Molecular Recognition of CXCR4 by a Dual Tropic HIV-1 gp120 V3 Loop

Supporting Material

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Supporting Text

Supporting Material on Methods, Step2 :

V3 loop: We employed 16 replicas with the following temperatures: 288, 300, 312, 325, 338, 352, 366, 381, 396, 412, 428, 445, 462, 480, 498, 517 K. Replica exchanges were attempted at 10-ps intervals and the total simulation length for all temperatures was equal to 0.8μs. We extracted 5000 snapshots (conformations), at 10-ps intervals, from the 50 ns replica simulations at 300 K. The peptide dielectric constant was set to $\varepsilon=2$ and a non-polar solvation energy surface term was included, with a surface-tension coefficient of 0.015 kcal/mol*Å^2; in addition, 7.5-Å cutoff was used for the non-bonded interactions in conjunction with the FACTS19 parametrization[1]. The peptide atomic charges, van der Waals and stereochemical parameters were taken from the CHARMM19 all-atom force field [2] in consistency with the FACTS 19 parametrization[1]. The equations of motion were integrated by the leap-frog algorithm, with a 2.0-fs timestep. Bonds involving hydrogen atoms were constrained to standard values with the SHAKE algorithm [3]. The temperature was controlled by the Langevin method; the friction coefficients were set to 5.0 ps^{-1} for heavy atoms and 0 ps^{-1} for hydrogen atoms.

CXCR4: Standard amino acids were described by the CHARMM27 all-atom topology and energy function [4] including the CMAP correction [5]. Sulfated tyrosine residues 7, 12, 21, denotes as "Tys", were parametrized using a combination of the standard tyrosine parameters and the methylsulfate parameters presented in CHARMM36 CGENFF force field [6]. A 16-Å cutoff distance was used for non-bonded interactions. The lengths of covalent bonds containing hydrogen atoms were constrained by the *SHAKE* algorithm [3], and the equations of motion were solved with an integration time step of 2.0 fs. The system was in contact with a Langevin heat bath at 300 K during the production and equilibration runs, and in addition, a friction coefficient of 5 ps^{-1} was used for heavy atoms. Prior to the production runs, four heating steps of total duration 400 ps were performed, and in addition, an equilibration procedure of a total duration of 1.7 ns was performed, during which the harmonic restraints were gradually removed. The production runs were performed at 300K with a total duration of 5 ns. The difference between the two independent simulations per complex was on the restraints imposed during the production runs: in the first simulation, no restraints were imposed on the system, whereas in the

second simulation, a weak harmonic force constant of 1 kcal/mol*A^2 was applied to the Cα atoms using the bestfit module in CHARMM [8].

Supporting Material on Methods, Step3 :

We merged the structures produced in the V3 loop replica exchange MD simulations in a single trajectory containing 5000 V3 loop structures. In addition, we merged the CXCR4 structures produced from the six independent aforesaid MD simulations in single trajectory containing 1500 CXCR4 structures. We employed the quality clustering method of WORDOM [7], to cluster independently the V3 loop and CXCR4 structures based on their Cα coordinates. For the V3 loop clustering, we included all Cα atoms and used a relatively large clustering radius of 2.0 Å, owing to the high flexibility of the V3 loop structures. We extracted the 20 most populated clusters for the V3 loop, with the smallest cluster acquiring a 0.09% percentage probability. For the CXCR4 clustering, we considered all Cα atoms with a z-coordinate value greater than 0 Å. The cluster analysis produced 17 clusters for CXCR4, including the initially modeled CXCR4 structure.

Supporting Material on Methods, Step5 :

In the PB calculations, we inserted the complex and protein in a membrane slab with a thickness of 31 Å (31≈36.0-2*(2.5), where 36.0 Å and 2.5 Å correspond to the membrane thickness and the half of membrane switching length, parameters used in the GBSW approximation). The membrane slab used in the PBSA calculations possessed a dielectric constant of 2, and was surrounded by water, with a dielectric constant of 80. The protein dielectric constant was set to 2. The PBSA calculations were performed with the Poisson-Boltzmann solver of the CHARMM program (PBEQ module) [8]. We used 250 grid points in each direction and a grid-spacing of 0.5 Å.

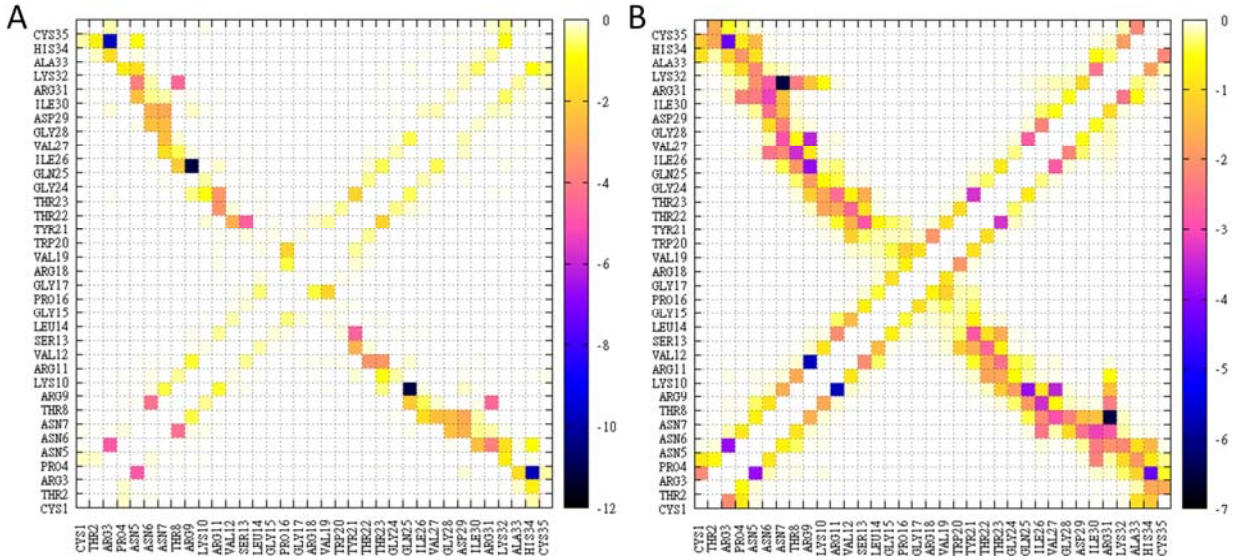
It is worth noting that in the initial set of 680,000 complexes, the docking of V3 loop performed by Zdock [9] was not in all cases in accordance with the experimentally defined binding pocket of CXCR4 [10]. Nevertheless, the binding free energy calculations showed that the binding free energies of the complex structures at which the V3 loop was outside of the binding pocket, was evidently higher compared to the binding free energy of the 17 complexes selected.

CXCR4 and V3 loop domains:

CXCR4 residues, denoted in brackets, can be approximately divided into the following domains: (i) N-terminal domain [1:37], (ii) Intramembrane helix 1 [38:65]; (iii) Intracellular loop 1 [66:71]; (iv) Intramembrane helix 2 [72:100], (v) Extracellular loop 1 (ECL1) [101:106]; (vi) Intramembrane helix 3 [107:137]; (vii) Intracellular loop 2 [138:146]; (viii) Intramembrane helix 4 [147:174]; (ix) Extracellular loop 2 (ECL2) [175:194]; (x) Intramembrane helix 5 [195:224]; (xi) Intracellular loop 3 [225:236]; (xii) Intramembrane helix 6 [237:265]; (xiii) Extracellular loop 3 (ECL3) [266:276]; (xiv) Intramembrane helix 7 [277:303]; (xv) C-terminal domain [304:352]. Regarding the V3 loop, the structure can be approximately divided into the following regions: (i) The base domain [1:4 and 31:35]; (ii) Stems [5:12 and 23:30] (iii) Tip [13:22]. According to the results of this study, the core region of the tip comprises residues 16-20.

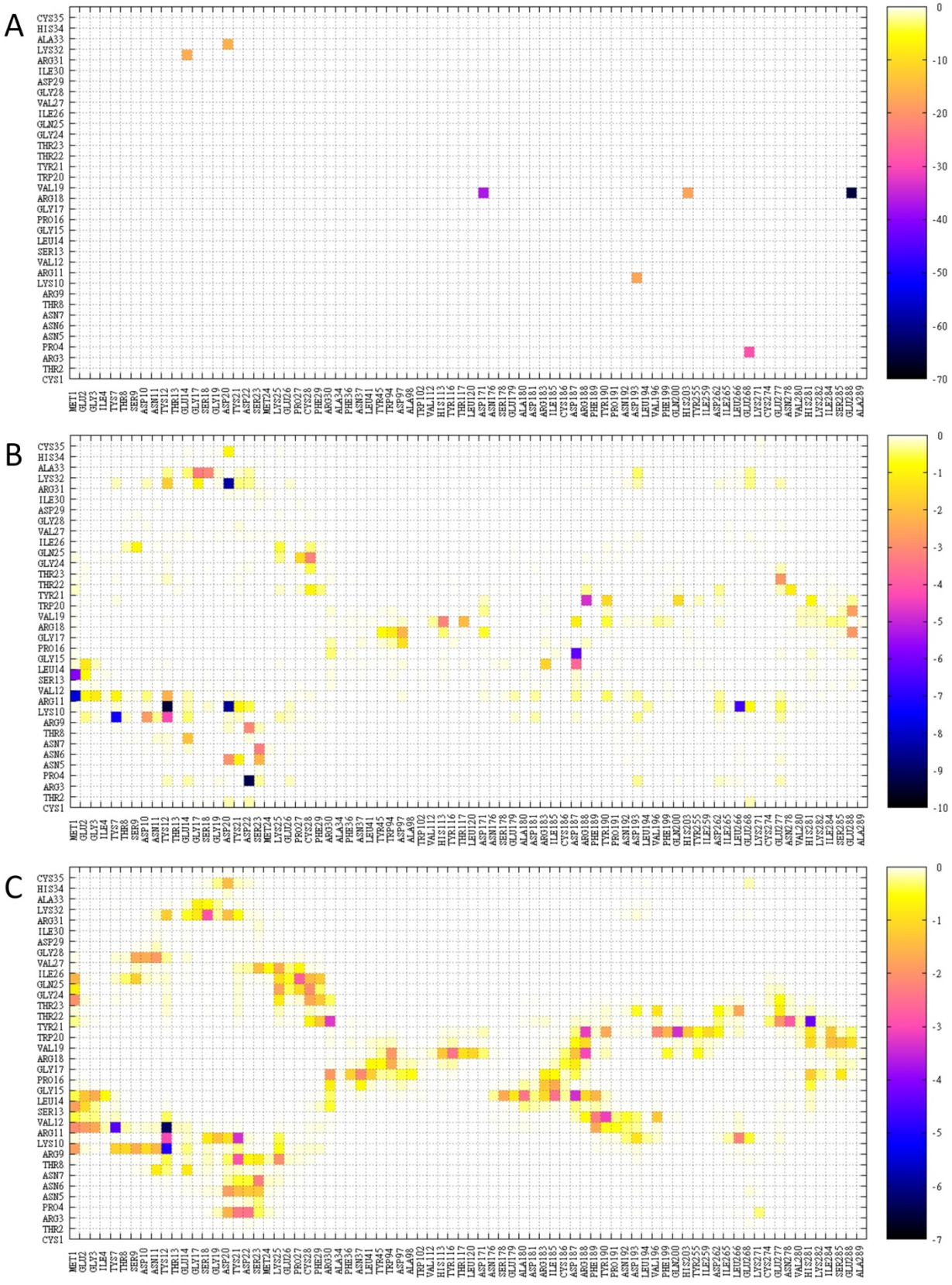
Supporting Figures

Supporting Figure 1:



Supporting Figure 1: Two dimensional density maps depicting the favorable (negative) average MM GBSA interaction free-energies for intramolecular V3 loop interacting residue pairs, within the simulation of the complex with the lowest average binding free energy. The left (A) and right (B) panels correspond, respectively, to polar and non-polar interactions. All energies are in kcal/mol. The color – interaction free energy correspondence is shown by the palette on the right-hand side of each panel. Interactions free energies were not calculated for pairs of covalently bonded residues. All values have been computed by analysis of 1000 snapshots, extracted from the 20-ns simulation of complex 1 at 20-ps intervals.

Supporting Figure 2:



Supporting Figure 2: Two dimensional density maps depicting the favorable (negative) average MM GBSA interaction free-energies for intermolecular V3 loop (y axis) : CXCR4 (x axis) interacting residue pairs, within the simulation of the complex with the lowest average binding free energy. The upper (A), middle (B) and bottom (C) panels correspond, respectively, to highly interacting polar [-70 kcal/mol : -10 kcal/mol], moderate interacting polar [-10 kcal/mol : 0 kcal/mol], and non-polar interactions. All energies are in kcal/mol. The color – interaction free energy correspondence is shown by the palette on the right-hand side of each panel. All values have been computed by analysis of 1000 snapshots, extracted from the 20-ns simulation of complex 1 at 20-ps intervals.

Supporting Tables

Supporting Table 1:

Binding free energies using the PBSA, MM GBSA and MM PBSA approximations for V3 loop : CXCR4 complexes in kcal/mol. All values have been computed by analysis of 1000 snapshots, extracted from the 20-ns simulation (of all complexes) at 20-ps intervals.

