

In the format provided by the authors and unedited.

Calicivirus VP2 forms a portal-like assembly following receptor engagement

Michaela J. Conley¹, Marion McElwee¹, Liyana Azmi², Mads Gabrielsen³, Olwyn Byron⁴, Ian G. Goodfellow⁵ & David Bhella^{1*}

¹Medical Research Council University of Glasgow Centre for Virus Research, Glasgow, UK. ²Institute of Infection, Immunity and Inflammation, University of Glasgow, Glasgow, UK. ³CRUK Beatson Institute, Glasgow, UK. ⁴School of Life Sciences, University of Glasgow, Glasgow, UK. ⁵Division of Virology, Department of Pathology, University of Cambridge, Cambridge, UK.
*e-mail: david.bhella@glasgow.ac.uk

Calicivirus VP2 forms a portal-like assembly following receptor engagement.

Michaela J. Conley, Marion McElwee, Liyana Azmi, Mads Gabrielsen, Olwyn Byron, Ian G. Goodfellow and David Bhella

Supplemental Data

Supplemental Data 1

VP1 protein sequence:

```
1 MCSTCANVLK YYNWDPHFRL VIDPNKFLSV GFCDNPLMCC YPELLPEFGT VWDCDQSPLQ
61 IYLESILGDD EWASTYEAI D PAVPPMHWDA AGKIFQPHPG VLMHHLIGEV AKAWDPNLPM
121 FRLEADGDGS ITAPEQGTPV GGVI AEP SAQ MSAAADMATG KSV DSEWEAF FSFHTSVNWS
181 TSETQ GKILF KQSLG PLLNP YLEHLAKLYV AWSGSIDVRF SISGSGVFGG KLAAIVVPPG
241 VDPVQST SML QYPHVLF DAR QVEPVIF SIP DLRSTLYHLM SDTDTTSLVI MVYNDLINPY
301 ANDSNSSGCI VTVETKPGAD FKFHLLKPPG SMLTHGSVPS DLIPKSSSLW IGNRHWT DIT
361 DFVIRPFV FQ ANRHFDNFQE TAGWSTPRYR PITITISEKN GAKLGIGVAT DYIVPGIPDG
421 WPDTTIPEKL TPAGDYAITN KSGNDITTA GYDGADVIVN NTNFKGMYIC GSLQRAWGDK
481 KISNTAFITT ATKVDNAIEP SNVIDMTKIA VYQDTHVGKE VQTSDDTL SL LGYTGIGEQA
541 IGS DRDRVVR ISVLPETGAR GGNHP IFYKN SIKLGYVIRS IDVFNSQILH TSRQLSLNHY
601 LLPPDSFAVY RIIDSNGSWF DIGIDSDGFS FVGVSSIGKL EFPLTASYMG IQLAKIRLAS
661 NIRSSMTKL
```

VP2 protein sequence

```
1 MNSILGLIDT VTNTIGKAQQ IELDKAALGQ QRELALKRMK LDHQALNNQV EQFNKILEQR
61 VQGPIQSVRL ARAAGFRVDP YSYTDQNFYD DQLNAIRLSY RNLFKN
```

SD 1

Protein sequences for FCV strain F9 major capsid protein VP1 and minor capsid protein VP2.

Supplemental Data 2

Table S2a

VP1 Chain A	% accessible area buried		fJAM-A ^A	% accessible area buried
LYS 399	10		TYR 31	30
ASN 400	50		SER 33	40
GLY 401	70		GLU 34	10
ALA 402	50		ARG 38	10
LYS 403	20		VAL 39	40
LYS 429	10		PRO 40	70
THR 431	90		ASP 42	10
PRO 432	70		LYS 43	70
ALA 433	80		PRO 44	90
GLY 434	50		ALA 45	80
ASP 435	50		LYS 46	90
TYR 436	10		SER 48	20
ALA 437	80		SER 50	70
ILE 438	20		TYR 51 (ASN 444)	100
THR 439	100		SER 52	50
LYS 441	10		GLY 53	20
SER 442	30		PHE 54	60
GLY 443	80		SER 55	20
ASN 444 (TYR 51)	60		ASN 56	10
ASP 445	70		PRO 57	60
ILE 446	80		THR 87	20
THR 448	20		SER 89	60
ASN 461	60		HIS 90	60
THR 462	40		SER 91	100
ASN 463	90		THR 94	80
ASP 495	30		PHE 95	70
ASN 496 (HIS 96)	90		HIS 96 (ASN 496)	60
ALA 497	100		SER 97	10
VAL 517	10		PRO 130	50
GLY 518	60		PRO 131	10
LYS 519	60		TYR 217	60
GLU 520	20		GLY 218	50
			MET 219	20
			MET 221	20

