



Full wwPDB NMR Structure Validation Report ⓘ

Oct 26, 2021 – 11:17 PM EDT

PDB ID : 6X63
Title : Atomic-Resolution Structure of HIV-1 Capsid Tubes by Magic Angle Spinning NMR
Authors : Lu, M.; Russell, R.W.; Bryer, A.; Quinn, C.M.; Hou, G.; Zhang, H.; Schwitters, C.D.; Perilla, J.R.; Gronenborn, A.M.; Polenova, T.
Deposited on : 2020-05-27

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance

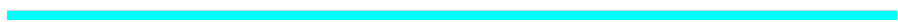
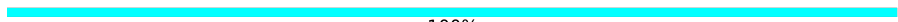
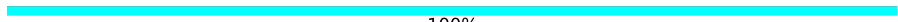
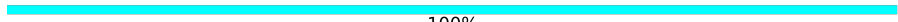
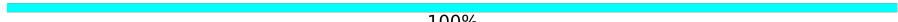
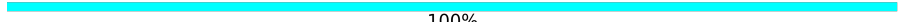
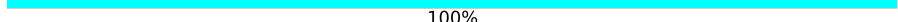
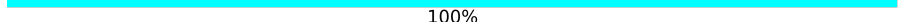
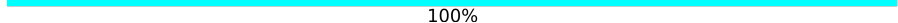
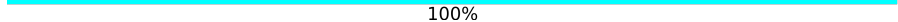
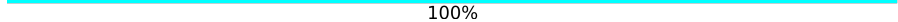
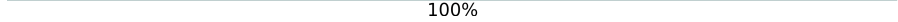
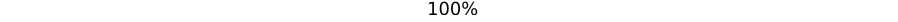
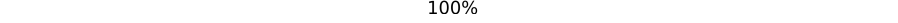
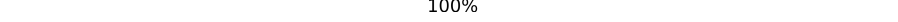
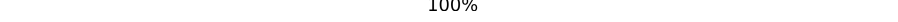
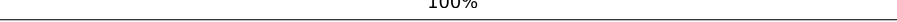
The following experimental techniques were used to determine the structure:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 0%.

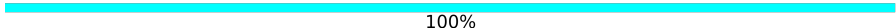
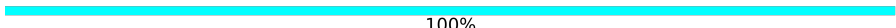
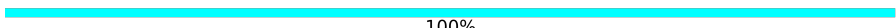
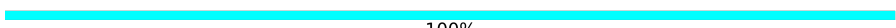
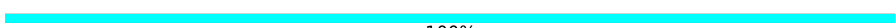








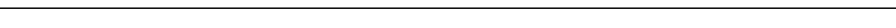

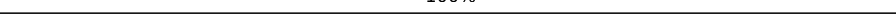
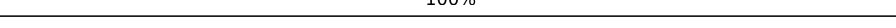
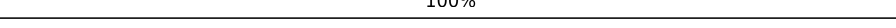
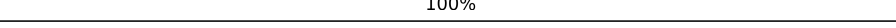
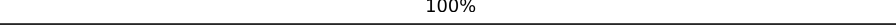
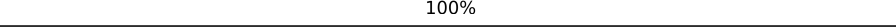
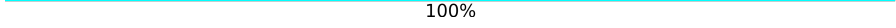
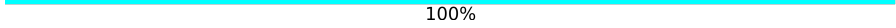
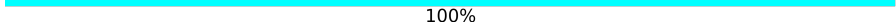
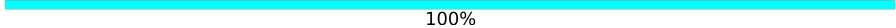
There are no overall percentile quality scores available for this entry.

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	0	231	 100%
1	0A	231	 100%
1	0B	231	 100%
1	0C	231	 100%
1	0D	231	 100%
1	0E	231	 100%
1	1	231	 100%
1	1A	231	 100%
1	1B	231	 100%
1	1C	231	 100%
1	1D	231	 100%
1	1E	231	 100%
1	2	231	 100%
1	2A	231	 100%
1	2B	231	 100%
1	2C	231	 100%
1	2D	231	 100%

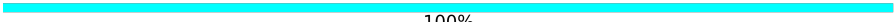
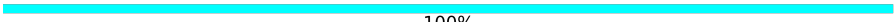
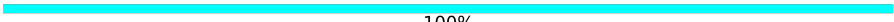
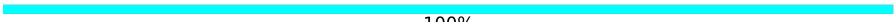
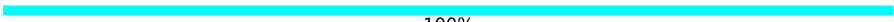
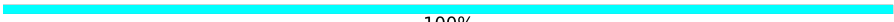
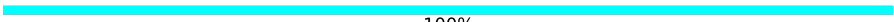
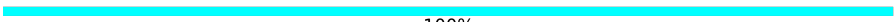
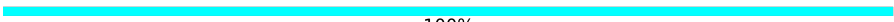
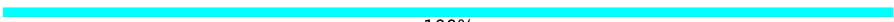




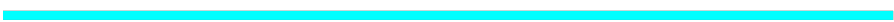
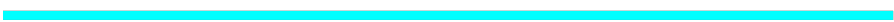
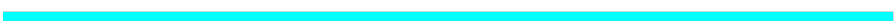








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Mol	Chain	Length	Quality of chain
1	2E	231	 100%
1	3	231	 100%
1	3A	231	 100%
1	3B	231	 100%
1	3C	231	 100%
1	3D	231	 100%
1	3E	231	 100%
1	4	231	 100%
1	4A	231	 100%
1	4B	231	 100%
1	4C	231	 100%
1	4D	231	 100%
1	4E	231	 100%
1	5	231	 100%
1	5A	231	 100%
1	5B	231	 100%
1	5C	231	 100%
1	5D	231	 100%
1	5E	231	 100%
1	6	231	 100%
1	6A	231	 100%
1	6B	231	 100%
1	6C	231	 100%
1	6D	231	 100%
1	6E	231	 100%

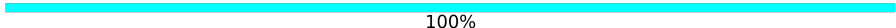
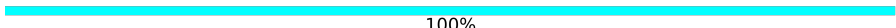
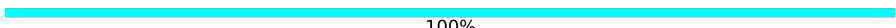
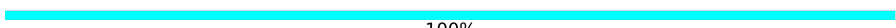
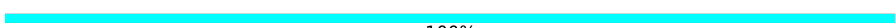








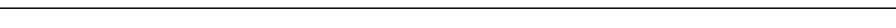

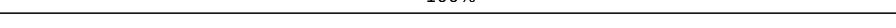
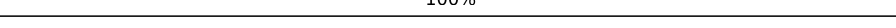
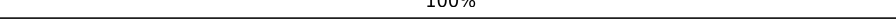
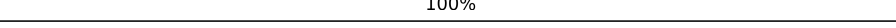
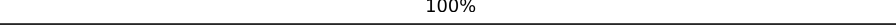
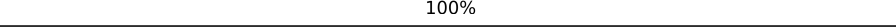
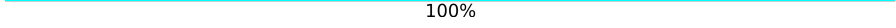
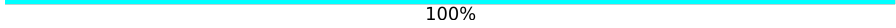
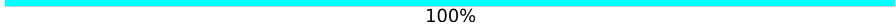
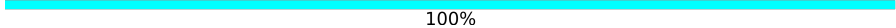
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Mol	Chain	Length	Quality of chain
1	7	231	 100%
1	7A	231	 100%
1	7B	231	 100%
1	7C	231	 100%
1	7D	231	 100%
1	7E	231	 100%
1	8	231	 100%
1	8A	231	 100%
1	8B	231	 100%
1	8C	231	 100%
1	8D	231	 100%
1	8E	231	 100%
1	9	231	 100%
1	9A	231	 100%
1	9B	231	 100%
1	9C	231	 100%
1	9D	231	 100%
1	9E	231	 100%
1	A	231	 100%
1	AA	231	 100%
1	AB	231	 100%
1	AC	231	 100%
1	AD	231	 100%
1	AE	231	 100%
1	AF	231	 100%

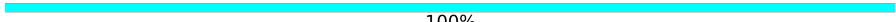
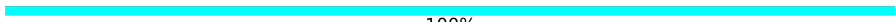
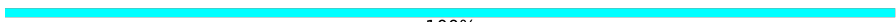
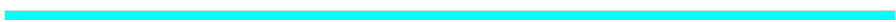











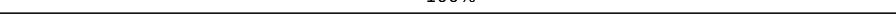
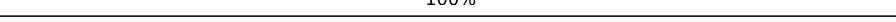
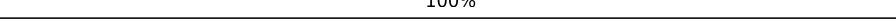

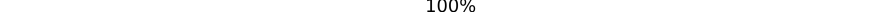
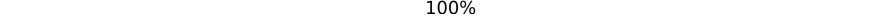
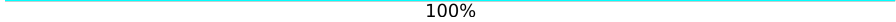
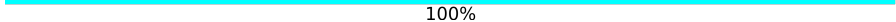

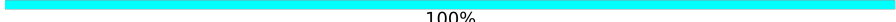
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Mol	Chain	Length	Quality of chain
1	B	231	 100%
1	BA	231	 100%
1	BB	231	 100%
1	BC	231	 100%
1	BD	231	 100%
1	BE	231	 100%
1	BF	231	 100%
1	C	231	 100%
1	CA	231	 100%
1	CB	231	 100%
1	CC	231	 100%
1	CD	231	 100%
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1	DD	231	 100%
1	DE	231	 100%
1	DF	231	 100%
1	E	231	 100%
1	EA	231	 100%
1	EB	231	 100%
1	EC	231	 100%

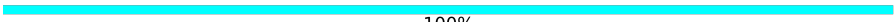
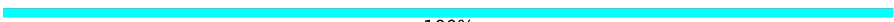












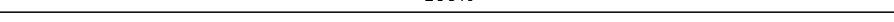
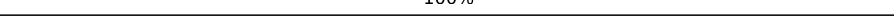
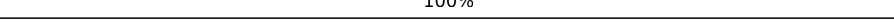
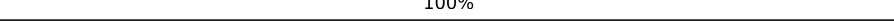
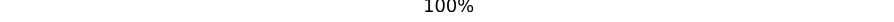
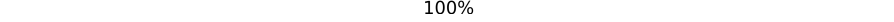
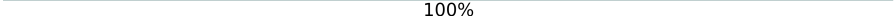
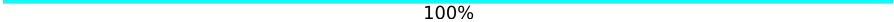
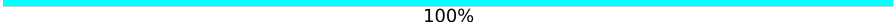
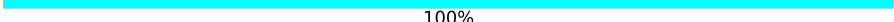
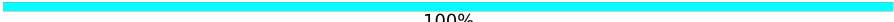
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Mol	Chain	Length	Quality of chain
1	ED	231	 100%
1	EE	231	 100%
1	EF	231	 100%
1	F	231	 100%
1	FA	231	 100%
1	FB	231	 100%
1	FC	231	 100%
1	FD	231	 100%
1	FE	231	 100%
1	FF	231	 100%
1	G	231	 100%
1	GA	231	 100%
1	GB	231	 100%
1	GC	231	 100%
1	GD	231	 100%
1	GE	231	 100%
1	H	231	 100%
1	HA	231	 100%
1	HB	231	 100%
1	HC	231	 100%
1	HD	231	 100%
1	HE	231	 100%
1	I	231	 100%
1	IA	231	 100%
1	IB	231	 100%

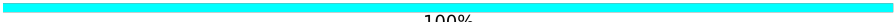
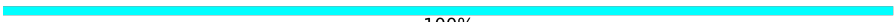
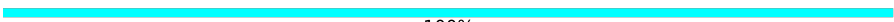
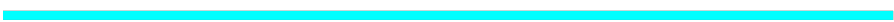











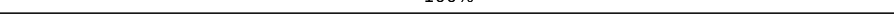
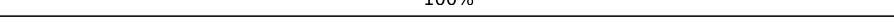
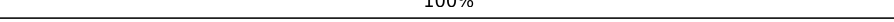
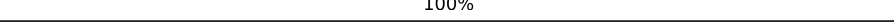
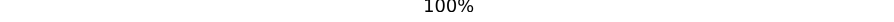
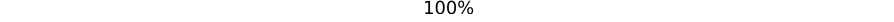
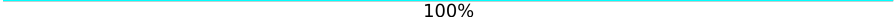
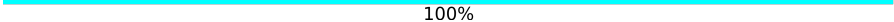
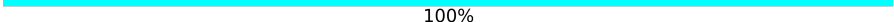
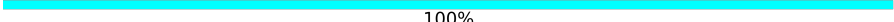
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Mol	Chain	Length	Quality of chain
1	IC	231	 100%
1	ID	231	 100%
1	IE	231	 100%
1	J	231	 100%
1	JA	231	 100%
1	JB	231	 100%
1	JC	231	 100%
1	JD	231	 100%
1	JE	231	 100%
1	K	231	 100%
1	KA	231	 100%
1	KB	231	 100%
1	KC	231	 100%
1	KD	231	 100%
1	KE	231	 100%
1	L	231	 100%
1	LA	231	 100%
1	LB	231	 100%
1	LC	231	 100%
1	LD	231	 100%
1	LE	231	 100%
1	M	231	 100%
1	MA	231	 100%
1	MB	231	 100%
1	MC	231	 100%

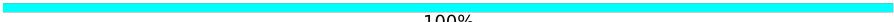
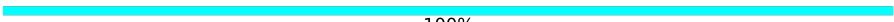
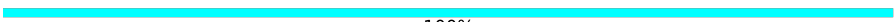
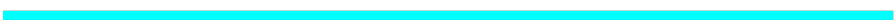











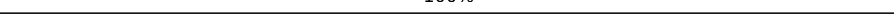
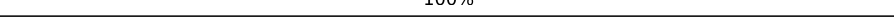
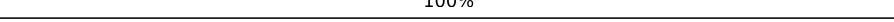
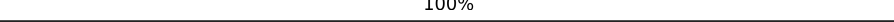
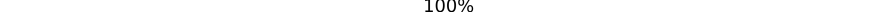
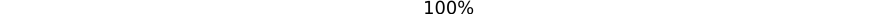
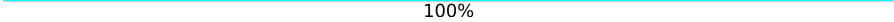
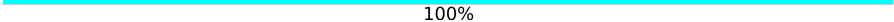
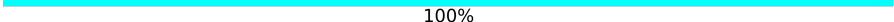
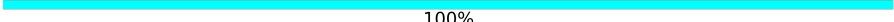
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Mol	Chain	Length	Quality of chain
1	MD	231	 100%
1	ME	231	 100%
1	N	231	 100%
1	NA	231	 100%
1	NB	231	 100%
1	NC	231	 100%
1	ND	231	 100%
1	NE	231	 100%
1	O	231	 100%
1	OA	231	 100%
1	OB	231	 100%
1	OC	231	 100%
1	OD	231	 100%
1	OE	231	 100%
1	P	231	 100%
1	PA	231	 100%
1	PB	231	 100%
1	PC	231	 100%
1	PD	231	 100%
1	PE	231	 100%
1	Q	231	 100%
1	QA	231	 100%
1	QB	231	 100%
1	QC	231	 100%
1	QD	231	 100%

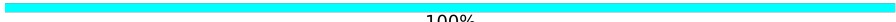
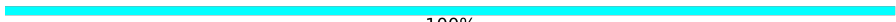
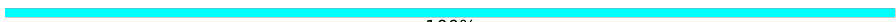
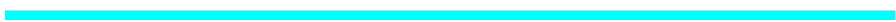











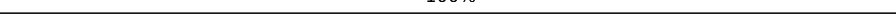
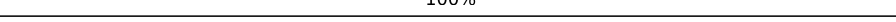
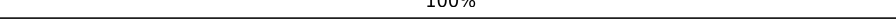

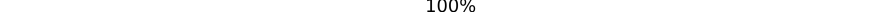
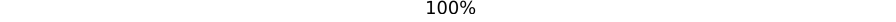
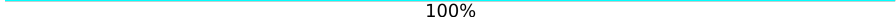
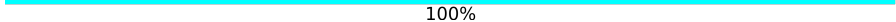

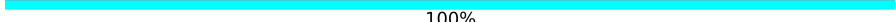
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Mol	Chain	Length	Quality of chain
1	QE	231	 100%
1	R	231	 100%
1	RA	231	 100%
1	RB	231	 100%
1	RC	231	 100%
1	RD	231	 100%
1	RE	231	 100%
1	S	231	 100%
1	SA	231	 100%
1	SB	231	 100%
1	SC	231	 100%
1	SD	231	 100%
1	SE	231	 100%
1	T	231	 100%
1	TA	231	 100%
1	TB	231	 100%
1	TC	231	 100%
1	TD	231	 100%
1	TE	231	 100%
1	U	231	 100%
1	UA	231	 100%
1	UB	231	 100%
1	UC	231	 100%
1	UD	231	 100%
1	UE	231	 100%

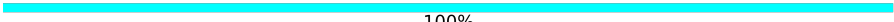
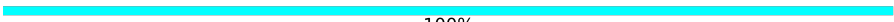
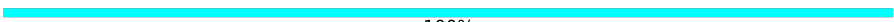
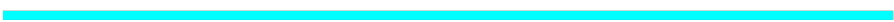











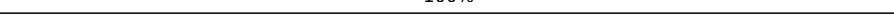
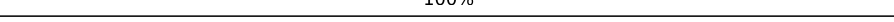
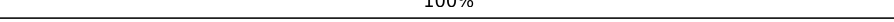
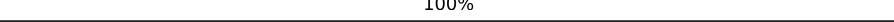
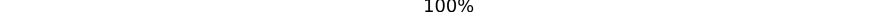
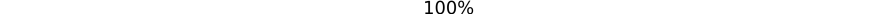
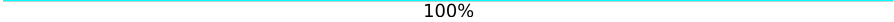
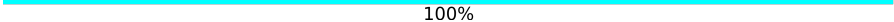
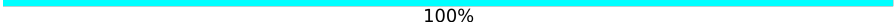
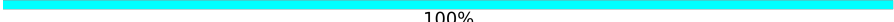
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Mol	Chain	Length	Quality of chain
1	V	231	 100%
1	VA	231	 100%
1	VB	231	 100%
1	VC	231	 100%
1	VD	231	 100%
1	VE	231	 100%
1	W	231	 100%
1	WA	231	 100%
1	WB	231	 100%
1	WC	231	 100%
1	WD	231	 100%
1	WE	231	 100%
1	X	231	 100%
1	XA	231	 100%
1	XB	231	 100%
1	XC	231	 100%
1	XD	231	 100%
1	XE	231	 100%
1	Y	231	 100%
1	YA	231	 100%
1	YB	231	 100%
1	YC	231	 100%
1	YD	231	 100%
1	YE	231	 100%
1	Z	231	 100%

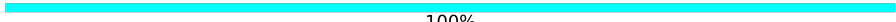
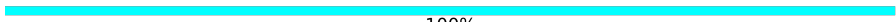
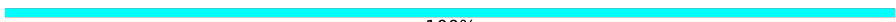
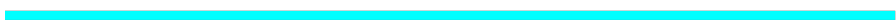











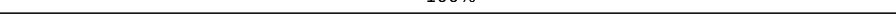
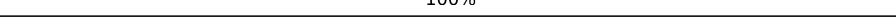
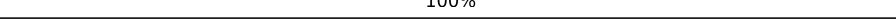

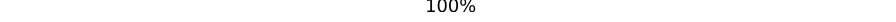
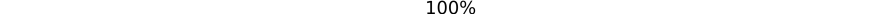
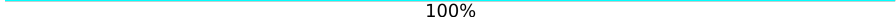
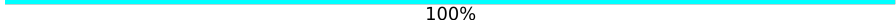

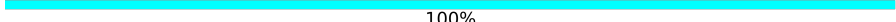
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Mol	Chain	Length	Quality of chain
1	ZA	231	 100%
1	ZB	231	 100%
1	ZC	231	 100%
1	ZD	231	 100%
1	ZE	231	 100%
1	a	231	 100%
1	aA	231	 100%
1	aB	231	 100%
1	aC	231	 100%
1	aD	231	 100%
1	aE	231	 100%
1	b	231	 100%
1	bA	231	 100%
1	bB	231	 100%
1	bC	231	 100%
1	bD	231	 100%
1	bE	231	 100%
1	c	231	 100%
1	cA	231	 100%
1	cB	231	 100%
1	cC	231	 100%
1	cD	231	 100%
1	cE	231	 100%
1	d	231	 100%
1	dA	231	 100%

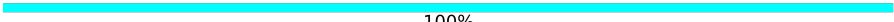
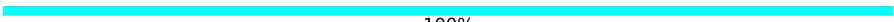
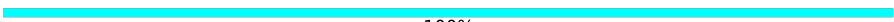
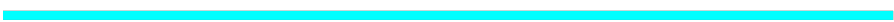











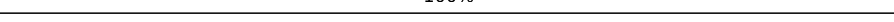
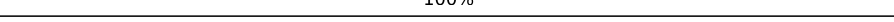
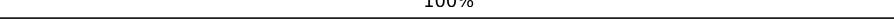
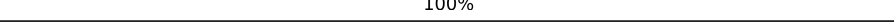
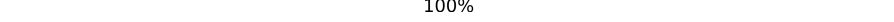
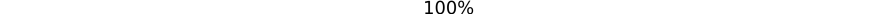
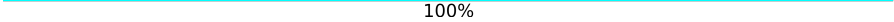
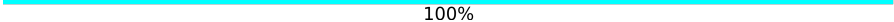
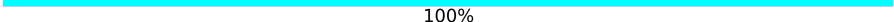
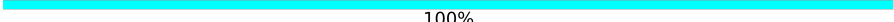
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Mol	Chain	Length	Quality of chain
1	dB	231	 100%
1	dC	231	 100%
1	dD	231	 100%
1	dE	231	 100%
1	e	231	 100%
1	eA	231	 100%
1	eB	231	 100%
1	eC	231	 100%
1	eD	231	 100%
1	eE	231	 100%
1	f	231	 100%
1	fA	231	 100%
1	fB	231	 100%
1	fC	231	 100%
1	fD	231	 100%
1	fE	231	 100%
1	g	231	 100%
1	gA	231	 100%
1	gB	231	 100%
1	gC	231	 100%
1	gD	231	 100%
1	gE	231	 100%
1	h	231	 100%
1	hA	231	 100%
1	hB	231	 100%

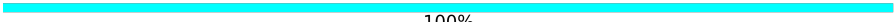
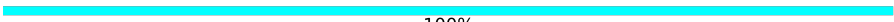
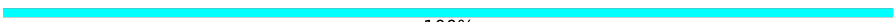
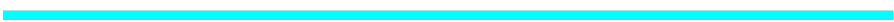











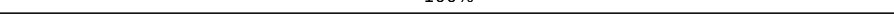
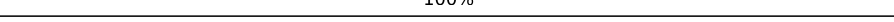
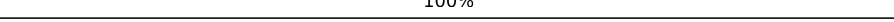
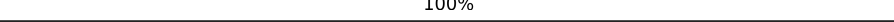
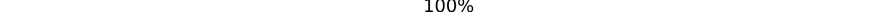
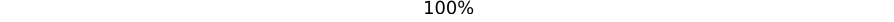
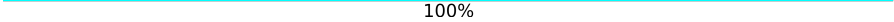
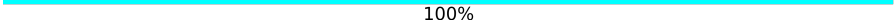
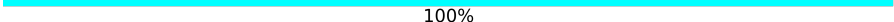
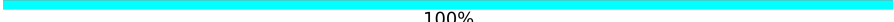
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Mol	Chain	Length	Quality of chain
1	hC	231	 100%
1	hD	231	 100%
1	hE	231	 100%
1	i	231	 100%
1	iA	231	 100%
1	iB	231	 100%
1	iC	231	 100%
1	iD	231	 100%
1	iE	231	 100%
1	j	231	 100%
1	jA	231	 100%
1	jB	231	 100%
1	jC	231	 100%
1	jD	231	 100%
1	jE	231	 100%
1	k	231	 100%
1	kA	231	 100%
1	kB	231	 100%
1	kC	231	 100%
1	kD	231	 100%
1	kE	231	 100%
1	l	231	 100%
1	lA	231	 100%
1	lB	231	 100%
1	lC	231	 100%

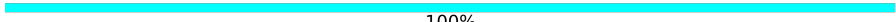
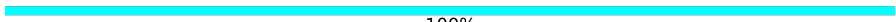
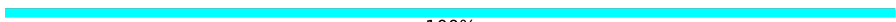
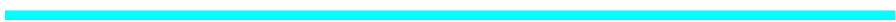











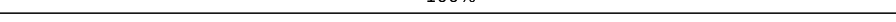
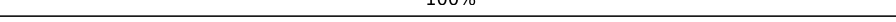
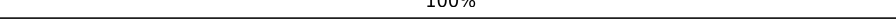

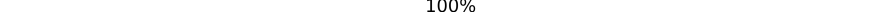
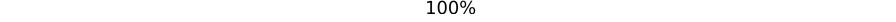
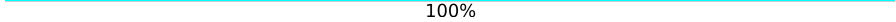
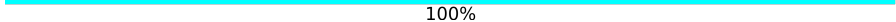

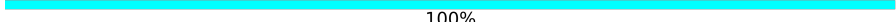
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Mol	Chain	Length	Quality of chain
1	lD	231	 100%
1	lE	231	 100%
1	m	231	 100%
1	mA	231	 100%
1	mB	231	 100%
1	mC	231	 100%
1	mD	231	 100%
1	mE	231	 100%
1	n	231	 100%
1	nA	231	 100%
1	nB	231	 100%
1	nC	231	 100%
1	nD	231	 100%
1	nE	231	 100%
1	o	231	 100%
1	oA	231	 100%
1	oB	231	 100%
1	oC	231	 100%
1	oD	231	 100%
1	oE	231	 100%
1	p	231	 100%
1	pA	231	 100%
1	pB	231	 100%
1	pC	231	 100%
1	pD	231	 100%

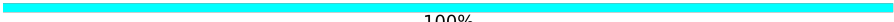
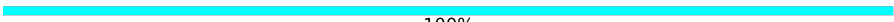
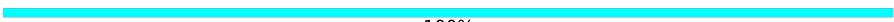
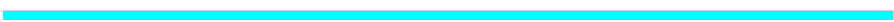











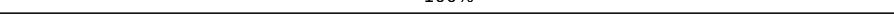
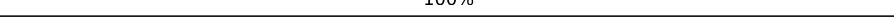
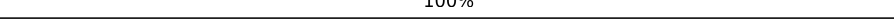
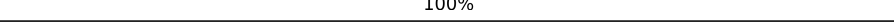
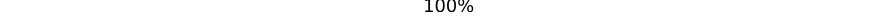
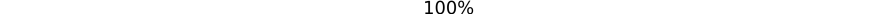
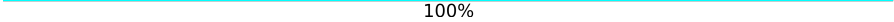
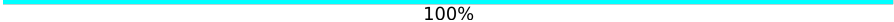
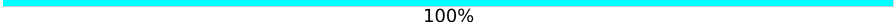
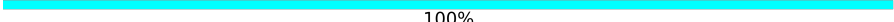
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Mol	Chain	Length	Quality of chain
1	pE	231	 100%
1	q	231	 100%
1	qA	231	 100%
1	qB	231	 100%
1	qC	231	 100%
1	qD	231	 100%
1	qE	231	 100%
1	r	231	 100%
1	rA	231	 100%
1	rB	231	 100%
1	rC	231	 100%
1	rD	231	 100%
1	rE	231	 100%
1	s	231	 100%
1	sA	231	 100%
1	sB	231	 100%
1	sC	231	 100%
1	sD	231	 100%
1	sE	231	 100%
1	t	231	 100%
1	tA	231	 100%
1	tB	231	 100%
1	tC	231	 100%
1	tD	231	 100%
1	tE	231	 100%

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Mol	Chain	Length	Quality of chain
1	u	231	 100%
1	uA	231	 100%
1	uB	231	 100%
1	uC	231	 100%
1	uD	231	 100%
1	uE	231	 100%
1	v	231	 100%
1	vA	231	 100%
1	vB	231	 100%
1	vC	231	 100%
1	vD	231	 100%
1	vE	231	 100%
1	w	231	 100%
1	wA	231	 100%
1	wB	231	 100%
1	wC	231	 100%
1	wD	231	 100%
1	wE	231	 100%
1	x	231	 100%
1	xA	231	 100%
1	xB	231	 100%
1	xC	231	 100%
1	xD	231	 100%
1	xE	231	 100%
1	y	231	 100%

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Mol	Chain	Length	Quality of chain
1	yA	231	 100%
1	yB	231	 100%
1	yC	231	 100%
1	yD	231	 100%
1	yE	231	 100%
1	z	231	 100%
1	zA	231	 100%
1	zB	231	 100%
1	zC	231	 100%
1	zD	231	 100%
1	zE	231	 100%

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1359288 atoms, of which 680778 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called HIV-1 capsid protein.

Mol	Chain	Residues	Atoms						Trace
1	A	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	B	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	C	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	D	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	E	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	F	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	G	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	H	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	I	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	J	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	K	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	L	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	M	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	N	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	O	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	P	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	Q	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	R	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	S	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	

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Mol	Chain	Residues	Atoms						Trace
1	T	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	U	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	V	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	W	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	X	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	Y	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	Z	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	a	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	b	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	c	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	d	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	e	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	f	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	g	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	h	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	i	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	j	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	k	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	l	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	m	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	n	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0

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Mol	Chain	Residues	Atoms						Trace
1	o	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	p	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	q	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	r	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	s	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	t	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	u	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	v	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	w	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	x	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	y	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	z	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	0	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	1	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	2	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	3	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	4	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	5	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	6	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	7	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	8	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0

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Mol	Chain	Residues	Atoms						Trace
1	9	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	AA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	BA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	CA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	DA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	EA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	FA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	GA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	HA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	IA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	JA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	KA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	LA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	MA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	NA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	OA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	PA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	QA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	RA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	SA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	TA	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	

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Mol	Chain	Residues	Atoms						Trace
1	UA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	VA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	WA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	XA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	YA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	ZA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	aA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	bA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	cA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	dA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	eA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	fA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	gA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	hA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	iA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	jA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	kA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	lA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	mA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	nA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	oA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0

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Mol	Chain	Residues	Atoms						Trace
1	pA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	qA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	rA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	sA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	tA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	uA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	vA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	wA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	xA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	yA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	zA	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	0A	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	1A	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	2A	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	3A	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	4A	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	5A	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	6A	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	7A	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	8A	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	9A	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0

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Mol	Chain	Residues	Atoms						Trace
1	AB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	BB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	CB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	DB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	EB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	FB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	GB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	HB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	IB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	JB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	KB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	LB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	MB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	NB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	OB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	PB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	QB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	RB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	SB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	TB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	UB	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0

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Mol	Chain	Residues	Atoms						Trace
1	VB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	WB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	XB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	YB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	ZB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	aB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	bB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	cB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	dB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	eB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	fB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	gB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	hB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	iB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	jB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	kB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	lB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	mB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	nB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	oB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	pB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	

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Mol	Chain	Residues	Atoms						Trace
1	qB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	rB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	sB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	tB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	uB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	vB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	wB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	xB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	yB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	zB	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	0B	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	1B	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	2B	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	3B	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	4B	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	5B	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	6B	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	7B	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	8B	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	9B	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	AC	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	

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Mol	Chain	Residues	Atoms						Trace
1	BC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	CC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	DC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	EC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	FC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	GC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	HC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	IC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	JC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	KC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	LC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	MC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	NC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	OC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	PC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	QC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	RC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	SC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	TC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	UC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	VC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0

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Mol	Chain	Residues	Atoms						Trace
1	WC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	XC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	YC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	ZC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	aC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	bC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	cC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	dC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	eC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	fC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	gC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	hC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	iC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	jC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	kC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	lC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	mC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	nC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	oC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	pC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	qC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0

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Mol	Chain	Residues	Atoms						Trace
1	rC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	sC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	tC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	uC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	vC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	wC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	xC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	yC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	zC	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	0C	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	1C	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	2C	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	3C	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	4C	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	5C	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	6C	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	7C	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	8C	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	9C	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	AD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	BD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0

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Mol	Chain	Residues	Atoms						Trace
1	CD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	DD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	ED	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	FD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	GD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	HD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	ID	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	JD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	KD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	LD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	MD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	ND	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	OD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	PD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	QD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	RD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	SD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	TD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	UD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	VD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	WD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0

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Mol	Chain	Residues	Atoms						Trace
1	XD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	YD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	ZD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	aD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	bD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	cD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	dD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	eD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	fD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	gD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	hD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	iD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	jD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	kD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	lD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	mD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	nD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	oD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	pD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	qD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	rD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0

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Mol	Chain	Residues	Atoms						Trace
1	sD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	tD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	uD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	vD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	wD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	xD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	yD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	zD	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	0D	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	1D	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	2D	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	3D	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	4D	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	5D	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	6D	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	7D	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	8D	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	9D	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	AE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	BE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	CE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0

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Mol	Chain	Residues	Atoms						Trace
1	DE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	EE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	FE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	GE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	HE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	IE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	JE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	KE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	LE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	ME	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	NE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	OE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	PE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	QE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	RE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	SE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	TE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	UE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	VE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	WE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	XE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0

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Mol	Chain	Residues	Atoms						Trace
1	YE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	ZE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	aE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	bE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	cE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	dE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	eE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	fE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	gE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	hE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	iE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	jE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	kE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	lE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	mE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	nE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	oE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	pE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	qE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	rE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	sE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0

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Mol	Chain	Residues	Atoms						Trace
1	tE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	uE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	vE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	wE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	xE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	yE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	zE	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	0E	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	1E	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	2E	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	3E	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	4E	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	5E	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	6E	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	7E	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	8E	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	9E	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	AF	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	BF	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	CF	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0
1	DF	231	Total 3596	C 1131	H 1801	N 317	O 334	S 13	0

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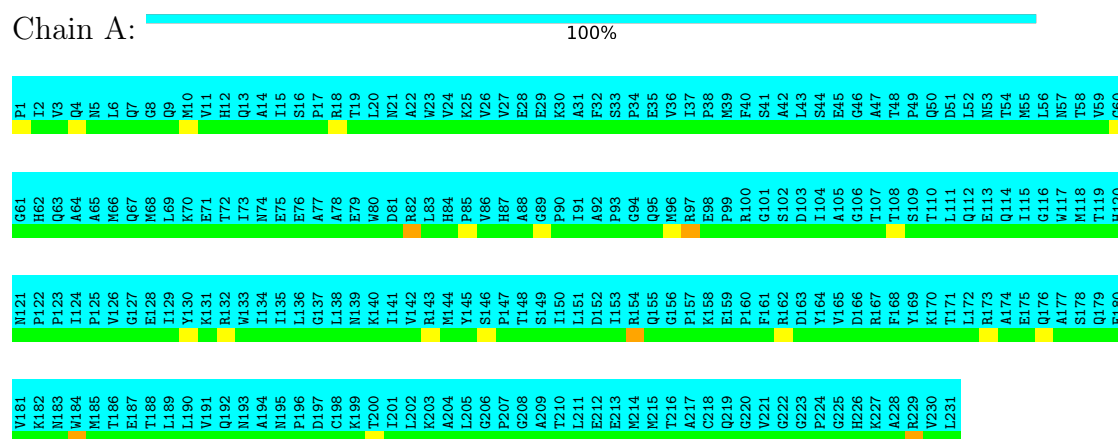
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Mol	Chain	Residues	Atoms						Trace
1	EF	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	
1	FF	231	Total	C	H	N	O	S	0
			3596	1131	1801	317	334	13	

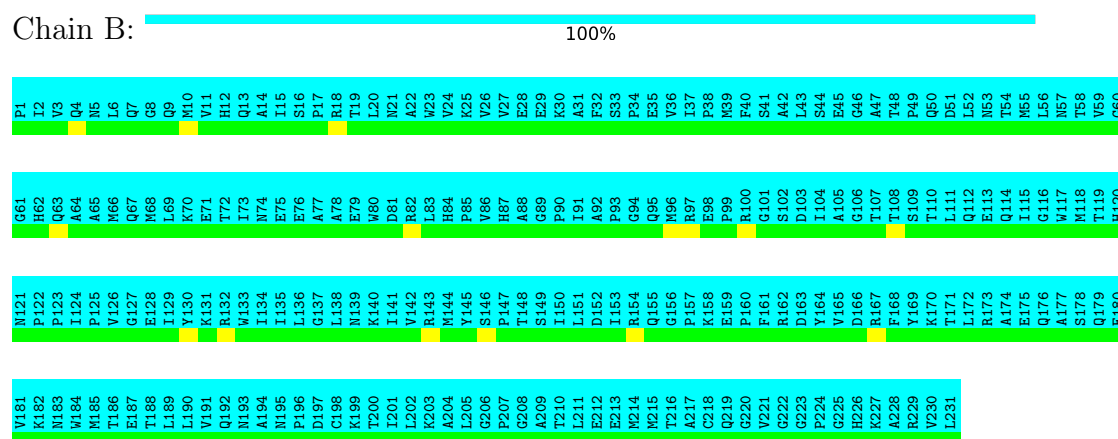
4 Residue-property plots

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

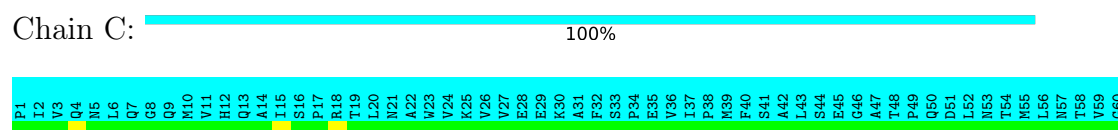
- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein



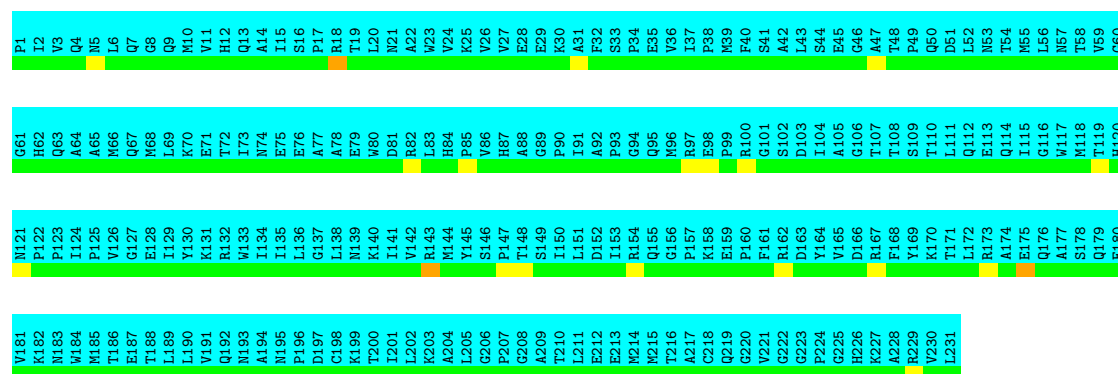
- Molecule 1: HIV-1 capsid protein





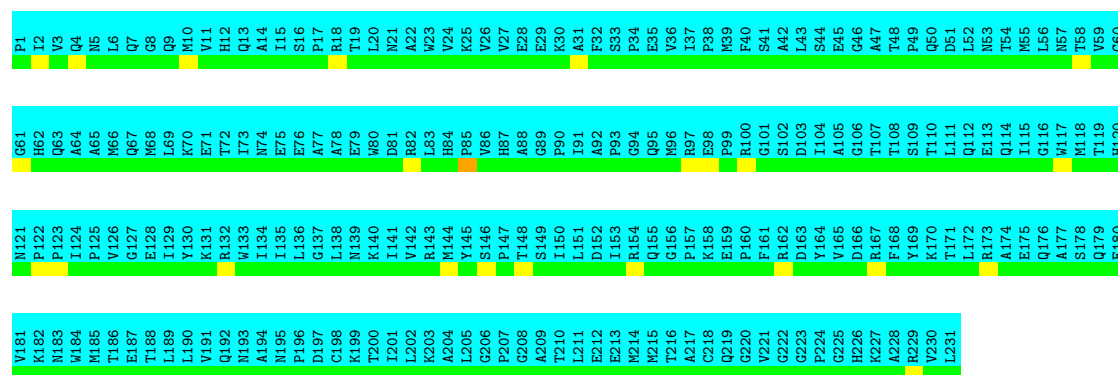
• Molecule 1: HIV-1 capsid protein

Chain D: 100%



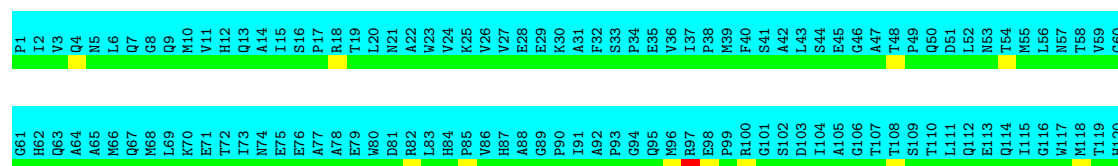
• Molecule 1: HIV-1 capsid protein

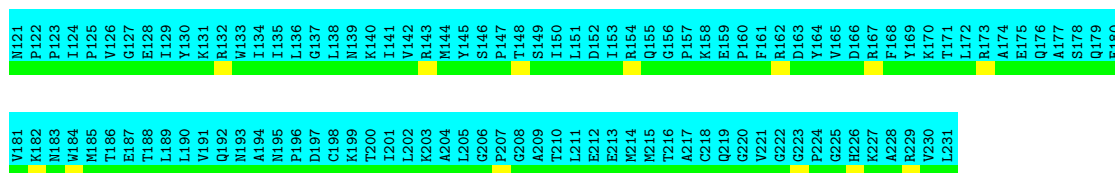
Chain E: 100%



• Molecule 1: HIV-1 capsid protein

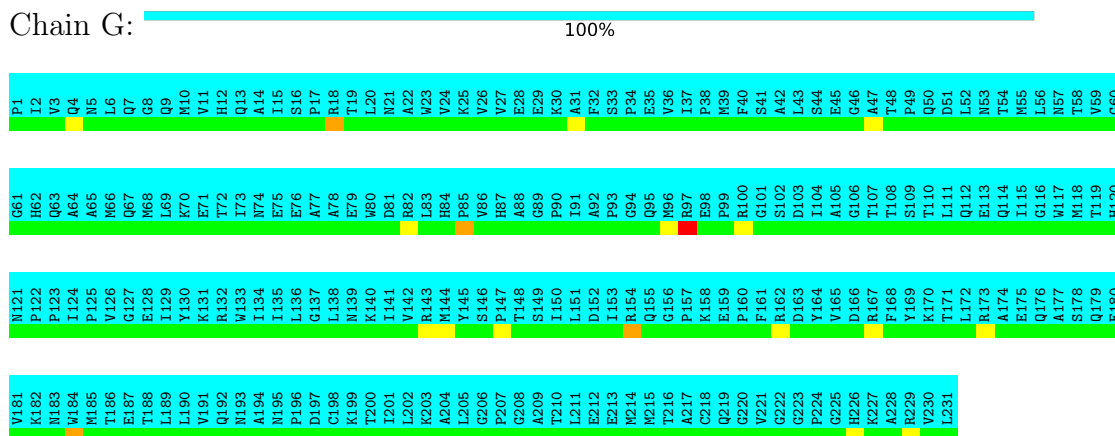
Chain F: 100%





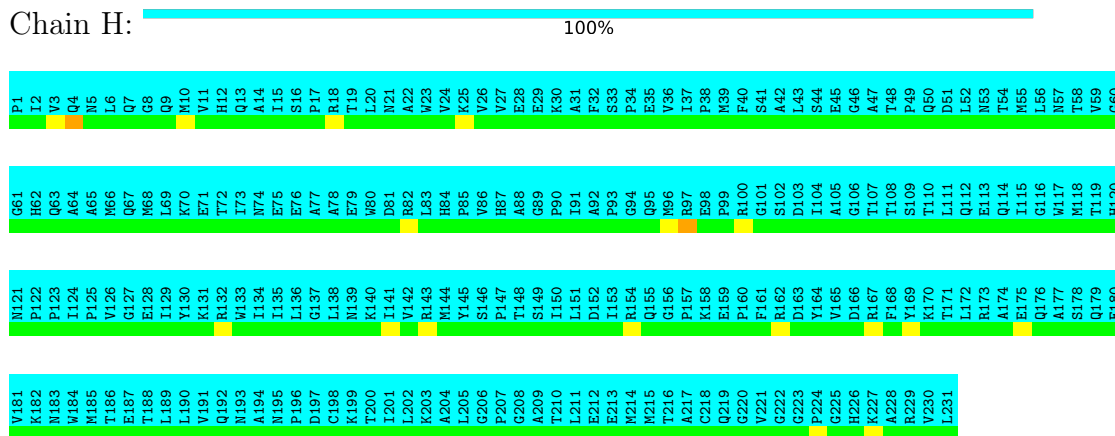
- Molecule 1: HIV-1 capsid protein

Chain G:



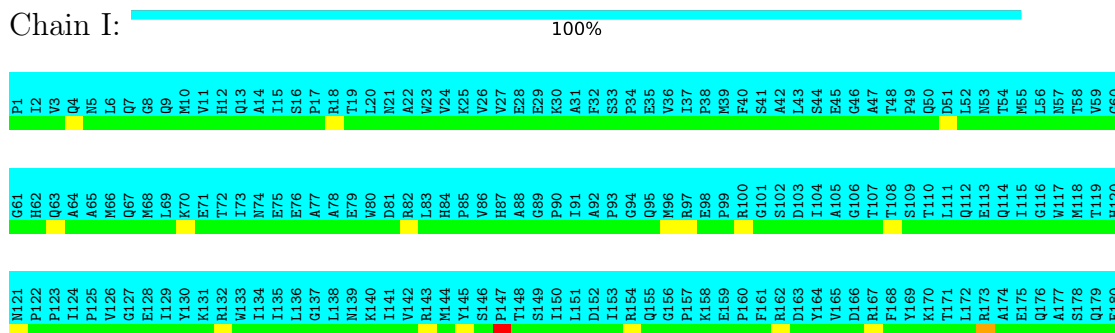
- Molecule 1: HIV-1 capsid protein

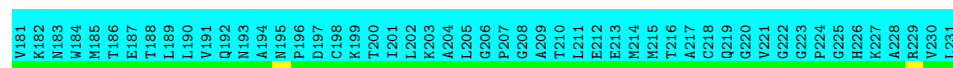
Chain H:



- Molecule 1: HIV-1 capsid protein

Chain I:

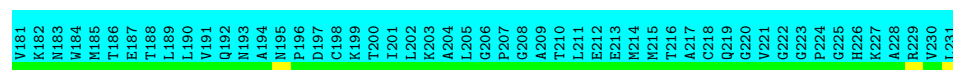
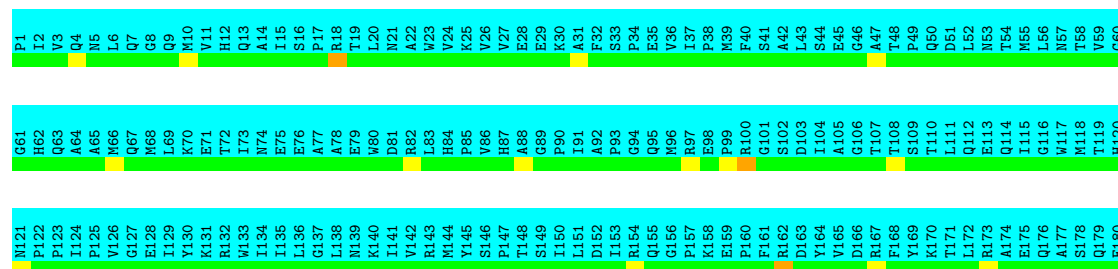




- Molecule 1: HIV-1 capsid protein

Chain J:

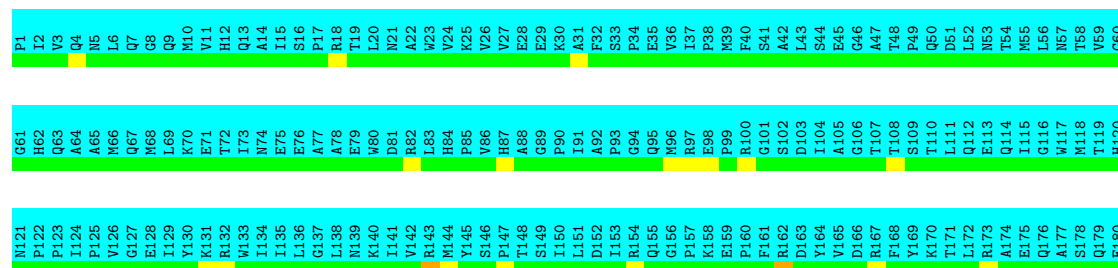
100%



- Molecule 1: HIV-1 capsid protein

Chain K:

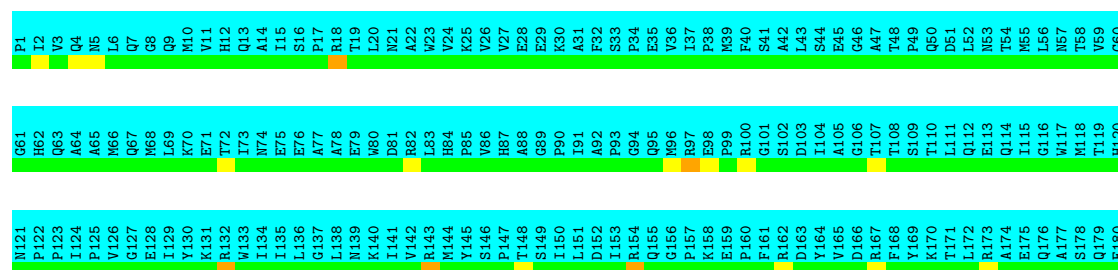
100%



- Molecule 1: HIV-1 capsid protein

Chain L:

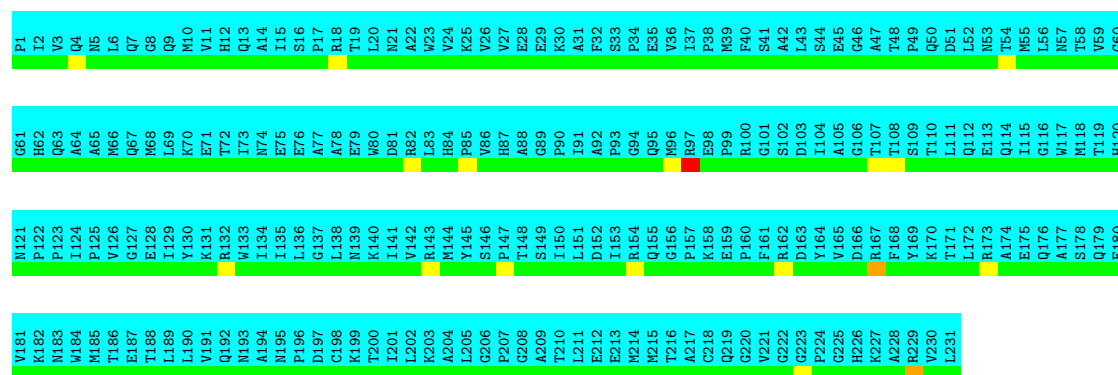
100%



- Molecule 1: HIV-1 capsid protein

Chain M:

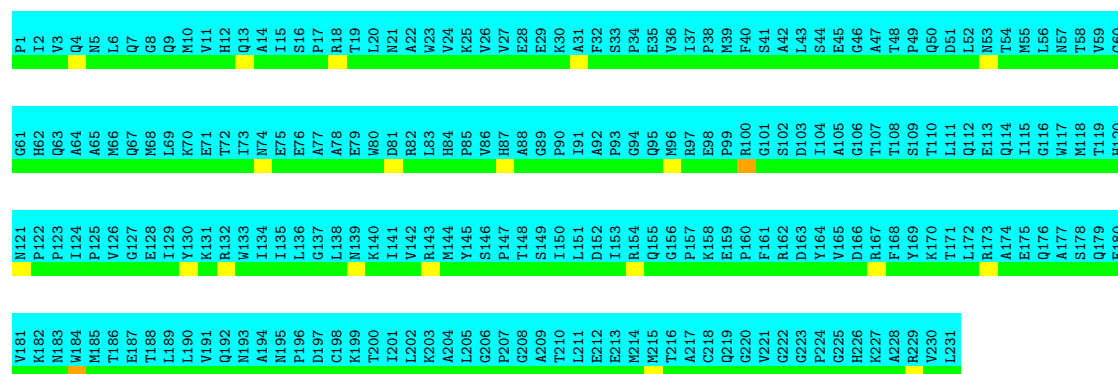
100%



- Molecule 1: HIV-1 capsid protein

Chain N:

100%



- Molecule 1: HIV-1 capsid protein

Chain O:

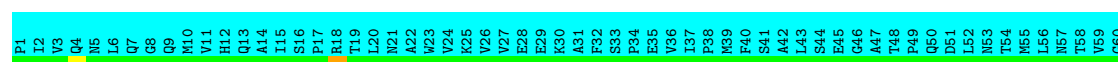
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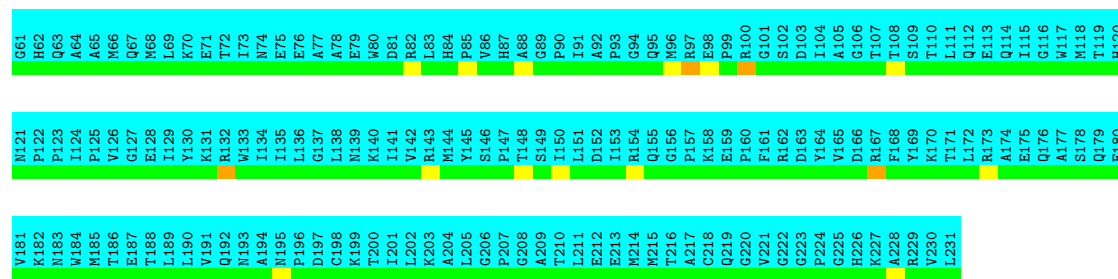