	Docking and Minimization[¶]			MD Simulations[†]				
	PBSA			MM PB/GBSA (Non-Polar)[‡]	MM GBSA[ǂ] (Polar and Total)		MM PBSA[#] (Polar and Total)	
	Non-Polar	Polar	Total	Non- polar	Polar	Total	Polar	Total
1[§]	-134.3	-10.0	-144.2	-269.0 (10.2)	-157.9 (19.8)	**-427.0 (22.4)**	-98.1 (11.1)	**-367.2 (12.9)**
2	-124.0	-19.8	-143.8	-230.7 (19.9)	-99.3 (11.4)	-330.1 (22.1)	-47.8 (16.1)	-278.5 (15.5)
3	-98.9	-44.7	-143.5	-210.8 (16.1)	-123.8 (13.4)	-334.6 (19.6)	-105.5 (9.3)	-316.3 (16.3)
4	-130.4	-12.2	-142.6	-269.3 (12.3)	-124.6 (13.8)	-393.8 (13.9)	-86.2 (10.5)	-355.5 (12.4)
5	-138.3	-4.0	-142.3	-225.5 (11.5)	-111.3 (22.0)	-336.9 (28.2)	-49.7 (9.8)	-275.2 (10.5)
6	-121.3	-19.9	-141.2	-225.7 (10.9)	-122.4 (14.7)	-348.2 (14.8)	-73.0 (9.1)	-298.7 (12.3)
7	-94.3	-46.6	-140.9	-229.2 (15.2)	-102.7 (16.7)	-331.9 (21.7)	-85.9 (10.2)	-315.1 (15.6)
8	-99.4	-39.5	-138.9	-231.8 (14.3)	-96.3 (15.2)	-328.2 (16.3)	-43.9 (15.4)	-275.8 (12.6)
9	-108.4	-28.4	-136.8	-233.6 (16.6)	-105.1 (13.3)	-338.6 (17.8)	-80.9 (12.5)	-314.4 (19.0)
10	-138.1	1.6	-136.5	-223.1 (10.0)	-62.3 (15.9)	-285.4 (19.5)	-25.8 (10.5)	-248.9 (13.6)
11	-119.6	-16.6	-136.2	-253.1 (10.4)	-107.3 (16.8)	-360.5 (16.0)	-80.1 (12.0)	-333.3 (13.9)
12	-123.5	-12.3	-135.8	-245.0 (12.4)	-134.9 (14.4)	-379.9 (16.2)	-109.6 (13.1)	-354.6 (16.2)
13	-137.8	2.0	-135.8	-235.0 (13.5)	-142.3 (18.3)	-377.3 (23.8)	-63.3 (21.0)	-298.2 (16.0)
14	-98.2	-37.3	-135.5	-217.2 (14.3)	-142.4 (16.8)	-359.6 (23.7)	-102.5 (10.4)	-319.7 (18.6)
15	-125.4	-9.9	-135.4	-239.7 (8.8)	-112.5 (15.8)	-352.2 (16.4)	-67.5 (8.7)	-307.2 (11.0)
16	-136.6	2.0	-134.6	-246.9 (12.8)	-109.1 (14.7)	-356 (18.0)	-49.1 (9.7)	-296.0 (15.1)
17	-136.5	2.5	-134.1	-233.0 (12.3)	-113.4 (14.3)	-346.4 (20.0)	-59.9 (9.8)	-292.9 (10.9)

The binding free energies are calculated as described in Methods. The numbering[§] (1-17) is sorted according to the total binding free energy, using the PBSA approximation, of the docked complexes after minimization, referred as step 5[¶]; the total binding free energy is the sum of non-polar and polar contributions of step 5. The MD simulation[†] results correspond the average binding free energies of the 17 complexes based on 20-ns MD simulation runs, referred as step 7, and were calculated both using MM PBSA[ǂ] and MM GBSA[#] methods.; the standard deviation is shown in parentheses. The non-polar component[‡] is the same in MM PBSA[ǂ] and MM GBSA[#]. For each calculation, MM GBSA[ǂ] or MM PBSA[#], the polar component is calculated using a different approach, thus, the total binding free energy, which is the sum of polar and non-polar

components for each approach is different, as well. According to both methods, the average total binding free energy of the first complex, marked in **bold** face, is the lowest.

Supporting Table 2:

Average and standard deviation values of Root Mean Square Deviation (RMSD) between the simulation coordinates of main-chain heavy atoms (N, Cα, and C) and their corresponding coordinates from the first simulation frame after equilibration. All values have been computed by analysis of 1000 snapshots (per complex), extracted from the 20-ns simulations at 20-ps intervals.

Complex	Protein Intramembrane		Protein N-terminal, residues 1 -37		V3 loop		V3 loop, residues: 8-26	
	Average	St. Deviation	Average	St. Deviation	Average	St. Deviation	Average	St. Deviation
1	1.31	0.03	3.65	0.29	3.86	0.27	2.9	0.14
2	1.09	0.01	3.34	0.28	4.99	0.91	3.57	0.31
3	1.32	0.07	4.5	0.65	5.61	0.75	3.15	1.44
4	1.16	0.02	2.92	0.1	2.12	0.16	1.56	0.04
5	0.93	0.01	2.06	0.11	5.14	0.36	1.79	0.07
6	1.11	0.02	3.3	0.4	3.5	0.29	2.77	0.18
7	1.33	0.03	7.43	0.59	7.02	1.76	3.04	0.42
8	1.19	0.02	2.96	0.25	8.01	0.86	2.52	0.15
9	1.17	0.01	3.96	0.35	6.8	0.48	5	0.29
10	0.95	0.02	3.51	0.45	4.34	2.41	1.71	0.15
11	1.06	0.01	3.76	0.15	4.48	0.24	3.53	0.2
12	1.09	0.02	2.39	0.1	4.27	0.51	2.73	0.09
13	1.22	0.02	3.78	0.43	5.42	3.69	1.58	0.09
14	1.29	0.05	4.63	0.39	5.27	0.47	4.62	0.52
15	1.04	0.01	2.99	0.14	5.43	1.29	1.78	0.08
16	1.16	0.01	2.04	0.07	8.05	2.36	1.32	0.04
17	1.09	0.01	1.87	0.05	3.82	0.16	2.23	0.07

The coordinates of the simulated systems are aligned with regard to the intramembrane backbone CXCR4 atoms of the first simulation frame. All values corresponding to protein N-terminal, V3 loop and V3 loop residues 8-26, are computed without any additional rotation/translation and are averaged over the 20 ns of the simulation trajectories. All values are reported in Å.

Supporting Table 3:

Percentage (%) hydrogen bond occupancy of important intermolecular hydrogen-bonding atom pairs within the 17 simulated complexes. Hydrogen bonding atom pairs with less than 10% are not reported. We present the hydrogen bond occupancies for each complex in a separate table and sort the hydrogen bonding atom pairs, firstly, with respect to the residue number of the V3 loop atom, and secondly, the residue number of the CXCR4 atom. All values have been computed by analysis of 1000 snapshots (per complex), extracted from the 20-ns simulations at 20-ps intervals. A hydrogen bond was present if the donor (D)–acceptor (A) distance was less than 3.5 Å and the corresponding angle (D–H ··· A) was larger than 90°. Hydrogen bond interactions associated with salt-bridge formation are highlighted in grey background.

Complex 1:

V3 loop Residue	Number	Group	Atom	CXCR4 Residue	Number	Group	Atom	Occupancy (%)
ARG	3	Side	NH2	ASP	22	Side	OD1	40.86
ARG	3	Side	NH2	ASP	22	Side	OD2	40.66
ARG	3	Side	NH2	GLU	268	Side	OE2	87.81
ARG	3	Side	NH1	GLU	268	Side	OE1	87.21
ARG	3	Side	NH2	GLU	268	Side	OE1	64.54
ARG	3	Side	NH1	GLU	268	Side	OE2	60.94
ASN	5	Side	ND2	ASP	20	Side	OD1	52.75
ASN	5	Side	ND2	ASP	20	Side	OD2	12.79
ASN	5	Side	ND2	TYS	21	Main	O	23.08
ASN	6	Main	N	SER	23	Side	OG	68.73
ASN	6	Side	OD1	SER	23	Side	OG	18.08
ASN	6	Side	ND2	SER	23	Side	OG	9.69
ASN	7	Side	OD1	ASN	11	Side	ND2	11.39
ASN	7	Side	ND2	GLU	14	Side	OE1	35.16
ASN	7	Side	ND2	GLU	14	Side	OE2	18.98
THR	8	Side	OG1	ASP	22	Main	O	61.04
ARG	9	Side	NH1	TYS	7	Main	O	84.62
ARG	9	Side	NH2	TYS	7	Main	O	57.14
ARG	9	Side	NH1	ASP	10	Main	O	65.13
LYS	10	Main	N	TYS	12	Side	OS3	85.71
LYS	10	Main	N	TYS	12	Side	OS2	11.09
LYS	10	Side	NZ	ASP	20	Main	O	95.3
LYS	10	Side	NZ	ASP	193	Side	OD1	97.8
LYS	10	Side	NZ	LEU	266	Main	O	94.21
ARG	11	Side	NH1	MET	1	Main	O	92.61
ARG	11	Side	NH2	MET	1	Main	O	48.05
ARG	11	Side	NE	MET	1	Main	O	13.69
ARG	11	Side	NH1	GLU	2	Main	O	10.79

ARG	11	Main	N	TYS	12	Side	OS3	23.88
SER	13	Side	OG	MET	1	Main	N	51.95
LEU	14	Main	N	GLU	2	Main	O	24.88
LEU	14	Main	O	ARG	183	Side	NH1	41.26
LEU	14	Main	O	ARG	183	Side	NH2	32.57
GLY	15	Main	N	ASP	187	Side	OD1	56.64
GLY	15	Main	N	ASP	187	Side	OD2	42.06
PRO	16	Main	N	ASN	37	Side	ND2	11.89
GLY	17	Main	N	TYR	45	Side	OH	11.79
GLY	17	Main	N	ASP	97	Side	OD2	25.47
ARG	18	Side	NH1	THR	117	Side	OG1	84.12
ARG	18	Side	NH1	THR	117	Side	OG1	29.47
ARG	18	Side	NH1	ASP	171	Side	OD1	69.63
ARG	18	Side	NH1	ASP	171	Side	OD2	55.04
ARG	18	Main	O	ARG	188	Side	NH2	99.1
ARG	18	Main	O	ARG	188	Side	NE	93.61
ARG	18	Side	NH2	HIS	203	Side	NE2	94.71
ARG	18	Side	NH1	HIS	203	Side	NE2	88.51
ARG	18	Side	NH2	TYR	255	Side	OH	71.23
ARG	18	Side	NH2	GLU	288	Side	OE2	99.4
ARG	18	Side	NE	GLU	288	Side	OE1	94.51
ARG	18	Side	NE	GLU	288	Side	OE2	62.34
ARG	18	Side	NH2	GLU	288	Side	OE1	34.17
TRP	20	Side	NE1	ARG	188	Side	NH2	53.95
TRP	20	Side	NE1	ARG	188	Side	NH1	10.69
TRP	20	Side	NE1	TYR	190	Side	OH	52.85
TRP	20	Main	O	HIS	281	Side	ND1	21.18
TYR	21	Side	OH	ASN	278	Side	ND2	52.95
TYR	21	Side	OH	ASN	278	Side	ND2	33.17
TYR	21	Side	OH	ASN	278	Side	OD1	21.58
THR	22	Side	OG1	GLU	277	Side	OE1	27.17
THR	23	Side	OG1	CYS	28	Main	O	18.08
GLY	24	Main	O	CYS	28	Main	N	94.61
GLY	24	Main	N	CYS	28	Main	O	15.58
GLN	25	Side	NE2	CYS	28	Main	O	11.59
ARG	31	Side	NE	GLU	14	Side	OE1	71.43
ARG	31	Side	NH2	GLU	14	Side	OE1	67.33
ARG	31	Side	NE	GLU	14	Side	OE2	57.84
ARG	31	Side	NH2	GLU	14	Side	OE2	30.17
ARG	31	Side	NH1	SER	18	Side	OG	12.69
ARG	31	Side	NH1	ASP	20	Side	OD1	47.25
LYS	32	Side	NZ	GLY	17	Main	O	53.55
LYS	32	Side	NZ	SER	18	Main	O	52.45
LYS	32	Side	NZ	ASP	20	Side	OD2	84.12
LYS	32	Side	NZ	ASP	20	Side	OD1	46.65
HIS	34	Side	ND1	ASP	20	Side	OD2	14.19

Complex 2:

V3 loop Residue	Number	Group	Atom	CXCR4 Residue	Number	Group	Atom	Occupancy (%)
ARG	3	Side	NH2	THR	13	Main	O	20.78
ARG	3	Side	NH1	GLU	14	Side	OE1	50.45
ARG	3	Side	NH2	GLU	14	Side	OE1	44.66
ARG	3	Side	NH2	GLU	14	Side	OE2	41.06
ARG	3	Side	NH1	GLU	14	Side	OE2	36.66
ASN	5	Side	ND2	ASN	11	Main	O	16.48
ASN	5	Side	OD1	ASN	11	Side	ND2	27.7
ASN	5	Side	ND2	TYS	12	Main	O	52
ASN	6	Main	N	TYS	12	Main	O	21.58
ASN	6	Main	O	TYS	12	Main	N	13.79
ASN	6	Side	ND2	TYS	12	Main	O	10.99
ASN	6	Side	ND2	GLU	14	Side	OE2	16.88
ASN	6	Side	ND2	GLU	14	Side	OE1	14.19
THR	8	Main	O	THR	8	Side	OG1	19.78
THR	8	Side	OG1	SER	9	Main	N	13.29
THR	8	Side	OG1	ASP	10	Main	N	29.67
THR	8	Side	OG1	ASP	10	Side	OD1	47.25
THR	8	Main	N	ASN	11	Side	OD1	12.19
THR	8	Side	OG1	ASN	11	Main	N	13.39
ARG	9	Side	NH2	ASP	22	Main	O	28.07
ARG	9	Side	NH2	SER	23	Main	O	13.39
ARG	9	Side	NH1	MET	24	Main	O	17.28
ARG	9	Side	NH2	MET	24	Main	O	12.09
ARG	9	Side	NH2	LYS	25	Main	O	62.14
ARG	9	Side	NH1	LYS	25	Main	O	44.66
ARG	9	Side	NE	LYS	25	Main	O	14.59
LYS	10	Side	NZ	GLU	2	Side	OE2	27.57
LYS	10	Side	NZ	GLU	2	Side	OE1	22.98
LYS	10	Side	NZ	ILE	6	Main	O	17.58
ARG	11	Side	NH1	TYS	21	Side	OS3	43.46
ARG	11	Side	NH1	TYS	21	Side	OS2	42.16
ARG	11	Side	NH2	TYS	21	Side	OS2	29.27
ARG	11	Side	NH2	TYS	21	Side	OS3	25.37
ARG	11	Side	NH1	TYS	21	Side	OS4	14.39
ARG	11	Side	NH2	TYS	21	Side	OS4	9.89
ARG	11	Side	NH1	GLU	277	Side	OE1	81.72
ARG	11	Side	NH1	GLU	277	Side	OE2	62.54
ARG	11	Side	NE	GLU	277	Side	OE1	14.29
VAL	12	Main	N	CYS	28	Main	O	80.32
LEU	14	Main	N	GLU	277	Side	OE2	40.66
LEU	14	Main	N	GLU	277	Side	OE1	22.28
GLY	15	Main	O	HIS	281	Side	ND1	84.12
GLY	17	Main	O	ASN	37	Side	ND2	66.13
GLY	17	Main	O	ARG	183	Side	NH2	46.35
GLY	17	Main	N	SER	285	Side	OG	75.02

