5-6-2014

CONFORMATIONALLY STABILIZED HIV ENVELOPE IMMUNOGENS

Peter Kwong

John Mascola

Gary Nabel

Richard Wyatt

Barna Dey

See next page for additional authors

Authors

Peter Kwong, John Mascola, Gary Nabel, Richard Wyatt, Barna Dey, Ling Xu, Tongqing Zhou, Joseph Sodroski, Wen Yuan, and Shi-Hua Xiang

US008715686B2

(12) **United States Patent**
Kwong et al.

(10) **Patent No.: US 8,715,686 B2**
(45) **Date of Patent: *May 6, 2014**

(54) **CONFORMATIONALLY STABILIZED HIV ENVELOPE IMMUNOGENS**

(75) Inventors: **Peter Kwong**, Washington, DC (US); **John Mascola**, Rockville, MD (US); **Gary Nabel**, Washington, DC (US); **Richard Wyatt**, Rockville, MD (US); **Barna Dey**, Germantown, MD (US); **Ling Xu**, Potomac, MD (US); **Tongqing Zhou**, Boyds, MD (US); **Joseph Sodroski**, Boston, MA (US); **Wen Yuan**, Brighton, MA (US); **Shi-Hua Xiang**, Boston, MA (US)

(73) Assignees: **The United States of America, as represented by the Secretary, Department of Health and Human Services**, Washington, DC (US); **Dana-Faber Cancer Institute, Inc.**, Boston, MA (US)

(*) Notice: Subject to any disclaimer, the term of this patent is extended or adjusted under 35 U.S.C. 154(b) by 7 days.

This patent is subject to a terminal disclaimer.

(21) Appl. No.: **13/585,700**

(22) Filed: **Aug. 14, 2012**

(65) **Prior Publication Data**

US 2012/0328641 A1 Dec. 27, 2012

Related U.S. Application Data

(60) Continuation of application No. 13/232,775, filed on Sep. 14, 2011, now Pat. No. 8,268,323, which is a division of application No. 12/065,894, filed as application No. PCT/US2006/034681 on Sep. 6, 2006, now Pat. No. 8,044,185.

(60) Provisional application No. 60/713,725, filed on Sep. 6, 2005, provisional application No. 60/729,878, filed on Oct. 24, 2005, provisional application No. 60/731,627, filed on Oct. 28, 2005, provisional application No. 60/832,458, filed on Jul. 20, 2006.

(51) **Int. Cl.**
A61K 39/21 (2006.01)

(52) **U.S. Cl.**
USPC **424/188.1**; 424/208.1

(58) **Field of Classification Search**
None
See application file for complete search history.

(56) **References Cited**

U.S. PATENT DOCUMENTS

5,869,624	A	2/1999	Hasel et al.	
5,922,325	A	7/1999	Tilley et al.	
6,432,675	B1	8/2002	Crea	
6,710,173	B1	3/2004	Binley et al.	
6,716,429	B1	4/2004	Sodroski et al.	
6,908,617	B1	6/2005	Wyatt et al.	
7,022,324	B2	4/2006	Binley et al.	
7,048,929	B1	5/2006	Sodroski et al.	
8,268,323	B2 *	9/2012	Kwong et al.	424/188.1
2005/0025779	A1	2/2005	Berman et al.	

FOREIGN PATENT DOCUMENTS

WO	WO 99/24465	5/1999
WO	WO 99/24553	5/1999
WO	WO 00/58438	10/2000
WO	WO 01/72123	10/2001
WO	WO 2007/030637	3/2007

OTHER PUBLICATIONS

Ashish et al., "Binding of Full-length HIV-1 gp120 to CD4 Induces Structural Reorientation Around the gp120 Core," *Biophysical Journal-Biophysical Letters*, pp. L01-L03 (2006).
Burton et al., HIV vaccine design and the neutralizing antibody problem, *Nature Immunology*; 5(3):233-236 (2004).
Burton, Dennis R., "Antibodies, viruses and vaccines," *Nature Review*, 2:706-713 (2002).
Chen et al., "Determining the Structure of an Unliganded and Fully Glycosylated SIV gp120 Envelope Glycoprotein," *Structure, Current Biology Ltd.*, 13(2):197-211 (2005).
Desrosiers, "Prospects for an AIDS vaccine," *Nature Medicine*, vol. 10, pp. 221-223 (2004).
Dey et al., "Neutralizing of Human Immunodeficiency Virus Type 1 by sCD4-17b, a Single-Chain Chimeric Protein, Based on Sequential Interaction of gp120 with CD4 and Coreceptor," *Journal of Virology*, 77(5):2859-2865 (2003).
Huang et al., "Scorpion-Toxin Mimics of CD4 in Complex with Human Immunodeficiency Virus gp120: Crystal Structures, Molecular Mimicry, and Neutralization Breadth," *Structure*, 13:755-768 (2005).
Huang et al., "Structure of a V3-Containing HIV-1 gp120 Core," *Science*, 310:1025-1028 (2005).
Korber et al., "Numbering Positions in HIV Relative to HXB2CG," *Human Retroviruses and AIDS*, pp. III-102 to III-111 (1998).
Kwong et al., "HIV-1 GP120 Core Complexed with CD4 and a Neutralizing Human Antibody," *Nature*, 393(648):1-105 (1998).
Kwong et al., "Structure of an HIV GP 120 Envelope Glycoprotein in Complex with the CD4 Receptor and a Neutralizing Human Antibody," *Nature*, 393:648-659 (1998).
Kwong et al., "Structures of HIV-1 gp120 envelope glycoprotein from laboratory-adapted and primary isolates," *Structures, Current Biology Ltd.*, 8(12):1329-1339 (2000).
Moulard et al., "Broadly cross-reactive HIV-1-neutralizing human monocolonal Fab selected for binding to gp120-CD4-CCR5 complexes," *PNAS*, 99(10):6913-6918 (2002).
Myszka et al., "Energetics of the HIV gp120-CD4 binding reaction," *PNAS*, 97(16):9026-9031 (2000).
Pan et al., "CD4 Binding Partially Locks the Bridging Sheet in gp120 but Leaves the beta2/3 Strands Flexible," *Journal of Molecular Biology*, 350(3):514-527 (2005).

(Continued)

Primary Examiner — Jeffrey Parkin
(74) *Attorney, Agent, or Firm* — Klarquist Sparkman, LLP

(57) **ABSTRACT**

Isolated immunogens including a HIV-1 gp120 polypeptide or immunogenic fragment thereof stabilized in a CD4 bound confirmation by crosslinked cysteines, and methods of their use are disclosed. The immunogens are useful, for example, for generating an immune response to HIV-1 gp120 in a subject.

20 Claims, 32 Drawing Sheets

(56) **References Cited**

OTHER PUBLICATIONS

Reynard et al., "HIV-1 acute infection env glycomutants designed from 3D model: effects on processing, antigenicity, and neutralization sensitivity," *Virology*, 324(1):90-102 (2004).

Satoh et al., "Bioactive Peptide Design Based on Protein Surface Epitopes," *The Journal of Biological Chemistry*, 272(18): 12175-12180 (1997).

Schülke et al., "Oligomeric and Conformational Properties of a Proteolytically Mature Disulfide-Stabilized Human Immunodeficiency Virus Type 1 gp140 Envelope Glycoprotein," *Journal of Virology*, 76(15):7760-7776 (2002).

Stanfield et al., "Recurring conformation of the human immunodeficiency virus type 1 gp120 V3 loop," *Virology*, 315(1):159-173 (2003). Abstract only.

Wang et al., "Uncommon gp120 Cysteine Residues Found in Primary HIV-1 Isolates," *Aids Research and Human Retroviruses*, 11(1):185-188 (1995).

Wyatt et al., "Structure of the Core of the HIV-1 gp120 Exterior Envelope Glycoprotein," *Analysis*, pp. III-3-III-9 (1998).

Wyatt et al., "The Antigenic Structure of the HIV gp120 Envelope Glycoprotein," *Nature*, 393:705-711 (1998).

Xiang et al., "CD4-Bound Conformation of HIV-1 gp120 Improved by Introduced Disulfide Bonds," 9th Conference on Retroviruses and Opportunistic Infections, 2002 <http://www.retroconference.org/2002/Abstract/12607.htm>.

Xiang et al., "Mutagenic Stabilization and/or Disruption of a CD4-Bound State Reveals Distinct Conformations of the Human Immunodeficiency Virus Type 1 gp120 Envelope Glycoprotein," *Journal of Virology*, 76(19):9888-9899 (2002).

Yang et al., "Characterization of the Outer Domain of the gp120 Glycoprotein from Human Immunodeficiency Virus Type 1," *Journal of Virology*, 78(23):12975-12986 (2004).

* cited by examiner

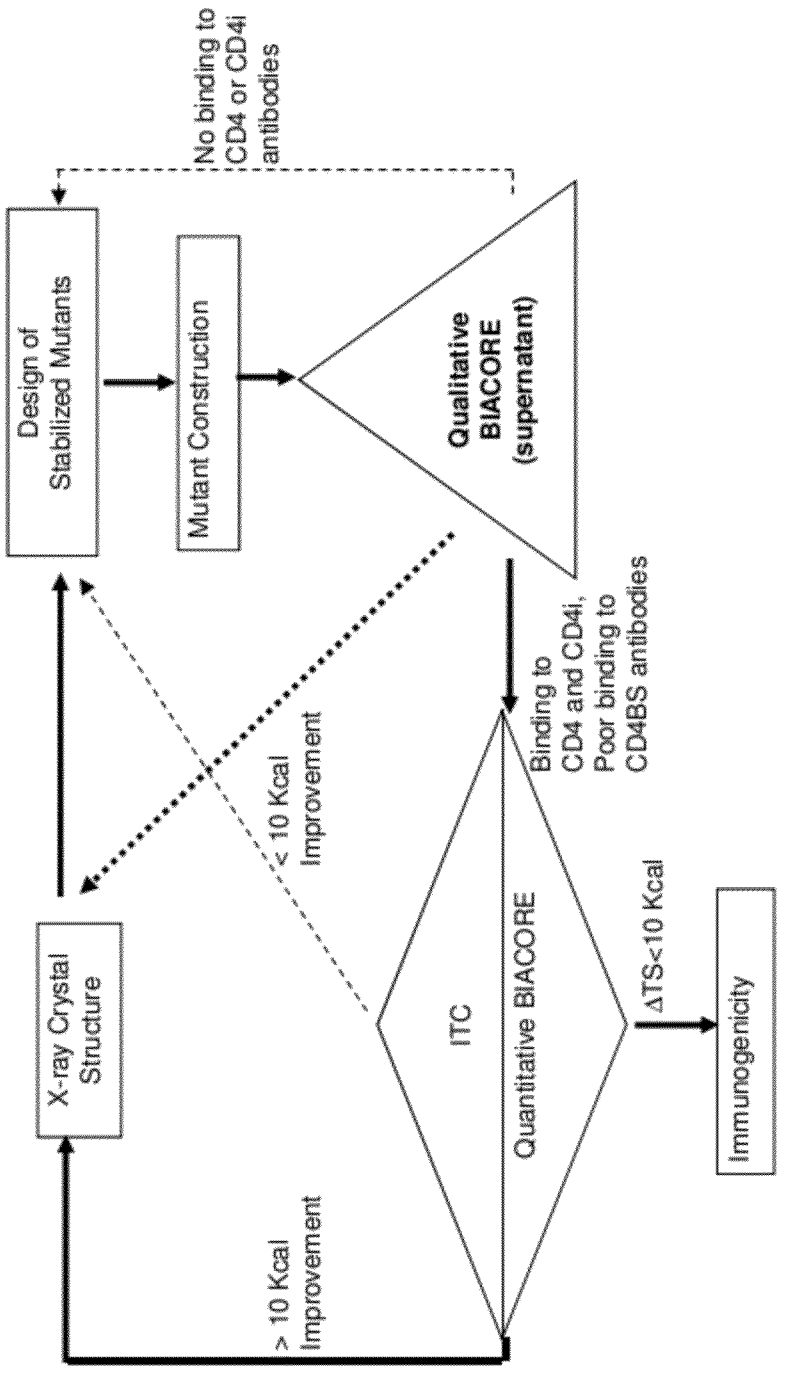

No binding to CD4 or CD4i antibodies
Design of Stabilized Mutants
Mutant Construction
Qualitative BIACORE (supernatant)
Binding to CD4 and CD4i, Poor binding to CD4BS antibodies
< 10 Kcal Improvement
X-ray Crystal Structure
ITC
Quantitative BIACORE
ΔTS<10 Kcal
Immunogenicity
> 10 Kcal Improvement

FIG. 1

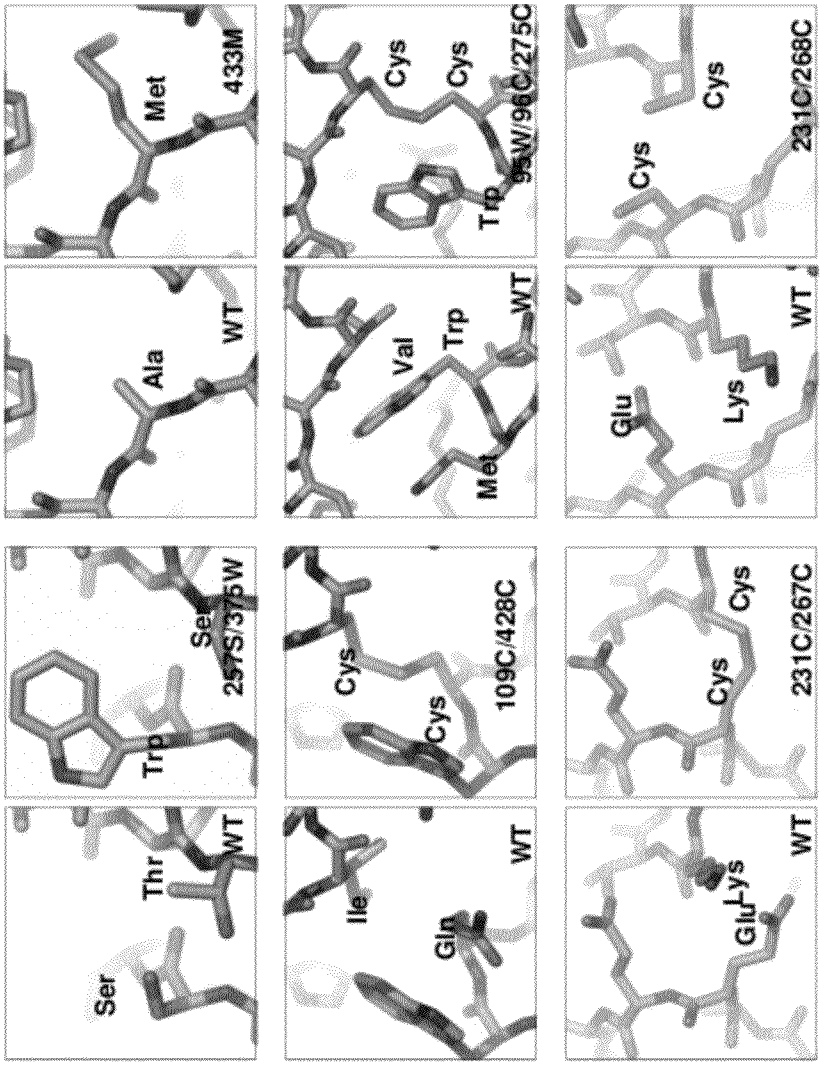

Ser
Thr
WT
Trp
Ser
257S/376W
Ile
Gln
WT
Cys
Cys
109C/428C
Glu
Lys
WT
Cys
Cys
231C/267C
Ala
WT
Val
Trp
Met
WT
Cys
Cys
Trp
95W/96C/275C
Glu
Lys
WT
Cys
Cys
231C/268C
Met
433M

FIG. 2

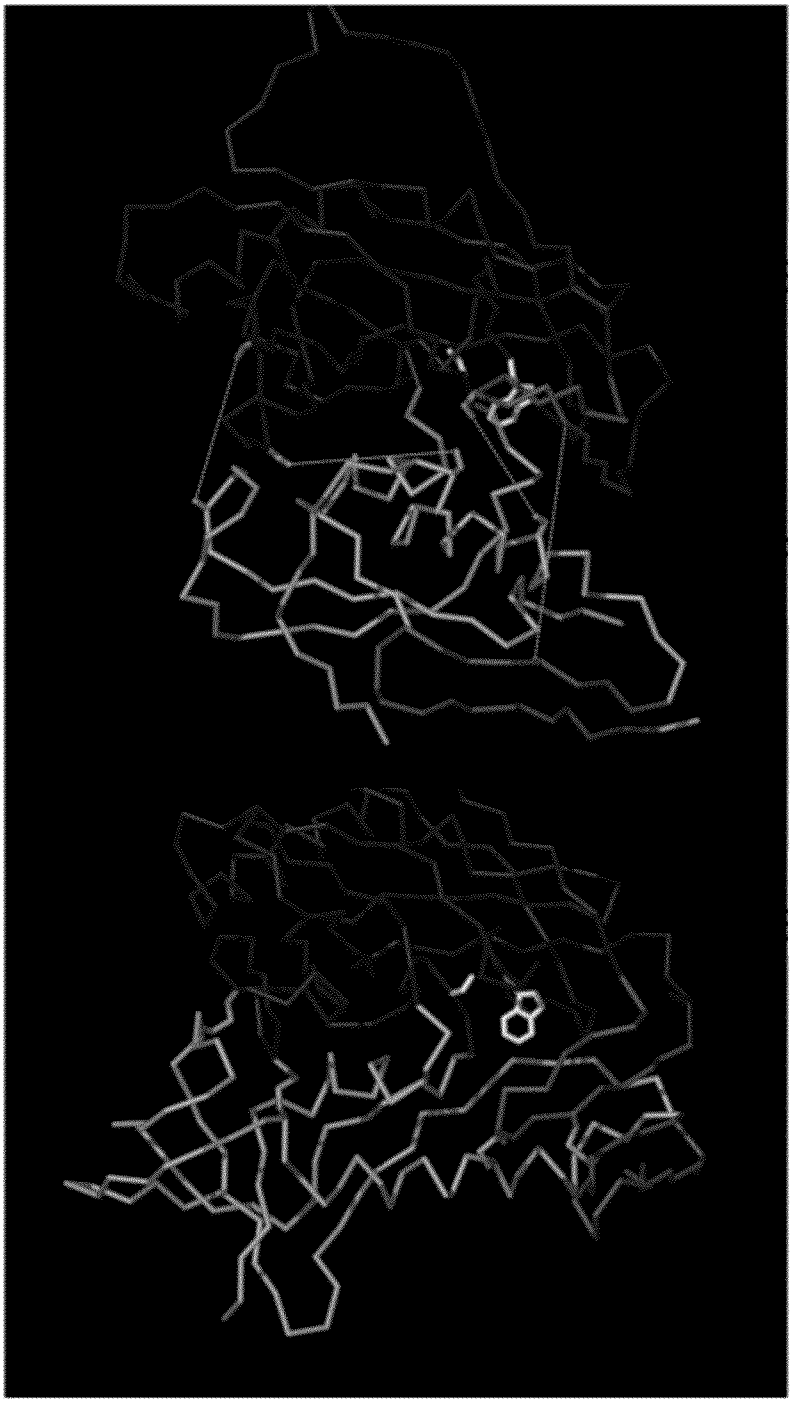


FIG. 3

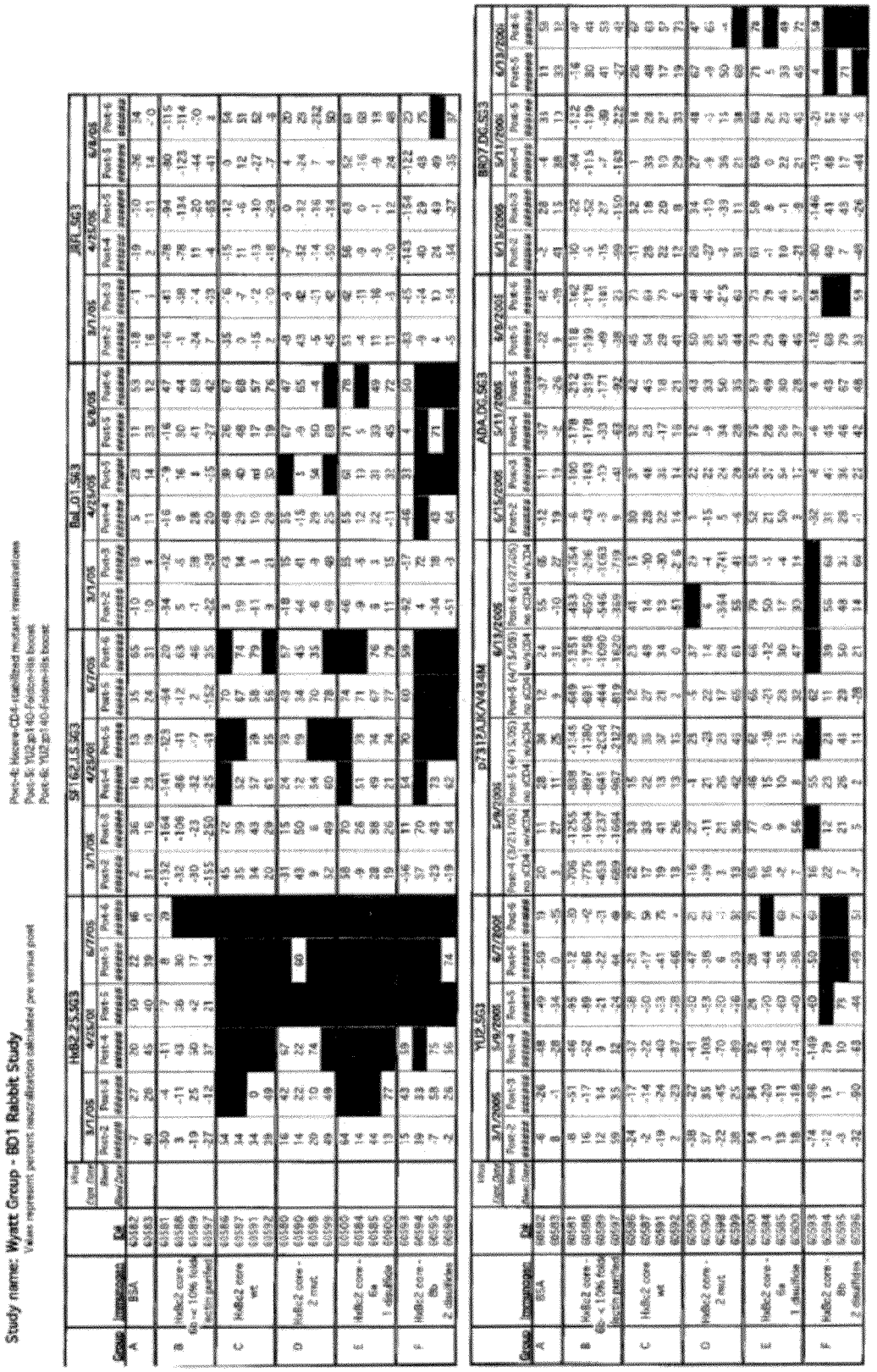

BD1 Rabbit Summary_full.xls
Study name: Wyatt Group - BD1 Rabbit Study
Values represent percent neutralization calculated pre versus post
Post-4: Hexavalent-CD4-stabilized mutant immunogens
Post-5: YU2.gp140-Fetzima-Alb boost
Post-6: YU2.gp140-Fetzima-Alb boost
SF162.LS.SG3
BaL.01.SG3
JRL.SG3
YU2.SG3
ADA.DC.SG3
BB07.DC.SG3

FIG. 4A

Group	Immunogen	ID#	Virus Exps. Date / Bleed / Bleed Date	BaL.26.SG3 6/22/2005 Post-2	Post-3	Post-4	Post-5	Post-6	6535.3.SG3 6/22/2005 Post-2	Post-3	Post-4	Post-5	Post-6	SS1196.01.SG3 6/22/2005 Post-2	Post-3	Post-4	Post-5	Post-6
A	BSA	60582		-3	0	-12	4	12	-14	17	-6	36	39	3	11	18	-8	16
		60583		6	15	-15	-11	-32	-27	-6	-16	3	-12	11	22	-2	-31	-58
E	HxBc2 core - 6b < 10% fold lectin purified	60581		12	13	-8	-32	29	-19	-17	-94	-73	-7	-39	-141	-159	-168	-118
		60588		5	-55	-22	-53	35	-34	-108	-104	-71	-44	-36	-184	-146	-217	-100
		60589		41	40	33	24	47	3	15	-8	-19	-3	-22	-58	-74	-92	-111
		60597		56	31	41	7	73	-149	-142	-104	-188	3	9	-39	3	-43	28
B	HxBc2 core wt	60586		28	42	33	27	[redacted]	36	54	43	49	64	21	27	33	10	71
		60587		-2	15	27	32		-3	26	38	48	16	26	19	31	43	60
		60591		39	43	15	24		52	53	36	49	49	26	28	10	-2	63
		60592		-18	-15	15	20		-26	3	41	51	65	8	3	15	2	37
C	HxBc2 core - 2 mut	60580		19	12	2	38	79	25	14	2	36	-7	-2	11	-11	16	41
		60590		-48	-33	-57	-31	71	-28	-25	-41	-26	46	2	12	-7	19	57
		60598		-2	12	30	61	44	-30	-11	44	51	-11	-6	10	14	41	-114
		60599		-41	-49	-37	71	[redacted]	10	-4	-32	8	56	5	3	33	69	77
D	HxBc2 core - 6a 1 disulfide	60600		33	11	38	43	[redacted]	53	39	67	75	72	33	19	51	48	70
		60584		26	28	27	36		27	31	22	41	61	-1	12	1	21	[redacted]
		60585		22	29	16	23		33	35	19	46	73	29	34	12	23	46
		60600		21	10	16	35		-7	28	56	63	50	33	11	15	9	71
F	HxBc2 core - 8b 2 disulfides	60593		-54	-40	0	56	[redacted]	-117	-57	-35	0	3	-22	-16	2	22	73
		60594		45	68	78	[redacted]		55	66	55	[redacted]		41	54	74	77	[redacted]
		60595		19	17	37			-2	22	23	49	76	29	39	43	64	
		60596		8	5	59			0	36	6	42	[redacted]	1	-21	58	78	

FIG. 4B

HxBc2 Core 8b=C123S12

Animal 60594

Serum Dilution	BD-1 Sera	Peptide	% Neut	fraction remain. virus	% Inhib	fold effect
1:10	30594 HxBc2 Core - 8b mutan	Mock	82	0.183		
		V3 Scr	79	0.214	4%	1.169
		YU2 V3 peptide	27	0.727	67%	3.977
		YU2 V1/2 pool 1	81	0.191	1%	1.046
		YU2 V1/2 pool 2	81	0.192	1%	1.050
1:40	30594 HxBc2 Core - 8b mutan	Mock	58	0.419		
		V3 Scr	58	0.424	1%	1.011
		YU2 V3 peptide	16	0.835	72%	1.994
		YU2 V1/2 pool 1	59	0.410	-2%	0.978
		YU2 V1/2 pool 2	57	0.429	2%	1.024
1:160	30594 HxBc2 Core - 8b mutan	Mock	29	0.713		
		V3 Scr	27	0.732	6%	97%
		YU2 V3 peptide	7	0.932	76%	97%
		YU2 V1/2 pool 1	32	0.678	-12%	98%
		YU2 V1/2 pool 2	28	0.716	1%	98%
1:640	30594 HxBc2 Core - 8b mutan	Mock	5	0.947		
		V3 Scr	10	0.896	-97%	0.946
		YU2 V3 peptide	8	0.923	-46%	0.974
		YU2 V1/2 pool 1	10	0.806	-265%	0.852
		YU2 V1/2 pool 2	13	0.868	-150%	0.916

Virus: YU2.SG3
Peptides: YU2 V3, YU2 V1/V2 Pools 1 and 2 all 20 µg/ml

Cells: TZM-BL cells
Sera: BD-1 Rabbit Sera Post-5

Animal 60595

Serum Dilution	BD-1 Sera	Peptide	% Neut	fraction remain. virus	% Inhib	fold effect
1:10	30595 HxBc2 Core - 8b mutan	Mock	73	0.269		
		V3 Scr	69	0.305	5%	1.133
		YU2 V3 peptide	26	0.743	65%	2.757
		YU2 V1/2 pool 1	69	0.306	5%	1.136
		YU2 V1/2 pool 2	70	0.298	4%	1.108
1:40	30595 HxBc2 Core - 8b mutan	Mock	44	0.563		
		V3 Scr	44	0.559	-1%	0.993
		YU2 V3 peptide	16	0.836	63%	1.485
		YU2 V1/2 pool 1	41	0.592	6%	1.050
		YU2 V1/2 pool 2	43	0.566	1%	1.006
		V3 Scr	8	0.918	50%	1.100
		YU2 V3 peptide	2	0.980	88%	1.174
		YU2 V1/2 pool 1	21	0.795	-24%	0.952
		YU2 V1/2 pool 2	17	0.833	-1%	0.998
1:640	30595 HxBc2 Core - 8b mutan	Mock	9	0.900		
		V3 Scr	8	0.923	16%	1.105
		YU2 V3 peptide	2	0.977	75%	1.170
		YU2 V1/2 pool 1	8	0.924	17%	1.107
		YU2 V1/2 pool 2	5	0.953	49%	1.141

FIG. 4C

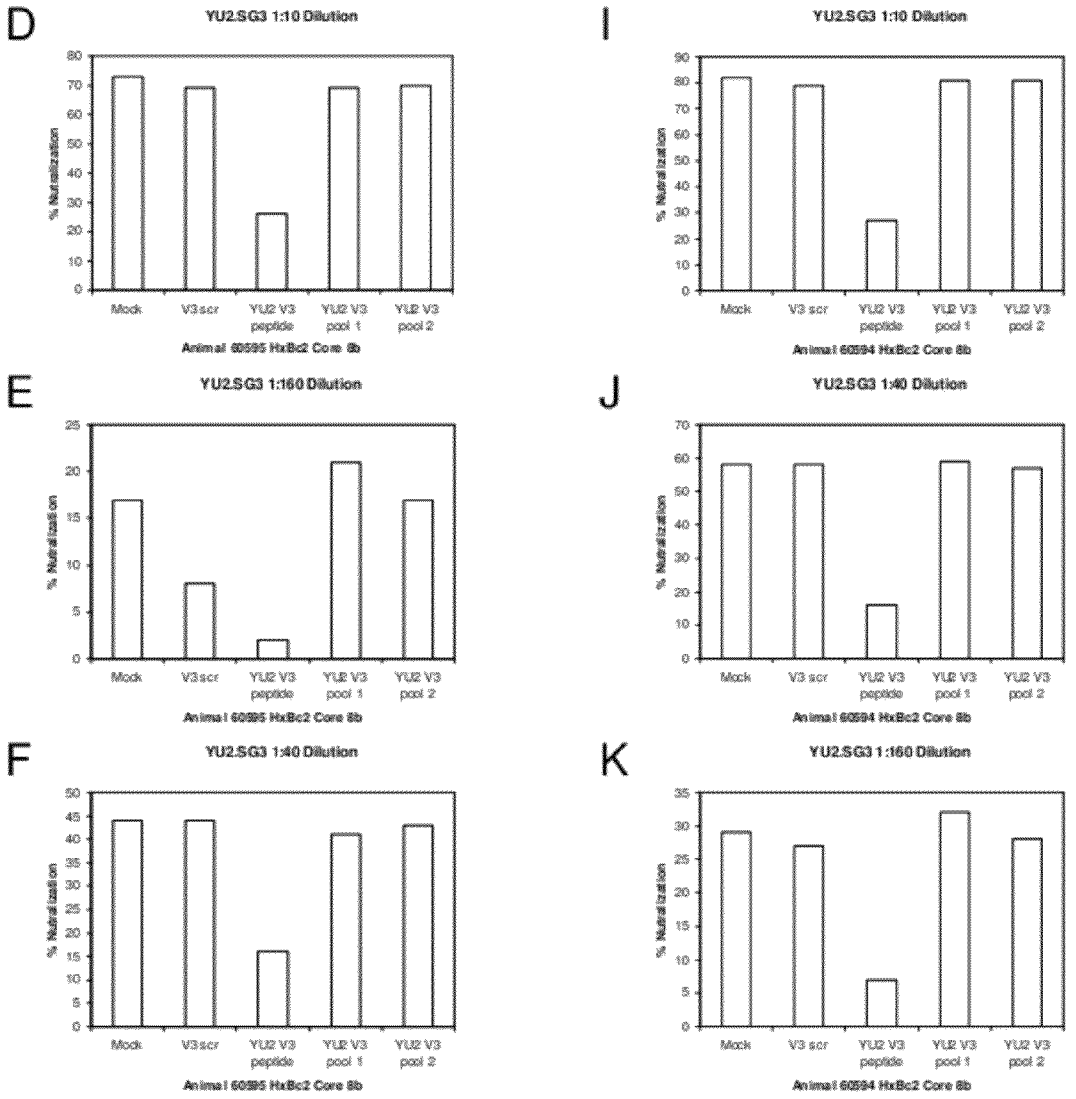

D
YU2.SG3 1:10 Dilution
% Neutralization
Mock
V3 scr
YU2 V3 peptide
YU2 V3 pool 1
YU2 V3 pool 2
Animal 60595 HxBc2 Core 8b
I
YU2.SG3 1:10 Dilution
Animal 60594 HxBc2 Core 8b
E
YU2.SG3 1:160 Dilution
J
YU2.SG3 1:40 Dilution
F
YU2.SG3 1:40 Dilution
K
YU2.SG3 1:160 Dilution

FIG. 4D-4K

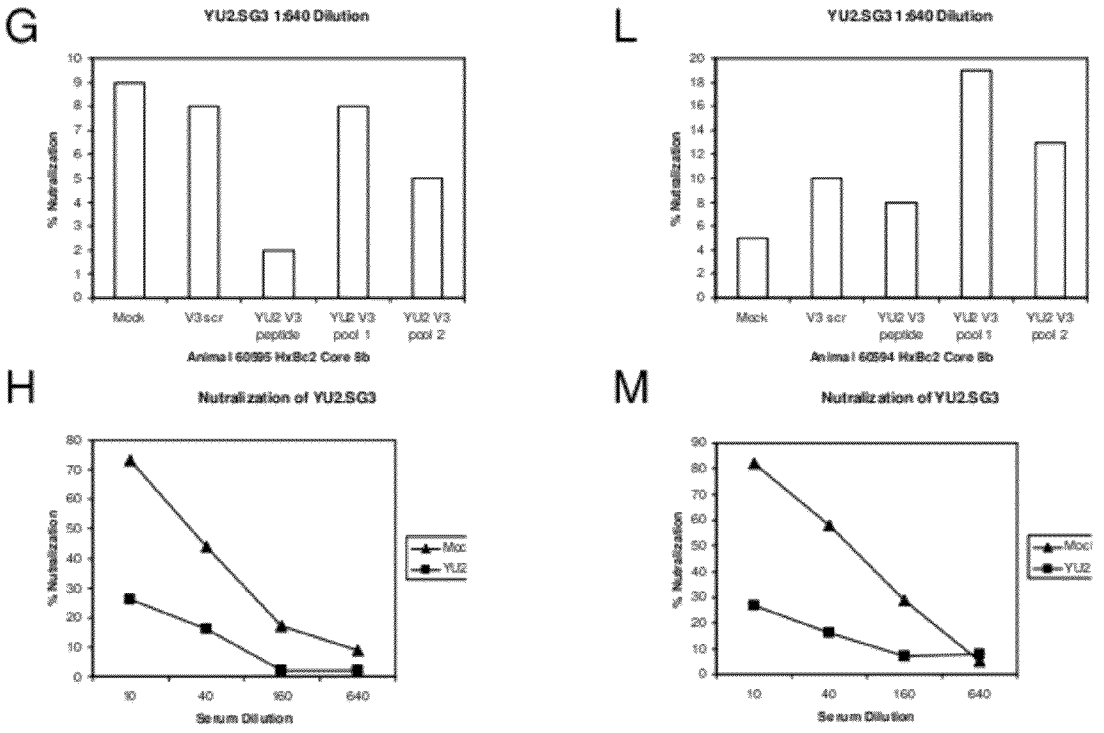

G
YU2.SG3 1:640 Dilution
% Nutralization
Mock
V3 scr
YU2 V3 peptide
YU2 V3 pool 1
YU2 V3 pool 2
Animal 60595 HxBc2 Core 8b
L
YU2.SG3 1:640 Dilution
% Nutralization
Mock
V3 scr
YU2 V3 peptide
YU2 V3 pool 1
YU2 V3 pool 2
Animal 60594 HxBc2 Core 8b
H
Nutralization of YU2.SG3
% Nutralization
10
40
160
640
Serum Dilution
M
Nutralization of YU2.SG3
% Nutralization
10
40
160
640
Serum Dilution

FIG. 4G-4M

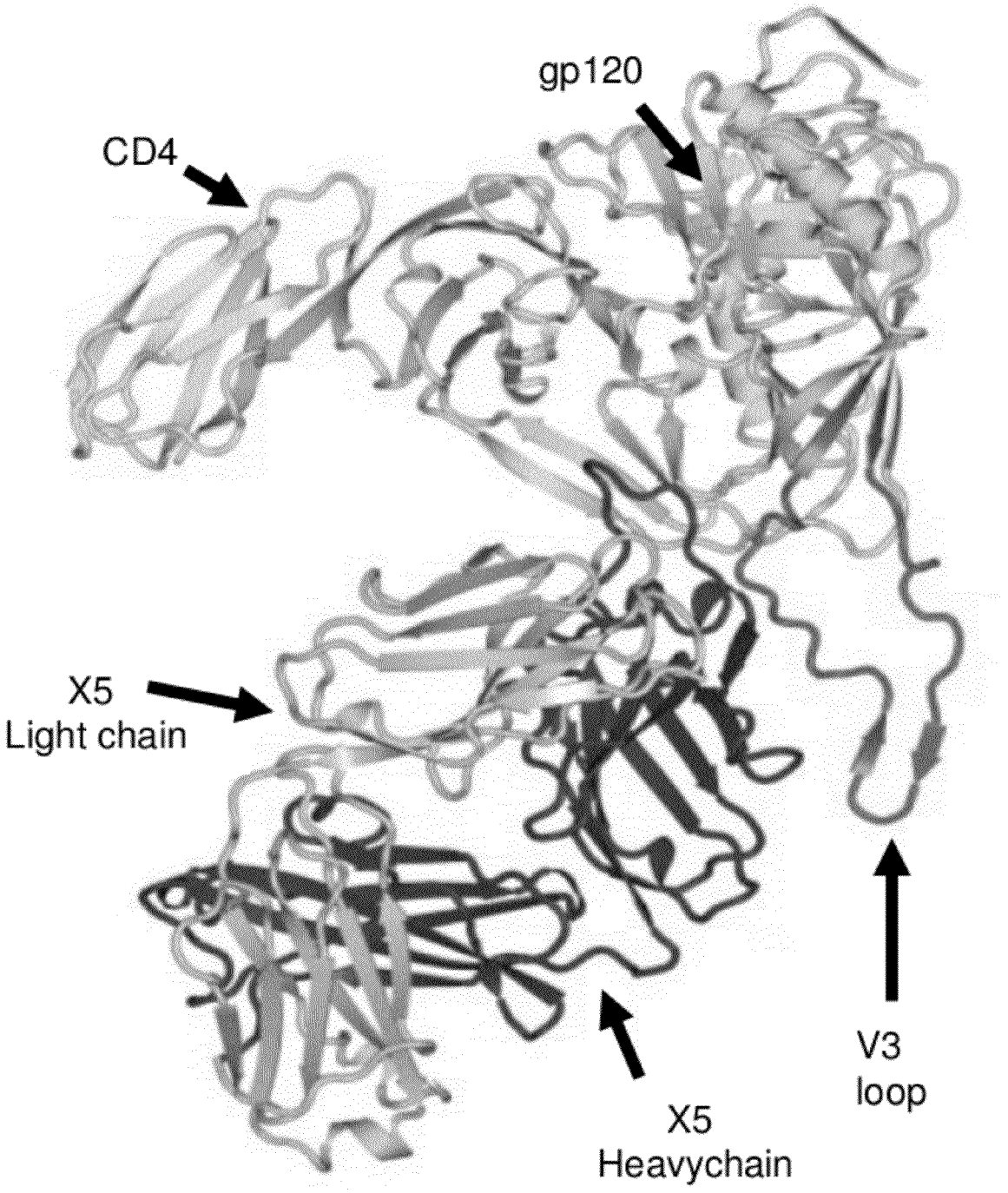


FIG. 5

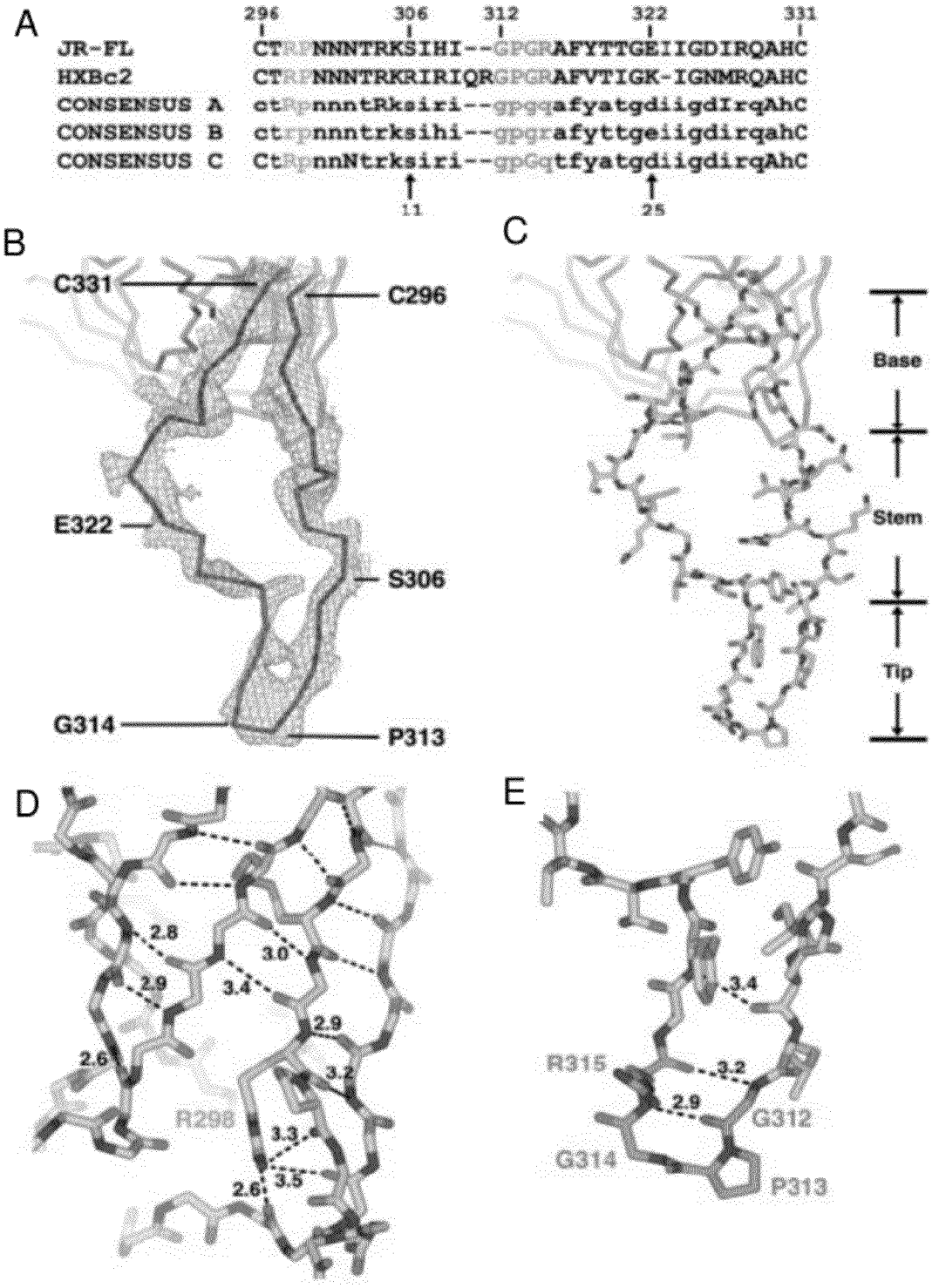

A
296
306
312
322
331
JR-FL CTRPNNNTRKSIHI--GPGRAFYTTGEIIGDIRQAHC
HXBc2 CTRPNNNTRKRIRIQRGPGRAFVTIGK-IGNMRQAHC
CONSENSUS A ctRpnnntRksiri--gpgqafyatgdiigdIrqAhC
CONSENSUS B ctrpnnntrksihi--gpgrafyttgeiigdirqahC
CONSENSUS C CtRpnnNtrksiri--gpGqtfyatgdiigdirqAhC
11
25
B
C331
C296
E322
S306
G314
P313
C
Base
Stem
Tip
D
2.8
3.0
2.9
3.4
2.9
2.6
3.2
R298
3.3
3.5
2.6
E
3.4
R315
3.2
2.9
G312
G314
P313

FIG. 6

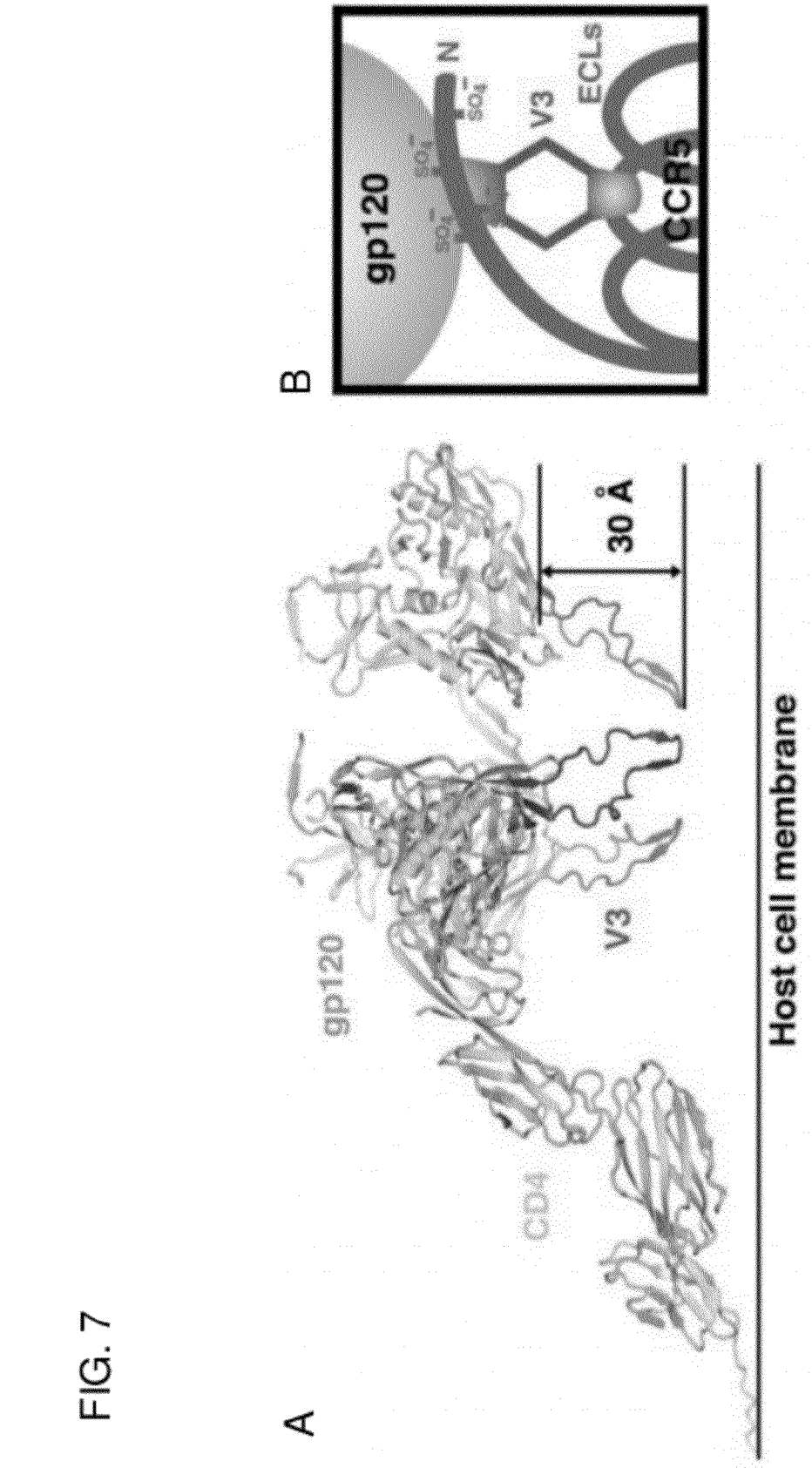


FIG. 7

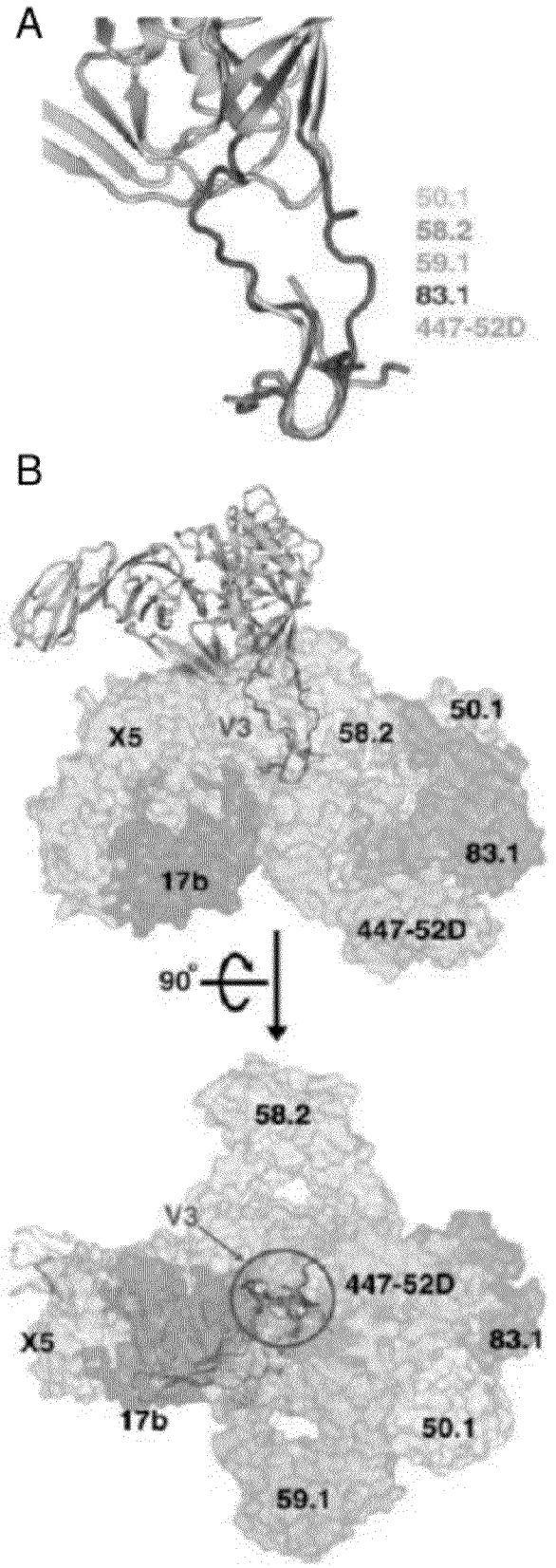

A
50.1
58.2
59.1
83.1
447-52D
B
X5
V3
58.2
50.1
83.1
17b
447-52D
90°
58.2
V3
447-52D
X5
83.1
17b
50.1
59.1

FIG. 8

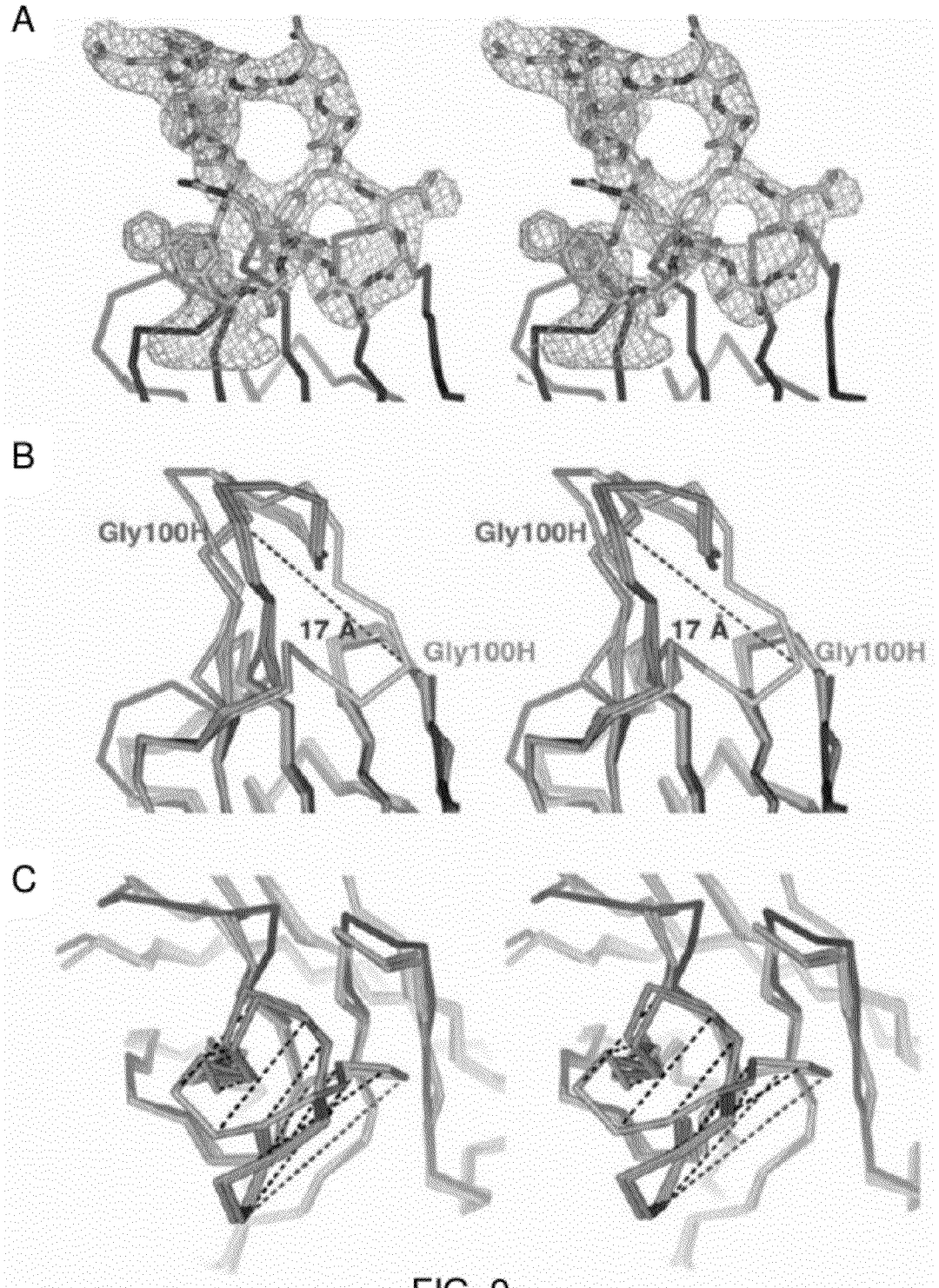


FIG. 9

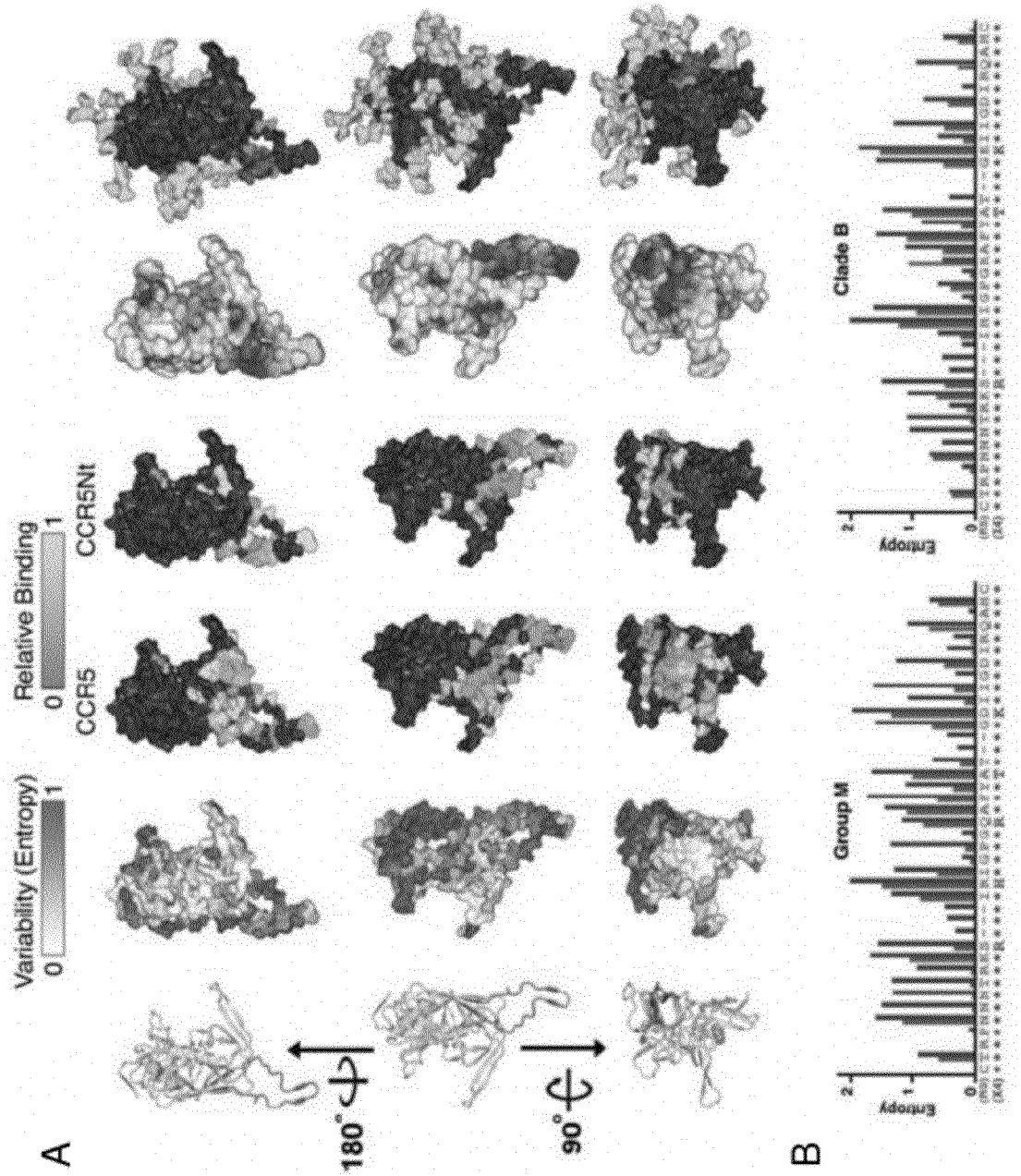

A
Variability (Entropy)
0
1
Relative Binding
0
1
CCR5
CCR5Nt
180°
90°
B
Group M
Clade B
Entropy
Entropy

FIG. 10

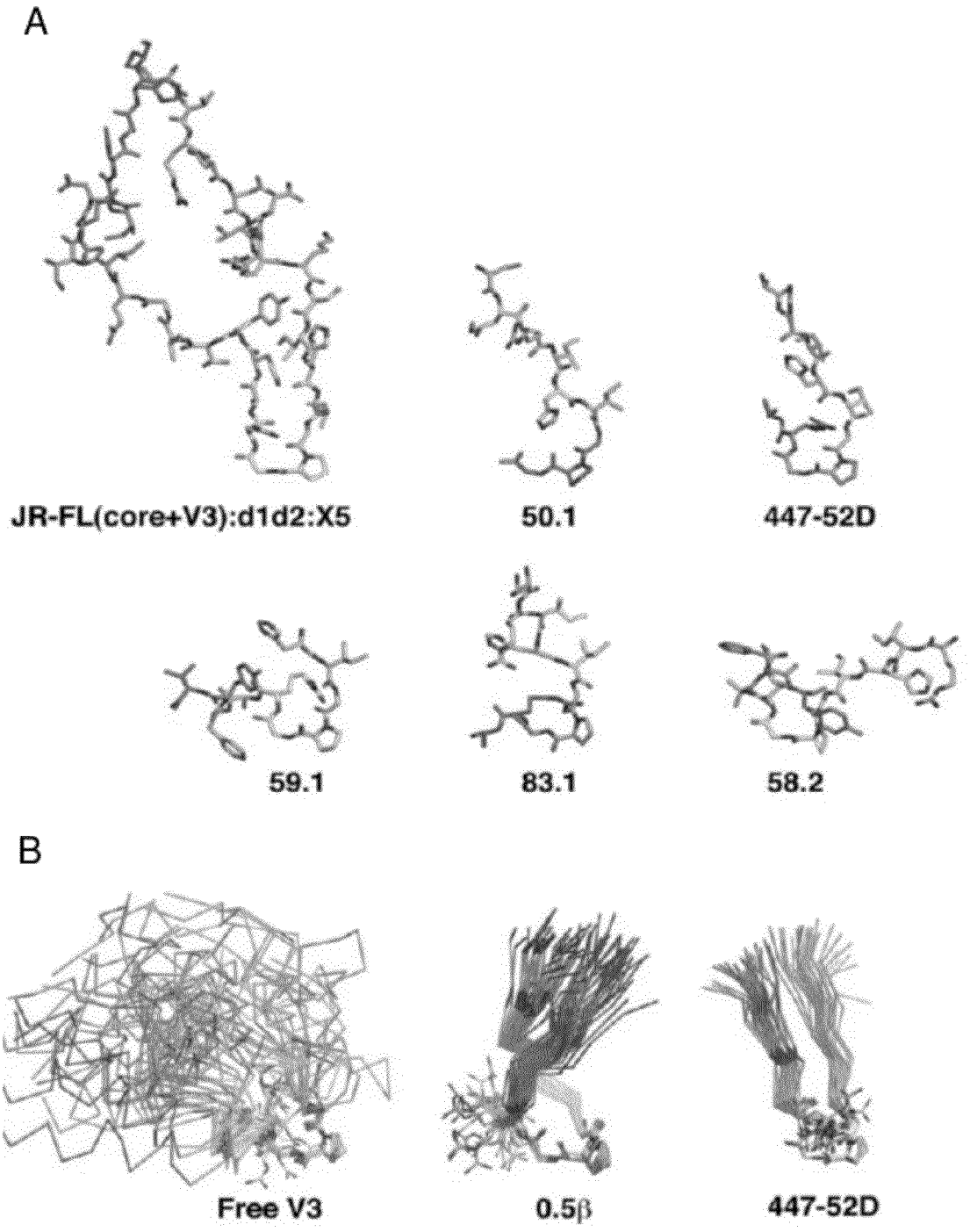
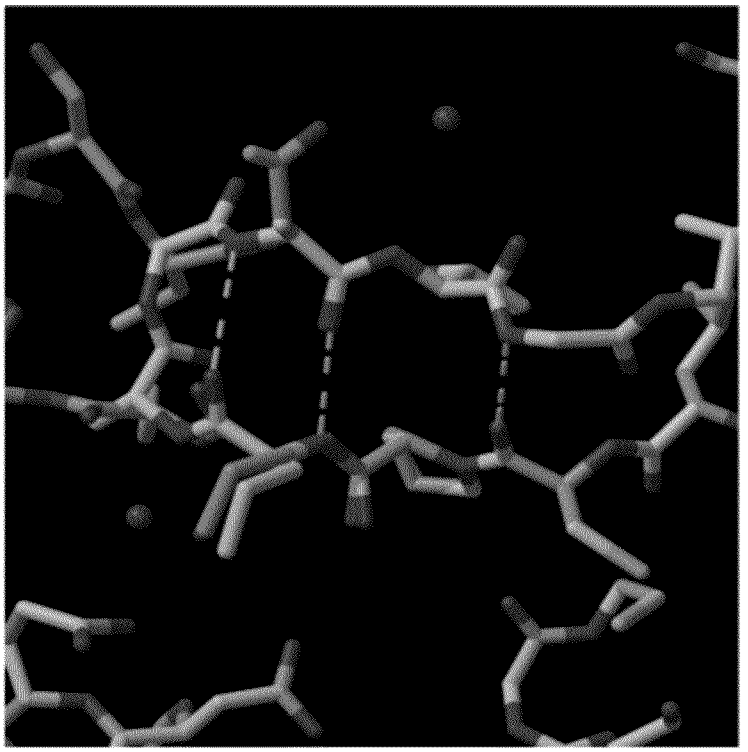

A
JR-FL(core+V3):d1d2:X5
50.1
447-52D
59.1
83.1
58.2
B
Free V3
0.5β
447-52D

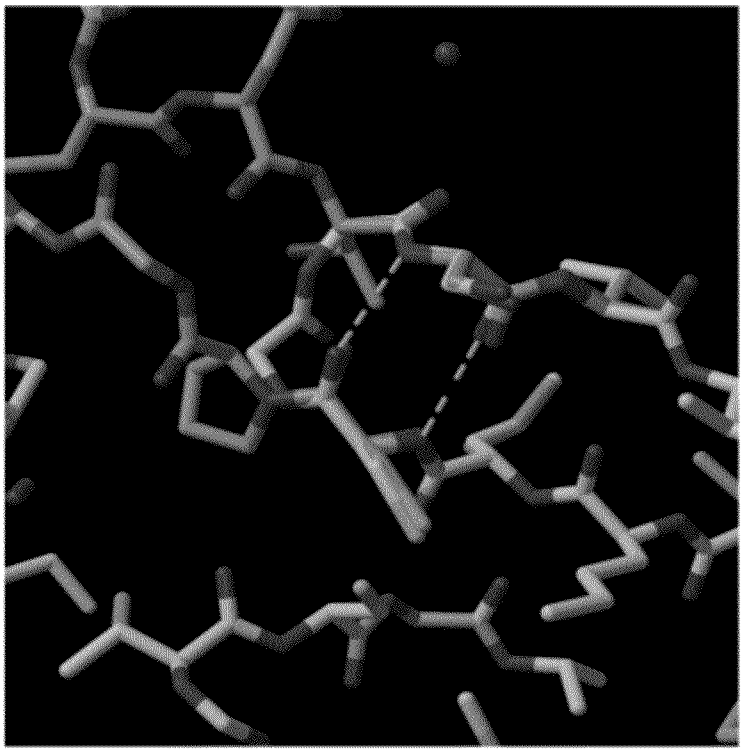
FIG. 11

FIG. 12

New V1/2 for HxBc2 9c mutant



B-turn after Leu125



B-turn right after Cys123

FIG. 13

```
New hxbc2 core gp120 with shorter V1/V1 and new V3

                                  9596          109           123
                                    ||           |             |
Hxbc2_core_       EVVLVNVTENFNMWKNDMVEQMHEDIISLWDQSLKPCVKLTPLCVGAGSCNTSVITQACP
New_9c_           EVVLVNVTENFNWCKNDMVEQMHEDICSLWDQSLKPCVKLCPLA-----GATSVITQACP
                  ************  ************ *************          *********
                                                                     257
                                                                     |
Hxbc2_core_       KVSFEPIPIHYCAPAGFAILKCNNKTFNGTGPCTNVSTVQCTHGIRPVVSTQLLLNGSLA
New_9c_           KVSFEPIPIHYCAPAGFAILKCNNKTFNGTGPCTNVSTVQCTHGIRPVVSSQLLLNGSLA
                  ****************************************************:*********
                         275
                          |
Hxbc2_core_       EEEVVIRSVNFTDNAKTIIVQLNTSVEINCT-------GAG------------------
New_9c_           EEEVVIRSCNFTDNAKTIIVQLNTSVEINCTRPNNGGSGSG-----------------GN
                  ******** ***********************       *:*
                                                          375
                                                           |
Hxbc2_core_       ----HCNISRAKWNNTLKQIASKLREQFGNNKTIIFKQSSGGDPEIVTHSFNCGGEFFYC
New_9c_           MRQAHCNISRAKWNNTLKQIASKLREQFGNNKTIIFKQSSGGDPEIVTHWFNCGGEFFYC
                      ********************************************* **********
                                                      428 431
                                                      |   |
Hxbc2_core_       NSTQLFNSTWFNSTWSTEGSNNTEGSDTITLPCRIKQIINMWQKVGKAMYAPPISGQIRC
New_9c_           NSTQLFNSTWFNSTWSTEGSNNTEGSDTITLPCRIKQIINMWCKVCKAMYAPPISGQIRC
                  ************************************** ** **************

Hxbc2_core_       SSNITGLLLTRDGGNSNNESEIFRPGGGDMRDNWRSELYKYKVVKIE
New_9c_           SSNITGLLLTRDGGNSNNESEIFRPGGGDMRDNWRSELYKYKVVKIE
                  ************************************************

Labels: 9c mutations, old core sequence, new design
```

DM or C2

Gtgaagagagggctctgctgtgtgctgctgctgtgtggagcagtcttcgtttcgcccagccaggaaatccatgc
ccgattcagaagaggagccagatctgaggtggtgctggtgaacgtgaccgagaacttcaacatgtggaagaacg
acatggtggagcagatgcacgaggacatcatcagcctgtgggaccagagcctgaagccctgcgtgaagctgacc
cccctgtgcgtgggcgccggcagctgcaacaccagcgtgatcacccaggcctgccccaaggtgagcttcgagcc
catccccatccactactgcgcccccgccggcttcgccatcctgaagtgcaacaacaagaccttcaacggcaccg
gcccctgcaccaacgtgagcaccgtgcagtgcacccacggcatccgccccgtggtgagcagtcagctgctgctg
aacggcagcctggccgaggaggaggtggtgatccgcagcgtgaacttcaccgacaacgccaagaccatcatcgt
gcagctgaacaccagcgtggagatcaactgcaccggcgccggccactgcaacatcgcccgcgccaagtggaaca
acaccctgaagcagatcgccagcaagctgcgcgagcagttcggcaacaacaagaccatcatcttcaagcagagc
agcggcggcgaccccgagatcgtgacccactggttcaactgcggcggcgagttcttctactgcaacagcaccca
gctgttcaacagcacctggttcaacagcacctggagcaccgagggcagcaacaacaccgagggcagcgacacca
tcaccctgccctgccgcatcaagcagatcatcaacatgtggcagaaggtgggcaaggccatgtacgccccccc
atcagcggccagatccgctgcagcagcaacatcaccggcctgctgctgacccgcgacggcggcaacagcaacaa
cgagagcgagatcttccgtccgggcggcggcgacatgcgcgacaactggcgcagcgagctgtacaagtacaagg
tggtgaagatcgagtga (SEQ ID NO:3)

4a or C2S2

Gtgaagagagggctctgctgtgtgctgctgctgtgtggagcagtcttcgtttcgcccagccaggaaatccatgc
ccgattcagaagaggagccagatctgaggtggtgctggtgaacgtgaccgagaacttcaacatgtggaagaacg
acatggtggagcagatgcacgaggacatctgtagcctgtgggaccagagcctgaagccctgcgtgaagctgacc
cccctgtgcgtgggcgccggcagctgcaacaccagcgtgatcacccaggcctgccccaaggtgagcttcgagcc
catccccatccactactgcgcccccgccggcttcgccatcctgaagtgcaacaacaagaccttcaacggcaccg
gcccctgcaccaacgtgagcaccgtgcagtgcacccacggcatccgccccgtggtgagcagtcagctgctgctg
aacggcagcctggccgaggaggaggtggtgatccgcagcgtgaacttcaccgacaacgccaagaccatcatcgt
gcagctgaacaccagcgtggagatcaactgcaccggcgccggccactgcaacatcgcccgcgccaagtggaaca
acaccctgaagcagatcgccagcaagctgcgcgagcagttcggcaacaacaagaccatcatcttcaagcagagc
agcggcggcgaccccgagatcgtgacccactggttcaactgcggcggcgagttcttctactgcaacagcaccca
gctgttcaacagcacctggttcaacagcacctggagcaccgagggcagcaacaacaccgagggcagcgacacca
tcaccctgccctgccgcatcaagcagatcatcaacatgtggtgtaaggtgggcaaggccatgtacgccccccc
atcagcggccagatccgctgcagcagcaacatcaccggcctgctgctgacccgcgacggcggcaacagcaacaa
cgagagcgagatcttccgtccgggcggcggcgacatgcgcgacaactggcgcagcgagctgtacaagtacaagg
tggtgaagatcgagtga (SEQ ID NO: 4)

4b or C2S4

Gtgaagagagggctctgctgtgtgctgctgctgtgtggagcagtcttcgtttcgcccagccaggaaatccatgc
ccgattcagaagaggagccagatctgaggtggtgctggtgaacgtgaccgagaacttcaacatgtggaagaacg
acatggtggagcagatgcacgaggacatcatcagcctgtgggaccagagcctgaagccctgcgtgaagctgacc
cccctgtgcgtgggcgccggcagctgcaacaccagcgtgatcacccaggcctgccccaaggtgagcttcgagcc
catccccatccactactgcgcccccgccggcttcgccatcctgaagtgcaacaactgtaccttcaacggtaccg
gcccctgcaccaacgtgagcaccgtgcagtgcacccacggcatccgccccgtggtgagcagtcagctgctgctg
aacggcagcctggcatgcgaggaggtggtgatccgcagcgtgaacttcaccgacaacgccaagaccatcatcgt
gcagctgaacaccagcgtggagatcaactgcaccggcgccggccactgcaacatcgcccgcgccaagtggaaca
acaccctgaagcagatcgccagcaagctgcgcgagcagttcggcaacaacaagaccatcatcttcaagcagagc
agcggcggcgaccccgagatcgtgacccactggttcaactgcggcggcgagttcttctactgcaacagcaccca
gctgttcaacagcacctggttcaacagcacctggagcaccgagggcagcaacaacaccgagggcagcgacacca
tcaccctgccctgccgcatcaagcagatcatcaacatgtggcagaaggtgggcaaggccatgtacgccccccc
atcagcggccagatccgctgcagcagcaacatcaccggcctgctgctgacccgcgacggcggcaacagcaacaa
cgagagcgagatcttccgtccgggcggcggcgacatgcgcgacaactggcgcagcgagctgtacaagtacaagg
tggtgaagatcgagtga (SEQ ID NO: 5)

FIG. 14A

4c or C2S3

Gtgaagagagggctctgctgtgtgctgctgctgtgtggagcagtcttcgtttcgcccagccaggaaatc
catgcccgattcagaagaggagccagatctgaggtggtgctggtgaacgtgaccgagaacttcaacatg
tggaagaacgacatggtggagcagatgcacgaggacatcatcagcctgtgggaccagagcctgaagccc
tgcgtgaagctgtgtcccctgtgcgtgggcgccggcagctgcaacaccagcgtgatcacccaggcctgc
cccaaggtgagcttcgagcccatccccatccactactgcgcccccgccggcttcgccatcctgaagtgc
aacaacaagaccttcaacggcaccggcccctgcaccaacgtgagcaccgtgcagtgcacccacggcatc
cgccccgtggtgagcagtcagctgctgctgaacggcagcctggccgaggaggaggtggtgatccgcagc
gtgaacttcaccgacaacgccaagaccatcatcgtgcagctgaacaccagcgtggagatcaactgcacc
ggcgccggccactgcaacatcgcccgcgccaagtggaacaacaccctgaagcagatcgccagcaagctg
cgcgagcagttcggcaacaacaagaccatcatcttcaagcagagcagcggcggcgaccccgagatcgtg
acccactggttcaactgcggcggcgagttcttctactgcaacagcacccagctgttcaacagcacctgg
ttcaacagcacctggagcaccgagggcagcaacaacaccgagggcagcgacaccatcaccctgccctgc
cgcatcaagcagatcatcaacatgtggcagaaggtgtgtaaggccatgtacgccccccccatcagcggc
cagatccgctgcagcagcaacatcaccggcctgctgctgacccgcgacggcggcaacagcaacaacgag
agcgagatcttccgtccgggcggcggcgacatgcgcgacaactggcgcagcgagctgtacaagtacaag
gtggtgaagatcgagtga (SEQ ID NO:6)

6a or C123S1

Gtgaagagagggctctgctgtgtgctgctgctgtgtggagcagtcttcgtttcgcccagccaggaaatc
catgcccgattcagaagaggagccagatctgaggtggtgctggtgaacgtgaccgagaacttcaactgg
tgcaagaacgacatggtggagcagatgcacgaggacatctgtagcctgtgggaccagagcctgaagccc
tgcgtgaagctgacccccctgtgcgtgggcgccggcagctgcaacaccagcgtgatcacccaggcctgc
cccaaggtgagcttcgagcccatccccatccactactgcgcccccgccggcttcgccatcctgaagtgc
aacaacaagaccttcaacggcaccggcccctgcaccaacgtgagcaccgtgcagtgcacccacggcatc
cgccccgtggtgagcagtcagctgctgctgaacggcagcctggccgaggaggaggtggtgatcagatct
tgcaacttcaccgacaacgccaagaccatcatcgtgcagctgaacaccagcgtggagatcaactgcacc
ggcgccggccactgcaacatcgcccgcgccaagtggaacaacaccctgaagcagatcgccagcaagctg
cgcgagcagttcggcaacaacaagaccatcatcttcaagcagagcagcggcggcgaccccgagatcgtg
acccactggttcaactgcggcggcgagttcttctactgcaacagcacccagctgttcaacagcacctgg
ttcaacagcacctggagcaccgagggcagcaacaacaccgagggcagcgacaccatcaccctgccctgc
cgcatcaagcagatcattaatatgtggtgtaaggtgggcaagatgatgtacgccccccccatcagcggc
cagatccgctgcagcagcaacatcaccggcctgctgctgacccgcgacggcggcaacagcaacaacgag
agcgagatcttccgtccgggcggcggcgacatgcgcgacaactggcgcagcgagctgtacaagtacaag
gtggtgaagatcgagtga (SEQ ID NO: 7)

6b or C2S24

Gtgaagagagggctctgctgtgtgctgctgctgtgtggagcagtcttcgtttcgcccagccaggaaatc
catgcccgattcagaagaggagccagatctgaggtggtgctggtgaacgtgaccgagaacttcaacatg
tggaagaacgacatggtggagcagatgcacgaggacatctgtagcctgtgggaccagagcctgaagccc
tgcgtgaagctgacccccctgtgcgtgggcgccggcagctgcaacaccagcgtgatcacccaggcctgc
cccaaggtgagcttcgagcccatccccatccactactgcgcccccgccggcttcgccatcctgaagtgc
aacaactgtaccttcaacggtaccggcccctgcaccaacgtgagcaccgtgcagtgcacccacggcatc
cgccccgtggtgagcagtcagctgctgctgaacggcagcctggcatgcgaggaggtggtgatccgcagc
gtgaacttcaccgacaacgccaagaccatcatcgtgcagctgaacaccagcgtggagatcaactgcacc
ggcgccggccactgcaacatcgcccgcgccaagtggaacaacaccctgaagcagatcgccagcaagctg
cgcgagcagttcggcaacaacaagaccatcatcttcaagcagagcagcggcggcgaccccgagatcgtg
acccactggttcaactgcggcggcgagttcttctactgcaacagcacccagctgttcaacagcacctgg
ttcaacagcacctggagcaccgagggcagcaacaacaccgagggcagcgacaccatcaccctgccctgc
cgcatcaagcagatcattaatatgtggtgtaaggtgggcaaggccatgtacgccccccccatcagcggc
cagatccgctgcagcagcaacatcaccggcctgctgctgacccgcgacggcggcaacagcaacaacgag
agcgagatcttccgtccgggcggcggcgacatgcgcgacaactggcgcagcgagctgtacaagtacaag
gtggtgaagatcgagtga (SEQ ID NO: 8)

FIG. 14B

8a or C123S14

Gtgaagagagggctctgctgtgtgctgctgctgtgtggagcagtcttcgtttcgcccagccaggaaatccatg
cccgattcagaagaggagccagatctgaggtggtgctggtgaacgtgaccgagaacttcaactggtgcaagaa
cgacatggtggagcagatgcacgaggacatcatcagcctgtgggaccagagcctgaagccctgcgtgaagctg
acccccctgtgcgtgggcgccggcagctgcaacaccagcgtgatcacccaggcctgccccaaggtgagcttcg
agcccatccccatccactactgcgcccccgccggcttcgccatcctgaagtgcaacaactgtaccttcaacgg
taccggcccctgcaccaacgtgagcaccgtgcagtgcacccacggcatccgccccgtggtgagcagtcagctg
ctgctgaacggcagcctggcatgcgaggaggtggtgatcagatcttgcaacttcaccgacaacgccaagacca
tcatcgtgcagctgaacaccagcgtggagatcaactgcaccggcgccggccactgcaacatcgcccgcgccaa
gtggaacaacaccctgaagcagatcgccagcaagctgcgcgagcagttcggcaacaacaagaccatcatcttc
aagcagagcagcggcggcgaccccgagatcgtgacccactggttcaactgcggcggcgagttcttctactgca
acagcacccagctgttcaacagcacctggttcaacagcacctggagcaccgagggcagcaacaacaccgaggg
cagcgacaccatcaccctgccctgccgcatcaagcagatcatcaatatgtggcagaaggtgggcaagatgatg
tacgccccccccatcagcggccagatccgctgcagcagcaacatcaccggcctgctgctgacccgcgacggcg
gcaacagcaacaacgagagcgagatcttccgtccgggcggcggcgacatgcgcgacaactggcgcagcgagct
gtacaagtacaaggtggtgaagatcgagtga (SEQ ID NO: 9)

8b or C123S12

Gtgaagagagggctctgctgtgtgctgctgctgtgtggagcagtcttcgtttcgcccagccaggaaatccatg
cccgattcagaagaggagccagatctgaggtggtgctggtgaacgtgaccgagaacttcaactggtgcaagaa
cgacatggtggagcagatgcacgaggacatctgtagcctgtgggaccagagcctgaagccctgcgtgaagctg
acccccctgtgcgtgggcgccggcagctgcaacaccagcgtgatcacccaggcctgccccaaggtgagcttcg
agcccatccccatccactactgcgcccccgccggcttcgccatcctgaagtgcaacaacaagaccttcaacgg
caccggcccctgcaccaacgtgagcaccgtgcagtgcacccacggcatccgccccgtggtgagcagtcagctg
ctgctgaacggcagcctggccgaggaggaggtggtgatcagatcttgcaacttcaccgacaacgccaagacca
tcatcgtgcagctgaacaccagcgtggagatcaactgcaccggcgccggccactgcaacatcgcccgcgccaa
gtggaacaacaccctgaagcagatcgccagcaagctgcgcgagcagttcggcaacaacaagaccatcatcttc
aagcagagcagcggcggcgaccccgagatcgtgacccactggttcaactgcggcggcgagttcttctactgca
acagcacccagctgttcaacagcacctggttcaacagcacctggagcaccgagggcagcaacaacaccgaggg
cagcgacaccatcaccctgccctgccgcatcaagcagatcattaatatgtggtgtaaggtgggcaagatgatg
tacgccccccccatcagcggccagatccgctgcagcagcaacatcaccggcctgctgctgacccgcgacggcg
gcaacagcaacaacgagagcgagatcttccgtccgggcggcggcgacatgcgcgacaactggcgcagcgagct
gtacaagtacaaggtggtgaagatcgagtga (SEQ ID NO: 10)

8c or C2S234

Gtgaagagagggctctgctgtgtgctgctgctgtgtggagcagtcttcgtttcgcccagccaggaaatccatg
cccgattcagaagaggagccagatctgaggtggtgctggtgaacgtgaccgagaacttcaacatgtggaagaa
cgacatggtggagcagatgcacgaggacatctgtagcctgtgggaccagagcctgaagccctgcgtgaagctt
tgtcccctgtgcgtgggcgccggcagctgcaacaccagcgtgatcacccaggcctgccccaaggtgagcttcg
agcccatccccatccactactgcgcccccgccggcttcgccatcctgaagtgcaacaactgtaccttcaacgg
taccggcccctgcaccaacgtgagcaccgtgcagtgcacccacggcatccgccccgtggtgagcagtcagctg
ctgctgaacggcagcctggcatgcgaggaggtggtgatccgcagcgtgaacttcaccgacaacgccaagacca
tcatcgtgcagctgaacaccagcgtggagatcaactgcaccggcgccggccactgcaacatcgcccgcgccaa
gtggaacaacaccctgaagcagatcgccagcaagctgcgcgagcagttcggcaacaacaagaccatcatcttc
aagcagagcagcggcggcgaccccgagatcgtgacccactggttcaactgcggcggcgagttcttctactgca
acagcacccagctgttcaacagcacctggttcaacagcacctggagcaccgagggcagcaacaacaccgaggg
cagcgacaccatcaccctgccctgccgcatcaagcagatcattaatatgtggtgtaaggtgtgtaaggccatg
tacgccccccccatcagcggccagatccgctgcagcagcaacatcaccggcctgctgctgacccgcgacggcg
gcaacagcaacaacgagagcgagatcttccgtccgggcggcggcgacatgcgcgacaactggcgcagcgagct
gtacaagtacaaggtggtgaagatcgagtga (SEQ ID NO: 11)

FIG. 14C

9a or C23S234

Gtgaagagagggctctgctgtgtgctgctgctgtgtggagcagtcttcgtttcgcccagccaggaaatcc
atgcccgattcagaagaggagccagatctgaggtggtgctggtgaacgtgaccgagaacttcaacatgtg
gaagaacgacatggtggagcagatgcacgaggacatctgtagcctgtgggaccagagcctgaagccctgc
gtgaagctttgtcccctgtgcgtgggcgccggcagctgcaacaccagcgtgatcacccaggcctgcccca
aggtgagcttcgagcccatccccatccactactgcgcccccgccggcttcgccatcctgaagtgcaacaa
ctgtaccttcaacggtaccggcccctgcaccaacgtgagcaccgtgcagtgcacccacggcatccgcccc
gtggtgagcagtcagctgctgctgaacggcagcctggcatgcgaggaggtggtgatccgcagcgtgaact
tcaccgacaacgccaagaccatcatcgtgcagctgaacaccagcgtggagatcaactgcaccggcgccgg
ccactgcaacatcgcccgcgccaagtggaacaacaccctgaagcagatcgccagcaagctgcgcgagcag
ttcggcaacaacaagaccatcatcttcaagcagagcagcggcggcgaccccgagatcgtgacccactggt
tcaactgcggcggcgagttcttctactgcaacagcacccagctgttcaacagcacctggttcaacagcac
ctggagcaccgagggcagcaacaacaccgagggcagcgacaccatcaccctgccctgccgcatcaagcag
atcattaatatgtggtgtaaggtgtgtaagatgatgtacgccccccgatatcaggccagatccgctgca
gcagcaacatcaccggcctgctgctgacccgcgacggcggcaacagcaacaacgagagcgagatcttccg
tccgggcggcggcgacatgcgcgacaactggcgcagcgagctgtacaagtacaaggtggtgaagatcgag
tga (SEQ ID NO:12)

9b or C12S134

Gtgaagagagggctctgctgtgtgctgctgctgtgtggagcagtcttcgtttcgcccagccaggaaatcc
atgcccgattcagaagaggagccagatctgaggtggtgctggtgaacgtgaccgagaacttcaactggtg
caagaacgacatggtggagcagatgcacgaggacatcatcagcctgtgggaccagagcctgaagccctgc
gtgaagctttgtcccctgtgcgtgggcgccggcagctgcaacaccagcgtgatcacccaggcctgcccca
aggtgagcttcgagcccatccccatccactactgcgcccccgccggcttcgccatcctgaagtgcaacaa
ctgtaccttcaacggtaccggcccctgcaccaacgtgagcaccgtgcagtgcacccacggcatccgcccc
gtggtgagcagtcagctgctgctgaacggcagcctggcatgcgaggaggtggtgatcagatcttgcaact
tcaccgacaacgccaagaccatcatcgtgcagctgaacaccagcgtggagatcaactgcaccggcgccgg
ccactgcaacatcgcccgcgccaagtggaacaacaccctgaagcagatcgccagcaagctgcgcgagcag
ttcggcaacaacaagaccatcatcttcaagcagagcagcggcggcgaccccgagatcgtgacccactggt
tcaactgcggcggcgagttcttctactgcaacagcacccagctgttcaacagcacctggttcaacagcac
ctggagcaccgagggcagcaacaacaccgagggcagcgacaccatcaccctgccctgccgcatcaagcag
atcatcaacatgtggcagaaggtgtgtaaggccatgtacgcccccccccatcagcggccagatccgctgca
gcagcaacatcaccggcctgctgctgacccgcgacggcggcaacagcaacaacgagagcgagatcttccg
tccgggcggcggcgacatgcgcgacaactggcgcagcgagctgtacaagtacaaggtggtgaagatcgag
tga (SEQ ID NO:13)

9c or C12S123

Gtgaagagagggctctgctgtgtgctgctgctgtgtggagcagtcttcgtttcgcccagccaggaaatcc
atgcccgattcagaagaggagccagatctgaggtggtgctggtgaacgtgaccgagaacttcaactggtg
caagaacgacatggtggagcagatgcacgaggacatctgtagcctgtgggaccagagcctgaagccctgc
gtgaagctgtgtcccctgtgcgtgggcgccggcagctgcaacaccagcgtgatcacccaggcctgcccca
aggtgagcttcgagcccatccccatccactactgcgcccccgctggcttcgccatcctgaagtgcaacaa
caagaccttcaacggcaccggcccctgcaccaacgtgagcaccgtgcagtgcacccacggcatccgcccc
gtggtgagcagtcagctgctgctgaacggcagcctggccgaggaggaggtggtgatcagatcttgcaact
tcaccgacaacgccaagaccatcatcgtgcagctgaacaccagcgtggagatcaactgcaccggcgccgg
ccactgcaacatcgcccgcgccaagtggaacaacaccctgaagcagatcgccagcaagctgcgcgagcag
ttcggcaacaacaagaccatcatcttcaagcagagcagcggcggcgaccccgagatcgtgacccactggt
tcaactgcggcggcgagttcttctactgcaacagcacccagctgttcaacagcacctggttcaacagcac
ctggagcaccgagggcagcaacaacaccgagggcagcgacaccatcaccctgccctgccgcatcaagcag
atcatcaacatgtggtgtaaggtgtgtaaggccatgtacgcccccccccatcagcggccagatccgctgca
gcagcaacatcaccggcctgctgctgacccgcgacggcggcaacagcaacaacgagagcgagatcttccg
tccgggcggcggcgacatgcgcgacaactggcgcagcgagctgtacaagtacaaggtggtgaagatcgag
tga (SEQ ID NO: 14)

FIG. 14D

10a or C123S124

Gtgaagagagggctctgctgtgtgctgctgctgtgtggagcagtcttcgtttcgcccagccaggaaatccatgcccgattcagaaga
ggagccagatctgaggtggtgctggtgaacgtgaccgagaacttcaactggtgcaagaacgacatggtggagcagatgcacga
ggacatctgtagcctgtgggaccagagcctgaagccctgcgtgaagctgacccccctgtgcgtgggcgccggcagctgcaacac
cagcgtgatcacccaggcctgccccaaggtgagcttcgagcccatccccatccactactgcgcccccgccggcttcgccatcctg
aagtgcaacaactgtaccttcaacggtaccggcccctgcaccaacgtgagcaccgtgcagtgcacccacggcatccgcccgtg
gtgagcagtcagctgctgctgaacggcagcctggcatgcgaggaggtggtgatcagatcttgcaacttcaccgacaacgccaag
accatcatcgtgcagctgaacaccagcgtggagatcaactgcaccggcgccggccactgcaacatcgcccgcgccaagtgga
acaacaccctgaagcagatcgccagcaagctgcgcgagcagttcggcaacaacaagaccatcatcttcaagcagagcagcg
gcggcgaccccgagatcgtgacccactggttcaactgcggcggcgagttcttctactgcaacagcacccagctgttcaacagcac
ctggttcaacagcacctggagcaccgagggcagcaacaacaccgagggcagcgacaccatcaccctgccctgccgcatcaa
gcagatcattaatatgtggtgtaaggtgggcaagatgatgtacgccccccccatcagcggccagatccgctgcagcagcaacatc
accggcctgctgctgacccgcgacggcggcaacagcaacaacgagagcgagatcttccgtccgggcggcggcgacatgcgc
gacaactggcgcagcgagctgtacaagtacaaggtggtgaagatcgagtga (SEQ ID NO: 15)

10b or C123S123

Atgaagagagggctctgctgtgtgctgctgctgtgtggagcagtcttcgtttcgcccagccaggaaatccatgcccgattcagaaga
ggagccagatctgaggtggtgctggtgaacgtgaccgagaacttcaactggtgcaagaacgacatggtggagcagatgcacga
ggacatctgtagcctgtgggaccagagcctgaagccctgcgtgaagctgtgtccctgtgcgtgggcgccggcagctgcaacacc
agcgtgatcacccaggcctgccccaaggtgagcttcgagcccatccccatccactactgcgcccccgctggcttcgccatcctga
agtgcaacaacaagaccttcaacggcaccggcccctgcaccaacgtgagcaccgtgcagtgcacccacggcatccgcccgt
ggtgagcagtcagctgctgctgaacggcagcctggccgaggaggaggtggtgatcagatcttgcaacttcaccgacaacgccaa
gaccatcatcgtgcagctgaacaccagcgtggagatcaactgcaccggcgccggccactgcaacatcgcccgcgccaagtgg
aacaacaccctgaagcagatcgccagcaagctgcgcgagcagttcggcaacaacaagaccatcatcttcaagcagagcagc
ggcggcgaccccgagatcgtgacccactggttcaactgcggcggcgagttcttctactgcaacagcacccagctgttcaacagca
cctggttcaacagcacctggagcaccgagggcagcaacaacaccgagggcagcgacaccatcaccctgccctgccgcatcaa
gcagatcatcaacatgtggtgtaaggtgtgtaagatgatgtacgccccccccatcagcggccagatccgctgcagcagcaacatc
accggcctgctgctgacccgcgacggcggcaacagcaacaacgagagcgagatcttccgtccgggcggcggcgacatgcgc
gacaactggcgcagcgagctgtacaagtacaaggtggtgaagatcgagtgag (SEQ ID NO: 16)

10c or C123S134

Gtgaagagagggctctgctgtgtgctgctgctgtgtggagcagtcttcgtttcgcccagccaggaaatccatgcccgattcagaaga
ggagccagatctgaggtggtgctggtgaacgtgaccgagaacttcaactggtgcaagaacgacatggtggagcagatgcacga
ggacatcatcagcctgtgggaccagagcctgaagccctgcgtgaagctttgtcccctgtgcgtgggcgccggcagctgcaacacc
agcgtgatcacccaggcctgccccaaggtgagcttcgagcccatccccatccactactgcgcccccgccggcttcgccatcctga
agtgcaacaactgtaccttcaacggtaccggcccctgcaccaacgtgagcaccgtgcagtgcacccacggcatccgcccgtgg
tgagcagtcagctgctgctgaacggcagcctggcatgcgaggaggtggtgatcagatcttgcaacttcaccgacaacgccaaga
ccatcatcgtgcagctgaacaccagcgtggagatcaactgcaccggcgccggccactgcaacatcgcccgcgccaagtggaa
caacaccctgaagcagatcgccagcaagctgcgcgagcagttcggcaacaacaagaccatcatcttcaagcagagcagcggc
ggcgaccccgagatcgtgacccactggttcaactgcggcggcgagttcttctactgcaacagcacccagctgttcaacagcacct
ggttcaacagcacctggagcaccgagggcagcaacaacaccgagggcagcgacaccatcaccctgccctgccgcatcaagc
agatcatcaatatgtggcagaaggtgtgtaaggccatgtacgccccccccatcagcggccagatccgctgcagcagcaacatca
ccggcctgctgctgacccgcgacggcggcaacagcaacaacgagagcgagatcttccgtccgggcggcggcgacatgcgcg
acaactggcgcagcgagctgtacaagtacaaggtggtgaagatcgagtga (SEQ ID NO: 17)

FIG. 14E

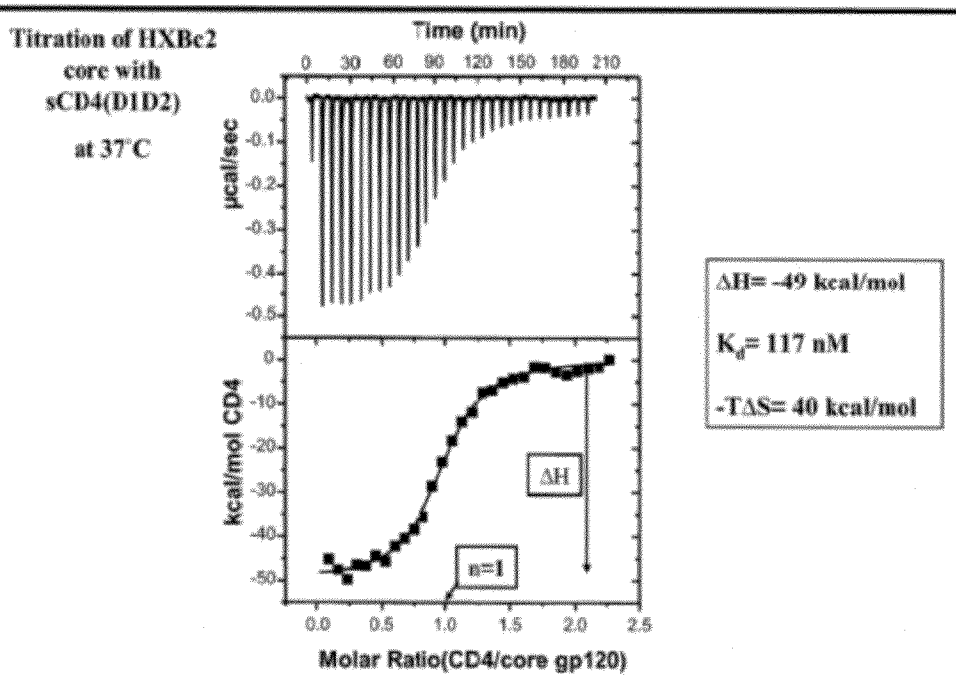
11a or C12S1234
Gtgaagagagggctctgctgtgtgctgctgctgtgtggagcagtcttcgtttcgcccagccaggaaat
ccatgcccgattcagaagaggagccagatctgaggtggtgctggtgaacgtgaccgagaacttcaact
ggtgcaagaacgacatggtggagcagatgcacgaggacatctgtagcctgtgggaccagagcctgaag
ccctgcgtgaagctgtgtccctgtgcgtgggcgccggcagctgcaacaccagcgtgatcacccaggc
ctgccccaaggtgagcttcgagcccatccccatccactactgcgcccccgccggcttcgccatcctga
agtgcaacaactgtaccttcaacggtaccggcccctgcaccaacgtgagcaccgtgcagtgcacccac
ggcatccgccccgtggtgagcagtcagctgctgctgaacggcagcctggcatgcgaggaggtggtgat
cagatcttgcaacttcaccgacaacgccaagaccatcatcgtgcagctgaacaccagcgtggagatca
actgcaccggcgccggccactgcaacatcgcccgcgccaagtggaacaacaccctgaagcagatcgcc
agcaagctgcgcgagcagttcggcaacaacaagaccatcatcttcaagcagagcagcggcggcgaccc
cgagatcgtgacccactggttcaactgcggcggcgagttcttctactgcaacagcacccagctgttca
acagcacctggttcaacagcacctggagcaccgagggcagcaacaacaccgagggcagcgacaccatc
accctgccctgccgcatcaagcagatcatcaacatgtggtgtaaggtgtgtaaggccatgtacgcccc
ccccatcagcggccagatccgctgcagcagcaacatcaccggcctgctgctgacccgcgacggcggca
acagcaacaacgagagcgagatcttccgtccgggcggcggcgacatgcgcgacaactggcgcagcgag
ctgtacaagtacaaggtggtgaagatcgagtga (SEQ ID NO: 18)

HxBc2Core wt
Gtgaagagagggctctgctgtgtgctgctgctgtgtggagcagtcttcgtttcgcccagccaggaaat
ccatgcccgattcagaagaggagccagatctgaggtggtgctggtgaacgtgaccgagaacttcaaca
tgtggaagaacgacatggtggagcagatgcacgaggacatcatcagcctgtgggaccagagcctgaag
ccctgcgtgaagctgacccccctgtgcgtgggcgccggcagctgcaacaccagcgtgatcacccaggc
ctgccccaaggtgagcttcgagcccatccccatccactactgcgcccccgccggcttcgccatcctga
agtgcaacaacaagaccttcaacggcaccggcccctgcaccaacgtgagcaccgtgcagtgcacccac
ggcatccgccccgtggtgagcacccagctgctgctgaacggcagcctggccgaggaggaggtggtgat
ccgcagcgtgaacttcaccgacaacgccaagaccatcatcgtgcagctgaacaccagcgtggagatca
actgcaccggcgccggccactgcaacatcgcccgcgccaagtggaacaacaccctgaagcagatcgcc
agcaagctgcgcgagcagttcggcaacaacaagaccatcatcttcaagcagagcagcggcggcgaccc
cgagatcgtgacccacagcttcaactgcggcggcgagttcttctactgcaacagcacccagctgttca
acagcacctggttcaacagcacctggagcaccgagggcagcaacaacaccgagggcagcgacaccatc
accctgccctgccgcatcaagcagatcatcaacatgtggcagaaggtgggcaaggccatgtacgcccc
ccccatcagcggccagatccgctgcagcagcaacatcaccggcctgctgctgacccgcgacggcggca
acagcaacaacgagagcgagatcttccgtccgggcggcggcgacatgcgcgacaactggcgcagcgag
ctgtacaagtacaaggtggtgaagatcgagtga (SEQ ID NO: 19)

New Core9c
Gtgaagagagggctctgctgtgtgctgctgctgtgtggagcagtcttcgtttcgcccagccaggaaat
ccatgcccgattcagaagaggagccagatctgaggtggtgctggtgaacgtgaccgagaacttcaact
ggtgcaagaacgacatggtggagcagatgcacgaggacatctgtagcctgtgggaccagagcctgaag
ccctgcgtgaagctgtgtcctctggccggcgccaccagcgtgatcacccaggcctgccccaaggtgag
cttcgagcccatccccatccactactgcgcccccgctggcttcgccatcctgaagtgcaacaacaaga
ccttcaacggcaccggcccctgcaccaacgtgagcaccgtgcagtgcacccacggcatccgccccgtg
gtgagcagtcagctgctgctgaacggcagcctggccgaggaggaggtggtgatcagatcttgcaactt
caccgacaacgccaagaccatcatcgtgcagctgaacaccagcgtggagatcaactgcacccgcccca
acaacggcggcagcggcagcggcggcaacatgcgccaggcccactgcaacatcagccgcgccaagtgg
aacaacaccctgaagcagatcgccagcaagctgcgcgagcagttcggcaacaacaagaccatcatctt
caagcagagcagcggcggcgaccccgagatcgtgacccactggttcaactgcggcggcgagttcttct
actgcaacagcacccagctgttcaacagcacctggttcaacagcacctggagcaccgagggcagcaac
aacaccgagggcagcgacaccatcaccctgccctgccgcatcaagcagatcatcaacatgtggtgtaa
ggtgtgtaaggccatgtacgccccccccatcagcggccagatccgctgcagcagcaacatcaccggcc
tgctgctgacccgcgacggcggcaacagcaacaacgagagcgagatcttccgtccgggcggcggcgac
atgcgcgacaactggcgcagcgagctgtacaagtacaaggtggtgaagatcgagtga (SEQ ID
NO: 26)

FIG. 14F

Measurement of thermodynamic properties of p120 upon ligand binding (by ITC)

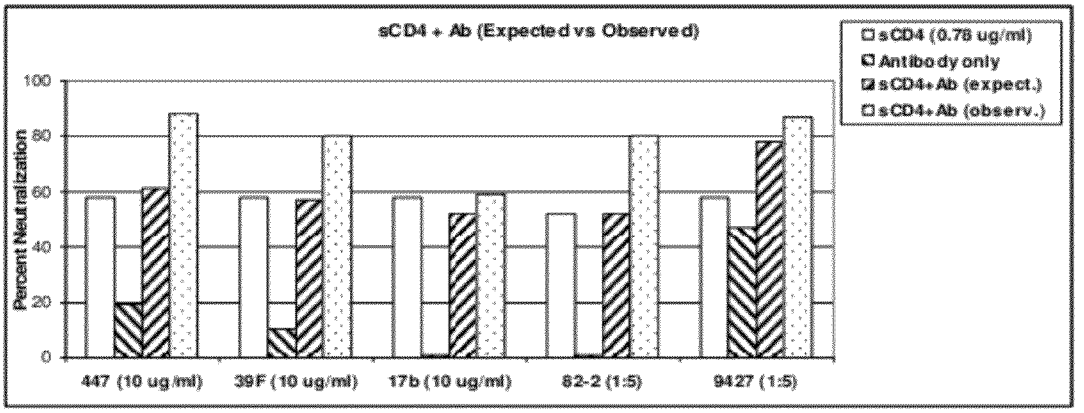


Comparison of thermodynamic values of CD4-gp10 binding

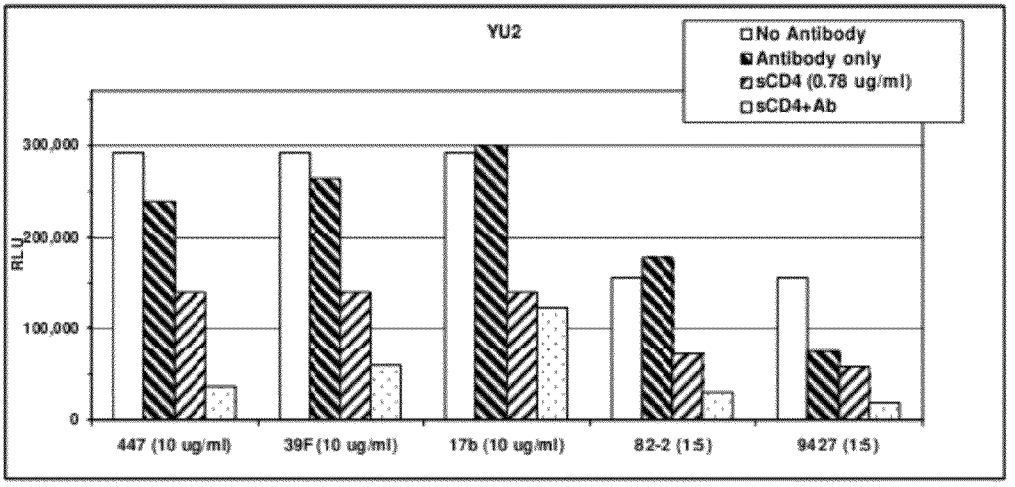
Protein	ΔH (kcal/mol)	$-T\Delta S$ (kcal/mol)	K_d (nM) to sCD4
HXcore WT	-49.7 +/- 1.77	40.0 +/- 1.77	87
C2	-51.3 +/- 1.82	39.0 +/- 1.81	1.5
C2S2	-29.3 +/- 1.04	17.2 +/- 1.04	2.5
C2S3	-46.4 +/- 1.97	26.8 +/- 1.97	1
C2S4	-39.4 +/- 2.32	34.2 +/- 2.32	3
C123S1	-38.8 +/- 2.06	28.3 +/- 2.06	35
C123S12	-30.0 +/- 1.07	18.5 +/- 1.08	6
C12S123	-31.4 +/- 1.60	18.9 +/- 1.60	1
New C12S123	-27.75 +/- 1.11	15.62 +/- 1.11	3
NewC12S1234	-27.47 +/- 1.39	15.24 +/- 1.39	2