Table S2b

VP1 Chain A	% accessible area buried		fJAM-A ^B	% accessible area buried
GLY 478	20		TYR 31	20
LYS 480	40		SER 33	70
LYS 481	30		GLU 34	10
			SER 50	40

Table S2c

VP1 Chain B	% accessible area buried		fJAM-A ^A	% accessible area buried
LYS 480 (SER 33)	50		TYR 31	20
LYS 481	30		THR 32	10
			SER 33 (LYS 480)	70
			GLU 34	10
			SER 50	40

Table S2d

VP1 Chain B	% accessible area buried	fJAM-A ^B	% accessible area buried
LYS 399	10	TYR 31	10
ASN 400	50	SER 33	20
GLY 401	70	GLU 34	20
ALA 402	70	PRO 40	80
LYS 429	10	GLU 41	10
THR 431	90	ASP 42	10
PRO 432	60	LYS 43	70
ALA 433	70	PRO 44	80
GLY 434	50	ALA 45	70
ASP 435	50	LYS 46 (ASN 463)	80
TYR 436	10	SER 48	10
ALA 437	50	SER 50	60
THR 439	100	TYR 51 (ASP 445)	100
LYS 441	10	SER 52	40
SER 442	60	GLY 53	20
GLY 443	90	PHE 54 (ASN 444)	90
ASN 444 (PHE 54)	70	SER 55	10
ASP 445 (TYR 51)	70	PRO 57	50
VAL 459	10	THR 87	30
ASN 461	80	SER 89	50
THR 462	10	HIS 90	60
ASN 463 (LYS 46)	70	SER 91	90
VAL 494	20	THR 94	90
ASP 495	10	PHE 95	50
ASN 496 (HIS 96)	80	HIS 96 (ASN 496)	70
ALA 497	100	SER 97	20
GLY 518	60	PRO 130	50
LYS 519	70	TYR 217	80
GLU 520	30	GLY 218	50
		MET 219	40
		MET 221	10

Table S2e

VP1 Chain C	% accessible area buried		fJAM-A ^C	% accessible area buried
ASN 400	40		TYR 31	10
GLY 401	70		SER 33	30
ALA 402	50		GLU 34	20
LEU 404	30		PRO 40	90
LYS 429	20		GLU 41	10
THR 431	90		ASP 42 (ASN 496)	30
PRO 432	60		LYS 43	70
ALA 433	80		PRO 44	90
GLY 434	40		ALA 45	60
ASP 435	40		LYS 46 (ASN 463)	90
TYR 436	10		SER 50	60
ALA 437	80		TYR 51 (ASP 445)	100
ILE 438	60		SER 52	40
THR 439	100		GLY 53 (ASN 444)	20
LYS 441	10		PHE 54 (ASN 444)	60
SER 442	60		SER 55	10
GLY 443	90		PRO 57	80
ASN 444 (GLY 53, PHE 54)	70		ASN 76	10
ASP 445 (TYR 51)	80		THR 87	20
THR 447	10		SER 89	60
VAL 459	10		HIS 90	70
ASN 461	80		SER 91	100
ASN 463 (LYS 46)	70		THR 94	100
VAL 494	20		PHE 95	80
ASP 495	10		HIS 96	70
ASN 496 (ASP 42)	100		SER 97	20
ALA 497	100		LEU 128	10
VAL 517	20		VAL 129	10
GLY 518	70		PRO 130	40
LYS 519	60		TYR 217	70
GLU 520	50		GLY 218	80
			MET 219	20

Table S2f

VP1 Chain C	% accessible area buried		fJAM-A ^D	% accessible area buried
GLY 478	10		TYR 31	20
LYS 480	40		SER 33 (LYS 481)	60
LYS 481 (SER 33, GLU 34)	40		GLU 34 (LYS 481)	20
			SER 48	10
			SER 50	30

Table S2g

VP1 Chain D	% accessible area buried		fJAM-A ^C	% accessible area buried
GLY 478	10		TYR 31	20
LYS 480	40		SER 33	70
LYS 481	40		GLU 34	30
			SER 50	20

