

Supporting Information

Baker et al. 10.1073/pnas.1309947110

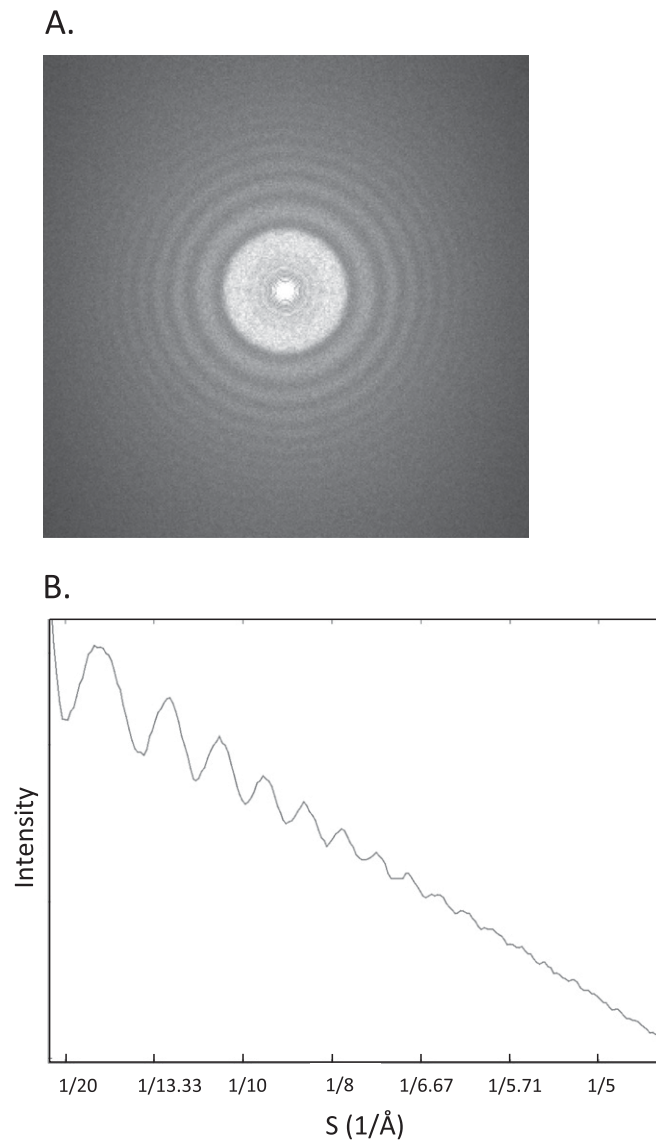


Fig. S1. Image quality assessment. (A) 2D average power spectra of ≈ 15 particles in a micrograph. (B) 1D rotational average of (A) showing signal beyond 5 \AA resolution.