FIG. 15

A **YU2 Percent neutralization**

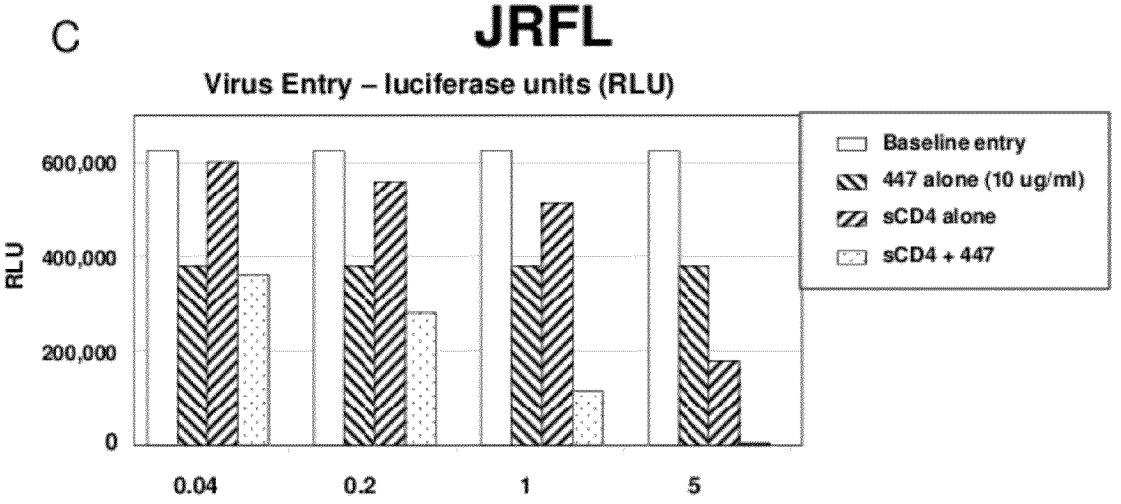


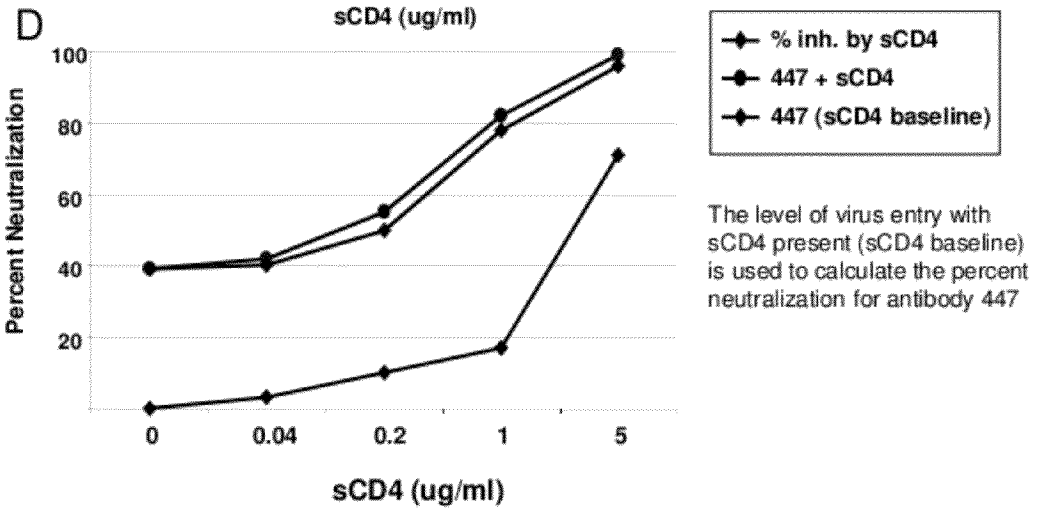
B **YU2 RLU Entry Data**

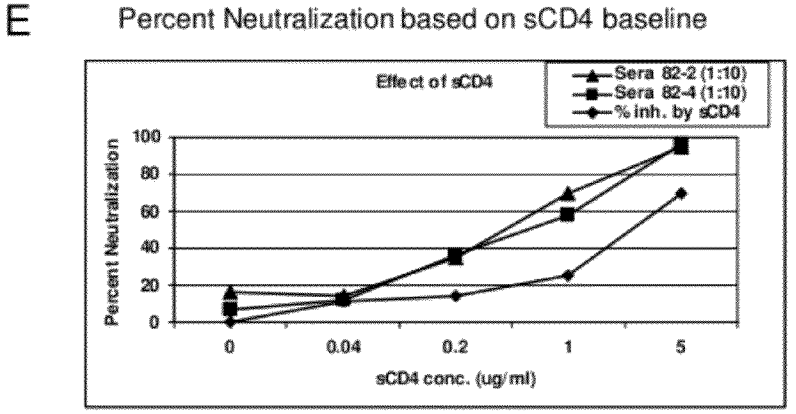


447 – V3 mAb
39F – V3 mAb
82-2 – GP sera from dCFldV12 clade (BaL)
9427 – Baboon sera; gp140GCN-4 (YU2)

FIGs. 16A-16B



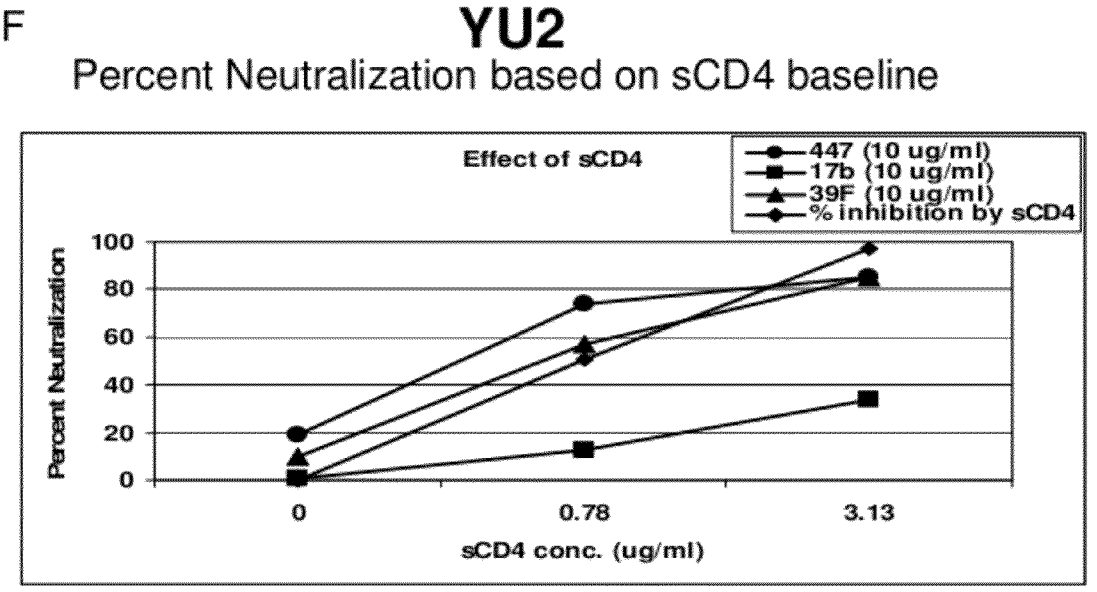




82-2, 82-4 are each GP sera from dCFldV12 clade (BaL)

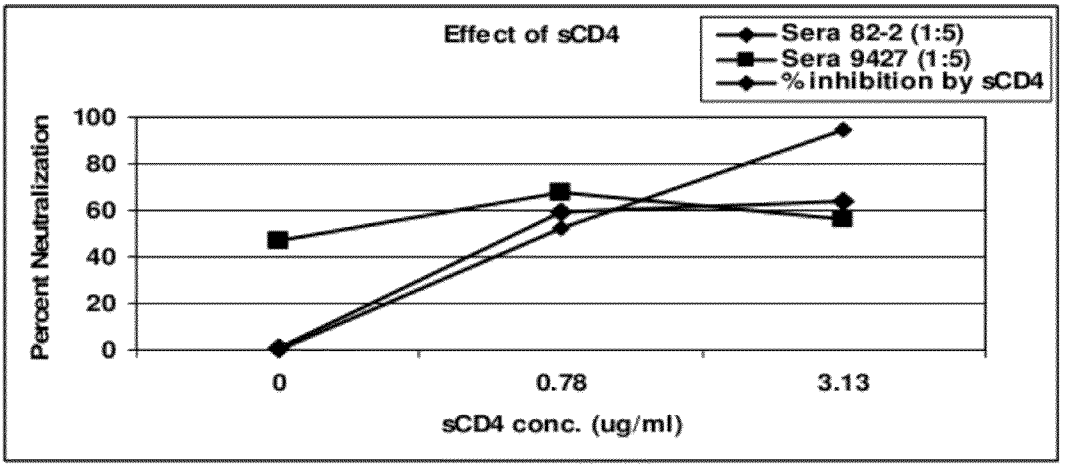
FIGs. 16C-16E

F



447 – V3 mAb
39F – V3 mAb
82-2 – GP sera from dCFldV12 clade (BaL)
9427 – Baboon sera; gp140GCN-4 (YU2)

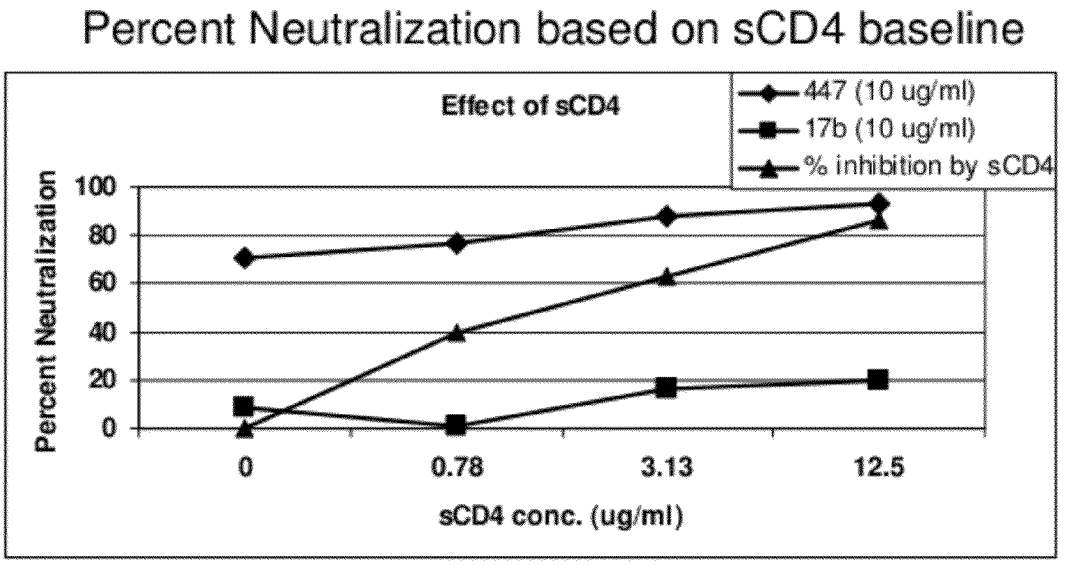
G



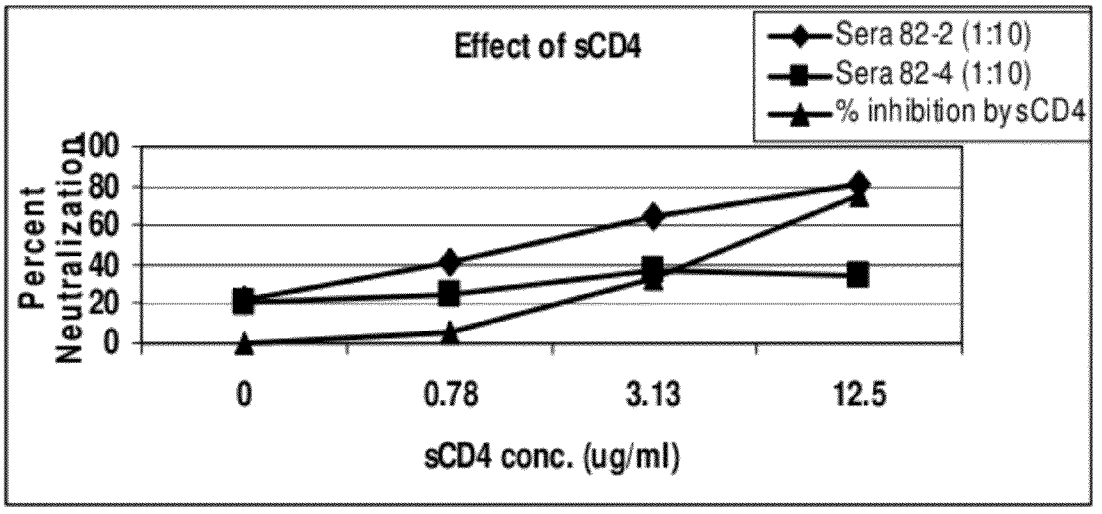
FIGs. 16F-16G

6535

H

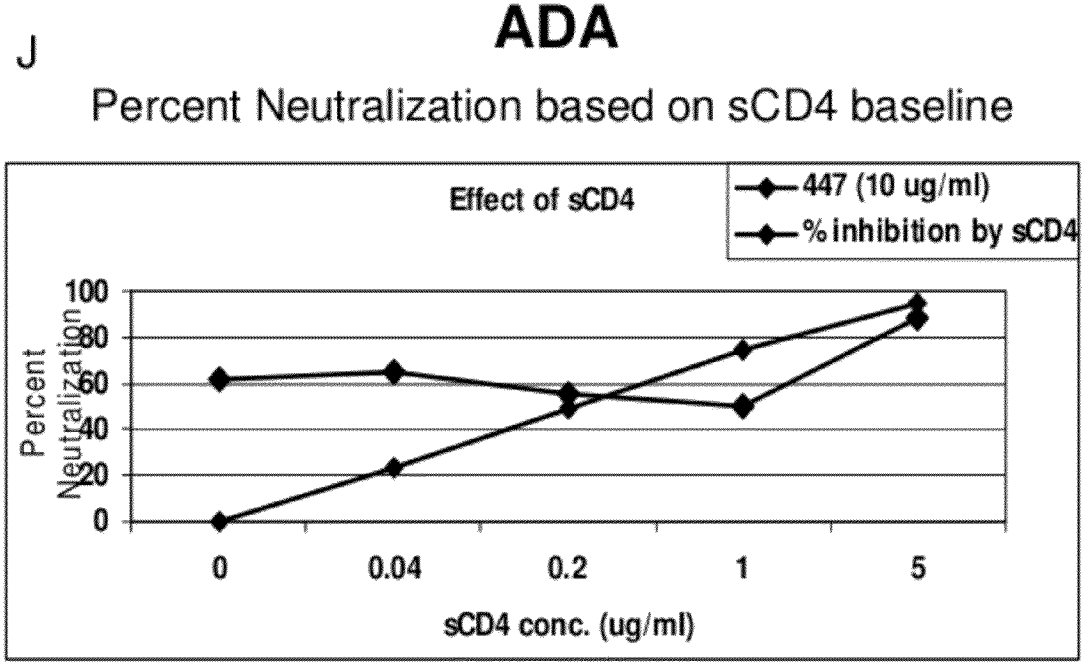


I

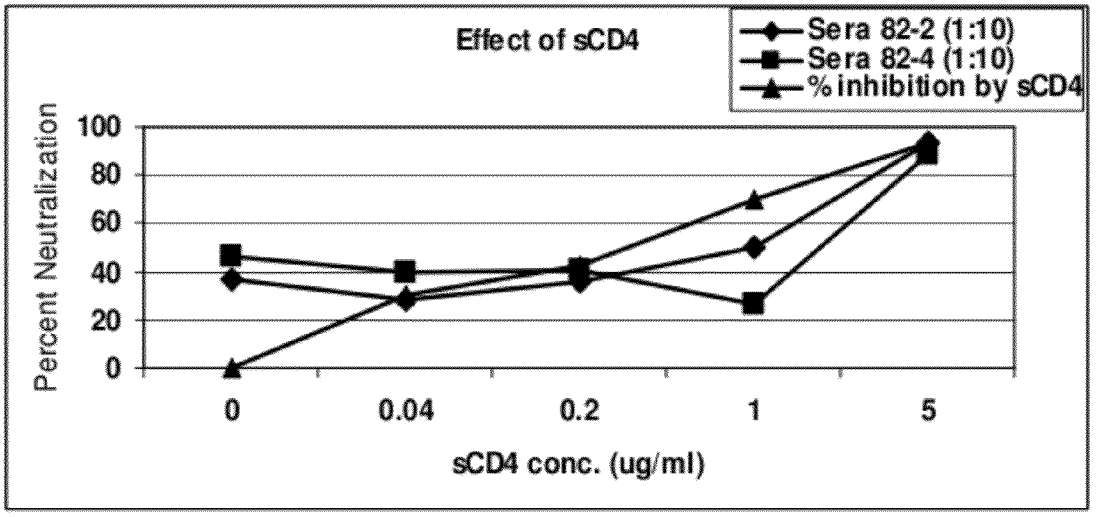


FIGs. 16H-16I

J



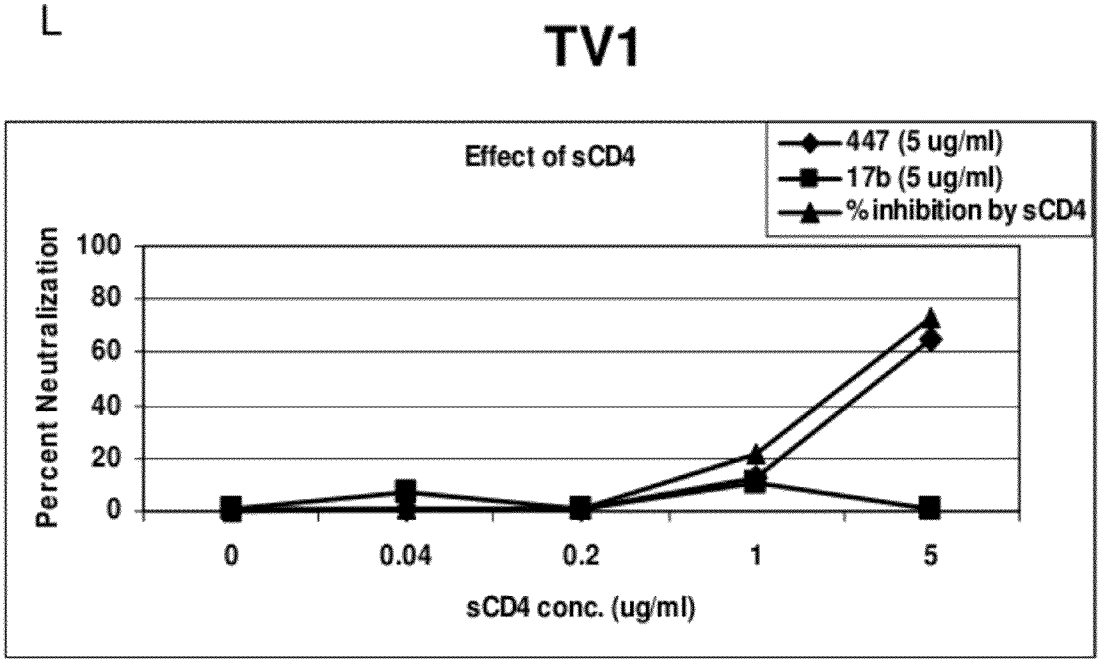
K



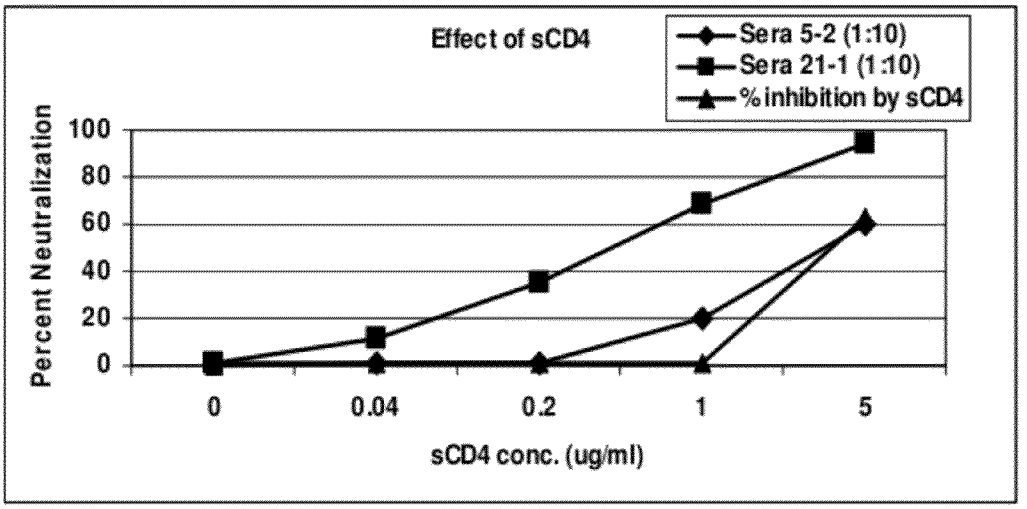
82-2, 82-4 are each GP sera from dCFIdV12 clade (BaL)

FIGs. 16J-16K

L



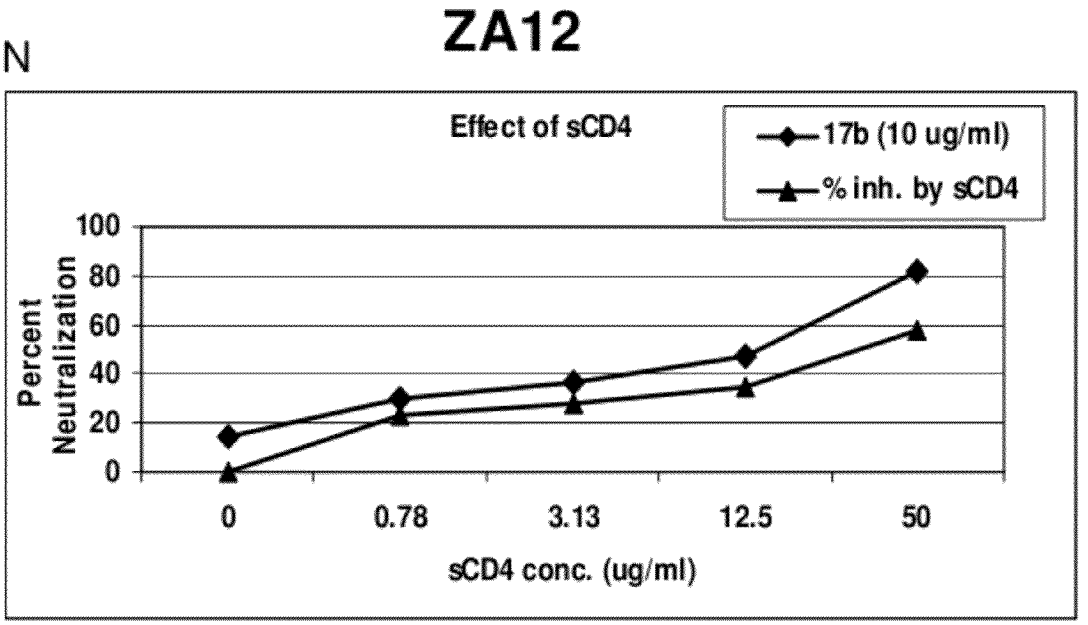
M



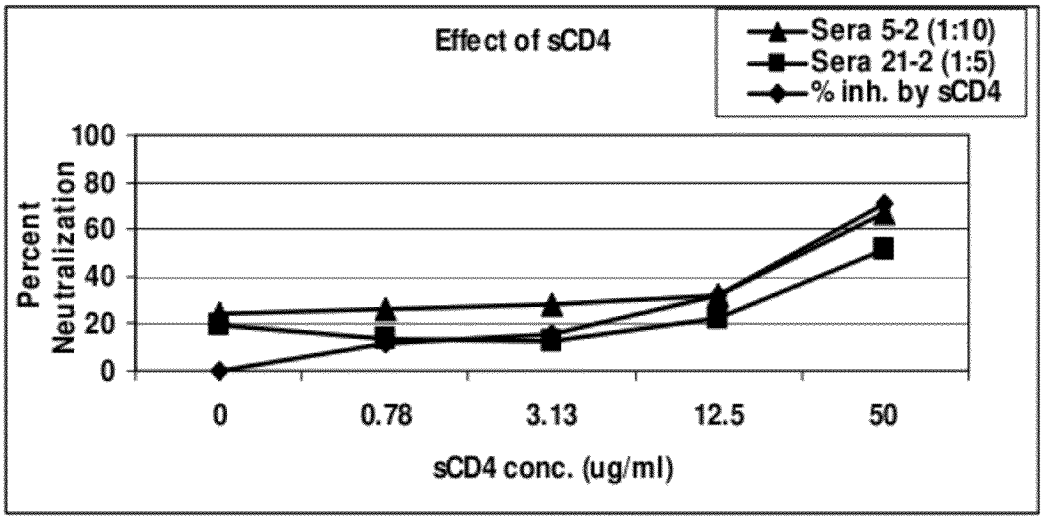
5-2, 21-4 are each GP sera from dCFI clade C

FIGs. 16L-16M

N



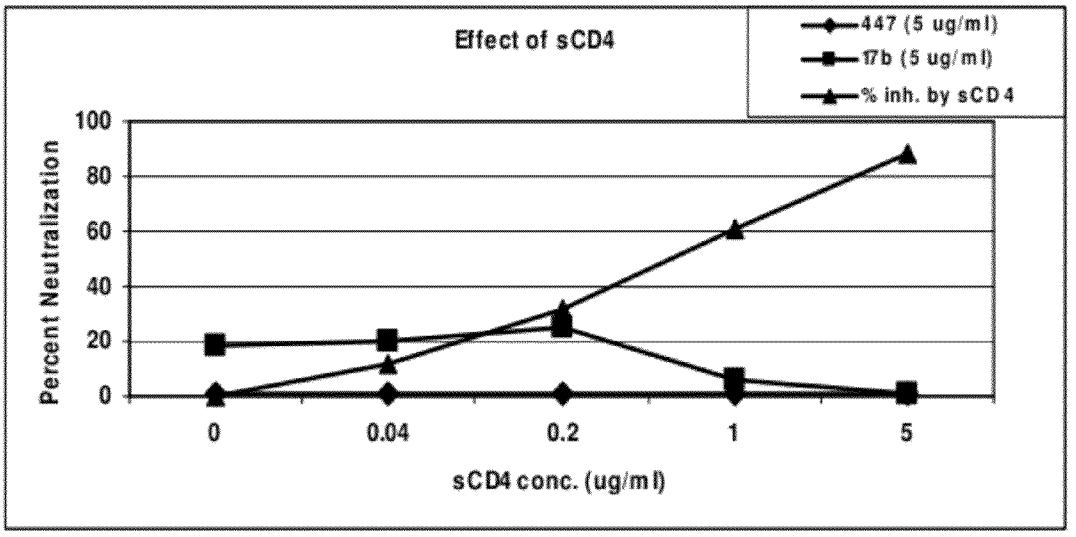
O



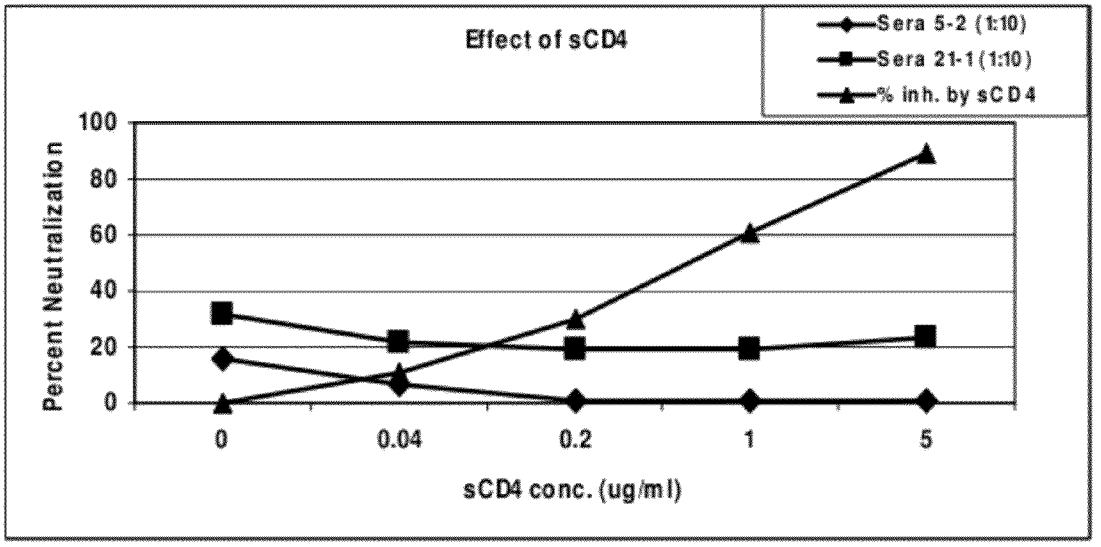
5-2, 21-4 are each GP sera from dCFI clade C

FIGs. 16N-16O

P



Q



5-2, 21-4 are each GP sera from dCFI clade C

FIGs. 16P-16Q

CONFORMATIONALLY STABILIZED HIV ENVELOPE IMMUNOGENS

CROSS REFERENCE TO RELATED APPLICATION

This application is a continuation application of U.S. patent application Ser. No. 13/232,775, filed Sep. 14, 2011, now U.S. Pat. No. 8,268,323, which is a divisional application of U.S. patent application Ser. No. 12/065,894, filed Mar. 5, 2008, now U.S. Pat. No. 8,044,185, which is the U.S. §371 National Stage of International Application No. PCT/US2006/034681, filed Sep. 6, 2006, published in English under PCT Article 21(2), which in turn claims the benefit of U.S. Provisional Application No: 60/713,725, filed Sep. 6, 2005; U.S. Provisional Application No: 60/729,878, filed Oct. 24, 2005; U.S. Provisional Application No: 60/731,627, filed Oct. 28, 2005; and U.S. Provisional Application No: 60/832,458, filed Jul. 20, 2006. All of the prior applications are incorporated by reference herein in their entirety.

FIELD

The present disclosure relates to stabilized forms of human immunodeficiency virus gp120 envelope protein, specifically to crystalline forms of gp120, high resolution structures obtained from these crystals, and use thereof.

BACKGROUND

The primary immunologic abnormality resulting from infection by human immunodeficiency virus (HIV) is the progressive depletion and functional impairment of T lymphocytes expressing the CD4 cell surface glycoprotein. The loss of CD4 helper/inducer T cell function probably underlies the profound defects in cellular and humoral immunity leading to the opportunistic infections and malignancies characteristic of the acquired immunodeficiency syndrome (AIDS) (Lane et al., *Ann. Rev. Immunol.* 3:477, 1985). Studies of HIV-1 infection of fractionated CD4 and CD8 T cells from normal donors and AIDS patients have revealed that depletion of CD4 T cells results from the ability of HIV-1 to selectively infect, replicate in, and ultimately destroy this T lymphocyte subset (Klatzmann et al., *Science* 225:59, 1984). The possibility that CD4 itself is an essential component of the cellular receptor for HIV-1 was first indicated by the observation that monoclonal antibodies directed against CD4 block HIV-1 infection and syncytia induction (Dalgleish et al., *Nature* 312:767, 1984; McDougal et al., *J. Immunol.* 135:3151, 1985). This hypothesis has been confirmed by the demonstration that a molecular complex forms between CD4 and the major envelope glycoprotein of HIV-1 (McDougal et al., *Science* 231:382, 1986)

The major envelope protein of HIV-1 is a glycoprotein of approximately 160 kD (160). During infection proteases of the host cell cleave gp160 into gp120 and gp41. gp41 is an integral membrane protein, while gp120 protrudes from the mature virus. Together gp120 and gp41 make up the HIV envelope spike.

The HIV envelope spike mediates binding to receptors and virus entry (Wyatt and Sodroski, *Science* 280:188, 1998). The spike is trimeric and composed of three gp120 exterior and three gp41 transmembrane envelope glycoproteins. CD4 binding to gp120 in the spike induces conformational changes that allow binding to a coreceptor, either CCR5 or CXCR4, which is required for viral entry (Dalgleish et al., *Nature* 312:763, 1984; Sattentau and Moore, *J. Exp. Med.* 174:407, 1991; Feng at al., *Science* 272:872, 1996; Wu et al., *Nature* 384:179, 1996; Trkola et al., *Nature* 384:184, 1996).

The mature gp120 glycoprotein is approximately 470-490 amino acids long depending on the HIV strain of origin. N-linked glycosylation at approximately 20-25 sites makes up nearly half of the mass of the molecule. Sequence analysis shows that the polypeptide is composed of five conserved regions (C1-C5) and five regions of high variability (V1-V5).

With the number of individuals infected by HIV-1 approaching 1% of the world's population, an effective vaccine is urgently needed. An enveloped virus, HIV-1 hides from humoral recognition behind a protective lipid bilayer. An available viral target for neutralizing antibodies is the envelope spike. Genetic, immunologic and structural studies of the HIV-1 envelope glycoproteins have revealed extraordinary diversity as well as multiple overlapping mechanisms of humoral evasion, including self-masquerading glycan, immunodominant variable loops, and conformational masking. These evolutionarily honed bathers of diversity and evasion have confounded traditional means of vaccine development. It is believed that immunization with effectively immunogenic HIV gp120 envelope glycoprotein can elicit a neutralizing response directed against gp120, and thus HIV. The need exists for immunogens that are capable of eliciting an immunogenic response in a suitable subject. In order to be effective, the antibodies raised must be capable of neutralizing a broad range of HIV strains and subtypes.

SUMMARY OF THE DISCLOSURE

Disclosed herein are gp120 polypeptides and nucleic acid molecules encoding gp120 polypeptides, which are useful to induce an immunogenic response to a lentivirus, such as SIV or HIV (for example HIV-1 and HIV-II) in a subject. In several embodiments, the gp120 polypeptides are stabilized in a CD4 bound conformation by the introduction of a plurality of non-naturally occurring cross-linking cysteine residues. In other examples, the gp120 polypeptide has the V3 loop in an extended conformation.

Immunogenic compositions containing a therapeutically effective amount of gp120 polypeptides and nucleic acid molecules encoding gp120 polypeptides are also disclosed. Also disclosed are methods for eliciting and/or enhancing an immune response in a subject, for example by administering an immunogenic composition.

Crystalline forms of gp120 are disclosed as are crystal structures of gp120 polypeptides obtained from these structures. Methods are also disclosed for identifying an immunogen that induces an immune response to gp120 using these crystal structures. Also provided by this disclosure is a machine readable data storage medium including a data storage material encoded with machine readable data corresponding to the coordinates of the crystal structures disclosed herein. A computer system is disclosed for displaying the coordinate data from these crystal structures of gp120, such as the atomic positions, surface, domain, or region of the gp120 polypeptide.

The foregoing and other objects, features, and advantages of the invention will become more apparent from the following detailed description, which proceeds with reference to the accompanying figures.

BRIEF DESCRIPTION OF THE DRAWINGS

FIG. **1** is a schematic representation of the development cycle for gp120 immunogens stabilized in the CD4-bound conformation. Qualitative Biacore analysis was used as an

initial screen to determine if CD4 and the CD4 induced (CD4i) antibodies still bound. Isothermal titration calorimetry (ITC) and crystal structure determination were used to refine the gp120 immunogens.

FIG. **2** is a set of computer generated images. The images show the modeled structures of wild-type gp120 compared with cavity-filling and double cysteine mutants. Each pair of panels shows the HXBc2 core wild-type structure (left panels) and the mutant structure (right panels). Data ranged from minimum Bragg spacings of 1.9 A to 2.5 A.

FIG. **3** is a set of computer generated images. The images show the positions of conformationally stabilizing mutations in the CD4-bound structure of HIV-1 (left) and the unliganded structure of SIV (right). Disulfide separations for each of the mutations in the CD4-bound and unliganded structure were calculated and are given in Table 3 below.

FIG. **4** is tabulated date and plots of neutralization data obtained from rabbits immunized with four prime cycles of BSA or the indicated gp120. FIGS. **4**A and **4**B are tables showing the percent neutralization of the indicated viruses by sera obtained from rabbits immunized with the indicated stabilized forms of gp120, followed by immunization with a stabilized gp140 trimer. FIG. **4**C is tabulated neutralization data from sera obtained from the indicated animals. The data show the effects of various peptides on the neutralization of HIV isolate YU2.SG3. This data demonstrates that the YU V3 peptide blocks neutralization of HIV isolate YU2.SG3 by antibodies produced by the boost prime immunization scheme described in Example 5. FIGS. **4**D-**4**M are graphical representations of the data shown in FIG. **4**C.

FIG. **5** is a computer generated image of the modeled structure of an HIV-1 gp120 core with V3 as defined by the coordinates in Table 2. The crystal structure of core gp120 with an intact V3 is shown bound to the membrane-distal two domains of the CD4 receptor and the Fab portion of the X5 antibody. In this orientation, the viral membrane would be positioned toward the top of the page and the target cell toward the bottom.

FIG. **6** is an alignment of the V3 sequence from the indicated HIV strains and clades and computer generated images of the structures of the V3 loop as set forth in Table 2. FIG. **6** (A) V3 sequence. The sequences of JR-FL (SEQ ID NO: 21) and HXBc2 (SEQ ID NO: 22) are shown along with the consensus sequence of clades A (SEQ ID NO: 23), B (SEQ ID NO: 24), and C (SEQ ID NO: 25). For the consensus sequences, absolutely conserved residues are shown in uppercase, with variable residues in lowercase. Single letter amino acid abbreviations: A, Ala; C, Cys; D, Asp; E, Glu; F, Phe; G, Gly; H, His; I, Ile; K, Lys; M, Met; N, Asn; P, Pro; Q, Gln; R, Arg; S, Ser; T, Thr; V, Val; Y, Tyr. The conserved (Arg-Pro) and (Gly-Pro-Gly-Arg) motifs indicated in grey FIG. **6** (D) and FIG. **6** (E). FIG. **6** (B) V3 electron density and B values. 2Fobs-Fcalc density is shown for the entire V3 region and contoured at 1 s. FIG. **6** (C) V3 structure. The entire V3 is shown. Regions corresponding to the fixed base, accordion-like stem, and b-hairpin tip are labeled. FIG. **6** (D) Close-up view of the V3 base. From its N terminus (Cys296), V3 extends the antiparallel sheet on the outer domain of gp120. After hydrogen bonding for three residues, additional sheet contacts are interrupted by two conserved residues: Arg298, whose side-chain hydrogen bonds to three carbonyl oxygens, including two on the neighboring outer domain strand; and Pro299, which initiates the separation of outgoing and returning V3 strands. In the returning strand, antiparallel b-sheet interactions with core gp120 recommence with the carbonyl of residue 297 and continue to the disulfide at Cys331. Main-chain atoms are shown for the core and V3 base. Hydrogen bonds are depicted with dashed lines, with select distances in Å. All atoms of the highly conserved Arg298, Pro299, and Cys296-Cys331 disulfide are shown, with Arg and Pro carbons highlighted in yellow and disulfide in orange. FIG. **6** (E) Conformation of the V3 tip. From Ser306 to Gly312, the main chain assumes a standard b-conformation, which terminates in a Gly-Pro-Gly-Arg b-turn (residues 312 to 315). After the turn, the returning density is less well defined, indicative of some disorder. All atoms of the tip are colored as in FIG. **6** (C), with carbon atoms of the conserved tip highlighted in green. Hydrogen bonds that stabilize the β hairpin are shown as in FIG. **6** (D).

FIG. **7** is a computer generated image of a modeled gp120 trimer and a coreceptor schematic. FIG. **7**(A) V3 in the context of a trimer at the target cell surface. The structure of the CD4-triggered gp120 with V3 was superimposed onto the structure of four-domain CD4 and the trimer model obtained by quantification of surface parameters. In this orientation, the target cell membrane and coreceptor are expected to be positioned toward the bottom of the page. FIG. **7** (B) Schematic of coreceptor interaction. CCR5 is shown with its tyrosine-sulfated N terminus (at residues 3, 10, 14, and 15) and three extracellular loops (ECLs). V3 is shown with its conserved base interacting with the sulfated CCR5 N terminus and its flexible legs allowing its conserved V3 tip to reach the second ECL of CCR5.

FIG. **8** is a set of computer generated images modeling of the V3 loop bound to the indicated antibodies. The images show the configuration of the loops and the accessibility of V3 to neutralizing antibodies. The molecular surfaces of neutralizing antibodies that block coreceptor binding are shown superimposed onto gp120 in the context of V3; antibodies 17b and X5 bind to the conserved coreceptor binding site on the core, whereas monoclonal antibodies 50.1, 58.2, 59.1, 83.1, and 447-52D bind to V3. FIG. **8** (A) Superposition of V3 structures. Core with V3 is shown with V3 peptides as extracted from peptide-anti-V3 neutralizing antibody complexes after superposition of the conserved V3 tip. FIG. **8** (B) Antibody accessibility of V3. Core gp120 with V3 (ribbon representation) is shown in two perpendicular views with Fab fragments (molecular surface representation) of antibodies that bind at the coreceptor binding site on either core or V3. V3 is completely surrounded by neutralizing antibodies, suggesting a high degree of accessibility for generating an immune response.

FIG. **9** is a set of computer generated images demonstrating the induced fit of the X5 CDR H3 loop. FIG. **9** (A) Bound X5 structure. A stereo depiction is shown for all atoms of the CDR H3 loop of X5. Electron density (Fo-Fc, 3σ) is shown for the loop after simulated annealing to remove model bias. FIG. **9** (B) Free versus bound conformations of X5. Stereo depictions of the Cα-traces are shown for the two conformations of the free X5 and of the X5 in the final refined structure of the complex with the V3-containing gp120 core. Cα-shifts are shown, with the 17 Å shift of Gly 100H labeled. (C) Same as (B), but rotated by 90°; dotted lines connect equivalent amino acids of free and bound X5.

FIG. **10** is a set of computer generated images and bar graphs showing the analysis of coreceptor binding to gp120. FIG. **10** (A) Surface chemistry. The gp120 core with V3 is shown in three orientations. The middle row shows an orientation similar to that in FIGS. **5** and **6**, an orientation in which the "outer" face of the V3 loop is closest to the viewer. The top row is rotated 180° about a vertical axis (showing the "inner" or core-proximal face) and the bottom row is rotated 90° about a horizontal axis. In the first column, a ribbon diagram shows gp120 colored in grey and V3 in red. The next columns

represent the surface of gp120 and V3 color-coded according to the properties of the underlying atoms. Column 2 shows the molecular surface colored according to the sequence variability of the underlying amino acids for Clade B, with variable regions in purple and conserved regions in white. Columns 3 and 4 show the mutational effect of varying amino acids on CCR5 binding (column 3) or on the binding of sulfated CCR5 Nterminal peptides (column 4). Black defines surfaces that were not tested, yellow regions that when altered do not affect binding, and green areas where alterations significantly affect binding. Column 5 depicts the electrostatic potential at the solvent accessible surface, with blue showing electropositive, red electronegative, and white apolar. Column 6 depicts the gp120 surface with modeled N-linked glycans [(Nacetylglucosamine) 2(mannose)3 cores] in orange-yellow, with the 301 glycan highlighted in purple. The molecular surface corresponding to positions "11" and "25", suggested to be important in distinguishing between CXCR4 and CCR5, are highlighted, as well as residue 440 which sequence analysis indicates is also of some significance in this regard. FIG. **10** (B) V3 sequence variation. The sequence variation was quantified (see methods) and is expressed as an entropy score: a score of zero indicates absolute conservation, a score of 4.4 indicates complete randomness. The V3 in B clade viruses which use CCR5 is comparable in terms of overall variation with other regions of gp120. The median entropy of each position within V3 is 0.21, and the interquartile range is 0-0.59. If one excludes the named variable domains, the rest of gp120 has a median entropy of 0.2, with an interquartile range of 0.-0.44. There is no statistical difference between these two distributions (Wilcoxon rank-sum p value=0.14). In contrast, V1, V2, V4 and V5 are much more variable (median entropy=1.24, interquartile range 0.67-1.70, p value compared to V3, <10-9.) Graphed in red and blue, respectively, are the position-dependent entropy score from 242 CCR5-using isolates (R5) and 47 CXCR4-using isolates (X4). Twenty positions were found to be significantly more variable in X4 than R5 viruses after correction for multiple tests. In particular, the N-linked glycosylation site (NNT) is highly conserved in R5 viruses, with 238/242 viruses reported to be R5 in the Los Alamos database carrying the potential glycosylation site at position 301, whereas only 17/47 X4 viruses retain the site (p<<10-10). This glycan has been previously observed to influence overall neutralization sensitivity. Finally, insertions were found with higher frequency in X4 viruses. The consensus R5 and X4 sequences are shown. The entropy scores from 64 R5 and 19 X4 Clade B isolates are shown, along with the respective consensus sequences. Asterisks denote where the consensus X4 sequence is the same as the consensus R5 sequence.

FIG. **11** is a set of computer generated images that show the alignment of V3 peptide:antibody structures with V3 in the context of core gp120. FIG. **11** (A) X-ray structures. The structures of V3 are shown either in the context of core gp120 or bound to antibody 50.1, 447-52D, 59.1, 83.1, or 58.2. FIG. **11** (B) Nuclear magnetic resonance (NMR) structures. The NMR ensembles are shown for free V3), as well as for V3 peptides bound to antibodies, 0.5β and 447-52D. All structures are aligned with the conserved Pro-Gly of the tip.

FIG. **12** is a set of computer generated images showing the modeled structure of the V1/2 for HXBc2 9c mutant.

FIG. **13** is an alignment of the amino acid sequences of the HXBc2 core (SEQ ID NO: 20) with the New HXBc2 9c (SEQ ID NO: 1).

FIG. **14** are nucleotide sequences that encode HXBc2 gp120 WT and stabilized forms thereof. FIG. **14**A is a nucleotide sequence of gp120 HXBc2 DM (SEQ ID NO: 3), a nucleotide sequence of gp120 HXBc2 Core4a (SEQ ID NO: 4), and a nucleotide sequence of gp120 HXBc2 Core 4b (SEQ ID NO: 5). FIG. **14** B is a nucleotide sequence of gp120 HXBc2 Core4c (SEQ ID NO: 6), a nucleotide sequence of gp120 HXBc2 Core6a (SEQ ID NO: 7), and a nucleotide sequence of gp120 HXBc2 Core6b (SEQ ID NO: 8). FIG. **14**C is a nucleotide sequence of gp120 HXBc2 Core8a (SEQ ID NO: 9), a nucleotide sequence of gp120 HXBc2 Core8b (SEQ ID NO: 10), and a nucleotide sequence of gp120 HXBc2 Core8c (SEQ ID NO: 11). FIG. **14**D is a nucleotide sequence of gp120 HXBc2 Core9a (SEQ ID NO: 12), a nucleotide sequence of gp120 HXBc2 Core9b (SEQ ID NO: 13), and a nucleotide sequence of gp120 HXBc2 Core9c (SEQ ID NO: 14). FIG. **14**E is a nucleotide sequence of gp120 HXBc2 Core10a (SEQ ID NO: 15), a nucleotide sequence of gp120 HXBc2 Core10b (SEQ ID NO: 16), and a nucleotide sequence of gp120 HXBc2 Core10c (SEQ ID NO: 17). FIG. **14**F is a nucleotide sequence of gp120 HXBc2 Core11a (SEQ ID NO: 18), a nucleotide sequence of wild type (WT) gp120 HXBc2 (SEQ ID NO: 19), and a nucleotide sequence of gp120 HXBc2 Core New 9c.

FIG. **15** is an example of an isothermal titration calorimetry curve for the binding of a soluble form of CD4 to a gp120 polypeptide. Thermodynamic properties describing this molecular interaction can be extracted from such a curve. The table shows the extracted thermodynamic parameters of a selected set of gp120 polypeptides binding to a soluble form of gp120. The collection of such data and the extraction thermodynamic parameters is well known in the art.

FIG. **16** is a set a plots of neutralization data for various HIV isolates in the presence and absence of CD4, showing the effect of CD4 triggering on viral neutralization. FIG. **16**A is a bar graph showing the percent neutralization by sCD4 triggering of the V3 loop epitope. Data shown are percent neutralization of pseudovirus YU2 by the monoclonal antibodies (mAb) or sera listed under each set of bar graphs. The white bar shows neutralization by sCD4 alone. The first hatched bar shows neutralization by the specified antibody alone. The second hatched bar shows the calculated (expected) neutralization by a combination of sCD4 and the specified antibody. The stippled bar shows the observed (actual) neutralization by the combination of sCD4 and the specified antibody. 447 and 39F are anti-V3 mAbs. 17b is a mAb to the co-receptor binding site. 82-2 is an individual guinea pig sera derived from immunization with dCFIdV12 (BaL). 9427 is an individual baboon sera derived from immunization with gp140GCN-4 (YU2). Observed is measured percent neutralization with sCD4+Antibody. Expected=calculated additive effect of the two antibodies assuming they act independently. This effect is the product of the fraction remaining virus for each Ab; e.g. an antibody that produces 50% neutralization leaves 0.5 virus remaining. A second antibody with 50% neutralization would reduce that by 50%, leaving 0.25 fraction remaining virus. Thus, the effect of the two antibodies is 0.5×0.5=0.25. And 0.25 remaining is 75% neutralization. FIG. **16**B is a bar graph of the actual luciferase (RLU) data plotted in FIG. **16**A. The figure legend describes each bar. The antibodies and sera used are as described for FIG. **16**A. FIG. **16**C is a bar graph of the actual luciferase (RLU) data for HIV strain JRFL. The antibodies tested are indicated. FIG. **16** D is a line graph shows percent neutralization of mAb 447 with the indicated amount of sCD4 present (x-axis), calculated after affect of sCD4 is taken into account. The diamonds (♦) show the affect of sCD4 alone. The circles (●) show the combined effect of sCD4 plus mAb 447. The diamonds (♦) show the percent neutralization calculated based on the level of virus entry with sCD4 present. FIG. **16**E is a line graph of the

neutralization of JRFL by two guinea pig sera as shown (▲, ■). The diamonds (♦) show the effect of sCD4 alone. The line graphs show the neutralization of each sera, calculated based on the virus entry with sCD4 present. FIG. **16**F is a line graph of the neutralization of YU2 by mAbs 447, 17b, and 39F. FIG. **16**G is a line graph of the neutralization of YU2 by the two animal sera that were described in FIG. **16**A. FIG. **16** H is a line graph of the neutralization of virus 6535 by mAbs 447 and 17b. FIG. **16**I is a line graph of the neutralization of virus 6535 by two guinea pig sera as shown (♦, ■). The diamonds (♦) show the effect of sCD4 alone. FIG. **16**J is a line graph of the neutralization of virus ADA by mAbs 447. FIG. **16**K is a line graph of the neutralization of virus ADA by two guinea pig sera as shown (♦, ■). FIG. **16**L is a line graph of the neutralization of the clade C virus TV1 by mAbs 447 and 17b. FIG. **16**M is a line graph of the neutralization of the clade C virus TV1 by guinea pig sera derived from animals immunized with clade C dCFI Env. FIG. **16**N is a line graph of the neutralization of the clade C virus ZA12 by mAb 17b. FIG. **16**O is a line graph of the neutralization of the clade C virus ZA12 by guinea pig sera derived from animals immunized with clade C dCFI Env. FIG. **16**P is a line graph of the neutralization of the clade C virus Z109 by mAbs 447 and 17b. FIG. **16**Q is a line graph of the neutralization of the clade C virus Z109 by guinea pig sera derived from animals immunized with clade C dCFI Env.

SEQUENCE LISTING AND NOMENCLATURE

The nucleic and amino acid sequences listed in the accompanying sequence listing are shown using standard letter abbreviations for nucleotide bases, and three letter code for amino acids, as defined in 37 C.F.R. 1.822. Only one strand of each nucleic acid sequence is shown, but the complementary strand is understood as included by any reference to the displayed strand.

SEQ ID NO: 1 is the amino acid sequence of gp120 HXBc2 Core New 9c.

SEQ ID NO: 2 the amino acid sequence of the gp120 with an extended V3 loop.

SEQ ID NO: 3 is a nucleotide sequence of gp120 HXBc2 DM.

SEQ ID NOs: 4-18 are nucleotide sequences of stabilized HXBc2 Core gp120.

SEQ ID NO: 19 is a nucleotide sequence of wild type (WT) HXBc2.

SEQ ID NO: 20 is the amino acid sequence of wild type (WT) HXBc2.

SEQ ID NO: 21-25 are amino acid sequences of V3 loops.

SEQ ID NO: 26 is a nucleotide sequence of gp120 HXBc2 Core New 9c.

SEQ ID NO: 27 is the amino acid sequence of gp120 HXB2CG.

Nomenclature Conversion for Conformationally Stabilized HXBc2 Mutants

		Mutant location						
Mutant Name WT core	New name WT core	T257S S375W C2	A433M C3	M95W W96C V275C C1S1	I109C Q428C S2	T123C G431C S3	K231C E267C S4	K231C E268C S5
2a	C2	x						
4-0	C2S5	x						x
4a	C2S2	x			x			
4b	C2S4	x					x	
4c	C2S3	x				x		
5mut	C12S1	x		x				
6a	C123S1	x	x	x				
6b	C2S24	x			x		x	
8a	C123S14	x	x	x			x	
8b	C123S12	x	x	x	x			
9a	C23S234	x	x		x	x	x	
8c	C2S234	x			x	x	x	
10a	C123S124	x	x	x	x		x	
9b	C12S134	x		x		x	x	
10c	C123S134	x	x	x		x	x	
9c	C12S123	x		x	x	x		
10b	C123S123	x	x	x	x	x		
11a	C12S1234	x		x	x	x	x	

DETAILED DESCRIPTION

I. Terms

Unless otherwise noted, technical terms are used according to conventional usage. Definitions of common terms in molecular biology can be found in Benjamin Lewin, Genes V, published by Oxford University Press, 1994 (ISBN 0-19-854287-9); Kendrew et al. (eds.), The Encyclopedia of Molecular Biology, published by Blackwell Science Ltd., 1994 (ISBN 0-632-02182-9); and Robert A. Meyers (ed.), Molecular Biology and Biotechnology: a Comprehensive Desk Reference, published by VCH Publishers, Inc., 1995 (ISBN 1-56081-569-8). Terms describing protein structure and structural elements of proteins can be found in Creighton, Proteins, Structures and Molecular Properties, W.H. Freeman & Co., New York, 1993 (ISBN 0-717-7030) which is incorporated by reference herein in its entirety.

Unless otherwise explained, all technical and scientific terms used herein have the same meaning as commonly understood by one of ordinary skill in the art to which this disclosure belongs. The singular terms "a," "an," and "the" include plural referents unless context clearly indicates otherwise. Similarly, the word "or" is intended to include "and" unless the context clearly indicates otherwise. It is further to be understood that all base sizes or amino acid sizes, and all molecular weight or molecular mass values, given for nucleic acids or polypeptides are approximate, and are provided for description. Although methods and materials similar or

equivalent to those described herein can be used in the practice or testing of this disclosure, suitable methods and materials are described below. The term "comprises" means "includes." The abbreviation, "e.g." is derived from the Latin exempli gratia, and is used herein to indicate a non-limiting example. Thus, the abbreviation "e.g." is synonymous with the term "for example."

All publications, patent applications, patents, and other references mentioned herein are incorporated by reference in their entirety. In case of conflict, the present specification, including explanations of terms, will control. In addition, all the materials, methods, and examples are illustrative and not intended to be limiting. In order to facilitate review of the various embodiments of the disclosure, the following explanations of specific terms are provided:

Adjuvant: A vehicle used to enhance antigenicity; such as a suspension of minerals (alum, aluminum hydroxide, aluminum phosphate) on which antigen is adsorbed; or water-in-oil emulsion in which antigen solution is emulsified in oil (MF-59, Freund's incomplete adjuvant), sometimes with the inclusion of killed mycobacteria (Freund's complete adjuvant) to further enhance antigenicity (inhibits degradation of antigen and/or causes influx of macrophages). Adjuvants also include immunostimulatory molecules, such as cytokines, costimulatory molecules, and for example, immunostimulatory DNA or RNA molecules, such as CpG oligonucleotides.

Administration: The introduction of a composition into a subject by a chosen route. For example, if the chosen route is intravenous, the composition is administered by introducing the composition into a vein of the subject.

Antibody: A polypeptide substantially encoded by an immunoglobulin gene or immunoglobulin genes, or fragments thereof, which specifically binds and recognizes an analyte (antigen) such as gp120 or an antigenic fragment of gp120. Immunoglobulin genes include the kappa, lambda, alpha, gamma, delta, epsilon and mu constant region genes, as well as the myriad immunoglobulin variable region genes.

Antibodies exist, for example as intact immunoglobulins and as a number of well characterized fragments produced by digestion with various peptidases. For instance, Fabs, Fvs, and single-chain Fvs (SCFvs) that bind to gp120 or fragments of gp120 would be gp120-specific binding agents. This includes intact immunoglobulins and the variants and portions of them well known in the art, such as Fab' fragments, $F(ab)'_2$ fragments, single chain Fv proteins ("scFv"), and disulfide stabilized Fv proteins ("dsFv"). A scFv protein is a fusion protein in which a light chain variable region of an immunoglobulin and a heavy chain variable region of an immunoglobulin are bound by a linker, while in dsFvs, the chains have been mutated to introduce a disulfide bond to stabilize the association of the chains. The term also includes genetically engineered forms such as chimeric antibodies (such as humanized murine antibodies), heteroconjugate antibodies such as bispecific antibodies). See also, *Pierce Catalog and Handbook,* 1994-1995 (Pierce Chemical Co., Rockford, Ill.); Kuby, J., *Immunology,* 3rd Ed., W.H. Freeman & Co., New York, 1997.

Antibody fragments are defined as follows: (1) Fab, the fragment which contains a monovalent antigen-binding fragment of an antibody molecule produced by digestion of whole antibody with the enzyme papain to yield an intact light chain and a portion of one heavy chain; (2) Fab', the fragment of an antibody molecule obtained by treating whole antibody with pepsin, followed by reduction, to yield an intact light chain and a portion of the heavy chain; two Fab' fragments are obtained per antibody molecule; (3) $(Fab')_2$, the fragment of the antibody obtained by treating whole antibody with the enzyme pepsin without subsequent reduction; (4) F(ab')2, a dimer of two Fab' fragments held together by two disulfide bonds; (5) Fv, a genetically engineered fragment containing the variable region of the light chain and the variable region of the heavy chain expressed as two chains; and (6) single chain antibody ("SCA"), a genetically engineered molecule containing the variable region of the light chain, the variable region of the heavy chain, linked by a suitable polypeptide linker as a genetically fused single chain molecule. The term "antibody," as used herein, also includes antibody fragments either produced by the modification of whole antibodies or those synthesized de novo using recombinant DNA methodologies.

Typically, a naturally occurring immunoglobulin has heavy (H) chains and light (L) chains interconnected by disulfide bonds. There are two types of light chain, lambda (λ) and kappa (κ). There are five main heavy chain classes (or isotypes) which determine the functional activity of an antibody molecule: IgM, IgD, IgG, IgA and IgE.

Each heavy and light chain contains a constant region and a variable region, (the regions are also known as "domains"). In combination, the heavy and the light chain variable regions specifically bind the antigen. Light and heavy chain variable regions contain a "framework" region interrupted by three hypervariable regions, also called "complementarity-determining regions" or "CDRs." The extent of the framework region and CDRs have been defined (see, Kabat et al., *Sequences of Proteins of Immunological Interest*, U.S. Department of Health and Human Services, 1991, which is hereby incorporated by reference). The Kabat database is now maintained online. The sequences of the framework regions of different light or heavy chains are relatively conserved within a species. The framework region of an antibody, that is the combined framework regions of the constituent light and heavy chains, serves to position and align the CDRs in three-dimensional space.

The CDRs are primarily responsible for binding to an epitope of an antigen. The CDRs of each chain are typically referred to as CDR1, CDR2, and CDR3, numbered sequentially starting from the N-terminus, and are also typically identified by the chain in which the particular CDR is located. Thus, a V_H CDR3 is located in the variable domain of the heavy chain of the antibody in which it is found, whereas a V_L CDR1 is the CDR1 from the variable domain of the light chain of the antibody in which it is found. Light chain CDRs are sometimes referred to as CDR L1, CDR L2, and CDR L3. Heavy chain CDRs are sometimes referred to as CDR H1, CDR H2, and CDR H3.

References to "V_H" or "VH" refer to the variable region of an immunoglobulin heavy chain, including that of an Fv, scFv, dsFv or Fab. References to "V_L" or "VL" refer to the variable region of an immunoglobulin light chain, including that of an Fv, scFv, dsFv or Fab.

A "monoclonal antibody" is an antibody produced by a single clone of B-lymphocytes or by a cell into which the light and heavy chain genes of a single antibody have been transfected. Monoclonal antibodies are produced by methods known to those of skill in the art, for instance by making hybrid antibody-forming cells from a fusion of myeloma cells with immune spleen cells. These fused cells and their progeny are termed "hybridomas." Monoclonal antibodies include humanized monoclonal antibodies.

A "humanized" immunoglobulin is an immunoglobulin including a human framework region and one or more CDRs from a non-human (such as a mouse, rat, or synthetic) immunoglobulin. The non-human immunoglobulin providing the CDRs is termed a "donor," and the human immunoglobulin

providing the framework is termed an "acceptor." In one embodiment, all the CDRs are from the donor immunoglobulin in a humanized immunoglobulin. Constant regions need not be present, but if they are, they must be substantially identical to human immunoglobulin constant regions, such as at least about 85-90%, such as about 95% or more identical. Hence, all parts of a humanized immunoglobulin, except possibly the CDRs, are substantially identical to corresponding parts of natural human immunoglobulin sequences. A "humanized antibody" is an antibody comprising a humanized light chain and a humanized heavy chain immunoglobulin. A humanized antibody binds to the same antigen as the donor antibody that provides the CDRs. The acceptor framework of a humanized immunoglobulin or antibody may have a limited number of substitutions by amino acids taken from the donor framework. Humanized or other monoclonal antibodies can have additional conservative amino acid substitutions which have substantially no effect on antigen binding or other immunoglobulin functions. Humanized immunoglobulins can be constructed by means of genetic engineering (for example, see U.S. Pat. No. 5,585,089).

Antigenic gp120 polypeptide: An "antigenic gp120 polypeptide" includes a gp120 molecule or a portion thereof that is capable of provoking an immune response in a mammal, such as a mammal with or without an HIV infection. Administration of an antigenic gp120 polypeptide that provokes an immune response preferably leads to protective immunity against HIV.

Antigenic surface: A surface of a molecule, for example a protein such as a gp120 protein or polypeptide, capable of eliciting an immune response. An antigenic surface includes the defining features of that surface, for example the three-dimensional shape and the surface charge. An antigenic surface includes both surfaces that occur on gp120 polypeptides as well as surfaces of compounds that mimic the surface of a gp120 polypeptide (mimetics).

CD4: Cluster of differentiation factor 4 polypeptide, a T-cell surface protein that mediates interaction with the MHC class II molecule. CD4 also serves as the primary receptor site for HIV on T-cells during HIV-1 infection.

The known sequence of the CD4 precursor has a hydrophobic signal peptide, an extracellular region of approximately 370 amino acids, a highly hydrophobic stretch with significant identity to the membrane-spanning domain of the class II MHC beta chain, and a highly charged intracellular sequence of 40 resides (Maddon, *Cell* 42:93, 1985).

The term "CD4" includes polypeptide molecules that are derived from CD4 include fragments of CD4, generated either by chemical (for example enzymatic) digestion or genetic engineering means. Such a fragment may be one or more entire CD4 protein domains. The extracellular domain of CD4 consists of four contiguous immunoglobulin-like regions (D1, D2, D3, and D4, see Sakihama et al., *Proc. Natl. Acad. Sci.* 92:6444, 1995; U.S. Pat. No. 6,117,655), and amino acids 1 to 183 have been shown to be involved in gp120 binding. For instance, a binding molecule or binding domain derived from CD4 would comprise a sufficient portion of the CD4 protein to mediate specific and functional interaction between the binding fragment and a native or viral binding site of CD4. One such binding fragment includes both the D1 and D2 extracellular domains of CD4 (D1D2 is also a fragment of soluble CD4 or sCD4 which is comprised of D1 D2 D3 and D4), although smaller fragments may also provide specific and functional CD4-like binding. The gp120-binding site has been mapped to D1 of CD4.

CD4 polypeptides also include "CD4-derived molecules" which encompasses analogs (non-protein organic molecules), derivatives (chemically functionalized protein molecules obtained starting with the disclosed protein sequences) or mimetics (three-dimensionally similar chemicals) of the native CD4 structure, as well as proteins sequence variants or genetic alleles that maintain the ability to functionally bind to a target molecule.

CD4BS antibodies: Antibodies that bind to or substantially overlap the CD4 binding surface of a gp120 polypeptide. The antibodies interfere with or prevent CD4 from binding to a gp120 polypeptide.

CD4i antibodies: Antibodies that bind to a conformation of gp120 induced by CD4 binding.

Contacting: Placement in direct physical association; includes both in solid and liquid form.

Computer readable media: Any medium or media, which can be read and accessed directly by a computer, so that the media is suitable for use in a computer system. Such media include, but are not limited to: magnetic storage media such as floppy discs, hard disc storage medium and magnetic tape; optical storage media such as optical discs or CD-ROM; electrical storage media such as RAM and ROM; and hybrids of these categories such as magnetic/optical storage media.

Computer system: Hardware that can be used to analyze atomic coordinate data. The minimum hardware of a computer-based system typically comprises a central processing unit (CPU), an input device, for example a mouse, keyboard, and the like, an output device, and a data storage device. Desirably a monitor is provided to visualize structure data. The data storage device may be RAM or other means for accessing computer readable. Examples of such systems are microcomputer workstations available from Silicon Graphics Incorporated and Sun Microsystems running Unix based Windows NT or IBM OS/2 operating systems.

Degenerate variant and conservative variant: A polynucleotide encoding a polypeptide or an antibody that includes a sequence that is degenerate as a result of the genetic code. For example, a polynucleotide encoding a gp120 polypeptide or an antibody that binds gp120 that includes a sequence that is degenerate as a result of the genetic code. There are 20 natural amino acids, most of which are specified by more than one codon. Therefore, all degenerate nucleotide sequences are included as long as the amino acid sequence of the gp120 polypeptide or antibody that binds gp120 encoded by the nucleotide sequence is unchanged. Because of the degeneracy of the genetic code, a large number of functionally identical nucleic acids encode any given polypeptide. For instance, the codons CGU, CGC, CGA, CGG, AGA, and AGG all encode the amino acid arginine. Thus, at every position where an arginine is specified within a protein encoding sequence, the codon can be altered to any of the corresponding codons described without altering the encoded protein. Such nucleic acid variations are "silent variations," which are one species of conservative variations. Each nucleic acid sequence herein that encodes a polypeptide also describes every possible silent variation. One of skill will recognize that each codon in a nucleic acid (except AUG, which is ordinarily the only codon for methionine) can be modified to yield a functionally identical molecule by standard techniques. Accordingly, each "silent variation" of a nucleic acid which encodes a polypeptide is implicit in each described sequence.

Furthermore, one of ordinary skill will recognize that individual substitutions, deletions or additions which alter, add or delete a single amino acid or a small percentage of amino acids (for instance less than 5%, in some embodiments less than 1%) in an encoded sequence are conservative variations

where the alterations result in the substitution of an amino acid with a chemically similar amino acid.

Conservative amino acid substitutions providing functionally similar amino acids are well known in the art. The following six groups each contain amino acids that are conservative substitutions for one another:

1) Alanine (A), Serine (S), Threonine (T);

2) Aspartic acid (D), Glutamic acid (E);

3) Asparagine (N), Glutamine (Q);

4) Arginine (R), Lysine (K);

5) Isoleucine (I), Leucine (L), Methionine (M), Valine (V); and

6) Phenylalanine (F), Tyrosine (Y), Tryptophan (W).

Not all residue positions within a protein will tolerate an otherwise "conservative" substitution. For instance, if an amino acid residue is essential for a function of the protein, even an otherwise conservative substitution may disrupt that activity.

Epitope: An antigenic determinant. These are particular chemical groups or peptide sequences on a molecule that are antigenic, such that they elicit a specific immune response. An antibody binds a particular antigenic epitope, such as an epitope of a gp120 polypeptide.

Expression: Translation of a nucleic acid into a protein. Proteins may be expressed and remain intracellular, become a component of the cell surface membrane, or be secreted into the extracellular matrix or medium.

Expression Control Sequences: Nucleic acid sequences that regulate the expression of a heterologous nucleic acid sequence to which it is operatively linked. Expression control sequences are operatively linked to a nucleic acid sequence when the expression control sequences control and regulate the transcription and, as appropriate, translation of the nucleic acid sequence. Thus expression control sequences can include appropriate promoters, enhancers, transcription terminators, a start codon (ATG) in front of a protein-encoding gene, splicing signal for introns, maintenance of the correct reading frame of that gene to permit proper translation of mRNA, and stop codons. The term "control sequences" is intended to include, at a minimum, components whose presence can influence expression, and can also include additional components whose presence is advantageous, for example, leader sequences and fusion partner sequences. Expression control sequences can include a promoter.

A promoter is a minimal sequence sufficient to direct transcription. Also included are those promoter elements which are sufficient to render promoter-dependent gene expression controllable for cell-type specific, tissue-specific, or inducible by external signals or agents; such elements may be located in the 5' or 3' regions of the gene. Both constitutive and inducible promoters are included (see for example, Bitter et al., *Methods in Enzymology* 153:516-544, 1987). For example, when cloning in bacterial systems, inducible promoters such as pL of bacteriophage lambda, plac, ptrp, ptac (ptrp-lac hybrid promoter) and the like may be used. In one embodiment, when cloning in mammalian cell systems, promoters derived from the genome of mammalian cells (such as metallothionein promoter) or from mammalian viruses (such as the retrovirus long terminal repeat; the adenovirus late promoter; the vaccinia virus 7.5K promoter) can be used. Promoters produced by recombinant DNA or synthetic techniques may also be used to provide for transcription of the nucleic acid sequences.

A polynucleotide can be inserted into an expression vector that contains a promoter sequence which facilitates the efficient transcription of the inserted genetic sequence of the host. The expression vector typically contains an origin of replication, a promoter, as well as specific nucleic acid sequences that allow phenotypic selection of the transformed cells.

gp120: The envelope protein from Human Immunodeficiency Virus (HIV). The envelope protein is initially synthesized as a longer precursor protein of 845-870 amino acids in size, designated gp160. Gp160 forms a homotrimer and undergoes glycosylation within the Golgi apparatus. It is then cleaved by a cellular protease into gp120 and gp41. Gp41 contains a transmembrane domain and remains in a trimeric configuration; it interacts with gp120 in a non-covalent manner. Gp120 contains most of the external, surface-exposed, domains of the envelope glycoprotein complex, and it is gp120 which binds both to the cellular CD4 receptor and to the cellular chemokine receptors (such as CCR5).

The mature gp120 wildtype polypeptides have about 500 amino acids in the primary sequence. Gp120 is heavily N-glycosylated giving rise to an apparent molecular weight of 120 kD. The polypeptide is comprised of five conserved regions (C1-C5) and five regions of high variability (V1-V5). Exemplary sequence of wt gp160 polypeptides are shown on GENBANK, for example accession numbers AAB05604 and AAD12142

The gp120 core has a unique molecular structure, which comprises two domains: an "inner" domain (which faces gp41) and an "outer" domain (which is mostly exposed on the surface of the oligomeric envelope glycoprotein complex). The two gp120 domains are separated by a "bridging sheet" that is not part of either domain. The gp120 core comprises 25 beta strands, 5 alpha helices, and 10 defined loop segments.

"Stabilized gp120" is a form of gp120 polypeptide from HIV-1, characterized by an increase in T_m over the wild type gp120. In some examples the gp120 is stabilized by the replacement of at least two amino acids of gp120 with cysteines such that a disulfide bond can form, wherein the gp120 protein has a T_m of greater than about 53.8° C. The stabilized gp120 mutants may contain amino acid substitutions that fill cavities present in the core of native gp120. The stabilized gp120 can bind CD4. Stabilized forms of gp120 may include forms that have synthetic amino acids. Several exemplary stabilized gp120 proteins are disclosed herein.

Gp120 polypeptides also include "gp120-derived molecules" which encompasses analogs (non-protein organic molecules), derivatives (chemically functionalized protein molecules obtained starting with the disclosed protein sequences) or mimetics (three-dimensionally similar chemicals) of the native gp120 structure, as well as proteins sequence variants (such as mutants), genetic alleles, fusions proteins of gp120, or combinations thereof.

The third variable region referred to herein as the V3 loop is a loop of about 35 amino acids critical for the binding of the co-receptor and determination of which of the co-receptors will bind. In certain examples the V3 loop comprises residues 296-331.

The numbering used in gp120 polypeptides disclosed herein is relative to the HXB2 numbering scheme as set forth in *Numbering Positions in HIV Relative to HXB2CG* Bette Korber et al., Human Retroviruses and AIDS 1998: A Compilation and Analysis of Nucleic Acid and Amino Acid Sequences. Korber B, Kuiken C L, Foley B, Hahn B, McCutchan F, Mellors J W, and Sodroski J, Eds. Theoretical Biology and Biophysics Group, Los Alamos National Laboratory, Los Alamos, N. Mex. which is incorporated by reference herein in its entirety. For reference, the amino acid sequence of HXB2CG is given below as SEQ ID NO: 27:

lwvtvyygvpvwkeatttlfcasdakaydtevhnvwathacvptdpnpqevv
lvnvtenfnmwkndmveqmhediislwdqslkpcvkltplcvslkctdlk

ndtntnsssgrmimekgeikncsfnistsirgkvqkeyaffykldiipidndtt sykltscntsvitqacpkvsfepipihycapagfailkcnnktfngtgpctnvstv qcthgirpvvstqlllngslaeeevvirsvnftdnaktiivqlntsveinctrpnnn trkririqrgpgrafvtigkignmrqahcnisrak wnntlkqiasklreqfgnnk-tiifkqssggdpeivthsfncggeffycnstqlfnstwfnstwstegsnntegsdt itlpcrikqiinmwqkvgkamyapp isgqircssnitglltrdggnsnnese-ifrpgggdmrdnwrselykykvvkieplgvaptkakrrvvqrekr (SEQ ID NO: 27). HXB2 is also known as: HXBc2, for HXB clone 2; HXB2R, in the Los Alamos HIV database, with the R for revised, as it was slightly revised relative to the original HXB2 sequence; and HXB2CG in GenBank, for HXB2 complete genome.

Heavy atom derivatization: A method of producing a chemically modified form of a protein crystal, for example a crystal containing gp120. In practice, a crystal is soaked in a solution containing heavy metal atom salts, or organometallic compounds, such as lead chloride, gold thiomalate, thimerosal or uranyl acetate, which can diffuse through the solvent channels of the crystal and bind the surface of the protein. The location(s) of the bound heavy metal atom(s) can be determined by X-ray diffraction analysis of the soaked crystal. This information, in turn, is used to generate the phase information used to construct three-dimensional structure of the enzyme (see Blundel and Johnson, Protein Crystallography, Academic Press (1976).

Host cells: Cells in which a vector can be propagated and its DNA expressed. The cell may be prokaryotic or eukaryotic. The term also includes any progeny of the subject host cell. It is understood that all progeny may not be identical to the parental cell since there may be mutations that occur during replication. However, such progeny are included when the term "host cell" is used.

In silico: A process performed virtually within a computer. For example, using a computer, a virtual compound can be screened for surface similarity or conversely surface complementarity to a virtual representation of the atomic positions at least a portion of a gp120 polypeptide, for example as stabilized gp120, such as defined in Table 1 or a gp120 with an extended V3 loop, such as defined in Table 2.

Immune response: A response of a cell of the immune system, such as a B cell, T cell, or monocyte, to a stimulus. In one embodiment, the response is specific for a particular antigen (an "antigen-specific response"). In one embodiment, an immune response is a T cell response, such as a CD4+ response or a CD8+ response. In another embodiment, the response is a B cell response, and results in the production of specific antibodies.

Immunogenic peptide: A peptide which comprises an allele-specific motif or other sequence, such as an N-terminal repeat, such that the peptide will bind an MHC molecule and induce a cytotoxic T lymphocyte ("CTL") response, or a B cell response (for example antibody production) against the antigen from which the immunogenic peptide is derived.

In one embodiment, immunogenic peptides are identified using sequence motifs or other methods, such as neural net or polynomial determinations known in the art. Typically, algorithms are used to determine the "binding threshold" of peptides to select those with scores that give them a high probability of binding at a certain affinity and will be immunogenic. The algorithms are based either on the effects on MHC binding of a particular amino acid at a particular position, the effects on antibody binding of a particular amino acid at a particular position, or the effects on binding of a particular substitution in a motif-containing peptide. Within the context of an immunogenic peptide, a "conserved residue" is one which appears in a significantly higher frequency than would be expected by random distribution at a particular position in a peptide. In one embodiment, a conserved residue is one where the MHC structure may provide a contact point with the immunogenic peptide. In one specific non-limiting example, an immunogenic polypeptide includes a region of gp120, or a fragment thereof.

Immunogenic composition: A composition comprising an immunogenic peptide that induces a measurable CTL response against virus expressing the immunogenic peptide, or induces a measurable B cell response (such as production of antibodies) against the immunogenic peptide. In one example an "immunogenic composition" is composition comprising a gp120 polypeptide that induces a measurable CTL response against virus expressing gp120 polypeptide, or induces a measurable B cell response (such as production of antibodies) against a gp120 polypeptide. It further refers to isolated nucleic acids encoding an immunogenic peptide, such as a nucleic acid that can be used to express the gp120 polypeptide (and thus be used to elicit an immune response against this polypeptide).

For in vitro use, an immunogenic composition may consist of the isolated protein, peptide epitope, or nucleic acid encoding the protein, or peptide epitope. For in vivo use, the immunogenic composition will typically comprise the protein or immunogenic peptide in pharmaceutically acceptable carriers, and/or other agents. Any particular peptide, such as a gp120 polypeptide, or nucleic acid encoding the polypeptide, can be readily tested for its ability to induce a CTL or B cell response by art-recognized assays. Immunogenic compositions can include adjuvants, which are well known to one of skill in the art.

Immunologically reactive conditions: Includes reference to conditions which allow an antibody raised against a particular epitope to bind to that epitope to a detectably greater degree than, and/or to the substantial exclusion of, binding to substantially all other epitopes. Immunologically reactive conditions are dependent upon the format of the antibody binding reaction and typically are those utilized in immunoassay protocols or those conditions encountered in vivo. The immunologically reactive conditions employed in the methods are "physiological conditions" which include reference to conditions (such as temperature, osmolarity, pH) that are typical inside a living mammal or a mammalian cell. While it is recognized that some organs are subject to extreme conditions, the intra-organismal and intracellular environment is normally about pH 7 (such as from pH 6.0 to pH 8.0, more typically pH 6.5 to 7.5), contains water as the predominant solvent, and exists at a temperature above 0° C. and below 50° C. Osmolarity is within the range that is supportive of cell viability and proliferation.

Immunotherapy: A method of evoking an immune response against a virus based on their production of target antigens. Immunotherapy based on cell-mediated immune responses involves generating a cell-mediated response to cells that produce particular antigenic determinants, while immunotherapy based on humoral immune responses involves generating specific antibodies to virus that produce particular antigenic determinants.

Inhibiting or treating a disease: Inhibiting the full development of a disease or condition, for example, in a subject who is at risk for a disease such as acquired immune deficiency syndrome (AIDS), AIDS related conditions, HIV-1 infection, or combinations thereof. "Treatment" refers to a therapeutic intervention that ameliorates a sign or symptom of a disease or pathological condition after it has begun to develop. The term "ameliorating," with reference to a disease or pathological condition, refers to any observable beneficial effect of the treatment. The beneficial effect can be evidenced, for

example, by a delayed onset of clinical symptoms of the disease in a susceptible subject, a reduction in severity of some or all clinical symptoms of the disease, a slower progression of the disease, a reduction in the number of metastases, an improvement in the overall health or well-being of the subject, or by other parameters well known in the art that are specific to the particular disease. A "prophylactic" treatment is a treatment administered to a subject who does not exhibit signs of a disease or exhibits only early signs for the purpose of decreasing the risk of developing pathology.

Isolated: An "isolated" biological component (such as a nucleic acid, peptide or protein) has been substantially separated, produced apart from, or purified away from other biological components in the cell of the organism in which the component naturally occurs, such as, other chromosomal and extrachromosomal DNA and RNA, and proteins. Nucleic acids, peptides and proteins which have been "isolated" thus include nucleic acids and proteins purified by standard purification methods. The term also embraces nucleic acids, peptides, and proteins prepared by recombinant expression in a host cell as well as chemically synthesized nucleic acids.

K_d: The dissociation constant for a given interaction, such as a polypeptide ligand interaction. For example, for the bimolecular interaction of CD4 and gp120 it is the concentration of the individual components of the bimolecular interaction divided by the concentration of the complex.

Leukocyte: Cells in the blood, also termed "white cells," that are involved in defending the body against infective organisms and foreign substances. Leukocytes are produced in the bone marrow. There are 5 main types of white blood cell, subdivided between 2 main groups: polymorphonuclear leukocytes (neutrophils, eosinophils, basophils) and mononuclear leukocytes (monocytes and lymphocytes).

Ligand: Any molecule which specifically binds a protein, such as a gp120 protein, and includes, inter alia, antibodies that specifically bind a gp120 protein. In alternative embodiments, the ligand is a protein or a small molecule (one with a molecular weight less than 6 kiloDaltons).

Mimetic: A molecule (such as an organic chemical compound) that mimics the activity of an agent, such as the activity of a gp120 protein, for example by inducing an immune response to gp120. Peptidomimetic and organomimetic embodiments are within the scope of this term, whereby the three-dimensional arrangement of the chemical constituents of such peptido- and organomimetics mimic the three-dimensional arrangement of the peptide backbone and component amino acid side chains in the peptide, resulting in such peptido- and organomimetics of the peptides having substantial specific activity. For computer modeling applications, a pharmacophore is an idealized, three-dimensional definition of the structural requirements for biological activity. Peptido- and organomimetics can be designed to fit each pharmacophore with computer modeling software (using computer assisted drug design or CADD). See Walters, "Computer-Assisted Modeling of Drugs", in Klegerman & Groves, eds., 1993, Pharmaceutical Biotechnology, Interpharm Press: Buffalo Grove, Ill., pp. 165-174 and Principles of Pharmacology (ed. Munson, 1995), chapter 102 for a description of techniques used in computer assisted drug design.

Molecular Replacement: A method that involves generating a preliminary model, such as a model of a gp120 polypeptide, whose structure coordinates are unknown, by orienting and positioning a molecule whose structure coordinates are known (such as coordinates from Table 1) within the unit cell of the unknown crystal so as best to account for the observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model and combined with the observed amplitudes to give an approximate Fourier synthesis of the structure whose coordinates are unknown. This, in turn, can be subject to any of the several forms of refinement to provide a final, accurate structure of the unknown molecule (see Lattman, Methods in Enzymology, 115:55-77, 1985; Rossmann, ed., "The Molecular Replacement Method", Int. Sci. Rev. Ser., No. 13, Gordon & Breach, New York, 1972). Using the structure coordinates of gp120, such as a stabilized gp120 provided herein; molecular replacement may be used to determine the structure coordinates of a crystalline mutant or homologue of gp120, a different crystal form of gp120, or gp120 in complex with another molecule, such as an antibody, cell surface receptor, or combination thereof.

Naturally Occurring Amino Acids: L-isomers of the naturally occurring amino acids. The naturally occurring amino acids are glycine, alanine, valine, leucine, isoleucine, serine, methionine, threonine, phenylalanine, tyrosine, tryptophan, cysteine, proline, histidine, aspartic acid, asparagine, glutamic acid, glutamine, gamma.-carboxyglutamic acid, arginine, ornithine and lysine. Unless specifically indicated, all amino acids referred to in this application are in the L-form. "Synthetic amino acids" refers to amino acids that are not naturally found in proteins. Examples of synthetic amino acids used herein, include racemic mixtures of selenocysteine and selenomethionine. In addition, unnatural amino acids include the D or L forms of nor-leucine, para-nitrophenylalanine, homophenylalanine, para-fluorophenylalanine, 3-amino-2-benzylpropionic acid, homoarginine, and D-phenylalanine. The term "positively charged amino acid" refers to any naturally occurring or synthetic amino acid having a positively charged side chain under normal physiological conditions. Examples of positively charged naturally occurring amino acids are arginine, lysine and histidine. The term "negatively charged amino acid" refers to any naturally occurring or synthetic amino acid having a negatively charged side chain under normal physiological conditions. Examples of negatively charged naturally occurring amino acids are aspartic acid and glutamic acid. The term "hydrophobic amino acid" refers to any amino acid having an uncharged, nonpolar side chain that is relatively insoluble in water. Examples of naturally occurring hydrophobic amino acids are alanine, leucine, isoleucine, valine, proline, phenylalanine, tryptophan and methionine. The term "hydrophilic amino acid" refers to any amino acid having an uncharged, polar side chain that is relatively soluble in water. Examples of naturally occurring hydrophilic amino acids are serine, threonine, tyrosine, asparagine, glutamine, and cysteine.

Nucleic acid: A polymer composed of nucleotide units (ribonucleotides, deoxyribonucleotides, related naturally occurring structural variants, and synthetic non-naturally occurring analogs thereof) linked via phosphodiester bonds, related naturally occurring structural variants, and synthetic non-naturally occurring analogs thereof. Thus, the term includes nucleotide polymers in which the nucleotides and the linkages between them include non-naturally occurring synthetic analogs, such as, for example and without limitation, phosphorothioates, phosphoramidates, methyl phosphonates, chiral-methyl phosphonates, 2-O-methyl ribonucleotides, peptide-nucleic acids (PNAs), and the like. Such polynucleotides can be synthesized, for example, using an automated DNA synthesizer. The term "oligonucleotide" typically refers to short polynucleotides, generally no greater than about 50 nucleotides. It will be understood that when a nucleotide sequence is represented by a DNA sequence (i.e., A, T, G, C), this also includes an RNA sequence (i.e., A, U, G, C) in which "U" replaces "T."

"Nucleotide" includes, but is not limited to, a monomer that includes a base linked to a sugar, such as a pyrimidine, purine or synthetic analogs thereof, or a base linked to an amino acid, as in a peptide nucleic acid (PNA). A nucleotide is one monomer in a polynucleotide. A nucleotide sequence refers to the sequence of bases in a polynucleotide. A gp120 polynucleotide is a nucleic acid encoding a gp120 polypeptide.

Conventional notation is used herein to describe nucleotide sequences: the left-hand end of a single-stranded nucleotide sequence is the 5'-end; the left-hand direction of a double-stranded nucleotide sequence is referred to as the 5'-direction. The direction of 5' to 3' addition of nucleotides to nascent RNA transcripts is referred to as the transcription direction. The DNA strand having the same sequence as an mRNA is referred to as the "coding strand;" sequences on the DNA strand having the same sequence as an mRNA transcribed from that DNA and which are located 5' to the 5'-end of the RNA transcript are referred to as "upstream sequences;" sequences on the DNA strand having the same sequence as the RNA and which are 3' to the 3' end of the coding RNA transcript are referred to as "downstream sequences."

"cDNA" refers to a DNA that is complementary or identical to an mRNA, in either single stranded or double stranded form.

"Encoding" refers to the inherent property of specific sequences of nucleotides in a polynucleotide, such as a gene, a cDNA, or an mRNA, to serve as templates for synthesis of other polymers and macromolecules in biological processes having either a defined sequence of nucleotides (for example, rRNA, tRNA and mRNA) or a defined sequence of amino acids and the biological properties resulting therefrom. Thus, a gene encodes a protein if transcription and translation of mRNA produced by that gene produces the protein in a cell or other biological system. Both the coding strand, the nucleotide sequence of which is identical to the mRNA sequence and is usually provided in sequence listings, and non-coding strand, used as the template for transcription, of a gene or cDNA can be referred to as encoding the protein or other product of that gene or cDNA. Unless otherwise specified, a "nucleotide sequence encoding an amino acid sequence" includes all nucleotide sequences that are degenerate versions of each other and that encode the same amino acid sequence. Nucleotide sequences that encode proteins and RNA may include introns.

"Recombinant nucleic acid" refers to a nucleic acid having nucleotide sequences that are not naturally joined together. This includes nucleic acid vectors comprising an amplified or assembled nucleic acid which can be used to transform a suitable host cell. A host cell that comprises the recombinant nucleic acid is referred to as a "recombinant host cell." The gene is then expressed in the recombinant host cell to produce, such as a "recombinant polypeptide." A recombinant nucleic acid may serve a non-coding function (such as a promoter, origin of replication, ribosome-binding site, etc.) as well.

A first sequence is an "antisense" with respect to a second sequence if a polynucleotide whose sequence is the first sequence specifically hybridizes with a polynucleotide whose sequence is the second sequence.

Terms used to describe sequence relationships between two or more nucleotide sequences or amino acid sequences include "reference sequence," "selected from," "comparison window," "identical," "percentage of sequence identity," "substantially identical," "complementary," and "substantially complementary."

For sequence comparison of nucleic acid sequences and amino acids sequences, typically one sequence acts as a reference sequence, to which test sequences are compared. When using a sequence comparison algorithm, test and reference sequences are entered into a computer, subsequence coordinates are designated, if necessary, and sequence algorithm program parameters are designated. Default program parameters are used. Methods of alignment of sequences for comparison are well known in the art. Optimal alignment of sequences for comparison can be conducted, for example, by the local homology algorithm of Smith & Waterman, *Adv. Appl. Math.* 2:482, 1981, by the homology alignment algorithm of Needleman & Wunsch, *J. Mol. Biol.* 48:443, 1970, by the search for similarity method of Pearson & Lipman, *Proc. Nat'l. Acad. Sci. USA* 85:2444, 1988, by computerized implementations of these algorithms (GAP, BESTFIT, FASTA, and TFASTA in the Wisconsin Genetics Software Package, Genetics Computer Group, 575 Science Dr., Madison, Wis.), or by manual alignment and visual inspection (see for example, *Current Protocols in Molecular Biology* (Ausubel et al., eds 1995 supplement)).

One example of a useful algorithm is PILEUP. PILEUP uses a simplification of the progressive alignment method of Feng & Doolittle, *J. Mol. Evol.* 35:351-360, 1987. The method used is similar to the method described by Higgins & Sharp, *CABIOS* 5:151-153, 1989. Using PILEUP, a reference sequence is compared to other test sequences to determine the percent sequence identity relationship using the following parameters: default gap weight (3.00), default gap length weight (0.10), and weighted end gaps. PILEUP can be obtained from the GCG sequence analysis software package, such as version 7.0 (Devereaux et al., *Nuc. Acids Res.* 12:387-395, 1984.

Another example of algorithms that are suitable for determining percent sequence identity and sequence similarity are the BLAST and the BLAST 2.0 algorithm, which are described in Altschul et al., *J. Mol. Biol.* 215:403-410, 1990 and Altschul et al., *Nucleic Acids Res.* 25:3389-3402, 1977. Software for performing BLAST analyses is publicly available through the National Center for Biotechnology Information (ncbi.nlm.nih.gov). The BLASTN program (for nucleotide sequences) uses as defaults a word length (W) of 11, alignments (B) of 50, expectation (E) of 10, M=5, N=−4, and a comparison of both strands. The BLASTP program (for amino acid sequences) uses as defaults a word length (W) of 3, and expectation (E) of 10, and the BLOSUM62 scoring matrix (see Henikoff & Henikoff, *Proc. Natl. Acad. Sci. USA* 89:10915, 1989).

Another indicia of sequence similarity between two nucleic acids is the ability to hybridize. The more similar are the sequences of the two nucleic acids, the more stringent the conditions at which they will hybridize. The stringency of hybridization conditions are sequence-dependent and are different under different environmental parameters. Thus, hybridization conditions resulting in particular degrees of stringency will vary depending upon the nature of the hybridization method of choice and the composition and length of the hybridizing nucleic acid sequences. Generally, the temperature of hybridization and the ionic strength (especially the Na^+ and/or Mg^{++} concentration) of the hybridization buffer will determine the stringency of hybridization, though wash times also influence stringency. Generally, stringent conditions are selected to be about 5° C. to 20° C. lower than the thermal melting point (T_m) for the specific sequence at a defined ionic strength and pH. The T_m is the temperature (under defined ionic strength and pH) at which 50% of the target sequence hybridizes to a perfectly matched probe. Con-

ditions for nucleic acid hybridization and calculation of stringencies can be found, for example, in Sambrook et al., *Molecular Cloning: A Laboratory Manual*, Cold Spring Harbor Laboratory Press, Cold Spring Harbor, N.Y., 2001; Tijssen, *Hybridization With Nucleic Acid Probes, Part I. Theory and Nucleic Acid Preparation*, Laboratory Techniques in Biochemistry and Molecular Biology, Elsevier Science Ltd., NY, N.Y., 1993 and Ausubel et al. *Short Protocols in Molecular Biology,* 4th ed., John Wiley & Sons, Inc., 1999.

"Stringent conditions" encompass conditions under which hybridization will only occur if there is less than 25% mismatch between the hybridization molecule and the target sequence. "Stringent conditions" may be broken down into particular levels of stringency for more precise definition. Thus, as used herein, "moderate stringency" conditions are those under which molecules with more than 25% sequence mismatch will not hybridize; conditions of "medium stringency" are those under which molecules with more than 15% mismatch will not hybridize, and conditions of "high stringency" are those under which sequences with more than 10% mismatch will not hybridize. Conditions of "very high stringency" are those under which sequences with more than 6% mismatch will not hybridize. In contrast nucleic acids that hybridize under "low stringency conditions include those with much less sequence identity, or with sequence identity over only short subsequences of the nucleic acid. For example, a nucleic acid construct can include a polynucleotide sequence that hybridizes under high stringency or very high stringency, or even higher stringency conditions to a polynucleotide sequence that encodes SEQ ID NO: 1.

Operably linked: A first nucleic acid sequence is operably linked with a second nucleic acid sequence when the first nucleic acid sequence is placed in a functional relationship with the second nucleic acid sequence. For instance, a promoter is operably linked to a coding sequence if the promoter affects the transcription or expression of the coding sequence. Generally, operably linked DNA sequences are contiguous and, where necessary to join two protein-coding regions, in the same reading frame.

Peptide Modifications: The present disclosure includes mutant gp120 peptides, as well as synthetic embodiments. In addition, analogues (non-peptide organic molecules), derivatives (chemically functionalized peptide molecules obtained starting with the disclosed peptide sequences) and variants (homologs) of gp120 can be utilized in the methods described herein. The peptides disclosed herein include a sequence of amino acids that can be either L- and/or D-amino acids, naturally occurring and otherwise.

Peptides can be modified by a variety of chemical techniques to produce derivatives having essentially the same activity as the unmodified peptides, and optionally having other desirable properties. For example, carboxylic acid groups of the protein, whether carboxyl-terminal or side chain, may be provided in the form of a salt of a pharmaceutically-acceptable cation or esterified to form a C_1-C_{16} ester, or converted to an amide of formula NR_1R_2 wherein R_1 and R_2 are each independently H or C_1-C_{16} alkyl, or combined to form a heterocyclic ring, such as a 5- or 6-membered ring. Amino groups of the peptide, whether amino-terminal or side chain, may be in the form of a pharmaceutically-acceptable acid addition salt, such as the HCl, HBr, acetic, benzoic, toluene sulfonic, maleic, tartaric and other organic salts, or may be modified to C_1-C_{16} alkyl or dialkyl amino or further converted to an amide.

Hydroxyl groups of the peptide side chains can be converted to C_1-C_{16} alkoxy or to a C_1-C_{16} ester using well-recognized techniques. Phenyl and phenolic rings of the peptide side chains can be substituted with one or more halogen atoms, such as F, Cl, Br or I, or with C_1-C_{16} alkyl, C_1-C_{16} alkoxy, carboxylic acids and esters thereof, or amides of such carboxylic acids. Methylene groups of the peptide side chains can be extended to homologous C_2-C_4 alkylenes. Thiols can be protected with any one of a number of well-recognized protecting groups, such as acetamide groups. Those skilled in the art will also recognize methods for introducing cyclic structures into the peptides of this disclosure to select and provide conformational constraints to the structure that result in enhanced stability. For example, a C- or N-terminal cysteine can be added to the peptide, so that when oxidized the peptide will contain a disulfide bond, generating a cyclic peptide. Other peptide cyclizing methods include the formation of thioethers and carboxyl- and amino-terminal amides and esters.

Peptidomimetic and organomimetic embodiments are also within the scope of the present disclosure, whereby the three-dimensional arrangement of the chemical constituents of such peptido- and organomimetics mimic the three-dimensional arrangement of the peptide backbone and component amino acid side chains, resulting in such peptido- and organomimetics of the proteins of this disclosure. For computer modeling applications, a pharmacophore is an idealized, three-dimensional definition of the structural requirements for biological activity. Peptido- and organomimetics can be designed to fit each pharmacophore with current computer modeling software (using computer assisted drug design or CADD). See Walters, "Computer-Assisted Modeling of Drugs", in Klegerman & Groves, eds., 1993, *Pharmaceutical Biotechnology*, Interpharm Press: Buffalo Grove, Ill., pp. 165-174 and *Principles of Pharmacology* Munson (ed.) 1995, Ch. 102, for descriptions of techniques used in CADD. Also included within the scope of the disclosure are mimetics prepared using such techniques. In one example, a mimetic mimics the antigenic activity generated by gp120 a mutant, a variant, fragment, or fusion thereof.

Pharmaceutical agent: A chemical compound or composition capable of inducing a desired therapeutic or prophylactic effect when properly administered to a subject or a cell. "Incubating" includes a sufficient amount of time for a drug to interact with a cell. "Contacting" includes incubating a drug in solid or in liquid form with a cell. An "anti-viral agent" or "anti-viral drug" is an agent that specifically inhibits a virus from replicating or infecting cells. Similarly, an "anti-retroviral agent" is an agent that specifically inhibits a retrovirus from replicating or infecting cells.

A "therapeutically effective amount" is a quantity of a chemical composition or an anti-viral agent sufficient to achieve a desired effect in a subject being treated. For instance, this can be the amount necessary to inhibit viral replication or to measurably alter outward symptoms of the viral infection, such as increase of T cell counts in the case of an HIV-1 infection. In general, this amount will be sufficient to measurably inhibit virus (for example, HIV) replication or infectivity. When administered to a subject, a dosage will generally be used that will achieve target tissue concentrations (for example, in lymphocytes) that has been shown to achieve in vitro inhibition of viral replication.

Pharmaceutically acceptable carriers: The pharmaceutically acceptable carriers of use are conventional. *Remington's Pharmaceutical Sciences*, by E. W. Martin, Mack Publishing Co., Easton, Pa., 15th Edition, 1975, describes compositions and formulations suitable for pharmaceutical delivery of the fusion proteins herein disclosed.

In general, the nature of the carrier will depend on the particular mode of administration being employed. For

instance, parenteral formulations usually comprise injectable fluids that include pharmaceutically and physiologically acceptable fluids such as water, physiological saline, balanced salt solutions, aqueous dextrose, glycerol or the like as a vehicle. For solid compositions (such as powder, pill, tablet, or capsule forms), conventional non-toxic solid carriers can include, for example, pharmaceutical grades of mannitol, lactose, starch, or magnesium stearate. In addition to biologically neutral carriers, pharmaceutical compositions to be administered can contain minor amounts of non-toxic auxiliary substances, such as wetting or emulsifying agents, preservatives, and pH buffering agents and the like, for example sodium acetate or sorbitan monolaurate.

Polypeptide: Any chain of amino acids, regardless of length or post-translational modification (such as glycosylation or phosphorylation). "Polypeptide" applies to amino acid polymers to naturally occurring amino acid polymers and non-naturally occurring amino acid polymer as well as in which one or more amino acid residue is a non-natural amino acid, for example an artificial chemical mimetic of a corresponding naturally occurring amino acid. In one embodiment, the polypeptide is a gp120 polypeptide, such as a stabilized gp120. A "residue" refers to an amino acid or amino acid mimetic incorporated in a polypeptide by an amide bond or amide bond mimetic. A polypeptide has an amino terminal (N-terminal) end and a carboxy terminal (C-terminal) end. "Polypeptide" is used interchangeably with peptide or protein, and is used interchangeably herein to refer to a polymer of amino acid residues.

Protein core: The protein core refers to the interior of a folded protein, which is substantially free of solvent exposure, such as solvent in the form of water molecules in solution. Typically, the protein core is predominately composed of hydrophobic or apolar amino acids. In some examples, a protein core may contain charged amino acids, for example aspartic acid, glutamic acid, arginine, and/or lysine. The inclusion of uncompensated charged amino acids (a compensated charged amino can be in the form of a salt bridge) in the protein core can lead to a destabilized protein. That is, a protein with a lower T_m then a similar protein without an uncompensated charged amino acid in the protein core. In other examples, a protein core may have a cavity with in the protein core. Cavities are essentially voids within a folded protein where amino acids or amino acid side chains are not present. Such cavities can also destabilize a protein relative to a similar protein without a cavity. Thus, when creating a stabilized form of a protein, for example a stabilized form of gp120, it may be advantageous to substitute amino acid residues within the core in order to fill cavities present in the wild-type protein.

Purified: The term purified does not require absolute purity; rather, it is intended as a relative term. Thus, for example, a purified protein is one in which the protein is more enriched than the protein is in its natural environment within a cell. Preferably, a preparation is purified such that the protein represents at least 50% of the protein content of the preparation.

The gp120 polypeptides disclosed herein, or antibodies that specifically bind gp120, can be purified by any of the means known in the art. See for example *Guide to Protein Purification*, ed. Deutscher, *Meth. Enzymol.* 185, Academic Press, San Diego, 1990; and Scopes, *Protein Purification: Principles and Practice*, Springer Verlag, New York, 1982. Substantial purification denotes purification from other proteins or cellular components. A substantially purified protein is at least 60%, 70%, 80%, 90%, 95% or 98% pure. Thus, in one specific, non-limiting example, a substantially purified protein is 90% free of other proteins or cellular components.

Space Group: The arrangement of symmetry elements of a crystal.

Structure coordinates: Mathematical coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) such as a gp120, a gp120:CD4 complex, a gp120:antibody complex, or combinations thereof in a crystal in crystal form. The diffraction data are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps are used to establish the positions of the individual atoms within the unit cell of the crystal. In one example, the term "structure coordinates" refers to Cartesian coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays, such as by the atoms of a stabilized form of gp120 in crystal form.

Atomic coordinate data, such as that in Table 1 and Table 2 lists each atom by a unique number (column 2); the atom name in the context of the residue to which it belongs (column 3), for example CA refers to the alpha carbon of the peptide backbone (detailed descriptions of the atom identifiers for each residue can be found for example in Creighton, Proteins, Structures and Molecular Properties, W.H. Freeman & Co., New York, 1993); the amino acid residue in which the atom is located (column 4); the chain identifier (column 4') which may or may not be included, the number of the residue (column 5); the coordinates (for example, X, Y, Z) which define with respect to the crystallographic axes the atomic position (in Å) of the respective atom (columns 6, 7, and 8); the occupancy of the atom in the respective position (column 9); the "B-factor", which is the isotropic displacement parameter (in $Å^2$) and accounts for movement of the atom around its atomic center (column 10).

Those of ordinary skill in the art understand that a set of structure coordinates determined by X-ray crystallography is not without standard error. For the purpose of this disclosure, any set of structure coordinates for a stabilized form of gp120 or a gp120 with an extended V3 loop that have a root mean square deviation of protein backbone atoms (N, Cα, C and 0) of less than about 1.0 Angstroms when superimposed, such as about 0.75, or about 0.5, or about 0.25 Angstroms, using backbone atoms, on the structure coordinates listed in Table 1 or Table 2 shall (in the absence of an explicit statement to the contrary) be considered identical.

Subject: Living multi-cellular vertebrate organisms, a category that includes both human and veterinary subjects, including human and non-human mammals.

T Cell: A white blood cell critical to the immune response. T cells include, but are not limited to, $CD4^+$ T cells and $CD8^+$ T cells. A $CD4^+$ T lymphocyte is an immune cell that carries a marker on its surface known as "cluster of differentiation 4" (CD4). These cells, also known as helper T cells, help orchestrate the immune response, including antibody responses as well as killer T cell responses. $CD8^+$ T cells carry the "cluster of differentiation 8" (CD8) marker. In one embodiment, a CD8 T cells is a cytotoxic T lymphocytes. In another embodiment, a CD8 cell is a suppressor T cell.

Therapeutic agent: Used in a generic sense, it includes treating agents, prophylactic agents, and replacement agents.

T_m: The temperature at which a change of state occurs. For example, the temperature at which gp120 undergoes a transition from the folded form to the unfolded form. Essentially this is the temperature at which the structure melts away.

Stabilized gp120 has a higher T_m than native gp120. Another example would be the temperature at which a DNA duplex melts.

Transformed: A transformed cell is a cell into which has been introduced a nucleic acid molecule by molecular biology techniques. As used herein, the term transformation encompasses all techniques by which a nucleic acid molecule might be introduced into such a cell, including transfection with viral vectors, transformation with plasmid vectors, and introduction of DNA by electroporation, lipofection, and particle gun acceleration.

Unit Cell: The smallest building block of a crystal. The entire volume of a crystal may be constructed by regular assembly of such blocks. Each unit cell comprises a complete representation of the unit of pattern, the repetition of which builds produces a crystal lattice

Vector: A nucleic acid molecule as introduced into a host cell, thereby producing a transformed host cell. Recombinant DNA vectors are vectors having recombinant DNA. A vector can include nucleic acid sequences that permit it to replicate in a host cell, such as an origin of replication. A vector can also include one or more selectable marker genes and other genetic elements known in the art. Viral vectors are recombinant DNA vectors having at least some nucleic acid sequences derived from one or more viruses.