Table S2h

VP1 Chain D	% accessible area buried		fJAM-A ^D	% accessible area buried
ASN 400	60		TYR 31	10
GLY 401	70		SER 33	30
ALA 402	40		GLU 34	20
LEU 404	10		PRO 40	80
LYS 429	10		GLU 41	10
THR 431	90		ASP 42	20
PRO 432	60		LYS 43	70
ALA 433	70		PRO 44	80
GLY 434	50		ALA 45	70
ASP 435	50		LYS 46	90
TYR 436	10		SER 48	20
ALA 437	70		SER 50	70
ILE 438	10		TYR 51	90
THR 439	100		SER 52	30
LYS 441	10		GLY 53	20
SER 442	20		PHE 54	50
GLY 443	90		SER 55	10
ASN 444	70		PRO 57	50
ASP 445	90		THR 87	20
THR 447	10		SER 89	
VAL 459	10		HIS 90	50
ASN 461	80		SER 91	80
THR 462	10		THR 94	100
ASN 463	70		PHE 95	100
VAL 494	10		HIS 96 (ASN 496)	80
ASP 495	10		SER 97	60
ASN 496 (HIS 96)	100		PRO 130	10
ALA 497	100		TYR 217	60
VAL 517	10		GLY 218	60
GLY 518	60		MET 219	50
LYS 519	40			20
GLU 520	10			

SD 2

Tables to show the amino-acid residues that contribute to the interfaces between FCV VP1 and the fJAM-A. The tables list amino acids contributing to contact interfaces in each column, rows do not indicate direct interactions between specific amino-acid residues. Interfaces are described for VP1 chain A bound to fJAM-A^A, the molecule primarily bound to chain A (3a), and to fJAM-A^B, the molecule primarily bound to VP1 chain B (3b). Similarly, we show interface data for VP1 chain B contacts with fJAM-A^A and fJAM-A^B (3c and 3d respectively), VP1 chain C contacting fJAM-A^C and fJAM-A^D (3e and 3f respectively) and VP1 chain D interfaces with fJAM-A^C and fJAM-A^D (3g and 3h respectively). Residues coloured blue are predicted to form a hydrogen bond with the residue in brackets, residues coloured red are predicted to form a salt-bridge.

Norwalk D-SFVVAGRVMTCPSPDFNFLFLVPPTVEQKTRPFTLPNLPSSLS---NSRAPLPSS 252
 MNV E-SFVVSGRLLSKPAADFNFVYLTPIPIERTIYRMVDLPVLPRLCT---HARWPAPIYG 251
 RHDV T--SAIQVTVETRPSEDFEFVMIKAPSSKTVDISIPAGLLTTPVLTGVGNDNRWNGQIVG 261
 Vesivirus2117 TTGTSCVTVEVTRGGTDFEHLKPPSRKMIFGADPSRLIPKKSMEFW--GNRHPGEFKG 398
 FB-NJ-13 SNSSGCIITVETKPGPDFKFHLLKPPGSMLVHGSIPSNLIPKSSSLWI--GNRHWSIDITD 360
 F4 SNSSGCIIVTVETKPGPDFKFHLLKPPGSLVTHGSIPSDLIPKSSSLWI--GNRYWTDITD 360
 F9 ANSSGCIIVTVETKPGPDFKFHLLKPPGSMVTHGSIPSDLIPKSSSLWI--GNRYWSDITD 360
 C6 SNSSGCIIVTVETKPGPDFKFHLLKPPGSMVTHGSIPSDLIPKSSSLWI--GNRFWSDITD 360
 FCV5_3M8L SNSSGCIIVTVETKPGPDFKFHLLKPPGSMVTHGSVPCLLIPKSSSLWI--GNRFWSDITD 232
 : : . **:* : *