GLY	17	Main	N	GLU	288	Side	OE2	19.37
ARG	18	Side	NE	TYR	45	Side	OH	12.29
ARG	18	Side	NH1	TRP	94	Side	NE1	24.68
ARG	18	Side	NH2	TYR	116	Side	OH	95
ARG	18	Main	O	ARG	183	Side	NH1	72.83
ARG	18	Main	O	ARG	183	Side	NH2	26.37
ARG	18	Side	NH2	TYR	255	Side	OH	55.14
ARG	18	Side	NH2	TYR	255	Side	OH	54.25
ARG	18	Side	NE	GLU	288	Side	OE1	99.7
ARG	18	Side	NH2	GLU	288	Side	OE2	99.5
ARG	18	Side	NE	GLU	288	Side	OE2	74.13
ARG	18	Side	NH2	GLU	288	Side	OE1	30.17
TRP	20	Side	NE1	ARG	183	Side	NH2	37.16
TRP	20	Main	N	ASP	187	Side	OD1	10.39
TRP	20	Side	NE1	HIS	281	Side	NE2	14.59
TYR	21	Side	OH	ARG	188	Side	NH2	45.05
TYR	21	Side	OH	TYR	190	Side	OH	10.79
TYR	21	Side	OH	GLN	200	Side	OE1	89.41
THR	22	Side	OG1	SER	178	Side	OG	70.53
THR	22	Main	N	ASP	187	Side	OD2	47.15
THR	22	Main	N	ASP	187	Side	OD1	29.27
THR	22	Side	OG1	ASP	187	Side	OD1	45.75
THR	22	Side	OG1	ASP	187	Side	OD2	44.36
THR	23	Side	OG1	ARG	188	Main	O	32.67
THR	23	Side	OG1	TYR	190	Main	N	69.43
GLN	25	Side	NE2	LYS	25	Main	O	16.08
GLN	25	Side	NE2	ASP	193	Side	OD1	10.29
ILE	26	Main	N	ASP	193	Side	OD2	26.07
ILE	26	Main	N	ASP	193	Side	OD1	18.68
GLY	28	Main	N	ASP	22	Main	O	52.05
GLY	28	Main	N	SER	23	Main	O	30.07
GLY	28	Main	N	SER	23	Side	OG	18.28
ASP	29	Main	N	SER	23	Main	O	33.97
ASP	29	Main	N	SER	23	Side	OG	15.58
ARG	31	Side	NH2	SER	23	Main	O	20.78
LYS	32	Side	NZ	GLU	14	Side	OE1	10.69

Complex 3:

V3 loop Residue	Number	Group	Atom	CXCR4 Residue	Number	Group	Atom	Occupancy (%)
ARG	3.00	Side	NH1	ASP	22.00	Main	O	43.36
ARG	3.00	Side	NH2	ASP	22.00	Side	OD2	99.30
ARG	3.00	Side	NH1	ASP	22.00	Side	OD1	95.70
ARG	3.00	Side	NH2	ASP	22.00	Side	OD1	77.42
ARG	3.00	Side	NH1	ASP	22.00	Side	OD2	22.78
ARG	3.00	Side	NH1	GLU	268.00	Side	OE1	81.62
ARG	3.00	Side	NE	GLU	268.00	Side	OE1	80.62
ARG	3.00	Side	NH1	GLU	268.00	Side	OE2	80.32
ARG	3.00	Side	NE	GLU	268.00	Side	OE2	14.39
ASN	6.00	Main	N	ASP	22.00	Side	OD2	90.21
ASN	6.00	Side	ND2	ASP	22.00	Side	OD1	14.29
ASN	7.00	Side	ND2	ASP	20.00	Side	OD2	19.28
ASN	7.00	Side	ND2	ASP	20.00	Side	OD1	15.68
THR	8.00	Main	N	ASP	20.00	Main	O	11.69
THR	8.00	Main	N	ASP	20.00	Side	OD1	41.96
THR	8.00	Main	N	ASP	20.00	Side	OD2	37.06
THR	8.00	Side	OG1	TYS	21.00	Main	O	58.94
THR	8.00	Side	OG1	TYS	21.00	Main	N	46.55
THR	8.00	Side	OG1	TYS	21.00	Main	N	18.58
ARG	9.00	Side	NH1	TYS	7.00	Main	O	13.09
ARG	9.00	Side	NH1	THR	8.00	Main	O	21.68
ARG	9.00	Side	NH2	ASP	10.00	Side	OD2	73.73
ARG	9.00	Side	NH2	ASP	10.00	Side	OD1	68.23
ARG	9.00	Side	NE	ASP	10.00	Side	OD1	64.54
ARG	9.00	Side	NE	ASP	10.00	Side	OD2	49.05
LYS	10.00	Side	NZ	GLY	19.00	Main	O	48.95
LYS	10.00	Side	NZ	TYS	21.00	Main	O	20.98
LYS	10.00	Side	NZ	TYR	190.00	Main	O	41.86
LYS	10.00	Side	NZ	ASN	192.00	Side	OD1	16.58
LYS	10.00	Side	NZ	ASP	193.00	Side	OD2	32.37
LYS	10.00	Side	NZ	ASP	193.00	Side	OD1	25.77
ARG	11.00	Side	NH1	GLU	2.00	Main	O	95.20
ARG	11.00	Side	NE	GLU	2.00	Main	O	84.72
ARG	11.00	Side	NH1	TYS	7.00	Side	OS2	54.05
ARG	11.00	Side	NH1	TYS	7.00	Side	OS4	43.76
ARG	11.00	Side	NH2	TYS	7.00	Side	OS2	38.06
ARG	11.00	Side	NH2	TYS	7.00	Side	OS4	12.99
ARG	11.00	Side	NH2	TYR	190.00	Main	O	32.37
ARG	11.00	Side	NH1	TYR	190.00	Main	O	26.37
SER	13.00	Side	OG	ASN	33.00	Side	ND2	27.27
SER	13.00	Side	OG	ASN	33.00	Side	OD1	10.09
SER	13.00	Side	OG	ASP	181.00	Side	OD2	11.19
SER	13.00	Side	OG	ARG	183.00	Side	NH1	11.29
LEU	14.00	Main	O	ARG	183.00	Side	NH1	78.62
LEU	14.00	Main	O	ARG	183.00	Side	NE	31.17

GLY	15.00	Main	N	ASP	187.00	Side	OD2	15.68
PRO	16.00	Main	O	SER	285.00	Side	OG	12.19
ARG	18.00	Side	NH1	HIS	113.00	Side	NE2	35.56
ARG	18.00	Side	NH1	TYR	116.00	Main	O	30.87
ARG	18.00	Side	NH2	TYR	116.00	Main	O	17.08
ARG	18.00	Side	NH1	THR	117.00	Side	OG1	76.92
ARG	18.00	Side	NH1	THR	117.00	Side	OG1	18.78
ARG	18.00	Side	NH1	ASP	171.00	Side	OD2	57.34
ARG	18.00	Side	NH1	ASP	171.00	Side	OD1	19.98
ARG	18.00	Main	O	ARG	188.00	Side	NH2	58.64
ARG	18.00	Main	O	ARG	188.00	Side	NE	42.36
ARG	18.00	Side	NH1	ARG	188.00	Side	NH1	18.88
ARG	18.00	Side	NH1	ARG	188.00	Side	NH1	10.79
ARG	18.00	Side	NH2	HIS	203.00	Side	NE2	52.75
ARG	18.00	Side	NH1	HIS	203.00	Side	NE2	16.18
ARG	18.00	Side	NH2	TYR	255.00	Side	OH	42.46
ARG	18.00	Side	NH2	TYR	255.00	Side	OH	23.68
ARG	18.00	Side	NE	TYR	255.00	Side	OH	20.48
ARG	18.00	Side	NE	TYR	255.00	Side	OH	19.08
ARG	18.00	Main	N	GLU	288.00	Side	OE2	67.73
ARG	18.00	Main	N	GLU	288.00	Side	OE1	26.07
ARG	18.00	Side	NE	GLU	288.00	Side	OE1	73.03
ARG	18.00	Side	NH2	GLU	288.00	Side	OE1	71.93
ARG	18.00	Side	NE	GLU	288.00	Side	OE2	44.56
ARG	18.00	Side	NH2	GLU	288.00	Side	OE2	28.37
TRP	20.00	Main	O	LYS	25.00	Side	NZ	34.67
TRP	20.00	Side	NE1	ASP	187.00	Side	OD1	11.49
TRP	20.00	Side	NE1	ARG	188.00	Main	O	59.54
TYR	21.00	Side	OH	CYS	28.00	Main	N	10.99
TYR	21.00	Side	OH	ASN	33.00	Side	ND2	20.08
TYR	21.00	Side	OH	SER	285.00	Side	OG	30.37
THR	22.00	Main	O	LYS	25.00	Main	N	10.39
THR	23.00	Side	OG1	CYS	28.00	Main	N	35.36
THR	23.00	Side	OG1	CYS	28.00	Main	O	17.08
GLY	24.00	Main	N	LYS	25.00	Main	O	24.38
GLY	24.00	Main	N	GLU	26.00	Main	O	56.44
ARG	31.00	Side	NH2	ASP	20.00	Main	O	84.32
ARG	31.00	Side	NE	ASP	20.00	Main	O	72.93
ARG	31.00	Side	NH2	TYS	21.00	Side	OS4	33.07
ARG	31.00	Side	NH2	TYS	21.00	Side	OS2	32.37
ARG	31.00	Side	NH1	TYS	21.00	Side	OS2	32.07
ARG	31.00	Side	NH1	TYS	21.00	Side	OS4	31.97
ARG	31.00	Side	NH1	TYS	21.00	Side	OS3	31.77
ARG	31.00	Side	NH2	TYS	21.00	Side	OS3	31.07
LYS	32.00	Side	NZ	TYS	21.00	Side	OS2	36.36
LYS	32.00	Side	NZ	TYS	21.00	Side	OS4	36.26
LYS	32.00	Side	NZ	TYS	21.00	Side	OS3	35.76

Complex 4:

V3 loop Residue	Number	Group	Atom	CXCR4 Residue	Number	Group	Atom	Occupancy (%)
ARG	3.00	Side	NH1	ASP	22.00	Main	O	36.16
ARG	3.00	Side	NH1	ASP	22.00	Side	OD2	10.49
ASN	5.00	Side	ND2	SER	23.00	Main	O	19.98
ASN	6.00	Main	N	SER	23.00	Main	O	35.76
ASN	7.00	Side	ND2	GLU	14.00	Side	OE2	29.77
ASN	7.00	Side	ND2	GLU	14.00	Side	OE1	17.18
THR	8.00	Side	OG1	LYS	25.00	Main	N	46.95
ARG	9.00	Side	NH1	ASP	10.00	Main	O	77.42
ARG	9.00	Side	NH1	ASN	11.00	Side	OD1	74.23
ARG	9.00	Side	NH2	ASN	11.00	Side	OD1	10.69
ARG	9.00	Side	NE	GLU	14.00	Side	OE2	50.15
ARG	9.00	Side	NH2	GLU	14.00	Side	OE2	49.45
ARG	9.00	Side	NE	GLU	14.00	Side	OE1	49.35
ARG	9.00	Side	NH2	GLU	14.00	Side	OE1	47.45
LYS	10.00	Main	N	TYS	12.00	Side	OS4	60.94
LYS	10.00	Main	N	TYS	12.00	Side	OS2	28.17
LYS	10.00	Side	NZ	GLY	19.00	Main	O	96.90
LYS	10.00	Side	NZ	ASP	20.00	Main	O	72.43
LYS	10.00	Side	NZ	ASP	193.00	Side	OD1	99.80
LYS	10.00	Side	NZ	GLU	268.00	Side	OE2	75.12
ARG	11.00	Side	NE	ASP	10.00	Side	OD2	95.10
ARG	11.00	Side	NH1	ASP	10.00	Side	OD2	91.51
ARG	11.00	Side	NH1	ASP	10.00	Side	OD1	10.19
ARG	11.00	Side	NH2	PRO	191.00	Main	O	89.71
SER	13.00	Side	OG	MET	1.00	Main	N	98.60
SER	13.00	Main	O	ARG	30.00	Side	NH1	18.08
LEU	14.00	Main	N	GLU	2.00	Main	O	75.12
LEU	14.00	Main	O	ARG	30.00	Side	NH1	36.56
LEU	14.00	Main	O	ARG	30.00	Side	NH2	19.28
GLY	15.00	Main	N	ASP	187.00	Side	OD2	53.75
GLY	15.00	Main	N	ASP	187.00	Side	OD1	44.96
ARG	18.00	Side	NH2	TYR	45.00	Side	OH	70.63
ARG	18.00	Side	NH1	TYR	45.00	Side	OH	16.88
ARG	18.00	Side	NH1	TRP	94.00	Side	NE1	76.12
ARG	18.00	Main	O	ARG	188.00	Side	NH2	94.31
ARG	18.00	Main	O	ARG	188.00	Side	NE	43.36
ARG	18.00	Side	NH2	TYR	255.00	Side	OH	10.39
ARG	18.00	Side	NH2	TYR	255.00	Side	OH	10.29
ARG	18.00	Main	N	GLU	288.00	Side	OE2	95.80
ARG	18.00	Side	NH2	GLU	288.00	Side	OE1	98.90
ARG	18.00	Side	NE	GLU	288.00	Side	OE1	80.32
ARG	18.00	Side	NE	GLU	288.00	Side	OE2	74.23
ARG	18.00	Side	NH2	GLU	288.00	Side	OE2	21.58
VAL	19.00	Main	N	GLU	288.00	Side	OE2	23.98
TRP	20.00	Side	NE1	ARG	188.00	Side	NE	15.78

TRP	20.00	Side	NE1	TYR	190.00	Side	OH	21.38
TYR	21.00	Side	OH	PHE	29.00	Main	O	20.78
TYR	21.00	Side	OH	ASN	278.00	Side	ND2	30.77
TYR	21.00	Side	OH	ASN	278.00	Side	ND2	27.57
THR	23.00	Side	OG1	MET	1.00	Main	N	54.95
GLY	24.00	Main	O	CYS	28.00	Main	N	30.67
GLN	25.00	Side	NE2	THR	8.00	Side	OG1	9.99
GLN	25.00	Side	OE1	SER	9.00	Main	N	73.83
GLN	25.00	Side	NE2	SER	9.00	Side	OG	20.98
ILE	26.00	Main	N	LYS	25.00	Main	O	54.75
ARG	31.00	Side	NH1	ASP	20.00	Side	OD1	50.55
ARG	31.00	Side	NH1	ASP	20.00	Side	OD2	38.56
ARG	31.00	Side	NH1	TYS	21.00	Main	O	81.72
ARG	31.00	Side	NH2	TYS	21.00	Main	O	70.63
ARG	31.00	Side	NH2	ASP	22.00	Main	O	10.59
ARG	31.00	Side	NH2	SER	23.00	Main	O	91.41
ARG	31.00	Side	NH1	SER	23.00	Main	O	12.29
LYS	32.00	Side	NZ	ASP	20.00	Side	OD1	45.85
LYS	32.00	Side	NZ	ASP	20.00	Side	OD2	44.76

Complex 5:

V3 loop Residue	Number	Group	Atom	CXCR4 Residue	Number	Group	Atom	Occupancy (%)
CYS	1	Main	N	MET	24	Main	O	33.57
CYS	1	Main	N	GLU	26	Side	OE1	71.83
CYS	1	Main	N	GLU	26	Side	OE2	69.53
ASN	7	Side	ND2	SER	23	Main	O	10.49
ARG	9	Side	NH1	ASP	20	Side	OD2	75.22
ARG	9	Side	NH1	ASP	20	Side	OD1	62.84
ARG	9	Side	NH2	ASP	20	Side	OD2	52.05
ARG	9	Side	NH2	ASP	20	Side	OD1	31.97
ARG	9	Side	NH1	TYS	21	Main	O	31.67
ARG	9	Side	NH1	ASP	22	Main	O	24.08
ARG	9	Side	NH2	ASP	193	Side	OD2	49.95
ARG	9	Side	NH2	ASP	193	Side	OD1	46.95
ARG	9	Side	NH1	ASP	193	Side	OD1	16.08
ARG	9	Side	NH1	ASP	193	Side	OD2	11.79
LYS	10	Side	NZ	CYS	28	Main	O	75.82
LYS	10	Side	NZ	PHE	29	Main	O	11.69
LYS	10	Side	NZ	GLU	277	Side	OE2	39.06
LYS	10	Side	NZ	GLU	277	Side	OE1	26.37
ARG	11	Side	NH2	ASP	10	Side	OD2	86.11
ARG	11	Side	NH1	ASP	10	Side	OD1	81.52
ARG	11	Side	NH1	ASP	10	Side	OD2	69.83
ARG	11	Side	NH2	ASP	10	Side	OD1	23.08
ARG	11	Side	NH2	PRO	191	Main	O	85.01
ARG	11	Side	NE	ASP	193	Side	OD2	12.79
ARG	11	Side	NH1	ASP	193	Side	OD1	9.69
SER	13	Side	OG	ARG	188	Main	O	97.10
SER	13	Side	OG	TYR	190	Main	N	61.84
LEU	14	Main	O	ARG	188	Side	NH2	99.90
LEU	14	Main	O	ARG	188	Side	NE	68.13
LEU	14	Main	N	GLN	200	Side	OE1	23.98
GLY	17	Main	O	SER	285	Side	OG	99.10
GLY	17	Main	N	GLU	288	Side	OE2	92.91
GLY	17	Main	N	GLU	288	Side	OE1	87.01
ARG	18	Side	NH1	ASP	181	Side	OD2	16.48
ARG	18	Side	NH2	ASP	181	Side	OD2	16.28
ARG	18	Side	NE	HIS	281	Side	NE2	42.56
ARG	18	Side	NH2	HIS	281	Side	NE2	20.58
VAL	19	Main	O	HIS	281	Side	ND1	11.29
TYR	21	Main	O	MET	1	Main	N	76.32
TYR	21	Side	OH	GLU	277	Main	O	57.74
TYR	21	Side	OH	ASN	278	Side	ND2	22.58
TYR	21	Side	OH	HIS	281	Side	ND1	12.39
THR	22	Side	OG1	MET	1	Main	N	77.42
THR	22	Side	OG1	ILE	6	Main	O	17.18
GLN	25	Main	N	THR	8	Side	OG1	20.48

GLN	25	Side	NE2	THR	8	Side	OG1	29.67
GLN	25	Side	NE2	SER	9	Side	OG	23.58
VAL	27	Main	N	TYS	12	Main	O	91.91
ILE	30	Main	O	SER	23	Side	OG	65.23
LYS	32	Side	NZ	ASP	22	Side	OD1	45.05
LYS	32	Side	NZ	ASP	22	Side	OD2	42.16
LYS	32	Main	N	SER	23	Side	OG	22.58
LYS	32	Main	N	SER	23	Side	OG	10.09
LYS	32	Side	NZ	SER	23	Side	OG	19.08

Complex 6:

V3 loop Residue	Number	Group	Atom	CXCR4 Residue	Number	Group	Atom	Occupancy (%)
CYS	1	Main	N	SER	23	Main	O	27.27
CYS	1	Main	N	SER	23	Side	OG	70.23
CYS	1	Main	O	SER	23	Side	OG	16.08
ASN	5	Side	ND2	SER	18	Side	OG	23.18
ASN	5	Side	ND2	ASP	20	Side	OD1	68.83
ASN	6	Main	N	ASP	20	Side	OD1	85.71
ASN	6	Main	N	ASP	20	Side	OD2	25.37
ASN	6	Side	ND2	ASP	20	Side	OD1	14.89
ASN	6	Side	ND2	TYS	21	Main	O	28.47
ASN	7	Side	ND2	TYS	12	Main	O	97.50
ASN	7	Side	ND2	GLU	14	Side	OE1	64.14
ASN	7	Side	ND2	GLU	14	Side	OE2	33.77
THR	8	Side	OG1	ASN	11	Main	N	35.26
THR	8	Side	OG1	ASN	11	Side	OD1	44.56
ARG	9	Main	O	SER	9	Main	N	39.26
ARG	9	Side	NH2	TYS	12	Side	OS2	93.11
ARG	9	Side	NH2	TYS	12	Side	OH	33.97
ARG	9	Side	NH2	TYS	12	Side	OS3	33.67
ARG	9	Side	NH1	TYS	12	Side	OS3	20.68
ARG	9	Side	NH1	TYS	12	Side	OS2	12.39
ARG	9	Side	NH2	GLY	19	Main	O	10.29
ARG	9	Side	NH1	ASP	20	Side	OD2	87.31
ARG	9	Side	NH2	ASP	20	Side	OD2	14.69
ARG	9	Side	NH2	ASP	193	Side	OD1	98.50
ARG	9	Side	NE	ASP	193	Side	OD2	97.00
ARG	9	Side	NH2	ASP	193	Side	OD2	73.43
ARG	9	Side	NE	ASP	193	Side	OD1	41.16
ARG	11	Main	N	TYS	7	Main	O	56.74
ARG	11	Side	NH1	ASP	10	Side	OD2	88.61
ARG	11	Side	NH1	ASP	10	Side	OD1	36.96
ARG	11	Side	NH2	ASP	10	Side	OD1	30.07
ARG	11	Side	NH2	TYR	190	Main	O	63.54
ARG	11	Side	NH1	TYR	190	Main	O	14.89
ARG	11	Side	NH2	PRO	191	Main	O	18.38
ARG	11	Side	NH1	PRO	191	Main	O	16.38
SER	13	Side	OG	MET	1	Main	N	14.09
SER	13	Side	OG	ASP	181	Main	N	14.79
SER	13	Side	OG	ASP	181	Side	OD1	30.47
SER	13	Side	OG	ASP	181	Side	OD2	19.88
SER	13	Side	OG	ARG	183	Side	NH2	20.58
GLY	15	Main	O	ASN	37	Side	ND2	27.17
PRO	16	Main	O	ASN	37	Side	ND2	15.48
PRO	16	Main	O	ARG	183	Side	NH1	39.76
GLY	17	Main	N	TYR	45	Side	OH	67.33
GLY	17	Main	N	GLU	288	Side	OE1	12.49

ARG	18	Side	NH2	TRP	94	Side	NE1	74.53
ARG	18	Side	NH1	HIS	113	Side	NE2	93.01
ARG	18	Side	NE	TYR	116	Side	OH	21.98
ARG	18	Side	NE	TYR	116	Side	OH	18.58
ARG	18	Side	NH2	GLU	288	Side	OE1	99.90
ARG	18	Side	NE	GLU	288	Side	OE2	99.80
ARG	18	Side	NE	GLU	288	Side	OE1	61.84
ARG	18	Side	NH2	GLU	288	Side	OE2	52.75
VAL	19	Main	N	ASP	187	Side	OD2	14.79
VAL	19	Main	O	TYR	190	Side	OH	30.97
TRP	20	Side	NE1	ARG	188	Side	NH1	18.98
TRP	20	Side	NE1	ARG	188	Side	NH1	16.68
TRP	20	Side	NE1	TYR	190	Side	OH	9.39
TYR	21	Side	OH	TYS	7	Side	OH	11.29
TYR	21	Side	OH	ASP	187	Side	OD1	96.60
TYR	21	Side	OH	ASP	187	Side	OD2	9.69
THR	22	Side	OG1	GLU	277	Side	OE2	93.41
THR	22	Side	OG1	GLU	277	Side	OE1	29.97
THR	23	Main	O	LYS	25	Side	NZ	90.71
THR	23	Side	OG1	LYS	25	Side	NZ	68.23
ARG	31	Side	NH1	GLU	14	Side	OE1	94.41
ARG	31	Side	NH1	GLU	14	Side	OE2	92.11
ARG	31	Side	NH2	GLU	14	Side	OE1	70.93
ARG	31	Side	NH2	GLU	14	Side	OE2	45.95

Complex 7:

V3 loop Residue	Number	Group	Atom	CXCR4 Residue	Number	Group	Atom	Occupancy (%)
ARG	3	Side	NH2	GLY	19	Main	O	15.08
ARG	3	Side	NH1	ASP	22	Side	OD1	30.57
ARG	3	Side	NH1	ASP	22	Side	OD2	24.78
ARG	3	Side	NE	ASP	22	Side	OD1	17.28
ARG	3	Side	NE	ASP	22	Side	OD2	16.58
ARG	3	Side	NH2	GLU	268	Side	OE1	52.95
ARG	3	Side	NH1	GLU	268	Side	OE2	48.45
ARG	3	Side	NH2	GLU	268	Side	OE2	44.26
ARG	3	Side	NH1	GLU	268	Side	OE1	18.38
ASN	7	Side	OD1	THR	13	Side	OG1	44.96
ASN	7	Side	ND2	THR	13	Side	OG1	12.99
THR	8	Main	N	THR	13	Side	OG1	21.78
THR	8	Main	O	THR	13	Side	OG1	14.39
THR	8	Main	O	GLU	14	Main	N	73.63
THR	8	Side	OG1	GLU	14	Side	OE2	38.46
ARG	9	Side	NH2	ASN	11	Side	OD1	17.88
ARG	9	Side	NE	TYS	12	Main	O	95.80
ARG	9	Side	NH2	TYS	12	Main	O	62.84
LYS	10	Side	NZ	GLU	14	Side	OE1	89.11
LYS	10	Side	NZ	GLU	14	Side	OE2	39.36
LYS	10	Side	NZ	SER	23	Main	O	28.27
LYS	10	Side	NZ	SER	23	Side	OG	10.29
LYS	10	Side	NZ	ASP	193	Side	OD1	63.04
LYS	10	Side	NZ	ASP	193	Side	OD2	44.56
ARG	11	Side	NH2	GLU	2	Side	OE2	35.66
ARG	11	Side	NH2	GLU	2	Side	OE1	12.89
ARG	11	Side	NH1	THR	8	Side	OG1	10.29
VAL	12	Main	N	GLU	2	Main	O	17.28
SER	13	Side	OG	ARG	30	Side	NE	10.19
GLY	15	Main	O	ASN	37	Side	ND2	19.58
GLY	15	Main	N	ASP	187	Side	OD2	65.03
GLY	15	Main	N	ASP	187	Side	OD1	16.18
GLY	17	Main	N	GLU	288	Side	OE2	68.03
GLY	17	Main	N	GLU	288	Side	OE1	47.45
ARG	18	Side	NH2	HIS	113	Side	ND1	16.98
ARG	18	Side	NH2	HIS	113	Side	ND1	16.88
ARG	18	Side	NE	TYR	116	Side	OH	26.57
ARG	18	Side	NH2	TYR	116	Side	OH	18.68
ARG	18	Side	NH1	THR	117	Side	OG1	85.81
ARG	18	Side	NH1	THR	117	Side	OG1	47.75
ARG	18	Side	NH2	THR	117	Side	OG1	25.27
ARG	18	Side	NH1	ASP	171	Side	OD1	95.40
ARG	18	Side	NH2	ASP	171	Side	OD2	92.81
ARG	18	Side	NH1	ASP	171	Side	OD2	73.93
ARG	18	Side	NH2	ASP	171	Side	OD1	39.16

ARG	18	Side	NH1	HIS	203	Side	NE2	51.65
ARG	18	Side	NH1	HIS	203	Side	ND1	33.37
ARG	18	Main	N	GLU	288	Side	OE1	64.34
ARG	18	Main	N	GLU	288	Side	OE2	62.14
TRP	20	Main	N	GLN	200	Side	OE1	13.89
TYR	21	Side	OH	CYS	28	Main	O	18.78
TYR	21	Side	OH	PHE	29	Main	O	19.58
TYR	21	Side	OH	GLU	277	Side	OE2	13.59
TYR	21	Side	OH	ASN	278	Side	ND2	58.34
TYR	21	Side	OH	ASN	278	Side	ND2	19.58
THR	22	Main	O	LYS	25	Side	NZ	35.46
THR	22	Side	OG1	LYS	25	Side	NZ	85.91
THR	23	Side	OG1	CYS	28	Main	O	86.21
THR	23	Side	OG1	CYS	28	Main	N	69.63
THR	23	Side	OG1	CYS	28	Main	N	44.36
GLY	24	Main	N	LYS	25	Main	O	20.78
GLY	24	Main	N	GLU	26	Main	O	51.65
GLN	25	Side	NE2	CYS	28	Main	O	9.79
ARG	31	Side	NH1	SER	18	Side	OG	17.78
ARG	31	Side	NH2	GLY	19	Main	O	21.08
ARG	31	Side	NH1	ASP	20	Side	OD1	75.12
ARG	31	Side	NH2	ASP	20	Side	OD2	72.73
ARG	31	Side	NH2	ASP	20	Side	OD1	57.24
ARG	31	Side	NH1	ASP	20	Side	OD2	49.15
LYS	32	Side	NZ	ASP	20	Side	OD2	60.64
LYS	32	Side	NZ	ASP	20	Side	OD1	54.35

Complex 8:

V3 loop Residue	Number	Group	Atom	CXCR4 Residue	Number	Group	Atom	Occupancy (%)
CYS	1	Main	N	MET	24	Main	O	53.85
CYS	1	Main	N	GLU	26	Side	OE1	26.47
CYS	1	Main	N	GLU	26	Side	OE2	23.18
ARG	3	Main	N	SER	23	Side	OG	30.87
ARG	3	Main	O	SER	23	Side	OG	14.49
THR	8	Side	OG1	TYS	12	Main	N	30.87
THR	8	Side	OG1	TYS	12	Main	O	22.28
THR	8	Side	OG1	ASP	20	Side	OD1	11.39
THR	8	Side	OG1	ASP	20	Side	OD2	9.69
ARG	9	Side	NH2	THR	8	Side	OG1	68.13
ARG	9	Side	NH1	THR	8	Side	OG1	61.04
ARG	9	Side	NH2	SER	9	Side	OG	78.02
LYS	10	Side	NZ	TYS	7	Main	O	13.19
LYS	10	Side	NZ	ASP	10	Side	OD1	55.64
LYS	10	Side	NZ	ASP	10	Side	OD2	42.36
LYS	10	Side	NZ	ASN	11	Main	O	52.45
ARG	11	Side	NH2	TYS	21	Side	OS4	25.97
ARG	11	Side	NH1	TYS	21	Side	OS4	25.77
ARG	11	Side	NH1	TYS	21	Side	OS3	15.08
ARG	11	Side	NH2	TYS	21	Side	OS3	14.09
ARG	11	Side	NH2	GLU	26	Main	O	10.59
VAL	12	Main	O	CYS	28	Main	N	82.62
SER	13	Side	OG	LYS	25	Side	NZ	13.69
SER	13	Side	OG	GLU	277	Side	OE2	14.99
SER	13	Side	OG	GLU	277	Side	OE1	12.29
GLY	15	Main	O	HIS	281	Side	ND1	97.40
PRO	16	Main	O	HIS	281	Side	ND1	60.94
GLY	17	Main	O	ARG	30	Side	NH1	69.23
GLY	17	Main	N	GLU	288	Side	OE1	77.02
ARG	18	Side	NH2	ASN	37	Side	OD1	87.11
ARG	18	Side	NH1	ASN	37	Side	OD1	29.67
ARG	18	Side	NE	TRP	94	Side	NE1	61.24
ARG	18	Side	NH1	ASP	97	Side	OD1	18.38
ARG	18	Main	N	GLU	288	Side	OE2	48.15
ARG	18	Main	N	GLU	288	Side	OE1	22.48
ARG	18	Side	NH2	GLU	288	Side	OE2	97.30
ARG	18	Side	NE	GLU	288	Side	OE2	40.56
TRP	20	Main	N	ASP	187	Side	OD1	45.15
TRP	20	Main	N	ASP	187	Side	OD2	14.69
TYR	21	Side	OH	GLN	200	Side	NE2	58.54
TYR	21	Side	OH	ASP	262	Side	OD1	53.85
TYR	21	Side	OH	ASP	262	Side	OD2	47.95
THR	22	Side	OG1	MET	1	Main	N	88.71
THR	22	Side	OG1	TYR	190	Main	O	14.09
GLY	24	Main	N	TYS	12	Side	OS4	86.21

GLY	24	Main	O	TYS	21	Main	N	29.77
GLY	24	Main	N	ASP	193	Side	OD2	21.28
GLN	25	Side	NE2	TYS	21	Main	O	12.99
GLN	25	Side	NE2	ASP	22	Main	O	41.36
GLN	25	Side	NE2	LYS	25	Main	O	19.98
ILE	26	Main	N	TYS	21	Main	O	50.65
ARG	31	Main	O	SER	9	Side	OG	13.19
HIS	34	Side	NE2	THR	8	Side	OG1	25.27
HIS	34	Side	ND1	LYS	25	Main	O	14.49

Complex 9:

V3 loop Residue	Number	Group	Atom	CXCR4 Residue	Number	Group	Atom	Occupancy (%)
ARG	3	Side	NH1	ASP	22	Side	OD2	83.62
ARG	3	Side	NE	ASP	22	Side	OD2	77.12
ARG	3	Side	NH1	ASP	22	Side	OD1	52.85
ARG	3	Side	NE	ASP	22	Side	OD1	14.19
ARG	3	Side	NH1	SER	23	Side	OG	56.34
ARG	3	Side	NH2	SER	23	Side	OG	39.26
ARG	3	Side	NH2	LEU	267	Main	O	54.95
ARG	3	Side	NH2	GLU	268	Side	OE1	32.97
ARG	3	Side	NH2	GLU	268	Side	OE2	21.48
THR	8	Main	N	GLY	19	Main	O	89.91
ARG	9	Side	NH2	ILE	4	Main	O	16.88
ARG	9	Side	NE	SER	5	Side	OG	0.10
ARG	9	Side	NH1	GLU	14	Side	OE2	63.94
ARG	9	Side	NH2	GLU	14	Side	OE2	56.94
ARG	9	Side	NH1	GLU	14	Side	OE1	55.64
ARG	9	Side	NH2	GLU	14	Side	OE1	44.26
ARG	9	Side	NH2	PRO	191	Main	O	64.24
ARG	9	Side	NE	PRO	191	Main	O	16.78
LYS	10	Side	NZ	GLY	19	Main	O	18.68
LYS	10	Side	NZ	TYS	21	Main	O	26.47
LYS	10	Side	NZ	SER	23	Main	O	89.01
LYS	10	Main	N	PRO	191	Main	O	14.89
LYS	10	Side	NZ	ASP	193	Side	OD2	99.10
ARG	11	Side	NH2	MET	1	Main	O	20.28
ARG	11	Side	NH2	GLU	2	Side	OE1	12.89
ARG	11	Side	NH2	GLU	2	Side	OE2	9.89
ARG	11	Side	NE	GLY	3	Main	O	24.18
VAL	12	Main	N	GLY	3	Main	O	17.68
LEU	14	Main	O	ARG	30	Side	NH2	11.79
PRO	16	Main	O	ARG	30	Side	NH1	32.07
PRO	16	Main	O	ASN	37	Side	ND2	21.28
GLY	17	Main	N	ASP	97	Side	OD1	32.97
GLY	17	Main	N	ASP	97	Side	OD2	24.78
GLY	17	Main	N	ALA	98	Main	O	9.89
ARG	18	Side	NH1	HIS	113	Side	NE2	58.34
ARG	18	Side	NH1	THR	117	Side	OG1	11.89
ARG	18	Side	NH2	HIS	203	Side	NE2	20.38
ARG	18	Side	NH1	HIS	203	Side	NE2	13.39
ARG	18	Side	NH2	TYR	255	Side	OH	30.37
ARG	18	Side	NH2	TYR	255	Side	OH	22.08
ARG	18	Side	NH2	GLU	288	Side	OE2	82.22
ARG	18	Side	NH2	GLU	288	Side	OE1	80.02
ARG	18	Side	NE	GLU	288	Side	OE1	77.52
ARG	18	Side	NE	GLU	288	Side	OE2	61.04
TRP	20	Side	NE1	HIS	113	Side	NE2	35.16

TRP	20	Side	NE1	ARG	188	Side	NH2	18.88
TRP	20	Side	NE1	ARG	188	Side	NH2	17.68
TRP	20	Side	NE1	ARG	188	Side	NE	12.09
TRP	20	Side	NE1	TYR	190	Side	OH	39.56
TRP	20	Main	O	HIS	281	Side	ND1	54.45
TYR	21	Side	OH	ARG	30	Side	NH1	29.47
TYR	21	Side	OH	GLU	31	Main	N	19.58
TYR	21	Side	OH	GLU	31	Main	O	9.69
TYR	21	Side	OH	ASN	33	Side	ND2	10.19
TYR	21	Side	OH	ASN	37	Side	ND2	44.66
THR	22	Main	O	LYS	25	Side	NZ	57.54
THR	22	Side	OG1	LYS	25	Side	NZ	85.51
THR	23	Side	OG1	GLU	26	Main	O	12.09
THR	23	Side	OG1	CYS	28	Main	N	67.43
THR	23	Side	OG1	CYS	28	Main	O	50.95
THR	23	Side	OG1	CYS	28	Main	N	19.88
GLY	24	Main	N	LYS	25	Main	O	26.77
GLY	24	Main	N	GLU	26	Main	O	44.46
GLN	25	Side	NE2	GLU	2	Main	O	29.97
ARG	31	Main	N	ASP	20	Side	OD1	46.05
ARG	31	Side	NH2	ASP	20	Side	OD2	99.30
ARG	31	Side	NE	ASP	20	Side	OD2	98.20
ARG	31	Side	NH2	TYS	21	Side	OS3	58.44
ARG	31	Side	NH2	TYS	21	Side	OS4	46.25
ARG	31	Side	NH2	TYS	21	Side	OS2	41.26
ARG	31	Side	NH1	TYS	21	Side	OS3	38.96
ARG	31	Side	NH1	TYS	21	Side	OS4	34.57
ARG	31	Side	NH1	TYS	21	Side	OS2	21.88
LYS	32	Side	NZ	TYS	21	Side	OS3	29.47
LYS	32	Side	NZ	TYS	21	Side	OS2	27.57
LYS	32	Side	NZ	TYS	21	Side	OS4	13.09
HIS	34	Side	ND1	ASP	20	Side	OD2	42.06

Complex 10:

V3 loop Residue	Number	Group	Atom	CXCR4 Residue	Number	Group	Atom	Occupancy (%)
CYS	1	Main	N	GLU	15	Side	OE1	26.87
CYS	1	Main	N	GLU	15	Side	OE2	23.28
CYS	1	Main	O	MET	16	Main	N	47.05
THR	2	Main	O	MET	16	Main	N	16.08
ASN	5	Side	ND2	TYS	12	Side	OS2	25.47
ASN	5	Side	ND2	TYS	12	Side	OS3	13.09
ASN	5	Main	N	GLU	14	Side	OE2	91.01
ASN	5	Main	N	GLU	14	Side	OE1	30.87
ASN	5	Side	ND2	GLU	14	Side	OE2	47.75
ASN	5	Side	ND2	GLU	14	Side	OE1	9.69
ASN	5	Side	ND2	MET	16	Main	O	14.19
ASN	5	Side	ND2	GLY	17	Main	O	15.38
THR	8	Main	O	ASP	10	Main	N	70.83
THR	8	Main	N	ASP	10	Side	OD1	18.38
THR	8	Side	OG1	TYS	12	Side	OS4	26.07
THR	8	Side	OG1	GLU	14	Side	OE1	13.99
ARG	9	Side	NH2	THR	8	Side	OG1	15.68
ARG	9	Side	NH2	SER	9	Side	OG	58.64
ARG	9	Side	NE	SER	9	Side	OG	13.59
ARG	9	Side	NH2	ASP	10	Side	OD1	16.58
ARG	9	Side	NH2	ASN	11	Side	OD1	10.19
LYS	10	Side	NZ	TYS	12	Side	OS4	31.97
LYS	10	Side	NZ	TYS	12	Side	OS3	24.08
LYS	10	Side	NZ	TYR	190	Main	O	47.05
LYS	10	Side	NZ	PRO	191	Main	O	25.37
LYS	10	Side	NZ	ASP	193	Side	OD2	54.75
LYS	10	Side	NZ	ASP	193	Side	OD1	40.96
ARG	11	Side	NH2	LYS	25	Main	O	38.36
ARG	11	Side	NH2	GLU	26	Main	O	60.94
ARG	11	Side	NH1	GLU	26	Main	O	34.67
ARG	11	Side	NH2	CYS	28	Main	O	17.38
SER	13	Side	OG	GLU	277	Side	OE2	35.86
SER	13	Side	OG	GLU	277	Side	OE1	20.28
GLY	15	Main	O	GLN	200	Side	NE2	32.77
GLY	17	Main	N	TYR	255	Side	OH	24.78
GLY	17	Main	N	TYR	255	Side	OH	12.39
ARG	18	Side	NH2	ASN	37	Side	ND2	71.73
ARG	18	Side	NH2	ASN	37	Side	ND2	20.88
ARG	18	Side	NH1	HIS	281	Side	NE2	96.60
ARG	18	Side	NH2	HIS	281	Side	NE2	27.77
ARG	18	Side	NH1	SER	285	Side	OG	99.80
ARG	18	Main	N	GLU	288	Side	OE2	98.20
TRP	20	Side	NE1	ASP	181	Side	OD1	25.47
TRP	20	Side	NE1	ASP	181	Side	OD2	23.48
TRP	20	Main	O	ARG	188	Main	N	73.63

TYR	21	Side	OH	GLN	200	Side	NE2	51.05
TYR	21	Side	OH	ASP	262	Side	OD2	69.73
TYR	21	Side	OH	ASP	262	Side	OD1	26.27
THR	22	Main	N	ARG	188	Main	O	18.98
THR	22	Side	OG1	TYR	190	Main	N	51.25
THR	23	Main	O	LYS	25	Side	NZ	10.69
THR	23	Side	OG1	LYS	25	Side	NZ	38.26
GLY	24	Main	O	LYS	25	Side	NZ	10.59
GLY	24	Main	N	ASP	193	Side	OD2	18.28
GLN	25	Side	NE2	SER	23	Main	O	15.38
GLN	25	Side	OE1	LYS	25	Main	N	80.72
ILE	26	Main	O	TYS	21	Main	N	29.97
ARG	31	Side	NH2	ASP	10	Side	OD1	71.73
ARG	31	Side	NH1	ASP	10	Side	OD2	61.44
ARG	31	Side	NH1	ASP	10	Side	OD1	42.26
ARG	31	Side	NH2	ASP	10	Side	OD2	20.68
ARG	31	Side	NH1	THR	13	Side	OG1	13.19

Complex 11:

V3 loop Residue	Number	Group	Atom	CXCR4 Residue	Number	Group	Atom	Occupancy (%)
CYS	1	Main	N	SER	23	Side	OG	55.64
CYS	1	Main	O	SER	23	Side	OG	11.19
ARG	3	Side	NH2	SER	23	Side	OG	12.99
ASN	5	Side	ND2	SER	18	Main	O	39.66
ASN	5	Side	ND2	GLY	19	Main	O	36.26
ASN	6	Main	N	ASP	20	Side	OD1	84.72
ASN	6	Main	N	ASP	20	Side	OD2	23.38
ASN	6	Side	ND2	ASP	20	Side	OD2	53.65
ASN	6	Side	ND2	ASP	20	Side	OD1	53.35
ASN	6	Side	ND2	ASP	22	Main	O	9.99
ASN	6	Side	OD1	SER	23	Side	OG	25.07
ASN	6	Side	ND2	SER	23	Side	OG	16.48
ASN	7	Side	ND2	TYS	12	Main	O	87.71
ASN	7	Side	ND2	TYS	12	Side	OS4	41.26
ASN	7	Side	ND2	TYS	12	Side	OS2	31.37
ASN	7	Side	ND2	TYS	12	Side	OS3	26.37
THR	8	Side	OG1	ASN	11	Side	ND2	94.51
ARG	9	Main	O	SER	9	Main	N	64.54
ARG	9	Side	NH1	TYS	12	Side	OH	50.45
ARG	9	Side	NH1	TYS	12	Side	OS3	37.16
ARG	9	Side	NH2	TYS	12	Side	OS4	27.87
ARG	9	Side	NH1	TYS	12	Side	OS4	24.98
ARG	9	Side	NH1	TYS	12	Side	OS2	24.38
ARG	9	Side	NH2	TYS	12	Side	OS2	20.68
ARG	9	Side	NH2	TYS	12	Side	OS3	17.58
ARG	9	Side	NH2	GLY	19	Main	O	79.82
ARG	9	Side	NH1	GLY	19	Main	O	30.27
ARG	9	Side	NH2	ASP	20	Main	O	13.79
ARG	9	Side	NH2	ASP	20	Side	OD1	34.47
ARG	9	Side	NH1	ASP	193	Side	OD1	88.91
ARG	9	Side	NH1	ASP	193	Side	OD2	78.72
LYS	10	Side	NZ	THR	8	Side	OG1	23.58
ARG	11	Main	N	TYS	7	Main	O	42.76
ARG	11	Side	NH1	TYS	7	Main	O	30.47
ARG	11	Side	NH2	ASP	10	Side	OD1	89.61
ARG	11	Side	NH1	ASP	10	Side	OD2	88.01
ARG	11	Side	NH2	ASP	10	Side	OD2	69.43
ARG	11	Side	NH1	ASP	10	Side	OD1	56.74
ARG	11	Side	NH2	PRO	191	Main	O	94.41
ARG	11	Side	NE	PRO	191	Main	O	44.76
SER	13	Side	OG	ASP	181	Main	N	15.78
SER	13	Side	OG	ASP	181	Side	OD1	74.53
SER	13	Side	OG	ASP	181	Side	OD2	61.54
GLY	15	Main	O	ARG	30	Side	NH2	80.82
GLY	15	Main	O	ARG	30	Side	NH1	69.13