Virus: Microscopic infectious organism that reproduces inside living cells. A virus consists essentially of a core of a single nucleic acid surrounded by a protein coat, and has the ability to replicate only inside a living cell. "Viral replication" is the production of additional virus by the occurrence of at least one viral life cycle. A virus may subvert the host cells' normal functions, causing the cell to behave in a manner determined by the virus. For example, a viral infection may result in a cell producing a cytokine, or responding to a cytokine, when the uninfected cell does not normally do so.

"Retroviruses" are RNA viruses wherein the viral genome is RNA. When a host cell is infected with a retrovirus, the genomic RNA is reverse transcribed into a DNA intermediate which is integrated very efficiently into the chromosomal DNA of infected cells. The integrated DNA intermediate is referred to as a provirus. The term "lentivirus" is used in its conventional sense to describe a genus of viruses containing reverse transcriptase. The lentiviruses include the "immunodeficiency viruses" which include human immunodeficiency virus (HIV) type 1 and type 2 (HIV-1 and HIV-2), simian immunodeficiency virus (SIV), and feline immunodeficiency virus (FIV).

HIV-1 is a retrovirus that causes immunosuppression in humans (HIV disease), and leads to a disease complex known as the acquired immunodeficiency syndrome (AIDS). "HIV disease" refers to a well-recognized constellation of signs and symptoms (including the development of opportunistic infections) in persons who are infected by an HIV virus, as determined by antibody or western blot studies. Laboratory findings associated with this disease are a progressive decline in T cells.

X5: An antibody that bonds a conformation of gp120 induced by the binding of CD4. Antibodies that bind to gp120 in a conformation induced by CD4 binding are termed CD4i antibodies.

ΔS: The change in entropy, such as the change in entropy upon the association of gp120 and CD4 or an antibody or antibody fragment, for example X5.

ΔH: The change in the enthalpy, such as the change enthalpy upon the association of gp120 and CD4 or an antibody.

II. Overview of Several Embodiments

Provided herein in various embodiments are gp120 polypeptides, which are useful to induce immunogenic response in vertebrate animals (such as mammals, for example primates, such as humans) to lentivirus, such as SIV or HIV (for example HIV-1 and HIV-2).

In several embodiments, the gp120 polypeptides are stabilized in a CD4 bound conformation. In several disclosed examples, the gp120 polypeptides are stabilized by modification. In certain examples, these modifications can be the introduction of a plurality of non-naturally occurring cross-linking cysteine residues. In certain examples, the modification can be the introduction of at least one amino acid substitution in the protein core of gp120.

In several disclosed examples, cysteines are introduced into the gp120 polypeptide at position 96, 109, 123, 231, 267, 275, 428, 431 or in combinations thereof. In some examples of gp120 polypeptides disclosed herein, the plurality of non-naturally occurring cross-linking cysteine residues are defined by the interaction and crosslinking of at least one of residue pairs 96 and 275; 109 and 428; 123 and 431; and 231 and 267. In some embodiments, all of the residue pairs 96 and 275; 109 and 428; 123 and 431; and 231 and 267 are crosslinked.

In some embodiments, the stabilized gp120 polypeptide contains one or more amino acid substitutions in the protein core. In several examples, the substitution is made at position 95, 257, 375, 433, or a combination thereof. In specific examples, the substitution is a serine to tryptophan substitution at position 95, a threonine to serine substitution at position 257, a serine to tryptophan substitution at position 375, an alanine to methionine substitution at position 433, or a combination thereof.

In specific examples, the stabilized gp120 polypeptide includes the amino acid sequence set forth as SEQ ID NO: 1 or is encoded by one of SEQ ID NO: 4, 5, 6, 7, 8, 10, 11, 12, 13, 14, 15, 16, 17, 18, or degenerate variants thereof. In still other embodiments, the stabilized gp120 contains a portion of the amino acid sequence set forth as SEQ ID NO: 1 or as encoded by any one of SEQ NOs: 4-18, for example, a domain such as the outer domain, or a contiguous stretch of about 5 or more amino acids, such as about 6, about 7, about 8, about 9, about 10, about 15, about 20, about 25, or more amino acids.

In other examples, the gp120 polypeptide has the V3 loop in an extended conformation. In one example, the gp120 polypeptide with the V3 loop in an extended conformation contains the amino acid sequence set forth as SEQ ID NO: 2. In other embodiments, the gp120 polypeptide with an extended v3 loop contains a portion of the amino acid sequence set forth as SED ID NO: 2, for example, a domain such as the outer domain, or a contiguous stretch of about 5 or more amino acids, such as about 6, about 7, about 8, about 9, about 10, about 15, about 20, about 25, or more amino acids wherein the domain or contiguous stretch of amino acids includes a portion of the V3 loop.

Other embodiments are compositions containing a therapeutically effective amount of at least one gp120 polypeptide, such as a stabilized gp120 polypeptide (such as set forth as SEQ ID NO: 1 or as encoded by the nucleotide sequence set forth as one of SEQ ID NO: 4, 5, 6, 7, 8, 10, 11, 12, 13, 14 15, 16, 17, and 18, or a degenerate variant thereof) or a gp120 polypeptide with the V3 loop in an extended conformation, such as the amino acid sequence set forth as SEQ NO: 2. In some embodiments, the composition can contain pharmaceutically acceptable carriers, adjuvants, or combinations thereof.

This disclosure further provides methods for eliciting and/or enhancing an immune response in a subject (such as a primate subject, for example a human subject). In some embodiments, these methods involve administering to the subject a composition including a gp120 polypeptide as disclosed herein, for example a stabilized gp120 such as set forth as SEQ ID NO: 1 or as encoded by the nucleotide sequence set forth as one of SEQ ID NO: 4, 5, 6, 7, 8, 10, 11, 12, 13, 14 15, 16, 17, and 18, or a degenerate variant thereof. In some embodiments, these methods involve administering to the subject a composition including a gp120 polypeptide with an extended V3 loop such as set forth as SEQ ID NO: 2. In one specific, non-limiting example, the subject is infected with a lentivirus, for example SIV or HIV, such as HIV-1 or HIV-2. In some embodiments, the immune response is a B cell response, a T cell response, or a combination thereof.

In other embodiments, the subject is further administered a therapeutically effective amount of a monomeric or trimeric gp140 polypeptide, an unmodified monomeric or trimeric gp120 polypeptide, or a combination thereof.

Other embodiments of this disclosure are isolated polynucleotides (nucleic acid molecules) which encode the gp120 polypeptides described herein. Specific examples of such nucleic acid molecules contain nucleic acids encoding the amino acid sequence set forth as one of SEQ ID NO: 1 or 2, the nucleotide sequences set forth as one of SEQ ID NOs: 4-18, or degenerate variants thereof. In other embodiments, the isolated polynucleotides consist of nucleic acid molecules encoding the amino acid sequence set forth as one of SEQ ID NO: 1 or 2, the nucleotide sequences set forth as one of SEQ ID NOs: 4-18, or degenerate variants thereof. In certain embodiments, the nucleic acid encoding a gp120 polypeptide is operably linked to a promoter. Vectors comprising such polynucleotides are also disclosed, as are host cells transformed with such vectors.

Other embodiments are compositions containing a therapeutically effective amount of a polynucleotide containing a nucleic acid encoding a gp120 polypeptide disclosed herein. In certain embodiments, the nucleic acid encodes the amino acid sequence set forth as SEQ ID NO: 1 and 2. In other embodiments the nucleic acid contains the one of the nucleotide sequences set forth as SEQ ID NO: 4-18 or a degenerate variant thereof. In some embodiments, the composition can contain pharmaceutically acceptable carriers, adjuvants, or combinations thereof.

This disclosure further provides methods for eliciting and/or enhancing an immune response in a subject (such as a primate subject, for example a human subject). The methods involve administering to the subject a composition containing a nucleic acid encoding a gp120 polypeptide of this disclosure. In one specific, non-limiting example, the subject is infected with a lentivirus, for example SIV or HIV, such as HIV-1 or HIV-2. In some embodiments, the immune response is a B cell response, a T cell response, or a combination thereof.

In other embodiments, the subject is further administered a therapeutically effective amount of a plasmid vector expressing a polypeptide containing a monomeric or trimeric gp140 polypeptide, an unmodified monomeric or trimeric gp120 polypeptide; or combination thereof.

Also disclosed herein are methods for identifying an immunogen that induces an immune response to gp120, for example gp120 from a lentivirus, such as SIV or HIV such as HIV-1 or HIV-2. Typically the immune response is a B cell response, a T cell response, or a combination thereof. These methods involve using a three-dimensional structure of gp120 as defined by atomic coordinates set forth in Table 1, Table 2, or a portion thereof to design or select the immunogen, synthesizing the immunogen, immunizing a subject with the immunogen; and determining if an immune response to gp120 is induced in the subject. In some embodiments, the immunogen is designed from the gp120 amino acid sequence. In certain embodiments, the immunogen is designed or selected using a three-dimensional structure of gp120 as defined by atomic coordinates set forth in Table 1, Table 2, or a portion thereof and an amino acid sequence is assembled to provide an immunogen, for example by synthesizing the amino acid sequence or producing a nucleic acid encoding the immunogen. In other embodiments the is selected from a database of compounds or is designed de novo.

Also provided by this disclosure is a machine readable data storage medium including a data storage material encoded with machine readable data corresponding to the coordinates of a stabilized form of gp120 as defined by Table 1 or a portion thereof or a form of gp120 having an extended conformation of the V3 loop as defined by Table 2 or a portion thereof.

Also provided for are computer systems including data and a data processor, wherein the system forms a representation of the three-dimensional structure gp120 protein as defined by Table 1, Table 2, or a portion thereof, such as the atomic positions, surface, domain, or region of the gp120 polypeptide.

Also disclosed herein is the use of stabilized gp120 molecules as crystallization tools. A crystalline form of a stabilized gp120 also is disclosed, for example the crystalline form of gp120 as defined by the coordinates as given in Table 1, or with coordinates having a root mean square deviation therefrom, wherein the distance between the residues is less than about 0.75 Å. A crystalline form of a gp120 with an extended V3 loop also is disclosed, for example the crystalline form of gp120 as defined by the coordinates as given in Table 2, or with coordinates having a root mean square deviation therefrom, wherein the distance between the residues is less than about 0.75 Å.

III. gp120 Immunogens and Nucleic Acids Encoding gp120 Immunogens

The present disclosure relates to gp120 polypeptides and nucleic acids encoding these gp120 polypeptides. The gp120 polypeptides of this disclosure are capable of eliciting an immune response to a gp120 protein in a subject, such as a human subject. In some embodiments, the gp120 polypeptides of this disclosure are stabilized in a CD4 bound conformation.

Using a combination of atomic level structural information with biophysical techniques novel gp120 polypeptides were designed that are stabilized in the conformation substantially identical to the CD4 bound polypeptide. For example, the three-dimensional structure of the wild-type polypeptide was analyzed to determine where cysteine residues could be introduced such that they would form disulfide bonds in the folded molecule. This methodology is not specific to cysteine residues; other natural or non-natural amino acids could be used. In some embodiments, the stabilized gp120 has a K_d for CD4 of less than or equal to about 10 nM, such as less than or equal to about 5 nM, less than or equal to about 3 nM, or less than or equal to about 1 nM. In some embodiments the stabilized gp120 has $-T\Delta S$ for CD4 binding of about less than or equal to 40 kcal/mol, such as about less than or equal to 30 kcal/mol, about less than or equal to 15 kcal/mol, or about less than or equal to 10 kcal/mol.

The stability of folded polypeptides can be measured using techniques such as thermal denaturation. The temperature of the unfolding transition (T_m) is an accepted measure of the stability of the folded polypeptide, where increases in T_m

indicate an increase in the stability of the folded polypeptide. In some embodiments, the stabilized gp120 polypeptides has a T_m value greater than about 52° C., such as greater than about 53° C., greater than about 54° C. (such as 53.8° C.), greater than about 55° C., greater than about 56° C., greater than about 57° C., greater than about 58° C., or even greater than about 59° C.

In some embodiments, the stabilized gp120 polypeptides are stabilized by a plurality of non-naturally occurring cross-linking cysteine residues. By plurality it is meant that there are at least 2, such as at least 4, at least 6, or at least 8 cysteines introduced by mutation into a gp120 polypeptide, such that pairs of cysteines form at least 1, such as at least 2, at least 3, or at least 4 disulfide bonds. Each disulfide bond is formed by a pair of cysteines.

In some embodiments, the mutationally introduced cysteines are introduced into the gp120 polypeptide at positions 96, 109, 123, 231, 267, 275, 428, 431, or in a sub-combination thereof. In some examples of the stabilized gp120 polypeptides, the plurality of non-naturally occurring cross-linking cysteine residues are defined by the interaction of at least one of residue pairs 96 and 275; 109 and 428; 123 and 431; and 231 and 267. Thus, the stabilized gp120 polypeptides of this disclosure may have any combination of the crosslinked cysteines defined by the interaction of 96 and 275; 109 and 428; 123 and 431; and 231 and 267.

In some embodiments, the stabilized gp120 polypeptide contains one or more amino acid substitutions in the protein core. In several disclosed examples, the substitution is made at position 95, 257, 375, 433, or a combination thereof. Thus, a stabilized gp120 polypeptide may have one, two, three, or four substitutions in the protein core. In specific examples, the substitution is a serine to tryptophan substitution at position 95, a threonine to serine substitution at position 257, a serine to tryptophan substitution at position 375, an alanine to methionine substitution at position 433, or various combinations thereof.

In one embodiment, the stabilized gp120 polypeptide (new_9c) includes the amino acid sequence set forth as:

(SEQ ID NO: 1)

EVVLVNVTENFNWCKNDMVEQMHEDICSLWDQSLKPCVKLCPLAGATSVITQACPKVSFEPIPIHY

CAPAGFAILKCNNKTFNGTGPCTNVSTVQCTHGIRPVVSSQLLLNGSLAEEEVVIRSCNFTDNAKTII

VQLNTSVEINCTRPNNGGSGSGGNMRQAHCNISRAKWNNTLKQIASKLREQFGNNKTIIFKQSSGG

DPEIVTHWFNCGGEFFYCNSTQLFNSTWFNSTWSTEGSNNTEGSDTITLPCRIKQIINMWCKVCKA

MYAPPISGQIRCSSNITGLLLTRDGGNSNNESEIFRPGGGDMRDNWRSELYKYKVVKIE.

In other embodiments, the stabilized gp120 includes the amino acid sequence encoded by one of SEQ ID NO: 4, 5, 6, 7, 8, 10, 11, 12, 13, 14 15, 16, 17, and 18, or degenerate variants thereof. In still other embodiments, the stabilized gp120 polypeptide consists of the amino acid sequence set forth as SEQ ID NO: 1 or as encoded by the nucleotide sequence set forth as one of SEQ ID NO: 4, 5, 6, 7, 8, 10, 11, 12, 13, 14 15, 16, 17, and 18, or a degenerate variant thereof. In some embodiments, a stabilized gp120 polypeptide is an immunogenic fragment of SEQ ID NO: 1 or as encoded by the nucleotide sequence set forth as one of SEQ ID NO: 4, 5, 6, 7, 8, 10, 11, 12, 13, 14 15, 16, 17, and 18, or a degenerate variant thereof, such that the immunogenic fragment is stabilized in a CD4 binding conformation. In some embodiments, the stabilized gp120 includes the outer-domain. In one example, the outer domain includes residues 255-421 and 436-474 of gp120. Thus, the outer domain can contain residues 109-246 and 261-299 of SEQ ID NO: 1, the amino acid sequence encoded by SEQ ID NO: 4-18 or a degenerate variant thereof. In some examples residues 246 and 261 are covalently linked, for example by a peptide linker. In some examples, the peptide linker is residues 247-260 of SEQ ID NO: 1, the amino acid sequence encoded by SEQ ID NO: 4-18 or a degenerate variant thereof. Ideally the linker should be of sufficient length such that the folded protein is a conformation that can be bound by CD4. In some embodiments, the linker is a peptide linker and the peptide linker is about 2 to about 20 amino acids in length, such as about 2, about 3, about 4, about 5, about 6, about 7, about 8, about 10, about 12, about 15, or about 20 amino acids in length. In some embodiments, the immunogenic fragment of gp120 consists of residues 109-246 and 261-299, and a linker In some embodiments the linker does not contain a sequence form gp120.

In other embodiments, the stabilized gp120 fragment is truncated on the carboxy terminal end. For example, the carboxy terminal end can be truncated to about amino acid residue 433. In addition, portions of the amino terminus of gp120 can also be eliminated from the stabilized gp120 fragment. The truncated gp120 sequence can be free from the carboxy terminus through amino acid residue 95. In one embodiment, the truncated gp120 sequence is free from the amino terminus of gp120 through residue 95 and residue 433 through the carboxy terminus of gp120. Thus, in some embodiments the stabilized gp120 contains a portion of the amino acid sequence set forth as SEQ ID NO: 1 or as encoded by any one of SED NOs:4-18.

In other embodiments, the gp120 polypeptide has the V3 loop in an extended conformation. An exemplary sequence of a gp120 with an extended loop is set forth as:

(SEQ ID NO: 2)

GARSEVVLENVTEHFNMWKNDMVEQMQEDIISLWDQSLKPCVKLTPLCVGAGSCDTSVITQACPKI

SFEPIPIHYCAPAGFAILKCNDKTFNGKGPCKNVSTVQCTHGIRPVVSTQLLLNGSLAEEEVVIRSDNF

TNNAKTIIVQLKESVEINCTRPNQNTRKSIHIGPGRAFYTTGEIIGDIRQAHCNISRAKWNDTLKQIVIK

LREQFENKTIVFNHSSGGDPEIVMHSFNCGGEFFYCNSAQLFNSTWNNNTEGSNNTEGNTITLPCRIK

QIINMWQEVGKAMYAPPIRGQIRCSSNITGLLLTRDGGINENGTEIFRPGGGDMRDNWRSELYKYKV

VKIE.

Thus, a gp120 polypeptide with an extended V3 loop can contain the amino acid sequence set forth as SEQ ID NO: 2 or a fragment thereof. In one example, the gp120 polypeptide with the V3 loop in an extended conformation consists of the amino acid sequence set forth as SEQ ID NO: 2 or a fragment thereof. In still other embodiments, the gp120 polypeptide with an extended V3 loop contains a portion of the amino acid sequence set forth as SED ID NO: 2. In some embodiments, the stabilized gp120 includes the outer-domain. In one example, the outer domain includes residues 255-421 and 436-474 of gp120. Thus, the outer domain can include residues 109-246 and 261-299 of SEQ ID NO: 2.

In other embodiments, the gp120 polypeptide has the V3 loop in an extended conformation is truncated on the carboxy terminal end. For example, the carboxy terminal end can be truncated to about amino acid residue 433. In addition, portions of the amino terminus of gp120 can also be eliminated from the gp120 polypeptide has the V3 loop in an extended conformation fragment. The truncated gp120 sequence can be free from the carboxy terminus through amino acid residue 95. In one embodiment, the truncated gp120 sequence is free from the amino terminus of gp120 through residue 95 and residue 433 through the carboxy terminus of gp120. Thus, in some embodiments the gp120 polypeptide has the V3 loop in an extended conformation contains a portion of the amino acid sequence set forth as SEQ ID NO: 2.

In other embodiments, the gp120 polypeptide has an amino acid sequence least 90% identical to SEQ ID NO: 1, SEQ ID NO: 2, or the amino acid sequence encoded by any one of SEQ ID NO: 4-18, for example a polypeptide that has about 91%, 92%, 93%, 94%, 95%, 96%, 97%, 98%, 99% or even higher sequence identity to SEQ ID NO: 1, SEQ ID NO: 2, or the amino acid sequence encoded by any one of SEQ ID NO: 4-18.

The immunogenic gp120 polypeptides or immunogenic fragments of the gp120 polypeptides disclosed herein can be chemically synthesized by standard methods, or can be produced recombinantly. An exemplary process for polypeptide production is described in Lu et al., *Federation of European Biochemical Societies Letters.* 429:31-35, 1998. They can also be isolated by methods including preparative chromatography and immunological separations.

In other embodiments, fusion proteins are provided including a first and second polypeptide moiety in which one of the protein moieties includes an amino acid sequence as set forth in SEQ ID NO: 1 or 2, or a fragment thereof. In other embodiments, fusion proteins are provided comprising a first and second polypeptide moiety in which one of the protein moieties includes an amino acid sequence encoded by one of the nucleotide sequences as set forth as SEQ ID NO: 4-18, or a fragment thereof. The other moiety is a heterologous protein such as can be a carrier protein and/or an immunogenic protein. Such fusions also are useful to evoke an immune response against gp120. In certain embodiments the gp120 polypeptides disclosed herein are covalent or non-covalent addition of TLR ligands or dendritic cell or B cell targeting moieties.

A gp120 polypeptide can be covalently linked to a carrier, which is an immunogenic macromolecule to which an antigenic molecule can be bound. When bound to a carrier, the bound polypeptide becomes more immunogenic. Carriers are chosen to increase the immunogenicity of the bound molecule and/or to elicit higher titers of antibodies against the carrier which are diagnostically, analytically, and/or therapeutically beneficial. Covalent linking of a molecule to a carrier can confer enhanced immunogenicity and T cell dependence (see Pozsgay et al., *PNAS* 96:5194-97, 1999; Lee et al., *J. Immunol.* 116:1711-18, 1976; Dintzis et al., *PNAS* 73:3671-75, 1976). Useful carriers include polymeric carriers, which can be natural (for example, polysaccharides, polypeptides or proteins from bacteria or viruses), semi-synthetic or synthetic materials containing one or more functional groups to which a reactant moiety can be attached. Bacterial products and viral proteins (such as hepatitis B surface antigen and core antigen) can also be used as carriers, as well as proteins from higher organisms such as keyhole limpet hemocyanin, horseshoe crab hemocyanin, edestin, mammalian serum albumins, and mammalian immunoglobulins. Additional bacterial products for use as carriers include bacterial wall proteins and other products (for example, streptococcal or staphylococcal cell walls and lipopolysaccharide (LPS)).

Most antigenic epitopes of HIV proteins are relatively small in size, such as about 5 to 100 amino acids in size, for example about 5, about 6, about 7, about 8, about 9, about 10, about 15, about 20, about 25, about 30, about 40, about 50, about 60, about 70, about 80, about 90, or about 100. Thus, fragments (for example, epitopes or other antigenic fragments) of a gp120 polypeptide, such as any of the gp120 polypeptides described herein or a fragment thereof, can be used as an immunogen.

In some embodiments, the disclosed gp120 polypeptides are modified by glycosylation, for example by N-linked glycans. Thus, the immune response can be focused on a region interest of a gp120 polypeptide by masking other regions with non-immunogenic glycans. Glycosylation sites can be introduced into the gp120 polypeptides by site directed mutagenesis. This straggly can be utilized to focus the immune response to regions of interest in the gp120 polypeptide, for example the CD4 binding site or the binding site for a neutralizing antibody, for example a the b12 antibody. Examples of glycan masking can be found in Pantophlet and Burton, *Trends Mol Med.* 9(11):468-73, 2003, which is incorporated by reference herein in its entirety.

Another strategy to focus the immune response on the CD4 binding region or b12 epitope region is to use SIV and HIVgp120 core glycoproteins (such as the stabilized gp120 polypeptides disclosed herein) that possess an endogenous CD4 binding site or to scaffold the heterologous HIV-1 CD4 binding region onto cores derived from selected SIV or HIV-2 strains. The gp120 core can be derived from the envelope glycoproteins of lentivirus, for example SIV such as SIV mac239 and HIV, such as HIV-2 7132A. The residues required for CD4BS antibody recognition, for example the site of b12 binding, are transplanted by site-directed mutagenesis of the appropriate codon-optimized plasmid sequences. In some embodiments, extra N-glycans are added to these cores to eliminate the elicitation of non-cross reactive antibodies directed against regions outside the antibody binding site, for example the binding site of a neutralizing antibody such as CD4BS antibody.

The present disclosure concerns nucleic acid constructs including polynucleotide sequences that encode antigenic gp120 polypeptides of HIV-1. These polynucleotides include DNA, cDNA and RNA sequences which encode the polypeptide of interest.

Methods for the manipulation and insertion of the nucleic acids of this disclosure into vectors are well known in the (see for example, Sambrook et al., *Molecular Cloning, a Laboratory Manual,* 2d edition, Cold Spring Harbor Press, Cold Spring Harbor, N.Y., 1989, and Ausubel et al., *Current Protocols in Molecular Biology*, Greene Publishing Associates and John Wiley & Sons, New York, N.Y., 1994).

Typically, the nucleic acid constructs encoding the gp120 polypeptides of this disclosure are plasmids. However, other vectors (for example, viral vectors, phage, cosmids, etc.) can be utilized to replicate the nucleic acids. In the context of this disclosure, the nucleic acid constructs typically are expression vectors that contain a promoter sequence which facilitates the efficient transcription of the inserted genetic sequence of the host. The expression vector typically contains an origin of replication, a promoter, as well as specific nucleic acid sequences that allow phenotypic selection of the transformed cells.

More generally, polynucleotide sequences encoding the gp120 polypeptides of this disclosure can be operably linked to any promoter and/or enhancer that is capable of driving expression of the nucleic acid following introduction into a host cell. A promoter is an array of nucleic acid control sequences that directs transcription of a nucleic acid. A promoter includes necessary nucleic acid sequences (which can be) near the start site of transcription, such as in the case of a polymerase II type promoter (a TATA element). A promoter also can include distal enhancer or repressor elements which can be located as much as several thousand base pairs from the start site of transcription. Both constitutive and inducible promoters are included (see, for example, Bitter et al., *Methods in Enzymology* 153:516-544, 1987).

To produce such nucleic acid constructs, polynucleotide sequences encoding gp120 polypeptides are inserted into a suitable expression vector, such as a plasmid expression vector. Procedures for producing polynucleotide sequences encoding gp120 polypeptides and for manipulating them in vitro are well known to those of skill in the art, and can be found, for example in Sambrook and Ausubel, supra.

In addition to the polynucleotide sequences encoding the polypeptides set forth as SEQ ID NOs:1-2 disclosed herein and nucleic acids encoding gp120 polypeptides as set forth as SEQ ID NOs:4-18 as disclosed herein, the nucleic acid constructs can include variant polynucleotide sequences that encode polypeptides that are substantially similar to SEQ ID NOs: 1-2 and nucleic acids encoding gp120 polypeptides as set forth as SEQ ID NOs: 4-18. Similarly, the nucleic acid constructs can include polynucleotides that encode chimeric polypeptides, for example fusion proteins. For enhanced immunogenicity, it may be advantageous to include the sequence encoding for heterologous T helper sequences derived from HIV or other heterologous sources.

The similarity between amino acid (and polynucleotide) sequences is expressed in terms of the similarity between the sequences, otherwise referred to as sequence identity. Sequence identity is frequently measured in terms of percentage identity (or similarity); the higher the percentage, the more similar are the primary structures of the two sequences. In general, the more similar the primary structures of two amino acid sequences, the more similar are the higher order structures resulting from folding and assembly. Thus, the nucleic acid constructs can include polynucleotides that encode polypeptides that are at least about 90%, or 95%, 98%, or 99% identical to one of SEQ ID NOs: 1-2 with respect to amino acid sequence, or that have at least about 90%, 95%, 98%, or 99% sequence identity to one or more of SEQ ID NOs: 4-18 and/or that differ from one of these sequences by the substitution of degenerate codons.

DNA sequences encoding an immunogenic gp120 polypeptide can be expressed in vitro by DNA transfer into a suitable host cell. The cell may be prokaryotic or eukaryotic. The term also includes any progeny of the subject host cell. It is understood that all progeny may not be identical to the parental cell since there may be mutations that occur during replication. Methods of stable transfer, meaning that the foreign DNA is continuously maintained in the host, are known in the art.

The polynucleotide sequences encoding an immunogenic gp120 polypeptide can be inserted into an expression vector including, but not limited to, a plasmid, virus or other vehicle that can be manipulated to allow insertion or incorporation of sequences and can be expressed in either prokaryotes or eukaryotes. Hosts can include microbial, yeast, insect, and mammalian organisms. Methods of expressing DNA sequences having eukaryotic or viral sequences in prokaryotes are well known in the art. Biologically functional viral and plasmid DNA vectors capable of expression and replication in a host are known in the art.

Transformation of a host cell with recombinant DNA can be carried out by conventional techniques that are well known to those of ordinary skill in the art. Where the host is prokaryotic, such as *E. coli*, competent cells which are capable of DNA uptake can be prepared from cells harvested after exponential growth phase and subsequently treated by the $CaCl_2$ method using procedures well known in the art. Alternatively, $MgCl_2$ or RbCl can be used. Transformation can also be performed after forming a protoplast of the host cell if desired, or by electroporation.

When the host is a eukaryote, such methods of transfection of DNA as calcium phosphate coprecipitates, conventional mechanical procedures such as microinjection, electroporation, insertion of a plasmid encased in liposomes, or virus vectors can be used. Eukaryotic cells can also be co-transformed with polynucleotide sequences encoding an immunogenic gp120 polypeptide, and a second foreign DNA molecule encoding a selectable phenotype, such as the herpes simplex thymidine kinase gene. Another method is to use a eukaryotic viral vector, such as simian virus 40 (SV40) or bovine papilloma virus, to transiently infect or transform eukaryotic cells and express the protein (see for example, *Eukaryotic Viral Vectors*, Cold Spring Harbor Laboratory, Gluzman ed., 1982).

IV. Immunogenic Compositions and Therapeutic Methods

Any of the gp120 polypeptides and nucleic acid molecules encoding the gp120 polypeptides disclosed herein can be used as immunogens, or to produce immunogens to elicit an immune response (immunogenic compositions) to gp120 such as to a gp120 expressing virus, for example to reduce HIV-1 infection or a symptom of HIV-1 infection. Following administration of a therapeutically effective amount of the disclosed therapeutic compositions, the subject can be monitored for HIV-1 infection, symptoms associated with HIV-1 infection, or both. Disclosed herein are methods of administering the therapeutic molecules disclosed herein (such as gp120 polypeptides and nucleic acids encoding gp120 polypeptides) to reduce HIV-1 infection. In several examples, a therapeutically effective amount of a gp120 polypeptide including SEQ ID NO: 1, a therapeutically effective amount of a gp120 polypeptide including SEQ ID NO: 2, a therapeutically effective amount of a gp120 polypeptide encoded by one of SEQ ID NOs: 4-18 or a degenerate variant thereof, or a combination thereof is administered to a subject.

In certain embodiments, the immunogenic composition includes an adjuvant. An adjuvant can be a suspension of minerals, such as alum, aluminum hydroxide, aluminum phosphate, on which antigen is adsorbed; or water-in-oil emulsion in which antigen solution is emulsified in oil (MF-59, Freund's incomplete adjuvant), sometimes with the inclusion of killed mycobacteria (Freund's complete adjuvant) to further enhance antigenicity (inhibits degradation of antigen and/or causes influx of macrophages). In one embodiment,

the adjuvant is a mixture of stabilizing detergents, micelle-forming agent, and oil available under the name PROVAX® (IDEC Pharmaceuticals, San Diego, Calif.). An adjuvant can also be an immunostimulatory nucleic acid, such as a nucleic acid including a CpG motif.

In one example, the immunogenic composition is mixed with an adjuvant containing two or more of a stabilizing detergent, a micelle-forming agent, and an oil. Suitable stabilizing detergents, micelle-forming agents, and oils are detailed in U.S. Pat. Nos. 5,585,103; 5,709,860; 5,270,202; and 5,695,770, all of which are incorporated by reference herein in their entirety. A stabilizing detergent is any detergent that allows the components of the emulsion to remain as a stable emulsion. Such detergents include polysorbate 80 (TWEEN) (Sorbitan-mono-9-octadecenoate-poly(oxy-1,2-ethanediyl; manufactured by ICI Americas, Wilmington, Del.), TWEEN 40™, TWEEN 20™, TWEEN 60™, ZWITTERGENT™ 3-12, TEEPOL HB7™, and SPAN 85™. These detergents are usually provided in an amount of approximately 0.05 to 0.5%, such as at about 0.2%. A micelle forming agent is an agent which is able to stabilize the emulsion formed with the other components such that a micelle-like structure is formed. Such agents generally cause some irritation at the site of injection in order to recruit macrophages to enhance the cellular response. Examples of such agents include polymer surfactants described by BASF Wyandotte publications, for example, Schmolka, *J. Am. Oil. Chem. Soc.* 54:110, 1977, and Hunter et al., *J. Immunol* 129:1244, 1981, PLURONIC™ L62LF, L101, and L64, PEG1000, and TETRONIC™ 1501, 150R1, 701, 901, 1301, and 130R1. The chemical structures of such agents are well known in the art. In one embodiment, the agent is chosen to have a hydrophile-lipophile balance (HLB) of between 0 and 2, as defined by Hunter and Bennett, *J. Immun.* 133:3167, 1984. The agent can be provided in an effective amount, for example between 0.5 and 10%, or in an amount between 1.25 and 5%.

The oil included in the composition is chosen to promote the retention of the antigen in oil-in-water emulsion, to provide a vehicle for the desired antigen, and preferably has a melting temperature of less than 65° C. such that emulsion is formed either at room temperature (about 20° C. to 25° C.), or once the temperature of the emulsion is brought down to room temperature. Examples of such oils include squalene, Squalane, EICOSANE™, tetratetracontane, glycerol, and peanut oil or other vegetable oils. In one specific, non-limiting example, the oil is provided in an amount between 1 and 10%, or between 2.5 and 5%. The oil should be both biodegradable and biocompatible so that the body can break down the oil over time, and so that no adverse effects, such as granulomas, are evident upon use of the oil.

Immunogenic compositions can be formulated with an appropriate solid or liquid carrier, depending upon the particular mode of administration chosen. If desired, the disclosed pharmaceutical compositions can also contain minor amounts of non-toxic auxiliary substances, such as wetting or emulsifying agents, preservatives, and pH buffering agents and the like, for example sodium acetate or sorbitan monolaurate. Excipients that can be included in the disclosed compositions include flow conditioners and lubricants, for example silicic acid, talc, stearic acid or salts thereof, such as magnesium or calcium stearate, and/or polyethylene glycol, or derivatives thereof.

Immunogenic compositions can be provided as parenteral compositions, such as for injection or infusion. Such compositions are formulated generally by mixing a disclosed therapeutic agent at the desired degree of purity, in a unit dosage injectable form (solution, suspension, or emulsion), with a pharmaceutically acceptable carrier, for example one that is non-toxic to recipients at the dosages and concentrations employed and is compatible with other ingredients of the formulation. In addition, a disclosed therapeutic agent can be suspended in an aqueous carrier, for example, in an isotonic buffer solution at a pH of about 3.0 to about 8.0, preferably at a pH of about 3.5 to about 7.4, 3.5 to 6.0, or 3.5 to about 5.0. Useful buffers include sodium citrate-citric acid and sodium phosphate-phosphoric acid, and sodium acetate/acetic acid buffers. The active ingredient, optionally together with excipients, can also be in the form of a lyophilisate and can be made into a solution prior to parenteral administration by the addition of suitable solvents. Solutions such as those that are used, for example, for parenteral administration can also be used as infusion solutions.

A form of repository or "depot" slow release preparation can be used so that therapeutically effective amounts of the preparation are delivered into the bloodstream over many hours or days following transdermal injection or delivery. Such long acting formulations can be administered by implantation (for example subcutaneously or intramuscularly) or by intramuscular injection. The compounds can be formulated with suitable polymeric or hydrophobic materials (for example as an emulsion in an acceptable oil) or ion exchange resins, or as sparingly soluble derivatives, for example, as a sparingly soluble salt.

Immunogenic compositions that include a disclosed therapeutic agent can be delivered by way of a pump (see Langer, supra; Sefton, *CRC Crit. Ref. Biomed. Eng.* 14:201, 1987; Buchwald et al., *Surgery* 88:507, 1980; Saudek et al., *N. Engl. J. Med.* 321:574, 1989) or by continuous subcutaneous infusions, for example, using a mini-pump. An intravenous bag solution can also be employed. One factor in selecting an appropriate dose is the result obtained, as measured by the methods disclosed here, as are deemed appropriate by the practitioner. Other controlled release systems are discussed in Langer (*Science* 249:1527-33, 1990).

In one example, a pump is implanted (for example see U.S. Pat. Nos. 6,436,091; 5,939,380; and 5,993,414). Implantable drug infusion devices are used to provide patients with a constant and long-term dosage or infusion of a therapeutic agent. Such device can be categorized as either active or passive.

Active drug or programmable infusion devices feature a pump or a metering system to deliver the agent into the patient's system. An example of such an active infusion device currently available is the Medtronic SYNCHROMED™ programmable pump. Passive infusion devices, in contrast, do not feature a pump, but rather rely upon a pressurized drug reservoir to deliver the agent of interest. An example of such a device includes the Medtronic ISOMED™.

In particular examples, immunogenic compositions including a disclosed therapeutic agent are administered by sustained-release systems. Suitable examples of sustained-release systems include suitable polymeric materials (such as, semi-permeable polymer matrices in the form of shaped articles, for example films, or microcapsules), suitable hydrophobic materials (for example as an emulsion in an acceptable oil) or ion exchange resins, and sparingly soluble derivatives (such as, for example, a sparingly soluble salt). Sustained-release compositions can be administered orally, parenterally, intracistemally, intraperitoneally, topically (as by powders, ointments, gels, drops or transdermal patch), or as an oral or nasal spray. Sustained-release matrices include polylactides (U.S. Pat. No. 3,773,919, EP 58,481), copolymers of L-glutamic acid and gamma-ethyl-L-glutamate (Sidman et

al., *Biopolymers* 22:547-556, 1983, poly(2-hydroxyethyl methacrylate)); (Langer et al., *J. Biomed. Mater. Res.* 15:167-277, 1981; Langer, *Chem. Tech.* 12:98-105, 1982, ethylene vinyl acetate (Langer et al., Id.) or poly-D-(−)-3-hydroxybutyric acid (EP 133,988).

Polymers can be used for ion-controlled release. Various degradable and nondegradable polymeric matrices for use in controlled drug delivery are known in the art (Langer, *Accounts Chem. Res.* 26:537, 1993). For example, the block copolymer, polaxamer 407 exists as a viscous yet mobile liquid at low temperatures but forms a semisolid gel at body temperature. It has shown to be an effective vehicle for formulation and sustained delivery of recombinant interleukin-2 and urease (Johnston et al., *Pharm. Res.* 9:425, 1992; and Pec, *J. Parent. Sci. Tech.* 44(2):58, 1990). Alternatively, hydroxyapatite has been used as a microcarrier for controlled release of proteins (Ijntema et al., *Int. J. Pharm.* 112:215, 1994). In yet another aspect, liposomes are used for controlled release as well as drug targeting of the lipid-capsulated drug (Betageri et al., *Liposome Drug Delivery Systems*, Technomic Publishing Co., Inc., Lancaster, Pa., 1993). Numerous additional systems for controlled delivery of therapeutic proteins are known (for example, U.S. Pat. Nos. 5,055,303; 5,188,837; 4,235,871; 4,501,728; 4,837,028; 4,957,735; 5,019,369; 5,055,303; 5,514,670; 5,413,797; 5,268,164; 5,004,697; 4,902,505; 5,506,206; 5,271,961; 5,254,342; and 5,534,496).

Immunogenic compositions can be administered for therapeutic treatments. In therapeutic applications, a therapeutically effective amount of the immunogenic composition is administered to a subject suffering from a disease, such as HIV-1 infection or AIDS. The immunogenic composition can be administered by any means known to one of skill in the art (see Banga, A., "Parenteral Controlled Delivery of Therapeutic Peptides and Proteins," in *Therapeutic Peptides and Proteins*, Technomic Publishing Co., Inc., Lancaster, Pa., 1995) such as by intramuscular, subcutaneous, or intravenous injection, but even oral, nasal, or anal administration is contemplated. To extend the time during which the peptide or protein is available to stimulate a response, the peptide or protein can be provided as an implant, an oily injection, or as a particulate system. The particulate system can be a microparticle, a microcapsule, a microsphere, a nanocapsule, or similar particle (see, for example, Banga, supra). A particulate carrier based on a synthetic polymer has been shown to act as an adjuvant to enhance the immune response, in addition to providing a controlled release. Aluminum salts can also be used as adjuvants to produce an immune response.

Immunogenic compositions can be formulated in unit dosage form, suitable for individual administration of precise dosages. In pulse doses, a bolus administration of an immunogenic composition that includes a disclosed immunogen is provided, followed by a time-period wherein no disclosed immunogen is administered to the subject, followed by a second bolus administration. A therapeutically effective amount of an immunogenic composition can be administered in a single dose, or in multiple doses, for example daily, during a course of treatment. In specific, non-limiting examples, pulse doses of an immunogenic composition that include a disclosed immunogen are administered during the course of a day, during the course of a week, or during the course of a month.

Immunogenic compositions can be administered whenever the effect (such as decreased signs, symptom, or laboratory results of HIV-1 infection) is desired. Generally, the dose is sufficient to treat or ameliorate symptoms or signs of disease without producing unacceptable toxicity to the subject. Systemic or local administration can be utilized.

Amounts effective for therapeutic use can depend on the severity of the disease and the age, weight, general state of the patient, and other clinical factors. Thus, the final determination of the appropriate treatment regimen will be made by the attending clinician. Typically, dosages used in vitro can provide useful guidance in the amounts useful for in situ administration of the pharmaceutical composition, and animal models may be used to determine effective dosages for treatment of particular disorders. Various considerations are described, for example in Gilman et al., eds., Goodman and Gilman: The Pharmacological Bases of Therapeutics, 8th ed., Pergamon Press, 1990; and Remington's Pharmaceutical Sciences, 17th ed., Mack Publishing Co., Easton, Pa., 1990. Typically, the dose range for a gp120 polypeptide is from about 0.1 μg/kg body weight to about 100 mg/kg body weight. Other suitable ranges include doses of from about 1 μg/kg to 10 mg/kg body weight. In one example, the dose is about 1.0 μg to about 50 mg, for example, 1 μg to 1 mg, such as 1 mg peptide per subject. The dosing schedule can vary from daily to as seldom as once a year, depending on clinical factors, such as the subject's sensitivity to the peptide and tempo of their disease. Therefore, a subject can receive a first dose of a disclosed therapeutic molecule, and then receive a second dose (or even more doses) at some later time(s), such as at least one day later, such as at least one week later.

The pharmaceutical compositions disclosed herein can be prepared and administered in dose units. Solid dose units include tablets, capsules, transdermal delivery systems, and suppositories. The administration of a therapeutic amount can be carried out both by single administration in the form of an individual dose unit or else several smaller dose units and also by multiple administrations of subdivided doses at specific intervals. Suitable single or divided doses include, but are not limited to about 0.01, 0.1, 0.5, 1, 3, 5, 10, 15, 30, or 50 μg protein/kg/day

The nucleic acid constructs encoding antigenic gp120 polypeptides described herein are used, for example, in combination, as pharmaceutical compositions (medicaments) for use in therapeutic, for example, prophylactic regimens (such as vaccines) and administered to subjects (for example, primate subjects such as human subjects) to elicit an immune response against one or more clade or strain of HIV. For example, the compositions described herein can be administered to a human (or non-human) subject prior to infection with HIV to inhibit infection by or replication of the virus. Thus, the pharmaceutical compositions described above can be administered to a subject to elicit a protective immune response against HIV. To elicit an immune response, a therapeutically effective (for example, immunologically effective) amount of the nucleic acid constructs are administered to a subject, such as a human (or non-human) subject.

Immunization by nucleic acid constructs is well known in the art and taught, for example, in U.S. Pat. No. 5,643,578 (which describes methods of immunizing vertebrates by introducing DNA encoding a desired antigen to elicit a cell-mediated or a humoral response), and U.S. Pat. Nos. 5,593,972 and 5,817,637 (which describe operably linking a nucleic acid sequence encoding an antigen to regulatory sequences enabling expression). U.S. Pat. No. 5,880,103 describes several methods of delivery of nucleic acids encoding immunogenic peptides or other antigens to an organism. The methods include liposomal delivery of the nucleic acids (or of the synthetic peptides themselves), and immune-stimulating constructs, or ISCOMS™, negatively charged cage-like structures of 30-40 nm in size formed spontaneously on mixing cholesterol and QUIL A™ (saponin).

For administration of gp120 nucleic acid molecules, the nucleic acid can be delivered intracellularly, for example by expression from an appropriate nucleic acid expression vector which is administered so that it becomes intracellular, such as by use of a retroviral vector (see U.S. Pat. No. 4,980,286), or by direct injection, or by use of microparticle bombardment (such as a gene gun; Biolistic, Dupont), or coating with lipids or cell-surface receptors or transfecting agents, or by administering it in linkage to a homeobox-like peptide which is known to enter the nucleus (for example Joliot et al., *Proc. Natl. Acad. Sci. USA* 1991, 88:1864-8). The present disclosure includes all forms of nucleic acid delivery, including synthetic oligos, naked DNA, plasmid and viral, integrated into the genome or not.

In another approach to using nucleic acids for immunization, an immunogenic gp120 polypeptide can also be expressed by attenuated viral hosts or vectors or bacterial vectors. Recombinant vaccinia virus, adeno-associated virus (AAV), herpes virus, retrovirus, or other viral vectors can be used to express the peptide or protein, thereby eliciting a CTL response. For example, vaccinia vectors and methods useful in immunization protocols are described in U.S. Pat. No. 4,722,848. BCG (Bacillus Calmette Guerin) provides another vector for expression of the peptides (see Stover, *Nature* 351:456-460, 1991).

In one example, a viral vector is utilized. These vectors include, but are not limited to, adenovirus, herpes virus, vaccinia, or an RNA virus such as a retrovirus. In one example, the retroviral vector is a derivative of a murine or avian retrovirus. Examples of retroviral vectors in which a single foreign gene can be inserted include, but are not limited to: Moloney murine leukemia virus (MoMuLV), Harvey murine sarcoma virus (HaMuSV), murine mammary tumor virus (MuMTV), and Rous Sarcoma Virus (RSV). When the subject is a human, a vector such as the gibbon ape leukemia virus (GaLV) can be utilized. A number of additional retroviral vectors can incorporate multiple genes. All of these vectors can transfer or incorporate a gene for a selectable marker so that transduced cells can be identified and generated. By inserting a nucleic acid sequence encoding a gp120 polypeptide into the viral vector, along with another gene that encodes the ligand for a receptor on a specific target cell, for example, the vector is now target specific. Retroviral vectors can be made target specific by attaching, for example, a sugar, a glycolipid, or a protein. Preferred targeting is accomplished by using an antibody to target the retroviral vector. Those of skill in the art will know of, or can readily ascertain without undue experimentation, specific polynucleotide sequences which can be inserted into the retroviral genome or attached to a viral envelope to allow target specific delivery of the retroviral vector containing the polynucleotide encoding a gp120 polypeptide.

Since recombinant retroviruses are defective, they need assistance in order to produce infectious vector particles. This assistance can be provided, for example, by using helper cell lines that contain plasmids encoding all of the structural genes of the retrovirus under the control of regulatory sequences within the LTR. These plasmids are missing a nucleotide sequence that enables the packaging mechanism to recognize an RNA transcript for encapsidation. Helper cell lines that have deletions of the packaging signal include, but are not limited to Q2, PA317, and PA12, for example. These cell lines produce empty virions, since no genome is packaged. If a retroviral vector is introduced into such cells in which the packaging signal is intact, but the structural genes are replaced by other genes of interest, the vector can be packaged and vector virion produced.

Suitable formulations for the nucleic acid constructs, include aqueous and non-aqueous solutions, isotonic sterile solutions, which can contain anti-oxidants, buffers, and bacteriostats, and aqueous and non-aqueous sterile suspensions that can include suspending agents, solubilizers, thickening agents, stabilizers, and preservatives. The formulations can be presented in unit-dose or multi-dose sealed containers, such as ampules and vials, and can be stored in a freeze-dried (lyophilized) condition requiring only the addition of the sterile liquid carrier, for example, water, immediately prior to use. Extemporaneous solutions and suspensions can be prepared from sterile powders, granules, and tablets. Preferably, the carrier is a buffered saline solution. More preferably, the composition for use in the inventive method is formulated to protect the nucleic acid constructs from damage prior to administration. For example, the composition can be formulated to reduce loss of the adenoviral vectors on devices used to prepare, store, or administer the expression vector, such as glassware, syringes, or needles. The compositions can be formulated to decrease the light sensitivity and/or temperature sensitivity of the components. To this end, the composition preferably comprises a pharmaceutically acceptable liquid carrier, such as, for example, those described above, and a stabilizing agent selected from the group consisting of polysorbate 80, L-arginine, polyvinylpyrrolidone, trehalose, and combinations thereof.

In therapeutic applications, a therapeutically effective amount of the composition is administered to a subject prior to or following exposure to or infection by HIV. When administered prior to exposure, the therapeutic application can be referred to as a prophylactic administration (such as in the form of a vaccine). Single or multiple administrations of the compositions are administered depending on the dosage and frequency as required and tolerated by the subject. In one embodiment, the dosage is administered once as a bolus, but in another embodiment can be applied periodically until a therapeutic result, such as a protective immune response, is achieved. Generally, the dose is sufficient to treat or ameliorate symptoms or signs of disease without producing unacceptable toxicity to the subject. Systemic or local administration can be utilized.

In the context of nucleic acid vaccines, naturally occurring or synthetic immunostimulatory compositions that bind to and stimulate receptors involved in innate immunity can be administered along with nucleic acid constructs encoding the gp120 polypeptides. For example, agents that stimulate certain Toll-like receptors (such as TLR7, TLR8 and TLR9) can be administered in combination with the nucleic acid constructs encoding gp120 polypeptides. In some embodiments, the nucleic acid construct is administered in combination with immunostimulatory CpG oligonucleotides.

Nucleic acid constructs encoding gp120 polypeptides can be introduced in vivo as naked DNA plasmids. DNA vectors can be introduced into the desired host cells by methods known in the art, including but not limited to transfection, electroporation (for example, transcutaneous electroporation), microinjection, transduction, cell fusion, DEAE dextran, calcium phosphate precipitation, use of a gene gun, or use of a DNA vector transporter (See for example, Wu et al. *J. Biol. Chem.,* 267:963-967, 1992; Wu and Wu *J. Biol. Chem.,* 263:14621-14624, 1988; and Williams et al. *Proc. Natl. Acad. Sci. USA* 88:2726-2730, 1991). As described in detail in the Examples, a needleless delivery device, such as a BIOJECTOR® needleless injection device can be utilized to introduce the therapeutic nucleic acid constructs in vivo. Receptor-mediated DNA delivery approaches can also be used (Curiel et al. *Hum. Gene Ther.,* 3:147-154, 1992; and Wu and

Wu, J. *Biol. Chem.,* 262:4429-4432, 1987). Methods for formulating and administering naked DNA to mammalian muscle tissue are disclosed in U.S. Pat. Nos. 5,580,859 and 5,589,466, both of which are herein incorporated by reference. Other molecules are also useful for facilitating transfection of a nucleic acid in vivo, such as a cationic oligopeptide (for example, WO95/21931), peptides derived from DNA binding proteins (for example, WO96/25508), or a cationic polymer (for example, WO95/21931).

Another well-known method that can be used to introduce nucleic acid constructs encoding gp120 immunogens into host cells is particle bombardment (also known as biolistic transformation). Biolistic transformation is commonly accomplished in one of several ways. One common method involves propelling inert or biologically active particles at cells. This technique is disclosed in, for example, U.S. Pat. Nos. 4,945,050, 5,036,006; and 5,100,792, all to Sanford et al., which are hereby incorporated by reference. Generally, this procedure involves propelling inert or biologically active particles at the cells under conditions effective to penetrate the outer surface of the cell and to be incorporated within the interior thereof. When inert particles are utilized, the plasmid can be introduced into the cell by coating the particles with the plasmid containing the exogenous DNA. Alternatively, the target cell can be surrounded by the plasmid so that the plasmid is carried into the cell by the wake of the particle.

Alternatively, the vector can be introduced in vivo by lipofection. For the past decade, there has been increasing use of liposomes for encapsulation and transfection of nucleic acids in vitro. Synthetic cationic lipids designed to limit the difficulties and dangers encountered with liposome mediated transfection can be used to prepare liposomes for in vivo transfection of a gene encoding a marker (Felgner et. al. *Proc. Natl. Acad. Sci. USA* 84:7413-7417, 1987; Mackey, et al. *Proc. Natl. Acad. Sci. USA* 85:8027-8031, 1988; Ulmer et al. *Science* 259:1745-1748, 1993). The use of cationic lipids can promote encapsulation of negatively charged nucleic acids, and also promote fusion with negatively charged cell membranes (Felgner and Ringoid *Science* 337:387-388, 1989). Particularly useful lipid compounds and compositions for transfer of nucleic acids are described in WO95/18863 and WO96/17823, and in U.S. Pat. No. 5,459,127, herein incorporated by reference.

As with the immunogenic polypeptide, the nucleic acid compositions may be administered in a single dose, or multiple doses separated by a time interval can be administered to elicit an immune response against HIV. For example, two doses, or three doses, or four doses, or five doses, or six doses or more can be administered to a subject over a period of several weeks, several months or even several years, to optimize the immune response.

It may be advantageous to administer the immunogenic compositions disclosed herein with other agents such as proteins, peptides, antibodies, and other anti-HIV agents. Examples of such anti-HIV therapeutic agents include nucleoside reverse transcriptase inhibitors, such as abacavir, AZT, didanosine, emtricitabine, lamivudine, stavudine, tenofovir, zalcitabine, zidovudine, and the like, non-nucleoside reverse transcriptase inhibitors, such as delavirdine, efavirenz, nevirapine, protease inhibitors such as amprenavir, atazanavir, indinavir, lopinavir, nelfinavir osamprenavir, ritonavir, saquinavir, tipranavir, and the like, and fusion protein inhibitors such as enfuvirtide and the like. In certain embodiments, immunonogenic compositions are administered concurrently with other anti-HIV therapeutic agents. In certain embodiments, the immunonogenic compositions are administered sequentially with other anti-HIV therapeutic agents, such as before or after the other agent. One of ordinary skill in the art would know that sequential administration can mean immediately following or after an appropriate period of time, such as hours days, weeks, months, or even years later.

While not being bound by theory, it is believed that CD4 binding to gp120 triggers the exposure of the immunodominant V3 loop. Thus, co-administration of soluble forms of CD4, such as the fragments described herein, or an antibody that binds to the CD4 binding site, can lead to enhanced elicitation of an immunogenic response to gp120.

In certain embodiments, immunonogenic compositions disclosed herein are administered with a soluble portion of CD4, for example a sufficient portion of the CD4 to bind to the CD4 binding site on gp120. Such soluble fragments typically include both the D1 and D2 extracellular domains of CD4 (D1D2) or sCD4 (which is comprised of D1 D2 D3 and D4 domains of CD4), although smaller fragments may also provide specific and functional CD4-like binding. In certain embodiments, the gp120 polypeptide with an extended V3 loop or a nucleic acid encoding the same is administered concurrently with a soluble portion of CD4. In other embodiments, the gp120 polypeptide with an extended V3 loop or a nucleic acid encoding the same is administered concurrently with an antibody that binds to the CD4 binding site on gp120.

The immunogenic gp120 polypeptides and nucleic acid encoding these polypeptides (such as stabilized gp120 polypeptides, gp120 polypeptides with an extended V3 loop) can be used in a novel multistep immunization regime. Typically, this regime includes administering to a subject a therapeutically effective amount of a gp120 polypeptide as disclosed herein (the prime) and boosting the immunogenic response with stabilized gp140 trimer (Yang et al. *J Virol.* 76(9):4634-42, 2002) after an appropriate period of time. The method of eliciting such an immune reaction is what is known as "prime-boost." In this method, a gp120 polypeptide is initially administered to a subject and at periodic times thereafter stabilized gp140 trimer boosts are administered. Examples of stabilized gp140 or gp120 trimers can be found for example in U.S. Pat. No. 6,911,205 which is incorporated herein in its entirely.

The prime can be administered as a single dose or multiple doses, for example two doses, three doses, four doses, five doses, six doses or more can be administered to a subject over day week or months. The boost can be administered as a single dose or multiple doses, for example two to six doses, or more can be administered to a subject over a day, a week or months. Multiple boosts can also be given, such one to five, or more.

The boosts can be an identical molecule or a somewhat different, but related, molecule. For example, one preferred strategy with the gp120 polypeptides of the present disclosure would be to prime using a stabilized gp120 polypeptide or a gp120 polypeptide with an extended V3 and boosting periodically with stabilized trimers where the gp120 units are designed to come closer and closer to the wild type gp120 over the succession of boosts. For example, the first prime could be a stabilized gp120 polypeptide, with a boost by a stabilized trimer form with the same stabilized gp120 or a trimer with less deletions or changes from the native gp120 conformation, with subsequent boosts using trimers that had still less deletions or changes from the native gp120 conformation until the boosts were finally being given by trimers with a gp120 portion based on the native wild type HIV gp120.

One can also use cocktails containing a variety of different HIV strains to prime and boost with trimers from a variety of different HIV strains or with trimers that are a mixture of

multiple HIV strains For example, the first prime could be with a gp120 polypeptide from one primary HIV isolate, with subsequent boosts using trimers from different primary isolates.

In certain embodiments, the prime is a nucleic acid construct comprising a nucleic acid sequence encoding a gp120 immunogen as disclosed herein, for example an nucleotide sequence encoding the amino acid sequence set forth as SEQ ID NO: 1 or SEQ ID NO: 2, or the nucleotide sequence as set forth as one of SEQ ID NO: 4-18 or a degenerate variant thereof. In certain embodiments the boost comprises a nucleic acid sequence encoding a stabilized gp140 trimer.

V. Crystal Structures

The stabilized gp120 polypeptides and the gp120 polypeptides with an extended V3 loop disclosed herein can be used to produce detailed models of gp120 polypeptide atomic structure. Exemplary coordinate data is given in Table 1 and Table 2. The atomic coordinate data is disclosed herein, or the coordinate data derived from homologous proteins may be used to build a three-dimensional model of a gp120 polypeptide or a portion thereof, for example by providing a sufficient number of atoms of the stabilized form of gp120 or the gp120 with the V3 loop in the extended conformation as defined by the coordinates of Table 1 or Table 2 which represent a surface or three-dimensional region of interest, such as an antigenic surface or ligand binding site. Thus, there can be provided the coordinates of at least about 5, such at least about 10, at least about 20, at least about 30, at least at least about 40, at least about 50, at least about 60, at least about 70, at least about 80, at least about 90, at least about 100, at least about 150, at least about 200, at least about 250, at least about 300, at least about 350, at least about 400, at least about 450, at least about 500 or more atoms of the structure, such as defined by the coordinates of Table 1 or Table 2. Thus, a sub-domain, region, or fragment of interest of the stabilized form of gp120 or the gp120 with the extended V3 loop which is in the vicinity of the antigenic surface, can be provided for identifying or rationally designing a compound or drug, such as an immunogen. A "sub-domain," "region," or "fragment" can mean at least one, for example, one, two, three, four, or more, element(s) of secondary structure of particular regions of the stabilized form of gp120 or the gp120 with the extended V3 loop gp120 with the extended V3 loop, and includes those set forth in Table 1 and Table 2.

Any available computational methods may be used to build the three dimensional model. As a starting point, the X-ray diffraction pattern obtained from the assemblage of the molecules or atoms in a crystalline version of a gp120 polypeptide can be used to build an electron density map using tools well known to those skilled in the art of crystallography and X-ray diffraction techniques. Additional phase information extracted either from the diffraction data and available in the published literature and/or from supplementing experiments may then used to complete the reconstruction.

For an overview of the procedures of collecting, analyzing, and utilizing X-ray diffraction data for the construction of electron densities see, for example, Campbell et al., *Biological Spectroscopy*, The Benjamin/Cummings Publishing Co., Inc., Menlo Park, Calif., 1984; Cantor et al., Biophysical Chemistry, Part II: Techniques for the study of biological structure and function, W.H. Freeman and Co., San Francisco, Calif. 1980; A. T. Brunger, X-plor Version 3.1: A system for X-ray crystallography and NMR, Yale Univ. Pr., New Haven, Conn. 1993; M. M. Woolfson, An Introduction to X-ray Crystallography, Cambridge Univ. Pr., Cambridge, UK, 1997; J. Drenth, Principles of Protein X-ray Crystallography (Springer Advanced Texts in Chemistry), Springer Verlag; Berlin, 1999; Tsirelson et al, Electron Density and Bonding in Crystals: Principles, Theory and X-ray Diffraction Experiments in Solid State Physics and Chemistry, Inst. of Physics Pub., 1996; each of which is herein specifically incorporated by reference in their entirety.

Information on molecular modeling can be found for example in, M. Schlecht, Molecular Modeling on the PC, 1998, John Wiley & Sons; Gans et al., Fundamental Principals of Molecular Modeling, Plenum Pub. Corp., 1996; N.C. Cohen (editor), Guidebook on Molecular Modeling in Drug Design, Academic Press, 1996; and W. B. Smith, Introduction to Theoretical Organic Chemistry and Molecular Modeling, 1996.

Typically, a well-ordered crystal that will diffract x-rays strongly is used to solve the three-dimensional structure of a protein by x-ray crystallography. The crystallographic method directs a beam of x-rays onto a regular, repeating array of many identical molecules. The x-rays are diffracted from it in a pattern from which the atomic positions of the atom that make up the molecule of interest can be determined.

Substantially pure and homogeneous protein samples are usually used for crystallization. Typically, crystals form when molecules are precipitated very slowly from supersaturated solutions. A typical procedure for making protein crystals is the hanging-drop method, in which a drop of protein solution is brought very gradually to supersaturation by loss of water from the droplet to the larger reservoir that contains salt, polyethylene glycol, or other solution that functions as a hydroattractant, although any other method that generates diffraction quality crystals can be used. In some examples diffraction quality crystals are obtained by seeding the supersaturated solution with smaller crystals that serve as templates.

Powerful x-ray beams can be produced from synchrotron storage rings where electrons (or positrons) travel close to the speed of light. These particles emit very strong radiation at all wavelengths from short gamma rays to visible light. When used as an x-ray source, only radiation within a window of suitable wavelengths is channeled from the storage ring.

In diffraction experiments a narrow and parallel beam of x-rays is taken out from the x-ray source and directed onto the crystal to produce diffracted beams. The incident x-ray beam causes damage to both protein and solvent molecules. The crystal is, therefore, usually cooled to prolong its lifetime (for example to −220° to −50° C.). In some examples, single crystals are used to obtain a data set, while in other examples, multiple crystals are used to obtain a data set. The x-ray beam must strike the crystal from many different directions to produce all possible diffraction spots, thereby creating a complete data set. Therefore, the crystal is rotated relative to the beam during data collection. The diffracted spots are recorded either on a film, or by an electronic detector, both of which are commercially available.

When the primary beam from an x-ray source strikes the crystal, x-rays interact with the electrons on each atom in the crystal and cause them to oscillate. The oscillating electrons serve as a new source of x-rays, which are emitted in almost all directions in a process referred to as scattering. When atoms (and hence their electrons) are arranged in a regular three-dimensional array, as in a crystal, the x-rays emitted from the oscillating electrons interfere with one another. In most cases, these x-rays, colliding from different directions, cancel each other out; those from certain directions, however, will add together to produce diffracted beams of radiation that can be recorded as a pattern on a photographic plate or detector.

The diffraction pattern obtained in an x-ray experiment is related to the crystal that caused the diffraction. X-rays that are reflected from adjacent planes travel different distances, and diffraction only occurs when the difference in distance is equal to the wavelength of the x-ray beam. This distance is dependent on the reflection angle, which is equal to the angle between the primary beam and the planes.

Each atom in a crystal scatters x-rays in all directions, and only those that positively interfere with one another, according to Bragg's law ($2d \sin \theta = \lambda$), give rise to diffracted beams that can be recorded as a distinct diffraction spot above background. Each diffraction spot is the result of interference of all x-rays with the same diffraction angle emerging from all atoms. To extract information about individual atoms from such a system requires considerable computation. The mathematical tool that is used to handle such problems is called the Fourier transform.

Each diffracted beam, which is recorded as a spot on the film, is defined by three properties: the amplitude, which is measured as the intensity of the spot; the wavelength, which is determined by the x-ray source; and the phase information, which is lost in x-ray experiments and must be calculated. All three properties are used for all of the diffracted beams, in order to determine the position of the atoms giving rise to the diffracted beams. Methods of determining the phases are well known in the art.

For example, phase differences between diffracted spots can be determined from intensity changes following heavy atom derivatization. Another example would be determining the phases by molecular replacement.

The amplitudes and the phases of the diffraction data from the protein crystals are used to calculate an electron-density map of the repeating unit of the crystal. A model of the particular amino acid sequence is built to approximate the electron density map.

The initial model will contain some errors. Provided the protein crystals diffract to high enough resolution (e.g., better than 3.5 Å), most or substantially all of the errors can be removed by crystallographic refinement of the model using computer algorithms. In this process, the model is changed to minimize the difference between the experimentally observed diffraction amplitudes and those calculated for a hypothetical crystal containing the model. This difference is expressed as an R factor (residual disagreement) which is 0.0 for exact agreement and about 0.59 for total disagreement.

Typically, the R factor of a refined model is preferably between 0.15 and 0.35 (such as less than about 0.24-0.28) for a well-determined protein structure. The residual difference is a consequence of errors and imperfections in the data. These derive from various sources, including slight variations in the conformation of the protein molecules, as well as inaccurate corrections both for the presence of solvent and for differences in the orientation of the microcrystals from which the crystal is built. Thus, the final model represents an average of molecules that are slightly different in both conformation and orientation.

In refined structures at high resolution, there are usually no major errors in the orientation of individual residues, and the estimated errors in atomic positions are usually around 0.1-0.2 Å, provided the amino acid sequence is known.

Most x-ray structures are determined to a resolution between 1.7 Å. and 3.5 Å. Electron-density maps with this resolution range are preferably interpreted by fitting the known amino acid sequences into regions of electron density in which individual atoms are not resolved.

VI. Crystals Structure of Stabilized gp120

The present disclosure also relates to the crystals obtained from stabilized forms of gp120, the crystal structures of the stabilized forms of gp120, the three-dimensional coordinates of the stabilized forms of gp120 polypeptide and three-dimensional structures of models of stabilized forms of gp120. Table 1 provides the atomic coordinates of the crystal structure of the polypeptide encoded by SEQ ID NO: 14.

TABLE 1

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	1	CB	GLU	83	18.617	−44.257	86.334	1.00	108.57
ATOM	2	CG	GLU	83	17.192	−44.735	86.515	1.00	108.41
ATOM	3	CD	GLU	83	16.205	−43.880	85.755	1.00	108.12
ATOM	4	OE1	GLU	83	16.358	−43.762	84.524	1.00	108.57
ATOM	5	OE2	GLU	83	15.280	−43.327	86.385	1.00	107.50
ATOM	6	C	GLU	83	19.772	−46.457	86.717	1.00	109.62
ATOM	7	O	GLU	83	18.985	−47.321	87.117	1.00	110.00
ATOM	8	N	GLU	83	20.954	−44.298	87.129	1.00	108.79
ATOM	9	CA	GLU	83	19.642	−45.003	87.189	1.00	109.16
ATOM	10	N	VAL	84	20.768	−46.714	85.869	1.00	109.52
ATOM	11	CA	VAL	84	21.044	−48.053	85.341	1.00	109.11
ATOM	12	CB	VAL	84	20.172	−48.376	84.093	1.00	108.87
ATOM	13	CG1	VAL	84	18.713	−48.542	84.498	1.00	108.27
ATOM	14	CG2	VAL	84	20.302	−47.271	83.061	1.00	109.39
ATOM	15	C	VAL	84	22.526	−48.185	84.964	1.00	108.77
ATOM	16	O	VAL	84	22.925	−47.846	83.851	1.00	108.35
ATOM	17	N	VAL	85	23.332	−48.684	85.900	1.00	108.71
ATOM	18	CA	VAL	85	24.774	−48.848	85.689	1.00	108.45
ATOM	19	CB	VAL	85	25.515	−49.032	87.038	1.00	108.05
ATOM	20	CG1	VAL	85	25.521	−47.724	87.807	1.00	108.41
ATOM	21	CG2	VAL	85	24.837	−50.110	87.862	1.00	107.81
ATOM	22	C	VAL	85	25.175	−49.994	84.754	1.00	108.29
ATOM	23	O	VAL	85	24.757	−51.138	84.941	1.00	108.64
ATOM	24	N	LEU	86	25.997	−49.670	83.755	1.00	107.51
ATOM	25	CA	LEU	86	26.483	−50.644	82.774	1.00	106.03
ATOM	26	CB	LEU	86	26.839	−49.943	81.458	1.00	104.36
ATOM	27	CG	LEU	86	25.737	−49.391	80.552	1.00	103.07
ATOM	28	CD1	LEU	86	24.750	−48.544	81.333	1.00	102.61
ATOM	29	CD2	LEU	86	26.390	−48.575	79.450	1.00	101.71
ATOM	30	C	LEU	86	27.720	−51.369	83.298	1.00	105.81
ATOM	31	O	LEU	86	28.354	−50.916	84.254	1.00	105.88

TABLE 1-continued

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	32	N	VAL	87	28.065	−52.490	82.668	1.00	105.43
ATOM	33	CA	VAL	87	29.231	−53.263	83.083	1.00	104.73
ATOM	34	CB	VAL	87	28.827	−54.553	83.805	1.00	104.68
ATOM	35	CG1	VAL	87	28.000	−54.214	85.032	1.00	104.54
ATOM	36	CG2	VAL	87	28.057	−55.462	82.857	1.00	105.03
ATOM	37	C	VAL	87	30.119	−53.643	81.910	1.00	104.29
ATOM	38	O	VAL	87	29.635	−53.933	80.813	1.00	103.86
ATOM	39	N	ASN	88	31.425	−53.652	82.166	1.00	104.01
ATOM	40	CA	ASN	88	32.428	−53.982	81.155	1.00	103.78
ATOM	41	CB	ASN	88	32.360	−55.474	80.781	1.00	104.65
ATOM	42	CG	ASN	88	32.859	−56.393	81.902	1.00	105.20
ATOM	43	OD1	ASN	88	33.953	−56.199	82.445	1.00	104.86
ATOM	44	ND2	ASN	88	32.056	−57.399	82.235	1.00	104.99
ATOM	45	C	ASN	88	32.252	−53.117	79.909	1.00	102.44
ATOM	46	O	ASN	88	32.505	−53.561	78.787	1.00	101.94
ATOM	47	N	VAL	89	31.822	−51.875	80.122	1.00	100.88
ATOM	48	CA	VAL	89	31.614	−50.931	79.032	1.00	98.81
ATOM	49	CB	VAL	89	30.231	−50.258	79.127	1.00	98.28
ATOM	50	CG1	VAL	89	30.035	−49.322	77.953	1.00	97.33
ATOM	51	CG2	VAL	89	29.139	−51.310	79.151	1.00	98.08
ATOM	52	C	VAL	89	32.679	−49.841	79.051	1.00	97.94
ATOM	53	O	VAL	89	33.180	−49.461	80.113	1.00	97.43
ATOM	54	N	THR	90	33.020	−49.348	77.864	1.00	96.73
ATOM	55	CA	THR	90	34.020	−48.295	77.724	1.00	95.18
ATOM	56	CB	THR	90	35.403	−48.891	77.319	1.00	95.36
ATOM	57	OG1	THR	90	36.380	−47.845	77.263	1.00	95.05
ATOM	58	CG2	THR	90	35.324	−49.591	75.962	1.00	95.57
ATOM	59	C	THR	90	33.551	−47.260	76.686	1.00	93.85
ATOM	60	O	THR	90	33.505	−47.539	75.481	1.00	93.47
ATOM	61	N	GLU	91	33.196	−46.069	77.177	1.00	91.35
ATOM	62	CA	GLU	91	32.707	−44.963	76.347	1.00	87.86
ATOM	63	CB	GLU	91	31.343	−44.504	76.865	1.00	88.15
ATOM	64	CG	GLU	91	30.189	−44.701	75.899	1.00	89.11
ATOM	65	CD	GLU	91	30.231	−43.732	74.737	1.00	90.17
ATOM	66	OE1	GLU	91	29.248	−43.679	73.968	1.00	90.39
ATOM	67	OE2	GLU	91	31.249	−43.023	74.591	1.00	90.88
ATOM	68	C	GLU	91	33.676	−43.781	76.358	1.00	85.11
ATOM	69	O	GLU	91	34.317	−43.509	77.369	1.00	85.37
ATOM	70	N	ASN	92	33.783	−43.076	75.235	1.00	81.78
ATOM	71	CA	ASN	92	34.683	−41.928	75.151	1.00	78.41
ATOM	72	CB	ASN	92	35.342	−41.832	73.778	1.00	79.10
ATOM	73	CG	ASN	92	36.358	−42.903	73.549	1.00	79.88
ATOM	74	OD1	ASN	92	36.973	−43.404	74.492	1.00	80.64
ATOM	75	ND2	ASN	92	36.568	−43.252	72.285	1.00	80.59
ATOM	76	C	ASN	92	34.001	−40.602	75.405	1.00	75.77
ATOM	77	O	ASN	92	33.114	−40.198	74.650	1.00	75.80
ATOM	78	N	PHE	93	34.426	−39.915	76.455	1.00	71.82
ATOM	79	CA	PHE	93	33.870	−38.608	76.751	1.00	68.48
ATOM	80	CB	PHE	93	33.622	−38.429	78.244	1.00	67.44
ATOM	81	CG	PHE	93	32.495	−39.245	78.781	1.00	67.39
ATOM	82	CD1	PHE	93	32.554	−40.629	78.775	1.00	68.23
ATOM	83	CD2	PHE	93	31.396	−38.629	79.358	1.00	68.44
ATOM	84	CE1	PHE	93	31.537	−41.393	79.346	1.00	68.02
ATOM	85	CE2	PHE	93	30.373	−39.382	79.931	1.00	69.14
ATOM	86	CZ	PHE	93	30.446	−40.768	79.926	1.00	68.02
ATOM	87	C	PHE	93	34.888	−37.568	76.319	1.00	66.64
ATOM	88	O	PHE	93	36.094	−37.801	76.418	1.00	66.70
ATOM	89	N	ASN	94	34.405	−36.436	75.821	1.00	63.67
ATOM	90	CA	ASN	94	35.277	−35.344	75.439	1.00	61.19
ATOM	91	CB	ASN	94	35.618	−35.387	73.950	1.00	61.27
ATOM	92	CG	ASN	94	36.609	−34.300	73.550	1.00	61.92
ATOM	93	OD1	ASN	94	37.602	−34.062	74.241	1.00	61.52
ATOM	94	ND2	ASN	94	36.351	−33.647	72.422	1.00	61.78
ATOM	95	C	ASN	94	34.442	−34.119	75.767	1.00	59.74
ATOM	96	O	ASN	94	33.882	−33.482	74.893	1.00	60.53
ATOM	97	N	TRP	95	34.345	−33.831	77.055	1.00	57.77
ATOM	98	CA	TRP	95	33.579	−32.719	77.567	1.00	55.79
ATOM	99	CB	TRP	95	33.948	−32.471	79.030	1.00	53.78
ATOM	100	CG	TRP	95	35.277	−31.803	79.223	1.00	49.89
ATOM	101	CD2	TRP	95	35.534	−30.615	79.971	1.00	50.17
ATOM	102	CE2	TRP	95	36.913	−30.357	79.903	1.00	49.60
ATOM	103	CE3	TRP	95	34.727	−29.734	80.707	1.00	50.04
ATOM	104	CD1	TRP	95	36.474	−32.211	78.737	1.00	49.33
ATOM	105	NE1	TRP	95	37.468	−31.354	79.134	1.00	49.08
ATOM	106	CZ2	TRP	95	37.513	−29.263	80.533	1.00	49.33
ATOM	107	CZ3	TRP	95	35.316	−28.650	81.335	1.00	49.36
ATOM	108	CH2	TRP	95	36.696	−28.424	81.246	1.00	50.29
ATOM	109	C	TRP	95	33.733	−31.432	76.782	1.00	55.51

TABLE 1-continued

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	110	O	TRP	95	32.832	−30.588	76.793	1.00	55.05
ATOM	111	N	CYS	96	34.876	−31.286	76.114	1.00	55.79
ATOM	112	CA	CYS	96	35.183	−30.109	75.309	1.00	56.39
ATOM	113	C	CYS	96	34.565	−30.210	73.922	1.00	55.35
ATOM	114	O	CYS	96	35.144	−29.765	72.935	1.00	55.34
ATOM	115	CB	CYS	96	36.705	−29.935	75.183	1.00	59.56
ATOM	116	SG	CYS	96	37.516	−29.511	76.772	1.00	65.71
ATOM	117	N	LYS	97	33.370	−30.781	73.863	1.00	54.38
ATOM	118	CA	LYS	97	32.641	−30.968	72.619	1.00	53.06
ATOM	119	CB	LYS	97	33.439	−31.832	71.655	1.00	54.39
ATOM	120	CG	LYS	97	34.407	−31.101	70.750	1.00	57.02
ATOM	121	CD	LYS	97	35.090	−32.103	69.834	1.00	59.38
ATOM	122	CE	LYS	97	36.181	−31.488	68.980	1.00	60.34
ATOM	123	NZ	LYS	97	36.872	−32.554	68.187	1.00	60.06
ATOM	124	C	LYS	97	31.366	−31.691	72.967	1.00	52.61
ATOM	125	O	LYS	97	31.042	−32.698	72.363	1.00	53.46
ATOM	126	N	ASN	98	30.653	−31.195	73.965	1.00	52.56
ATOM	127	CA	ASN	98	29.410	−31.833	74.362	1.00	52.14
ATOM	128	CB	ASN	98	29.300	−31.911	75.889	1.00	50.77
ATOM	129	CG	ASN	98	28.087	−32.706	76.342	1.00	49.63
ATOM	130	OD1	ASN	98	26.961	−32.405	75.957	1.00	48.41
ATOM	131	ND2	ASN	98	28.314	−33.723	77.168	1.00	48.49
ATOM	132	C	ASN	98	28.232	−31.056	73.788	1.00	52.73
ATOM	133	O	ASN	98	28.181	−29.825	73.873	1.00	52.21
ATOM	134	N	ASP	99	27.286	−31.780	73.202	1.00	53.95
ATOM	135	CA	ASP	99	26.107	−31.160	72.601	1.00	55.38
ATOM	136	CB	ASP	99	25.354	−32.184	71.745	1.00	58.50
ATOM	137	CG	ASP	99	25.615	−32.009	70.253	1.00	60.48
ATOM	138	OD1	ASP	99	25.206	−32.892	69.462	1.00	61.59
ATOM	139	OD2	ASP	99	26.222	−30.982	69.877	1.00	61.09
ATOM	140	C	ASP	99	25.142	−30.546	73.608	1.00	54.26
ATOM	141	O	ASP	99	24.342	−29.676	73.260	1.00	54.68
ATOM	142	N	MET	100	25.208	−31.008	74.851	1.00	51.85
ATOM	143	CA	MET	100	24.331	−30.496	75.889	1.00	49.13
ATOM	144	CB	MET	100	24.357	−31.424	77.094	1.00	48.72
ATOM	145	CG	MET	100	24.159	−32.873	76.743	1.00	49.12
ATOM	146	SD	MET	100	24.699	−33.947	78.077	1.00	48.08
ATOM	147	CE	MET	100	23.233	−33.971	79.064	1.00	49.17
ATOM	148	C	MET	100	24.783	−29.110	76.308	1.00	47.86
ATOM	149	O	MET	100	23.969	−28.274	76.678	1.00	48.48
ATOM	150	N	VAL	101	26.085	−28.867	76.253	1.00	46.25
ATOM	151	CA	VAL	101	26.616	−27.569	76.641	1.00	45.39
ATOM	152	CB	VAL	101	28.145	−27.522	76.472	1.00	45.11
ATOM	153	CG1	VAL	101	28.654	−26.126	76.755	1.00	44.71
ATOM	154	CG2	VAL	101	28.801	−28.517	77.401	1.00	43.94
ATOM	155	C	VAL	101	25.994	−26.455	75.800	1.00	45.33
ATOM	156	O	VAL	101	25.579	−25.426	76.318	1.00	45.54
ATOM	157	N	GLU	102	25.918	−26.676	74.498	1.00	45.19
ATOM	158	CA	GLU	102	25.371	−25.685	73.599	1.00	46.23
ATOM	159	CB	GLU	102	25.770	−26.016	72.167	1.00	49.62
ATOM	160	CG	GLU	102	27.168	−26.621	72.070	1.00	55.61
ATOM	161	CD	GLU	102	28.245	−25.679	72.588	1.00	59.03
ATOM	162	OE1	GLU	102	29.297	−26.166	73.077	1.00	59.85
ATOM	163	OE2	GLU	102	28.034	−24.448	72.489	1.00	60.10
ATOM	164	C	GLU	102	23.869	−25.627	73.715	1.00	45.67
ATOM	165	O	GLU	102	23.278	−24.568	73.567	1.00	45.84
ATOM	166	N	GLN	103	23.244	−26.764	73.982	1.00	45.79
ATOM	167	CA	GLN	103	21.795	−26.786	74.101	1.00	47.31
ATOM	168	CB	GLN	103	21.271	−28.220	74.156	1.00	48.93
ATOM	169	CG	GLN	103	19.750	−28.313	74.345	1.00	52.63
ATOM	170	CD	GLN	103	18.929	−27.662	73.216	1.00	53.89
ATOM	171	OE1	GLN	103	17.703	−27.566	73.309	1.00	54.70
ATOM	172	NE2	GLN	103	19.600	−27.222	72.154	1.00	52.85
ATOM	173	C	GLN	103	21.416	−26.066	75.363	1.00	47.02
ATOM	174	O	GLN	103	20.494	−25.260	75.390	1.00	46.84
ATOM	175	N	MET	104	22.146	−26.369	76.418	1.00	48.58
ATOM	176	CA	MET	104	21.902	−25.752	77.703	1.00	49.89
ATOM	177	CB	MET	104	22.985	−26.182	78.694	1.00	52.33
ATOM	178	CG	MET	104	22.741	−25.743	80.137	1.00	56.81
ATOM	179	SD	MET	104	22.286	−27.119	81.216	1.00	60.04
ATOM	180	CE	MET	104	20.594	−27.574	80.517	1.00	58.09
ATOM	181	C	MET	104	21.975	−24.255	77.483	1.00	49.53
ATOM	182	O	MET	104	20.998	−23.535	77.676	1.00	50.52
ATOM	183	N	HIS	105	23.146	−23.808	77.048	1.00	48.30
ATOM	184	CA	HIS	105	23.409	−22.403	76.807	1.00	47.10
ATOM	185	CB	HIS	105	24.712	−22.250	76.031	1.00	46.50
ATOM	186	CG	HIS	105	25.181	−20.836	75.913	1.00	45.38
ATOM	187	CD2	HIS	105	25.468	−20.082	74.828	1.00	44.97

TABLE 1-continued

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	188	ND1	HIS	105	25.431	−20.044	77.010	1.00	45.09
ATOM	189	CE1	HIS	105	25.855	−18.859	76.607	1.00	45.28
ATOM	190	NE2	HIS	105	25.887	−18.858	75.289	1.00	45.84
ATOM	191	C	HIS	105	22.306	−21.664	76.077	1.00	47.03
ATOM	192	O	HIS	105	22.185	−20.458	76.222	1.00	47.98
ATOM	193	N	GLU	106	21.506	−22.362	75.283	1.00	47.46
ATOM	194	CA	GLU	106	20.439	−21.680	74.564	1.00	48.81
ATOM	195	CB	GLU	106	20.203	−22.323	73.203	1.00	51.42
ATOM	196	CG	GLU	106	21.432	−22.305	72.320	1.00	57.65
ATOM	197	CD	GLU	106	21.126	−22.632	70.870	1.00	61.26
ATOM	198	OE1	GLU	106	20.441	−23.656	70.619	1.00	63.05
ATOM	199	OE2	GLU	106	21.583	−21.866	69.985	1.00	62.41
ATOM	200	C	GLU	106	19.153	−21.679	75.356	1.00	48.72
ATOM	201	O	GLU	106	18.369	−20.731	75.281	1.00	47.67
ATOM	202	N	ASP	107	18.928	−22.747	76.109	1.00	49.07
ATOM	203	CA	ASP	107	17.733	−22.828	76.921	1.00	49.88
ATOM	204	CB	ASP	107	17.606	−24.210	77.535	1.00	52.08
ATOM	205	CG	ASP	107	17.469	−25.283	76.484	1.00	55.84
ATOM	206	OD1	ASP	107	16.638	−25.099	75.569	1.00	56.69
ATOM	207	OD2	ASP	107	18.186	−26.304	76.566	1.00	58.55
ATOM	208	C	ASP	107	17.834	−21.775	78.000	1.00	49.32
ATOM	209	O	ASP	107	16.845	−21.127	78.340	1.00	50.32
ATOM	210	N	ILE	108	19.043	−21.595	78.524	1.00	48.00
ATOM	211	CA	ILE	108	19.285	−20.600	79.562	1.00	46.04
ATOM	212	CB	ILE	108	20.713	−20.686	80.102	1.00	45.64
ATOM	213	CG2	ILE	108	20.891	−19.691	81.234	1.00	43.75
ATOM	214	CG1	ILE	108	21.024	−22.119	80.550	1.00	46.19
ATOM	215	CD1	ILE	108	20.330	−22.579	81.803	1.00	46.61
ATOM	216	C	ILE	108	19.082	−19.204	78.979	1.00	45.89
ATOM	217	O	ILE	108	18.185	−18.483	79.396	1.00	47.43
ATOM	218	N	CYS	109	19.913	−18.824	78.015	1.00	44.32
ATOM	219	CA	CYS	109	19.773	−17.518	77.413	1.00	43.51
ATOM	220	C	CYS	109	18.334	−17.218	77.154	1.00	41.47
ATOM	221	O	CYS	109	17.860	−16.135	77.471	1.00	40.35
ATOM	222	CB	CYS	109	20.550	−17.422	76.110	1.00	46.91
ATOM	223	SG	CYS	109	22.213	−16.826	76.488	1.00	54.67
ATOM	224	N	SER	110	17.643	−18.198	76.585	1.00	41.43
ATOM	225	CA	SER	110	16.227	−18.094	76.252	1.00	42.22
ATOM	226	CB	SER	110	15.780	−19.377	75.551	1.00	43.14
ATOM	227	OG	SER	110	14.365	−19.448	75.485	1.00	46.83
ATOM	228	C	SER	110	15.347	−17.839	77.473	1.00	41.93
ATOM	229	O	SER	110	14.414	−17.037	77.438	1.00	40.88
ATOM	230	N	LEU	111	15.646	−18.534	78.557	1.00	42.29
ATOM	231	CA	LEU	111	14.881	−18.369	79.773	1.00	43.38
ATOM	232	CB	LEU	111	15.370	−19.376	80.807	1.00	41.89
ATOM	233	CG	LEU	111	14.309	−19.802	81.813	1.00	42.18
ATOM	234	CD1	LEU	111	13.052	−20.245	81.083	1.00	42.84
ATOM	235	CD2	LEU	111	14.863	−20.926	82.659	1.00	43.66
ATOM	236	C	LEU	111	15.061	−16.935	80.279	1.00	45.09
ATOM	237	O	LEU	111	14.095	−16.253	80.633	1.00	44.96
ATOM	238	N	TRP	112	16.307	−16.476	80.290	1.00	46.31
ATOM	239	CA	TRP	112	16.613	−15.131	80.744	1.00	48.17
ATOM	240	CB	TRP	112	18.126	−14.922	80.779	1.00	49.91
ATOM	241	CG	TRP	112	18.747	−15.516	82.010	1.00	52.44
ATOM	242	CD2	TRP	112	19.544	−14.840	82.984	1.00	53.45
ATOM	243	CE2	TRP	112	19.851	−15.778	83.999	1.00	53.54
ATOM	244	CE3	TRP	112	20.031	−13.532	83.102	1.00	54.72
ATOM	245	CD1	TRP	112	18.613	−16.796	82.453	1.00	52.57
ATOM	246	NE1	TRP	112	19.269	−16.964	83.647	1.00	51.79
ATOM	247	CZ2	TRP	112	20.619	−15.454	85.121	1.00	55.71
ATOM	248	CZ3	TRP	112	20.797	−13.204	84.217	1.00	56.51
ATOM	249	CH2	TRP	112	21.083	−14.165	85.215	1.00	57.71
ATOM	250	C	TRP	112	15.951	−14.044	79.914	1.00	49.45
ATOM	251	O	TRP	112	15.497	−13.047	80.459	1.00	50.46
ATOM	252	N	ASP	113	15.889	−14.222	78.603	1.00	50.27
ATOM	253	CA	ASP	113	15.257	−13.220	77.765	1.00	51.73
ATOM	254	CB	ASP	113	15.386	−13.594	76.291	1.00	53.23
ATOM	255	CG	ASP	113	16.821	−13.541	75.807	1.00	55.73
ATOM	256	OD1	ASP	113	17.504	−12.529	76.078	1.00	56.27
ATOM	257	OD2	ASP	113	17.270	−14.506	75.152	1.00	57.05
ATOM	258	C	ASP	113	13.788	−13.064	78.125	1.00	52.99
ATOM	259	O	ASP	113	13.250	−11.953	78.091	1.00	52.81
ATOM	260	N	GLN	114	13.144	−14.173	78.483	1.00	54.06
ATOM	261	CA	GLN	114	11.727	−14.145	78.837	1.00	54.67
ATOM	262	CB	GLN	114	11.018	−15.408	78.318	1.00	56.60
ATOM	263	CG	GLN	114	11.793	−16.710	78.507	1.00	61.03
ATOM	264	CD	GLN	114	11.135	−17.906	77.812	1.00	63.04
ATOM	265	OE1	GLN	114	10.062	−18.362	78.210	1.00	64.12

TABLE 1-continued

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	266	NE2	GLN	114	11.780	−18.411	76.764	1.00	63.49
ATOM	267	C	GLN	114	11.441	−13.953	80.321	1.00	53.71
ATOM	268	O	GLN	114	10.316	−14.158	80.766	1.00	54.68
ATOM	269	N	SER	115	12.449	−13.547	81.086	1.00	52.50
ATOM	270	CA	SER	115	12.265	−13.308	82.519	1.00	51.69
ATOM	271	CB	SER	115	13.038	−14.336	83.348	1.00	51.04
ATOM	272	OG	SER	115	12.621	−15.652	83.056	1.00	52.93
ATOM	273	C	SER	115	12.746	−11.913	82.901	1.00	51.57
ATOM	274	O	SER	115	12.011	−11.142	83.520	1.00	52.69
ATOM	275	N	LEU	116	13.989	−11.604	82.532	1.00	49.90
ATOM	276	CA	LEU	116	14.603	−10.315	82.825	1.00	48.45
ATOM	277	CB	LEU	116	16.022	−10.529	83.343	1.00	47.47
ATOM	278	CG	LEU	116	16.268	−10.161	84.806	1.00	48.17
ATOM	279	CD1	LEU	116	17.715	−10.461	85.176	1.00	47.96
ATOM	280	CD2	LEU	116	15.955	−8.686	85.019	1.00	47.70
ATOM	281	C	LEU	116	14.645	−9.431	81.581	1.00	48.28
ATOM	282	O	LEU	116	15.644	−9.414	80.858	1.00	48.83
ATOM	283	N	LYS	117	13.571	−8.682	81.345	1.00	46.85
ATOM	284	CA	LYS	117	13.479	−7.817	80.170	1.00	45.19
ATOM	285	CB	LYS	117	12.012	−7.662	79.768	1.00	45.35
ATOM	286	CG	LYS	117	11.377	−8.958	79.341	1.00	45.38
ATOM	287	CD	LYS	117	9.987	−8.733	78.809	1.00	45.69
ATOM	288	CE	LYS	117	9.621	−9.864	77.882	1.00	45.39
ATOM	289	NZ	LYS	117	10.704	−10.041	76.876	1.00	44.68
ATOM	290	C	LYS	117	14.100	−6.440	80.351	1.00	43.15
ATOM	291	O	LYS	117	14.002	−5.846	81.410	1.00	43.84
ATOM	292	N	PRO	118	14.764	−5.920	79.315	1.00	41.84
ATOM	293	CD	PRO	118	15.467	−6.711	78.301	1.00	41.18
ATOM	294	CA	PRO	118	15.377	−4.594	79.428	1.00	42.68
ATOM	295	CB	PRO	118	16.611	−4.708	78.532	1.00	41.64
ATOM	296	CG	PRO	118	16.852	−6.184	78.446	1.00	41.32
ATOM	297	C	PRO	118	14.452	−3.444	78.977	1.00	44.00
ATOM	298	O	PRO	118	13.547	−3.631	78.155	1.00	43.14
ATOM	299	N	CYS	119	14.688	−2.258	79.528	1.00	44.26
ATOM	300	CA	CYS	119	13.911	−1.082	79.177	1.00	45.33
ATOM	301	C	CYS	119	14.328	−0.688	77.776	1.00	44.84
ATOM	302	O	CYS	119	13.536	−0.157	76.996	1.00	45.02
ATOM	303	CB	CYS	119	14.212	0.059	80.148	1.00	48.41
ATOM	304	SG	CYS	119	14.000	−0.390	81.904	1.00	55.41
ATOM	305	N	VAL	120	15.595	−0.946	77.476	1.00	43.63
ATOM	306	CA	VAL	120	16.165	−0.669	76.166	1.00	42.72
ATOM	307	CB	VAL	120	16.807	0.719	76.110	1.00	40.94
ATOM	308	CG1	VAL	120	17.494	0.914	74.784	1.00	38.51
ATOM	309	CG2	VAL	120	15.740	1.773	76.293	1.00	40.48
ATOM	310	C	VAL	120	17.217	−1.734	75.897	1.00	43.68
ATOM	311	O	VAL	120	17.932	−2.162	76.811	1.00	42.94
ATOM	312	N	LYS	121	17.292	−2.168	74.643	1.00	44.39
ATOM	313	CA	LYS	121	18.232	−3.197	74.237	1.00	45.78
ATOM	314	CB	LYS	121	17.498	−4.530	74.119	1.00	46.75
ATOM	315	CG	LYS	121	18.292	−5.667	73.498	1.00	48.39
ATOM	316	CD	LYS	121	17.477	−6.942	73.525	1.00	49.47
ATOM	317	CE	LYS	121	18.214	−8.075	72.855	1.00	52.19
ATOM	318	NZ	LYS	121	17.391	−9.321	72.815	1.00	54.57
ATOM	319	C	LYS	121	18.834	−2.829	72.897	1.00	46.81
ATOM	320	O	LYS	121	18.119	−2.708	71.913	1.00	47.70
ATOM	321	N	LEU	122	20.146	−2.641	72.864	1.00	48.66
ATOM	322	CA	LEU	122	20.828	−2.293	71.629	1.00	51.53
ATOM	323	CB	LEU	122	21.795	−1.138	71.841	1.00	50.96
ATOM	324	CG	LEU	122	21.169	0.187	72.235	1.00	51.52
ATOM	325	CD1	LEU	122	22.202	1.272	72.015	1.00	52.75
ATOM	326	CD2	LEU	122	19.930	0.468	71.403	1.00	51.31
ATOM	327	C	LEU	122	21.613	−3.454	71.075	1.00	54.29
ATOM	328	O	LEU	122	22.385	−4.069	71.794	1.00	55.82
ATOM	329	N	CYS	123	21.422	−3.756	69.796	1.00	57.66
ATOM	330	CA	CYS	123	22.156	−4.844	69.161	1.00	61.99
ATOM	331	C	CYS	123	22.651	−4.401	67.790	1.00	65.95
ATOM	332	O	CYS	123	21.868	−3.977	66.952	1.00	66.42
ATOM	333	CB	CYS	123	21.261	−6.068	69.001	1.00	61.14
ATOM	334	SG	CYS	123	20.636	−6.863	70.520	1.00	64.65
ATOM	335	N	PRO	124	23.962	−4.486	67.543	1.00	70.34
ATOM	336	CD	PRO	124	25.032	−4.644	68.538	1.00	71.39
ATOM	337	CA	PRO	124	24.526	−4.079	66.255	1.00	74.44
ATOM	338	CB	PRO	124	25.915	−3.586	66.640	1.00	73.49
ATOM	339	CG	PRO	124	26.298	−4.577	67.678	1.00	72.11
ATOM	340	C	PRO	124	24.600	−5.151	65.170	1.00	78.68
ATOM	341	O	PRO	124	25.007	−6.289	65.435	1.00	78.97
ATOM	342	N	LEU	125	24.216	−4.754	63.952	1.00	83.43
ATOM	343	CA	LEU	125	24.246	−5.602	62.755	1.00	87.97

TABLE 1-continued

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	344	CB	LEU	125	22.826	−5.802	62.199	1.00	85.90
ATOM	345	CG	LEU	125	22.682	−6.595	60.892	1.00	85.01
ATOM	346	CD1	LEU	125	23.501	−7.878	60.933	1.00	84.72
ATOM	347	CD2	LEU	125	21.223	−6.908	60.673	1.00	84.26
ATOM	348	C	LEU	125	25.136	−4.880	61.723	1.00	91.79
ATOM	349	O	LEU	125	24.645	−4.294	60.751	1.00	92.07
ATOM	350	N	CYS	126	26.449	−4.932	61.963	1.00	95.81
ATOM	351	CA	CYS	126	27.456	−4.274	61.128	1.00	99.93
ATOM	352	C	CYS	126	27.478	−4.610	59.639	1.00	101.72
ATOM	353	O	CYS	126	26.500	−5.115	59.075	1.00	101.70
ATOM	354	CB	CYS	126	28.860	−4.525	61.702	1.00	101.65
ATOM	355	SG	CYS	126	29.830	−3.024	62.094	1.00	105.44
ATOM	356	N	VAL	127	28.627	−4.317	59.026	1.00	103.91
ATOM	357	CA	VAL	127	28.873	−4.528	57.601	1.00	105.90
ATOM	358	CB	VAL	127	29.149	−6.029	57.278	1.00	105.47
ATOM	359	CG1	VAL	127	29.583	−6.188	55.822	1.00	104.28
ATOM	360	CG2	VAL	127	30.240	−6.563	58.196	1.00	104.81
ATOM	361	C	VAL	127	27.668	−4.011	56.817	1.00	107.53
ATOM	362	O	VAL	127	27.187	−2.905	57.086	1.00	107.44
ATOM	363	N	GLY	128	27.171	−4.801	55.869	1.00	108.79
ATOM	364	CA	GLY	128	26.041	−4.358	55.076	1.00	110.07
ATOM	365	C	GLY	128	26.390	−3.033	54.422	1.00	111.37
ATOM	366	O	GLY	128	25.543	−2.144	54.318	1.00	111.70
ATOM	367	N	ALA	129	27.653	−2.909	54.007	1.00	112.10
ATOM	368	CA	ALA	129	28.187	−1.712	53.350	1.00	112.06
ATOM	369	CB	ALA	129	27.246	−1.268	52.213	1.00	112.16
ATOM	370	C	ALA	129	28.491	−0.520	54.272	1.00	111.66
ATOM	371	O	ALA	129	27.895	0.551	54.125	1.00	111.99
ATOM	372	N	GLY	194	29.418	−0.709	55.215	1.00	110.69
ATOM	373	CA	GLY	194	29.815	0.358	56.129	1.00	108.83
ATOM	374	C	GLY	194	28.806	0.894	57.136	1.00	107.51
ATOM	375	O	GLY	194	29.136	1.040	58.316	1.00	106.82
ATOM	376	N	SER	195	27.596	1.212	56.672	1.00	106.32
ATOM	377	CA	SER	195	26.529	1.737	57.529	1.00	104.42
ATOM	378	CB	SER	195	25.342	2.211	56.684	1.00	104.28
ATOM	379	OG	SER	195	25.728	3.205	55.752	1.00	103.83
ATOM	380	C	SER	195	26.050	0.664	58.497	1.00	103.36
ATOM	381	O	SER	195	24.927	0.164	58.381	1.00	103.62
ATOM	382	N	CYS	196	26.917	0.317	59.446	1.00	101.48
ATOM	383	CA	CYS	196	26.631	−0.696	60.461	1.00	98.25
ATOM	384	C	CYS	196	25.391	−0.331	61.275	1.00	93.82
ATOM	385	O	CYS	196	25.496	0.258	62.352	1.00	93.50
ATOM	386	CB	CYS	196	27.846	−0.843	61.390	1.00	100.91
ATOM	387	SG	CYS	196	29.301	−1.683	60.659	1.00	104.77
ATOM	388	N	ASN	197	24.219	−0.688	60.758	1.00	88.40
ATOM	389	CA	ASN	197	22.973	−0.380	61.444	1.00	82.77
ATOM	390	CB	ASN	197	21.770	−0.728	60.566	1.00	85.03
ATOM	391	CG	ASN	197	21.187	0.494	59.868	1.00	87.21
ATOM	392	OD1	ASN	197	20.801	1.465	60.529	1.00	88.02
ATOM	393	ND2	ASN	197	21.120	0.450	58.539	1.00	88.02
ATOM	394	C	ASN	197	22.863	−1.088	62.780	1.00	77.50
ATOM	395	O	ASN	197	23.334	−2.210	62.943	1.00	77.29
ATOM	396	N	THR	198	22.227	−0.413	63.730	1.00	71.01
ATOM	397	CA	THR	198	22.048	−0.929	65.075	1.00	63.96
ATOM	398	CB	THR	198	22.715	0.006	66.085	1.00	64.25
ATOM	399	OG1	THR	198	24.118	0.085	65.802	1.00	64.31
ATOM	400	CG2	THR	198	22.496	−0.496	67.500	1.00	64.07
ATOM	401	C	THR	198	20.575	−1.056	65.427	1.00	58.97
ATOM	402	O	THR	198	19.859	−0.065	65.448	1.00	58.60
ATOM	403	N	SER	199	20.136	−2.279	65.709	1.00	53.41
ATOM	404	CA	SER	199	18.747	−2.559	66.067	1.00	48.39
ATOM	405	CB	SER	199	18.470	−4.051	65.915	1.00	47.89
ATOM	406	OG	SER	199	17.306	−4.425	66.627	1.00	48.16
ATOM	407	C	SER	199	18.439	−2.134	67.495	1.00	45.34
ATOM	408	O	SER	199	19.174	−2.470	68.403	1.00	45.45
ATOM	409	N	VAL	200	17.340	−1.414	67.691	1.00	42.99
ATOM	410	CA	VAL	200	16.955	−0.932	69.016	1.00	40.63
ATOM	411	CB	VAL	200	16.927	0.610	69.046	1.00	39.79
ATOM	412	CG1	VAL	200	16.500	1.098	70.404	1.00	39.65
ATOM	413	CG2	VAL	200	18.290	1.164	68.702	1.00	38.60
ATOM	414	C	VAL	200	15.583	−1.440	69.449	1.00	40.29
ATOM	415	O	VAL	200	14.629	−1.400	68.678	1.00	40.35
ATOM	416	N	ILE	201	15.482	−1.905	70.689	1.00	40.20
ATOM	417	CA	ILE	201	14.217	−2.417	71.219	1.00	41.32
ATOM	418	CB	ILE	201	14.249	−3.956	71.405	1.00	42.65
ATOM	419	CG2	ILE	201	12.921	−4.441	71.989	1.00	41.02
ATOM	420	CG1	ILE	201	14.543	−4.646	70.070	1.00	43.17
ATOM	421	CD1	ILE	201	14.834	−6.135	70.211	1.00	44.46

TABLE 1-continued

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	422	C	ILE	201	13.874	−1.810	72.577	1.00	41.94
ATOM	423	O	ILE	201	14.654	−1.896	73.532	1.00	41.41
ATOM	424	N	THR	202	12.690	−1.214	72.657	1.00	41.95
ATOM	425	CA	THR	202	12.226	−0.601	73.889	1.00	42.08
ATOM	426	CB	THR	202	11.969	0.892	73.696	1.00	41.25
ATOM	427	OG1	THR	202	13.082	1.490	73.027	1.00	40.91
ATOM	428	CG2	THR	202	11.788	1.560	75.031	1.00	41.52
ATOM	429	C	THR	202	10.918	−1.251	74.318	1.00	43.20
ATOM	430	O	THR	202	9.948	−1.241	73.563	1.00	43.24
ATOM	431	N	GLN	203	10.890	−1.818	75.524	1.00	44.57
ATOM	432	CA	GLN	203	9.679	−2.464	76.037	1.00	45.88
ATOM	433	CB	GLN	203	9.752	−3.978	75.850	1.00	45.18
ATOM	434	CG	GLN	203	10.718	−4.635	76.792	1.00	46.99
ATOM	435	CD	GLN	203	11.663	−5.579	76.093	1.00	48.26
ATOM	436	OE1	GLN	203	11.253	−6.602	75.541	1.00	47.41
ATOM	437	NE2	GLN	203	12.945	−5.236	76.109	1.00	49.20
ATOM	438	C	GLN	203	9.526	−2.169	77.515	1.00	46.24
ATOM	439	O	GLN	203	10.416	−1.575	78.126	1.00	46.33
ATOM	440	N	ALA	204	8.395	−2.576	78.086	1.00	46.69
ATOM	441	CA	ALA	204	8.169	−2.376	79.510	1.00	47.75
ATOM	442	CB	ALA	204	6.754	−2.731	79.869	1.00	47.77
ATOM	443	C	ALA	204	9.155	−3.326	80.193	1.00	49.20
ATOM	444	O	ALA	204	9.282	−4.492	79.799	1.00	50.45
ATOM	445	N	CYS	205	9.854	−2.830	81.209	1.00	49.03
ATOM	446	CA	CYS	205	10.870	−3.618	81.895	1.00	47.82
ATOM	447	C	CYS	205	10.596	−3.914	83.372	1.00	47.00
ATOM	448	O	CYS	205	11.342	−3.464	84.244	1.00	47.48
ATOM	449	CB	CYS	205	12.214	−2.899	81.749	1.00	49.40
ATOM	450	SG	CYS	205	12.089	−1.097	82.038	1.00	52.40
ATOM	451	N	PRO	206	9.535	−4.692	83.671	1.00	45.36
ATOM	452	CD	PRO	206	8.592	−5.258	82.690	1.00	44.00
ATOM	453	CA	PRO	206	9.142	−5.069	85.037	1.00	43.93
ATOM	454	CB	PRO	206	8.083	−6.135	84.797	1.00	42.82
ATOM	455	CG	PRO	206	7.423	−5.660	83.552	1.00	42.86
ATOM	456	C	PRO	206	10.294	−5.603	85.890	1.00	43.70
ATOM	457	O	PRO	206	11.013	−6.495	85.458	1.00	43.27
ATOM	458	N	LYS	207	10.471	−5.059	87.094	1.00	44.28
ATOM	459	CA	LYS	207	11.533	−5.521	87.992	1.00	45.36
ATOM	460	CB	LYS	207	11.664	−4.626	89.235	1.00	43.66
ATOM	461	CG	LYS	207	12.061	−3.179	89.019	1.00	42.40
ATOM	462	CD	LYS	207	13.436	−3.046	88.429	1.00	41.07
ATOM	463	CE	LYS	207	14.481	−3.725	89.264	1.00	40.58
ATOM	464	NZ	LYS	207	15.758	−3.685	88.510	1.00	40.89
ATOM	465	C	LYS	207	11.157	−6.913	88.481	1.00	47.60
ATOM	466	O	LYS	207	10.126	−7.086	89.126	1.00	49.38
ATOM	467	N	VAL	208	11.975	−7.910	88.185	1.00	49.19
ATOM	468	CA	VAL	208	11.669	−9.248	88.654	1.00	50.40
ATOM	469	CB	VAL	208	11.317	−10.192	87.512	1.00	49.17
ATOM	470	CG1	VAL	208	10.947	−11.548	88.072	1.00	48.47
ATOM	471	CG2	VAL	208	10.171	−9.621	86.720	1.00	49.94
ATOM	472	C	VAL	208	12.867	−9.800	89.379	1.00	52.48
ATOM	473	O	VAL	208	13.950	−9.895	88.820	1.00	53.30
ATOM	474	N	SER	209	12.667	−10.153	90.638	1.00	55.82
ATOM	475	CA	SER	209	13.744	−10.701	91.442	1.00	59.23
ATOM	476	CB	SER	209	14.271	−9.657	92.433	1.00	60.00
ATOM	477	OG	SER	209	13.294	−9.300	93.397	1.00	59.59
ATOM	478	C	SER	209	13.251	−11.912	92.205	1.00	60.56
ATOM	479	O	SER	209	12.328	−11.819	93.015	1.00	61.51
ATOM	480	N	PHE	210	13.863	−13.054	91.927	1.00	61.88
ATOM	481	CA	PHE	210	13.509	−14.293	92.596	1.00	62.55
ATOM	482	CB	PHE	210	12.163	−14.831	92.088	1.00	62.36
ATOM	483	CG	PHE	210	12.173	−15.247	90.645	1.00	62.80
ATOM	484	CD1	PHE	210	12.312	−14.303	89.634	1.00	63.22
ATOM	485	CD2	PHE	210	12.044	−16.588	90.295	1.00	63.02
ATOM	486	CE1	PHE	210	12.321	−14.690	88.294	1.00	62.99
ATOM	487	CE2	PHE	210	12.052	−16.980	88.957	1.00	63.02
ATOM	488	CZ	PHE	210	12.191	−16.027	87.956	1.00	62.16
ATOM	489	C	PHE	210	14.624	−15.285	92.317	1.00	62.59
ATOM	490	O	PHE	210	15.231	−15.266	91.245	1.00	62.81
ATOM	491	N	GLU	211	14.908	−16.138	93.291	1.00	62.66
ATOM	492	CA	GLU	211	15.963	−17.120	93.127	1.00	62.85
ATOM	493	CB	GLU	211	16.274	−17.768	94.490	1.00	63.27
ATOM	494	CG	GLU	211	17.354	−16.985	95.278	1.00	65.06
ATOM	495	CD	GLU	211	17.291	−17.160	96.800	1.00	65.99
ATOM	496	OE1	GLU	211	17.055	−18.299	97.267	1.00	66.91
ATOM	497	OE2	GLU	211	17.497	−16.153	97.528	1.00	63.93
ATOM	498	C	GLU	211	15.645	−18.161	92.036	1.00	61.85
ATOM	499	O	GLU	211	14.538	−18.703	91.965	1.00	61.07