- Molecule 1: HIV-1 capsid protein

Chain P:

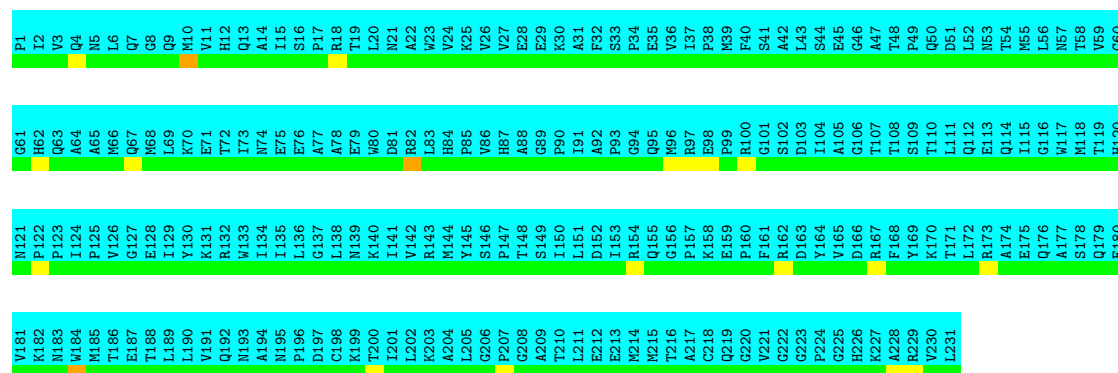
100%





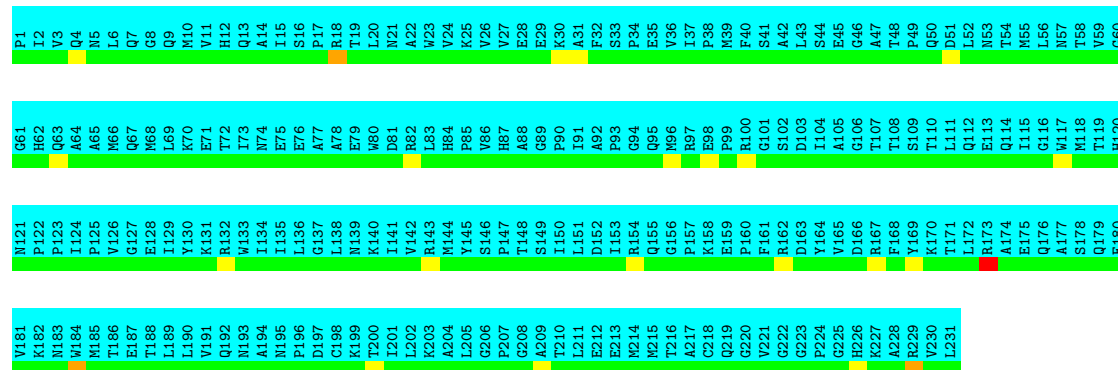
- Molecule 1: HIV-1 capsid protein

Chain Q:  100%



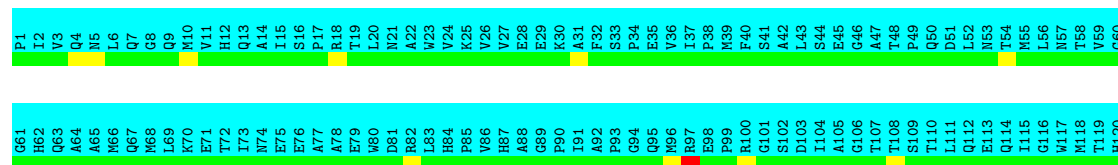
- Molecule 1: HIV-1 capsid protein

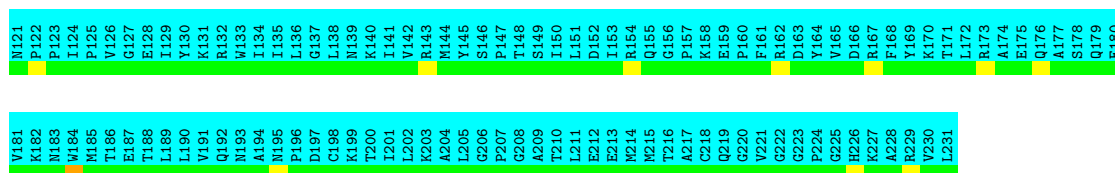
Chain R:  100%



- Molecule 1: HIV-1 capsid protein

Chain S:  100%

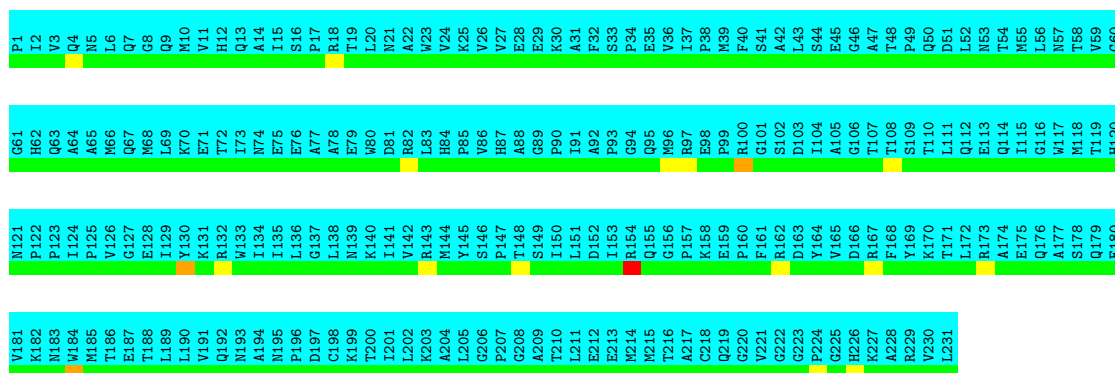




• Molecule 1: HIV-1 capsid protein

Chain T:

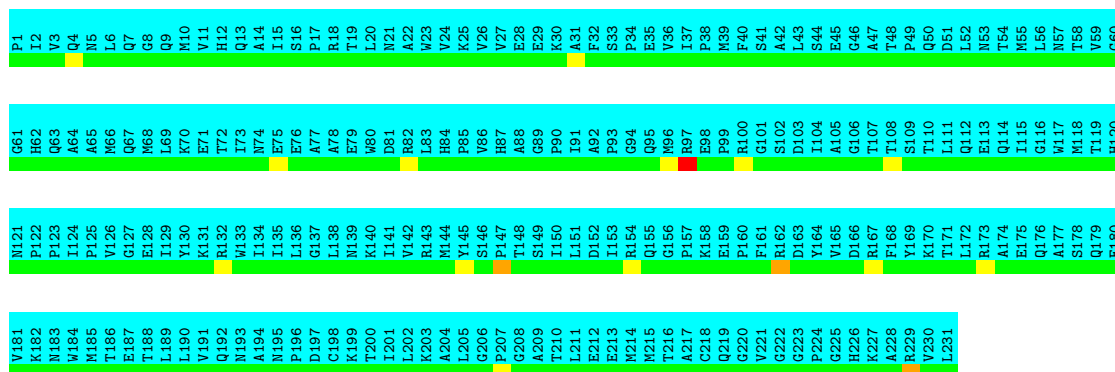
100%



• Molecule 1: HIV-1 capsid protein

Chain U:

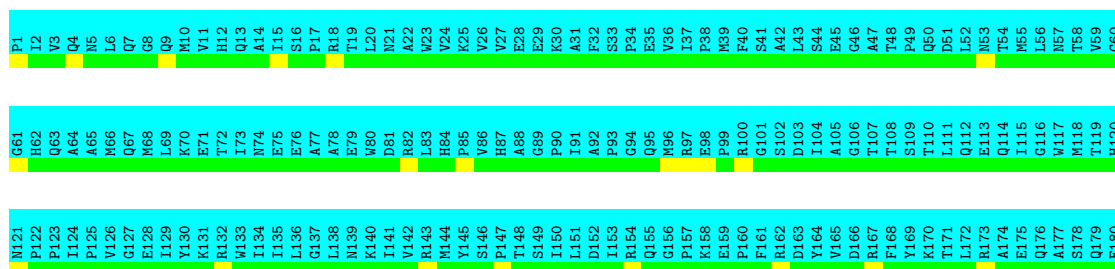
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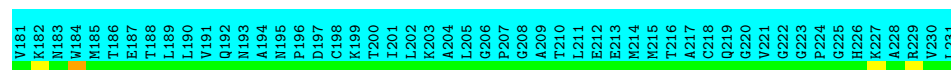


• Molecule 1: HIV-1 capsid protein

Chain V:

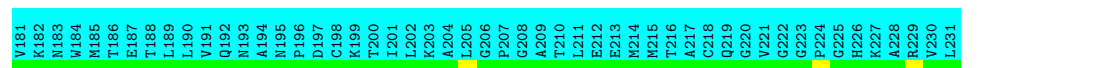
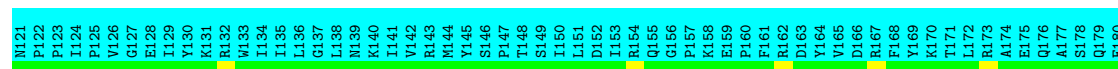
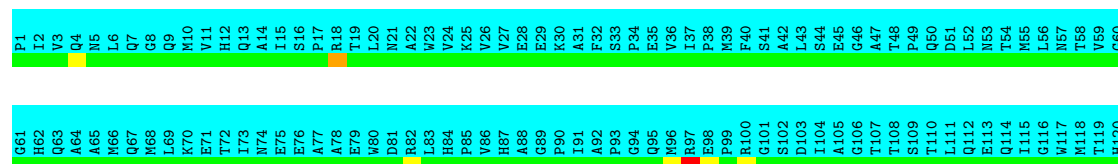
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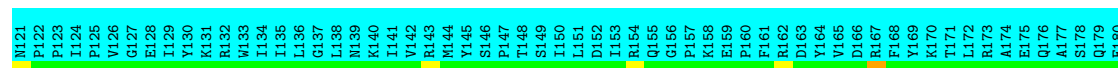
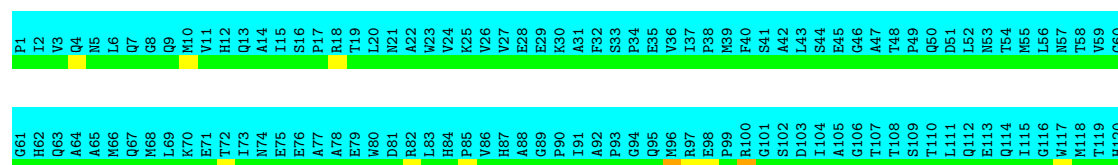
- Molecule 1: HIV-1 capsid protein

Chain W: 100%



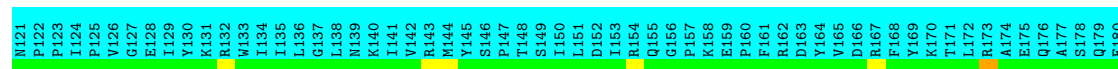
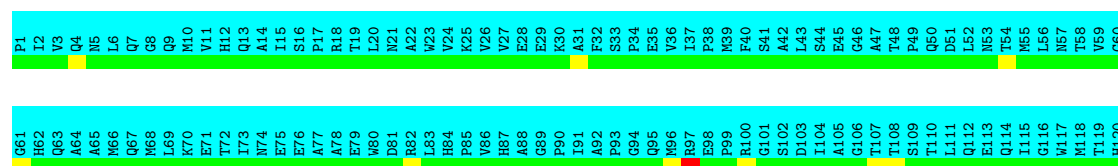
- Molecule 1: HIV-1 capsid protein

Chain X: 100%



- Molecule 1: HIV-1 capsid protein

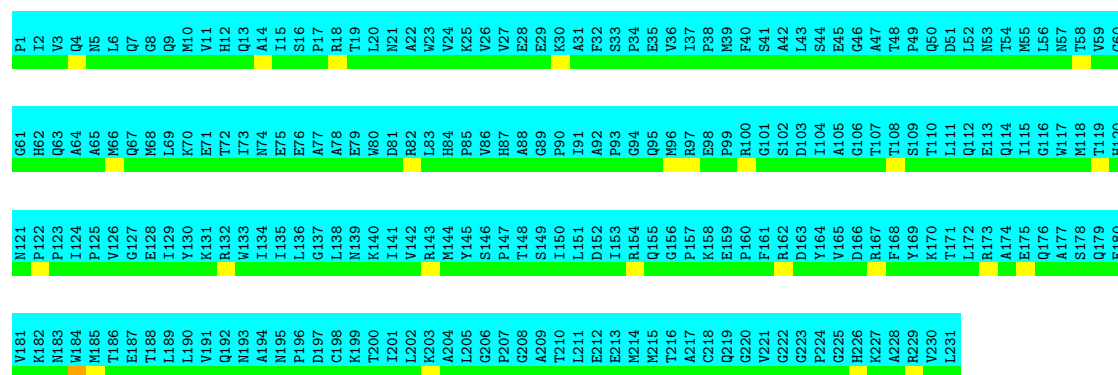
Chain Y: 100%



- Molecule 1: HIV-1 capsid protein

Chain Z:

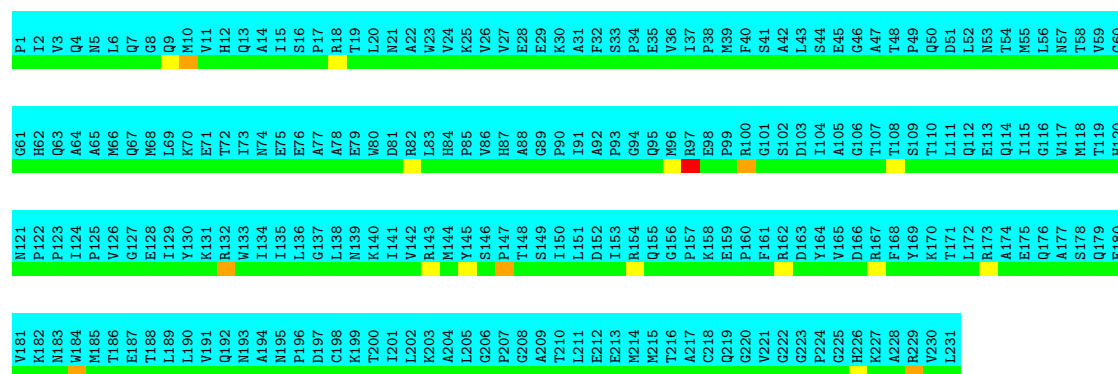
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- Molecule 1: HIV-1 capsid protein

Chain a:

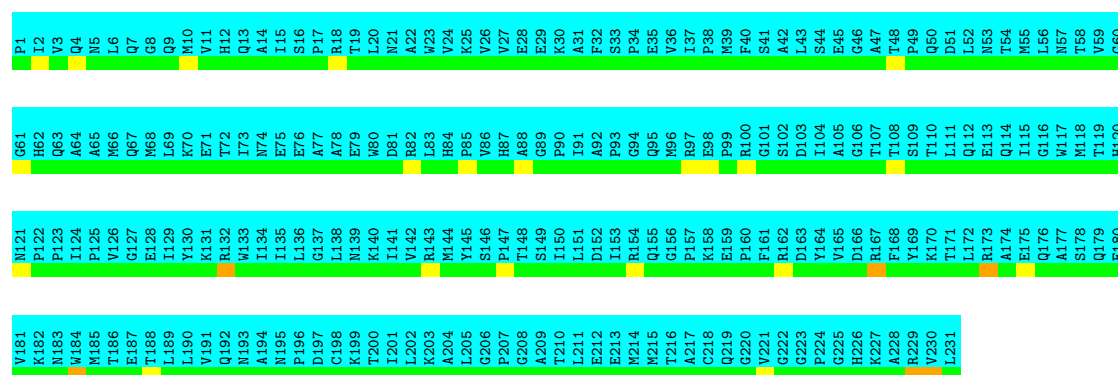
100%



- Molecule 1: HIV-1 capsid protein

Chain b:

100%

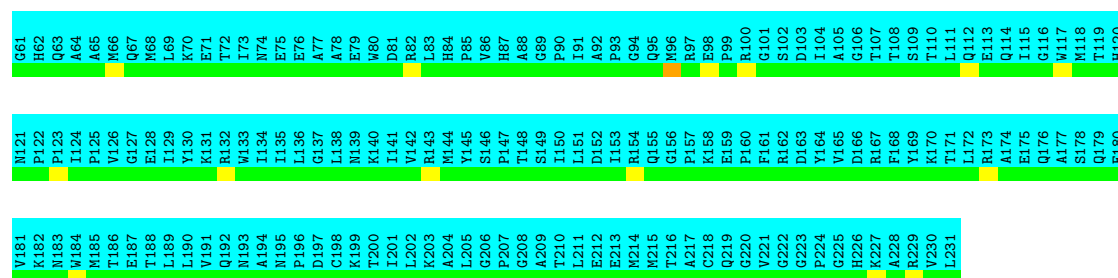


- Molecule 1: HIV-1 capsid protein

Chain c:

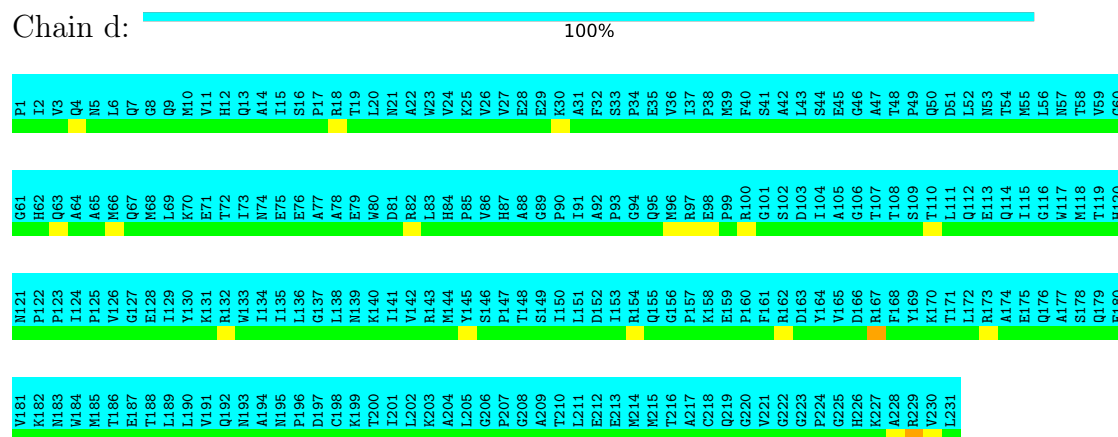
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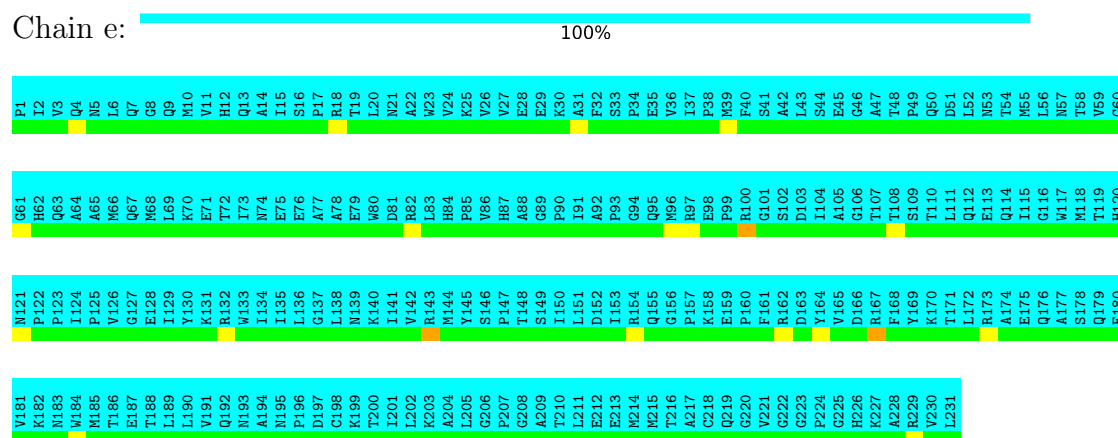
- Molecule 1: HIV-1 capsid protein

Chain d:



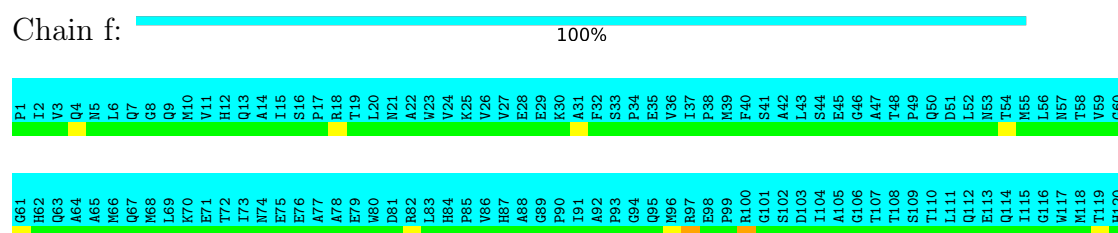
- Molecule 1: HIV-1 capsid protein

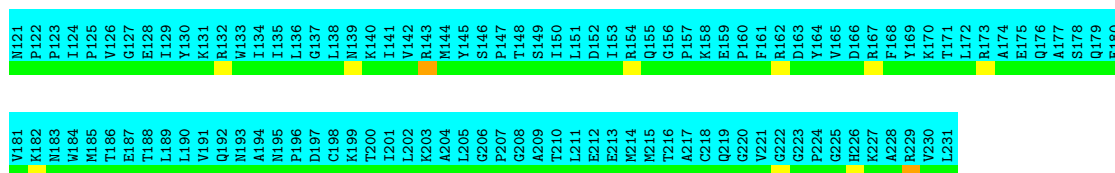
Chain e:



- Molecule 1: HIV-1 capsid protein

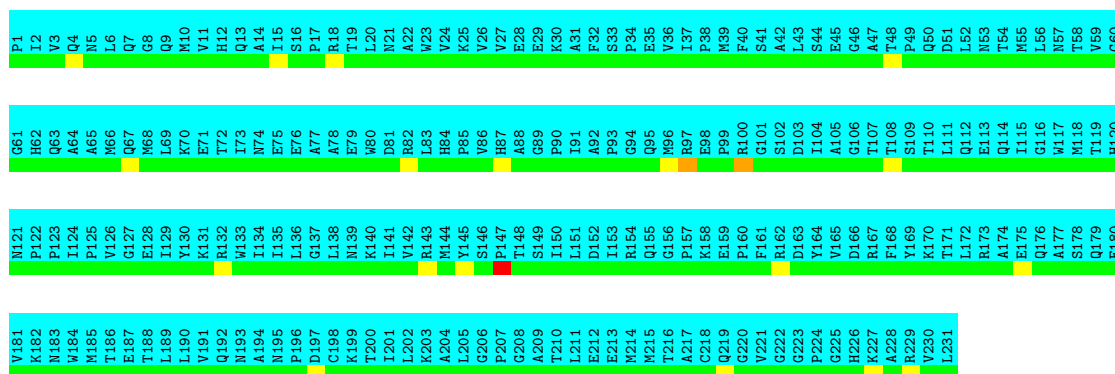
Chain f:





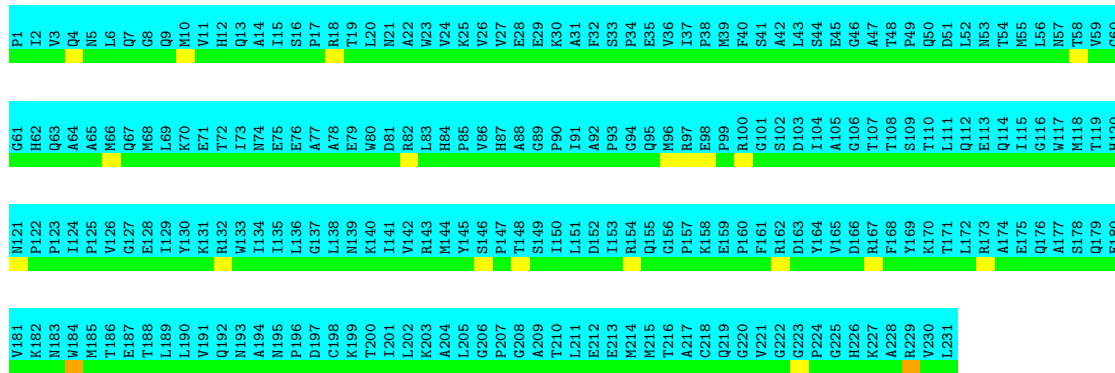
- Molecule 1: HIV-1 capsid protein

Chain g:



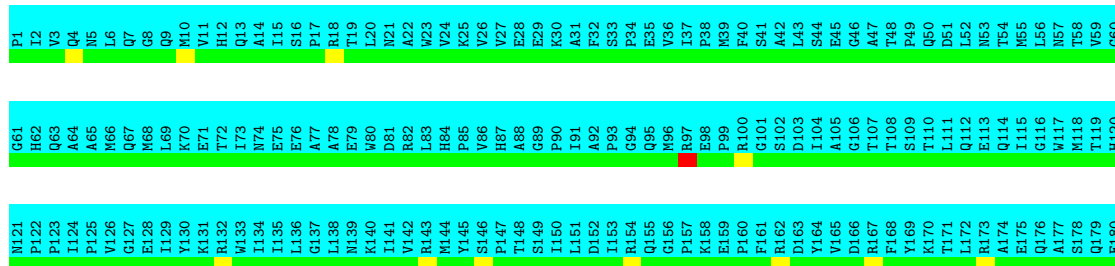
- Molecule 1: HIV-1 capsid protein

Chain h:



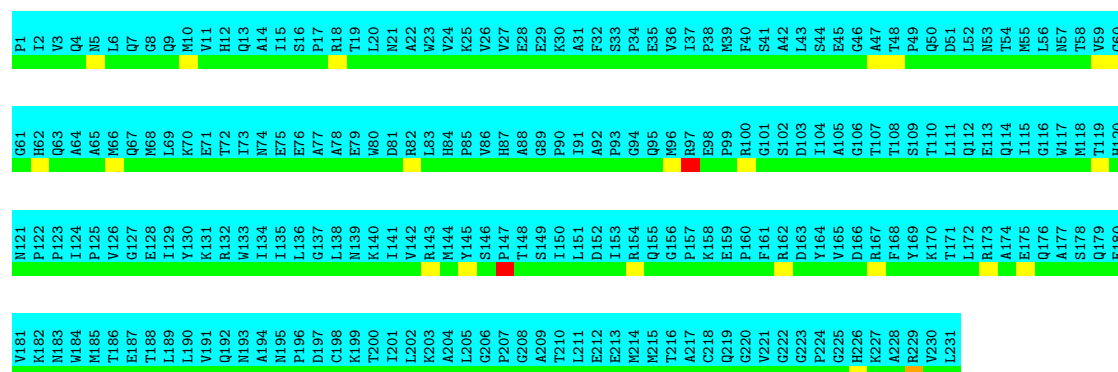
- Molecule 1: HIV-1 capsid protein

Chain i:



Chain m:

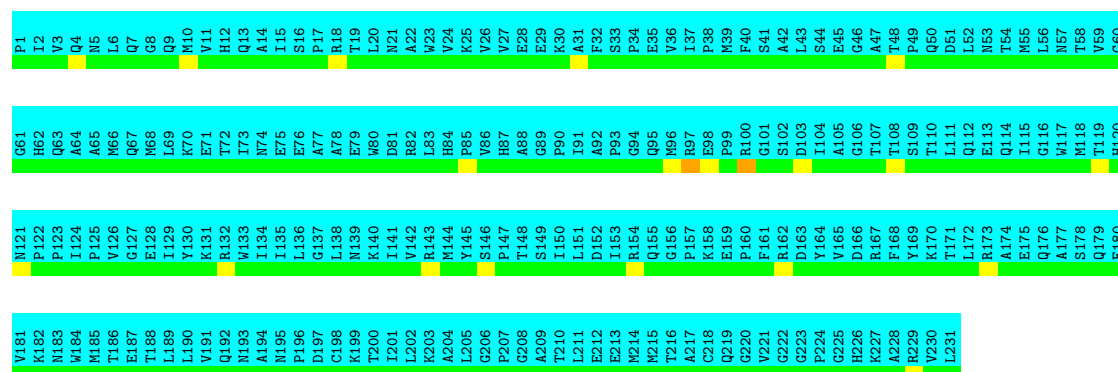
100%



• Molecule 1: HIV-1 capsid protein

Chain n:

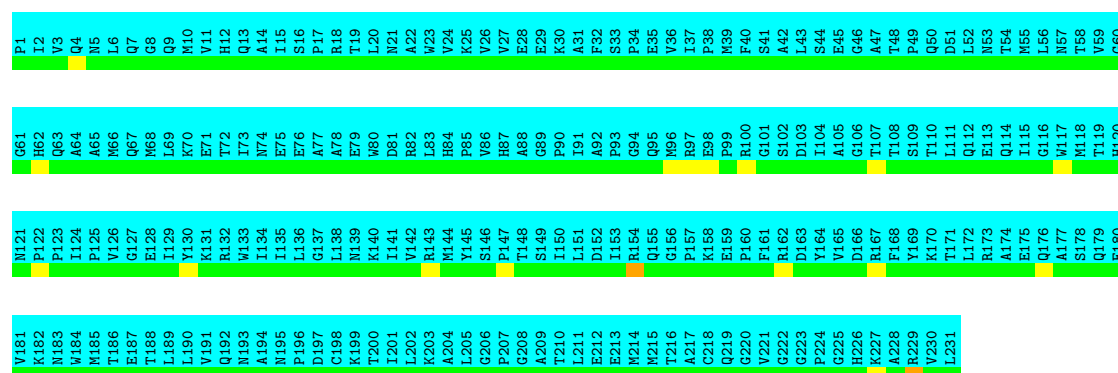
100%



• Molecule 1: HIV-1 capsid protein

Chain o:

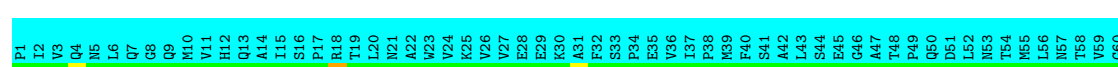
100%

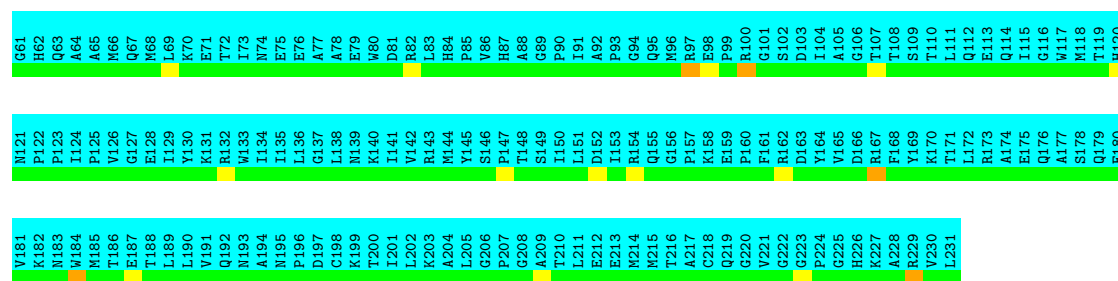


• Molecule 1: HIV-1 capsid protein

Chain p:

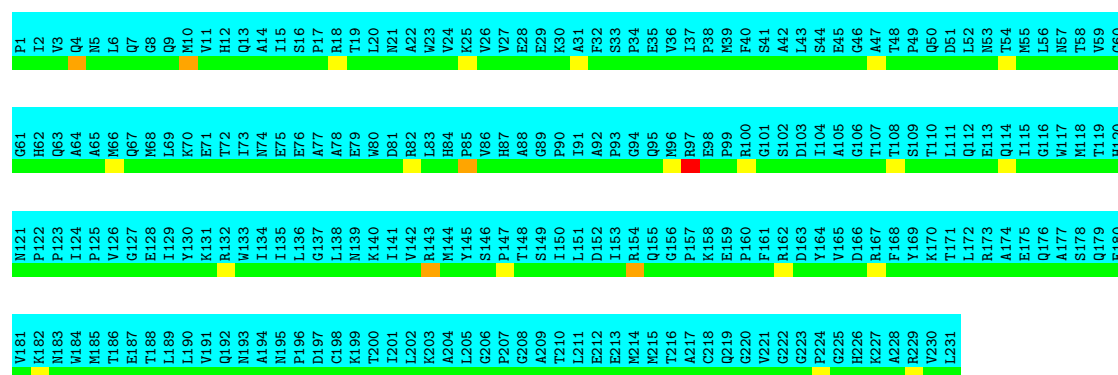
100%





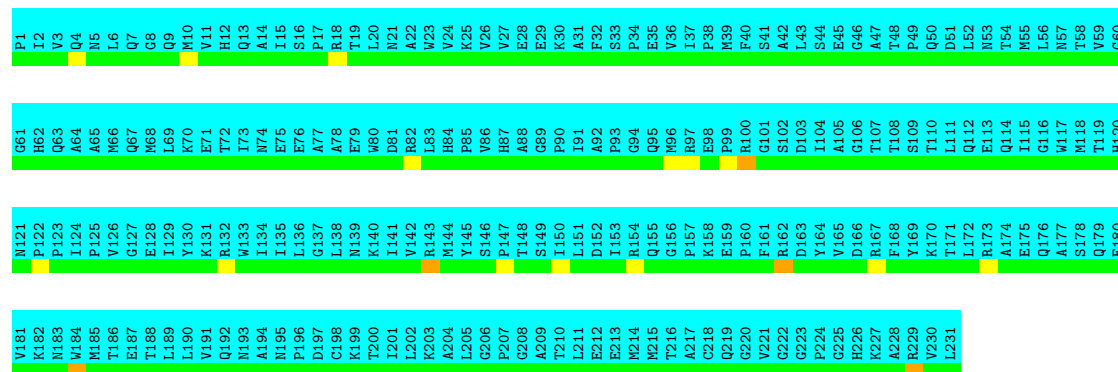
- Molecule 1: HIV-1 capsid protein

Chain q:  100%



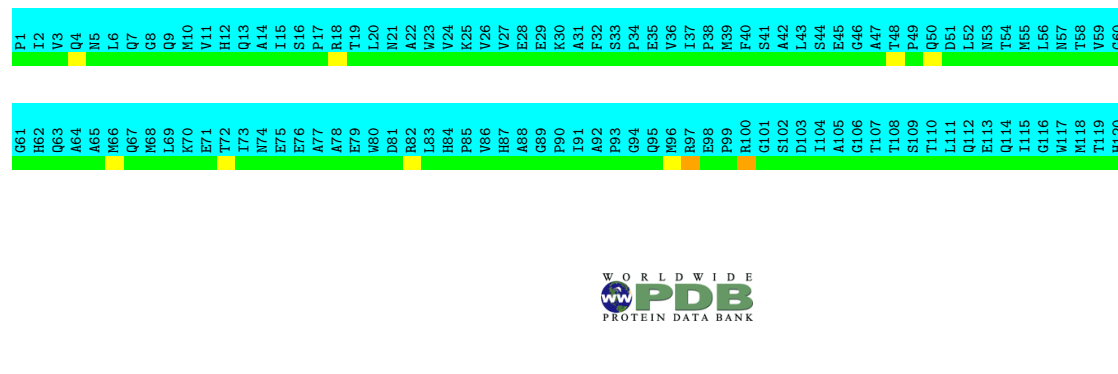
- Molecule 1: HIV-1 capsid protein

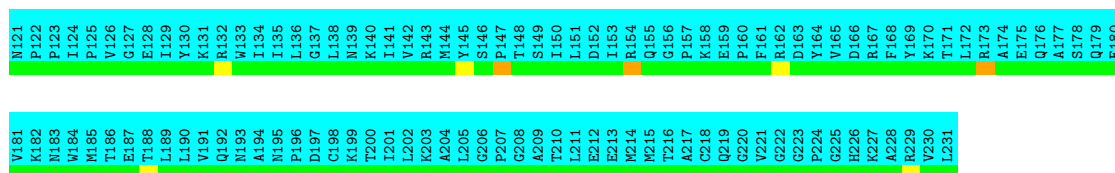
Chain r:  100%



- Molecule 1: HIV-1 capsid protein

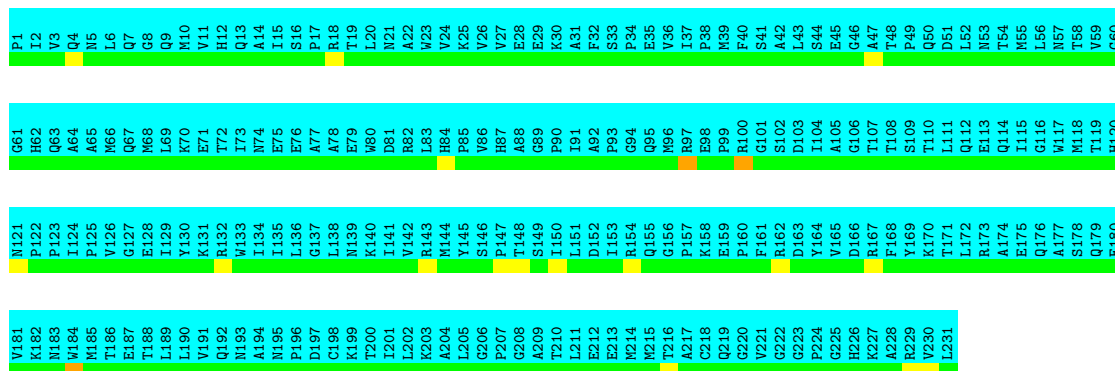
Chain s:  100%





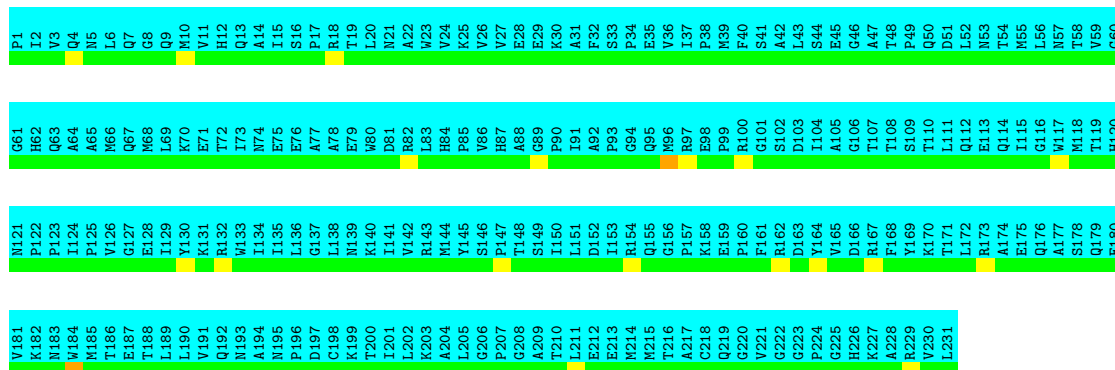
• Molecule 1: HIV-1 capsid protein

Chain t: 100%



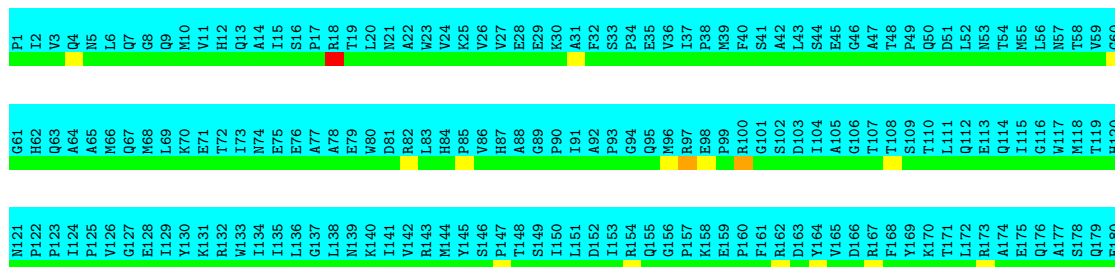
• Molecule 1: HIV-1 capsid protein

Chain u: 100%



• Molecule 1: HIV-1 capsid protein

Chain v: 100%

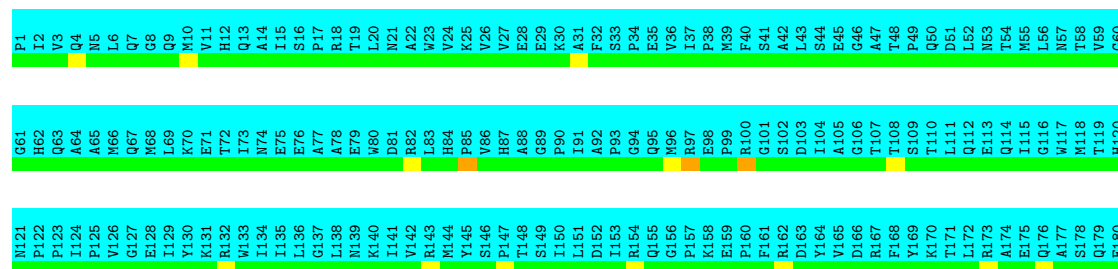




• Molecule 1: HIV-1 capsid protein

Chain w:

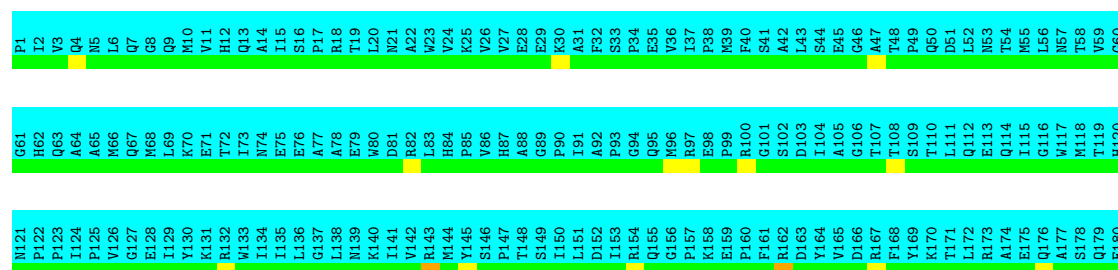
100%



• Molecule 1: HIV-1 capsid protein

Chain x:

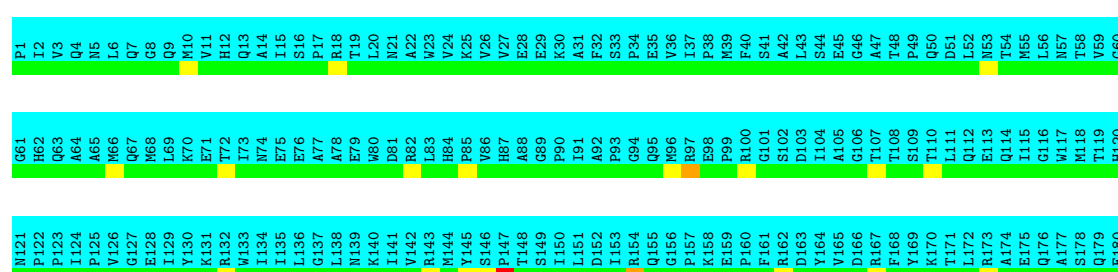
100%



• Molecule 1: HIV-1 capsid protein

Chain y:

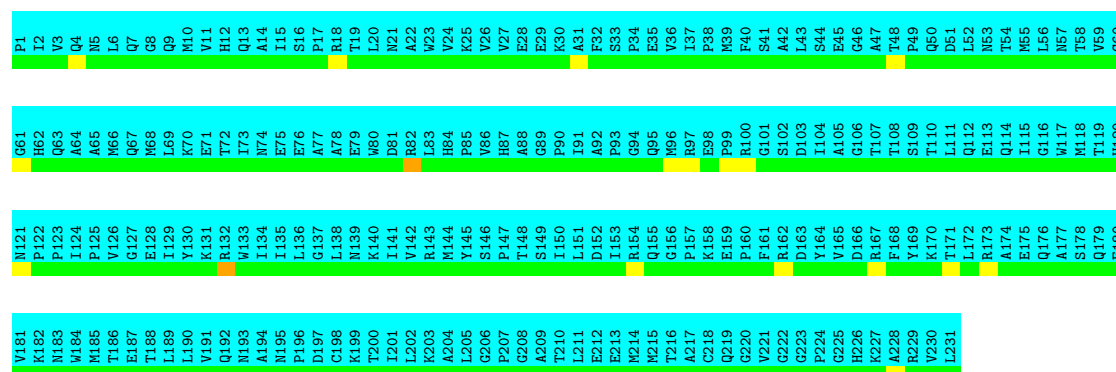
100%



• Molecule 1: HIV-1 capsid protein

Chain z:

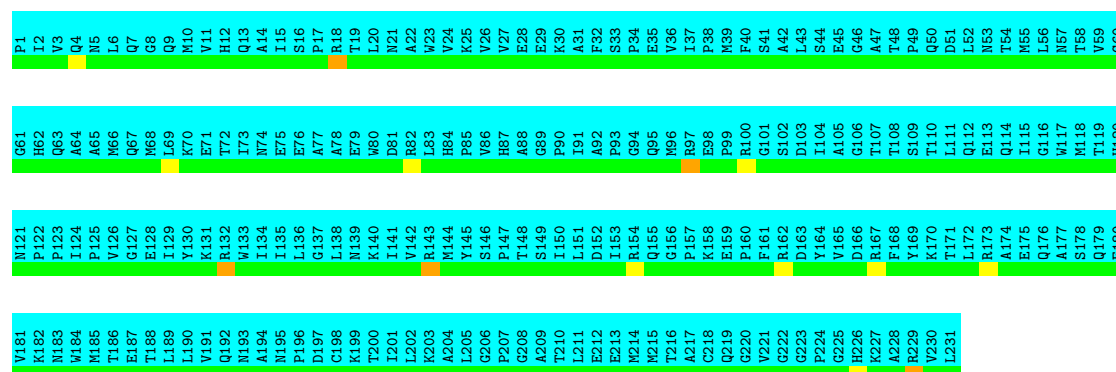
100%



• Molecule 1: HIV-1 capsid protein

Chain 0:

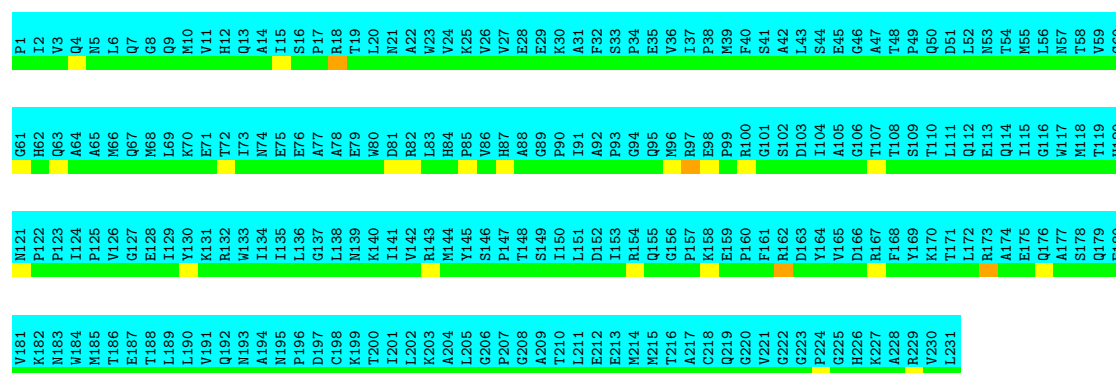
100%



• Molecule 1: HIV-1 capsid protein

Chain 1:

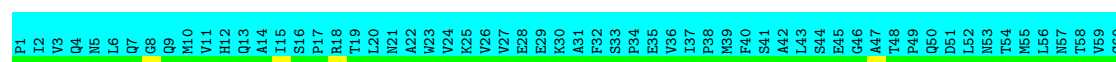
100%



• Molecule 1: HIV-1 capsid protein

Chain 2:

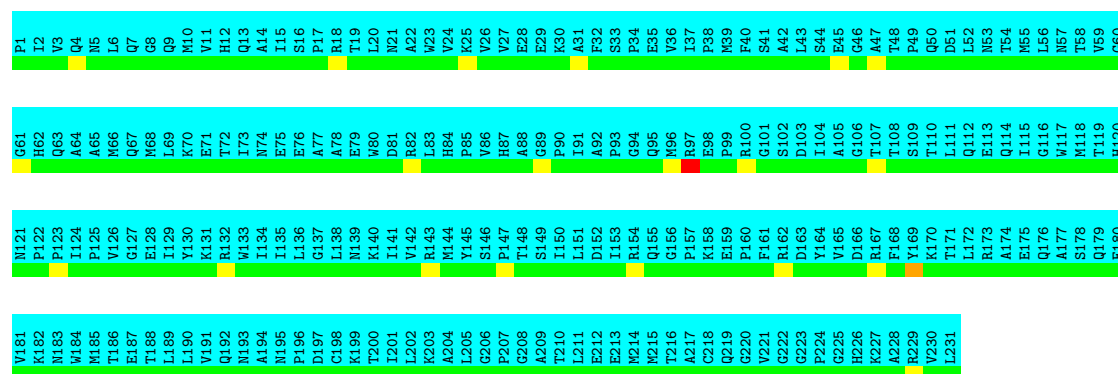
100%





• Molecule 1: HIV-1 capsid protein

Chain 3:  100%



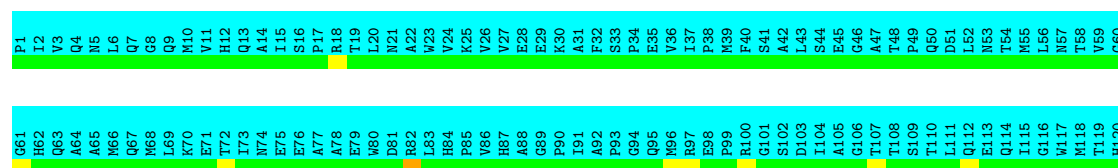
• Molecule 1: HIV-1 capsid protein

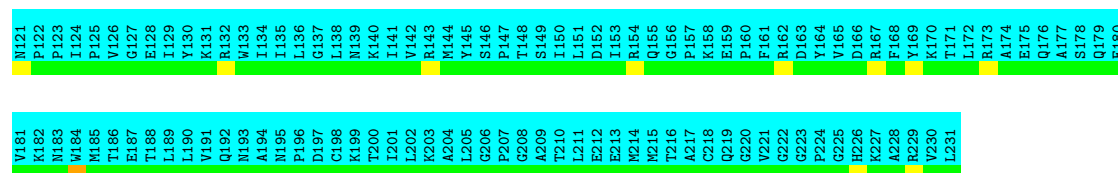
Chain 4:  100%



• Molecule 1: HIV-1 capsid protein

Chain 5:  100%

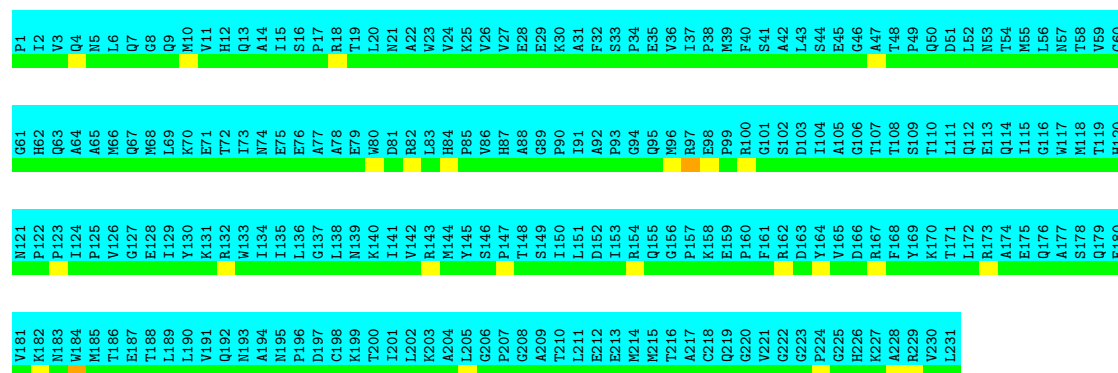




• Molecule 1: HIV-1 capsid protein

Chain 6:

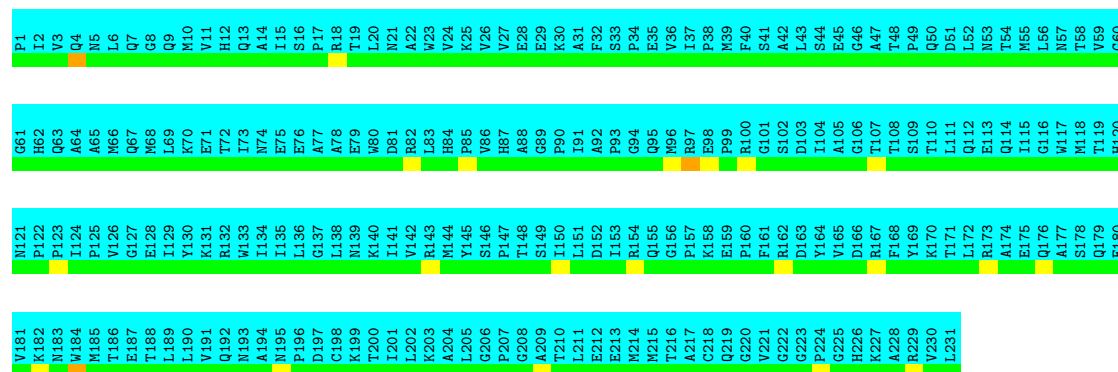
100%



• Molecule 1: HIV-1 capsid protein

Chain 7:

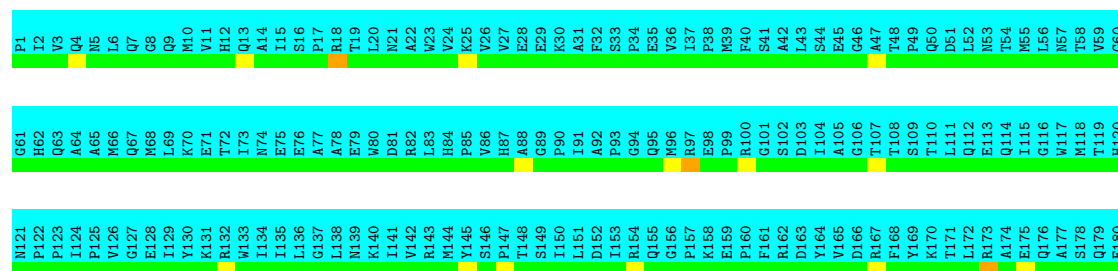
100%



• Molecule 1: HIV-1 capsid protein

Chain 8:

100%

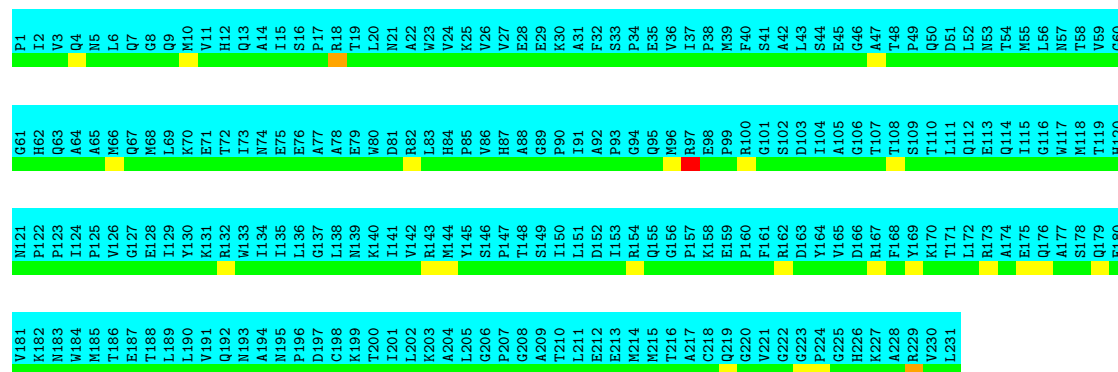




- Molecule 1: HIV-1 capsid protein

Chain 9:

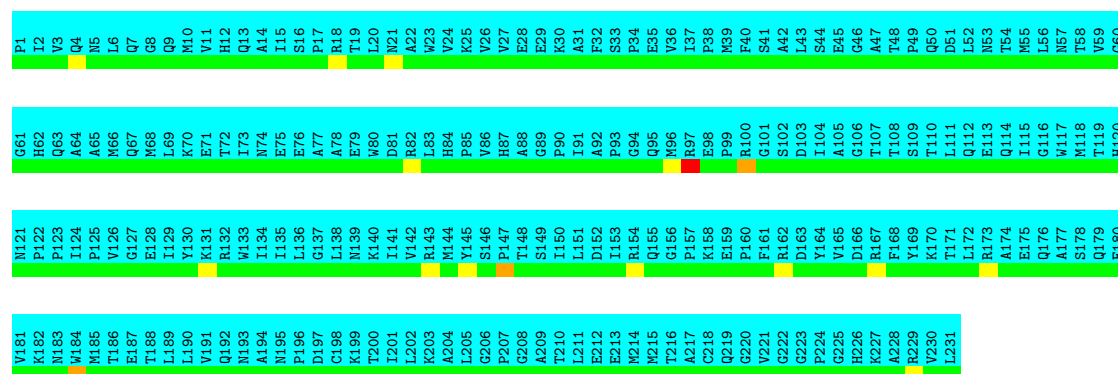
100%



- Molecule 1: HIV-1 capsid protein

Chain AA:

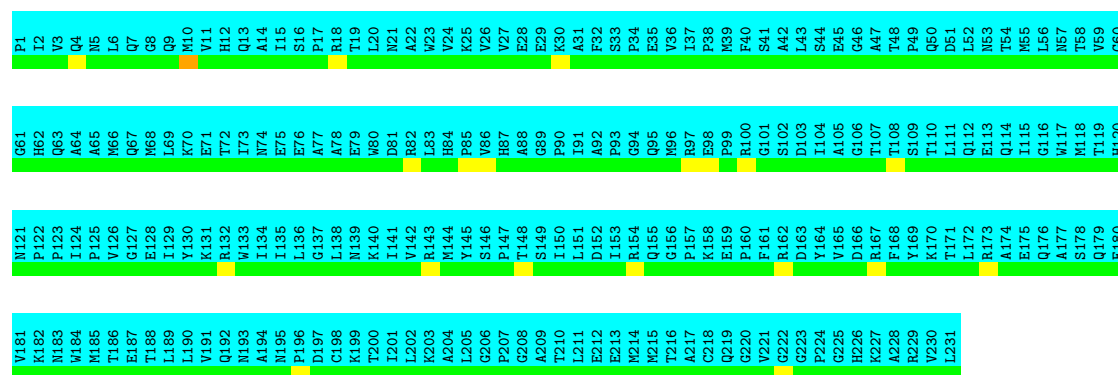
100%



- Molecule 1: HIV-1 capsid protein

Chain BA:

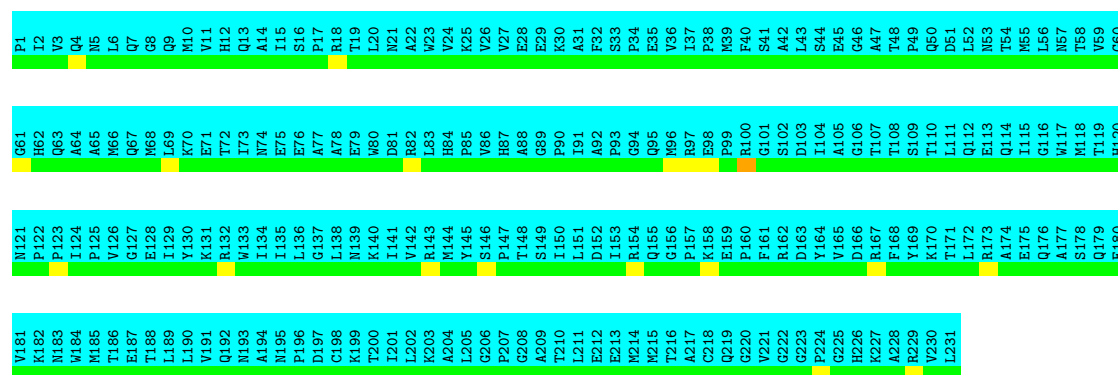
100%



- Molecule 1: HIV-1 capsid protein

Chain CA:

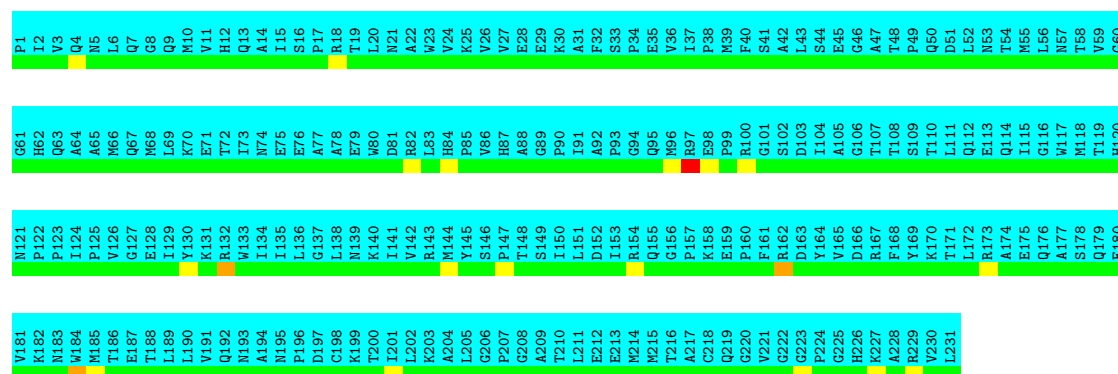
100%



- Molecule 1: HIV-1 capsid protein

Chain DA:

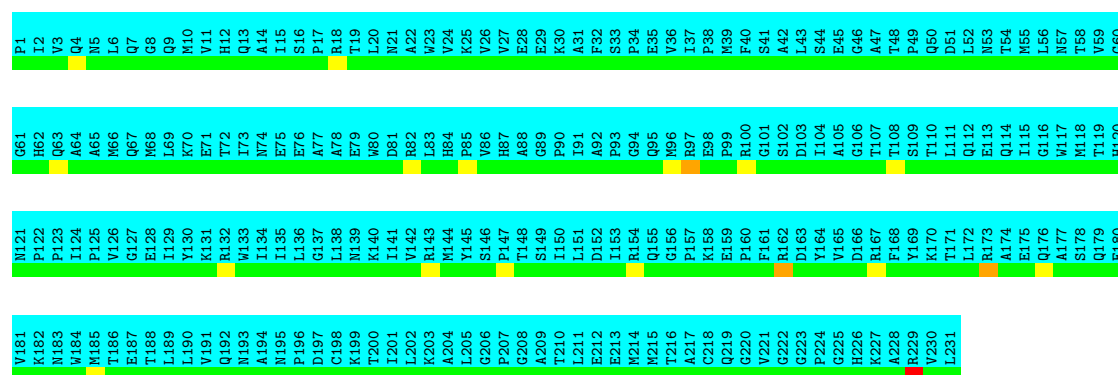
100%



- Molecule 1: HIV-1 capsid protein

Chain EA:

100%

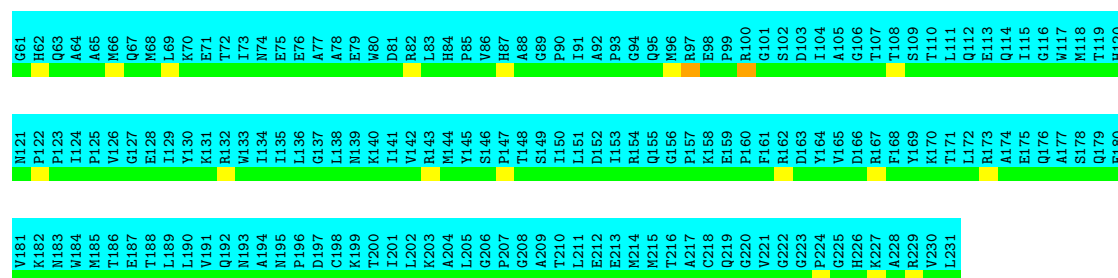


- Molecule 1: HIV-1 capsid protein

Chain FA:

100%

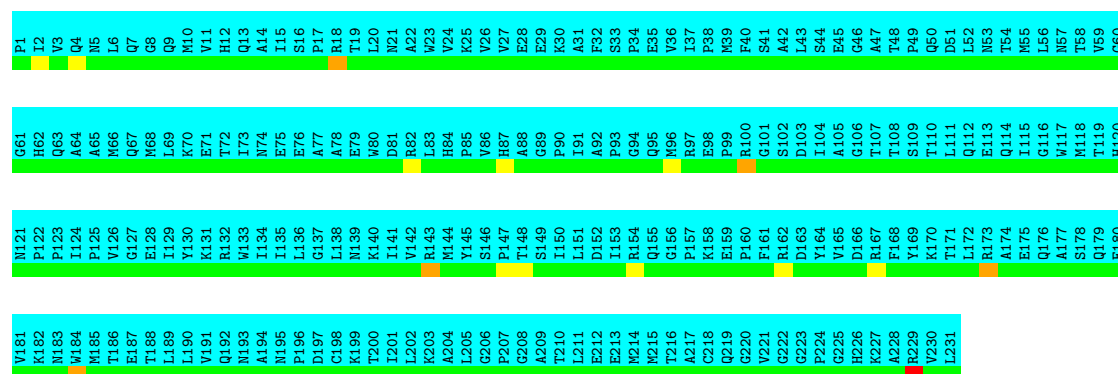




- Molecule 1: HIV-1 capsid protein

Chain GA:

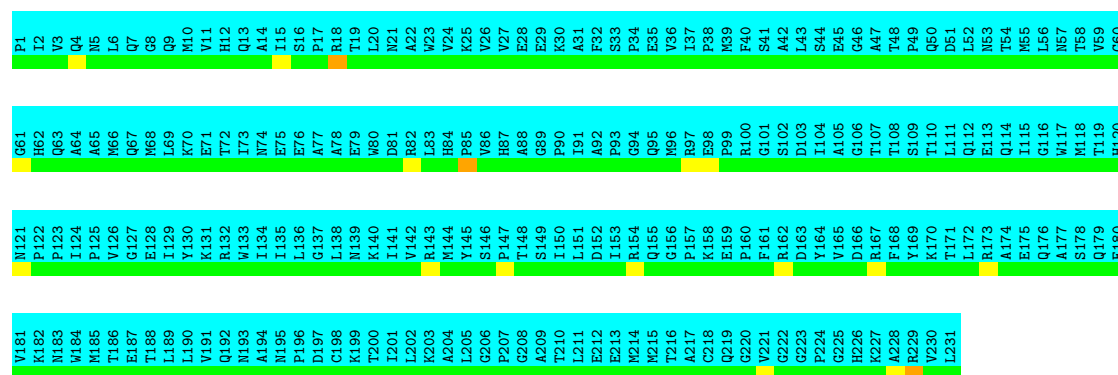
100%



- Molecule 1: HIV-1 capsid protein

Chain HA:

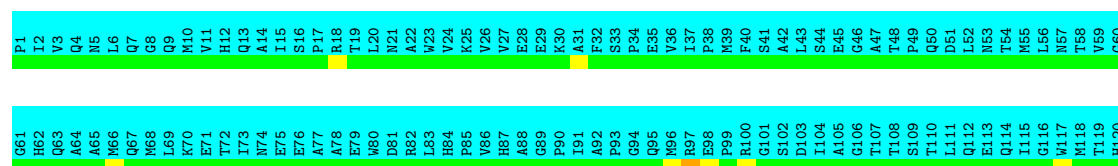
100%

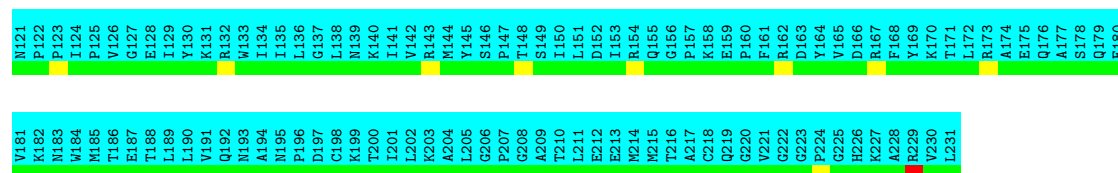


- Molecule 1: HIV-1 capsid protein

Chain IA:

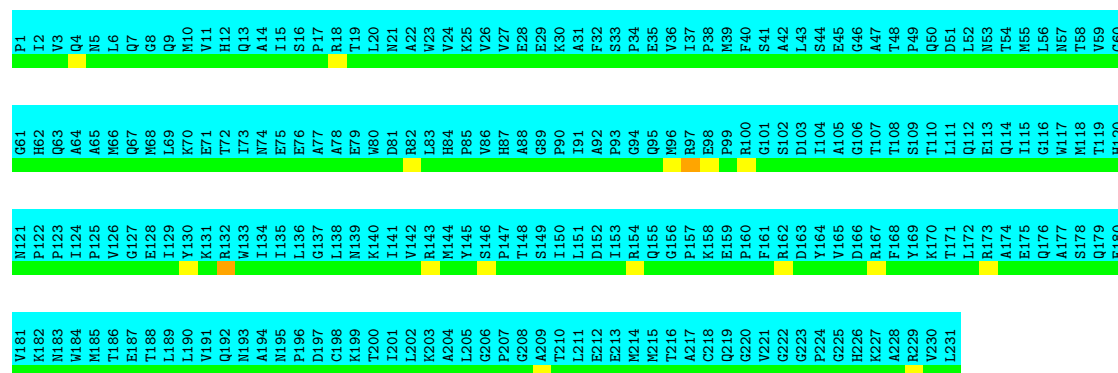
100%





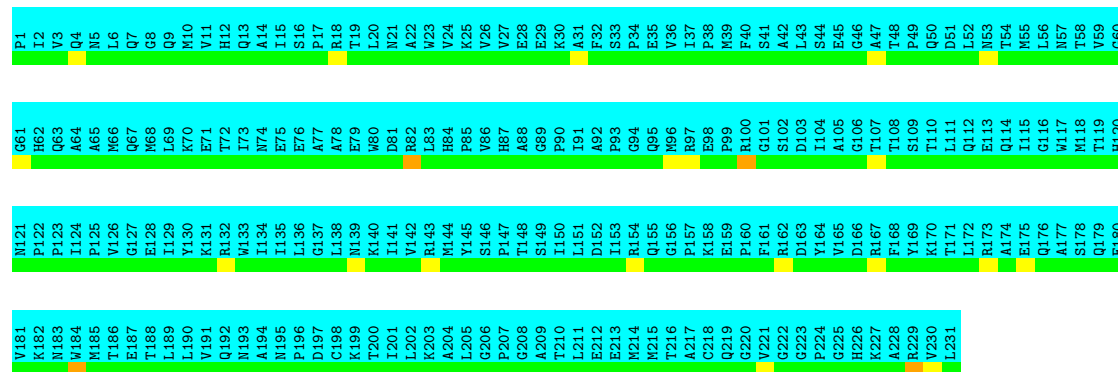
• Molecule 1: HIV-1 capsid protein

Chain JA:



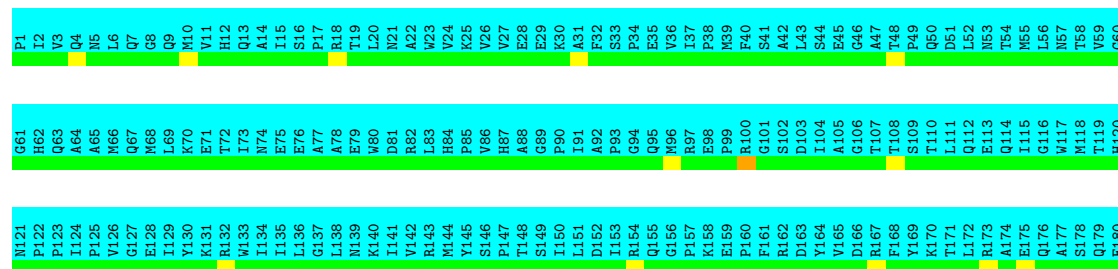
• Molecule 1: HIV-1 capsid protein

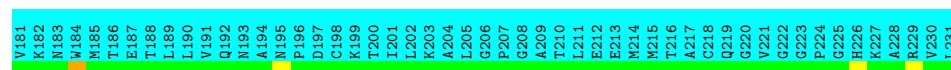
Chain KA:



• Molecule 1: HIV-1 capsid protein

Chain LA:





- Molecule 1: HIV-1 capsid protein

Chain MA:

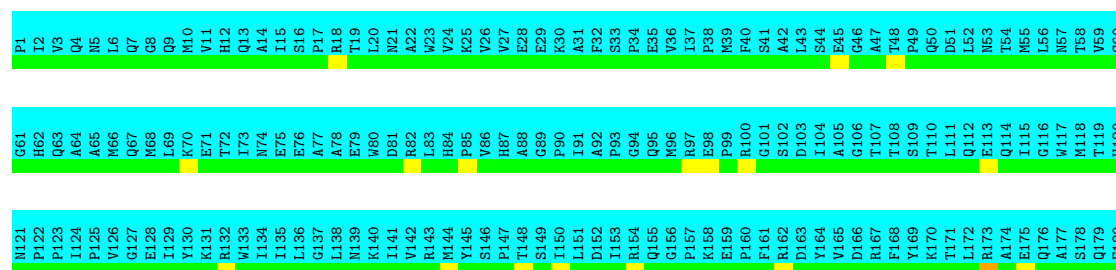
100%



- Molecule 1: HIV-1 capsid protein

Chain NA:

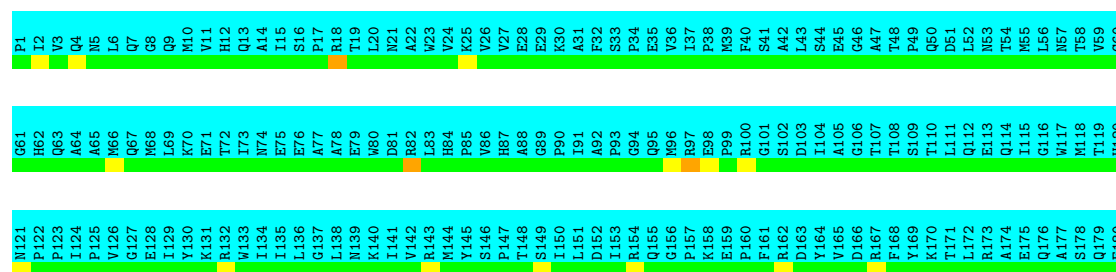
100%



- Molecule 1: HIV-1 capsid protein

Chain OA:

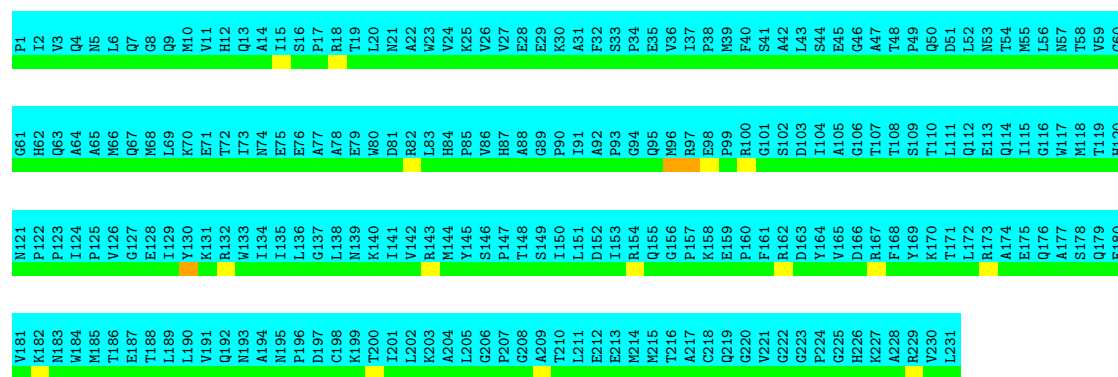
100%



- Molecule 1: HIV-1 capsid protein

Chain PA:

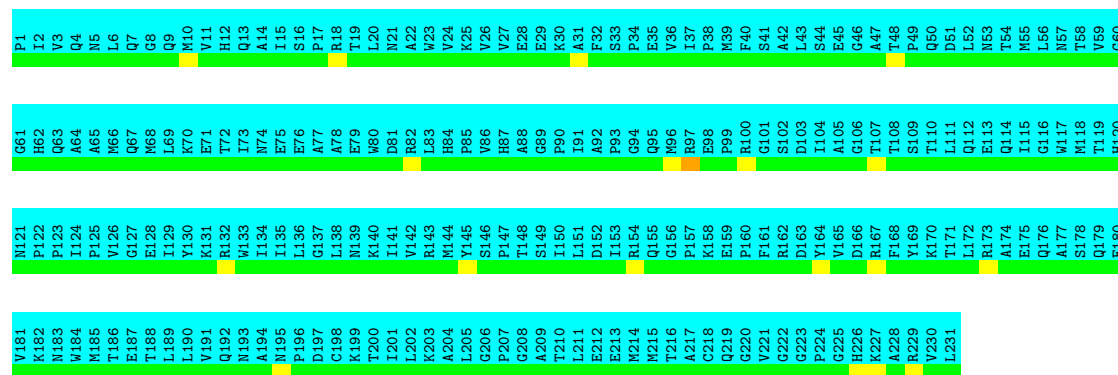
100%



- Molecule 1: HIV-1 capsid protein

Chain QA:

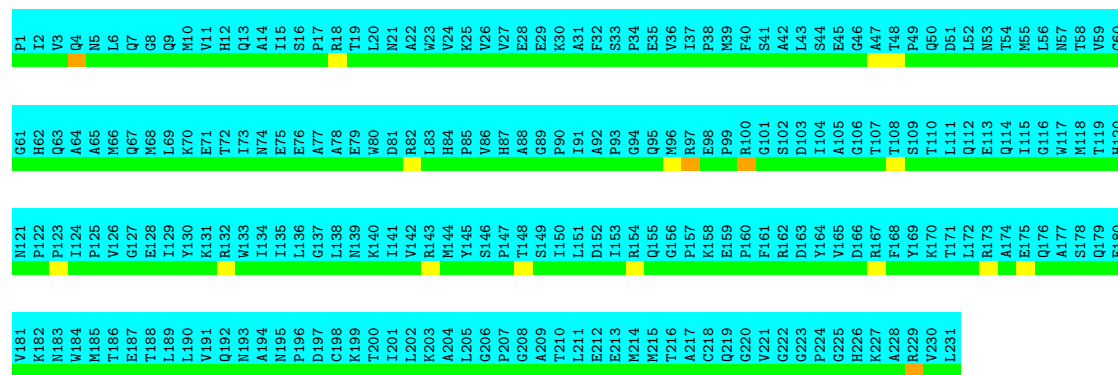
100%



- Molecule 1: HIV-1 capsid protein

Chain RA:

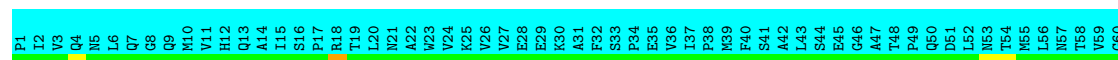
100%



- Molecule 1: HIV-1 capsid protein

Chain SA:

100%

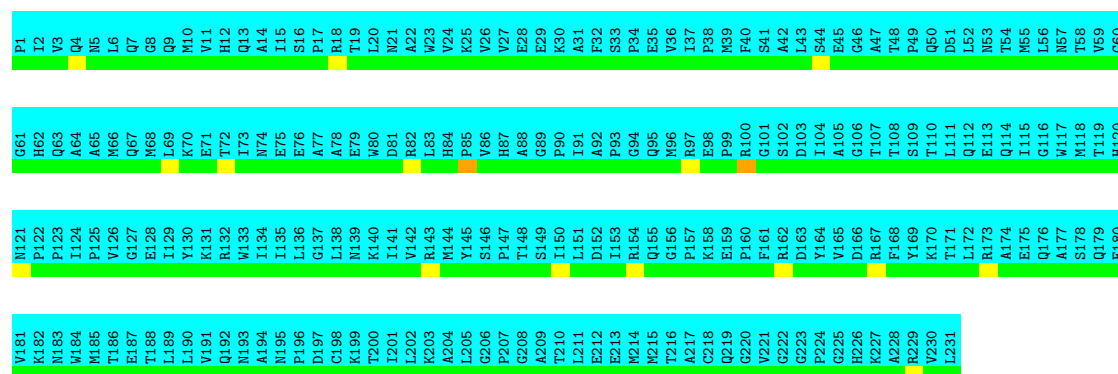




- Molecule 1: HIV-1 capsid protein

Chain TA:

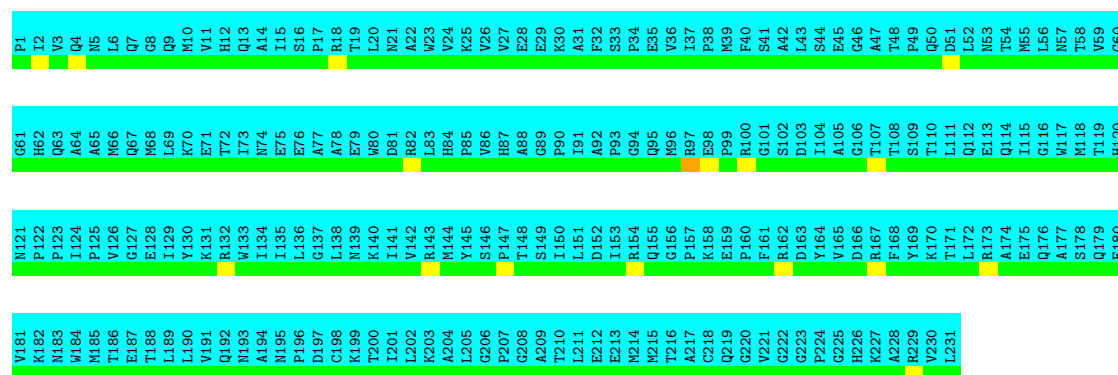
100%



- Molecule 1: HIV-1 capsid protein

Chain UA:

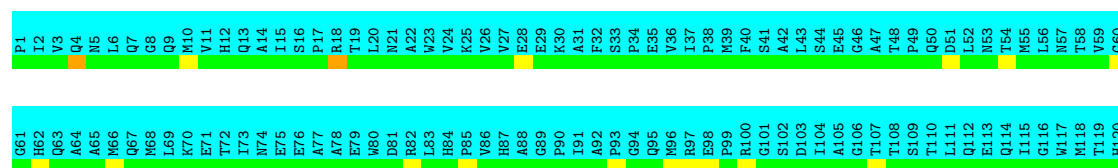
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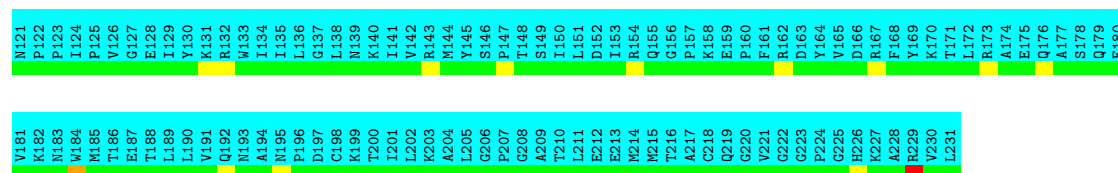


- Molecule 1: HIV-1 capsid protein

Chain VA:

100%





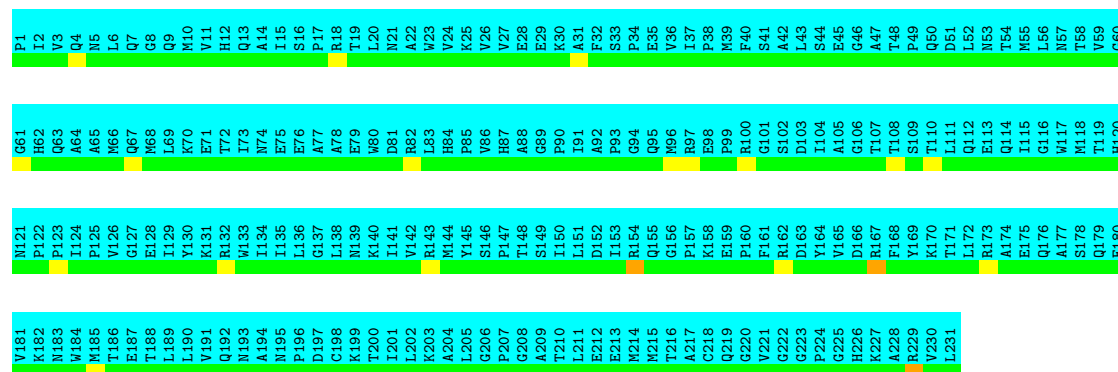
• Molecule 1: HIV-1 capsid protein

Chain WA:



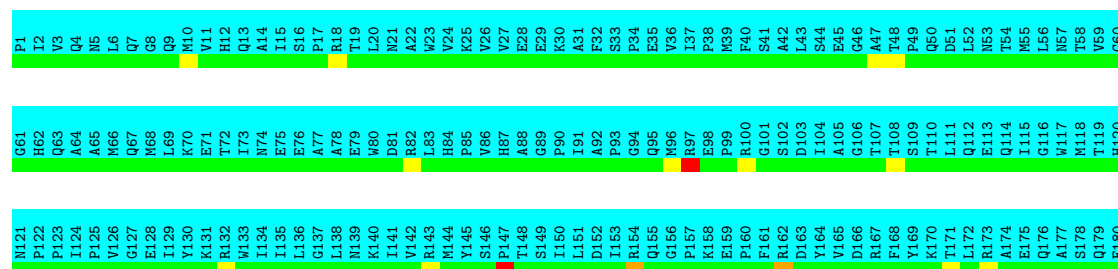
• Molecule 1: HIV-1 capsid protein

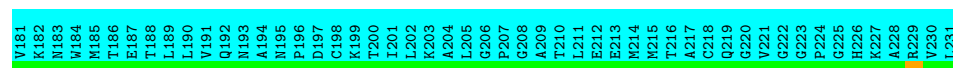
Chain XA:



• Molecule 1: HIV-1 capsid protein

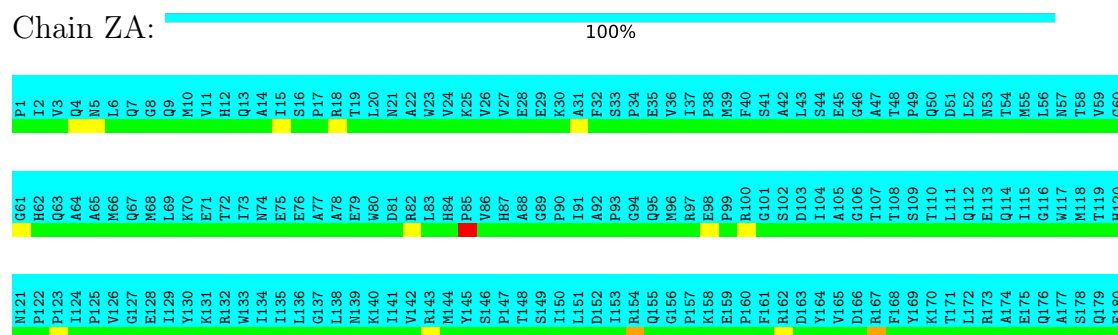
Chain YA:





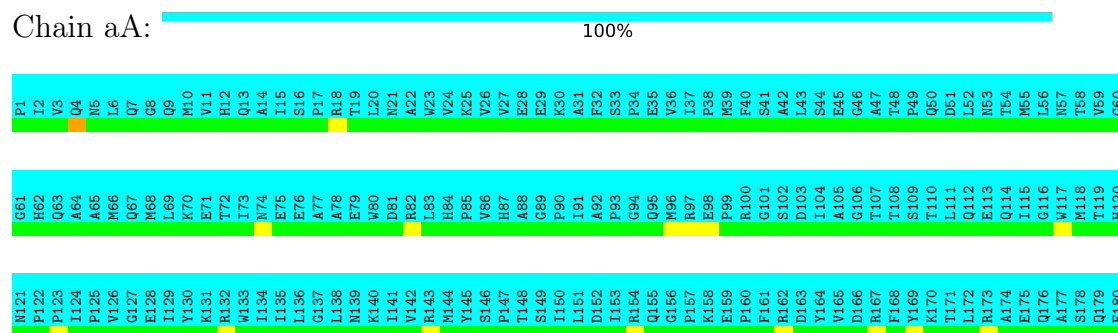
- Molecule 1: HIV-1 capsid protein

Chain ZA:



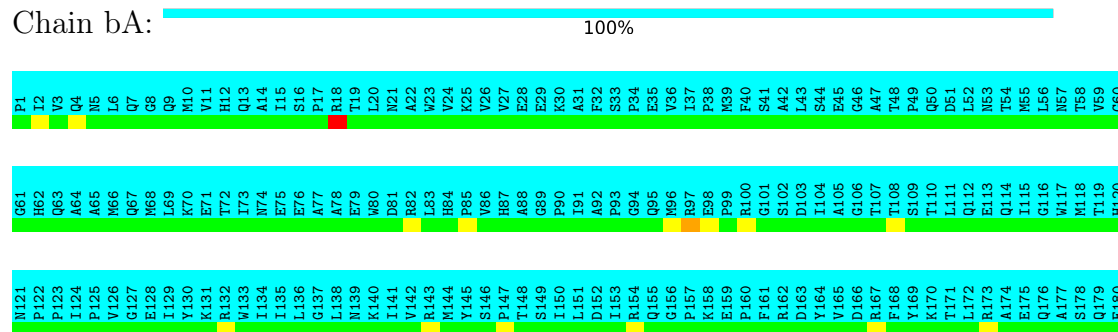
- Molecule 1: HIV-1 capsid protein

Chain aA:



- Molecule 1: HIV-1 capsid protein

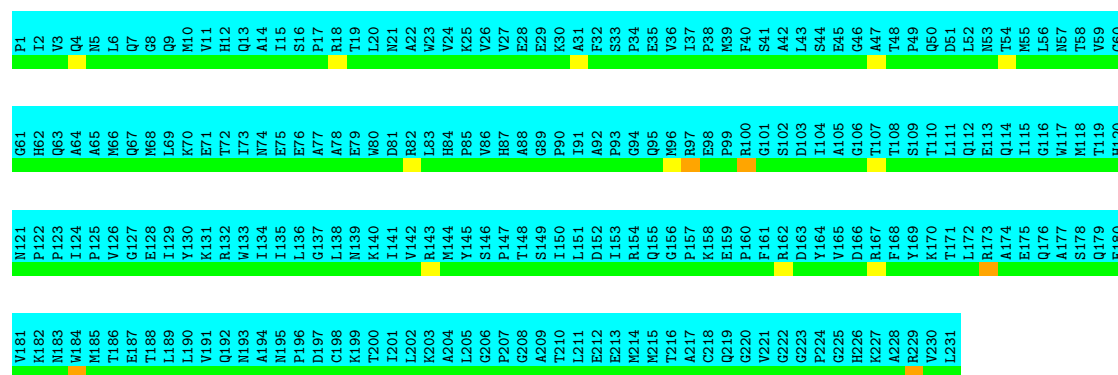
Chain bA:



- Molecule 1: HIV-1 capsid protein

Chain cA:

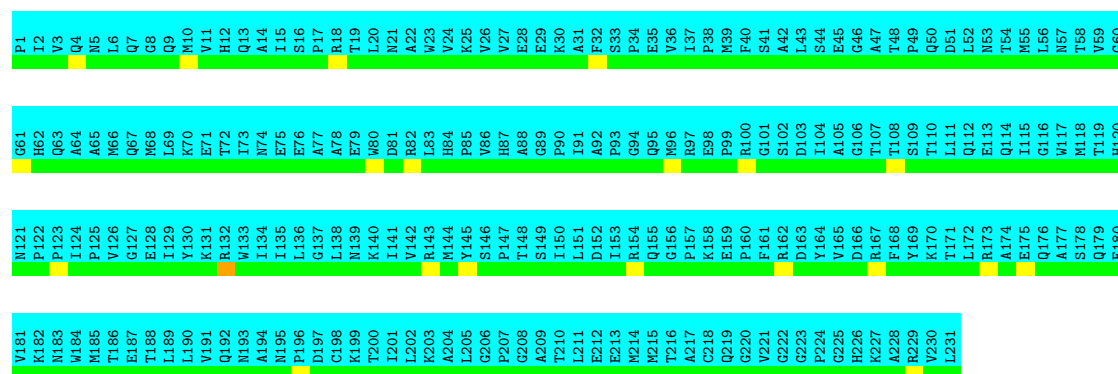
100%



- Molecule 1: HIV-1 capsid protein

Chain dA:

100%



- Molecule 1: HIV-1 capsid protein

Chain eA:

100%

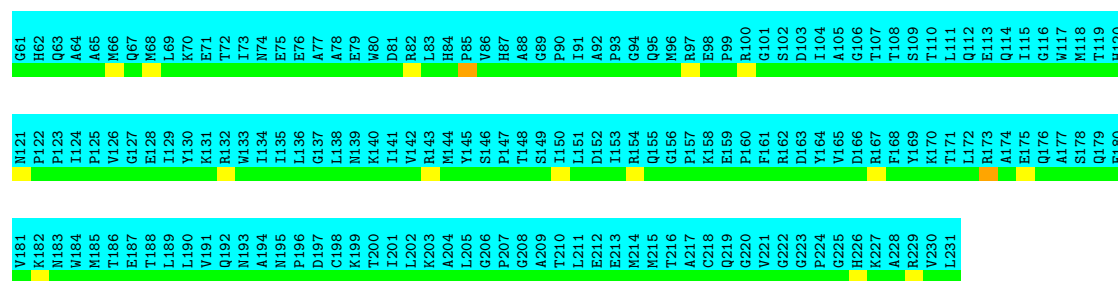


- Molecule 1: HIV-1 capsid protein

Chain fA:

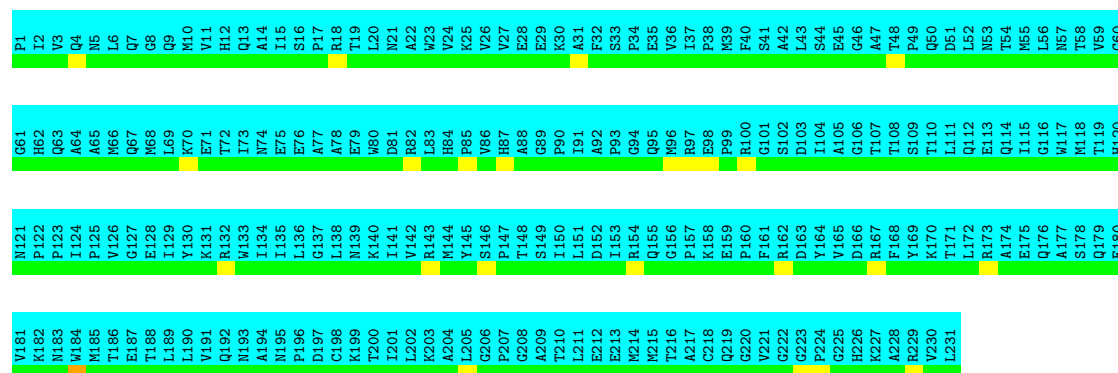
100%





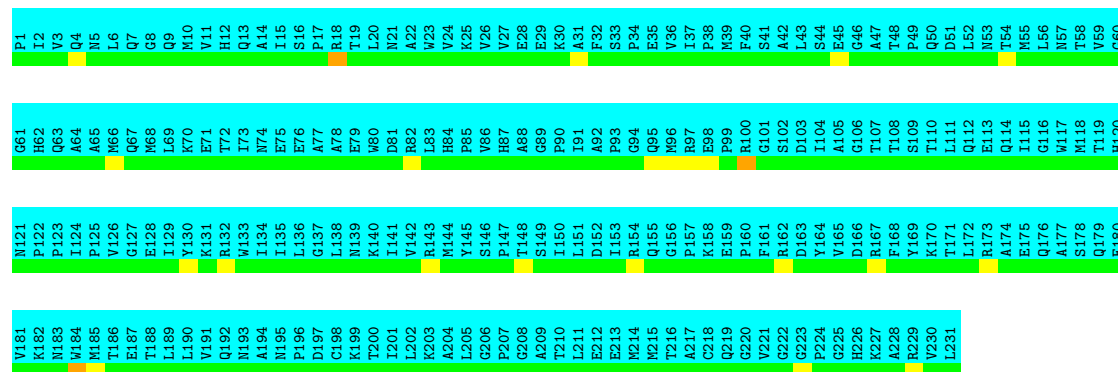
- Molecule 1: HIV-1 capsid protein

Chain gA: 100%



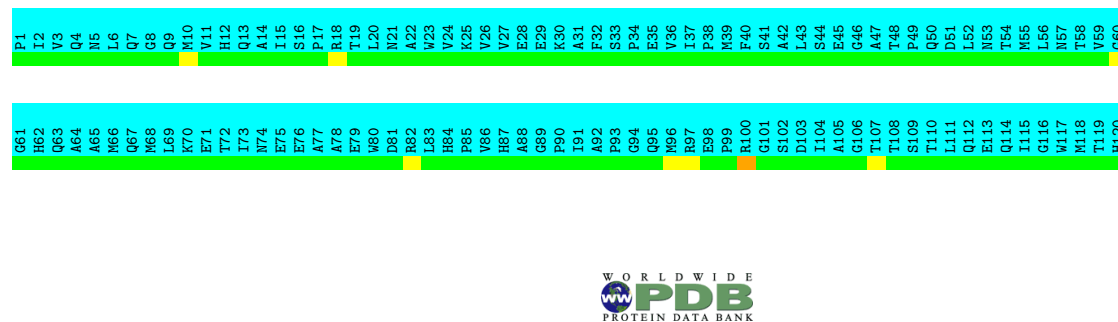
- Molecule 1: HIV-1 capsid protein

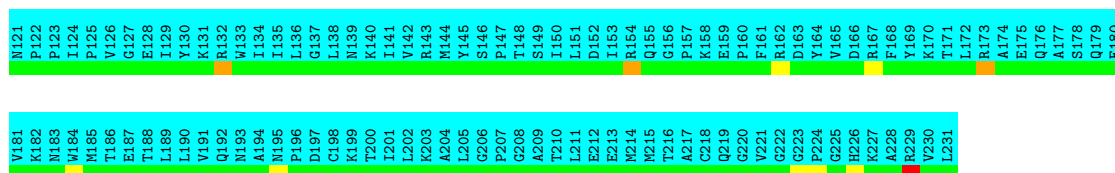
Chain hA: 100%



- Molecule 1: HIV-1 capsid protein

Chain iA: 100%

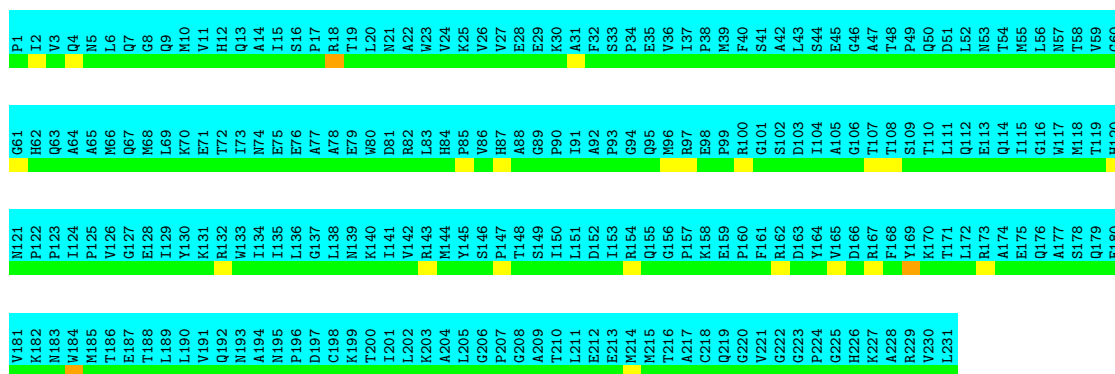




- Molecule 1: HIV-1 capsid protein

Chain jA:

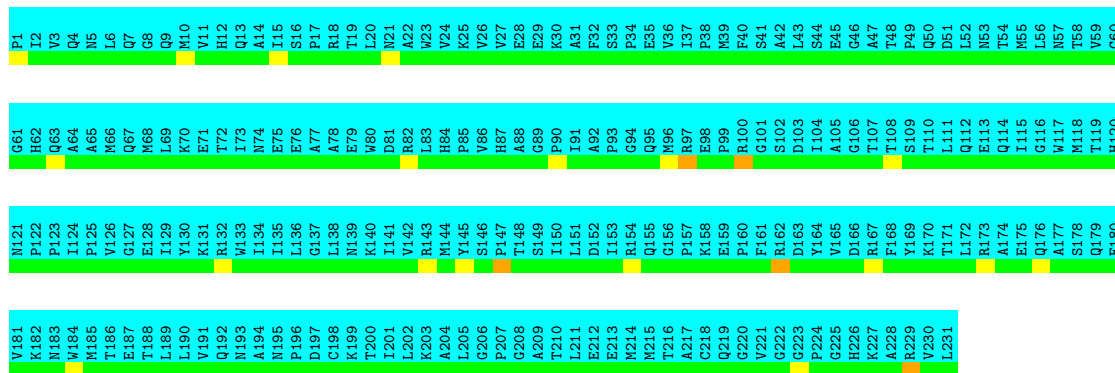
100%



- Molecule 1: HIV-1 capsid protein

Chain kA:

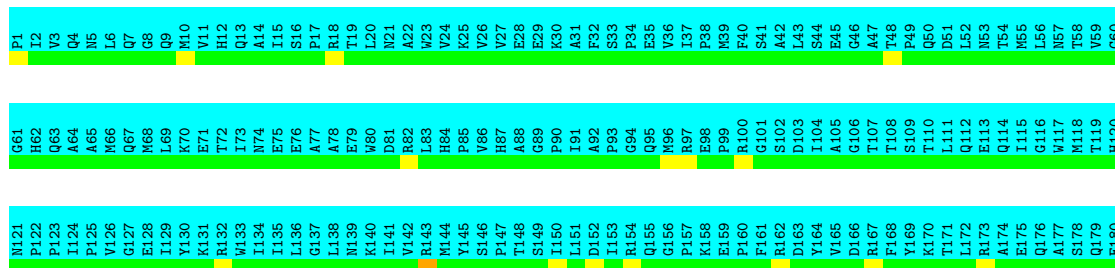
100%

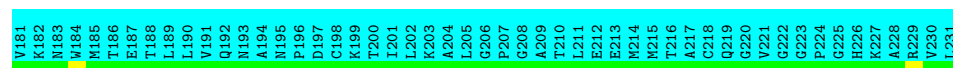


- Molecule 1: HIV-1 capsid protein

Chain lA:

100%

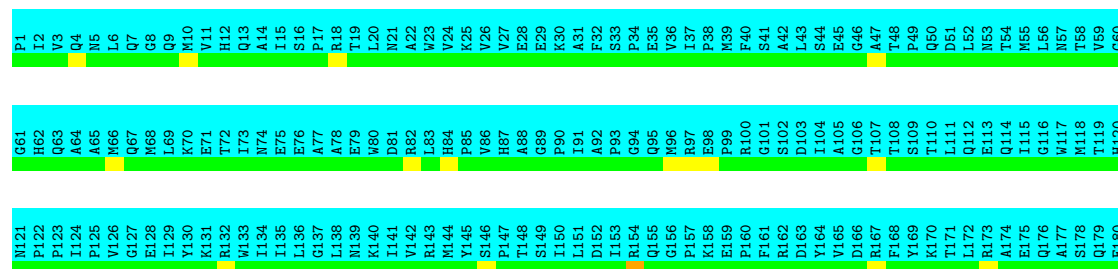




• Molecule 1: HIV-1 capsid protein

Chain mA:

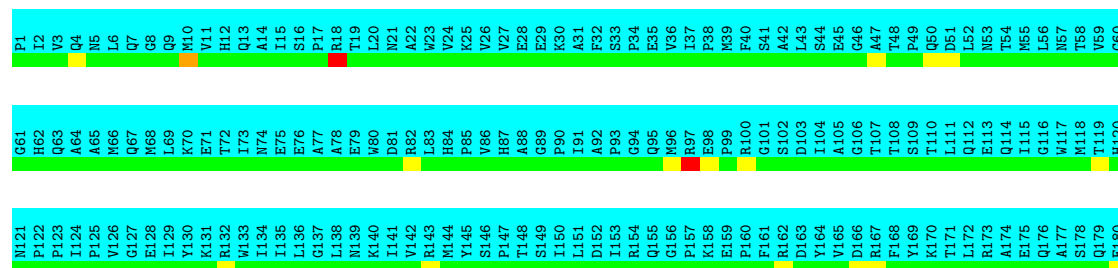
100%



• Molecule 1: HIV-1 capsid protein

Chain nA:

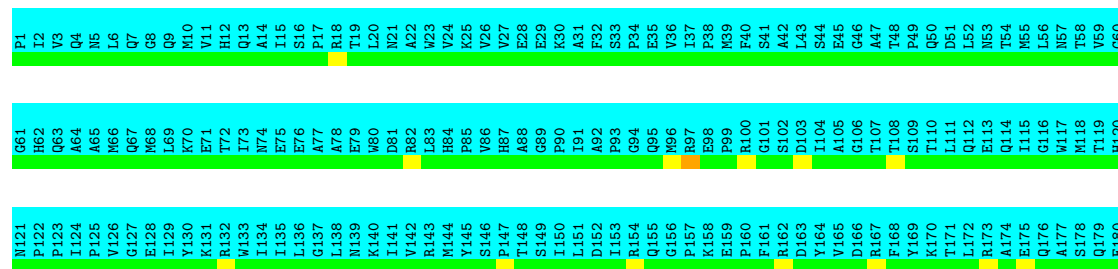
100%



• Molecule 1: HIV-1 capsid protein

Chain oA:

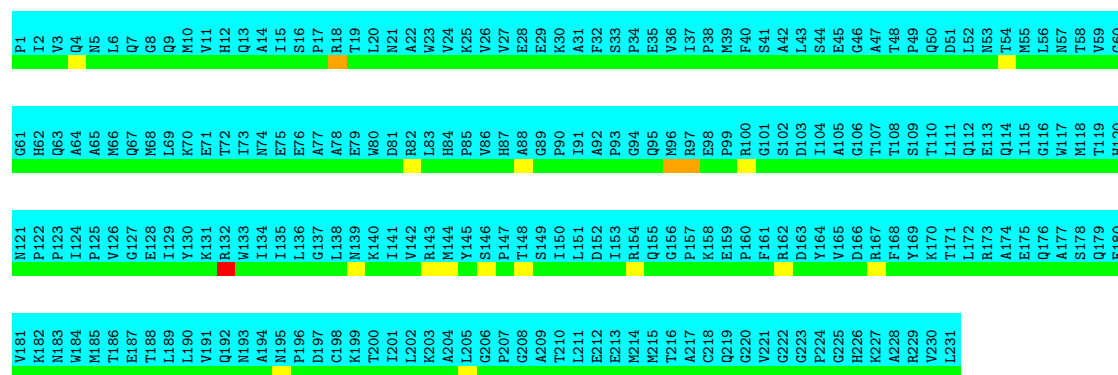
100%



• Molecule 1: HIV-1 capsid protein

Chain pA:

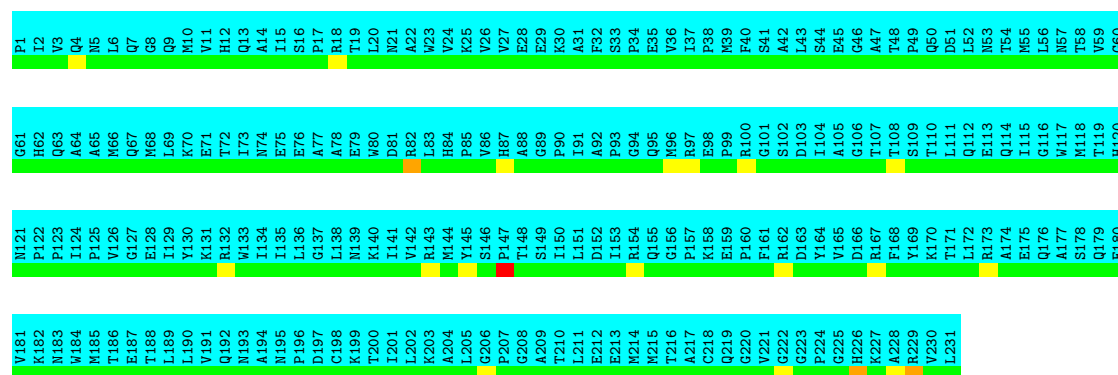
100%



• Molecule 1: HIV-1 capsid protein

Chain qA:

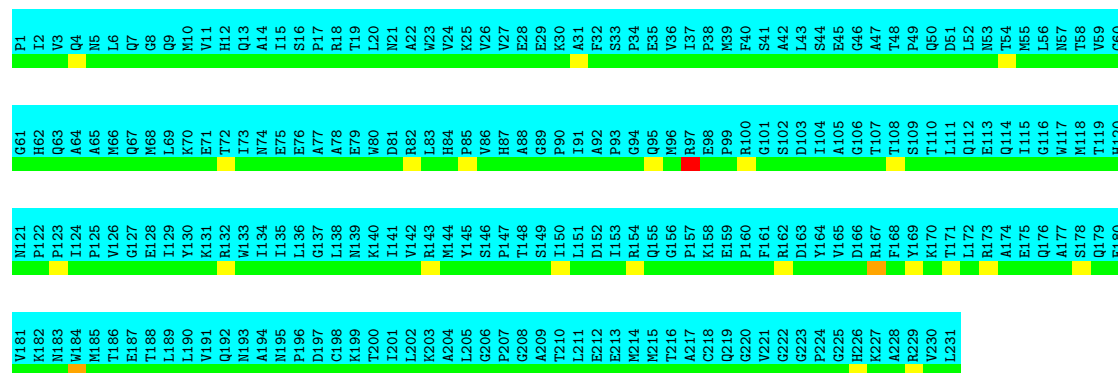
100%



• Molecule 1: HIV-1 capsid protein

Chain rA:

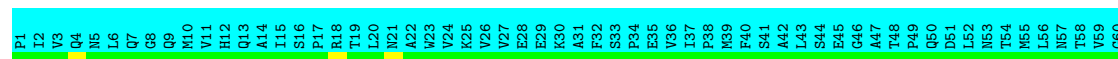
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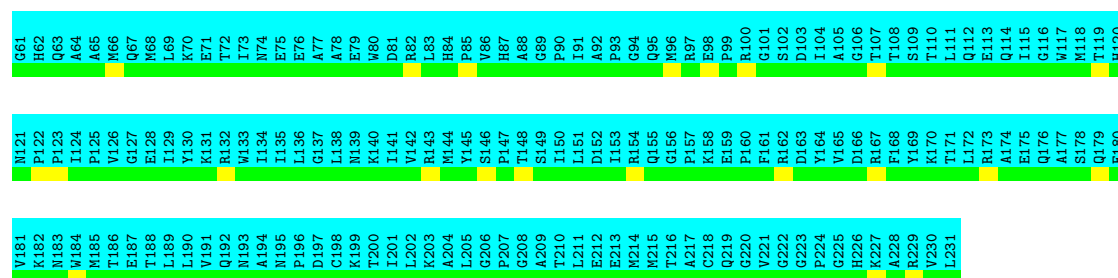


• Molecule 1: HIV-1 capsid protein

Chain sA:

100%

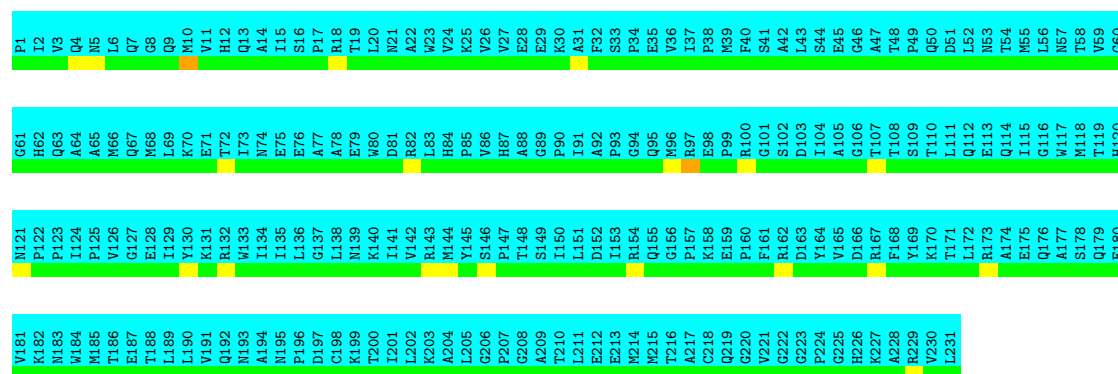




• Molecule 1: HIV-1 capsid protein

Chain tA:

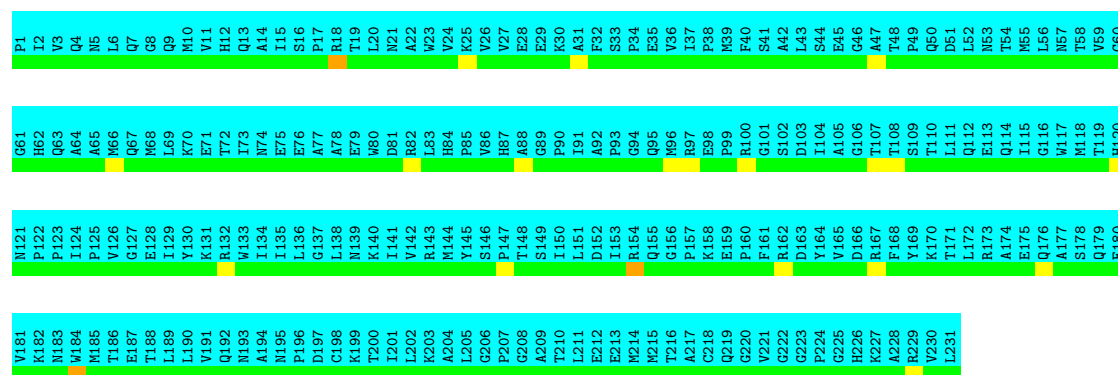
100%



• Molecule 1: HIV-1 capsid protein

Chain uA:

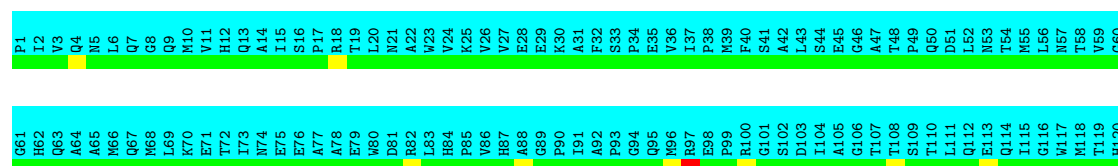
100%

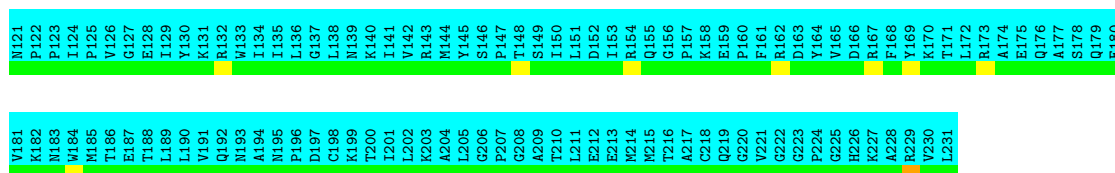


• Molecule 1: HIV-1 capsid protein

Chain vA:

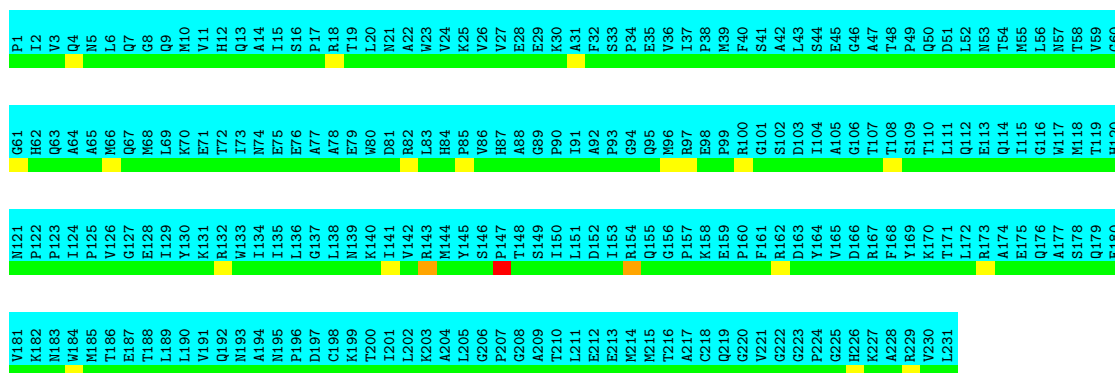
100%





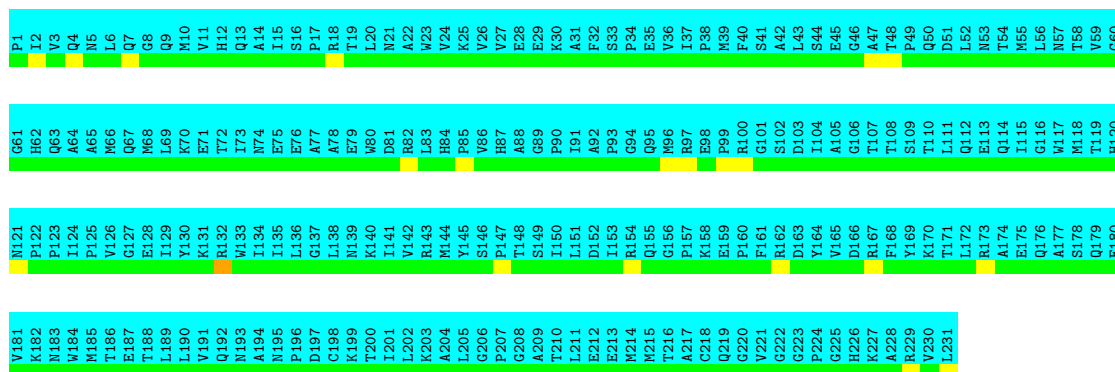
• Molecule 1: HIV-1 capsid protein

Chain wA:  100%



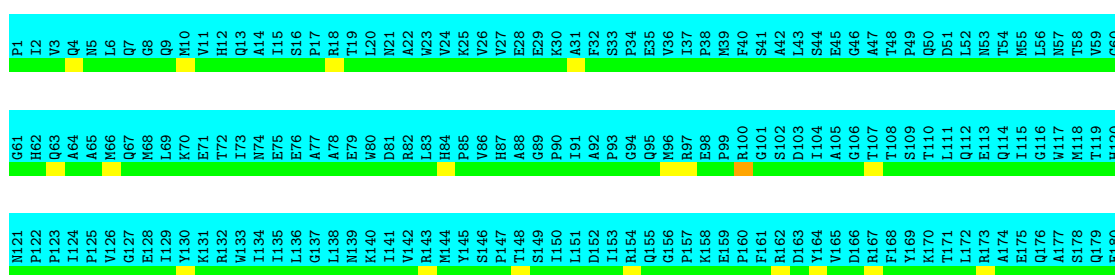
• Molecule 1: HIV-1 capsid protein

Chain xA:  100%



• Molecule 1: HIV-1 capsid protein

Chain yA:  100%

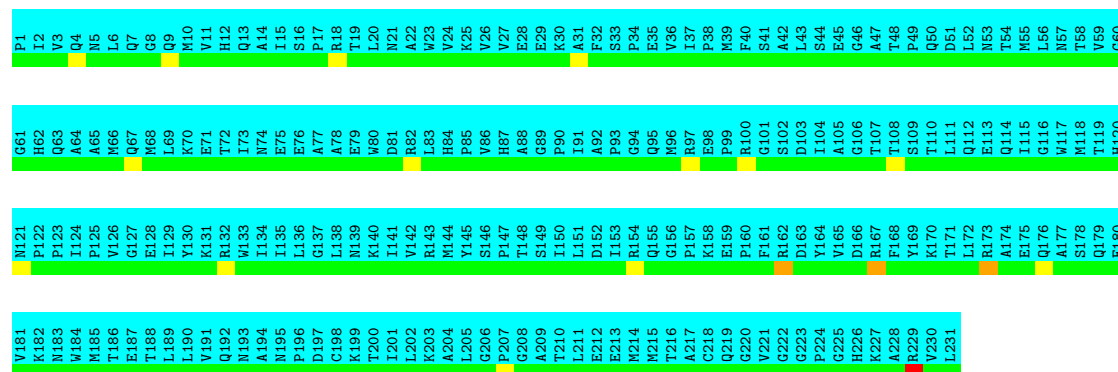




- Molecule 1: HIV-1 capsid protein

Chain zA:

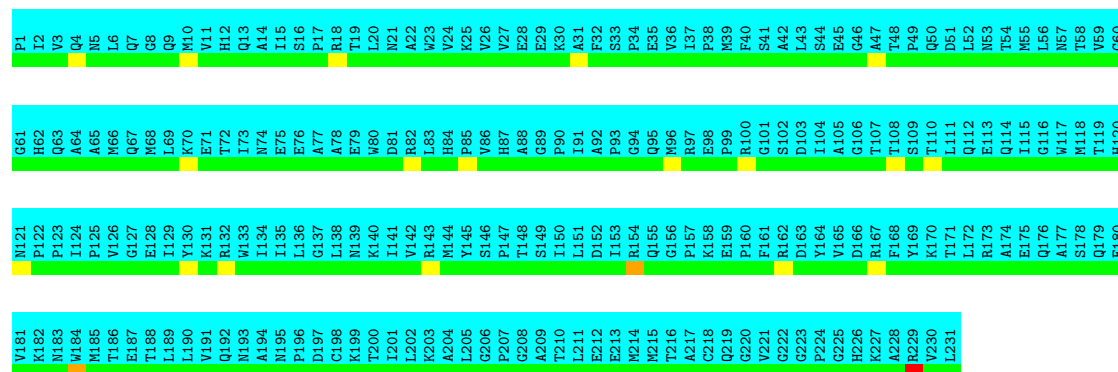
100%



- Molecule 1: HIV-1 capsid protein

Chain 0A:

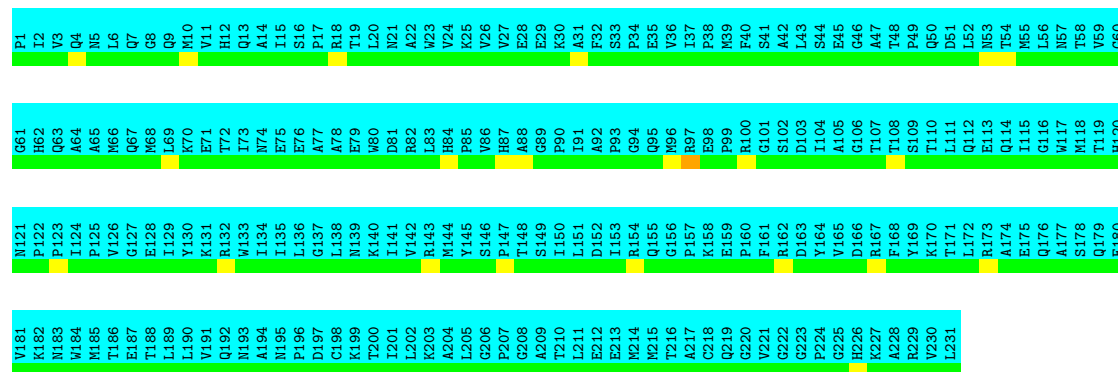
100%



- Molecule 1: HIV-1 capsid protein

Chain 1A:

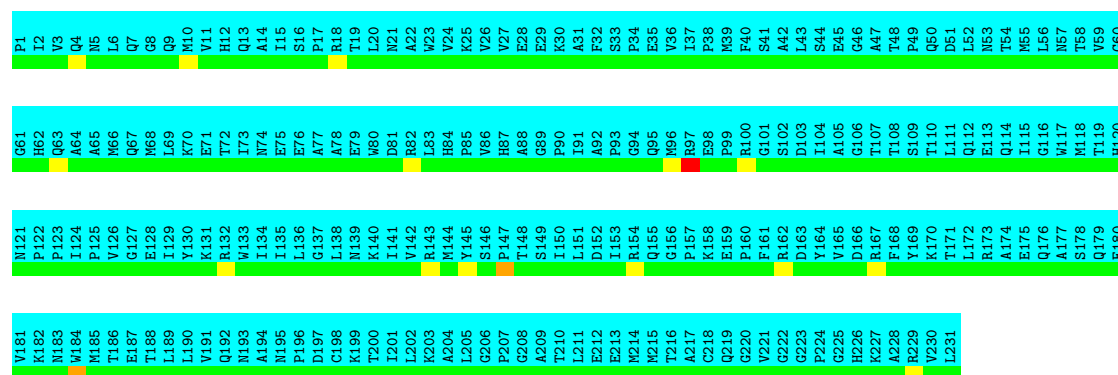
100%



- Molecule 1: HIV-1 capsid protein

Chain 2A:

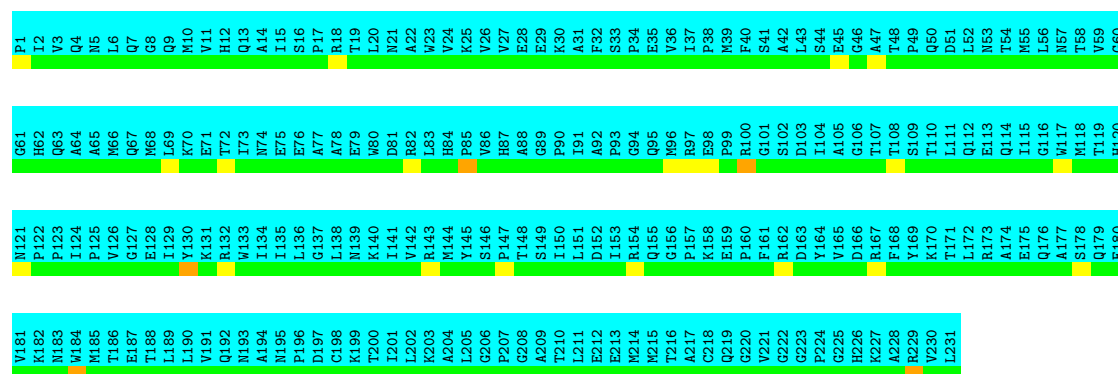
100%



- Molecule 1: HIV-1 capsid protein

Chain 3A:

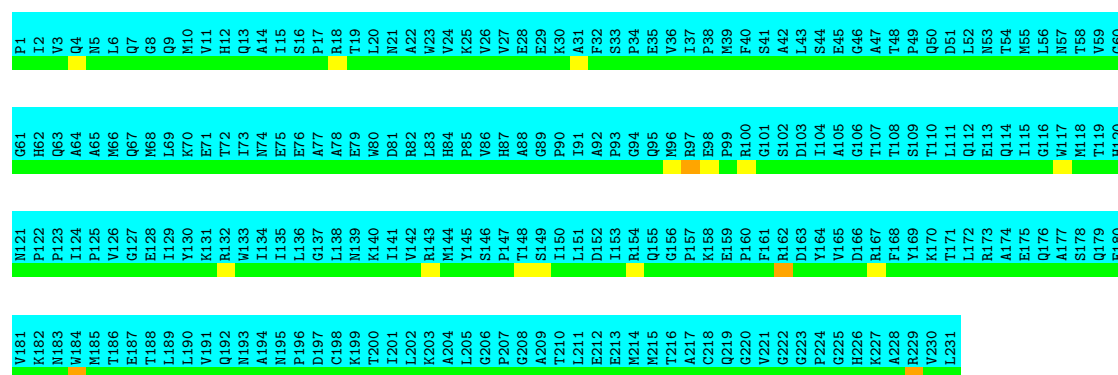
100%



- Molecule 1: HIV-1 capsid protein

Chain 4A:

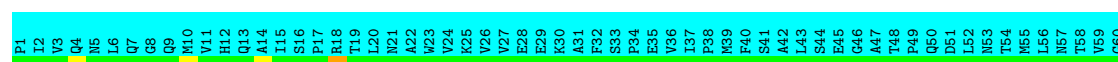
100%

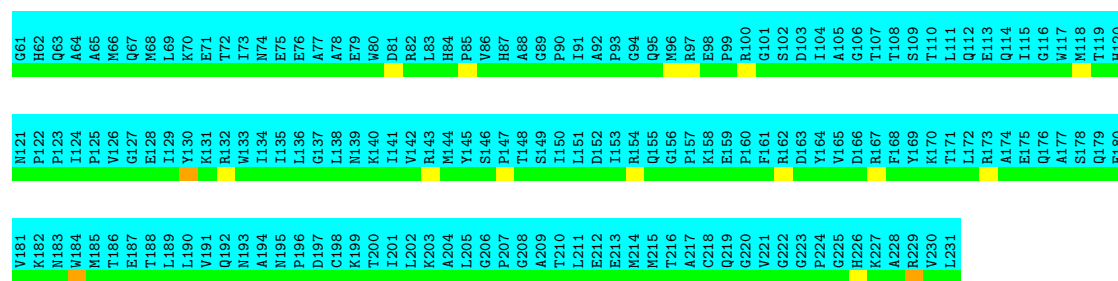


- Molecule 1: HIV-1 capsid protein

Chain 5A:

100%

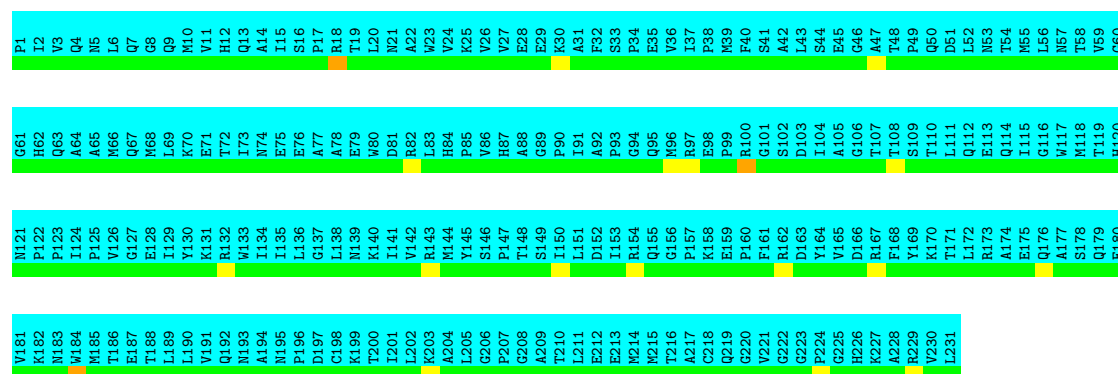




- Molecule 1: HIV-1 capsid protein

Chain 6A:

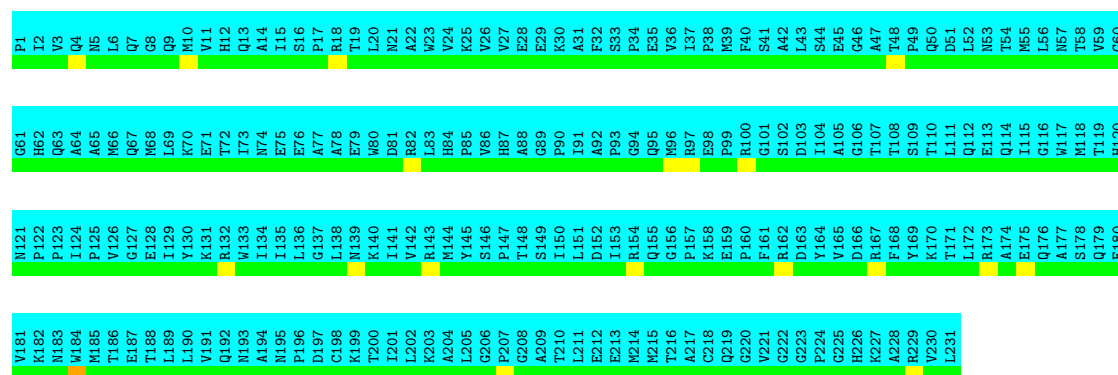
100%



- Molecule 1: HIV-1 capsid protein

Chain 7A:

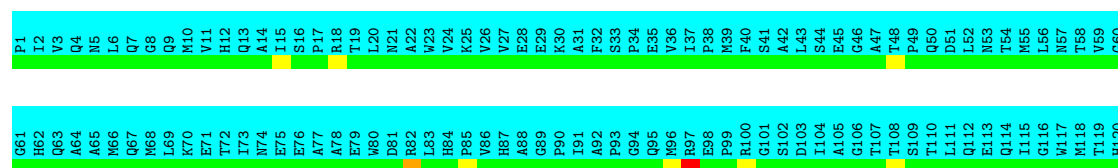
100%

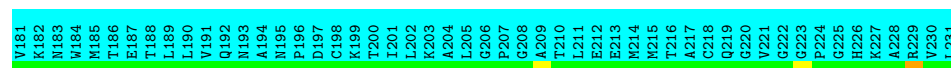


- Molecule 1: HIV-1 capsid protein

Chain 8A:

100%

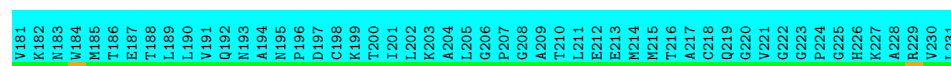
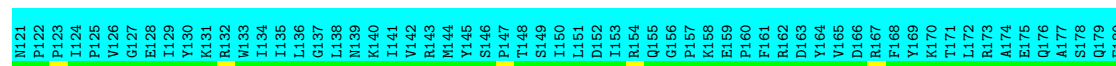
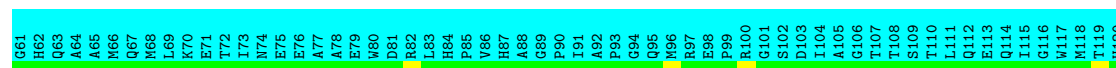
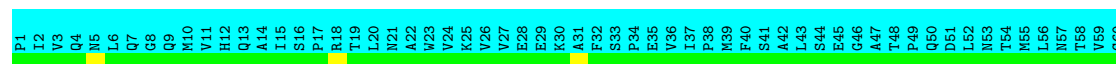




- Molecule 1: HIV-1 capsid protein

Chain CB:

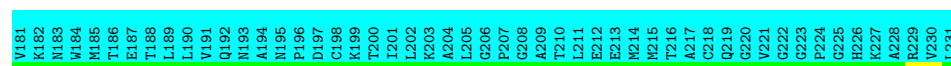
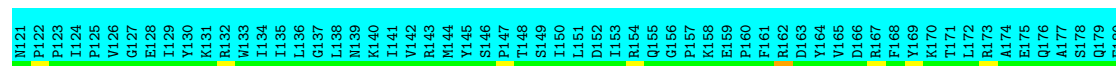
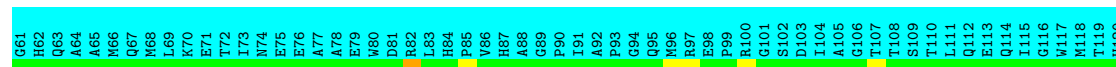
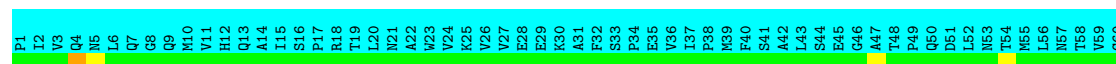
100%



- Molecule 1: HIV-1 capsid protein

Chain DB:

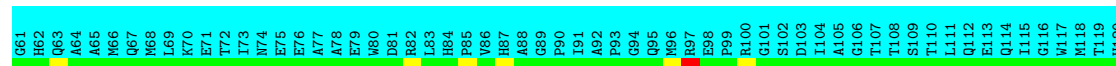
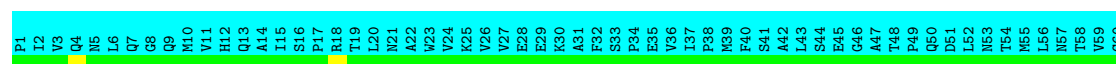
100%



- Molecule 1: HIV-1 capsid protein

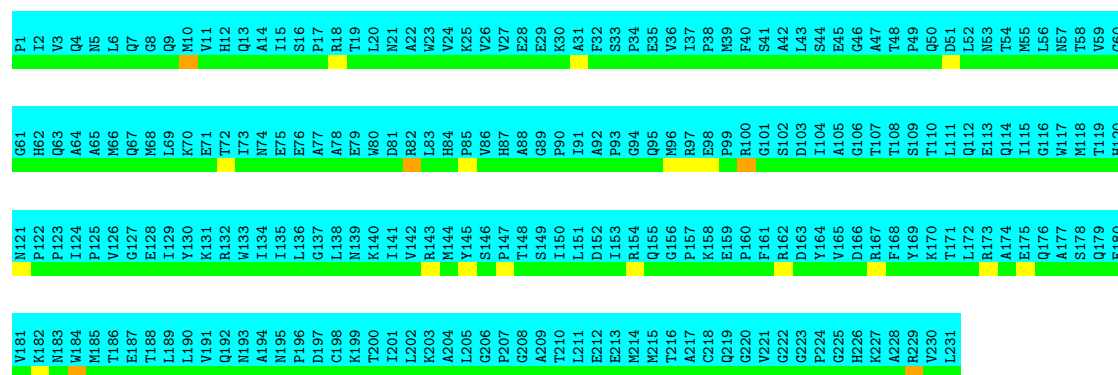
Chain EB:

100%



Chain FB:

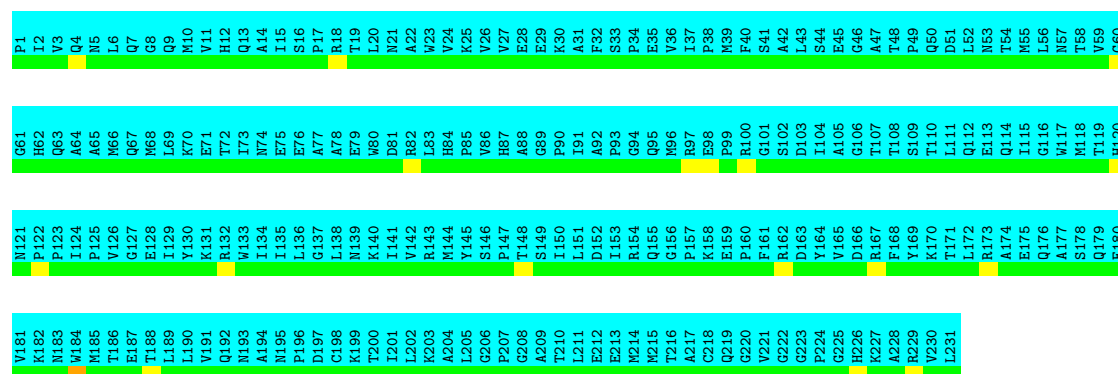
100%



- Molecule 1: HIV-1 capsid protein

Chain GB:

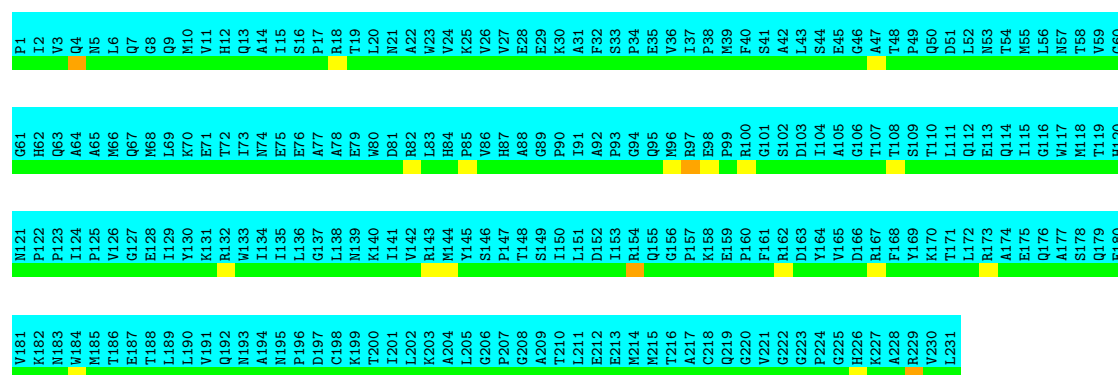
100%



- Molecule 1: HIV-1 capsid protein

Chain HB:

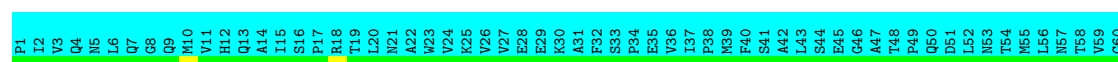
100%

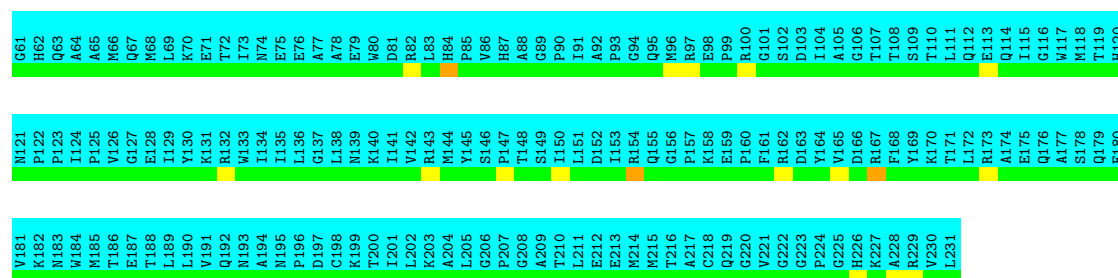


- Molecule 1: HIV-1 capsid protein

Chain IB:

100%

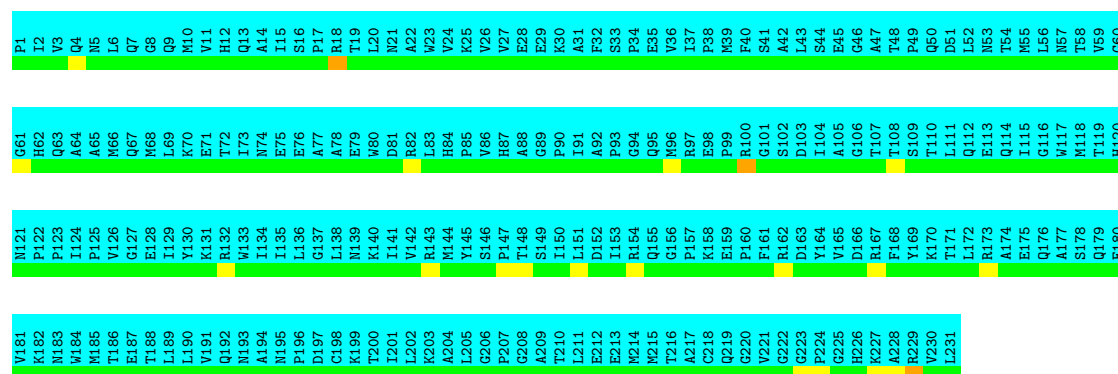




- Molecule 1: HIV-1 capsid protein

Chain JB:

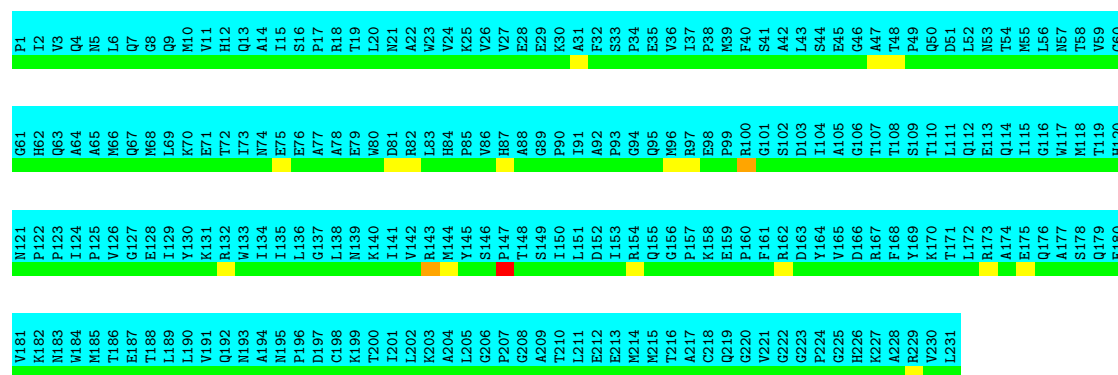
100%



- Molecule 1: HIV-1 capsid protein

Chain KB:

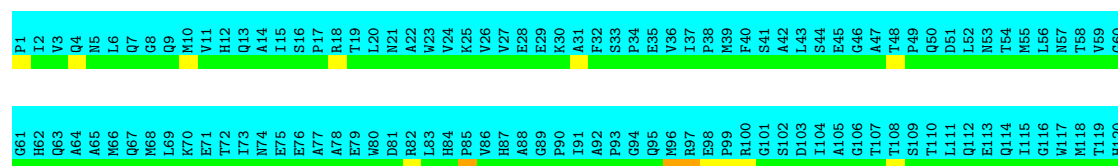
100%

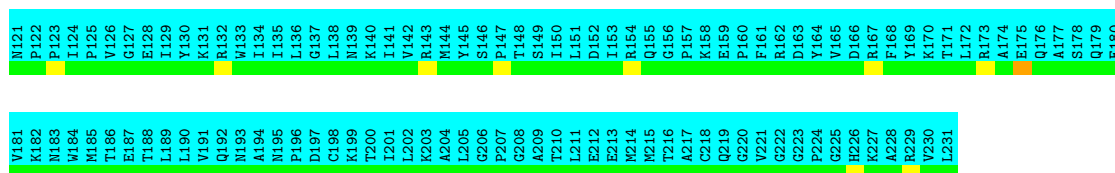


- Molecule 1: HIV-1 capsid protein

Chain LB:

100%

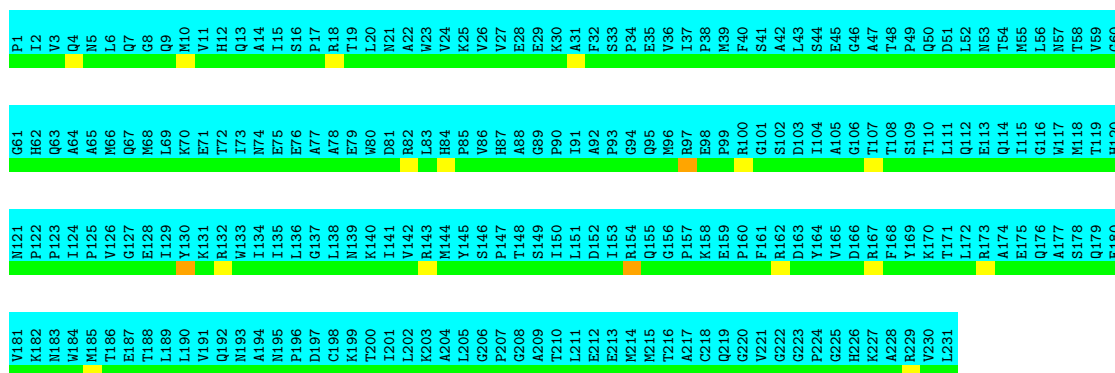




• Molecule 1: HIV-1 capsid protein

Chain MB:

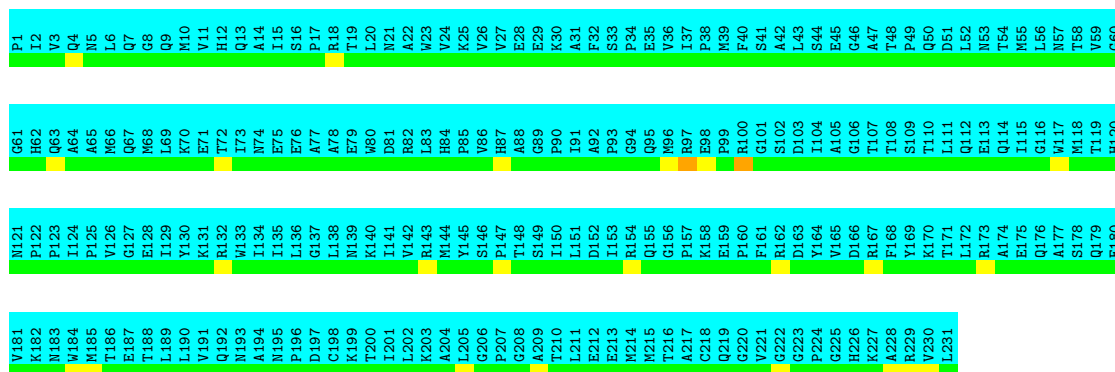
100%



• Molecule 1: HIV-1 capsid protein

Chain NB:

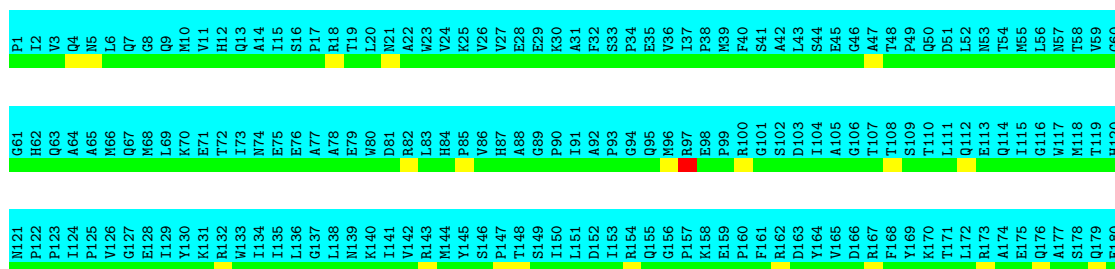
100%



• Molecule 1: HIV-1 capsid protein

Chain OB:

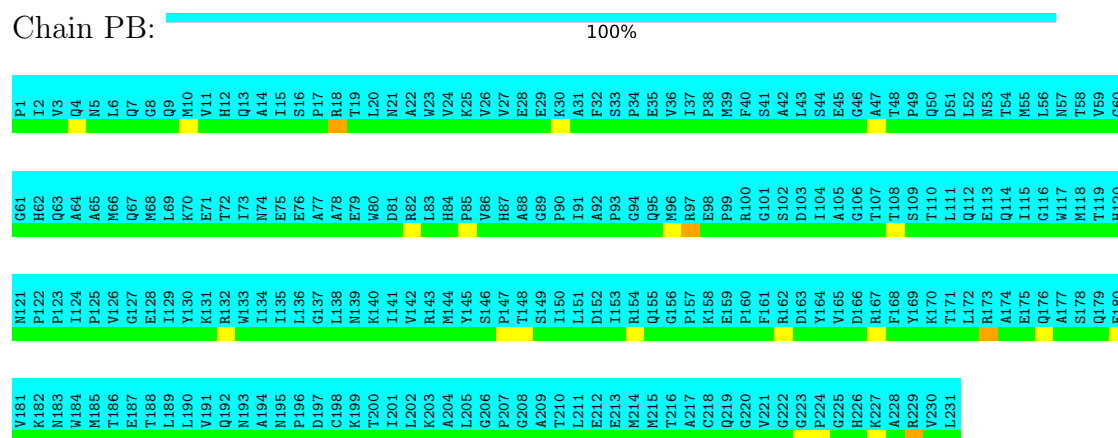
100%



V181	K182	M183	W184	M185	T186	E187	T188	L189	K190	V191	Q192	N193	A194	M195	P196	D197	C198	K199	T200	I201	L202	K203	A204	L205	G206	P207	G208	A209	T210	L211	E212	E213	M214	M215	T216	A217	C218	Q219	G220	V221	G222	G223	P224	G225	H226	K227	A228	R229	V230	L231
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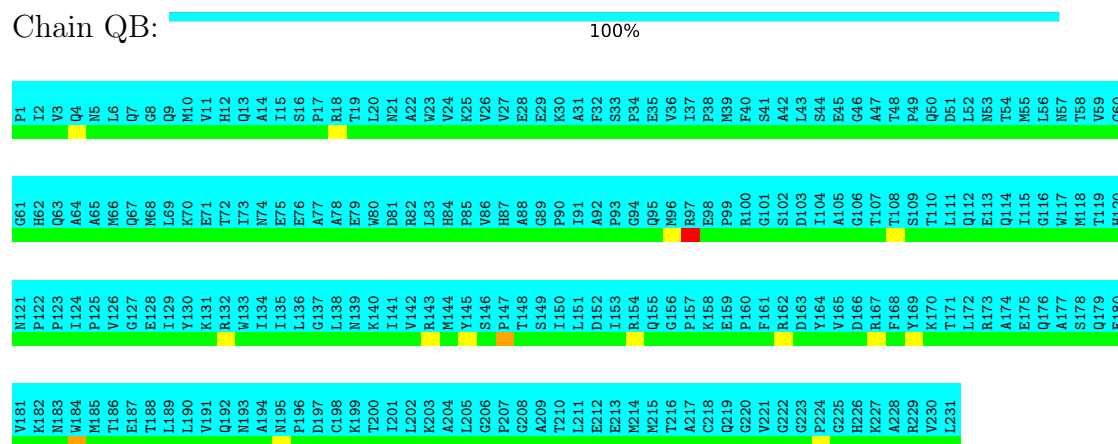
• Molecule 1: HIV-1 capsid protein

Chain PB:



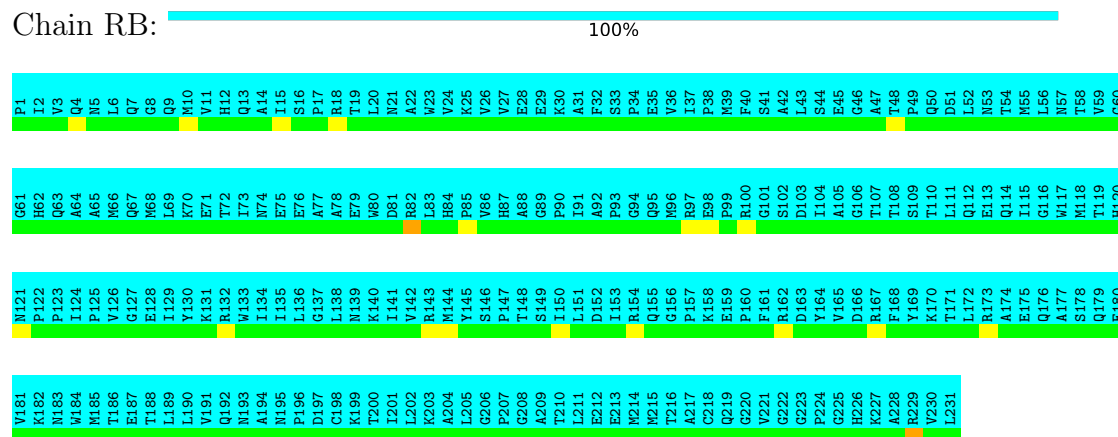
• Molecule 1: HIV-1 capsid protein

Chain QB:



• Molecule 1: HIV-1 capsid protein

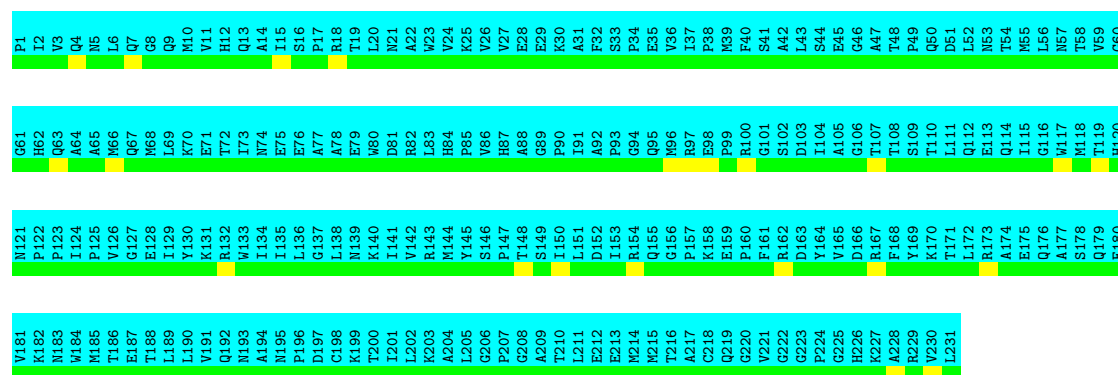
Chain RB:



• Molecule 1: HIV-1 capsid protein

Chain SB:

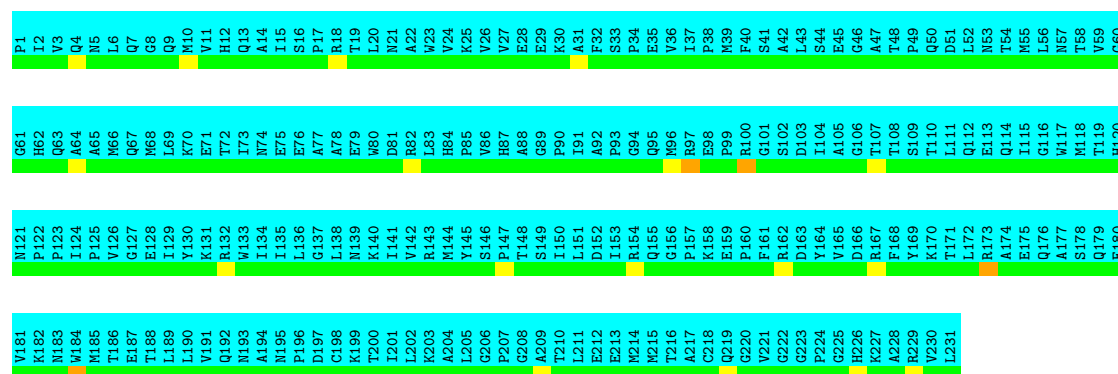
100%



- Molecule 1: HIV-1 capsid protein

Chain TB:

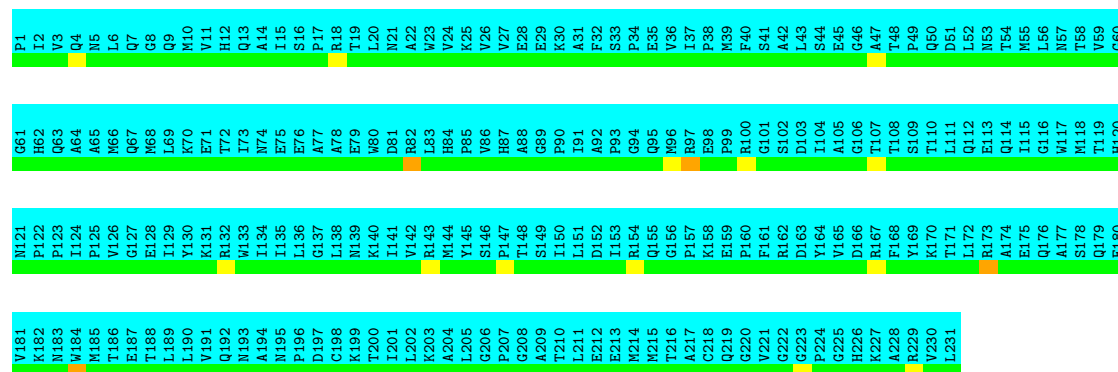
100%



- Molecule 1: HIV-1 capsid protein

Chain UB:

100%

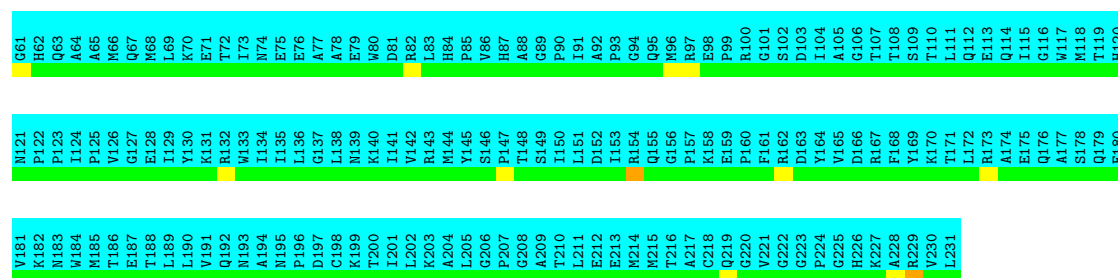


- Molecule 1: HIV-1 capsid protein

Chain VB:

100%

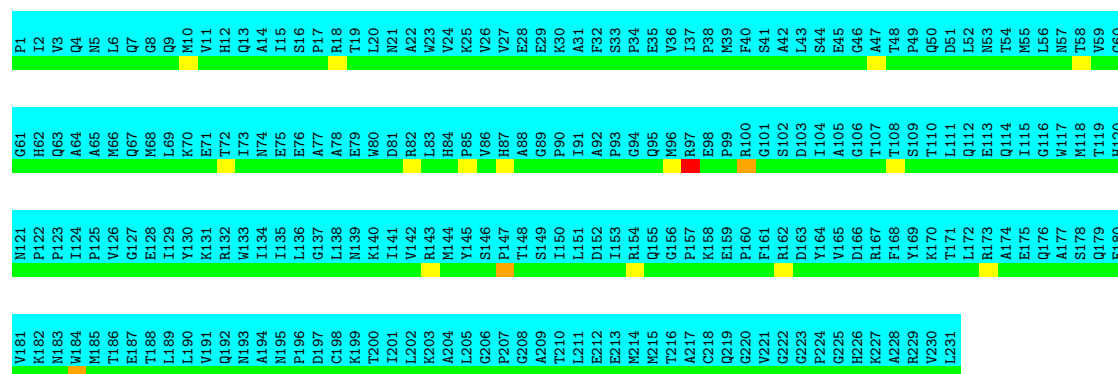




- Molecule 1: HIV-1 capsid protein

Chain WB:

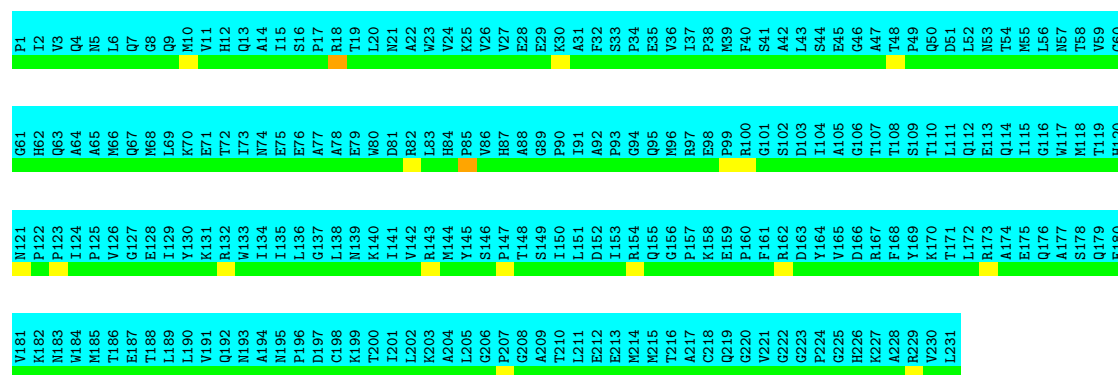
100%



- Molecule 1: HIV-1 capsid protein

Chain XB:

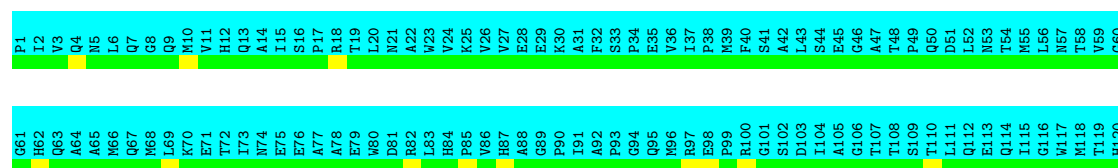
100%

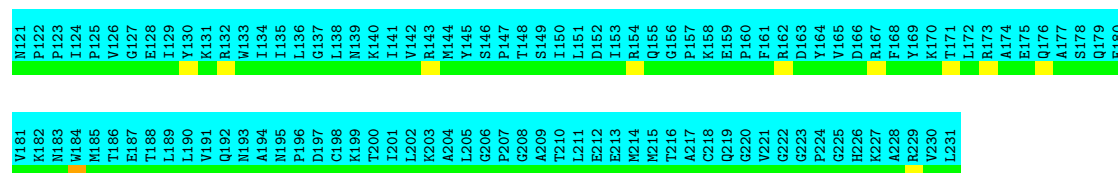


- Molecule 1: HIV-1 capsid protein

Chain YB:

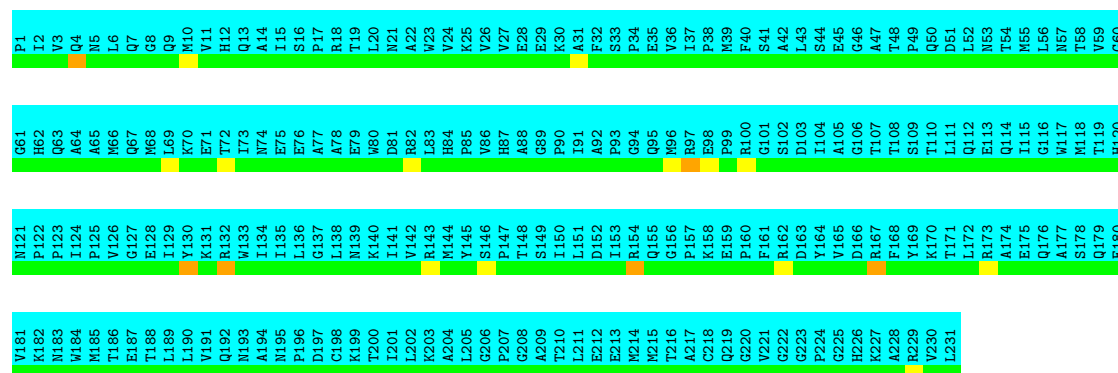
100%





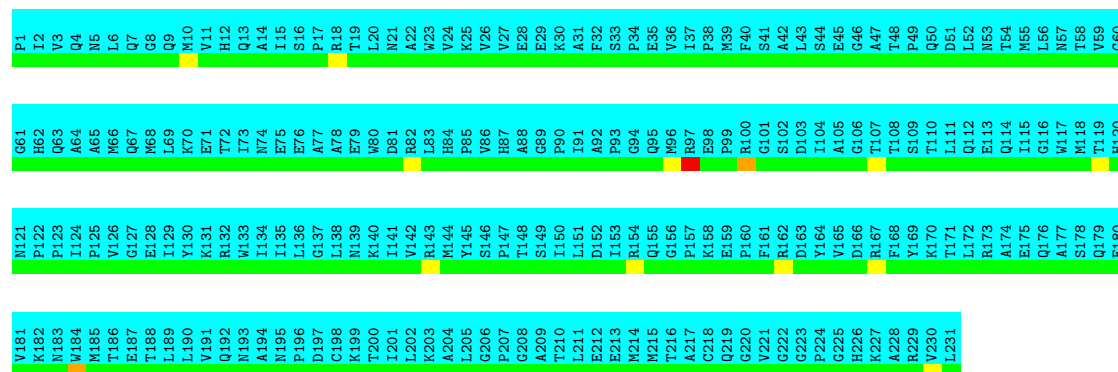
• Molecule 1: HIV-1 capsid protein

Chain ZB:



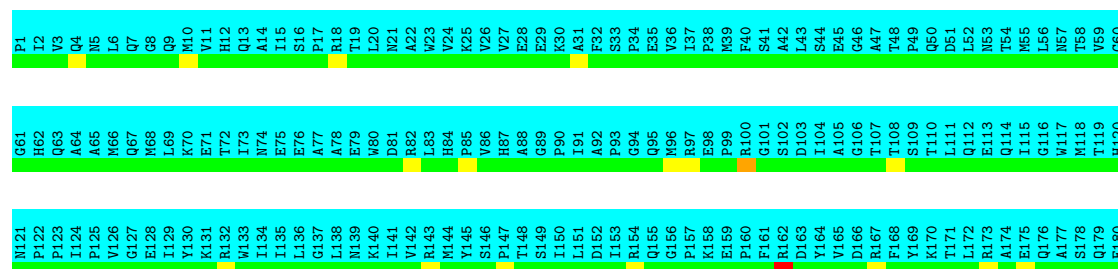
• Molecule 1: HIV-1 capsid protein

Chain aB:



• Molecule 1: HIV-1 capsid protein

Chain bB:



V181	K182	M183	W184	M185	T186	E187	T188	L189	L190	V191	Q192	N193	A194	M195	P196	D197	C198	K199	T200	I201	L202	K203	A204	L205	G206	P207	G208	A209	T210	L211	E212	S213	M214	N215	T216	A217	C218	Q219	G220	V221	G222	D223	P224	G225	H226	K227	A228	R229	V230	L231
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- Molecule 1: HIV-1 capsid protein

Chain cB:

100%

P1	I2	V3	Q4	N5	L6	Q7	G8	Q9	M10	E11	H12	Q13	A14	I15	S16	P17	R18	T19	L20	N21	A22	W23	V24	K25	V26	V27	E28	E29	K30	A31	F32	S33	P34	Q35	E36	V37	I38	P39	M40	F41	S42	A43	L44	E45	G46	A47	T48	P49	Q50	D51	L52	N53	T54	L56	N57	T58	V59	G60
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G61	H62	Q63	I64	A65	M66	G67	M68	L69	K70	E71	T72	W73	N74	E75	S76	A77	R78	E79	W80	D81	A82	L83	H84	P85	V86	H87	A88	G89	P90	I91	A92	P93	G94	Q95	M96	R97	E98	P99	R100	G101	S102	R103	D104	A105	G106	T107	T108	S109	T110	L111	Q112	E113	Q114	I115	G116	W117	M118	Q119	H120
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M121	P122	P123	I124	P125	V126	G127	E128	L129	Y130	K131	R132	W133	I134	I135	L136	G137	L138	N139	K140	I141	V142	R143	M144	Y145	S146	P147	T148	S149	I150	L151	D152	I153	R154	Q155	G156	P157	K158	E159	P160	F161	R162	D163	Y164	V165	D166	R167	F168	Y169	K170	T171	L172	R173	A174	E175	Q176	A177	Q178	Q179	E180
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V181	K182	M183	W184	M185	T186	E187	T188	L189	L190	V191	Q192	N193	A194	M195	P196	D197	C198	K199	T200	I201	L202	K203	A204	L205	G206	P207	G208	A209	T210	L211	E212	S213	M214	N215	T216	A217	C218	Q219	G220	V221	G222	D223	P224	G225	H226	K227	A228	R229	V230	L231
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- Molecule 1: HIV-1 capsid protein

Chain dB:

100%

P1	I2	V3	Q4	N5	L6	Q7	G8	Q9	M10	E11	H12	Q13	A14	I15	S16	P17	R18	T19	L20	N21	A22	W23	V24	K25	V26	V27	E28	E29	K30	A31	F32	S33	P34	Q35	E36	V37	I38	P39	M40	F41	S42	A43	L44	E45	G46	A47	T48	P49	Q50	D51	L52	N53	T54	L56	N57	T58	V59	G60
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G61	H62	Q63	I64	A65	M66	G67	M68	L69	K70	E71	T72	W73	N74	E75	S76	A77	R78	E79	W80	D81	A82	L83	H84	P85	V86	H87	A88	G89	P90	I91	A92	P93	G94	Q95	M96	R97	E98	P99	R100	G101	S102	R103	D104	A105	G106	T107	T108	S109	T110	L111	Q112	E113	Q114	I115	G116	W117	M118	Q119	H120
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M121	P122	P123	I124	P125	V126	G127	E128	L129	Y130	K131	R132	W133	I134	I135	L136	G137	L138	N139	K140	I141	V142	R143	M144	Y145	S146	P147	T148	S149	I150	L151	D152	I153	R154	Q155	G156	P157	K158	E159	P160	F161	R162	D163	Y164	V165	D166	R167	F168	Y169	K170	T171	L172	R173	A174	E175	Q176	A177	Q178	Q179	E180
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V181	K182	M183	W184	M185	T186	E187	T188	L189	L190	V191	Q192	N193	A194	M195	P196	D197	C198	K199	T200	I201	L202	K203	A204	L205	G206	P207	G208	A209	T210	L211	E212	S213	M214	N215	T216	A217	C218	Q219	G220	V221	G222	D223	P224	G225	H226	K227	A228	R229	V230	L231
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- Molecule 1: HIV-1 capsid protein

Chain eB:

100%

P1	I2	V3	Q4	N5	L6	Q7	G8	Q9	M10	E11	H12	Q13	A14	I15	S16	P17	R18	T19	L20	N21	A22	W23	V24	K25	V26	V27	E28	E29	K30	A31	F32	S33	P34	Q35	E36	V37	I38	P39	M40	F41	S42	A43	L44	E45	G46	A47	T48	P49	Q50	D51	L52	N53	T54	L56	N57	T58	V59	G60
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G61	H62	Q63	I64	A65	M66	G67	M68	L69	K70	E71	T72	W73	N74	E75	S76	A77	R78	E79	W80	D81	A82	L83	H84	P85	V86	H87	A88	G89	P90	I91	A92	P93	G94	Q95	M96	R97	E98	P99	R100	G101	S102	R103	D104	A105	G106	T107	T108	S109	T110	L111	Q112	E113	Q114	I115	G116	W117	M118	Q119	H120
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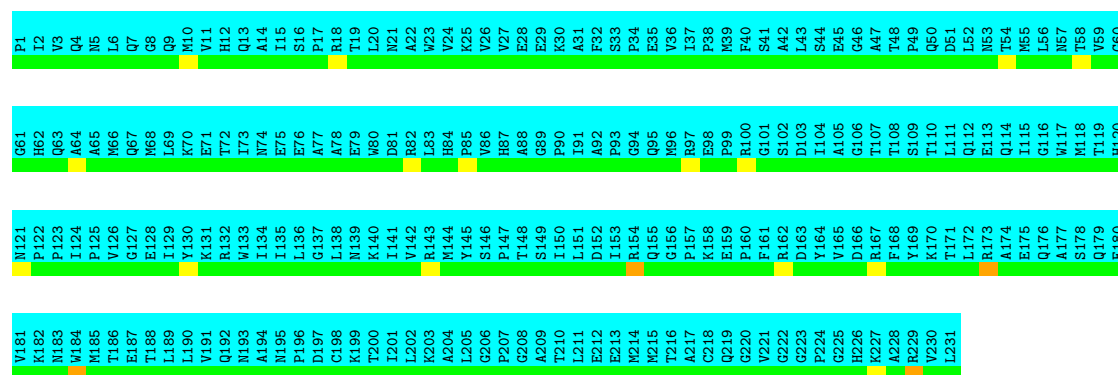
M121	P122	P123	I124	P125	V126	G127	E128	L129	Y130	K131	R132	W133	I134	I135	L136	G137	L138	N139	K140	I141	V142	R143	M144	Y145	S146	P147	T148	S149	I150	L151	D152	I153	R154	Q155	G156	P157	K158	E159	P160	F161	R162	D163	Y164	V165	D166	R167	F168	Y169	K170	T171	L172	R173	A174	E175	Q176	A177	Q178	Q179	E180
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V181	K182	M183	W184	M185	T186	E187	T188	L189	L190	V191	Q192	N193	A194	M195	P196	D197	C198	K199	T200	I201	L202	K203	A204	L205	G206	P207	G208	A209	T210	L211	E212	S213	M214	N215	T216	A217	C218	Q219	G220	V221	G222	D223	P224	G225	H226	K227	A228	R229	V230	L231
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- Molecule 1: HIV-1 capsid protein

Chain fB:

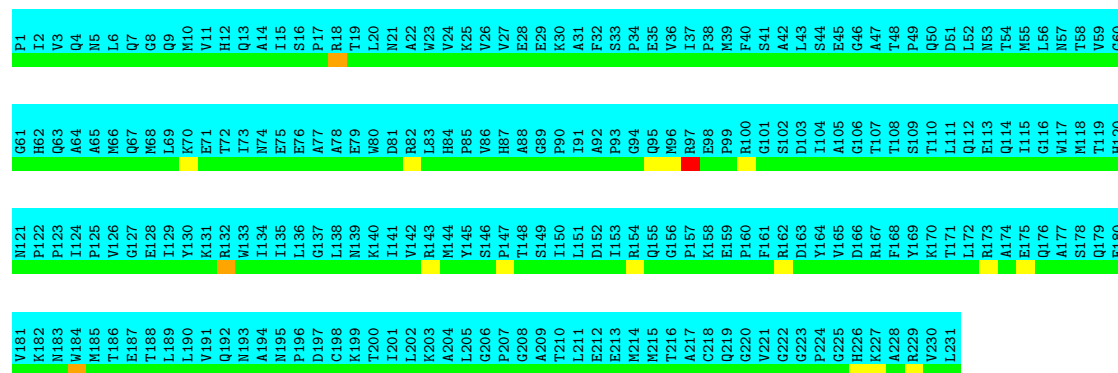
100%



• Molecule 1: HIV-1 capsid protein

Chain gB:

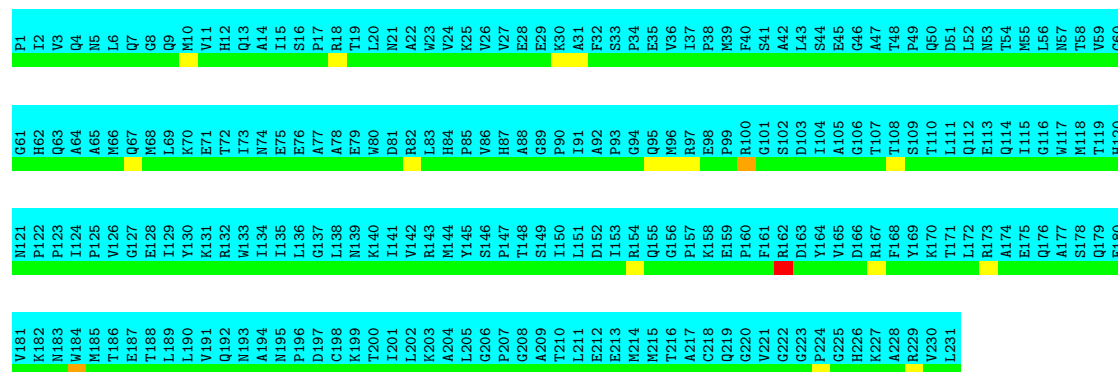
100%



• Molecule 1: HIV-1 capsid protein

Chain hB:

100%



• Molecule 1: HIV-1 capsid protein

Chain iB:

100%

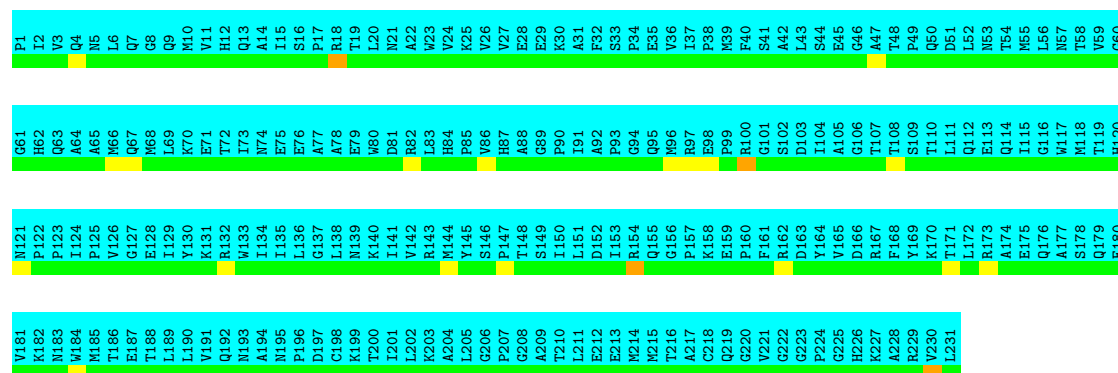




- Molecule 1: HIV-1 capsid protein

Chain jB:

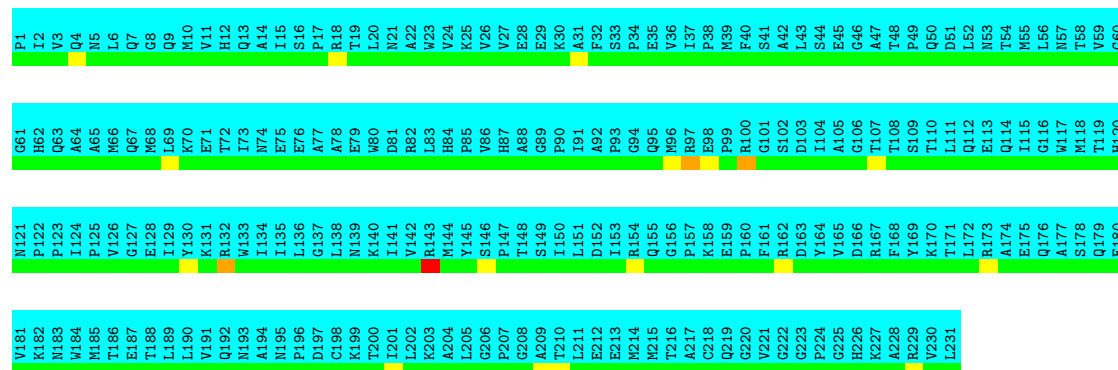
100%



- Molecule 1: HIV-1 capsid protein

Chain kB:

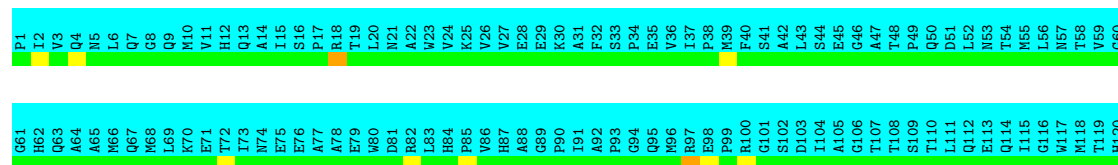
100%

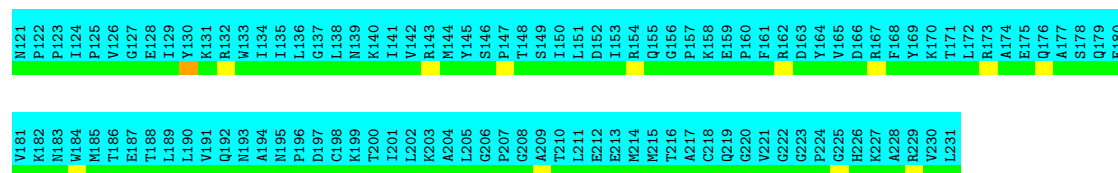


- Molecule 1: HIV-1 capsid protein

Chain lB:

100%

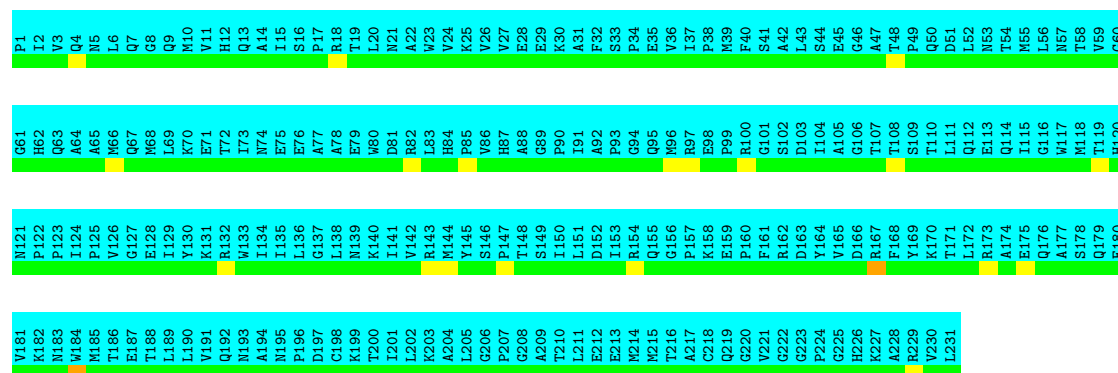




• Molecule 1: HIV-1 capsid protein

Chain mB:

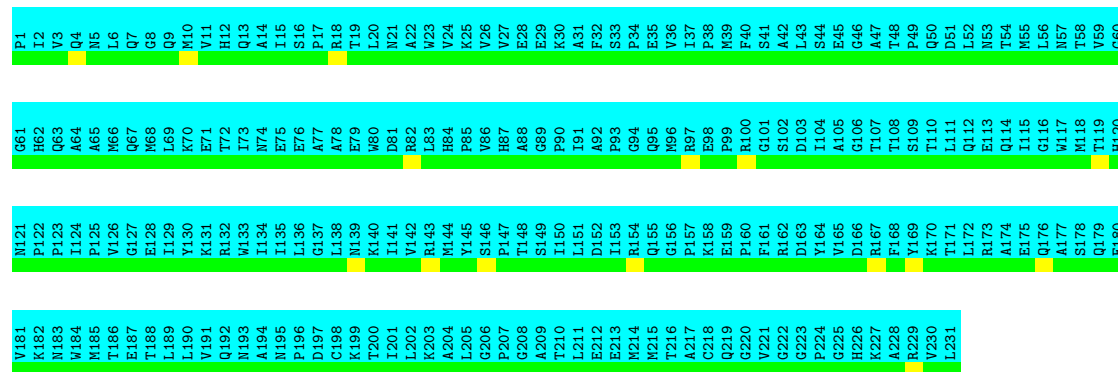
100%



• Molecule 1: HIV-1 capsid protein

Chain nB:

100%



• Molecule 1: HIV-1 capsid protein

Chain oB:

100%

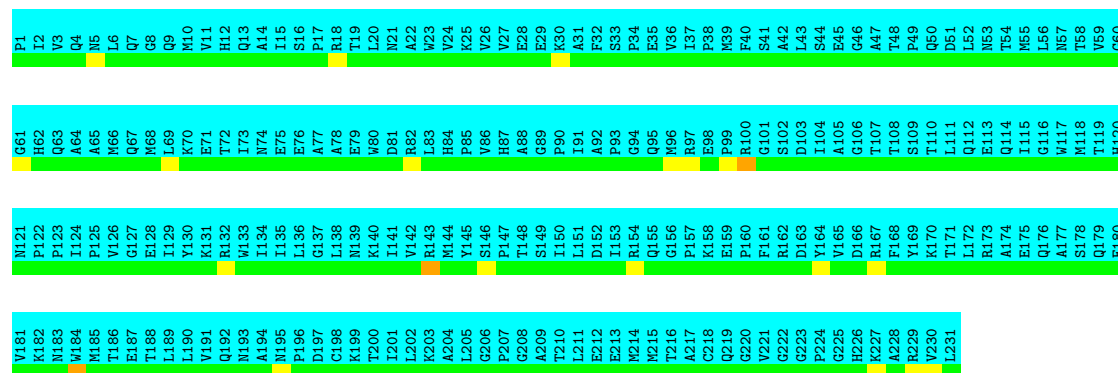




• Molecule 1: HIV-1 capsid protein

Chain pB:

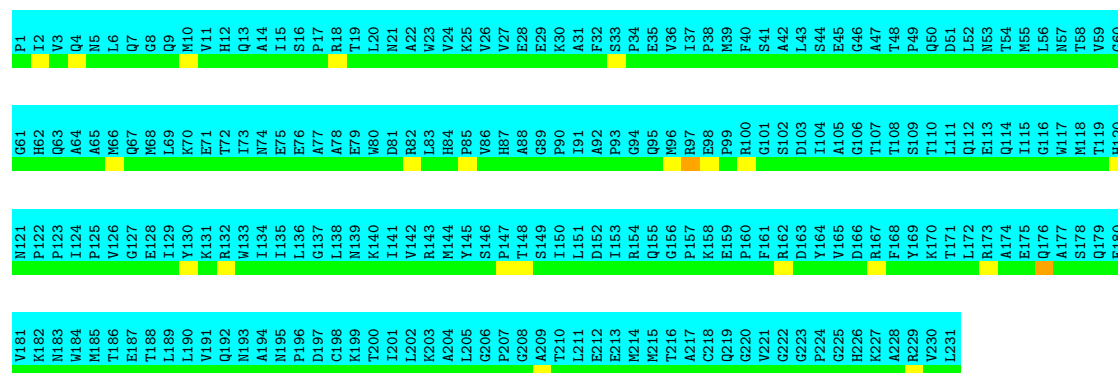
100%



• Molecule 1: HIV-1 capsid protein

Chain qB:

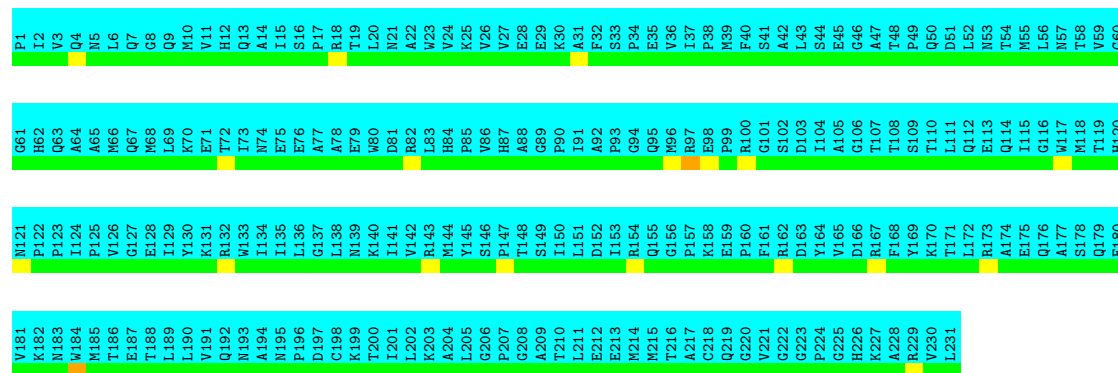
100%



• Molecule 1: HIV-1 capsid protein

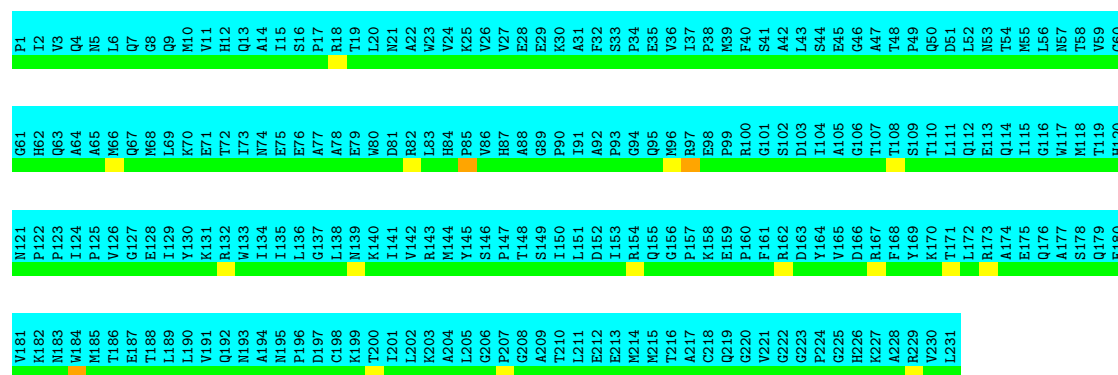
Chain rB:

100%



Chain sB:

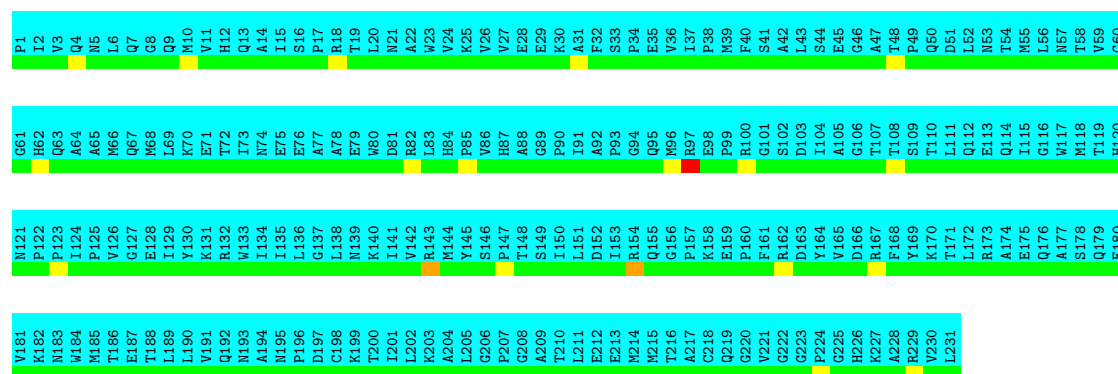
100%



- Molecule 1: HIV-1 capsid protein

Chain tB:

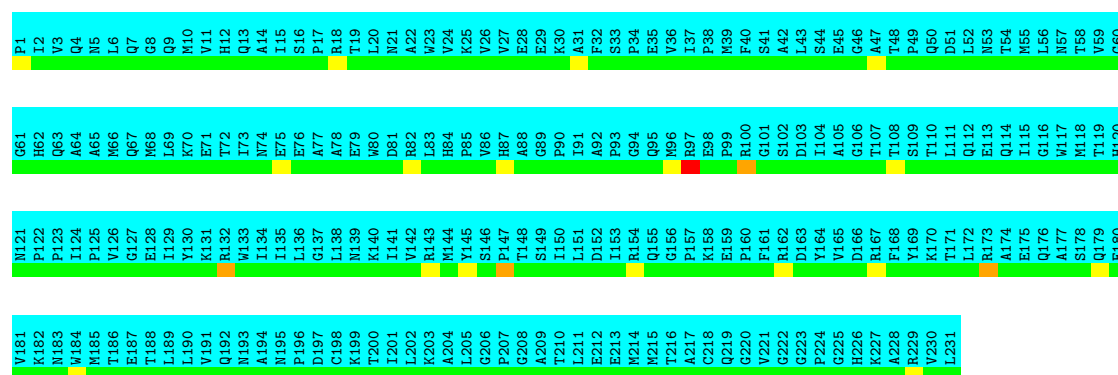
100%



- Molecule 1: HIV-1 capsid protein

Chain uB:

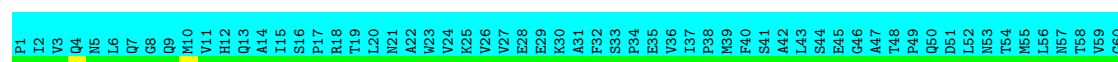
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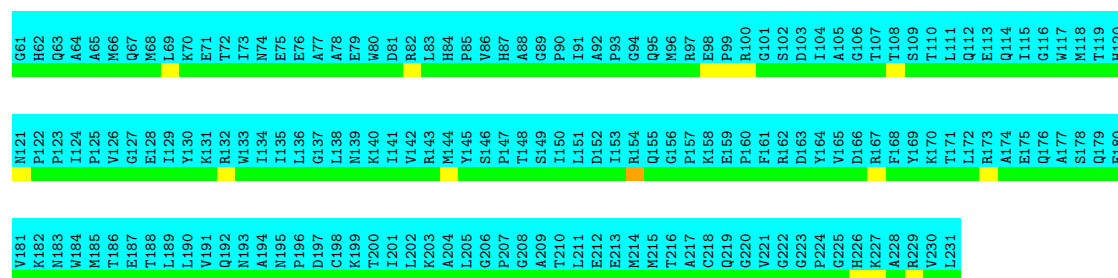


- Molecule 1: HIV-1 capsid protein

Chain vB:

100%

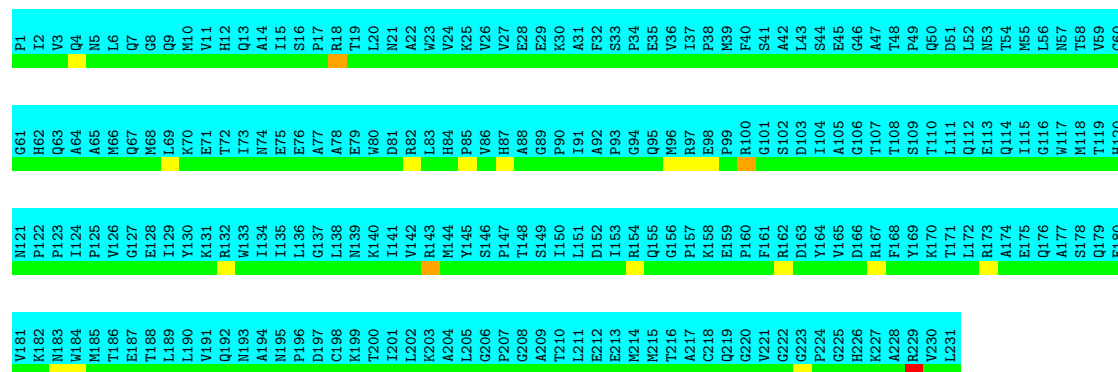




- Molecule 1: HIV-1 capsid protein

Chain wB:

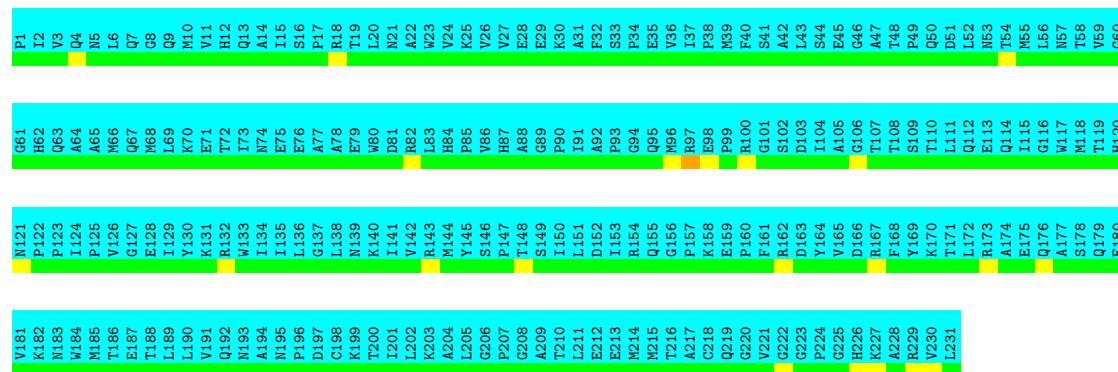
100%



- Molecule 1: HIV-1 capsid protein

Chain xB:

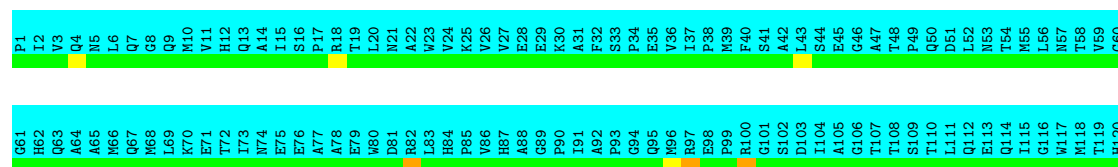
100%



- Molecule 1: HIV-1 capsid protein

Chain yB:

100%



V181	K182	M183	W184	M185	T186	E187	T188	L189	L190	V191	Q192	Q193	N194	A194	P196	D197	C198	K199	T200	L201	L202	K203	A204	L205	G206	P207	G208	A209	T210	L211	E212	E213	M214	Q215	T216	A217	C218	Q219	G220	V221	G222	G223	P224	G225	H226	K227	A228	R229	V230	L231
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- Molecule 1: HIV-1 capsid protein

Chain 2B: 100%

P1	I2	V3	Q4	N5	L6	Q7	G8	Q9	M10	V11	H12	Q13	Q14	A15	E16	P17	R18	T19	L20	N21	A22	W23	H24	P25	V26	V27	H28	G29	P30	K31	A32	F33	G34	Q35	E36	V37	I38	P39	M40	F41	S42	A43	L44	S45	G46	T47	T48	P49	S50	D51	L52	N53	T54	L55	N56	T58	V59	G60
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G61	H62	Q63	A64	A65	M66	Q67	M68	L69	K70	E71	T72	W73	N74	E75	S76	A77	C78	E79	W80	D81	A82	L83	H84	P85	V86	H87	A88	G89	E90	P91	L92	P93	G94	Q95	M96	R97	E98	P99	R100	G101	S102	D103	L104	A105	G106	T107	T108	S109	T110	L111	Q112	E113	Q114	I115	G116	W117	M118	T119	H120
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M121	P122	P123	I124	P125	V126	G127	E128	L129	Y130	K131	R132	W133	I134	I135	L136	G137	L138	N139	K140	I141	V142	R143	M144	Y145	S146	P147	T148	S149	I150	P151	D152	I153	R154	Q155	G156	P157	K158	E159	P160	F161	R162	D163	Y164	V165	D166	R167	F168	Y169	K170	T171	L172	R173	A174	E175	Q176	A177	S178	Q179	E180
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- Molecule 1: HIV-1 capsid protein

Chain 3B: 100%

P1	I2	V3	Q4	N5	L6	Q7	G8	Q9	M10	V11	H12	Q13	Q14	A15	E16	P17	R18	T19	L20	N21	A22	W23	H24	P25	V26	V27	H28	G29	P30	K31	A32	F33	G34	Q35	E36	V37	I38	P39	M40	F41	S42	A43	L44	S45	G46	T47	T48	P49	S50	D51	L52	N53	T54	L55	N56	T58	V59	G60
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G61	H62	Q63	A64	A65	M66	Q67	M68	L69	K70	E71	T72	W73	N74	E75	S76	A77	C78	E79	W80	D81	A82	L83	H84	P85	V86	H87	A88	G89	E90	P91	L92	P93	G94	Q95	M96	R97	E98	P99	R100	G101	S102	D103	L104	A105	G106	T107	T108	S109	T110	L111	Q112	E113	Q114	I115	G116	W117	M118	T119	H120
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M121	P122	P123	I124	P125	V126	G127	E128	L129	Y130	K131	R132	W133	I134	I135	L136	G137	L138	N139	K140	I141	V142	R143	M144	Y145	S146	P147	T148	S149	I150	P151	D152	I153	R154	Q155	G156	P157	K158	E159	P160	F161	R162	D163	Y164	V165	D166	R167	F168	Y169	K170	T171	L172	R173	A174	E175	Q176	A177	S178	Q179	E180
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- Molecule 1: HIV-1 capsid protein

Chain 4B: 100%

P1	I2	V3	Q4	N5	L6	Q7	G8	Q9	M10	V11	H12	Q13	Q14	A15	E16	P17	R18	T19	L20	N21	A22	W23	H24	P25	V26	V27	H28	G29	P30	K31	A32	F33	G34	Q35	E36	V37	I38	P39	M40	F41	S42	A43	L44	S45	G46	T47	T48	P49	S50	D51	L52	N53	T54	L55	N56	T58	V59	G60
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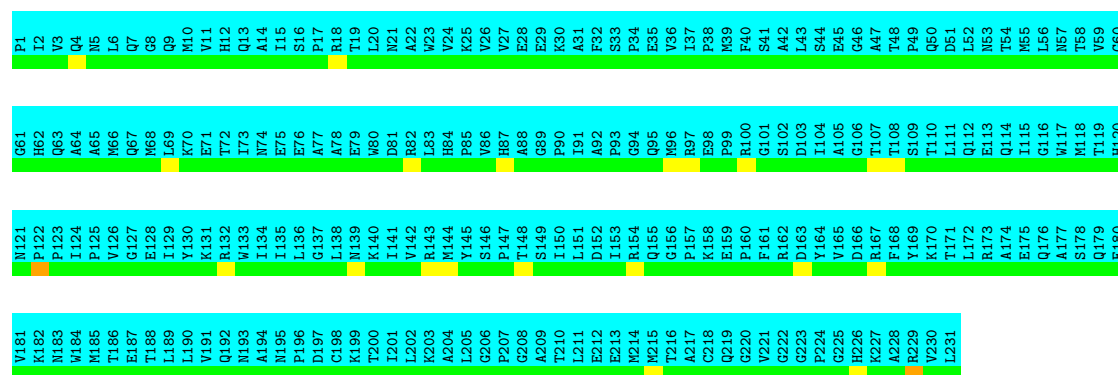
G61	H62	Q63	A64	A65	M66	Q67	M68	L69	K70	E71	T72	W73	N74	E75	S76	A77	C78	E79	W80	D81	A82	L83	H84	P85	V86	H87	A88	G89	E90	P91	L92	P93	G94	Q95	M96	R97	E98	P99	R100	G101	S102	D103	L104	A105	G106	T107	T108	S109	T110	L111	Q112	E113	Q114	I115	G116	W117	M118	T119	H120
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M121	P122	P123	I124	P125	V126	G127	E128	L129	Y130	K131	R132	W133	I134	I135	L136	G137	L138	N139	K140	I141	V142	R143	M144	Y145	S146	P147	T148	S149	I150	P151	D152	I153	R154	Q155	G156	P157	K158	E159	P160	F161	R162	D163	Y164	V165	D166	R167	F168	Y169	K170	T171	L172	R173	A174	E175	Q176	A177	S178	Q179	E180
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- Molecule 1: HIV-1 capsid protein

Chain 5B:

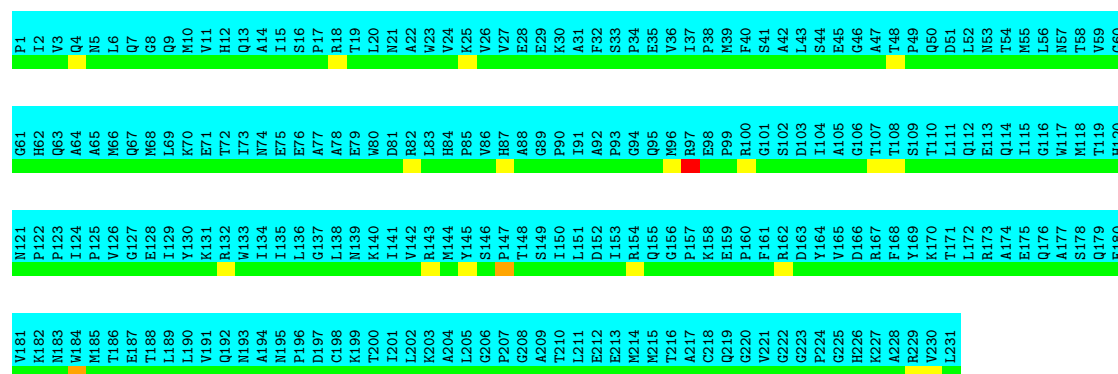
100%



- Molecule 1: HIV-1 capsid protein

Chain 6B:

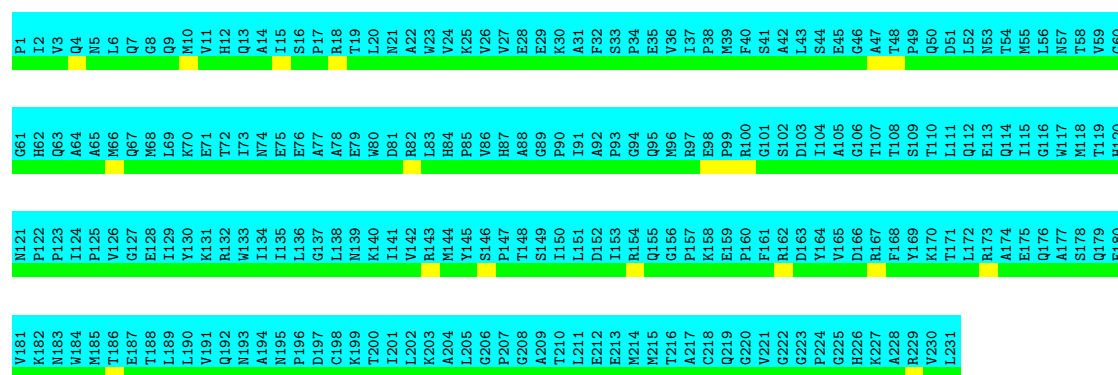
100%



- Molecule 1: HIV-1 capsid protein

Chain 7B:

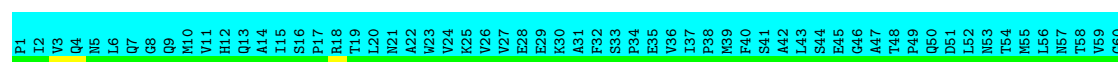
100%

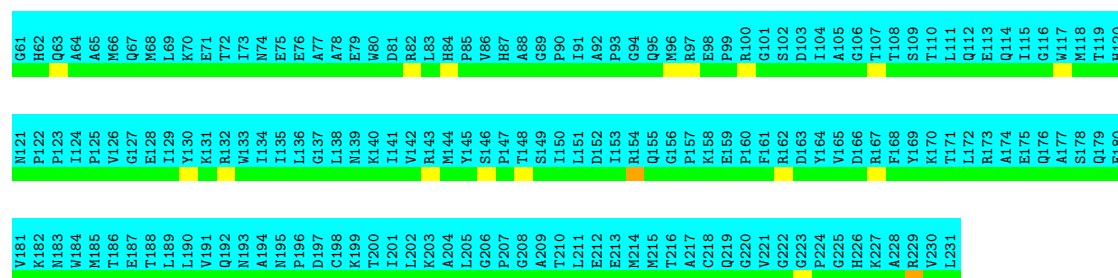


- Molecule 1: HIV-1 capsid protein

Chain 8B:

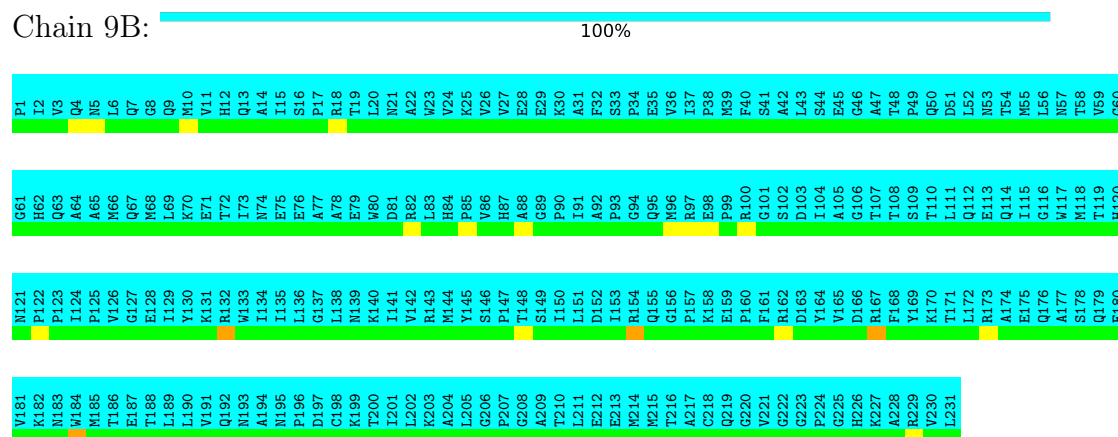
100%





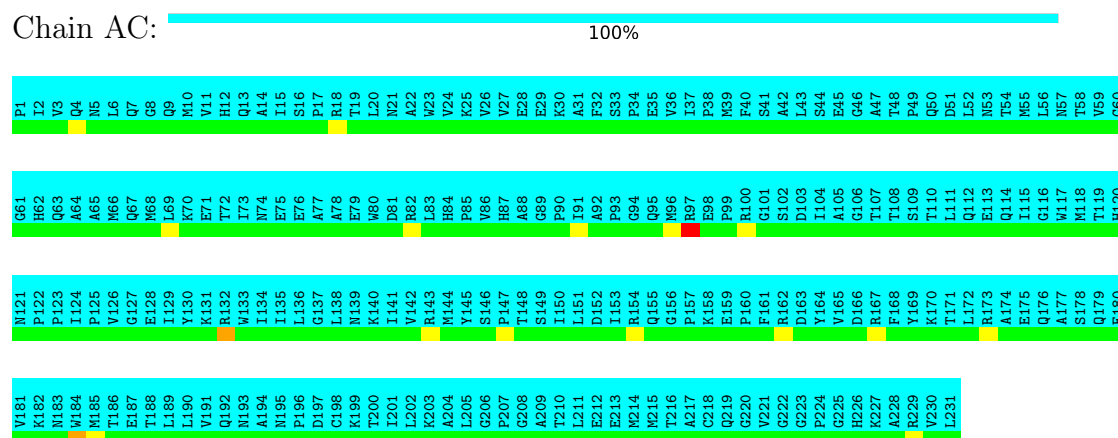
- Molecule 1: HIV-1 capsid protein

Chain 9B:



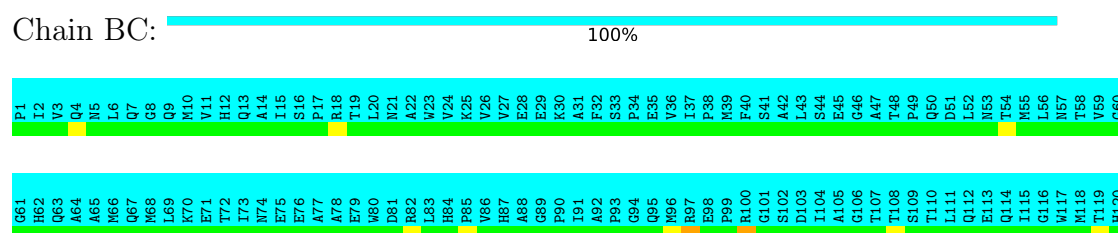
- Molecule 1: HIV-1 capsid protein

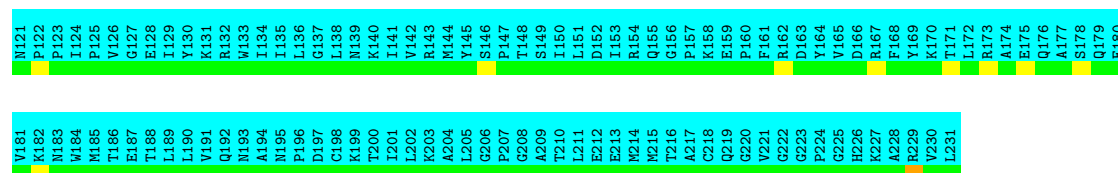
Chain AC:



- Molecule 1: HIV-1 capsid protein

Chain BC:





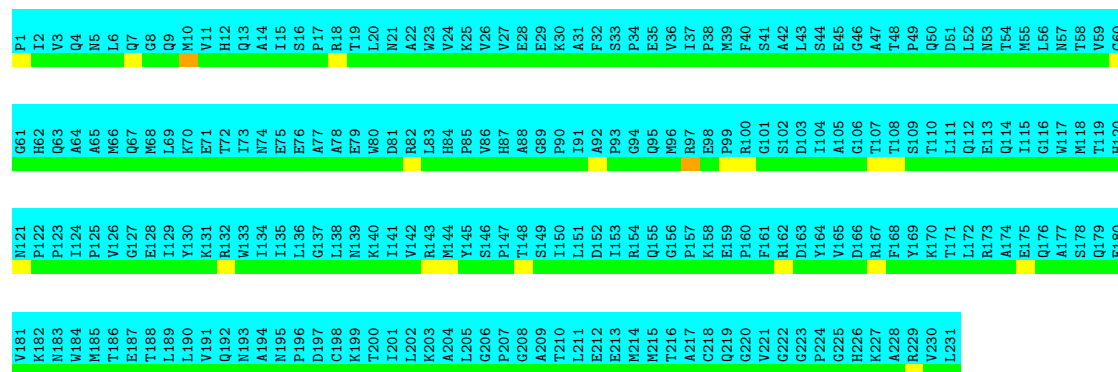
• Molecule 1: HIV-1 capsid protein

Chain CC:  100%



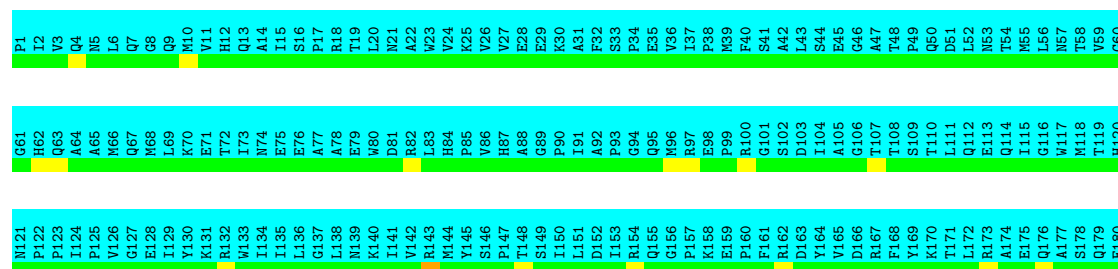
• Molecule 1: HIV-1 capsid protein

Chain DC:  100%



• Molecule 1: HIV-1 capsid protein

Chain EC:  100%

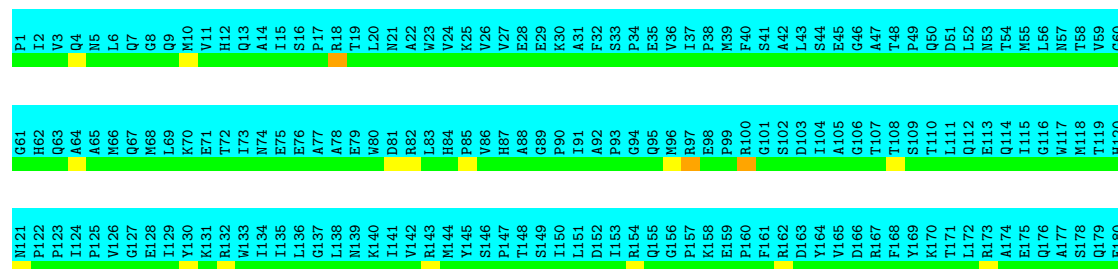




- Molecule 1: HIV-1 capsid protein

Chain FC:

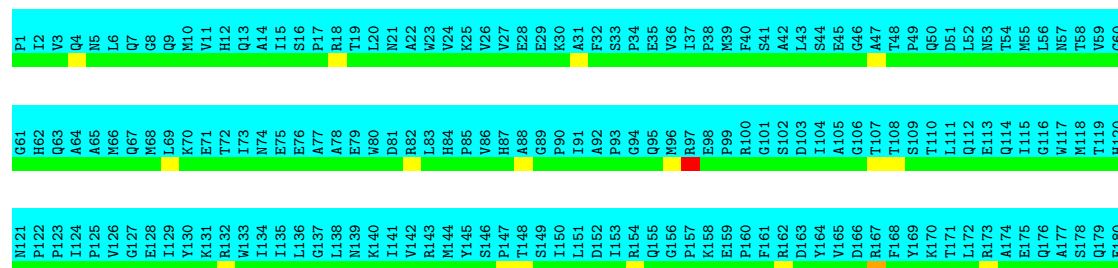
100%



- Molecule 1: HIV-1 capsid protein

Chain GC:

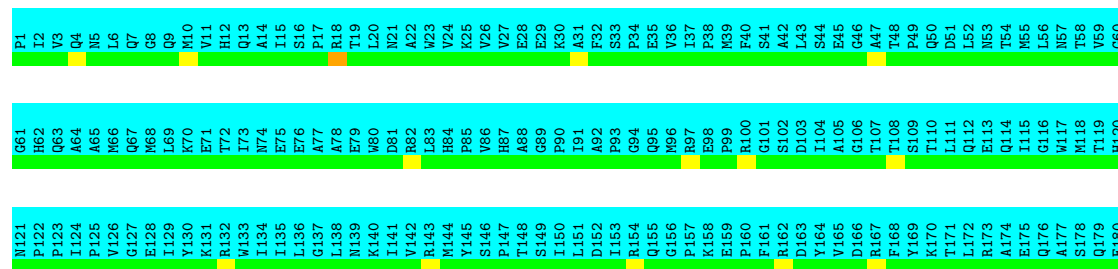
100%



- Molecule 1: HIV-1 capsid protein

Chain HC:

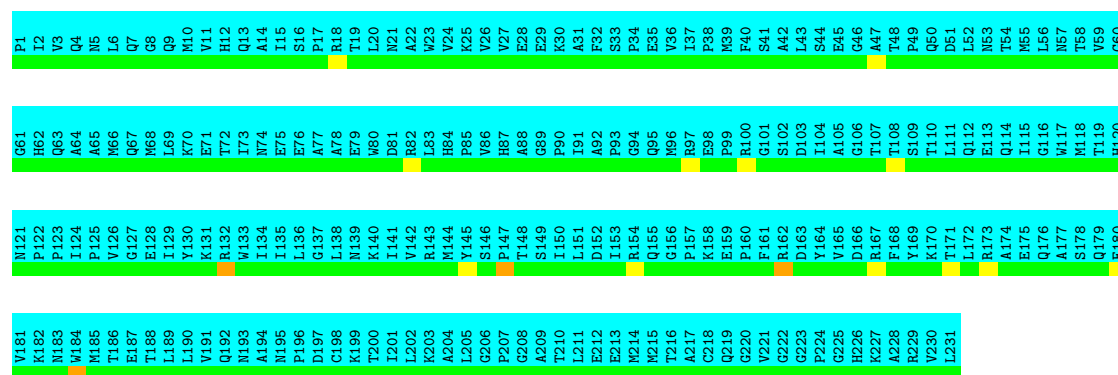
100%



- Molecule 1: HIV-1 capsid protein

Chain IC:

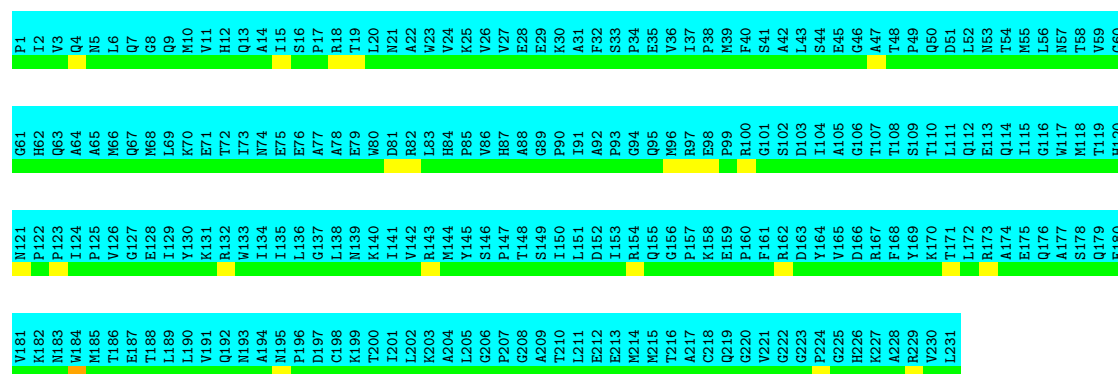
100%



- Molecule 1: HIV-1 capsid protein

Chain JC:

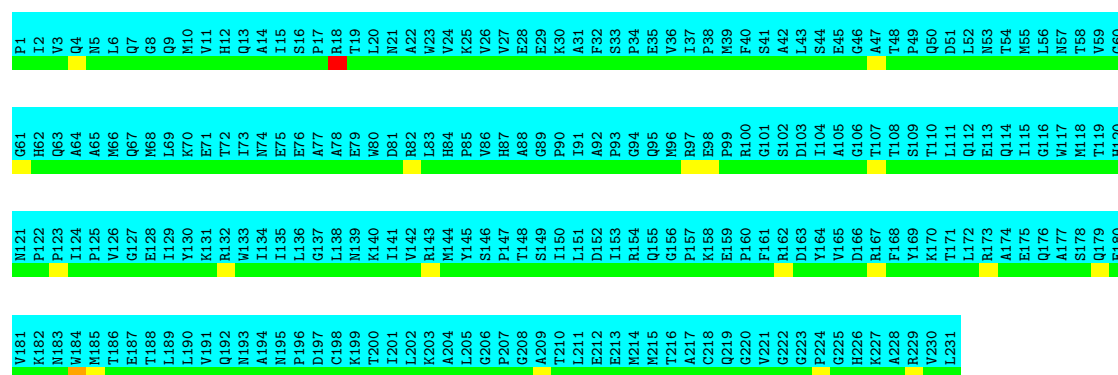
100%



- Molecule 1: HIV-1 capsid protein

Chain KC:

100%

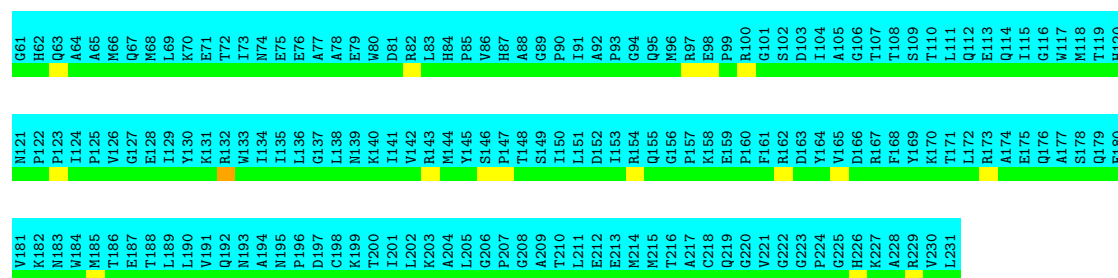


- Molecule 1: HIV-1 capsid protein

Chain LC:

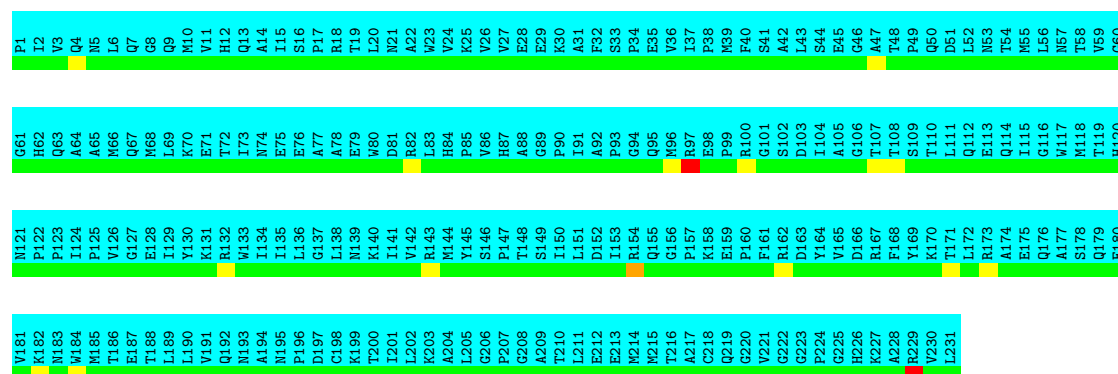
100%





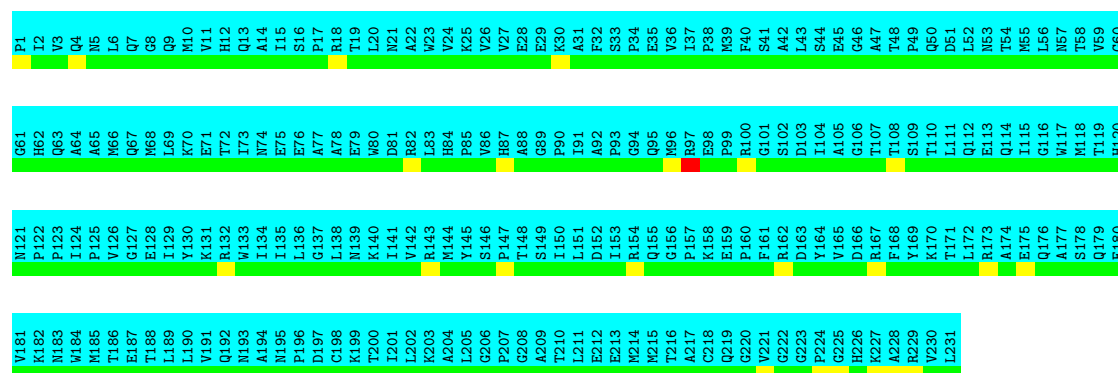
- Molecule 1: HIV-1 capsid protein

Chain MC:  100%



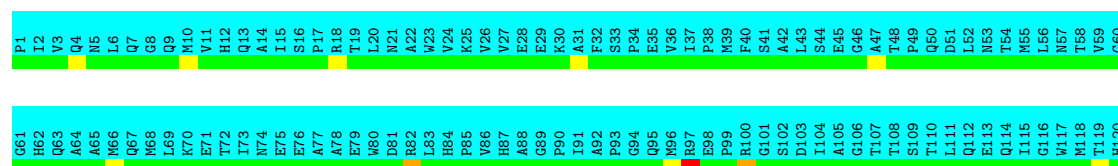
- Molecule 1: HIV-1 capsid protein

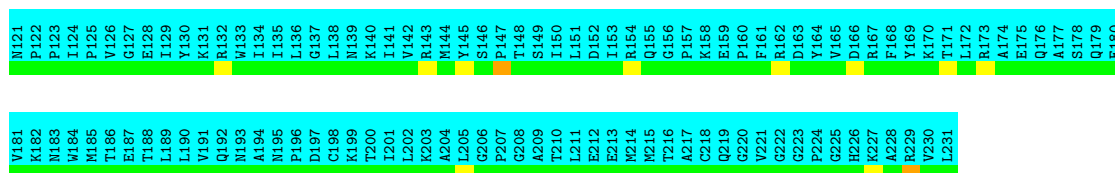
Chain NC:  100%



- Molecule 1: HIV-1 capsid protein

Chain OC:  100%

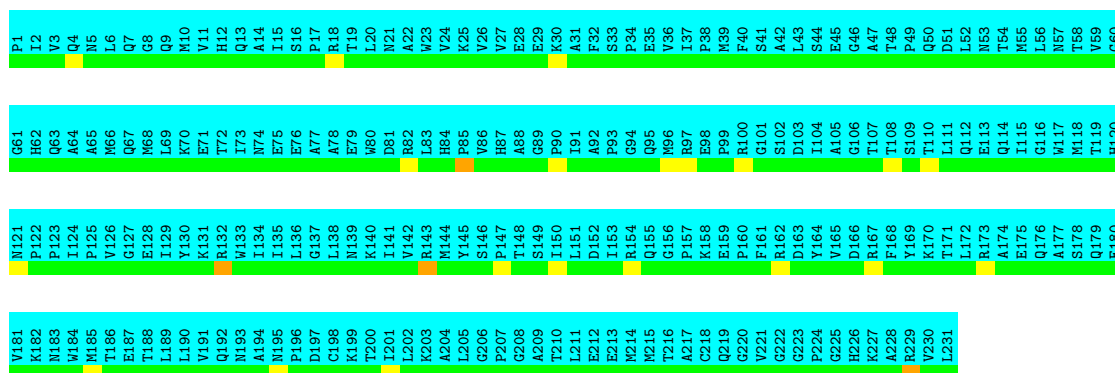




• Molecule 1: HIV-1 capsid protein

Chain PC:

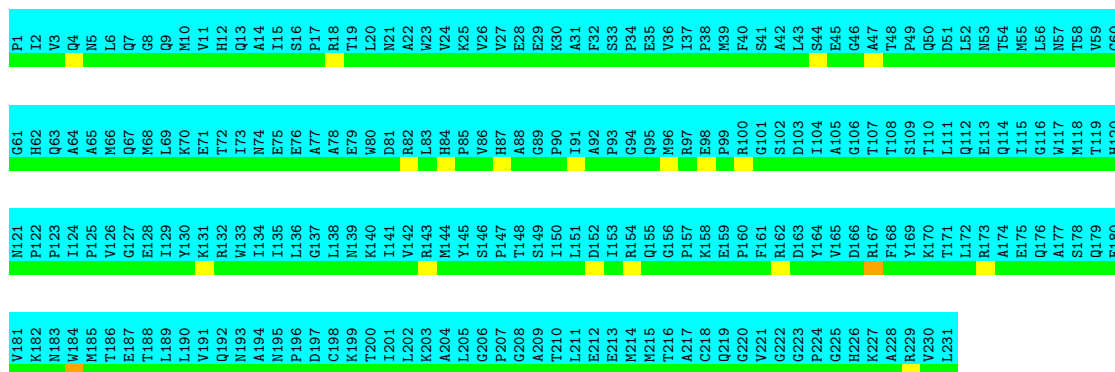
100%



• Molecule 1: HIV-1 capsid protein

Chain QC:

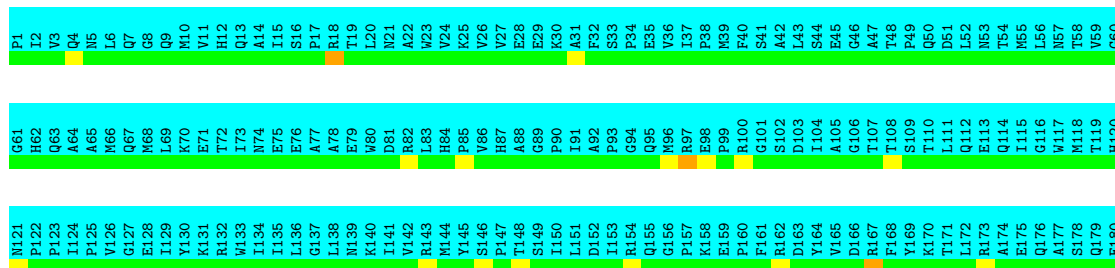
100%

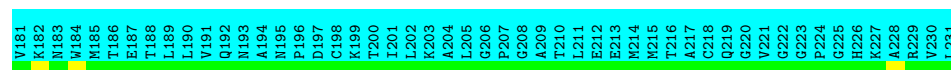


• Molecule 1: HIV-1 capsid protein

Chain RC:

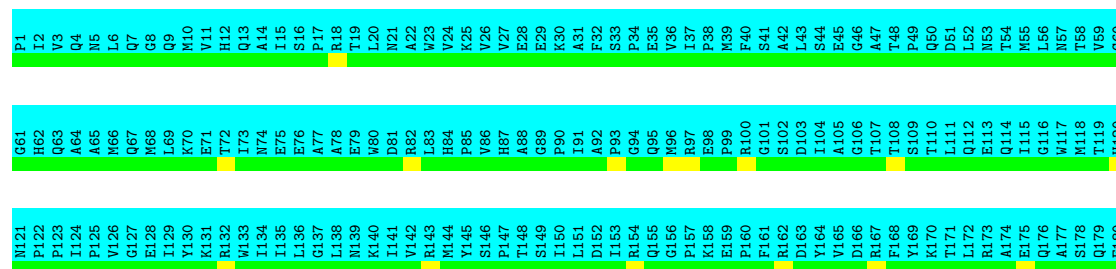
100%





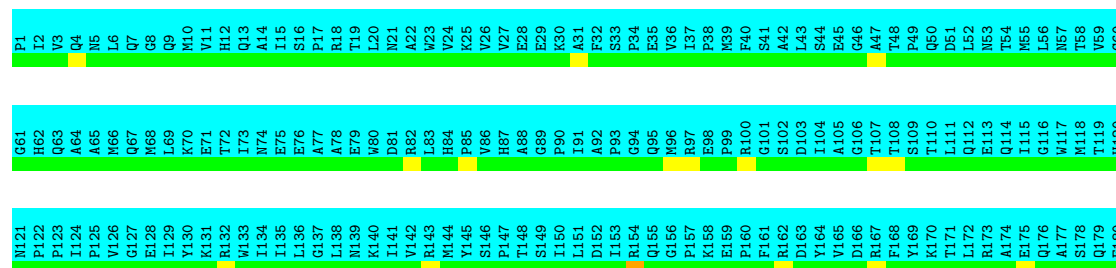
- Molecule 1: HIV-1 capsid protein

Chain SC: 100%



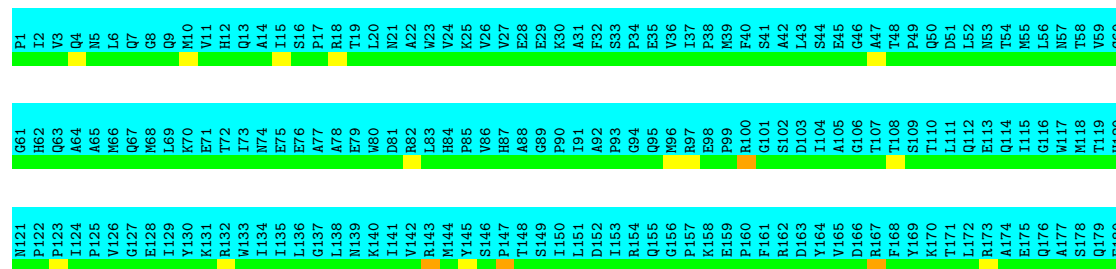
- Molecule 1: HIV-1 capsid protein

Chain TC: 100%



- Molecule 1: HIV-1 capsid protein

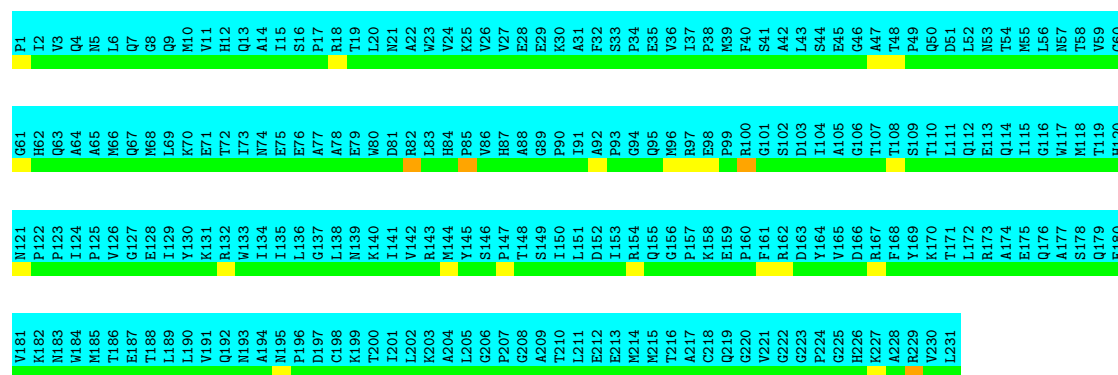
Chain UC: 100%



- Molecule 1: HIV-1 capsid protein

Chain VC:

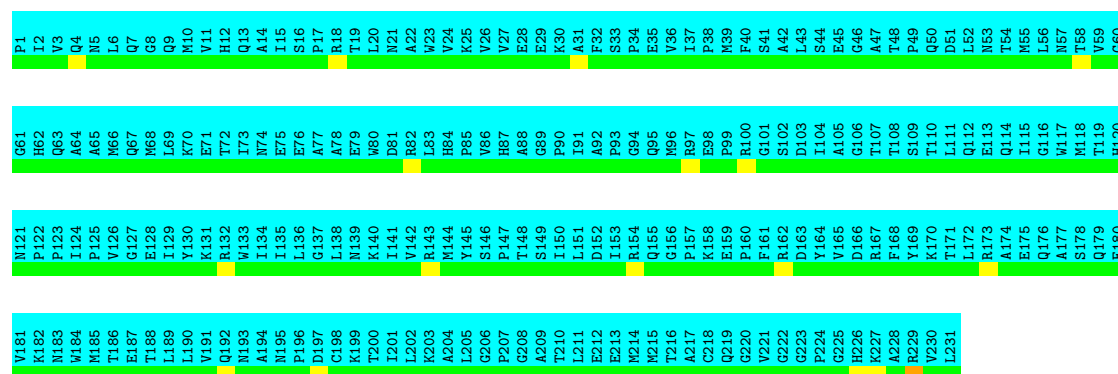
100%



- Molecule 1: HIV-1 capsid protein

Chain WC:

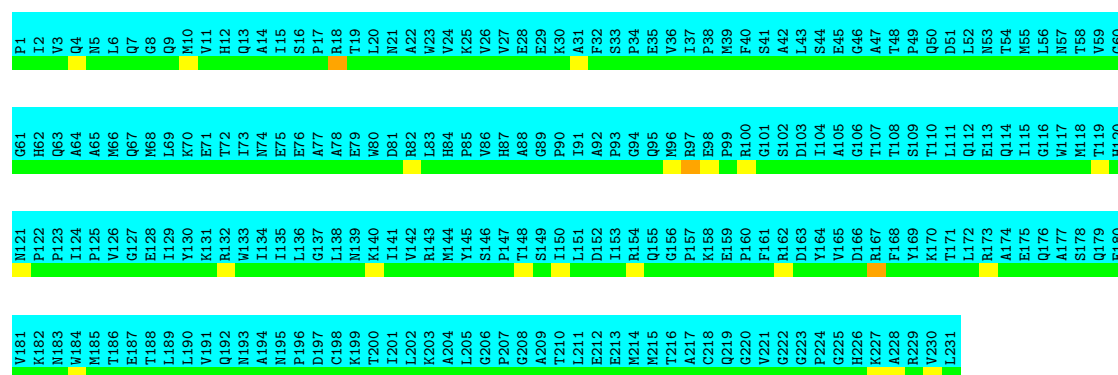
100%



- Molecule 1: HIV-1 capsid protein

Chain XC:

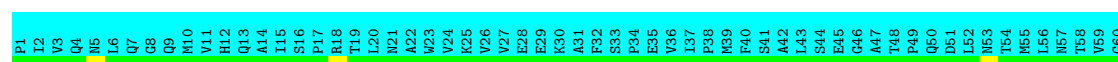
100%

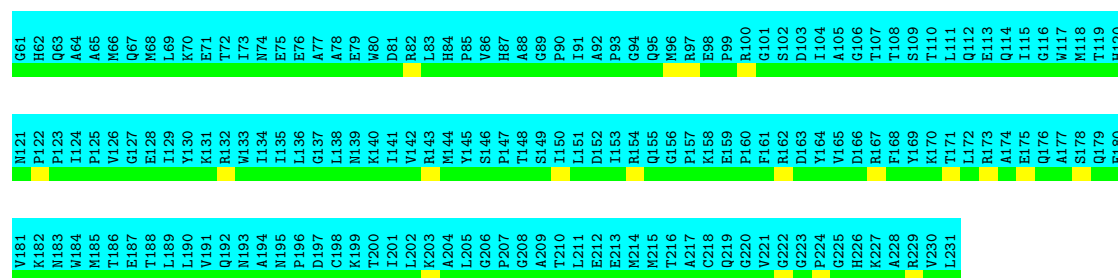


- Molecule 1: HIV-1 capsid protein

Chain YC:

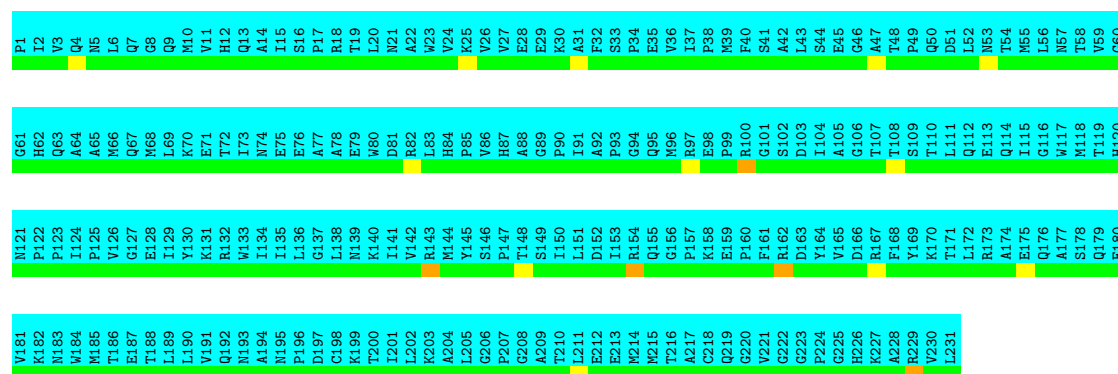
100%





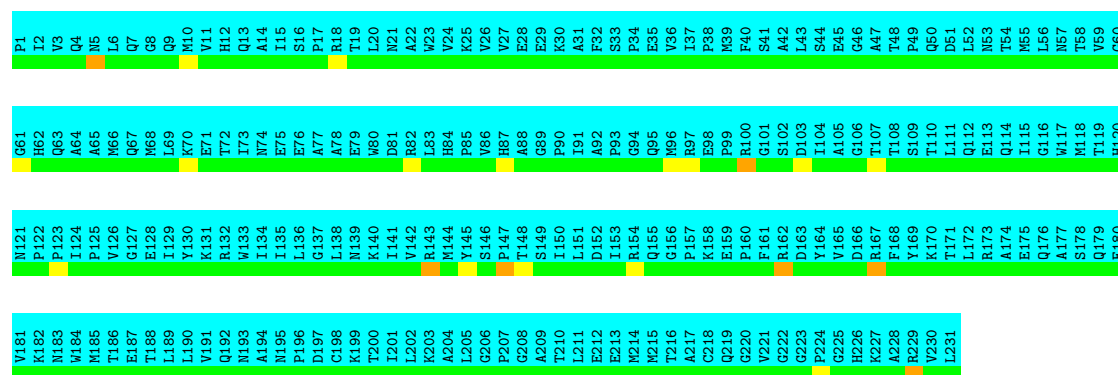
- Molecule 1: HIV-1 capsid protein

Chain ZC: 100%



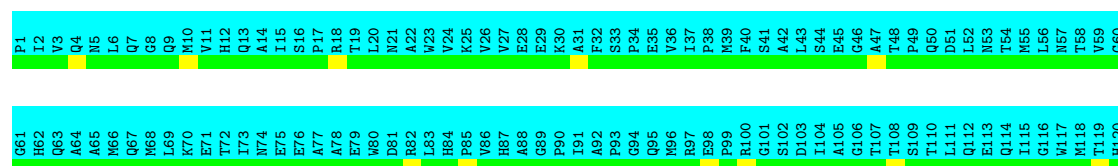
- Molecule 1: HIV-1 capsid protein

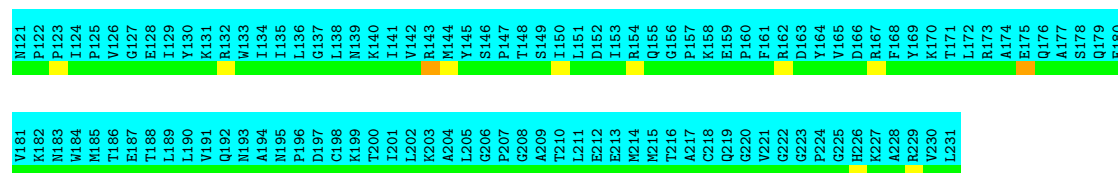
Chain aC: 100%



- Molecule 1: HIV-1 capsid protein

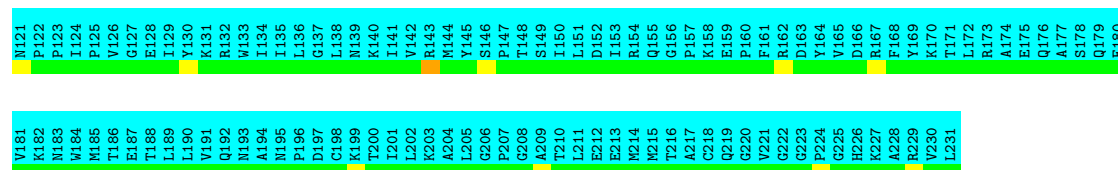
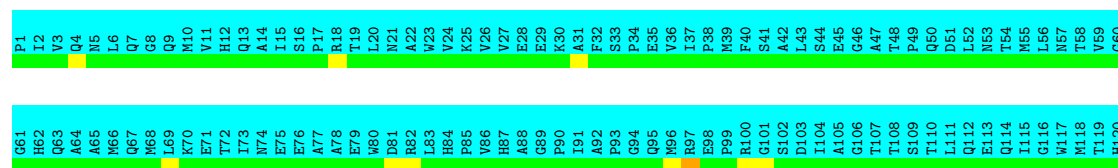
Chain bC: 100%





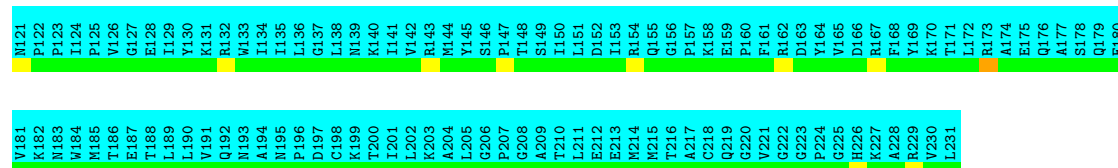
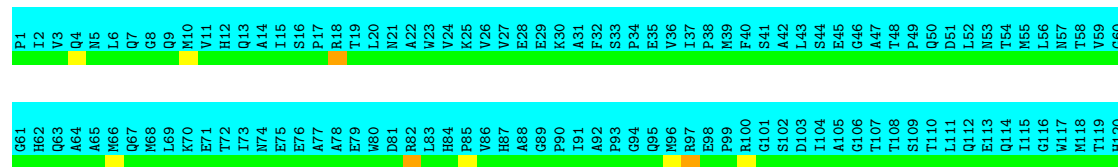
• Molecule 1: HIV-1 capsid protein

Chain cC: 100%



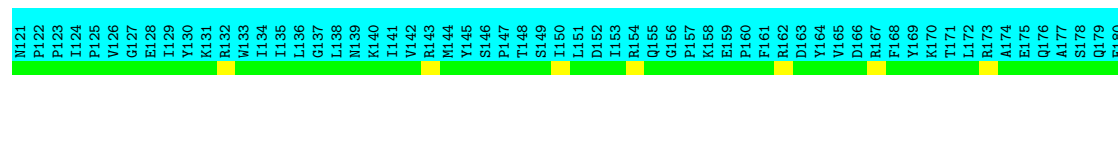
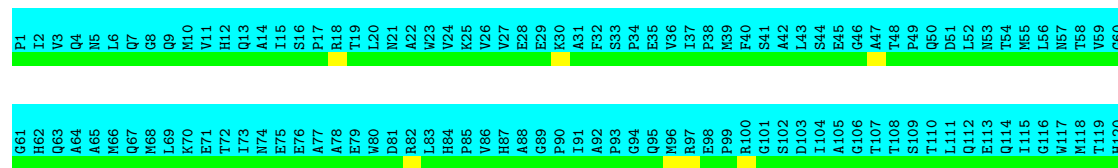
• Molecule 1: HIV-1 capsid protein

Chain dC: 100%



• Molecule 1: HIV-1 capsid protein

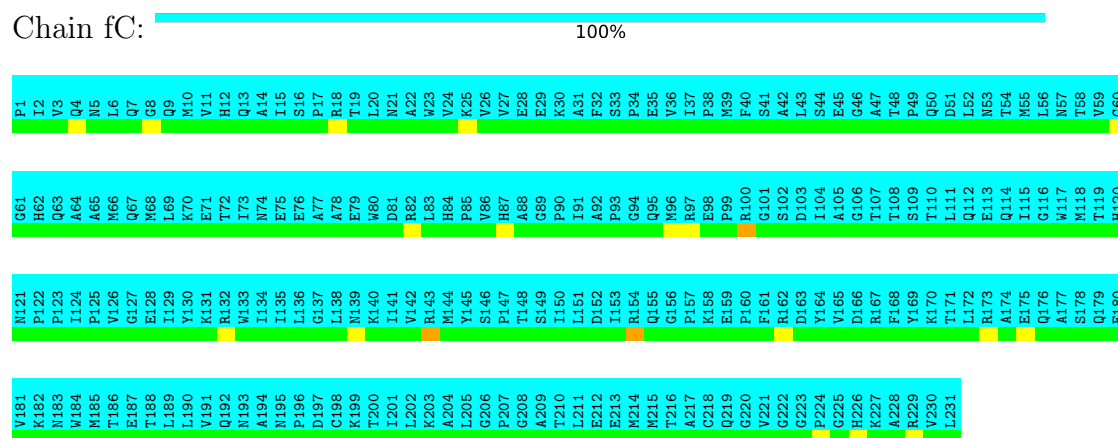
Chain eC: 100%





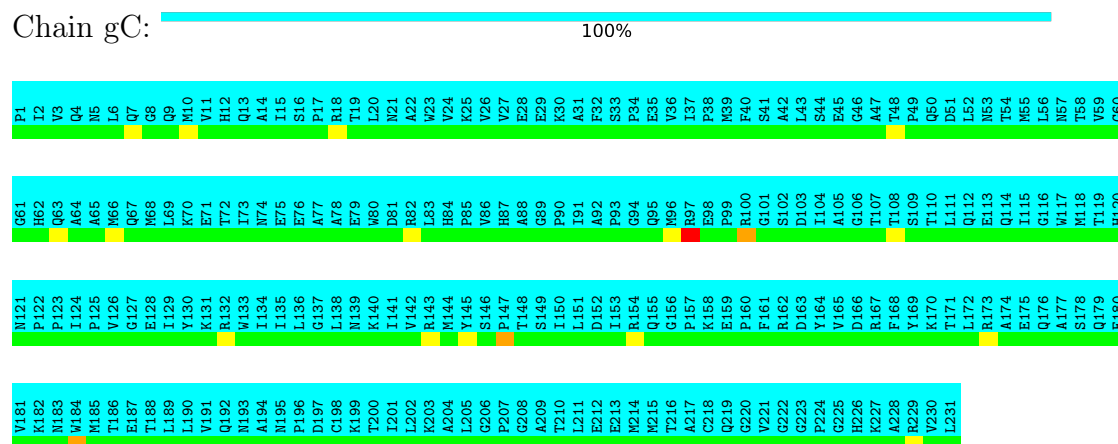
• Molecule 1: HIV-1 capsid protein

Chain fC:



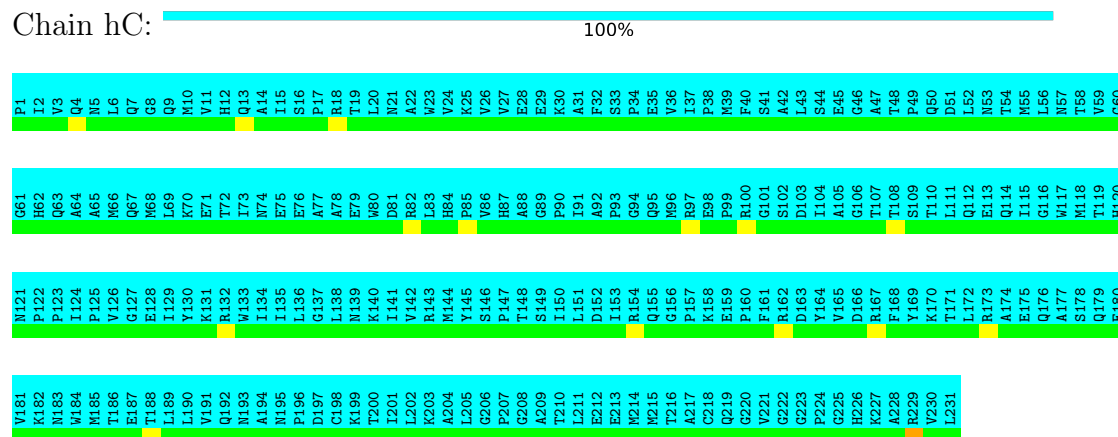
• Molecule 1: HIV-1 capsid protein

Chain gC:



• Molecule 1: HIV-1 capsid protein

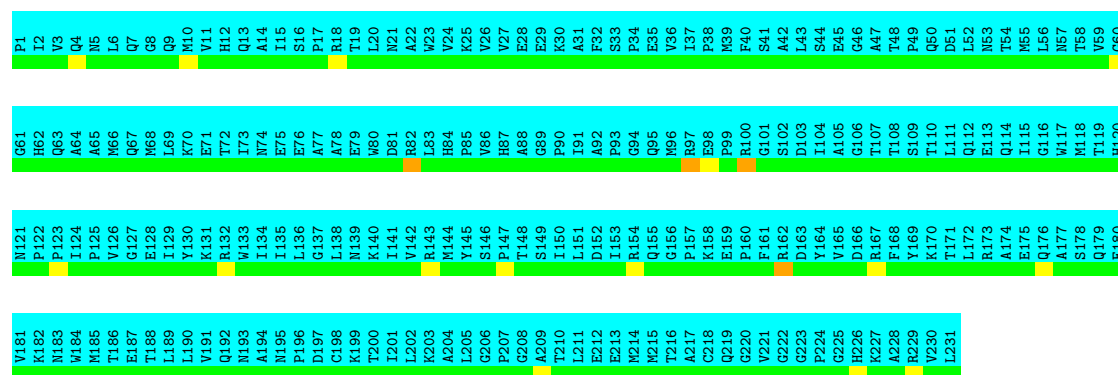
Chain hC:



• Molecule 1: HIV-1 capsid protein

Chain iC:

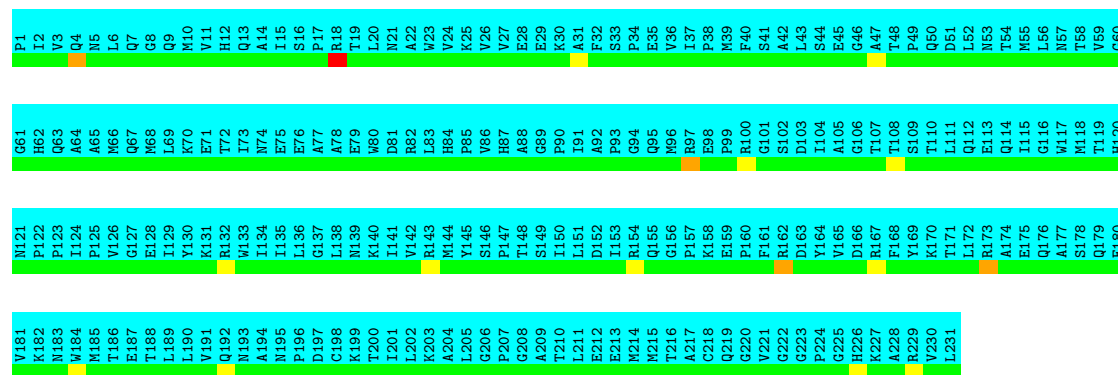
100%



- Molecule 1: HIV-1 capsid protein

Chain jC:

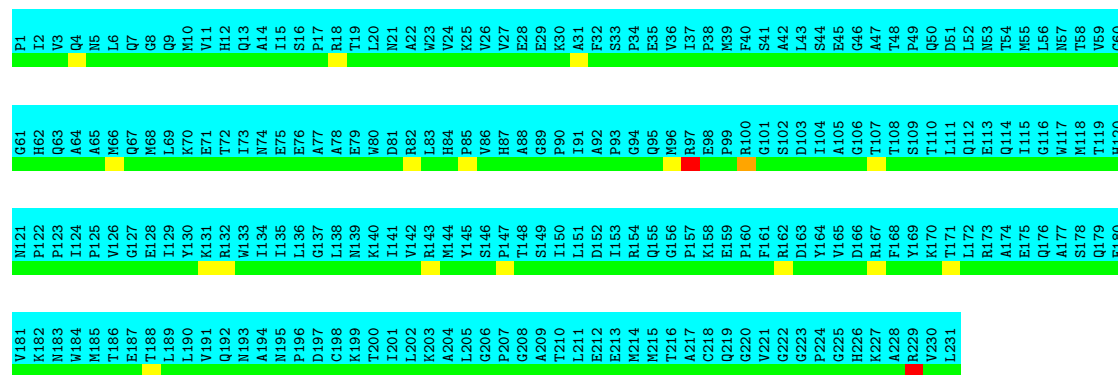
100%



- Molecule 1: HIV-1 capsid protein

Chain kC:

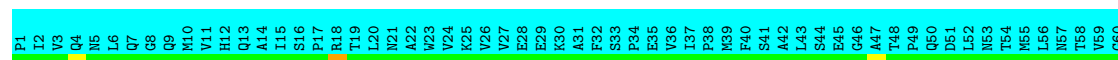
100%

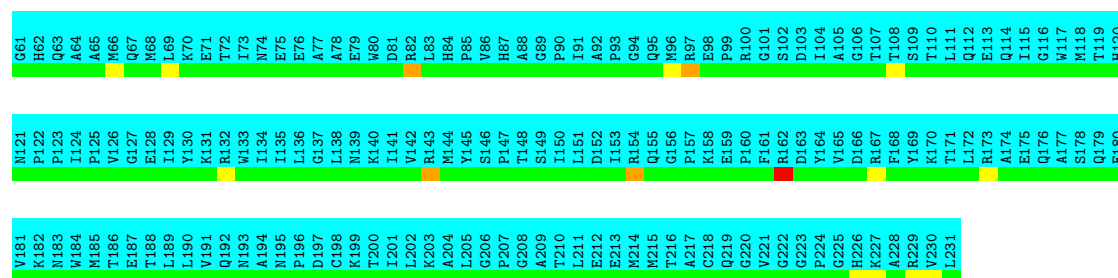


- Molecule 1: HIV-1 capsid protein

Chain lC:

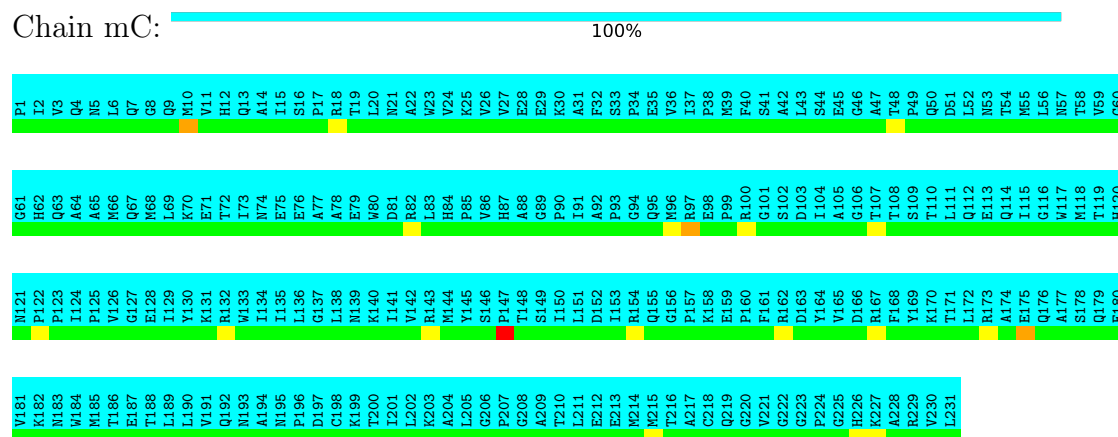
100%





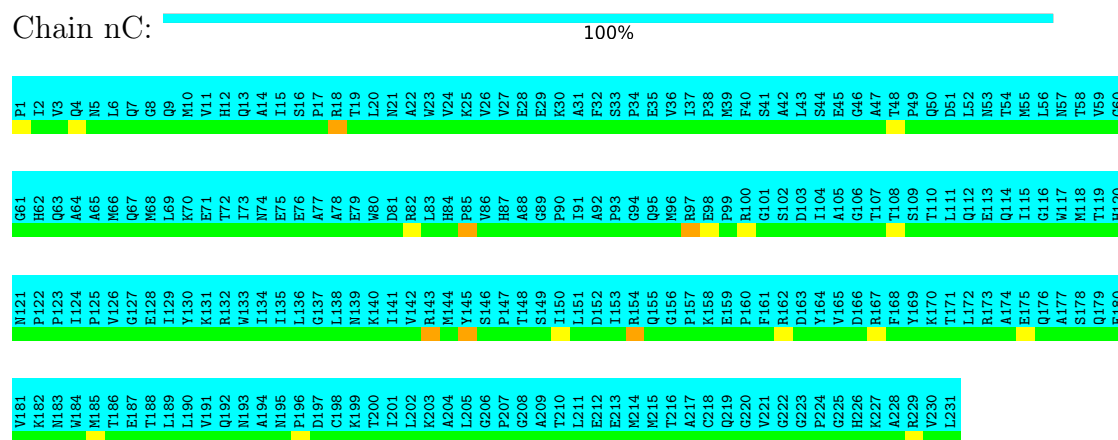
- Molecule 1: HIV-1 capsid protein

Chain mC:



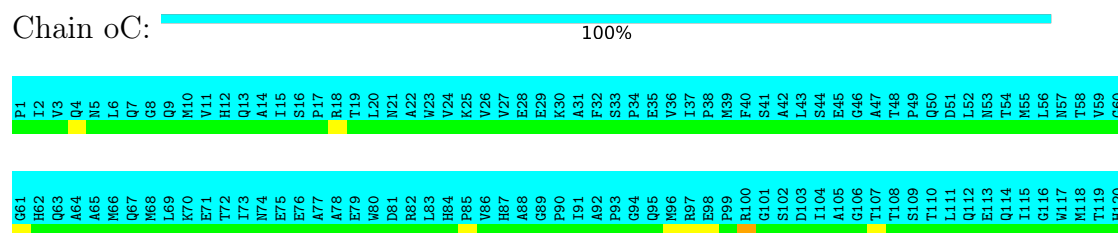
- Molecule 1: HIV-1 capsid protein

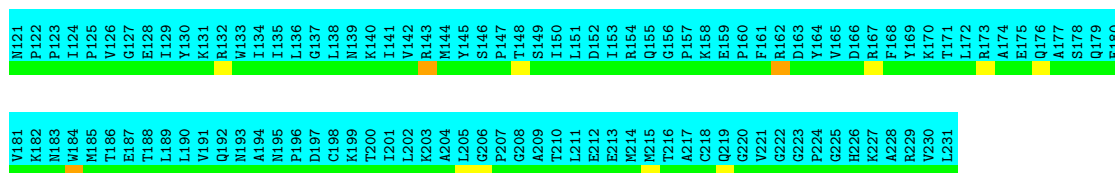
Chain nC:



