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Supplementary Table 1 | Interface of gp120 and gp41 in the HIV-1 viral spike.

a. gp120-gp41 interface within the same protomer.

Disulfide bond, Hydrogen bonds and salt bridges							
Type	**gp120**	**Dist.[Å]**	**gp41**	**Type**	**gp120**	**Dist.[Å]**	**gp41**
D*	G:CYS501[SG]	2.03	B:CYS605[SG]	H	G:VAL36[O]	3.44	B:THR606[N]
H	G:VAL36[N]	3.23	B:VAL608[O]	H	G:VAL38[O]	3.44	B:CYS604[N]
H	G:VAL38[N]	3.23	B:CYS604[O]	H	G:GLY41[O]	2.85	B:GLN540[NE2]
H	G:TYR40[N]	2.78	B:LEU602[O]	H	G:ILE491[O]	2.47	B:ARG585[NH2]
H	G:GLY222[N]	3.32	B:LEU544[O]	H	G:LEU494[O]	3.69	B:TYR643[OH]
H	G:CYS501[SG]	2.03	B:CYS605[SG]	H	G:VAL496[O]	3.01	B:TRP631[NE1]
H	G:ARG503[N]	3.69	B:ASN607[OD1]	H	G:PRO498[O]	3.22	B:TRP623[NE1]
H	G:ARG503[NE]	2.77	B:CYS605[O]	S	G:ARG503[NH1]	3.66	B:GLU654[OE1]
H	G:ARG503[NH1]	3.66	B:GLU654[OE1]	S	G:ARG503[NH1]	3.77	B:GLU654[OE2]
H	G:ARG503[NH2]	3.88	B:ASN651[OD1]	S	G:ARG503[NH2]	3.31	B:GLU654[OE2]
H	G:ARG503[NH2]	3.31	B:GLU654[OE2]	S	G:ASP107[OD1]	3.88	B:LYS574[NZ]
H	G:LEU34[O]	3.27	B:TRP610[N]				

List of interface residues (the residues on each row are not matched interactive partners)									
gp120	**HSD***	**ASA**	**BSA**	**ΔiG**	**gp41**	**HSD**	**ASA**	**BSA**	**ΔiG**
G:GLU32		159.45	4.30|	-0.05	B:LEU520		121.69	21.75||	-0.12
G:ASN33		89.08	2.66|	0.01	B:GLY521		26.76	8.18||||	0.13
G:LEU34	H	110.93	77.87||||||||	0.76	B:PHE522		97.67	71.75||||||||	0.51
G:TRP35		100.83	63.15|||||||	1.01	B:LEU523		109.67	109.67||||||||||	1.53
G:VAL36	H	114.66	114.66||||||||||	1.46	B:GLY524		27.66	25.36|||||||||	-0.07
G:THR37		30.75	25.23|||||||||	0.40	B:ALA525		10.37	5.95||||||	0.03
G:VAL38	H	106.47	104.98||||||||||	0.87	B:ALA526		41.11	39.96||||||||||	0.64
G:TYR39		105.81	81.77||||||||	1.01	B:GLY527		69.79	56.29|||||||||	0.37
G:TYR40	H	179.40	176.84||||||||||	0.80	B:SER528		36.71	6.97||	0.02
G:GLY41	H	56.83	56.83||||||||||	0.14	B:MET530		4.02	4.02||||||||||	0.06
G:VAL42		35.68	35.68|||||||||	0.53	B:ALA533		9.35	9.35||||||||||	0.10
G:PRO43		120.19	120.19||||||||||	1.42	B:SER534		34.69	8.52|||	0.07
G:VAL44		65.52	61.67||||||||||	0.99	B:THR536		14.87	0.67|	0.01
G:TRP45		54.65	44.97|||||||||	0.41	B:LEU537		55.20	46.56|||||||||	0.64
G:LYS46		120.67	43.68||||	-0.47	B:GLN540	H	43.31	43.31|||||||||	0.39
G:THR50		25.14	5.03|||	-0.06	B:ALA541		51.42	26.04||||||	0.38
G:THR51		113.45	69.78|||||||	0.90	B:ASN543		67.50	4.04|	-0.05
G:LEU52		17.22	12.82||||||||	-0.13	B:LEU544	H	101.31	92.14||||||||||	0.99
G:PHE53		85.28	39.95|||||	0.64	B:LEU545		73.00	8.28||	-0.06
G:CYS54		42.46	32.07||||||||	0.95	B:SER546		84.70	8.33|	0.08
G:ALA70		37.95	31.06|||||||||	0.24	B:THR569		176.82	10.29|	0.01
G:THR71		14.13	1.57||	0.00	B:VAL570		125.76	35.73|||	0.57
G:HIS72		121.47	5.88|	0.06	B:TRP571		220.73	156.50||||||||	1.92
G:ALA73		96.56	29.12||||	0.24	B:GLY572		37.57	18.36|||||	0.29
G:CYS74		23.63	7.73||||	0.17	B:LYS574	S	152.09	82.95||||||	0.70
G:VAL75		78.47	11.55||	0.18	B:GLN575		92.61	41.82|||||	0.67
G:ILE84		99.58	66.43|||||||	1.06	B:GLN577		134.10	6.02|	0.10
G:HIS85		78.96	1.35|	-0.02	B:ALA578		57.70	53.73|||||||||	0.71
G:LEU86		30.31	29.33|||||||||	0.47	B:ARG579		151.60	3.66|	0.05
G:GLU87		119.82	18.20||	-0.05	B:LEU581		110.03	27.96|||	0.45
G:ASN88		153.77	33.19|||	0.03	B:ALA582		40.33	33.52|||||||||	0.50
G:VAL89		37.55	31.55|||||||||	0.50	B:ARG585	H	143.40	111.70||||||||	-1.49
G:GLU91		30.92	4.37||	-0.07	B:TYR586		44.47	4.86||	0.07
G:GLN103		36.99	3.93||	0.03	B:ARG588		110.32	8.29|	-0.25
G:THR106		80.82	1.23|	-0.01	B:ASP589		57.71	54.89|||||||||	0.08
G:ASP107	S	61.19	45.56||||||||	-0.27	B:GLN590		43.04	13.39||||	-0.15
G:SER110		55.55	0.37|	-0.00	B:LEU592		49.31	7.70||	0.12
G:LEU111		27.14	6.17|||	0.10	B:LEU593		45.47	42.80|||||||||	0.68
G:GLN114		120.33	31.88|||	-0.10	B:TRP596		31.12	29.58|||||||||	0.47
G:ILE215		13.89	7.54|||||	0.12	B:GLY597		27.87	21.33||||||||	0.10
G:PRO220		41.14	34.13|||||||||	0.55	B:CYS598		28.15	7.27|||	0.30
G:ALA221		100.15	84.00|||||||||	0.92	B:LYS601		100.71	9.72|	0.16
G:GLY222	H	45.99	42.17|||||||||	0.36	B:LEU602	H	109.20	36.90||||	-0.19
G:PHE223		53.56	40.21||||||||	0.53	B:ILE603		132.63	27.62|||	0.44
G:ALA224		16.56	15.06|||||||||	0.24	B:CYS604	H	51.21	33.54|||||||	0.02
G:LEU226		2.85	2.85|||||||||	0.05	B:CYS605	HD	122.91	92.60||||||||	2.38

