

## SUPPLEMENTARY MATERIALS

### **Experimental structures of antibody/MHC-I complexes reveal details of epitopes overlooked by computational prediction**

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SUPPLEMENTARY FIGURE 1. Fab Sequence Alignments and CDR ranges.

SUPPLEMENTARY TABLE 1. Buried surface area (BSA) at interface between Fab and pMHC.

SUPPLEMENTARY TABLE 2. Comparison of elbow angles of X-ray and AF-M structural models.

Supplementary Figure 1.

**A**

**H-Chain**

Fab3458-H	-----EESGPELGKPGASVKMSCTA <b>SGYFTSY</b> VMHWVMQKPGQGLEWIGY <b>FNPYNDAG</b>	58
Fab34212-H	---VQLQQSGPELVKPGASVKISCS <b>SGYTI</b> SN <b>SMN</b> WVQRPGKGLEWIGRI <b>YPGDGD</b> T	58
Fab2814S-H	-----QQSGAELAKPGASVKMSCKA <b>SGYNFTTY</b> MMHWVRQKPGQGLEWIGY <b>INPSSGYT</b>	58
FabS19-H	---VQLQQSGPVLVKPGASVKMSCKA <b>SGYFTFDHY</b> MNHWKQSPGK <b>SL</b> EWIGGI <b>INPYNGGI</b>	58
Fab3458-H	KYNAKFKGKATLTSDKSSNTAYMELSSLTSESDSTVYY <b>CARA--Y-FSKGPFAY</b> WGQGT <b>LV</b>	115
Fab34212-H	HYNGKFRKAKATLTADRSSSTAYMHLSSLTSESDSAIYFC <b>ARSTA-----AWFPY</b> WGRGT <b>LV</b>	113
Fab2814S-H	EFNQKFKGKATLTADKSSNTAYIQLTSLTSDSDSAIY <b>CARSF-----YFPDY</b> WGQGT <b>LV</b>	112
FabS19-H	SYNQKFKGMATLTADKSSSTAYMELSSLTSESDSAVYCV <b>RIGY-YPSYFFD</b> YWQGT <b>LV</b>	116

**B**

**L-Chain**

Fab3458-L	----TQTPASLAVSLGQRATISCR <b>ASVDRHGNSF</b> MHWYQQKPGQPPKLLI <b>YRASNLDS</b>	60
Fab34212-L	---TTVTQTPKFMSTSVGDRVSVTCTA <b>SNQV----</b> DTN <b>AWY</b> QKPGQSPKPLI <b>IFSASSRYT</b>	56
Fab2814S-L	----TQTPSSLSASLGDRVTISCR <b>ASQDI----</b> SNY <b>NWY</b> QKPGDPVKLLI <b>YYSRLHS</b>	56
FabS19-L	---TTVTQSPASLSVATGEKVTIRCI <b>FTSDI----</b> DD <b>MN</b> WYQKPGEPKLLI <b>SEGNTLRP</b>	56
Fab3458-L	GIPARFSGSGSRTDFTLTINPVEADDVATYYC <b>QSNEDPPWTF</b> GGG <b>T</b> KLEIKRADA <b>APT</b>	120
Fab34212-L	GIPDRFGSGSGTDFAL <b>TIS</b> NVQSEDLAEYFC <b>QYH-SFPYTF</b> GGG <b>T</b> RL <b>EIKRADAAPT</b>	115
Fab2814S-L	GVPSRFSGSGSDYSL <b>TIS</b> NLEQED <b>IATYFCQGN-TFPWTF</b> GGG <b>T</b> KLEIKRADA <b>APT</b>	115
FabS19-L	GVPSRFSSSGFGTDFVFT <b>IENT</b> LS <b>EDFADYCLQSD-DMPLTF</b> GAG <b>T</b> KLEIKRADA <b>APT</b>	115

**C**

8TQ8		8TQ7	
CDR	34-5-8	CDR	34-2-12
CDRH1	S25-V33	CDRH1	S25-M33
CDRH2	N52-D56	CDRH2	Y52-D57
CDRH3	R98-Y108	CDRH3	R98-Y106
CDRL1	S26-F36	CDRL1	S26-V33
CDRL2	R54-L58	CDRL2	F49-S53
CDRL3	Q94-W101	CDRL3	Q90-Y96

  

8TQA		8TQ9	
CDR	28-14-8	CDR	S19.8
CDRH1	S25-W33	CDRH1	S25-Y33
CDRH2	N52-G56	CDRH2	N52-G56
CDRH3	R98-Y105	CDRH3	R99-F107
CDRL1	A25-L33	CDRL1	T25-N32
CDRL2	Y49-R53	CDRL2	S49-T53
CDRL3	Q90-W96	CDRL3	Q90-L96

Supplementary Figure 1. Fab Sequence Alignments and CDR ranges. Amino acid sequences of the indicated Fab H and L chains, as deduced from their respective nucleotide sequences and confirmed structurally were aligned with Clustal Omega <https://www.ebi.ac.uk/seqdb/confluence/display/JDSAT/Clustal+Omega+Help+and+Documentation> (94). These are shown for the  $V_H$  (A) and  $V_L$  (B) regions of the indicated antibodies. Dashes indicate amino acid residues that were not observed in electron density maps. Color highlights indicate structurally defined loops corresponding to the CDRs tabulated in panel C.

<b>Complex</b>	<b>PDB</b>	<b>Chains</b>	<b>BSA-H</b>	<b>BSA-L</b>	<b>BSA-(H+L)</b>
Fab34-5-8/D <sup>d</sup> _A	8TQ8	A (H,L)	710	210	920
Fab34-5-8/D <sup>d</sup> _B	8TQ8	B (H,L)	0	0	0
Fab34-2-12/D <sup>d</sup> _A	8TQ7	A (H,L)	680	80	760
Fab34-2-12/D <sup>d</sup> _B	8TQ7	B (H,L)	0	0	0
Fab28-14-8/D <sup>b</sup> _A	8TQA	A (H,L)	500	350	850
Fab28-14-8/D <sup>b</sup> _B	8TQA	B (H,L)	10	0	10
FabS19.8/D <sup>d</sup> _A	8TQ9	A (H,L)	140	50	190
FabS19.8/D <sup>d</sup> _B	8TQ9	B (H,L)	660	240	900

Supplementary Table 1. Buried surface area (BSA) at interface between Fab and pMHC. Buried surface areas for each of the indicated interfaces were calculated with PDBePISA (51). Values are in Å<sup>2</sup>, rounded to the nearest 10.

<b>Fab</b>	X-ray Model (PDB)	AF-M Model	X-ray Elbow Angle (°)	AF-M Elbow Angle (°)	<b>Δ Elbow Angle (°)</b>	Limit-l	Limit-h
<b>34-5-8</b>	8TQ8	8TQ8-AF	150	136	<b>14.0</b>	113	119
<b>34-2-12</b>	8TQ7	8TQ7-AF	135	136	<b>1.0</b>	109	117
<b>28-14-8</b>	8TQA	8TQAAF	173	145	<b>28.0</b>	107	116
<b>S19.8</b>	8TQ9	8TQ9AF	152	168	<b>16.0</b>	107	116

Supplementary Table 2. Comparison of elbow angles of X-ray and AF-M structural models.

“Limit\_l” and “limit\_h” indicate the residues defining the ends of variable domain of the light chain and the heavy chain respectively. The measurement of elbow angle is calculated by using the Python Script of “elbow\_angle.py” imported to PyMol (48).