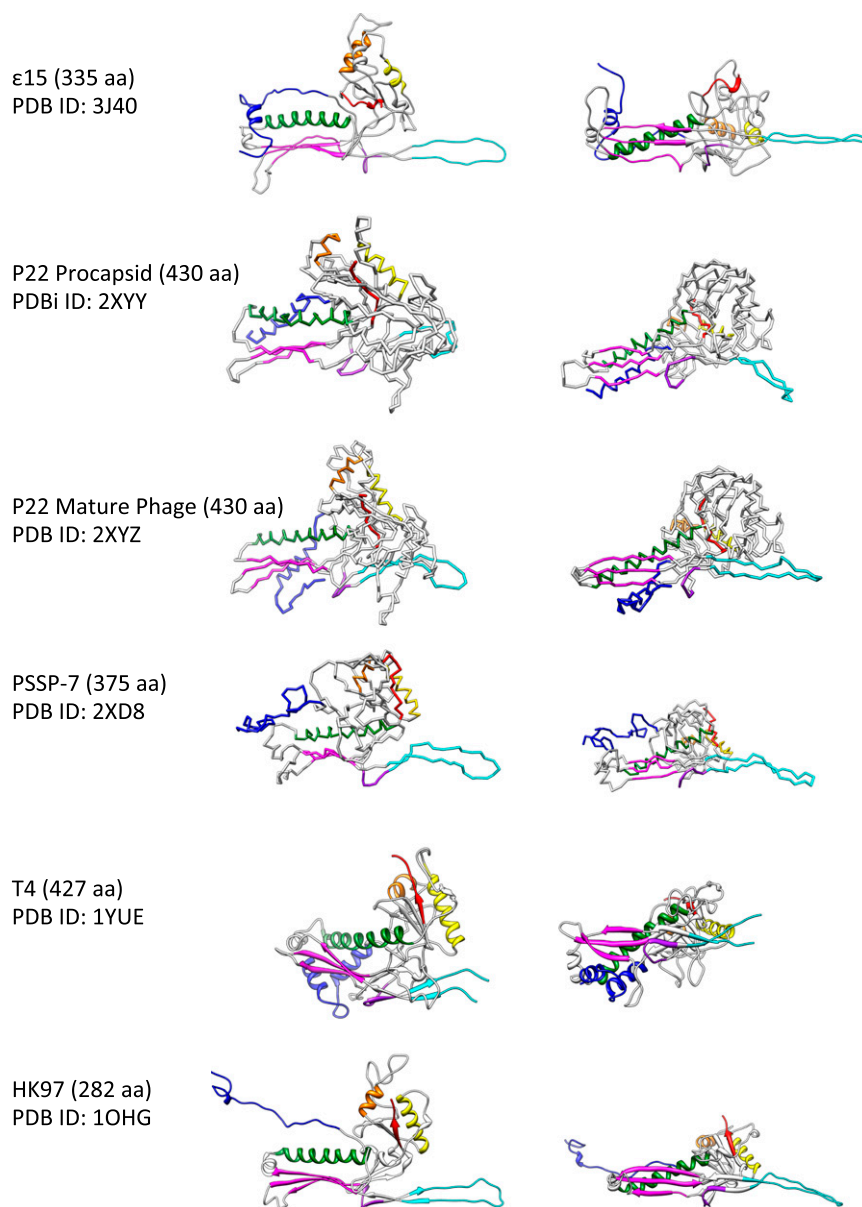


Fig. S6. Structural homologs of gp7. Two views of bacteriophage capsid protein structures are shown, colored by their functional domains. These functional domains are shown in Fig. 2B.