PRO	16	Main	O	ARG	183	Side	NH1	35.86
GLY	17	Main	N	TYR	45	Side	OH	21.08
GLY	17	Main	N	GLU	288	Side	OE1	49.75
ARG	18	Side	NH2	TYR	45	Side	OH	13.49
ARG	18	Side	NH1	TRP	94	Side	NE1	22.48
ARG	18	Side	NH2	TRP	94	Side	NE1	13.79
ARG	18	Side	NH1	HIS	113	Side	NE2	82.82
ARG	18	Side	NE	TYR	116	Side	OH	23.78
ARG	18	Side	NE	TYR	116	Side	OH	22.58
ARG	18	Main	O	TYR	190	Side	OH	14.89
ARG	18	Main	N	GLU	288	Side	OE1	31.37
ARG	18	Side	NE	GLU	288	Side	OE2	97.80
ARG	18	Side	NH2	GLU	288	Side	OE1	97.40
ARG	18	Side	NE	GLU	288	Side	OE1	68.63
ARG	18	Side	NH2	GLU	288	Side	OE2	41.26
VAL	19	Main	O	TYR	190	Side	OH	14.59
TRP	20	Side	NE1	ARG	188	Side	NH2	22.08
TRP	20	Side	NE1	ARG	188	Side	NH2	20.28
TRP	20	Side	NE1	TYR	190	Side	OH	34.47
TYR	21	Side	OH	SER	178	Side	OG	9.59
TYR	21	Side	OH	ASP	187	Side	OD1	47.25
THR	22	Side	OG1	GLU	277	Side	OE2	89.21
THR	23	Main	O	LYS	25	Side	NZ	89.71
THR	23	Side	OG1	LYS	25	Side	NZ	64.44
GLY	24	Main	O	CYS	28	Main	N	95.80
ILE	26	Main	O	LYS	25	Main	N	88.81
ILE	26	Main	N	LYS	25	Main	O	63.84
GLY	28	Main	N	SER	23	Main	O	26.87
ASP	29	Side	OD2	ASN	11	Side	ND2	65.23
ASP	29	Side	OD1	ASN	11	Side	ND2	63.14
ARG	31	Side	NE	ASN	11	Side	OD1	23.88
ARG	31	Side	NH1	GLU	14	Side	OE1	81.92
ARG	31	Side	NH1	GLU	14	Side	OE2	80.52
ARG	31	Side	NH2	GLU	14	Side	OE1	56.64
ARG	31	Side	NH2	GLU	14	Side	OE2	56.14
LYS	32	Side	NZ	GLU	14	Side	OE1	17.28
LYS	32	Side	NZ	GLU	14	Side	OE2	10.69

Complex 12:

V3 loop Residue	Number	Group	Atom	CXCR4 Residue	Number	Group	Atom	Occupancy (%)
ARG	3	Side	NH2	ASP	22	Side	OD1	64.44
ARG	3	Side	NH2	ASP	22	Side	OD2	24.38
ARG	3	Side	NH1	ASP	22	Side	OD1	17.98
ARG	3	Side	NH2	GLU	268	Side	OE1	32.97
ARG	3	Side	NH2	GLU	268	Side	OE2	27.77
ARG	3	Side	NH1	GLU	268	Side	OE1	26.47
ARG	3	Side	NH1	GLU	268	Side	OE2	23.48
ASN	5	Side	ND2	TYS	21	Main	O	23.48
ASN	5	Side	ND2	ASP	22	Main	O	24.68
ASN	5	Side	ND2	SER	23	Main	O	36.76
ASN	6	Main	N	SER	23	Main	O	80.32
ASN	6	Side	ND2	SER	23	Main	O	25.67
THR	8	Side	OG1	LYS	25	Main	N	44.16
ARG	9	Side	NH1	SER	9	Side	OG	39.36
ARG	9	Side	NH2	SER	9	Side	OG	32.17
ARG	9	Side	NH1	ASP	10	Side	OD2	22.48
ARG	9	Side	NH2	ASP	10	Side	OD2	19.38
ARG	9	Side	NH1	ASN	11	Main	O	14.19
ARG	9	Side	NE	ASN	11	Side	OD1	50.65
ARG	9	Side	NH2	ASN	11	Side	OD1	48.75
LYS	10	Main	N	TYS	12	Side	OS3	37.26
LYS	10	Side	NZ	TYS	12	Side	OS2	27.27
LYS	10	Side	NZ	TYS	12	Side	OS4	25.97
LYS	10	Side	NZ	TYS	12	Side	OS3	16.98
LYS	10	Side	NZ	ASP	20	Main	O	96.90
LYS	10	Side	NZ	ASP	193	Side	OD1	97.00
LYS	10	Side	NZ	ASP	193	Side	OD2	60.24
LYS	10	Side	NZ	GLU	268	Side	OE1	32.17
LYS	10	Side	NZ	GLU	268	Side	OE2	14.99
ARG	11	Main	O	MET	1	Main	N	15.18
ARG	11	Side	NE	MET	1	Main	O	54.85
ARG	11	Side	NH1	MET	1	Main	O	53.15
ARG	11	Side	NH1	ASP	10	Side	OD2	76.82
ARG	11	Side	NH1	ASP	10	Side	OD1	60.24
ARG	11	Side	NH2	ASP	10	Side	OD1	56.34
ARG	11	Side	NE	ASP	10	Side	OD2	28.57
ARG	11	Side	NH2	ASP	10	Side	OD2	26.87
ARG	11	Side	NE	ASP	10	Side	OD1	20.88
ARG	11	Side	NH2	ASN	11	Main	O	14.49
ARG	11	Side	NH2	TYR	190	Main	O	38.46
ARG	11	Side	NH1	TYR	190	Main	O	12.89
VAL	12	Main	O	MET	1	Main	N	20.08
SER	13	Side	OG	MET	1	Main	N	97.20
SER	13	Side	OG	GLU	2	Main	O	17.08
LEU	14	Main	N	ASP	187	Side	OD2	47.95

LEU	14	Main	N	ASP	187	Side	OD1	46.15
GLY	15	Main	O	ARG	183	Side	NH1	14.79
ARG	18	Side	NH1	THR	117	Side	OG1	92.71
ARG	18	Side	NH1	THR	117	Side	OG1	38.76
ARG	18	Side	NH1	ASP	171	Side	OD2	75.42
ARG	18	Main	O	ARG	188	Side	NH2	99.20
ARG	18	Side	NH1	HIS	203	Side	NE2	99.00
ARG	18	Side	NH2	HIS	203	Side	NE2	97.00
ARG	18	Side	NH2	TYR	255	Side	OH	90.61
ARG	18	Side	NH2	TYR	255	Side	OH	68.73
ARG	18	Main	N	GLU	288	Side	OE2	35.56
ARG	18	Side	NH2	GLU	288	Side	OE1	97.30
ARG	18	Side	NE	GLU	288	Side	OE2	61.24
ARG	18	Side	NH2	GLU	288	Side	OE2	45.35
ARG	18	Side	NE	GLU	288	Side	OE1	30.37
TRP	20	Side	NE1	ARG	188	Side	NH2	74.53
TRP	20	Side	NE1	TYR	190	Side	OH	52.75
TRP	20	Side	NE1	TYR	190	Side	OH	13.29
TRP	20	Main	O	HIS	281	Side	ND1	78.02
TYR	21	Side	OH	ARG	30	Main	N	24.08
TYR	21	Side	OH	ASN	278	Side	ND2	42.46
TYR	21	Side	OH	ASN	278	Side	ND2	22.68
THR	23	Side	OG1	MET	1	Main	N	77.42
GLY	24	Main	O	CYS	28	Main	N	81.52
GLY	24	Main	N	CYS	28	Main	O	58.44
GLN	25	Side	OE1	SER	9	Main	N	13.69
GLN	25	Side	NE2	SER	9	Side	OG	15.18
ARG	31	Side	NH2	TYS	12	Side	OS4	47.05
ARG	31	Side	NH1	TYS	12	Side	OH	40.46
ARG	31	Side	NH1	TYS	12	Side	OS4	29.67
ARG	31	Side	NH2	TYS	12	Side	OS2	25.17
ARG	31	Side	NH1	TYS	12	Side	OS2	12.49
ARG	31	Side	NH2	TYS	12	Side	OS3	11.49
ARG	31	Side	NH2	ASP	20	Side	OD2	16.08
ARG	31	Side	NH2	SER	23	Main	O	11.79
LYS	32	Side	NZ	TYS	12	Side	OS3	11.49
LYS	32	Side	NZ	ASP	20	Side	OD2	53.35
LYS	32	Side	NZ	ASP	20	Side	OD1	51.75
HIS	34	Side	ND1	TYS	21	Main	O	29.57

Complex 13:

V3 loop Residue	Number	Group	Atom	CXCR4 Residue	Number	Group	Atom	Occupancy (%)
CYS	1	Main	N	GLU	31	Side	OE2	37.56
CYS	1	Main	N	GLU	31	Side	OE1	37.06
THR	2	Main	N	PRO	27	Main	O	33.37
THR	8	Main	N	MET	24	Side	SD	19.28
THR	8	Main	O	LYS	25	Main	N	92.41
ARG	9	Side	NH2	TYS	12	Side	OS3	24.58
ARG	9	Side	NH2	TYS	12	Side	OS4	16.08
ARG	9	Side	NH1	TYS	12	Side	OS4	12.59
ARG	9	Side	NH2	TYS	12	Side	OS2	10.19
ARG	9	Side	NH1	GLU	14	Side	OE2	55.44
ARG	9	Side	NH1	GLU	14	Side	OE1	12.09
ARG	9	Side	NH1	GLU	15	Main	O	35.96
ARG	9	Side	NH2	ASP	20	Side	OD1	94.71
ARG	9	Side	NH2	ASP	20	Side	OD2	92.41
ARG	9	Side	NH1	ASP	20	Side	OD1	50.85
ARG	9	Side	NH1	ASP	20	Side	OD2	28.67
ARG	9	Side	NH1	TYS	21	Main	O	25.87
ARG	9	Side	NH1	ASP	22	Main	O	18.38
ARG	9	Side	NH2	ASP	193	Side	OD1	99.70
ARG	9	Side	NE	ASP	193	Side	OD2	88.21
ARG	9	Side	NH2	ASP	193	Side	OD2	67.83
ARG	9	Side	NE	ASP	193	Side	OD1	40.76
LYS	10	Side	NZ	GLU	2	Side	OE1	9.79
LYS	10	Side	NZ	GLU	2	Side	OE2	9.69
LYS	10	Side	NZ	CYS	28	Main	O	94.51
ARG	11	Side	NH1	TYS	7	Main	O	17.08
ARG	11	Side	NH1	ASP	10	Side	OD2	76.72
ARG	11	Side	NH1	ASP	10	Side	OD1	57.14
ARG	11	Side	NH2	ASP	10	Side	OD1	40.46
ARG	11	Side	NH2	ASP	10	Side	OD2	30.87
ARG	11	Side	NH2	TYR	190	Main	O	71.63
ARG	11	Side	NH2	PRO	191	Main	O	47.95
SER	13	Side	OG	ARG	188	Main	O	32.97
LEU	14	Main	O	ARG	188	Side	NH2	99.70
LEU	14	Main	O	ARG	188	Side	NE	42.16
LEU	14	Main	N	GLN	200	Side	OE1	66.43
GLY	17	Main	O	ASN	37	Side	ND2	39.86
GLY	17	Main	O	SER	285	Side	OG	93.11
GLY	17	Main	N	GLU	288	Side	OE1	94.81
GLY	17	Main	N	GLU	288	Side	OE2	79.92
ARG	18	Side	NH2	ASP	181	Side	OD2	25.57
ARG	18	Side	NH1	ASP	181	Side	OD2	13.09
VAL	19	Main	N	HIS	281	Side	NE2	62.24
VAL	19	Main	O	HIS	281	Side	ND1	19.08
VAL	19	Main	N	HIS	281	Side	ND1	15.98

TYR	21	Main	O	GLU	2	Main	N	17.08
TYR	21	Side	OH	GLU	277	Main	O	46.65
TYR	21	Side	OH	ASN	278	Side	OD1	18.48
TYR	21	Side	OH	ASN	278	Side	ND2	15.58
TYR	21	Side	OH	HIS	281	Side	ND1	51.85
THR	22	Side	OG1	MET	1	Main	N	75.92
THR	23	Main	N	MET	1	Main	O	16.78
THR	23	Side	OG1	GLU	2	Side	OE2	51.75
THR	23	Side	OG1	GLU	2	Side	OE1	49.45
GLN	25	Side	NE2	ILE	6	Main	O	23.68
GLN	25	Main	N	TYS	7	Main	O	28.57
GLN	25	Side	NE2	THR	8	Side	OG1	13.49
GLN	25	Main	O	SER	9	Main	N	66.53
GLN	25	Main	O	ASP	10	Main	N	53.75
VAL	27	Main	N	ASP	10	Main	O	13.79
VAL	27	Main	N	ASN	11	Side	OD1	38.26
VAL	27	Main	O	ASN	11	Side	ND2	24.58
ARG	31	Side	NH1	GLU	14	Side	OE1	85.51
ARG	31	Side	NH2	GLU	14	Side	OE2	81.82
ARG	31	Side	NH2	GLU	14	Side	OE1	67.83
ARG	31	Side	NH1	GLU	14	Side	OE2	46.65
ARG	31	Side	NH2	SER	23	Main	O	96.30
ARG	31	Side	NE	SER	23	Main	O	49.85
LYS	32	Side	NZ	ASP	22	Side	OD2	79.02
LYS	32	Side	NZ	ASP	22	Side	OD1	78.42
LYS	32	Side	NZ	SER	23	Side	OG	32.77