TABLE 1-continued

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	500	N	PRO	212	16.617	−18.406	91.136	1.00	60.73
ATOM	501	CD	PRO	212	17.853	−17.606	91.033	1.00	60.13
ATOM	502	CA	PRO	212	16.529	−19.355	90.019	1.00	60.07
ATOM	503	CB	PRO	212	17.865	−19.151	89.295	1.00	60.56
ATOM	504	CG	PRO	212	18.190	−17.724	89.579	1.00	58.99
ATOM	505	C	PRO	212	16.318	−20.824	90.424	1.00	59.13
ATOM	506	O	PRO	212	17.062	−21.371	91.241	1.00	58.14
ATOM	507	N	ILE	213	15.308	−21.454	89.834	1.00	58.39
ATOM	508	CA	ILE	213	14.999	−22.851	90.111	1.00	57.51
ATOM	509	CB	ILE	213	13.582	−23.226	89.634	1.00	57.45
ATOM	510	CG2	ILE	213	12.936	−24.123	90.645	1.00	58.00
ATOM	511	CG1	ILE	213	12.716	−21.978	89.461	1.00	58.13
ATOM	512	CD1	ILE	213	12.426	−21.230	90.750	1.00	58.27
ATOM	513	C	ILE	213	15.995	−23.705	89.330	1.00	57.45
ATOM	514	O	ILE	213	16.398	−23.335	88.225	1.00	57.51
ATOM	515	N	PRO	214	16.406	−24.863	89.888	1.00	56.69
ATOM	516	CD	PRO	214	16.153	−25.380	91.240	1.00	55.47
ATOM	517	CA	PRO	214	17.361	−25.729	89.193	1.00	55.78
ATOM	518	CB	PRO	214	17.614	−26.845	90.197	1.00	54.06
ATOM	519	CG	PRO	214	17.405	−26.184	91.489	1.00	54.24
ATOM	520	C	PRO	214	16.789	−26.257	87.894	1.00	56.50
ATOM	521	O	PRO	214	15.620	−26.637	87.820	1.00	55.06
ATOM	522	N	ILE	215	17.640	−26.271	86.878	1.00	58.07
ATOM	523	CA	ILE	215	17.286	−26.745	85.555	1.00	58.99
ATOM	524	CB	ILE	215	17.892	−25.815	84.461	1.00	60.28
ATOM	525	CG2	ILE	215	17.752	−26.442	83.088	1.00	61.12
ATOM	526	CG1	ILE	215	17.218	−24.435	84.499	1.00	61.06
ATOM	527	CD1	ILE	215	15.713	−24.448	84.230	1.00	60.70
ATOM	528	C	ILE	215	17.846	−28.153	85.391	1.00	59.41
ATOM	529	O	ILE	215	18.987	−28.418	85.754	1.00	58.13
ATOM	530	N	HIS	216	17.019	−29.051	84.866	1.00	61.77
ATOM	531	CA	HIS	216	17.403	−30.436	84.617	1.00	63.93
ATOM	532	CB	HIS	216	16.393	−31.403	85.235	1.00	64.72
ATOM	533	CG	HIS	216	16.375	−31.414	86.730	1.00	67.28
ATOM	534	CD2	HIS	216	15.441	−30.977	87.609	1.00	67.94
ATOM	535	ND1	HIS	216	17.375	−31.987	87.483	1.00	68.72
ATOM	536	CE1	HIS	216	17.057	−31.908	88.766	1.00	68.43
ATOM	537	NE2	HIS	216	15.890	−31.300	88.868	1.00	69.02
ATOM	538	C	HIS	216	17.378	−30.655	83.105	1.00	65.39
ATOM	539	O	HIS	216	16.331	−30.504	82.474	1.00	65.51
ATOM	540	N	TYR	217	18.517	−31.002	82.517	1.00	66.95
ATOM	541	CA	TYR	217	18.562	−31.260	81.081	1.00	67.77
ATOM	542	CB	TYR	217	19.964	−30.971	80.530	1.00	69.80
ATOM	543	CG	TYR	217	20.183	−31.360	79.076	1.00	72.85
ATOM	544	CD1	TYR	217	20.066	−32.688	78.656	1.00	73.62
ATOM	545	CE1	TYR	217	20.306	−33.062	77.332	1.00	73.91
ATOM	546	CD2	TYR	217	20.543	−30.408	78.124	1.00	74.21
ATOM	547	CE2	TYR	217	20.787	−30.774	76.791	1.00	75.39
ATOM	548	CZ	TYR	217	20.664	−32.105	76.407	1.00	75.03
ATOM	549	OH	TYR	217	20.905	−32.476	75.101	1.00	75.25
ATOM	550	C	TYR	217	18.198	−32.726	80.881	1.00	67.53
ATOM	551	O	TYR	217	18.779	−33.611	81.512	1.00	66.37
ATOM	552	N	CYS	218	17.220	−32.977	80.021	1.00	68.26
ATOM	553	CA	CYS	218	16.801	−34.345	79.736	1.00	69.95
ATOM	554	C	CYS	218	17.146	−34.676	78.291	1.00	70.18
ATOM	555	O	CYS	218	17.368	−33.768	77.483	1.00	71.00
ATOM	556	CB	CYS	218	15.299	−34.515	79.952	1.00	70.79
ATOM	557	SG	CYS	218	14.717	−34.185	81.647	1.00	73.86
ATOM	558	N	ALA	219	17.190	−35.969	77.972	1.00	69.23
ATOM	559	CA	ALA	219	17.525	−36.418	76.622	1.00	67.68
ATOM	560	CB	ALA	219	17.950	−37.874	76.651	1.00	68.44
ATOM	561	C	ALA	219	16.367	−36.224	75.644	1.00	66.31
ATOM	562	O	ALA	219	15.224	−36.577	75.937	1.00	64.91
ATOM	563	N	PRO	220	16.657	−35.652	74.462	1.00	65.58
ATOM	564	CD	PRO	220	17.955	−35.074	74.079	1.00	65.63
ATOM	565	CA	PRO	220	15.657	−35.394	73.420	1.00	64.40
ATOM	566	CB	PRO	220	16.352	−34.386	72.500	1.00	64.51
ATOM	567	CG	PRO	220	17.515	−33.858	73.317	1.00	65.89
ATOM	568	C	PRO	220	15.298	−36.670	72.676	1.00	63.38
ATOM	569	O	PRO	220	16.095	−37.609	72.625	1.00	63.61
ATOM	570	N	ALA	221	14.104	−36.691	72.090	1.00	61.61
ATOM	571	CA	ALA	221	13.645	−37.852	71.345	1.00	59.16
ATOM	572	CB	ALA	221	12.397	−37.503	70.558	1.00	57.25
ATOM	573	C	ALA	221	14.751	−38.323	70.407	1.00	58.51
ATOM	574	O	ALA	221	15.303	−37.532	69.645	1.00	58.11
ATOM	575	N	GLY	222	15.092	−39.608	70.492	1.00	58.44
ATOM	576	CA	GLY	222	16.121	−40.163	69.632	1.00	58.13
ATOM	577	C	GLY	222	17.508	−40.316	70.229	1.00	58.27

TABLE 1-continued

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	578	O	GLY	222	18.405	−40.830	69.560	1.00	57.97
ATOM	579	N	PHE	223	17.700	−39.888	71.475	1.00	58.69
ATOM	580	CA	PHE	223	19.020	−39.989	72.102	1.00	58.31
ATOM	581	CB	PHE	223	19.711	−38.625	72.073	1.00	59.64
ATOM	582	CG	PHE	223	20.030	−38.136	70.690	1.00	60.13
ATOM	583	CD1	PHE	223	19.032	−37.613	69.873	1.00	59.78
ATOM	584	CD2	PHE	223	21.330	−38.222	70.197	1.00	59.77
ATOM	585	CE1	PHE	223	19.323	−37.182	68.588	1.00	60.31
ATOM	586	CE2	PHE	223	21.632	−37.797	68.919	1.00	60.24
ATOM	587	CZ	PHE	223	20.626	−37.273	68.107	1.00	61.40
ATOM	588	C	PHE	223	19.052	−40.530	73.527	1.00	57.51
ATOM	589	O	PHE	223	18.016	−40.708	74.165	1.00	56.31
ATOM	590	N	ALA	224	20.261	−40.787	74.021	1.00	57.34
ATOM	591	CA	ALA	224	20.447	−41.309	75.373	1.00	58.31
ATOM	592	CB	ALA	224	20.842	−42.773	75.311	1.00	58.16
ATOM	593	C	ALA	224	21.517	−40.514	76.116	1.00	58.54
ATOM	594	O	ALA	224	22.404	−39.945	75.491	1.00	59.61
ATOM	595	N	ILE	225	21.436	−40.486	77.444	1.00	57.96
ATOM	596	CA	ILE	225	22.401	−39.751	78.255	1.00	57.94
ATOM	597	CB	ILE	225	21.699	−38.763	79.225	1.00	58.15
ATOM	598	CG2	ILE	225	22.734	−38.081	80.114	1.00	58.23
ATOM	599	CG1	ILE	225	20.904	−37.712	78.444	1.00	58.02
ATOM	600	CD1	ILE	225	20.136	−36.737	79.329	1.00	55.55
ATOM	601	C	ILE	225	23.278	−40.666	79.101	1.00	58.42
ATOM	602	O	ILE	225	22.794	−41.341	80.006	1.00	59.16
ATOM	603	N	LEU	226	24.572	−40.686	78.815	1.00	58.75
ATOM	604	CA	LEU	226	25.484	−41.509	79.597	1.00	59.39
ATOM	605	CB	LEU	226	26.569	−42.109	78.699	1.00	57.81
ATOM	606	CG	LEU	226	26.083	−42.866	77.461	1.00	56.08
ATOM	607	CD1	LEU	226	27.257	−43.550	76.802	1.00	55.05
ATOM	608	CD2	LEU	226	25.039	−43.886	77.838	1.00	55.26
ATOM	609	C	LEU	226	26.101	−40.612	80.667	1.00	60.63
ATOM	610	O	LEU	226	26.257	−39.412	80.453	1.00	60.94
ATOM	611	N	LYS	227	26.448	−41.197	81.810	1.00	62.31
ATOM	612	CA	LYS	227	27.022	−40.452	82.930	1.00	63.91
ATOM	613	CB	LYS	227	25.940	−40.230	84.000	1.00	63.10
ATOM	614	CG	LYS	227	26.440	−39.783	85.373	1.00	62.19
ATOM	615	CD	LYS	227	25.292	−39.708	86.391	1.00	61.38
ATOM	616	CE	LYS	227	25.767	−39.220	87.765	1.00	61.56
ATOM	617	NZ	LYS	227	24.653	−39.044	88.746	1.00	59.42
ATOM	618	C	LYS	227	28.208	−41.169	83.560	1.00	65.80
ATOM	619	O	LYS	227	28.038	−42.199	84.205	1.00	67.24
ATOM	620	N	CYS	228	29.409	−40.631	83.387	1.00	68.12
ATOM	621	CA	CYS	228	30.578	−41.262	83.983	1.00	70.64
ATOM	622	C	CYS	228	30.444	−41.156	85.496	1.00	70.41
ATOM	623	O	CYS	228	30.085	−40.107	86.019	1.00	70.19
ATOM	624	CB	CYS	228	31.871	−40.590	83.511	1.00	73.46
ATOM	625	SG	CYS	228	33.366	−41.502	84.026	1.00	78.70
ATOM	626	N	ASN	229	30.733	−42.243	86.200	1.00	71.33
ATOM	627	CA	ASN	229	30.600	−42.255	87.647	1.00	71.92
ATOM	628	CB	ASN	229	29.857	−43.508	88.082	1.00	72.45
ATOM	629	CG	ASN	229	28.411	−43.492	87.652	1.00	73.11
ATOM	630	OD1	ASN	229	27.647	−42.610	88.051	1.00	72.87
ATOM	631	ND2	ASN	229	28.022	−44.465	86.830	1.00	72.92
ATOM	632	C	ASN	229	31.867	−42.109	88.469	1.00	72.51
ATOM	633	O	ASN	229	31.785	−42.025	89.688	1.00	72.22
ATOM	634	N	ASN	230	33.033	−42.089	87.829	1.00	74.40
ATOM	635	CA	ASN	230	34.272	−41.910	88.582	1.00	76.62
ATOM	636	CB	ASN	230	35.455	−41.654	87.648	1.00	77.04
ATOM	637	CG	ASN	230	35.879	−42.887	86.894	1.00	78.06
ATOM	638	OD1	ASN	230	36.745	−42.818	86.020	1.00	78.68
ATOM	639	ND2	ASN	230	35.278	−44.024	87.232	1.00	78.86
ATOM	640	C	ASN	230	34.064	−40.685	89.458	1.00	77.81
ATOM	641	O	ASN	230	33.496	−39.687	89.010	1.00	78.44
ATOM	642	N	LYS	231	34.507	−40.754	90.706	1.00	79.00
ATOM	643	CA	LYS	231	34.338	−39.623	91.608	1.00	80.19
ATOM	644	CB	LYS	231	34.648	−40.048	93.049	1.00	81.06
ATOM	645	CG	LYS	231	33.678	−41.098	93.576	1.00	81.81
ATOM	646	CD	LYS	231	34.028	−41.600	94.968	1.00	82.80
ATOM	647	CE	LYS	231	33.081	−42.740	95.376	1.00	83.45
ATOM	648	NZ	LYS	231	33.385	−43.321	96.720	1.00	82.56
ATOM	649	C	LYS	231	35.235	−38.474	91.169	1.00	80.35
ATOM	650	O	LYS	231	35.008	−37.321	91.536	1.00	80.46
ATOM	651	N	THR	232	36.245	−38.803	90.368	1.00	80.83
ATOM	652	CA	THR	232	37.188	−37.817	89.843	1.00	81.48
ATOM	653	CB	THR	232	38.552	−37.900	90.545	1.00	81.81
ATOM	654	OG1	THR	232	38.381	−37.665	91.947	1.00	82.72
ATOM	655	CG2	THR	232	39.515	−36.865	89.965	1.00	81.15

TABLE 1-continued

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	656	C	THR	232	37.399	−38.103	88.367	1.00	81.71
ATOM	657	O	THR	232	38.174	−38.987	87.998	1.00	82.58
ATOM	658	N	PHE	233	36.706	−37.350	87.526	1.00	81.77
ATOM	659	CA	PHE	233	36.807	−37.537	86.089	1.00	81.98
ATOM	660	CB	PHE	233	35.426	−37.881	85.532	1.00	80.95
ATOM	661	CG	PHE	233	35.448	−38.347	84.117	1.00	80.20
ATOM	662	CD1	PHE	233	36.242	−39.423	83.746	1.00	79.86
ATOM	663	CD2	PHE	233	34.675	−37.713	83.153	1.00	80.45
ATOM	664	CE1	PHE	233	36.269	−39.865	82.434	1.00	80.01
ATOM	665	CE2	PHE	233	34.692	−38.145	81.840	1.00	80.85
ATOM	666	CZ	PHE	233	35.493	−39.226	81.477	1.00	80.97
ATOM	667	C	PHE	233	37.351	−36.276	85.428	1.00	82.46
ATOM	668	O	PHE	233	36.918	−35.172	85.749	1.00	82.61
ATOM	669	N	ASN	234	38.304	−36.432	84.513	1.00	83.24
ATOM	670	CA	ASN	234	38.874	−35.271	83.841	1.00	84.16
ATOM	671	CB	ASN	234	40.354	−35.499	83.532	1.00	86.83
ATOM	672	CG	ASN	234	40.574	−36.548	82.469	1.00	90.05
ATOM	673	OD1	ASN	234	39.934	−36.527	81.421	1.00	91.19
ATOM	674	ND2	ASN	234	41.507	−37.457	82.725	1.00	92.74
ATOM	675	C	ASN	234	38.117	−34.914	82.559	1.00	83.56
ATOM	676	O	ASN	234	38.633	−34.196	81.697	1.00	83.14
ATOM	677	N	GLY	235	36.897	−35.433	82.444	1.00	82.91
ATOM	678	CA	GLY	235	36.049	−35.147	81.300	1.00	81.77
ATOM	679	C	GLY	235	36.479	−35.646	79.936	1.00	80.76
ATOM	680	O	GLY	235	35.687	−35.623	78.996	1.00	80.76
ATOM	681	N	THR	236	37.722	−36.095	79.808	1.00	79.92
ATOM	682	CA	THR	236	38.203	−36.583	78.521	1.00	78.75
ATOM	683	CB	THR	236	39.368	−35.722	77.992	1.00	79.46
ATOM	684	OG1	THR	236	39.526	−35.948	76.586	1.00	79.72
ATOM	685	CG2	THR	236	40.671	−36.091	78.698	1.00	79.62
ATOM	686	C	THR	236	38.676	−38.020	78.618	1.00	77.39
ATOM	687	O	THR	236	38.821	−38.564	79.706	1.00	77.35
ATOM	688	N	GLY	237	38.926	−38.628	77.469	1.00	76.80
ATOM	689	CA	GLY	237	39.390	−39.998	77.455	1.00	76.72
ATOM	690	C	GLY	237	38.283	−40.994	77.729	1.00	76.45
ATOM	691	O	GLY	237	37.106	−40.659	77.589	1.00	76.57
ATOM	692	N	PRO	238	38.634	−42.235	78.113	1.00	75.99
ATOM	693	CD	PRO	238	40.000	−42.777	78.002	1.00	75.67
ATOM	694	CA	PRO	238	37.689	−43.311	78.413	1.00	75.71
ATOM	695	CB	PRO	238	38.456	−44.544	77.980	1.00	75.43
ATOM	696	CG	PRO	238	39.824	−44.215	78.454	1.00	75.46
ATOM	697	C	PRO	238	37.247	−43.404	79.876	1.00	75.60
ATOM	698	O	PRO	238	38.014	−43.116	80.795	1.00	74.29
ATOM	699	N	CYS	239	35.996	−43.811	80.065	1.00	76.23
ATOM	700	CA	CYS	239	35.401	−43.978	81.386	1.00	77.64
ATOM	701	C	CYS	239	35.078	−45.462	81.561	1.00	77.75
ATOM	702	O	CYS	239	34.724	−46.151	80.602	1.00	77.99
ATOM	703	CB	CYS	239	34.114	−43.136	81.511	1.00	78.55
ATOM	704	SG	CYS	239	33.201	−43.307	83.092	1.00	79.98
ATOM	705	N	THR	240	35.205	−45.950	82.789	1.00	77.99
ATOM	706	CA	THR	240	34.936	−47.352	83.086	1.00	77.29
ATOM	707	CB	THR	240	36.156	−47.984	83.808	1.00	77.48
ATOM	708	OG1	THR	240	36.642	−47.088	84.817	1.00	77.79
ATOM	709	CG2	THR	240	37.276	−48.253	82.812	1.00	76.21
ATOM	710	C	THR	240	33.651	−47.555	83.914	1.00	76.52
ATOM	711	O	THR	240	32.878	−48.482	83.653	1.00	76.31
ATOM	712	N	ASN	241	33.427	−46.683	84.898	1.00	74.90
ATOM	713	CA	ASN	241	32.239	−46.740	85.760	1.00	72.80
ATOM	714	CB	ASN	241	32.617	−46.258	87.171	1.00	72.80
ATOM	715	CG	ASN	241	31.621	−46.691	88.241	1.00	72.83
ATOM	716	OD1	ASN	241	30.404	−46.657	88.031	1.00	73.02
ATOM	717	ND2	ASN	241	32.142	−47.079	89.402	1.00	71.56
ATOM	718	C	ASN	241	31.195	−45.797	85.132	1.00	71.45
ATOM	719	O	ASN	241	31.185	−44.601	85.419	1.00	70.59
ATOM	720	N	VAL	242	30.323	−46.333	84.278	1.00	69.95
ATOM	721	CA	VAL	242	29.319	−45.512	83.591	1.00	68.27
ATOM	722	CB	VAL	242	29.779	−45.171	82.153	1.00	68.44
ATOM	723	CG1	VAL	242	30.532	−46.343	81.548	1.00	68.10
ATOM	724	CG2	VAL	242	28.574	−44.842	81.286	1.00	68.72
ATOM	725	C	VAL	242	27.911	−46.091	83.494	1.00	66.92
ATOM	726	O	VAL	242	27.736	−47.279	83.258	1.00	67.05
ATOM	727	N	SER	243	26.908	−45.231	83.650	1.00	65.86
ATOM	728	CA	SER	243	25.513	−45.657	83.568	1.00	65.72
ATOM	729	CB	SER	243	24.911	−45.773	84.975	1.00	64.61
ATOM	730	OG	SER	243	25.167	−44.631	85.765	1.00	62.69
ATOM	731	C	SER	243	24.655	−44.729	82.700	1.00	65.75
ATOM	732	O	SER	243	25.138	−43.719	82.195	1.00	66.44
ATOM	733	N	THR	244	23.386	−45.089	82.523	1.00	65.22

TABLE 1-continued

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	734	CA	THR	244	22.440	−44.307	81.722	1.00	64.94
ATOM	735	CB	THR	244	21.692	−45.202	80.714	1.00	65.14
ATOM	736	OG1	THR	244	22.448	−45.286	79.501	1.00	65.13
ATOM	737	CG2	THR	244	20.294	−44.655	80.422	1.00	64.17
ATOM	738	C	THR	244	21.408	−43.644	82.614	1.00	65.03
ATOM	739	O	THR	244	20.913	−44.262	83.550	1.00	66.14
ATOM	740	N	VAL	245	21.065	−42.397	82.310	1.00	64.75
ATOM	741	CA	VAL	245	20.089	−41.669	83.112	1.00	64.42
ATOM	742	CB	VAL	245	20.777	−40.574	83.939	1.00	64.72
ATOM	743	CG1	VAL	245	21.922	−41.172	84.732	1.00	64.56
ATOM	744	CG2	VAL	245	21.291	−39.477	83.019	1.00	65.00
ATOM	745	C	VAL	245	19.008	−41.016	82.264	1.00	64.37
ATOM	746	O	VAL	245	19.148	−40.887	81.052	1.00	62.59
ATOM	747	N	GLN	246	17.927	−40.600	82.910	1.00	65.67
ATOM	748	CA	GLN	246	16.839	−39.947	82.195	1.00	67.31
ATOM	749	CB	GLN	246	15.528	−40.083	82.972	1.00	69.55
ATOM	750	CG	GLN	246	15.009	−41.514	83.055	1.00	72.91
ATOM	751	CD	GLN	246	14.973	−42.189	81.691	1.00	74.79
ATOM	752	OE1	GLN	246	14.414	−41.645	80.737	1.00	76.33
ATOM	753	NE2	GLN	246	15.568	−43.381	81.593	1.00	74.80
ATOM	754	C	GLN	246	17.174	−38.477	81.991	1.00	67.14
ATOM	755	O	GLN	246	17.049	−37.952	80.887	1.00	67.40
ATOM	756	N	CYS	247	17.603	−37.819	83.064	1.00	67.11
ATOM	757	CA	CYS	247	17.981	−36.408	83.009	1.00	66.41
ATOM	758	C	CYS	247	19.173	−36.223	83.942	1.00	64.14
ATOM	759	O	CYS	247	19.394	−37.048	84.834	1.00	63.44
ATOM	760	CB	CYS	247	16.821	−35.516	83.465	1.00	68.57
ATOM	761	SG	CYS	247	15.192	−35.863	82.704	1.00	72.95
ATOM	762	N	THR	248	19.943	−35.155	83.736	1.00	61.65
ATOM	763	CA	THR	248	21.115	−34.882	84.571	1.00	58.60
ATOM	764	CB	THR	248	22.015	−33.789	83.953	1.00	58.51
ATOM	765	OG1	THR	248	21.401	−32.506	84.118	1.00	58.42
ATOM	766	CG2	THR	248	22.224	−34.048	82.472	1.00	57.39
ATOM	767	C	THR	248	20.649	−34.404	85.938	1.00	56.78
ATOM	768	O	THR	248	19.460	−34.479	86.248	1.00	56.77
ATOM	769	N	HIS	249	21.575	−33.914	86.759	1.00	54.48
ATOM	770	CA	HIS	249	21.204	−33.423	88.085	1.00	52.32
ATOM	771	CB	HIS	249	22.408	−33.455	89.036	1.00	50.67
ATOM	772	CG	HIS	249	23.557	−32.617	88.581	1.00	50.88
ATOM	773	CD2	HIS	249	23.960	−31.378	88.951	1.00	51.06
ATOM	774	ND1	HIS	249	24.418	−33.016	87.582	1.00	52.07
ATOM	775	CE1	HIS	249	25.300	−32.059	87.354	1.00	52.55
ATOM	776	NE2	HIS	249	25.043	−31.053	88.171	1.00	51.62
ATOM	777	C	HIS	249	20.648	−31.997	88.000	1.00	51.12
ATOM	778	O	HIS	249	20.672	−31.366	86.943	1.00	50.41
ATOM	779	N	GLY	250	20.120	−31.504	89.112	1.00	50.12
ATOM	780	CA	GLY	250	19.589	−30.158	89.128	1.00	48.39
ATOM	781	C	GLY	250	20.738	−29.188	89.013	1.00	47.71
ATOM	782	O	GLY	250	21.720	−29.274	89.754	1.00	47.82
ATOM	783	N	ILE	251	20.631	−28.262	88.075	1.00	47.08
ATOM	784	CA	ILE	251	21.692	−27.295	87.898	1.00	47.14
ATOM	785	CB	ILE	251	22.386	−27.494	86.533	1.00	46.53
ATOM	786	CG2	ILE	251	23.380	−26.363	86.268	1.00	46.08
ATOM	787	CG1	ILE	251	23.100	−28.845	86.534	1.00	46.01
ATOM	788	CD1	ILE	251	23.697	−29.231	85.209	1.00	46.76
ATOM	789	C	ILE	251	21.222	−25.856	88.050	1.00	47.08
ATOM	790	O	ILE	251	20.219	−25.439	87.479	1.00	46.45
ATOM	791	N	ARG	252	21.953	−25.114	88.868	1.00	47.74
ATOM	792	CA	ARG	252	21.651	−23.722	89.101	1.00	48.23
ATOM	793	CB	ARG	252	22.398	−23.209	90.335	1.00	49.56
ATOM	794	CG	ARG	252	21.642	−23.363	91.631	1.00	52.05
ATOM	795	CD	ARG	252	21.428	−24.816	91.987	1.00	55.46
ATOM	796	NE	ARG	252	20.534	−24.934	93.127	1.00	58.57
ATOM	797	CZ	ARG	252	20.800	−24.438	94.330	1.00	61.06
ATOM	798	NH1	ARG	252	21.942	−23.796	94.547	1.00	61.62
ATOM	799	NH2	ARG	252	19.917	−24.568	95.313	1.00	62.98
ATOM	800	C	ARG	252	22.125	−22.965	87.877	1.00	47.35
ATOM	801	O	ARG	252	23.322	−22.949	87.577	1.00	48.58
ATOM	802	N	PRO	253	21.194	−22.354	87.134	1.00	45.23
ATOM	803	CD	PRO	253	19.728	−22.423	87.233	1.00	44.55
ATOM	804	CA	PRO	253	21.595	−21.604	85.949	1.00	43.24
ATOM	805	CB	PRO	253	20.288	−21.483	85.179	1.00	42.38
ATOM	806	CG	PRO	253	19.293	−21.350	86.272	1.00	43.19
ATOM	807	C	PRO	253	22.182	−20.256	86.375	1.00	41.47
ATOM	808	O	PRO	253	21.744	−19.199	85.926	1.00	42.48
ATOM	809	N	VAL	254	23.179	−20.305	87.255	1.00	39.38
ATOM	810	CA	VAL	254	23.822	−19.092	87.751	1.00	37.91
ATOM	811	CB	VAL	254	24.819	−19.384	88.879	1.00	37.89

TABLE 1-continued

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	812	CG1	VAL	254	25.491	−18.100	89.330	1.00	36.95
ATOM	813	CG2	VAL	254	24.107	−20.023	90.030	1.00	40.36
ATOM	814	C	VAL	254	24.589	−18.384	86.661	1.00	36.14
ATOM	815	O	VAL	254	25.346	−19.000	85.913	1.00	37.64
ATOM	816	N	VAL	255	24.399	−17.078	86.588	1.00	32.62
ATOM	817	CA	VAL	255	25.090	−16.278	85.607	1.00	30.04
ATOM	818	CB	VAL	255	24.103	−15.366	84.867	1.00	31.25
ATOM	819	CG1	VAL	255	24.783	−14.073	84.437	1.00	31.11
ATOM	820	CG2	VAL	255	23.571	−16.105	83.654	1.00	32.07
ATOM	821	C	VAL	255	26.165	−15.463	86.298	1.00	26.49
ATOM	822	O	VAL	255	25.878	−14.632	87.144	1.00	24.49
ATOM	823	N	SER	256	27.412	−15.706	85.931	1.00	24.46
ATOM	824	CA	SER	256	28.486	−14.982	86.556	1.00	23.46
ATOM	825	CB	SER	256	28.585	−15.389	88.010	1.00	22.73
ATOM	826	OG	SER	256	29.018	−16.727	88.096	1.00	21.19
ATOM	827	C	SER	256	29.846	−15.182	85.915	1.00	23.86
ATOM	828	O	SER	256	30.047	−16.034	85.038	1.00	22.73
ATOM	829	N	SER	257	30.787	−14.384	86.401	1.00	23.62
ATOM	830	CA	SER	257	32.159	−14.423	85.941	1.00	23.31
ATOM	831	CB	SER	257	32.559	−13.053	85.417	1.00	22.82
ATOM	832	OG	SER	257	32.592	−12.107	86.466	1.00	20.86
ATOM	833	C	SER	257	33.063	−14.804	87.106	1.00	23.53
ATOM	834	O	SER	257	32.629	−14.829	88.250	1.00	23.12
ATOM	835	N	GLN	258	34.313	−15.119	86.792	1.00	24.34
ATOM	836	CA	GLN	258	35.327	−15.475	87.785	1.00	26.23
ATOM	837	CB	GLN	258	35.699	−14.223	88.565	1.00	25.47
ATOM	838	CG	GLN	258	35.659	−13.014	87.684	1.00	25.81
ATOM	839	CD	GLN	258	36.430	−11.876	88.256	1.00	26.39
ATOM	840	OE1	GLN	258	36.368	−11.623	89.454	1.00	27.90
ATOM	841	NE2	GLN	258	37.163	−11.168	87.407	1.00	23.70
ATOM	842	C	GLN	258	34.995	−16.601	88.757	1.00	26.10
ATOM	843	O	GLN	258	35.661	−17.630	88.785	1.00	27.43
ATOM	844	N	LEU	259	33.965	−16.397	89.559	1.00	26.43
ATOM	845	CA	LEU	259	33.563	−17.382	90.538	1.00	25.71
ATOM	846	CB	LEU	259	33.304	−16.692	91.865	1.00	25.10
ATOM	847	CG	LEU	259	34.388	−15.692	92.261	1.00	24.45
ATOM	848	CD1	LEU	259	33.952	−14.868	93.466	1.00	20.24
ATOM	849	CD2	LEU	259	35.672	−16.457	92.530	1.00	26.19
ATOM	850	C	LEU	259	32.295	−18.068	90.083	1.00	26.56
ATOM	851	O	LEU	259	31.402	−17.423	89.533	1.00	27.02
ATOM	852	N	LEU	260	32.236	−19.377	90.310	1.00	26.59
ATOM	853	CA	LEU	260	31.076	−20.199	89.977	1.00	25.55
ATOM	854	CB	LEU	260	31.528	−21.570	89.490	1.00	21.73
ATOM	855	CG	LEU	260	32.353	−21.522	88.222	1.00	20.50
ATOM	856	CD1	LEU	260	32.904	−22.888	87.902	1.00	21.75
ATOM	857	CD2	LEU	260	31.485	−21.036	87.102	1.00	19.68
ATOM	858	C	LEU	260	30.306	−20.347	91.282	1.00	26.59
ATOM	859	O	LEU	260	30.823	−20.923	92.233	1.00	28.36
ATOM	860	N	LEU	261	29.076	−19.847	91.330	1.00	27.70
ATOM	861	CA	LEU	261	28.283	−19.905	92.557	1.00	28.07
ATOM	862	CB	LEU	261	27.611	−18.555	92.769	1.00	28.66
ATOM	863	CG	LEU	261	28.555	−17.374	92.533	1.00	28.66
ATOM	864	CD1	LEU	261	27.784	−16.071	92.672	1.00	28.33
ATOM	865	CD2	LEU	261	29.722	−17.433	93.517	1.00	28.00
ATOM	866	C	LEU	261	27.233	−21.004	92.632	1.00	28.30
ATOM	867	O	LEU	261	26.633	−21.362	91.635	1.00	27.56
ATOM	868	N	ASN	262	27.022	−21.538	93.831	1.00	30.19
ATOM	869	CA	ASN	262	26.026	−22.589	94.062	1.00	30.65
ATOM	870	CB	ASN	262	24.627	−21.988	93.972	1.00	30.68
ATOM	871	CG	ASN	262	24.446	−20.825	94.915	1.00	32.60
ATOM	872	OD1	ASN	262	25.131	−20.716	95.937	1.00	32.65
ATOM	873	ND2	ASN	262	23.506	−19.952	94.590	1.00	33.30
ATOM	874	C	ASN	262	26.107	−23.820	93.158	1.00	29.62
ATOM	875	O	ASN	262	25.084	−24.400	92.777	1.00	27.50
ATOM	876	N	GLY	263	27.328	−24.226	92.835	1.00	29.42
ATOM	877	CA	GLY	263	27.501	−25.384	91.983	1.00	30.33
ATOM	878	C	GLY	263	27.889	−26.635	92.734	1.00	29.97
ATOM	879	O	GLY	263	27.951	−26.638	93.954	1.00	30.00
ATOM	880	N	SER	264	28.148	−27.704	91.991	1.00	31.78
ATOM	881	CA	SER	264	28.540	−28.977	92.579	1.00	32.91
ATOM	882	CB	SER	264	28.367	−30.119	91.576	1.00	32.66
ATOM	883	OG	SER	264	27.014	−30.289	91.197	1.00	33.12
ATOM	884	C	SER	264	29.992	−28.926	92.992	1.00	33.65
ATOM	885	O	SER	264	30.813	−28.339	92.288	1.00	34.68
ATOM	886	N	LEU	265	30.301	−29.537	94.133	1.00	34.04
ATOM	887	CA	LEU	265	31.667	−29.588	94.627	1.00	34.32
ATOM	888	CB	LEU	265	31.689	−29.585	96.155	1.00	32.99
ATOM	889	CG	LEU	265	31.346	−28.271	96.859	1.00	33.66

TABLE 1-continued

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	890	CD1	LEU	265	31.307	−28.477	98.352	1.00	34.03
ATOM	891	CD2	LEU	265	32.379	−27.219	96.520	1.00	34.44
ATOM	892	C	LEU	265	32.297	−30.869	94.098	1.00	35.56
ATOM	893	O	LEU	265	31.596	−31.751	93.607	1.00	34.43
ATOM	894	N	ALA	266	33.622	−30.951	94.176	1.00	38.30
ATOM	895	CA	ALA	266	34.352	−32.128	93.725	1.00	40.59
ATOM	896	CB	ALA	266	35.769	−31.751	93.302	1.00	38.89
ATOM	897	C	ALA	266	34.372	−33.070	94.920	1.00	43.62
ATOM	898	O	ALA	266	34.755	−32.677	96.026	1.00	44.02
ATOM	899	N	GLU	267	33.961	−34.314	94.691	1.00	46.39
ATOM	900	CA	GLU	267	33.868	−35.303	95.754	1.00	49.11
ATOM	901	CB	GLU	267	33.263	−36.593	95.198	1.00	51.72
ATOM	902	CG	GLU	267	32.103	−36.352	94.222	1.00	56.02
ATOM	903	CD	GLU	267	31.126	−37.527	94.130	1.00	57.75
ATOM	904	OE1	GLU	267	30.292	−37.680	95.053	1.00	58.56
ATOM	905	OE2	GLU	267	31.190	−38.294	93.139	1.00	58.03
ATOM	906	C	GLU	267	35.125	−35.625	96.554	1.00	49.70
ATOM	907	O	GLU	267	35.031	−35.933	97.736	1.00	50.00
ATOM	908	N	GLU	268	36.299	−35.552	95.944	1.00	51.35
ATOM	909	CA	GLU	268	37.510	−35.879	96.691	1.00	53.41
ATOM	910	CB	GLU	268	38.332	−36.923	95.940	1.00	55.13
ATOM	911	CG	GLU	268	37.589	−38.222	95.692	1.00	59.90
ATOM	912	CD	GLU	268	38.264	−39.115	94.650	1.00	61.80
ATOM	913	OE1	GLU	268	37.689	−40.179	94.332	1.00	62.83
ATOM	914	OE2	GLU	268	39.358	−38.756	94.154	1.00	62.29
ATOM	915	C	GLU	268	38.381	−34.672	96.964	1.00	53.78
ATOM	916	O	GLU	268	38.293	−34.046	98.023	1.00	54.54
ATOM	917	N	GLU	269	39.232	−34.355	96.000	1.00	53.53
ATOM	918	CA	GLU	269	40.139	−33.231	96.132	1.00	53.58
ATOM	919	CB	GLU	269	41.564	−33.689	95.841	1.00	55.20
ATOM	920	CG	GLU	269	41.923	−35.009	96.487	1.00	57.76
ATOM	921	CD	GLU	269	43.335	−35.450	96.151	1.00	59.84
ATOM	922	OE1	GLU	269	43.678	−36.621	96.416	1.00	59.87
ATOM	923	OE2	GLU	269	44.109	−34.623	95.626	1.00	62.07
ATOM	924	C	GLU	269	39.746	−32.126	95.162	1.00	52.41
ATOM	925	O	GLU	269	38.749	−32.252	94.452	1.00	53.19
ATOM	926	N	VAL	270	40.530	−31.049	95.138	1.00	50.34
ATOM	927	CA	VAL	270	40.269	−29.926	94.241	1.00	48.54
ATOM	928	CB	VAL	270	41.091	−28.663	94.633	1.00	47.63
ATOM	929	CG1	VAL	270	41.172	−27.707	93.467	1.00	45.74
ATOM	930	CG2	VAL	270	40.424	−27.950	95.806	1.00	47.67
ATOM	931	C	VAL	270	40.631	−30.337	92.823	1.00	47.45
ATOM	932	O	VAL	270	41.651	−30.994	92.606	1.00	47.66
ATOM	933	N	VAL	271	39.790	−29.948	91.864	1.00	45.27
ATOM	934	CA	VAL	271	40.012	−30.290	90.461	1.00	42.45
ATOM	935	CB	VAL	271	38.878	−31.202	89.925	1.00	41.54
ATOM	936	CG1	VAL	271	39.220	−31.677	88.530	1.00	39.33
ATOM	937	CG2	VAL	271	38.663	−32.380	90.857	1.00	40.44
ATOM	938	C	VAL	271	40.123	−29.071	89.535	1.00	40.87
ATOM	939	O	VAL	271	39.324	−28.132	89.623	1.00	41.07
ATOM	940	N	ILE	272	41.130	−29.096	88.662	1.00	37.99
ATOM	941	CA	ILE	272	41.342	−28.035	87.691	1.00	35.44
ATOM	942	CB	ILE	272	42.724	−27.352	87.867	1.00	32.95
ATOM	943	CG2	ILE	272	42.894	−26.892	89.302	1.00	30.53
ATOM	944	CG1	ILE	272	43.857	−28.308	87.528	1.00	30.50
ATOM	945	CD1	ILE	272	45.218	−27.694	87.759	1.00	28.89
ATOM	946	C	ILE	272	41.226	−28.705	86.329	1.00	36.01
ATOM	947	O	ILE	272	41.804	−29.760	86.104	1.00	36.26
ATOM	948	N	ARG	273	40.436	−28.100	85.444	1.00	36.70
ATOM	949	CA	ARG	273	40.173	−28.629	84.107	1.00	36.68
ATOM	950	CB	ARG	273	38.711	−29.077	83.996	1.00	34.08
ATOM	951	CG	ARG	273	38.209	−30.035	85.056	1.00	32.56
ATOM	952	CD	ARG	273	36.708	−30.273	84.871	1.00	32.51
ATOM	953	NE	ARG	273	36.253	−31.508	85.502	1.00	31.47
ATOM	954	CZ	ARG	273	36.149	−31.672	86.811	1.00	32.01
ATOM	955	NH1	ARG	273	36.458	−30.672	87.615	1.00	34.75
ATOM	956	NH2	ARG	273	35.771	−32.835	87.323	1.00	30.95
ATOM	957	C	ARG	273	40.409	−27.566	83.030	1.00	39.20
ATOM	958	O	ARG	273	40.272	−26.364	83.288	1.00	41.19
ATOM	959	N	SER	274	40.757	−28.013	81.823	1.00	40.06
ATOM	960	CA	SER	274	40.969	−27.114	80.691	1.00	40.76
ATOM	961	CB	SER	274	42.332	−26.436	80.763	1.00	36.80
ATOM	962	OG	SER	274	42.480	−25.540	79.681	1.00	32.87
ATOM	963	C	SER	274	40.867	−27.899	79.399	1.00	43.92
ATOM	964	O	SER	274	41.114	−29.100	79.372	1.00	45.39
ATOM	965	N	CYS	275	40.480	−27.230	78.325	1.00	47.15
ATOM	966	CA	CYS	275	40.377	−27.916	77.055	1.00	51.92
ATOM	967	C	CYS	275	41.737	−27.968	76.403	1.00	52.82

TABLE 1-continued

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	968	O	CYS	275	41.890	−28.485	75.303	1.00	54.44
ATOM	969	CB	CYS	275	39.375	−27.207	76.154	1.00	55.95
ATOM	970	SG	CYS	275	37.681	−27.472	76.771	1.00	66.91
ATOM	971	N	ASN	276	42.730	−27.439	77.106	1.00	53.33
ATOM	972	CA	ASN	276	44.104	−27.397	76.624	1.00	52.97
ATOM	973	CB	ASN	276	44.161	−26.855	75.186	1.00	55.96
ATOM	974	CG	ASN	276	45.584	−26.683	74.685	1.00	61.01
ATOM	975	OD1	ASN	276	46.331	−25.861	75.210	1.00	63.58
ATOM	976	ND2	ASN	276	45.980	−27.485	73.701	1.00	64.98
ATOM	977	C	ASN	276	44.864	−26.475	77.571	1.00	51.50
ATOM	978	O	ASN	276	44.876	−25.251	77.398	1.00	50.11
ATOM	979	N	PHE	277	45.483	−27.074	78.584	1.00	49.28
ATOM	980	CA	PHE	277	46.235	−26.309	79.570	1.00	47.85
ATOM	981	CB	PHE	277	46.763	−27.231	80.675	1.00	46.32
ATOM	982	CG	PHE	277	45.689	−27.794	81.567	1.00	44.69
ATOM	983	CD1	PHE	277	45.136	−29.050	81.321	1.00	43.74
ATOM	984	CD2	PHE	277	45.235	−27.070	82.667	1.00	43.64
ATOM	985	CE1	PHE	277	44.149	−29.577	82.163	1.00	41.58
ATOM	986	CE2	PHE	277	44.249	−27.590	83.511	1.00	42.49
ATOM	987	CZ	PHE	277	43.707	−28.848	83.258	1.00	40.91
ATOM	988	C	PHE	277	47.397	−25.526	78.959	1.00	47.27
ATOM	989	O	PHE	277	47.758	−24.456	79.451	1.00	46.87
ATOM	990	N	THR	278	47.972	−26.069	77.890	1.00	47.46
ATOM	991	CA	THR	278	49.103	−25.462	77.189	1.00	48.47
ATOM	992	CB	THR	278	49.612	−26.414	76.092	1.00	48.42
ATOM	993	OG1	THR	278	50.438	−27.415	76.691	1.00	48.33
ATOM	994	CG2	THR	278	50.410	−25.659	75.038	1.00	49.75
ATOM	995	C	THR	278	48.784	−24.103	76.562	1.00	48.99
ATOM	996	O	THR	278	49.596	−23.168	76.609	1.00	48.80
ATOM	997	N	ASP	279	47.600	−24.021	75.964	1.00	48.66
ATOM	998	CA	ASP	279	47.094	−22.816	75.315	1.00	48.23
ATOM	999	CB	ASP	279	45.819	−23.178	74.547	1.00	50.23
ATOM	1000	CG	ASP	279	45.261	−22.025	73.742	1.00	51.68
ATOM	1001	OD1	ASP	279	44.294	−22.275	72.986	1.00	51.77
ATOM	1002	OD2	ASP	279	45.778	−20.890	73.870	1.00	51.55
ATOM	1003	C	ASP	279	46.792	−21.801	76.414	1.00	47.12
ATOM	1004	O	ASP	279	45.827	−21.958	77.168	1.00	47.67
ATOM	1005	N	ASN	280	47.609	−20.758	76.507	1.00	43.96
ATOM	1006	CA	ASN	280	47.410	−19.775	77.559	1.00	41.43
ATOM	1007	CB	ASN	280	48.671	−18.910	77.722	1.00	39.74
ATOM	1008	CG	ASN	280	49.007	−18.101	76.485	1.00	36.68
ATOM	1009	OD1	ASN	280	48.755	−18.525	75.364	1.00	36.56
ATOM	1010	ND2	ASN	280	49.604	−16.931	76.692	1.00	33.53
ATOM	1011	C	ASN	280	46.174	−18.916	77.364	1.00	41.24
ATOM	1012	O	ASN	280	45.970	−17.927	78.058	1.00	40.99
ATOM	1013	N	ALA	281	45.321	−19.315	76.434	1.00	41.19
ATOM	1014	CA	ALA	281	44.117	−18.547	76.192	1.00	40.89
ATOM	1015	CB	ALA	281	44.119	−18.045	74.777	1.00	42.27
ATOM	1016	C	ALA	281	42.859	−19.356	76.463	1.00	40.32
ATOM	1017	O	ALA	281	41.764	−18.949	76.090	1.00	41.07
ATOM	1018	N	LYS	282	43.012	−20.500	77.115	1.00	39.16
ATOM	1019	CA	LYS	282	41.864	−21.334	77.423	1.00	38.60
ATOM	1020	CB	LYS	282	42.116	−22.773	76.970	1.00	39.99
ATOM	1021	CG	LYS	282	41.897	−22.990	75.479	1.00	41.46
ATOM	1022	CD	LYS	282	40.523	−22.473	75.048	1.00	43.09
ATOM	1023	CE	LYS	282	40.172	−22.875	73.625	1.00	41.82
ATOM	1024	NZ	LYS	282	39.986	−24.349	73.519	1.00	42.86
ATOM	1025	C	LYS	282	41.488	−21.310	78.897	1.00	37.93
ATOM	1026	O	LYS	282	42.336	−21.477	79.777	1.00	38.22
ATOM	1027	N	THR	283	40.200	−21.110	79.149	1.00	36.68
ATOM	1028	CA	THR	283	39.648	−21.049	80.494	1.00	35.31
ATOM	1029	CB	THR	283	38.117	−20.944	80.447	1.00	34.66
ATOM	1030	OG1	THR	283	37.745	−19.702	79.850	1.00	37.62
ATOM	1031	CG2	THR	283	37.523	−21.018	81.833	1.00	34.32
ATOM	1032	C	THR	283	39.982	−22.263	81.340	1.00	35.03
ATOM	1033	O	THR	283	39.808	−23.396	80.896	1.00	35.94
ATOM	1034	N	ILE	284	40.461	−22.026	82.558	1.00	33.55
ATOM	1035	CA	ILE	284	40.750	−23.115	83.481	1.00	32.06
ATOM	1036	CB	ILE	284	42.087	−22.926	84.220	1.00	29.94
ATOM	1037	CG2	ILE	284	42.264	−24.025	85.253	1.00	25.00
ATOM	1038	CG1	ILE	284	43.234	−22.964	83.225	1.00	28.55
ATOM	1039	CD1	ILE	284	44.563	−22.787	83.859	1.00	28.55
ATOM	1040	C	ILE	284	39.609	−23.124	84.502	1.00	33.37
ATOM	1041	O	ILE	284	39.398	−22.149	85.237	1.00	32.79
ATOM	1042	N	ILE	285	38.867	−24.227	84.516	1.00	33.28
ATOM	1043	CA	ILE	285	37.740	−24.413	85.412	1.00	32.89
ATOM	1044	CB	ILE	285	36.657	−25.259	84.734	1.00	31.95
ATOM	1045	CG2	ILE	285	35.537	−25.555	85.697	1.00	32.46

TABLE 1-continued

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	1046	CG1	ILE	285	36.113	−24.517	83.527	1.00	32.81
ATOM	1047	CD1	ILE	285	34.981	−25.242	82.844	1.00	35.28
ATOM	1048	C	ILE	285	38.158	−25.122	86.695	1.00	34.13
ATOM	1049	O	ILE	285	38.440	−26.313	86.690	1.00	35.08
ATOM	1050	N	VAL	286	38.206	−24.398	87.799	1.00	34.62
ATOM	1051	CA	VAL	286	38.566	−25.024	89.056	1.00	34.98
ATOM	1052	CB	VAL	286	39.403	−24.051	89.931	1.00	34.50
ATOM	1053	CG1	VAL	286	39.593	−24.600	91.335	1.00	31.43
ATOM	1054	CG2	VAL	286	40.743	−23.843	89.292	1.00	34.26
ATOM	1055	C	VAL	286	37.276	−25.413	89.788	1.00	36.26
ATOM	1056	O	VAL	286	36.276	−24.683	89.736	1.00	36.24
ATOM	1057	N	GLN	287	37.290	−26.581	90.425	1.00	35.78
ATOM	1058	CA	GLN	287	36.151	−27.041	91.210	1.00	36.32
ATOM	1059	CB	GLN	287	35.441	−28.214	90.547	1.00	35.89
ATOM	1060	CG	GLN	287	34.369	−28.830	91.444	1.00	35.81
ATOM	1061	CD	GLN	287	33.732	−30.067	90.834	1.00	35.51
ATOM	1062	OE1	GLN	287	34.394	−30.838	90.141	1.00	34.61
ATOM	1063	NE2	GLN	287	32.446	−30.269	91.102	1.00	34.71
ATOM	1064	C	GLN	287	36.673	−27.444	92.595	1.00	36.79
ATOM	1065	O	GLN	287	37.691	−28.131	92.728	1.00	35.75
ATOM	1066	N	LEU	288	35.955	−27.011	93.623	1.00	37.06
ATOM	1067	CA	LEU	288	36.357	−27.248	94.996	1.00	37.17
ATOM	1068	CB	LEU	288	36.146	−25.962	95.805	1.00	34.97
ATOM	1069	CG	LEU	288	36.614	−24.630	95.206	1.00	32.83
ATOM	1070	CD1	LEU	288	35.969	−23.494	95.955	1.00	31.53
ATOM	1071	CD2	LEU	288	38.120	−24.514	95.268	1.00	31.88
ATOM	1072	C	LEU	288	35.653	−28.405	95.707	1.00	38.46
ATOM	1073	O	LEU	288	34.553	−28.817	95.334	1.00	38.22
ATOM	1074	N	ASN	289	36.322	−28.898	96.748	1.00	39.95
ATOM	1075	CA	ASN	289	35.855	−29.984	97.605	1.00	40.45
ATOM	1076	CB	ASN	289	37.057	−30.772	98.117	1.00	40.55
ATOM	1077	CG	ASN	289	38.027	−29.893	98.867	1.00	42.68
ATOM	1078	OD1	ASN	289	38.080	−28.692	98.600	1.00	43.84
ATOM	1079	ND2	ASN	289	38.797	−30.451	99.798	1.00	45.54
ATOM	1080	C	ASN	289	35.136	−29.342	98.793	1.00	40.56
ATOM	1081	O	ASN	289	34.426	−30.011	99.534	1.00	41.39
ATOM	1082	N	THR	290	35.334	−28.037	98.971	1.00	40.82
ATOM	1083	CA	THR	290	34.716	−27.293	100.075	1.00	39.80
ATOM	1084	CB	THR	290	35.738	−26.968	101.168	1.00	40.22
ATOM	1085	OG1	THR	290	36.425	−28.160	101.564	1.00	40.45
ATOM	1086	CG2	THR	290	35.038	−26.345	102.361	1.00	40.96
ATOM	1087	C	THR	290	34.141	−25.953	99.630	1.00	38.45
ATOM	1088	O	THR	290	34.790	−25.211	98.898	1.00	38.51
ATOM	1089	N	SER	291	32.941	−25.626	100.093	1.00	37.41
ATOM	1090	CA	SER	291	32.334	−24.349	99.735	1.00	36.56
ATOM	1091	CB	SER	291	30.834	−24.367	100.019	1.00	37.11
ATOM	1092	OG	SER	291	30.126	−25.014	98.978	1.00	40.14
ATOM	1093	C	SER	291	32.965	−23.232	100.537	1.00	35.66
ATOM	1094	O	SER	291	33.504	−23.480	101.604	1.00	36.84
ATOM	1095	N	VAL	292	32.919	−22.012	100.002	1.00	35.35
ATOM	1096	CA	VAL	292	33.432	−20.806	100.682	1.00	34.01
ATOM	1097	CB	VAL	292	34.734	−20.239	100.018	1.00	32.71
ATOM	1098	CG1	VAL	292	35.059	−18.859	100.597	1.00	27.63
ATOM	1099	CG2	VAL	292	35.907	−21.193	100.257	1.00	29.57
ATOM	1100	C	VAL	292	32.306	−19.784	100.537	1.00	33.54
ATOM	1101	O	VAL	292	31.983	−19.374	99.426	1.00	33.35
ATOM	1102	N	GLU	293	31.691	−19.379	101.639	1.00	33.37
ATOM	1103	CA	GLU	293	30.580	−18.440	101.519	1.00	34.15
ATOM	1104	CB	GLU	293	29.834	−18.262	102.846	1.00	37.09
ATOM	1105	CG	GLU	293	29.612	−19.536	103.649	1.00	44.11
ATOM	1106	CD	GLU	293	30.893	−20.000	104.321	1.00	50.19
ATOM	1107	OE1	GLU	293	31.452	−19.216	105.135	1.00	53.93
ATOM	1108	OE2	GLU	293	31.350	−21.131	104.033	1.00	51.72
ATOM	1109	C	GLU	293	31.013	−17.077	101.036	1.00	32.44
ATOM	1110	O	GLU	293	32.131	−16.632	101.270	1.00	32.48
ATOM	1111	N	ILE	294	30.112	−16.419	100.334	1.00	31.24
ATOM	1112	CA	ILE	294	30.371	−15.080	99.858	1.00	31.02
ATOM	1113	CB	ILE	294	30.909	−15.060	98.407	1.00	28.57
ATOM	1114	CG2	ILE	294	29.896	−15.631	97.459	1.00	28.94
ATOM	1115	CG1	ILE	294	31.228	−13.627	97.999	1.00	26.61
ATOM	1116	CD1	ILE	294	31.771	−13.513	96.622	1.00	26.35
ATOM	1117	C	ILE	294	29.018	−14.391	99.953	1.00	32.34
ATOM	1118	O	ILE	294	28.050	−14.785	99.293	1.00	31.74
ATOM	1119	N	ASN	295	28.943	−13.381	100.811	1.00	33.69
ATOM	1120	CA	ASN	295	27.694	−12.666	101.002	1.00	36.46
ATOM	1121	CB	ASN	295	27.305	−12.678	102.484	1.00	36.40
ATOM	1122	CG	ASN	295	27.390	−14.059	103.099	1.00	36.18
ATOM	1123	OD1	ASN	295	26.783	−15.025	102.619	1.00	32.60

TABLE 1-continued

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	1124	ND2	ASN	295	28.148	−14.155	104.180	1.00	37.07
ATOM	1125	C	ASN	295	27.801	−11.230	100.513	1.00	37.74
ATOM	1126	O	ASN	295	28.729	−10.512	100.889	1.00	37.01
ATOM	1127	N	CYS	296	26.852	−10.822	99.672	1.00	39.54
ATOM	1128	CA	CYS	296	26.853	−9.467	99.142	1.00	40.74
ATOM	1129	C	CYS	296	25.546	−8.761	99.438	1.00	39.17
ATOM	1130	O	CYS	296	24.554	−9.388	99.804	1.00	37.88
ATOM	1131	CB	CYS	296	27.051	−9.468	97.637	1.00	43.38
ATOM	1132	SG	CYS	296	28.393	−10.504	96.984	1.00	50.13
ATOM	1133	N	THR	297	25.548	−7.450	99.241	1.00	38.11
ATOM	1134	CA	THR	297	24.368	−6.654	99.498	1.00	38.11
ATOM	1135	CB	THR	297	24.326	−6.200	100.953	1.00	39.36
ATOM	1136	OG1	THR	297	23.087	−5.522	101.209	1.00	40.89
ATOM	1137	CG2	THR	297	25.500	−5.261	101.241	1.00	37.42
ATOM	1138	C	THR	297	24.348	−5.412	98.629	1.00	37.88
ATOM	1139	O	THR	297	25.400	−4.820	98.356	1.00	37.71
ATOM	1140	N	GLY	298	23.144	−5.011	98.218	1.00	36.98
ATOM	1141	CA	GLY	298	22.990	−3.829	97.389	1.00	36.14
ATOM	1142	C	GLY	298	23.541	−2.583	98.058	1.00	35.80
ATOM	1143	O	GLY	298	23.479	−1.486	97.499	1.00	35.86
ATOM	1144	N	ALA	299	24.079	−2.752	99.262	1.00	35.67
ATOM	1145	CA	ALA	299	24.648	−1.644	100.018	1.00	34.99
ATOM	1146	CB	ALA	299	24.757	−2.001	101.506	1.00	35.85
ATOM	1147	C	ALA	299	26.014	−1.346	99.450	1.00	34.21
ATOM	1148	O	ALA	299	26.628	−0.354	99.809	1.00	34.18
ATOM	1149	N	GLY	329	26.503	−2.232	98.591	1.00	34.17
ATOM	1150	CA	GLY	329	27.785	−1.988	97.965	1.00	35.52
ATOM	1151	C	GLY	329	28.940	−2.931	98.199	1.00	36.98
ATOM	1152	O	GLY	329	30.059	−2.611	97.805	1.00	37.25
ATOM	1153	N	HIS	330	28.709	−4.086	98.817	1.00	39.63
ATOM	1154	CA	HIS	330	29.827	−5.002	99.058	1.00	40.25
ATOM	1155	CB	HIS	330	30.600	−4.559	100.305	1.00	39.30
ATOM	1156	CG	HIS	330	29.818	−4.666	101.578	1.00	40.80
ATOM	1157	CD2	HIS	330	30.171	−5.105	102.807	1.00	42.00
ATOM	1158	ND1	HIS	330	28.516	−4.227	101.693	1.00	41.71
ATOM	1159	CE1	HIS	330	28.105	−4.386	102.936	1.00	41.88
ATOM	1160	NE2	HIS	330	29.090	−4.918	103.636	1.00	42.53
ATOM	1161	C	HIS	330	29.536	−6.504	99.162	1.00	40.37
ATOM	1162	O	HIS	330	28.388	−6.961	99.125	1.00	38.87
ATOM	1163	N	CYS	331	30.630	−7.255	99.255	1.00	41.78
ATOM	1164	CA	CYS	331	30.620	−8.702	99.394	1.00	42.53
ATOM	1165	C	CYS	331	31.656	−9.068	100.444	1.00	41.74
ATOM	1166	O	CYS	331	32.783	−8.569	100.418	1.00	40.56
ATOM	1167	CB	CYS	331	31.022	−9.387	98.105	1.00	44.95
ATOM	1168	SG	CYS	331	29.923	−9.199	96.679	1.00	48.68
ATOM	1169	N	ASN	332	31.273	−9.945	101.359	1.00	40.38
ATOM	1170	CA	ASN	332	32.189	−10.364	102.386	1.00	40.12
ATOM	1171	CB	ASN	332	31.556	−10.224	103.766	1.00	42.37
ATOM	1172	CG	ASN	332	31.322	−8.777	104.151	1.00	44.33
ATOM	1173	OD1	ASN	332	32.169	−7.911	103.909	1.00	44.82
ATOM	1174	ND2	ASN	332	30.175	−8.509	104.768	1.00	44.71
ATOM	1175	C	ASN	332	32.586	−11.795	102.141	1.00	39.72
ATOM	1176	O	ASN	332	31.793	−12.607	101.661	1.00	38.64
ATOM	1177	N	ILE	333	33.834	−12.088	102.472	1.00	40.00
ATOM	1178	CA	ILE	333	34.387	−13.416	102.317	1.00	40.51
ATOM	1179	CB	ILE	333	35.109	−13.544	100.985	1.00	40.85
ATOM	1180	CG2	ILE	333	35.936	−14.821	100.957	1.00	42.34
ATOM	1181	CG1	ILE	333	34.089	−13.520	99.855	1.00	40.11
ATOM	1182	CD1	ILE	333	34.709	−13.314	98.515	1.00	41.51
ATOM	1183	C	ILE	333	35.381	−13.647	103.432	1.00	40.36
ATOM	1184	O	ILE	333	36.201	−12.780	103.723	1.00	40.87
ATOM	1185	N	ALA	334	35.299	−14.812	104.060	1.00	39.60
ATOM	1186	CA	ALA	334	36.204	−15.156	105.147	1.00	38.54
ATOM	1187	CB	ALA	334	35.762	−16.471	105.757	1.00	41.22
ATOM	1189	C	ALA	334	37.614	−15.275	104.590	1.00	36.87
ATOM	1190	O	ALA	334	37.883	−16.097	103.715	1.00	33.76
ATOM	1191	N	ARG	335	38.510	−14.444	105.102	1.00	36.58
ATOM	1192	CA	ARG	335	39.883	−14.434	104.628	1.00	37.37
ATOM	1193	CB	ARG	335	40.669	−13.333	105.326	1.00	36.39
ATOM	1194	CG	ARG	335	42.094	−13.213	104.847	1.00	38.55
ATOM	1195	CD	ARG	335	42.801	−12.047	105.516	1.00	42.33
ATOM	1196	NE	ARG	335	42.268	−10.762	105.079	1.00	44.44
ATOM	1197	CZ	ARG	335	42.375	−10.305	103.837	1.00	45.53
ATOM	1198	NH1	ARG	335	42.999	−11.034	102.924	1.00	46.03
ATOM	1199	NH2	ARG	335	41.856	−9.127	103.509	1.00	46.38
ATOM	1200	C	ARG	335	40.558	−15.774	104.855	1.00	38.44
ATOM	1201	O	ARG	335	41.318	−16.259	104.012	1.00	39.73
ATOM	1202	N	ALA	336	40.276	−16.375	106.000	1.00	38.31

TABLE 1-continued

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	1203	CA	ALA	336	40.849	−17.664	106.347	1.00	38.08
ATOM	1204	CB	ALA	336	40.436	−18.025	107.750	1.00	38.47
ATOM	1205	C	ALA	336	40.393	−18.754	105.371	1.00	38.68
ATOM	1206	O	ALA	336	41.214	−19.420	104.728	1.00	37.19
ATOM	1207	N	LYS	337	39.078	−18.934	105.271	1.00	39.27
ATOM	1208	CA	LYS	337	38.523	−19.932	104.376	1.00	39.56
ATOM	1209	CB	LYS	337	37.003	−19.839	104.339	1.00	40.15
ATOM	1210	CG	LYS	337	36.316	−20.161	105.642	1.00	42.29
ATOM	1211	CD	LYS	337	34.875	−20.564	105.373	1.00	44.78
ATOM	1212	CE	LYS	337	34.130	−20.917	106.647	1.00	46.19
ATOM	1213	NZ	LYS	337	32.829	−21.580	106.331	1.00	47.33
ATOM	1214	C	LYS	337	39.066	−19.744	102.974	1.00	39.65
ATOM	1215	O	LYS	337	39.464	−20.699	102.329	1.00	39.54
ATOM	1216	N	TRP	338	39.086	−18.506	102.501	1.00	41.16
ATOM	1217	CA	TRP	338	39.585	−18.252	101.159	1.00	43.17
ATOM	1218	CB	TRP	338	39.319	−16.817	100.725	1.00	40.60
ATOM	1219	CG	TRP	338	39.685	−16.593	99.290	1.00	37.38
ATOM	1220	CD2	TRP	338	38.950	−17.042	98.154	1.00	36.44
ATOM	1221	CE2	TRP	338	39.646	−16.608	97.004	1.00	36.35
ATOM	1222	CE3	TRP	338	37.765	−17.774	97.993	1.00	35.17
ATOM	1223	CD1	TRP	338	40.777	−15.928	98.803	1.00	36.91
ATOM	1224	NE1	TRP	338	40.761	−15.930	97.427	1.00	35.85
ATOM	1225	CZ2	TRP	338	39.194	−16.878	95.714	1.00	36.13
ATOM	1226	CZ3	TRP	338	37.316	−18.044	96.712	1.00	34.19
ATOM	1227	CH2	TRP	338	38.028	−17.596	95.588	1.00	35.36
ATOM	1228	C	TRP	338	41.069	−18.515	101.032	1.00	46.01
ATOM	1229	O	TRP	338	41.523	−19.094	100.045	1.00	46.74
ATOM	1230	N	ASN	339	41.836	−18.083	102.020	1.00	48.56
ATOM	1231	CA	ASN	339	43.260	−18.298	101.949	1.00	51.16
ATOM	1232	CB	ASN	339	43.957	−17.688	103.143	1.00	56.16
ATOM	1233	CG	ASN	339	45.435	−17.890	103.080	1.00	63.56
ATOM	1234	OD1	ASN	339	46.073	−17.445	102.132	1.00	64.19
ATOM	1235	ND2	ASN	339	45.995	−18.566	104.079	1.00	71.86
ATOM	1236	C	ASN	339	43.605	−19.777	101.860	1.00	50.86
ATOM	1237	O	ASN	339	44.597	−20.144	101.242	1.00	50.87
ATOM	1238	N	ASN	340	42.800	−20.634	102.478	1.00	50.99
ATOM	1239	CA	ASN	340	43.071	−22.067	102.407	1.00	51.70
ATOM	1240	CB	ASN	340	42.192	−22.862	103.371	1.00	54.49
ATOM	1241	CG	ASN	340	42.634	−22.724	104.808	1.00	58.41
ATOM	1242	OD1	ASN	340	43.787	−23.014	105.151	1.00	60.24
ATOM	1243	ND2	ASN	340	41.719	−22.288	105.666	1.00	60.46
ATOM	1244	C	ASN	340	42.781	−22.540	101.004	1.00	50.85
ATOM	1245	O	ASN	340	43.537	−23.331	100.433	1.00	51.84
ATOM	1246	N	THR	341	41.669	−22.058	100.456	1.00	48.01
ATOM	1247	CA	THR	341	41.269	−22.434	99.116	1.00	45.14
ATOM	1248	CB	THR	341	39.989	−21.678	98.686	1.00	44.64
ATOM	1249	OG1	THR	341	38.964	−21.883	99.667	1.00	42.76
ATOM	1250	CG2	THR	341	39.488	−22.189	97.334	1.00	42.30
ATOM	1251	C	THR	341	42.416	−22.124	98.163	1.00	44.38
ATOM	1252	O	THR	341	42.821	−22.977	97.377	1.00	42.42
ATOM	1253	N	LEU	342	42.959	−20.911	98.249	1.00	44.37
ATOM	1254	CA	LEU	342	44.061	−20.531	97.373	1.00	44.41
ATOM	1255	CB	LEU	342	44.506	−19.087	97.635	1.00	43.85
ATOM	1256	CG	LEU	342	43.507	−17.950	97.335	1.00	44.37
ATOM	1257	CD1	LEU	342	44.162	−16.606	97.623	1.00	43.63
ATOM	1258	CD2	LEU	342	43.050	−17.996	95.894	1.00	43.05
ATOM	1259	C	LEU	342	45.245	−21.489	97.514	1.00	44.72
ATOM	1260	O	LEU	342	45.858	−21.851	96.515	1.00	45.32
ATOM	1261	N	LYS	343	45.567	−21.917	98.735	1.00	44.30
ATOM	1262	CA	LYS	343	46.678	−22.854	98.921	1.00	43.59
ATOM	1263	CB	LYS	343	46.928	−23.141	100.406	1.00	44.40
ATOM	1264	CG	LYS	343	48.240	−23.898	100.658	1.00	46.15
ATOM	1265	CD	LYS	343	48.413	−24.323	102.114	1.00	49.16
ATOM	1266	CE	LYS	343	48.578	−23.136	103.080	1.00	52.93
ATOM	1267	NZ	LYS	343	49.893	−22.400	103.011	1.00	53.31
ATOM	1268	C	LYS	343	46.388	−24.173	98.206	1.00	42.93
ATOM	1269	O	LYS	343	47.242	−24.709	97.493	1.00	42.92
ATOM	1270	N	GLN	344	45.179	−24.693	98.396	1.00	42.56
ATOM	1271	CA	GLN	344	44.778	−25.957	97.777	1.00	42.99
ATOM	1272	CB	GLN	344	43.385	−26.373	98.241	1.00	41.89
ATOM	1273	CG	GLN	344	43.168	−26.344	99.725	1.00	42.51
ATOM	1274	CD	GLN	344	41.735	−26.664	100.081	1.00	43.88
ATOM	1275	OE1	GLN	344	41.243	−27.736	99.755	1.00	45.09
ATOM	1276	NE2	GLN	344	41.052	−25.728	100.744	1.00	44.66
ATOM	1277	C	GLN	344	44.762	−25.908	96.254	1.00	43.37
ATOM	1278	O	GLN	344	44.870	−26.952	95.612	1.00	44.99
ATOM	1279	N	ILE	345	44.602	−24.714	95.679	1.00	43.39
ATOM	1280	CA	ILE	345	44.559	−24.567	94.218	1.00	42.52

TABLE 1-continued

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	1281	CB	ILE	345	43.705	−23.359	93.765	1.00	40.62
ATOM	1282	CG2	ILE	345	43.479	−23.434	92.280	1.00	39.28
ATOM	1283	CG1	ILE	345	42.332	−23.377	94.419	1.00	40.32
ATOM	1284	CD1	ILE	345	41.517	−22.134	94.104	1.00	40.02
ATOM	1285	C	ILE	345	45.946	−24.394	93.611	1.00	43.06
ATOM	1286	O	ILE	345	46.281	−25.050	92.626	1.00	42.31
ATOM	1287	N	ALA	346	46.745	−23.496	94.184	1.00	44.37
ATOM	1288	CA	ALA	346	48.097	−23.273	93.683	1.00	45.42
ATOM	1289	CB	ALA	346	48.836	−22.275	94.556	1.00	43.26
ATOM	1290	C	ALA	346	48.771	−24.630	93.743	1.00	46.84
ATOM	1291	O	ALA	346	49.582	−24.981	92.886	1.00	47.39
ATOM	1292	N	SER	347	48.408	−25.396	94.765	1.00	47.70
ATOM	1293	CA	SER	347	48.950	−26.722	94.934	1.00	49.50
ATOM	1294	CB	SER	347	48.337	−27.376	96.160	1.00	51.28
ATOM	1295	OG	SER	347	48.850	−28.685	96.317	1.00	56.57
ATOM	1296	C	SER	347	48.662	−27.558	93.683	1.00	49.94
ATOM	1297	O	SER	347	49.586	−28.029	93.030	1.00	50.34
ATOM	1298	N	LYS	348	47.382	−27.728	93.351	1.00	50.78
ATOM	1299	CA	LYS	348	46.962	−28.494	92.170	1.00	51.63
ATOM	1300	CB	LYS	348	45.432	−28.577	92.098	1.00	51.50
ATOM	1301	CG	LYS	348	44.791	−29.584	93.032	1.00	51.75
ATOM	1302	CD	LYS	348	45.064	−30.988	92.556	1.00	50.85
ATOM	1303	CE	LYS	348	44.542	−32.004	93.543	1.00	50.69
ATOM	1304	NZ	LYS	348	44.944	−33.375	93.137	1.00	50.94
ATOM	1305	C	LYS	348	47.463	−27.869	90.869	1.00	52.28
ATOM	1306	O	LYS	348	47.585	−28.535	89.840	1.00	52.16
ATOM	1307	N	LEU	349	47.738	−26.579	90.908	1.00	53.08
ATOM	1308	CA	LEU	349	48.203	−25.921	89.713	1.00	55.10
ATOM	1309	CB	LEU	349	48.002	−24.402	89.824	1.00	53.88
ATOM	1310	CG	LEU	349	46.572	−23.855	89.720	1.00	50.78
ATOM	1311	CD1	LEU	349	46.600	−22.369	89.985	1.00	49.11
ATOM	1312	CD2	LEU	349	45.977	−24.134	88.345	1.00	47.99
ATOM	1313	C	LEU	349	49.655	−26.259	89.402	1.00	57.08
ATOM	1314	O	LEU	349	49.959	−26.620	88.270	1.00	57.54
ATOM	1315	N	ARG	350	50.555	−26.159	90.383	1.00	59.82
ATOM	1316	CA	ARG	350	51.961	−26.476	90.114	1.00	63.18
ATOM	1317	CB	ARG	350	52.866	−26.042	91.266	1.00	64.31
ATOM	1318	CG	ARG	350	52.410	−26.471	92.624	1.00	68.34
ATOM	1319	CD	ARG	350	53.595	−26.540	93.563	1.00	72.56
ATOM	1320	NE	ARG	350	54.525	−25.427	93.375	1.00	76.31
ATOM	1321	CZ	ARG	350	55.714	−25.343	93.974	1.00	78.63
ATOM	1322	NH1	ARG	350	56.113	−26.308	94.798	1.00	78.98
ATOM	1323	NH2	ARG	350	56.511	−24.301	93.751	1.00	79.29
ATOM	1324	C	ARG	350	52.125	−27.968	89.851	1.00	64.33
ATOM	1325	O	ARG	350	53.102	−28.405	89.234	1.00	65.71
ATOM	1326	N	GLU	351	51.148	−28.741	90.312	1.00	64.55
ATOM	1327	CA	GLU	351	51.126	−30.180	90.112	1.00	63.62
ATOM	1328	CB	GLU	351	49.963	−30.778	90.898	1.00	66.10
ATOM	1329	CG	GLU	351	49.896	−32.290	90.914	1.00	70.44
ATOM	1330	CD	GLU	351	48.652	−32.811	91.628	1.00	72.67
ATOM	1331	OE1	GLU	351	47.536	−32.631	91.090	1.00	74.72
ATOM	1332	OE2	GLU	351	48.787	−33.397	92.726	1.00	73.74
ATOM	1333	C	GLU	351	50.941	−30.456	88.615	1.00	61.98
ATOM	1334	O	GLU	351	51.096	−31.588	88.162	1.00	61.55
ATOM	1335	N	GLN	352	50.602	−29.409	87.861	1.00	60.65
ATOM	1336	CA	GLN	352	50.397	−29.505	86.415	1.00	59.13
ATOM	1337	CB	GLN	352	48.942	−29.191	86.053	1.00	56.49
ATOM	1338	CG	GLN	352	48.699	−29.115	84.545	1.00	53.84
ATOM	1339	CD	GLN	352	47.501	−29.931	84.092	1.00	52.61
ATOM	1340	OE1	GLN	352	47.280	−30.122	82.895	1.00	49.99
ATOM	1341	NE2	GLN	352	46.722	−30.416	85.048	1.00	52.71
ATOM	1342	C	GLN	352	51.320	−28.619	85.563	1.00	59.46
ATOM	1343	O	GLN	352	51.494	−28.873	84.375	1.00	58.99
ATOM	1344	N	PHE	353	51.908	−27.585	86.152	1.00	60.32
ATOM	1345	CA	PHE	353	52.796	−26.714	85.390	1.00	62.07
ATOM	1346	CB	PHE	353	52.262	−25.277	85.366	1.00	61.62
ATOM	1347	CG	PHE	353	50.957	−25.129	84.641	1.00	61.43
ATOM	1348	CD1	PHE	353	49.752	−25.258	85.316	1.00	61.91
ATOM	1349	CD2	PHE	353	50.930	−24.905	83.268	1.00	62.10
ATOM	1350	CE1	PHE	353	48.532	−25.168	84.633	1.00	62.04
ATOM	1351	CE2	PHE	353	49.717	−24.815	82.576	1.00	61.69
ATOM	1352	CZ	PHE	353	48.516	−24.948	83.261	1.00	61.58
ATOM	1353	C	PHE	353	54.229	−26.713	85.915	1.00	64.18
ATOM	1354	O	PHE	353	55.046	−25.880	85.511	1.00	65.29
ATOM	1355	N	GLY	354	54.540	−27.642	86.812	1.00	64.51
ATOM	1356	CA	GLY	354	55.888	−27.697	87.340	1.00	65.83
ATOM	1357	C	GLY	354	55.948	−27.501	88.838	1.00	67.15
ATOM	1358	O	GLY	354	55.746	−26.395	89.346	1.00	67.01

TABLE 1-continued

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	1359	N	ASN	355	56.237	−28.589	89.544	1.00	67.83
ATOM	1360	CA	ASN	355	56.329	−28.576	90.994	1.00	68.59
ATOM	1361	CB	ASN	355	56.573	−29.995	91.513	1.00	70.55
ATOM	1362	CG	ASN	355	55.301	−30.841	91.533	1.00	72.72
ATOM	1363	OD1	ASN	355	55.353	−32.048	91.776	1.00	74.24
ATOM	1364	ND2	ASN	355	54.155	−30.208	91.290	1.00	72.93
ATOM	1365	C	ASN	355	57.413	−27.644	91.509	1.00	68.43
ATOM	1366	O	ASN	355	57.574	−27.480	92.716	1.00	69.01
ATOM	1367	N	ASN	356	58.155	−27.032	90.597	1.00	67.89
ATOM	1368	CA	ASN	356	59.214	−26.114	90.988	1.00	67.81
ATOM	1369	CB	ASN	356	60.495	−26.427	90.209	1.00	68.67
ATOM	1370	CG	ASN	356	61.021	−27.836	90.475	1.00	68.82
ATOM	1371	OD1	ASN	356	62.067	−28.223	89.956	1.00	68.37
ATOM	1372	ND2	ASN	356	60.294	−28.605	91.282	1.00	69.10
ATOM	1373	C	ASN	356	58.756	−24.690	90.698	1.00	67.61
ATOM	1374	O	ASN	356	59.399	−23.719	91.109	1.00	68.06
ATOM	1375	N	LYS	357	57.632	−24.588	89.989	1.00	66.72
ATOM	1376	CA	LYS	357	57.028	−23.308	89.603	1.00	64.44
ATOM	1377	CB	LYS	357	55.979	−23.528	88.503	1.00	65.55
ATOM	1378	CG	LYS	357	56.524	−23.915	87.138	1.00	66.86
ATOM	1379	CD	LYS	357	57.287	−22.758	86.511	1.00	68.57
ATOM	1380	CE	LYS	357	57.563	−22.990	85.033	1.00	69.07
ATOM	1381	NZ	LYS	357	56.297	−23.017	84.250	1.00	69.35
ATOM	1382	C	LYS	357	56.353	−22.582	90.769	1.00	61.58
ATOM	1383	O	LYS	357	55.735	−23.211	91.630	1.00	61.43
ATOM	1384	N	THR	358	56.463	−21.257	90.778	1.00	57.89
ATOM	1385	CA	THR	358	55.851	−20.434	91.817	1.00	54.10
ATOM	1386	CB	THR	358	56.721	−19.218	92.155	1.00	53.27
ATOM	1387	OG1	THR	358	57.983	−19.666	92.659	1.00	52.66
ATOM	1388	CG2	THR	358	56.045	−18.358	93.202	1.00	53.26
ATOM	1389	C	THR	358	54.500	−19.944	91.317	1.00	51.75
ATOM	1390	O	THR	358	54.412	−19.332	90.257	1.00	51.73
ATOM	1391	N	ILE	359	53.452	−20.221	92.084	1.00	48.72
ATOM	1392	CA	ILE	359	52.100	−19.832	91.707	1.00	45.84
ATOM	1393	CB	ILE	359	51.054	−20.849	92.247	1.00	44.27
ATOM	1394	CG2	ILE	359	49.667	−20.470	91.782	1.00	43.26
ATOM	1395	CG1	ILE	359	51.387	−22.258	91.767	1.00	42.29
ATOM	1396	CD1	ILE	359	51.461	−22.383	90.264	1.00	42.14
ATOM	1397	C	ILE	359	51.732	−18.450	92.228	1.00	45.04
ATOM	1398	O	ILE	359	51.703	−18.231	93.438	1.00	44.85
ATOM	1399	N	ILE	360	51.451	−17.528	91.309	1.00	44.16
ATOM	1400	CA	ILE	360	51.058	−16.163	91.667	1.00	43.62
ATOM	1401	CB	ILE	360	51.930	−15.086	90.968	1.00	41.87
ATOM	1402	CG2	ILE	360	51.486	−13.711	91.399	1.00	41.80
ATOM	1403	CG1	ILE	360	53.401	−15.280	91.297	1.00	40.00
ATOM	1404	CD1	ILE	360	54.176	−15.839	90.143	1.00	41.00
ATOM	1405	C	ILE	360	49.620	−15.898	91.231	1.00	43.95
ATOM	1406	O	ILE	360	49.205	−16.302	90.139	1.00	43.81
ATOM	1407	N	PHE	361	48.859	−15.215	92.076	1.00	43.88
ATOM	1408	CA	PHE	361	47.486	−14.886	91.721	1.00	45.05
ATOM	1409	CB	PHE	361	46.510	−15.333	92.818	1.00	44.55
ATOM	1410	CG	PHE	361	46.421	−16.832	92.991	1.00	43.16
ATOM	1411	CD1	PHE	361	47.047	−17.463	94.059	1.00	41.83
ATOM	1412	CD2	PHE	361	45.723	−17.609	92.074	1.00	41.08
ATOM	1413	CE1	PHE	361	46.978	−18.835	94.207	1.00	39.99
ATOM	1414	CE2	PHE	361	45.650	−18.978	92.216	1.00	39.19
ATOM	1415	CZ	PHE	361	46.280	−19.591	93.284	1.00	39.63
ATOM	1416	C	PHE	361	47.370	−13.381	91.521	1.00	45.78
ATOM	1417	O	PHE	361	47.599	−12.619	92.456	1.00	48.15
ATOM	1418	N	LYS	362	47.032	−12.946	90.310	1.00	44.97
ATOM	1419	CA	LYS	362	46.880	−11.519	90.044	1.00	45.08
ATOM	1420	CB	LYS	362	47.836	−11.058	88.946	1.00	46.05
ATOM	1421	CG	LYS	362	49.297	−11.075	89.307	1.00	46.12
ATOM	1422	CD	LYS	362	50.116	−10.559	88.147	1.00	44.35
ATOM	1423	CE	LYS	362	51.572	−10.516	88.524	1.00	45.15
ATOM	1424	NZ	LYS	362	51.752	−9.677	89.742	1.00	45.33
ATOM	1425	C	LYS	362	45.461	−11.179	89.611	1.00	45.45
ATOM	1426	O	LYS	362	44.719	−12.042	89.138	1.00	45.50
ATOM	1427	N	GLN	363	45.102	−9.907	89.759	1.00	45.24
ATOM	1428	CA	GLN	363	43.781	−9.411	89.380	1.00	44.82
ATOM	1429	CB	GLN	363	43.639	−7.954	89.818	1.00	44.59
ATOM	1430	CG	GLN	363	44.807	−7.064	89.415	1.00	45.02
ATOM	1431	CD	GLN	363	44.428	−5.595	89.372	1.00	45.87
ATOM	1432	OE1	GLN	363	43.555	−5.199	88.600	1.00	47.42
ATOM	1433	NE2	GLN	363	45.079	−4.780	90.199	1.00	44.92
ATOM	1434	C	GLN	363	43.527	−9.506	87.872	1.00	45.01
ATOM	1435	O	GLN	363	44.459	−9.717	87.090	1.00	44.87
ATOM	1436	N	SER	364	42.263	−9.350	87.470	1.00	44.60

TABLE 1-continued

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	1437	CA	SER	364	41.895	−9.394	86.052	1.00	43.07
ATOM	1438	CB	SER	364	40.444	−8.956	85.850	1.00	41.38
ATOM	1439	OG	SER	364	40.073	−9.076	84.487	1.00	39.74
ATOM	1440	C	SER	364	42.803	−8.436	85.297	1.00	43.26
ATOM	1441	O	SER	364	43.104	−7.347	85.793	1.00	43.43
ATOM	1442	N	SER	365	43.234	−8.829	84.102	1.00	42.44
ATOM	1443	CA	SER	365	44.116	−7.979	83.312	1.00	41.33
ATOM	1444	CB	SER	365	45.140	−8.846	82.566	1.00	41.58
ATOM	1445	OG	SER	365	44.530	−10.000	82.013	1.00	44.41
ATOM	1446	C	SER	365	43.445	−6.996	82.328	1.00	40.25
ATOM	1447	O	SER	365	44.132	−6.413	81.491	1.00	42.93
ATOM	1448	N	GLY	366	42.130	−6.794	82.424	1.00	36.76
ATOM	1449	CA	GLY	366	41.473	−5.860	81.524	1.00	32.05
ATOM	1450	C	GLY	366	40.321	−6.445	80.741	1.00	31.17
ATOM	1451	O	GLY	366	40.099	−7.652	80.762	1.00	31.00
ATOM	1452	N	GLY	367	39.581	−5.585	80.044	1.00	30.27
ATOM	1453	CA	GLY	367	38.441	−6.040	79.258	1.00	29.70
ATOM	1454	C	GLY	367	37.117	−5.504	79.777	1.00	29.80
ATOM	1455	O	GLY	367	37.087	−4.691	80.702	1.00	31.08
ATOM	1456	N	ASP	368	36.015	−5.954	79.192	1.00	29.13
ATOM	1457	CA	ASP	368	34.699	−5.507	79.626	1.00	31.89
ATOM	1458	CB	ASP	368	33.604	−6.305	78.909	1.00	35.79
ATOM	1459	CG	ASP	368	33.588	−6.073	77.397	1.00	39.65
ATOM	1460	OD1	ASP	368	32.826	−6.784	76.700	1.00	40.00
ATOM	1461	OD2	ASP	368	34.328	−5.187	76.908	1.00	42.73
ATOM	1462	C	ASP	368	34.527	−5.663	81.144	1.00	32.13
ATOM	1463	O	ASP	368	35.139	−6.527	81.757	1.00	32.82
ATOM	1464	N	PRO	369	33.684	−4.821	81.766	1.00	31.85
ATOM	1465	CD	PRO	369	32.993	−3.693	81.120	1.00	30.96
ATOM	1466	CA	PRO	369	33.404	−4.838	83.207	1.00	31.36
ATOM	1467	CB	PRO	369	32.265	−3.842	83.337	1.00	31.63
ATOM	1468	CG	PRO	369	32.613	−2.833	82.289	1.00	31.18
ATOM	1469	C	PRO	369	33.007	−6.203	83.739	1.00	30.91
ATOM	1470	O	PRO	369	33.485	−6.649	84.778	1.00	31.90
ATOM	1471	N	GLU	370	32.112	−6.858	83.023	1.00	30.62
ATOM	1472	CA	GLU	370	31.627	−8.162	83.415	1.00	31.59
ATOM	1473	CB	GLU	370	30.534	−8.585	82.440	1.00	32.54
ATOM	1474	CG	GLU	370	29.303	−7.659	82.445	1.00	34.81
ATOM	1475	CD	GLU	370	29.452	−6.366	81.622	1.00	34.63
ATOM	1476	OE1	GLU	370	28.495	−5.567	81.601	1.00	34.16
ATOM	1477	OE2	GLU	370	30.503	−6.142	80.991	1.00	35.90
ATOM	1478	C	GLU	370	32.718	−9.245	83.519	1.00	32.22
ATOM	1479	O	GLU	370	32.528	−10.259	84.194	1.00	33.09
ATOM	1480	N	ILE	371	33.857	−9.016	82.864	1.00	31.32
ATOM	1481	CA	ILE	371	34.999	−9.943	82.861	1.00	28.31
ATOM	1482	CB	ILE	371	35.579	−10.085	81.422	1.00	28.08
ATOM	1483	CG2	ILE	371	37.098	−10.089	81.437	1.00	27.78
ATOM	1484	CG1	ILE	371	35.037	−11.343	80.779	1.00	28.02
ATOM	1485	CD1	ILE	371	33.555	−11.407	80.819	1.00	30.47
ATOM	1486	C	ILE	371	36.133	−9.506	83.797	1.00	27.21
ATOM	1487	O	ILE	371	36.974	−10.315	84.191	1.00	26.14
ATOM	1488	N	VAL	372	36.158	−8.224	84.138	1.00	26.33
ATOM	1489	CA	VAL	372	37.194	−7.676	85.007	1.00	27.67
ATOM	1490	CB	VAL	372	37.487	−6.200	84.678	1.00	27.14
ATOM	1491	CG1	VAL	372	38.468	−5.636	85.687	1.00	24.67
ATOM	1492	CG2	VAL	372	38.035	−6.078	83.258	1.00	26.38
ATOM	1493	C	VAL	372	36.807	−7.739	86.467	1.00	28.75
ATOM	1494	O	VAL	372	37.662	−7.792	87.355	1.00	29.82
ATOM	1495	N	THR	373	35.506	−7.734	86.709	1.00	29.47
ATOM	1496	CA	THR	373	34.983	−7.770	88.066	1.00	28.66
ATOM	1497	CB	THR	373	34.079	−6.554	88.296	1.00	27.96
ATOM	1498	OG1	THR	373	32.916	−6.668	87.472	1.00	28.85
ATOM	1499	CG2	THR	373	34.801	−5.285	87.888	1.00	26.32
ATOM	1500	C	THR	373	34.166	−9.042	88.221	1.00	28.00
ATOM	1501	O	THR	373	33.806	−9.658	87.211	1.00	28.23
ATOM	1502	N	HIS	374	33.902	−9.453	89.466	1.00	27.55
ATOM	1503	CA	HIS	374	33.075	−10.642	89.723	1.00	26.55
ATOM	1504	CB	HIS	374	33.245	−11.149	91.162	1.00	25.93
ATOM	1505	CG	HIS	374	32.187	−12.121	91.591	1.00	26.09
ATOM	1506	CD2	HIS	374	31.358	−12.121	92.663	1.00	26.47
ATOM	1507	ND1	HIS	374	31.866	−13.243	90.863	1.00	27.70
ATOM	1508	CE1	HIS	374	30.881	−13.892	91.463	1.00	25.87
ATOM	1509	NE2	HIS	374	30.555	−13.232	92.557	1.00	25.26
ATOM	1510	C	HIS	374	31.654	−10.153	89.476	1.00	25.07
ATOM	1511	O	HIS	374	31.071	−9.423	90.268	1.00	25.98
ATOM	1512	N	TRP	375	31.132	−10.546	88.332	1.00	24.08
ATOM	1513	CA	TRP	375	29.829	−10.142	87.866	1.00	24.74
ATOM	1514	CB	TRP	375	29.960	−9.781	86.383	1.00	25.04

TABLE 1-continued

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	1515	CG	TRP	375	28.702	−9.478	85.662	1.00	25.75
ATOM	1516	CD2	TRP	375	28.096	−10.271	84.645	1.00	25.29
ATOM	1517	CE2	TRP	375	26.916	−9.609	84.235	1.00	24.75
ATOM	1518	CE3	TRP	375	28.430	−11.488	84.037	1.00	26.21
ATOM	1519	CD1	TRP	375	27.896	−8.390	85.828	1.00	26.87
ATOM	1520	NE1	TRP	375	26.819	−8.457	84.972	1.00	25.73
ATOM	1521	CZ2	TRP	375	26.075	−10.111	83.256	1.00	25.28
ATOM	1522	CZ3	TRP	375	27.591	−11.996	83.057	1.00	25.89
ATOM	1523	CH2	TRP	375	26.424	−11.307	82.678	1.00	26.36
ATOM	1524	C	TRP	375	28.844	−11.268	88.060	1.00	26.93
ATOM	1525	O	TRP	375	29.098	−12.411	87.687	1.00	27.40
ATOM	1526	N	PHE	376	27.707	−10.946	88.646	1.00	28.62
ATOM	1527	CA	PHE	376	26.693	−11.954	88.863	1.00	31.15
ATOM	1528	CB	PHE	376	26.989	−12.736	90.130	1.00	30.11
ATOM	1529	CG	PHE	376	27.135	−11.877	91.332	1.00	30.51
ATOM	1530	CD1	PHE	376	28.310	−11.162	91.547	1.00	30.86
ATOM	1531	CD2	PHE	376	26.090	−11.754	92.241	1.00	30.19
ATOM	1532	CE1	PHE	376	28.448	−10.331	92.652	1.00	29.71
ATOM	1533	CE2	PHE	376	26.209	−10.929	93.352	1.00	30.22
ATOM	1534	CZ	PHE	376	27.393	−10.213	93.560	1.00	30.89
ATOM	1535	C	PHE	376	25.355	−11.279	88.996	1.00	32.83
ATOM	1536	O	PHE	376	25.280	−10.086	89.252	1.00	33.02
ATOM	1537	N	ASN	377	24.299	−12.051	88.809	1.00	35.69
ATOM	1538	CA	ASN	377	22.963	−11.521	88.929	1.00	40.61
ATOM	1539	CB	ASN	377	22.046	−12.178	87.913	1.00	44.38
ATOM	1540	CG	ASN	377	20.647	−11.597	87.940	1.00	48.66
ATOM	1541	OD1	ASN	377	20.426	−10.443	87.542	1.00	48.26
ATOM	1542	ND2	ASN	377	19.689	−12.393	88.420	1.00	51.13
ATOM	1543	C	ASN	377	22.491	−11.855	90.327	1.00	42.23
ATOM	1544	O	ASN	377	22.892	−12.864	90.876	1.00	44.30
ATOM	1545	N	CYS	378	21.643	−11.009	90.901	1.00	44.55
ATOM	1546	CA	CYS	378	21.117	−11.220	92.251	1.00	45.14
ATOM	1547	C	CYS	378	19.934	−10.282	92.488	1.00	43.00
ATOM	1548	O	CYS	378	20.075	−9.066	92.377	1.00	41.28
ATOM	1549	CB	CYS	378	22.203	−10.950	93.302	1.00	49.09
ATOM	1550	SG	CYS	378	21.506	−11.015	94.982	1.00	57.12
ATOM	1551	N	GLY	379	18.773	−10.842	92.819	1.00	41.22
ATOM	1552	CA	GLY	379	17.600	−10.011	93.025	1.00	40.83
ATOM	1553	C	GLY	379	17.246	−9.244	91.753	1.00	40.79
ATOM	1554	O	GLY	379	16.556	−8.222	91.784	1.00	41.26
ATOM	1555	N	GLY	380	17.718	−9.738	90.619	1.00	39.72
ATOM	1556	CA	GLY	380	17.442	−9.059	89.372	1.00	39.79
ATOM	1557	C	GLY	380	18.461	−7.986	89.005	1.00	39.81
ATOM	1558	O	GLY	380	18.544	−7.578	87.842	1.00	39.98
ATOM	1559	N	GLU	381	19.243	−7.524	89.979	1.00	39.10
ATOM	1560	CA	GLU	381	20.244	−6.489	89.712	1.00	38.16
ATOM	1561	CB	GLU	381	20.440	−5.607	90.940	1.00	38.52
ATOM	1562	CG	GLU	381	19.162	−5.139	91.601	1.00	41.28
ATOM	1563	CD	GLU	381	18.327	−4.226	90.728	1.00	43.40
ATOM	1564	OE1	GLU	381	18.904	−3.420	89.963	1.00	44.79
ATOM	1565	OE2	GLU	381	17.083	−4.303	90.827	1.00	44.94
ATOM	1566	C	GLU	381	21.583	−7.123	89.353	1.00	36.75
ATOM	1567	O	GLU	381	21.890	−8.228	89.796	1.00	34.31
ATOM	1568	N	PHE	382	22.382	−6.421	88.556	1.00	34.93
ATOM	1569	CA	PHE	382	23.684	−6.937	88.174	1.00	34.11
ATOM	1570	CB	PHE	382	23.955	−6.685	86.699	1.00	35.03
ATOM	1571	CG	PHE	382	23.062	−7.450	85.796	1.00	35.63
ATOM	1572	CD1	PHE	382	21.868	−6.901	85.351	1.00	37.48
ATOM	1573	CD2	PHE	382	23.392	−8.740	85.415	1.00	37.08
ATOM	1574	CE1	PHE	382	21.007	−7.628	84.534	1.00	38.27
ATOM	1575	CE2	PHE	382	22.543	−9.482	84.600	1.00	38.30
ATOM	1576	CZ	PHE	382	21.343	−8.924	84.156	1.00	38.80
ATOM	1577	C	PHE	382	24.800	−6.316	88.992	1.00	33.85
ATOM	1578	O	PHE	382	25.066	−5.122	88.892	1.00	33.66
ATOM	1579	N	PHE	383	25.463	−7.145	89.788	1.00	33.72
ATOM	1580	CA	PHE	383	26.557	−6.694	90.628	1.00	33.09
ATOM	1581	CB	PHE	383	26.646	−7.546	91.895	1.00	34.99
ATOM	1582	CG	PHE	383	25.462	−7.409	92.806	1.00	38.33
ATOM	1583	CD1	PHE	383	24.183	−7.730	92.364	1.00	39.48
ATOM	1584	CD2	PHE	383	25.619	−6.928	94.103	1.00	40.16
ATOM	1585	CE1	PHE	383	23.079	−7.568	93.195	1.00	39.96
ATOM	1586	CE2	PHE	383	24.517	−6.762	94.942	1.00	39.80
ATOM	1587	CZ	PHE	383	23.247	−7.082	94.484	1.00	40.07
ATOM	1588	C	PHE	383	27.876	−6.775	89.887	1.00	31.86
ATOM	1589	O	PHE	383	28.064	−7.627	89.024	1.00	30.97
ATOM	1590	N	TYR	384	28.779	−5.870	90.233	1.00	31.42
ATOM	1591	CA	TYR	384	30.102	−5.818	89.646	1.00	32.51
ATOM	1592	CB	TYR	384	30.197	−4.673	88.643	1.00	33.51

TABLE 1-continued

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	1593	CG	TYR	384	29.350	−4.850	87.399	1.00	35.33
ATOM	1594	CD1	TYR	384	27.961	−4.728	87.451	1.00	36.88
ATOM	1595	CE1	TYR	384	27.177	−4.891	86.311	1.00	36.38
ATOM	1596	CD2	TYR	384	29.938	−5.145	86.170	1.00	35.34
ATOM	1597	CE2	TYR	384	29.165	−5.311	85.023	1.00	36.36
ATOM	1598	CZ	TYR	384	27.784	−5.185	85.102	1.00	37.21
ATOM	1599	OH	TYR	384	27.008	−5.351	83.971	1.00	37.53
ATOM	1600	C	TYR	384	31.033	−5.558	90.815	1.00	33.55
ATOM	1601	O	TYR	384	31.207	−4.404	91.217	1.00	32.94
ATOM	1602	N	CYS	385	31.619	−6.631	91.356	1.00	34.77
ATOM	1603	CA	CYS	385	32.509	−6.549	92.525	1.00	34.65
ATOM	1604	C	CYS	385	33.971	−6.626	92.216	1.00	34.20
ATOM	1605	O	CYS	385	34.433	−7.558	91.565	1.00	35.22
ATOM	1606	CB	CYS	385	32.217	−7.658	93.521	1.00	34.87
ATOM	1607	SG	CYS	385	30.526	−7.663	94.168	1.00	40.52
ATOM	1608	N	ASN	386	34.705	−5.653	92.727	1.00	33.25
ATOM	1609	CA	ASN	386	36.129	−5.598	92.521	1.00	33.13
ATOM	1610	CB	ASN	386	36.645	−4.259	93.011	1.00	35.09
ATOM	1611	CG	ASN	386	38.103	−4.104	92.775	1.00	39.37
ATOM	1612	OD1	ASN	386	38.880	−4.983	93.117	1.00	41.53
ATOM	1613	ND2	ASN	386	38.506	−2.990	92.194	1.00	43.99
ATOM	1614	C	ASN	386	36.802	−6.744	93.280	1.00	32.07
ATOM	1615	O	ASN	386	36.891	−6.718	94.507	1.00	33.16
ATOM	1616	N	SER	387	37.288	−7.746	92.555	1.00	30.06
ATOM	1617	CA	SER	387	37.922	−8.895	93.196	1.00	29.26
ATOM	1618	CB	SER	387	37.505	−10.178	92.478	1.00	28.12
ATOM	1619	OG	SER	387	37.730	−10.093	91.087	1.00	26.31
ATOM	1620	C	SER	387	39.443	−8.867	93.337	1.00	29.50
ATOM	1621	O	SER	387	40.063	−9.889	93.624	1.00	29.39
ATOM	1622	N	THR	388	40.045	−7.702	93.159	1.00	29.97
ATOM	1623	CA	THR	388	41.488	−7.586	93.273	1.00	31.62
ATOM	1624	CB	THR	388	41.929	−6.116	93.190	1.00	32.80
ATOM	1625	OG1	THR	388	41.734	−5.630	91.849	1.00	31.68
ATOM	1626	CG2	THR	388	43.392	−5.980	93.590	1.00	31.85
ATOM	1627	C	THR	388	42.038	−8.194	94.561	1.00	33.05
ATOM	1628	O	THR	388	43.100	−8.816	94.553	1.00	33.91
ATOM	1629	N	GLN	389	41.320	−8.027	95.667	1.00	34.67
ATOM	1630	CA	GLN	389	41.792	−8.574	96.944	1.00	37.35
ATOM	1631	CB	GLN	389	40.957	−8.065	98.124	1.00	36.04
ATOM	1632	CG	GLN	389	40.860	−6.578	98.266	1.00	34.05
ATOM	1633	CD	GLN	389	39.773	−6.202	99.241	1.00	34.91
ATOM	1634	OE1	GLN	389	39.964	−6.271	100.451	1.00	37.19
ATOM	1635	NE2	GLN	389	38.609	−5.826	98.720	1.00	36.20
ATOM	1636	C	GLN	389	41.779	−10.101	97.011	1.00	38.08
ATOM	1637	O	GLN	389	42.422	−10.687	97.882	1.00	40.01
ATOM	1638	N	LEU	390	41.042	−10.752	96.124	1.00	37.43
ATOM	1639	CA	LEU	390	40.994	−12.199	96.175	1.00	38.01
ATOM	1640	CB	LEU	390	39.663	−12.699	95.613	1.00	37.92
ATOM	1641	CG	LEU	390	38.396	−12.318	96.392	1.00	37.01
ATOM	1642	CD1	LEU	390	37.175	−12.765	95.614	1.00	35.68
ATOM	1643	CD2	LEU	390	38.399	−12.959	97.764	1.00	35.67
ATOM	1644	C	LEU	390	42.163	−12.816	95.415	1.00	39.31
ATOM	1645	O	LEU	390	42.692	−13.863	95.801	1.00	40.54
ATOM	1646	N	PHE	391	42.583	−12.150	94.347	1.00	39.70
ATOM	1647	CA	PHE	391	43.680	−12.644	93.528	1.00	38.54
ATOM	1648	CB	PHE	391	43.206	−12.794	92.092	1.00	37.22
ATOM	1649	CG	PHE	391	41.913	−13.532	91.984	1.00	37.31
ATOM	1650	CD1	PHE	391	40.707	−12.871	92.177	1.00	38.01
ATOM	1651	CD2	PHE	391	41.897	−14.907	91.784	1.00	37.44
ATOM	1652	CE1	PHE	391	39.507	−13.565	92.179	1.00	37.83
ATOM	1653	CE2	PHE	391	40.699	−15.613	91.786	1.00	37.13
ATOM	1654	CZ	PHE	391	39.501	−14.939	91.986	1.00	38.34
ATOM	1655	C	PHE	391	44.848	−11.691	93.622	1.00	39.15
ATOM	1656	O	PHE	391	45.093	−10.874	92.724	1.00	37.81
ATOM	1657	N	ASN	392	45.554	−11.808	94.742	1.00	40.04
ATOM	1658	CA	ASN	392	46.709	−10.980	95.038	1.00	40.61
ATOM	1659	CB	ASN	392	46.243	−9.647	95.650	1.00	40.52
ATOM	1660	CG	ASN	392	47.401	−8.713	95.990	1.00	42.11
ATOM	1661	OD1	ASN	392	48.388	−8.643	95.255	1.00	42.90
ATOM	1662	ND2	ASN	392	47.272	−7.978	97.093	1.00	42.11
ATOM	1663	C	ASN	392	47.615	−11.736	96.006	1.00	40.17
ATOM	1664	O	ASN	392	47.771	−11.336	97.148	1.00	40.62
ATOM	1665	N	SER	393	48.205	−12.837	95.558	1.00	40.28
ATOM	1666	CA	SER	393	49.085	−13.598	96.436	1.00	41.43
ATOM	1667	CB	SER	393	48.261	−14.448	97.403	1.00	40.63
ATOM	1668	OG	SER	393	47.328	−15.262	96.718	1.00	40.80
ATOM	1669	C	SER	393	50.077	−14.479	95.687	1.00	42.79
ATOM	1670	O	SER	393	49.819	−14.908	94.556	1.00	42.31