Norwalk MGISPDNVQ--SVQFQNGRCTLDRGLVGTTPVSLSHVAKIR-----GTSNGTVINL 301
 MNV LLVDPSPS--NPQWQNGRVVDGTLGTTPISGSWVSCFAAEAAEFQSGIGEVATFSL 309
 RHDV LQVPVGGFSTCNRHWNLNGSTYGWSSPRFGDIDHR-----RGSASYSGSNA--TNVLQFWY 315
 Vesivirus2117 FSIKPLVF-QANRHFDCKRQTFGWSTPEHAGVKLN-----IQRQLDTEDEK--TD-IGVH- 449
 FB-NJ-13 FVIRPSVF-QANRHFDKQETAGWSTPRFRPMTIT-----ISQKQSA-----K-LGI-- 405
 F4 FVIRPFVF-QANRHFDNQEETAGWSTPRFRPITIT-----ISEKNGS-----K-LGI-- 405
 F9 FVIRPFVF-QANRHFDNQEETAGWSTPRFRPISVT-----ITEQNGA-----K-LGI-- 405
 C6 FVIRPFVF-QANRHFDNQEETAGWSTPRFRPITIT-----ISVKESA-----K-LGI-- 405
 FCV5_3M8L FVIRPFVF-QANRHFDNQEETAGWSTPRFRPITVT-----ISQKEGE-----M-LGI-- 277
 : * . : : : . :

Norwalk TELDGTGTP-FHPFEGPAPIGFDDLGGCDWH---INMTQ---FG---HSSQTQYVDVT---- 347
 MNV VEQDGSAYVPGDRAAPLGYPDFSGQLEI---XVQTE---TT---K-SGDKLVVTT---F 355
 RHDV AN-AGSAIDNPISQVAPDGFDMFVFPNGGIPAAGWVGFAGIWNNSNGAPNVTTVQAY 374
 Vesivirus2117 ---LVTG-LKTIKSOVDPGWPDYGRNII---LANTT-ASFG-----EVSEAMLGTVVY 496
 FB-NJ-13 ---AVA-LESIVPGIPDGWPDTTIDSNL---IPAGD-YAIT---NQADNDITTAMEY 451
 F4 ---GVA-TDYIIPGIPDGWPDTTIADKL---IPAGD-YSIT---TGEENDIKTAQAY 451
 F9 ---GVA-TDYIVPGIPDGWPDTTIPGEL---IPAGD-YAIT---NGTGNNDITTATGY 451
 C6 ---GVA-TDYIVPGIPDGWPDTTIPGEL---VPVGD-YAIT---NGTNNNDITTAAQY 451
 FCV5_3M8L ---GVA-TDYIVPGIPDGWPDTTIPNEL---IPAGD-YAIT---NQSGNDIQTKEYE 323
 * * : ** :

Norwalk -----TPDTFVPHLGSIQA---NGIGSGNYV---GVLSWI---SPPSHPSGSQVD 388
 MNV EMV--LGPTTNDQTPYXGKVYA---SVTAASSLD---LVDGRV--RAVPRSVYGFQ-- 402
 RHDV ELGFATGAPGNLQPTT-----NTSGAQTVAKSIY---AVVTGTA-----QN 412
 Vesivirus2117 RVSGK---LEWRHLP---EIAFASGTAKNSTIVCGKHLTG---NFYVGG---NFTQ 540
 FB-NJ-13 DAATEIKNNTNFRSMYICGALQRAWGDKKVSNTAFITADLDG---NTIKPN---NVIN 504
 F4 DTAADVKNNTNFRSMYICGSLQRAWGDKKISNTAFITTAIRDG---NEIKPS---NTID 504
 F9 DTADIIKNNTNFRSMYICGSLQRAWGDKKISNTAFITATLDGDNKINPC---NTID 507
 C6 DAATEIRNNTNFRSMYICGSLQRAWGDKKISNTAFITTTGTVDG---AKLIPS---NTID 504
 FCV5_3M8L ESAMIISNNTNFRSMYICGSLQRAWGNKKVSNTAFITATVKE---NKLIPS---NTID 376
 .

Norwalk LWKIPNYGS-----S-----ITEATHLAPSVPYPPGFGEV 417
 MNV -DALPEYND-----G-----LL--FPLAPPIGPFLPGEI 428
 RHDV PAGLFVMAS-----GIISTPNASAITYPQDRIVTTPGTPAAAPVG-KNT 457
 Vesivirus2117 QGNVVVYPAFW-----TSKHGDTKCIGEDEDMVKRIDVLPQAQTG-GNY 584
 FB-NJ-13 QSRRIIVYQDNHVNLOVQTSSEVTLAMLGYTGIGEEVIGANRDRVVRINVLPEVSARG-GNH 563
 F4 MTKLAVYQDTHVEQEVQTSDDTLALLGYTGIGEEAIGSNRDRVVRISVLPEAGARG-GNH 563
 F9 QSKIVVFQDNHVGKKAQTSDDTLALLGYTGIGEEAIGSDRDRVVRISTLPEAGARG-GNH 566
 C6 QTKIAVFQDTHANKHVQTSDDTLALLGYTGIGEEAIGADRDRVVRISVLPERGARG-GNH 563
 FCV5_3M8L QTKIAIFQDNHVRDVQTSDDTLALLGYTGIGEEAIGADREKVVRIIGVLPEAGARG-GNH 435
 : * :