*. D: Disulfide bond, H: Hydrogen bond, S: Salt bridge.
ASA: Accessible Surface Area, Å², BSA: Buried Surface Area, Å², ΔiG: Solvation energy effect, kcal/mol, ||||: Buried area percentage, one bar per 10%.

gp120	HSD*	ASA	BSA	ΔiG	gp41	HSD	ASA	BSA	ΔiG
G:THR244		24.69	21.63||||||||	0.25	B:THR606	H	50.11	49.65|||||||||	-0.26
G:GLN246		85.27	1.22|	-0.02	B:ASN607	H	124.12	79.55||||||	-0.46
G:VAL489		0.34	0.34||||||||||	0.01	B:VAL608	H	37.64	31.45||||||||	-0.08
G:LYS490		73.37	17.59|||	0.25	B:PRO609		117.67	28.85|||	0.45
G:ILE491	H	61.56	61.56|||||||||	0.58	B:TRP610	H	120.54	93.20||||||||	1.27
G:GLU492		66.22	16.94|||	0.16	B:TRP614		17.78	1.72|	0.03
G:PRO493		36.83	35.49|||||||||	0.57	B:ARG617		120.66	11.78|	-0.13
G:LEU494	H	126.36	110.93||||||||	1.37	B:ASN618		90.29	5.61|	-0.03
G:GLY495		22.28	16.59|||||||	0.26	B:LEU619		122.62	80.84|||||||	1.19
G:VAL496	H	111.77	105.32|||||||||	1.09	B:ILE622		19.73	18.90|||||||||	0.30
G:ALA497		40.47	40.47|||||||||	0.64	B:TRP623	H	88.48	63.25||||||||	0.83
G:PRO498	H	85.23	85.23|||||||||	0.85	B:TRP628		104.58	102.71|||||||||	1.60
G:THR499		44.62	19.72|||||	0.20	B:LEU629		134.49	88.15||||||	1.41
G:ARG500		189.46	32.79||	-0.35	B:TRP631	H	28.70	24.25||||||||	-0.01
G:CYS501	HD	74.02	24.28||||	0.81	B:ASP632		83.43	62.02||||||||	-0.30
G:LYS502		140.46	28.75|||	0.46	B:LYS633		159.78	16.90||	0.27
G:ARG503	HS	206.15	158.06||||||||	-1.47	B:ILE635		7.69	5.85||||||||	0.09
G:ARG504		207.48	14.46|	-0.16	B:SER636		54.68	6.70||	0.11
G:VAL505		195.08	15.78|	0.23	B:THR639		37.06	7.68|||	0.12
					B:ILE642		28.01	28.01|||||||||	0.45
					B:TYR643	H	80.82	41.37||||||	-0.04
					B:LEU646		21.93	21.76|||||||||	0.35
					B:GLN650		19.52	1.36|	-0.01
					B:ASN651	H	21.14	1.12|	-0.01
					B:GLU654	HS	92.77	24.69|||	-0.32
					B:LEU661		124.01	16.57||	0.27

Glycan-peptide interactions (interactive partners are shaded)

gp120	HSD*	ASA	BSA	ΔiG	gp41	HSD	ASA	BSA	ΔiG
G:NAG1088	H	361.66	73.01|||	-1.75	B:LEU520		121.69	16.40||	0.26
					B:GLY524		27.66	1.84|	-0.02
					B:GLY527		69.79	11.56||	0.01
					B:SER528	H	36.71	27.04||||||||	-0.12
G:NAG1089		351.65	3.07|	-0.04	B:THR529		40.42	0.86|	-0.01
					B:ALA532		46.96	2.35|	0.04
G:GLU32		159.45	39.08|||	-0.38	B:NAG1618		364.26	36.79||	-0.53
G:ARG500		189.46	4.52|	-0.05					

b. gp41-gp41 interface between two protomers.

