

Supplementary material to

Molecular simulations to rationalize humanized Ab2/3H6 activity

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Table S1. Average number of hydrogen bonds in the interface region during the 2F5/3H6 crystal simulation. For each hydrogen bond which was observed more than 50% of the time during one of the 8 copies (2 simulations, each with 4 copies of the complex) the acceptor and donor residues, the average number of hydrogen bonds between the residues over all 8 copies, the standard deviation of the average and the number of copies for which the hydrogen bond is seen for more than 50% of the time are shown. The columns labeled with atom indicate whether the hydrogen bonds involve the backbone (bb) or side chain (sc) atoms.

	Donor			Acceptor			Nr. Hbonds	
	Chain	Residue	Atom	Chain	Residue	Atom	avg (stdev)	#
Inter face	2F5_H	THR67	sc	3H6_H	THR30	bb	0.98 (0.01)	8
	2F5_H	ASN66	sc	3H6_H	ASP31	bb	0.92 (0.13)	8
	3H6_H	GLY102	bb	2F5_H	ASN66	sc	0.79 (0.12)	8
	3H6_H	GLY104	bb	2F5_H	ASN66	sc	0.71 (0.35)	6
	2F5_H	TYR61	bb	3H6_H	GLY102	bb	0.41 (0.26)	5
	3H6_H	ASN52	sc	2F5_H	THR67	bb	0.37 (0.26)	3
	2F5_H	ARG86	sc	3H6_H	TYR54	sc	0.27 (0.33)	2
	2F5_H	ARG60	sc	3H6_H	ASP50	sc	0.24 (0.32)	2
	3H6_H	ASN93	sc	2F5_H	ASP57	sc	0.21 (0.33)	1
2F5	2F5_H	ARG60	bb	2F5_H	ILE52	bb	0.96 (0.01)	8
	2F5_H	THR70	bb	2F5_H	VAL83	bb	0.95 (0.03)	8
	2F5_L	PHE93	bb	2F5_L	GLN90	sc	0.94 (0.03)	8
	2F5_H	ILE111	bb	2F5_H	THR104	bb	0.82 (0.12)	8
	2F5_H	VAL87	bb	2F5_H	GLN16	bb	0.67 (0.15)	7
	2F5_H	ARG68	sc	2F5_H	THR85	bb	0.65 (0.33)	5
	2F5_H	SER62	bb	2F5_H	LEU50	bb	0.63 (0.40)	6
	2F5_H	LEU69	bb	2F5_H	LEU65	bb	0.60 (0.38)	5
	2F5_H	THR85	bb	2F5_H	ARG68	bb	0.59 (0.15)	5
	2F5_H	ARG68	sc	2F5_H	ARG86	bb	0.57 (0.22)	5
	2F5_H	LYSH59	sc	2F5_H	ASP57	bb	0.52 (0.28)	5
	2F5_H	ARG60	sc	2F5_H	ASP58	sc	0.50 (0.43)	4
	2F5_H	ARG68	sc	2F5_H	ASP91	sc	0.49 (0.53)	4
	2F5_H	ARG113	sc	2F5_H	ALA112	bb	0.30 (0.12)	1
	2F5_H	VAL109	bb	2F5_H	LEU106	bb	0.27 (0.20)	1
	2F5_H	ASP57	bb	2F5_H	ASP56	sc	0.23 (0.43)	2
2F5_H	ASP58	bb	2F5_H	TYR54	bb	0.22 (0.29)	2	

	2F5_H	ARG86	sc	2F5_H	THR15	bb	0.21 (0.26)	1
	2F5_H	ARG113	bb	2F5_H	THR104	sc	0.17 (0.31)	1
	2F5_H	ASP57	bb	2F5_H	SER55	bb	0.13 (0.24)	1
	2F5_H	ARG60	sc	2F5_H	LYSH59	bb	0.10 (0.24)	1
	2F5_H	ASP58	bb	2F5_H	ASP56	sc	0.07 (0.18)	1
3H6	3H6_H	TYR103	sc	3H6_L	ASP50	sc	1.22 (0.14)	8
	3H6_L	ASN93	bb	3H6_L	ASP92	sc	0.94 (0.05)	8
	3H6_H	TYR50	bb	3H6_H	ASN59	bb	0.90 (0.07)	8
	3H6_H	ASN52	bb	3H6_H	ALA57	bb	0.87 (0.10)	8
	3H6_H	THR55	bb	3H6_H	ASN52	sc	0.86 (0.16)	8
	3H6_L	THR53	bb	3H6_L	SER49	bb	0.84 (0.27)	7
	3H6_H	SER106	bb	3H6_H	TYR103	bb	0.71 (0.12)	8
	3H6_H	THR99	sc	3H6_H	GLY104	bb	0.70 (0.45)	6
	3H6_H	TYR54	bb	3H6_H	ASN52	bb	0.70 (0.23)	7
	3H6_H	TYR32	bb	3H6_H	PHE29	bb	0.64 (0.10)	7
	3H6_L	LEU94	bb	3H6_L	ASN93	sc	0.61 (0.26)	6
	3H6_H	THR99	bb	3H6_H	PHE33	bb	0.61 (0.32)	5
	3H6_L	SER91	sc	3H6_L	ASP32	sc	0.59 (0.40)	4
	3H6_L	GLY51	bb	3H6_L	ASP32	sc	0.58 (0.47)	4
	3H6_H	TYR103	bb	3H6_H	SER100	bb	0.57 (0.28)	6
	3H6_L	THR53	sc	3H6_L	ASP50	bb	0.47 (0.38)	4
	3H6_H	CYSH53	sc	3H6_H	TYR32	bb	0.44 (0.27)	3
	3H6_L	TYR67	bb	3H6_L	ASP70	bb	0.36 (0.23)	2
	3H6_H	SER100	bb	3H6_H	PRO108	bb	0.35 (0.31)	3
	3H6_L	SER91	bb	3H6_L	ASP32	bb	0.30 (0.37)	3
	3H6_L	ASP31	bb	3H6_L	ASP30	sc	0.29 (0.27)	1
	3H6_L	TYR96	sc	3H6_L	ASP92	bb	0.28 (0.41)	2
	3H6_L	TYR67	sc	3H6_L	ASP30	sc	0.24 (0.42)	2
	3H6_L	ASP32	bb	3H6_L	ASP30	sc	0.19 (0.28)	1
	3H6_L	ASP50	bb	3H6_L	ASN34	sc	0.18 (0.24)	1
	3H6_L	ASP32	bb	3H6_L	ASP30	bb	0.16 (0.26)	1
	3H6_L	GLY51	bb	3H6_L	ASP31	sc	0.14 (0.29)	1
	3H6_H	GLY56	bb	3H6_H	ASN52	sc	0.11 (0.26)	1
	3H6_H	TYR54	bb	3H6_H	ASN52	sc	0.10 (0.21)	1
	3H6_H	CYSH53	bb	3H6_H	GLY56	bb	0.10 (0.24)	1
	3H6_H	TYR50	sc	3H6_L	TYR96	sc	0.09 (0.26)	1
	3H6_H	THR99	sc	3H6_H	PHE33	bb	0.09 (0.18)	1
	3H6_L	ASN93	sc	3H6_L	ASP92	sc	0.08 (0.23)	1
	3H6_H	SER105	sc	3H6_L	TYR96	sc	0.07 (0.19)	1
	3H6_L	SER91	sc	3H6_L	ASP32	bb	0.07 (0.18)	1
	3H6_H	PHE29	bb	3H6_H	ASN77	sc	0.07 (0.18)	1