Norwalk LVFFMSKM-----PGPGAYNLPCLLPQEYISHLASEQAPT-----VGEAALLH 460
 MNV LLRFRTYMRRVDSTDTSAQALDCALPQEFVSWFANNSFTV-----QSEXLLLX 476
 RHDV PIMFASVVRRTGDNVATAGSA-----NGTQYGTGSQPLPVTIGLSLNYYSSALMPGQFFV 512
 Vesivirus2117 PIYYVTEFPAAALP-----APRVYNSQLLWTSRLLAQDVYD--IGPEALAV 628
 FB-NJ-13 PIYYKNSLKLGYVIR-----SIDVFNSQLLHTSRQLALNNYL--LDPDCFVAV 608
 F4 PIFYKNSIKLGYVIR-----SIDVFNSQLLHTSRQLSLNHYL--LPPDSFAV 608
 F9 PIFYKNSIKLGYVIR-----SIDVFNSQLLHTSRQLSLNHYL--LPPDSFAV 611
 C6 PIFHKNSIKLGYVIR-----SIDVFNSQLLHTSRQLSLNHYL--LSPDSFAV 608
 FCV5_3M8L PIFYRNSMKLGYVIK-----SIDVFNSQLLHTSRQLSLNNYL--LSPDSFAV 480
 : . . . : :

Norwalk	YVDPDTGRNLGEFKAYPDGFLTCVPNGA-SSGPQQLPINGVVFVSWVSRFYQLKPVGTA	519
MNV	YRNTLTGQLLFECKLYSEGYIALSYS---GSGPLTFPXDGFFXVVSWPRLYQLTSVGS	533
RHDV	WQLTF-ASGFMEIGLSVDGYFYAGTGASTTLIDLTELIDVRPVGPPSKSTLVFN-LGGT	570
Vesivirus2117	FKIKDSAGNWFDIGISCEGFSFVGASTLP-FSSLQFPLEASYVGMASAHNKLQHN-IAGT	686
FB-NJ-13	YRITDSNGSWFDIGIDYSGFSFVGVS---IGALEFPLTASYTGIQLAKIRLASN-IRSS	664
F4	YRIIDSNGSWFDIGIDSEGFSAFVGVS---IGKLEFPLSASYMGIQLAKIRLASN-IRSR	664
F9	YRIIDSNGSWFDIGIDSDGFSFVGVS---FGKLEFPLSASYMGIQLAKIRLASN-IRSP	667
C6	YRIIDSNGSWFDIGIDNDGFSFVGVS---IGKLEFPLTASYMGIQLAKIRLASN-IRSV	664
FCV5_3M8L	YRIIDSNGSWFDIGIDSDGFSFVGVS---IGKLEFPLTASYMGNQLAKIRLASN-IR--	534
	: : .*: . . :	
Norwalk	SSARGRLGLRR	530
MNV	XTGRSLKS---	541
RHDV	ANGFSYV----	577
Vesivirus2117	SVTL-----	690
FB-NJ-13	MTKL-----	668
F4	MTKL-----	668
F9	MTKL-----	671
C6	MTKL-----	668
FCV5_3M8L	-----	534

SD 3

Protein sequence alignment for VP1 proteins of Norwalk virus, Murine norovirus, Rabbit haemorrhagic disease virus, Vesivirus 2117 and several strains of FCV. Highlighted in yellow are the aromatic amino-acid residues that are arranged about the icosahedral three-fold symmetry axes of these viruses.