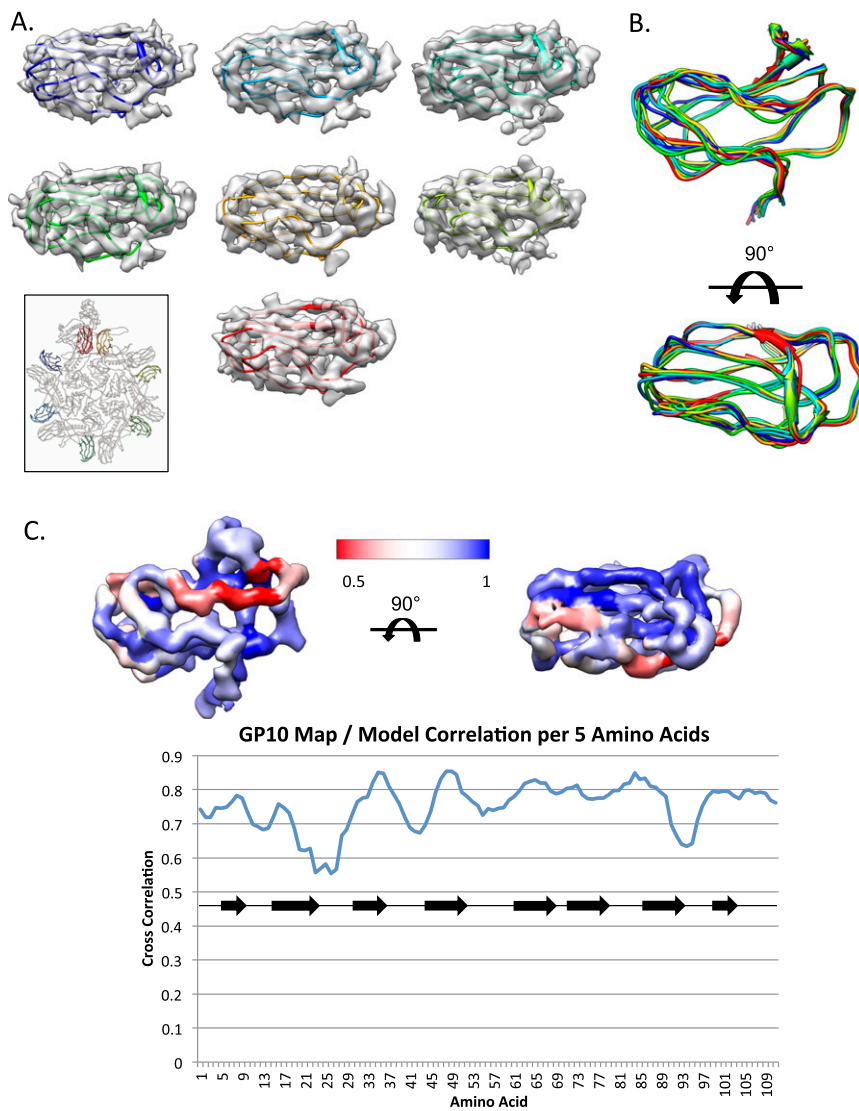


Fig. S7. Structure of gp10. (A) Seven individual gp10 subunits from an asymmetric unit are shown with the corresponding density. (B) Two views of the seven gp10 subunits are shown superimposed. (C) The average density map and model correlation (five amino acids window) for gp10 is shown. The correlation values are mapped on to the density map (Left), where red indicates poor correlation and blue indicates good correlation. These values are shown in the plot on the right.

Table S1. Cont.

