43	1046	4.5e-7	-8.66	298.0	7.5	ITC	10
3LVK_AC:B	E	3LVM_AB	Cysteine desulfurase IscS	1DCJ_A(12)	Sulfurtransferase tusA	0.81	1609	3.04e-7	-8.89	298.0	7.4	SPR	11
3L89_ABC:M	OR	3L88_ABC	Ad21 fiber knob	1CKL_A	CD46 SCR1 and SCR2 domains	2.51	2167	2.84e-7	-8.93	298.0	7.4	SPR	12
4IZ7_A:B	EI	1ERK_A	Non-phosphorylated ERK	2LS7_A(1)	PEA-15 Death Effector Domain	1.56	1202	1.33e-7	-9.44	300.0	7.5	SA	13
3K75_D:B	ER	1BPB_A	DNA polymerase beta	3K77_A	Reduced XRCC1, N-terminal domain	0.64	1195	1.1e-7	-9.49		7.5	SA	14
3PC8_A:C	ER	3PC6_A	DNA repair protein XRCC1	3PC7_A	DNA ligase III-alpha BRCT domain	0.5	1240	1.02e-7	-9.54		7.5	SPR	15
3BIW_A:E	OX	3BIX_A	Neuroligin-1	2R1D_A	Neuroligin-1-beta	0.39	1191	9.7e-8	-9.41	293.0	7.2	ITC	16
3SZK_DE:F	OX	3ODQ_AB	MetHaemoglobin	2H3K_A	ISDH-N1	2.1	1263	9.01e-8	-9.45	293.0	7.5	ITC	17
3AAA_AB:C	OX	3AA7_AB	Actin capping protein	1MYO_A(30)	Myotrophin	1.78	1686	2.1e-8	-10.30	293.0	7	SPR	18
3RVW_CD:A	A	3RVT_CD	4C1 Fab	3F5V_A	DER P 1 allergen	0.5	1383	1.9e-8	-10.53	298.0	7.5	ITC	19
3BX7_A:C	OX	3BX8_A	Lipocalin 2	3OSK_A	CTLA-4 extracellular domain	1.63	2349	9e-9	-10.98	298.0	7.4	SPR	20
3MXW_LH:A	A	3MXV_LH	Anti-Shh 5E1 chimera Fab fragment	3M1N_A	Sonic Hedgehog N-terminal domain	0.48	1696	7e-9	-11.31	303.0	7.2	ITC	21
4GXU_MN:ABEFCD	A	4GXV_HL	1F1 antibody	1RUZ_HIJKLM	1918 H1 Hemagglutinin	0.78	1830	6.2e-9	-11.20			BLI	22
4G6J_HL:A	A	4G5Z_HL	Canakinumab antibody fragment	4I1B_A	Interleukin-1 beta	0.61	1893	4.1e-9	-11.44	298.0	7.4	TP	23
3V6Z_AB:F	A	3V6F_AB	Fab E6	3KXS_F	Capsid protein assembly domain	1.83	1922	3.3e-9	-11.57		7.4	SPR	24
3S9D_B:A	OR	1N6U_A(15)	IFNAR2	1ITF_A(9)	IFNa2	1.69	1841	3e-9	-11.63		7.5	SA	25
3EOA_LH:I	A	3EO9_LH	Efalizumab Fab fragment	3F74_A	Integrin alpha-L I domain	0.39	1272	2.2e-9	-11.81	298.0	7.4	SPR	26
2GAF_D:A	ER	3OWG_A	Poly(A) polymerase VP55	1VPT_A	Vaccinia protein VP39	0.69	3368	1.2e-9	-12.17		7	SPR	27
4FQI_HL:ABEFCD	A	4FQH_HL	CR9114 Fab	2FK0_ABCDEF	H5N1 influenza virus hemagglutinin	1.08	1459	9e-10	-12.55	303.0	7.4	BLI	28
2VXT_HL:I	A	2VXU_HL	Murine reference antibody 125-2H Fab	1J0S_A(6)	Interleukin-18	1.33	2163	5.33e-10	-12.65			SPR	29
4G6M_HL:A	A	4G6K_HL	Gevokizumab antibody fragment	4I1B_A	Interleukin-1 beta	0.49	1673	2.9e-10	-13.01	298.0	7.4	TP	23
2W9E_HL:A	A	2W9D_HL	ICSM 18 Fab fragment	1QM1_A	Prion protein fragment	1.13	1677	1.3e-10	-13.49		9.6	ELISA	30
3L5W_LH:I	A	3L7E_LH	C836 Fab	1IK0_A(11)	Interleukin-13	0.48	1138	5.4e-11	-14.01	298.0	7.4	SPR	31