Supplemental Data 4

Table S4a

VP2 Chain I Conformer 2	% accessible area buried		VP1 Chain D	% accessible area buried
LEU 70	10		ARG 365	50
ARG 72	10		VAL 457	10
ALA 73	40		GLN 539	40
ALA 74	90		ALA 540	50
GLY 75	60		SER 543	80
PHE 76	20		ASP 544	40
			ARG 545	10
			PHE 584	10

Table S4b

VP2 Chain J Conformer 1	% accessible area buried		VP1 Chain A	% accessible area buried
ARG 97 (THR 410)	50		PHE 375	70
TYR 100	80		ASN 378 (ASN 106)	10
ARG 101 (TYR 412)	80		GLN 379	60
LEU 103	30		GLU 380 (ASN 106)	30
PHE 104	100		THR 386	100
LYS 105	10		PRO 387	70
ASN 106 (GLU 380, ASN 378)	50		ARG 388	40
			ARG 390	10
			THR 393	10
			THR 410 (ARG 97)	50
			ASP 411	70
			TYR 412 (ARG 101)	50
			ILE 413	70
			ASP 419	20
			SER 596	100
			LEU 597	40

Table S4c

VP2 Chain J Conformer 1	% accessible area buried		VP1 Chain B	% accessible area buried
THR 84	20		SER 346	30
ASP 85	20		SER 347	20
GLN 86	70		SER 348	100
ASN 87	40		LEU 349	30
TYR 89	30		ASP 358	40
GLN 92	70		ILE 359	90
ALA 95	60		THR 360	70
ILE 96	80		ASP 361	10
SER 99	60		LYS 569	10
TYR 100	30		SER 571	50
LEU 103	40		SER 580	10
			ASN 616	20
			LYS 639	30
			LEU 640	40
			GLU 641	80
			PHE 642	100
			PRO 643	60

Table S4d

VP2 Chain J Conformer 1	% accessible area buried	VP1 Chain D	% accessible area buried
LYS 55	20	THR 360 (ARG 77)	40
GLN 59 (ASP 456)	50	ASP 361	100
GLN 62	50	PHE 362	20
ILE 65	40	VAL 363	100
GLN 66	40	ILE 364	100
VAL 68	30	ARG 365 (TYR 81)	60
ARG 69 (ASP 453, ALA 455)	100	PRO 366	100
LEU 70	10	PHE 367	100
ARG 72 (ASP 582)	60	LYS 441	10
ALA 73	70	TYR 452	40
PHE 76	10	ASP 453 (ARG 69)	70
ARG 77 (LEU 640, THR 360)	60	ALA 455 (ARG 69)	90
VAL 78	30	ASP 456 (GLN 59)	70
ASP 79	80	VAL 457	60
TYR 81 (ARG 365)	70	ILE 458	50
SER 82	60	GLN 539	80
TYR 83	50	ALA 540	50
THR 84	90	SER 543	10
ASP 85	10	ARG 545	30
GLN 86	20	VAL 553	10
ASP 91	60	GLU 556	60
ASN 94	60	THR 557	50
ALA 95	40	GLY 558	40
LEU 98	80	ALA 559	10
ASN 102	20	HIS 564	50
LYS 105	10	LYS 569	70
		ARG 579	30
		SER 580	20
		ILE 581	70
		ASP 582	90
		PHE 584	100
		GLU 627	10
		VAL 634	20
		SER 635	30
		SER 636	10
		ILE 637	10
		GLY 638	10
		LYS 639	50
		LEU 640 (ARG 77)	50
		PHE 642	20

Table S4e

VP2 Chain K Conformer 2	% accessible area buried		VP1 Chain B	% accessible area buried
LEU 70	10		ARG 365	40
ARG 72	10		VAL 457	20
ALA 73	40		GLN 539	50
ALA 74	90		ALA 540	40
GLY 75	60		SER 543	50
PHE 76	20		ASP 544	40
			ARG 545	10
			PHE 584	10

Table S4f

VP2 Chain L Conformer 1	% accessible area buried		VP1 Chain C	% accessible area buried
ARG 97 (THR 410, ASP 411)	60		PHE 375	60
TYR 100	80		ASN 378	10
ARG 101	60		GLN 379	40
LEU 103	30		GLU 380 (ASN 106)	30
PHE 104	100		THR 386	100
ASN 106 (GLU 380)	50		PRO 387	70
			ARG 388	50
			ARG 390	10
			THR 393	10
			THR 410 (ARG 97)	40
			ASP 411 (ARG 97)	60
			TYR 412	50
			ILE 413	70
			ASP 419	10
			ARG 593	10
			SER 596	100
			LEU 597	30