Chain	Z	rmsd	lali	Nres	%id	Description
1wme-A	4.1	3.4	94	434	5	PROTEASE
4acq-A	4.1	3.6	85	1,270	6	ALPHA-2-MACROGLOBULIN
1k5m-A	4.1	3.6	89	283	7	COAT PROTEIN VP1 (P1D)
2jd9-A	4.1	3.6	87	139	2	YEGBM32
3km5-B	4	2.8	90	173	10	LYSINE SPECIFIC CYSTEINE PROTEASE
1ule-B	4	2.9	85	150	2	GALECTIN-2
3nap-C	4	3	94	276	5	CAPSID PROTEIN
2w87-B	4	3	87	138	11	ESTERASE D
2ygm-A	4	3.1	91	351	5	BLOOD GROUP A-AND B-CLEAVING ENDO-BETA-GALACTOSID
2vng-B	4	3.1	90	173	10	CPE0329
4d8m-A	4	3.4	95	585	6	PESTICIDAL CRYSTAL PROTEIN CRY5BA
4aw7-A	4	3.5	86	565	2	GH86A BETA-PORPHYRANASE
2zs6-B	4	3.6	83	420	6	HEMAGGLUTININ COMPONENTS HA3
1c3h-E	3.9	2.6	81	137	10	30 KD ADIPOCYTE COMPLEMENT-RELATED PROTEIN
2qfe-A	3.9	3	84	139	2	CALPAIN-7
1fpn-3	3.9	3.1	93	237	4	COAT PROTEIN VP1
2w47-A	3.9	3.2	83	135	11	LIPOLYTIC ENZYME, G-D-S-L
3k75-B	3.9	3.3	84	151	6	DNA REPAIR PROTEIN XRCC1
1hn0-A	3.9	3.4	91	971	7	CHONDROITIN ABC LYASEI
3km9-B	3.9	3.4	83	1,459	11	COMPLEMENT C5
1gr3-A	3.8	2.8	81	132	7	COLLAGEN X
1o91-A	3.8	2.9	82	131	5	COLLAGEN ALPHA 1(VIII) CHAIN
2vtx-D	3.8	3	75	89	4	NPM-A PROTEIN
1b35-C	3.8	3	93	282	5	PROTEIN (CRICKET PARALYSIS VIRUS, VP1)
4bcu-A	3.8	3.1	90	188	9	COAT PROTEIN
2w91-A	3.8	3.1	93	635	10	ENDO-BETA-N-ACETYLGLUCOSAMINIDASE D
3jr0-A	3.8	3.1	85	156	6	GENE 9 PROTEIN
1w8x-N	3.8	3.2	81	114	7	MAJOR CAPSID PROTEIN(PROTEIN P3)
2buk-A	3.8	3.4	91	184	8	COAT PROTEIN
1ciy-A	3.8	3.5	89	577	4	CRYIA(A)
2cdo-A	3.8	3.6	81	138	10	BETA-AGARASE 1
3cih-A	3.8	3.7	85	714	7	PUTATIVE ALPHA-RHAMNOSIDASE
3g6j-B	3.8	4.2	86	903	5	COMPLEMENT C3 BETA CHAIN
2wq4-A	3.7	2.7	82	134	11	LECTIN
2wdb-A	3.7	2.9	83	139	6	HYALURONOGLUCOSAMINIDASE
2k46-A	3.7	3.2	90	190	4	MGC80075 PROTEIN
3afk-A	3.7	3.3	84	168	2	ANTI-TUMOR LECTIN
1u5i-A	3.7	3.3	94	625	2	CALPAIN 2, LARGE [CATALYTIC] SUBUNIT PRECURSOR
2w3j-A	3.7	3.3	83	137	5	CARBOHYDRATE BINDINGMODULE
1d4m-1	3.7	3.3	90	284	4	PROTEIN (COXSACKIEVIRUS A9)
1zba-2	3.7	3.4	95	207	14	COAT PROTEIN VP1
2vzp-B	3.7	3.4	86	127	7	EXO-BETA-D-GLUCOSAMINIDASE
1aym-1	3.7	3.4	90	285	6	HUMAN RHINOVIRUS 16 COAT PROTEIN
1qxp-B	3.7	3.4	97	788	8	MU-LIKE CALPAIN
2v5d-A	3.7	3.4	89	722	4	O-GLCNACASE NAGJ
3rjr-C	3.7	3.5	91	343	9	TRANSFORMING GROWTH FACTOR BETA-1
2quo-A	3.7	3.6	85	123	1	HEAT-LABILE ENTEROTOXIN B CHAIN
1dlc-A	3.7	3.7	89	584	7	DELTA-ENDOTOXIN CRYIIIA
1ddl-A	3.7	3.8	91	188	5	RNA (5'-R(P*UP*UP*UP*UP*UP*U)-3')
2obe-A	3.7	3.9	88	915	1	HEXON
2xom-A	3.6	3	83	145	10	ARABINO GALACTAN ENDO-1,4-BETA-GALACTOSIDASE
1df0-A	3.6	3.1	90	624	2	M-CALPAIN
4gh4-B	3.6	3.4	94	207	13	CAPSID PROTEIN VP1
1gqp-B	3.6	3.4	95	188	5	DOC1/APC10
3pof-B	3.6	3.4	77	114	6	MANNAN-BINDING LECTIN SERINE PROTEASE 1
2p1b-A	3.6	3.4	76	100	4	NUCLEOPHOSMIN
1wmx-B	3.6	3.5	94	195	7	COG3291; FOG: PKD REPEAT
3toj-B	3.6	3.7	93	197	5	SET1/ASH2 HISTONE METHYLTRANSFERASE COMPLEX SUBUN
1wck-A	3.5	2.8	77	136	6	BCLA PROTEIN
1gmm-A	3.5	2.9	78	126	6	CBM6
2qdn-A	3.5	2.9	81	123	10	GITR LIGAND
1iqa-A	3.5	2.9	85	156	11	RECEPTOR ACTIVATOR OF NUCLEAR FACTOR KAPPA B

Table S1. Cont.