TABLE 1-continued

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	1671	N	THR	394	51.212	−14.737	96.333	1.00	43.79
ATOM	1672	CA	THR	394	52.277	−15.551	95.756	1.00	45.04
ATOM	1673	CB	THR	394	53.574	−14.737	95.642	1.00	45.96
ATOM	1674	OG1	THR	394	53.333	−13.573	94.833	1.00	46.10
ATOM	1675	CG2	THR	394	54.688	−15.584	95.026	1.00	45.27
ATOM	1676	C	THR	394	52.541	−16.790	96.602	1.00	45.64
ATOM	1677	O	THR	394	52.906	−16.684	97.769	1.00	44.76
ATOM	1678	N	TRP	395	52.378	−17.964	95.996	1.00	47.09
ATOM	1679	CA	TRP	395	52.548	−19.228	96.705	1.00	47.76
ATOM	1680	CB	TRP	395	51.288	−20.068	96.527	1.00	41.92
ATOM	1681	CG	TRP	395	50.107	−19.326	96.976	1.00	38.28
ATOM	1682	CD2	TRP	395	49.405	−19.506	98.205	1.00	36.22
ATOM	1683	CE2	TRP	395	48.415	−18.503	98.268	1.00	36.46
ATOM	1684	CE3	TRP	395	49.514	−20.414	99.258	1.00	33.85
ATOM	1685	CD1	TRP	395	49.532	−18.258	96.357	1.00	37.38
ATOM	1686	NE1	TRP	395	48.517	−17.754	97.126	1.00	36.41
ATOM	1687	CZ2	TRP	395	47.539	−18.387	99.348	1.00	34.01
ATOM	1688	CZ3	TRP	395	48.647	−20.297	100.324	1.00	33.66
ATOM	1689	CH2	TRP	395	47.670	−19.290	100.361	1.00	33.40
ATOM	1690	C	TRP	395	53.761	−20.066	96.339	1.00	51.43
ATOM	1691	O	TRP	395	54.159	−20.124	95.170	1.00	52.73
ATOM	1692	N	PHE	396	54.339	−20.710	97.358	1.00	54.22
ATOM	1693	CA	PHE	396	55.491	−21.589	97.190	1.00	56.04
ATOM	1694	CB	PHE	396	55.138	−22.681	96.186	1.00	54.94
ATOM	1695	CG	PHE	396	53.790	−23.305	96.422	1.00	55.63
ATOM	1696	CD1	PHE	396	53.083	−23.883	95.373	1.00	56.03
ATOM	1697	CD2	PHE	396	53.226	−23.325	97.699	1.00	56.08
ATOM	1698	CE1	PHE	396	51.830	−24.480	95.591	1.00	56.77
ATOM	1699	CE2	PHE	396	51.974	−23.917	97.930	1.00	56.41
ATOM	1700	CZ	PHE	396	51.275	−24.495	96.872	1.00	56.06
ATOM	1701	C	PHE	396	56.708	−20.813	96.713	1.00	58.81
ATOM	1702	O	PHE	396	57.523	−21.322	95.938	1.00	59.35
ATOM	1703	N	ASN	397	56.815	−19.570	97.172	1.00	61.45
ATOM	1704	CA	ASN	397	57.932	−18.717	96.802	1.00	63.89
ATOM	1705	CB	ASN	397	57.462	−17.262	96.713	1.00	65.82
ATOM	1706	CG	ASN	397	58.568	−16.310	96.270	1.00	68.51
ATOM	1707	OD1	ASN	397	58.333	−15.112	96.075	1.00	69.99
ATOM	1708	ND2	ASN	397	59.782	−16.839	96.110	1.00	68.62
ATOM	1709	C	ASN	397	59.052	−18.854	97.837	1.00	64.94
ATOM	1710	O	ASN	397	59.583	−19.946	98.065	1.00	64.91
ATOM	1711	N	GLY	410	45.948	−11.180	107.879	1.00	61.02
ATOM	1712	CA	GLY	410	45.413	−9.847	107.656	1.00	62.50
ATOM	1713	C	GLY	410	44.155	−9.569	108.466	1.00	62.44
ATOM	1714	O	GLY	410	44.097	−9.849	109.668	1.00	63.35
ATOM	1715	N	SER	411	43.145	−9.007	107.814	1.00	61.14
ATOM	1716	CA	SER	411	41.893	−8.720	108.488	1.00	60.04
ATOM	1717	CB	SER	411	41.252	−7.461	107.913	1.00	61.29
ATOM	1718	OG	SER	411	39.982	−7.232	108.499	1.00	62.93
ATOM	1719	C	SER	411	40.959	−9.902	108.295	1.00	59.15
ATOM	1720	O	SER	411	40.857	−10.448	107.197	1.00	59.05
ATOM	1721	N	ASP	412	40.278	−10.285	109.369	1.00	57.82
ATOM	1722	CA	ASP	412	39.338	−11.406	109.376	1.00	56.24
ATOM	1723	CB	ASP	412	38.360	−11.213	110.532	1.00	59.37
ATOM	1724	CG	ASP	412	37.032	−11.908	110.298	1.00	63.07
ATOM	1725	OD1	ASP	412	37.031	−13.136	110.041	1.00	64.07
ATOM	1726	OD2	ASP	412	35.990	−11.214	110.371	1.00	65.25
ATOM	1727	C	ASP	412	38.556	−11.681	108.082	1.00	53.55
ATOM	1728	O	ASP	412	38.694	−12.746	107.475	1.00	52.85
ATOM	1729	N	THR	413	37.715	−10.735	107.680	1.00	50.45
ATOM	1730	CA	THR	413	36.918	−10.892	106.472	1.00	46.99
ATOM	1731	CB	THR	413	35.415	−10.527	106.742	1.00	46.65
ATOM	1732	OG1	THR	413	34.929	−9.666	105.703	1.00	46.90
ATOM	1733	CG2	THR	413	35.247	−9.813	108.078	1.00	44.53
ATOM	1734	C	THR	413	37.456	−10.014	105.337	1.00	44.78
ATOM	1735	O	THR	413	38.021	−8.954	105.580	1.00	45.19
ATOM	1736	N	ILE	414	37.311	−10.471	104.099	1.00	41.90
ATOM	1737	CA	ILE	414	37.744	−9.684	102.949	1.00	39.73
ATOM	1738	CB	ILE	414	38.299	−10.564	101.813	1.00	38.13
ATOM	1739	CG2	ILE	414	38.798	−9.697	100.690	1.00	36.56
ATOM	1740	CG1	ILE	414	39.464	−11.408	102.316	1.00	37.94
ATOM	1741	CD1	ILE	414	39.966	−12.403	101.300	1.00	34.67
ATOM	1742	C	ILE	414	36.474	−9.007	102.444	1.00	39.45
ATOM	1743	O	ILE	414	35.541	−9.682	102.008	1.00	38.16
ATOM	1744	N	THR	415	36.420	−7.683	102.526	1.00	39.33
ATOM	1745	CA	THR	415	35.237	−6.956	102.071	1.00	39.02
ATOM	1746	CB	THR	415	34.868	−5.782	103.045	1.00	40.55
ATOM	1747	OG1	THR	415	34.451	−6.313	104.313	1.00	41.85
ATOM	1748	CG2	THR	415	33.731	−4.942	102.483	1.00	39.85

TABLE 1-continued

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	1749	C	THR	415	35.487	−6.410	100.671	1.00	37.52
ATOM	1750	O	THR	415	36.386	−5.592	100.458	1.00	36.96
ATOM	1751	N	LEU	416	34.683	−6.887	99.722	1.00	35.70
ATOM	1752	CA	LEU	416	34.772	−6.480	98.323	1.00	33.93
ATOM	1753	CB	LEU	416	34.459	−7.669	97.422	1.00	35.45
ATOM	1754	CG	LEU	416	35.609	−8.553	96.946	1.00	36.03
ATOM	1755	CD1	LEU	416	36.708	−8.616	98.004	1.00	35.17
ATOM	1756	CD2	LEU	416	35.046	−9.933	96.610	1.00	35.12
ATOM	1757	C	LEU	416	33.831	−5.340	97.949	1.00	31.99
ATOM	1758	O	LEU	416	32.631	−5.392	98.222	1.00	31.87
ATOM	1759	N	PRO	417	34.366	−4.285	97.319	1.00	29.92
ATOM	1760	CD	PRO	417	35.782	−3.965	97.067	1.00	27.19
ATOM	1761	CA	PRO	417	33.507	−3.169	96.929	1.00	28.26
ATOM	1762	CB	PRO	417	34.509	−2.052	96.705	1.00	24.49
ATOM	1763	CG	PRO	417	35.678	−2.776	96.162	1.00	23.69
ATOM	1764	C	PRO	417	32.747	−3.548	95.654	1.00	28.94
ATOM	1765	O	PRO	417	33.305	−4.215	94.781	1.00	29.04
ATOM	1766	N	CYS	418	31.476	−3.166	95.553	1.00	30.16
ATOM	1767	CA	CYS	418	30.702	−3.472	94.348	1.00	33.10
ATOM	1768	C	CYS	418	29.782	−2.338	93.978	1.00	32.71
ATOM	1769	O	CYS	418	29.610	−1.387	94.731	1.00	33.13
ATOM	1770	CB	CYS	418	29.808	−4.704	94.510	1.00	35.70
ATOM	1771	SG	CYS	418	30.459	−6.095	95.454	1.00	40.35
ATOM	1772	N	ARG	419	29.167	−2.479	92.812	1.00	33.12
ATOM	1773	CA	ARG	419	28.226	−1.499	92.315	1.00	33.48
ATOM	1774	CB	ARG	419	28.937	−0.474	91.418	1.00	35.57
ATOM	1775	CG	ARG	419	28.028	0.673	91.009	1.00	42.11
ATOM	1776	CD	ARG	419	28.395	1.296	89.654	1.00	47.71
ATOM	1777	NE	ARG	419	29.270	2.464	89.754	1.00	50.54
ATOM	1778	CZ	ARG	419	30.576	2.412	90.009	1.00	50.62
ATOM	1779	NH1	ARG	419	31.178	1.240	90.189	1.00	50.07
ATOM	1780	NH2	ARG	419	31.279	3.538	90.093	1.00	49.54
ATOM	1781	C	ARG	419	27.163	−2.223	91.501	1.00	31.21
ATOM	1782	O	ARG	419	27.453	−3.223	90.848	1.00	28.57
ATOM	1783	N	ILE	420	25.929	−1.736	91.567	1.00	30.97
ATOM	1784	CA	ILE	420	24.845	−2.301	90.759	1.00	31.92
ATOM	1785	CB	ILE	420	23.459	−2.255	91.482	1.00	31.58
ATOM	1786	CG2	ILE	420	22.341	−2.527	90.491	1.00	29.56
ATOM	1787	CG1	ILE	420	23.396	−3.308	92.583	1.00	32.48
ATOM	1788	CD1	ILE	420	24.525	−3.201	93.579	1.00	35.47
ATOM	1789	C	ILE	420	24.793	−1.378	89.542	1.00	31.56
ATOM	1790	O	ILE	420	24.866	−0.161	89.687	1.00	31.84
ATOM	1791	N	LYS	421	24.687	−1.938	88.349	1.00	30.80
ATOM	1792	CA	LYS	421	24.626	−1.104	87.163	1.00	31.04
ATOM	1793	CB	LYS	421	25.808	−1.418	86.259	1.00	32.69
ATOM	1794	CG	LYS	421	27.164	−1.194	86.883	1.00	32.84
ATOM	1795	CD	LYS	421	28.220	−1.316	85.790	1.00	33.11
ATOM	1796	CE	LYS	421	29.583	−0.872	86.271	1.00	32.74
ATOM	1797	NZ	LYS	421	30.553	−0.859	85.147	1.00	32.81
ATOM	1798	C	LYS	421	23.320	−1.330	86.401	1.00	30.54
ATOM	1799	O	LYS	421	22.720	−2.408	86.503	1.00	30.70
ATOM	1800	N	GLN	422	22.879	−0.319	85.651	1.00	29.64
ATOM	1801	CA	GLN	422	21.652	−0.428	84.859	1.00	30.52
ATOM	1802	CB	GLN	422	20.803	0.838	84.969	1.00	30.67
ATOM	1803	CG	GLN	422	20.065	0.997	86.279	1.00	32.13
ATOM	1804	CD	GLN	422	20.998	1.157	87.466	1.00	33.77
ATOM	1805	OE1	GLN	422	21.823	2.081	87.514	1.00	30.92
ATOM	1806	NE2	GLN	422	20.869	0.255	88.438	1.00	34.85
ATOM	1807	C	GLN	422	21.989	−0.669	83.395	1.00	31.34
ATOM	1808	O	GLN	422	21.162	−1.159	82.630	1.00	31.50
ATOM	1809	N	ILE	423	23.213	−0.321	83.017	1.00	32.09
ATOM	1810	CA	ILE	423	23.681	−0.501	81.650	1.00	31.47
ATOM	1811	CB	ILE	423	24.220	0.825	81.125	1.00	30.44
ATOM	1812	CG2	ILE	423	24.767	0.662	79.725	1.00	29.43
ATOM	1813	CG1	ILE	423	23.084	1.842	81.151	1.00	29.90
ATOM	1814	CD1	ILE	423	23.454	3.193	80.628	1.00	30.47
ATOM	1815	C	ILE	423	24.727	−1.625	81.564	1.00	32.00
ATOM	1816	O	ILE	423	25.905	−1.453	81.856	1.00	33.10
ATOM	1817	N	ILE	424	24.241	−2.785	81.149	1.00	33.21
ATOM	1818	CA	ILE	424	24.995	−4.022	81.017	1.00	33.92
ATOM	1819	CB	ILE	424	24.055	−5.212	81.346	1.00	34.97
ATOM	1820	CG2	ILE	424	24.828	−6.487	81.526	1.00	35.83
ATOM	1821	CG1	ILE	424	23.264	−4.900	82.605	1.00	37.56
ATOM	1822	CD1	ILE	424	24.141	−4.483	83.764	1.00	40.47
ATOM	1823	C	ILE	424	25.529	−4.276	79.609	1.00	33.77
ATOM	1824	O	ILE	424	25.094	−3.670	78.644	1.00	34.71
ATOM	1825	N	ASN	425	26.481	−5.194	79.515	1.00	34.13
ATOM	1826	CA	ASN	425	27.033	−5.649	78.244	1.00	33.45

TABLE 1-continued

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	1827	CB	ASN	425	28.559	−5.655	78.279	1.00	33.20
ATOM	1828	CG	ASN	425	29.174	−4.556	77.438	1.00	32.66
ATOM	1829	OD1	ASN	425	28.619	−4.149	76.414	1.00	30.45
ATOM	1830	ND2	ASN	425	30.346	−4.087	77.855	1.00	32.53
ATOM	1831	C	ASN	425	26.536	−7.081	78.347	1.00	33.79
ATOM	1832	O	ASN	425	27.053	−7.826	79.167	1.00	33.77
ATOM	1833	N	MET	426	25.539	−7.471	77.554	1.00	35.05
ATOM	1834	CA	MET	426	24.974	−8.827	77.653	1.00	36.48
ATOM	1835	CB	MET	426	23.788	−8.980	76.698	1.00	37.46
ATOM	1836	CG	MET	426	22.690	−7.954	76.921	1.00	42.17
ATOM	1837	SD	MET	426	21.033	−8.496	76.443	1.00	47.19
ATOM	1838	CE	MET	426	21.110	−8.248	74.701	1.00	47.57
ATOM	1839	C	MET	426	25.928	−10.006	77.447	1.00	37.83
ATOM	1840	O	MET	426	27.017	−9.867	76.885	1.00	37.54
ATOM	1841	N	TRP	427	25.506	−11.176	77.916	1.00	39.73
ATOM	1842	CA	TRP	427	26.304	−12.386	77.770	1.00	41.17
ATOM	1843	CB	TRP	427	26.323	−13.179	79.085	1.00	42.99
ATOM	1844	CG	TRP	427	24.959	−13.556	79.621	1.00	45.82
ATOM	1845	CD2	TRP	427	24.303	−14.822	79.485	1.00	46.80
ATOM	1846	CE2	TRP	427	23.034	−14.709	80.100	1.00	47.00
ATOM	1847	CE3	TRP	427	24.662	−16.044	78.899	1.00	47.97
ATOM	1848	CD1	TRP	427	24.087	−12.748	80.300	1.00	47.03
ATOM	1849	NE1	TRP	427	22.929	−13.434	80.591	1.00	47.49
ATOM	1850	CZ2	TRP	427	22.124	−15.763	80.143	1.00	47.71
ATOM	1851	CZ3	TRP	427	23.756	−17.097	78.944	1.00	48.88
ATOM	1852	CH2	TRP	427	22.500	−16.947	79.562	1.00	49.07
ATOM	1853	C	TRP	427	25.812	−13.284	76.632	1.00	41.19
ATOM	1854	O	TRP	427	26.607	−13.964	76.000	1.00	41.60
ATOM	1855	N	CYS	428	24.509	−13.272	76.363	1.00	42.00
ATOM	1856	CA	CYS	428	23.922	−14.101	75.308	1.00	44.36
ATOM	1857	C	CYS	428	24.410	−13.749	73.917	1.00	44.00
ATOM	1858	O	CYS	428	24.887	−14.616	73.176	1.00	44.48
ATOM	1859	CB	CYS	428	22.394	−14.023	75.381	1.00	47.62
ATOM	1860	SG	CYS	428	21.874	−14.854	76.914	1.00	57.16
ATOM	1861	N	LYS	429	24.290	−12.479	73.557	1.00	43.21
ATOM	1862	CA	LYS	429	24.750	−12.015	72.263	1.00	41.60
ATOM	1863	CB	LYS	429	23.569	−11.882	71.307	1.00	42.35
ATOM	1864	CG	LYS	429	22.384	−11.156	71.883	1.00	43.72
ATOM	1865	CD	LYS	429	21.248	−11.148	70.901	1.00	45.78
ATOM	1866	CE	LYS	429	20.053	−10.418	71.475	1.00	47.56
ATOM	1867	NZ	LYS	429	18.901	−10.405	70.517	1.00	50.92
ATOM	1868	C	LYS	429	25.423	−10.673	72.495	1.00	40.41
ATOM	1869	O	LYS	429	25.256	−10.073	73.553	1.00	40.49
ATOM	1870	N	VAL	430	26.193	−10.213	71.521	1.00	39.52
ATOM	1871	CA	VAL	430	26.879	−8.944	71.645	1.00	39.11
ATOM	1872	CB	VAL	430	27.937	−8.791	70.532	1.00	37.84
ATOM	1873	CG1	VAL	430	28.489	−7.380	70.507	1.00	39.67
ATOM	1874	CG2	VAL	430	29.073	−9.761	70.743	1.00	35.62
ATOM	1875	C	VAL	430	25.914	−7.764	71.573	1.00	40.33
ATOM	1876	O	VAL	430	25.783	−7.136	70.539	1.00	42.24
ATOM	1877	N	CYS	431	25.211	−7.470	72.657	1.00	41.16
ATOM	1878	CA	CYS	431	24.291	−6.326	72.682	1.00	43.40
ATOM	1879	C	CYS	431	24.499	−5.530	73.970	1.00	42.17
ATOM	1880	O	CYS	431	25.000	−6.062	74.964	1.00	43.09
ATOM	1881	CB	CYS	431	22.835	−6.780	72.668	1.00	48.10
ATOM	1882	SG	CYS	431	22.257	−7.836	71.299	1.00	60.95
ATOM	1883	N	LYS	432	24.119	−4.257	73.960	1.00	38.87
ATOM	1884	CA	LYS	432	24.226	−3.454	75.164	1.00	36.15
ATOM	1885	CB	LYS	432	24.860	−2.104	74.846	1.00	35.67
ATOM	1886	CG	LYS	432	25.975	−1.723	75.807	1.00	37.19
ATOM	1887	CD	LYS	432	26.857	−0.647	75.192	1.00	39.70
ATOM	1888	CE	LYS	432	28.075	−0.335	76.058	1.00	42.82
ATOM	1889	NZ	LYS	432	28.992	−1.509	76.255	1.00	42.87
ATOM	1890	C	LYS	432	22.794	−3.297	75.680	1.00	35.02
ATOM	1891	O	LYS	432	21.888	−3.024	74.909	1.00	35.60
ATOM	1892	N	ALA	433	22.574	−3.497	76.972	1.00	33.36
ATOM	1893	CA	ALA	433	21.226	−3.385	77.500	1.00	33.09
ATOM	1894	CB	ALA	433	20.714	−4.753	77.881	1.00	33.61
ATOM	1895	C	ALA	433	21.156	−2.460	78.696	1.00	34.02
ATOM	1896	O	ALA	433	22.129	−2.309	79.420	1.00	35.31
ATOM	1897	N	MET	434	20.006	−1.830	78.908	1.00	34.39
ATOM	1898	CA	MET	434	19.853	−0.927	80.043	1.00	34.19
ATOM	1899	CB	MET	434	19.688	0.522	79.577	1.00	34.29
ATOM	1900	CG	MET	434	19.537	1.519	80.722	1.00	35.19
ATOM	1901	SD	MET	434	18.772	3.088	80.230	1.00	38.57
ATOM	1902	CE	MET	434	17.017	2.778	80.598	1.00	37.43
ATOM	1903	C	MET	434	18.626	−1.328	80.841	1.00	34.05
ATOM	1904	O	MET	434	17.522	−1.387	80.307	1.00	35.74

TABLE 1-continued

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	1905	N	TYR	435	18.817	−1.602	82.123	1.00	32.51
ATOM	1906	CA	TYR	435	17.709	−1.984	82.973	1.00	30.96
ATOM	1907	CB	TYR	435	18.106	−3.184	83.822	1.00	29.29
ATOM	1908	CG	TYR	435	18.339	−4.417	82.992	1.00	25.84
ATOM	1909	CD1	TYR	435	19.560	−4.636	82.365	1.00	25.45
ATOM	1910	CE1	TYR	435	19.745	−5.711	81.524	1.00	24.61
ATOM	1911	CD2	TYR	435	17.311	−5.314	82.760	1.00	23.29
ATOM	1912	CE2	TYR	435	17.482	−6.382	81.924	1.00	24.52
ATOM	1913	CZ	TYR	435	18.699	−6.581	81.305	1.00	24.68
ATOM	1914	OH	TYR	435	18.847	−7.648	80.450	1.00	26.95
ATOM	1915	C	TYR	435	17.313	−0.828	83.859	1.00	32.33
ATOM	1916	O	TYR	435	18.001	0.195	83.892	1.00	33.56
ATOM	1917	N	ALA	436	16.203	−0.984	84.576	1.00	32.62
ATOM	1918	CA	ALA	436	15.736	0.067	85.473	1.00	33.64
ATOM	1919	CB	ALA	436	14.236	−0.064	85.698	1.00	31.13
ATOM	1920	C	ALA	436	16.494	−0.003	86.813	1.00	35.55
ATOM	1921	O	ALA	436	17.025	−1.058	87.199	1.00	36.85
ATOM	1922	N	PRO	437	16.580	1.132	87.527	1.00	35.03
ATOM	1923	CD	PRO	437	16.171	2.473	87.084	1.00	34.29
ATOM	1924	CA	PRO	437	17.270	1.198	88.817	1.00	34.44
ATOM	1925	CB	PRO	437	17.150	2.665	89.182	1.00	35.20
ATOM	1926	CG	PRO	437	17.130	3.339	87.833	1.00	35.19
ATOM	1927	C	PRO	437	16.572	0.287	89.825	1.00	35.06
ATOM	1928	O	PRO	437	15.471	−0.200	89.562	1.00	36.23
ATOM	1929	N	PRO	438	17.188	0.051	90.994	1.00	33.79
ATOM	1930	CD	PRO	438	18.576	0.364	91.356	1.00	33.35
ATOM	1931	CA	PRO	438	16.587	−0.820	92.008	1.00	34.09
ATOM	1932	CB	PRO	438	17.729	−1.028	92.994	1.00	33.97
ATOM	1933	CG	PRO	438	18.947	−0.849	92.167	1.00	33.01
ATOM	1934	C	PRO	438	15.343	−0.263	92.694	1.00	35.40
ATOM	1935	O	PRO	438	15.116	0.945	92.706	1.00	35.71
ATOM	1936	N	ILE	439	14.524	−1.151	93.253	1.00	36.30
ATOM	1937	CA	ILE	439	13.333	−0.707	93.962	1.00	36.39
ATOM	1938	CB	ILE	439	12.008	−1.142	93.261	1.00	34.37
ATOM	1939	CG2	ILE	439	12.003	−0.699	91.836	1.00	34.23
ATOM	1940	CG1	ILE	439	11.845	−2.653	93.288	1.00	35.39
ATOM	1941	CD1	ILE	439	10.469	−3.098	92.843	1.00	34.29
ATOM	1942	C	ILE	439	13.367	−1.242	95.393	1.00	37.68
ATOM	1943	O	ILE	439	12.507	−0.911	96.204	1.00	39.13
ATOM	1944	N	SER	440	14.364	−2.062	95.705	1.00	37.37
ATOM	1945	CA	SER	440	14.491	−2.584	97.057	1.00	39.32
ATOM	1946	CB	SER	440	14.604	−4.104	97.054	1.00	40.44
ATOM	1947	OG	SER	440	14.933	−4.568	98.362	1.00	40.66
ATOM	1948	C	SER	440	15.707	−2.011	97.774	1.00	40.33
ATOM	1949	O	SER	440	16.679	−1.597	97.135	1.00	41.36
ATOM	1950	N	GLY	441	15.646	−1.994	99.102	1.00	40.54
ATOM	1951	CA	GLY	441	16.752	−1.482	99.890	1.00	42.17
ATOM	1952	C	GLY	441	17.425	−2.604	100.659	1.00	43.06
ATOM	1953	O	GLY	441	18.367	−2.392	101.437	1.00	42.78
ATOM	1954	N	GLN	442	16.920	−3.811	100.439	1.00	43.64
ATOM	1955	CA	GLN	442	17.445	−4.997	101.085	1.00	44.67
ATOM	1956	CB	GLN	442	16.475	−5.475	102.175	1.00	45.38
ATOM	1957	CG	GLN	442	16.864	−5.030	103.587	1.00	47.90
ATOM	1958	CD	GLN	442	15.750	−5.219	104.621	1.00	49.44
ATOM	1959	OE1	GLN	442	14.751	−4.495	104.599	1.00	50.66
ATOM	1960	NE2	GLN	442	15.921	−6.190	105.530	1.00	47.39
ATOM	1961	C	GLN	442	17.679	−6.080	100.035	1.00	44.84
ATOM	1962	O	GLN	442	16.909	−7.032	99.904	1.00	44.57
ATOM	1963	N	ILE	443	18.755	−5.908	99.278	1.00	45.49
ATOM	1964	CA	ILE	443	19.132	−6.851	98.236	1.00	46.47
ATOM	1965	CB	ILE	443	19.492	−6.092	96.941	1.00	45.56
ATOM	1966	CG2	ILE	443	20.064	−7.039	95.908	1.00	44.09
ATOM	1967	CG1	ILE	443	18.238	−5.392	96.411	1.00	45.07
ATOM	1968	CD1	ILE	443	18.433	−4.604	95.153	1.00	44.19
ATOM	1969	C	ILE	443	20.328	−7.651	98.744	1.00	47.21
ATOM	1970	O	ILE	443	21.449	−7.142	98.782	1.00	47.84
ATOM	1971	N	ARG	444	20.087	−8.899	99.135	1.00	47.05
ATOM	1972	CA	ARG	444	21.150	−9.732	99.681	1.00	48.36
ATOM	1973	CB	ARG	444	20.856	−10.036	101.152	1.00	50.00
ATOM	1974	CG	ARG	444	20.436	−8.837	101.994	1.00	52.86
ATOM	1975	CD	ARG	444	21.439	−8.535	103.105	1.00	55.04
ATOM	1976	NE	ARG	444	20.951	−7.500	104.017	1.00	59.88
ATOM	1977	CZ	ARG	444	20.629	−6.255	103.659	1.00	61.86
ATOM	1978	NH1	ARG	444	20.193	−5.391	104.570	1.00	62.57
ATOM	1979	NH2	ARG	444	20.741	−5.862	102.395	1.00	62.40
ATOM	1980	C	ARG	444	21.361	−11.052	98.948	1.00	48.73
ATOM	1981	O	ARG	444	20.405	−11.671	98.481	1.00	49.67
ATOM	1982	N	CYS	445	22.619	−11.479	98.849	1.00	48.63

TABLE 1-continued

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	1983	CA	CYS	445	22.956	−12.749	98.212	1.00	47.62
ATOM	1984	C	CYS	445	24.029	−13.502	98.946	1.00	45.78
ATOM	1985	O	CYS	445	25.207	−13.129	98.931	1.00	45.76
ATOM	1986	CB	CYS	445	23.392	−12.574	96.762	1.00	50.80
ATOM	1987	SG	CYS	445	21.966	−12.871	95.692	1.00	57.24
ATOM	1988	N	SER	446	23.595	−14.574	99.589	1.00	42.24
ATOM	1989	CA	SER	446	24.471	−15.438	100.339	1.00	39.56
ATOM	1990	CB	SER	446	23.764	−15.885	101.600	1.00	40.45
ATOM	1991	OG	SER	446	22.870	−14.868	102.024	1.00	43.28
ATOM	1992	C	SER	446	24.667	−16.613	99.417	1.00	37.50
ATOM	1993	O	SER	446	23.767	−17.424	99.252	1.00	37.85
ATOM	1994	N	SER	447	25.833	−16.693	98.795	1.00	34.81
ATOM	1995	CA	SER	447	26.095	−17.780	97.881	1.00	33.45
ATOM	1996	CB	SER	447	26.331	−17.227	96.485	1.00	34.56
ATOM	1997	OG	SER	447	25.323	−16.307	96.128	1.00	36.68
ATOM	1998	C	SER	447	27.300	−18.588	98.300	1.00	32.91
ATOM	1999	O	SER	447	28.088	−18.178	99.151	1.00	33.16
ATOM	2000	N	ASN	448	27.432	−19.755	97.697	1.00	32.65
ATOM	2001	CA	ASN	448	28.561	−20.620	97.970	1.00	33.16
ATOM	2002	CB	ASN	448	28.088	−22.019	98.361	1.00	35.97
ATOM	2003	CG	ASN	448	27.950	−22.184	99.852	1.00	41.24
ATOM	2004	OD1	ASN	448	28.938	−22.162	100.574	1.00	42.95
ATOM	2005	ND2	ASN	448	26.727	−22.357	100.331	1.00	46.28
ATOM	2006	C	ASN	448	29.444	−20.706	96.731	1.00	31.71
ATOM	2007	O	ASN	448	29.005	−21.162	95.668	1.00	30.58
ATOM	2008	N	ILE	449	30.675	−20.222	96.862	1.00	29.84
ATOM	2009	CA	ILE	449	31.645	−20.292	95.772	1.00	27.37
ATOM	2010	CB	ILE	449	32.980	−19.595	96.137	1.00	25.12
ATOM	2011	CG2	ILE	449	34.005	−19.817	95.040	1.00	24.87
ATOM	2012	CG1	ILE	449	32.766	−18.110	96.374	1.00	22.91
ATOM	2013	CD1	ILE	449	34.006	−17.435	96.882	1.00	20.04
ATOM	2014	C	ILE	449	31.929	−21.784	95.734	1.00	27.61
ATOM	2015	O	ILE	449	32.203	−22.373	96.785	1.00	29.12
ATOM	2016	N	THR	450	31.854	−22.409	94.567	1.00	25.09
ATOM	2017	CA	THR	450	32.134	−23.836	94.501	1.00	24.31
ATOM	2018	CB	THR	450	30.832	−24.667	94.295	1.00	24.01
ATOM	2019	OG1	THR	450	30.135	−24.223	93.121	1.00	23.07
ATOM	2020	CG2	THR	450	29.927	−24.523	95.489	1.00	22.78
ATOM	2021	C	THR	450	33.108	−24.109	93.368	1.00	24.60
ATOM	2022	O	THR	450	33.469	−25.248	93.088	1.00	23.80
ATOM	2023	N	GLY	451	33.542	−23.042	92.718	1.00	25.04
ATOM	2024	CA	GLY	451	34.470	−23.200	91.620	1.00	26.73
ATOM	2025	C	GLY	451	34.924	−21.855	91.118	1.00	26.65
ATOM	2026	O	GLY	451	34.370	−20.828	91.505	1.00	27.30
ATOM	2027	N	LEU	452	35.945	−21.851	90.273	1.00	26.29
ATOM	2028	CA	LEU	452	36.439	−20.592	89.739	1.00	27.72
ATOM	2029	CB	LEU	452	37.798	−20.211	90.351	1.00	25.03
ATOM	2030	CG	LEU	452	37.865	−19.937	91.850	1.00	23.22
ATOM	2031	CD1	LEU	452	37.792	−21.248	92.592	1.00	22.91
ATOM	2032	CD2	LEU	452	39.150	−19.225	92.198	1.00	22.12
ATOM	2033	C	LEU	452	36.602	−20.720	88.249	1.00	27.91
ATOM	2034	O	LEU	452	36.381	−21.784	87.678	1.00	30.44
ATOM	2035	N	LEU	453	36.983	−19.620	87.626	1.00	25.60
ATOM	2036	CA	LEU	453	37.223	−19.605	86.211	1.00	24.90
ATOM	2037	CB	LEU	453	36.071	−18.936	85.473	1.00	21.07
ATOM	2038	CG	LEU	453	34.724	−19.652	85.532	1.00	16.96
ATOM	2039	CD1	LEU	453	33.754	−18.930	84.649	1.00	17.51
ATOM	2040	CD2	LEU	453	34.850	−21.061	85.077	1.00	13.58
ATOM	2041	C	LEU	453	38.485	−18.790	86.124	1.00	27.06
ATOM	2042	O	LEU	453	38.458	−17.568	86.262	1.00	28.02
ATOM	2043	N	LEU	454	39.602	−19.480	85.936	1.00	28.63
ATOM	2044	CA	LEU	454	40.889	−18.809	85.862	1.00	30.83
ATOM	2045	CB	LEU	454	41.898	−19.483	86.789	1.00	29.19
ATOM	2046	CG	LEU	454	41.646	−19.667	88.277	1.00	28.21
ATOM	2047	CD1	LEU	454	42.802	−20.460	88.863	1.00	28.15
ATOM	2048	CD2	LEU	454	41.527	−18.331	88.961	1.00	28.25
ATOM	2049	C	LEU	454	41.474	−18.815	84.465	1.00	32.86
ATOM	2050	O	LEU	454	41.103	−19.631	83.622	1.00	33.87
ATOM	2051	N	THR	455	42.415	−17.904	84.248	1.00	34.41
ATOM	2052	CA	THR	455	43.123	−17.791	82.984	1.00	37.13
ATOM	2053	CB	THR	455	42.759	−16.519	82.250	1.00	38.41
ATOM	2054	OG1	THR	455	41.340	−16.467	82.075	1.00	41.71
ATOM	2055	CG2	THR	455	43.438	−16.491	80.893	1.00	38.74
ATOM	2056	C	THR	455	44.591	−17.716	83.344	1.00	38.29
ATOM	2057	O	THR	455	44.943	−17.138	84.367	1.00	38.34
ATOM	2058	N	ARG	456	45.450	−18.289	82.508	1.00	39.99
ATOM	2059	CA	ARG	456	46.881	−18.277	82.783	1.00	41.61
ATOM	2060	CB	ARG	456	47.424	−19.698	82.719	1.00	42.00

TABLE 1-continued

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	2061	CG	ARG	456	48.889	−19.811	83.063	1.00	44.96
ATOM	2062	CD	ARG	456	49.323	−21.250	82.973	1.00	47.06
ATOM	2063	NE	ARG	456	49.147	−21.774	81.621	1.00	49.39
ATOM	2064	CZ	ARG	456	50.117	−21.842	80.714	1.00	50.82
ATOM	2065	NH1	ARG	456	49.857	−22.331	79.506	1.00	52.13
ATOM	2066	NH2	ARG	456	51.348	−21.439	81.019	1.00	49.94
ATOM	2067	C	ARG	456	47.664	−17.389	81.825	1.00	42.48
ATOM	2068	O	ARG	456	47.665	−17.626	80.624	1.00	41.96
ATOM	2069	N	ASP	457	48.333	−16.371	82.362	1.00	44.50
ATOM	2070	CA	ASP	457	49.124	−15.451	81.541	1.00	46.62
ATOM	2071	CB	ASP	457	49.969	−14.515	82.414	1.00	45.79
ATOM	2072	CG	ASP	457	49.169	−13.352	82.978	1.00	46.16
ATOM	2073	OD1	ASP	457	49.798	−12.434	83.549	1.00	44.86
ATOM	2074	OD2	ASP	457	47.921	−13.355	82.853	1.00	44.91
ATOM	2075	C	ASP	457	50.051	−16.199	80.597	1.00	48.50
ATOM	2076	O	ASP	457	49.941	−16.088	79.378	1.00	48.45
ATOM	2077	N	GLY	458	50.975	−16.959	81.168	1.00	51.31
ATOM	2078	CA	GLY	458	51.898	−17.712	80.346	1.00	54.51
ATOM	2079	C	GLY	458	52.751	−16.795	79.499	1.00	57.29
ATOM	2080	O	GLY	458	53.043	−15.659	79.886	1.00	56.35
ATOM	2081	N	GLY	459	53.145	−17.288	78.332	1.00	60.01
ATOM	2082	CA	GLY	459	53.980	−16.494	77.454	1.00	63.76
ATOM	2083	C	GLY	459	55.443	−16.727	77.769	1.00	66.68
ATOM	2084	O	GLY	459	55.830	−16.889	78.932	1.00	66.19
ATOM	2085	N	ASN	460	56.254	−16.735	76.716	1.00	69.80
ATOM	2086	CA	ASN	460	57.694	−16.954	76.813	1.00	73.18
ATOM	2087	CB	ASN	460	58.357	−16.575	75.486	1.00	73.04
ATOM	2088	CG	ASN	460	57.866	−17.426	74.325	1.00	73.09
ATOM	2089	OD1	ASN	460	56.884	−18.161	74.450	1.00	73.18
ATOM	2090	ND2	ASN	460	58.543	−17.323	73.186	1.00	72.64
ATOM	2091	C	ASN	460	58.409	−16.242	77.965	1.00	75.44
ATOM	2092	O	ASN	460	58.412	−15.010	78.062	1.00	75.19
ATOM	2093	N	SER	461	59.021	−17.051	78.828	1.00	77.97
ATOM	2094	CA	SER	461	59.771	−16.582	79.987	1.00	80.75
ATOM	2095	CB	SER	461	58.858	−15.820	80.955	1.00	80.97
ATOM	2096	OG	SER	461	59.608	−15.227	82.007	1.00	81.02
ATOM	2097	C	SER	461	60.368	−17.804	80.689	1.00	82.74
ATOM	2098	O	SER	461	59.649	−18.579	81.332	1.00	82.67
ATOM	2099	N	ASN	462	61.682	−17.979	80.545	1.00	84.51
ATOM	2100	CA	ASN	462	62.399	−19.101	81.160	1.00	85.75
ATOM	2101	CB	ASN	462	63.877	−19.043	80.770	1.00	86.14
ATOM	2102	CG	ASN	462	64.408	−17.626	80.735	1.00	86.77
ATOM	2103	OD1	ASN	462	64.320	−16.891	81.723	1.00	87.52
ATOM	2104	ND2	ASN	462	64.963	−17.230	79.594	1.00	86.09
ATOM	2105	C	ASN	462	62.248	−19.078	82.681	1.00	85.99
ATOM	2106	O	ASN	462	62.664	−20.014	83.377	1.00	86.05
ATOM	2107	N	ASN	463	61.648	−17.992	83.172	1.00	85.36
ATOM	2108	CA	ASN	463	61.379	−17.775	84.591	1.00	84.11
ATOM	2109	CB	ASN	463	60.737	−16.395	84.774	1.00	86.07
ATOM	2110	CG	ASN	463	60.656	−15.967	86.227	1.00	88.02
ATOM	2111	OD1	ASN	463	60.296	−16.757	87.101	1.00	90.17
ATOM	2112	ND2	ASN	463	60.976	−14.703	86.490	1.00	88.10
ATOM	2113	C	ASN	463	60.392	−18.861	85.012	1.00	82.29
ATOM	2114	O	ASN	463	59.372	−19.058	84.351	1.00	82.70
ATOM	2115	N	GLU	464	60.684	−19.569	86.098	1.00	79.57
ATOM	2116	CA	GLU	464	59.788	−20.631	86.542	1.00	76.54
ATOM	2117	CB	GLU	464	60.598	−21.833	87.058	1.00	79.45
ATOM	2118	CG	GLU	464	61.323	−22.608	85.943	1.00	82.50
ATOM	2119	CD	GLU	464	62.120	−23.814	86.448	1.00	85.16
ATOM	2120	OE1	GLU	464	62.812	−24.457	85.620	1.00	85.88
ATOM	2121	OE2	GLU	464	62.055	−24.121	87.663	1.00	85.82
ATOM	2122	C	GLU	464	58.765	−20.185	87.583	1.00	72.60
ATOM	2123	O	GLU	464	58.986	−20.303	88.788	1.00	71.55
ATOM	2124	N	SER	465	57.639	−19.677	87.081	1.00	68.78
ATOM	2125	CA	SER	465	56.516	−19.200	87.893	1.00	64.10
ATOM	2126	CB	SER	465	56.918	−17.974	88.715	1.00	63.31
ATOM	2127	OG	SER	465	57.130	−16.853	87.880	1.00	60.85
ATOM	2128	C	SER	465	55.356	−18.818	86.968	1.00	60.87
ATOM	2129	O	SER	465	55.526	−18.016	86.049	1.00	59.72
ATOM	2130	N	GLU	466	54.184	−19.397	87.215	1.00	57.26
ATOM	2131	CA	GLU	466	52.994	−19.126	86.410	1.00	53.95
ATOM	2132	CB	GLU	466	52.200	−20.413	86.211	1.00	54.65
ATOM	2133	CG	GLU	466	52.956	−21.470	85.438	1.00	56.85
ATOM	2134	CD	GLU	466	53.221	−21.049	84.011	1.00	57.73
ATOM	2135	OE1	GLU	466	54.153	−21.608	83.395	1.00	58.80
ATOM	2136	OE2	GLU	466	52.492	−20.165	83.506	1.00	57.31
ATOM	2137	C	GLU	466	52.110	−18.087	87.080	1.00	51.49
ATOM	2138	O	GLU	466	52.057	−18.015	88.306	1.00	51.94

TABLE 1-continued

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	2139	N	ILE	467	51.419	−17.276	86.283	1.00	47.68
ATOM	2140	CA	ILE	467	50.543	−16.254	86.850	1.00	44.16
ATOM	2141	CB	ILE	467	50.903	−14.837	86.354	1.00	42.54
ATOM	2142	CG2	ILE	467	50.189	−13.805	87.209	1.00	41.04
ATOM	2143	CG1	ILE	467	52.410	−14.601	86.454	1.00	41.74
ATOM	2144	CD1	ILE	467	52.829	−13.208	86.044	1.00	40.72
ATOM	2145	C	ILE	467	49.100	−16.539	86.466	1.00	42.71
ATOM	2146	O	ILE	467	48.817	−16.864	85.315	1.00	43.08
ATOM	2147	N	PHE	468	48.187	−16.421	87.423	1.00	39.98
ATOM	2148	CA	PHE	468	46.793	−16.684	87.129	1.00	38.70
ATOM	2149	CB	PHE	468	46.347	−17.953	87.827	1.00	39.01
ATOM	2150	CG	PHE	468	47.216	−19.127	87.541	1.00	40.09
ATOM	2151	CD1	PHE	468	48.465	−19.243	88.145	1.00	40.16
ATOM	2152	CD2	PHE	468	46.789	−20.127	86.670	1.00	41.47
ATOM	2153	CE1	PHE	468	49.280	−20.334	87.891	1.00	40.98
ATOM	2154	CE2	PHE	468	47.596	−21.229	86.404	1.00	42.44
ATOM	2155	CZ	PHE	468	48.847	−21.333	87.018	1.00	42.97
ATOM	2156	C	PHE	468	45.863	−15.552	87.515	1.00	38.30
ATOM	2157	O	PHE	468	46.022	−14.928	88.563	1.00	39.47
ATOM	2158	N	ARG	469	44.876	−15.305	86.664	1.00	36.77
ATOM	2159	CA	ARG	469	43.912	−14.250	86.897	1.00	35.74
ATOM	2160	CB	ARG	469	44.139	−13.121	85.907	1.00	34.66
ATOM	2161	CG	ARG	469	45.560	−12.642	85.831	1.00	33.62
ATOM	2162	CD	ARG	469	45.735	−11.760	84.620	1.00	33.99
ATOM	2163	NE	ARG	469	47.111	−11.330	84.426	1.00	32.62
ATOM	2164	CZ	ARG	469	47.721	−10.426	85.179	1.00	32.46
ATOM	2165	NH1	ARG	469	47.083	−9.851	86.182	1.00	32.30
ATOM	2166	NH2	ARG	469	48.968	−10.089	84.918	1.00	33.90
ATOM	2167	C	ARG	469	42.522	−14.811	86.690	1.00	35.90
ATOM	2168	O	ARG	469	42.344	−15.782	85.968	1.00	37.30
ATOM	2169	N	PRO	470	41.512	−14.196	87.316	1.00	36.11
ATOM	2170	CD	PRO	470	41.626	−13.004	88.173	1.00	37.74
ATOM	2171	CA	PRO	470	40.117	−14.628	87.205	1.00	35.55
ATOM	2172	CB	PRO	470	39.425	−13.835	88.306	1.00	37.42
ATOM	2173	CG	PRO	470	40.181	−12.546	88.299	1.00	37.79
ATOM	2174	C	PRO	470	39.572	−14.304	85.826	1.00	34.84
ATOM	2175	O	PRO	470	39.664	−13.163	85.350	1.00	32.79
ATOM	2176	N	GLY	471	39.009	−15.318	85.182	1.00	34.39
ATOM	2177	CA	GLY	471	38.481	−15.126	83.849	1.00	34.12
ATOM	2178	C	GLY	471	37.014	−15.447	83.762	1.00	33.66
ATOM	2179	O	GLY	471	36.250	−15.157	84.681	1.00	32.21
ATOM	2180	N	GLY	472	36.630	−16.054	82.646	1.00	34.79
ATOM	2181	CA	GLY	472	35.242	−16.408	82.433	1.00	36.19
ATOM	2182	C	GLY	472	34.526	−15.361	81.600	1.00	37.07
ATOM	2183	O	GLY	472	35.141	−14.417	81.090	1.00	37.63
ATOM	2184	N	GLY	473	33.218	−15.516	81.471	1.00	36.43
ATOM	2185	CA	GLY	473	32.451	−14.578	80.687	1.00	36.25
ATOM	2186	C	GLY	473	31.703	−15.393	79.669	1.00	37.28
ATOM	2187	O	GLY	473	30.653	−14.982	79.179	1.00	37.79
ATOM	2188	N	ASP	474	32.253	−16.562	79.351	1.00	37.46
ATOM	2189	CA	ASP	474	31.620	−17.455	78.396	1.00	38.13
ATOM	2190	CB	ASP	474	32.666	−18.142	77.528	1.00	39.46
ATOM	2191	CG	ASP	474	32.042	−18.956	76.420	1.00	41.78
ATOM	2192	OD1	ASP	474	30.863	−19.345	76.567	1.00	41.80
ATOM	2193	OD2	ASP	474	32.726	−19.215	75.408	1.00	43.88
ATOM	2194	C	ASP	474	30.842	−18.501	79.179	1.00	37.74
ATOM	2195	O	ASP	474	31.350	−19.584	79.445	1.00	38.81
ATOM	2196	N	MET	475	29.609	−18.166	79.543	1.00	37.28
ATOM	2197	CA	MET	475	28.741	−19.049	80.318	1.00	36.81
ATOM	2198	CB	MET	475	27.297	−18.559	80.213	1.00	36.74
ATOM	2199	CG	MET	475	26.718	−18.082	81.529	1.00	37.69
ATOM	2200	SD	MET	475	27.926	−17.234	82.557	1.00	38.71
ATOM	2201	CE	MET	475	28.119	−15.706	81.638	1.00	38.89
ATOM	2202	C	MET	475	28.814	−20.542	79.979	1.00	37.19
ATOM	2203	O	MET	475	28.382	−21.382	80.773	1.00	37.30
ATOM	2204	N	ARG	476	29.353	−20.878	78.809	1.00	36.64
ATOM	2205	CA	ARG	476	29.484	−22.273	78.420	1.00	34.96
ATOM	2206	CB	ARG	476	29.919	−22.392	76.973	1.00	37.33
ATOM	2207	CG	ARG	476	28.879	−21.935	75.991	1.00	39.91
ATOM	2208	CD	ARG	476	29.264	−22.348	74.595	1.00	43.35
ATOM	2209	NE	ARG	476	28.644	−21.475	73.610	1.00	48.16
ATOM	2210	CZ	ARG	476	29.072	−20.246	73.339	1.00	50.83
ATOM	2211	NH1	ARG	476	30.130	−19.751	73.978	1.00	50.44
ATOM	2212	NH2	ARG	476	28.434	−19.508	72.438	1.00	52.09
ATOM	2213	C	ARG	476	30.505	−22.950	79.309	1.00	34.15
ATOM	2214	O	ARG	476	30.466	−24.155	79.495	1.00	33.39
ATOM	2215	N	ASP	477	31.437	−22.175	79.846	1.00	33.97
ATOM	2216	CA	ASP	477	32.428	−22.731	80.748	1.00	34.21

TABLE 1-continued

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	2217	CB	ASP	477	33.497	−21.702	81.091	1.00	34.12
ATOM	2218	CG	ASP	477	34.475	−21.478	79.971	1.00	35.39
ATOM	2219	OD1	ASP	477	34.800	−22.449	79.256	1.00	36.22
ATOM	2220	OD2	ASP	477	34.937	−20.326	79.823	1.00	37.07
ATOM	2221	C	ASP	477	31.696	−23.120	82.030	1.00	35.79
ATOM	2222	O	ASP	477	31.977	−24.157	82.640	1.00	36.61
ATOM	2223	N	ASN	478	30.753	−22.278	82.440	1.00	35.81
ATOM	2224	CA	ASN	478	29.992	−22.539	83.647	1.00	35.64
ATOM	2225	CB	ASN	478	29.160	−21.315	84.029	1.00	37.76
ATOM	2226	CG	ASN	478	29.987	−20.040	84.081	1.00	39.41
ATOM	2227	OD1	ASN	478	29.613	−19.070	84.748	1.00	40.06
ATOM	2228	ND2	ASN	478	31.108	−20.029	83.363	1.00	37.85
ATOM	2229	C	ASN	478	29.096	−23.756	83.478	1.00	34.88
ATOM	2230	O	ASN	478	28.958	−24.550	84.389	1.00	34.09
ATOM	2231	N	TRP	479	28.479	−23.906	82.316	1.00	34.86
ATOM	2232	CA	TRP	479	27.641	−25.070	82.078	1.00	36.03
ATOM	2233	CB	TRP	479	26.892	−24.932	80.760	1.00	37.78
ATOM	2234	CG	TRP	479	26.218	−23.624	80.555	1.00	40.26
ATOM	2235	CD2	TRP	479	25.541	−22.847	81.536	1.00	40.78
ATOM	2236	CE2	TRP	479	25.028	−21.702	80.883	1.00	41.01
ATOM	2237	CE3	TRP	479	25.314	−23.002	82.904	1.00	41.79
ATOM	2238	CD1	TRP	479	26.095	−22.943	79.374	1.00	41.62
ATOM	2239	NE1	TRP	479	25.380	−21.787	79.562	1.00	41.25
ATOM	2240	CZ2	TRP	479	24.307	−20.719	81.552	1.00	40.72
ATOM	2241	CZ3	TRP	479	24.595	−22.023	83.569	1.00	43.55
ATOM	2242	CH2	TRP	479	24.099	−20.894	82.889	1.00	42.51
ATOM	2243	C	TRP	479	28.576	−26.270	81.972	1.00	35.96
ATOM	2244	O	TRP	479	28.297	−27.346	82.476	1.00	37.65
ATOM	2245	N	ARG	480	29.700	−26.070	81.304	1.00	36.48
ATOM	2246	CA	ARG	480	30.685	−27.126	81.108	1.00	37.20
ATOM	2247	CB	ARG	480	31.863	−26.576	80.284	1.00	39.00
ATOM	2248	CG	ARG	480	32.614	−27.615	79.462	1.00	40.70
ATOM	2249	CD	ARG	480	33.888	−27.058	78.807	1.00	42.07
ATOM	2250	NE	ARG	480	33.624	−25.883	77.995	1.00	41.84
ATOM	2251	CZ	ARG	480	32.745	−25.850	77.002	1.00	41.61
ATOM	2252	NH1	ARG	480	32.044	−26.937	76.691	1.00	41.31
ATOM	2253	NH2	ARG	480	32.552	−24.720	76.337	1.00	41.06
ATOM	2254	C	ARG	480	31.202	−27.706	82.428	1.00	36.72
ATOM	2255	O	ARG	480	31.560	−28.869	82.495	1.00	37.82
ATOM	2256	N	SER	481	31.236	−26.899	83.479	1.00	36.72
ATOM	2257	CA	SER	481	31.738	−27.367	84.765	1.00	37.00
ATOM	2258	CB	SER	481	32.088	−26.182	85.645	1.00	36.50
ATOM	2259	OG	SER	481	30.897	−25.619	86.144	1.00	33.89
ATOM	2260	C	SER	481	30.742	−28.243	85.516	1.00	37.55
ATOM	2261	O	SER	481	31.024	−28.717	86.616	1.00	36.47
ATOM	2262	N	GLU	482	29.575	−28.453	84.933	1.00	38.59
ATOM	2263	CA	GLU	482	28.572	−29.269	85.583	1.00	40.68
ATOM	2264	CB	GLU	482	27.350	−28.418	85.922	1.00	42.64
ATOM	2265	CG	GLU	482	27.521	−27.504	87.131	1.00	44.81
ATOM	2266	CD	GLU	482	26.957	−28.100	88.412	1.00	46.18
ATOM	2267	OE1	GLU	482	25.726	−28.318	88.481	1.00	47.32
ATOM	2268	OE2	GLU	482	27.744	−28.348	89.353	1.00	46.06
ATOM	2269	C	GLU	482	28.163	−30.428	84.697	1.00	41.36
ATOM	2270	O	GLU	482	27.733	−31.472	85.188	1.00	43.64
ATOM	2271	N	LEU	483	28.304	−30.255	83.391	1.00	40.45
ATOM	2272	CA	LEU	483	27.919	−31.303	82.459	1.00	40.92
ATOM	2273	CB	LEU	483	27.182	−30.673	81.283	1.00	40.20
ATOM	2274	CG	LEU	483	25.928	−29.921	81.723	1.00	40.80
ATOM	2275	CD1	LEU	483	25.420	−29.072	80.587	1.00	41.63
ATOM	2276	CD2	LEU	483	24.874	−30.909	82.175	1.00	41.17
ATOM	2277	C	LEU	483	29.096	−32.132	81.951	1.00	41.69
ATOM	2278	O	LEU	483	28.931	−33.000	81.092	1.00	41.28
ATOM	2279	N	TYR	484	30.282	−31.880	82.492	1.00	41.67
ATOM	2280	CA	TYR	484	31.463	−32.598	82.050	1.00	42.77
ATOM	2281	CB	TYR	484	32.684	−32.103	82.830	1.00	42.89
ATOM	2282	CG	TYR	484	32.695	−32.515	84.277	1.00	43.93
ATOM	2283	CD1	TYR	484	33.244	−33.735	84.668	1.00	44.09
ATOM	2284	CE1	TYR	484	33.210	−34.148	86.000	1.00	43.91
ATOM	2285	CD2	TYR	484	32.113	−31.714	85.255	1.00	43.24
ATOM	2286	CE2	TYR	484	32.074	−32.121	86.588	1.00	42.95
ATOM	2287	CZ	TYR	484	32.624	−33.337	86.950	1.00	42.55
ATOM	2288	OH	TYR	484	32.605	−33.739	88.263	1.00	43.56
ATOM	2289	C	TYR	484	31.316	−34.120	82.176	1.00	43.44
ATOM	2290	O	TYR	484	31.810	−34.877	81.327	1.00	42.64
ATOM	2291	N	LYS	485	30.622	−34.562	83.221	1.00	43.25
ATOM	2292	CA	LYS	485	30.424	−35.989	83.449	1.00	44.97
ATOM	2293	CB	LYS	485	30.249	−36.265	84.946	1.00	46.94
ATOM	2294	CG	LYS	485	29.083	−35.540	85.606	1.00	49.26

TABLE 1-continued

The structural coordinates of an exemplary stabilized form of gp120 at atomic resolution

ATOM	2295	CD	LYS	485	29.109	−35.779	87.115	1.00	53.35
ATOM	2296	CE	LYS	485	28.091	−34.913	87.862	1.00	55.98
ATOM	2297	NZ	LYS	485	28.190	−35.067	89.350	1.00	55.85
ATOM	2298	C	LYS	485	29.230	−36.557	82.686	1.00	44.79
ATOM	2299	O	LYS	485	28.637	−37.547	83.105	1.00	45.03
ATOM	2300	N	TYR	486	28.876	−35.931	81.568	1.00	43.62
ATOM	2301	CA	TYR	486	27.750	−36.389	80.767	1.00	41.82
ATOM	2302	CB	TYR	486	26.523	−35.492	80.970	1.00	38.82
ATOM	2303	CG	TYR	486	25.915	−35.521	82.350	1.00	36.43
ATOM	2304	CD1	TYR	486	26.240	−34.550	83.299	1.00	37.04
ATOM	2305	CE1	TYR	486	25.677	−34.577	84.576	1.00	36.71
ATOM	2306	CD2	TYR	486	25.011	−36.514	82.709	1.00	34.16
ATOM	2307	CE2	TYR	486	24.445	−36.550	83.979	1.00	33.33
ATOM	2308	CZ	TYR	486	24.777	−35.583	84.904	1.00	34.49
ATOM	2309	OH	TYR	486	24.220	−35.624	86.158	1.00	34.00
ATOM	2310	C	TYR	486	28.089	−36.382	79.291	1.00	42.66
ATOM	2311	O	TYR	486	29.078	−35.796	78.866	1.00	44.53
ATOM	2312	N	LYS	487	27.249	−37.041	78.509	1.00	43.23
ATOM	2313	CA	LYS	487	27.413	−37.090	77.070	1.00	43.39
ATOM	2314	CB	LYS	487	28.638	−37.915	76.670	1.00	42.59
ATOM	2315	CG	LYS	487	28.399	−39.401	76.615	1.00	42.82
ATOM	2316	CD	LYS	487	29.518	−40.088	75.855	1.00	45.58
ATOM	2317	CE	LYS	487	29.612	−39.594	74.405	1.00	46.48
ATOM	2318	NZ	LYS	487	30.745	−40.213	73.638	1.00	44.44
ATOM	2319	C	LYS	487	26.149	−37.724	76.527	1.00	43.48
ATOM	2320	O	LYS	487	25.597	−38.640	77.128	1.00	43.29
ATOM	2321	N	VAL	488	25.682	−37.217	75.400	1.00	44.12
ATOM	2322	CA	VAL	488	24.475	−37.729	74.790	1.00	45.91
ATOM	2323	CB	VAL	488	23.558	−36.554	74.409	1.00	44.11
ATOM	2324	CG1	VAL	488	24.209	−35.720	73.338	1.00	44.27
ATOM	2325	CG2	VAL	488	22.214	−37.056	73.966	1.00	44.39
ATOM	2326	C	VAL	488	24.864	−38.554	73.557	1.00	48.36
ATOM	2327	O	VAL	488	25.888	−38.290	72.927	1.00	48.88
ATOM	2328	N	VAL	489	24.070	−39.570	73.223	1.00	51.09
ATOM	2329	CA	VAL	489	24.383	−40.403	72.060	1.00	53.62
ATOM	2330	CB	VAL	489	25.341	−41.573	72.438	1.00	53.16
ATOM	2331	CG1	VAL	489	24.659	−42.513	73.409	1.00	51.07
ATOM	2332	CG2	VAL	489	25.783	−42.316	71.178	1.00	52.29
ATOM	2333	C	VAL	489	23.161	−40.983	71.344	1.00	55.28
ATOM	2334	O	VAL	489	22.115	−41.249	71.956	1.00	55.15
ATOM	2335	N	LYS	490	23.317	−41.163	70.033	1.00	56.80
ATOM	2336	CA	LYS	490	22.272	−41.708	69.179	1.00	58.05
ATOM	2337	CB	LYS	490	22.757	−41.833	67.729	1.00	59.78
ATOM	2338	CG	LYS	490	23.172	−40.539	67.031	1.00	63.37
ATOM	2339	CD	LYS	490	24.493	−39.974	67.570	1.00	66.32
ATOM	2340	CE	LYS	490	25.132	−38.975	66.597	1.00	66.85
ATOM	2341	NZ	LYS	490	24.183	−37.926	66.111	1.00	68.56
ATOM	2342	C	LYS	490	21.928	−43.094	69.671	1.00	57.96
ATOM	2343	O	LYS	490	22.825	−43.917	69.873	1.00	58.39
ATOM	2344	N	ILE	491	20.642	−43.364	69.868	1.00	57.59
ATOM	2345	CA	ILE	491	20.237	−44.697	70.303	1.00	56.42
ATOM	2346	CB	ILE	491	18.861	−44.685	70.982	1.00	53.57
ATOM	2347	CG2	ILE	491	18.641	−45.994	71.698	1.00	52.55
ATOM	2348	CG1	ILE	491	18.776	−43.545	71.983	1.00	52.06
ATOM	2349	CD1	ILE	491	17.409	−43.403	72.594	1.00	50.94
ATOM	2350	C	ILE	491	20.144	−45.570	69.045	1.00	57.42
ATOM	2351	O	ILE	491	19.728	−45.038	67.989	1.00	57.28
ATOM	2352	OXT	ILE	491	20.478	−46.769	69.127	1.00	58.91
END									

VII. Crystals of gp120 with an Extended V3 Loop

The present disclosure further relates to the crystal structure of gp120 in which the V3 loop is in an extended conformation. The present disclosure also relates to the crystals obtained from a gp120 polypeptide with an extended V3 loop. The three-dimensional coordinates of a gp120 polypeptide with an extended V3 loop, three-dimensional structures of models of a gp120 polypeptide with an extended V3 loop, and uses of these models. The amino acid sequence of a gp120 polypeptide with an extended V3 loop variant is set forth as SEQ ID NO: 2.

The structure of a gp120 polypeptide with an extended V3 loop was solved in complex with the X5 Fab and the d1d2 domain of the CD4 receptor. Analysis of the structure revealed that the V3 loop was present in an elongated conformation that was previously not seen in other complexes involving the gp120 protein. An advantageous feature of this crystal structure over previous structures is the organization of the V3 loop in an elongated conformation, compatible with the elicitation of immunodominant antibody response. Table 2 provides the atomic coordinates of the crystal structure of the polypeptide disclosed in SEQ ID NO: 2.

TABLE 2

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	1	N	VAL	G	84	83.090	−158.764	98.727	1.00	133.29
ATOM	2	CA	VAL	G	84	84.569	−158.842	98.897	1.00	133.95
ATOM	3	C	VAL	G	84	85.258	−158.165	97.714	1.00	134.16
ATOM	4	O	VAL	G	84	85.855	−158.828	96.866	1.00	134.41
ATOM	5	CB	VAL	G	84	85.039	−160.312	98.978	1.00	134.07
ATOM	6	CG1	VAL	G	84	86.507	−160.372	99.373	1.00	134.72
ATOM	7	CG2	VAL	G	84	84.181	−161.078	99.974	1.00	132.76
ATOM	8	N	VAL	G	85	85.169	−156.839	97.667	1.00	134.17
ATOM	9	CA	VAL	G	85	85.767	−156.061	96.587	1.00	133.97
ATOM	10	C	VAL	G	85	87.243	−155.768	96.832	1.00	134.16
ATOM	11	O	VAL	G	85	87.711	−155.788	97.971	1.00	134.47
ATOM	12	CB	VAL	G	85	85.026	−154.715	96.401	1.00	133.69
ATOM	13	CG1	VAL	G	85	85.141	−153.883	97.666	1.00	133.08
ATOM	14	CG2	VAL	G	85	85.601	−153.958	95.213	1.00	133.51
ATOM	15	N	LEU	G	86	87.971	−155.505	95.751	1.00	134.10
ATOM	16	CA	LEU	G	86	89.392	−155.192	95.827	1.00	134.30
ATOM	17	C	LEU	G	86	89.724	−154.045	94.874	1.00	134.27
ATOM	18	O	LEU	G	86	90.077	−154.264	93.714	1.00	134.21
ATOM	19	CB	LEU	G	86	90.235	−156.426	95.483	1.00	134.49
ATOM	20	CG	LEU	G	86	90.134	−157.616	96.446	1.00	134.44
ATOM	21	CD1	LEU	G	86	88.803	−158.331	96.264	1.00	134.35
ATOM	22	CD2	LEU	G	86	91.277	−158.581	96.183	1.00	134.28
ATOM	23	N	GLU	G	87	89.663	−152.780	95.269	1.00	136.00
ATOM	24	CA	GLU	G	87	89.975	−151.658	94.374	1.00	136.69
ATOM	25	C	GLU	G	87	91.472	−151.398	94.342	1.00	137.59
ATOM	26	O	GLU	G	87	92.122	−151.341	95.383	1.00	138.06
ATOM	27	CB	GLU	G	87	89.285	−150.383	94.827	1.00	135.94
ATOM	28	CG	GLU	G	87	87.799	−150.526	94.988	1.00	136.55
ATOM	29	CD	GLU	G	87	87.274	−149.713	96.220	1.00	137.15
ATOM	30	OE1	GLU	G	87	88.011	−149.739	97.285	1.00	138.80
ATOM	31	OE2	GLU	G	87	86.143	−149.072	96.141	1.00	137.57
ATOM	32	N	ASN	G	88	91.857	−151.247	93.247	1.00	136.70
ATOM	33	CA	ASN	G	88	93.272	−150.981	92.995	1.00	137.44
ATOM	34	C	ASN	G	88	93.532	−149.487	92.827	1.00	138.14
ATOM	35	O	ASN	G	88	93.615	−148.984	91.707	1.00	138.46
ATOM	36	CB	ASN	G	88	93.735	−151.732	91.741	1.00	137.16
ATOM	37	CG	ASN	G	88	95.046	−151.199	91.192	1.00	137.46
ATOM	38	OD1	ASN	G	88	96.022	−151.042	91.924	1.00	137.34
ATOM	39	ND2	ASN	G	88	95.074	−150.921	89.892	1.00	138.00
ATOM	40	N	VAL	G	89	93.664	−148.778	93.944	1.00	138.65
ATOM	41	CA	VAL	G	89	93.906	−147.342	93.893	1.00	138.82
ATOM	42	C	VAL	G	89	94.756	−146.842	95.059	1.00	139.51
ATOM	43	O	VAL	G	89	94.835	−147.483	96.108	1.00	139.82
ATOM	44	CB	VAL	G	89	92.570	−146.564	93.877	1.00	138.22
ATOM	45	CG1	VAL	G	89	91.797	−146.834	95.158	1.00	137.56
ATOM	46	CG2	VAL	G	89	92.830	−145.076	93.703	1.00	137.89
ATOM	47	N	THR	G	90	95.394	−145.693	94.856	1.00	139.18
ATOM	48	CA	THR	G	90	96.233	−145.076	95.874	1.00	138.77
ATOM	49	C	THR	G	90	95.355	−144.357	96.903	1.00	137.61
ATOM	50	O	THR	G	90	94.887	−143.241	96.671	1.00	137.17
ATOM	51	CB	THR	G	90	97.224	−144.075	95.229	1.00	139.07
ATOM	52	OG1	THR	G	90	97.906	−143.340	96.252	1.00	139.89
ATOM	53	CG2	THR	G	90	96.490	−143.113	94.303	1.00	138.94
ATOM	54	N	GLU	G	91	95.133	−145.015	98.038	1.00	136.88
ATOM	55	CA	GLU	G	91	94.302	−144.480	99.117	1.00	136.34
ATOM	56	C	GLU	G	91	94.989	−143.439	99.999	1.00	136.12
ATOM	57	O	GLU	G	91	95.991	−143.730	100.653	1.00	136.07
ATOM	58	CB	GLU	G	91	93.806	−145.627	100.002	1.00	135.71
ATOM	59	CG	GLU	G	91	92.609	−146.385	99.457	1.00	134.03
ATOM	60	CD	GLU	G	91	91.293	−145.844	99.980	1.00	132.56
ATOM	61	OE1	GLU	G	91	90.982	−144.661	99.725	1.00	131.44
ATOM	62	OE2	GLU	G	91	90.568	−146.606	100.653	1.00	131.61
ATOM	63	N	HIS	G	92	94.430	−142.231	100.027	1.00	135.50
ATOM	64	CA	HIS	G	92	94.973	−141.145	100.838	1.00	134.96
ATOM	65	C	HIS	G	92	94.490	−141.268	102.282	1.00	133.04
ATOM	66	O	HIS	G	92	93.411	−141.798	102.537	1.00	133.15
ATOM	67	CB	HIS	G	92	94.541	−139.793	100.266	1.00	138.44
ATOM	68	CG	HIS	G	92	95.064	−139.522	98.889	1.00	142.66
ATOM	69	ND1	HIS	G	92	94.870	−138.319	98.245	1.00	144.46
ATOM	70	CD2	HIS	G	92	95.775	−140.296	98.035	1.00	143.67
ATOM	71	CE1	HIS	G	92	95.441	−138.362	97.054	1.00	145.80
ATOM	72	NE2	HIS	G	92	95.997	−139.551	96.902	1.00	145.38
ATOM	73	N	PHE	G	93	95.289	−140.768	103.221	1.00	130.39
ATOM	74	CA	PHE	G	93	94.950	−140.836	104.640	1.00	126.69
ATOM	75	C	PHE	G	93	95.478	−139.628	105.413	1.00	125.30
ATOM	76	O	PHE	G	93	96.479	−139.026	105.033	1.00	125.23
ATOM	77	CB	PHE	G	93	95.534	−142.115	105.247	1.00	125.14
ATOM	78	CG	PHE	G	93	94.502	−143.095	105.721	1.00	123.03

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	79	CD1	PHE	G	93	93.494	−143.538	104.871	1.00	122.34
ATOM	80	CD2	PHE	G	93	94.558	−143.600	107.013	1.00	122.41
ATOM	81	CE1	PHE	G	93	92.556	−144.470	105.304	1.00	121.87
ATOM	82	CE2	PHE	G	93	93.626	−144.532	107.456	1.00	121.75
ATOM	83	CZ	PHE	G	93	92.623	−144.969	106.599	1.00	121.40
ATOM	84	N	ASN	G	94	94.800	−139.283	106.502	1.00	123.37
ATOM	85	CA	ASN	G	94	95.207	−138.158	107.336	1.00	121.13
ATOM	86	C	ASN	G	94	94.643	−138.370	108.735	1.00	120.97
ATOM	87	O	ASN	G	94	93.696	−139.136	108.918	1.00	121.62
ATOM	88	CB	ASN	G	94	94.677	−136.839	106.762	1.00	118.89
ATOM	89	CG	ASN	G	94	95.603	−135.670	107.034	1.00	116.56
ATOM	90	OD1	ASN	G	94	96.617	−135.501	106.358	1.00	115.47
ATOM	91	ND2	ASN	G	94	95.266	−134.863	108.033	1.00	115.47
ATOM	92	N	MET	G	95	95.217	−137.687	109.719	1.00	120.03
ATOM	93	CA	MET	G	95	94.754	−137.820	111.094	1.00	119.35
ATOM	94	C	MET	G	95	94.581	−136.459	111.751	1.00	118.97
ATOM	95	O	MET	G	95	93.918	−136.332	112.780	1.00	118.34
ATOM	96	CB	MET	G	95	95.750	−138.658	111.900	1.00	119.23
ATOM	97	CG	MET	G	95	97.163	−138.093	111.906	1.00	119.40
ATOM	98	SD	MET	G	95	98.323	−139.128	112.817	1.00	118.08
ATOM	99	CE	MET	G	95	98.176	−138.435	114.461	1.00	119.02
ATOM	100	N	TRP	G	96	95.175	−135.438	111.144	1.00	119.91
ATOM	101	CA	TRP	G	96	95.102	−134.087	111.683	1.00	121.52
ATOM	102	C	TRP	G	96	93.868	−133.346	111.184	1.00	123.34
ATOM	103	O	TRP	G	96	93.242	−132.601	111.935	1.00	123.67
ATOM	104	CB	TRP	G	96	96.371	−133.312	111.323	1.00	120.30
ATOM	105	CG	TRP	G	96	97.616	−134.122	111.530	1.00	119.93
ATOM	106	CD1	TRP	G	96	98.257	−134.889	110.599	1.00	119.95
ATOM	107	CD2	TRP	G	96	98.326	−134.309	112.761	1.00	119.57
ATOM	108	NE1	TRP	G	96	99.321	−135.544	111.174	1.00	119.53
ATOM	109	CE2	TRP	G	96	99.387	−135.204	112.498	1.00	119.10
ATOM	110	CE3	TRP	G	96	98.170	−133.805	114.058	1.00	119.39
ATOM	111	CZ2	TRP	G	96	100.285	−135.611	113.490	1.00	118.59
ATOM	112	CZ3	TRP	G	96	99.064	−134.210	115.043	1.00	117.94
ATOM	113	CH2	TRP	G	96	100.109	−135.103	114.751	1.00	117.96
ATOM	114	N	LYS	G	97	93.519	−133.549	109.919	1.00	125.13
ATOM	115	CA	LYS	G	97	92.338	−132.906	109.350	1.00	127.15
ATOM	116	C	LYS	G	97	91.243	−133.960	109.235	1.00	127.03
ATOM	117	O	LYS	G	97	90.591	−134.084	108.201	1.00	127.49
ATOM	118	CB	LYS	G	97	92.656	−132.324	107.965	1.00	128.56
ATOM	119	CG	LYS	G	97	92.419	−130.817	107.836	1.00	130.40
ATOM	120	CD	LYS	G	97	93.554	−129.998	108.449	1.00	131.70
ATOM	121	CE	LYS	G	97	94.673	−129.727	107.447	1.00	132.45
ATOM	122	NZ	LYS	G	97	94.251	−128.765	106.387	1.00	132.15
ATOM	123	N	ASN	G	98	91.056	−134.719	110.309	1.00	127.04
ATOM	124	CA	ASN	G	98	90.060	−135.781	110.347	1.00	127.06
ATOM	125	C	ASN	G	98	88.846	−135.370	111.174	1.00	126.76
ATOM	126	O	ASN	G	98	88.979	−134.956	112.325	1.00	127.98
ATOM	127	CB	ASN	G	98	90.692	−137.051	110.924	1.00	126.57
ATOM	128	CG	ASN	G	98	89.763	−138.242	110.877	1.00	125.98
ATOM	129	OD1	ASN	G	98	88.791	−138.254	110.124	1.00	126.75
ATOM	130	ND2	ASN	G	98	90.067	−139.262	111.670	1.00	125.44
ATOM	131	N	ASP	G	99	87.665	−135.494	110.580	1.00	125.41
ATOM	132	CA	ASP	G	99	86.426	−135.125	111.251	1.00	124.29
ATOM	133	C	ASP	G	99	86.042	−136.161	112.303	1.00	122.94
ATOM	134	O	ASP	G	99	85.313	−135.865	113.253	1.00	123.21
ATOM	135	CB	ASP	G	99	85.309	−134.984	110.213	1.00	125.07
ATOM	136	CG	ASP	G	99	84.039	−134.383	110.792	1.00	125.46
ATOM	137	OD1	ASP	G	99	83.255	−135.132	111.407	1.00	125.32
ATOM	138	OD2	ASP	G	99	83.839	−133.158	110.637	1.00	125.35
ATOM	139	N	MET	G	100	86.548	−137.376	112.128	1.00	121.29
ATOM	140	CA	MET	G	100	86.264	−138.472	113.044	1.00	120.02
ATOM	141	C	MET	G	100	86.815	−138.176	114.432	1.00	119.25
ATOM	142	O	MET	G	100	86.282	−138.649	115.436	1.00	118.87
ATOM	143	CB	MET	G	100	86.879	−139.768	112.510	1.00	119.67
ATOM	144	CG	MET	G	100	86.385	−141.023	113.205	1.00	120.23
ATOM	145	SD	MET	G	100	87.433	−142.456	112.875	1.00	121.05
ATOM	146	CE	MET	G	100	86.737	−143.078	111.340	1.00	122.33
ATOM	147	N	VAL	G	101	87.887	−137.395	114.482	1.00	118.47
ATOM	148	CA	VAL	G	101	88.514	−137.038	115.748	1.00	117.12
ATOM	149	C	VAL	G	101	87.713	−135.967	116.472	1.00	115.61
ATOM	150	O	VAL	G	101	87.466	−136.072	117.671	1.00	114.97
ATOM	151	CB	VAL	G	101	89.943	−136.515	115.529	1.00	117.83
ATOM	152	CG1	VAL	G	101	90.577	−136.163	116.863	1.00	119.14
ATOM	153	CG2	VAL	G	101	90.770	−137.564	114.807	1.00	118.81
ATOM	154	N	GLU	G	102	87.305	−134.938	115.738	1.00	115.04
ATOM	155	CA	GLU	G	102	86.523	−133.862	116.330	1.00	115.24
ATOM	156	C	GLU	G	102	85.146	−134.344	116.762	1.00	114.28

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	157	O	GLU	G	102	84.557	−133.812	117.702	1.00	113.48
ATOM	158	CB	GLU	G	102	86.367	−132.695	115.347	1.00	116.69
ATOM	159	CG	GLU	G	102	87.576	−131.763	115.267	1.00	118.95
ATOM	160	CD	GLU	G	102	88.647	−132.239	114.301	1.00	120.98
ATOM	161	OE1	GLU	G	102	88.576	−131.886	113.102	1.00	121.42
ATOM	162	OE2	GLU	G	102	89.561	−132.969	114.738	1.00	121.86
ATOM	163	N	GLN	G	103	84.634	−135.357	116.076	1.00	114.05
ATOM	164	CA	GLN	G	103	83.319	−135.893	116.395	1.00	114.16
ATOM	165	C	GLN	G	103	83.404	−136.708	117.681	1.00	113.15
ATOM	166	O	GLN	G	103	82.510	−136.657	118.525	1.00	113.27
ATOM	167	CB	GLN	G	103	82.824	−136.756	115.230	1.00	116.01
ATOM	168	CG	GLN	G	103	81.313	−136.831	115.089	1.00	118.46
ATOM	169	CD	GLN	G	103	80.887	−137.109	113.660	1.00	120.20
ATOM	170	OE1	GLN	G	103	81.169	−138.173	113.109	1.00	121.62
ATOM	171	NE2	GLN	G	103	80.208	−136.143	113.048	1.00	120.70
ATOM	172	N	MET	G	104	84.497	−137.450	117.823	1.00	112.25
ATOM	173	CA	MET	G	104	84.730	−138.274	119.004	1.00	111.54
ATOM	174	C	MET	G	104	84.838	−137.376	120.232	1.00	112.25
ATOM	175	O	MET	G	104	84.313	−137.689	121.299	1.00	112.78
ATOM	176	CB	MET	G	104	86.028	−139.071	118.840	1.00	110.90
ATOM	177	CG	MET	G	104	86.435	−139.867	120.071	1.00	109.19
ATOM	178	SD	MET	G	104	85.518	−141.402	120.304	1.00	108.60
ATOM	179	CE	MET	G	104	86.816	−142.479	120.947	1.00	106.86
ATOM	180	N	GLN	G	105	85.530	−136.256	120.063	1.00	112.10
ATOM	181	CA	GLN	G	105	85.726	−135.286	121.134	1.00	111.89
ATOM	182	C	GLN	G	105	84.399	−134.844	121.744	1.00	112.91
ATOM	183	O	GLN	G	105	84.246	−134.807	122.963	1.00	113.09
ATOM	184	CB	GLN	G	105	86.475	−134.064	120.588	1.00	110.93
ATOM	185	CG	GLN	G	105	86.461	−132.848	121.498	1.00	108.92
ATOM	186	CD	GLN	G	105	87.579	−132.849	122.518	1.00	108.26
ATOM	187	OE1	GLN	G	105	87.613	−132.002	123.408	1.00	108.65
ATOM	188	NE2	GLN	G	105	88.505	−133.792	122.388	1.00	108.60
ATOM	189	N	GLU	G	106	83.443	−134.516	120.882	1.00	113.95
ATOM	190	CA	GLU	G	106	82.123	−134.062	121.310	1.00	114.14
ATOM	191	C	GLU	G	106	81.423	−135.064	122.216	1.00	112.47
ATOM	192	O	GLU	G	106	80.694	−134.683	123.129	1.00	111.33
ATOM	193	CB	GLU	G	106	81.240	−133.790	120.085	1.00	117.22
ATOM	194	CG	GLU	G	106	81.847	−132.829	119.069	1.00	121.88
ATOM	195	CD	GLU	G	106	81.831	−131.385	119.534	1.00	124.83
ATOM	196	OE1	GLU	G	106	80.725	−130.827	119.702	1.00	127.31
ATOM	197	OE2	GLU	G	106	82.922	−130.809	119.731	1.00	125.75
ATOM	198	N	ASP	G	107	81.651	−136.347	121.961	1.00	112.07
ATOM	199	CA	ASP	G	107	81.025	−137.407	122.739	1.00	112.28
ATOM	200	C	ASP	G	107	81.683	−137.674	124.079	1.00	110.45
ATOM	201	O	ASP	G	107	81.034	−138.143	125.012	1.00	110.76
ATOM	202	CB	ASP	G	107	80.989	−138.693	121.918	1.00	114.84
ATOM	203	CG	ASP	G	107	79.945	−138.646	120.814	1.00	117.49
ATOM	204	OD1	ASP	G	107	78.775	−138.970	121.099	1.00	120.99
ATOM	205	OD2	ASP	G	107	80.294	−138.268	119.674	1.00	117.70
ATOM	206	N	ILE	G	108	82.972	−137.386	124.181	1.00	108.33
ATOM	207	CA	ILE	G	108	83.680	−137.603	125.432	1.00	106.57
ATOM	208	C	ILE	G	108	83.295	−136.515	126.419	1.00	104.72
ATOM	209	O	ILE	G	108	83.130	−136.771	127.611	1.00	105.07
ATOM	210	CB	ILE	G	108	85.194	−137.592	125.199	1.00	107.34
ATOM	211	CG1	ILE	G	108	85.570	−138.780	124.303	1.00	106.62
ATOM	212	CG2	ILE	G	108	85.931	−137.666	126.532	1.00	107.53
ATOM	213	CD1	ILE	G	108	86.711	−138.511	123.364	1.00	106.38
ATOM	214	N	ILE	G	109	83.140	−135.301	125.909	1.00	102.38
ATOM	215	CA	ILE	G	109	82.755	−134.174	126.740	1.00	100.25
ATOM	216	C	ILE	G	109	81.357	−134.416	127.284	1.00	99.75
ATOM	217	O	ILE	G	109	81.073	−134.128	128.443	1.00	100.09
ATOM	218	CB	ILE	G	109	82.758	−132.871	125.925	1.00	99.79
ATOM	219	CG1	ILE	G	109	84.181	−132.570	125.447	1.00	98.40
ATOM	220	CG2	ILE	G	109	82.219	−131.728	126.764	1.00	99.76
ATOM	221	CD1	ILE	G	109	84.271	−131.441	124.449	1.00	97.98
ATOM	222	N	SER	G	110	80.493	−134.963	126.436	1.00	99.49
ATOM	223	CA	SER	G	110	79.120	−135.258	126.819	1.00	99.12
ATOM	224	C	SER	G	110	79.098	−136.336	127.897	1.00	99.07
ATOM	225	O	SER	G	110	78.261	−136.317	128.797	1.00	98.54
ATOM	226	CB	SER	G	110	78.329	−135.732	125.601	1.00	99.18
ATOM	227	OG	SER	G	110	76.996	−136.053	125.961	1.00	99.12
ATOM	228	N	LEU	G	111	80.029	−137.276	127.793	1.00	99.33
ATOM	229	CA	LEU	G	111	80.135	−138.364	128.755	1.00	100.48
ATOM	230	C	LEU	G	111	80.790	−137.873	130.041	1.00	101.49
ATOM	231	O	LEU	G	111	80.609	−138.458	131.109	1.00	101.29
ATOM	232	CB	LEU	G	111	80.952	−139.511	128.155	1.00	100.12
ATOM	233	CG	LEU	G	111	80.176	−140.676	127.531	1.00	100.14
ATOM	234	CD1	LEU	G	111	80.992	−141.321	126.426	1.00	100.57

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	235	CD2	LEU	G	111	79.843	−141.684	128.621	1.00	100.82
ATOM	236	N	TRP	G	112	81.553	−136.791	129.928	1.00	103.03
ATOM	237	CA	TRP	G	112	82.238	−136.210	131.076	1.00	104.23
ATOM	238	C	TRP	G	112	81.265	−135.378	131.896	1.00	105.45
ATOM	239	O	TRP	G	112	81.329	−135.357	133.122	1.00	106.05
ATOM	240	CB	TRP	G	112	83.402	−135.326	130.612	1.00	103.46
ATOM	241	CG	TRP	G	112	84.730	−135.748	131.159	1.00	102.75
ATOM	242	CD1	TRP	G	112	85.403	−136.903	130.881	1.00	103.42
ATOM	243	CD2	TRP	G	112	85.550	−135.017	132.080	1.00	101.80
ATOM	244	NE1	TRP	G	112	86.593	−136.936	131.570	1.00	103.39
ATOM	245	CE2	TRP	G	112	86.708	−135.792	132.313	1.00	101.79
ATOM	246	CE3	TRP	G	112	85.418	−133.783	132.730	1.00	100.62
ATOM	247	CZ2	TRP	G	112	87.730	−135.371	133.171	1.00	100.65
ATOM	248	CZ3	TRP	G	112	86.435	−133.366	133.582	1.00	100.30
ATOM	249	CH2	TRP	G	112	87.576	−134.160	133.793	1.00	100.15
ATOM	250	N	ASP	G	113	80.361	−134.693	131.207	1.00	106.82
ATOM	251	CA	ASP	G	113	79.376	−133.862	131.879	1.00	108.44
ATOM	252	C	ASP	G	113	78.342	−134.672	132.643	1.00	108.41
ATOM	253	O	ASP	G	113	77.709	−134.157	133.563	1.00	108.64
ATOM	254	CB	ASP	G	113	78.673	−132.951	130.875	1.00	110.86
ATOM	255	CG	ASP	G	113	79.477	−131.700	130.566	1.00	113.42
ATOM	256	OD1	ASP	G	113	79.640	−130.866	131.479	1.00	116.27
ATOM	257	OD2	ASP	G	113	79.955	−131.560	129.420	1.00	115.26
ATOM	258	N	GLN	G	114	78.160	−135.936	132.273	1.00	107.17
ATOM	259	CA	GLN	G	114	77.188	−136.766	132.974	1.00	106.10
ATOM	260	C	GLN	G	114	77.874	−137.744	133.923	1.00	103.76
ATOM	261	O	GLN	G	114	77.242	−138.651	134.461	1.00	104.43
ATOM	262	CB	GLN	G	114	76.300	−137.527	131.980	1.00	109.06
ATOM	263	CG	GLN	G	114	77.005	−138.596	131.161	1.00	113.60
ATOM	264	CD	GLN	G	114	76.029	−139.502	130.422	1.00	116.46
ATOM	265	OE1	GLN	G	114	75.346	−139.076	129.488	1.00	118.64
ATOM	266	NE2	GLN	G	114	75.951	−140.758	130.850	1.00	116.28
ATOM	267	N	SER	G	115	79.172	−137.543	134.127	1.00	100.33
ATOM	268	CA	SER	G	115	79.956	−138.393	135.014	1.00	96.91
ATOM	269	C	SER	G	115	80.706	−137.560	136.051	1.00	93.15
ATOM	270	O	SER	G	115	80.543	−137.758	137.255	1.00	93.21
ATOM	271	CB	SER	G	115	80.946	−139.233	134.203	1.00	99.27
ATOM	272	OG	SER	G	115	80.275	−140.234	133.457	1.00	102.68
ATOM	273	N	LEU	G	116	81.527	−136.629	135.581	1.00	88.46
ATOM	274	CA	LEU	G	116	82.290	−135.766	136.475	1.00	84.39
ATOM	275	C	LEU	G	116	81.741	−134.347	136.459	1.00	82.46
ATOM	276	O	LEU	G	116	81.977	−133.591	135.519	1.00	82.86
ATOM	277	CB	LEU	G	116	83.767	−135.750	136.068	1.00	83.85
ATOM	278	CG	LEU	G	116	84.646	−136.857	136.656	1.00	82.12
ATOM	279	CD1	LEU	G	116	85.974	−136.902	135.922	1.00	82.50
ATOM	280	CD2	LEU	G	116	84.854	−136.596	138.144	1.00	80.96
ATOM	281	N	LYS	G	117	81.000	−133.995	137.503	1.00	80.71
ATOM	282	CA	LYS	G	117	80.407	−132.668	137.619	1.00	80.17
ATOM	283	C	LYS	G	117	81.100	−131.822	138.683	1.00	77.80
ATOM	284	O	LYS	G	117	81.342	−132.288	139.797	1.00	77.93
ATOM	285	CB	LYS	G	117	78.921	−132.780	137.955	1.00	82.16
ATOM	286	CG	LYS	G	117	77.997	−133.018	136.772	1.00	85.17
ATOM	287	CD	LYS	G	117	76.551	−132.954	137.242	1.00	87.66
ATOM	288	CE	LYS	G	117	75.607	−132.504	136.137	1.00	90.61
ATOM	289	NZ	LYS	G	117	74.283	−132.090	136.692	1.00	87.92
ATOM	290	N	PRO	G	118	81.420	−130.558	138.355	1.00	75.68
ATOM	291	CA	PRO	G	118	82.088	−129.645	139.284	1.00	74.22
ATOM	292	C	PRO	G	118	81.059	−129.021	140.206	1.00	73.71
ATOM	293	O	PRO	G	118	79.881	−128.947	139.863	1.00	75.64
ATOM	294	CB	PRO	G	118	82.709	−128.596	138.358	1.00	73.60
ATOM	295	CG	PRO	G	118	82.659	−129.228	136.975	1.00	74.73
ATOM	296	CD	PRO	G	118	81.352	−129.945	137.022	1.00	75.01
ATOM	297	N	CYS	G	119	81.481	−128.570	141.377	1.00	73.04
ATOM	298	CA	CYS	G	119	80.517	−127.953	142.264	1.00	73.80
ATOM	299	C	CYS	G	119	80.324	−126.491	141.888	1.00	72.46
ATOM	300	O	CYS	G	119	79.284	−125.907	142.171	1.00	73.82
ATOM	301	CB	CYS	G	119	80.944	−128.105	143.722	1.00	77.08
ATOM	302	SG	CYS	G	119	79.924	−129.360	144.564	1.00	86.22
ATOM	303	N	VAL	G	120	81.326	−125.907	141.241	1.00	69.39
ATOM	304	CA	VAL	G	120	81.247	−124.524	140.795	1.00	66.24
ATOM	305	C	VAL	G	120	81.939	−124.437	139.445	1.00	66.78
ATOM	306	O	VAL	G	120	83.008	−125.008	139.260	1.00	67.35
ATOM	307	CB	VAL	G	120	81.964	−123.562	141.757	1.00	65.45
ATOM	308	CG1	VAL	G	120	81.757	−122.128	141.292	1.00	64.25
ATOM	309	CG2	VAL	G	120	81.448	−123.745	143.167	1.00	65.16
ATOM	310	N	LYS	G	121	81.321	−123.744	138.498	1.00	68.69
ATOM	311	CA	LYS	G	121	81.903	−123.590	137.170	1.00	71.74
ATOM	312	C	LYS	G	121	82.060	−122.128	136.796	1.00	74.27

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	313	O	LYS	G	121	81.131	−121.337	136.959	1.00	76.19
ATOM	314	CB	LYS	G	121	81.033	−124.260	136.099	1.00	72.94
ATOM	315	CG	LYS	G	121	81.448	−125.664	135.700	1.00	75.20
ATOM	316	CD	LYS	G	121	80.779	−126.073	134.387	1.00	77.11
ATOM	317	CE	LYS	G	121	81.061	−127.533	134.049	1.00	78.09
ATOM	318	NZ	LYS	G	121	80.615	−127.906	132.674	1.00	79.45
ATOM	319	N	LEU	G	122	83.233	−121.767	136.290	1.00	76.38
ATOM	320	CA	LEU	G	122	83.473	−120.394	135.863	1.00	79.17
ATOM	321	C	LEU	G	122	83.757	−120.376	134.371	1.00	81.74
ATOM	322	O	LEU	G	122	84.701	−121.010	133.905	1.00	82.55
ATOM	323	CB	LEU	G	122	84.657	−119.785	136.611	1.00	79.45
ATOM	324	CG	LEU	G	122	84.274	−118.875	137.779	1.00	78.85
ATOM	325	CD1	LEU	G	122	83.608	−119.695	138.873	1.00	77.90
ATOM	326	CD2	LEU	G	122	85.521	−118.189	138.306	1.00	79.94
ATOM	327	N	THR	G	123	82.938	−119.641	133.629	1.00	85.43
ATOM	328	CA	THR	G	123	83.092	−119.563	132.186	1.00	90.13
ATOM	329	C	THR	G	123	83.058	−118.134	131.670	1.00	93.59
ATOM	330	O	THR	G	123	82.259	−117.321	132.126	1.00	94.38
ATOM	331	CB	THR	G	123	81.968	−120.333	131.489	1.00	91.32
ATOM	332	OG1	THR	G	123	81.834	−121.630	132.076	1.00	93.24
ATOM	333	CG2	THR	G	123	82.256	−120.494	130.011	1.00	91.25
ATOM	334	N	PRO	G	124	83.927	−117.810	130.700	1.00	97.34
ATOM	335	CA	PRO	G	124	83.953	−116.456	130.148	1.00	100.80
ATOM	336	C	PRO	G	124	82.656	−116.141	129.415	1.00	103.51
ATOM	337	O	PRO	G	124	82.392	−116.686	128.346	1.00	104.31
ATOM	338	CB	PRO	G	124	85.163	−116.493	129.211	1.00	100.91
ATOM	339	CG	PRO	G	124	86.068	−117.489	129.882	1.00	100.12
ATOM	340	CD	PRO	G	124	85.075	−118.584	130.199	1.00	98.73
ATOM	341	N	LEU	G	125	81.838	−115.271	129.994	1.00	107.90
ATOM	342	CA	LEU	G	125	80.575	−114.898	129.366	1.00	112.76
ATOM	343	C	LEU	G	125	80.861	−113.904	128.250	1.00	116.09
ATOM	344	O	LEU	G	125	80.624	−112.709	128.406	1.00	116.30
ATOM	345	CB	LEU	G	125	79.648	−114.256	130.398	1.00	113.40
ATOM	346	CG	LEU	G	125	78.192	−114.016	129.992	1.00	113.32
ATOM	347	CD1	LEU	G	125	77.403	−115.309	130.161	1.00	114.30
ATOM	348	CD2	LEU	G	125	77.599	−112.929	130.874	1.00	114.10
ATOM	349	N	CYS	G	126	81.378	−114.395	127.128	1.00	119.58
ATOM	350	CA	CYS	G	126	81.708	−113.515	126.016	1.00	122.95
ATOM	351	C	CYS	G	126	80.573	−113.191	125.057	1.00	125.81
ATOM	352	O	CYS	G	126	80.494	−113.734	123.953	1.00	126.35
ATOM	353	CB	CYS	G	126	82.901	−114.067	125.236	1.00	122.36
ATOM	354	SG	CYS	G	126	84.494	−113.726	126.046	1.00	121.90
ATOM	355	N	VAL	G	127	79.696	−112.296	125.497	1.00	129.15
ATOM	356	CA	VAL	G	127	78.566	−111.852	124.693	1.00	131.76
ATOM	357	C	VAL	G	127	78.834	−110.393	124.326	1.00	132.26
ATOM	358	O	VAL	G	127	79.182	−109.582	125.187	1.00	132.30
ATOM	359	CB	VAL	G	127	77.241	−111.952	125.483	1.00	132.38
ATOM	360	CG1	VAL	G	127	77.304	−111.072	126.721	1.00	133.33
ATOM	361	CG2	VAL	G	127	76.075	−111.553	124.595	1.00	133.20
ATOM	362	N	GLY	G	128	78.684	−110.063	123.048	1.00	131.94
ATOM	363	CA	GLY	G	128	78.941	−108.702	122.614	1.00	131.82
ATOM	364	C	GLY	G	128	80.436	−108.454	122.541	1.00	131.76
ATOM	365	O	GLY	G	128	81.051	−108.049	123.527	1.00	131.75
ATOM	366	N	ALA	G	129	81.009	−108.709	121.367	1.00	131.69
ATOM	367	CA	ALA	G	129	82.439	−108.541	121.102	1.00	131.75
ATOM	368	C	ALA	G	129	83.240	−107.898	122.232	1.00	132.17
ATOM	369	O	ALA	G	129	84.144	−108.523	122.787	1.00	132.86
ATOM	370	CB	ALA	G	129	82.632	−107.748	119.819	1.00	131.22
ATOM	371	N	GLY	G	130	82.913	−106.649	122.558	1.00	131.78
ATOM	372	CA	GLY	G	130	83.615	−105.949	123.621	1.00	130.67
ATOM	373	C	GLY	G	130	84.005	−106.869	124.763	1.00	130.19
ATOM	374	O	GLY	G	130	83.255	−107.782	125.104	1.00	130.65
ATOM	375	N	SER	G	195	85.182	−106.632	125.341	1.00	128.61
ATOM	376	CA	SER	G	195	85.705	−107.429	126.454	1.00	126.30
ATOM	377	C	SER	G	195	84.590	−108.085	127.275	1.00	125.16
ATOM	378	O	SER	G	195	83.538	−107.483	127.495	1.00	125.28
ATOM	379	CB	SER	G	195	86.570	−106.538	127.345	1.00	125.36
ATOM	380	OG	SER	G	195	87.524	−105.831	126.567	1.00	121.97
ATOM	381	N	CYS	G	196	84.830	−109.311	127.740	1.00	122.96
ATOM	382	CA	CYS	G	196	83.821	−110.058	128.490	1.00	120.58
ATOM	383	C	CYS	G	196	83.992	−110.143	130.010	1.00	118.42
ATOM	384	O	CYS	G	196	84.973	−109.664	130.580	1.00	117.88
ATOM	385	CB	CYS	G	196	83.720	−111.480	127.931	1.00	120.97
ATOM	386	SG	CYS	G	196	84.469	−111.710	126.286	1.00	122.59
ATOM	387	N	ASP	G	197	83.008	−110.771	130.649	1.00	115.33
ATOM	388	CA	ASP	G	197	82.992	−110.960	132.095	1.00	112.91
ATOM	389	C	ASP	G	197	82.935	−112.461	132.366	1.00	111.21
ATOM	390	O	ASP	G	197	82.951	−113.257	131.431	1.00	111.48

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	391	CB	ASP	G	197	81.766	−110.273	132.701	1.00	114.40
ATOM	392	CG	ASP	G	197	81.916	−110.021	134.191	1.00	116.21
ATOM	393	OD1	ASP	G	197	82.826	−109.253	134.563	1.00	118.31
ATOM	394	OD2	ASP	G	197	81.132	−110.590	134.980	1.00	116.81
ATOM	395	N	THR	G	198	82.848	−112.849	133.633	1.00	108.94
ATOM	396	CA	THR	G	198	82.796	−114.265	133.987	1.00	106.71
ATOM	397	C	THR	G	198	81.395	−114.729	134.392	1.00	104.11
ATOM	398	O	THR	G	198	80.627	−113.974	134.988	1.00	105.56
ATOM	399	CB	THR	G	198	83.760	−114.574	135.144	1.00	108.19
ATOM	400	OG1	THR	G	198	83.441	−113.738	136.263	1.00	109.13
ATOM	401	CG2	THR	G	198	85.190	−114.315	134.729	1.00	108.79
ATOM	402	N	SER	G	199	81.071	−115.978	134.068	1.00	101.10
ATOM	403	CA	SER	G	199	79.765	−116.555	134.395	1.00	98.61
ATOM	404	C	SER	G	199	79.905	−117.657	135.444	1.00	96.43
ATOM	405	O	SER	G	199	80.584	−118.661	135.216	1.00	96.37
ATOM	406	CB	SER	G	199	79.113	−117.124	133.130	1.00	98.18
ATOM	407	OG	SER	G	199	77.821	−117.635	133.406	1.00	96.50
ATOM	408	N	VAL	G	200	79.247	−117.479	136.584	1.00	92.80
ATOM	409	CA	VAL	G	200	79.331	−118.454	137.664	1.00	89.88
ATOM	410	C	VAL	G	200	78.074	−119.310	137.797	1.00	87.32
ATOM	411	O	VAL	G	200	76.954	−118.798	137.747	1.00	86.48
ATOM	412	CB	VAL	G	200	79.568	−117.749	139.012	1.00	90.70
ATOM	413	CG1	VAL	G	200	80.051	−118.755	140.045	1.00	90.81
ATOM	414	CG2	VAL	G	200	80.568	−116.621	138.831	1.00	91.35
ATOM	415	N	ILE	G	201	78.270	−120.614	137.976	1.00	84.68
ATOM	416	CA	ILE	G	201	77.164	−121.552	138.132	1.00	81.86
ATOM	417	C	ILE	G	201	77.483	−122.552	139.234	1.00	79.73
ATOM	418	O	ILE	G	201	78.516	−123.210	139.197	1.00	79.56
ATOM	419	CB	ILE	G	201	76.904	−122.366	136.840	1.00	82.08
ATOM	420	CG1	ILE	G	201	76.600	−121.432	135.666	1.00	85.27
ATOM	421	CG2	ILE	G	201	75.733	−123.311	137.055	1.00	78.87
ATOM	422	CD1	ILE	G	201	77.830	−120.796	135.047	1.00	89.69
ATOM	423	N	THR	G	202	76.600	−122.667	140.216	1.00	78.11
ATOM	424	CA	THR	G	202	76.812	−123.613	141.299	1.00	79.05
ATOM	425	C	THR	G	202	75.852	−124.794	141.137	1.00	80.92
ATOM	426	O	THR	G	202	74.653	−124.609	140.906	1.00	81.00
ATOM	427	CB	THR	G	202	76.575	−122.964	142.667	1.00	78.00
ATOM	428	OG1	THR	G	202	75.243	−122.452	142.725	1.00	79.43
ATOM	429	CG2	THR	G	202	77.549	−121.842	142.901	1.00	77.99
ATOM	430	N	GLN	G	203	76.384	−126.007	141.249	1.00	81.69
ATOM	431	CA	GLN	G	203	75.571	−127.207	141.104	1.00	81.90
ATOM	432	C	GLN	G	203	76.077	−128.353	141.977	1.00	83.87
ATOM	433	O	GLN	G	203	77.208	−128.325	142.457	1.00	84.27
ATOM	434	CB	GLN	G	203	75.548	−127.628	139.635	1.00	80.36
ATOM	435	CG	GLN	G	203	76.918	−127.643	138.979	1.00	79.24
ATOM	436	CD	GLN	G	203	76.859	−128.040	137.514	1.00	80.19
ATOM	437	OE1	GLN	G	203	76.167	−127.412	136.714	1.00	79.78
ATOM	438	NE2	GLN	G	203	77.589	−129.090	137.157	1.00	80.36
ATOM	439	N	ALA	G	204	75.232	−129.359	142.181	1.00	86.42
ATOM	440	CA	ALA	G	204	75.593	−130.514	143.003	1.00	87.19
ATOM	441	C	ALA	G	204	76.718	−131.315	142.355	1.00	87.49
ATOM	442	O	ALA	G	204	76.692	−131.563	141.156	1.00	85.76
ATOM	443	CB	ALA	G	204	74.366	−131.405	143.209	1.00	86.04
ATOM	444	N	CYS	G	205	77.702	−131.728	143.149	1.00	89.57
ATOM	445	CA	CYS	G	205	78.808	−132.510	142.609	1.00	93.38
ATOM	446	C	CYS	G	205	79.087	−133.832	143.328	1.00	96.85
ATOM	447	O	CYS	G	205	79.822	−133.876	144.314	1.00	96.56
ATOM	448	CB	CYS	G	205	80.083	−131.668	142.558	1.00	92.11
ATOM	449	SG	CYS	G	205	80.806	−131.144	144.146	1.00	93.23
ATOM	450	N	PRO	G	206	78.506	−134.938	142.826	1.00	100.89
ATOM	451	CA	PRO	G	206	78.691	−136.266	143.416	1.00	105.01
ATOM	452	C	PRO	G	206	80.095	−136.768	143.099	1.00	109.65
ATOM	453	O	PRO	G	206	80.606	−136.538	142.004	1.00	110.64
ATOM	454	CB	PRO	G	206	77.621	−137.107	142.719	1.00	103.87
ATOM	455	CG	PRO	G	206	76.607	−136.099	142.253	1.00	102.48
ATOM	456	CD	PRO	G	206	77.497	−135.000	141.757	1.00	102.04
ATOM	457	N	LYS	G	207	80.719	−137.456	144.044	1.00	114.22
ATOM	458	CA	LYS	G	207	82.064	−137.960	143.823	1.00	119.19
ATOM	459	C	LYS	G	207	82.101	−139.371	143.241	1.00	123.01
ATOM	460	O	LYS	G	207	82.701	−140.267	143.830	1.00	124.82
ATOM	461	CB	LYS	G	207	82.851	−137.922	145.139	1.00	119.60
ATOM	462	CG	LYS	G	207	83.462	−136.565	145.466	1.00	119.01
ATOM	463	CD	LYS	G	207	84.876	−136.473	144.916	1.00	118.82
ATOM	464	CE	LYS	G	207	85.454	−135.076	145.044	1.00	117.77
ATOM	465	NZ	LYS	G	207	84.868	−134.134	144.051	1.00	116.94
ATOM	466	N	ILE	G	208	81.466	−139.574	142.091	1.00	127.08
ATOM	467	CA	ILE	G	208	81.482	−140.893	141.466	1.00	131.24
ATOM	468	C	ILE	G	208	82.668	−141.008	140.512	1.00	132.68