Hydrogen bonds and salt bridges

Type	Protomer 1	Dist.[Å]	Protomer 2	Type	Protomer 1	Dist.[Å]	Protomer 2
H*	B:THR538[N]	3.25	N:GLN652[OE1]	H	B:ARG542[O]	3.70	N:GLN591[NE2]
H	B:THR538[OG1]	3.34	N:GLU647[O]	H	B:LYS601[O]	2.99	N:LYS655[NZ]
H	B:ARG579[NH2]	3.66	N:GLN577[O]	S	B:ARG579[NE]	3.91	N:GLU584[OE1]
H	B:SER534[O]	3.04	N:GLN652[NE2]	S	B:ARG579[NE]	3.81	N:GLU584[OE2]
H	B:MET535[SD]	3.18	N:ASN656[ND2]	S	B:ARG579[NH1]	3.66	N:GLU584[OE1]
H	B:ALA541[O]	2.60	N:GLN591[NE2]				

List of interface residues (the residues on each row are not matched interactive partners)

Protomer 1	HSD*	ASA	BSA	ΔiG	Protomer 2	HSD	ASA	BSA	ΔiG
B:PHE519		186.83	42.66|||	0.68	N:VAL570		126.21	2.34|	0.04
B:SER534	H	34.69	13.07||||	-0.07	N:ILE573		93.94	22.94|||	0.37
B:MET535	H	156.91	40.14|||	0.81	N:LEU576		82.58	20.67|||	0.33
B:LEU537		55.20	6.31||	0.09	N:GLN577	H	134.57	53.69||||	0.09
B:THR538	H	75.83	69.24|||||||||	0.30	N:VAL580		67.81	44.79|||||||	0.72
B:ALA541	H	51.42	23.75|||||	0.04	N:LEU581		110.02	15.40||	0.25
B:ARG542	H	146.72	59.48|||||	0.51	N:VAL583		66.78	10.55||	0.17
B:LEU545		73.00	56.46||||||||	0.90	N:GLU584	S	106.22	87.36|||||||||	-0.21
B:SER546		84.70	0.73|	-0.01	N:ARG585		143.08	0.17|	0.00
B:GLY547		117.72	55.99|||||	0.31	N:LEU587		110.12	85.18||||||||	1.31

*. D: Disulfide bond, H: Hydrogen bond, S: Salt bridge.
ASA: Accessible Surface Area, Å², BSA: Buried Surface Area, Å², ΔiG: Solvation energy effect, kcal/mol, ||||: Buried area percentage, one bar per 10%.

Protomer 1	HSD*	ASA	BSA	ΔiG	Protomer 2	HSD	ASA	BSA	ΔiG
B:THR569		176.82	2.47|	-0.03	N:ARG588		110.89	34.82||||	0.55
B:GLY572		37.57	0.61|	-0.01	N:GLN590		42.98	2.39|	-0.02
B:ILE573		94.88	15.39||	0.25	N:GLN591	H	117.50	107.20||||||||||	-0.48
B:GLN575		92.61	12.96||	-0.15	N:LEU592		48.64	3.52|	0.06
B:LEU576		83.59	62.75||||||||	1.00	N:GLY594		29.76	21.20||||||||	0.21
B:ARG579	HS	151.60	91.09|||||||	-0.97	N:ILE595		63.30	59.10|||||||||	0.89
B:VAL580		68.80	23.47||||	0.38	N:SER599		77.41	18.41|||	-0.01
B:VAL583		66.76	51.19||||||||	0.82	N:GLU647	H	69.63	48.68|||||||	-0.26
B:TYR586		44.47	28.29|||||||	0.11	N:GLU648		126.06	52.30|||||	0.16
B:LEU587		110.38	25.61|||	0.41	N:ASN651		20.57	11.32||||||	0.05
B:SER599		76.87	6.95|	-0.05	N:GLN652	H	118.71	94.27||||||||	-0.62
B:GLY600		48.68	17.81||||	0.29	N:LYS655	H	119.03	86.36||||||||	-0.78
B:LYS601	H	100.71	68.22|||||||	-0.56	N:ASN656	H	84.63	43.02||||||	-0.41
B:LEU602		109.20	68.18|||||||	1.09	N:GLN658		112.11	4.37|	0.02
B:ILE603		132.63	71.19||||||	1.04	N:ASP659		92.31	28.16||||	-0.10
B:CYS605		122.91	30.32|||	1.24	N:ALA662		81.10	14.85||	0.24

c. gp120-gp120 interface between two protomers.

Hydrogen bonds

Type	Protomer 1	Dist.[Å]	Protomer 2	Type	Protomer 1	Dist.[Å]	Protomer 2
H*	G:ARG166[N]	3.53	M:CYS126[O]	H	G:ARG308[NH2]	2.51	M:ASN197[O]
H	G:ARG166[NH1]	3.12	M:THR162[OG1]	H	G:ASP167[OD1]	2.82	M:THR128[N]

List of interface residues (the residues on each row are not matched interactive partners)

Protomer 1	HSD*	ASA	BSA	ΔiG	Protomer 2	HSD	ASA	BSA	ΔiG
G:LYS121		125.83	1.05|	-0.04	M:LYS121		124.12	1.05|	-0.04
G:GLU164		60.11	32.69|||||	0.27	M:THR123		86.16	17.50|||	0.04
G:LEU165		121.56	88.67|||||||	1.42	M:PRO124		50.39	29.08|||||	0.47
G:ARG166	H	232.85	96.11|||||	0.02	M:CYS126	H	58.84	57.67|||||||||	0.69
G:ASP167	H	112.65	53.43|||||	-0.30	M:VAL127		50.15	40.17||||||||	0.64
G:LYS168		169.18	6.94|	0.03	M:THR128	H	84.95	48.41||||||	0.61
G:ARG308	H	154.00	41.66|||	-0.61	M:ASN160		66.98	1.80|	-0.01
G:PRO313		113.91	95.17||||||||	1.22	M:THR162	H	61.82	28.15|||||	-0.17
G:GLY314		80.10	34.53|||||	0.35	M:ILE184		86.42	10.72||	0.17
G:GLN315		69.99	5.43|	-0.06	M:GLU190		65.42	1.60|	-0.05
					M:TYR191		11.33	0.24|	-0.00
					M:ARG192		53.70	22.11|||||	0.35
					M:CYS196		37.27	36.90|||||||||	-0.17
					M:ASN197	H	100.94	44.59|||||	0.18
					M:THR198		75.16	6.04|	-0.02
					M:SER199		23.86	21.46||||||||	0.23
					M:ALA200		72.04	35.32|||||	0.43
					M:ILE201		6.81	1.97|||	0.02