Complex 14:

V3 loop Residue	Number	Group	Atom	CXCR4 Residue	Number	Group	Atom	Occupancy (%)
ARG	3	Side	NH1	ASP	22	Side	OD2	91.11
ARG	3	Side	NH2	ASP	22	Side	OD1	87.61
ARG	3	Side	NH2	ASP	22	Side	OD2	74.93
ARG	3	Side	NH1	ASP	22	Side	OD1	18.48
ASN	5	Side	ND2	ASP	20	Main	O	90.71
ASN	5	Side	ND2	ASP	22	Side	OD2	84.32
ASN	5	Side	ND2	ASP	22	Side	OD1	79.02
ASN	6	Main	N	ASP	22	Side	OD1	42.16
ASN	7	Side	ND2	ASP	20	Side	OD1	55.34
ASN	7	Side	ND2	ASP	20	Side	OD2	37.06
THR	8	Main	N	ASP	20	Side	OD1	53.55
THR	8	Main	N	ASP	20	Side	OD2	32.97
THR	8	Side	OG1	ASP	20	Main	O	11.59
THR	8	Side	OG1	TYS	21	Main	O	22.98
ARG	9	Side	NH1	SER	5	Side	OG	21.38
ARG	9	Side	NH2	PRO	191	Main	O	95.30
ARG	9	Side	NH1	PRO	191	Main	O	74.83
LYS	10	Side	NZ	GLY	19	Main	O	88.81
LYS	10	Side	NZ	TYS	21	Main	O	97.90
LYS	10	Side	NZ	SER	23	Main	O	50.45
LYS	10	Side	NZ	ASP	193	Side	OD2	95.90
LYS	10	Side	NZ	ASP	193	Side	OD1	23.98
ARG	11	Side	NH1	GLU	2	Side	OE2	70.43
ARG	11	Side	NH1	GLU	2	Side	OE1	64.54
ARG	11	Side	NH2	GLU	2	Side	OE2	62.64
ARG	11	Side	NH2	GLU	2	Side	OE1	58.94
ARG	11	Side	NH1	TYS	7	Side	OS4	81.32
VAL	12	Main	N	TYS	7	Side	OS2	95.90
VAL	12	Main	N	TYS	7	Side	OS4	10.29
SER	13	Main	O	ARG	30	Side	NH2	38.16
SER	13	Side	OG	ARG	30	Side	NH2	19.58
LEU	14	Main	O	ARG	30	Side	NH2	54.65
PRO	16	Main	O	ASN	37	Side	ND2	38.26
GLY	17	Main	N	ASP	97	Side	OD1	91.21
ARG	18	Side	NH1	HIS	113	Side	NE2	98.40
ARG	18	Side	NH2	TYR	116	Side	OH	11.79
ARG	18	Side	NH2	HIS	203	Side	NE2	97.10
ARG	18	Side	NH1	HIS	203	Side	NE2	78.62
ARG	18	Side	NH2	TYR	255	Side	OH	89.21
ARG	18	Side	NH2	TYR	255	Side	OH	68.73
ARG	18	Side	NE	GLU	288	Side	OE2	91.21
ARG	18	Side	NH2	GLU	288	Side	OE1	83.02
ARG	18	Side	NH2	GLU	288	Side	OE2	63.54
ARG	18	Side	NE	GLU	288	Side	OE1	62.24
TRP	20	Side	NE1	TYR	190	Side	OH	22.88

TRP	20	Side	NE1	TYR	190	Side	OH	21.18
TRP	20	Side	NE1	GLN	200	Side	OE1	25.07
TRP	20	Side	NE1	GLN	200	Side	NE2	18.38
TRP	20	Main	O	HIS	281	Side	ND1	67.33
TRP	20	Main	N	SER	285	Side	OG	19.78
TYR	21	Side	OH	ASN	33	Side	ND2	10.49
TYR	21	Side	OH	ASN	37	Side	ND2	18.48
THR	22	Main	O	LYS	25	Side	NZ	37.76
THR	22	Side	OG1	LYS	25	Side	NZ	79.02
THR	23	Side	OG1	CYS	28	Main	N	35.76
THR	23	Side	OG1	CYS	28	Main	O	26.17
GLY	24	Main	N	LYS	25	Main	O	46.05
GLY	24	Main	N	GLU	26	Main	O	13.79
GLN	25	Side	NE2	THR	8	Side	OG1	10.49
ARG	31	Side	NH1	GLU	14	Side	OE1	31.67
ARG	31	Side	NH1	GLU	14	Side	OE2	29.67
ARG	31	Side	NH1	SER	18	Side	OG	41.96
ARG	31	Side	NH1	SER	18	Side	OG	31.17
ARG	31	Side	NH2	TYS	21	Side	OS3	47.95
ARG	31	Side	NH1	TYS	21	Side	OS3	47.35
ARG	31	Side	NH2	TYS	21	Side	OS2	43.26
ARG	31	Side	NH2	TYS	21	Side	OS4	37.86
ARG	31	Side	NH1	TYS	21	Side	OS2	35.16
ARG	31	Side	NH1	TYS	21	Side	OS4	34.07
LYS	32	Side	NZ	TYS	21	Side	OS2	29.77
LYS	32	Side	NZ	TYS	21	Side	OS3	26.87
LYS	32	Side	NZ	TYS	21	Side	OS4	23.28

Complex 15:

V3 loop Residue	Number	Group	Atom	CXCR4 Residue	Number	Group	Atom	Occupancy (%)
CYS	1	Main	N	ASP	20	Main	O	58.84
CYS	1	Main	N	ASP	20	Side	OD2	81.52
CYS	1	Main	N	ASP	20	Side	OD1	41.26
CYS	1	Main	N	TYS	21	Main	O	58.04
CYS	1	Main	N	GLU	268	Side	OE1	43.76
CYS	1	Main	N	GLU	268	Side	OE2	15.88
ASN	5	Side	ND2	TYS	12	Side	OS2	39.56
ASN	6	Main	N	TYS	12	Side	OS4	45.45
ASN	6	Main	N	TYS	12	Side	OS2	21.18
ASN	7	Main	O	ASN	11	Main	N	22.88
ASN	7	Main	O	ASN	11	Side	ND2	18.38
ASN	7	Main	O	TYS	12	Main	N	36.76
ASN	7	Side	ND2	TYS	12	Main	O	22.08
ASN	7	Side	ND2	GLU	14	Side	OE1	17.68
ASN	7	Side	ND2	GLU	14	Side	OE2	14.69
THR	8	Main	O	SER	9	Main	N	45.75
THR	8	Side	OG1	ASN	11	Side	OD1	22.98
THR	8	Side	OG1	ASN	11	Side	ND2	18.98
ARG	9	Side	NE	TYS	12	Side	OS4	90.61
ARG	9	Side	NH2	TYS	12	Side	OS4	23.68
ARG	9	Side	NE	TYS	12	Side	OS3	14.89
ARG	9	Side	NH2	ASP	20	Side	OD1	22.98
ARG	9	Side	NH2	TYS	21	Main	O	17.38
ARG	9	Side	NH1	TYS	21	Main	O	13.39
ARG	9	Side	NH1	ASP	22	Main	O	30.27
ARG	9	Side	NH2	ASP	22	Main	O	13.29
LYS	10	Side	NZ	ILE	6	Main	O	25.37
LYS	10	Side	NZ	THR	8	Side	OG1	29.17
LYS	10	Side	NZ	SER	9	Side	OG	15.28
ARG	11	Main	O	MET	1	Main	N	28.97
ARG	11	Side	NH1	TYS	7	Main	O	15.88
ARG	11	Side	NH2	ASP	10	Side	OD1	99.30
ARG	11	Side	NH1	ASP	10	Side	OD2	99.30
ARG	11	Side	NH1	ASP	10	Side	OD1	54.65
ARG	11	Side	NH2	ASP	10	Side	OD2	41.26
ARG	11	Side	NH2	PRO	191	Main	O	46.75
ARG	11	Side	NE	PRO	191	Main	O	40.86
SER	13	Side	OG	MET	1	Main	N	62.04
PRO	16	Main	O	ASN	37	Side	ND2	10.79
PRO	16	Main	O	ARG	183	Side	NH1	84.12
PRO	16	Main	O	ARG	183	Side	NH2	52.35
GLY	17	Main	N	GLU	288	Side	OE1	78.02
ARG	18	Side	NH2	TYR	45	Side	OH	98.30
ARG	18	Side	NH1	TYR	45	Side	OH	43.46
ARG	18	Side	NH1	TRP	94	Side	NE1	50.85

ARG	18	Side	NH2	TYR	116	Side	OH	12.09
ARG	18	Main	O	ARG	188	Side	NE	35.86
ARG	18	Main	O	ARG	188	Side	NH2	32.67
ARG	18	Main	N	GLU	288	Side	OE1	98.60
ARG	18	Side	NH2	GLU	288	Main	O	28.87
ARG	18	Side	NH2	GLU	288	Side	OE2	97.80
ARG	18	Side	NE	GLU	288	Side	OE2	94.01
ARG	18	Side	NE	GLU	288	Side	OE1	44.46
ARG	18	Side	NH2	GLU	288	Side	OE1	13.09
VAL	19	Main	O	ARG	188	Side	NH2	34.97
VAL	19	Main	O	TYR	190	Side	OH	89.51
TRP	20	Side	NE1	ARG	188	Side	NH2	86.51
TRP	20	Side	NE1	ARG	188	Side	NH2	42.26
TRP	20	Side	NE1	HIS	203	Side	NE2	23.68
TYR	21	Side	OH	MET	1	Main	N	39.66
TYR	21	Side	OH	ASP	187	Side	OD2	37.06
TYR	21	Side	OH	ASP	187	Side	OD1	15.98
TYR	21	Side	OH	ARG	188	Main	O	20.98
THR	22	Side	OG1	GLU	277	Side	OE2	60.54
THR	23	Main	O	LYS	25	Side	NZ	98.50
THR	23	Side	OG1	ASP	193	Side	OD2	30.97
THR	23	Side	OG1	ASP	193	Side	OD1	19.28
GLY	24	Main	O	CYS	28	Main	N	27.47
ILE	26	Main	N	LYS	25	Main	O	57.04
CYS	35	Main	N	SER	23	Main	O	37.56

Complex 16:

V3 loop Residue	Number	Group	Atom	CXCR4 Residue	Number	Group	Atom	Occupancy (%)
ARG	3	Side	NE	SER	23	Side	OG	10.19
ARG	3	Side	NE	SER	23	Side	OG	9.79
ASN	6	Side	ND2	ASN	11	Side	OD1	20.08
ASN	7	Side	ND2	ASP	22	Main	O	10.09
ASN	7	Side	ND2	SER	23	Main	O	21.88
ASN	7	Side	OD1	LYS	25	Main	N	25.67
THR	8	Main	O	LYS	25	Main	N	24.18
ARG	9	Side	NH1	GLU	14	Side	OE1	62.74
ARG	9	Side	NH1	GLU	14	Side	OE2	53.75
ARG	9	Side	NH2	ASP	20	Main	O	10.59
ARG	9	Side	NH1	ASP	193	Side	OD2	82.32
ARG	9	Side	NH2	ASP	193	Side	OD2	61.74
ARG	9	Side	NH1	ASP	193	Side	OD1	56.84
ARG	9	Side	NH2	ASP	193	Side	OD1	11.89
ARG	9	Side	NH2	LEU	266	Main	O	17.38
LYS	10	Side	NZ	CYS	28	Main	O	34.07
ARG	11	Side	NH1	TYS	12	Side	OS2	43.16
ARG	11	Side	NH2	TYS	12	Side	OS2	36.56
ARG	11	Side	NH1	TYS	12	Side	OS3	30.57
ARG	11	Side	NH1	TYS	12	Side	OS4	23.48
ARG	11	Side	NH2	TYS	12	Side	OS4	21.58
ARG	11	Side	NH2	TYS	12	Side	OS3	12.59
ARG	11	Side	NH1	GLU	14	Side	OE2	68.23
ARG	11	Side	NE	GLU	14	Side	OE2	40.76
ARG	11	Side	NH2	PRO	191	Main	O	58.54
ARG	11	Side	NE	ASP	193	Side	OD1	23.78
ARG	11	Side	NH1	ASP	193	Side	OD1	22.98
SER	13	Side	OG	ARG	188	Main	O	59.54
LEU	14	Main	O	ARG	188	Side	NH2	99.30
LEU	14	Main	O	ARG	188	Side	NE	57.34
LEU	14	Main	N	GLN	200	Side	OE1	28.77
GLY	17	Main	O	SER	285	Side	OG	93.51
GLY	17	Main	N	GLU	288	Side	OE1	96.20
GLY	17	Main	N	GLU	288	Side	OE2	88.51
ARG	18	Side	NH2	ARG	30	Side	NH2	33.47
ARG	18	Side	NH1	ARG	30	Side	NH2	31.77
ARG	18	Side	NH1	ARG	30	Side	NH2	11.79
ARG	18	Side	NH2	ASP	181	Side	OD2	86.51
ARG	18	Side	NH1	ASP	181	Side	OD2	26.47
ARG	18	Side	NH1	ARG	183	Side	NH2	17.08
ARG	18	Side	NH1	ARG	183	Side	NH2	16.38
TYR	21	Main	O	MET	1	Main	N	61.44
TYR	21	Main	N	MET	1	Side	SD	20.18
TYR	21	Side	OH	GLU	277	Main	O	45.35
TYR	21	Side	OH	ASN	278	Side	OD1	15.98

THR	22	Side	OG1	MET	1	Main	N	96.10
THR	22	Side	OG1	MET	1	Main	O	20.48
GLN	25	Main	N	THR	8	Side	OG1	16.18
GLN	25	Side	OE1	SER	9	Main	N	13.19
GLN	25	Main	O	ASP	10	Main	N	57.24
GLN	25	Main	N	ASP	10	Side	OD2	10.69
GLN	25	Side	OE1	ASP	10	Main	N	19.18
GLN	25	Main	O	ASN	11	Main	N	70.63
GLN	25	Side	OE1	ASN	11	Main	N	22.08
GLN	25	Side	NE2	ASN	11	Side	OD1	37.86
VAL	27	Main	N	TYS	12	Main	O	70.03
VAL	27	Main	N	GLU	14	Side	OE1	16.38
VAL	27	Main	N	GLU	14	Side	OE2	14.99
ASP	29	Side	OD1	SER	18	Side	OG	11.59
ASP	29	Main	N	SER	23	Side	OG	71.33
ILE	30	Main	N	ASP	20	Side	OD1	12.19
ARG	31	Side	NH1	ASP	20	Main	O	14.69
ARG	31	Side	NH1	ASP	20	Side	OD1	16.78
ARG	31	Side	NH1	ASP	20	Side	OD2	15.38
ARG	31	Side	NH2	TYS	21	Main	O	16.58
ARG	31	Side	NH1	GLU	268	Side	OE1	73.13
ARG	31	Side	NH2	GLU	268	Side	OE1	72.23
ARG	31	Side	NH2	GLU	268	Side	OE2	70.53
ARG	31	Side	NH1	GLU	268	Side	OE2	41.66
LYS	32	Side	NZ	ASP	22	Side	OD1	55.54
LYS	32	Side	NZ	ASP	22	Side	OD2	37.56