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	469	O	ILE	G	208	83.143	−140.004	139.984	1.00	133.21
ATOM	470	CB	ILE	G	208	80.184	−141.174	140.682	1.00	132.20
ATOM	471	CG1	ILE	G	208	79.995	−140.133	139.584	1.00	132.98
ATOM	472	CG2	ILE	G	208	78.995	−141.165	141.622	1.00	132.23
ATOM	473	CD1	ILE	G	208	78.847	−140.446	138.655	1.00	134.64
ATOM	474	N	SER	G	209	83.138	−142.234	140.295	1.00	134.15
ATOM	475	CA	SER	G	209	84.284	−142.480	139.429	1.00	135.70
ATOM	476	C	SER	G	209	83.970	−142.546	137.938	1.00	137.12
ATOM	477	O	SER	G	209	83.009	−143.192	137.517	1.00	138.29
ATOM	478	CB	SER	G	209	84.979	−143.779	139.850	1.00	134.98
ATOM	479	OG	SER	G	209	84.086	−144.875	139.771	1.00	135.08
ATOM	480	N	PHE	G	210	84.798	−141.869	137.146	1.00	137.24
ATOM	481	CA	PHE	G	210	84.660	−141.858	135.694	1.00	137.12
ATOM	482	C	PHE	G	210	85.467	−143.033	135.152	1.00	138.23
ATOM	483	O	PHE	G	210	86.687	−142.950	135.018	1.00	138.35
ATOM	484	CB	PHE	G	210	85.200	−140.546	135.121	1.00	136.15
ATOM	485	CG	PHE	G	210	85.309	−140.538	133.623	1.00	135.14
ATOM	486	CD1	PHE	G	210	84.170	−140.630	132.828	1.00	134.46
ATOM	487	CD2	PHE	G	210	86.550	−140.429	133.003	1.00	134.03
ATOM	488	CE1	PHE	G	210	84.266	−140.612	131.436	1.00	133.36
ATOM	489	CE2	PHE	G	210	86.657	−140.409	131.614	1.00	133.27
ATOM	490	CZ	PHE	G	210	85.513	−140.499	130.829	1.00	133.06
ATOM	491	N	GLU	G	211	84.774	−144.126	134.852	1.00	139.29
ATOM	492	CA	GLU	G	211	85.408	−145.342	134.347	1.00	140.31
ATOM	493	C	GLU	G	211	85.710	−145.289	132.849	1.00	140.01
ATOM	494	O	GLU	G	211	84.856	−144.906	132.049	1.00	139.77
ATOM	495	CB	GLU	G	211	84.515	−146.543	134.648	1.00	141.10
ATOM	496	CG	GLU	G	211	84.410	−146.875	136.128	1.00	143.21
ATOM	497	CD	GLU	G	211	83.070	−147.479	136.492	1.00	144.76
ATOM	498	OE1	GLU	G	211	82.970	−148.106	137.568	1.00	145.16
ATOM	499	OE2	GLU	G	211	82.114	−147.317	135.704	1.00	146.11
ATOM	500	N	PRO	G	212	86.933	−145.685	132.452	1.00	139.56
ATOM	501	CA	PRO	G	212	87.358	−145.686	131.050	1.00	139.07
ATOM	502	C	PRO	G	212	86.618	−146.766	130.271	1.00	138.18
ATOM	503	O	PRO	G	212	87.206	−147.771	129.876	1.00	138.23
ATOM	504	CB	PRO	G	212	88.858	−145.974	131.143	1.00	139.58
ATOM	505	CG	PRO	G	212	89.224	−145.516	132.532	1.00	139.85
ATOM	506	CD	PRO	G	212	88.063	−146.041	133.324	1.00	139.87
ATOM	507	N	ILE	G	213	85.327	−146.555	130.049	1.00	136.58
ATOM	508	CA	ILE	G	213	84.515	−147.525	129.329	1.00	134.44
ATOM	509	C	ILE	G	213	84.844	−147.553	127.836	1.00	133.16
ATOM	510	O	ILE	G	213	84.751	−146.535	127.154	1.00	133.40
ATOM	511	CB	ILE	G	213	83.025	−147.221	129.538	1.00	134.18
ATOM	512	CG1	ILE	G	213	82.170	−148.233	128.780	1.00	133.60
ATOM	513	CG2	ILE	G	213	82.728	−145.797	129.093	1.00	134.56
ATOM	514	CD1	ILE	G	213	80.713	−148.192	129.175	1.00	134.43
ATOM	515	N	PRO	G	214	85.234	−148.730	127.316	1.00	131.77
ATOM	516	CA	PRO	G	214	85.590	−148.929	125.907	1.00	130.01
ATOM	517	C	PRO	G	214	84.603	−148.292	124.933	1.00	128.02
ATOM	518	O	PRO	G	214	83.390	−148.418	125.097	1.00	126.87
ATOM	519	CB	PRO	G	214	85.637	−150.449	125.787	1.00	130.90
ATOM	520	CG	PRO	G	214	86.169	−150.848	127.130	1.00	131.42
ATOM	521	CD	PRO	G	214	85.294	−150.012	128.043	1.00	131.68
ATOM	522	N	ILE	G	215	85.131	−147.609	123.922	1.00	126.22
ATOM	523	CA	ILE	G	215	84.297	−146.949	122.928	1.00	124.39
ATOM	524	C	ILE	G	215	84.606	−147.439	121.517	1.00	123.82
ATOM	525	O	ILE	G	215	85.758	−147.432	121.089	1.00	123.83
ATOM	526	CB	ILE	G	215	84.498	−145.419	122.972	1.00	124.52
ATOM	527	CG1	ILE	G	215	83.798	−144.853	124.204	1.00	124.66
ATOM	528	CG2	ILE	G	215	83.946	−144.775	121.712	1.00	123.95
ATOM	529	CD1	ILE	G	215	82.301	−145.085	124.207	1.00	126.40
ATOM	530	N	HIS	G	216	83.567	−147.855	120.801	1.00	122.91
ATOM	531	CA	HIS	G	216	83.707	−148.337	119.436	1.00	122.26
ATOM	532	C	HIS	G	216	83.005	−147.378	118.487	1.00	122.82
ATOM	533	O	HIS	G	216	81.782	−147.263	118.512	1.00	122.59
ATOM	534	CB	HIS	G	216	83.064	−149.719	119.279	1.00	121.11
ATOM	535	CG	HIS	G	216	83.602	−150.756	120.212	1.00	120.49
ATOM	536	ND1	HIS	G	216	84.919	−151.164	120.198	1.00	120.39
ATOM	537	CD2	HIS	G	216	82.988	−151.501	121.161	1.00	120.37
ATOM	538	CE1	HIS	G	216	85.091	−152.118	121.096	1.00	120.82
ATOM	539	NE2	HIS	G	216	83.935	−152.341	121.694	1.00	120.97
ATOM	540	N	TYR	G	217	83.767	−146.678	117.657	1.00	124.13
ATOM	541	CA	TYR	G	217	83.154	−145.780	116.686	1.00	126.48
ATOM	542	C	TYR	G	217	82.753	−146.675	115.523	1.00	129.20
ATOM	543	O	TYR	G	217	83.591	−147.022	114.699	1.00	129.59
ATOM	544	CB	TYR	G	217	84.159	−144.736	116.202	1.00	124.57
ATOM	545	CG	TYR	G	217	83.551	−143.677	115.308	1.00	123.48
ATOM	546	CD1	TYR	G	217	82.990	−142.522	115.849	1.00	123.73

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	547	CD2	TYR	G	217	83.531	−143.831	113.921	1.00	123.00
ATOM	548	CE1	TYR	G	217	82.427	−141.541	115.033	1.00	123.68
ATOM	549	CE2	TYR	G	217	82.969	−142.858	113.096	1.00	123.64
ATOM	550	CZ	TYR	G	217	82.420	−141.715	113.658	1.00	123.44
ATOM	551	OH	TYR	G	217	81.865	−140.755	112.843	1.00	122.11
ATOM	552	N	CYS	G	218	81.486	−147.070	115.462	1.00	132.82
ATOM	553	CA	CYS	G	218	81.054	−147.947	114.380	1.00	136.36
ATOM	554	C	CYS	G	218	80.480	−147.158	113.202	1.00	137.85
ATOM	555	O	CYS	G	218	80.050	−146.011	113.357	1.00	138.46
ATOM	556	CB	CYS	G	218	79.996	−148.934	114.866	1.00	137.77
ATOM	557	SG	CYS	G	218	80.410	−149.952	116.317	1.00	141.47
ATOM	558	N	ALA	G	219	80.464	−147.790	112.031	1.00	138.84
ATOM	559	CA	ALA	G	219	79.953	−147.180	110.806	1.00	139.87
ATOM	560	C	ALA	G	219	78.437	−147.322	110.652	1.00	140.76
ATOM	561	O	ALA	G	219	77.887	−148.416	110.788	1.00	140.94
ATOM	562	CB	ALA	G	219	80.656	−147.793	109.599	1.00	139.80
ATOM	563	N	PRO	G	220	77.747	−146.211	110.347	1.00	141.32
ATOM	564	CA	PRO	G	220	76.292	−146.186	110.168	1.00	142.02
ATOM	565	C	PRO	G	220	75.880	−146.886	108.878	1.00	142.66
ATOM	566	O	PRO	G	220	76.725	−147.227	108.052	1.00	143.05
ATOM	567	CB	PRO	G	220	75.973	−144.688	110.128	1.00	141.53
ATOM	568	CG	PRO	G	220	77.147	−144.054	110.841	1.00	141.13
ATOM	569	CD	PRO	G	220	78.287	−144.845	110.277	1.00	140.75
ATOM	570	N	ALA	G	221	74.580	−147.099	108.708	1.00	143.48
ATOM	571	CA	ALA	G	221	74.079	−147.743	107.503	1.00	143.71
ATOM	572	C	ALA	G	221	74.302	−146.806	106.325	1.00	142.82
ATOM	573	O	ALA	G	221	73.748	−145.708	106.284	1.00	142.96
ATOM	574	CB	ALA	G	221	72.603	−148.056	107.654	1.00	144.82
ATOM	575	N	GLY	G	222	75.115	−147.243	105.370	1.00	140.94
ATOM	576	CA	GLY	G	222	75.396	−146.417	104.209	1.00	138.32
ATOM	577	C	GLY	G	222	76.792	−145.835	104.279	1.00	136.29
ATOM	578	O	GLY	G	222	77.201	−145.050	103.424	1.00	136.34
ATOM	579	N	PHE	G	223	77.526	−146.238	105.311	1.00	134.39
ATOM	580	CA	PHE	G	223	78.890	−145.777	105.537	1.00	132.34
ATOM	581	C	PHE	G	223	79.777	−146.927	106.001	1.00	130.44
ATOM	582	O	PHE	G	223	79.291	−147.921	106.542	1.00	130.04
ATOM	583	CB	PHE	G	223	78.894	−144.670	106.592	1.00	132.84
ATOM	584	CG	PHE	G	223	78.252	−143.397	106.134	1.00	133.73
ATOM	585	CD1	PHE	G	223	78.935	−142.528	105.292	1.00	133.66
ATOM	586	CD2	PHE	G	223	76.967	−143.061	106.547	1.00	134.47
ATOM	587	CE1	PHE	G	223	78.352	−141.337	104.868	1.00	134.19
ATOM	588	CE2	PHE	G	223	76.371	−141.871	106.128	1.00	135.20
ATOM	589	CZ	PHE	G	223	77.067	−141.007	105.287	1.00	135.04
ATOM	590	N	ALA	G	224	81.081	−146.784	105.788	1.00	128.35
ATOM	591	CA	ALA	G	224	82.038	−147.806	106.189	1.00	126.17
ATOM	592	C	ALA	G	224	83.350	−147.160	106.618	1.00	124.72
ATOM	593	O	ALA	G	224	83.741	−146.125	106.083	1.00	124.65
ATOM	594	CB	ALA	G	224	82.280	−148.763	105.033	1.00	126.68
ATOM	595	N	ILE	G	225	84.028	−147.771	107.583	1.00	122.82
ATOM	596	CA	ILE	G	225	85.296	−147.238	108.062	1.00	121.00
ATOM	597	C	ILE	G	225	86.481	−148.096	107.630	1.00	119.79
ATOM	598	O	ILE	G	225	86.477	−149.316	107.801	1.00	119.03
ATOM	599	CB	ILE	G	225	85.293	−147.094	109.603	1.00	121.03
ATOM	600	CG1	ILE	G	225	84.767	−148.369	110.258	1.00	120.98
ATOM	601	CG2	ILE	G	225	84.438	−145.910	110.010	1.00	120.24
ATOM	602	CD1	ILE	G	225	85.843	−149.311	110.722	1.00	120.08
ATOM	603	N	LEU	G	226	87.488	−147.442	107.061	1.00	118.45
ATOM	604	CA	LEU	G	226	88.692	−148.108	106.575	1.00	117.87
ATOM	605	C	LEU	G	226	89.778	−148.170	107.644	1.00	117.93
ATOM	606	O	LEU	G	226	90.048	−147.181	108.320	1.00	117.78
ATOM	607	CB	LEU	G	226	89.233	−147.360	105.355	1.00	117.84
ATOM	608	CG	LEU	G	226	88.416	−147.465	104.067	1.00	117.99
ATOM	609	CD1	LEU	G	226	88.412	−146.134	103.329	1.00	117.75
ATOM	610	CD2	LEU	G	226	89.000	−148.571	103.202	1.00	118.64
ATOM	611	N	LYS	G	227	90.405	−149.333	107.784	1.00	118.28
ATOM	612	CA	LYS	G	227	91.465	−149.518	108.766	1.00	119.16
ATOM	613	C	LYS	G	227	92.802	−149.761	108.070	1.00	120.69
ATOM	614	O	LYS	G	227	93.016	−150.822	107.486	1.00	121.36
ATOM	615	CB	LYS	G	227	91.137	−150.710	109.674	1.00	117.69
ATOM	616	CG	LYS	G	227	92.124	−150.907	110.812	1.00	116.17
ATOM	617	CD	LYS	G	227	92.021	−152.297	111.418	1.00	115.50
ATOM	618	CE	LYS	G	227	93.166	−152.535	112.389	1.00	114.84
ATOM	619	NZ	LYS	G	227	93.253	−153.948	112.850	1.00	113.75
ATOM	620	N	CYS	G	228	93.701	−148.782	108.125	1.00	122.52
ATOM	621	CA	CYS	G	228	95.013	−148.931	107.494	1.00	124.88
ATOM	622	C	CYS	G	228	95.858	−149.909	108.317	1.00	125.15
ATOM	623	O	CYS	G	228	96.285	−149.591	109.427	1.00	125.31
ATOM	624	CB	CYS	G	228	95.704	−147.560	107.380	1.00	127.78

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	625	SG	CYS	G	228	97.401	−147.576	106.702	1.00	132.08
ATOM	626	N	ASN	G	229	96.082	−151.103	107.768	1.00	125.50
ATOM	627	CA	ASN	G	229	96.859	−152.135	108.452	1.00	126.07
ATOM	628	C	ASN	G	229	98.350	−152.104	108.155	1.00	126.43
ATOM	629	O	ASN	G	229	99.019	−153.135	108.224	1.00	126.40
ATOM	630	CB	ASN	G	229	96.331	−153.533	108.114	1.00	127.05
ATOM	631	CG	ASN	G	229	95.052	−153.874	108.855	1.00	128.07
ATOM	632	OD1	ASN	G	229	93.960	−153.472	108.455	1.00	129.09
ATOM	633	ND2	ASN	G	229	95.185	−154.612	109.953	1.00	128.62
ATOM	634	N	ASP	G	230	98.873	−150.931	107.822	1.00	127.09
ATOM	635	CA	ASP	G	230	100.298	−150.803	107.541	1.00	128.18
ATOM	636	C	ASP	G	230	101.112	−151.040	108.808	1.00	129.06
ATOM	637	O	ASP	G	230	100.792	−150.501	109.867	1.00	129.47
ATOM	638	CB	ASP	G	230	100.611	−149.413	106.994	1.00	128.04
ATOM	639	CG	ASP	G	230	100.772	−149.400	105.486	1.00	128.21
ATOM	640	OD1	ASP	G	230	99.829	−149.813	104.784	1.00	129.16
ATOM	641	OD2	ASP	G	230	101.844	−148.972	105.012	1.00	127.80
ATOM	642	N	LYS	G	231	102.174	−151.832	108.693	1.00	130.19
ATOM	643	CA	LYS	G	231	103.034	−152.142	109.833	1.00	131.50
ATOM	644	C	LYS	G	231	103.705	−150.890	110.406	1.00	132.11
ATOM	645	O	LYS	G	231	103.862	−150.762	111.620	1.00	132.26
ATOM	646	CB	LYS	G	231	104.103	−153.164	109.420	1.00	131.22
ATOM	647	CG	LYS	G	231	103.545	−154.525	108.994	1.00	131.29
ATOM	648	CD	LYS	G	231	102.981	−155.296	110.185	1.00	131.06
ATOM	649	CE	LYS	G	231	102.249	−156.559	109.747	1.00	130.17
ATOM	650	NZ	LYS	G	231	101.640	−157.279	110.904	1.00	128.78
ATOM	651	N	THR	G	232	104.100	−149.970	109.531	1.00	132.72
ATOM	652	CA	THR	G	232	104.750	−148.738	109.960	1.00	133.16
ATOM	653	C	THR	G	232	104.170	−147.577	109.173	1.00	133.64
ATOM	654	O	THR	G	232	104.627	−147.283	108.072	1.00	134.29
ATOM	655	CB	THR	G	232	106.264	−148.791	109.698	1.00	133.30
ATOM	656	OG1	THR	G	232	106.807	−149.976	110.286	1.00	133.19
ATOM	657	CG2	THR	G	232	106.956	−147.583	110.304	1.00	134.01
ATOM	658	N	PHE	G	233	103.162	−146.923	109.741	1.00	133.70
ATOM	659	CA	PHE	G	233	102.506	−145.798	109.086	1.00	134.07
ATOM	660	C	PHE	G	233	102.979	−144.482	109.689	1.00	133.22
ATOM	661	O	PHE	G	233	103.185	−144.394	110.897	1.00	133.97
ATOM	662	CB	PHE	G	233	100.990	−145.927	109.240	1.00	135.95
ATOM	663	CG	PHE	G	233	100.211	−145.067	108.293	1.00	138.56
ATOM	664	CD1	PHE	G	233	100.413	−145.170	106.922	1.00	139.24
ATOM	665	CD2	PHE	G	233	99.267	−144.163	108.766	1.00	139.44
ATOM	666	CE1	PHE	G	233	99.687	−144.386	106.031	1.00	140.27
ATOM	667	CE2	PHE	G	233	98.534	−143.372	107.885	1.00	140.80
ATOM	668	CZ	PHE	G	233	98.744	−143.485	106.513	1.00	140.90
ATOM	669	N	ASN	G	234	103.137	−143.455	108.857	1.00	132.11
ATOM	670	CA	ASN	G	234	103.606	−142.163	109.353	1.00	131.12
ATOM	671	C	ASN	G	234	102.497	−141.209	109.789	1.00	130.16
ATOM	672	O	ASN	G	234	102.776	−140.083	110.195	1.00	130.18
ATOM	673	CB	ASN	G	234	104.479	−141.463	108.305	1.00	131.40
ATOM	674	CG	ASN	G	234	103.667	−140.844	107.184	1.00	131.18
ATOM	675	OD1	ASN	G	234	103.832	−139.666	106.859	1.00	130.27
ATOM	676	ND2	ASN	G	234	102.791	−141.636	106.581	1.00	130.32
ATOM	677	N	GLY	G	235	101.246	−141.649	109.711	1.00	128.79
ATOM	678	CA	GLY	G	235	100.152	−140.784	110.119	1.00	127.79
ATOM	679	C	GLY	G	235	99.372	−140.177	108.967	1.00	127.12
ATOM	680	O	GLY	G	235	98.186	−140.456	108.808	1.00	126.69
ATOM	681	N	LYS	G	236	100.023	−139.334	108.171	1.00	126.63
ATOM	682	CA	LYS	G	236	99.361	−138.704	107.031	1.00	126.89
ATOM	683	C	LYS	G	236	100.036	−139.113	105.726	1.00	128.87
ATOM	684	O	LYS	G	236	101.238	−139.357	105.693	1.00	129.74
ATOM	685	CB	LYS	G	236	99.386	−137.177	107.169	1.00	124.81
ATOM	686	CG	LYS	G	236	100.774	−136.597	107.412	1.00	122.07
ATOM	687	CD	LYS	G	236	100.770	−135.068	107.512	1.00	120.19
ATOM	688	CE	LYS	G	236	100.766	−134.390	106.146	1.00	118.90
ATOM	689	NZ	LYS	G	236	100.848	−132.901	106.254	1.00	116.47
ATOM	690	N	GLY	G	237	99.254	−139.183	104.654	1.00	130.44
ATOM	691	CA	GLY	G	237	99.797	−139.569	103.364	1.00	132.18
ATOM	692	C	GLY	G	237	99.066	−140.755	102.767	1.00	133.46
ATOM	693	O	GLY	G	237	97.921	−141.018	103.138	1.00	134.02
ATOM	694	N	PRO	G	238	99.693	−141.487	101.838	1.00	133.68
ATOM	695	CA	PRO	G	238	99.075	−142.651	101.200	1.00	133.81
ATOM	696	C	PRO	G	238	99.297	−143.951	101.985	1.00	133.94
ATOM	697	O	PRO	G	238	100.427	−144.267	102.353	1.00	133.93
ATOM	698	CB	PRO	G	238	99.759	−142.702	99.827	1.00	133.77
ATOM	699	CG	PRO	G	238	100.463	−141.336	99.685	1.00	134.36
ATOM	700	CD	PRO	G	238	100.886	−141.069	101.093	1.00	134.13
ATOM	701	N	CYS	G	239	98.228	−144.703	102.245	1.00	134.81
ATOM	702	CA	CYS	G	239	98.361	−145.976	102.959	1.00	136.32

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	703	C	CYS	G	239	98.399	−147.104	101.926	1.00	136.72
ATOM	704	O	CYS	G	239	97.640	−147.086	100.958	1.00	136.38
ATOM	705	CB	CYS	G	239	97.187	−146.196	103.935	1.00	136.44
ATOM	706	SG	CYS	G	239	97.192	−147.860	104.696	1.00	136.59
ATOM	707	N	LYS	G	240	99.274	−148.086	102.136	1.00	138.05
ATOM	708	CA	LYS	G	240	99.405	−149.212	101.207	1.00	139.87
ATOM	709	C	LYS	G	240	98.342	−150.286	101.428	1.00	139.47
ATOM	710	O	LYS	G	240	97.436	−150.447	100.613	1.00	139.04
ATOM	711	CB	LYS	G	240	100.802	−149.837	101.324	1.00	141.13
ATOM	712	CG	LYS	G	240	101.941	−148.901	100.918	1.00	142.81
ATOM	713	CD	LYS	G	240	103.310	−149.526	101.173	1.00	143.74
ATOM	714	CE	LYS	G	240	104.429	−148.549	100.835	1.00	143.78
ATOM	715	NZ	LYS	G	240	105.786	−149.103	101.110	1.00	143.33
ATOM	716	N	ASN	G	241	98.458	−151.020	102.530	1.00	139.54
ATOM	717	CA	ASN	G	241	97.499	−152.070	102.850	1.00	139.69
ATOM	718	C	ASN	G	241	96.445	−151.535	103.811	1.00	139.92
ATOM	719	O	ASN	G	241	96.774	−151.092	104.908	1.00	139.69
ATOM	720	CB	ASN	G	241	98.207	−153.257	103.505	1.00	139.80
ATOM	721	CG	ASN	G	241	97.305	−154.468	103.640	1.00	140.13
ATOM	722	OD1	ASN	G	241	97.503	−155.314	104.512	1.00	139.63
ATOM	723	ND2	ASN	G	241	96.312	−154.563	102.763	1.00	139.93
ATOM	724	N	VAL	G	242	95.182	−151.588	103.405	1.00	139.96
ATOM	725	CA	VAL	G	242	94.098	−151.102	104.249	1.00	140.28
ATOM	726	C	VAL	G	242	92.840	−151.950	104.097	1.00	140.63
ATOM	727	O	VAL	G	242	92.326	−152.114	102.991	1.00	141.19
ATOM	728	CB	VAL	G	242	93.759	−149.631	103.905	1.00	140.31
ATOM	729	CG1	VAL	G	242	93.609	−149.479	102.400	1.00	139.72
ATOM	730	CG2	VAL	G	242	92.476	−149.210	104.607	1.00	140.48
ATOM	731	N	SER	G	243	92.350	−152.486	105.211	1.00	140.58
ATOM	732	CA	SER	G	243	91.149	−153.322	105.211	1.00	140.55
ATOM	733	C	SER	G	243	89.925	−152.489	105.588	1.00	140.69
ATOM	734	O	SER	G	243	90.002	−151.264	105.656	1.00	140.64
ATOM	735	CB	SER	G	243	91.308	−154.467	106.213	1.00	140.83
ATOM	736	OG	SER	G	243	91.381	−153.972	107.536	1.00	140.52
ATOM	737	N	THR	G	244	88.804	−153.157	105.845	1.00	141.03
ATOM	738	CA	THR	G	244	87.582	−152.460	106.212	1.00	141.52
ATOM	739	C	THR	G	244	86.765	−153.217	107.244	1.00	142.08
ATOM	740	O	THR	G	244	86.149	−154.231	106.927	1.00	141.97
ATOM	741	CB	THR	G	244	86.683	−152.231	104.983	1.00	141.57
ATOM	742	OG1	THR	G	244	87.375	−151.421	104.032	1.00	142.02
ATOM	743	CG2	THR	G	244	85.395	−151.532	105.384	1.00	140.17
ATOM	744	N	VAL	G	245	86.769	−152.726	108.476	1.00	142.71
ATOM	745	CA	VAL	G	245	86.005	−153.338	109.549	1.00	143.44
ATOM	746	C	VAL	G	245	84.747	−152.503	109.763	1.00	143.75
ATOM	747	O	VAL	G	245	84.627	−151.413	109.204	1.00	143.15
ATOM	748	CB	VAL	G	245	86.821	−153.377	110.853	1.00	144.12
ATOM	749	CG1	VAL	G	245	87.881	−154.460	110.778	1.00	144.77
ATOM	750	CG2	VAL	G	245	87.479	−152.032	111.086	1.00	144.53
ATOM	751	N	GLN	G	246	83.808	−153.006	110.557	1.00	144.36
ATOM	752	CA	GLN	G	246	82.577	−152.266	110.799	1.00	144.77
ATOM	753	C	GLN	G	246	82.652	−151.364	112.024	1.00	144.15
ATOM	754	O	GLN	G	246	82.087	−150.272	112.025	1.00	143.24
ATOM	755	CB	GLN	G	246	81.392	−153.227	110.918	1.00	146.20
ATOM	756	CG	GLN	G	246	81.220	−154.117	109.699	1.00	148.95
ATOM	757	CD	GLN	G	246	81.195	−153.327	108.400	1.00	150.00
ATOM	758	OE1	GLN	G	246	80.344	−152.461	108.202	1.00	150.67
ATOM	759	NE2	GLN	G	246	82.136	−153.623	107.510	1.00	149.89
ATOM	760	N	CYS	G	247	83.338	−151.814	113.069	1.00	143.81
ATOM	761	CA	CYS	G	247	83.474	−150.999	114.274	1.00	143.17
ATOM	762	C	CYS	G	247	84.949	−150.785	114.595	1.00	142.65
ATOM	763	O	CYS	G	247	85.796	−151.613	114.255	1.00	142.71
ATOM	764	CB	CYS	G	247	82.810	−151.662	115.485	1.00	142.99
ATOM	765	SG	CYS	G	247	80.988	−151.740	115.542	1.00	143.43
ATOM	766	N	THR	G	248	85.247	−149.676	115.262	1.00	141.73
ATOM	767	CA	THR	G	248	86.613	−149.336	115.640	1.00	140.76
ATOM	768	C	THR	G	248	87.070	−150.095	116.883	1.00	140.31
ATOM	769	O	THR	G	248	86.258	−150.456	117.731	1.00	140.20
ATOM	770	CB	THR	G	248	86.725	−147.838	115.923	1.00	140.39
ATOM	771	OG1	THR	G	248	86.168	−147.112	114.824	1.00	141.14
ATOM	772	CG2	THR	G	248	88.169	−147.433	116.094	1.00	140.10
ATOM	773	N	HIS	G	249	88.375	−150.325	116.991	1.00	139.86
ATOM	774	CA	HIS	G	249	88.932	−151.035	118.138	1.00	139.38
ATOM	775	C	HIS	G	249	88.597	−150.355	119.464	1.00	137.88
ATOM	776	O	HIS	G	249	88.282	−149.167	119.501	1.00	138.46
ATOM	777	CB	HIS	G	249	90.449	−151.170	117.990	1.00	140.83
ATOM	778	CG	HIS	G	249	90.872	−152.257	117.049	1.00	143.17
ATOM	779	ND1	HIS	G	249	90.448	−152.316	115.739	1.00	143.35
ATOM	780	CD2	HIS	G	249	91.689	−153.323	117.227	1.00	143.40

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	781	CE1	HIS	G	249	90.986	−153.371	115.151	1.00	143.13
ATOM	782	NE2	HIS	G	249	91.743	−153.998	116.032	1.00	143.09
ATOM	783	N	GLY	G	250	88.672	−151.119	120.550	1.00	135.79
ATOM	784	CA	GLY	G	250	88.359	−150.585	121.865	1.00	132.31
ATOM	785	C	GLY	G	250	89.255	−149.450	122.328	1.00	129.65
ATOM	786	O	GLY	G	250	90.404	−149.674	122.714	1.00	129.34
ATOM	787	N	ILE	G	251	88.723	−148.232	122.302	1.00	126.82
ATOM	788	CA	ILE	G	251	89.464	−147.053	122.729	1.00	123.65
ATOM	789	C	ILE	G	251	89.083	−146.696	124.159	1.00	121.43
ATOM	790	O	ILE	G	251	87.906	−146.528	124.468	1.00	121.14
ATOM	791	CB	ILE	G	251	89.145	−145.841	121.836	1.00	123.65
ATOM	792	CG1	ILE	G	251	89.420	−146.199	120.375	1.00	124.47
ATOM	793	CG2	ILE	G	251	89.983	−144.643	122.259	1.00	122.65
ATOM	794	CD1	ILE	G	251	90.843	−146.656	120.116	1.00	125.76
ATOM	795	N	ARG	G	252	90.082	−146.581	125.025	1.00	119.23
ATOM	796	CA	ARG	G	252	89.857	−146.237	126.422	1.00	117.32
ATOM	797	C	ARG	G	252	89.886	−144.713	126.553	1.00	114.89
ATOM	798	O	ARG	G	252	90.918	−144.088	126.322	1.00	114.47
ATOM	799	CB	ARG	G	252	90.959	−146.854	127.291	1.00	119.04
ATOM	800	CG	ARG	G	252	91.398	−148.252	126.860	1.00	120.89
ATOM	801	CD	ARG	G	252	90.441	−149.350	127.320	1.00	123.64
ATOM	802	NE	ARG	G	252	90.658	−149.735	128.715	1.00	125.39
ATOM	803	CZ	ARG	G	252	90.032	−150.741	129.319	1.00	125.75
ATOM	804	NH1	ARG	G	252	89.145	−151.468	128.653	1.00	126.03
ATOM	805	NH2	ARG	G	252	90.296	−151.025	130.589	1.00	124.96
ATOM	806	N	PRO	G	253	88.749	−144.093	126.923	1.00	113.15
ATOM	807	CA	PRO	G	253	88.674	−142.635	127.073	1.00	112.07
ATOM	808	C	PRO	G	253	89.467	−142.080	128.254	1.00	111.17
ATOM	809	O	PRO	G	253	88.925	−141.891	129.346	1.00	111.86
ATOM	810	CB	PRO	G	253	87.178	−142.389	127.228	1.00	111.80
ATOM	811	CG	PRO	G	253	86.754	−143.589	128.011	1.00	112.54
ATOM	812	CD	PRO	G	253	87.441	−144.700	127.232	1.00	113.08
ATOM	813	N	VAL	G	254	90.746	−141.807	128.022	1.00	109.24
ATOM	814	CA	VAL	G	254	91.622	−141.274	129.057	1.00	106.74
ATOM	815	C	VAL	G	254	92.049	−139.851	128.722	1.00	106.15
ATOM	816	O	VAL	G	254	92.714	−139.615	127.712	1.00	105.35
ATOM	817	CB	VAL	G	254	92.894	−142.136	129.198	1.00	106.43
ATOM	818	CG1	VAL	G	254	93.815	−141.539	130.252	1.00	105.45
ATOM	819	CG2	VAL	G	254	92.516	−143.559	129.568	1.00	105.32
ATOM	820	N	VAL	G	255	91.659	−138.906	129.567	1.00	105.48
ATOM	821	CA	VAL	G	255	92.020	−137.511	129.363	1.00	104.38
ATOM	822	C	VAL	G	255	93.205	−137.137	130.244	1.00	102.82
ATOM	823	O	VAL	G	255	93.042	−136.827	131.423	1.00	103.17
ATOM	824	CB	VAL	G	255	90.835	−136.573	129.684	1.00	103.63
ATOM	825	CG1	VAL	G	255	89.960	−136.398	128.452	1.00	102.60
ATOM	826	CG2	VAL	G	255	90.013	−137.153	130.821	1.00	103.74
ATOM	827	N	SER	G	256	94.399	−137.177	129.664	1.00	101.35
ATOM	828	CA	SER	G	256	95.619	−136.849	130.391	1.00	100.45
ATOM	829	C	SER	G	256	96.587	−136.050	129.530	1.00	99.76
ATOM	830	O	SER	G	256	96.492	−136.053	128.304	1.00	99.01
ATOM	831	CB	SER	G	256	96.298	−138.133	130.875	1.00	100.56
ATOM	832	OG	SER	G	256	96.534	−139.020	129.799	1.00	100.95
ATOM	833	N	THR	G	257	97.529	−135.379	130.182	1.00	99.86
ATOM	834	CA	THR	G	257	98.513	−134.566	129.479	1.00	100.65
ATOM	835	C	THR	G	257	99.914	−135.174	129.524	1.00	101.63
ATOM	836	O	THR	G	257	100.217	−136.011	130.380	1.00	101.64
ATOM	837	CB	THR	G	257	98.581	−133.145	130.078	1.00	99.95
ATOM	838	OG1	THR	G	257	98.775	−133.230	131.496	1.00	97.28
ATOM	839	CG2	THR	G	257	97.307	−132.392	129.795	1.00	100.77
ATOM	840	N	GLN	G	258	100.762	−134.744	128.591	1.00	101.38
ATOM	841	CA	GLN	G	258	102.140	−135.218	128.506	1.00	101.30
ATOM	842	C	GLN	G	258	102.259	−136.706	128.194	1.00	101.52
ATOM	843	O	GLN	G	258	102.841	−137.083	127.180	1.00	101.61
ATOM	844	CB	GLN	G	258	102.879	−134.899	129.807	1.00	102.03
ATOM	845	CG	GLN	G	258	102.869	−133.420	130.152	1.00	104.23
ATOM	846	CD	GLN	G	258	103.675	−133.098	131.394	1.00	105.40
ATOM	847	OE1	GLN	G	258	103.500	−133.721	132.440	1.00	106.32
ATOM	848	NE2	GLN	G	258	104.560	−132.114	131.286	1.00	107.50
ATOM	849	N	LEU	G	259	101.713	−137.546	129.068	1.00	101.69
ATOM	850	CA	LEU	G	259	101.768	−138.993	128.881	1.00	102.17
ATOM	851	C	LEU	G	259	100.423	−139.538	128.414	1.00	102.41
ATOM	852	O	LEU	G	259	99.373	−139.022	128.788	1.00	102.52
ATOM	853	CB	LEU	G	259	102.160	−139.681	130.196	1.00	101.92
ATOM	854	CG	LEU	G	259	103.530	−139.358	130.810	1.00	101.73
ATOM	855	CD1	LEU	G	259	103.500	−139.663	132.298	1.00	99.97
ATOM	856	CD2	LEU	G	259	104.617	−140.161	130.111	1.00	101.60
ATOM	857	N	LEU	G	260	100.465	−140.582	127.593	1.00	102.49
ATOM	858	CA	LEU	G	260	99.251	−141.217	127.088	1.00	102.67

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	859	C	LEU	G	260	99.110	−142.568	127.778	1.00	103.61
ATOM	860	O	LEU	G	260	99.966	−143.437	127.621	1.00	103.69
ATOM	861	CB	LEU	G	260	99.353	−141.409	125.576	1.00	101.68
ATOM	862	CG	LEU	G	260	99.448	−140.122	124.752	1.00	101.95
ATOM	863	CD1	LEU	G	260	99.953	−140.434	123.355	1.00	104.05
ATOM	864	CD2	LEU	G	260	98.086	−139.457	124.703	1.00	102.22
ATOM	865	N	LEU	G	261	98.030	−142.748	128.533	1.00	105.17
ATOM	866	CA	LEU	G	261	97.815	−143.991	129.276	1.00	106.41
ATOM	867	C	LEU	G	261	96.661	−144.836	128.744	1.00	107.21
ATOM	868	O	LEU	G	261	95.708	−144.314	128.167	1.00	106.94
ATOM	869	CB	LEU	G	261	97.549	−143.661	130.743	1.00	105.72
ATOM	870	CG	LEU	G	261	98.232	−142.392	131.272	1.00	104.79
ATOM	871	CD1	LEU	G	261	97.660	−142.057	132.637	1.00	105.02
ATOM	872	CD2	LEU	G	261	99.741	−142.577	131.340	1.00	103.55
ATOM	873	N	ASN	G	262	96.752	−146.147	128.959	1.00	108.66
ATOM	874	CA	ASN	G	262	95.724	−147.091	128.515	1.00	110.01
ATOM	875	C	ASN	G	262	95.280	−146.877	127.074	1.00	112.35
ATOM	876	O	ASN	G	262	94.183	−146.376	126.822	1.00	113.39
ATOM	877	CB	ASN	G	262	94.502	−147.021	129.432	1.00	108.26
ATOM	878	CG	ASN	G	262	94.817	−147.452	130.846	1.00	107.34
ATOM	879	OD1	ASN	G	262	95.692	−148.294	131.054	1.00	106.57
ATOM	880	ND2	ASN	G	262	94.093	−146.901	131.819	1.00	107.98
ATOM	881	N	GLY	G	263	96.129	−147.276	126.132	1.00	114.75
ATOM	882	CA	GLY	G	263	95.801	−147.115	124.728	1.00	117.52
ATOM	883	C	GLY	G	263	96.326	−148.237	123.856	1.00	119.64
ATOM	884	O	GLY	G	263	96.747	−149.284	124.354	1.00	119.72
ATOM	885	N	SER	G	264	96.308	−148.008	122.547	1.00	121.07
ATOM	886	CA	SER	G	264	96.771	−148.992	121.578	1.00	122.04
ATOM	887	C	SER	G	264	98.291	−149.038	121.482	1.00	123.78
ATOM	888	O	SER	G	264	98.949	−148.003	121.362	1.00	123.31
ATOM	889	CB	SER	G	264	96.178	−148.678	120.201	1.00	120.42
ATOM	890	OG	SER	G	264	96.593	−149.632	119.242	1.00	120.43
ATOM	891	N	LEU	G	265	98.844	−150.244	121.540	1.00	126.40
ATOM	892	CA	LEU	G	265	100.286	−150.421	121.448	1.00	129.15
ATOM	893	C	LEU	G	265	100.693	−150.823	120.037	1.00	130.72
ATOM	894	O	LEU	G	265	99.983	−151.573	119.368	1.00	130.95
ATOM	895	CB	LEU	G	265	100.764	−151.493	122.433	1.00	130.79
ATOM	896	CG	LEU	G	265	100.641	−151.191	123.929	1.00	132.07
ATOM	897	CD1	LEU	G	265	99.572	−152.079	124.562	1.00	132.65
ATOM	898	CD2	LEU	G	265	101.988	−151.433	124.590	1.00	131.38
ATOM	899	N	ALA	G	266	101.838	−150.322	119.586	1.00	132.23
ATOM	900	CA	ALA	G	266	102.339	−150.651	118.259	1.00	134.12
ATOM	901	C	ALA	G	266	102.910	−152.065	118.269	1.00	135.84
ATOM	902	O	ALA	G	266	103.783	−152.381	119.077	1.00	136.72
ATOM	903	CB	ALA	G	266	103.413	−149.656	117.848	1.00	133.87
ATOM	904	N	GLU	G	267	102.417	−152.911	117.370	1.00	137.31
ATOM	905	CA	GLU	G	267	102.878	−154.294	117.286	1.00	138.28
ATOM	906	C	GLU	G	267	104.287	−154.420	116.704	1.00	138.43
ATOM	907	O	GLU	G	267	104.941	−155.449	116.877	1.00	138.51
ATOM	908	CB	GLU	G	267	101.913	−155.128	116.435	1.00	139.08
ATOM	909	CG	GLU	G	267	101.055	−156.140	117.199	1.00	140.98
ATOM	910	CD	GLU	G	267	100.029	−155.491	118.109	1.00	142.29
ATOM	911	OE1	GLU	G	267	100.397	−155.083	119.230	1.00	143.33
ATOM	912	OE2	GLU	G	267	98.855	−155.381	117.696	1.00	142.39
ATOM	913	N	GLU	G	268	104.752	−153.384	116.011	1.00	138.17
ATOM	914	CA	GLU	G	268	106.084	−153.414	115.408	1.00	137.57
ATOM	915	C	GLU	G	268	107.102	−152.595	116.197	1.00	136.57
ATOM	916	O	GLU	G	268	107.669	−153.080	117.175	1.00	135.78
ATOM	917	CB	GLU	G	268	106.017	−152.915	113.959	1.00	137.43
ATOM	918	CG	GLU	G	268	105.211	−153.810	113.019	1.00	137.50
ATOM	919	CD	GLU	G	268	105.925	−155.107	112.673	1.00	136.95
ATOM	920	OE1	GLU	G	268	106.938	−155.053	111.943	1.00	136.48
ATOM	921	OE2	GLU	G	268	105.474	−156.178	113.133	1.00	135.94
ATOM	922	N	GLU	G	269	107.332	−151.358	115.767	1.00	136.24
ATOM	923	CA	GLU	G	269	108.289	−150.478	116.434	1.00	135.49
ATOM	924	C	GLU	G	269	107.654	−149.157	116.855	1.00	134.06
ATOM	925	O	GLU	G	269	106.488	−148.888	116.558	1.00	133.72
ATOM	926	CB	GLU	G	269	109.470	−150.193	115.500	1.00	136.19
ATOM	927	CG	GLU	G	269	110.272	−151.422	115.099	1.00	136.58
ATOM	928	CD	GLU	G	269	111.252	−151.862	116.170	1.00	136.55
ATOM	929	OE1	GLU	G	269	112.182	−151.086	116.479	1.00	136.08
ATOM	930	OE2	GLU	G	269	111.095	−152.982	116.700	1.00	136.04
ATOM	931	N	VAL	G	270	108.431	−148.335	117.553	1.00	132.32
ATOM	932	CA	VAL	G	270	107.958	−147.031	117.994	1.00	130.76
ATOM	933	C	VAL	G	270	107.775	−146.124	116.783	1.00	129.81
ATOM	934	O	VAL	G	270	108.685	−145.973	115.968	1.00	130.00
ATOM	935	CB	VAL	G	270	108.966	−146.377	118.966	1.00	131.35
ATOM	936	CG1	VAL	G	270	108.937	−144.860	118.811	1.00	131.66

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	937	CG2	VAL	G	270	108.621	−146.755	120.395	1.00	130.81
ATOM	938	N	VAL	G	271	106.598	−145.520	116.668	1.00	128.20
ATOM	939	CA	VAL	G	271	106.313	−144.636	115.547	1.00	126.00
ATOM	940	C	VAL	G	271	105.937	−143.226	115.975	1.00	123.76
ATOM	941	O	VAL	G	271	104.888	−143.009	116.581	1.00	123.89
ATOM	942	CB	VAL	G	271	105.168	−145.198	114.680	1.00	127.31
ATOM	943	CG1	VAL	G	271	105.713	−146.225	113.699	1.00	127.47
ATOM	944	CG2	VAL	G	271	104.117	−145.838	115.573	1.00	128.06
ATOM	945	N	ILE	G	272	106.804	−142.272	115.656	1.00	121.03
ATOM	946	CA	ILE	G	272	106.572	−140.872	115.990	1.00	118.57
ATOM	947	C	ILE	G	272	105.975	−140.139	114.795	1.00	116.72
ATOM	948	O	ILE	G	272	106.352	−140.394	113.652	1.00	116.74
ATOM	949	CB	ILE	G	272	107.887	−140.177	116.415	1.00	118.70
ATOM	950	CG1	ILE	G	272	109.042	−140.617	115.512	1.00	119.92
ATOM	951	CG2	ILE	G	272	108.203	−140.507	117.860	1.00	118.21
ATOM	952	CD1	ILE	G	272	109.082	−139.944	114.157	1.00	120.90
ATOM	953	N	ARG	G	273	105.040	−139.232	115.052	1.00	114.52
ATOM	954	CA	ARG	G	273	104.405	−138.500	113.967	1.00	112.62
ATOM	955	C	ARG	G	273	103.923	−137.100	114.334	1.00	112.88
ATOM	956	O	ARG	G	273	103.487	−136.845	115.455	1.00	113.04
ATOM	957	CB	ARG	G	273	103.254	−139.339	113.401	1.00	110.31
ATOM	958	CG	ARG	G	273	102.587	−140.260	114.417	1.00	106.44
ATOM	959	CD	ARG	G	273	102.311	−141.625	113.795	1.00	104.49
ATOM	960	NE	ARG	G	273	101.683	−142.560	114.726	1.00	102.80
ATOM	961	CZ	ARG	G	273	101.400	−143.826	114.433	1.00	101.53
ATOM	962	NH1	ARG	G	273	101.691	−144.310	113.234	1.00	99.91
ATOM	963	NH2	ARG	G	273	100.825	−144.607	115.337	1.00	100.38
ATOM	964	N	SER	G	274	104.018	−136.199	113.363	1.00	113.32
ATOM	965	CA	SER	G	274	103.618	−134.810	113.531	1.00	114.33
ATOM	966	C	SER	G	274	103.131	−134.296	112.184	1.00	115.69
ATOM	967	O	SER	G	274	103.519	−134.816	111.140	1.00	115.97
ATOM	968	CB	SER	G	274	104.814	−133.974	114.003	1.00	114.12
ATOM	969	OG	SER	G	274	104.457	−132.617	114.198	1.00	114.92
ATOM	970	N	ASP	G	275	102.285	−133.274	112.205	1.00	117.50
ATOM	971	CA	ASP	G	275	101.764	−132.718	110.966	1.00	119.82
ATOM	972	C	ASP	G	275	102.906	−132.161	110.109	1.00	122.54
ATOM	973	O	ASP	G	275	102.898	−132.283	108.885	1.00	123.77
ATOM	974	CB	ASP	G	275	100.742	−131.626	111.284	1.00	119.48
ATOM	975	CG	ASP	G	275	99.978	−131.168	110.059	1.00	119.15
ATOM	976	OD1	ASP	G	275	100.457	−130.241	109.380	1.00	119.47
ATOM	977	OD2	ASP	G	275	98.907	−131.748	109.774	1.00	119.52
ATOM	978	N	ASN	G	276	103.885	−131.547	110.766	1.00	124.54
ATOM	979	CA	ASN	G	276	105.053	−130.984	110.095	1.00	126.17
ATOM	980	C	ASN	G	276	106.182	−130.957	111.116	1.00	126.16
ATOM	981	O	ASN	G	276	106.209	−130.097	111.996	1.00	127.07
ATOM	982	CB	ASN	G	276	104.764	−129.565	109.575	1.00	127.69
ATOM	983	CG	ASN	G	276	105.951	−128.957	108.826	1.00	130.48
ATOM	984	OD1	ASN	G	276	106.983	−128.684	109.436	1.00	131.45
ATOM	985	ND2	ASN	G	276	105.817	−128.752	107.512	1.00	133.41
ATOM	986	N	PHE	G	277	107.098	−131.915	111.001	1.00	125.51
ATOM	987	CA	PHE	G	277	108.223	−132.013	111.917	1.00	124.73
ATOM	988	C	PHE	G	277	109.164	−130.820	111.885	1.00	124.32
ATOM	989	O	PHE	G	277	109.851	−130.543	112.869	1.00	124.52
ATOM	990	CB	PHE	G	277	109.021	−133.282	111.645	1.00	124.97
ATOM	991	CG	PHE	G	277	108.616	−134.440	112.498	1.00	124.70
ATOM	992	CD1	PHE	G	277	107.662	−135.352	112.061	1.00	124.33
ATOM	993	CD2	PHE	G	277	109.177	−134.606	113.758	1.00	125.19
ATOM	994	CE1	PHE	G	277	107.274	−136.416	112.872	1.00	124.54
ATOM	995	CE2	PHE	G	277	108.797	−135.661	114.575	1.00	125.18
ATOM	996	CZ	PHE	G	277	107.843	−136.568	114.132	1.00	124.26
ATOM	997	N	THR	G	278	109.205	−130.113	110.763	1.00	123.74
ATOM	998	CA	THR	G	278	110.082	−128.954	110.660	1.00	123.33
ATOM	999	C	THR	G	278	109.545	−127.821	111.522	1.00	122.48
ATOM	1000	O	THR	G	278	110.298	−126.961	111.974	1.00	122.37
ATOM	1001	CB	THR	G	278	110.194	−128.471	109.208	1.00	123.77
ATOM	1002	OG1	THR	G	278	110.512	−129.583	108.363	1.00	122.39
ATOM	1003	CG2	THR	G	278	111.299	−127.432	109.076	1.00	124.71
ATOM	1004	N	ASN	G	279	108.237	−127.836	111.752	1.00	121.41
ATOM	1005	CA	ASN	G	279	107.588	−126.823	112.569	1.00	120.64
ATOM	1006	C	ASN	G	279	107.553	−127.290	114.019	1.00	119.86
ATOM	1007	O	ASN	G	279	107.075	−128.384	114.316	1.00	119.77
ATOM	1008	CB	ASN	G	279	106.168	−126.570	112.060	1.00	122.36
ATOM	1009	CG	ASN	G	279	105.527	−125.362	112.703	1.00	123.19
ATOM	1010	OD1	ASN	G	279	106.104	−124.276	112.716	1.00	124.95
ATOM	1011	ND2	ASN	G	279	104.322	−125.540	113.228	1.00	123.66
ATOM	1012	N	ASN	G	280	108.059	−126.451	114.917	1.00	118.87
ATOM	1013	CA	ASN	G	280	108.107	−126.780	116.336	1.00	118.01
ATOM	1014	C	ASN	G	280	106.785	−126.592	117.075	1.00	117.08

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	1015	O	ASN	G	280	106.615	−127.104	118.181	1.00	117.55
ATOM	1016	CB	ASN	G	280	109.187	−125.943	117.019	1.00	118.90
ATOM	1017	CG	ASN	G	280	109.006	−124.457	116.781	1.00	119.84
ATOM	1018	OD1	ASN	G	280	108.992	−124.001	115.638	1.00	119.58
ATOM	1019	ND2	ASN	G	280	108.865	−123.694	117.859	1.00	121.00
ATOM	1020	N	ALA	G	281	105.851	−125.862	116.472	1.00	115.19
ATOM	1021	CA	ALA	G	281	104.557	−125.612	117.102	1.00	112.13
ATOM	1022	C	ALA	G	281	103.663	−126.842	117.077	1.00	109.69
ATOM	1023	O	ALA	G	281	102.802	−127.010	117.937	1.00	109.86
ATOM	1024	CB	ALA	G	281	103.859	−124.453	116.409	1.00	113.29
ATOM	1025	N	LYS	G	282	103.865	−127.693	116.078	1.00	106.77
ATOM	1026	CA	LYS	G	282	103.078	−128.911	115.939	1.00	104.34
ATOM	1027	C	LYS	G	282	103.510	−129.937	116.979	1.00	102.27
ATOM	1028	O	LYS	G	282	104.699	−130.197	117.147	1.00	101.74
ATOM	1029	CB	LYS	G	282	103.260	−129.495	114.534	1.00	104.78
ATOM	1030	CG	LYS	G	282	102.841	−128.579	113.392	1.00	105.16
ATOM	1031	CD	LYS	G	282	101.326	−128.507	113.226	1.00	107.10
ATOM	1032	CE	LYS	G	282	100.956	−127.757	111.947	1.00	107.70
ATOM	1033	NZ	LYS	G	282	99.493	−127.777	111.657	1.00	108.40
ATOM	1034	N	THR	G	283	102.542	−130.523	117.671	1.00	100.94
ATOM	1035	CA	THR	G	283	102.848	−131.514	118.693	1.00	100.59
ATOM	1036	C	THR	G	283	103.256	−132.850	118.076	1.00	99.16
ATOM	1037	O	THR	G	283	102.777	−133.227	117.003	1.00	98.27
ATOM	1038	CB	THR	G	283	101.643	−131.751	119.620	1.00	102.18
ATOM	1039	OG1	THR	G	283	100.523	−132.185	118.843	1.00	103.66
ATOM	1040	CG2	THR	G	283	101.276	−130.478	120.352	1.00	102.55
ATOM	1041	N	ILE	G	284	104.135	−133.567	118.767	1.00	97.96
ATOM	1042	CA	ILE	G	284	104.616	−134.855	118.292	1.00	97.14
ATOM	1043	C	ILE	G	284	104.064	−136.005	119.123	1.00	97.31
ATOM	1044	O	ILE	G	284	104.344	−136.110	120.318	1.00	97.07
ATOM	1045	CB	ILE	G	284	106.157	−134.899	118.331	1.00	96.52
ATOM	1046	CG1	ILE	G	284	106.714	−133.841	117.375	1.00	96.20
ATOM	1047	CG2	ILE	G	284	106.656	−136.293	117.964	1.00	96.59
ATOM	1048	CD1	ILE	G	284	108.195	−133.608	117.509	1.00	96.44
ATOM	1049	N	ILE	G	285	103.276	−136.863	118.485	1.00	98.01
ATOM	1050	CA	ILE	G	285	102.685	−138.013	119.158	1.00	99.80
ATOM	1051	C	ILE	G	285	103.602	−139.229	119.071	1.00	101.17
ATOM	1052	O	ILE	G	285	103.975	−139.661	117.980	1.00	100.52
ATOM	1053	CB	ILE	G	285	101.312	−138.386	118.537	1.00	99.80
ATOM	1054	CG1	ILE	G	285	100.246	−137.372	118.961	1.00	100.25
ATOM	1055	CG2	ILE	G	285	100.903	−139.782	118.977	1.00	100.16
ATOM	1056	CD1	ILE	G	285	100.455	−135.980	118.409	1.00	102.53
ATOM	1057	N	VAL	G	286	103.955	−139.782	120.224	1.00	103.62
ATOM	1058	CA	VAL	G	286	104.831	−140.943	120.282	1.00	106.86
ATOM	1059	C	VAL	G	286	104.055	−142.192	120.683	1.00	109.26
ATOM	1060	O	VAL	G	286	103.311	−142.176	121.663	1.00	109.45
ATOM	1061	CB	VAL	G	286	105.953	−140.727	121.314	1.00	107.59
ATOM	1062	CG1	VAL	G	286	106.960	−141.865	121.236	1.00	108.43
ATOM	1063	CG2	VAL	G	286	106.621	−139.385	121.074	1.00	107.25
ATOM	1064	N	GLN	G	287	104.222	−143.270	119.923	1.00	112.10
ATOM	1065	CA	GLN	G	287	103.540	−144.527	120.225	1.00	115.20
ATOM	1066	C	GLN	G	287	104.575	−145.549	120.675	1.00	116.64
ATOM	1067	O	GLN	G	287	105.564	−145.779	119.982	1.00	117.12
ATOM	1068	CB	GLN	G	287	102.803	−145.057	118.992	1.00	116.06
ATOM	1069	CG	GLN	G	287	101.378	−145.514	119.275	1.00	117.17
ATOM	1070	CD	GLN	G	287	100.932	−146.653	118.378	1.00	117.46
ATOM	1071	OE1	GLN	G	287	101.086	−146.600	117.158	1.00	116.74
ATOM	1072	NE2	GLN	G	287	100.366	−147.692	118.984	1.00	117.73
ATOM	1073	N	LEU	G	288	104.338	−146.170	121.825	1.00	119.08
ATOM	1074	CA	LEU	G	288	105.270	−147.150	122.375	1.00	122.20
ATOM	1075	C	LEU	G	288	104.788	−148.588	122.203	1.00	124.20
ATOM	1076	O	LEU	G	288	103.594	−148.867	122.309	1.00	124.85
ATOM	1077	CB	LEU	G	288	105.479	−146.874	123.862	1.00	121.50
ATOM	1078	CG	LEU	G	288	105.844	−145.433	124.231	1.00	121.43
ATOM	1079	CD1	LEU	G	288	105.637	−145.233	125.720	1.00	122.39
ATOM	1080	CD2	LEU	G	288	107.281	−145.134	123.832	1.00	123.19
ATOM	1081	N	LYS	G	289	105.721	−149.503	121.953	1.00	126.07
ATOM	1082	CA	LYS	G	289	105.380	−150.912	121.782	1.00	127.42
ATOM	1083	C	LYS	G	289	105.478	−151.682	123.097	1.00	127.68
ATOM	1084	O	LYS	G	289	104.856	−152.732	123.258	1.00	126.88
ATOM	1085	CB	LYS	G	289	106.285	−151.552	120.723	1.00	128.03
ATOM	1086	CG	LYS	G	289	107.441	−150.673	120.252	1.00	129.35
ATOM	1087	CD	LYS	G	289	108.782	−151.209	120.736	1.00	130.44
ATOM	1088	CE	LYS	G	289	109.966	−150.519	120.051	1.00	130.23
ATOM	1089	NZ	LYS	G	289	110.464	−149.301	120.754	1.00	131.22
ATOM	1090	N	GLU	G	290	106.263	−151.159	124.033	1.00	128.43
ATOM	1091	CA	GLU	G	290	106.416	−151.788	125.341	1.00	128.96
ATOM	1092	C	GLU	G	290	105.619	−150.998	126.375	1.00	127.87

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	1093	O	GLU	G	290	105.837	−149.800	126.553	1.00	127.30
ATOM	1094	CB	GLU	G	290	107.894	−151.843	125.744	1.00	131.22
ATOM	1095	CG	GLU	G	290	108.714	−152.872	124.974	1.00	134.12
ATOM	1096	CD	GLU	G	290	110.117	−153.047	125.532	1.00	135.56
ATOM	1097	OE1	GLU	G	290	110.924	−152.097	125.442	1.00	136.25
ATOM	1098	OE2	GLU	G	290	110.412	−154.138	126.064	1.00	135.63
ATOM	1099	N	SER	G	291	104.697	−151.673	127.052	1.00	126.04
ATOM	1100	CA	SER	G	291	103.856	−151.030	128.053	1.00	124.60
ATOM	1101	C	SER	G	291	104.589	−150.693	129.344	1.00	124.35
ATOM	1102	O	SER	G	291	105.113	−151.577	130.025	1.00	125.69
ATOM	1103	CB	SER	G	291	102.656	−151.922	128.379	1.00	123.78
ATOM	1104	OG	SER	G	291	103.084	−153.161	128.915	1.00	123.88
ATOM	1105	N	VAL	G	292	104.615	−149.408	129.679	1.00	123.16
ATOM	1106	CA	VAL	G	292	105.263	−148.941	130.898	1.00	121.87
ATOM	1107	C	VAL	G	292	104.192	−148.750	131.968	1.00	121.23
ATOM	1108	O	VAL	G	292	103.399	−147.813	131.897	1.00	120.89
ATOM	1109	CB	VAL	G	292	105.968	−147.595	130.662	1.00	121.78
ATOM	1110	CG1	VAL	G	292	106.742	−147.191	131.907	1.00	121.71
ATOM	1111	CG2	VAL	G	292	106.886	−147.697	129.461	1.00	120.71
ATOM	1112	N	GLU	G	293	104.169	−149.640	132.952	1.00	120.89
ATOM	1113	CA	GLU	G	293	103.178	−149.574	134.015	1.00	121.29
ATOM	1114	C	GLU	G	293	103.474	−148.476	135.031	1.00	121.55
ATOM	1115	O	GLU	G	293	104.568	−148.408	135.591	1.00	121.80
ATOM	1116	CB	GLU	G	293	103.086	−150.933	134.723	1.00	121.08
ATOM	1117	CG	GLU	G	293	102.116	−150.988	135.893	1.00	121.19
ATOM	1118	CD	GLU	G	293	101.966	−152.394	136.445	1.00	122.13
ATOM	1119	OE1	GLU	G	293	102.946	−153.167	136.371	1.00	122.07
ATOM	1120	OE2	GLU	G	293	100.876	−152.722	136.961	1.00	123.25
ATOM	1121	N	ILE	G	294	102.493	−147.610	135.258	1.00	121.87
ATOM	1122	CA	ILE	G	294	102.637	−146.524	136.217	1.00	121.70
ATOM	1123	C	ILE	G	294	101.621	−146.720	137.333	1.00	121.42
ATOM	1124	O	ILE	G	294	100.433	−146.917	137.076	1.00	121.27
ATOM	1125	CB	ILE	G	294	102.418	−145.160	135.536	1.00	122.02
ATOM	1126	CG1	ILE	G	294	102.578	−144.033	136.557	1.00	122.87
ATOM	1127	CG2	ILE	G	294	101.048	−145.125	134.884	1.00	121.44
ATOM	1128	CD1	ILE	G	294	102.714	−142.660	135.931	1.00	122.60
ATOM	1129	N	ASN	G	295	102.097	−146.674	138.573	1.00	121.00
ATOM	1130	CA	ASN	G	295	101.238	−146.874	139.736	1.00	121.44
ATOM	1131	C	ASN	G	295	101.204	−145.674	140.677	1.00	121.01
ATOM	1132	O	ASN	G	295	102.134	−145.462	141.457	1.00	121.03
ATOM	1133	CB	ASN	G	295	101.710	−148.103	140.517	1.00	122.74
ATOM	1134	CG	ASN	G	295	101.810	−149.344	139.651	1.00	122.92
ATOM	1135	OD1	ASN	G	295	100.819	−149.793	139.075	1.00	122.88
ATOM	1136	ND2	ASN	G	295	103.011	−149.905	139.555	1.00	122.92
ATOM	1137	N	CYS	G	296	100.124	−144.901	140.605	1.00	120.25
ATOM	1138	CA	CYS	G	296	99.960	−143.728	141.456	1.00	118.86
ATOM	1139	C	CYS	G	296	98.928	−144.045	142.537	1.00	117.99
ATOM	1140	O	CYS	G	296	97.835	−144.528	142.236	1.00	117.00
ATOM	1141	CB	CYS	G	296	99.466	−142.537	140.636	1.00	119.34
ATOM	1142	SG	CYS	G	296	100.316	−142.227	139.052	1.00	119.64
ATOM	1143	N	THR	G	297	99.268	−143.765	143.791	1.00	117.75
ATOM	1144	CA	THR	G	297	98.356	−144.042	144.895	1.00	117.96
ATOM	1145	C	THR	G	297	98.386	−142.956	145.967	1.00	117.03
ATOM	1146	O	THR	G	297	99.224	−142.055	145.933	1.00	115.96
ATOM	1147	CB	THR	G	297	98.692	−145.394	145.560	1.00	118.94
ATOM	1148	OG1	THR	G	297	99.992	−145.325	146.159	1.00	120.18
ATOM	1149	CG2	THR	G	297	98.688	−146.509	144.524	1.00	119.76
ATOM	1150	N	ARG	G	298	97.459	−143.050	146.916	1.00	116.66
ATOM	1151	CA	ARG	G	298	97.369	−142.092	148.010	1.00	116.73
ATOM	1152	C	ARG	G	298	96.753	−142.780	149.228	1.00	118.95
ATOM	1153	O	ARG	G	298	95.710	−143.426	149.124	1.00	118.61
ATOM	1154	CB	ARG	G	298	96.521	−140.888	147.585	1.00	114.49
ATOM	1155	CG	ARG	G	298	96.550	−139.720	148.564	1.00	112.45
ATOM	1156	CD	ARG	G	298	95.473	−139.831	149.632	1.00	110.20
ATOM	1157	NE	ARG	G	298	94.138	−139.603	149.085	1.00	108.71
ATOM	1158	CZ	ARG	G	298	93.026	−139.566	149.812	1.00	107.87
ATOM	1159	NH1	ARG	G	298	93.082	−139.742	151.125	1.00	107.98
ATOM	1160	NH2	ARG	G	298	91.857	−139.349	149.227	1.00	107.62
ATOM	1161	N	PRO	G	299	97.402	−142.651	150.399	1.00	121.18
ATOM	1162	CA	PRO	G	299	96.984	−143.233	151.681	1.00	123.48
ATOM	1163	C	PRO	G	299	95.484	−143.182	151.977	1.00	125.98
ATOM	1164	O	PRO	G	299	94.700	−142.658	151.186	1.00	126.15
ATOM	1165	CB	PRO	G	299	97.805	−142.442	152.691	1.00	123.50
ATOM	1166	CG	PRO	G	299	99.092	−142.253	151.958	1.00	122.94
ATOM	1167	CD	PRO	G	299	98.621	−141.841	150.576	1.00	121.50
ATOM	1168	N	ASN	G	300	95.092	−143.724	153.127	1.00	127.96
ATOM	1169	CA	ASN	G	300	93.684	−143.752	153.502	1.00	130.21
ATOM	1170	C	ASN	G	300	93.364	−143.237	154.905	1.00	131.51

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	1171	O	ASN	G	300	93.985	−142.292	155.394	1.00	131.18
ATOM	1172	CB	ASN	G	300	93.137	−145.173	153.341	1.00	130.07
ATOM	1173	CG	ASN	G	300	93.919	−146.194	154.142	1.00	130.57
ATOM	1174	OD1	ASN	G	300	95.139	−146.299	154.015	1.00	130.10
ATOM	1175	ND2	ASN	G	300	93.216	−146.958	154.969	1.00	131.18
ATOM	1176	N	GLN	G	301	92.384	−143.877	155.537	1.00	133.80
ATOM	1177	CA	GLN	G	301	91.912	−143.514	156.871	1.00	135.82
ATOM	1178	C	GLN	G	301	92.716	−144.156	158.004	1.00	137.01
ATOM	1179	O	GLN	G	301	92.448	−143.903	159.180	1.00	136.35
ATOM	1180	CB	GLN	G	301	90.436	−143.911	157.001	1.00	135.35
ATOM	1181	CG	GLN	G	301	89.724	−143.404	158.248	1.00	135.28
ATOM	1182	CD	GLN	G	301	89.563	−141.897	158.258	1.00	134.83
ATOM	1183	OE1	GLN	G	301	89.785	−141.230	157.247	1.00	134.19
ATOM	1184	NE2	GLN	G	301	89.160	−141.353	159.402	1.00	133.96
ATOM	1185	N	ASN	G	302	93.701	−144.979	157.656	1.00	138.83
ATOM	1186	CA	ASN	G	302	94.522	−145.651	158.662	1.00	140.81
ATOM	1187	C	ASN	G	302	95.302	−144.706	159.574	1.00	141.45
ATOM	1188	O	ASN	G	302	96.112	−145.155	160.387	1.00	141.13
ATOM	1189	CB	ASN	G	302	95.494	−146.633	157.997	1.00	141.80
ATOM	1190	CG	ASN	G	302	94.851	−147.975	157.690	1.00	143.04
ATOM	1191	OD1	ASN	G	302	94.307	−148.632	158.579	1.00	142.23
ATOM	1192	ND2	ASN	G	302	94.919	−148.392	156.431	1.00	142.70
ATOM	1193	N	THR	G	303	95.063	−143.404	159.440	1.00	142.24
ATOM	1194	CA	THR	G	303	95.745	−142.423	160.278	1.00	142.95
ATOM	1195	C	THR	G	303	95.430	−142.755	161.734	1.00	143.18
ATOM	1196	O	THR	G	303	96.274	−143.285	162.457	1.00	143.28
ATOM	1197	CB	THR	G	303	95.263	−140.990	159.969	1.00	143.28
ATOM	1198	OG1	THR	G	303	95.502	−140.691	158.588	1.00	143.23
ATOM	1199	CG2	THR	G	303	96.006	−139.980	160.831	1.00	144.01
ATOM	1200	N	ARG	G	304	94.208	−142.441	162.154	1.00	143.39
ATOM	1201	CA	ARG	G	304	93.762	−142.731	163.512	1.00	143.68
ATOM	1202	C	ARG	G	304	92.770	−143.886	163.431	1.00	143.18
ATOM	1203	O	ARG	G	304	92.051	−144.019	162.441	1.00	143.86
ATOM	1204	CB	ARG	G	304	93.108	−141.495	164.138	1.00	144.11
ATOM	1205	CG	ARG	G	304	94.084	−140.349	164.381	1.00	145.32
ATOM	1206	CD	ARG	G	304	95.261	−140.809	165.238	1.00	147.31
ATOM	1207	NE	ARG	G	304	96.271	−139.770	165.421	1.00	147.56
ATOM	1208	CZ	ARG	G	304	97.419	−139.953	166.067	1.00	147.68
ATOM	1209	NH1	ARG	G	304	97.706	−141.136	166.593	1.00	146.72
ATOM	1210	NH2	ARG	G	304	98.283	−138.953	166.187	1.00	146.63
ATOM	1211	N	LYS	G	305	92.728	−144.722	164.464	1.00	141.97
ATOM	1212	CA	LYS	G	305	91.836	−145.874	164.442	1.00	140.98
ATOM	1213	C	LYS	G	305	90.851	−145.964	165.606	1.00	140.38
ATOM	1214	O	LYS	G	305	89.921	−146.771	165.565	1.00	140.91
ATOM	1215	CB	LYS	G	305	92.668	−147.159	164.384	1.00	141.00
ATOM	1216	CG	LYS	G	305	91.930	−148.361	163.818	1.00	140.99
ATOM	1217	CD	LYS	G	305	91.633	−148.169	162.338	1.00	141.06
ATOM	1218	CE	LYS	G	305	90.967	−149.397	161.741	1.00	141.85
ATOM	1219	NZ	LYS	G	305	90.730	−149.243	160.279	1.00	140.37
ATOM	1220	N	SER	G	306	91.042	−145.149	166.638	1.00	139.15
ATOM	1221	CA	SER	G	306	90.143	−145.193	167.788	1.00	137.47
ATOM	1222	C	SER	G	306	89.922	−143.845	168.466	1.00	136.43
ATOM	1223	O	SER	G	306	90.820	−143.005	168.518	1.00	136.13
ATOM	1224	CB	SER	G	306	90.663	−146.198	168.818	1.00	137.39
ATOM	1225	OG	SER	G	306	90.732	−147.502	168.267	1.00	136.71
ATOM	1226	N	ILE	G	307	88.713	−143.654	168.985	1.00	135.40
ATOM	1227	CA	ILE	G	307	88.345	−142.424	169.678	1.00	135.12
ATOM	1228	C	ILE	G	307	87.998	−142.771	171.124	1.00	133.50
ATOM	1229	O	ILE	G	307	87.697	−143.924	171.433	1.00	133.64
ATOM	1230	CB	ILE	G	307	87.122	−141.754	169.013	1.00	135.24
ATOM	1231	CG1	ILE	G	307	87.410	−141.505	167.531	1.00	136.04
ATOM	1232	CG2	ILE	G	307	86.802	−140.437	169.709	1.00	135.56
ATOM	1233	CD1	ILE	G	307	86.248	−140.899	166.770	1.00	137.26
ATOM	1234	N	HIS	G	308	88.042	−141.777	172.005	1.00	132.91
ATOM	1235	CA	HIS	G	308	87.739	−141.997	173.416	1.00	132.86
ATOM	1236	C	HIS	G	308	86.709	−141.003	173.946	1.00	130.36
ATOM	1237	O	HIS	G	308	86.915	−139.791	173.887	1.00	130.34
ATOM	1238	CB	HIS	G	308	89.023	−141.899	174.244	1.00	133.35
ATOM	1239	CG	HIS	G	308	90.081	−142.878	173.836	1.00	134.57
ATOM	1240	ND1	HIS	G	308	90.588	−142.935	172.557	1.00	135.10
ATOM	1241	CD2	HIS	G	308	90.726	−143.837	174.541	1.00	134.82
ATOM	1242	CE1	HIS	G	308	91.501	−143.889	172.490	1.00	135.21
ATOM	1243	NE2	HIS	G	308	91.604	−144.451	173.680	1.00	134.93
ATOM	1244	N	ILE	G	309	85.593	−141.524	174.451	1.00	129.66
ATOM	1245	CA	ILE	G	309	84.535	−140.678	174.996	1.00	132.96
ATOM	1246	C	ILE	G	309	84.853	−140.335	176.442	1.00	129.06
ATOM	1247	O	ILE	G	309	85.368	−141.163	177.189	1.00	130.20
ATOM	1248	CB	ILE	G	309	83.150	−141.381	174.982	1.00	129.80

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	1249	CG1	ILE	G	309	82.794	−141.842	173.567	1.00	129.99
ATOM	1250	CG2	ILE	G	309	82.079	−140.427	175.513	1.00	129.45
ATOM	1251	CD1	ILE	G	309	82.707	−140.721	172.551	1.00	131.16
ATOM	1252	N	AGLY	G	312	84.519	−139.106	176.817	0.50	130.34
ATOM	1253	N	BGLY	G	312	84.580	−139.093	176.821	0.50	130.54
ATOM	1254	CA	AGLY	G	312	84.745	−138.635	178.168	0.50	130.62
ATOM	1255	CA	BGLY	G	312	84.870	−138.668	178.175	0.50	132.03
ATOM	1256	C	AGLY	G	312	83.667	−137.629	178.521	0.50	130.49
ATOM	1257	C	BGLY	G	312	84.057	−137.472	178.615	0.50	132.56
ATOM	1258	O	AGLY	G	312	83.395	−136.719	177.734	0.50	129.55
ATOM	1259	O	BGLY	G	312	83.971	−136.469	177.901	0.50	132.01
ATOM	1260	N	APRO	G	313	83.028	−137.767	179.695	0.50	130.44
ATOM	1261	N	BPRO	G	313	83.443	−137.553	179.805	0.50	133.04
ATOM	1262	CA	APRO	G	313	81.972	−136.840	180.115	0.50	131.53
ATOM	1263	CA	BPRO	G	313	82.628	−136.463	180.344	0.50	134.04
ATOM	1264	C	APRO	G	313	82.413	−135.375	180.098	0.50	132.66
ATOM	1265	C	BPRO	G	313	83.434	−135.170	180.483	0.50	134.58
ATOM	1266	O	APRO	G	313	81.581	−134.468	180.030	0.50	132.16
ATOM	1267	O	BPRO	G	313	84.184	−134.985	181.445	0.50	133.93
ATOM	1268	CB	APRO	G	313	81.618	−137.333	181.522	0.50	130.68
ATOM	1269	CB	BPRO	G	313	82.148	−137.021	181.686	0.50	133.44
ATOM	1270	CG	APRO	G	313	82.890	−137.969	181.999	0.50	130.40
ATOM	1271	CG	BPRO	G	313	83.237	−137.955	182.081	0.50	133.35
ATOM	1272	CD	APRO	G	313	83.349	−138.718	180.774	0.50	130.35
ATOM	1273	CD	BPRO	G	313	83.569	−138.649	180.783	0.50	133.12
ATOM	1274	N	AGLY	G	314	83.726	−135.158	180.147	0.50	133.78
ATOM	1275	N	BGLY	G	314	83.279	−134.282	179.508	0.50	135.23
ATOM	1276	CA	AGLY	G	314	84.259	−133.808	180.140	0.50	135.11
ATOM	1277	CA	BGLY	G	314	84.005	−133.028	179.539	0.50	136.68
ATOM	1278	C	AGLY	G	314	85.185	−133.514	178.973	0.50	136.46
ATOM	1279	C	BGLY	G	314	85.217	−133.071	178.633	0.50	137.64
ATOM	1280	O	AGLY	G	314	85.779	−132.436	178.916	0.50	136.65
ATOM	1281	O	BGLY	G	314	86.040	−132.151	178.641	0.50	137.68
ATOM	1282	N	AARG	G	315	85.317	−134.464	178.047	0.50	137.71
ATOM	1283	N	BARG	G	315	85.330	−134.146	177.855	0.50	138.87
ATOM	1284	CA	AARG	G	315	86.179	−134.280	176.881	0.50	138.32
ATOM	1285	CA	BARG	G	315	86.445	−134.302	176.934	0.50	139.12
ATOM	1286	C	AARG	G	315	86.103	−135.394	175.835	0.50	139.46
ATOM	1287	C	BARG	G	315	86.339	−135.478	175.969	0.50	140.02
ATOM	1288	O	AARG	G	315	85.308	−136.326	175.960	0.50	140.02
ATOM	1289	O	BARG	G	315	85.746	−136.513	176.268	0.50	140.48
ATOM	1290	CB	AARG	G	315	87.634	−134.069	177.327	0.50	138.97
ATOM	1291	CB	BARG	G	315	87.766	−134.388	177.707	0.50	140.03
ATOM	1292	CG	AARG	G	315	88.095	−134.926	178.501	0.50	138.68
ATOM	1293	CG	BARG	G	315	87.860	−135.517	178.714	0.50	140.27
ATOM	1294	CD	AARG	G	315	89.381	−134.354	179.103	0.50	138.38
ATOM	1295	CD	BARG	G	315	89.207	−135.465	179.420	0.50	140.88
ATOM	1296	NE	AARG	G	315	89.824	−135.078	180.294	0.50	138.70
ATOM	1297	NE	BARG	G	315	89.349	−136.496	180.445	0.50	140.22
ATOM	1298	CZ	AARG	G	315	90.845	−134.703	181.062	0.50	138.42
ATOM	1299	CZ	BARG	G	315	90.422	−136.637	181.219	0.50	139.80
ATOM	1300	NH1	AARG	G	315	91.530	−133.607	180.768	0.50	138.28
ATOM	1301	NH1	BARG	G	315	91.454	−135.813	181.085	0.50	138.98
ATOM	1302	NH2	AARG	G	315	91.181	−135.424	182.125	0.50	138.35
ATOM	1303	NH2	BARG	G	315	90.466	−137.604	182.126	0.50	138.56
ATOM	1304	N	ALA	G	316	86.934	−135.273	174.800	1.00	144.80
ATOM	1305	CA	ALA	G	316	86.989	−136.226	173.690	1.00	143.79
ATOM	1306	C	ALA	G	316	88.432	−136.339	173.191	1.00	146.46
ATOM	1307	O	ALA	G	316	89.285	−135.522	173.549	1.00	147.07
ATOM	1308	CB	ALA	G	316	86.065	−135.774	172.553	1.00	144.31
ATOM	1309	N	PHE	G	317	88.701	−137.350	172.366	1.00	149.66
ATOM	1310	CA	PHE	G	317	90.048	−137.578	171.852	1.00	151.88
ATOM	1311	C	PHE	G	317	90.071	−137.825	170.343	1.00	152.98
ATOM	1312	O	PHE	G	317	89.095	−138.305	169.765	1.00	153.44
ATOM	1313	CB	PHE	G	317	90.693	−138.774	172.565	1.00	151.95
ATOM	1314	CG	PHE	G	317	90.978	−138.541	174.025	1.00	152.25
ATOM	1315	CD1	PHE	G	317	89.940	−138.387	174.940	1.00	151.95
ATOM	1316	CD2	PHE	G	317	92.290	−138.486	174.487	1.00	152.28
ATOM	1317	CE1	PHE	G	317	90.204	−138.181	176.293	1.00	151.79
ATOM	1318	CE2	PHE	G	317	92.565	−138.281	175.838	1.00	152.38
ATOM	1319	CZ	PHE	G	317	91.519	−138.129	176.742	1.00	152.23
ATOM	1320	N	TYR	G	318	91.199	−137.492	169.720	1.00	154.53
ATOM	1321	CA	TYR	G	318	91.406	−137.676	168.283	1.00	155.71
ATOM	1322	C	TYR	G	318	90.427	−136.911	167.391	1.00	155.64
ATOM	1323	O	TYR	G	318	89.646	−137.520	166.659	1.00	155.52
ATOM	1324	CB	TYR	G	318	91.340	−139.165	167.919	1.00	156.48
ATOM	1325	CG	TYR	G	318	92.267	−140.063	168.711	1.00	157.82
ATOM	1326	CD1	TYR	G	318	92.044	−140.309	170.065	1.00	158.34

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	1327	CD2	TYR	G	318	93.353	−140.689	168.099	1.00	158.59
ATOM	1328	CE1	TYR	G	318	92.875	−141.159	170.791	1.00	158.85
ATOM	1329	CE2	TYR	G	318	94.192	−141.542	168.817	1.00	159.15
ATOM	1330	CZ	TYR	G	318	93.945	−141.772	170.162	1.00	159.22
ATOM	1331	OH	TYR	G	318	94.765	−142.615	170.877	1.00	159.77
ATOM	1332	N	THR	G	319	90.474	−135.583	167.440	1.00	155.30
ATOM	1333	CA	THR	G	319	89.589	−134.763	166.616	1.00	155.09
ATOM	1334	C	THR	G	319	90.251	−133.430	166.269	1.00	154.62
ATOM	1335	O	THR	G	319	89.683	−132.611	165.545	1.00	153.91
ATOM	1336	CB	THR	G	319	88.246	−134.485	167.334	1.00	155.83
ATOM	1337	OG1	THR	G	319	87.669	−135.722	167.771	1.00	156.26
ATOM	1338	CG2	THR	G	319	87.265	−133.797	166.389	1.00	155.64
ATOM	1339	N	THR	G	320	91.460	−133.223	166.783	1.00	154.50
ATOM	1340	CA	THR	G	320	92.199	−131.990	166.532	1.00	154.03
ATOM	1341	C	THR	G	320	93.278	−132.162	165.463	1.00	153.67
ATOM	1342	O	THR	G	320	94.420	−131.734	165.646	1.00	153.56
ATOM	1343	CB	THR	G	320	92.867	−131.467	167.823	1.00	154.73
ATOM	1344	OG1	THR	G	320	93.762	−132.462	168.338	1.00	154.90
ATOM	1345	CG2	THR	G	320	91.814	−131.143	168.874	1.00	154.48
ATOM	1346	N	GLY	G	321	92.912	−132.791	164.350	1.00	152.75
ATOM	1347	CA	GLY	G	321	93.861	−132.995	163.270	1.00	151.08
ATOM	1348	C	GLY	G	321	94.014	−131.729	162.449	1.00	150.38
ATOM	1349	O	GLY	G	321	93.119	−131.365	161.685	1.00	149.77
ATOM	1350	N	GLU	G	322	95.150	−131.056	162.605	1.00	149.39
ATOM	1351	CA	GLU	G	322	95.405	−129.814	161.884	1.00	148.29
ATOM	1352	C	GLU	G	322	96.649	−129.909	161.008	1.00	147.73
ATOM	1353	O	GLU	G	322	96.564	−130.249	159.827	1.00	146.53
ATOM	1354	CB	GLU	G	322	95.572	−128.662	162.877	1.00	148.27
ATOM	1355	CG	GLU	G	322	94.503	−128.616	163.956	1.00	148.79
ATOM	1356	CD	GLU	G	322	94.707	−127.471	164.928	1.00	148.76
ATOM	1357	OE1	GLU	G	322	95.819	−127.354	165.485	1.00	148.26
ATOM	1358	OE2	GLU	G	322	93.753	−126.693	165.138	1.00	148.68
ATOM	1359	N	ILE	G	322A	97.801	−129.607	161.603	1.00	147.61
ATOM	1360	CA	ILE	G	322A	99.087	−129.634	160.910	1.00	147.08
ATOM	1361	C	ILE	G	322A	98.968	−129.223	159.444	1.00	146.30
ATOM	1362	O	ILE	G	322A	98.978	−130.067	158.548	1.00	145.89
ATOM	1363	CB	ILE	G	322A	99.755	−131.036	161.003	1.00	147.76
ATOM	1364	CG1	ILE	G	322A	98.807	−132.120	160.480	1.00	148.35
ATOM	1365	CG2	ILE	G	322A	100.149	−131.324	162.446	1.00	147.20
ATOM	1366	CD1	ILE	G	322A	99.408	−133.513	160.469	1.00	146.09
ATOM	1367	N	ILE	G	323	98.854	−127.917	159.214	1.00	145.42
ATOM	1368	CA	ILE	G	323	98.728	−127.370	157.865	1.00	144.18
ATOM	1369	C	ILE	G	323	99.759	−127.991	156.928	1.00	143.58
ATOM	1370	O	ILE	G	323	100.878	−127.492	156.799	1.00	143.84
ATOM	1371	CB	ILE	G	323	98.919	−125.833	157.864	1.00	143.68
ATOM	1372	CG1	ILE	G	323	97.919	−125.179	158.823	1.00	142.95
ATOM	1373	CG2	ILE	G	323	98.743	−125.285	156.452	1.00	142.76
ATOM	1374	CD1	ILE	G	323	96.462	−125.431	158.476	1.00	141.08
ATOM	1375	N	GLY	G	324	99.371	−129.082	156.275	1.00	142.21
ATOM	1376	CA	GLY	G	324	100.273	−129.759	155.363	1.00	139.77
ATOM	1377	C	GLY	G	324	99.607	−130.172	154.067	1.00	137.92
ATOM	1378	O	GLY	G	324	98.645	−129.543	153.622	1.00	137.70
ATOM	1379	N	ASP	G	325	100.119	−131.238	153.461	1.00	136.00
ATOM	1380	CA	ASP	G	325	99.579	−131.735	152.203	1.00	133.50
ATOM	1381	C	ASP	G	325	98.873	−133.076	152.378	1.00	131.01
ATOM	1382	O	ASP	G	325	99.517	−134.125	152.420	1.00	130.01
ATOM	1383	CB	ASP	G	325	100.701	−131.883	151.168	1.00	134.89
ATOM	1384	CG	ASP	G	325	101.463	−130.587	150.937	1.00	135.71
ATOM	1385	OD1	ASP	G	325	100.829	−129.577	150.563	1.00	136.06
ATOM	1386	OD2	ASP	G	325	102.698	−130.580	151.125	1.00	134.58
ATOM	1387	N	ILE	G	326	97.549	−133.035	152.488	1.00	129.15
ATOM	1388	CA	ILE	G	326	96.752	−134.248	152.636	1.00	127.17
ATOM	1389	C	ILE	G	326	96.181	−134.612	151.270	1.00	125.06
ATOM	1390	O	ILE	G	326	95.556	−135.660	151.097	1.00	123.58
ATOM	1391	CB	ILE	G	326	95.585	−134.060	153.642	1.00	128.41
ATOM	1392	CG1	ILE	G	326	94.645	−132.942	153.173	1.00	129.82
ATOM	1393	CG2	ILE	G	326	96.140	−133.766	155.028	1.00	127.42
ATOM	1394	CD1	ILE	G	326	95.235	−131.542	153.236	1.00	130.42
ATOM	1395	N	ARG	G	327	96.405	−133.725	150.305	1.00	123.14
ATOM	1396	CA	ARG	G	327	95.941	−133.924	148.939	1.00	121.11
ATOM	1397	C	ARG	G	327	97.147	−134.327	148.100	1.00	120.61
ATOM	1398	O	ARG	G	327	97.188	−134.076	146.897	1.00	120.79
ATOM	1399	CB	ARG	G	327	95.358	−132.627	148.372	1.00	120.85
ATOM	1400	CG	ARG	G	327	94.459	−131.843	149.317	1.00	118.55
ATOM	1401	CD	ARG	G	327	93.929	−130.592	148.622	1.00	116.19
ATOM	1402	NE	ARG	G	327	93.320	−129.641	149.549	1.00	114.20
ATOM	1403	CZ	ARG	G	327	92.253	−129.896	150.299	1.00	112.97
ATOM	1404	NH1	ARG	G	327	91.661	−131.080	150.241	1.00	112.39

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	1405	NH2	ARG	G	327	91.777	−128.963	151.111	1.00	111.25
ATOM	1406	N	GLN	G	328	98.134	−134.943	148.743	1.00	120.56
ATOM	1407	CA	GLN	G	328	99.349	−135.363	148.056	1.00	120.47
ATOM	1408	C	GLN	G	328	99.300	−136.818	147.602	1.00	120.52
ATOM	1409	O	GLN	G	328	98.731	−137.676	148.278	1.00	119.31
ATOM	1410	CB	GLN	G	328	100.564	−135.158	148.965	1.00	120.86
ATOM	1411	CG	GLN	G	328	101.888	−135.560	148.330	1.00	121.32
ATOM	1412	CD	GLN	G	328	103.053	−135.494	149.302	1.00	121.93
ATOM	1413	OE1	GLN	G	328	104.192	−135.792	148.942	1.00	121.20
ATOM	1414	NE2	GLN	G	328	102.771	−135.104	150.541	1.00	121.27
ATOM	1415	N	ALA	G	329	99.909	−137.081	146.451	1.00	120.97
ATOM	1416	CA	ALA	G	329	99.961	−138.422	145.883	1.00	121.52
ATOM	1417	C	ALA	G	329	101.311	−138.622	145.204	1.00	122.43
ATOM	1418	O	ALA	G	329	102.079	−137.673	145.043	1.00	122.38
ATOM	1419	CB	ALA	G	329	98.836	−138.606	144.877	1.00	121.15
ATOM	1420	N	HIS	G	330	101.600	−139.858	144.811	1.00	123.54
ATOM	1421	CA	HIS	G	330	102.861	−140.168	144.150	1.00	124.36
ATOM	1422	C	HIS	G	330	102.701	−141.357	143.210	1.00	124.92
ATOM	1423	O	HIS	G	330	101.851	−142.221	143.431	1.00	124.23
ATOM	1424	CB	HIS	G	330	103.943	−140.473	145.189	1.00	124.54
ATOM	1425	CG	HIS	G	330	103.653	−141.680	146.028	1.00	125.33
ATOM	1426	ND1	HIS	G	330	102.556	−141.764	146.858	1.00	125.66
ATOM	1427	CD2	HIS	G	330	104.317	−142.852	146.162	1.00	125.46
ATOM	1428	CE1	HIS	G	330	102.556	−142.937	147.467	1.00	125.67
ATOM	1429	NE2	HIS	G	330	103.614	−143.617	147.061	1.00	125.50
ATOM	1430	N	CYS	G	331	103.519	−141.392	142.162	1.00	125.98
ATOM	1431	CA	CYS	G	331	103.471	−142.479	141.187	1.00	127.16
ATOM	1432	C	CYS	G	331	104.763	−143.292	141.212	1.00	129.17
ATOM	1433	O	CYS	G	331	105.756	−142.883	141.814	1.00	129.56
ATOM	1434	CB	CYS	G	331	103.263	−141.931	139.777	1.00	124.83
ATOM	1435	SG	CYS	G	331	101.784	−140.903	139.514	1.00	121.39
ATOM	1436	N	ASN	G	332	104.744	−144.441	140.542	1.00	131.21
ATOM	1437	CA	ASN	G	332	105.907	−145.317	140.491	1.00	133.03
ATOM	1438	C	ASN	G	332	106.019	−146.059	139.161	1.00	132.94
ATOM	1439	O	ASN	G	332	105.054	−146.665	138.696	1.00	133.74
ATOM	1440	CB	ASN	G	332	105.845	−146.346	141.625	1.00	135.06
ATOM	1441	CG	ASN	G	332	106.883	−146.090	142.699	1.00	138.61
ATOM	1442	OD1	ASN	G	332	108.036	−145.797	142.379	1.00	140.34
ATOM	1443	ND2	ASN	G	332	106.492	−146.199	143.969	1.00	141.14
ATOM	1444	N	ILE	G	333	107.205	−146.016	138.562	1.00	132.27
ATOM	1445	CA	ILE	G	333	107.458	−146.705	137.305	1.00	131.40
ATOM	1446	C	ILE	G	333	108.827	−147.371	137.344	1.00	131.17
ATOM	1447	O	ILE	G	333	109.685	−146.991	138.138	1.00	130.59
ATOM	1448	CB	ILE	G	333	107.438	−145.738	136.110	1.00	130.99
ATOM	1449	CG1	ILE	G	333	108.336	−144.541	136.416	1.00	131.41
ATOM	1450	CG2	ILE	G	333	106.013	−145.321	135.796	1.00	130.08
ATOM	1451	CD1	ILE	G	333	108.808	−143.797	135.194	1.00	130.71
ATOM	1452	N	SER	G	334	109.027	−148.362	136.482	1.00	130.80
ATOM	1453	CA	SER	G	334	110.298	−149.071	136.417	1.00	130.47
ATOM	1454	C	SER	G	334	111.379	−148.202	135.781	1.00	129.18
ATOM	1455	O	SER	G	334	111.253	−147.785	134.630	1.00	128.30
ATOM	1456	CB	SER	G	334	110.137	−150.366	135.620	1.00	131.53
ATOM	1457	OG	SER	G	334	109.185	−151.224	136.226	1.00	134.33
ATOM	1458	N	ARG	G	335	112.441	−147.938	136.537	1.00	128.40
ATOM	1459	CA	ARG	G	335	113.550	−147.114	136.062	1.00	127.88
ATOM	1460	C	ARG	G	335	114.232	−147.713	134.831	1.00	127.39
ATOM	1461	O	ARG	G	335	114.594	−146.992	133.901	1.00	125.90
ATOM	1462	CB	ARG	G	335	114.588	−146.944	137.174	1.00	128.63
ATOM	1463	CG	ARG	G	335	115.721	−145.986	136.839	1.00	130.03
ATOM	1464	CD	ARG	G	335	115.354	−144.549	137.175	1.00	131.46
ATOM	1465	NE	ARG	G	335	116.464	−143.631	136.927	1.00	133.64
ATOM	1466	CZ	ARG	G	335	116.796	−143.164	135.728	1.00	135.08
ATOM	1467	NH1	ARG	G	335	116.102	−143.521	134.655	1.00	135.62
ATOM	1468	NH2	ARG	G	335	117.828	−142.340	135.600	1.00	136.66
ATOM	1469	N	ALA	G	336	114.409	−149.030	134.831	1.00	127.56
ATOM	1470	CA	ALA	G	336	115.060	−149.712	133.717	1.00	127.56
ATOM	1471	C	ALA	G	336	114.193	−149.726	132.462	1.00	127.53
ATOM	1472	O	ALA	G	336	114.702	−149.613	131.347	1.00	127.19
ATOM	1473	CB	ALA	G	336	115.419	−151.140	134.121	1.00	127.32
ATOM	1474	N	LYS	G	337	112.884	−149.870	132.653	1.00	127.34
ATOM	1475	CA	LYS	G	337	111.929	−149.897	131.547	1.00	126.12
ATOM	1476	C	LYS	G	337	111.697	−148.511	130.952	1.00	125.19
ATOM	1477	O	LYS	G	337	111.525	−148.370	129.742	1.00	125.25
ATOM	1478	CB	LYS	G	337	110.590	−150.483	132.019	1.00	125.26
ATOM	1479	CG	LYS	G	337	110.486	−152.006	131.948	1.00	125.56
ATOM	1480	CD	LYS	G	337	110.195	−152.482	130.524	1.00	125.22
ATOM	1481	CE	LYS	G	337	110.096	−154.003	130.442	1.00	125.33
ATOM	1482	NZ	LYS	G	337	109.878	−154.486	129.045	1.00	122.70

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	1483	N	TRP	G	338	111.693	−147.488	131.802	1.00	123.88
ATOM	1484	CA	TRP	G	338	111.471	−146.120	131.343	1.00	122.35
ATOM	1485	C	TRP	G	338	112.656	−145.584	130.551	1.00	122.08
ATOM	1486	O	TRP	G	338	112.482	−144.934	129.521	1.00	121.22
ATOM	1487	CB	TRP	G	338	111.188	−145.199	132.535	1.00	121.06
ATOM	1488	CG	TRP	G	338	111.092	−143.744	132.172	1.00	119.31
ATOM	1489	CD1	TRP	G	338	111.853	−142.726	132.669	1.00	119.14
ATOM	1490	CD2	TRP	G	338	110.185	−143.145	131.235	1.00	118.77
ATOM	1491	NE1	TRP	G	338	111.479	−141.531	132.103	1.00	119.01
ATOM	1492	CE2	TRP	G	338	110.458	−141.758	131.220	1.00	118.35
ATOM	1493	CE3	TRP	G	338	109.170	−143.644	130.409	1.00	118.58
ATOM	1494	CZ2	TRP	G	338	109.751	−140.864	130.408	1.00	117.90
ATOM	1495	CZ3	TRP	G	338	108.467	−142.753	129.601	1.00	118.02
ATOM	1496	CH2	TRP	G	338	108.763	−141.378	129.609	1.00	117.53
ATOM	1497	N	ASN	G	339	113.860	−145.865	131.034	1.00	122.65
ATOM	1498	CA	ASN	G	339	115.068	−145.399	130.367	1.00	123.64
ATOM	1499	C	ASN	G	339	115.247	−146.081	129.015	1.00	122.72
ATOM	1500	O	ASN	G	339	115.779	−145.490	128.079	1.00	120.87
ATOM	1501	CB	ASN	G	339	116.292	−145.661	131.249	1.00	126.14
ATOM	1502	CG	ASN	G	339	117.430	−144.705	130.960	1.00	128.79
ATOM	1503	OD1	ASN	G	339	117.338	−143.511	131.247	1.00	129.26
ATOM	1504	ND2	ASN	G	339	118.508	−145.223	130.384	1.00	130.45
ATOM	1505	N	ASP	G	340	114.805	−147.331	128.922	1.00	122.55
ATOM	1506	CA	ASP	G	340	114.913	−148.080	127.676	1.00	122.48
ATOM	1507	C	ASP	G	340	113.925	−147.552	126.654	1.00	121.75
ATOM	1508	O	ASP	G	340	114.254	−147.398	125.482	1.00	121.24
ATOM	1509	CB	ASP	G	340	114.651	−149.569	127.913	1.00	123.36
ATOM	1510	CG	ASP	G	340	115.932	−150.373	128.021	1.00	124.46
ATOM	1511	OD1	ASP	G	340	116.606	−150.547	126.987	1.00	124.57
ATOM	1512	OD2	ASP	G	340	116.263	−150.820	129.138	1.00	124.24
ATOM	1513	N	THR	G	341	112.709	−147.277	127.107	1.00	121.23
ATOM	1514	CA	THR	G	341	111.678	−146.760	126.223	1.00	120.37
ATOM	1515	C	THR	G	341	112.005	−145.321	125.864	1.00	120.04
ATOM	1516	O	THR	G	341	111.571	−144.813	124.833	1.00	119.85
ATOM	1517	CB	THR	G	341	110.292	−146.798	126.885	1.00	119.50
ATOM	1518	OG1	THR	G	341	110.387	−146.310	128.227	1.00	118.81
ATOM	1519	CG2	THR	G	341	109.738	−148.202	126.892	1.00	119.32
ATOM	1520	N	LEU	G	342	112.780	−144.668	126.719	1.00	118.58
ATOM	1521	CA	LEU	G	342	113.172	−143.285	126.488	1.00	117.21
ATOM	1522	C	LEU	G	342	114.214	−143.283	125.372	1.00	117.06
ATOM	1523	O	LEU	G	342	114.277	−142.363	124.557	1.00	116.61
ATOM	1524	CB	LEU	G	342	113.757	−142.700	127.780	1.00	116.17
ATOM	1525	CG	LEU	G	342	113.453	−141.242	128.147	1.00	115.99
ATOM	1526	CD1	LEU	G	342	113.803	−141.014	129.608	1.00	115.86
ATOM	1527	CD2	LEU	G	342	114.230	−140.299	127.247	1.00	115.38
ATOM	1528	N	LYS	G	343	115.021	−144.340	125.341	1.00	117.43
ATOM	1529	CA	LYS	G	343	116.071	−144.497	124.340	1.00	117.14
ATOM	1530	C	LYS	G	343	115.481	−144.739	122.957	1.00	116.27
ATOM	1531	O	LYS	G	343	115.931	−144.159	121.970	1.00	114.89
ATOM	1532	CB	LYS	G	343	116.988	−145.668	124.720	1.00	118.24
ATOM	1533	CG	LYS	G	343	118.124	−145.916	123.741	1.00	119.11
ATOM	1534	CD	LYS	G	343	118.999	−147.081	124.184	1.00	118.05
ATOM	1535	CE	LYS	G	343	120.143	−147.321	123.205	1.00	117.07
ATOM	1536	NZ	LYS	G	343	121.015	−148.456	123.624	1.00	118.22
ATOM	1537	N	GLN	G	344	114.466	−145.594	122.890	1.00	115.18
ATOM	1538	CA	GLN	G	344	113.828	−145.899	121.617	1.00	114.37
ATOM	1539	C	GLN	G	344	113.146	−144.685	121.009	1.00	114.01
ATOM	1540	O	GLN	G	344	112.888	−144.642	119.807	1.00	113.70
ATOM	1541	CB	GLN	G	344	112.838	−147.051	121.780	1.00	113.68
ATOM	1542	CG	GLN	G	344	113.519	−148.414	121.728	1.00	114.75
ATOM	1543	CD	GLN	G	344	113.191	−149.300	122.912	1.00	115.83
ATOM	1544	OE1	GLN	G	344	112.072	−149.795	123.044	1.00	116.37
ATOM	1545	NE2	GLN	G	344	114.172	−149.505	123.784	1.00	116.57
ATOM	1546	N	ILE	G	345	112.858	−143.694	121.839	1.00	113.81
ATOM	1547	CA	ILE	G	345	112.241	−142.472	121.349	1.00	113.74
ATOM	1548	C	ILE	G	345	113.341	−141.701	120.641	1.00	114.51
ATOM	1549	O	ILE	G	345	113.143	−141.157	119.555	1.00	114.50
ATOM	1550	CB	ILE	G	345	111.689	−141.630	122.513	1.00	113.46
ATOM	1551	CG1	ILE	G	345	110.481	−142.345	123.133	1.00	113.45
ATOM	1552	CG2	ILE	G	345	111.291	−140.246	122.018	1.00	112.53
ATOM	1553	CD1	ILE	G	345	109.980	−141.716	124.407	1.00	114.16
ATOM	1554	N	VAL	G	346	114.509	−141.680	121.271	1.00	115.23
ATOM	1555	CA	VAL	G	346	115.670	−140.996	120.729	1.00	116.13
ATOM	1556	C	VAL	G	346	116.128	−141.657	119.439	1.00	116.56
ATOM	1557	O	VAL	G	346	116.491	−140.980	118.476	1.00	115.69
ATOM	1558	CB	VAL	G	346	116.836	−141.021	121.727	1.00	116.71
ATOM	1559	CG1	VAL	G	346	118.063	−140.394	121.104	1.00	116.76
ATOM	1560	CG2	VAL	G	346	116.444	−140.284	122.999	1.00	117.56