Glycan-peptide interactions (interactive partners are shaded)

Protomer 1	HSD*	ASA	BSA	ΔiG	Protomer 2	HSD	ASA	BSA	ΔiG
G:ASP167		112.65	11.41||	-0.19	M:NAG1160		357.88	10.91|	-0.36
G:ARG308		154.00	36.82|||	-0.89	M:NAG1197		357.46	36.02||	-1.02

d. gp120-gp41 interface between two protomers.

List of interface residues (the residues on each row are not matched interactive partners)

Protomer 1	HSD*	ASA	BSA	ΔiG	Protomer 2	HSD	ASA	BSA	ΔiG
G:ALA31		96.84	2.91|	-0.00	N:GLN591		117.50	1.89|	-0.02
G:THR37		30.75	3.85||	0.06	N:GLN658		112.11	21.55||	-0.25
G:TYR39		105.81	8.33|	-0.10	N:ASP659		92.31	47.80||||||	-0.54
G:TYR40		179.40	2.13|	-0.00	N:ALA662		81.10	39.46|||||	0.21
G:THR499		44.62	12.18|||	0.00	N:LEU663		135.17	73.02||||||	0.91
G:ARG500		189.46	55.45|||	-0.49					
G:CYS501		74.02	49.74|||||||	1.65					

*. D: Disulfide bond, H: Hydrogen bond, S: Salt bridge.
ASA: Accessible Surface Area, Å², BSA: Buried Surface Area, Å², ΔiG: Solvation energy effect, kcal/mol, ||||: Buried area percentage, one bar per 10%.

Protomer 1	HSD*	ASA	BSA	ΔiG	Protomer 2	HSD	ASA	BSA	ΔiG

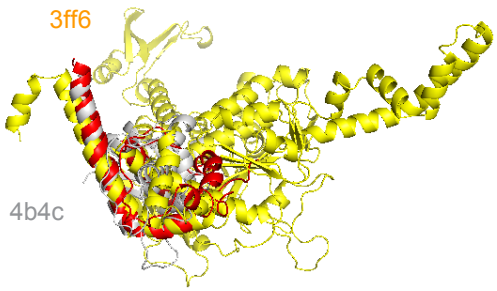
G:LYS502	140.46	19.36||	-0.22
G:ARG503	206.15	0.17|	0.00
G:ARG504	207.48	22.43||	-0.52

*. D: Disulfide bond, H: Hydrogen bond, S: Salt bridge.
ASA: Accessible Surface Area, Å², BSA: Buried Surface Area, Å², ΔiG: Solvation energy effect, kcal/mol, ||||: Buried area percentage, one bar per 10%.

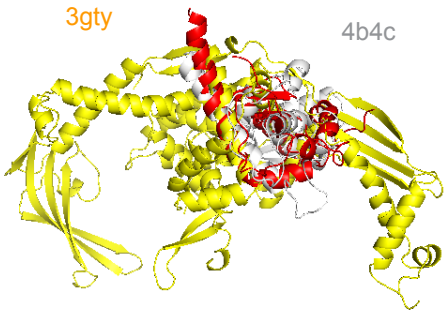
Supplementary Table 2 | DALI structural comparison.

Target	Chain	Z	rmsd	lali	nres	%id PDB	Description
gp41 monomer	3FF6-D	3	4.9	74	733	9 PDB	ACETYL-COA CARBOXYLASE 2
	4JLE-B	2.6	8.1	66	159	6 PDB	PHIST
	4B4C-A	2.3	4.1	66	187	6 PDB	CHROMODOMAIN-HELICASE-DNA-BINDING
gp41+gp120 N and C (monomer)	4B4C-A	2.1	3.8	66	187	6 PDB	CHROMODOMAIN-HELICASE-DNA-BINDING
	3GTY-X	2	6.3	89	412	7 PDB	TRIGGER FACTOR
gp41+gp120 N and C (trimer)	1QOY-A	2.6	4.5	114	303	6 PDB	HEMOLYSIN E
	3ZYM-C	2.5	5.1	110	280	7 PDB	PHOSPHATIDYLINOSITOL-BINDING CLATHRIN ASSEMBLY
	1HX8-A	2.1	9	104	270	8 PDB	SYNAPSE-ENRICHED CLATHRIN ADAPTOR PROTEIN LAP
	3ZYK-A	2	4.5	109	269	5 PDB	PHOSPHATIDYLINOSITOL-BINDING CLATHRIN ASSEMBLY

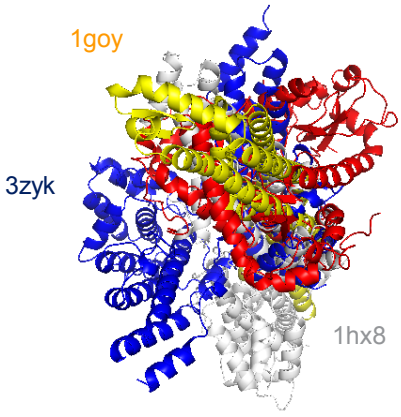
Target: gp41



Target: gp41+gp120 N and C



Target: gp41+gp120 N and C (Trimer)



