Supplemental Material

Suppl. Table Notable interatomic contacts between poliovirus and VHH

PV-PVSP6A		PV residues	VHH residues	VHH-structure	Interaction type
North	VP1 (LP)[a] EF-loop	CG1:Val166	CE1:Phe109	FG-loop	hydrophobic
West	VP1 (LP) H-strand	CG2:Ile:239	CE:Met108	FG-loop	hydrophobic
	VP1 (LP) C-strand (and vicinity)	OD1:Asp102	NE2:Gln3	A-strand	H-bond
		N:Phe105	OE1:Gln1	N-term	H-bond
		O:Phe105	N:Gln1	N-term	H-bond
		CG1:Val107	CZ:Phe109	FG-loop	hydrophobic
		O:Val107	N: Phe27	BC-loop	proximity
		CD1:Trp108	CZ:Phe29	BC-loop	hydrophobic
		OD2:Asp114	CE2:Phe29	BC-loop	vanderWaals
Southwest	VP1 (LP) C-term prox.[a] loop	CA:Gly281	NE2:His31	BC-loop	vanderWaals
		CD:Pro282	CG:His31	BC-loop	hydrophobic
	VP2 (LP) EF-loop tip	CG2:Thr139	CG2:Thr53	C’-strand	hydrophobic
		OG1:Thr139	CA:Gly55	C’C”-strand	vanderWaals
		O:Thr140	NH2:Arg52	C’-strand	H-bond
		OG1:Thr140	ND1:His31	BC-loop	vanderWaals
		O:Gln167	C:Val56	C’C”-strand	vanderWaals
		CG:Pro170	CG:Ser57	C”-strand	hydrophobic
South	VP1 (LP) GH-loop	NZ:Lys214	OG:Ser105	FG-loop	H-bond
		CE:Lys214	CB:Cys103	FG-loop	hydrophobic
		CD1:Leu228	CB:Ser102	FG-loop	hydrophobic
		CD1:Leu234	CA:Gly106	FG-loop	hydrophobic
		CD2:Leu234	C:Ser100	FG-loop	hydrophobic
		CG:Asn235	CE:Met108	FG-loop	hydrophobic
East	VP1 (RP)[a] C-term dist.ext.[a]	CB:Thr296	C:Lys43	CC’-loop	hydrophobic
		NZ:Lys297	OE1:Glu44	CC’-loop	Salt link
		N:Asp298	OE2:Glu44	CC’-loop	H-bond
	VP3 (RP) B-strand knob insertion	CB:Ala59	CB:Glu42	CC’-loop	hydrophobic
		NZ:Lys62	OE1:Glu42	CC’-loop	Salt link

PV-PVSS8A		PV residues	VHH residues	VHH-structure	Interaction type
North	VP1 (LP) EF-loop	CG1:Val166	CZ:Tyr27	BC-loop	hydrophobic
		O:Glu168	N:Gln1	N-term	H-bond
		OE2:Glu168	OH:Tyr1115	G-strand	proximity
		OE2:Glu168	NH2:Arg100	FG-loop	proximity
		NZ:Lys169	OE1:Gln1	N-term	proximity
West	VP1 (LP) C-strand	CG1:Val107	CD1:Tyr27	BC-loop	hydrophobic
	VP1 (LP) GH-loop prox. end	CG:Asp236	CG:Phe103	FG-loop	hydrophobic
Southwest	VP1 (LP) C-term ext. prox. end	CG:Pro282	CZ:Tyr54	C’C”-loop	hydrophobic
	VP2 (LP) EF-loop	CG2:Thr139	CG:Asn55	C’C”-loop	short
		O:Thr140	ND2:Asn55	C’C”-loop	H-bond
		N:Thr140	OD1:Asn55	C’C”-loop	H-bond
		CD2:His142	CB:Ala57	C’C”-loop	hydrophobic
		O:Gln167	SD:Met58	C’C”-loop	vanderWaals
		O:Gln167	OH:Tyr60	C”-strand	H-bond
		CG2:Thr168	CA:Gly66	C”D-loop	proximity
		CG:Pro170	SD:Met58	C’C”-loop	proximity
South	VP1 (LP) GH-loop dist. end	NZ:Lys214	OD2:Asp105	FG-loop	salt link
		OD2:Asp226	NH2:Arg59	C”-strand	salt link

		O:Ser227	CD1:Ile106	FG-loop	vanderWaals
		N:Leu228	O:Gly104	FG-loop	H-bond
		CD2:Leu228	CG1:Ile106	FG-loop	hydrophobic
		CD1:Leu228	CD1:Tyr54	C'C"-loop	hydrophobic
		CD1:Leu228	CD1:Tyr54	C'C"-loop	hydrophobic
Center	VP3 (RP) GH-loop	O:Asp181	NH1:Arg102	FG-loop	H-bond
		OD2:Asp181	NH2:Arg102	FG-loop	proximity