Table S4g

VP2 Chain L Conformer 1	% accessible area buried		VP1 Chain D	% accessible area buried
THR 84	20		SER 346	40
ASP 85	30		SER 347	30
GLN 86	100		SER 348	100
ASN 87 (LYS 639)	40		LEU 349	30
TYR 89	40		ASP 358	30
GLN 92	70		ILE 359	70
ALA 95	50		THR 360	90
ILE 96	70		LYS 569	20
SER 99	50		SER 571	50
TYR 100	30		ASN 616	20
LEU 103	40		LYS 639 (ASN 87)	40
PHE 104	10		LEU 640	30
			GLU 641	70
			PHE 642	100
			PRO 643	60

Table S4h

VP2 Chain L Conformer 1	% accessible area buried	VP1 Chain B	% accessible area buried
LYS 55	20	THR 360	40
GLN 59	30	ASP 361	100
GLN 62	60	PHE 362	50
ILE 65	20	VAL 363	100
GLN 66	30	ILE 364	100
VAL 68	40	ARG 365	70
ARG 69 (TYR 452, ALA 455)	100	PRO 366	90
LEU 70	10	PHE 367	100
ARG 72 (ASP 582)	60	LYS 441	30
ALA 73	60	TYR 452 (ARG 69)	30
PHE 76	10	ASP 453	80
ARG 77 (LYS 639)	60	ALA 455 (ARG 69)	70
VAL 78	30	ASP 456	70
ASP 79	80	VAL 457	70
PRO 80	10	ILE 458	80
TYR 81 (ASP 582)	80	GLY 537	10
SER 82	70	GLN 539	60
TYR 83	50	ILE 541	20
THR 84	90	ARG 545	40
ASP 85	10	LEU 554	10
GLN 86	20	GLU 556	100
ASP 90	10	THR 557	40
ASP 91	60	GLY 558	30
ASN 94	80	HIS 564	50
ALA 95	40	LYS 569	50
LEU 98	80	ARG 579	20
ARG 101	10	SER 580	20
ASN 102	10	ILE 581	40
		ASP 582 (ARG 72)	90
		PHE 584	80
		GLU 627	10
		SER 635	30
		SER 636	20
		ILE 637	30
		GLY 638	30
		LYS 639 (ARG 77)	50
		LEU 640	70
		PHE 642	20

SD 4

Tables to show the amino-acid residues that contribute to the interfaces between FCV VP1 and the portal protein VP2. The tables list amino acids contributing to contact interfaces in each column, rows do not indicate direct interactions between specific amino-acid residues.

Residues coloured blue are predicted to form a hydrogen bond with the residue in brackets, residues coloured red are predicted to form a salt-bridge.

Supplemental Data 5

	pH3	pH4	pH5	pH6	pH7	pH8	pH9
Central tendency	178935	76897	51651	48826	82787	43448	31503
Variation (SD)	51311	31468	7331	11953	10387	7272	7147
F	369.6	389.7	42.35	-95.83	-19.77	-39.32	-75.39
Confidence Intervals	178 to 561.2	346 to 433.4	-4.138 to 88.84	-182.7 to -8.942	-107.2 to 67.65	-88.36 to 9.707	-117.9 to -32.9
Effect sizes (R²)	0.1324	0.6819	0.03294	0.03173	0.001376	0.01703	0.07818
Degrees of Freedom	1, 145	1, 145	1, 145	1, 145	1, 145	1, 145	1, 145
P value	0.0002	<0.0001	0.0737	0.0309	0.6556	0.1151	0.0006

SD 5 Statistical analysis of RNA release assay data for FCV in the presence of fJAM-A and at varying pH values. Linear regression was used to evaluate whether the slope for each plot of fluorescence against time under different pH conditions was non-zero.