Supplementary Table 3 | 3502 interface with HIV-1 Env.

a. 3502 heavy chain (chain D) and light chain (chain E) interface with gp41 (chain B)

Hydrogen bonds							
	gp41	Dist.[Å]	3502		gp41	Dist.[Å]	3502
1	B:ASN625[ND2]	3.68	D:LEU96[O]	3	B:ASP624[O]	3.04	D:ARG98[N]
2	B:ASN625[OD1]	2.44	D:TYR32[OH]	4	B:ASP624[O]	3.20	D:ASP99[N]

List of heavy chain-gp41 interface residues (the residues on each row are not matched interactive partners)									
gp41	HSD*	ASA	BSA	ΔiG	3502	HSD	ASA	BSA	ΔiG
B:GLY527		69.79	18.98|||	-0.13	D:GLN1		192.89	29.65||	-0.35
B:SER528		36.71	4.59||	0.07	D:PHE31		63.18	12.09||	0.19
B:THR529		40.42	37.31|||||||||	0.24	D:TYR32	H	53.73	25.90|||||	-0.26
B:ALA532		46.96	3.52|	0.06	D:PHE72H		169.27	95.44||||||	1.53
B:ARG617		120.66	26.65|||	-0.70	D:LEU96	H	56.05	5.65||	-0.06
B:SER620		73.21	21.28|||	-0.18	D:LEU97		90.59	68.55||||||||	1.10
B:GLU621		86.31	8.52|	0.14	D:ARG98	H	153.80	71.96|||||	-0.38
B:ASP624	H	98.64	66.75|||||||	-0.11	D:ASP99	H	118.53	47.77|||||	0.22
B:ASN625	H	112.81	73.74|||||||	-0.54	D:GLY100		52.83	5.97||	0.10
B:MET626		7.75	2.28|||	0.02					
B:THR627		29.84	21.28||||||||	0.24					
B:LEU629		134.49	18.20||	0.21					
B:GLN630		99.10	36.41||||	0.35					

List of light chain-gp41 interface residues (the residues on each row are not matched interactive partners)									
gp41	HSD	ASA	BSA	ΔiG	3502	HSD	ASA	BSA	ΔiG
B:LYS633		159.78	17.24||	-0.05	E:TYR49		74.12	32.70|||||	-0.26
B:ARG617		120.66	2.47|	-0.09	E:GLU50		85.57	7.34|	-0.10
B:ASN618		90.29	18.66|||	-0.16	E:GLU53		71.21	16.28|||	-0.02
B:SER620		73.21	36.85||||||	0.27	E:ARG54		115.05	11.48|	-0.13
B:GLU621		86.31	58.39|||||||	-0.27	E:PRO56		129.25	36.15|||	0.58

b. 3502 interface with gp41 glycans (chain B)

Light chain residues interacting with gp41 glycan NAG1618									
3502	HSD	ASA	BSA	ΔiG	gp41	HSD	ASA	BSA	ΔiG
E:TYR49		74.12	2.84|	-0.03	B:NAG1618		364.26	155.97|||||	-2.95
E:ASN52		101.39	14.60||	-0.07					
E:GLU53		71.21	40.20||||||	0.28					
E:ARG54		115.05	60.92||||||	-1.06					
E:ALA55		8.17	3.50|||||	-0.03					
E:PRO56		129.25	1.01|	0.02					
E:ILE58		36.63	3.56|	-0.04					

c. 3502 heavy chain (chain D) and light chain (chain E) interface with gp120 (chain G)

Hydrogen bonds							
	gp120	Dist.[Å]	3502		gp120	Dist.[Å]	3502
1	G:GLU87[OE2]	3.47	D:TYR53[OH]	4	G:THR90[O]	2.67	D:SER72G[OG]
2	G:ASN88[O]	3.52	D:ARG28[NH1]	5	G:THR90[OG1]	3.19	D:ARG28[NH1]
3	G:ASN88[O]	3.57	D:ARG28[NH2]	6	G:GLU92[OE2]	3.66	D:SER72G[N]

List of heavy chain-gp120 interface residues (the residues on each row are not matched interactive partners)									
gp120	HSD*	ASA	BSA	ΔiG	3502	HSD	ASA	BSA	ΔiG
G:GLU87	H	119.82	30.03|||	-0.04	D:ARG28	H	61.56	41.29|||||||	-0.86
G:ASN88	H	153.77	76.82|||||	-0.45	D:ASN30		36.89	0.67|	0.01
G:VAL89		37.55	0.16|	0.00	D:PHE31		63.18	29.42|||||	0.47
G:THR90	H	84.18	78.15|||||||||	0.06	D:TYR53	H	174.22	57.23||||	0.43
G:GLU91		30.92	6.18||	-0.07	D:GLU72B		31.31	3.07|	-0.05
G:GLU92	H	120.15	37.29||||	-0.20	D:PRO72D		100.81	68.72|||||||	0.94
G:PRO238		84.68	52.14|||||||	0.79	D:VAL72E		95.12	16.09||	-0.14
G:PRO240		94.84	25.90|||	0.41	D:THR72F		81.85	25.64||||	0.19
					D:SER72G	H	84.96	55.39|||||||	0.12
					D:ARG98		153.80	14.44|	-0.15

*. D: Disulfide bond, H: Hydrogen bond, S: Salt bridge.
ASA: Accessible Surface Area, Å², BSA: Buried Surface Area, Å², ΔiG: Solvation energy effect, kcal/mol, ||||: Buried area percentage, one bar per 10%.

d. 35O22 heavy chain (chain D) and light chain (chain E) interface with gp120 glycans (chain G)