4DN4_LH:M	A	4DN3_LH	CNTO888 Fab	1DOL_A	MCP-1	0.81	1317	3.8e-11	-14.22	298.0	7.1	SPR	32
1JTD_B:A	EI	3QI0_A	BLIP-II	1BTL_A	TEM-1 beta-lactamase	0.44	2180	2.72e-11	-14.41	298.0	7	SA	33
3G6D_LH:A	A	3G6A_LH	CNTO607 Fab	1IK0_A(10)	Interleukin-13	1.86	1793	1.84e-11	-14.65	298.0	7.3	SPR	34

Supporting Table 1: New interactions in version 2 of the structural affinity benchmark. Notes: (a) PDB entry with the chain codes noted AB:C to represent a complex where chains A and B make up component 1, chain C, component 2. Some of the unbound components have NMR structures; the number in parentheses refers to a model in the NMR ensemble. The processed coordinate files may be downloaded from http://zlab.umassmed.edu/benchmark/ (b) Functional classes: A antigen/antibody; EI enzyme/inhibitor; ER enzyme complex with a regulatory or accessory chain; OR receptor containing; OX miscellaneous. (c) Root-mean-square displacement of the Cα atoms of interface residues of the two partners after the unbound and the bound interfaces have been superimposed by least-square. (d) Change in accessible surface area (ASA) between the complex and its components in bound conformation. (e) $\Delta G = -RT \ln K$; temperatures are as reported, with "ambient" or "not stated" set to 298 K. Additional kinetic and thermodynamic are available online at http://bmm.cancerresearchuk.org/~bmmadmin/Affinity (f) Method used to determine affinity: ITC isothermal titration calorimetry; SA spectroscopic assay; SPR surface plasmon resonance; BLI biolayer interferometry; TP thermophoresis; ELISA enzyme-linked immunosorbent assay. (g) Primary citation as listed below. Additional references and corroborating data are available online at http://bmm.cancerresearchuk.org/~bmmadmin/Affinity

Complex	ΔG (kcal/mol)	ΔASA	DComplex	DOPE	pyDock	SIPPER	FireDock	DDG_CU	DDG_CW	DDG_AU	DDG_AW	DDG_V	MARS	RF	RBF	M5'	ConsBind	SolveBind	ZAPP	IRAD	ZRANK	ZDOCK	ΔASA/RMSD
1M27	−7.45	799	−9.27	−499	−36.20	2.72	−21.15	−9.56	−8.72	−11.29	−10.84	−10.56	−8.61	−8.01	−6.25	−7.75	−7.65	6.30	−8.23	−138.84	−82.13	644.2	6.61
3PC8	−9.54	1240	−14.67	−770	−28.96	6.09	−60.48	−3.87	−6.28	−9.05	−15.47	−20.36	−9.62	−8.82	−9.33	−7.91	−8.92	5.55	−9.46	−215.42	−103.27	1108.4	10.39
3BIW	−9.41	1191	−9.66	−681	−18.71	0.66	−18.34	−0.13	−3.14	−3.21	−7.69	−12.41	−7.87	−7.83	−6.42	−10.72	−8.21	7.25	−9.69	−120.07	−69.44	516.8	10.37
3F1P	−7.85	1919	−18.28	−1521	−44.79	14.04	−50.20	−2.11	−4.61	−9.28	−18.02	−29.53	−8.87	−10.64	−14.22	−17.52	−12.82	8.93	−10.89	−233.74	−87.55	1299.3	9.57