Chain	Z	rmsd	lali	Nres	%id	Description
1rj7-F	3.5	3	85	144	9	ECTODYSPLASIN A
1c28-A	3.5	3	81	123	4	PROTEIN (30 KD ADIPOCYTE COMPLEMENT-RELATED
2qe3-A	3.5	3	85	140	5	TNF SUPERFAMILY LIGAND TL1A
1sfp-A	3.5	3.1	76	111	9	ASFP
1nt0-A	3.5	3.1	78	257	5	MANNOSE-BINDING PROTEIN ASSOCIATED SERINE PROTEAS
3jyb-A	3.5	3.1	81	138	2	SENSOR PROTEIN
1dg6-A	3.5	3.2	87	149	6	APO2L/TNF-RELATED APOPTOSIS INDUCING LIGAND (TRAIL
1wky-A	3.5	3.2	86	446	5	ENDO-BETA-1,4-MANNANASE
2v24-A	3.5	3.2	91	197	3	SPRY DOMAIN-CONTAINING SOCS BOX PROTEIN 4
1a6c-A	3.5	3.2	88	513	7	TOBACCO RINGSPOT VIRUS CAPSID PROTEIN
4a6o-A	3.5	3.3	82	144	7	ALPHA-N-ACETYLGALACTOSAMINIDASE FAMILY PROTEIN
1gff-2	3.5	3.3	89	177	9	BACTERIOPHAGE G4 CAPSID PROTEINS GPF, GPG, GPJ
1mec-3	3.5	3.3	95	231	5	MENGO VIRUS COAT PROTEIN (SUBUNIT VP1)
1tmf-3	3.5	3.3	96	232	3	THEILER'S MURINE ENCEPHALOMYELITIS VIRUS
1opo-C	3.5	3.4	91	268	12	COAT PROTEIN
1qqp-2	3.5	3.4	96	216	11	PROTEIN (GENOME POLYPROTEIN)
1ihm-B	3.5	3.5	94	511	4	CAPSID PROTEIN
2y26-A	3.5	3.5	96	504	4	COAT PROTEIN
2ypj-A	3.5	3.6	87	122	2	ENDOGLUCANASE CEL5A
3see-A	3.4	2.7	91	214	2	HYPOTHETICAL SUGAR BINDING PROTEIN
1bev-1	3.4	3.1	89	268	7	BOVINE ENTEROVIRUS COAT PROTEINS VP1 TO VP4
1m06-G	3.4	3.1	89	187	2	CAPSID PROTEIN
1nzi-B	3.4	3.1	75	156	8	COMPLEMENT C1S COMPONENT
1k5j-A	3.4	3.1	76	94	5	NUCLEOPLASMIN CORE
1y4w-A	3.4	3.2	86	517	6	EXO-INULINASE
1f49-A	3.4	3.3	89	1,021	3	BETA-GALACTOSIDASE
3m8l-A	3.4	3.3	92	534	4	CAPSID PROTEIN
3ecq-B	3.4	3.3	89	1,347	9	ENDO-ALPHA-N-ACETYLGALACTOSAMINIDASE
4dzc-A	3.4	3.3	82	114	7	PLIG