Hydrogen bonds

	35O22	Dist.[Å]	gp120		35O22	Dist.[Å]	gp120
1	D:ARG98[NH1]	3.15	G:NAG1088[O5]	12	E:HIS93[ND1]	3.70	G:BMA1090[O4]
2	D:ARG98[NH1]	3.20	G:NAG1088[O6]	13	E:ASN94[ND2]	2.90	G:MAN1092[O5]
3	D:HIS33[NE2]	3.19	G:NAG1089[O3]	14	E:ASN94[ND2]	2.98	G:MAN1092[O6]
4	D:THR100C[OG1]	3.79	G:NAG1089[O3]				
5	D:SER52[OG]	2.81	G:NAG1089[O7]				
6	D:ASP99[OD2]	2.69	G:NAG1089[O6]				
7	D:THR100C[OG1]	3.64	G:BMA1090[O2				
8	D:GLY100[N]	3.81	G:MAN1091[O6]				
9	D:ASP99[OD2]	2.89	G:MAN1091[O6]				
10	D:ASN58[ND2]	2.75	G:MAN1093[O5]				
11	D:LYS57[O]	2.83	G:MAN1093[O6]				

Heavy chain residues interacting with gp120 glycans (interactive partners are shaded)

35O22	HSD*	ASA	BSA	ΔiG	gp120	HSD	ASA	BSA	ΔiG
D:ASN30		36.89	3.80||	-0.04	G:NAG1088	H	361.66	152.80|||||	-2.90
D:PHE31		63.18	14.73|||	0.21					
D:SER52		14.76	4.10|||	-0.05					
D:TYR53		174.22	56.84||||	0.60					
D:ARG98	H	153.80	34.95|||	0.09					
D:ASN30		36.89	3.30|	-0.04	G:NAG1089	H	351.65	208.97||||||	-3.87
D:PHE31		63.18	6.93||	0.03					
D:TYR32		53.73	2.88|	0.04					
D:HIS33	H	31.99	27.65|||||||||	-0.34					
D:SER52	H	14.76	10.65|||||||	-0.10					
D:PRO52A		21.95	0.17|	0.00					
D:TYR53		174.22	15.13|	0.24					
D:SER54		79.25	0.49|	-0.01					
D:LEU97		90.59	0.34|	-0.00					
D:ARG98		153.80	29.55||	0.07					
D:ASP99	H	118.53	28.74|||	-0.23					
D:GLY100		52.83	1.75|	-0.02					
D:THR100C	H	23.46	9.80|||||	0.07					
D:HIS33		31.99	0.87|	-0.03	G:BMA1090	H	290.20	66.73|||	-1.33
D:TRP50		35.25	6.06||	0.10					
D:ASP56		82.09	5.52|	-0.03					
D:ARG98		153.80	2.90|	-0.03					
D:ASP99		118.53	8.40|	-0.05					
D:GLY100		52.83	16.78||||	-0.19					
D:SER100A		115.04	3.65|	0.06					
D:THR100C	H	23.46	13.65||||||	0.07					
D:TRP100D		96.11	0.78|	0.01					
D:ASP99	H	118.53	22.92||	-0.26	G:MAN1091	H	291.06	83.96|||	-1.30
D:GLY100	H	52.83	24.33|||||	-0.02					
D:SER100A		115.04	21.29||	0.32					
D:TRP50		35.25	13.76||||	0.22	G:MAN1092		291.10	71.20|||	-1.09
D:ASP56		82.09	35.67|||||	-0.24					
D:LYS57		97.21	1.59|	-0.02					
D:ASN58		70.22	15.87|||	-0.07					
D:TRP50		35.25	1.77|	0.03	G:MAN1093	H	291.76	65.49|||	-0.59
D:ASP56		82.09	6.71|	-0.08					
D:LYS57	H	97.21	14.49||	-0.17					
D:ASN58	H	70.22	37.81||||||	-0.30					
D:GLN64		112.58	0.14|	-0.00					
D:SER54		79.25	9.66||	0.15	G:MAN1094		291.56	44.25||	-1.07
D:GLY55		40.15	0.00	0.00					
D:ASP56		82.09	30.40||||	0.18					

*. D: Disulfide bond, H: Hydrogen bond, S: Salt bridge.
ASA: Accessible Surface Area, Å², BSA: Buried Surface Area, Å², ΔiG: Solvation energy effect, kcal/mol, ||||: Buried area percentage, one bar per 10%.

35O22	HSD*	ASA	BSA	ΔiG	gp120	HSD	ASA	BSA	ΔiG
D:PRO72D		100.81	2.52|	-0.03	G:NAG1234		364.49	2.64|	-0.03
D:VAL72C		88.44	0.84|	0.01	G:NAG1235		364.33	52.98||	-1.74
D:PRO72D		100.81	12.83||	-0.15					
D:VAL72E		95.12	21.29|||	0.10					

Light chain residues interacting with gp120 glycans (interactive partners are shaded)

35O22	HSD	ASA	BSA	ΔiG	gp120	HSD	ASA	BSA	ΔiG
E:HIS93	H	185.68	48.93|||	0.03	G:BMA1090	H	290.20	51.57||	-0.37
E:ASN94		129.52	10.53|	-0.04					
E:HIS93		185.68	46.93|||	0.38	G:MAN1091		291.06	49.91||	-1.43
E:HIS93		185.68	8.20|	-0.08	G:MAN1092	H	291.10	52.50||	-0.66
E:ASN94	H	129.52	50.11||||	-0.48					
E:ASN94		129.52	43.33||||	-0.57	G:MAN1093		291.76	44.67||	-1.35
E:SER95		60.35	0.34|	0.01					

*. D: Disulfide bond, H: Hydrogen bond, S: Salt bridge.
ASA: Accessible Surface Area, Å², BSA: Buried Surface Area, Å², ΔiG: Solvation energy effect, kcal/mol, ||||: Buried area percentage, one bar per 10%.