3A4S	−7.57	1116	−11.30	−643	−37.00	2.85	−29.43	−10.00	−11.97	−9.54	−14.03	−11.81	−10.28	−7.99	−6.82	−6.08	−7.79	5.58	−8.03	−177.25	−109.72	902.0	9.46
2X9A	−7.31	1571	−17.03	−945	−21.02	1.64	−82.03	−10.36	−18.63	−16.73	−27.46	−22.05	−11.31	−12.30	−11.89	−14.39	−12.47	7.24	−10.15	−222.07	−116.17	1302.4	9.06
3L89	−8.93	2167	−13.68	−1446	−21.95	8.68	−45.87	−3.72	−6.21	−10.31	−19.61	−27.60	−9.57	−9.93	−8.90	−10.35	−9.69	10.19	−12.05	−218.08	−127.60	1238.1	10.51
4HX3	−7.41	2086	−16.70	−1372	−29.60	4.68	−41.56	−7.70	−3.84	−7.07	−18.38	−23.96	−8.61	−10.73	−13.63	−10.35	−10.83	10.03	−12.80	−221.45	−118.88	1235.4	12.65
3H2V	−6.31	1263	−9.53	−712	−13.64	−0.29	2.30	−1.86	−3.44	−6.85	−9.37	−13.35	−8.58	−8.22	−8.89	−7.75	−8.36	5.99	−7.45	−114.67	−58.88	672.5	9.81
3AAA	−10.30	1686	−13.84	−1123	−43.31	0.45	−60.77	−6.54	−7.19	−15.89	−20.28	−19.73	−11.36	−11.28	−10.45	−8.67	−10.44	7.01	−9.90	−244.97	−131.67	1257.6	8.68
4IZ7	−9.44	1202	−10.75	−717	−26.59	5.03	−37.98	−7.02	−5.37	−10.06	−13.26	−19.02	−8.74	−8.82	−9.29	−9.36	−9.05	6.76	−9.98	−160.50	−81.94	881.3	6.84
3SZK	−9.45	1263	−11.16	−1128	−19.30	1.27	−7.58	−12.35	−13.07	−9.10	−15.60	−16.95	−9.16	−9.36	−11.27	−11.47	−10.31	6.34	−9.53	−135.20	−69.74	704.4	7.07
1JTD	−14.41	2180	−19.50	−1910	−48.40	12.04	−53.71	−8.29	−17.27	−19.10	−29.19	−29.32	−13.64	−12.42	−12.65	−11.34	−12.51	8.88	−13.51	−234.03	−99.64	1729.0	14.05
3S9D	−11.63	1841	−15.52	−1082	−32.77	10.16	−56.36	−11.61	−14.45	−10.30	−16.87	−25.54	−11.23	−10.68	−12.58	−11.34	−11.46	8.14	−11.41	−186.75	−92.79	1262.9	9.27
2GAF	−12.17	3368	−19.44	−1949	−41.41	7.73	−48.72	−13.37	−18.50	−16.22	−36.96	−39.10	−9.00	−12.29	−11.42	−8.67	−10.34	11.58	−10.01	−292.91	−150.15	1622.0	18.09
3K75	−9.49	1195	−12.43	−1011	−36.98	2.73	−51.09	−3.08	−10.34	−5.05	−12.58	−18.86	−9.77	−8.73	−11.27	−7.75	−9.38	6.10	−10.46	−142.06	−69.75	817.7	9.94
3R9A	−7.44	1926	−15.28	−959	−17.93	−2.26	−30.09	2.71	1.23	−8.52	−24.01	−25.80	−7.54	−10.59	−7.36	−10.22	−8.92	7.47	−9.05	−180.61	−105.48	1007.7	9.59
3LVK	−8.89	1609	−11.46	−902	−43.02	11.12	−43.88	−4.24	−5.90	−13.58	−25.16	−17.49	−9.85	−9.23	−10.09	−7.75	−9.23	6.25	−7.27	−235.72	−122.70	1524.6	11.10
3BX7	−10.98	2349	−21.48	−1627	−44.46	10.31	−75.21	−7.48	−10.34	−7.30	−19.53	−37.80	−10.80	−11.75	−12.00	−14.39	−12.24	9.57	−11.00	−268.18	−129.98	1697.1	11.20
3DAW	−6.41	2323	−19.23	−1519	−28.45	9.75	−107.16	−9.62	−11.75	−16.94	−25.66	−33.67	−10.66	−12.17	−12.60	−10.42	−11.46	8.47	−11.28	−319.66	−161.42	1650.0	11.15