1ns-A	3.4	3.3	88	763	3	X-PROLYL DIPEPTIDYL AMINOPETIDASE
2wzr-2	3.4	3.4	94	207	9	POLYPROTEIN
3cmg-A	3.4	3.4	87	661	3	PUTATIVE BETA-GALACTOSIDASE
2ii7-B	3.4	3.5	79	115	3	ANABAENA SENSORY RHODOPSIN TRANSDUCER PROTEIN
3mo4-A	3.4	3.6	88	456	9	ALPHA-1,3/4-FUCOSIDASE
2qkg-A	3.4	3.6	90	589	3	INSECTICIDAL DELTA-ENDOTOXIN CRY8EA1
1xna-A	3.4	3.6	88	151	6	PROTEIN (DNA-REPAIR PROTEIN XRCC1)
4es8-A	3.4	3.7	91	302	5	EPF
1oq1-A	3.4	3.7	93	223	4	PROTEIN YESU
1sdd-B	3.4	4	88	601	2	COAGULATION FACTOR V
2r32-A	3.3	2.8	71	140	7	GCN4-PII/TUMOR NECROSIS FACTOR LIGAND
1rb8-F	3.3	3.1	93	422	9	CAPSID PROTEIN
3b7m-A	3.3	3.1	91	216	5	CELLULASE
3ggl-A	3.3	3.2	85	161	12	PUTATIVE CHITOBIASE
1d2q-A	3.3	3.2	85	134	8	TNF-RELATED APOPTOSISINDUCING LIGAND
3cji-B	3.3	3.3	93	238	8	POLYPROTEIN
1rud-1	3.3	3.3	83	273	7	RHINOVIRUS 14
1c8n-C	3.3	3.4	95	219	5	COAT PROTEIN
1h8t-B	3.3	3.4	96	252	4	ECHOVIRUS 11 COAT PROTEIN VP1
4ag4-A	3.3	3.4	86	340	0	EPITHELIAL DISCOIDINDOMAIN-CONTAINING RECEPTOR 1
3ut0-A	3.3	3.5	95	804	9	EXO-1,3/1,4-BETA-GLUCANASE
1al0-G	3.3	3.5	95	175	7	SCAFFOLDING PROTEIN GPD
1tnv-B	3.3	3.5	93	186	0	TOBACCO NECROSIS VIRUS (SUBUNIT VP1)
1yjl-A	3.3	3.6	84	285	7	PEPTIDYL-GLYCINE ALPHA-AMIDATING MONOOXYGENASE
2r0f-A	3.3	3.7	87	163	5	CGL3 LECTIN
1xpw-A	3.3	3.7	80	143	6	LOC51668 PROTEIN
4gz9-A	3.2	3	80	562	6	NEUROFILIN-1
1k3i-A	3.2	3.1	81	651	7	GALACTOSE OXIDASE PRECURSOR
1poq-A	3.2	3.1	79	118	5	YPM
2y38-A	3.2	3.2	84	341	8	LAMININ SUBUNIT ALPHA-5
1spp-A	3.2	3.2	74	109	5	MAJOR SEMINAL PLASMA GLYCOPROTEIN PSP-1
2yue-A	3.2	3.2	87	168	3	PROTEIN NEURALIZED
2fnj-A	3.2	3.3	92	217	5	CG2944-PF, ISOFORM F