Supplementary Table 4 | PGT122 interface with HIV-1 Env.

a. PGT122 heavy chain (chain H) and light chain (chain L) interface with gp120 (chain G)

Hydrogen bonds							
Type	**gp120**	**Dist.[Å]**	**PGT122**	**Type**	**gp120**	**Dist.[Å]**	**PGT122**
H*	G:ARG327[NH2]	3.42	H:TYR100B[O]	H	G:THR135[O]	2.42	L:ARG94[NE]
H	G:ARG327[NE]	3.36	H:GLU100I[OE1]	H	G:ILE322[O]	3.16	L:ARG94[NH1]
H	G:GLN328[N]	3.29	H:GLU100I[OE2]	H	G:GLY324[O]	2.60	L:ARG94[NH1]
H	G:ARG327[NE]	3.36	H:GLU100I[OE1]	H	G:ASP325[OD1]	2.68	L:SER30[N]
				H	G:ASP325[OD1]	2.95	L:SER30[OG]
				H	G:ASP325[OD1]	2.80	L:SER93[OG]

List of heavy chain-gp120 interface residues (the residues on each row are not matched interactive partners)									
gp120	**HSD***	**ASA**	**BSA**	**ΔiG**	**PGT122**	**HSD**	**ASA**	**BSA**	**ΔiG**
G:ASN137		123.15	1.70|	-0.02	H:TYR100B	H	139.30	66.62|||||	0.57
G:THR139		89.34	2.51|	-0.01	H:GLY100C		29.03	7.47|||	0.08
G:ASP141		125.06	0.61|	-0.01	H:VAL100D		88.88	34.67||||	0.55
G:MET150		82.97	8.11|	0.33	H:ALA100F		91.59	3.32|	0.05
G:ASP325		109.50	35.59||||	0.02	H:PHE100G		159.25	111.47|||||||	1.57
G:ILE326		52.34	10.65|||	-0.12	H:LYS100H		166.63	8.38|	0.10
G:ARG327	HS	131.02	76.40||||||	-0.25	H:GLU100I	HS	64.86	54.78||||||||	-0.50
G:GLN328	H	104.59	55.71||||||	-0.12	H:PHE100K		110.10	1.55|	0.02
G:ALA329		6.63	0.61|	-0.01					
G:HIS330		41.10	18.00|||||	-0.05					
G:THR415		80.97	31.04||||	0.47					
G:PRO417		73.74	25.67||||	0.40					

List of light chain-gp120 interface residues (the residues on each row are not matched interactive partners)									
gp120	**HSD***	**ASA**	**BSA**	**ΔiG**	**PGT122**	**HSD**	**ASA**	**BSA**	**ΔiG**
G:VAL134		15.62	3.68|||	0.06	L:LEU28		75.20	24.09||||	0.18
G:THR135	H	128.22	67.20||||||	0.77	L:GLY29		8.25	8.01|||||||||	0.13
G:ASN136		70.11	25.75||||	0.23	L:SER30	H	62.08	13.05|||	0.02
G:ASN137		123.15	68.20||||||	0.14	L:PHE67C		139.10	58.57|||||	0.84
G:ILE138		121.22	1.51|	0.02	L:ASP92		12.79	0.50|	-0.01
G:ASP321A		84.62	2.96|	0.03	L:SER93	H	81.90	27.48||||	-0.17
G:ILE322	H	26.29	20.49||||||||	-0.19	L:ARG94	H	157.44	141.21||||||||	-1.53
G:ILE323		97.31	28.13|||	0.38	L:ARG95		110.87	19.10||	-0.38
G:GLY324	H	62.68	61.10|||||||||	0.21	L:PRO95A		108.78	26.57|||	0.41
G:ASP325	H	109.50	63.14||||||	-0.45	L:THR95B		60.91	5.62|	-0.06
G:ILE326		52.34	13.09|||	0.16					

b. PGT122 heavy chain (chain H) and light chain (chain L) interface with gp120 glycans (chain G)

Hydrogen bonds							
	PGT122	**Dist.[Å]**	**gp120**		**PGT122**	**Dist.[Å]**	**gp120**
1	H:THR100L[OG1]	3.06	G:NAG1138[O6]	11	L:THR95B[OG1]	3.38	G:NAG1137[N2]
2	H:ASN58[ND2]	2.96	G:NAG1138[O7]	12	L:ASN51[ND2]	2.95	G:MAN1338[O3]
3	H:ARG99[NE]	3.73	G:MAN1140[O4]	13	L:GLY67[N]	3.37	G:MAN1338[O3]
4	H:ARG99[NH2]	3.28	G:MAN1140[O3]	14	L:ASN51[ND2]	2.79	G:MAN1338[O4]
5	H:TYR33[OH]	3.14	G:MAN1140[O2]	15	L:ASN50[ND2]	3.49	G:MAN1338[O6]
6	H:GLY100C[O]	3.89	G:NAG1332[O6]	16	L:ASN52[ND2]	3.83	G:MAN1339[O2]
7	H:ARG100[NH2]	3.89	G:MAN1337[O2]				
8	H:ARG100[NH1]	3.35	G:MAN1337[O5]				
9	H:ARG100[NH2]	3.22	G:MAN1337[O6]				
10	H:ARG100[NE]	3.17	G:MAN1338[O4]				

*. D: Disulfide bond, H: Hydrogen bond, S: Salt bridge.
ASA: Accessible Surface Area, Å², BSA: Buried Surface Area, Å², ΔiG: Solvation energy effect, kcal/mol, ||||: Buried area percentage, one bar per 10%.