4M76	−8.66	1046	−9.68	−499	−8.15	0.39	−10.81	−4.46	−7.06	−6.59	−14.49	−8.76	−7.93	−7.18	−5.88	−6.08	−6.77	5.18	−7.31	−94.73	−44.33	577.8	9.76
3G6D	−14.65	1793	−16.16	−1238	−57.10	15.33	−61.34	−8.25	−12.70	−16.31	−19.21	−25.67	−12.58	−12.60	−12.90	−16.35	−13.61	9.14	−11.30	−278.12	−141.04	1423.9	12.66
3L5W	−14.01	1138	−11.06	−895	−31.50	4.88	−48.21	−12.59	−14.66	−14.92	−17.09	−18.31	−10.50	−10.15	−9.53	−13.83	−11.00	7.87	−9.67	−174.44	−78.23	1098.7	10.03
3V6Z	−11.57	1922	−15.10	−1746	−43.74	16.11	−62.69	−4.34	−10.90	−13.36	−19.06	−29.90	−13.08	−12.28	−10.79	−14.39	−12.63	9.61	−14.09	−223.07	−111.87	1344.4	9.58
4G6J	−11.44	1893	−16.10	−1463	−27.70	2.01	−60.16	−13.75	−15.62	−19.27	−26.18	−23.01	−11.21	−10.90	−13.65	−8.67	−11.11	9.18	−12.03	−215.20	−104.43	1282.9	12.66
4G6M	−13.01	1673	−14.66	−1488	−18.48	1.07	−45.44	−12.94	−10.05	−22.64	−22.54	−21.79	−9.71	−10.78	−13.89	−12.39	−11.69	8.78	−12.98	−232.79	−117.86	1249.9	12.05
2VXT	−12.65	2163	−21.28	−1457	−46.26	4.89	−76.01	−19.35	−20.28	−25.99	−35.82	−31.97	−13.03	−12.44	−11.99	−12.59	−12.51	9.30	−12.55	−318.30	−160.11	1687.4	11.31
3EOA	−11.81	1272	−12.46	−892	−33.64	5.73	−43.08	−6.65	−8.06	−9.68	−13.72	−17.16	−10.31	−9.57	−9.54	−9.36	−9.69	7.36	−9.66	−167.36	−82.97	1148.2	10.68
3HI6	−7.27	1871	−16.41	−1391	−51.66	8.12	−51.64	−3.84	−9.37	−11.10	−22.10	−26.79	−13.50	−10.39	−9.57	−10.35	−10.95	9.15	−11.88	−235.06	−113.86	1455.8	9.38
3RVW	−10.53	1383	−13.96	−1174	−29.63	7.10	−9.45	−6.13	−7.48	−7.18	−8.46	−18.17	−8.68	−9.94	−13.56	−9.36	−10.39	9.05	−10.61	−169.67	−74.46	1233.7	10.93
2W9E	−13.49	1677	−16.05	−1471	−37.82	5.58	−35.00	−5.81	−9.27	−9.17	−14.17	−18.96	−10.54	−10.90	−15.97	−12.39	−12.45	9.38	−10.82	−234.13	−98.88	1353.8	10.30
3MXW	−11.31	1696	−18.63	−1405	−44.13	5.25	−68.89	−11.60	−10.56	−20.70	−15.80	−20.11	−11.06	−11.22	−12.15	−13.83	−12.06	8.79	−10.17	−300.39	−150.62	1503.3	12.15
4DN4	−14.22	1317	−13.77	−779	−23.25	8.64	−74.64	−11.24	−15.81	−15.04	−24.80	−20.32	−11.03	−11.01	−10.02	−13.83	−11.47	7.57	−10.96	−235.64	−112.60	1236.6	9.99
4FQI	−12.55	1459	−13.65	−1220	−46.91	8.34	−63.13	−8.36	−11.33	−11.22	−23.76	−22.07	−12.64	−11.43	−12.32	−7.88	−11.07	7.78	−11.25	−201.69	−93.54	1405.9	9.66
4GXU	−11.20	1830	−11.56	−1089	−5.61	−2.46	−6.52	−6.36	−9.91	−5.61	−20.73	−21.64	−8.88	−10.18	−8.83	−10.22	−9.53	9.00	−7.83	−105.82	−48.78	798.7	12.02

Supporting Table 2: Predicted affinities. See main text for descriptions of the scoring functions.