PV-PVSP19B		**PV residues**	**VHH residues**	**VHH-structure**	**Interaction type**
North	VP1 (LP) EF-loop	N:Gly163	CZ3:Trp97	FG-loop	vanderWaals
		CG2:Val166	CB:Trp97	FG-loop	hydrophobic
		O:Val166	NE2:Gln109	FG-loop	H-bond
		OE2:Glu168	NE2:Gln109	FG-loop	proximity
		OE2:Glu168	NE:Arg98	FG-loop	proximity
Northwest	VP1 (LP) C-strand	CD2:Phe105	CB:Gln1	N-term	proximity
		O:Phe105	CB:Gln1	N-term	vanderWaals
		CB:Val107	CE:Met31	BC-loop	hydrophobic
West	VP1 (LP) C-strand	NZ:Lys109	OD1:Asn51	C'C"-loop	proximity
		N:Lys109	SG:Cys30	BC-loop	vanderWaals
	VP1 (LP) GH-loop (proximate)	OD2:Asp236	ND2:Asn51	C'C"-loop	H-bond
		CG2:Ile239	NE1:Trp97	FG-loop	vanderWaals
Southwest	VP1 (LP) C-term prox.	CA:Gly281	CB:Ala72	DE-loop	hydrophobic
		CD:Pro282	CB:His71	DE-loop	hydrophobic
	VP2 (LP) EF-loop	OG1:Thr140	OD1:Asn70	DE-loop	proximity
		CE:Met141	CD2:His71	DE-loop	hydrophobic
South	VP1 (LP) GH-loop (dist.)	OG:Ser213	N:Gly53	C'C"-loop	proximity
		CD1:Leu228	O:Gly53	C'C"-loop	vanderWaals
		CB:Ala231	CA:Asp52	C'C"-loop	hydrophobic
Center	VP3 (RP) GH-loop	CB:Ile180	CZ2:Trp99	FG-loop	hydrophobic
		O:Asp181	NZ:Lys49	C'-strand	H-bond
		OD1:Asp182	OD2:Asp52	C'C"-loop	vanderWaals

PV-PVSS21E		**PV residues**	**VHH residues**	**VHH-structure**	**Interaction type**
North	VP1 (LP) EF-loop	CG2:Val166	CE1:Tyr55	C'C"-loop	hydrophobic
		O:Pro167	NE1:Trp57	C"-strand	H-bond
Northwest	VP1 (LP) BC-loop (twisted)	OG1:Thr99	OE2:Glu43	CC'-loop	proximity
		ND1:Asn100	O:Arg44	C'-strand	proximity
		CD:Lys101	CE3:Trp46	C'-strand	hydrophobic
		CD:Lys101	CB:Trp46	C'-strand	hydrophobic
		CG:Lys103	CZ3:Trp46	C'-strand	hydrophobic
West	VP1 (LP) C-strand	O:Phe105	N:Gly102	FG-loop	long H-bond
		CZ:Phe105	NE1:Trp57	C"-strand	hydrophobic
		CB:Val107	CG:Pro101	FG-loop	hydrophobic
		O:Val107	OG1:Thr99	FG-loop	H-bond
		CD1:Trp108	OG1:Thr99	FG-loop	vanderWaals
Southwest	VP1 (LP) C-term prox.	CE1:Tyr280	CD2:Tyr27	BC-loop	hydrophobic
		CD1:Tyr280	CG:Pro29	BC-loop	proximity
		CA:Gly281	CB:Pro29	BC-loop	proximity
	VP2 (LP) EF-loop	O:Asn137	N:Tyr27	BC-loop	H-bond
		CG2:Thr139	CA:Lys74	DE-loop	hydrophobic
		CG2:Thr139	CB:Ala73	DE-loop	hydrophobic
		OG1:Thr140	OH:Tyr27	BC-loop	H-bond
		CG2:Thr140	CE2:Tyr27	BC-loop	hydrophobic
		CD2:His142	CB:Ala73	DE-loop	hydrophobic
		OE1:Gln167	NZ:Lys74	DE-loop	H-bond
South	VP1 (LP) GH-loop	CD2:Leu228	CB:Ala73	DE-loop	hydrophobic

	dist.				

PV-PVSP29F		**PV residues**	**VHH residues**	**VHH-structure**	**Interaction type**
North	VP1 (LP) EF-loop	CA:Pro162	NE2:Gln29	BC-loop	proximity
		CB:Val166	CE1:Tyr27	BC-loop	hydrophobic
		OE1:Glu168	OD1:Asn77	DE-loop	proximity
Northwest	VP1 (LP) C-strand	CD:Lys109	CD1:Leu103	FG-loop	hydrophobic
Southwest	VP2 (LP) EF-loop	CG2:Thr139	CA:Ala108	FG-loop	hydrophobic
		CD2:His142	CZ:Tyr113	FG-loop	hydrophobic
South	VP1 (LP) GH-loop dist.	NZ:Lys214	OD1:Asn116	FG-loop	salt link
		CA:Leu224	CH2:Trp118	G-strand	hydrophobic
		OD1:Asp226	CA:Tyr113	FG-loop	vanderWaals
		CD2:Leu228	CB:Tyr113	FG-loop	hydrophobic
Center	VP3 (RP) GH-loop	OD2:Asp181	N:Gln1	N-term	H-bond
		O:Asp181	ND2:Asn116	FG-loop	H-bond
East	VP1 (RP) C-term ext.	OG:Ser295	NE2:Gln1	N-term	H-bond
	VP3 (RP) CD-helix	O:Ser91	N:Gln1	N-term	H-bond
Northeast	VP1 (RP) C-term ext. (prox.)	CB:Pro282	CG:Gln107	FG-loop	hydrophobic

[a]: LP (leftmost protomer) and RP (rightmost protomer) indicate the protomer to which the poliovirus structure involved in binding belongs. ext. stands for extension and prox. and dist. for proximal and distal, respectively.