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	1561	N	ILE	G	347	116.105	−142.984	119.423	1.00	116.67
ATOM	1562	CA	ILE	G	347	116.513	−143.735	118.246	1.00	117.05
ATOM	1563	C	ILE	G	347	115.693	−143.356	117.022	1.00	117.43
ATOM	1564	O	ILE	G	347	116.235	−143.207	115.928	1.00	117.11
ATOM	1565	CB	ILE	G	347	116.366	−145.248	118.488	1.00	118.09
ATOM	1566	CG1	ILE	G	347	117.391	−145.700	119.527	1.00	118.82
ATOM	1567	CG2	ILE	G	347	116.546	−146.012	117.186	1.00	117.63
ATOM	1568	CD1	ILE	G	347	118.828	−145.515	119.081	1.00	120.24
ATOM	1569	N	LYS	G	348	114.387	−143.199	117.215	1.00	118.10
ATOM	1570	CA	LYS	G	348	113.492	−142.836	116.125	1.00	119.28
ATOM	1571	C	LYS	G	348	113.477	−141.331	115.880	1.00	120.01
ATOM	1572	O	LYS	G	348	113.158	−140.883	114.780	1.00	119.90
ATOM	1573	CB	LYS	G	348	112.069	−143.326	116.416	1.00	119.85
ATOM	1574	CG	LYS	G	348	111.895	−144.844	116.394	1.00	120.97
ATOM	1575	CD	LYS	G	348	112.020	−145.410	114.980	1.00	122.36
ATOM	1576	CE	LYS	G	348	111.989	−146.937	114.982	1.00	123.02
ATOM	1577	NZ	LYS	G	348	112.225	−147.510	113.623	1.00	121.99
ATOM	1578	N	LEU	G	349	113.815	−140.550	116.903	1.00	120.97
ATOM	1579	CA	LEU	G	349	113.837	−139.098	116.757	1.00	122.27
ATOM	1580	C	LEU	G	349	115.045	−138.660	115.947	1.00	124.05
ATOM	1581	O	LEU	G	349	114.973	−137.710	115.170	1.00	124.00
ATOM	1582	CB	LEU	G	349	113.876	−138.406	118.122	1.00	121.94
ATOM	1583	CG	LEU	G	349	112.543	−138.095	118.810	1.00	122.12
ATOM	1584	CD1	LEU	G	349	112.808	−137.386	120.131	1.00	122.10
ATOM	1585	CD2	LEU	G	349	111.696	−137.209	117.900	1.00	122.34
ATOM	1586	N	ARG	G	350	116.161	−139.356	116.134	1.00	126.82
ATOM	1587	CA	ARG	G	350	117.382	−139.020	115.411	1.00	129.77
ATOM	1588	C	ARG	G	350	117.297	−139.583	114.004	1.00	130.79
ATOM	1589	O	ARG	G	350	118.100	−139.246	113.138	1.00	130.39
ATOM	1590	CB	ARG	G	350	118.618	−139.578	116.136	1.00	131.03
ATOM	1591	CG	ARG	G	350	118.728	−141.100	116.172	1.00	134.23
ATOM	1592	CD	ARG	G	350	119.545	−141.557	117.385	1.00	136.50
ATOM	1593	NE	ARG	G	350	120.947	−141.131	117.377	1.00	137.14
ATOM	1594	CZ	ARG	G	350	121.944	−141.836	116.849	1.00	137.25
ATOM	1595	NH1	ARG	G	350	121.700	−143.008	116.276	1.00	136.86
ATOM	1596	NH2	ARG	G	350	123.190	−141.381	116.914	1.00	136.51
ATOM	1597	N	GLU	G	351	116.307	−140.440	113.783	1.00	131.73
ATOM	1598	CA	GLU	G	351	116.108	−141.051	112.477	1.00	131.78
ATOM	1599	C	GLU	G	351	115.426	−140.024	111.574	1.00	131.64
ATOM	1600	O	GLU	G	351	115.425	−140.150	110.352	1.00	130.89
ATOM	1601	CB	GLU	G	351	115.250	−142.319	112.618	1.00	132.20
ATOM	1602	CG	GLU	G	351	115.735	−143.503	111.787	1.00	133.83
ATOM	1603	CD	GLU	G	351	114.933	−144.778	112.033	1.00	134.12
ATOM	1604	OE1	GLU	G	351	114.970	−145.303	113.165	1.00	133.27
ATOM	1605	OE2	GLU	G	351	114.267	−145.261	111.092	1.00	133.23
ATOM	1606	N	GLN	G	352	114.851	−138.998	112.197	1.00	131.55
ATOM	1607	CA	GLN	G	352	114.174	−137.930	111.469	1.00	131.20
ATOM	1608	C	GLN	G	352	115.029	−136.667	111.583	1.00	131.74
ATOM	1609	O	GLN	G	352	115.015	−135.810	110.703	1.00	131.22
ATOM	1610	CB	GLN	G	352	112.775	−137.684	112.055	1.00	129.40
ATOM	1611	CG	GLN	G	352	111.683	−137.483	111.010	1.00	128.29
ATOM	1612	CD	GLN	G	352	111.760	−136.141	110.302	1.00	128.13
ATOM	1613	OE1	GLN	G	352	111.325	−136.007	109.158	1.00	128.02
ATOM	1614	NE2	GLN	G	352	112.296	−135.137	110.986	1.00	127.02
ATOM	1615	N	PHE	G	353	115.781	−136.567	112.675	1.00	132.98
ATOM	1616	CA	PHE	G	353	116.654	−135.423	112.911	1.00	135.12
ATOM	1617	C	PHE	G	353	118.045	−135.862	113.357	1.00	136.10
ATOM	1618	O	PHE	G	353	118.362	−135.841	114.547	1.00	136.53
ATOM	1619	CB	PHE	G	353	116.054	−134.490	113.969	1.00	135.78
ATOM	1620	CG	PHE	G	353	114.963	−133.605	113.447	1.00	137.46
ATOM	1621	CD1	PHE	G	353	113.645	−133.786	113.853	1.00	137.80
ATOM	1622	CD2	PHE	G	353	115.255	−132.586	112.544	1.00	137.80
ATOM	1623	CE1	PHE	G	353	112.631	−132.963	113.365	1.00	138.59
ATOM	1624	CE2	PHE	G	353	114.249	−131.759	112.050	1.00	138.17
ATOM	1625	CZ	PHE	G	353	112.935	−131.948	112.461	1.00	138.87
ATOM	1626	N	GLU	G	354	118.871	−136.261	112.397	1.00	137.05
ATOM	1627	CA	GLU	G	354	120.224	−136.707	112.687	1.00	137.91
ATOM	1628	C	GLU	G	354	121.203	−135.540	112.616	1.00	137.70
ATOM	1629	O	GLU	G	354	120.881	−134.475	112.085	1.00	137.66
ATOM	1630	CB	GLU	G	354	120.615	−137.825	111.716	1.00	138.86
ATOM	1631	CG	GLU	G	354	121.921	−138.512	112.053	1.00	139.85
ATOM	1632	CD	GLU	G	354	122.022	−138.871	113.521	1.00	140.14
ATOM	1633	OE1	GLU	G	354	121.152	−139.618	114.017	1.00	140.78
ATOM	1634	OE2	GLU	G	354	122.976	−138.403	114.175	1.00	139.52
ATOM	1635	N	ASN	G	355	122.406	−135.754	113.142	1.00	137.40
ATOM	1636	CA	ASN	G	355	123.425	−134.703	113.192	1.00	136.85
ATOM	1637	C	ASN	G	355	122.937	−133.573	114.098	1.00	136.44
ATOM	1638	O	ASN	G	355	123.254	−132.412	113.913	1.00	137.04

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	1639	CB	ASN	G	355	123.740	−134.195	111.776	1.00	136.54
ATOM	1640	CG	ASN	G	355	124.508	−135.220	110.949	1.00	135.79
ATOM	1641	OD1	ASN	G	355	124.035	−136.328	110.725	1.00	135.13
ATOM	1642	ND2	ASN	G	355	125.715	−134.853	110.514	1.00	135.21
ATOM	1643	N	LYS	G	357	122.152	−133.950	115.096	1.00	135.07
ATOM	1644	CA	LYS	G	357	121.606	−133.017	116.079	1.00	133.42
ATOM	1645	C	LYS	G	357	121.698	−133.716	117.421	1.00	131.94
ATOM	1646	O	LYS	G	357	121.977	−134.913	117.471	1.00	131.61
ATOM	1647	CB	LYS	G	357	120.137	−132.700	115.770	1.00	133.82
ATOM	1648	CG	LYS	G	357	119.862	−132.151	114.378	1.00	134.32
ATOM	1649	CD	LYS	G	357	119.821	−130.635	114.369	1.00	135.18
ATOM	1650	CE	LYS	G	357	119.478	−130.113	112.987	1.00	135.74
ATOM	1651	NZ	LYS	G	357	119.344	−128.636	112.997	1.00	135.57
ATOM	1652	N	THR	G	358	121.466	−132.974	118.499	1.00	130.25
ATOM	1653	CA	THR	G	358	121.499	−133.557	119.832	1.00	128.54
ATOM	1654	C	THR	G	358	120.142	−133.485	120.532	1.00	127.66
ATOM	1655	O	THR	G	358	119.636	−132.395	120.811	1.00	127.33
ATOM	1656	CB	THR	G	358	122.531	−132.868	120.749	1.00	127.87
ATOM	1657	OG1	THR	G	358	123.852	−133.126	120.269	1.00	127.40
ATOM	1658	CG2	THR	G	358	122.406	−133.397	122.167	1.00	127.41
ATOM	1659	N	ILE	G	359	119.558	−134.647	120.813	1.00	126.20
ATOM	1660	CA	ILE	G	359	118.258	−134.718	121.480	1.00	125.26
ATOM	1661	C	ILE	G	359	118.360	−134.591	123.005	1.00	124.58
ATOM	1662	O	ILE	G	359	118.904	−135.468	123.681	1.00	124.63
ATOM	1663	CB	ILE	G	359	117.528	−136.050	121.154	1.00	124.56
ATOM	1664	CG1	ILE	G	359	117.243	−136.142	119.654	1.00	124.71
ATOM	1665	CG2	ILE	G	359	116.212	−136.130	121.922	1.00	124.84
ATOM	1666	CD1	ILE	G	359	118.474	−136.371	118.804	1.00	124.99
ATOM	1667	N	VAL	G	360	117.816	−133.503	123.541	1.00	123.68
ATOM	1668	CA	VAL	G	360	117.841	−133.248	124.977	1.00	122.86
ATOM	1669	C	VAL	G	360	116.417	−133.181	125.520	1.00	122.77
ATOM	1670	O	VAL	G	360	115.532	−132.627	124.874	1.00	122.31
ATOM	1671	CB	VAL	G	360	118.535	−131.907	125.278	1.00	122.10
ATOM	1672	CG1	VAL	G	360	118.861	−131.806	126.759	1.00	121.81
ATOM	1673	CG2	VAL	G	360	119.783	−131.772	124.427	1.00	122.35
ATOM	1674	N	PHE	G	361	116.201	−133.746	126.702	1.00	122.89
ATOM	1675	CA	PHE	G	361	114.881	−133.744	127.323	1.00	122.88
ATOM	1676	C	PHE	G	361	114.852	−132.840	128.544	1.00	123.80
ATOM	1677	O	PHE	G	361	115.619	−133.024	129.490	1.00	124.18
ATOM	1678	CB	PHE	G	361	114.486	−135.169	127.705	1.00	121.54
ATOM	1679	CG	PHE	G	361	114.075	−136.008	126.536	1.00	120.64
ATOM	1680	CD1	PHE	G	361	112.802	−135.884	125.995	1.00	121.67
ATOM	1681	CD2	PHE	G	361	114.967	−136.901	125.954	1.00	120.34
ATOM	1682	CE1	PHE	G	361	112.419	−136.638	124.889	1.00	122.25
ATOM	1683	CE2	PHE	G	361	114.596	−137.660	124.847	1.00	120.52
ATOM	1684	CZ	PHE	G	361	113.319	−137.528	124.314	1.00	121.45
ATOM	1685	N	ASN	G	362	113.954	−131.864	128.516	1.00	124.73
ATOM	1686	CA	ASN	G	362	113.837	−130.906	129.602	1.00	125.55
ATOM	1687	C	ASN	G	362	112.401	−130.831	130.118	1.00	124.88
ATOM	1688	O	ASN	G	362	111.485	−131.370	129.499	1.00	124.87
ATOM	1689	CB	ASN	G	362	114.294	−129.537	129.097	1.00	127.19
ATOM	1690	CG	ASN	G	362	114.691	−128.608	130.215	1.00	130.61
ATOM	1691	OD1	ASN	G	362	113.874	−128.287	131.083	1.00	131.85
ATOM	1692	ND2	ASN	G	362	115.948	−128.168	130.199	1.00	133.40
ATOM	1693	N	HIS	G	363	112.207	−130.159	131.248	1.00	124.22
ATOM	1694	CA	HIS	G	363	110.878	−130.014	131.826	1.00	123.37
ATOM	1695	C	HIS	G	363	110.003	−129.081	130.986	1.00	122.33
ATOM	1696	O	HIS	G	363	110.445	−128.552	129.965	1.00	123.35
ATOM	1697	CB	HIS	G	363	110.986	−129.485	133.261	1.00	123.55
ATOM	1698	CG	HIS	G	363	111.789	−128.228	133.388	1.00	123.69
ATOM	1699	ND1	HIS	G	363	111.430	−127.051	132.769	1.00	123.31
ATOM	1700	CD2	HIS	G	363	112.933	−127.966	134.063	1.00	124.89
ATOM	1701	CE1	HIS	G	363	112.319	−126.118	133.056	1.00	123.86
ATOM	1702	NE2	HIS	G	363	113.242	−126.646	133.839	1.00	125.14
ATOM	1703	N	SER	G	364	108.763	−128.876	131.419	1.00	119.87
ATOM	1704	CA	SER	G	364	107.853	−128.002	130.691	1.00	117.00
ATOM	1705	C	SER	G	364	108.279	−126.547	130.857	1.00	115.19
ATOM	1706	O	SER	G	364	108.577	−126.102	131.964	1.00	115.16
ATOM	1707	CB	SER	G	364	106.422	−128.192	131.192	1.00	116.69
ATOM	1708	OG	SER	G	364	105.495	−127.562	130.324	1.00	116.92
ATOM	1709	N	SER	G	365	108.307	−125.811	129.752	1.00	113.25
ATOM	1710	CA	SER	G	365	108.711	−124.411	129.770	1.00	112.58
ATOM	1711	C	SER	G	365	107.797	−123.480	130.566	1.00	112.63
ATOM	1712	O	SER	G	365	108.216	−122.389	130.949	1.00	113.24
ATOM	1713	CB	SER	G	365	108.848	−123.897	128.341	1.00	112.43
ATOM	1714	OG	SER	G	365	107.754	−124.318	127.550	1.00	112.84
ATOM	1715	N	GLY	G	366	106.559	−123.895	130.823	1.00	112.08
ATOM	1716	CA	GLY	G	366	105.661	−123.044	131.591	1.00	111.71

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	1717	C	GLY	G	366	104.224	−123.031	131.111	1.00	111.01
ATOM	1718	O	GLY	G	366	103.920	−123.550	130.041	1.00	111.21
ATOM	1719	N	GLY	G	367	103.339	−122.439	131.908	1.00	110.29
ATOM	1720	CA	GLY	G	367	101.935	−122.374	131.538	1.00	109.86
ATOM	1721	C	GLY	G	367	101.013	−122.876	132.633	1.00	109.09
ATOM	1722	O	GLY	G	367	101.382	−122.880	133.806	1.00	110.03
ATOM	1723	N	ASP	G	368	99.810	−123.300	132.255	1.00	107.77
ATOM	1724	CA	ASP	G	368	98.847	−123.813	133.219	1.00	106.93
ATOM	1725	C	ASP	G	368	99.347	−125.117	133.825	1.00	105.42
ATOM	1726	O	ASP	G	368	99.888	−125.969	133.122	1.00	105.22
ATOM	1727	CB	ASP	G	368	97.490	−124.046	132.551	1.00	109.08
ATOM	1728	CG	ASP	G	368	96.754	−122.749	132.246	1.00	110.72
ATOM	1729	OD1	ASP	G	368	96.346	−122.063	133.204	1.00	112.84
ATOM	1730	OD2	ASP	G	368	96.587	−122.420	131.052	1.00	110.53
ATOM	1731	N	PRO	G	369	99.161	−125.290	135.143	1.00	104.21
ATOM	1732	CA	PRO	G	369	99.587	−126.484	135.874	1.00	103.74
ATOM	1733	C	PRO	G	369	99.165	−127.797	135.227	1.00	102.96
ATOM	1734	O	PRO	G	369	99.756	−128.842	135.495	1.00	103.69
ATOM	1735	CB	PRO	G	369	98.955	−126.279	137.243	1.00	104.51
ATOM	1736	CG	PRO	G	369	99.051	−124.796	137.406	1.00	104.97
ATOM	1737	CD	PRO	G	369	98.530	−124.330	136.063	1.00	104.21
ATOM	1738	N	GLU	G	370	98.148	−127.745	134.376	1.00	101.68
ATOM	1739	CA	GLU	G	370	97.676	−128.949	133.707	1.00	100.29
ATOM	1740	C	GLU	G	370	98.665	−129.450	132.663	1.00	99.24
ATOM	1741	O	GLU	G	370	98.741	−130.650	132.396	1.00	100.20
ATOM	1742	CB	GLU	G	370	96.316	−128.699	133.049	1.00	101.70
ATOM	1743	CG	GLU	G	370	95.129	−128.747	134.007	1.00	101.29
ATOM	1744	CD	GLU	G	370	94.927	−127.459	134.790	1.00	101.71
ATOM	1745	OE1	GLU	G	370	94.058	−127.440	135.687	1.00	101.10
ATOM	1746	OE2	GLU	G	370	95.628	−126.465	134.508	1.00	102.45
ATOM	1747	N	ILE	G	371	99.424	−128.532	132.077	1.00	97.76
ATOM	1748	CA	ILE	G	371	100.401	−128.891	131.058	1.00	96.84
ATOM	1749	C	ILE	G	371	101.755	−129.144	131.702	1.00	95.29
ATOM	1750	O	ILE	G	371	102.455	−130.104	131.369	1.00	94.66
ATOM	1751	CB	ILE	G	371	100.563	−127.756	130.041	1.00	96.73
ATOM	1752	CG1	ILE	G	371	99.189	−127.193	129.678	1.00	96.23
ATOM	1753	CG2	ILE	G	371	101.254	−128.276	128.792	1.00	98.30
ATOM	1754	CD1	ILE	G	371	99.236	−125.769	129.192	1.00	96.31
ATOM	1755	N	VAL	G	372	102.111	−128.273	132.637	1.00	92.31
ATOM	1756	CA	VAL	G	372	103.376	−128.378	133.340	1.00	89.48
ATOM	1757	C	VAL	G	372	103.503	−129.702	134.081	1.00	87.73
ATOM	1758	O	VAL	G	372	104.586	−130.277	134.150	1.00	88.58
ATOM	1759	CB	VAL	G	372	103.533	−127.237	134.352	1.00	89.89
ATOM	1760	CG1	VAL	G	372	104.936	−127.246	134.926	1.00	91.74
ATOM	1761	CG2	VAL	G	372	103.233	−125.906	133.683	1.00	89.58
ATOM	1762	N	MET	G	373	102.395	−130.187	134.631	1.00	86.24
ATOM	1763	CA	MET	G	373	102.411	−131.444	135.364	1.00	86.32
ATOM	1764	C	MET	G	373	101.540	−132.498	134.689	1.00	86.85
ATOM	1765	O	MET	G	373	100.541	−132.174	134.051	1.00	86.82
ATOM	1766	CB	MET	G	373	101.930	−131.220	136.805	1.00	86.15
ATOM	1767	CG	MET	G	373	102.616	−130.059	137.512	1.00	85.92
ATOM	1768	SD	MET	G	373	103.120	−130.448	139.200	1.00	87.98
ATOM	1769	CE	MET	G	373	101.830	−129.658	140.161	1.00	88.57
ATOM	1770	N	HIS	G	374	101.930	−133.762	134.823	1.00	87.56
ATOM	1771	CA	HIS	G	374	101.161	−134.857	134.244	1.00	88.76
ATOM	1772	C	HIS	G	374	99.810	−134.931	134.944	1.00	90.65
ATOM	1773	O	HIS	G	374	99.699	−135.514	136.019	1.00	93.49
ATOM	1774	CB	HIS	G	374	101.905	−136.181	134.422	1.00	87.35
ATOM	1775	CG	HIS	G	374	101.079	−137.385	134.096	1.00	85.69
ATOM	1776	ND1	HIS	G	374	100.563	−137.614	132.839	1.00	85.77
ATOM	1777	CD2	HIS	G	374	100.677	−138.425	134.863	1.00	85.18
ATOM	1778	CE1	HIS	G	374	99.881	−138.745	132.845	1.00	87.31
ATOM	1779	NE2	HIS	G	374	99.934	−139.257	134.061	1.00	86.65
ATOM	1780	N	SER	G	375	98.788	−134.346	134.330	1.00	91.35
ATOM	1781	CA	SER	G	375	97.454	−134.327	134.918	1.00	91.01
ATOM	1782	C	SER	G	375	96.531	−135.438	134.431	1.00	90.01
ATOM	1783	O	SER	G	375	96.426	−135.685	133.233	1.00	90.38
ATOM	1784	CB	SER	G	375	96.796	−132.978	134.636	1.00	93.11
ATOM	1785	OG	SER	G	375	96.788	−132.708	133.244	1.00	93.88
ATOM	1786	N	PHE	G	376	95.860	−136.101	135.368	1.00	90.06
ATOM	1787	CA	PHE	G	376	94.920	−137.166	135.037	1.00	93.27
ATOM	1788	C	PHE	G	376	93.895	−137.317	136.156	1.00	95.94
ATOM	1789	O	PHE	G	376	94.034	−136.702	137.212	1.00	95.54
ATOM	1790	CB	PHE	G	376	95.649	−138.495	134.805	1.00	92.86
ATOM	1791	CG	PHE	G	376	96.283	−139.076	136.037	1.00	93.02
ATOM	1792	CD1	PHE	G	376	97.542	−138.660	136.454	1.00	93.40
ATOM	1793	CD2	PHE	G	376	95.628	−140.065	136.766	1.00	92.09
ATOM	1794	CE1	PHE	G	376	98.144	−139.223	137.581	1.00	93.87

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	1795	CE2	PHE	G	376	96.218	−140.634	137.892	1.00	92.28
ATOM	1796	CZ	PHE	G	376	97.479	−140.214	138.300	1.00	94.05
ATOM	1797	N	ASN	G	377	92.870	−138.132	135.930	1.00	99.59
ATOM	1798	CA	ASN	G	377	91.825	−138.327	136.931	1.00	104.81
ATOM	1799	C	ASN	G	377	91.355	−139.774	137.059	1.00	107.26
ATOM	1800	O	ASN	G	377	91.034	−140.429	136.068	1.00	107.33
ATOM	1801	CB	ASN	G	377	90.625	−137.442	136.598	1.00	107.57
ATOM	1802	CG	ASN	G	377	90.145	−137.635	135.176	1.00	110.35
ATOM	1803	OD1	ASN	G	377	90.827	−137.256	134.223	1.00	112.46
ATOM	1804	ND2	ASN	G	377	88.974	−138.242	135.023	1.00	111.65
ATOM	1805	N	CYS	G	378	91.313	−140.259	138.296	1.00	110.71
ATOM	1806	CA	CYS	G	378	90.878	−141.621	138.595	1.00	113.87
ATOM	1807	C	CYS	G	378	90.247	−141.634	139.988	1.00	114.07
ATOM	1808	O	CYS	G	378	90.894	−141.266	140.966	1.00	113.69
ATOM	1809	CB	CYS	G	378	92.069	−142.601	138.540	1.00	116.89
ATOM	1810	SG	CYS	G	378	93.430	−142.309	139.720	1.00	121.15
ATOM	1811	N	GLY	G	379	88.985	−142.047	140.080	1.00	113.75
ATOM	1812	CA	GLY	G	379	88.320	−142.076	141.373	1.00	112.55
ATOM	1813	C	GLY	G	379	87.547	−140.800	141.651	1.00	111.47
ATOM	1814	O	GLY	G	379	86.731	−140.736	142.570	1.00	112.00
ATOM	1815	N	GLY	G	380	87.809	−139.776	140.849	1.00	109.49
ATOM	1816	CA	GLY	G	380	87.123	−138.513	141.024	1.00	107.11
ATOM	1817	C	GLY	G	380	88.074	−137.401	141.410	1.00	105.53
ATOM	1818	O	GLY	G	380	87.672	−136.246	141.521	1.00	106.59
ATOM	1819	N	GLU	G	381	89.342	−137.743	141.611	1.00	102.89
ATOM	1820	CA	GLU	G	381	90.339	−136.749	141.989	1.00	100.20
ATOM	1821	C	GLU	G	381	91.269	−136.414	140.832	1.00	97.39
ATOM	1822	O	GLU	G	381	91.658	−137.291	140.062	1.00	97.65
ATOM	1823	CB	GLU	G	381	91.165	−137.252	143.174	1.00	101.99
ATOM	1824	CG	GLU	G	381	90.341	−137.669	144.376	1.00	104.32
ATOM	1825	CD	GLU	G	381	89.409	−136.574	144.853	1.00	106.86
ATOM	1826	OE1	GLU	G	381	89.884	−135.439	145.071	1.00	108.66
ATOM	1827	OE2	GLU	G	381	88.201	−136.853	145.014	1.00	108.04
ATOM	1828	N	PHE	G	382	91.629	−135.140	140.719	1.00	93.73
ATOM	1829	CA	PHE	G	382	92.513	−134.697	139.648	1.00	89.57
ATOM	1830	C	PHE	G	382	93.963	−134.629	140.104	1.00	88.33
ATOM	1831	O	PHE	G	382	94.338	−133.753	140.882	1.00	88.16
ATOM	1832	CB	PHE	G	382	92.073	−133.326	139.134	1.00	86.63
ATOM	1833	CG	PHE	G	382	90.700	−133.321	138.523	1.00	84.43
ATOM	1834	CD1	PHE	G	382	89.570	−133.512	139.313	1.00	82.70
ATOM	1835	CD2	PHE	G	382	90.536	−133.130	137.155	1.00	83.85
ATOM	1836	CE1	PHE	G	382	88.298	−133.513	138.749	1.00	80.29
ATOM	1837	CE2	PHE	G	382	89.268	−133.130	136.584	1.00	82.03
ATOM	1838	CZ	PHE	G	382	88.149	−133.321	137.383	1.00	80.22
ATOM	1839	N	PHE	G	383	94.777	−135.555	139.607	1.00	87.21
ATOM	1840	CA	PHE	G	383	96.190	−135.607	139.965	1.00	86.08
ATOM	1841	C	PHE	G	383	97.049	−134.663	139.136	1.00	85.60
ATOM	1842	O	PHE	G	383	96.735	−134.368	137.984	1.00	85.11
ATOM	1843	CB	PHE	G	383	96.727	−137.032	139.805	1.00	85.28
ATOM	1844	CG	PHE	G	383	96.120	−138.022	140.755	1.00	85.57
ATOM	1845	CD1	PHE	G	383	94.790	−138.408	140.627	1.00	85.90
ATOM	1846	CD2	PHE	G	383	96.880	−138.571	141.782	1.00	85.81
ATOM	1847	CE1	PHE	G	383	94.226	−139.327	141.508	1.00	85.70
ATOM	1848	CE2	PHE	G	383	96.326	−139.489	142.667	1.00	85.26
ATOM	1849	CZ	PHE	G	383	94.997	−139.868	142.530	1.00	84.70
ATOM	1850	N	TYR	G	384	98.135	−134.190	139.736	1.00	85.21
ATOM	1851	CA	TYR	G	384	99.071	−133.295	139.061	1.00	86.70
ATOM	1852	C	TYR	G	384	100.504	−133.685	139.415	1.00	89.54
ATOM	1853	O	TYR	G	384	101.132	−133.047	140.255	1.00	90.93
ATOM	1854	CB	TYR	G	384	98.812	−131.845	139.473	1.00	85.32
ATOM	1855	CG	TYR	G	384	97.548	−131.256	138.895	1.00	83.12
ATOM	1856	CD1	TYR	G	384	96.321	−131.416	139.533	1.00	82.42
ATOM	1857	CD2	TYR	G	384	97.579	−130.555	137.690	1.00	81.60
ATOM	1858	CE1	TYR	G	384	95.153	−130.891	138.983	1.00	82.41
ATOM	1859	CE2	TYR	G	384	96.422	−130.029	137.132	1.00	81.05
ATOM	1860	CZ	TYR	G	384	95.214	−130.200	137.782	1.00	81.32
ATOM	1861	OH	TYR	G	384	94.070	−129.681	137.223	1.00	78.86
ATOM	1862	N	CYS	G	385	101.010	−134.733	138.764	1.00	93.00
ATOM	1863	CA	CYS	G	385	102.358	−135.249	139.016	1.00	96.10
ATOM	1864	C	CYS	G	385	103.432	−134.478	138.255	1.00	98.98
ATOM	1865	O	CYS	G	385	103.284	−134.196	137.064	1.00	100.31
ATOM	1866	CB	CYS	G	385	102.448	−136.727	138.625	1.00	96.17
ATOM	1867	SG	CYS	G	385	101.237	−137.831	139.415	1.00	97.03
ATOM	1868	N	ASN	G	386	104.522	−134.158	138.944	1.00	101.88
ATOM	1869	CA	ASN	G	386	105.630	−133.416	138.351	1.00	105.68
ATOM	1870	C	ASN	G	386	106.483	−134.318	137.460	1.00	109.06
ATOM	1871	O	ASN	G	386	107.126	−135.249	137.940	1.00	110.00
ATOM	1872	CB	ASN	G	386	106.488	−132.802	139.464	1.00	104.65

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	1873	CG	ASN	G	386	107.278	−131.592	138.997	1.00	104.49
ATOM	1874	OD1	ASN	G	386	107.793	−130.826	139.811	1.00	105.86
ATOM	1875	ND2	ASN	G	386	107.380	−131.417	137.682	1.00	103.57
ATOM	1876	N	SER	G	387	106.489	−134.033	136.161	1.00	112.28
ATOM	1877	CA	SER	G	387	107.255	−134.828	135.204	1.00	115.20
ATOM	1878	C	SER	G	387	108.613	−134.207	134.897	1.00	117.38
ATOM	1879	O	SER	G	387	109.080	−134.244	133.756	1.00	118.83
ATOM	1880	CB	SER	G	387	106.468	−134.982	133.901	1.00	114.78
ATOM	1881	OG	SER	G	387	106.259	−133.722	133.290	1.00	115.93
ATOM	1882	N	ALA	G	388	109.242	−133.635	135.916	1.00	118.94
ATOM	1883	CA	ALA	G	388	110.543	−133.004	135.747	1.00	120.08
ATOM	1884	C	ALA	G	388	111.650	−134.046	135.640	1.00	120.63
ATOM	1885	O	ALA	G	388	112.518	−133.955	134.776	1.00	121.23
ATOM	1886	CB	ALA	G	388	110.821	−132.064	136.915	1.00	120.48
ATOM	1887	N	GLN	G	389	111.612	−135.038	136.523	1.00	121.07
ATOM	1888	CA	GLN	G	389	112.616	−136.094	136.531	1.00	121.87
ATOM	1889	C	GLN	G	389	112.436	−137.082	135.383	1.00	121.47
ATOM	1890	O	GLN	G	389	113.415	−137.619	134.864	1.00	122.53
ATOM	1891	CB	GLN	G	389	112.584	−136.833	137.870	1.00	123.58
ATOM	1892	CG	GLN	G	389	111.184	−137.051	138.405	1.00	127.91
ATOM	1893	CD	GLN	G	389	111.168	−137.823	139.708	1.00	130.19
ATOM	1894	OE1	GLN	G	389	111.948	−137.547	140.620	1.00	132.91
ATOM	1895	NE2	GLN	G	389	110.266	−138.791	139.806	1.00	131.56
ATOM	1896	N	LEU	G	390	111.189	−137.319	134.987	1.00	120.77
ATOM	1897	CA	LEU	G	390	110.899	−138.241	133.892	1.00	119.93
ATOM	1898	C	LEU	G	390	111.556	−137.810	132.589	1.00	119.16
ATOM	1899	O	LEU	G	390	112.076	−138.639	131.843	1.00	119.29
ATOM	1900	CB	LEU	G	390	109.392	−138.349	133.667	1.00	120.27
ATOM	1901	CG	LEU	G	390	108.609	−139.237	134.633	1.00	120.93
ATOM	1902	CD1	LEU	G	390	107.122	−139.075	134.385	1.00	122.76
ATOM	1903	CD2	LEU	G	390	109.028	−140.682	134.437	1.00	121.13
ATOM	1904	N	PHE	G	391	111.525	−136.512	132.312	1.00	117.95
ATOM	1905	CA	PHE	G	391	112.116	−135.993	131.088	1.00	116.69
ATOM	1906	C	PHE	G	391	113.329	−135.117	131.375	1.00	116.29
ATOM	1907	O	PHE	G	391	113.311	−133.915	131.123	1.00	116.61
ATOM	1908	CB	PHE	G	391	111.076	−135.193	130.296	1.00	115.47
ATOM	1909	CG	PHE	G	391	109.902	−136.012	129.830	1.00	113.79
ATOM	1910	CD1	PHE	G	391	108.889	−136.372	130.713	1.00	112.00
ATOM	1911	CD2	PHE	G	391	109.814	−136.430	128.504	1.00	113.65
ATOM	1912	CE1	PHE	G	391	107.806	−137.138	130.284	1.00	111.30
ATOM	1913	CE2	PHE	G	391	108.735	−137.197	128.066	1.00	112.65
ATOM	1914	CZ	PHE	G	391	107.730	−137.550	128.959	1.00	111.37
ATOM	1915	N	ASN	G	392	114.386	−135.730	131.900	1.00	116.37
ATOM	1916	CA	ASN	G	392	115.614	−135.010	132.219	1.00	116.90
ATOM	1917	C	ASN	G	392	116.832	−135.861	131.881	1.00	117.22
ATOM	1918	O	ASN	G	392	117.371	−136.552	132.746	1.00	117.20
ATOM	1919	CB	ASN	G	392	115.653	−134.660	133.710	1.00	117.23
ATOM	1920	CG	ASN	G	392	116.788	−133.711	134.059	1.00	117.04
ATOM	1921	OD1	ASN	G	392	117.373	−133.793	135.141	1.00	116.31
ATOM	1922	ND2	ASN	G	392	117.091	−132.792	133.148	1.00	115.97
ATOM	1923	N	SER	G	393	117.264	−135.811	130.628	1.00	117.25
ATOM	1924	CA	SER	G	393	118.420	−136.587	130.199	1.00	117.84
ATOM	1925	C	SER	G	393	118.898	−136.099	128.838	1.00	118.76
ATOM	1926	O	SER	G	393	118.091	−135.750	127.979	1.00	118.46
ATOM	1927	CB	SER	G	393	118.059	−138.076	130.130	1.00	117.40
ATOM	1928	OG	SER	G	393	116.915	−138.287	129.323	1.00	117.90
ATOM	1929	N	THR	G	394	120.213	−136.069	128.648	1.00	120.79
ATOM	1930	CA	THR	G	394	120.788	−135.615	127.390	1.00	122.12
ATOM	1931	C	THR	G	394	121.239	−136.811	126.565	1.00	123.64
ATOM	1932	O	THR	G	394	121.846	−137.738	127.096	1.00	123.04
ATOM	1933	CB	THR	G	394	122.003	−134.711	127.640	1.00	121.38
ATOM	1934	OG1	THR	G	394	121.701	−133.792	128.694	1.00	121.49
ATOM	1935	CG2	THR	G	394	122.347	−133.924	126.390	1.00	120.33
ATOM	1936	N	TRP	G	395	120.938	−136.791	125.271	1.00	125.53
ATOM	1937	CA	TRP	G	395	121.324	−137.885	124.389	1.00	127.71
ATOM	1938	C	TRP	G	395	122.040	−137.385	123.138	1.00	130.76
ATOM	1939	O	TRP	G	395	121.444	−136.713	122.296	1.00	130.73
ATOM	1940	CB	TRP	G	395	120.092	−138.696	123.976	1.00	124.98
ATOM	1941	CG	TRP	G	395	119.330	−139.263	125.127	1.00	122.80
ATOM	1942	CD1	TRP	G	395	118.578	−138.573	126.032	1.00	122.44
ATOM	1943	CD2	TRP	G	395	119.259	−140.641	125.511	1.00	121.88
ATOM	1944	NE1	TRP	G	395	118.041	−139.435	126.957	1.00	122.03
ATOM	1945	CE2	TRP	G	395	118.442	−140.710	126.662	1.00	121.61
ATOM	1946	CE3	TRP	G	395	119.804	−141.823	124.995	1.00	122.03
ATOM	1947	CZ2	TRP	G	395	118.159	−141.918	127.308	1.00	121.03
ATOM	1948	CZ3	TRP	G	395	119.521	−143.024	125.638	1.00	121.12
ATOM	1949	CH2	TRP	G	395	118.705	−143.061	126.782	1.00	120.35
ATOM	1950	N	ASN	G	396	123.322	−137.722	123.023	1.00	134.68

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	1951	CA	ASN	G	396	124.132	−137.319	121.877	1.00	138.49
ATOM	1952	C	ASN	G	396	125.278	−138.306	121.699	1.00	140.34
ATOM	1953	O	ASN	G	396	126.028	−138.237	120.723	1.00	140.16
ATOM	1954	CB	ASN	G	396	124.702	−135.914	122.091	1.00	139.54
ATOM	1955	CG	ASN	G	396	125.710	−135.858	123.225	1.00	140.48
ATOM	1956	OD1	ASN	G	396	125.396	−136.194	124.367	1.00	140.41
ATOM	1957	ND2	ASN	G	396	126.929	−135.431	122.914	1.00	139.91
ATOM	1958	N	ASN	G	397	125.405	−139.223	122.653	1.00	142.71
ATOM	1959	CA	ASN	G	397	126.461	−140.225	122.616	1.00	145.52
ATOM	1960	C	ASN	G	397	126.235	−141.263	123.712	1.00	147.30
ATOM	1961	O	ASN	G	397	126.975	−141.314	124.696	1.00	147.83
ATOM	1962	CB	ASN	G	397	127.820	−139.546	122.804	1.00	145.45
ATOM	1963	CG	ASN	G	397	128.980	−140.452	122.449	1.00	146.09
ATOM	1964	OD1	ASN	G	397	130.135	−140.031	122.478	1.00	147.69
ATOM	1965	ND2	ASN	G	397	128.680	−141.700	122.109	1.00	146.44
ATOM	1966	N	ASN	G	401	125.206	−142.087	123.536	1.00	148.95
ATOM	1967	CA	ASN	G	401	124.874	−143.125	124.505	1.00	150.19
ATOM	1968	C	ASN	G	401	124.087	−144.258	123.850	1.00	151.32
ATOM	1969	O	ASN	G	401	122.864	−144.187	123.729	1.00	151.15
ATOM	1970	CB	ASN	G	401	124.057	−142.526	125.654	1.00	149.72
ATOM	1971	CG	ASN	G	401	123.716	−143.547	126.723	1.00	150.07
ATOM	1972	OD1	ASN	G	401	123.043	−144.543	126.455	1.00	150.13
ATOM	1973	ND2	ASN	G	401	124.180	−143.304	127.943	1.00	150.04
ATOM	1974	N	THR	G	402	124.798	−145.301	123.431	1.00	152.32
ATOM	1975	CA	THR	G	402	124.171	−146.452	122.790	1.00	152.72
ATOM	1976	C	THR	G	402	124.884	−147.746	123.178	1.00	152.78
ATOM	1977	O	THR	G	402	125.762	−148.222	122.457	1.00	152.62
ATOM	1978	CB	THR	G	402	124.193	−146.315	121.249	1.00	152.55
ATOM	1979	OG1	THR	G	402	123.528	−145.105	120.864	1.00	152.61
ATOM	1980	CG2	THR	G	402	123.489	−147.498	120.597	1.00	152.80
ATOM	1981	N	GLU	G	403	124.503	−148.307	124.322	1.00	153.02
ATOM	1982	CA	GLU	G	403	125.102	−149.547	124.806	1.00	153.40
ATOM	1983	C	GLU	G	403	124.013	−150.508	125.281	1.00	153.32
ATOM	1984	O	GLU	G	403	123.311	−151.112	124.468	1.00	152.98
ATOM	1985	CB	GLU	G	403	126.074	−149.251	125.952	1.00	153.38
ATOM	1986	CG	GLU	G	403	126.971	−150.422	126.323	1.00	154.46
ATOM	1987	CD	GLU	G	403	127.851	−150.127	127.522	1.00	155.23
ATOM	1988	OE1	GLU	G	403	128.568	−149.104	127.499	1.00	155.71
ATOM	1989	OE2	GLU	G	403	127.828	−150.921	128.486	1.00	155.97
ATOM	1990	N	GLY	G	404	123.875	−150.647	126.597	1.00	153.51
ATOM	1991	CA	GLY	G	404	122.862	−151.531	127.148	1.00	153.40
ATOM	1992	C	GLY	G	404	123.409	−152.822	127.728	1.00	153.73
ATOM	1993	O	GLY	G	404	123.831	−153.715	126.991	1.00	153.69
ATOM	1994	N	SER	G	405	123.400	−152.922	129.054	1.00	153.35
ATOM	1995	CA	SER	G	405	123.888	−154.112	129.745	1.00	152.70
ATOM	1996	C	SER	G	405	123.183	−154.291	131.086	1.00	152.14
ATOM	1997	O	SER	G	405	122.394	−155.221	131.259	1.00	151.89
ATOM	1998	CB	SER	G	405	125.401	−154.021	129.962	1.00	152.88
ATOM	1999	OG	SER	G	405	126.096	−154.051	128.728	1.00	152.70
ATOM	2000	N	ASN	G	406	123.473	−153.398	132.031	1.00	151.38
ATOM	2001	CA	ASN	G	406	122.864	−153.445	133.359	1.00	150.36
ATOM	2002	C	ASN	G	406	123.489	−152.410	134.294	1.00	149.65
ATOM	2003	O	ASN	G	406	124.666	−152.503	134.641	1.00	149.18
ATOM	2004	CB	ASN	G	406	123.020	−154.842	133.970	1.00	150.31
ATOM	2005	CG	ASN	G	406	122.212	−155.018	135.243	1.00	150.00
ATOM	2006	OD1	ASN	G	406	122.418	−154.308	136.227	1.00	150.04
ATOM	2007	ND2	ASN	G	406	121.284	−155.970	135.228	1.00	148.55
ATOM	2008	N	ASN	G	407	122.691	−151.425	134.696	1.00	149.20
ATOM	2009	CA	ASN	G	407	123.153	−150.371	135.596	1.00	148.98
ATOM	2010	C	ASN	G	407	122.039	−149.959	136.557	1.00	148.75
ATOM	2011	O	ASN	G	407	120.905	−149.720	136.141	1.00	148.64
ATOM	2012	CB	ASN	G	407	123.622	−149.154	134.792	1.00	148.85
ATOM	2013	CG	ASN	G	407	124.837	−149.454	133.934	1.00	148.15
ATOM	2014	OD1	ASN	G	407	125.883	−149.861	134.440	1.00	147.21
ATOM	2015	ND2	ASN	G	407	124.704	−149.252	132.627	1.00	146.76
ATOM	2016	N	THR	G	408	122.372	−149.876	137.843	1.00	148.42
ATOM	2017	CA	THR	G	408	121.400	−149.505	138.866	1.00	147.81
ATOM	2018	C	THR	G	408	121.620	−148.095	139.413	1.00	147.62
ATOM	2019	O	THR	G	408	122.740	−147.710	139.750	1.00	147.36
ATOM	2020	CB	THR	G	408	121.433	−150.503	140.047	1.00	147.47
ATOM	2021	OG1	THR	G	408	121.128	−151.820	139.570	1.00	146.97
ATOM	2022	CG2	THR	G	408	120.415	−150.110	141.110	1.00	147.04
ATOM	2023	N	GLU	G	409	120.532	−147.333	139.497	1.00	147.14
ATOM	2024	CA	GLU	G	409	120.563	−145.965	140.005	1.00	146.36
ATOM	2025	C	GLU	G	409	119.161	−145.527	140.417	1.00	145.32
ATOM	2026	O	GLU	G	409	118.354	−145.122	139.579	1.00	145.40
ATOM	2027	CB	GLU	G	409	121.116	−145.012	138.938	1.00	146.73
ATOM	2028	CG	GLU	G	409	120.856	−143.531	139.211	1.00	147.62

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	2029	CD	GLU	G	409	121.396	−143.060	140.552	1.00	148.32
ATOM	2030	OE1	GLU	G	409	121.186	−141.875	140.891	1.00	147.74
ATOM	2031	OE2	GLU	G	409	122.029	−143.866	141.267	1.00	149.23
ATOM	2032	N	GLY	G	410	118.878	−145.613	141.713	1.00	143.74
ATOM	2033	CA	GLY	G	410	117.570	−145.228	142.210	1.00	141.66
ATOM	2034	C	GLY	G	410	116.524	−146.283	141.903	1.00	140.56
ATOM	2035	O	GLY	G	410	115.851	−146.210	140.874	1.00	140.48
ATOM	2036	N	ASN	G	412	116.401	−147.261	142.799	1.00	138.86
ATOM	2037	CA	ASN	G	412	115.446	−148.363	142.670	1.00	136.44
ATOM	2038	C	ASN	G	412	114.351	−148.049	141.651	1.00	134.58
ATOM	2039	O	ASN	G	412	114.474	−148.377	140.470	1.00	133.27
ATOM	2040	CB	ASN	G	412	114.818	−148.658	144.038	1.00	137.07
ATOM	2041	CG	ASN	G	412	114.127	−150.009	144.090	1.00	138.01
ATOM	2042	OD1	ASN	G	412	113.251	−150.306	143.279	1.00	138.79
ATOM	2043	ND2	ASN	G	412	114.519	−150.835	145.055	1.00	137.47
ATOM	2044	N	THR	G	413	113.283	−147.412	142.121	1.00	132.39
ATOM	2045	CA	THR	G	413	112.167	−147.028	141.264	1.00	129.59
ATOM	2046	C	THR	G	413	111.876	−145.553	141.502	1.00	127.51
ATOM	2047	O	THR	G	413	111.733	−145.116	142.645	1.00	127.21
ATOM	2048	CB	THR	G	413	110.899	−147.848	141.575	1.00	129.45
ATOM	2049	OG1	THR	G	413	110.560	−147.703	142.959	1.00	130.30
ATOM	2050	CG2	THR	G	413	111.125	−149.319	141.259	1.00	129.33
ATOM	2051	N	ILE	G	414	111.792	−144.788	140.418	1.00	125.10
ATOM	2052	CA	ILE	G	414	111.543	−143.356	140.515	1.00	122.12
ATOM	2053	C	ILE	G	414	110.120	−143.022	140.958	1.00	119.27
ATOM	2054	O	ILE	G	414	109.151	−143.618	140.489	1.00	118.60
ATOM	2055	CB	ILE	G	414	111.838	−142.653	139.169	1.00	121.95
ATOM	2056	CG1	ILE	G	414	111.801	−141.138	139.358	1.00	122.52
ATOM	2057	CG2	ILE	G	414	110.830	−143.086	138.118	1.00	121.32
ATOM	2058	CD1	ILE	G	414	112.797	−140.620	140.384	1.00	122.64
ATOM	2059	N	THR	G	415	110.003	−142.060	141.866	1.00	115.70
ATOM	2060	CA	THR	G	415	108.704	−141.642	142.387	1.00	111.52
ATOM	2061	C	THR	G	415	108.362	−140.206	141.981	1.00	109.61
ATOM	2062	O	THR	G	415	109.175	−139.293	142.141	1.00	109.81
ATOM	2063	CB	THR	G	415	108.676	−141.739	143.923	1.00	110.78
ATOM	2064	OG1	THR	G	415	109.874	−141.165	144.460	1.00	110.36
ATOM	2065	CG2	THR	G	415	108.569	−143.179	144.369	1.00	109.69
ATOM	2066	N	LEU	G	416	107.150	−140.018	141.463	1.00	106.18
ATOM	2067	CA	LEU	G	416	106.684	−138.706	141.012	1.00	103.07
ATOM	2068	C	LEU	G	416	105.914	−137.919	142.070	1.00	101.81
ATOM	2069	O	LEU	G	416	104.998	−138.443	142.708	1.00	101.50
ATOM	2070	CB	LEU	G	416	105.775	−138.847	139.791	1.00	101.73
ATOM	2071	CG	LEU	G	416	106.344	−139.279	138.433	1.00	101.54
ATOM	2072	CD1	LEU	G	416	107.506	−138.367	138.062	1.00	100.93
ATOM	2073	CD2	LEU	G	416	106.797	−140.724	138.497	1.00	102.75
ATOM	2074	N	PRO	G	417	106.269	−136.638	142.261	1.00	100.49
ATOM	2075	CA	PRO	G	417	105.601	−135.778	143.242	1.00	99.11
ATOM	2076	C	PRO	G	417	104.244	−135.385	142.674	1.00	97.27
ATOM	2077	O	PRO	G	417	104.181	−134.634	141.706	1.00	96.57
ATOM	2078	CB	PRO	G	417	106.539	−134.573	143.338	1.00	99.33
ATOM	2079	CG	PRO	G	417	107.875	−135.120	142.895	1.00	100.96
ATOM	2080	CD	PRO	G	417	107.462	−135.964	141.726	1.00	101.14
ATOM	2081	N	CYS	G	418	103.158	−135.878	143.255	1.00	96.07
ATOM	2082	CA	CYS	G	418	101.840	−135.543	142.722	1.00	95.36
ATOM	2083	C	CYS	G	418	100.974	−134.814	143.737	1.00	94.31
ATOM	2084	O	CYS	G	418	101.186	−134.933	144.941	1.00	93.95
ATOM	2085	CB	CYS	G	418	101.124	−136.816	142.273	1.00	96.19
ATOM	2086	SG	CYS	G	418	100.205	−136.655	140.711	1.00	99.96
ATOM	2087	N	ARG	G	419	99.992	−134.065	143.243	1.00	93.30
ATOM	2088	CA	ARG	G	419	99.085	−133.325	144.112	1.00	92.31
ATOM	2089	C	ARG	G	419	97.658	−133.284	143.571	1.00	90.72
ATOM	2090	O	ARG	G	419	97.433	−132.982	142.396	1.00	90.53
ATOM	2091	CB	ARG	G	419	99.596	−131.890	144.314	1.00	93.73
ATOM	2092	CG	ARG	G	419	98.698	−131.006	145.181	1.00	95.93
ATOM	2093	CD	ARG	G	419	99.220	−129.571	145.236	1.00	99.25
ATOM	2094	NE	ARG	G	419	98.204	−128.611	145.670	1.00	100.53
ATOM	2095	CZ	ARG	G	419	97.837	−128.412	146.933	1.00	100.92
ATOM	2096	NH1	ARG	G	419	98.402	−129.102	147.916	1.00	100.24
ATOM	2097	NH2	ARG	G	419	96.900	−127.517	147.214	1.00	100.94
ATOM	2098	N	ILE	G	420	96.699	−133.601	144.436	1.00	88.67
ATOM	2099	CA	ILE	G	420	95.283	−133.579	144.078	1.00	86.76
ATOM	2100	C	ILE	G	420	94.765	−132.157	144.276	1.00	86.13
ATOM	2101	O	ILE	G	420	95.033	−131.530	145.302	1.00	86.62
ATOM	2102	CB	ILE	G	420	94.463	−134.540	144.969	1.00	85.30
ATOM	2103	CG1	ILE	G	420	94.795	−135.997	144.627	1.00	84.63
ATOM	2104	CG2	ILE	G	420	92.977	−134.295	144.768	1.00	85.53
ATOM	2105	CD1	ILE	G	420	96.188	−136.429	145.018	1.00	84.54
ATOM	2106	N	LYS	G	421	94.021	−131.645	143.302	1.00	84.49

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	2107	CA	LYS	G	421	93.523	−130.279	143.400	1.00	83.10
ATOM	2108	C	LYS	G	421	92.006	−130.151	143.259	1.00	83.34
ATOM	2109	O	LYS	G	421	91.341	−131.023	142.702	1.00	83.53
ATOM	2110	CB	LYS	G	421	94.224	−129.405	142.343	1.00	82.25
ATOM	2111	CG	LYS	G	421	95.756	−129.478	142.395	1.00	82.29
ATOM	2112	CD	LYS	G	421	96.428	−128.598	141.347	1.00	81.95
ATOM	2113	CE	LYS	G	421	97.882	−128.375	141.743	1.00	84.09
ATOM	2114	NZ	LYS	G	421	98.489	−127.187	141.078	1.00	83.94
ATOM	2115	N	GLN	G	422	91.471	−129.045	143.768	1.00	83.63
ATOM	2116	CA	GLN	G	422	90.040	−128.764	143.702	1.00	82.61
ATOM	2117	C	GLN	G	422	89.728	−127.802	142.565	1.00	80.65
ATOM	2118	O	GLN	G	422	88.823	−128.044	141.770	1.00	78.92
ATOM	2119	CB	GLN	G	422	89.553	−128.181	145.033	1.00	84.13
ATOM	2120	CG	GLN	G	422	89.286	−129.228	146.109	1.00	88.24
ATOM	2121	CD	GLN	G	422	88.821	−128.620	147.421	1.00	91.10
ATOM	2122	OE1	GLN	G	422	89.614	−128.054	148.174	1.00	92.63
ATOM	2123	NE2	GLN	G	422	87.527	−128.731	147.699	1.00	91.83
ATOM	2124	N	ILE	G	423	90.474	−126.706	142.493	1.00	79.69
ATOM	2125	CA	ILE	G	423	90.276	−125.734	141.431	1.00	79.70
ATOM	2126	C	ILE	G	423	91.021	−126.251	140.208	1.00	79.36
ATOM	2127	O	ILE	G	423	92.238	−126.436	140.240	1.00	81.30
ATOM	2128	CB	ILE	G	423	90.807	−124.356	141.858	1.00	79.75
ATOM	2129	CG1	ILE	G	423	89.917	−123.811	142.982	1.00	80.64
ATOM	2130	CG2	ILE	G	423	90.841	−123.411	140.668	1.00	79.15
ATOM	2131	CD1	ILE	G	423	90.446	−122.563	143.643	1.00	83.89
ATOM	2132	N	ILE	G	424	90.275	−126.493	139.138	1.00	78.23
ATOM	2133	CA	ILE	G	424	90.833	−127.038	137.915	1.00	77.77
ATOM	2134	C	ILE	G	424	90.580	−126.185	136.690	1.00	77.60
ATOM	2135	O	ILE	G	424	89.543	−125.539	136.576	1.00	78.36
ATOM	2136	CB	ILE	G	424	90.208	−128.401	137.631	1.00	78.68
ATOM	2137	CG1	ILE	G	424	90.294	−129.256	138.885	1.00	80.96
ATOM	2138	CG2	ILE	G	424	90.893	−129.069	136.451	1.00	80.04
ATOM	2139	CD1	ILE	G	424	89.310	−130.360	138.897	1.00	85.27
ATOM	2140	N	ASN	G	425	91.533	−126.182	135.766	1.00	78.21
ATOM	2141	CA	ASN	G	425	91.356	−125.444	134.521	1.00	79.38
ATOM	2142	C	ASN	G	425	90.717	−126.445	133.562	1.00	81.00
ATOM	2143	O	ASN	G	425	91.281	−127.506	133.291	1.00	82.92
ATOM	2144	CB	ASN	G	425	92.697	−124.946	133.978	1.00	78.48
ATOM	2145	CG	ASN	G	425	93.007	−123.526	134.408	1.00	79.22
ATOM	2146	OD1	ASN	G	425	92.243	−122.601	134.123	1.00	78.79
ATOM	2147	ND2	ASN	G	425	94.136	−123.341	135.080	1.00	80.19
ATOM	2148	N	MET	G	426	89.534	−126.112	133.057	1.00	82.44
ATOM	2149	CA	MET	G	426	88.803	−127.010	132.169	1.00	83.15
ATOM	2150	C	MET	G	426	89.441	−127.260	130.810	1.00	82.81
ATOM	2151	O	MET	G	426	89.996	−126.349	130.194	1.00	81.41
ATOM	2152	CB	MET	G	426	87.378	−126.496	131.982	1.00	84.29
ATOM	2153	CG	MET	G	426	86.668	−126.263	133.303	1.00	83.67
ATOM	2154	SD	MET	G	426	84.893	−126.182	133.114	1.00	83.84
ATOM	2155	CE	MET	G	426	84.500	−127.928	133.137	1.00	84.40
ATOM	2156	N	TRP	G	427	89.355	−128.509	130.353	1.00	82.00
ATOM	2157	CA	TRP	G	427	89.909	−128.910	129.063	1.00	81.18
ATOM	2158	C	TRP	G	427	88.857	−128.872	127.963	1.00	80.45
ATOM	2159	O	TRP	G	427	89.182	−128.678	126.793	1.00	80.26
ATOM	2160	CB	TRP	G	427	90.501	−130.323	129.142	1.00	81.81
ATOM	2161	CG	TRP	G	427	89.522	−131.397	129.531	1.00	82.28
ATOM	2162	CD1	TRP	G	427	89.242	−131.834	130.794	1.00	82.98
ATOM	2163	CD2	TRP	G	427	88.708	−132.181	128.646	1.00	81.40
ATOM	2164	NE1	TRP	G	427	88.310	−132.843	130.751	1.00	82.68
ATOM	2165	CE2	TRP	G	427	87.964	−133.076	129.447	1.00	81.58
ATOM	2166	CE3	TRP	G	427	88.536	−132.213	127.256	1.00	80.71
ATOM	2167	CZ2	TRP	G	427	87.061	−133.996	128.902	1.00	81.39
ATOM	2168	CZ3	TRP	G	427	87.637	−133.130	126.715	1.00	80.74
ATOM	2169	CH2	TRP	G	427	86.912	−134.007	127.539	1.00	80.83
ATOM	2170	N	GLN	G	428	87.596	−129.059	128.341	1.00	80.48
ATOM	2171	CA	GLN	G	428	86.509	−129.047	127.370	1.00	80.94
ATOM	2172	C	GLN	G	428	86.367	−127.664	126.752	1.00	80.28
ATOM	2173	O	GLN	G	428	86.432	−127.507	125.534	1.00	80.34
ATOM	2174	CB	GLN	G	428	85.192	−129.450	128.033	1.00	82.24
ATOM	2175	CG	GLN	G	428	85.271	−130.727	128.850	1.00	84.02
ATOM	2176	CD	GLN	G	428	85.490	−130.459	130.327	1.00	85.70
ATOM	2177	OE1	GLN	G	428	86.450	−129.794	130.718	1.00	86.37
ATOM	2178	NE2	GLN	G	428	84.593	−130.976	131.157	1.00	88.20
ATOM	2179	N	GLU	G	429	86.168	−126.661	127.599	1.00	79.28
ATOM	2180	CA	GLU	G	429	86.028	−125.290	127.128	1.00	79.36
ATOM	2181	C	GLU	G	429	86.891	−124.365	127.975	1.00	77.22
ATOM	2182	O	GLU	G	429	87.281	−124.718	129.088	1.00	77.49
ATOM	2183	CB	GLU	G	429	84.558	−124.850	127.196	1.00	82.15
ATOM	2184	CG	GLU	G	429	84.005	−124.666	128.603	1.00	82.38

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	2185	CD	GLU	G	429	82.538	−124.263	128.606	1.00	83.05
ATOM	2186	OE1	GLU	G	429	82.199	−123.225	127.998	1.00	81.83
ATOM	2187	OE2	GLU	G	429	81.723	−124.988	129.215	1.00	83.79
ATOM	2188	N	VAL	G	430	87.199	−123.187	127.449	1.00	74.05
ATOM	2189	CA	VAL	G	430	88.009	−122.237	128.193	1.00	72.33
ATOM	2190	C	VAL	G	430	87.291	−121.876	129.491	1.00	72.05
ATOM	2191	O	VAL	G	430	86.126	−121.489	129.473	1.00	73.40
ATOM	2192	CB	VAL	G	430	88.240	−120.955	127.377	1.00	72.15
ATOM	2193	CG1	VAL	G	430	89.157	−120.012	128.135	1.00	70.59
ATOM	2194	CG2	VAL	G	430	88.826	−121.304	126.022	1.00	72.50
ATOM	2195	N	GLY	G	431	87.983	−122.013	130.616	1.00	71.44
ATOM	2196	CA	GLY	G	431	87.367	−121.693	131.891	1.00	70.65
ATOM	2197	C	GLY	G	431	87.947	−122.483	133.046	1.00	69.99
ATOM	2198	O	GLY	G	431	88.954	−123.168	132.884	1.00	72.09
ATOM	2199	N	LYS	G	432	87.319	−122.386	134.214	1.00	68.32
ATOM	2200	CA	LYS	G	432	87.785	−123.103	135.397	1.00	66.54
ATOM	2201	C	LYS	G	432	86.663	−123.912	136.026	1.00	64.43
ATOM	2202	O	LYS	G	432	85.510	−123.822	135.611	1.00	66.65
ATOM	2203	CB	LYS	G	432	88.344	−122.123	136.434	1.00	68.76
ATOM	2204	CG	LYS	G	432	89.580	−121.362	135.973	1.00	71.24
ATOM	2205	CD	LYS	G	432	90.008	−120.336	137.012	1.00	72.43
ATOM	2206	CE	LYS	G	432	91.167	−119.486	136.515	1.00	74.60
ATOM	2207	NZ	LYS	G	432	92.391	−120.287	136.230	1.00	76.20
ATOM	2208	N	ALA	G	433	87.008	−124.700	137.036	1.00	61.60
ATOM	2209	CA	ALA	G	433	86.031	−125.529	137.721	1.00	60.62
ATOM	2210	C	ALA	G	433	86.467	−125.778	139.156	1.00	61.66
ATOM	2211	O	ALA	G	433	87.655	−125.757	139.464	1.00	65.08
ATOM	2212	CB	ALA	G	433	85.872	−126.850	136.989	1.00	59.62
ATOM	2213	N	MET	G	434	85.495	−126.019	140.027	1.00	61.86
ATOM	2214	CA	MET	G	434	85.756	−126.272	141.439	1.00	62.17
ATOM	2215	C	MET	G	434	85.099	−127.572	141.885	1.00	63.75
ATOM	2216	O	MET	G	434	83.884	−127.727	141.762	1.00	65.83
ATOM	2217	CB	MET	G	434	85.203	−125.123	142.283	1.00	61.94
ATOM	2218	CG	MET	G	434	84.957	−125.495	143.737	1.00	62.90
ATOM	2219	SD	MET	G	434	86.262	−125.005	144.862	1.00	64.78
ATOM	2220	CE	MET	G	434	85.342	−123.924	145.974	1.00	64.90
ATOM	2221	N	TYR	G	435	85.890	−128.501	142.413	1.00	63.38
ATOM	2222	CA	TYR	G	435	85.343	−129.777	142.874	1.00	61.59
ATOM	2223	C	TYR	G	435	85.401	−129.929	144.388	1.00	62.48
ATOM	2224	O	TYR	G	435	86.030	−129.129	145.079	1.00	62.27
ATOM	2225	CB	TYR	G	435	86.079	−130.945	142.219	1.00	58.59
ATOM	2226	CG	TYR	G	435	85.750	−131.133	140.759	1.00	54.66
ATOM	2227	CD1	TYR	G	435	86.207	−130.237	139.798	1.00	52.26
ATOM	2228	CD2	TYR	G	435	84.967	−132.206	140.340	1.00	57.11
ATOM	2229	CE1	TYR	G	435	85.893	−130.406	138.453	1.00	54.48
ATOM	2230	CE2	TYR	G	435	84.646	−132.384	138.999	1.00	57.17
ATOM	2231	CZ	TYR	G	435	85.110	−131.482	138.062	1.00	55.72
ATOM	2232	OH	TYR	G	435	84.781	−131.663	136.738	1.00	55.13
ATOM	2233	N	ALA	G	436	84.747	−130.967	144.897	1.00	64.73
ATOM	2234	CA	ALA	G	436	84.713	−131.229	146.331	1.00	69.52
ATOM	2235	C	ALA	G	436	86.048	−131.755	146.862	1.00	73.34
ATOM	2236	O	ALA	G	436	86.882	−132.251	146.104	1.00	74.12
ATOM	2237	CB	ALA	G	436	83.598	−132.225	146.645	1.00	68.49
ATOM	2238	N	PRO	G	437	86.266	−131.648	148.184	1.00	77.56
ATOM	2239	CA	PRO	G	437	87.501	−132.114	148.818	1.00	80.89
ATOM	2240	C	PRO	G	437	87.721	−133.611	148.599	1.00	85.07
ATOM	2241	O	PRO	G	437	86.766	−134.365	148.413	1.00	86.90
ATOM	2242	CB	PRO	G	437	87.285	−131.754	150.285	1.00	79.74
ATOM	2243	CG	PRO	G	437	86.421	−130.527	150.197	1.00	78.93
ATOM	2244	CD	PRO	G	437	85.409	−130.972	149.171	1.00	77.85
ATOM	2245	N	PRO	G	438	88.988	−134.058	148.617	1.00	88.61
ATOM	2246	CA	PRO	G	438	89.362	−135.460	148.416	1.00	91.38
ATOM	2247	C	PRO	G	438	88.540	−136.458	149.225	1.00	95.06
ATOM	2248	O	PRO	G	438	88.062	−136.149	150.318	1.00	94.95
ATOM	2249	CB	PRO	G	438	90.840	−135.467	148.790	1.00	89.15
ATOM	2250	CG	PRO	G	438	91.284	−134.125	148.301	1.00	87.77
ATOM	2251	CD	PRO	G	438	90.189	−133.240	148.859	1.00	88.31
ATOM	2252	N	ILE	G	439	88.379	−137.655	148.672	1.00	99.51
ATOM	2253	CA	ILE	G	439	87.615	−138.713	149.320	1.00	105.19
ATOM	2254	C	ILE	G	439	88.361	−139.228	150.546	1.00	110.13
ATOM	2255	O	ILE	G	439	89.590	−139.212	150.581	1.00	110.70
ATOM	2256	CB	ILE	G	439	87.395	−139.884	148.354	1.00	104.20
ATOM	2257	CG1	ILE	G	439	87.009	−139.347	146.973	1.00	103.55
ATOM	2258	CG2	ILE	G	439	86.297	−140.795	148.882	1.00	104.68
ATOM	2259	CD1	ILE	G	439	87.025	−140.395	145.894	1.00	105.15
ATOM	2260	N	ARG	G	440	87.613	−139.688	151.544	1.00	116.12
ATOM	2261	CA	ARG	G	440	88.200	−140.192	152.779	1.00	122.02
ATOM	2262	C	ARG	G	440	89.016	−141.478	152.623	1.00	124.42

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	2263	O	ARG	G	440	90.028	−141.660	153.300	1.00	125.60
ATOM	2264	CB	ARG	G	440	87.096	−140.376	153.833	1.00	124.40
ATOM	2265	CG	ARG	G	440	85.821	−141.037	153.316	1.00	128.47
ATOM	2266	CD	ARG	G	440	85.962	−142.547	153.275	1.00	132.51
ATOM	2267	NE	ARG	G	440	85.509	−143.111	152.007	1.00	135.84
ATOM	2268	CZ	ARG	G	440	85.710	−144.374	151.643	1.00	137.31
ATOM	2269	NH1	ARG	G	440	86.354	−145.200	152.456	1.00	137.16
ATOM	2270	NH2	ARG	G	440	85.275	−144.810	150.467	1.00	136.49
ATOM	2271	N	GLY	G	441	88.592	−142.358	151.721	1.00	125.98
ATOM	2272	CA	GLY	G	441	89.305	−143.609	151.521	1.00	127.56
ATOM	2273	C	GLY	G	441	90.602	−143.502	150.739	1.00	128.74
ATOM	2274	O	GLY	G	441	91.025	−142.412	150.347	1.00	128.11
ATOM	2275	N	GLN	G	442	91.230	−144.653	150.518	1.00	129.91
ATOM	2276	CA	GLN	G	442	92.483	−144.745	149.780	1.00	130.78
ATOM	2277	C	GLN	G	442	92.234	−144.787	148.275	1.00	131.13
ATOM	2278	O	GLN	G	442	91.299	−145.438	147.805	1.00	130.50
ATOM	2279	CB	GLN	G	442	93.251	−145.997	150.219	1.00	132.26
ATOM	2280	CG	GLN	G	442	93.839	−146.801	149.072	1.00	134.25
ATOM	2281	CD	GLN	G	442	95.123	−147.506	149.454	1.00	135.13
ATOM	2282	OE1	GLN	G	442	95.125	−148.447	150.248	1.00	136.02
ATOM	2283	NE2	GLN	G	442	96.233	−147.040	148.897	1.00	134.96
ATOM	2284	N	ILE	G	443	93.084	−144.096	147.524	1.00	131.67
ATOM	2285	CA	ILE	G	443	92.961	−144.041	146.073	1.00	132.30
ATOM	2286	C	ILE	G	443	94.142	−144.725	145.398	1.00	131.73
ATOM	2287	O	ILE	G	443	95.271	−144.238	145.452	1.00	131.38
ATOM	2288	CB	ILE	G	443	92.890	−142.582	145.591	1.00	133.10
ATOM	2289	CG1	ILE	G	443	91.729	−141.871	146.291	1.00	133.63
ATOM	2290	CG2	ILE	G	443	92.701	−142.535	144.080	1.00	134.13
ATOM	2291	CD1	ILE	G	443	91.703	−140.384	146.055	1.00	133.79
ATOM	2292	N	ARG	G	444	93.874	−145.856	144.759	1.00	131.74
ATOM	2293	CA	ARG	G	444	94.909	−146.629	144.078	1.00	131.48
ATOM	2294	C	ARG	G	444	94.593	−146.714	142.583	1.00	129.69
ATOM	2295	O	ARG	G	444	93.492	−147.113	142.205	1.00	129.68
ATOM	2296	CB	ARG	G	444	94.964	−148.037	144.693	1.00	133.90
ATOM	2297	CG	ARG	G	444	96.261	−148.390	145.433	1.00	136.43
ATOM	2298	CD	ARG	G	444	96.037	−149.515	146.449	1.00	138.19
ATOM	2299	NE	ARG	G	444	97.247	−150.283	146.748	1.00	139.51
ATOM	2300	CZ	ARG	G	444	98.290	−149.830	147.441	1.00	140.29
ATOM	2301	NH1	ARG	G	444	98.294	−148.595	147.929	1.00	140.09
ATOM	2302	NH2	ARG	G	444	99.338	−150.619	147.647	1.00	140.64
ATOM	2303	N	CYS	G	445	95.543	−146.334	141.732	1.00	127.32
ATOM	2304	CA	CYS	G	445	95.316	−146.391	140.286	1.00	124.83
ATOM	2305	C	CYS	G	445	96.544	−146.962	139.558	1.00	123.33
ATOM	2306	O	CYS	G	445	97.684	−146.679	139.926	1.00	123.02
ATOM	2307	CB	CYS	G	445	94.974	−144.987	139.740	1.00	124.31
ATOM	2308	SG	CYS	G	445	93.684	−144.087	140.680	1.00	124.41
ATOM	2309	N	SER	G	446	96.299	−147.780	138.536	1.00	121.97
ATOM	2310	CA	SER	G	446	97.366	−148.402	137.752	1.00	119.88
ATOM	2311	C	SER	G	446	97.031	−148.373	136.262	1.00	117.92
ATOM	2312	O	SER	G	446	95.924	−148.733	135.859	1.00	117.72
ATOM	2313	CB	SER	G	446	97.574	−149.853	138.202	1.00	120.03
ATOM	2314	OG	SER	G	446	96.407	−150.627	137.986	1.00	120.27
ATOM	2315	N	SER	G	447	97.994	−147.955	135.448	1.00	114.74
ATOM	2316	CA	SER	G	447	97.790	−147.875	134.008	1.00	112.04
ATOM	2317	C	SER	G	447	99.096	−148.079	133.241	1.00	108.70
ATOM	2318	O	SER	G	447	100.182	−147.987	133.812	1.00	108.62
ATOM	2319	CB	SER	G	447	97.173	−146.518	133.655	1.00	113.67
ATOM	2320	OG	SER	G	447	97.856	−145.468	134.314	1.00	114.63
ATOM	2321	N	ASN	G	448	98.975	−148.359	131.946	1.00	104.80
ATOM	2322	CA	ASN	G	448	100.127	−148.587	131.084	1.00	101.05
ATOM	2323	C	ASN	G	448	100.392	−147.407	130.161	1.00	98.08
ATOM	2324	O	ASN	G	448	99.549	−147.048	129.342	1.00	97.79
ATOM	2325	CB	ASN	G	448	99.908	−149.848	130.235	1.00	102.67
ATOM	2326	CG	ASN	G	448	100.039	−151.126	131.038	1.00	103.58
ATOM	2327	OD1	ASN	G	448	101.140	−151.519	131.422	1.00	103.71
ATOM	2328	ND2	ASN	G	448	98.912	−151.781	131.299	1.00	103.79
ATOM	2329	N	ILE	G	449	101.566	−146.804	130.294	1.00	94.94
ATOM	2330	CA	ILE	G	449	101.935	−145.676	129.449	1.00	92.96
ATOM	2331	C	ILE	G	449	102.228	−146.206	128.054	1.00	92.14
ATOM	2332	O	ILE	G	449	103.343	−146.635	127.757	1.00	91.85
ATOM	2333	CB	ILE	G	449	103.182	−144.975	129.987	1.00	93.15
ATOM	2334	CG1	ILE	G	449	102.947	−144.584	131.449	1.00	94.25
ATOM	2335	CG2	ILE	G	449	103.494	−143.747	129.141	1.00	91.79
ATOM	2336	CD1	ILE	G	449	104.181	−144.084	132.146	1.00	94.95
ATOM	2337	N	THR	G	450	101.214	−146.178	127.201	1.00	91.70
ATOM	2338	CA	THR	G	450	101.349	−146.681	125.845	1.00	92.19
ATOM	2339	C	THR	G	450	101.910	−145.647	124.876	1.00	91.91
ATOM	2340	O	THR	G	450	102.164	−145.955	123.714	1.00	92.23

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	2341	CB	THR	G	450	99.992	−147.171	125.312	1.00	92.87
ATOM	2342	OG1	THR	G	450	99.044	−146.101	125.374	1.00	94.60
ATOM	2343	CG2	THR	G	450	99.480	−148.328	126.147	1.00	91.70
ATOM	2344	N	GLY	G	451	102.101	−144.421	125.350	1.00	92.40
ATOM	2345	CA	GLY	G	451	102.631	−143.373	124.493	1.00	93.12
ATOM	2346	C	GLY	G	451	102.795	−142.059	125.232	1.00	93.74
ATOM	2347	O	GLY	G	451	102.551	−141.983	126.434	1.00	94.94
ATOM	2348	N	LEU	G	452	103.208	−141.020	124.516	1.00	93.32
ATOM	2349	CA	LEU	G	452	103.394	−139.708	125.121	1.00	94.48
ATOM	2350	C	LEU	G	452	103.370	−138.597	124.077	1.00	96.43
ATOM	2351	O	LEU	G	452	103.383	−138.862	122.875	1.00	97.24
ATOM	2352	CB	LEU	G	452	104.717	−139.660	125.898	1.00	94.99
ATOM	2353	CG	LEU	G	452	105.989	−140.116	125.174	1.00	94.35
ATOM	2354	CD1	LEU	G	452	107.082	−139.061	125.305	1.00	93.41
ATOM	2355	CD2	LEU	G	452	106.447	−141.441	125.767	1.00	94.53
ATOM	2356	N	LEU	G	453	103.339	−137.353	124.546	1.00	97.31
ATOM	2357	CA	LEU	G	453	103.312	−136.191	123.662	1.00	97.97
ATOM	2358	C	LEU	G	453	104.537	−135.317	123.900	1.00	99.02
ATOM	2359	O	LEU	G	453	104.923	−135.080	125.044	1.00	98.34
ATOM	2360	CB	LEU	G	453	102.045	−135.374	123.919	1.00	100.23
ATOM	2361	CG	LEU	G	453	100.710	−136.088	123.684	1.00	102.44
ATOM	2362	CD1	LEU	G	453	99.780	−135.831	124.857	1.00	104.66
ATOM	2363	CD2	LEU	G	453	100.089	−135.602	122.384	1.00	104.74
ATOM	2364	N	LEU	G	454	105.144	−134.835	122.821	1.00	101.32
ATOM	2365	CA	LEU	G	454	106.335	−133.995	122.925	1.00	104.16
ATOM	2366	C	LEU	G	454	106.287	−132.786	122.002	1.00	105.43
ATOM	2367	O	LEU	G	454	105.683	−132.829	120.935	1.00	104.92
ATOM	2368	CB	LEU	G	454	107.587	−134.810	122.590	1.00	107.11
ATOM	2369	CG	LEU	G	454	108.124	−135.787	123.640	1.00	109.52
ATOM	2370	CD1	LEU	G	454	109.036	−136.808	122.980	1.00	110.38
ATOM	2371	CD2	LEU	G	454	108.870	−135.011	124.718	1.00	110.90
ATOM	2372	N	THR	G	455	106.940	−131.710	122.423	1.00	107.87
ATOM	2373	CA	THR	G	455	107.007	−130.483	121.639	1.00	111.93
ATOM	2374	C	THR	G	455	108.450	−129.979	121.669	1.00	113.34
ATOM	2375	O	THR	G	455	108.941	−129.532	122.708	1.00	113.32
ATOM	2376	CB	THR	G	455	106.087	−129.392	122.216	1.00	112.59
ATOM	2377	OG1	THR	G	455	106.172	−129.403	123.643	1.00	113.78
ATOM	2378	CG2	THR	G	455	104.650	−129.615	121.796	1.00	113.67
ATOM	2379	N	ARG	G	456	109.126	−130.057	120.526	1.00	115.82
ATOM	2380	CA	ARG	G	456	110.520	−129.638	120.426	1.00	117.80
ATOM	2381	C	ARG	G	456	110.714	−128.126	120.336	1.00	118.96
ATOM	2382	O	ARG	G	456	109.853	−127.405	119.834	1.00	118.29
ATOM	2383	CB	ARG	G	456	111.177	−130.305	119.212	1.00	117.97
ATOM	2384	CG	ARG	G	456	110.748	−129.740	117.864	1.00	119.08
ATOM	2385	CD	ARG	G	456	111.533	−130.384	116.728	1.00	119.35
ATOM	2386	NE	ARG	G	456	111.439	−129.607	115.496	1.00	119.68
ATOM	2387	CZ	ARG	G	456	112.130	−128.496	115.257	1.00	119.75
ATOM	2388	NH1	ARG	G	456	112.977	−128.027	116.165	1.00	120.37
ATOM	2389	NH2	ARG	G	456	111.968	−127.847	114.112	1.00	119.93
ATOM	2390	N	ASP	G	457	111.860	−127.656	120.823	1.00	119.85
ATOM	2391	CA	ASP	G	457	112.189	−126.233	120.793	1.00	120.75
ATOM	2392	C	ASP	G	457	112.749	−125.857	119.427	1.00	122.23
ATOM	2393	O	ASP	G	457	113.723	−126.451	118.964	1.00	122.14
ATOM	2394	CB	ASP	G	457	113.226	−125.903	121.869	1.00	120.14
ATOM	2395	CG	ASP	G	457	112.739	−126.229	123.267	1.00	120.03
ATOM	2396	OD1	ASP	G	457	113.374	−125.778	124.243	1.00	119.43
ATOM	2397	OD2	ASP	G	457	111.721	−126.943	123.378	1.00	119.90
ATOM	2398	N	GLY	G	458	112.139	−124.865	118.787	1.00	123.91
ATOM	2399	CA	GLY	G	458	112.597	−124.440	117.475	1.00	126.39
ATOM	2400	C	GLY	G	458	113.689	−123.387	117.531	1.00	128.56
ATOM	2401	O	GLY	G	458	114.703	−123.567	118.205	1.00	128.30
ATOM	2402	N	GLY	G	459	113.487	−122.284	116.817	1.00	130.42
ATOM	2403	CA	GLY	G	459	114.472	−121.222	116.807	1.00	132.58
ATOM	2404	C	GLY	G	459	115.502	−121.403	115.712	1.00	134.70
ATOM	2405	O	GLY	G	459	116.070	−122.485	115.552	1.00	134.58
ATOM	2406	N	ILE	G	460	115.751	−120.338	114.959	1.00	137.83
ATOM	2407	CA	ILE	G	460	116.726	−120.379	113.875	1.00	140.76
ATOM	2408	C	ILE	G	460	118.138	−120.321	114.468	1.00	142.81
ATOM	2409	O	ILE	G	460	119.123	−120.606	113.792	1.00	142.92
ATOM	2410	CB	ILE	G	460	116.497	−119.194	112.903	1.00	140.96
ATOM	2411	CG1	ILE	G	460	116.933	−119.570	111.484	1.00	141.22
ATOM	2412	CG2	ILE	G	460	117.259	−117.970	113.383	1.00	141.19
ATOM	2413	CD1	ILE	G	460	118.421	−119.766	111.310	1.00	140.88
ATOM	2414	N	ASN	G	461	118.223	−119.963	115.746	1.00	145.09
ATOM	2415	CA	ASN	G	461	119.506	−119.878	116.443	1.00	147.66
ATOM	2416	C	ASN	G	461	120.070	−121.289	116.632	1.00	149.02
ATOM	2417	O	ASN	G	461	119.393	−122.161	117.178	1.00	148.11
ATOM	2418	CB	ASN	G	461	119.309	−119.186	117.800	1.00	148.39

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	2419	CG	ASN	G	461	120.581	−118.560	118.329	1.00	149.53
ATOM	2420	OD1	ASN	G	461	121.509	−119.257	118.737	1.00	149.19
ATOM	2421	ND2	ASN	G	461	120.631	−117.233	118.323	1.00	148.79
ATOM	2422	N	GLU	G	462	121.303	−121.511	116.179	1.00	151.28
ATOM	2423	CA	GLU	G	462	121.931	−122.826	116.284	1.00	153.22
ATOM	2424	C	GLU	G	462	122.706	−123.073	117.578	1.00	153.57
ATOM	2425	O	GLU	G	462	123.216	−122.143	118.202	1.00	153.46
ATOM	2426	CB	GLU	G	462	122.859	−123.067	115.085	1.00	153.86
ATOM	2427	CG	GLU	G	462	124.074	−122.139	114.989	1.00	156.71
ATOM	2428	CD	GLU	G	462	123.763	−120.798	114.342	1.00	157.61
ATOM	2429	OE1	GLU	G	462	123.171	−119.922	115.006	1.00	157.89
ATOM	2430	OE2	GLU	G	462	124.110	−120.625	113.154	1.00	158.13
ATOM	2431	N	ASN	G	463	122.794	−124.342	117.965	1.00	153.66
ATOM	2432	CA	ASN	G	463	123.507	−124.735	119.172	1.00	153.40
ATOM	2433	C	ASN	G	463	123.918	−126.200	119.044	1.00	152.49
ATOM	2434	O	ASN	G	463	124.772	−126.690	119.784	1.00	152.48
ATOM	2435	CB	ASN	G	463	122.608	−124.525	120.400	1.00	154.12
ATOM	2436	CG	ASN	G	463	123.375	−124.598	121.707	1.00	155.58
ATOM	2437	OD1	ASN	G	463	123.613	−125.679	122.245	1.00	156.54
ATOM	2438	ND2	ASN	G	463	123.780	−123.439	122.217	1.00	156.41
ATOM	2439	N	GLY	G	464	123.311	−126.886	118.081	1.00	150.94
ATOM	2440	CA	GLY	G	464	123.614	−128.286	117.858	1.00	149.00
ATOM	2441	C	GLY	G	464	122.693	−129.184	118.658	1.00	147.53
ATOM	2442	O	GLY	G	464	122.652	−130.397	118.450	1.00	147.66
ATOM	2443	N	THR	G	465	121.937	−128.577	119.566	1.00	145.51
ATOM	2444	CA	THR	G	465	121.012	−129.311	120.416	1.00	142.98
ATOM	2445	C	THR	G	465	119.561	−128.931	120.146	1.00	140.93
ATOM	2446	O	THR	G	465	119.208	−127.752	120.074	1.00	140.82
ATOM	2447	CB	THR	G	465	121.305	−129.042	121.903	1.00	143.71
ATOM	2448	OG1	THR	G	465	121.216	−127.633	122.153	1.00	144.71
ATOM	2449	CG2	THR	G	465	122.691	−129.520	122.266	1.00	143.31
ATOM	2450	N	GLU	G	466	118.730	−129.951	119.981	1.00	137.84
ATOM	2451	CA	GLU	G	466	117.304	−129.762	119.750	1.00	134.60
ATOM	2452	C	GLU	G	466	116.586	−130.315	120.976	1.00	132.23
ATOM	2453	O	GLU	G	466	116.495	−131.530	121.155	1.00	131.65
ATOM	2454	CB	GLU	G	466	116.866	−130.515	118.492	1.00	134.81
ATOM	2455	CG	GLU	G	466	117.430	−129.969	117.182	1.00	135.55
ATOM	2456	CD	GLU	G	466	116.756	−128.681	116.729	1.00	136.34
ATOM	2457	OE1	GLU	G	466	117.195	−128.100	115.711	1.00	136.05
ATOM	2458	OE2	GLU	G	466	115.785	−128.250	117.386	1.00	137.26
ATOM	2459	N	ILE	G	467	116.080	−129.417	121.814	1.00	129.25
ATOM	2460	CA	ILE	G	467	115.400	−129.801	123.047	1.00	126.01
ATOM	2461	C	ILE	G	467	113.989	−130.338	122.826	1.00	123.54
ATOM	2462	O	ILE	G	467	113.261	−129.848	121.966	1.00	122.31
ATOM	2463	CB	ILE	G	467	115.299	−128.602	124.008	1.00	125.82
ATOM	2464	CG1	ILE	G	467	116.509	−127.686	123.827	1.00	125.39
ATOM	2465	CG2	ILE	G	467	115.262	−129.091	125.449	1.00	124.63
ATOM	2466	CD1	ILE	G	467	117.829	−128.361	124.104	1.00	125.46
ATOM	2467	N	PHE	G	468	113.609	−131.345	123.610	1.00	121.29
ATOM	2468	CA	PHE	G	468	112.277	−131.939	123.518	1.00	119.38
ATOM	2469	C	PHE	G	468	111.562	−131.923	124.866	1.00	117.84
ATOM	2470	O	PHE	G	468	111.904	−132.687	125.768	1.00	118.28
ATOM	2471	CB	PHE	G	468	112.360	−133.382	123.005	1.00	119.43
ATOM	2472	CG	PHE	G	468	112.625	−133.488	121.533	1.00	119.45
ATOM	2473	CD1	PHE	G	468	113.909	−133.319	121.028	1.00	119.08
ATOM	2474	CD2	PHE	G	468	111.584	−133.738	120.645	1.00	119.65
ATOM	2475	CE1	PHE	G	468	114.154	−133.397	119.660	1.00	119.36
ATOM	2476	CE2	PHE	G	468	111.818	−133.817	119.274	1.00	119.82
ATOM	2477	CZ	PHE	G	468	113.105	−133.647	118.781	1.00	119.73
ATOM	2478	N	ARG	G	469	110.564	−131.053	124.991	1.00	115.90
ATOM	2479	CA	ARG	G	469	109.789	−130.924	126.224	1.00	113.44
ATOM	2480	C	ARG	G	469	108.427	−131.610	126.079	1.00	112.22
ATOM	2481	O	ARG	G	469	107.896	−131.719	124.975	1.00	112.65
ATOM	2482	CB	ARG	G	469	109.598	−129.441	126.557	1.00	113.09
ATOM	2483	CG	ARG	G	469	110.898	−128.670	126.770	1.00	111.90
ATOM	2484	CD	ARG	G	469	110.656	−127.167	126.817	1.00	111.27
ATOM	2485	NE	ARG	G	469	111.891	−126.413	127.024	1.00	110.94
ATOM	2486	CZ	ARG	G	469	112.337	−126.009	128.210	1.00	111.59
ATOM	2487	NH1	ARG	G	469	111.650	−126.282	129.311	1.00	111.63
ATOM	2488	NH2	ARG	G	469	113.474	−125.331	128.297	1.00	111.19
ATOM	2489	N	PRO	G	470	107.846	−132.080	127.196	1.00	110.32
ATOM	2490	CA	PRO	G	470	106.544	−132.757	127.180	1.00	109.56
ATOM	2491	C	PRO	G	470	105.415	−131.804	126.802	1.00	109.38
ATOM	2492	O	PRO	G	470	105.184	−130.810	127.487	1.00	109.40
ATOM	2493	CB	PRO	G	470	106.404	−133.268	128.615	1.00	108.27
ATOM	2494	CG	PRO	G	470	107.830	−133.391	129.083	1.00	109.61
ATOM	2495	CD	PRO	G	470	108.422	−132.120	128.547	1.00	110.06
ATOM	2496	N	GLY	G	471	104.716	−132.104	125.712	1.00	109.49

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	2497	CA	GLY	G	471	103.619	−131.252	125.285	1.00	109.11
ATOM	2498	C	GLY	G	471	102.315	−131.685	125.924	1.00	108.92
ATOM	2499	O	GLY	G	471	102.257	−131.939	127.126	1.00	108.60
ATOM	2500	N	GLY	G	472	101.265	−131.772	125.119	1.00	109.42
ATOM	2501	CA	GLY	G	472	99.979	−132.193	125.638	1.00	110.45
ATOM	2502	C	GLY	G	472	99.070	−131.040	126.004	1.00	111.45
ATOM	2503	O	GLY	G	472	99.502	−129.891	126.097	1.00	111.96
ATOM	2504	N	GLY	G	473	97.796	−131.351	126.209	1.00	111.01
ATOM	2505	CA	GLY	G	473	96.835	−130.322	126.562	1.00	110.43
ATOM	2506	C	GLY	G	473	95.576	−130.471	125.741	1.00	109.88
ATOM	2507	O	GLY	G	473	94.491	−130.678	126.277	1.00	109.70
ATOM	2508	N	ASP	G	474	95.730	−130.366	124.428	1.00	109.83
ATOM	2509	CA	ASP	G	474	94.608	−130.513	123.516	1.00	110.37
ATOM	2510	C	ASP	G	474	94.250	−131.993	123.454	1.00	110.43
ATOM	2511	O	ASP	G	474	95.003	−132.796	122.907	1.00	110.70
ATOM	2512	CB	ASP	G	474	94.996	−129.990	122.135	1.00	111.19
ATOM	2513	CG	ASP	G	474	93.885	−130.137	121.121	1.00	111.06
ATOM	2514	OD1	ASP	G	474	92.726	−129.834	121.465	1.00	110.92
ATOM	2515	OD2	ASP	G	474	94.180	−130.541	119.977	1.00	111.81
ATOM	2516	N	MET	G	475	93.102	−132.346	124.024	1.00	109.99
ATOM	2517	CA	MET	G	475	92.659	−133.732	124.061	1.00	108.99
ATOM	2518	C	MET	G	475	92.325	−134.343	122.706	1.00	108.30
ATOM	2519	O	MET	G	475	91.989	−135.524	122.634	1.00	108.27
ATOM	2520	CB	MET	G	475	91.454	−133.873	124.992	1.00	110.06
ATOM	2521	CG	MET	G	475	91.742	−133.498	126.443	1.00	110.69
ATOM	2522	SD	MET	G	475	93.014	−134.548	127.161	1.00	111.79
ATOM	2523	CE	MET	G	475	93.387	−133.671	128.688	1.00	111.72
ATOM	2524	N	ARG	G	476	92.409	−133.560	121.633	1.00	107.84
ATOM	2525	CA	ARG	G	476	92.113	−134.093	120.302	1.00	107.39
ATOM	2526	C	ARG	G	476	93.218	−135.060	119.904	1.00	105.79
ATOM	2527	O	ARG	G	476	92.979	−136.056	119.224	1.00	105.68
ATOM	2528	CB	ARG	G	476	92.034	−132.961	119.271	1.00	108.90
ATOM	2529	CG	ARG	G	476	90.927	−131.951	119.512	1.00	110.95
ATOM	2530	CD	ARG	G	476	91.060	−130.754	118.578	1.00	112.58
ATOM	2531	NE	ARG	G	476	90.086	−129.707	118.883	1.00	114.24
ATOM	2532	CZ	ARG	G	476	90.079	−128.499	118.323	1.00	115.25
ATOM	2533	NH1	ARG	G	476	90.997	−128.170	117.422	1.00	114.91
ATOM	2534	NH2	ARG	G	476	89.151	−127.616	118.668	1.00	115.36
ATOM	2535	N	ASP	G	477	94.430	−134.748	120.345	1.00	103.73
ATOM	2536	CA	ASP	G	477	95.599	−135.558	120.051	1.00	101.54
ATOM	2537	C	ASP	G	477	95.552	−136.903	120.752	1.00	99.60
ATOM	2538	O	ASP	G	477	96.155	−137.864	120.286	1.00	98.87
ATOM	2539	CB	ASP	G	477	96.863	−134.813	120.473	1.00	103.36
ATOM	2540	CG	ASP	G	477	96.918	−133.399	119.918	1.00	105.17
ATOM	2541	OD1	ASP	G	477	96.905	−133.252	118.680	1.00	105.96
ATOM	2542	OD2	ASP	G	477	96.965	−132.441	120.720	1.00	106.74
ATOM	2543	N	ASN	G	478	94.844	−136.972	121.875	1.00	98.58
ATOM	2544	CA	ASN	G	478	94.741	−138.220	122.628	1.00	98.61
ATOM	2545	C	ASN	G	478	93.974	−139.286	121.862	1.00	99.30
ATOM	2546	O	ASN	G	478	94.303	−140.468	121.926	1.00	99.94
ATOM	2547	CB	ASN	G	478	94.058	−137.984	123.977	1.00	97.49
ATOM	2548	CG	ASN	G	478	94.911	−137.180	124.928	1.00	96.81
ATOM	2549	OD1	ASN	G	478	95.228	−136.022	124.666	1.00	95.84
ATOM	2550	ND2	ASN	G	478	95.289	−137.792	126.044	1.00	97.25
ATOM	2551	N	TRP	G	479	92.945	−138.861	121.141	1.00	99.87
ATOM	2552	CA	TRP	G	479	92.131	−139.788	120.370	1.00	100.66
ATOM	2553	C	TRP	G	479	92.738	−139.936	118.980	1.00	102.34
ATOM	2554	O	TRP	G	479	92.442	−140.887	118.259	1.00	102.87
ATOM	2555	CB	TRP	G	479	90.692	−139.267	120.263	1.00	98.97
ATOM	2556	CG	TRP	G	479	90.253	−138.426	121.434	1.00	96.33
ATOM	2557	CD1	TRP	G	479	89.768	−137.150	121.384	1.00	94.67
ATOM	2558	CD2	TRP	G	479	90.275	−138.791	122.823	1.00	94.42
ATOM	2559	NE1	TRP	G	479	89.491	−136.696	122.651	1.00	92.78
ATOM	2560	CE2	TRP	G	479	89.795	−137.680	123.553	1.00	92.98
ATOM	2561	CE3	TRP	G	479	90.660	−139.944	123.520	1.00	93.84
ATOM	2562	CZ2	TRP	G	479	89.681	−137.691	124.948	1.00	92.68
ATOM	2563	CZ3	TRP	G	479	90.547	−139.954	124.910	1.00	93.85
ATOM	2564	CH2	TRP	G	479	90.063	−138.831	125.606	1.00	93.88
ATOM	2565	N	ARG	G	480	93.588	−138.984	118.607	1.00	103.86
ATOM	2566	CA	ARG	G	480	94.246	−139.015	117.304	1.00	105.08
ATOM	2567	C	ARG	G	480	95.281	−140.125	117.271	1.00	105.26
ATOM	2568	O	ARG	G	480	95.594	−140.668	116.215	1.00	105.84
ATOM	2569	CB	ARG	G	480	94.922	−137.670	117.013	1.00	106.56
ATOM	2570	CG	ARG	G	480	94.125	−136.768	116.090	1.00	107.60
ATOM	2571	CD	ARG	G	480	94.632	−135.333	116.100	1.00	109.95
ATOM	2572	NE	ARG	G	480	93.740	−134.452	115.346	1.00	114.38
ATOM	2573	CZ	ARG	G	480	93.766	−133.122	115.392	1.00	117.10
ATOM	2574	NH1	ARG	G	480	94.645	−132.492	116.162	1.00	118.14

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	2575	NH2	ARG	G	480	92.901	−132.421	114.671	1.00	119.32
ATOM	2576	N	SER	G	481	95.807	−140.461	118.440	1.00	105.09
ATOM	2577	CA	SER	G	481	96.810	−141.506	118.545	1.00	105.78
ATOM	2578	C	SER	G	481	96.169	−142.872	118.346	1.00	106.98
ATOM	2579	O	SER	G	481	96.853	−143.854	118.069	1.00	107.51
ATOM	2580	CB	SER	G	481	97.483	−141.448	119.918	1.00	105.86
ATOM	2581	OG	SER	G	481	96.531	−141.636	120.949	1.00	102.63
ATOM	2582	N	GLU	G	482	94.850	−142.925	118.487	1.00	108.44
ATOM	2583	CA	GLU	G	482	94.112	−144.173	118.341	1.00	110.31
ATOM	2584	C	GLU	G	482	93.359	−144.249	117.016	1.00	111.16
ATOM	2585	O	GLU	G	482	93.213	−145.324	116.438	1.00	111.61
ATOM	2586	CB	GLU	G	482	93.123	−144.327	119.501	1.00	110.81
ATOM	2587	CG	GLU	G	482	93.759	−144.254	120.883	1.00	110.72
ATOM	2588	CD	GLU	G	482	94.577	−145.485	121.225	1.00	110.51
ATOM	2589	OE1	GLU	G	482	93.977	−146.563	121.425	1.00	109.50
ATOM	2590	OE2	GLU	G	482	95.819	−145.375	121.292	1.00	110.56
ATOM	2591	N	LEU	G	483	92.883	−143.103	116.540	1.00	111.84
ATOM	2592	CA	LEU	G	483	92.130	−143.046	115.294	1.00	112.60
ATOM	2593	C	LEU	G	483	92.979	−142.608	114.107	1.00	113.68
ATOM	2594	O	LEU	G	483	92.449	−142.122	113.108	1.00	114.27
ATOM	2595	CB	LEU	G	483	90.949	−142.083	115.440	1.00	112.17
ATOM	2596	CG	LEU	G	483	89.872	−142.442	116.469	1.00	111.13
ATOM	2597	CD1	LEU	G	483	88.927	−141.266	116.650	1.00	110.76
ATOM	2598	CD2	LEU	G	483	89.115	−143.677	116.003	1.00	111.73
ATOM	2599	N	TYR	G	484	94.292	−142.782	114.206	1.00	114.79
ATOM	2600	CA	TYR	G	484	95.186	−142.383	113.125	1.00	115.54
ATOM	2601	C	TYR	G	484	95.019	−143.284	111.912	1.00	115.88
ATOM	2602	O	TYR	G	484	95.102	−142.827	110.774	1.00	115.90
ATOM	2603	CB	TYR	G	484	96.644	−142.409	113.602	1.00	115.90
ATOM	2604	CG	TYR	G	484	97.250	−143.791	113.733	1.00	116.80
ATOM	2605	CD1	TYR	G	484	98.038	−144.328	112.714	1.00	116.77
ATOM	2606	CD2	TYR	G	484	97.042	−144.560	114.878	1.00	118.01
ATOM	2607	CE1	TYR	G	484	98.608	−145.597	112.836	1.00	117.84
ATOM	2608	CE2	TYR	G	484	97.606	−145.828	115.008	1.00	118.60
ATOM	2609	CZ	TYR	G	484	98.388	−146.339	113.985	1.00	118.39
ATOM	2610	OH	TYR	G	484	98.956	−147.587	114.115	1.00	118.31
ATOM	2611	N	LYS	G	485	94.780	−144.566	112.160	1.00	116.57
ATOM	2612	CA	LYS	G	485	94.606	−145.525	111.082	1.00	117.94
ATOM	2613	C	LYS	G	485	93.136	−145.765	110.752	1.00	119.33
ATOM	2614	O	LYS	G	485	92.749	−146.883	110.413	1.00	119.55
ATOM	2615	CB	LYS	G	485	95.282	−146.851	111.451	1.00	116.62
ATOM	2616	CG	LYS	G	485	94.855	−147.425	112.794	1.00	114.79
ATOM	2617	CD	LYS	G	485	95.577	−148.736	113.075	1.00	113.85
ATOM	2618	CE	LYS	G	485	95.207	−149.299	114.438	1.00	112.32
ATOM	2619	NZ	LYS	G	485	95.894	−150.593	114.708	1.00	112.53
ATOM	2620	N	TYR	G	486	92.321	−144.718	110.849	1.00	121.24
ATOM	2621	CA	TYR	G	486	90.895	−144.831	110.549	1.00	123.65
ATOM	2622	C	TYR	G	486	90.356	−143.638	109.763	1.00	125.80
ATOM	2623	O	TYR	G	486	90.761	−142.499	109.986	1.00	126.52
ATOM	2624	CB	TYR	G	486	90.077	−144.979	111.836	1.00	122.26
ATOM	2625	CG	TYR	G	486	90.279	−146.286	112.559	1.00	120.89
ATOM	2626	CD1	TYR	G	486	91.272	−146.426	113.527	1.00	120.39
ATOM	2627	CD2	TYR	G	486	89.478	−147.389	112.271	1.00	120.13
ATOM	2628	CE1	TYR	G	486	91.461	−147.636	114.192	1.00	119.39
ATOM	2629	CE2	TYR	G	486	89.660	−148.600	112.927	1.00	119.78
ATOM	2630	CZ	TYR	G	486	90.651	−148.717	113.885	1.00	119.20
ATOM	2631	OH	TYR	G	486	90.829	−149.916	114.531	1.00	118.81
ATOM	2632	N	LYS	G	487	89.433	−143.912	108.848	1.00	127.78
ATOM	2633	CA	LYS	G	487	88.820	−142.869	108.041	1.00	129.98
ATOM	2634	C	LYS	G	487	87.421	−143.315	107.641	1.00	131.14
ATOM	2635	O	LYS	G	487	87.261	−144.328	106.959	1.00	131.65
ATOM	2636	CB	LYS	G	487	89.660	−142.592	106.786	1.00	130.89
ATOM	2637	CG	LYS	G	487	89.250	−141.325	106.044	1.00	132.86
ATOM	2638	CD	LYS	G	487	90.086	−141.091	104.791	1.00	134.47
ATOM	2639	CE	LYS	G	487	89.712	−139.769	104.131	1.00	134.86
ATOM	2640	NZ	LYS	G	487	90.540	−139.468	102.931	1.00	133.70
ATOM	2641	N	VAL	G	488	86.408	−142.571	108.072	1.00	132.54
ATOM	2642	CA	VAL	G	488	85.031	−142.915	107.737	1.00	134.39
ATOM	2643	C	VAL	G	488	84.808	−142.655	106.245	1.00	135.42
ATOM	2644	O	VAL	G	488	85.382	−141.719	105.682	1.00	135.33
ATOM	2645	CB	VAL	G	488	84.047	−142.072	108.571	1.00	134.46
ATOM	2646	CG1	VAL	G	488	84.146	−140.608	108.170	1.00	134.65
ATOM	2647	CG2	VAL	G	488	82.638	−142.599	108.401	1.00	134.22
ATOM	2648	N	VAL	G	489	83.982	−143.470	105.600	1.00	137.04
ATOM	2649	CA	VAL	G	489	83.762	−143.293	104.173	1.00	139.05
ATOM	2650	C	VAL	G	489	82.330	−143.585	103.707	1.00	140.08
ATOM	2651	O	VAL	G	489	81.606	−144.357	104.338	1.00	140.02
ATOM	2652	CB	VAL	G	489	84.732	−144.207	103.383	1.00	139.34

TABLE 2-continued

The structural coordinates of an exemplary gp120 with an extended V3 loop

ATOM	2653	CG1	VAL	G	489	83.998	−145.432	102.860	1.00	140.18
ATOM	2654	CG2	VAL	G	489	85.385	−143.422	102.267	1.00	139.74
ATOM	2655	N	LYS	G	490	81.934	−142.966	102.597	1.00	142.79
ATOM	2656	CA	LYS	G	490	80.607	−143.179	102.032	1.00	145.45
ATOM	2657	C	LYS	G	490	80.669	−144.502	101.281	1.00	147.18
ATOM	2658	O	LYS	G	490	81.655	−144.786	100.598	1.00	146.18
ATOM	2659	CB	LYS	G	490	80.247	−142.036	101.070	1.00	145.83
ATOM	2660	CG	LYS	G	490	78.752	−141.852	100.807	1.00	146.99
ATOM	2661	CD	LYS	G	490	78.501	−140.629	99.928	1.00	148.09
ATOM	2662	CE	LYS	G	490	77.034	−140.213	99.934	1.00	148.60
ATOM	2663	NZ	LYS	G	490	76.795	−138.971	99.143	1.00	149.62
ATOM	2664	N	ILE	G	491	79.626	−145.312	101.399	1.00	149.88
ATOM	2665	CA	ILE	G	491	79.617	−146.604	100.731	1.00	153.14
ATOM	2666	C	ILE	G	491	79.546	−146.484	99.202	1.00	154.50
ATOM	2667	O	ILE	G	491	78.688	−147.084	98.550	1.00	154.54
ATOM	2668	CB	ILE	G	491	78.451	−147.475	101.262	1.00	153.49
ATOM	2669	CG1	ILE	G	491	78.722	−148.946	100.955	1.00	154.55
ATOM	2670	CG2	ILE	G	491	77.126	−147.000	100.685	1.00	153.61
ATOM	2671	CD1	ILE	G	491	79.857	−149.529	101.778	1.00	154.67
ATOM	2672	N	GLU	G	492	80.465	−145.699	98.645	1.00	156.47
ATOM	2673	CA	GLU	G	492	80.561	−145.474	97.201	1.00	158.38
ATOM	2674	C	GLU	G	492	81.994	−145.101	96.827	1.00	159.02
ATOM	2675	O	GLU	G	492	82.890	−145.919	97.028	1.00	158.59
ATOM	2676	CB	GLU	G	492	79.624	−144.345	96.762	1.00	159.61
ATOM	2677	CG	GLU	G	492	78.521	−144.781	95.808	1.00	162.25
ATOM	2678	CD	GLU	G	492	77.654	−143.621	95.352	1.00	162.67
ATOM	2679	OE1	GLU	G	492	78.173	−142.729	94.645	1.00	163.05
ATOM	2680	OE2	GLU	G	492	76.455	−143.599	95.704	1.00	162.15
ATOM	2681	OXT	GLU	G	492	82.208	−143.994	96.336	1.00	158.19
TER	2682		GLU	G	492					
END										

The present disclosure also provides for a machine-readable data storage medium which comprises a data storage material encoded with machine readable data defined by the structure coordinates of a stabilized gp120 polypeptide or gp120 polypeptide with an extended V3 loop as define in Table 1 or Table 2 respectively, or a subset thereof, such as at least about 5, such at least about 10, at least about 20, at least about 30, at least at least about 40, at least about 50, at least about 60, at least about 70, at least about 80, at least about 90, at least about 100, at least about 150, at least about 200, at least about 250, at least about 300, at least about 350, at least about 400, at least about 450, at least about 500 or more atoms of the structure, such as defined by the coordinates of Table 1 or Table 2.

Those of skill in the art will understand that a set of structure coordinates for a gp120 polypeptide, for example a stabilized gp120 polypeptide, a gp120 polypeptide with an extended V3 loop, or a portion thereof, is a relative set of points that define a shape in three dimensions. Thus, it is possible that an entirely different set of coordinates could define a similar or identical shape. Moreover, slight variations in the individual coordinates will have little effect on overall shape. The variations in coordinates discussed above may be generated because of mathematical manipulations of the structure coordinates. For example, the structure coordinates set forth in Table 1 or Table 2, or a portion thereof could be manipulated by crystallographic permutations of the structure coordinates, fractionalization of the structure coordinates; integer additions or subtractions to sets of the structure coordinates, deletion of a portion of the coordinates, inversion of the structure coordinates, or any combination of the above.

This disclosure further provides systems, such as computer systems, intended to generate structures and/or perform rational drug or compound design for an antigenic compound capable of eliciting an immune response in a subject. The system can contain one or more or all of: atomic co-ordinate data according to Table 1, Table 2, or a subset thereof and the Figures derived therefrom by homology modeling, the data defining the three-dimensional structure of a gp120 or at least one sub-domain thereof, or structure factor data for gp120, the structure factor data being derivable from the atomic co-ordinate data of Table 1 or Table 2 or a subset thereof and the Figures. This disclosure also involves computer readable media with: atomic co-ordinate data according to Table 1, Table 2 or a subset thereof and/or the Figures or derived therefrom by homology modeling, the data defining the three-dimensional structure of a gp120 or at least one sub-domain thereof; or structure factor data for a gp120, the structure factor data being derivable from the atomic co-ordinate data of Table 1, Table 2, or a subset thereof and/or the Figures. By providing such computer readable media, the atomic co-ordinate data can be routinely accessed to the gp120 or a sub-domain thereof. For example RASMOL (Sayle et al., TIBS vol. 20 (1995), 374) is a publicly available software package which allows access and analysis of atomic co-ordinate data for structural determination and/or rational drug design. Structure factor data, which are derivable from atomic co-ordinate data (see, for example, Blundell et al., in *Protein Crystallography*, Academic Press, NY, London and San Francisco (1976)), are particularly useful for calculating electron density maps, for example, difference Fourier electron density maps. Thus, there are additional uses for the computer readable media and/or computer systems and/or atomic co-ordinate data and additional reasons to provide them to users.