Supplemental Data 6

fJAM-A:VP1 ratio	Dye only	1:1	1:2	1:5	1:7	1:9
Central tendency	9768	22308	26204	23988	12096	16671
Variation (SD)	3659	7353	5921	6791	4872	4158
F	-44.8	85.83	67.99	64.48	52.39	45.13
Confidence Intervals	-49.25 to -39.71	72.4 to 99.25	48.23 to 87.75	42.21 to 86.75	35.48 to 69.31	31.87 to 58.38
Effect sizes (R ²)	0.7008	0.5241	0.2417	0.1843	0.2053	0.2379
Degrees of Freedom	1, 145	1, 145	1, 145	1, 145	1, 145	1, 145
P value	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
	1:11	1:14	1:16	1:18	1:20	1:22
Central tendency	15158	16406	4355	3702	9267	12301
Variation (SD)	3732	4883	1857	1863	4485	1132
F	0.583	47.03	-3.222	5.4	17.12	8.194
Confidence Intervals	-20.65 to 21.81	33.8 to 60.26	-12.06 to 5.62	-8.314 to 19.11	4.075 to 30.17	-12.73 to 29.12
Effect sizes (R ²)	0.000002	0.2539	0.003564	0.004159	0.06602	0.007533
Degrees of Freedom	1, 145	1, 145	1, 145	1, 145	1, 145	1, 145
P value	0.9568	<0.0001	0.4726	0.4377	0.0106	0.4381

SD 6

Statistical analysis of RNA release assay data showing the RNA released by virions at low pH and in the presence of varying ratios of fJAM-A to VP1. Linear regression was used to evaluate whether the slope for each plot of fluorescence against time was non-zero.

Supplemental Data 7

Table S7a

PDB 1NBQ Human JAM-A Chain A	% accessible area buried		PDB 1NBQ Human JAM-A Chain B	% accessible area buried
MET 26	30		MET 26	30
ARG 59 (GLU 61, ASN 76)	90		ARG 59 (GLU 61, ASN 76)	90
GLU 61 (ARG 59)	80		GLU 61 (ARG 59)	80
LYS 63 (GLU 121)	70		LYS 63 (GLU 121)	70
ASP 68	10		ASP 68	10
THR 69	20		THR 69	20
THR 70	70		THR 70	70
ARG 71	40		ARG 71	40
LEU 72	100		LEU 72	100
TYR 75 (GLU 114)	100		TYR 75 (GLU 114)	100
ASN 76 (ARG 59)	10		ASN 76 (ARG 59)	10
THR 80	90		THR 80	90
ALA 81	30		ALA 81	30
SER 82	10		SER 82	10
MET 110	60		MET 110	60
SER 112	100		SER 112	100
GLU 113	20		GLU 113	20
GLU 114 (TYR 75)	20		GLU 114 (TYR 75)	20
GLY 115	50		GLY 115	50
GLY 116	100		GLY 116	100
ASN 117	40		ASN 117	40
SER 118	40		SER 118	40
TYR 119	100		TYR 119	100
GLY 120	20		GLY 120	20
GLU 121 (LYS 63)	30		GLU 121 (LYS 63)	30

Table S7b

fJAM-A Chain G (FCV bound)	% accessible area buried	fJAM-A Chain H (FCV bound)	% accessible area buried
ARG 58	50	ARG 58	60
LYS 62 (GLU 175)	50	GLU 60	30
THR 107	30	LYS 62 (GLU 175)	50
MET 109	60	THR 107	20
VAL 110	50	MET 109 (ARG 180)	80
SER 111	50	VAL 110	50
ASN 116	20	SER 111	80
THR 117	20	GLY 115	40
TYR 118 (ARG 180)	70	ASN 116	20
GLY 119	70	THR 117	30
GLU 120 (ARG 180)	100	TYR 118 (ARG 180)	90
VAL 121	10	GLY 119	70
SER 122	10	GLU 120	100
VAL 170	60	VAL 121	10
ARG 171	80	SER 122	10
PRO 173	100	VAL 170	50
LEU 174	30	ARG 171	70
GLU 175 (LYS 62)	50	PRO 173	100
ASN 179	30	LEU 174	30
ARG 180 (MET 109, TYR 118)	100	GLU 175 (LYS 62)	60
ALA 181	20	ASN 179	20
		ARG 180 (TYR 118, GLU 120)	80

SD 7 Tables to show the amino-acid residues that contribute to the interfaces between junctional adhesion molecule A. Human JAM-A forms homodimers via an interface in D1 (a). fJAM-A forms similarly shaped homodimers in solution, but when bound to FCV a second interaction disrupts the D1-D1 interface, leading to a new set of contacts between D1 and D2 of symmetry related molecules (b). The tables list amino acids contributing to contact interfaces in each column, rows do not indicate direct interactions between specific amino-acid residues. Residues coloured blue are predicted to form a hydrogen bond with the residue in brackets, residues coloured red are predicted to form a salt-bridge.