Complex 17:

V3 loop Residue	Number	Group	Atom	CXCR4 Residue	Number	Group	Atom	Occupancy (%)
ARG	3	Side	NH2	TYS	21	Main	O	27.47
ARG	3	Side	NH1	TYS	21	Main	O	14.79
ARG	3	Side	NH2	ASP	22	Main	O	40.36
ARG	3	Side	NH2	SER	23	Main	O	10.49
ARG	9	Side	NH2	TYS	12	Side	OS3	19.28
ARG	9	Side	NH2	TYS	12	Side	OS2	13.09
ARG	9	Side	NH2	ASP	193	Side	OD1	22.28
ARG	9	Side	NE	ASP	193	Side	OD1	11.99
LYS	10	Side	NZ	GLU	2	Side	OE1	41.66
LYS	10	Side	NZ	GLU	2	Side	OE2	40.36
LYS	10	Main	O	LYS	25	Side	NZ	68.73
ARG	11	Side	NH2	TYS	12	Side	OS2	90.81
ARG	11	Side	NH2	TYS	12	Side	OS4	44.76
ARG	11	Side	NH2	TYS	12	Side	OS3	19.28
ARG	11	Side	NH2	ASP	193	Side	OD1	93.91
SER	13	Side	OG	ASP	187	Side	OD2	99.20
SER	13	Side	OG	ASP	187	Side	OD1	60.94
SER	13	Side	OG	PHE	189	Main	N	72.23
SER	13	Side	OG	PHE	189	Main	N	68.63
SER	13	Side	OG	TYR	190	Main	N	87.41
LEU	14	Main	O	ARG	188	Side	NE	91.81
LEU	14	Main	O	ARG	188	Side	NH2	88.91
GLY	17	Main	N	TYR	45	Side	OH	16.68
GLY	17	Main	O	SER	285	Side	OG	80.62
GLY	17	Main	N	GLU	288	Side	OE1	95.70
GLY	17	Main	N	GLU	288	Side	OE2	84.92
ARG	18	Side	NH1	ASP	181	Side	OD1	91.51
ARG	18	Side	NH2	ASP	181	Side	OD1	85.71
ARG	18	Side	NH2	HIS	281	Side	NE2	47.75
ARG	18	Side	NE	HIS	281	Side	NE2	46.75
ARG	18	Side	NH2	HIS	281	Side	ND1	29.27
TRP	20	Side	NE1	ARG	183	Side	NH2	27.47
TRP	20	Side	NE1	ARG	183	Side	NH2	25.57
TRP	20	Side	NE1	ARG	183	Side	NH1	9.59
TYR	21	Main	N	ASP	181	Side	OD2	19.18
TYR	21	Main	N	ASP	181	Side	OD1	14.99
TYR	21	Side	OH	GLU	277	Side	OE2	46.05
TYR	21	Side	OH	GLU	277	Side	OE1	34.97
TYR	21	Side	OH	ASN	278	Side	ND2	12.59
TYR	21	Side	OH	HIS	281	Side	ND1	10.79
THR	22	Side	OG1	TYR	190	Main	O	91.91
THR	23	Main	O	MET	1	Main	N	94.91
THR	23	Main	N	MET	1	Main	O	39.96
THR	23	Side	OG1	GLU	2	Side	OE2	47.95
THR	23	Side	OG1	GLU	2	Side	OE1	46.25

GLN	25	Side	NE2	SER	9	Side	OG	37.66
GLN	25	Main	O	ASN	11	Side	ND2	24.38
GLN	25	Side	OE1	ASN	11	Side	ND2	34.67
GLN	25	Side	NE2	ASN	11	Side	OD1	19.48
GLN	25	Main	O	TYS	12	Main	N	57.84
ILE	26	Main	O	ASN	11	Side	ND2	11.89
VAL	27	Main	N	ASN	11	Side	OD1	10.89
VAL	27	Main	N	TYS	12	Main	O	52.95
GLY	28	Main	N	GLU	14	Side	OE2	17.28
GLY	28	Main	N	GLU	14	Side	OE1	11.09
ARG	31	Side	NH1	GLU	14	Side	OE1	34.07
ARG	31	Side	NH1	GLU	14	Side	OE2	22.28
ARG	31	Side	NH2	GLU	14	Side	OE1	20.08
ARG	31	Side	NH2	SER	18	Side	OG	11.59
ARG	31	Side	NH2	SER	18	Side	OG	11.59
ARG	31	Side	NH2	ASP	20	Side	OD1	87.21
ARG	31	Side	NH1	ASP	20	Side	OD2	79.12
ARG	31	Side	NH2	ASP	20	Side	OD2	58.34
ARG	31	Side	NH1	ASP	20	Side	OD1	35.06
LYS	32	Side	NZ	GLU	268	Side	OE1	77.42
LYS	32	Side	NZ	GLU	268	Side	OE2	62.34

Supporting Table 4: The table consists of three individual panels divided by thick black frames. The left panel presents the average interaction energy per V3 loop residue in descending order, by summing up the interaction energies of the specific residue with all of its possible CXCR4 interacting residues. The middle and right panels present the (%) residue propensity per V3 loop position for all 35-residue CXCR4 and CXCR/CCR5 V3 loops, respectively, deposited in the Los Alamos National Laboratory database (http://www.hiv.lanl.gov). All values have been computed by analysis of 1000 snapshots, extracted from the 20-ns simulation of complex 1 at 20-ps intervals.

	Interaction Free Energies per V3-loop residue (kcal/mol)			Residue (%) Propensity for CXCR4 V3 loops				Residue (%) Propensity for CXCR4/CCR5 V3 loops			
Residue	Total	Polar	Non-Polar	Residue 1:	Residue 2:	Residue 3:	Residue 4:	Residue 1:	Residue 2:	Residue 3:	Residue 4:
Arg18	-124.03	-111.61	-12.42	Arg(60)	Gln(31)	Lys(4)	Gly(2)	Arg(57)	Gln(35)	Gly(2)	Lys(2)
Lys10	-57.74	-42.30	-15.44	Lys(63)	Arg(15)	Thr(12)	Gln(7)	Lys(68)	Arg(15)	Gln(9)	Thr(6)
Arg3	-42.21	-37.32	-4.89	Arg(100)	Ile(0)	Met(0)	Ser(0)	Arg(100)	Ile(0)	Met(0)	Ser(0)
Arg31	-37.87	-29.54	-8.33	Arg(96)	Lys(2)	Gly(1)	Ile(1)	Arg(98)	Ile(1)	Lys(1)	Val(0)
Arg11	-37.58	-15.91	-21.67	Ser(42)	Arg(30)	Gly(24)	Asp(1)	Ser(47)	Gly(27)	Arg(22)	Asp(1)
Arg9	-32.58	-16.99	-15.59	Arg(88)	Ile(4)	Lys(3)	Ala(2)	Arg(89)	Ala(3)	Ile(3)	Lys(3)
Trp20	-28.95	-8.94	-20.01	Phe(59)	Trp(10)	Val(9)	Leu(8)	Phe(60)	Trp(10)	Leu(9)	Val(8)
Leu14	-27.42	-7.00	-20.42	Ile(65)	Leu(18)	Met(11)	Ala(1)	Ile(70)	Leu(16)	Met(10)	Ala(1)
Lys32	-26.28	-24.74	-1.54	Gln(50)	Lys(31)	Arg(18)	Ile(0)	Gln(55)	Lys(28)	Arg(15)	His(1)
Tyr21	-19.79	-2.61	-17.18	Tyr(82)	Phe(8)	His(6)	Ser(2)	Tyr(81)	Phe(10)	His(7)	Val(0)
Pro16	-13.58	-0.73	-12.85	Pro(91)	Gln(4)	Gly(2)	Leu(1)	Pro(94)	Gln(3)	Gly(2)	Ala(0)
Gly15	-12.67	-6.48	-6.20	Gly(95)	Ile(2)	Ser(2)	Ala(0)	Gly(97)	Ile(2)	Ser(1)	Ala(0)
Ser13	-12.49	-6.72	-5.77	Arg(29)	His(27)	Thr(15)	Ser(14)	His(35)	Arg(28)	Thr(12)	Ser(10)
Asn5	-12.48	-6.14	-6.34	Asn(60)	Gly(17)	Ser(11)	Tyr(6)	Asn(62)	Gly(20)	Ser(11)	Tyr(5)
Gly17	-12.11	-6.12	-6.00	Gly(96)	Pro(1)	Gln(1)	Arg(1)	Gly(97)	Pro(1)	Arg(1)	Ala(0)
Gln25	-11.96	-1.05	-10.91	Asp(21)	Glu(19)	Gln(18)	Arg(12)	Asp(22)	Glu(18)	Gln(14)	Lys(13)
Gly24	-11.49	-4.43	-7.07	Gly(66)	Glu(8)	Arg(7)	Thr(6)	Gly(68)	Glu(8)	Thr(7)	Lys(4)
Val12	-10.31	0.50	-10.82	Ile(56)	Val(29)	Thr(5)	Leu(4)	Ile(59)	Val(29)	Thr(6)	Phe(2)
Thr8	-10.22	-1.96	-8.26	Thr(84)	Ile(9)	Lys(3)	Met(1)	Thr(92)	Ile(4)	Lys(1)	Arg(1)
Val19	-9.52	-0.98	-8.53	Ala(49)	Val(28)	Thr(15)	Arg(2)	Ala(50)	Val(23)	Thr(21)	Tyr(2)
Thr22	-8.33	-1.94	-6.4	Thr(43)	Ala(40)	Lys(7)	Arg(5)	Ala(48)	Thr(42)	Arg(3)	His(2)
Thr23	-8.32	-0.19	-8.13	Thr(87)	Ala(6)	Met(2)	His(1)	Thr(86)	Ala(7)	Arg(2)	Ser(2)
Asn6	-7.40	-3.53	-3.87	Asn(90)	Lys(4)	Tyr(2)	Asp(1)	Asn(95)	Asp(1)	Glu(1)	Lys(1)
Val27	-6.38	-0.22	-6.15	Ile(71)	Val(13)	Thr(11)	Glu(1)	Ile(80)	Val(12)	Thr(7)	Met(1)
Ile26	-5.90	-0.33	-5.57	Ile(95)	Val(3)	Gly(1)	Lys(1)	Ile(95)	Val(3)	Gly(1)	Lys(0)
Asn7	-4.90	-2.14	-2.76	Asn(84)	Lys(5)	Tyr(3)	Thr(2)	Asn(93)	Lys(2)	Tyr(2)	Ile(1)
His34	-2.99	-0.71	-2.28	His(65)	Tyr(34)	Arg(0)	Ile(0)	His(72)	Tyr(27)	Val(0)	His(0)
Cys1	-0.71	-0.68	-0.04	Cys(100)	-	-	-	Cys(100)	-	-	-
Pro4	-0.67	-0.07	-0.61	Pro(100)	Ile(0)	Met(0)	Ser(0)	Pro(100)	Ile(0)	Met(0)	Ser(0)
Ile30	-0.44	-0.15	-0.29	Ile(96)	Met(1)	Asn(1)	Thr(1)	Ile(97)	Asn(1)	Thr(1)	Val(1)
Gly28	-0.32	0.06	-0.38	Gly(99)	Lys(1)	Thr(0)	Glu(0)	Gly(99)	Lys(1)	Thr(0)	Met(0)
Thr2	-0.19	-0.03	-0.16	Thr(79)	Ile(9)	Met(3)	Ser(3)	Thr(74)	Ile(12)	Met(4)	Ser(4)
Ala33	-0.16	0.02	-0.18	Ala(98)	Pro(1)	Arg(0)	Ile(0)	Ala(98)	Pro(1)	Val(1)	His(0)
Cys35	0.98	1.03	-0.06	Cys(100)	-	-	-	Cys(100)	-	-	-
Asp29	1.04	1.25	-0.21	Asp(83)	Asn(11)	Tyr(2)	Gly(1)	Asp(85)	Asn(13)	Gly(1)	Met(0)

Left panel: The interaction energies are decomposed into polar and non-polar components. Middle and right panels: The four most probable V3 loop residues per position (according to the descending order of the left panel) are presented, and the corresponding residue propensity is

shown in parenthesis. If a residue in the middle and right panels, matches the corresponding residue of the left panel (V3 loop of this study), it is highlighted in grey background. If a residue in the middle and right panels, possesses similar physicochemical properties to the corresponding residue of left panel (V3 loop of this study), it is highlighted in light green background.

Supporting Coordinates

The MD coordinates, extracted every 2 are provided as Supporting Information in PDB format. The structures are aligned with regard to the backbone of the CXCR4 intramembrane helical region. The correspondence of PDB files and time in the MD simulation is as follows:

PDB file	Time (ns)
v3loop_cxcr4.1.pdb	2
v3loop_cxcr4.2.pdb	4
v3loop_cxcr4.3.pdb	6
v3loop_cxcr4.4.pdb	8
v3loop_cxcr4.5.pdb	10
v3loop_cxcr4.6.pdb	12
v3loop_cxcr4.7.pdb	14
v3loop_cxcr4.8.pdb	16
v3loop_cxcr4.9.pdb	18
v3loop_cxcr4.10.pdb	20

Supporting Video

A video demonstrating the simulation trajectory of the V3 loop : CXCR4 complex structure, and depicting the gradual stabilization and preservation of the key salt bridges is provided as Supporting Video.

The V3 loop is shown in tube and in red color, and its 16-20 residue moiety is shown in fat tube representation. The CXCR4 is shown in light gray transparent tube representation. The salt bridge and hydrogen bonds in panels (A) and (B) are denoted in dashed lines, the corresponding heavy atom distances are denoted in Å, and the participating V3 loop and CXCR4 residue moieties are shown in licorice. The Cα atoms of V3 loop and CXCR4 salt bridge participating residues are annotated. Hydrogen atoms are omitted for clarity and the V3 loop disulfide bridge is shown in fat transparent licorice representation.

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