PDB code*	Light Chain L1	Light Chain L2	Light Chain L3	Heavy Chain H1	Heavy Chain H2	Heavy Chain H3
3G6D_LH	26, 27, 28, 29, 30, 31, 32, 33	45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55	88, 89, 90, 91, 92, 93, 94, 95, 96	27, 28, 29, 30, 31, 32, 33, 34, 35	47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60	98, 99, 100, 101, 102, 103, 104, 105, 106, 107, 108, 109, 110, 111
3L5W_LH	27, 28, 29, 30, 31, 32, 33, 34	46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56	89, 90, 91, 92, 93, 94, 95, 96	27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37	49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61	99, 100, 101, 102, 103, 104, 105, 106, 107, 108, 109, 110
3V6Z_BA	27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40	52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62	95, 96, 97, 98, 99, 100, 101, 102, 103	27, 28, 29, 30, 31, 32, 33, 34, 35	47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60	98, 99, 100, 101, 102, 103, 104, 105, 106, 107, 108, 109, 110, 111, 112
4G6J_LH	27, 28, 29, 30, 31, 32, 33, 34	46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56	89, 90, 91, 92, 93, 94, 95, 96	27, 28, 29, 30, 31, 32, 33, 34, 35	47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60	98, 99, 100, 101, 102, 103, 104, 105, 106, 107
4G6M_LH	27, 28, 29, 30, 31, 32, 33, 34	46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56	89, 90, 91, 92, 93, 94, 95, 96	27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37	49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61	99, 100, 101, 102, 103, 104, 105, 106, 107, 108, 109
2VXT_LH	27, 28, 29, 30, 31, 32, 33, 34	46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56	89, 90, 91, 92, 93, 94, 95, 96	27, 28, 29, 30, 31, 32, 33, 34, 35	47, 48, 49, 50, 51, 52, 52A, 53, 54, 55, 56, 57, 58, 59	94, 95, 96, 101, 102
3EOA_LH	27, 28, 29, 30, 31, 32, 33, 34	46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56	89, 90, 91, 92, 93, 94, 95, 96	27, 28, 29, 30, 31, 32, 33, 34, 35	47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60	98, 99, 100, 101, 102, 103, 104, 105, 106, 107, 108, 109, 110
3HI6_LH	27, 28, 29, 30, 31, 32, 33, 34	46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56	89, 90, 91, 92, 93, 94, 95	27, 28, 29, 30, 31, 32, 33, 34, 35	47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60	98, 99, 100, 101, 102, 103, 104, 105, 106, 107, 108, 109
3RVW_CD	27, 28, 29, 30, 31, 32, 33, 34	46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56	89, 90, 91, 92, 93, 94, 95	27, 28, 29, 30, 31, 32, 33, 34, 35, 36	48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60	98, 99, 100, 101, 102, 103, 104, 105, 106, 107, 108, 109, 110
2W9E_LH	27, 28, 29, 30, 31, 32, 33	45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55	88, 89, 90, 91, 92, 93, 94, 95	27, 28, 29, 30, 31, 32, 33, 34, 35	47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60	98, 99, 100, 101, 102, 103, 104, 105
3MXW_LH	27, 28, 29, 30, 31, 32, 33, 34	46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56	89, 90, 91, 92, 93, 94, 95, 96	27, 28, 29, 30, 31, 32, 33, 34, 35	47, 48, 49, 50, 51, 52, 53, 54, 55, 55A, 56, 57, 58, 59	94, 95, 96, 97, 98, 99, 100, 100A, 100K, 101, 102
4DN4_LH	27, 28, 29, 30, 31, 32, 33, 34, 35	47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57	90, 91, 92, 93, 94, 95, 96, 97, 98	27, 28, 29, 30, 31, 32, 33, 34, 35	47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60	98, 99, 100, 101, 102, 103, 104, 105, 106, 107, 108
3EO1_AB	27, 28, 29, 30, 31, 32, 33, 34, 35	47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57	90, 91, 92, 93, 94, 95, 96, 97	27, 28, 29, 30, 31, 32, 33, 34, 35	47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60	98, 99, 100, 101, 102, 103, 104, 105, 106, 107, 108, 109
3HMX_LH	27, 28, 29, 30, 31, 32, 33, 34	46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56	89, 90, 91, 92, 93, 94, 95, 96	27, 28, 29, 30, 31, 32, 33, 34, 35	47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60	98, 99, 100, 101, 102, 103, 104, 105, 106, 107, 108
4FQI_LH	27, 27A, 27B, 28, 29, 30, 31, 32, 33, 34	46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56	89, 90, 91, 92, 93, 94, 95, 95A, 95B, 96	27, 28, 29, 30, 31, 32, 33, 34, 35	47, 48, 49, 50, 51, 52, 52A, 53, 54, 55, 56, 57, 58, 59	94, 95, 96, 97, 98, 99, 100, 100A, 100B, 100C, 100D, 101, 102
4GXU_NM	27, 27A, 27B, 28, 29, 30, 31, 32, 33, 34	46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56	89, 90, 91, 92, 93, 94, 95, 95A, 95B, 95C, 96	27, 28, 29, 30, 31, 32, 33, 34, 35	47, 48, 49, 50, 51, 52, 52A, 53, 54, 55, 56, 57, 58, 59	94, 95, 96, 97, 98, 99, 100, 100A, 100B, 100C, 100D, 100E, 100F, 100G, 100H, 100I, 101, 102

* PDB code and chain identifiers are reported, in the order light/heavy chain.

Supporting Table 3: List of antibodies complementarity-determining regions (CDRs) in antibody/antigen complexes used to drive docking simulation in HADDOCK; data calculated by PARATOME webserver. For the other type of complexes, restraints to drive the docking were derived from bioinformatics predictions by CPORT (`http://haddock.chem.uu.nl/services/CPORT/`). The full list of the CPORT predicted residues is reported in the online set of HADDOCK decoys provided.

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