Table S1. Cont.

Chain	Z	rmsd	lali	Nres	%id	Description
4h7m-A	3.2	3.3	91	226	5	ENDO-1,4-BETA-GLUCANASE
1z7s-3	3.2	3.3	94	239	3	HUMAN COXSACKIEVIRUSA21
3iyp-C	3.2	3.4	97	252	4	CAPSID PROTEIN
1cov-3	3.2	3.4	97	238	3	COXSACKIEVIRUS COAT PROTEIN
1ev1-2	3.2	3.4	98	254	5	ECHOVIRUS 1
3vbf-B	3.2	3.4	96	245	7	GENOME POLYPROTEIN, CAPSID PROTEIN VP1
1eah-2	3.2	3.4	97	262	6	POLIOVIRUS TYPE 2 COAT PROTEINS VP1 TO VP4
1qkq-A	3.2	3.5	78	141	3	EOSINOPHIL LYSOPHOSPHOLIPASE
1mqt-B	3.2	3.5	98	254	4	POLYPROTEIN
3skv-A	3.2	3.5	78	354	8	SSFX3
4fy1-1	3.2	3.7	97	217	8	CAPSID PROTEIN
1ncq-A	3.2	3.7	91	273	8	COAT PROTEIN VP1
3sam-B	3.2	3.8	82	544	2	RIFAMPICIN RESISTANCEPROTEIN
1auy-B	3.2	4.4	96	189	4	TURNIP YELLOW MOSAICVIRUS
4g3y-C	3.1	2.9	76	147	9	INFLIXIMAB FAB L
4rhv-1	3.1	3.3	88	273	9	HUMAN RHINOVIRUS 14 C
3frl-B	3.1	3.3	91	232	2	LIPL32
1bzw-A	3.1	3.3	95	232	3	PROTEIN (PEANUT LECTIN)
1lgn-A	3.1	3.3	86	204	10	SERUM AMYLOID P COMPONENT
1o59-A	3.1	3.4	83	318	10	ALLANTOICASE
2zah-C	3.1	3.4	94	331	6	COAT PROTEIN
2gh8-A	3.1	3.5	89	544	8	CAPSID PROTEIN
1o8p-A	3.1	3.5	81	131	7	PUTATIVE ENDO-XYLANASE
4dy5-A	3.1	3.6	75	111	9	GIFS-1 PROPHAGE PROTEIN
3iii-A	3.1	3.8	86	556	5	COCE/NOND FAMILY HYDROLASE
3kb5-A	3.1	3.8	89	193	7	TRIPARTITE MOTIF-CONTAINING PROTEIN 72
3kq4-B	3	2.9	74	457	11	GASTRIC INTRINSIC FACTOR
1ovp-A	3	2.9	71	114	3	HYPOTHETICAL PROTEINLECB
3nv1-A	3	3	75	136	1	GALECTIN 9 SHORT ISOFORM VARIANT
1vbc-3	3	3.2	92	235	4	POLIOVIRUS TYPE 3
2wzp-P	3	3.3	77	298	6	PUTATIVE RECEPTOR BINDING PROTEIN
2w0c-L	3	3.5	102	335	7	MAJOR CAPSID PROTEINP2
3k94-B	3	3.5	72	216	1	THIAMIN PYROPHOSPHOKINASE
3a0n-A	3	3.5	93	242	5	VAL-1
2tbv-C	3	3.6	95	320	4	TOMATO BUSHY STUNT VIRUS
4dmi-B	3	3.7	75	169	11	CAPSID PROTEIN
1qjz-B	3	3.7	94	188	5	PHYSALIS MOTTLE VIRUS
2okx-B	3	3.7	86	954	2	RHAMNOSIDASE B
2v73-A	3	3.8	92	183	4	PUTATIVE EXO-ALPHA-SIALIDASE
2fbe-C	3	3.9	88	199	11	PREDICTED: SIMILAR TORET FINGER PROTEIN-LIKE 1
1p30-A	3	4.1	91	891	4	HEXON PROTEIN

A nonredundant list of the top DALI hits above 3.0 for gp10 are shown. "Chain" represents the four letter PDB ID and associated chain ID, "Z" is the DALI Z-score, "rmsd" is the root mean squared deviation between gp10 and the DALI hit over the aligned residues ("lali"). The sequence identity of the aligned residues is shown in the "%id" column; total domain length for the DALI hit is shown in the "nres" column. A short description of the hit is listed under the "Description" column.

Table S2. Potential salt bridges

gp7	gp7	gp10	Location	Density observed
Ser10	—	Lys2	N-arm	+++
Lys20	Asp48	—	N-arm:F-loop	+++
Lys33	Asp232	—	N-arm:A-domain	++
Lys51	—	Asp107	F-loop	+++
Arg57	Glu113	—	E-loop:long helix	+++
Glu62	Lys124	—	E-loop:long helix	+
Arg66	Asp96	—	E-loop:P-domain	—
Arg102	Asp225	—	P-domain:P-domain	—
Asp135	—	Arg41	A-domain	+++
His199	Glu200	—	P-domain:P-domain	—
Arg216	Glu221	—	P-domain:P-domain	+++
Asp263	Lys292	—	A-domain:A-domain	—
Asp269	Lys284	—	A-domain:A-domain	—
Glu-305	Lys310	—	A-domain	+++

A list of potential salt bridges was identified using PDBe PISA webserver. Residues for the relevant gp7 and gp10 subunits are indicated. A general location is given for the interaction (relative to gp10 in the case of gp7–gp10 interactions). Interactions across capsomeres are highlighted in red text in the location column. Visible density at the potential salt bridge locations is indicated with a rank for “–” (no density present) to “+++” where clear density is seen.