Heavy chain residues interacting with gp120 glycans (interactive partners are shaded)									
PGT122	**HSD***	**ASA**	**BSA**	**ΔiG**	**gp120**	**HSD**	**ASA**	**BSA**	**ΔiG**
H:ASN58		82.39	3.34|	-0.04	G:NAG1137		363.36	64.91||	-1.28
H:PHE100K		110.10	40.05||||	0.64					
H:THR100L		71.33	13.33||	-0.15					
H:TYR50		32.44	9.89||||	-0.11	G:NAG1138	H	361.16	67.39||	-1.08
H:ASN58	H	82.39	28.86||||	-0.24					
H:PHE100K		110.10	0.15|	0.00					
H:THR100L	H	71.33	23.27||||	-0.14					
H:TYR50		32.44	2.21|	-0.03	G:BMA1139		292.42	52.46||	-0.60
H:SER54		102.04	1.96|	-0.02					
H:GLY55		70.18	7.22||	-0.04					
H:ASP56		55.22	39.30||||||||	0.01					
H:THR57		50.88	1.31|	-0.01					
H:TYR33	H	39.27	19.22|||||	-0.22	G:MAN1140	H	288.49	124.68|||||	-2.12
H:ASP56		55.22	15.93|||	0.02					
H:HIS97		81.98	2.93|	0.02					
H:ARG99	H	137.04	37.65|||	-0.72					
H:TRP100J		93.30	12.76||	0.17					
H:THR100L		71.33	24.31||||	0.24					
H:GLY100C		29.03	1.81|	-0.02	G:NAG1331		363.56	46.79||	-0.22
H:VAL100D		88.88	32.79||||	0.41					
H:ILE100A		78.65	11.05||	0.18	G:NAG1332	H	355.60	104.64|||	-1.96
H:TYR100B		139.30	8.08|	-0.06					
H:GLY100C	H	29.03	14.32|||||	-0.14					
H:VAL100D		88.88	21.43|||	0.24					
H:VAL100E		71.06	21.76||||	0.35					
H:ARG100		126.64	6.29|	-0.07	G:BMA1333		287.56	71.78|||	-1.82
H:ILE100A		78.65	45.03||||||	0.30					
H:TYR100B		139.30	8.75|	0.03					
H:GLY100C		29.03	5.44||	-0.06					
H:VAL100E		71.06	0.17|	0.00					
H:ILE100A		78.65	12.91||	0.21	G:MAN1334		289.35	14.25|	-0.37
H:ARG100	H	126.64	26.73|||	-0.73	G:MAN1337	H	290.72	69.38|||	-0.95
H:ILE100A		78.65	7.44|	-0.08					
H:TYR100B		139.30	19.66||	0.14					
H:ARG100	H	126.64	36.72|||	-0.38	G:MAN1338	H	290.85	50.03||	-0.94
H:ILE100A		78.65	2.22|	-0.03					

Light chain residues interacting with gp120 glycans (interactive partners are shaded)									
PGT122	**HSD**	**ASA**	**BSA**	**ΔiG**	**gp120**	**HSD**	**ASA**	**BSA**	**ΔiG**
L:TRP91		109.68	21.87||	0.35	G:NAG1137	H	363.36	114.45||||	-3.21
L:ASP92		12.79	9.29||||||||	-0.07					
L:SER93		81.90	10.84||	0.14					
L:ARG94		157.44	0.00	0.00					
L:ARG95		110.87	8.22|	-0.09					
L:PRO95A		108.78	9.06|	0.14					
L:THR95B	H	60.91	28.01|||||	-0.27					
L:TRP96		223.52	0.31|	0.00	G:NAG1138		361.16	0.24|	-0.00
L:ARG94		157.44	16.23||	-0.36	G:NAG1156		362.08	16.35|	-0.54
L:ARG95		110.87	6.55|	-0.07	G:NAG1157		363.82	6.38|	-0.07
L:GLU25		83.84	1.35|	-0.02	G:MAN1159		289.29	1.28|	-0.04

*. D: Disulfide bond, H: Hydrogen bond, S: Salt bridge.
ASA: Accessible Surface Area, Å², BSA: Buried Surface Area, Å², ΔiG: Solvation energy effect, kcal/mol, ||||: Buried area percentage, one bar per 10%.

PGT122	HSD	ASA	BSA	ΔiG	gp120	HSD	ASA	BSA	ΔiG
L:SER30		62.08	10.76||	0.17	G:MAN1337		290.72	62.39|||	-0.82
L:GLY67		13.30	0.98|	-0.01					
L:SER67A		77.94	44.21||||||	0.62					
L:PHE67C		139.10	7.35|	0.12					
L:ARG31		14.38	0.98|	-0.01	G:MAN1338	H	290.85	104.08||||	-1.04
L:ASN50	H	71.14	33.52|||||	-0.41					
L:ASN51	H	18.57	11.39||||||	-0.05					
L:ASN52		72.55	1.17|	0.02					
L:ASP53		60.91	0.61|	-0.01					
L:PRO66		83.14	12.23||	0.20					
L:GLY67	H	13.30	3.86|||	0.00					
L:SER67A		77.94	14.20||	0.20					
L:ASN51		18.57	2.74||	0.03	G:MAN1339	H	287.69	77.17|||	-1.13
L:ASN52	H	72.55	23.68||||	0.09					
L:ASP53		60.91	5.04|	-0.09					
L:PRO66		83.14	28.74||||	0.46					
L:GLY67		13.30	0.58|	-0.01					
L:SER67A		77.94	7.10|	-0.06					

*. D: Disulfide bond, H: Hydrogen bond, S: Salt bridge.
ASA: Accessible Surface Area, Å², BSA: Buried Surface Area, Å², ΔiG: Solvation energy effect, kcal/mol, ||||: Buried area percentage, one bar per 10%.