VIII. Identification of Immunogens

The crystals of this disclosure and particularly the atomic structure coordinates obtained from these crystals are particularly useful for identifying compounds elicit neutralizing antibodies, for example CD4BS and CD4i antibodies. The compounds identified are useful in eliciting antibodies to gp120, such as antibodies to lentivirus, such as SIV, or HIV, for example HIV-1 or HIV-2.

The crystal structure of a stabilized form of gp120 or a gp120 with the V3 loop in the extended conformation allows a novel approach for drug or compound discovery, identification, and design of compounds that mimic the antigenic surfaces of gp120 that bind neutralizing antibodies. Such compound can be useful as immunogens to illicit an immune response to HIV when administered to a subject, for example by eliciting anti-HIV antibodies, such as neutralizing antibodies, for example CD4BD or CD4i antibodies. Compounds that elicit anti-HIV antibodies are useful in diagnosis, treatment, or prevention of HIV-1 in a subject in need thereof.

The disclosure provides a computer-based method of rational drug, compound design, or identification which comprises: providing the structure of a stabilized form of gp120 (for example as defined by the coordinates or a subset of the coordinates in Table 1 and/or in the Figures) or a gp120 with the V3 loop in the extended conformation (for example as defined by the coordinates or subset of the coordinates in Table 2 and/or in the Figures); providing a structure of a candidate compound; and fitting the structure of the candidate compound to the structure of the stabilized form of gp120 (for example as defined by the coordinates or a subset of the coordinates in Table 1 and/or in the Figures) or the gp120 with the V3 loop in the extended conformation (for example as defined by the coordinates or a subset of the coordinates in Table 2 and/or in the Figures.

In certain embodiments, the coordinates of atoms of interest of the stabilized form of gp120 or the gp120 with the V3 loop in the extended conformation in the vicinity of the antigenic surface are used to model the antigenic surface to which as antibody binds, such as a neutralizing antibody, for example a CD4i or CD4BS antibody. These coordinates may be used to define a space which is then screened "in silico" against a candidate compound. Thus, the disclosure provides a computer-based method of rational drug or compound design or identification which comprises: providing the coordinates of at least two atoms of Table 1 or Table 2; providing the structure of a candidate compound; and fitting the structure of the candidate to the coordinates of at least two atoms of Table 1 or Table 2.

In practice, it may be desirable to model a sufficient number of atoms of the stabilized form of gp120 or the gp120 with the V3 loop in the extended conformation as defined by the coordinates of Table 1 or Table 2 which represent the active site or binding region. Thus, there can be provided the coordinates of at least about 5, such at least about 10, at least about 20, at least about 30, at least at least about 40, at least about 50, at least about 60, at least about 70, at least about 80, at least about 90, at least about 100, at least about 150, at least about 200, at least about 250, at least about 300, at least about 350, at least about 400, at least about 450, or at least about 500 atoms of the structure.

The methods disclosed herein can employ a sub-domain, region, or fragment of interest of the stabilized form of gp120 or the gp120 with the extended V3 loop which is in the vicinity of the antigenic surface, and providing a computer-based method for identifying or rationally designing a compound or drug, such as an immunogen which includes: providing the coordinates of at least a sub-domain, region, or fragment of the stabilized form of gp120 or the gp120 with the extended V3 loop; providing the structure of a candidate compound that mimics the antigenic surface of the gp120 with the extended V3 loop; and fitting the structure of the candidate compound to the coordinates of the stabilized form of gp120 or the gp120 with the extended V3 loop sub-domain, region, or fragment provided. A "sub-domain", "region", or "fragment" can mean at least one, for example, one, two, three, four, or more, element(s) of secondary structure of particular regions of the stabilized form of gp120 or the gp120 with the extended V3 loop gp120 with the extended V3 loop, and includes those set forth in Table 1 and Table 2.

These methods can optionally include synthesizing the candidate compound, (such as an immunogen) and/or administering the candidate compound to an animal capable of eliciting antibodies and testing whether the candidate compound elicits anti-HIV antibodies. Compounds which elicit anti-HIV antibodies are useful for diagnostic purposes, as well as for immunogenic, immunological or even vaccine compositions, as well as pharmaceutical compositions.

In some embodiments, the candidate compound is designed from the gp120 amino acid sequence, for example an amino acid sequence is assembled to provide a candidate compound, for example by synthesizing the amino acid sequence or producing a nucleic acid encoding the candidate compound.

The step of providing the structure of a candidate compound may involve selecting the candidate compound by computationally screening a database of compounds for surface similarity with an epitope on the stabilized form of gp120 or the gp120 with the extended V3 loop. For example, a 3-D descriptor for the candidate compound may be derived, the descriptor including geometric and functional constraints derived from the architecture and chemical nature of the epitope. The descriptor may then be used to interrogate the compound database, a candidate compound being a compound that has a good match to the features of the descriptor. In effect, the descriptor can be a type of virtual pharmacophore.

The determination of the three-dimensional structure of the gp120 with the extended V3 loop provides a basis for the design of new and specific compounds that are useful for eliciting an immune response. For example, from knowing the three-dimensional structure the stabilized form of gp120 or the gp120 with the extended V3 loop, computer modeling programs may be used to design or identify different molecules expected to interact with possible or confirmed active sites such as binding sites or other structural or functional features of neutralizing antibodies.

By way of example, a compound that potentially mimics the antigenic surface of the stabilized form of gp120 or the gp120 with the extended V3 loop can be examined through the use of computer modeling using a docking program such as GRAM, DOCK or AUTODOCK (see for example, Walters et al. *Drug Discovery Today,* 3(4):160-178, 1998; Dunbrack et al. *Folding and Design* 2:27-42, 1997). This procedure can include computer fitting of potential immunogens to ascertain how well the shape and the chemical structure of the potential binder will mimic the antigenic surface. Various other computer programs such as AMBER or CHARM may be used to further refine the dynamic and electrostatic characteristics of a candidate compound. Programs such as GRID (Goodford, *J. Med. Chem,* 28:849-57, 1985) may also be used to analyze the antigenic surfaces to predict immunogenic compounds. Alternatively, computer-assisted, manual examination can be used to predict immunogenic compounds from antigenic surfaces.

IX. Stabilized gp120 Polypeptides as Crystallization Tools

One problem with the formation of crystals containing wild-type gp120 is that conformationally variable molecules are not amenable to crystallization. For an ordered crystal to form the molecules forming the crystal must be essential locked in place. Molecules that are unstable or "floppy" such as wild-type gp120 must overcome large entropic (ΔS) costs to form a crystal lattice. By using conformationally stabilized

forms of gp120 this entropic cost of becoming ordered is lessened and crystals form more easily. Those skilled in the art can take advantage of this by crystallizing their complex of interest with a stabilized form of gp120. For example, stabilized forms of gp120 can be used to crystallize previously uncrystallizable broadly neutralizing antibodies. In one embodiment, the broadly neutralizing antibody does not induce conformational stabilization as measured by $-T\Delta S$ of less than 28 kcal/mol upon antibody binding to gp120. The use of broadly neutralizing antibodies is disclosed, for example, in Burton, Nature Re. 2:706-713, 2002, herein incorporated by reference. One example of how this can be accomplished is by forming complexes of a stabilized form of gp120 and the antibody of interest in the presence of CD4.

The following examples are provided to illustrate certain particular features and/or embodiments. These examples should not be construed to limit the invention to the particular features or embodiments described.

EXAMPLES

Example 1

Structure-Assisted Stabilization of gp120 in its CD4-Bound Conformation

This example describes the methods used to design stabilized forms of gp120 disclosed herein.

Thermodynamic analysis showed that the conformation of gp120 prior to CD4 binding was highly flexible (Myszka et al., *Proc Natl Acad Sci USA.* 97(16):9026-31, 2000). The CD4-bound state of gp120 consists of an inner domain (containing the N and C termini), an outer domain, and a four-stranded bridging sheet minidomain. Two-thirds of the CD4 contact surface is with the outer domain, the remaining one-third with the bridging sheet. In the unliganded state, the inner domain is radically altered, with most of its secondary structural elements repositioned. The bridging sheet is pulled apart with the two β-hairpins of the sheet separated by 20 Å. The outer domain, by contrast, remains virtually unchanged.

An initial series of mutants was constructed and analyzed. Initial antigenic analysis suggested that a single mutation, 375 S to W, was able to partially stabilize gp120 in the CD4-bound state. Thermodynamic analysis (ITC) confirmed this result, showing that the entropy ($-T\Delta S$) of gp120 binding to CD4 had reduced from 40 kcal/mol to roughly 25 kcal/mol (Xiang et al., *J Virol.* 76(19):9888-99, 2002).

To further reduce the entropy of CD4 binding to a range typical of antibody recognition (5-10 kcal/mol), precise characterization was used to confirm the mutational stabilization of conformation including: (1) crystallographic determination of the gp120 mutant structure (2) isothermotitration calorimetric analysis of the entropy of CD4 binding, and (3) precise surface-plasmon resonance analysis of the on/off rates of antibodies to the modified gp120 glycoproteins. This design cycle is shown in FIG. **1**. Initial isothermotitration calorimetry demonstrated that cavity-filling mutants, such as 375 S to W, did not significantly reduce the entropy of CD4 gp120 binding in the context of core HXBc2.

Additional cavity-filling mutations and five different disulfides were modeled. The cavity-filling mutants increased hydrophobic interactions at domain interfaces. The disulfides either tied together the inner domain, outer domain and bridging sheet, or were internal to the bridging sheet. Crystallographic analysis on five of these disulfides showed that four of them formed disulfide bonds. Two of these showed minimal perturbation in structure: 96-275 which tied together the inner and outer domain, 109-428 which tied together the bridging sheet and outer domain. The 231-267 disulfide, which tied together the inner domain and outer domain and the 123-431 disulfide, which tied together two strands of the bridging sheet, both showed local perturbations of structure. The potential disulfide formed by mutating 231 to C and 268 to C did not form (FIG. **2**). The recently solved crystal structure of the unliganded gp120 core from SIV (Chen et al, Structure, 13(2):197-211, 2005) allowed the position of each disulfide to be modeled in the unliganded structure (FIG. **3**). This mapping showed that even a single disulfide would be incompatible with the conformation of the unliganded gp120 seen in the SIV crystal structure (Table 3).

TABLE 3

Relative disulfide distances in the CD4-bound conformation and in the unliganded SIV conformation.

Category	HIV Mutation	SIV Equivalent	Cα-Cα Distance (Å)	Cα-Cα Distance (Å)
Category	HIV Mutation	SIV Equivalent	HIV	SIV
S-S	96-275	78-290	6.4	21.9
S-S	109-428	91-441	6.1	16.2
S-S	123-431	105-444	4.4	23.5
S-S	231-267	245-282	6.0	16.8
Cavity	257/375	271/391	5.2	5.6

In the core context, each single inter-domain disulfide reduced the entropy of CD4 interaction by roughly 10 kcal/mol, as measured by isothermotitration calorimetry (ITC). Combinations of disulfides were tested. Two disulfide combinations showed similar antigenic phenotypes suggesting a partially stabilized gp120 conformation; ITC analysis for several of the different two disulfide combinations showed the entropy of CD4 interaction was reduced by roughly 20 kcal/mol. Combinations of three and four disulfides were also tested, although most of these only expressed poorly, perhaps due to complications of folding so many cysteines into the correct disulfide bonds. Removal of additional core disulfide (such as the second conserved disulfide in the V1/V2 region) and stabilization of the V3 region may enhance folding. A summary of the qualitative Biacore and ITC results for 17 mutants is shown in Table 4.

TABLE 4

Qualitative BIACORE on Supernatant and ITC results

Mutant	Mutant location							CD4/CD4i			CD4BS							DSC/T_M
Name	C2	C3	C1S1	S2	S3	S4	S5	CD4	17B	M6	b12	F105	F91	15e	m14	m18	SS	folding	° C.
WT core*								A	A	A	AA	AA	AA	AA	AA	AA	0	FFFF	50.6
2a*	x							AAA	AA	AA	AA	N	N	A/N	A/N	AA	0	FFFF	50.6

TABLE 4-continued

Qualitative BIACORE on Supernatant and ITC results

Mutant	Mutant location							CD4/CD4i			CD4BS							DSC/T_M
Name	C2	C3	C1S1	S2	S3	S4	S5	CD4	17B	M6	b12	F105	F91	15e	m14	m18	SS	folding	° C.
4-0*	x						x	AAA	AA	AA	AA	N	N	A/N	A/N	AA	0	FFFF	55.7
4a*	x			x				A	A	nd	A/N	N	N	N	N	A	1	FFF	53.8
4b*	x					x		A	A	nd	AA	N	A/N	N	N	AA	1	FFF	56.4
4c*	x				X			A	A	nd	A	N	N	N	N	AA	1	FFF	
5mut	x		x					A	A	nd	A	N	N	N	N	AA	1	FFF	
6a*	x	x	x					A	A	nd	AA	N	A	N	N	AA	1	FFF	
6b	x			x		x		AA	A	nd	N	N	N	N	N	N	2	FFF	59.0
8a	x	x	x			x		AA	A	nd	A	N	N	N	N	AA	2	F	
8b*	x	x	x	x				AA	A	nd	A	N	N	N	N	A/N	2	FF	
9a	x	x		x	X	x		A	N	N	A/N	N	N	N	N	N	3	F/N	
8c	x			x	X	x		A	A	A	A/N	N	N	N	N	N	3	F/N	
10a	x	x	x	x		x		N	N	nd	N	N	N	N	N	N	3	N	
9b	x		x		X	x		A	A	A	A/N	N	N	N	N	AA	3	F/N	
10c	x	x	x		X	x		A	N	N	A/N	N	N	N	N	AA	3	F/N	
9c*	x		x	x	X			AA	AA	AAA	A	N	N	N	N	A/N	3	F	
10b	x	x	x	x	X			A	A	A/N	A	N	N	N	N	A/N	3	F/N	
11a	x		x	x	X	x		A	A	A	A	N	N	N	N	N	4	F/N	

Note:
Cavity-filling mutants: C1: M95W, C2: T257S/S375W; C3: A433M;
Disulfide bond mutants: S1: W96C/V275C; S2: I109C/Q428C; S3: T123C/G431C; S4: K231C/E267C; S5: K231C/E268C

Qualitative Biacore analysis and ITC of conformationally stabilized mutants. Biacore analyses were carried out on transfected cell supernatants or with purified protein at 10 ug/ml. Yellow rows represent mutants with structures determined by X-ray crystallography. "A" indicates binding, "F" indicates folding, and "N" indicates no binding or folding. The mutants are indicated with the wildtype residue and position followed by the substituted residue as follows, C1:M95W; C2:T275S/S375W; C3:A433M; S1:W96C/V275C; S2:I109C/Q428C; S3:T123C/G431C; S4K231C/E267C, for example A433M means that a methionine has been substituted for an alanine to create a C3 mutant protein.

Quantitative surface-plasmon resonance characterization of the binding of the various mutants to CD4, to 17b in the absence of CD4 and to 17b in the presence of CD4 allowed the degree of conformational stabilization to be assessed (Table 5).

TABLE 5

Quantitative Surface-Plasmon Resonance Characterization of Mutant gp120 Kinetic Parameters.

	CD4			17b without CD4			17b with CD4			CD4
Mutant	on	off	KD	on	off	KD	on	off	KD	Induction
WT core	4.95E+04	1.46E−03	2.95E−08	9.81E+03	4.33E−03	4.41E−07	7.84E+05	2.07E−03	2.64E−09	7.99E+01
2a	1.19E+05	1.78E−04	1.49E−09	1.03E+05	1.66E−02	1.61E−07	1.62E+06	9.98E−03	6.14E−09	1.57E+01
4-0	1.10E+05	1.39E−04	1.26E−09	1.54E+05	0.0196	1.28E−07	1.76E+06	0.0101	5.73E−09	1.14E+01
4a	1.23E+05	2.81E−04	2.28E−09	3.75E+05	0.0212	5.66E−08	2.51E+06	0.014	5.56E−09	6.69E+00
4b	1.08E+05	1.62E−04	1.50E−09	1.06E+05	0.0192	1.81E−07	1.48E+06	0.01	6.76E−09	1.40E+01
4c	1.07E+05	1.20E−04	1.12E−09	2.98E+05	0.0114	3.82E−08	2.05E+06	9.14E−03	4.45E−09	6.88E+00
5mut	3.08E+04	4.14E−04	1.35E−08	7.06E+04	0.0168	2.37E−07	1.31E+06	1.02E−02	7.78E−09	1.86E+01
6a	6.56E+04	4.47E−04	6.82E−09	8.94E+04	8.42E−03	9.41E−08	2.83E+05	7.46E−03	2.64E−08	3.17E+00
6b	7.89E+04	3.08E−04	3.91E−09	2.08E+05	0.0225	1.08E−07	9.27E+05	0.0126	1.36E−08	4.46E+00
8a	141000	0.00062	4.4E−09	354000	0.00712	2.01E−08	240000	0.0106	4.42E−08	0.677966
8b	83000	0.000484	5.83E−09	135000	0.00403	3.01E−08	310000	0.0151	4.88E−08	2.296296
9c	6.78E+04	1.45E−04	2.14E−09	1.04E+06	0.011	1.05E−08	1.28E+06	8.53E−03	6.69E−09	1.23E+00

CD4-on rate did not change much, indicating that initial CD4 occurs without conformational stabilization. The off-rate did decrease relative to wild-type, however, indicating that once CD4 bound, the conformational change was able to lock CD4 into place. A very different effect was seen with the CD4i antibody 17b. With 17b, conformational stabilization greatly increased the "on-rate" of binding, with little effect on the off-rate. This indicated that 17b cannot bind to its site, without the conformational change induced by CD4. In contrast, the initial binding even of CD4 must occur without the conformational change.

Surface-plasmon resonance (SPR) experiments were performed on a Biacore biosensor system at 25° C. Antibody (17b or m6 for the CD4i antibodies; F105, b12, 1.5e, etc. for CD4BS antibodies; b3, b3, b11 etc. for Fab fragments of CD4BS antibodies; and 2-domain CD4 for CD4) were immobilized on research grade CM5 sensor chips using the recommended standard amine coupling. Binding experiments were carried out in HBSP buffer (10 mM HEPES, pH 7.4, 150 mM NaCl and 0.005% surfactant P-20).

During the association phase, gp120 were passed over the buffer-equilibrated chip surface at a rate of 30 ul/min. After the association phase, bound analytes were allowed to dissociate for 5 min. The chip surface was then regenerated by two 25 ul injections of 10 mM Glycine/HCl (pH 3.0) at a flow rate of 50 ul/min. Association and dissociation values were calculated by numerical integration and global fitting to a 1:1 interaction model using BIAevaluation 3.0 software (Biacore, Inc.)

Example 2

Atomic Level Structure Determination of gp120

This example describes the methods used to obtain crystals of a gp120 with an extended V3 loop.

Variational Crystallization and Robotic Screening

To increase the probability of obtaining crystals suitable for X-ray structural analysis, 13 different complexes of HIV-1 envelope glycoprotein gp120 core with intact V3 were prepared and screened for crystallization. To ensure that gp120 was in its coreceptor binding conformation, all complexes contained CD4 (2-domain).

1) Protein Production, Purification, and Complex Preparation

Constructs of core+V3 gp120 from clade B HIV-1 isolates, YU2, JR-FL, and HXBc2, were prepared as previously described (Wu et al., *Nature* 384:179, 1996; Grundner et al., *Virology* 330:233, 2004). Truncations of the N-terminus, C-terminus, and substitution of the tripeptide GAG for the V1/V2 region were identical to those previously described (Grundner et al., *Virology* 330:233, 2004). Wild-type isolates were used for YU2 and HXBc2. For JR-FL, a functional 2-glycan deletion variant was used with mutations, 301N/Q and 388T/A (Koch et al., *Virology* 313:387, 2003). This CCR5-using JR-FL variant was more susceptible to neutralization by CD4-binding site antibodies, but not to CD4-induced antibodies (Koch et al., *Virology* 313: 387, 2003. Constructs were expressed in *Drosophila* Schneider 2 cells under an inducible metallothionein promoter. The 2-domain CD4 (d1d2), antigen-binding fragments (Fabs) and single-chain variable fragments (scFv) of CD4-induced (CD4i) antibodies, 17b, 48d, 412d, m6, m9 and X5, were prepared as previously described (Ryu et al., *Nature* 348:419, 1990; Kwong et al., *J. Biol. Chem.* 274:4115, 1999; Huang et al., *Proc. Natl. Acad. Sci. USA* 101:2706, 2004; Zhang et al., *J. Mol. Biol.* 335:209, 2004; Moulard et al., *Proc. Natl. Acad. Sci. USA* 99:6913, 2002). Preparations of gp120 complexes followed procedures that were essentially the same as previously described (Kwong et al., *J. Biol. Chem.* 274:4115, 1999). Briefly, glycans were removed by digestion with endoglycosidases H and D to leave only the protein proximal N-acetylglucosamine and 1,6 fucose residues. The 2-domain CD4 was added, the binary complexes passed through a concanavalin A column to remove any gp120 proteins with uncleaved N-linked glycan, and the complexes further purified by gel filtration (Hiload 26/60 Superdex S200 prep grad, Amersham). Fab or scFv of CD4-induced (CD4i) antibodies were added and the ternary complexes purified by Superdex S200 chromatography. Purified complexes in 0.35 M NaCl, 2.5 mM Tris pH 7.0, 0.02% NaN3 were concentrated to 5-8 mg/ml. The following complexes were made (specified by strain of core+V3 gp120:soluble CD4 domain fragment: CD4-induced antibody type and fragment):

JR-FL:d1d2:17b Fab
JR-FL:d1d2:48d Fab
JR-FL:d1d2:412d Fab
JR-FL:d1d2:X5 Fab
JR-FL:d1d2
YU2:d1d2:48d Fab
YU2:d1d2:X5 Fab
HXBc2:d1d2:17b Fab
HXBc2:d1d2:48d Fab
HXBc2:d1d2:412d Fab
HXBc2:d1d2:X5 Fab
HXBc2:d1d2:m6 scFv
HXBc2:d1d2:m9 scFv

2) Robotic Screening of Crystallization Conditions

The gp120 complexes were screened robotically using vapor-diffusion sitting droplets composed of 50 nl protein combined with 50 nl crystallization solution (Lesley et al., *Proc. Natl. Acad. Sci. USA* 99:11664, 2002). 576 different commercially available crystallization solutions were used in each screen. JRFL complexes were screened with Hampton Research Screen I/II, Emerald Wizard Screen I/II, Emerald Wizard Cryo Screen I/II, Hampton Crystal Screen Cryo, Hampton PEG/Ion Screen, Hampton Grid Screens (ammonium sulfate, PEG 6000, MPD, and PEG/LiCl), and Syrrx Polymer Screen. YU2 and HXBc2 complexes were screened in the same manner except that the Hampton Research Index screen was substituted for the Emerald Wizard Cryo Screens. Pictures of crystallization drops were taken at 0, 1, 3, 7, 14, and 21 days after set-up, and the images inspected visually for protein crystals.

3) Crystallization Optimization

Initial crystals observed from robotic screens were reproduced and optimized manually using vapor-diffusion hanging droplets. A total of eight different crystal forms were grown to sizes suitable for testing diffraction quality. While most of the crystals diffracted to at best only 6-10 Å, one crystal consisting of JR-FL:d1d2:X5 Fab diffracted to at least 5 Å and was chosen for further optimization. Larger single crystals were produced by macroseeding (Thaller et al., *J. Mol. Biol.* 147: 465, 1981): 1.5 μl of 5 mg/ml JR-FL:d1d2:X5 Fab was mixed with an equal volume of 1.3 M ammonium sulfate and placed over a 0.5 ml reservoir of 1.3 M ammonium sulfate; after 30 minutes, a single crystal was transferred directly to the droplet. Macroseeded crystals grew to 0.1×0.1×0.2 mm in 5-7 days.

Example 3

Structure Determination of gp120 with an Extended V3 Loop

This example describes the methods used to determine the structure of a gp120 with an extended loop to atomic resolution.

Data Collection

Crystals were dehydrated (Heras et al., *Structure* 11:139, 2003) over 3 M ammonium sulfate reservoirs for 2-3 days. Dehydrated crystals were cross-linked over 20 μl of 1.5% glutaraldehyde for 1.5 hr using the procedure of Lusty (Lusty, *J. Appl. Cryst.* 32:106, 1999), transferred to a cryoprotectant solution containing 2 M ammonium sulfate, 60% (w/v) xylitol, 10% (w/v) erythritol and 5% (v/v) ethylene glycol for 1-2 minutes, covered with paratone-N, loop mounted, and flash-cooled to 100° K. for data collection. X-ray data were collected at a wavelength of 1.00 Å, using the intense 3rd generation undulator beam-line (SER-CAT) at the Advanced Photon Source, and processed and reduced with HKL2000 (Otwinowski and Minor, *Methods Enymol.* 276:307, 1997). The crystals were found to belong to space group P622 and to contain one complex per asymmetric unit. The diffraction was anisotropic, with stronger diffraction along the 6-fold axis. The crystal structure of JR-FL:d1d2:X5 Fab was solved by molecular replacement with CNS (Brunger et al., *Acta Crystallogr. D* 54:905, 1998). For gp120:CD4, a binary search model was constructed from YU2 core gp120 complexed to d1d2 as extracted from the previously determined ternary complex with 17b (pdb accession number, 1RZK) (Kwong et al., *Structure* 8:1329, 2000), with gp120 N-terminus (residues 83-86) and V4 region (residues 399-406) deleted. For X5 Fab, the structure of free X5 was used (pdb

accession number, 1RHH) (Darbha et al., *Biochemistry* 43:1410, 2004). Cross-rotation and translation search with 15-4 Å data yielded Patterson correlation coefficients of 22.3% and 31.1% for YU2core:d1d2 and X5 Fab, respectively. The combined solution gave a Patterson correlation coefficient of 51.7%. By using the programs, O (Jones et al., *Acta Crystallogr. A* 47:110, 1991) for model building and CNS (Brunger et al., *Acta Crystallogr. D*54:905, 1998) for refinement, side-chains of the initial models were corrected, and the models subjected to torsion angle simulated annealing with slow cooling. Iterative manual fittings were carried out in B-value sharpened maps (−75 $Å^2$; 2Fo-Fc) to enhance visual recognition of protein sidechain definition. Refinement in CNS, however, used unsharpened data, with strong 3 geometric constraints to maintain idealized stereochemistry. Statistics summarizing the X-ray crystallographic data and refinement are shown in Table 6.

TABLE 6

X-ray crystallographic data and refinement statistics

Data collection	
Space group	P622
Molecules per ASU	1
Wavelength, Å	1.00
Unit cell dimensions	a = b = 226.0 Å, c = 98.0 Å
Resolution, Å*	50-3.30 (3.71-3.55, 3.55-3.42, 3.42-3.30)
Completeness, %*	86.6 (91.4, 50.7, 20.9)
No. of total reflections	186,823
No. of unique reflections	19,372
Redundancy*	9.6 (5.1, 4.3, 3.1)
I/σ*	26.2 (2.3, 1.5, 1.3)
Rsym, %*, ‡	8.2 (38.8, 47.3, 50.5)
Refinement statistics (|F| > 0 σ)	
Resolution, Å	20.0-3.30
No. of reflections	19,364
Rcryst, %*, §	31.7
Rfree, %*, §, ||	34.7
Rmsd bond length, Å	0.0043#
Rmsd bond angles, °	0.978#
Luzzatti error, Å	0.64
Average B-value, Å2	125
Ramachandran plot	
Most favored, %	83.3
Additionally allowed, %	15.8
Generously allowed, %	0.8
Disallowed, %	0.1

*Values in parentheses are for the last three highest resolution shells.

‡ Rsym = Σ|I − <I>|/Σ<I>, where I is the observed intensity, and <I> is the average intensity of multiple observations of symmetry related reflections.

§ R = Σhkl||Fobs| − |Fcalc||/Σhkl|Fobs|

|| Rfree is calculated from 10% of the reflections excluded from refinement.

#The geometry was tightly restrained, as this was observed to improve the Rfree.

Model Analysis

All superpositions were performed using lsqkab in CCP4 (Collaborative Computational Project, *Acta Crystallogr. D*50:760, 1994). Molecular surface interactions were calculated using MS (Connolly, *J. Mol. Graph.* 11:139, 1993). Figures were prepared using PyMOL (DeLano Scientific, San Carlos, Calif., 2002) and GRASP (Nicholls et al, *Proteins Struct. Funct. Genet.* 11:281, 1991).

Glycan Modeling

Asn-(N-acetylglucosamine)2(mannose)3 N-linked sugar cores were modeled following procedures described previously for the HXBc2 core (Wyatt et al., *Nature* 393:705, 1998). Briefly, JR-FL core with V3 and the HXBc2 core with modeled glycan were superimposed. Conserved sites of Nlinked glycan were transferred, and other sites were built manually, including glycans at 301 and 386. The core was fixed and the Asn and attached glycan were subjected to molecular dynamics.

Sequence Analysis

Analyses were carried out with only sequences with complete V3, limited to one sequence per individual, extracted from the Los Alamos HIV sequence database (www.hiv.lanl.gov/content/hiv-db.) for all M group sequences that had coreceptor usage specified as either CCR5 or CXCR4. The B clade subset of the M group had the most coreceptor usage information for a single clade, and so it was also analyzed separately. Alignments were made from constant to variable regions, with the β-turn (GPGR analog) of the tip forced into alignment. The Shannon entropy (Shannon, *Bell System Tech.* 27:379, 1948) was calculated for each site, treating gaps inserted to maintain alignment and distinct amino acids as characters, and statistical analysis of the variation at each site comparing R5 and X4 viruses was performed by using a Monte Carlo randomization of the two data sets (Korber et al., *J. Virol.* 68:7467, 1994), with a Bonferroni correction to contend with multiple tests. An entropy score is actually a simple measure of the information content of a data set: when considered in this context, as a measure of amino acid diversity in the column of an alignment, it has the virtue of capturing both the range and distribution of observed amino acids. Zero indicates absolute conservation, and a score of 4.4 indicates complete randomness.

Example 4

This example describes the analysis of the structural details of a gp120 with an extended loop.

The third variable region (V3) of the HIV-1 gp120 envelope glycoprotein is immunodominant and contains features essential for coreceptor binding. Disclosed herein is the structure of the V3 loop in the context of an HIV-1 gp120 core complexed to the CD4 receptor and to the X5 antibody at 3.5 angstrom resolution. Binding of gp120 to cell-surface CD4 positions V3 so that its coreceptor-binding tip protrudes 30 angstroms from the core toward the target cell membrane. The extended nature and antibody accessibility of V3 explain its immunodominance. Snapshots of the gp120 entry mechanism have been visualized through crystal structures of unliganded and CD4-bound states (Chen et al., *Nature* 433:834, 2005; Kwong et al., *Nature* 393:648, 1998). Prior to this disclosure an essential component of the coreceptor binding site, the third variable region (V3), was been absent from structural characterizations of the gp120 core. The structure of V3 in the context of core gp120 bound to CD4, described herein, reveals the entire coreceptor binding site. The V3 appears to act as a molecular hook, not only for snaring coreceptor but also for modulating subunit associations within the viral spike. Its extended nature is compatible with the elicitation of an immunodominant antibody response and the generation of broadly neutralizing antibodies to V3 epitopes.

The extreme glycosylation and conformational flexibility of gp120 inhibit crystallization. Variational crystallization and various technologies adapted from structural genomics were used to obtain crystals suitable for x-ray structural analysis (Kwong et al., *J. Biol. Chem.* 274:4115, 1999; Stevens and Wilson, *Science* 293:519 (2001). The gp120 core with V3 from JR-FL The crystallized JR-FL was derived from a JR-FL variant with two point mutants, Asn301Gln and Thr388Ala. These mutations removed two Nlinked glycans, and the resultant virus was more sensitive to neutralization but was otherwise functional (Koch et al., *Virology* 313:387, 2003), when complexed to CD4 (two domain) and the antigen-binding fragment (Fab) of the X5 antibody (Koch et al., *Virology* 313:387, 2003), formed hexagonal crystals that dif-

fracted to approximately 3.5 Å resolution with x-rays provided by an Advanced Photon Source undulator beam line (SER-CAT) (Table 5). The structure was solved by molecular replacement and is shown in FIG. **5**.

The overall assembly of CD4, X5, and core gp120 resembled the previously determined individual structures of CD4 (Ryu et al., *Nature* 34:419, 1990; Wang et al., *Nature* 348:411, 1990) and of free X5 (Darbha et al., *Biochemistry* 43:1410, 2004) as well as the complex of core gp120 bound to CD4 (Kwong et al., *Nature* 393:648, 1998; Kwong et al., *Structure* 8:1329, 2000). For core gp120, some differences were observed in the variable loops and also at the N terminus, regions where variations in gp120 have previously been observed (Chen et al., *Nature* 433:834, 2005; Kwong et al., *Nature* 393:648, 1998; Kwong et al., *Structure* 8:1329, 2000; Huang et al., *Structure* 13:755, 2005). Structural resemblance was maintained around the base of V3, indicating that the previous truncation (Chen et al., *Nature* 433:834, 2005; Kwong et al., *Nature* 393:648, 1998; Kwong et al., *Structure* 8:1329, 2000; Huang et al., *Structure* 13:755, 2005) did not distort this region of the core. In X5, a large structural difference was observed for the third complementarity determining loop of the X5 heavy chain (CDR H3). Comparison of the refined structures of free X5 (Darbha et al., *Biochemistry* 43:1410, 2004) and bound X5 showed Ca movements of up to 17 Å, one of the largest induced fits observed for an antibody (FIG. **9**). The gp120 envelope protein is composed of inner and outer domains, named for their expected orientation in the oligomeric viral spike (Kwong et al., *Nature* 393:648, 1998). V3 emanates from neighboring staves of the stacked double barrel that makes up the outer domain; it is almost 50 Å long from the disulfide bridge at its base to its conserved tip, but is otherwise only 15 Å wide and 5 Å deep (FIG. **6**). Overall, it can be subdivided into three structural regions: a conserved base, which forms an integral portion of the core; a flexible stem, which extends away from the core; and a b-hairpin tip. In the crystal structure, the flexibility and position of the V3 tip may be influenced by a lattice contact, in which hydrogen bonds are made to the exposed backbone of the V3 b ribbon between Ile307 and Ile309. Tenuous side-chain contacts are also observed for the returning strand in the V3 stem with X5, as well as with V4 of a symmetry-related gp120 molecule, but these side-chain contacts are unlikely to influence its conformation. Features of gp120 important for coreceptor binding have been mapped by mutagenesis to two regions: (i) the V3 tip, and (ii) the gp120 core around the bridging sheet, the V3 base, and neighboring residues (Rizzuto et al., *Science* 280:1949, 1998; Rizzuto and Sodroski, *AIDS Res. Hum. Retroviruses* 16:741, 2000; Cormier et al., *J. Virol.* 75:5541, 2001; Cormier et al., *J. Virol.* 76:8953, 2002). Analysis of these two regions on this new structure indicates that they are conserved in both sequence and structure (FIGS. **10**A and **11**). The structural conservation of the V3 tip was surprising here in light of the apparent flexibility of the intervening stem, but we found the V3 tip to be strikingly similar in the context of the core, in antibody-V3 peptide complexes, and as a free peptide; such similarity is consistent with previous reports of recurring conformations for the V3 tip in antibody:peptide complexes (Stanfield et al., *Virology* 315: 159, 2003). The structure shows that conserved regions important for coreceptor binding are separated by 10 to 20 Å and by portions of the V3 stem with moderate to high sequence variation (FIG. **10**). Emerging data on the structures of the coreceptors indicate that the regions identified as being important for binding gp120—the coreceptor N terminus and the second extracellular loop—may also be spatially separated (Klco, et al., *Nat. Struct. Mol. Biol.* 12:320, 2005).

By integrating the two-site gp120 binding site on the coreceptor with the two-site coreceptor binding site that it is observe in the structure of V3 gp120 with an extended V3 loop, that the N terminus of the coreceptor reaches up and binds to the core and V3 base while the V3 tip of gp120 reaches down to interact with the second extracellular loop of the coreceptor (FIG. **7**B). Support for this model comes from several sources: (i) Biochemical studies show that the binding of CCR5 Nterminal peptides to gp120 is affected by gp120 alterations only on the core and around the base of V3 (Cormier and Dragic, *J. Virol.* 76:8953, 2002); and (ii) small-molecule inhibitors of HIV entry that bind to the second extracellular loop of the coreceptor are observed to no longer affect mutant viruses with V3 truncations. Despite general tolerance of the V3 stem to changes in sequence, there is less tolerance for insertions or deletions than in other gp120 variable loops. Superimposition of the core gp120 V3 structure on the modeled gp120 core trimer that previously obtained by optimization of quantifiable surface parameters (Kwong, et al., *J. Virol.* 74:1961, 2000) orients gp120 in the context of both cell-surface CD4 and the target cell membrane. Such a superposition projects the highly conserved Pro-Gly of the V3 tip 30 Å toward the target cell membrane (FIG. **7**A). Different coreceptors, primarily CXCR4 or CCR5, can support HIV-1 entry. Sequence analysis has defined an 11/25 rule: If the 11th or 25th positions of V3 are positively charged, viruses will use CXCR4; otherwise they use CCR5 (Resch et al., *Virology* 288:51, 2001). In addition, V3 sequences are more conserved for CCR5-using viruses (FIG. **10**). The structure of the V3 loop disclosed herein shows that positions 11 and 25 (residues 306 and 322) are within the variable stem. They each project about the same distance away from the core but are separated by a Ca distance of 17 Å (FIG. **10**). This separation suggests that positions 11 and 25 recognize different portions of the coreceptor. CD4 induces large conformational changes in gp120. Before CD4 binding, V3 may not protrude precisely as observed here for the CD4-triggered coreceptor binding state of gp120 (Sattentau and Moore, *J. Exp. Med.* 174:407, 1991; Werner and Levy, *J. Virol.* 67:2566, 1993). However, structural comparison of unliganded versus CD4-bound conformations of gp120 (Kwong et al., *Nature* 393:648, 1998; Hartley et al., *AIDS Res. Hum. Retroviruses* 21:171, 2005) reveals that the local conformation of the region of the outer domain from which V3 emanates is mostly unchanged. Thus, the extended structure of V3 that we observe here should be generally representative of V3. Immunization with gp120 or gp120/gp41 in various contexts may elicit an immune response in which HXB2CG

virtually all of the neutralizing activity is directed at V3. The conformation of crystal and nuclear magnetic resonance structures of V3-reactive antibody-peptide complexes was examined for clues to this immunodominant response (FIG. **11**). Although the conformation of V3 peptides in these antibody-peptide complexes varies somewhat, the Pro-Gly tip is more conserved. Superimposing the conserved tip in the peptides with the V3 tip in the core+V3 structure permits the V3 peptide-binding antibodies to be placed in the context of the gp120 core. The antibodies completely surround V3 (FIG. **8**). Although the accessibility of V3 may be quite different on a primary isolate in its pre-CD4 trimeric state, the extended nature of V3 as disclosed herein, when coupled to mechanisms that cloak the rest of the HIV envelope from antibody binding (Wyatt and Sodroski, *Science* 280:1884, 1998; Wyatt et al., *Nature* 393:705, 1998; Wei et al., *Nature* 422:307, 2003), is consistent with its ability to generate an immunodominant response. The attributes observed for V3 (such as, high relative surface area, chemically reactive backbone, conformational flexibility, and overall extended nature) may allow V3 to serve as a general molecular hook. Before CD4 binding, these attributes would enhance the ability of V3 to grasp neighboring protomers on the viral spike. Such quaternary interactions would explain V3's influence on overall neutralization sensitivity, for example, its ability to transfer

neutralization resistance from YU2 to HXBc2 (Sullivan et al., *J. Virol.* 72:6332, 1998). After CD4 binding, the coreceptor binding site forms and V3 would jut prominently toward the target cell membrane. In this context, binding at the V3 tip may act as a ripcord to initiate gp41-mediated fusion.

Example 5

Prime-Boost Immunization with Stabilized gp120 and gp140 Trimer

This example describes the "prime-boost" immunization scheme used to generate a heightened immune response in a subject.

Based on the biophysical characterization of gp120 stabilized in the CD4 bound conformation performed an immunization scheme was performed whereby HXBc2 strain wild-type or cysteine-stabilized core gp120 proteins were used to prime the immune response for subsequent immunization with soluble, stabilized trimeric YU2 strain gp140-foldon molecules (Yang et al. *J Virol.* 76(9):4634-42, 2002). B-cells primed by the stabilized cores were primed for epitopes displayed preferentially only on the stabilized HX core CD4 binding site, or to other stabilized surfaces, efficiently presented only by the cysteine-stabilized cores.

Boosting with the gp140 trimeric molecules "immunofocuses" primed B cells on shared and conserved determinants between the two immunogens and altering strains would not boost B cells directed at HX- or YU2-specific epitopes. Thus, the only B-cells boosted selectively by the trimer would be those that could bind efficiently both the stabilized core as well as the trimer. Thus, stabilized cores can stimulate B cells that could induce the CD4-bound or the b12 conformation in the gp140 trimers.

Based upon this scheme, HIV gp120 core and trimer proteins were expressed by transient transfection of 293 cells with the relevant plasmid DNA. Soluble proteins were purified from culture supernatants by affinity chromatography and maintained in PBS, pH 7.4. Each rabbit was injected at two sites by the intramuscular route in the hind leg with 50 ug of protein emulsified at 1:1 ratio in GSK AS01B adjuvant in a total volume of 1 ml. The rabbits were inoculated four times with emulsified HX wild-type or stabilized core proteins followed by two injections with the emulsified YU2 gp140 trimeric proteins. Inoculations were performed at approximate four week intervals and the immune sera were collected ten days following each injection. The presence of high-titer anti-gp120 antibodies were confirmed by ELISA. The ability to neutralize viral particles derived from selected HIV strains was determined in a luciferase-based HIV entry assay. Virus was incubated with pre- or post-immune sera and the percent neutralization in the immune sera was calculated as the decrease in entry relative to virus incubated with pre-immune sera or an irrelevant BSA protein-emulsified control. The tabulated results of the immunogenicity-neutralization are shown in FIG. **4**A-B.

Example 6

Virus Neutralization

This example describes the neutralization of various HIV isolates with CD4 induced triggering.

Construction of DNA and Recombinant Adenoviruses

Plasmid DNA and Ad5-based first-generation (ΔE1, ΔE3) recombinant adenoviruses expressing different V loop deletions of gp140(ΔCFI) were constructed. HIV envelope genes encoding gp145(ΔCFI) (BaL) (Genbank accession No. M68893), gp145(ΔCFI) (clade C) (Genbank accession No. AF286227), gp145(ΔCFI) (CN54) (Genbank accession No. AX149771), and gp145(ΔCFI) (clade A) (Genbank accession No. U08794) were synthesized using human-preferred codons. gp145(ΔCFI)(B)(V3/C/1AB) and gp145(ΔCFI)(B)(V3/A/1AB) were made by replacing Bal V3 loop with shortened clade C V3(1AB) and clade A V3(1AB) sequences respectively.

Vaccination

Guinea pigs were intramuscularly immunized with 500 μg (in 400 μl PBS) of the gp145 version of plasmid DNA at week 0, 2, and 6. At week 14, the guinea pigs were boosted with 10^{11} particles (in 400 μl PBS) of recombinant replication defective adenovirus (rAd) expressing the corresponding gp140 version of the protein. Serum was collected at week −2 and week 16, aliquotted, and frozen at −20° C.

Virus Neutralization Assay

Single round of infection HIV-1 Env pseudoviruses were prepared by cotransfecting 293T cells with an Env expression plasmid containing a full gp160 env gene and an env-deficient HIV-1 backbone vector (pSG3ΔEnv). Virus-containing culture supernatants were harvested 2 days after transfection, centrifuged and filtered through 0.45-micron filter, and stored at −80° C. Pseudovirus neutralization was measured as a function of Tat-induced luciferase reporter gene expression after a single round of infection in TZM-bl cells. TZM-bl cells express CD4, CXCR4 and CCR5 and contain and integrated reporter gene for firefly luciferase under the control of an HIV-1 LTR. The level of viral infection was quantified by measurement of relative luciferase units (RLU) that are directly proportion to the amount of virus inputs. Briefly, 40 ul of virus was incubated for 30 minutes at 37° C. with serial dilutions of test serum samples (10 ul) in duplicate wells of a 96-well flat bottom culture plate. The final serum dilution was defined at the point of incubation with virus supernatant. 10,000 TZM-bl cells were then added to each well in a total volume of 20 ul and plates were incubated overnight at 37° C. in a 5% CO2 incubator. One set of eight wells received mock antibody followed by virus and cells (controls wells for virus entry) and a set of eight wells received cells with mock virus (to control for luciferase background). Viral input was set at a multiplicity of infection (moi) of approximately 0.1, which generally results in 100,000 to 400,00 0RLU. After over night incubation, 150 ul of fresh medium was added to each well and incubated for 24 hours at 37° C. in a 5% CO_2 incubator. To determine RLU, cell culture medium was aspirated from wells followed by addition of 50 ul of cell lysis buffer (Promega, Madison, Wis.). 30 ul of cell lysate was transferred to wells of a black Optiplate (PerkinElmer) for measurement of luminescence using a Perkin-Elmer Victor-light luminometer that injects 50 ul of luciferase substrate reagent to each well just prior to reading RLU. To test for sCD4 triggering, two-domain sCD4 was added to the virus just prior to the addition of sera.

Example 7

Identification of Immunogenic Fragments of gp120

This example describes the selection of immunogenic fragments of stabilized gp120.

A nucleic acid molecule encoding a stabilized p120 fragment is expressed in a host using standard techniques (see above; see Sambrook et al., Molecular Cloning; A Laboratory Manual, Cold Spring Harbor Press, Cold Spring Harbor, N.Y.: 1989). Preferable gp120 fragment is expressed such that the gp120 fragment can be isolated or purified in sufficient quantity. The stabilized gp120 fragment that are expressed are analyzed by various techniques known in the art, such as immunoblot, and ELISA, and for binding to CD4 and mAbs directed to the CD4 binding site, for example the b12 antibody.

To determine the antigenic potential of stabilized p120 fragments, subjects such as mice, rabbits or other suitable subjects are immunized with stabilized p120 fragments. Sera from such immunized subjects are tested for antibody activity for example by ELISA with the expressed polypeptide. They are also tested in a CD4 binding assay, for example by qualitative biacore, and the binding of neutralizing antibodies, for example by using the b12 antibody. Thus, antigenic fragments of stabilized forms are selected to archive broadly reactive neutralizing antibody responses.

Example 8

Conformational Masking of Stabilized Immunogens

This example describes the strategies to mask portions of a stabilized gp120 polypeptide from non-neutralizing antibodies.

The polypeptide "new 9c" as set forth as SEQ ID NO: 1 includes residues at the base of the V3 loop, and restores recognition of the core by the CD4-induced antibodies, such as 17b. Individual and combination glycan mutations were designed in the context of the stabilized gp120 polypeptides disclosed herein (for example, such as set forth in SEQ ID NO: 2 or encoded by SEQ ID NO: 4-18) to prevent the elicitation of non-neutralizing antibodies. Using site-directed mutagenesis, specific Asn and Ser/Thr residues are incorporated into the 8b core. The Asn-X-Ser/Thr residues mediate the attachment of glycans to the designated asparagine residues by mammalian cell glycosylating enzymes in the endoplasmic reticulum. This scheme is used to mask the immunogenic but non-neutralizing surfaces present in gp120.

Typically, wild-type gp120 cores elicit antibodies in rabbits that bind more efficiently to the core proteins than to full length gp120 glycoproteins. It is likely that the cores, via their truncated loops and N- and C-termini, elicit antibodies to surfaces that are not exposed in monomeric gp120.

As another aspect of an overall strategy to optimize the stabilized core priming of a trimer boost, glycans are designed at selected densities on the stabilized core to dampen or eliminate unwanted core-specific responses based upon the 8b core-b12 structure disclosed herein. The optimized and proteins are expressed, purified, analyzed and tested for immunogenicity by themselves or in sequential prime-boost with the YU2 gp140 trimers.

To mask the surface recognized by 17b and other CD4-induced antibodies the following mutations were designed:

Mutation 1	Mutation 2
a. R419N	K421S
b. I420N	Q422S
c. Q422N	I424T
d. I423N	N425T
and one additional mutant to add 2 glycans	
e. R419N	K421S + I423N	N425T

To mask surfaces other than the CD4 binding site, which includes the b12 epitope region, the following N-glycan addition sites were designed:

Glycan	Location	Mutation 1	Mutation 2
1	246	Q246N	
2	267	E267N	E269T
3	97	K97N	D99T
4	103	Q103N	H105S
5	92		N94T
6	114	Q114N	L116T
7	222	G222N	A224T
8	201	I201N	Q203T
9	206	P206N	V208T
10	423	I423N	N425T
11	434	M434N	A436S
12	442	Q442N	R444T
13	210	F210N	P212T
		Density 2	
1	246	Q246N	
2	97	K97N	D99T
3	103	Q103N	H105S
4	201	I201N	Q203T
5	206	P206N	V208T
6	434	M434N	A436S
7	442	Q442N	R444T
8	210	F210N	P212T
9	114	Q114N	L116T
		Density 3	
1	206	P206N	V208T
2	442	Q442N	R444T
3	114	Q114N	L116T
4	246	Q246N	
5	434	M434N	A436S

Mutation 1 and Mutation 2 correspond to the N glycosylation consensus sequence: NxT/S where x is anything except proline. T is better than S for glycosylation. Blanks indicate positions where no mutations are necessary. These glysolated peptides are used to induce a immune response in a subject.

In view of the many possible embodiments to which the principles of the disclosed invention may be applied, it should be recognized that the illustrated embodiments are only preferred examples of the invention and should not be taken as limiting the scope of the invention. Rather, the scope of the invention is defined by the following claims. We therefore claim as our invention all that comes within the scope and spirit of these claims.

SEQUENCE LISTING

<160> NUMBER OF SEQ ID NOS: 27

<210> SEQ ID NO 1
<211> LENGTH: 324
<212> TYPE: PRT
<213> ORGANISM: Human immunodeficiency virus type 1

<400> SEQUENCE: 1

-continued

```
Val Val Leu Val Asn Val Thr Glu Asn Phe Asn Trp Cys Lys Asn Asp
1               5                   10                  15

Met Val Glu Gln Met His Glu Asp Ile Cys Ser Leu Trp Asp Gln Ser
            20                  25                  30

Leu Lys Pro Cys Val Lys Leu Cys Pro Leu Ala Gly Ala Thr Ser Val
        35                  40                  45

Ile Thr Gln Ala Cys Pro Lys Val Ser Phe Glu Pro Ile Pro Ile His
    50                  55                  60

Tyr Cys Ala Pro Ala Gly Phe Ala Ile Leu Lys Cys Asn Asn Lys Thr
65                  70                  75                  80

Phe Asn Gly Thr Gly Pro Cys Thr Asn Val Ser Thr Val Gln Cys Thr
                85                  90                  95

His Gly Ile Arg Pro Val Val Ser Ser Gln Leu Leu Leu Asn Gly Ser
            100                 105                 110

Leu Ala Glu Glu Glu Val Val Ile Arg Ser Cys Asn Phe Thr Asp Asn
        115                 120                 125

Ala Lys Thr Ile Ile Val Gln Leu Asn Thr Ser Val Glu Ile Asn Cys
    130                 135                 140

Thr Arg Pro Asn Asn Gly Gly Ser Gly Ser Gly Gly Asn Met Arg Gln
145                 150                 155                 160

Ala His Cys Asn Ile Ser Arg Ala Lys Trp Asn Asn Thr Leu Lys Gln
                165                 170                 175

Ile Ala Ser Lys Leu Arg Glu Gln Phe Gly Asn Asn Lys Thr Ile Ile
            180                 185                 190

Phe Lys Gln Ser Ser Gly Gly Asp Pro Glu Ile Val Thr His Trp Phe
        195                 200                 205

Asn Cys Gly Gly Glu Phe Phe Tyr Cys Asn Ser Thr Gln Leu Phe Asn
    210                 215                 220

Ser Thr Trp Phe Asn Ser Thr Trp Ser Thr Glu Gly Ser Asn Asn Thr
225                 230                 235                 240

Glu Gly Ser Asp Thr Ile Thr Leu Pro Cys Arg Ile Lys Gln Ile Ile
                245                 250                 255

Asn Met Trp Cys Lys Val Cys Lys Ala Met Tyr Ala Pro Pro Ile Ser
            260                 265                 270

Gly Gln Ile Arg Cys Ser Ser Asn Ile Thr Gly Leu Leu Leu Thr Arg
        275                 280                 285

Asp Gly Gly Asn Ser Asn Asn Glu Ser Glu Ile Phe Arg Pro Gly Gly
    290                 295                 300

Gly Asp Met Arg Asp Asn Trp Arg Ser Glu Leu Tyr Lys Tyr Lys Val
305                 310                 315                 320

Val Lys Ile Glu


<210> SEQ ID NO 2
<211> LENGTH: 344
<212> TYPE: PRT
<213> ORGANISM: Human immunodeficiency virus type 1

<400> SEQUENCE: 2

Gly Ala Arg Ser Glu Val Val Leu Glu Asn Val Thr Glu His Phe Asn
1               5                   10                  15

Met Trp Lys Asn Asp Met Val Glu Gln Met Gln Glu Asp Ile Ile Ser
            20                  25                  30

Leu Trp Asp Gln Ser Leu Lys Pro Cys Val Lys Leu Thr Pro Leu Cys
        35                  40                  45
```

-continued

```
Val Gly Ala Gly Ser Cys Asp Thr Ser Val Ile Thr Gln Ala Cys Pro
    50                  55                  60

Lys Ile Ser Phe Glu Pro Ile Pro Ile His Tyr Cys Ala Pro Ala Gly
65                  70                  75                  80

Phe Ala Ile Leu Lys Cys Asn Asp Lys Thr Phe Asn Gly Lys Gly Pro
                85                  90                  95

Cys Lys Asn Val Ser Thr Val Gln Cys Thr His Gly Ile Arg Pro Val
            100                 105                 110

Val Ser Thr Gln Leu Leu Leu Asn Gly Ser Leu Ala Glu Glu Glu Val
        115                 120                 125

Val Ile Arg Ser Asp Asn Phe Thr Asn Asn Ala Lys Thr Ile Ile Val
    130                 135                 140

Gln Leu Lys Glu Ser Val Glu Ile Asn Cys Thr Arg Pro Asn Gln Asn
145                 150                 155                 160

Thr Arg Lys Ser Ile His Ile Gly Pro Gly Arg Ala Phe Tyr Thr Thr
                165                 170                 175

Gly Glu Ile Ile Gly Asp Ile Arg Gln Ala His Cys Asn Ile Ser Arg
            180                 185                 190

Ala Lys Trp Asn Asp Thr Leu Lys Gln Ile Val Ile Lys Leu Arg Glu
        195                 200                 205

Gln Phe Glu Asn Lys Thr Ile Val Phe Asn His Ser Ser Gly Gly Asp
    210                 215                 220

Pro Glu Ile Val Met His Ser Phe Asn Cys Gly Gly Glu Phe Phe Tyr
225                 230                 235                 240

Cys Asn Ser Ala Gln Leu Phe Asn Ser Thr Trp Asn Asn Asn Thr Glu
                245                 250                 255

Gly Ser Asn Asn Thr Glu Gly Asn Thr Ile Thr Leu Pro Cys Arg Ile
            260                 265                 270

Lys Gln Ile Ile Asn Met Trp Gln Glu Val Gly Lys Ala Met Tyr Ala
        275                 280                 285

Pro Pro Ile Arg Gly Gln Ile Arg Cys Ser Ser Asn Ile Thr Gly Leu
    290                 295                 300

Leu Leu Thr Arg Asp Gly Gly Ile Asn Glu Asn Gly Thr Glu Ile Phe
305                 310                 315                 320

Arg Pro Gly Gly Gly Asp Met Arg Asp Asn Trp Arg Ser Glu Leu Tyr
                325                 330                 335

Lys Tyr Lys Val Val Lys Ile Glu
            340
```

<210> SEQ ID NO 3
<211> LENGTH: 1053
<212> TYPE: DNA
<213> ORGANISM: Human immunodeficiency virus type 1

<400> SEQUENCE: 3

```
atgaagagag ggctctgctg tgtgctgctg ctgtgtggag cagtcttcgt ttcgcccagc     60

caggaaatcc atgcccgatt cagaagagga gccagatctg aggtggtgct ggtgaacgtg    120

accgagaact tcaacatgtg gaagaacgac atggtggagc agatgcacga ggacatcatc    180

agcctgtggg accagagcct gaagccctgc gtgaagctga ccccctgtg cgtgggcgcc    240

ggcagctgca acaccagcgt gatcacccag gcctgcccca aggtgagctt cgagcccatc    300

cccatccact actgcgcccc cgccggcttc gccatcctga agtgcaacaa caagaccttc    360

aacggcaccg gcccctgcac caacgtgagc accgtgcagt gcacccacgg catccgcccc    420

gtggtgagca gtcagctgct gctgaacggc agcctggccg aggaggaggt ggtgatccgc    480
```

-continued

agcgtgaact tcaccgacaa cgccaagacc atcatcgtgc agctgaacac cagcgtggag 540

atcaactgca ccggcgccgg ccactgcaac atcgcccgcg ccaagtggaa caacaccctg 600

aagcagatcg ccagcaagct gcgcgagcag ttcggcaaca acaagaccat catcttcaag 660

cagagcagcg gcggcgaccc cgagatcgtg acccactggt tcaactgcgg cggcgagttc 720

ttctactgca acagcaccca gctgttcaac agcacctggt tcaacagcac ctggagcacc 780

gagggcagca acaacaccga gggcagcgac accatcaccc tgccctgccg catcaagcag 840

atcatcaaca tgtggcagaa ggtgggcaag gccatgtacg ccccccccat cagcggccag 900

atccgctgca gcagcaacat caccggcctg ctgctgaccc gcgacggcgg caacagcaac 960

aacgagagcg agatcttccg tccgggcggc ggcgacatgc gcgacaactg gcgcagcgag 1020

ctgtacaagt acaaggtggt gaagatcgag tga 1053

<210> SEQ ID NO 4
<211> LENGTH: 1053
<212> TYPE: DNA
<213> ORGANISM: Human immunodeficiency virus type 1

<400> SEQUENCE: 4

atgaagagag ggctctgctg tgtgctgctg ctgtgtggag cagtcttcgt ttcgcccagc 60

caggaaatcc atgcccgatt cagaagagga gccagatctg aggtggtgct ggtgaacgtg 120

accgagaact tcaacatgtg gaagaacgac atggtggagc agatgcacga ggacatctgt 180

agcctgtggg accagagcct gaagccctgc gtgaagctga cccccctgtg cgtgggcgcc 240

ggcagctgca acaccagcgt gatcacccag gcctgcccca aggtgagctt cgagcccatc 300

cccatccact actgcgcccc cgccggcttc gccatcctga agtgcaacaa caagaccttc 360

aacggcaccg gcccctgcac caacgtgagc accgtgcagt gcacccacgg catccgcccc 420

gtggtgagca gtcagctgct gctgaacggc agcctggccg aggaggaggt ggtgatccgc 480

agcgtgaact tcaccgacaa cgccaagacc atcatcgtgc agctgaacac cagcgtggag 540

atcaactgca ccggcgccgg ccactgcaac atcgcccgcg ccaagtggaa caacaccctg 600

aagcagatcg ccagcaagct gcgcgagcag ttcggcaaca acaagaccat catcttcaag 660

cagagcagcg gcggcgaccc cgagatcgtg acccactggt tcaactgcgg cggcgagttc 720

ttctactgca acagcaccca gctgttcaac agcacctggt tcaacagcac ctggagcacc 780

gagggcagca acaacaccga gggcagcgac accatcaccc tgccctgccg catcaagcag 840

atcatcaaca tgtggtgtaa ggtgggcaag gccatgtacg ccccccccat cagcggccag 900

atccgctgca gcagcaacat caccggcctg ctgctgaccc gcgacggcgg caacagcaac 960

aacgagagcg agatcttccg tccgggcggc ggcgacatgc gcgacaactg gcgcagcgag 1020

ctgtacaagt acaaggtggt gaagatcgag tga 1053

<210> SEQ ID NO 5
<211> LENGTH: 1053
<212> TYPE: DNA
<213> ORGANISM: Human immunodeficiency virus type 1

<400> SEQUENCE: 5

atgaagagag ggctctgctg tgtgctgctg ctgtgtggag cagtcttcgt ttcgcccagc 60

caggaaatcc atgcccgatt cagaagagga gccagatctg aggtggtgct ggtgaacgtg 120

accgagaact tcaacatgtg gaagaacgac atggtggagc agatgcacga ggacatcatc 180

agcctgtggg accagagcct gaagccctgc gtgaagctga cccccctgtg cgtgggcgcc 240

-continued

ggcagctgca acaccagcgt gatcacccag gcctgcccca aggtgagctt cgagcccatc 300

cccatccact actgcgcccc cgccggcttc gccatcctga agtgcaacaa ctgtaccttc 360

aacggtaccg gcccctgcac caacgtgagc accgtgcagt gcacccacgg catccgcccc 420

gtggtgagca gtcagctgct gctgaacggc agcctggcat gcgaggaggt ggtgatccgc 480

agcgtgaact tcaccgacaa cgccaagacc atcatcgtgc agctgaacac cagcgtggag 540

atcaactgca ccggcgccgg ccactgcaac atcgcccgcg ccaagtggaa caacaccctg 600

aagcagatcg ccagcaagct gcgcgagcag ttcggcaaca acaagaccat catcttcaag 660

cagagcagcg gcggcgaccc cgagatcgtg acccactggt tcaactgcgg cggcgagttc 720

ttctactgca acagcaccca gctgttcaac agcacctggt tcaacagcac ctggagcacc 780

gagggcagca acaacaccga gggcagcgac accatcaccc tgccctgccg catcaagcag 840

atcatcaaca tgtggcagaa ggtgggcaag gccatgtacg cccccccat cagcggccag 900

atccgctgca gcagcaacat caccggcctg ctgctgaccc gcgacggcgg caacagcaac 960

aacgagagcg agatcttccg tccgggcggc ggcgacatgc gcgacaactg gcgcagcgag 1020

ctgtacaagt acaaggtggt gaagatcgag tga 1053

<210> SEQ ID NO 6
<211> LENGTH: 1053
<212> TYPE: DNA
<213> ORGANISM: Human immunodeficiency virus type 1

<400> SEQUENCE: 6

atgaagagag ggctctgctg tgtgctgctg ctgtgtggag cagtcttcgt ttcgcccagc 60

caggaaatcc atgcccgatt cagaagagga gccagatctg aggtggtgct ggtgaacgtg 120

accgagaact tcaacatgtg gaagaacgac atggtggagc agatgcacga ggacatcatc 180

agcctgtggg accagagcct gaagccctgc gtgaagctgt gtccctgtg cgtgggcgcc 240

ggcagctgca acaccagcgt gatcacccag gcctgcccca aggtgagctt cgagcccatc 300

cccatccact actgcgcccc cgccggcttc gccatcctga agtgcaacaa caagaccttc 360

aacggcaccg gcccctgcac caacgtgagc accgtgcagt gcacccacgg catccgcccc 420

gtggtgagca gtcagctgct gctgaacggc agcctggccg aggaggaggt ggtgatccgc 480

agcgtgaact tcaccgacaa cgccaagacc atcatcgtgc agctgaacac cagcgtggag 540

atcaactgca ccggcgccgg ccactgcaac atcgcccgcg ccaagtggaa caacaccctg 600

aagcagatcg ccagcaagct gcgcgagcag ttcggcaaca acaagaccat catcttcaag 660

cagagcagcg gcggcgaccc cgagatcgtg acccactggt tcaactgcgg cggcgagttc 720

ttctactgca acagcaccca gctgttcaac agcacctggt tcaacagcac ctggagcacc 780

gagggcagca acaacaccga gggcagcgac accatcaccc tgccctgccg catcaagcag 840

atcatcaaca tgtggcagaa ggtgtgtaag gccatgtacg cccccccat cagcggccag 900

atccgctgca gcagcaacat caccggcctg ctgctgaccc gcgacggcgg caacagcaac 960

aacgagagcg agatcttccg tccgggcggc ggcgacatgc gcgacaactg gcgcagcgag 1020

ctgtacaagt acaaggtggt gaagatcgag tga 1053

<210> SEQ ID NO 7
<211> LENGTH: 1053
<212> TYPE: DNA
<213> ORGANISM: Human immunodeficiency virus type 1

<400> SEQUENCE: 7

-continued

atgaagagag ggctctgctg tgtgctgctg ctgtgtggag cagtcttcgt ttcgcccagc 60

caggaaatcc atgcccgatt cagaagagga gccagatctg aggtggtgct ggtgaacgtg 120

accgagaact tcaactggtg caagaacgac atggtggagc agatgcacga ggacatctgt 180

agcctgtggg accagagcct gaagccctgc gtgaagctga ccccccctgtg cgtgggcgcc 240

ggcagctgca acaccagcgt gatcacccag gcctgcccca aggtgagctt cgagcccatc 300

cccatccact actgcgcccc cgccggcttc gccatcctga agtgcaacaa caagaccttc 360

aacggcaccg gcccctgcac caacgtgagc accgtgcagt gcacccacgg catccgcccc 420

gtggtgagca gtcagctgct gctgaacggc agcctggccg aggaggaggt ggtgatcaga 480

tcttgcaact tcaccgacaa cgccaagacc atcatcgtgc agctgaacac cagcgtggag 540

atcaactgca ccggcgccgg ccactgcaac atcgcccgcg ccaagtggaa caacaccctg 600

aagcagatcg ccagcaagct gcgcgagcag ttcggcaaca acaagaccat catcttcaag 660

cagagcagcg gcggcgaccc cgagatcgtg acccactggt tcaactgcgg cggcgagttc 720

ttctactgca acagcaccca gctgttcaac agcacctggt tcaacagcac ctggagcacc 780

gagggcagca acaacaccga gggcagcgac accatcaccc tgccctgccg catcaagcag 840

atcattaata tgtggtgtaa ggtgggcaag atgatgtacg ccccccccat cagcggccag 900

atccgctgca gcagcaacat caccggcctg ctgctgaccc gcgacggcgg caacagcaac 960

aacgagagcg agatcttccg tccgggcggc ggcgacatgc gcgacaactg gcgcagcgag 1020

ctgtacaagt acaaggtggt gaagatcgag tga 1053

<210> SEQ ID NO 8
<211> LENGTH: 1053
<212> TYPE: DNA
<213> ORGANISM: Human immunodeficiency virus type 1

<400> SEQUENCE: 8

atgaagagag ggctctgctg tgtgctgctg ctgtgtggag cagtcttcgt ttcgcccagc 60

caggaaatcc atgcccgatt cagaagagga gccagatctg aggtggtgct ggtgaacgtg 120

accgagaact tcaacatgtg gaagaacgac atggtggagc agatgcacga ggacatctgt 180

agcctgtggg accagagcct gaagccctgc gtgaagctga ccccccctgtg cgtgggcgcc 240

ggcagctgca acaccagcgt gatcacccag gcctgcccca aggtgagctt cgagcccatc 300

cccatccact actgcgcccc cgccggcttc gccatcctga agtgcaacaa ctgtaccttc 360

aacggtaccg gcccctgcac caacgtgagc accgtgcagt gcacccacgg catccgcccc 420

gtggtgagca gtcagctgct gctgaacggc agcctggcat gcgaggaggt ggtgatccgc 480

agcgtgaact tcaccgacaa cgccaagacc atcatcgtgc agctgaacac cagcgtggag 540

atcaactgca ccggcgccgg ccactgcaac atcgcccgcg ccaagtggaa caacaccctg 600

aagcagatcg ccagcaagct gcgcgagcag ttcggcaaca acaagaccat catcttcaag 660

cagagcagcg gcggcgaccc cgagatcgtg acccactggt tcaactgcgg cggcgagttc 720

ttctactgca acagcaccca gctgttcaac agcacctggt tcaacagcac ctggagcacc 780

gagggcagca acaacaccga gggcagcgac accatcaccc tgccctgccg catcaagcag 840

atcattaata tgtggtgtaa ggtgggcaag gccatgtacg ccccccccat cagcggccag 900

atccgctgca gcagcaacat caccggcctg ctgctgaccc gcgacggcgg caacagcaac 960

aacgagagcg agatcttccg tccgggcggc ggcgacatgc gcgacaactg gcgcagcgag 1020

ctgtacaagt acaaggtggt gaagatcgag tga 1053

<210> SEQ ID NO 9
<211> LENGTH: 1053
<212> TYPE: DNA
<213> ORGANISM: Human immunodeficiency virus type 1

<400> SEQUENCE: 9

atgaagagag ggctctgctg tgtgctgctg ctgtgtggag cagtcttcgt ttcgcccagc 60

caggaaatcc atgcccgatt cagaagagga gccagatctg aggtggtgct ggtgaacgtg 120

accgagaact tcaactggtg caagaacgac atggtggagc agatgcacga ggacatcatc 180

agcctgtggg accagagcct gaagccctgc gtgaagctga ccccccctgtg cgtgggcgcc 240

ggcagctgca acaccagcgt gatcacccag gcctgcccca aggtgagctt cgagcccatc 300

cccatccact actgcgcccc cgccggcttc gccatcctga agtgcaacaa ctgtaccttc 360

aacggtaccg gcccctgcac caacgtgagc accgtgcagt gcacccacgg catccgcccc 420

gtggtgagca gtcagctgct gctgaacggc agcctggcat gcgaggaggt ggtgatcaga 480

tcttgcaact tcaccgacaa cgccaagacc atcatcgtgc agctgaacac cagcgtggag 540

atcaactgca ccggcgccgg ccactgcaac atcgcccgcg ccaagtggaa caacaccctg 600

aagcagatcg ccagcaagct gcgcgagcag ttcggcaaca acaagaccat catcttcaag 660

cagagcagcg gcggcgaccc cgagatcgtg acccactggt tcaactgcgg cggcgagttc 720

ttctactgca acagcaccca gctgttcaac agcacctggt tcaacagcac ctggagcacc 780

gagggcagca acaacaccga gggcagcgac accatcaccc tgccctgccg catcaagcag 840

atcatcaata tgtggcagaa ggtgggcaag atgatgtacg ccccccccat cagcggccag 900

atccgctgca gcagcaacat caccggcctg ctgctgaccc gcgacggcgg caacagcaac 960

aacgagagcg agatcttccg tccgggcggc ggcgacatgc gcgacaactg gcgcagcgag 1020

ctgtacaagt acaaggtggt gaagatcgag tga 1053

<210> SEQ ID NO 10
<211> LENGTH: 1053
<212> TYPE: DNA
<213> ORGANISM: Human immunodeficiency virus type 1

<400> SEQUENCE: 10

atgaagagag ggctctgctg tgtgctgctg ctgtgtggag cagtcttcgt ttcgcccagc 60

caggaaatcc atgcccgatt cagaagagga gccagatctg aggtggtgct ggtgaacgtg 120

accgagaact tcaactggtg caagaacgac atggtggagc agatgcacga ggacatctgt 180

agcctgtggg accagagcct gaagccctgc gtgaagctga ccccccctgtg cgtgggcgcc 240

ggcagctgca acaccagcgt gatcacccag gcctgcccca aggtgagctt cgagcccatc 300

cccatccact actgcgcccc cgccggcttc gccatcctga agtgcaacaa caagaccttc 360

aacggcaccg gcccctgcac caacgtgagc accgtgcagt gcacccacgg catccgcccc 420

gtggtgagca gtcagctgct gctgaacggc agcctggccg aggaggaggt ggtgatcaga 480

tcttgcaact tcaccgacaa cgccaagacc atcatcgtgc agctgaacac cagcgtggag 540

atcaactgca ccggcgccgg ccactgcaac atcgcccgcg ccaagtggaa caacaccctg 600

aagcagatcg ccagcaagct gcgcgagcag ttcggcaaca acaagaccat catcttcaag 660

cagagcagcg gcggcgaccc cgagatcgtg acccactggt tcaactgcgg cggcgagttc 720

ttctactgca acagcaccca gctgttcaac agcacctggt tcaacagcac ctggagcacc 780

gagggcagca acaacaccga gggcagcgac accatcaccc tgccctgccg catcaagcag 840

-continued

atcattaata tgtggtgtaa ggtgggcaag atgatgtacg ccccccccat cagcggccag 900

atccgctgca gcagcaacat caccggcctg ctgctgaccc gcgacggcgg caacagcaac 960

aacgagagcg agatcttccg tccgggcggc ggcgacatgc gcgacaactg gcgcagcgag 1020

ctgtacaagt acaaggtggt gaagatcgag tga 1053

<210> SEQ ID NO 11
<211> LENGTH: 1053
<212> TYPE: DNA
<213> ORGANISM: Human immunodeficiency virus type 1

<400> SEQUENCE: 11

atgaagagag ggctctgctg tgtgctgctg ctgtgtggag cagtcttcgt ttcgcccagc 60

caggaaatcc atgcccgatt cagaagagga gccagatctg aggtggtgct ggtgaacgtg 120

accgagaact tcaacatgtg gaagaacgac atggtggagc agatgcacga ggacatctgt 180

agcctgtggg accagagcct gaagccctgc gtgaagcttt gtcccctgtg cgtgggcgcc 240

ggcagctgca acaccagcgt gatcacccag gcctgcccca aggtgagctt cgagcccatc 300

cccatccact actgcgcccc cgccggcttc gccatcctga agtgcaacaa ctgtaccttc 360

aacggtaccg gcccctgcac caacgtgagc accgtgcagt gcacccacgg catccgcccc 420

gtggtgagca gtcagctgct gctgaacggc agcctggcat gcgaggaggt ggtgatccgc 480

agcgtgaact tcaccgacaa cgccaagacc atcatcgtgc agctgaacac cagcgtggag 540

atcaactgca ccggcgccgg ccactgcaac atcgcccgcg ccaagtggaa caacaccctg 600

aagcagatcg ccagcaagct gcgcgagcag ttcggcaaca acaagaccat catcttcaag 660

cagagcagcg gcggcgaccc cgagatcgtg acccactggt tcaactgcgg cggcgagttc 720

ttctactgca acagcaccca gctgttcaac agcacctggt tcaacagcac ctggagcacc 780

gagggcagca acaacaccga gggcagcgac accatcaccc tgccctgccg catcaagcag 840

atcattaata tgtggtgtaa ggtgtgtaag gccatgtacg ccccccccat cagcggccag 900

atccgctgca gcagcaacat caccggcctg ctgctgaccc gcgacggcgg caacagcaac 960

aacgagagcg agatcttccg tccgggcggc ggcgacatgc gcgacaactg gcgcagcgag 1020

ctgtacaagt acaaggtggt gaagatcgag tga 1053

<210> SEQ ID NO 12
<211> LENGTH: 1053
<212> TYPE: DNA
<213> ORGANISM: Human immunodeficiency virus type 1

<400> SEQUENCE: 12

atgaagagag ggctctgctg tgtgctgctg ctgtgtggag cagtcttcgt ttcgcccagc 60

caggaaatcc atgcccgatt cagaagagga gccagatctg aggtggtgct ggtgaacgtg 120

accgagaact tcaacatgtg gaagaacgac atggtggagc agatgcacga ggacatctgt 180

agcctgtggg accagagcct gaagccctgc gtgaagcttt gtcccctgtg cgtgggcgcc 240

ggcagctgca acaccagcgt gatcacccag gcctgcccca aggtgagctt cgagcccatc 300

cccatccact actgcgcccc cgccggcttc gccatcctga agtgcaacaa ctgtaccttc 360

aacggtaccg gcccctgcac caacgtgagc accgtgcagt gcacccacgg catccgcccc 420

gtggtgagca gtcagctgct gctgaacggc agcctggcat gcgaggaggt ggtgatccgc 480

agcgtgaact tcaccgacaa cgccaagacc atcatcgtgc agctgaacac cagcgtggag 540

atcaactgca ccggcgccgg ccactgcaac atcgcccgcg ccaagtggaa caacaccctg 600

-continued

aagcagatcg ccagcaagct gcgcgagcag ttcggcaaca acaagaccat catcttcaag 660

cagagcagcg gcggcgaccc cgagatcgtg acccactggt tcaactgcgg cggcgagttc 720

ttctactgca acagcaccca gctgttcaac agcacctggt tcaacagcac ctggagcacc 780

gagggcagca acaacaccga gggcagcgac accatcaccc tgccctgccg catcaagcag 840

atcattaata tgtggtgtaa ggtgtgtaag atgatgtacg cccccccgat atcaggccag 900

atccgctgca gcagcaacat caccggcctg ctgctgaccc gcgacggcgg caacagcaac 960

aacgagagcg agatcttccg tccgggcggc ggcgacatgc gcgacaactg gcgcagcgag 1020

ctgtacaagt acaaggtggt gaagatcgag tga 1053

<210> SEQ ID NO 13
<211> LENGTH: 1053
<212> TYPE: DNA
<213> ORGANISM: Human immunodeficiency virus type 1

<400> SEQUENCE: 13

atgaagagag ggctctgctg tgtgctgctg ctgtgtggag cagtcttcgt ttcgcccagc 60

caggaaatcc atgcccgatt cagaagagga gccagatctg aggtggtgct ggtgaacgtg 120

accgagaact tcaactggtg caagaacgac atggtggagc agatgcacga ggacatcatc 180

agcctgtggg accagagcct gaagccctgc gtgaagcttt gtcccctgtg cgtgggcgcc 240

ggcagctgca acaccagcgt gatcacccag gcctgcccca aggtgagctt cgagcccatc 300

cccatccact actgcgcccc cgccggcttc gccatcctga agtgcaacaa ctgtaccttc 360

aacggtaccg gcccctgcac caacgtgagc accgtgcagt gcacccacgg catccgcccc 420

gtggtgagca gtcagctgct gctgaacggc agcctggcat gcgaggaggt ggtgatcaga 480

tcttgcaact tcaccgacaa cgccaagacc atcatcgtgc agctgaacac cagcgtggag 540

atcaactgca ccggcgccgg ccactgcaac atcgcccgcg ccaagtggaa caacaccctg 600

aagcagatcg ccagcaagct gcgcgagcag ttcggcaaca acaagaccat catcttcaag 660

cagagcagcg gcggcgaccc cgagatcgtg acccactggt tcaactgcgg cggcgagttc 720

ttctactgca acagcaccca gctgttcaac agcacctggt tcaacagcac ctggagcacc 780

gagggcagca acaacaccga gggcagcgac accatcaccc tgccctgccg catcaagcag 840

atcatcaaca tgtggcagaa ggtgtgtaag gccatgtacg ccccccccat cagcggccag 900

atccgctgca gcagcaacat caccggcctg ctgctgaccc gcgacggcgg caacagcaac 960

aacgagagcg agatcttccg tccgggcggc ggcgacatgc gcgacaactg gcgcagcgag 1020

ctgtacaagt acaaggtggt gaagatcgag tga 1053

<210> SEQ ID NO 14
<211> LENGTH: 1053
<212> TYPE: DNA
<213> ORGANISM: Human immunodeficiency virus type 1

<400> SEQUENCE: 14

atgaagagag ggctctgctg tgtgctgctg ctgtgtggag cagtcttcgt ttcgcccagc 60

caggaaatcc atgcccgatt cagaagagga gccagatctg aggtggtgct ggtgaacgtg 120

accgagaact tcaactggtg caagaacgac atggtggagc agatgcacga ggacatctgt 180

agcctgtggg accagagcct gaagccctgc gtgaagctgt gtcccctgtg cgtgggcgcc 240

ggcagctgca acaccagcgt gatcacccag gcctgcccca aggtgagctt cgagcccatc 300

cccatccact actgcgcccc cgctggcttc gccatcctga agtgcaacaa caagaccttc 360

-continued

aacggcaccg gcccctgcac caacgtgagc accgtgcagt gcacccacgg catccgcccc 420

gtggtgagca gtcagctgct gctgaacggc agcctggccg aggaggaggt ggtgatcaga 480

tcttgcaact tcaccgacaa cgccaagacc atcatcgtgc agctgaacac cagcgtggag 540

atcaactgca ccggcgccgg ccactgcaac atcgcccgcg ccaagtggaa caacaccctg 600

aagcagatcg ccagcaagct gcgcgagcag ttcggcaaca acaagaccat catcttcaag 660

cagagcagcg gcggcgaccc cgagatcgtg acccactggt tcaactgcgg cggcgagttc 720

ttctactgca acagcaccca gctgttcaac agcacctggt tcaacagcac ctggagcacc 780

gagggcagca acaacaccga gggcagcgac accatcaccc tgccctgccg catcaagcag 840

atcatcaaca tgtggtgtaa ggtgtgtaag gccatgtacg cccccccccat cagcggccag 900

atccgctgca gcagcaacat caccggcctg ctgctgaccc gcgacggcgg caacagcaac 960

aacgagagcg agatcttccg tccgggcggc ggcgacatgc gcgacaactg gcgcagcgag 1020

ctgtacaagt acaaggtggt gaagatcgag tga 1053

<210> SEQ ID NO 15
<211> LENGTH: 1053
<212> TYPE: DNA
<213> ORGANISM: Human immunodeficiency virus type 1

<400> SEQUENCE: 15

atgaagagag ggctctgctg tgtgctgctg ctgtgtggag cagtcttcgt ttcgcccagc 60

caggaaatcc atgcccgatt cagaagagga gccagatctg aggtggtgct ggtgaacgtg 120

accgagaact tcaactggtg caagaacgac atggtggagc agatgcacga ggacatctgt 180

agcctgtggg accagagcct gaagccctgc gtgaagctga cccccctgtg cgtgggcgcc 240

ggcagctgca acaccagcgt gatcacccag gcctgcccca aggtgagctt cgagcccatc 300

cccatccact actgcgcccc cgccggcttc gccatcctga agtgcaacaa ctgtaccttc 360

aacggtaccg gcccctgcac caacgtgagc accgtgcagt gcacccacgg catccgcccc 420

gtggtgagca gtcagctgct gctgaacggc agcctggcat gcgaggaggt ggtgatcaga 480

tcttgcaact tcaccgacaa cgccaagacc atcatcgtgc agctgaacac cagcgtggag 540

atcaactgca ccggcgccgg ccactgcaac atcgcccgcg ccaagtggaa caacaccctg 600

aagcagatcg ccagcaagct gcgcgagcag ttcggcaaca acaagaccat catcttcaag 660

cagagcagcg gcggcgaccc cgagatcgtg acccactggt tcaactgcgg cggcgagttc 720

ttctactgca acagcaccca gctgttcaac agcacctggt tcaacagcac ctggagcacc 780

gagggcagca acaacaccga gggcagcgac accatcaccc tgccctgccg catcaagcag 840

atcattaata tgtggtgtaa ggtgggcaag atgatgtacg cccccccccat cagcggccag 900

atccgctgca gcagcaacat caccggcctg ctgctgaccc gcgacggcgg caacagcaac 960

aacgagagcg agatcttccg tccgggcggc ggcgacatgc gcgacaactg gcgcagcgag 1020

ctgtacaagt acaaggtggt gaagatcgag tga 1053

<210> SEQ ID NO 16
<211> LENGTH: 1054
<212> TYPE: DNA
<213> ORGANISM: Human immunodeficiency virus type 1

<400> SEQUENCE: 16

atgaagagag ggctctgctg tgtgctgctg ctgtgtggag cagtcttcgt ttcgcccagc 60

caggaaatcc atgcccgatt cagaagagga gccagatctg aggtggtgct ggtgaacgtg 120

accgagaact tcaactggtg caagaacgac atggtggagc agatgcacga ggacatctgt 180

agcctgtggg accagagcct gaagccctgc gtgaagctgt gtcccctgtg cgtgggcgcc 240

ggcagctgca acaccagcgt gatcacccag gcctgcccca aggtgagctt cgagcccatc 300

cccatccact actgcgcccc cgctggcttc gccatcctga agtgcaacaa caagaccttc 360

aacggcaccg gcccctgcac caacgtgagc accgtgcagt gcacccacgg catccgcccc 420

gtggtgagca gtcagctgct gctgaacggc agcctggccg aggaggaggt ggtgatcaga 480

tcttgcaact tcaccgacaa cgccaagacc atcatcgtgc agctgaacac cagcgtggag 540

atcaactgca ccggcgccgg ccactgcaac atcgcccgcg ccaagtggaa caacaccctg 600

aagcagatcg ccagcaagct gcgcgagcag ttcggcaaca acaagaccat catcttcaag 660

cagagcagcg gcggcgaccc cgagatcgtg acccactggt tcaactgcgg cggcgagttc 720

ttctactgca acagcaccca gctgttcaac agcacctggt tcaacagcac ctggagcacc 780

gagggcagca acaacaccga gggcagcgac accatcaccc tgccctgccg catcaagcag 840

atcatcaaca tgtggtgtaa ggtgtgtaag atgatgtacg cccccccat cagcggccag 900

atccgctgca gcagcaacat caccggcctg ctgctgaccc gcgacggcgg caacagcaac 960

aacgagagcg agatcttccg tccgggcggc ggcgacatgc gcgacaactg gcgcagcgag 1020

ctgtacaagt acaaggtggt gaagatcgag tgag 1054

<210> SEQ ID NO 17
<211> LENGTH: 1053
<212> TYPE: DNA
<213> ORGANISM: Human immunodeficiency virus type 1

<400> SEQUENCE: 17

atgaagagag ggctctgctg tgtgctgctg ctgtgtggag cagtcttcgt ttcgcccagc 60

caggaaatcc atgcccgatt cagaagagga gccagatctg aggtggtgct ggtgaacgtg 120

accgagaact tcaactggtg caagaacgac atggtggagc agatgcacga ggacatcatc 180

agcctgtggg accagagcct gaagccctgc gtgaagcttt gtcccctgtg cgtgggcgcc 240

ggcagctgca acaccagcgt gatcacccag gcctgcccca aggtgagctt cgagcccatc 300

cccatccact actgcgcccc cgccggcttc gccatcctga agtgcaacaa ctgtaccttc 360

aacggtaccg gcccctgcac caacgtgagc accgtgcagt gcacccacgg catccgcccc 420

gtggtgagca gtcagctgct gctgaacggc agcctggcat gcgaggaggt ggtgatcaga 480

tcttgcaact tcaccgacaa cgccaagacc atcatcgtgc agctgaacac cagcgtggag 540

atcaactgca ccggcgccgg ccactgcaac atcgcccgcg ccaagtggaa caacaccctg 600

aagcagatcg ccagcaagct gcgcgagcag ttcggcaaca acaagaccat catcttcaag 660

cagagcagcg gcggcgaccc cgagatcgtg acccactggt tcaactgcgg cggcgagttc 720

ttctactgca acagcaccca gctgttcaac agcacctggt tcaacagcac ctggagcacc 780

gagggcagca acaacaccga gggcagcgac accatcaccc tgccctgccg catcaagcag 840

atcatcaata tgtggcagaa ggtgtgtaag gccatgtacg cccccccat cagcggccag 900

atccgctgca gcagcaacat caccggcctg ctgctgaccc gcgacggcgg caacagcaac 960

aacgagagcg agatcttccg tccgggcggc ggcgacatgc gcgacaactg gcgcagcgag 1020

ctgtacaagt acaaggtggt gaagatcgag tga 1053

<210> SEQ ID NO 18
<211> LENGTH: 1053

-continued

<212> TYPE: DNA
<213> ORGANISM: Human immunodeficiency virus type 1

<400> SEQUENCE: 18

atgaagagag ggctctgctg tgtgctgctg ctgtgtggag cagtcttcgt ttcgcccagc 60

caggaaatcc atgcccgatt cagaagagga gccagatctg aggtggtgct ggtgaacgtg 120

accgagaact tcaactggtg caagaacgac atggtggagc agatgcacga ggacatctgt 180

agcctgtggg accagagcct gaagccctgc gtgaagctgt gtcccctgtg cgtgggcgcc 240

ggcagctgca acaccagcgt gatcacccag gcctgcccca aggtgagctt cgagcccatc 300

cccatccact actgcgcccc cgccggcttc gccatcctga agtgcaacaa ctgtaccttc 360

aacggtaccg gcccctgcac caacgtgagc accgtgcagt gcacccacgg catccgcccc 420

gtggtgagca gtcagctgct gctgaacggc agcctggcat gcgaggaggt ggtgatcaga 480

tcttgcaact tcaccgacaa cgccaagacc atcatcgtgc agctgaacac cagcgtggag 540

atcaactgca ccggcgccgg ccactgcaac atcgcccgcg ccaagtggaa caacaccctg 600

aagcagatcg ccagcaagct gcgcgagcag ttcggcaaca acaagaccat catcttcaag 660

cagagcagcg gcggcgaccc cgagatcgtg acccactggt tcaactgcgg cggcgagttc 720

ttctactgca acagcaccca gctgttcaac agcacctggt tcaacagcac ctggagcacc 780

gagggcagca acaacaccga gggcagcgac accatcaccc tgccctgccg catcaagcag 840

atcatcaaca tgtggtgtaa ggtgtgtaag gccatgtacg ccccccccat cagcggccag 900

atccgctgca gcagcaacat caccggcctg ctgctgaccc gcgacggcgg caacagcaac 960

aacgagagcg agatcttccg tccgggcggc ggcgacatgc gcgacaactg gcgcagcgag 1020

ctgtacaagt acaaggtggt gaagatcgag tga 1053

<210> SEQ ID NO 19
<211> LENGTH: 1053
<212> TYPE: DNA
<213> ORGANISM: Human immunodeficiency virus type 1

<400> SEQUENCE: 19

atgaagagag ggctctgctg tgtgctgctg ctgtgtggag cagtcttcgt ttcgcccagc 60

caggaaatcc atgcccgatt cagaagagga gccagatctg aggtggtgct ggtgaacgtg 120

accgagaact tcaacatgtg gaagaacgac atggtggagc agatgcacga ggacatcatc 180

agcctgtggg accagagcct gaagccctgc gtgaagctga cccccctgtg cgtgggcgcc 240

ggcagctgca acaccagcgt gatcacccag gcctgcccca aggtgagctt cgagcccatc 300

cccatccact actgcgcccc cgccggcttc gccatcctga agtgcaacaa caagaccttc 360

aacggcaccg gcccctgcac caacgtgagc accgtgcagt gcacccacgg catccgcccc 420

gtggtgagca cccagctgct gctgaacggc agcctggccg aggaggaggt ggtgatccgc 480

agcgtgaact tcaccgacaa cgccaagacc atcatcgtgc agctgaacac cagcgtggag 540

atcaactgca ccggcgccgg ccactgcaac atcgcccgcg ccaagtggaa caacaccctg 600

aagcagatcg ccagcaagct gcgcgagcag ttcggcaaca acaagaccat catcttcaag 660

cagagcagcg gcggcgaccc cgagatcgtg acccacagct tcaactgcgg cggcgagttc 720

ttctactgca acagcaccca gctgttcaac agcacctggt tcaacagcac ctggagcacc 780

gagggcagca acaacaccga gggcagcgac accatcaccc tgccctgccg catcaagcag 840

atcatcaaca tgtggcagaa ggtgggcaag gccatgtacg ccccccccat cagcggccag 900

atccgctgca gcagcaacat caccggcctg ctgctgaccc gcgacggcgg caacagcaac 960

-continued

aacgagagcg agatcttccg tccgggcggc ggcgacatgc gcgacaactg gcgcagcgag 1020

ctgtacaagt acaaggtggt gaagatcgag tga 1053

<210> SEQ ID NO 20
<211> LENGTH: 317
<212> TYPE: PRT
<213> ORGANISM: Human immunodeficiency virus type 1

<400> SEQUENCE: 20

Glu Val Val Leu Val Asn Val Thr Glu Asn Phe Asn Met Trp Lys Asn
1 5 10 15

Asp Met Val Glu Gln Met His Glu Asp Ile Ile Ser Leu Trp Asp Gln
20 25 30

Ser Leu Lys Pro Cys Val Lys Leu Thr Pro Leu Cys Val Gly Ala Gly
35 40 45

Ser Cys Asn Thr Ser Val Ile Thr Gln Ala Cys Pro Lys Val Ser Phe
50 55 60

Glu Pro Ile Pro Ile His Tyr Cys Ala Pro Ala Gly Phe Ala Ile Leu
65 70 75 80

Lys Cys Asn Asn Lys Thr Phe Asn Gly Thr Gly Pro Cys Thr Asn Val
85 90 95

Ser Thr Val Gln Cys Thr His Gly Ile Arg Pro Val Val Ser Thr Gln
100 105 110

Leu Leu Leu Asn Gly Ser Leu Ala Glu Glu Glu Val Val Ile Arg Ser
115 120 125

Val Asn Phe Thr Asp Asn Ala Lys Thr Ile Ile Val Gln Leu Asn Thr
130 135 140

Ser Val Glu Ile Asn Cys Thr Gly Ala Gly His Cys Asn Ile Ser Arg
145 150 155 160

Ala Lys Trp Asn Asn Thr Leu Lys Gln Ile Ala Ser Lys Leu Arg Glu
165 170 175

Gln Phe Gly Asn Asn Lys Thr Ile Ile Phe Lys Gln Ser Ser Gly Gly
180 185 190

Asp Pro Glu Ile Val Thr His Ser Phe Asn Cys Gly Gly Glu Phe Phe
195 200 205

Tyr Cys Asn Ser Thr Gln Leu Phe Asn Ser Thr Trp Phe Asn Ser Thr
210 215 220

Trp Ser Thr Glu Gly Ser Asn Asn Thr Glu Gly Ser Asp Thr Ile Thr
225 230 235 240

Leu Pro Cys Arg Ile Lys Gln Ile Ile Asn Met Trp Gln Lys Val Gly
245 250 255

Lys Ala Met Tyr Ala Pro Pro Ile Ser Gly Gln Ile Arg Cys Ser Ser
260 265 270

Asn Ile Thr Gly Leu Leu Leu Thr Arg Asp Gly Gly Asn Ser Asn Asn
275 280 285

Glu Ser Glu Ile Phe Arg Pro Gly Gly Gly Asp Met Arg Asp Asn Trp
290 295 300

Arg Ser Glu Leu Tyr Lys Tyr Lys Val Val Lys Ile Glu
305 310 315

<210> SEQ ID NO 21
<211> LENGTH: 35
<212> TYPE: PRT
<213> ORGANISM: Human immunodeficiency virus type 1

<400> SEQUENCE: 21

Cys Thr Arg Pro Asn Asn Asn Thr Arg Lys Ser Ile His Ile Gly Pro
1 5 10 15

Gly Arg Ala Phe Tyr Thr Thr Gly Glu Ile Ile Gly Asp Ile Arg Gln
20 25 30

Ala His Cys
35

<210> SEQ ID NO 22
<211> LENGTH: 36
<212> TYPE: PRT
<213> ORGANISM: Human immunodeficiency virus type 1

<400> SEQUENCE: 22

Cys Thr Arg Pro Asn Asn Asn Thr Arg Lys Arg Ile Arg Ile Gln Arg
1 5 10 15

Gly Pro Gly Arg Ala Phe Val Thr Ile Gly Lys Ile Gly Asn Met Arg
20 25 30

Gln Ala His Cys
35

<210> SEQ ID NO 23
<211> LENGTH: 35
<212> TYPE: PRT
<213> ORGANISM: Human immunodeficiency virus type 1

<400> SEQUENCE: 23

Cys Thr Arg Pro Asn Asn Asn Thr Arg Lys Ser Ile Arg Ile Gly Pro
1 5 10 15

Gly Gln Ala Phe Tyr Ala Thr Gly Asp Ile Ile Gly Asp Ile Arg Gln
20 25 30

Ala His Cys
35

<210> SEQ ID NO 24
<211> LENGTH: 35
<212> TYPE: PRT
<213> ORGANISM: Human immunodeficiency virus type 1

<400> SEQUENCE: 24

Cys Thr Arg Pro Asn Asn Asn Thr Arg Lys Ser Ile His Ile Gly Pro
1 5 10 15

Gly Arg Ala Phe Tyr Thr Thr Gly Glu Ile Ile Gly Asp Ile Arg Gln
20 25 30

Ala His Cys
35

<210> SEQ ID NO 25
<211> LENGTH: 35
<212> TYPE: PRT
<213> ORGANISM: Human immunodeficiency virus type 1

<400> SEQUENCE: 25

Cys Thr Arg Pro Asn Asn Asn Thr Arg Lys Ser Ile Arg Ile Gly Pro
1 5 10 15

Gly Gln Thr Phe Tyr Ala Thr Gly Asp Ile Ile Gly Asp Ile Arg Gln
20 25 30

Ala His Cys
35

<210> SEQ ID NO 26

-continued

<211> LENGTH: 1077
<212> TYPE: DNA
<213> ORGANISM: Human immunodeficiency virus type 1

<400> SEQUENCE: 26

atgaagagag ggctctgctg tgtgctgctg ctgtgtggag cagtcttcgt ttcgcccagc 60

caggaaatcc atgcccgatt cagaagagga gccagatctg aggtggtgct ggtgaacgtg 120

accgagaact tcaactggtg caagaacgac atggtggagc agatgcacga ggacatctgt 180

agcctgtggg accagagcct gaagccctgc gtgaagctgt gtcctctggc cggcgccacc 240

agcgtgatca cccaggcctg ccccaaggtg agcttcgagc ccatccccat ccactactgc 300

gcccccgctg gcttcgccat cctgaagtgc aacaacaaga ccttcaacgg caccggcccc 360

tgcaccaacg tgagcaccgt gcagtgcacc cacggcatcc gccccgtggt gagcagtcag 420

ctgctgctga acggcagcct ggccgaggag gaggtggtga tcagatcttg caacttcacc 480

gacaacgcca agaccatcat cgtgcagctg aacaccagcg tggagatcaa ctgcacccgc 540

cccaacaacg gcggcagcgg cagcggcggc aacatgcgcc aggcccactg caacatcagc 600

cgcgccaagt ggaacaacac cctgaagcag atcgccagca agctgcgcga gcagttcggc 660

aacaacaaga ccatcatctt caagcagagc agcggcggcg accccgagat cgtgacccac 720

tggttcaact gcggcggcga gttcttctac tgcaacagca cccagctgtt caacagcacc 780

tggttcaaca gcacctggag caccgagggc agcaacaaca ccgagggcag cgacaccatc 840

accctgccct gccgcatcaa gcagatcatc aacatgtggt gtaaggtgtg taaggccatg 900

tacgcccccc ccatcagcgg ccagatccgc tgcagcagca acatcaccgg cctgctgctg 960

acccgcgacg gcggcaacag caacaacgag agcgagatct tccgtccggg cggcggcgac 1020

atgcgcgaca actggcgcag cgagctgtac aagtacaagg tggtgaagat cgagtga 1077

<210> SEQ ID NO 27
<211> LENGTH: 478
<212> TYPE: PRT
<213> ORGANISM: Human immunodeficiency virus

<400> SEQUENCE: 27

Leu Trp Val Thr Val Tyr Tyr Gly Val Pro Val Trp Lys Glu Ala Thr
1 5 10 15

Thr Thr Leu Phe Cys Ala Ser Asp Ala Lys Ala Tyr Asp Thr Glu Val
20 25 30

His Asn Val Trp Ala Thr His Ala Cys Val Pro Thr Asp Pro Asn Pro
35 40 45

Gln Glu Val Val Leu Val Asn Val Thr Glu Asn Phe Asn Met Trp Lys
50 55 60

Asn Asp Met Val Glu Gln Met His Glu Asp Ile Ile Ser Leu Trp Asp
65 70 75 80

Gln Ser Leu Lys Pro Cys Val Lys Leu Thr Pro Leu Cys Val Ser Leu
85 90 95

Lys Cys Thr Asp Leu Lys Asn Asp Thr Asn Thr Asn Ser Ser Ser Gly
100 105 110

Arg Met Ile Met Glu Lys Gly Glu Ile Lys Asn Cys Ser Phe Asn Ile
115 120 125

Ser Thr Ser Ile Arg Gly Lys Val Gln Lys Glu Tyr Ala Phe Phe Tyr
130 135 140

Lys Leu Asp Ile Ile Pro Ile Asp Asn Asp Thr Thr Ser Tyr Lys Leu
145 150 155 160

-continued

```
Thr Ser Cys Asn Thr Ser Val Ile Thr Gln Ala Cys Pro Lys Val Ser
                165                 170                 175

Phe Glu Pro Ile Pro Ile His Tyr Cys Ala Pro Ala Gly Phe Ala Ile
            180                 185                 190

Leu Lys Cys Asn Asn Lys Thr Phe Asn Gly Thr Gly Pro Cys Thr Asn
        195                 200                 205

Val Ser Thr Val Gln Cys Thr His Gly Ile Arg Pro Val Val Ser Thr
    210                 215                 220

Gln Leu Leu Leu Asn Gly Ser Leu Ala Glu Glu Glu Val Val Ile Arg
225                 230                 235                 240

Ser Val Asn Phe Thr Asp Asn Ala Lys Thr Ile Ile Val Gln Leu Asn
                245                 250                 255

Thr Ser Val Glu Ile Asn Cys Thr Arg Pro Asn Asn Asn Thr Arg Lys
            260                 265                 270

Arg Ile Arg Ile Gln Arg Gly Pro Gly Arg Ala Phe Val Thr Ile Gly
        275                 280                 285

Lys Ile Gly Asn Met Arg Gln Ala His Cys Asn Ile Ser Arg Ala Lys
    290                 295                 300

Trp Asn Asn Thr Leu Lys Gln Ile Ala Ser Lys Leu Arg Glu Gln Phe
305                 310                 315                 320

Gly Asn Asn Lys Thr Ile Ile Phe Lys Gln Ser Ser Gly Gly Asp Pro
                325                 330                 335

Glu Ile Val Thr His Ser Phe Asn Cys Gly Gly Glu Phe Phe Tyr Cys
            340                 345                 350

Asn Ser Thr Gln Leu Phe Asn Ser Thr Trp Phe Asn Ser Thr Trp Ser
        355                 360                 365

Thr Glu Gly Ser Asn Asn Thr Glu Gly Ser Asp Thr Ile Thr Leu Pro
    370                 375                 380

Cys Arg Ile Lys Gln Ile Ile Asn Met Trp Gln Lys Val Gly Lys Ala
385                 390                 395                 400

Met Tyr Ala Pro Pro Ile Ser Gly Gln Ile Arg Cys Ser Ser Asn Ile
                405                 410                 415

Thr Gly Leu Leu Leu Thr Arg Asp Gly Gly Asn Ser Asn Asn Glu Ser
            420                 425                 430

Glu Ile Phe Arg Pro Gly Gly Gly Asp Met Arg Asp Asn Trp Arg Ser
        435                 440                 445

Glu Leu Tyr Lys Tyr Lys Val Val Lys Ile Glu Pro Leu Gly Val Ala
    450                 455                 460

Pro Thr Lys Ala Lys Arg Arg Val Val Gln Arg Glu Lys Arg
465                 470                 475
```

We claim:

1. An isolated immunogen comprising a HIV-1 gp120 polypeptide or immunogenic fragment thereof stabilized in a CD4-bound conformation by crosslinked cysteines, wherein the gp120polypeptide or immunogenic fragment thereof comprises cysteines for the amino acids in at least one of residue pairs 96 and 275; 109 and 428; 123 and 431; and 231 and 267, and amino acid substitutions at positions 257 and 375, and wherein the residue numbers correspond to amino acid positions in the amino acid sequence set forth as SEQ ID NO: 27.

2. The isolated immunogen of claim **1**, having a substitution of serine for the amino acid at position 257 and a substitution of tryptophan for the amino acid at position 375.

3. The isolated immunogen of claim **1**, further comprising an amino acid substitution at position 95, 433, or a combination thereof.

4. The isolated immunogen of claim **3**, wherein the substitution at position 95 is a tryptophan substitution and the substitution at position 433 is a methionine substitution.

5. The isolated immunogen of claim **1**, wherein the gp120 polypeptide or immunogenic fragment thereof is encoded by a nucleic acid sequence set forth as one of SEQ ID NOs: 4-9 and 11-18, or any degenerate variant of SEQ ID NOs: 4-9 and 11-18.

6. The isolated immunogen of claim **1**, wherein the gp120 polypeptide or immunogenic fragment thereof is encoded by a nucleic acid sequence set forth as SEQ ID NO: 10, or a degenerate variant of SEQ ID NO: 10.

7. The isolated immunogen according to claim 1, wherein the gp120 polypeptide or immunogenic fragment thereof comprises the gp120 Hxbc core of SEQ ID NO: 20, having substitutions of cysteines for the amino acids at positions 96, 109, 275, and 428.

8. The isolated immunogen according to claim 1, wherein the gp120 polypeptide or immunogenic fragment thereof comprises the gp120 Hxbc core of SEQ ID NO: 20having substitutions of cysteines for the amino acids at positions 96, 109, 275, and 428, a tryptophan for the amino acid at position 95, a serine for the amino acid at position 257, a tryptophan for the amino acid at position 375, and a methionine for the amino acid at position 433.

9. The isolated immunogen according to claim 1, wherein the immunogenic fragment comprises residues 255-421 and 436-474 of gp120 covalently linked at residues 421 and 436.

10. The isolated immunogen according to claim 9, wherein residues 421 and 436 of the immunogenic fragment are covalently linked by a peptide linker.

11. The isolated immunogen according to claim 1, wherein the gp120 polypeptide comprises at least two pairs of crosslinked cysteine residues.

12. The isolated immunogen according to claim 1, wherein the gp120 polypeptide comprises at least three pairs of crosslinked cysteine residues.

13. The isolated immunogen according to claim 1, wherein the gp120 polypeptide comprises at least four pairs of crosslinked cysteine residues.

14. The isolated immunogen according to claim 1, wherein the immunogen is further covalently linked to a carrier, Toll like receptor ligand, dendritic cell, or B cell targeting moiety.

15. The isolated immunogen according to claim 1, wherein the immunogen is glycosylated.

16. The isolated immunogen according to claim 15, wherein the immunogen is glycosylated at one or more of amino acid residue positions 92, 97, 103, 114, 201, 206, 210, 222, 246, 267, 419, 420, 422, 423, 434, or 442 of the gp120 polypeptide.

17. A composition comprising the immunogen of claim 1 and a pharmaceutically acceptable carrier.

18. A method for generating an immune response in a subject, comprising administering to the subject a therapeutically effective amount of the immunogen of claim 1, thereby generating the immune response.

19. The method of claim 18, further comprising administering a therapeutically effective amount of a polypeptide comprising:

a) a monomeric or trimeric gp140 polypeptide;

b) an monomeric or trimeric gp120 polypeptide; or

c) a soluble form of CD4; or

d) any combination of a-c, above.

20. The method of claim 18, wherein the subject is a human subject.

* * * * *