- Molecule 1: HIV-1 capsid protein

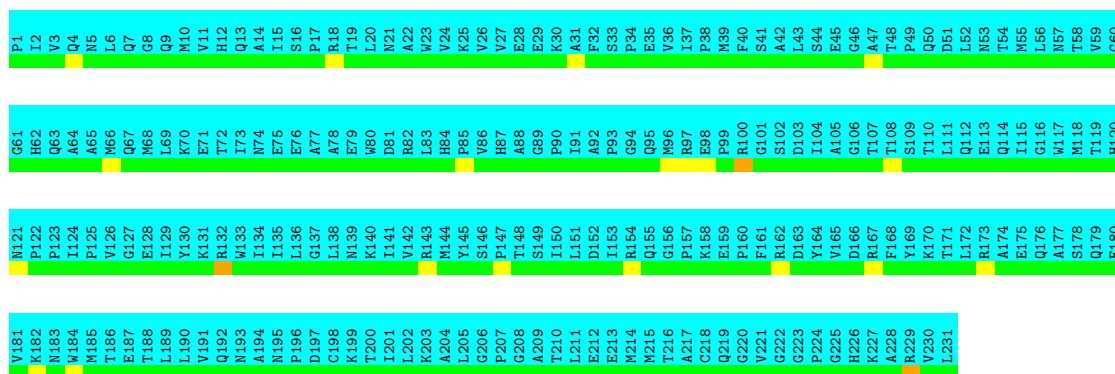
Chain oC:





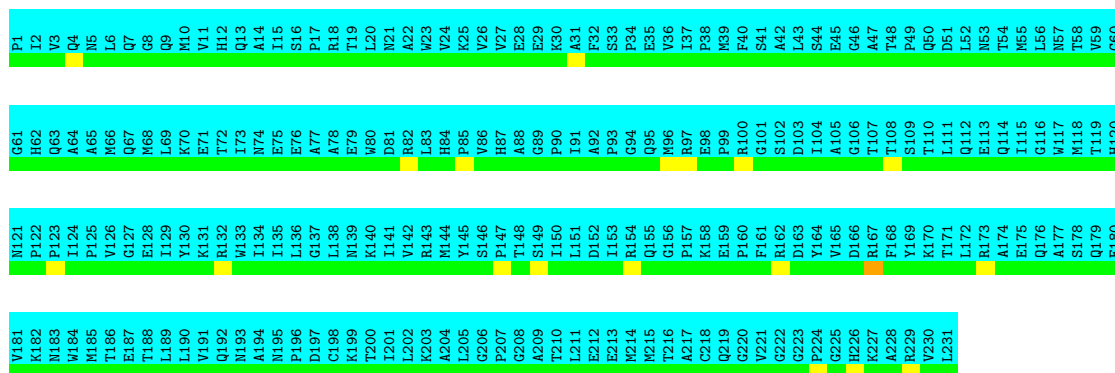
- Molecule 1: HIV-1 capsid protein

Chain pC:  100%



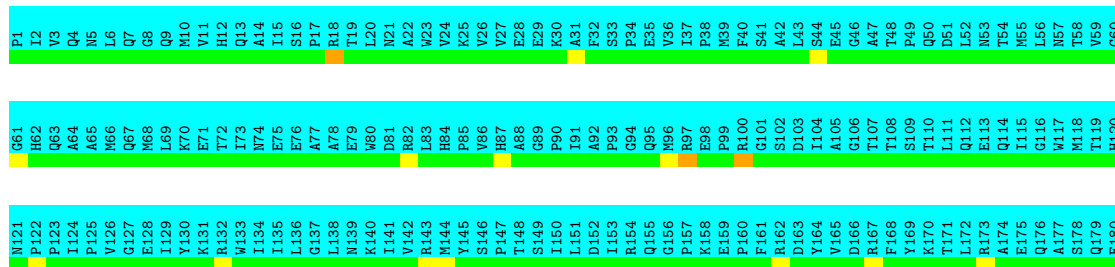
- Molecule 1: HIV-1 capsid protein

Chain qC:  100%



- Molecule 1: HIV-1 capsid protein

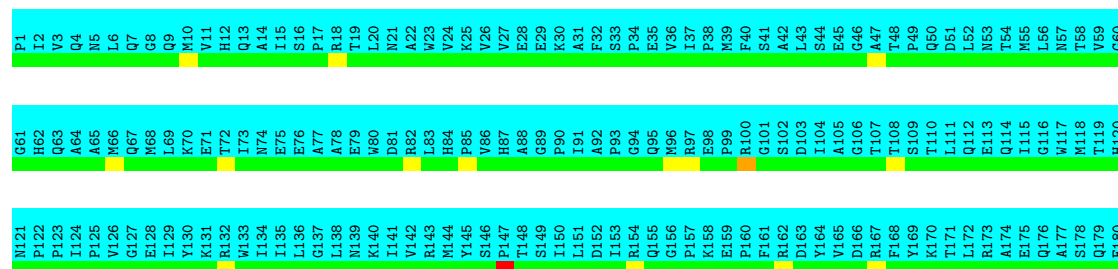
Chain rC:  100%





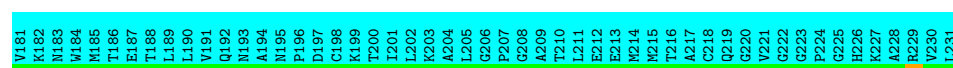
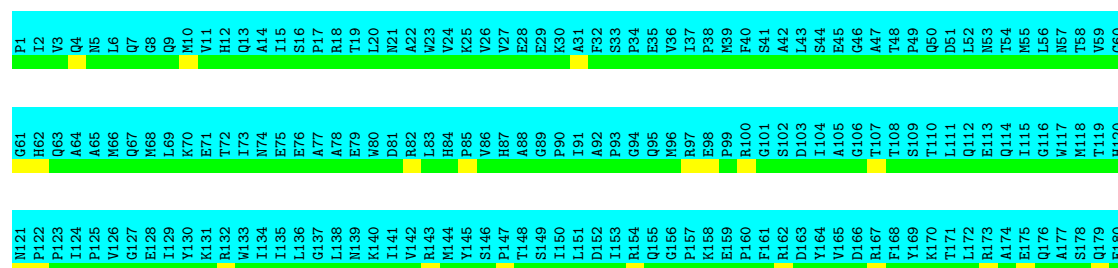
- Molecule 1: HIV-1 capsid protein

Chain sC: 100%



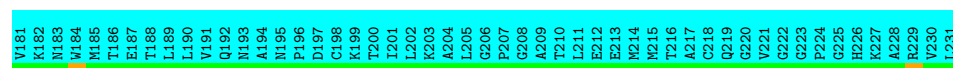
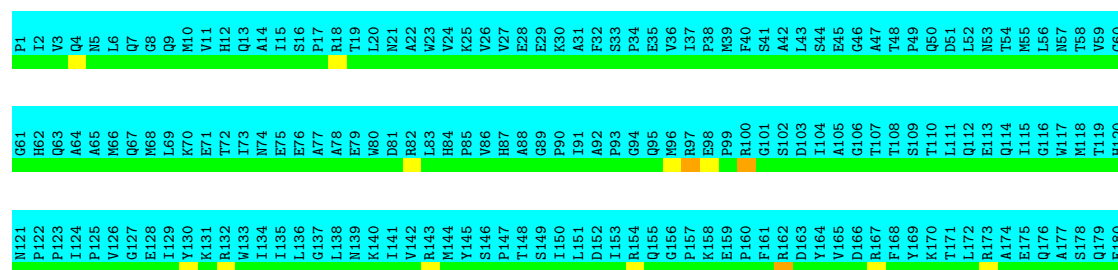
- Molecule 1: HIV-1 capsid protein

Chain tC: 100%



- Molecule 1: HIV-1 capsid protein

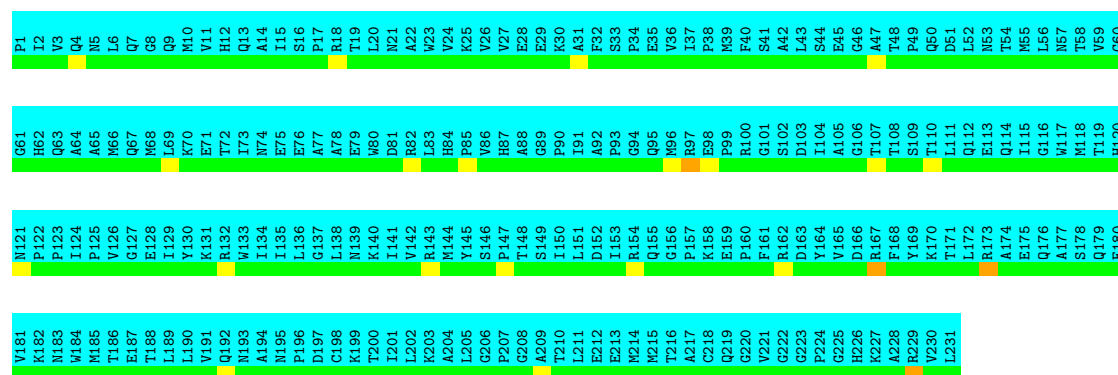
Chain uC: 100%



- Molecule 1: HIV-1 capsid protein

Chain vC:

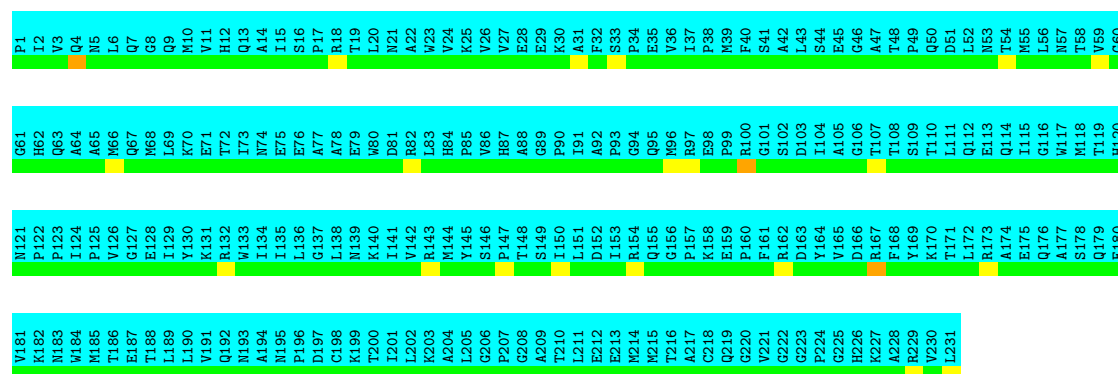
100%



• Molecule 1: HIV-1 capsid protein

Chain wC:

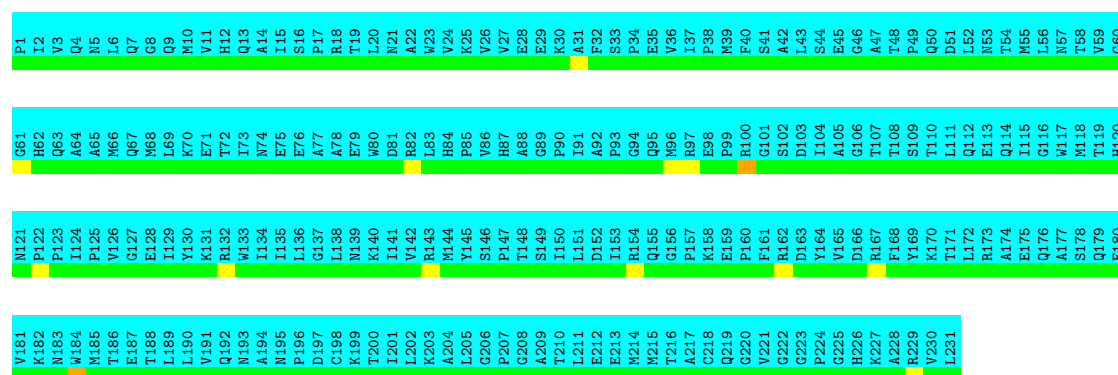
100%



• Molecule 1: HIV-1 capsid protein

Chain xC:

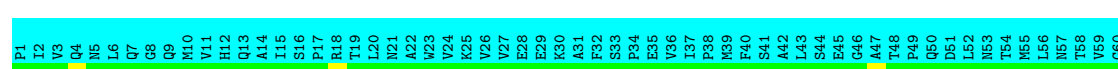
100%



• Molecule 1: HIV-1 capsid protein

Chain yC:

100%

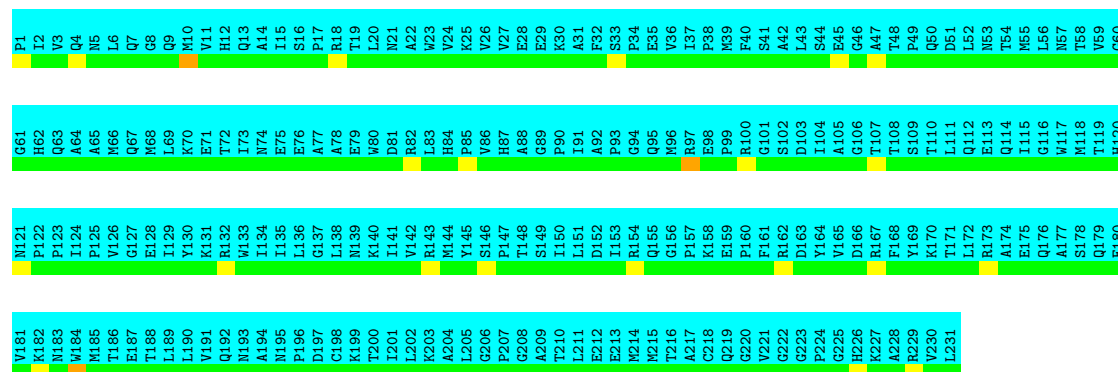




- Molecule 1: HIV-1 capsid protein

Chain zC:

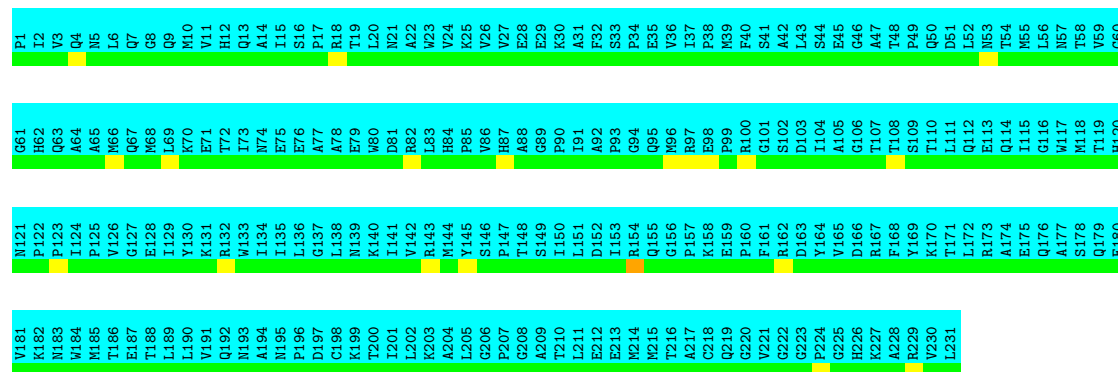
100%



- Molecule 1: HIV-1 capsid protein

Chain 0C:

100%

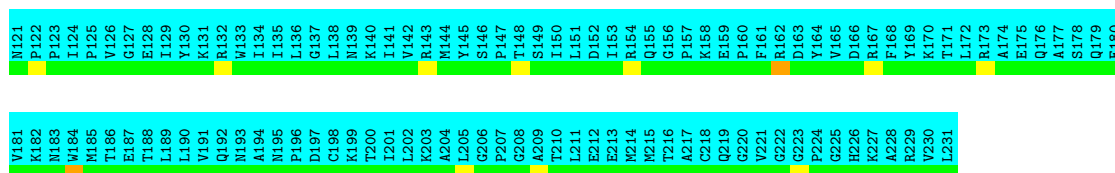


- Molecule 1: HIV-1 capsid protein

Chain 1C:

100%

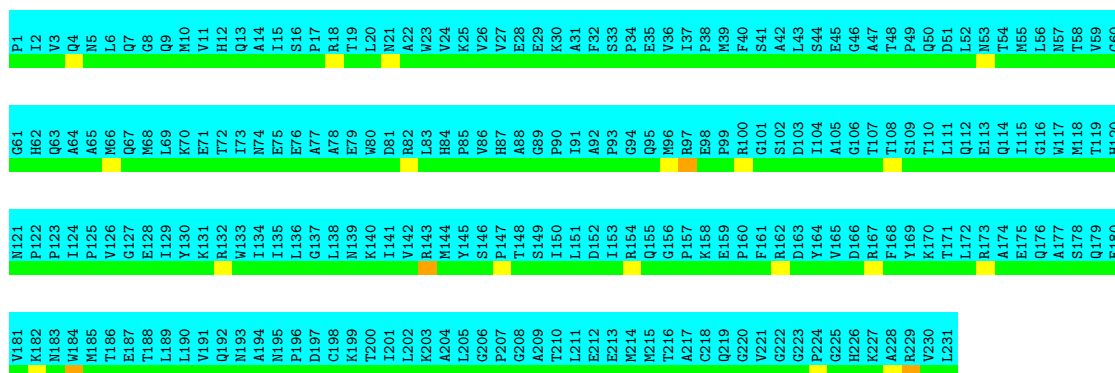




- Molecule 1: HIV-1 capsid protein

Chain 2C:

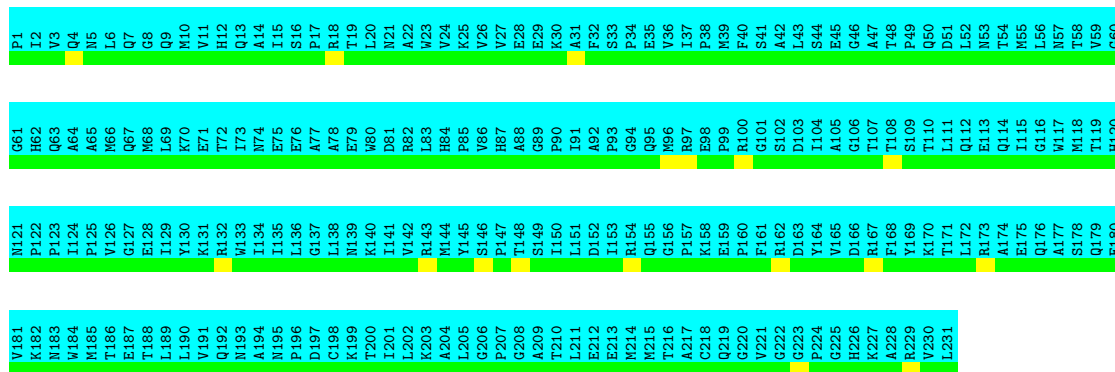
100%



- Molecule 1: HIV-1 capsid protein

Chain 3C:

100%

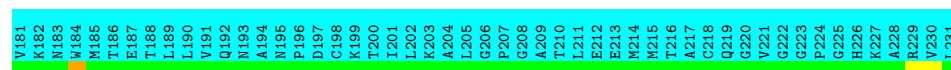


- Molecule 1: HIV-1 capsid protein

Chain 4C:

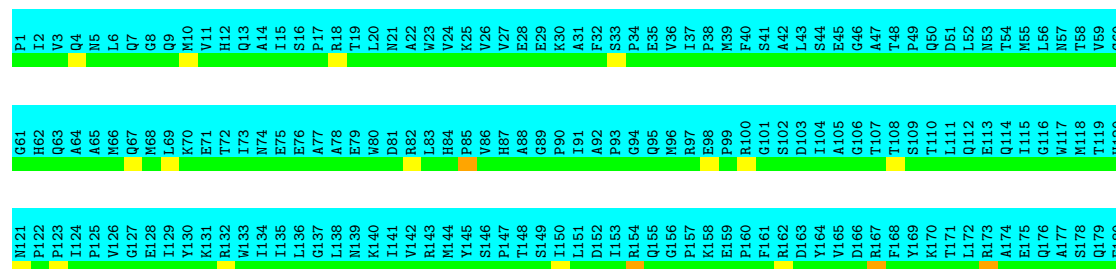
100%





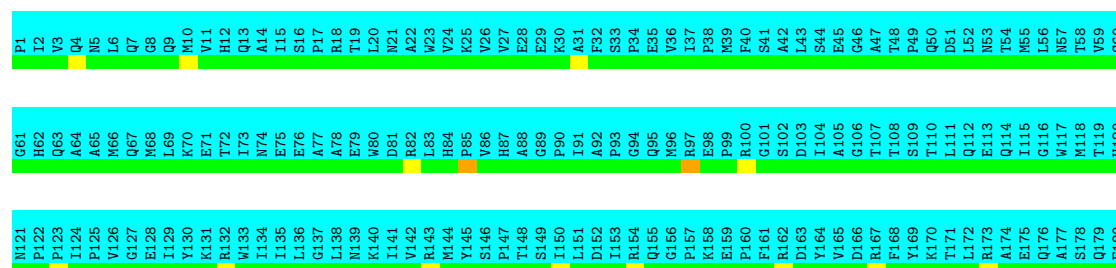
- Molecule 1: HIV-1 capsid protein

Chain 5C: 100%



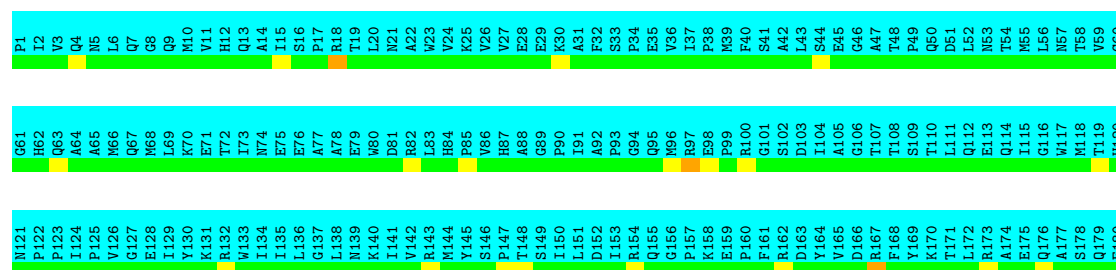
- Molecule 1: HIV-1 capsid protein

Chain 6C: 100%



- Molecule 1: HIV-1 capsid protein

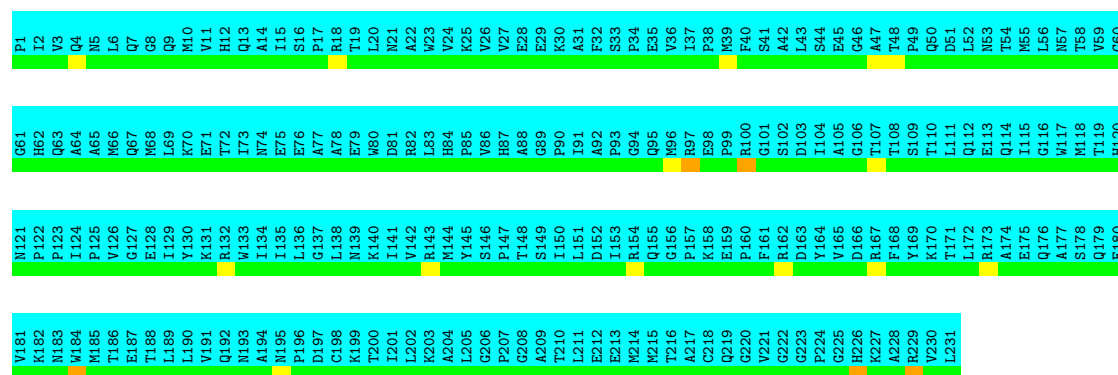
Chain 7C: 100%



- Molecule 1: HIV-1 capsid protein

Chain 8C:

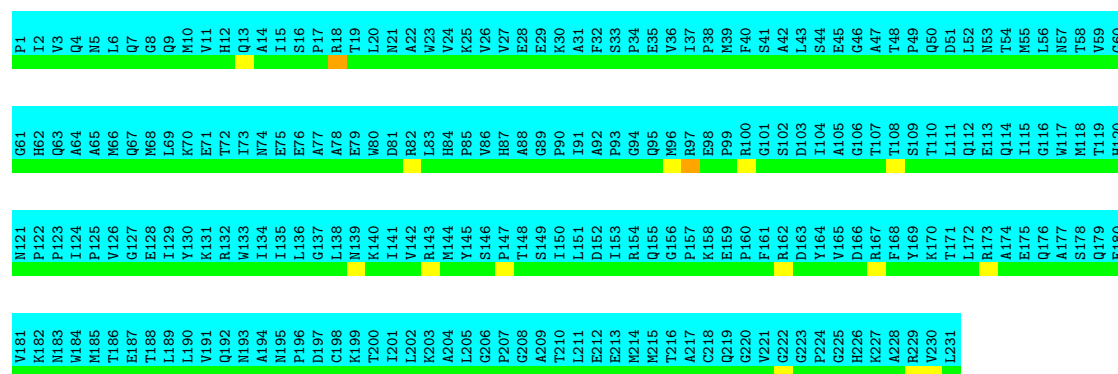
100%



- Molecule 1: HIV-1 capsid protein

Chain 9C:

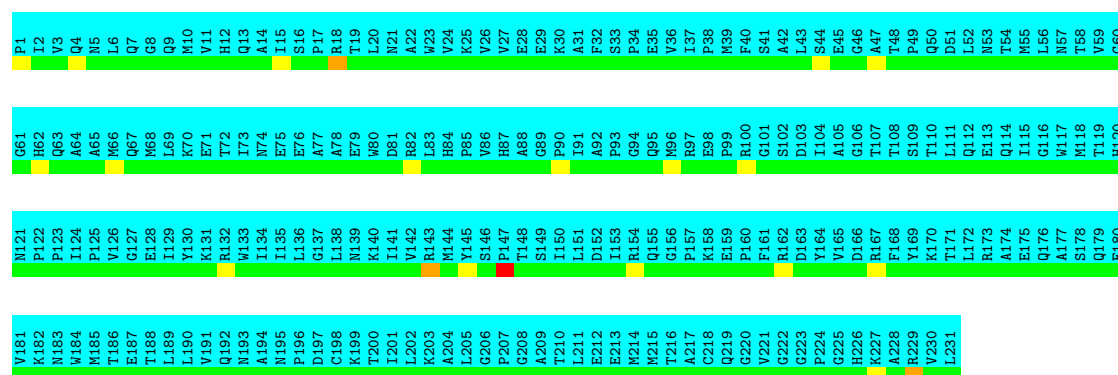
100%



- Molecule 1: HIV-1 capsid protein

Chain AD:

100%

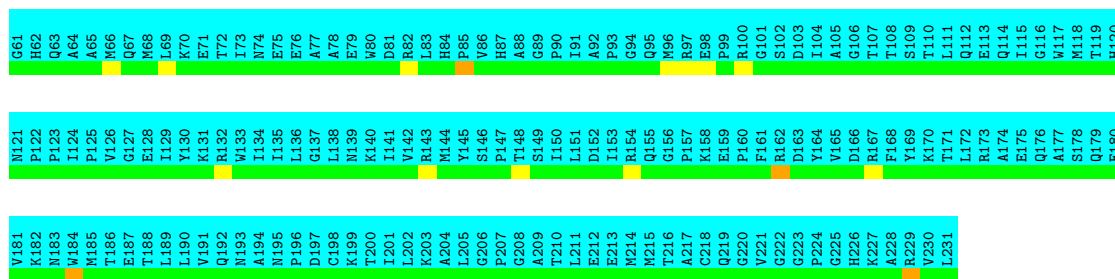


- Molecule 1: HIV-1 capsid protein

Chain BD:

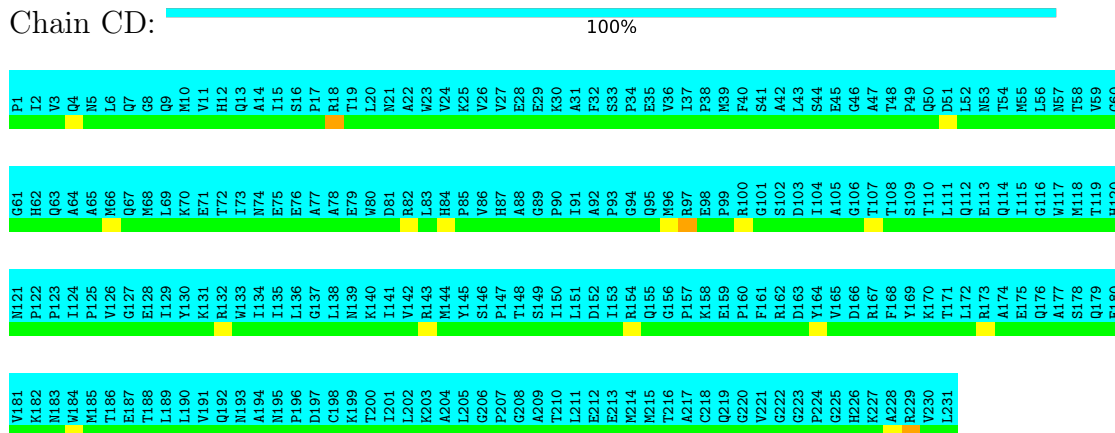
100%





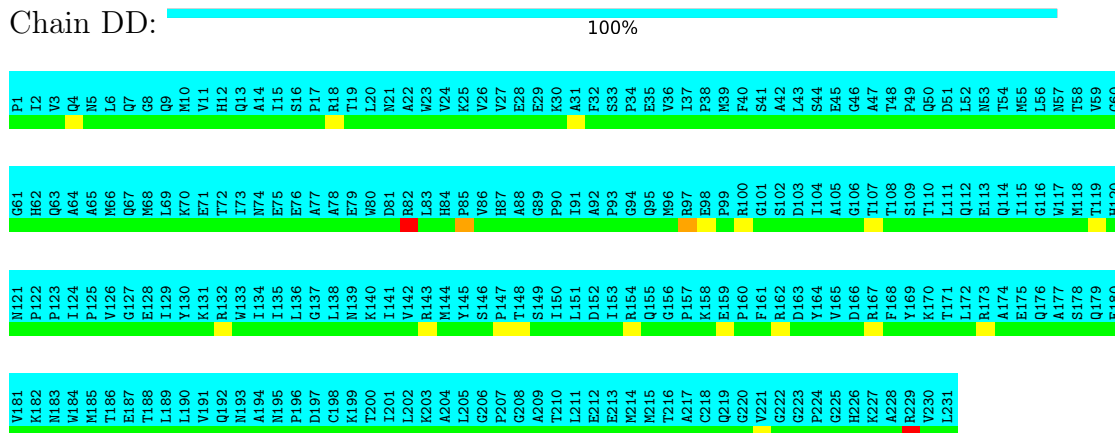
• Molecule 1: HIV-1 capsid protein

Chain CD:



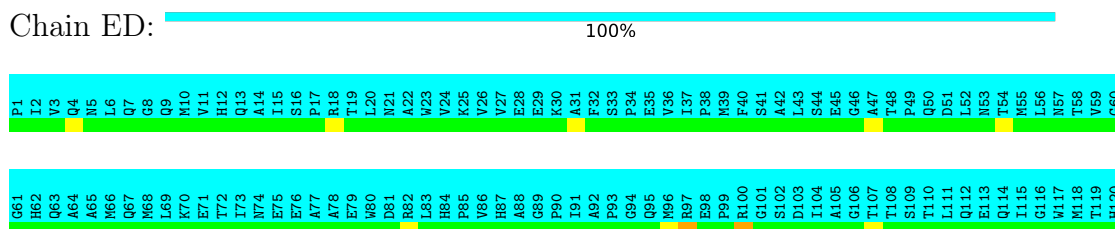
• Molecule 1: HIV-1 capsid protein

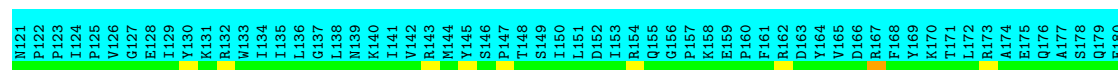
Chain DD:



• Molecule 1: HIV-1 capsid protein

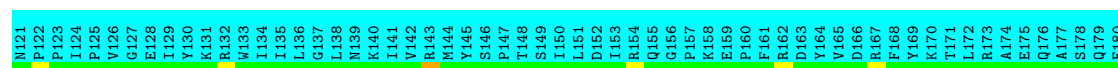
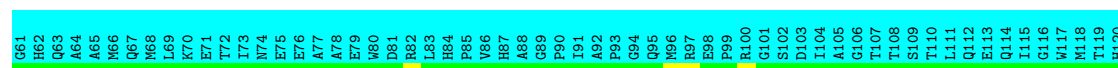
Chain ED:





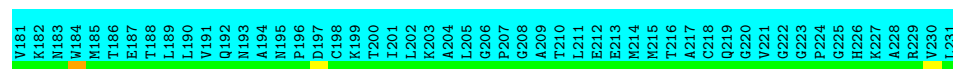
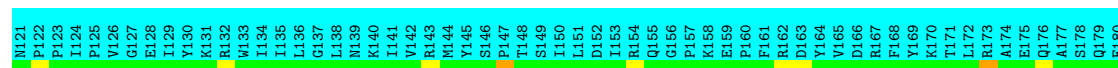
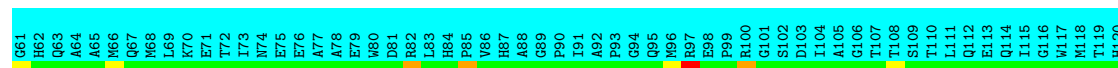
• Molecule 1: HIV-1 capsid protein

Chain FD:  100%



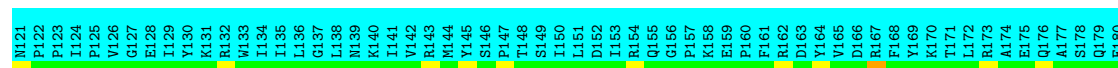
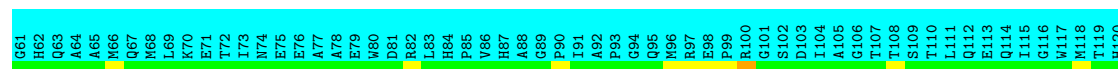
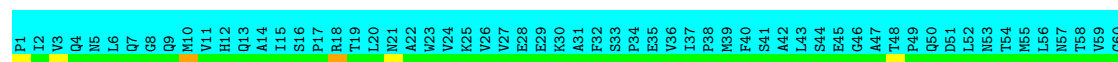
• Molecule 1: HIV-1 capsid protein

Chain GD:  100%



• Molecule 1: HIV-1 capsid protein

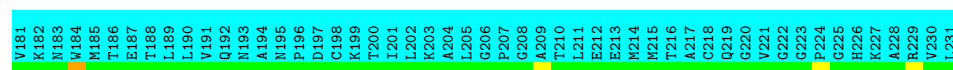
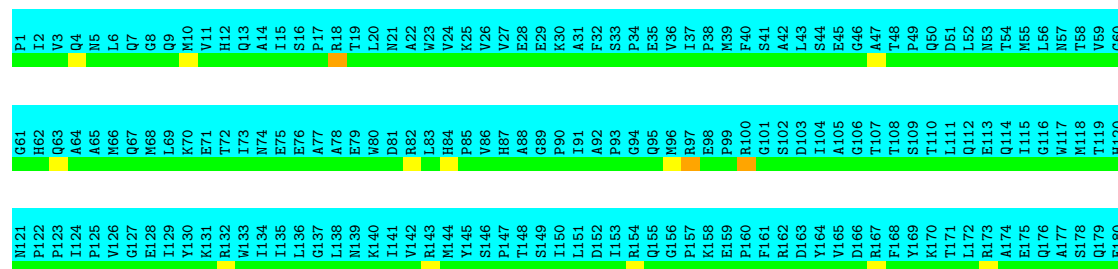
Chain HD:  100%





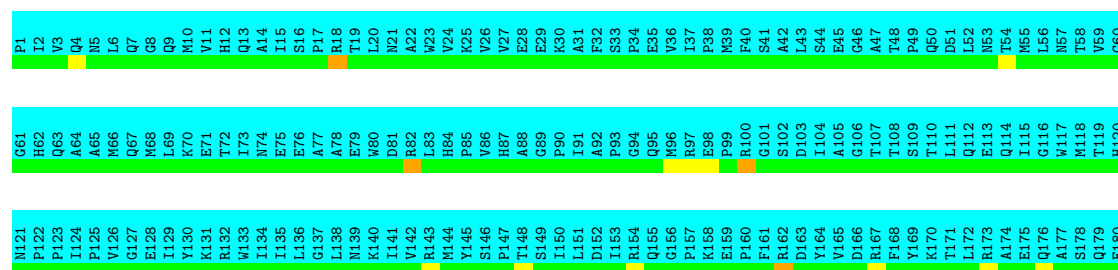
- Molecule 1: HIV-1 capsid protein

Chain ID:  100%



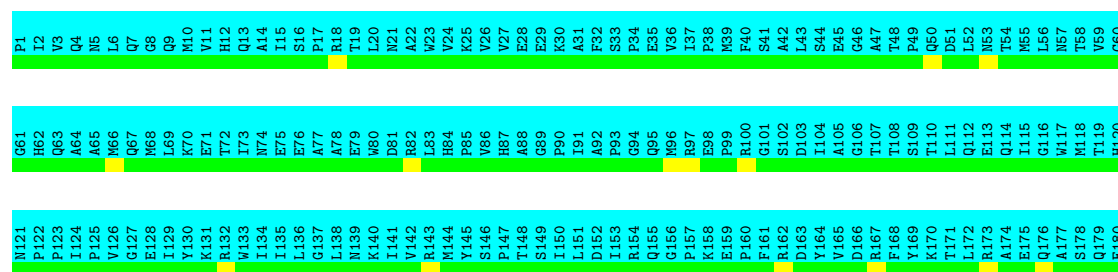
- Molecule 1: HIV-1 capsid protein

Chain JD:  100%



- Molecule 1: HIV-1 capsid protein

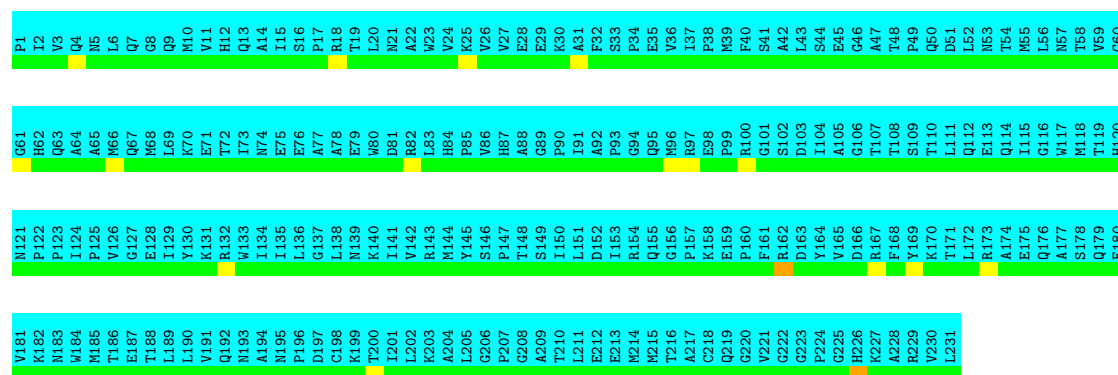
Chain KD:  100%



- Molecule 1: HIV-1 capsid protein

Chain LD:

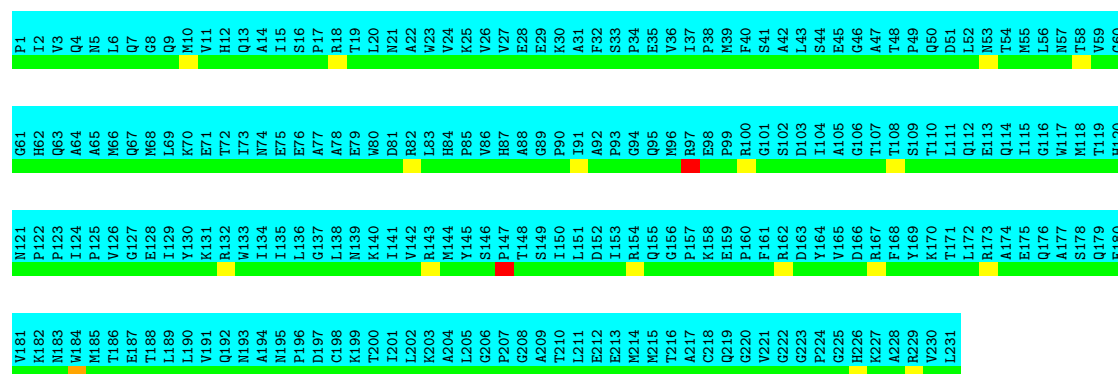
100%



- Molecule 1: HIV-1 capsid protein

Chain MD:

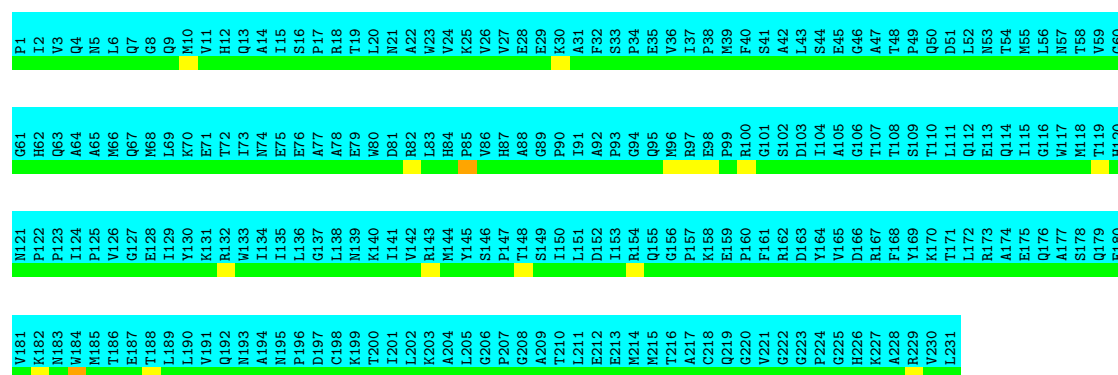
100%



- Molecule 1: HIV-1 capsid protein

Chain ND:

100%

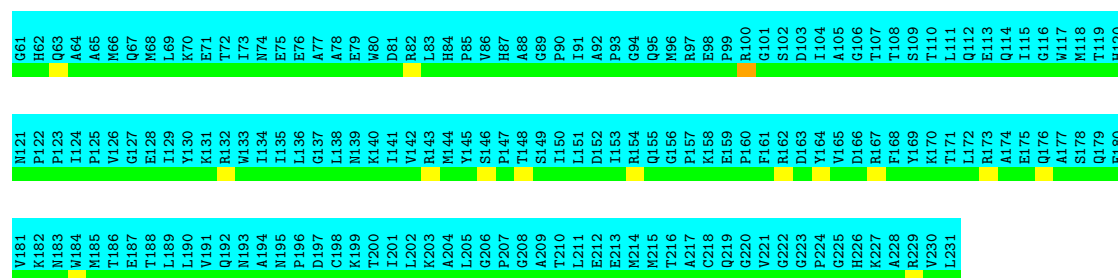


- Molecule 1: HIV-1 capsid protein

Chain OD:

100%

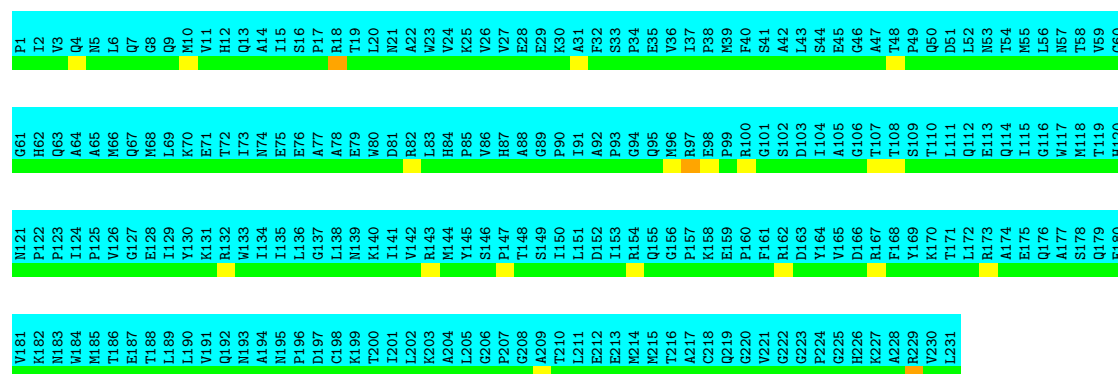




- Molecule 1: HIV-1 capsid protein

Chain PD:

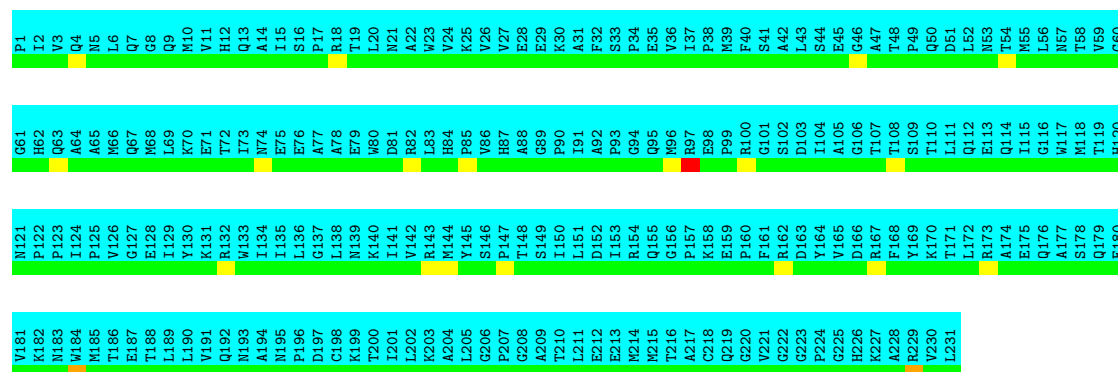
100%



- Molecule 1: HIV-1 capsid protein

Chain QD:

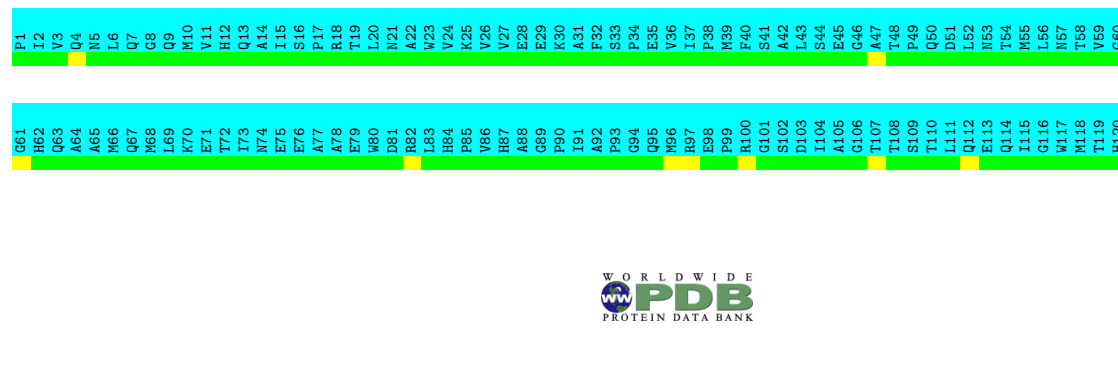
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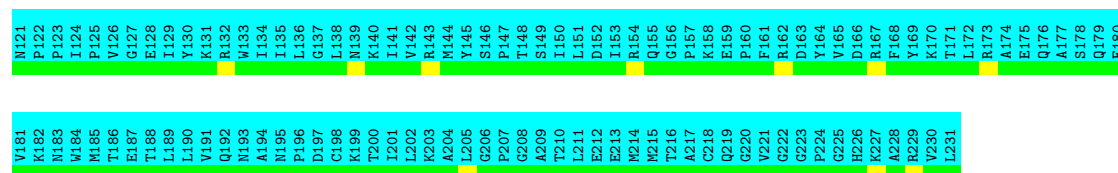


- Molecule 1: HIV-1 capsid protein

Chain RD:

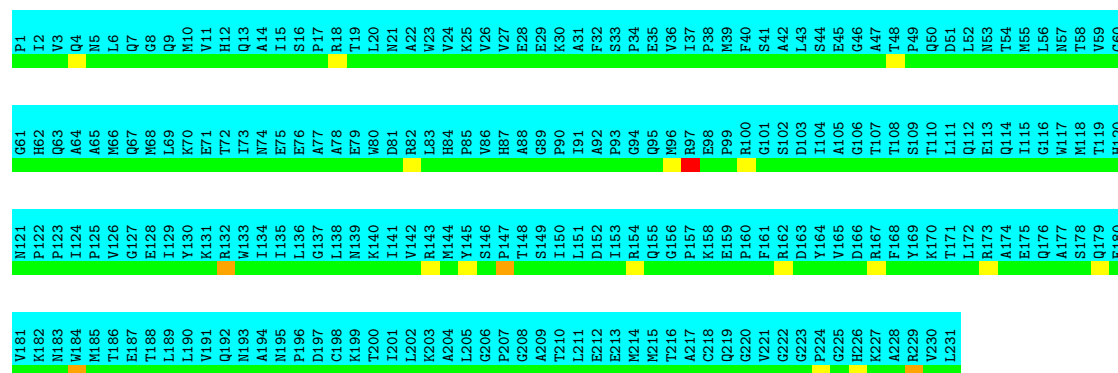
100%





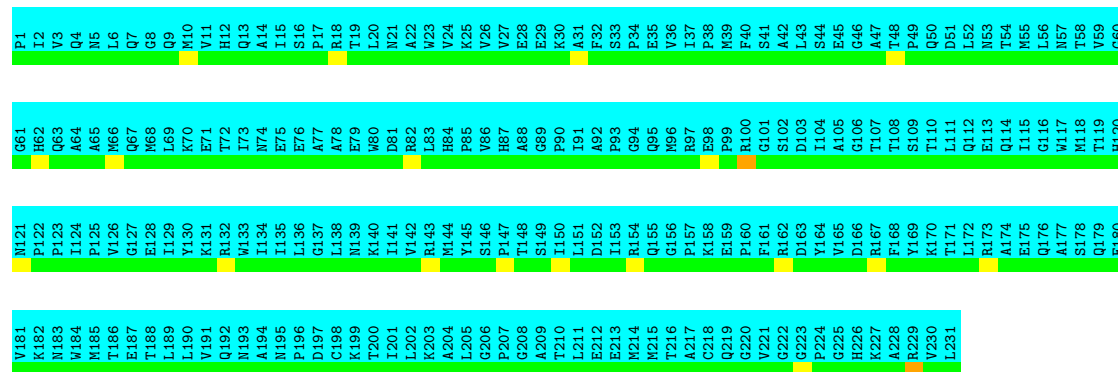
• Molecule 1: HIV-1 capsid protein

Chain SD:



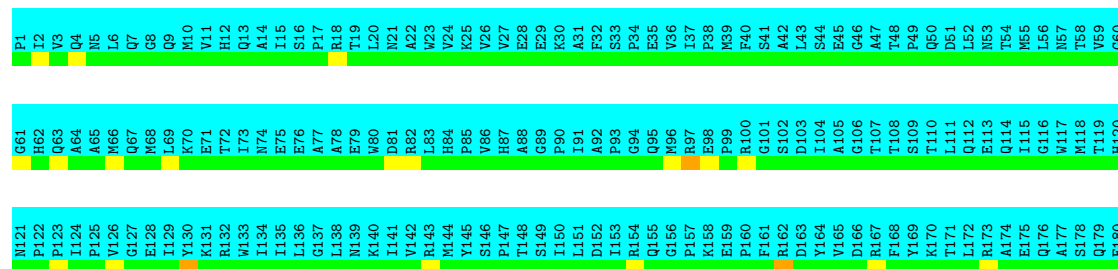
• Molecule 1: HIV-1 capsid protein

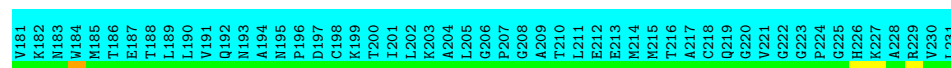
Chain TD:



• Molecule 1: HIV-1 capsid protein

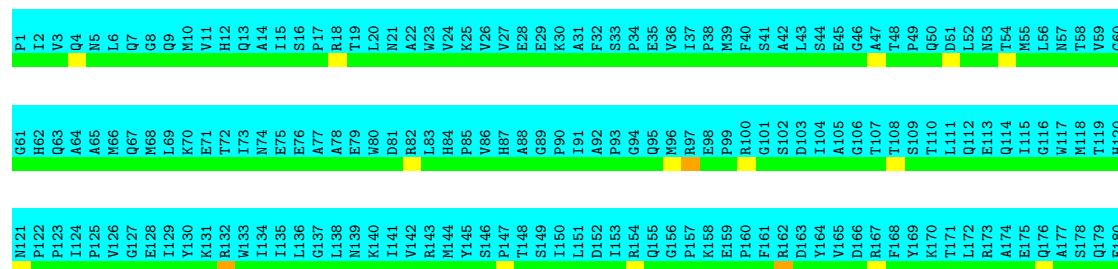
Chain UD:





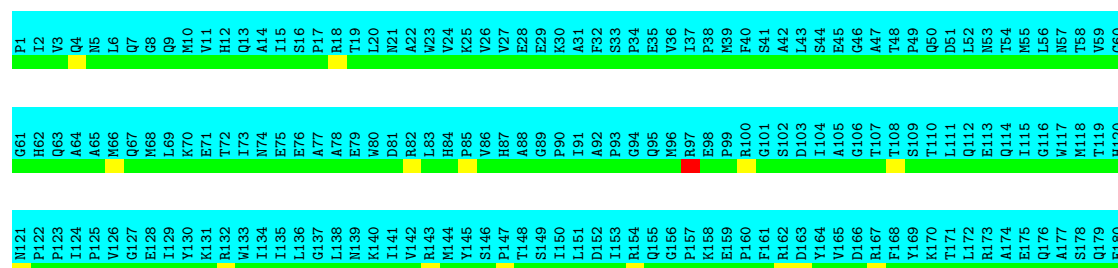
- Molecule 1: HIV-1 capsid protein

Chain VD: 100%



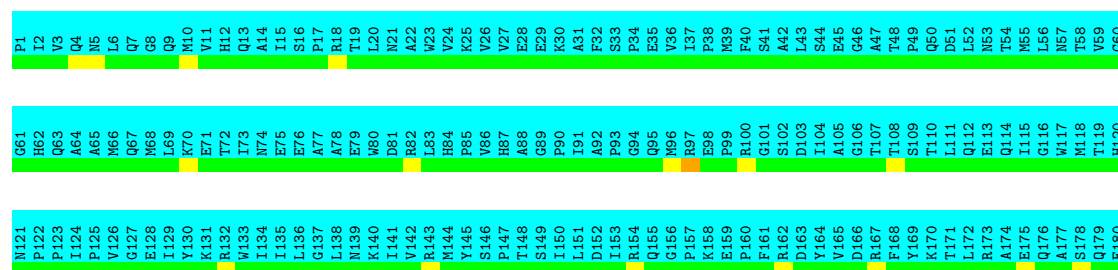
- Molecule 1: HIV-1 capsid protein

Chain WD: 100%



- Molecule 1: HIV-1 capsid protein

Chain XD: 100%



- Molecule 1: HIV-1 capsid protein

Chain YD:

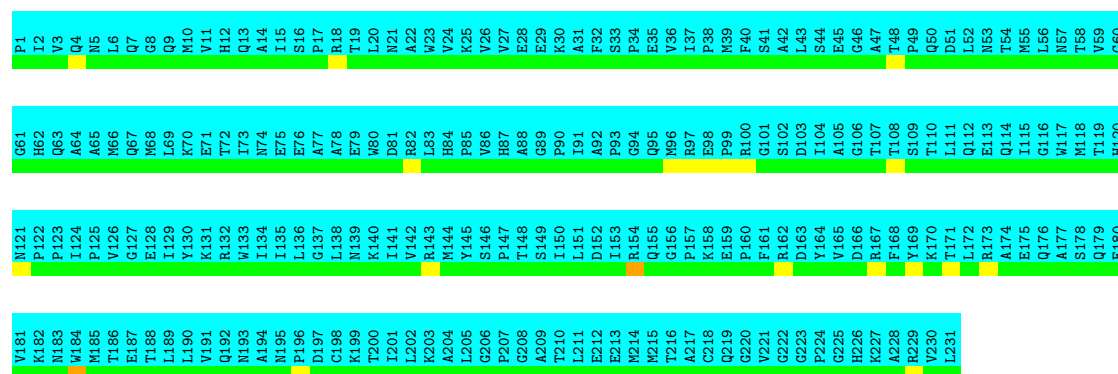
100%



- Molecule 1: HIV-1 capsid protein

Chain ZD:

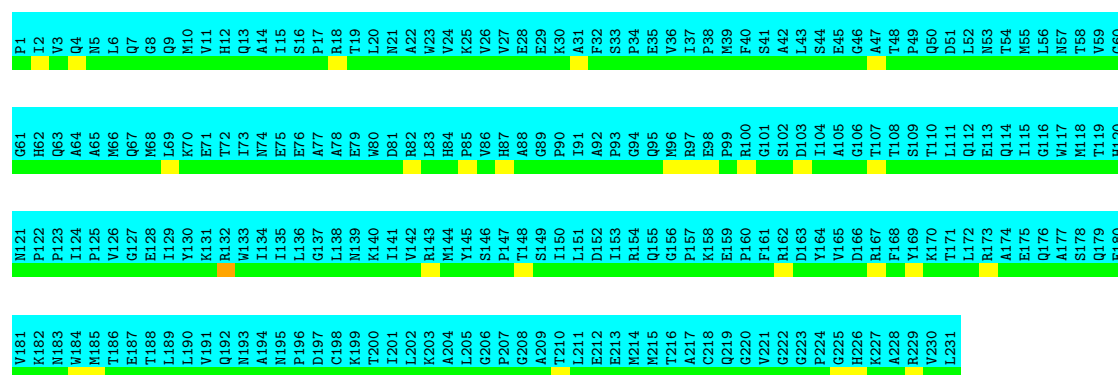
100%



- Molecule 1: HIV-1 capsid protein

Chain aD:

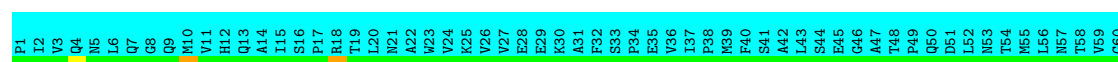
100%

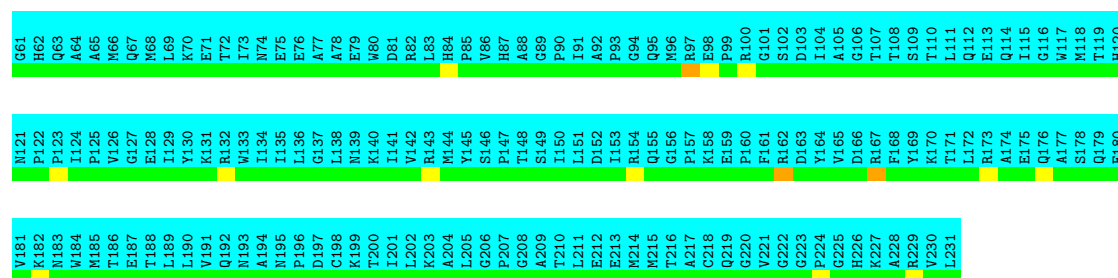


- Molecule 1: HIV-1 capsid protein

Chain bD:

100%

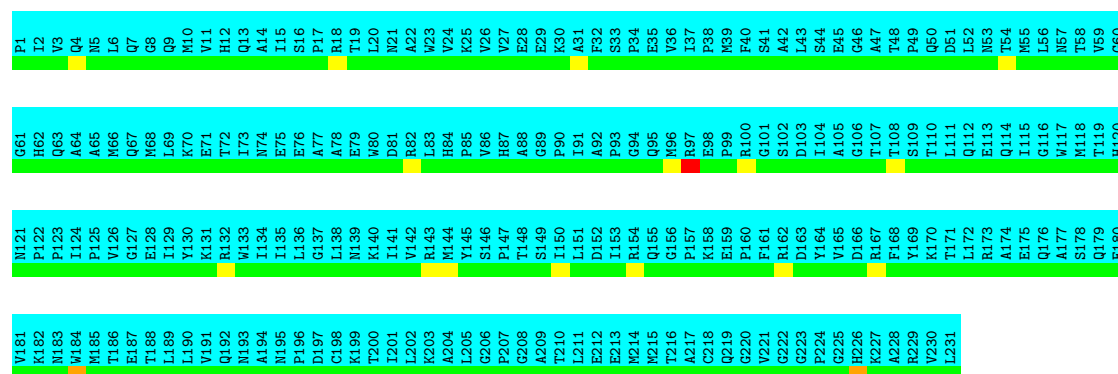




- Molecule 1: HIV-1 capsid protein

Chain cD:

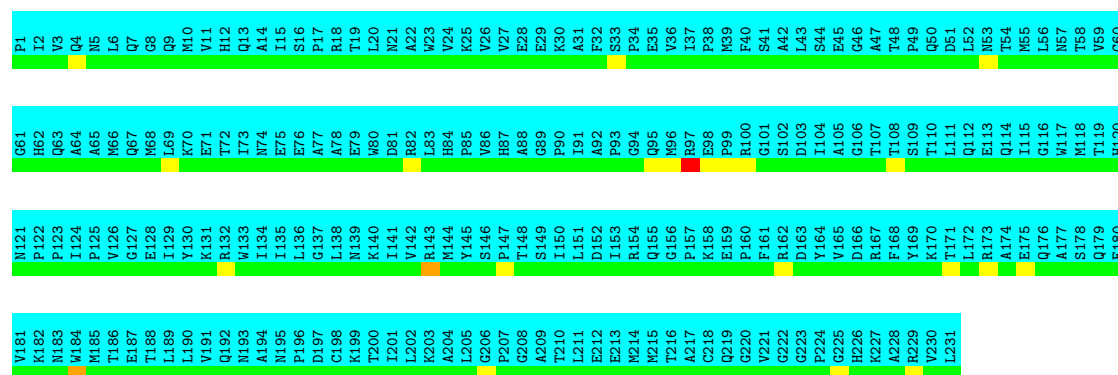
100%



- Molecule 1: HIV-1 capsid protein

Chain dD:

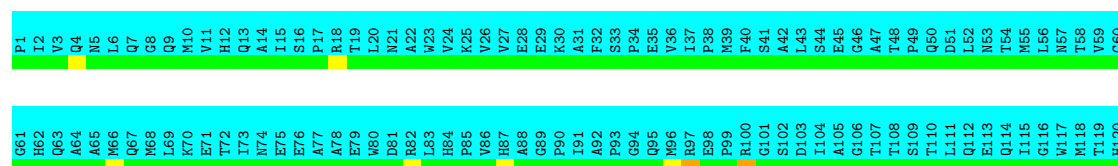
100%

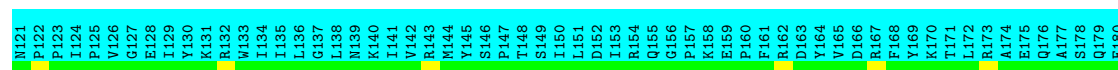


- Molecule 1: HIV-1 capsid protein

Chain eD:

100%

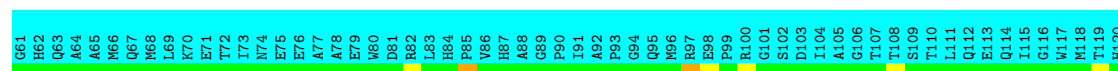
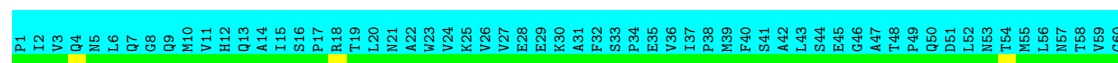




• Molecule 1: HIV-1 capsid protein

Chain fD:

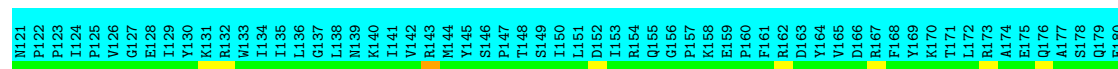
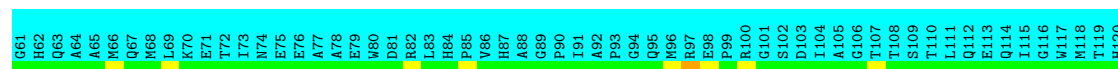
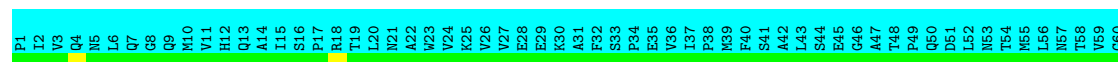
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• Molecule 1: HIV-1 capsid protein

Chain gD:

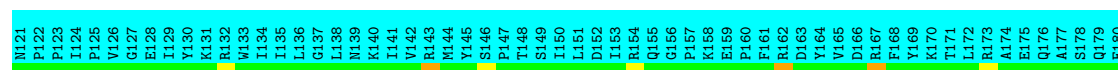
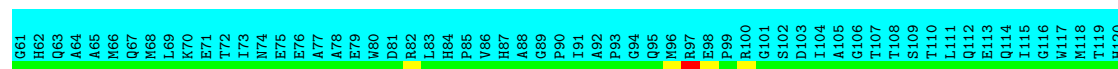
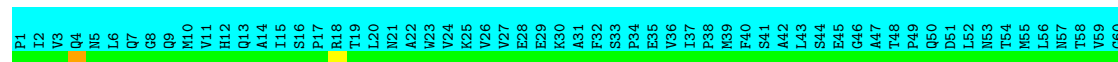
100%



• Molecule 1: HIV-1 capsid protein

Chain hD:

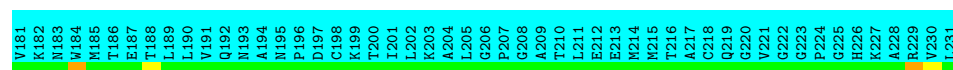
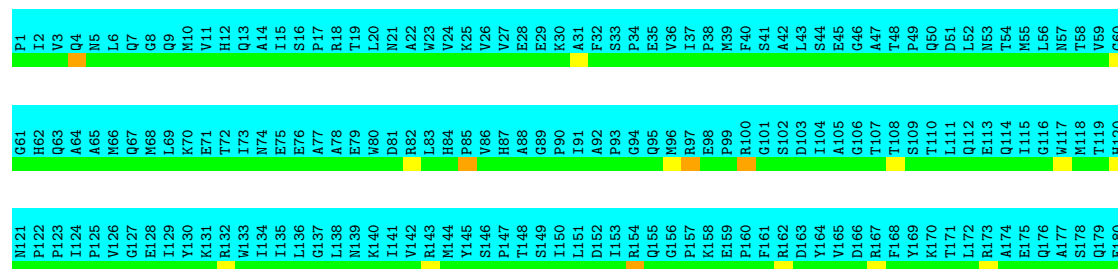
100%





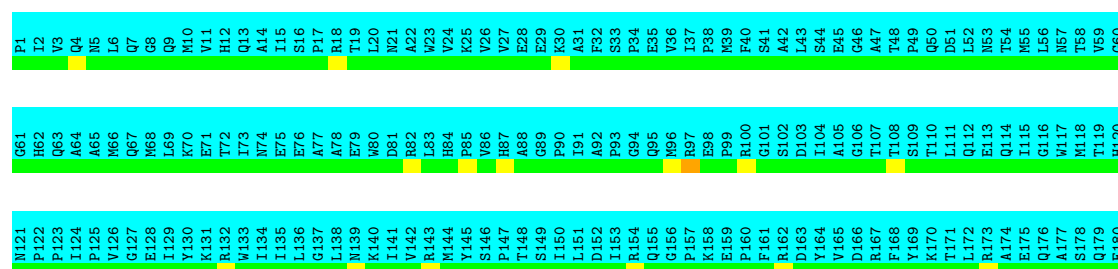
- Molecule 1: HIV-1 capsid protein

Chain iD:  100%



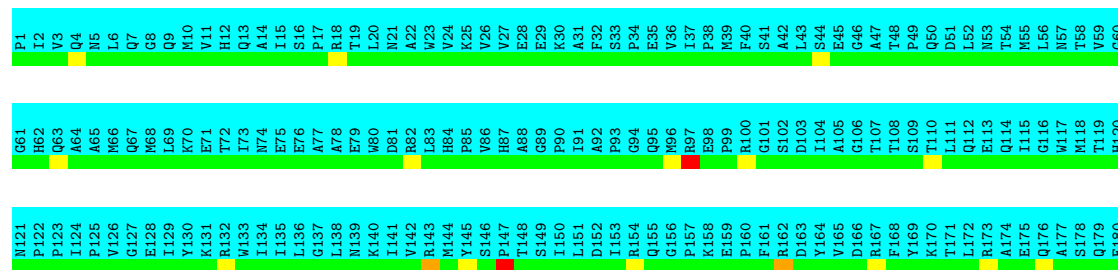
- Molecule 1: HIV-1 capsid protein

Chain jD:  100%



- Molecule 1: HIV-1 capsid protein

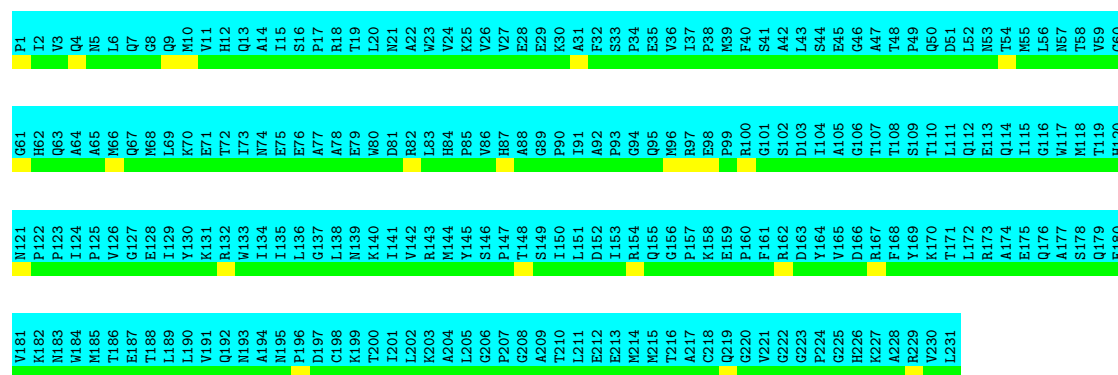
Chain kD:  100%



- Molecule 1: HIV-1 capsid protein

Chain ID:

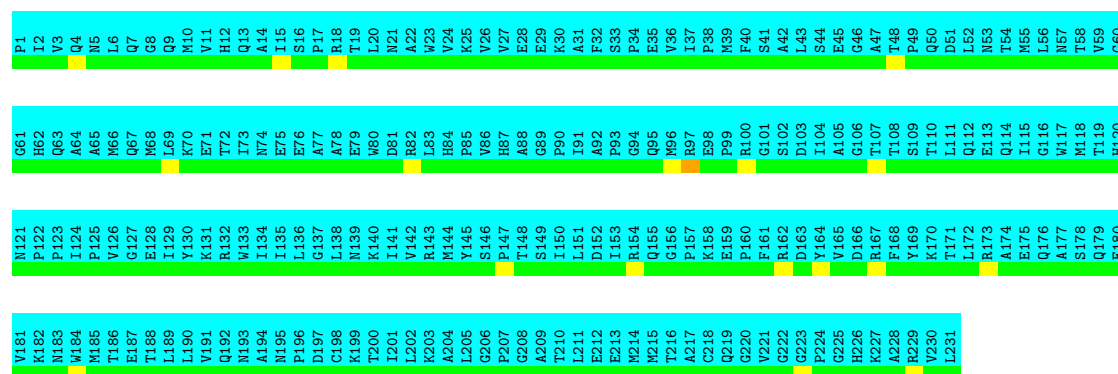
100%



- Molecule 1: HIV-1 capsid protein

Chain mD:

100%



- Molecule 1: HIV-1 capsid protein

Chain nD:

100%

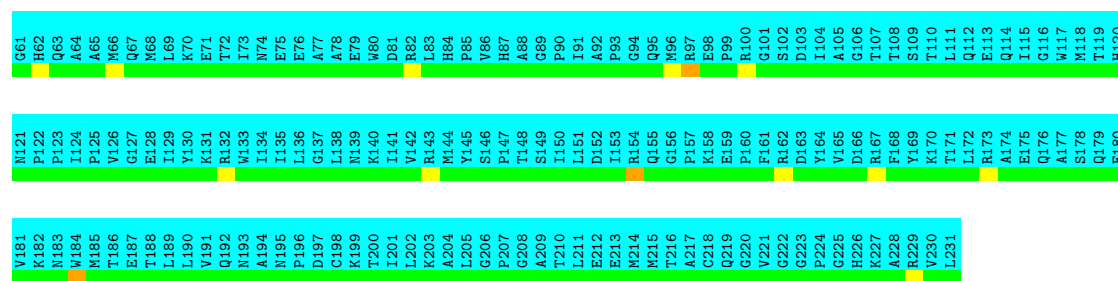


- Molecule 1: HIV-1 capsid protein

Chain oD:

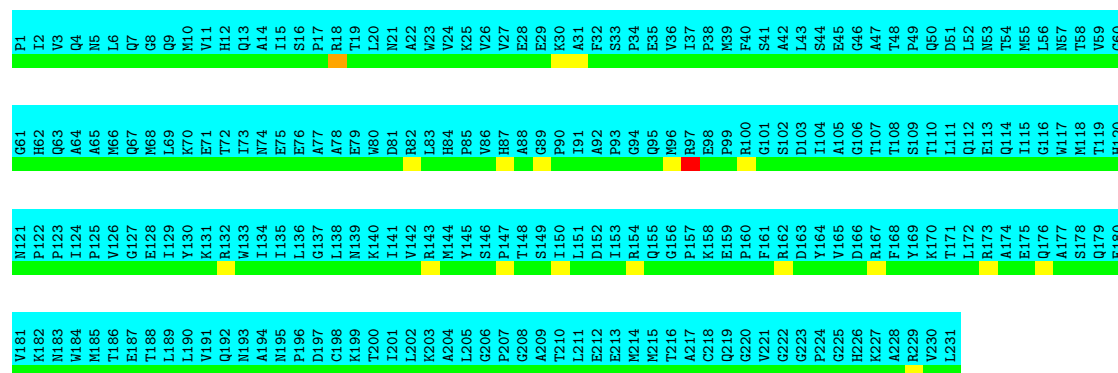
100%





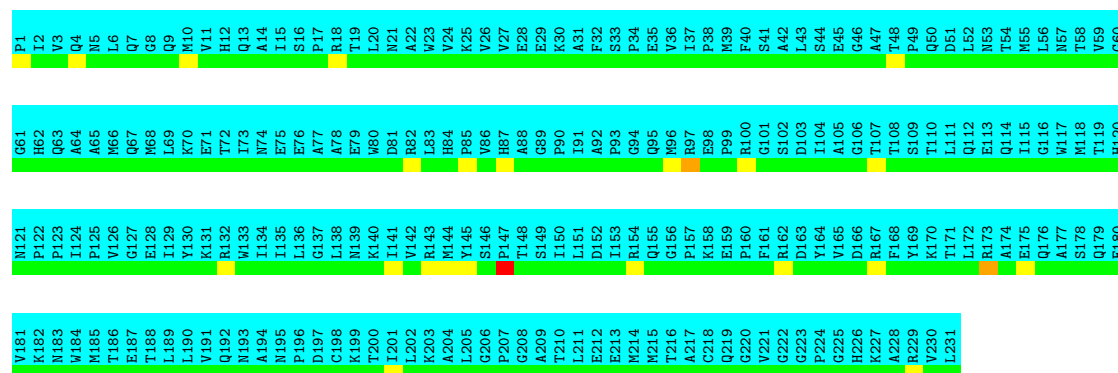
- Molecule 1: HIV-1 capsid protein

Chain pD:  100%



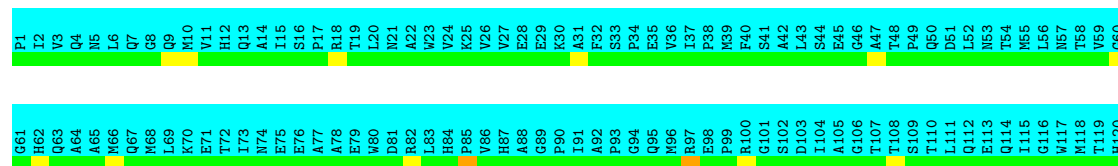
- Molecule 1: HIV-1 capsid protein

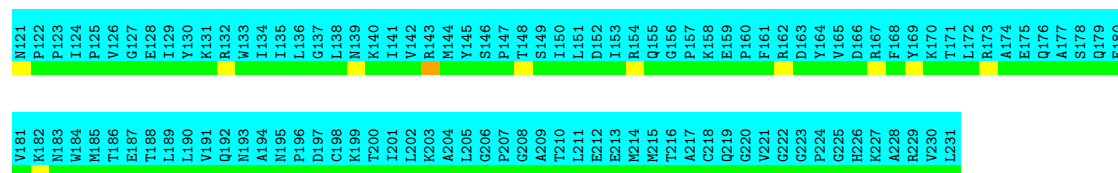
Chain qD:  100%



- Molecule 1: HIV-1 capsid protein

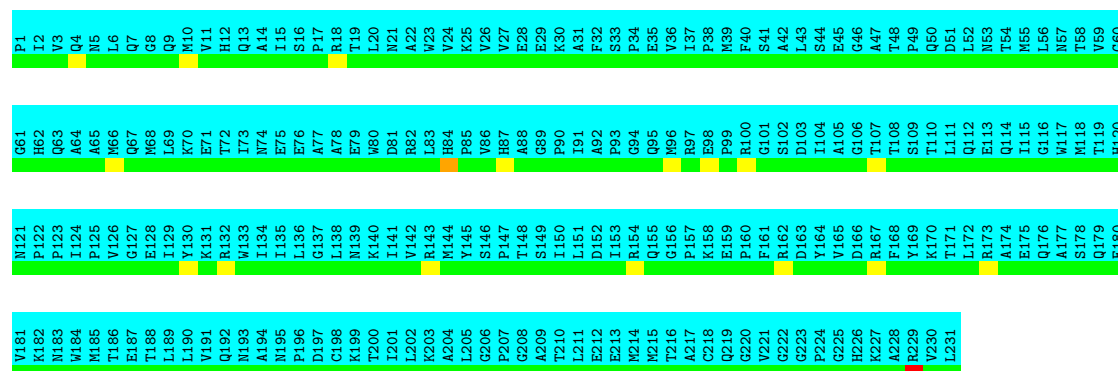
Chain rD:  100%





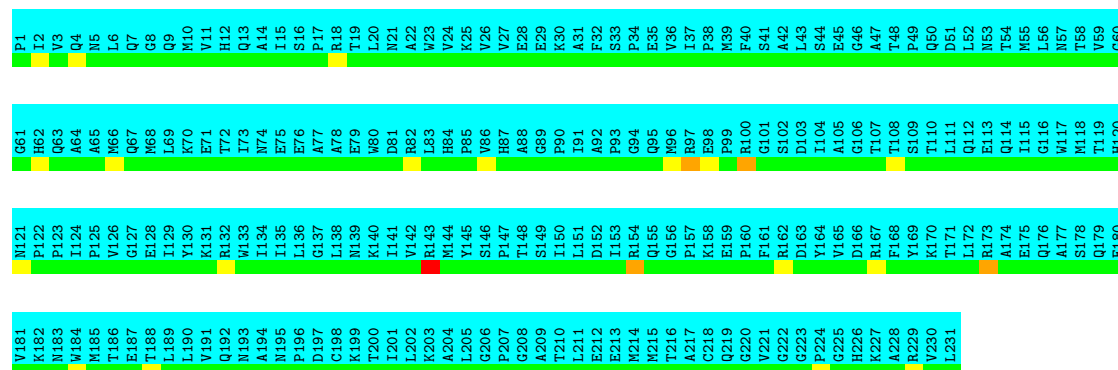
• Molecule 1: HIV-1 capsid protein

Chain sD:



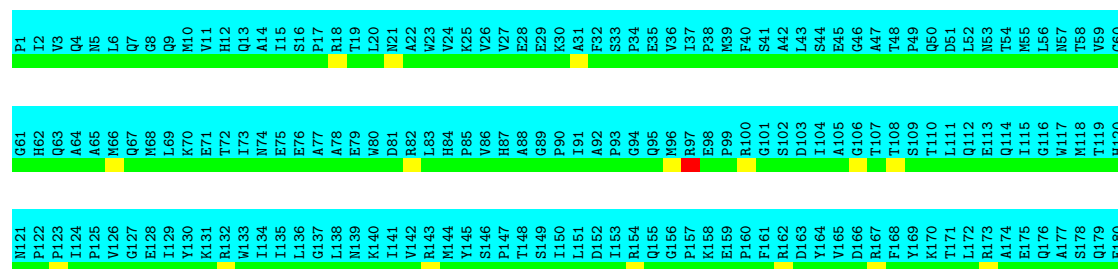
• Molecule 1: HIV-1 capsid protein

Chain tD:



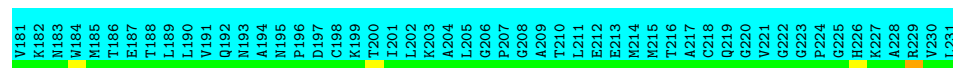
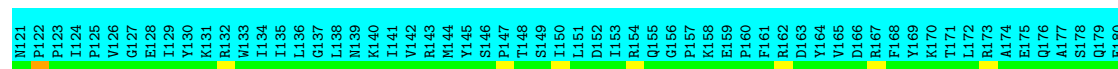
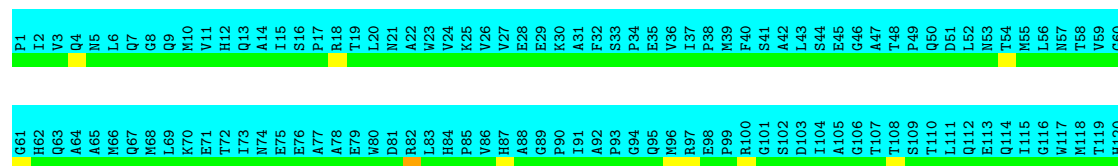
• Molecule 1: HIV-1 capsid protein

Chain uD:

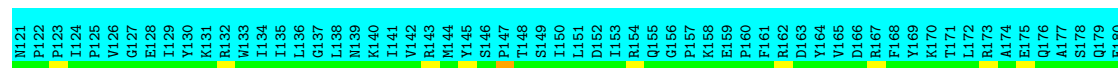
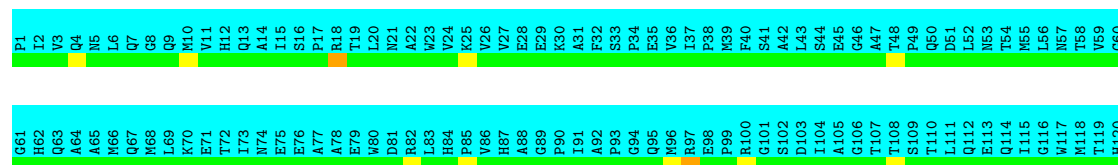




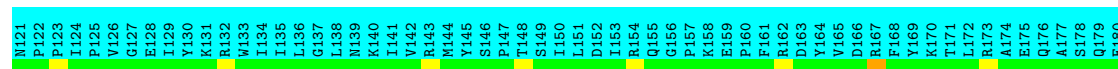
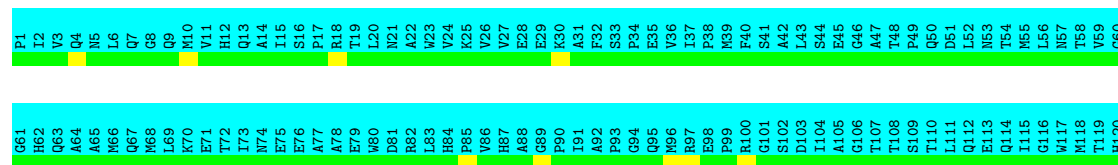
• Molecule 1: HIV-1 capsid protein



• Molecule 1: HIV-1 capsid protein



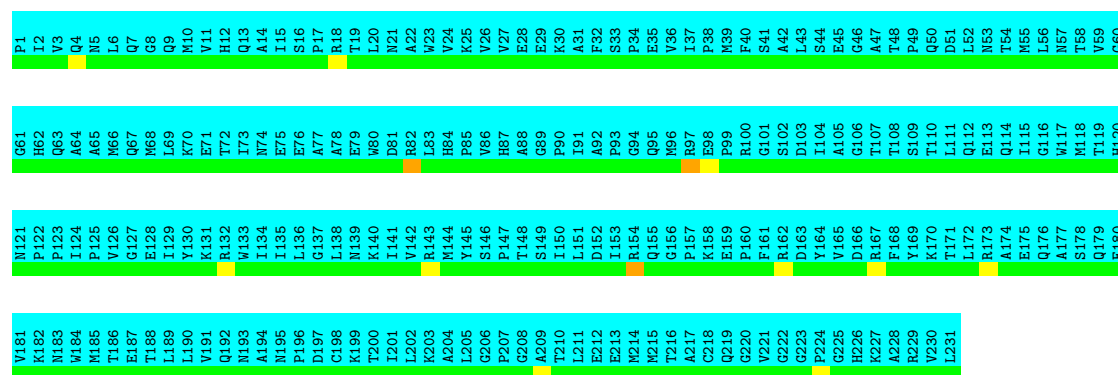
• Molecule 1: HIV-1 capsid protein



• Molecule 1: HIV-1 capsid protein

Chain yD:

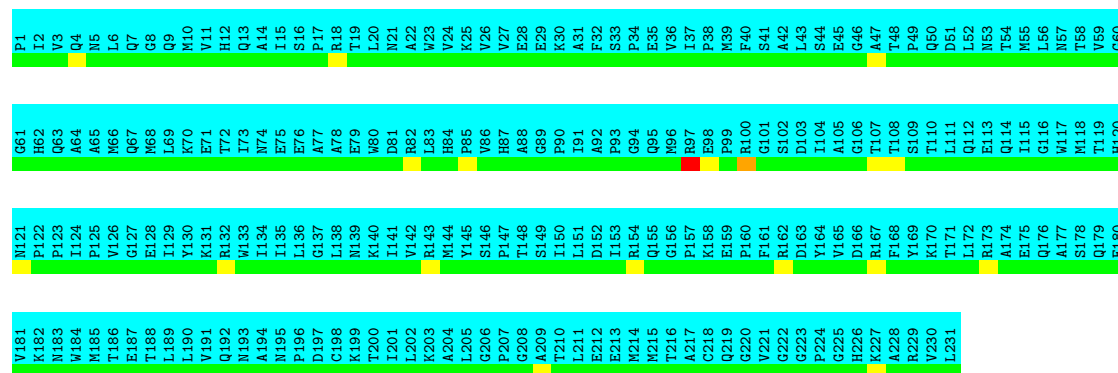
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● Molecule 1: HIV-1 capsid protein

Chain zD:

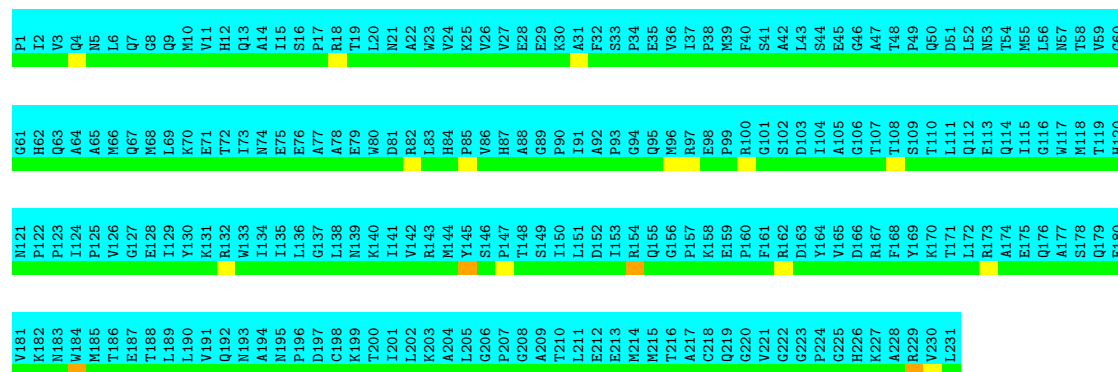
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● Molecule 1: HIV-1 capsid protein

Chain 0D:

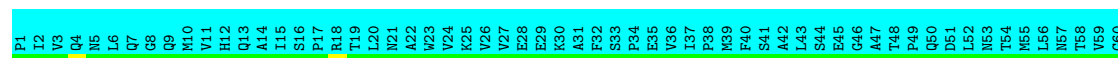
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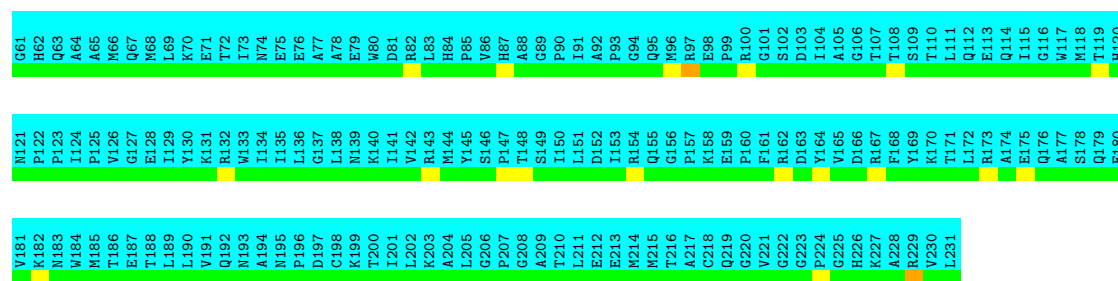


● Molecule 1: HIV-1 capsid protein

Chain 1D:

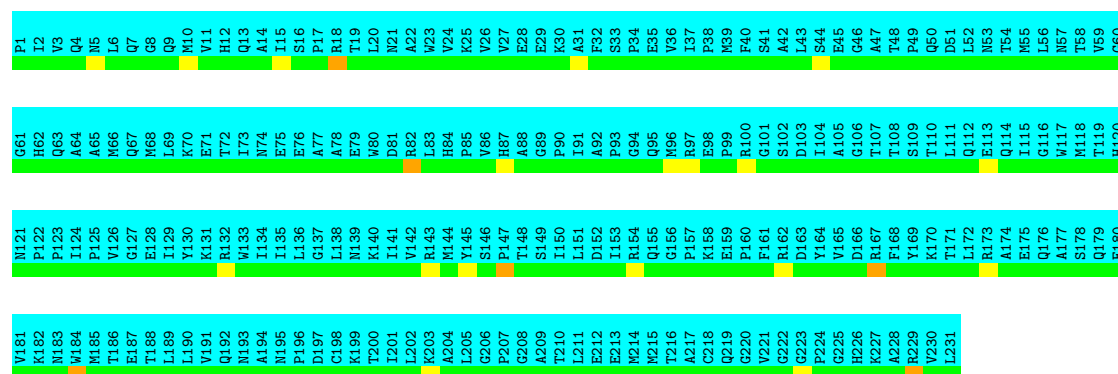
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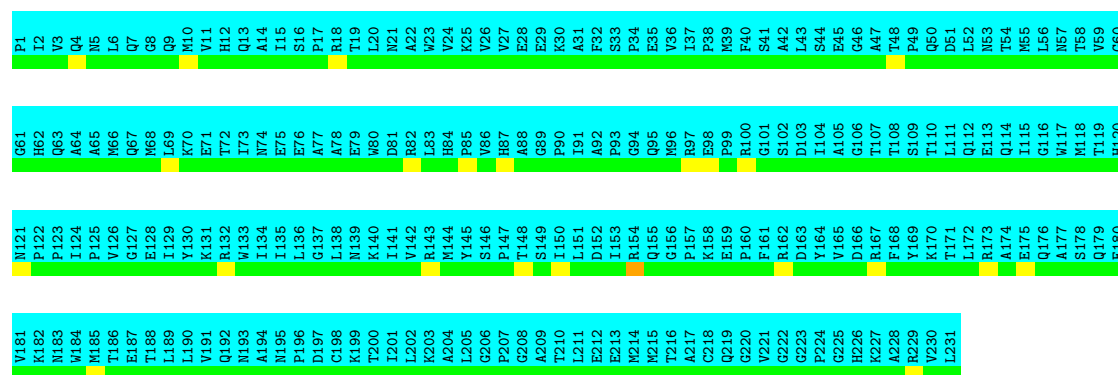
- Molecule 1: HIV-1 capsid protein

Chain 2D: 100%



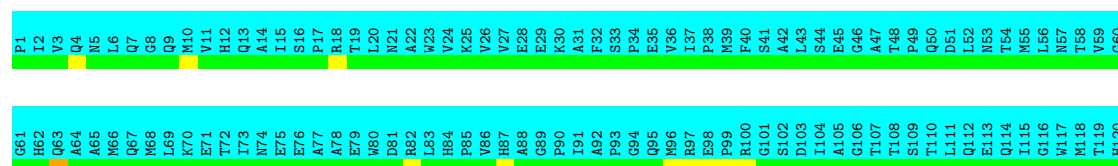
- Molecule 1: HIV-1 capsid protein

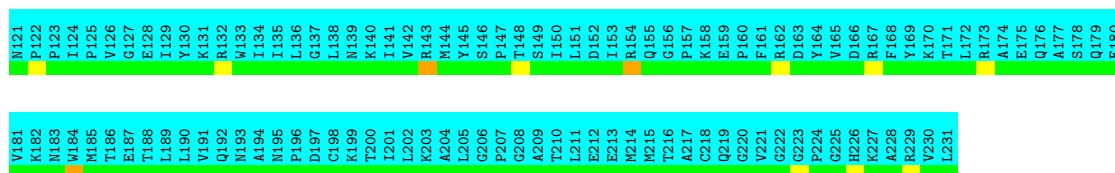
Chain 3D: 100%



- Molecule 1: HIV-1 capsid protein

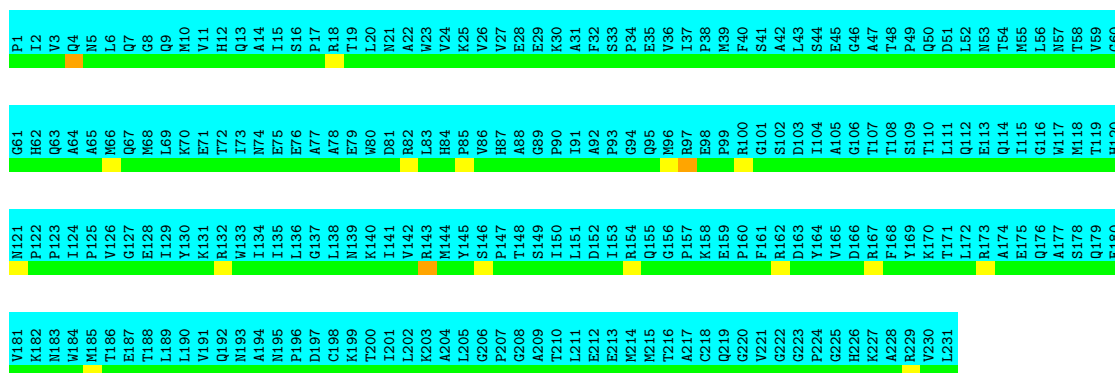
Chain 4D: 100%





• Molecule 1: HIV-1 capsid protein

Chain 5D: 100%



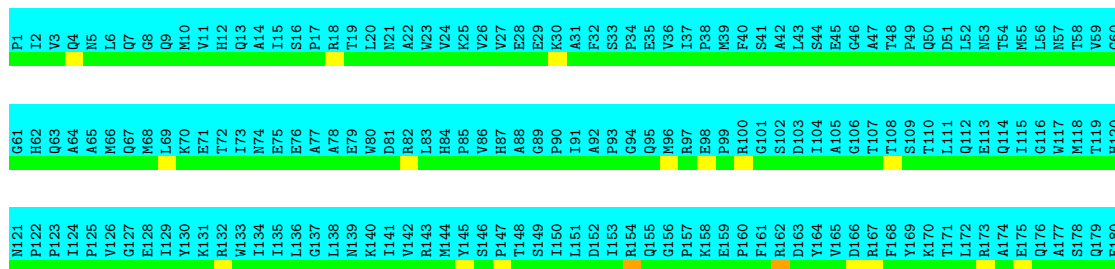
• Molecule 1: HIV-1 capsid protein

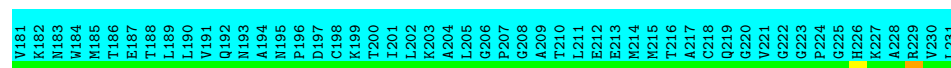
Chain 6D: 100%



• Molecule 1: HIV-1 capsid protein

Chain 7D: 100%





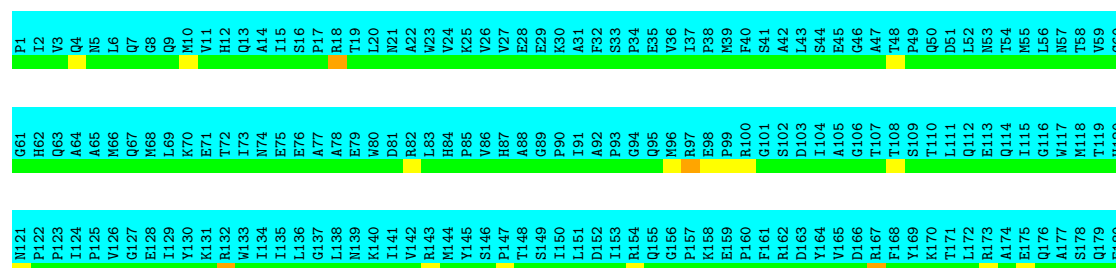
- Molecule 1: HIV-1 capsid protein

Chain 8D: 100%



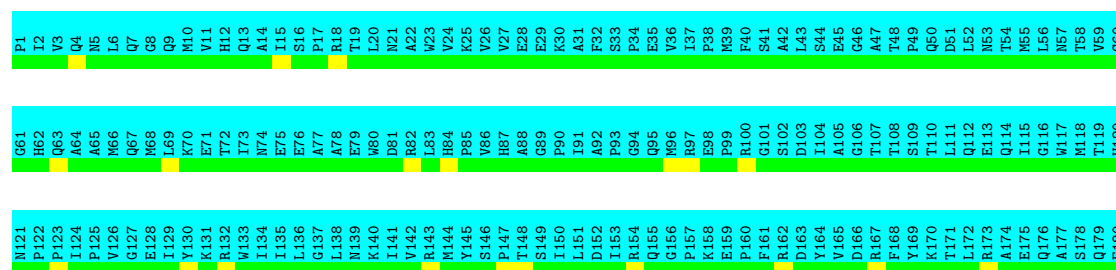
- Molecule 1: HIV-1 capsid protein

Chain 9D: 100%



- Molecule 1: HIV-1 capsid protein

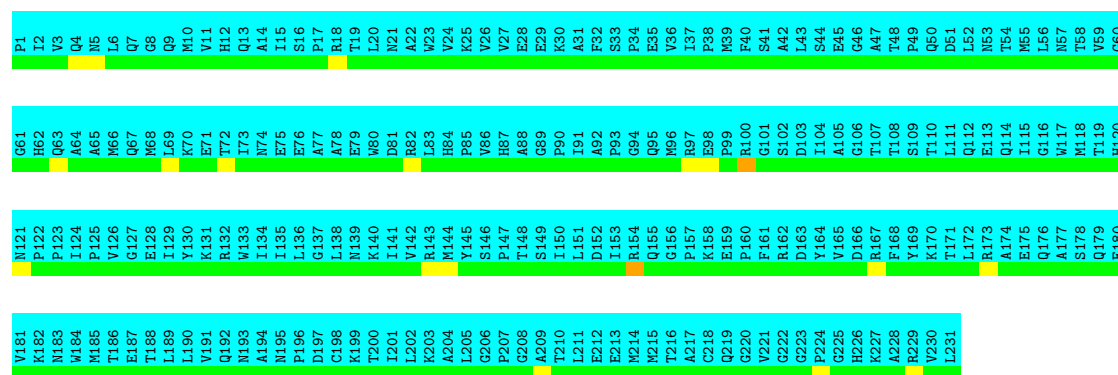
Chain AE: 100%



- Molecule 1: HIV-1 capsid protein

Chain BE:

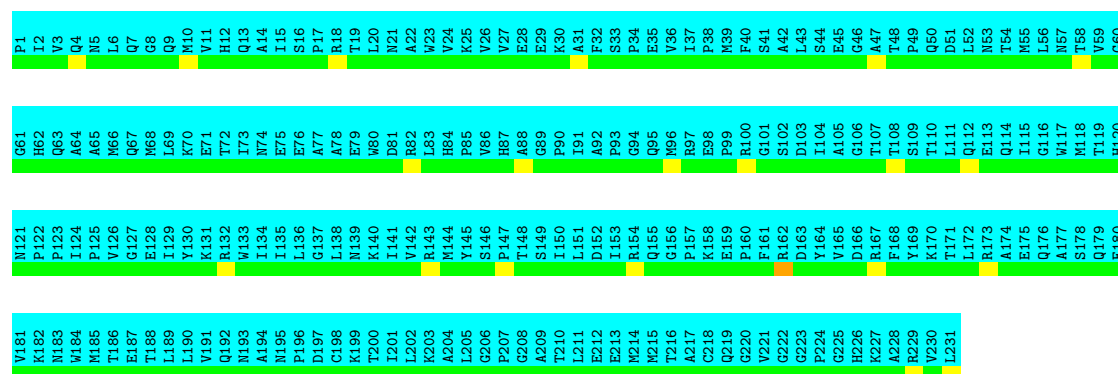
100%



- Molecule 1: HIV-1 capsid protein

Chain CE:

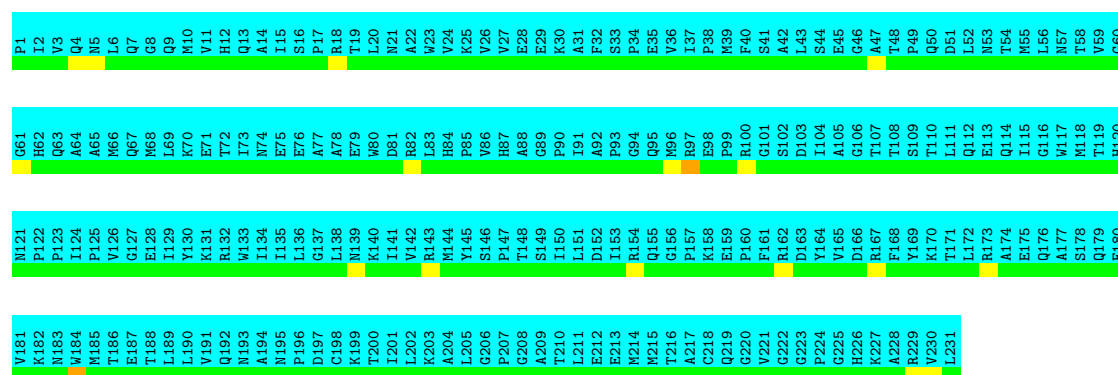
100%



- Molecule 1: HIV-1 capsid protein

Chain DE:

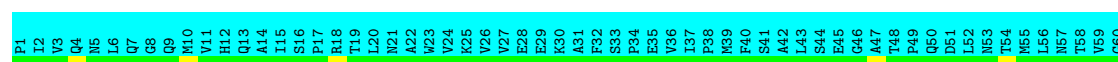
100%



- Molecule 1: HIV-1 capsid protein

Chain EE:

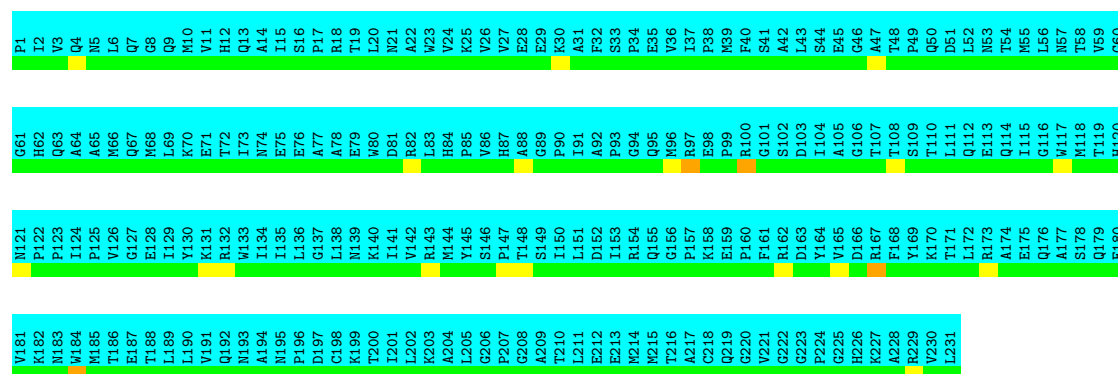
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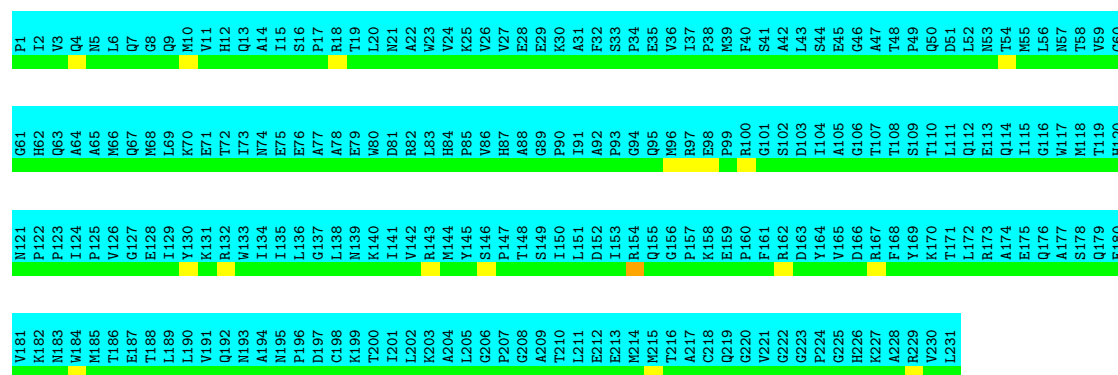
• Molecule 1: HIV-1 capsid protein

Chain FE: 100%



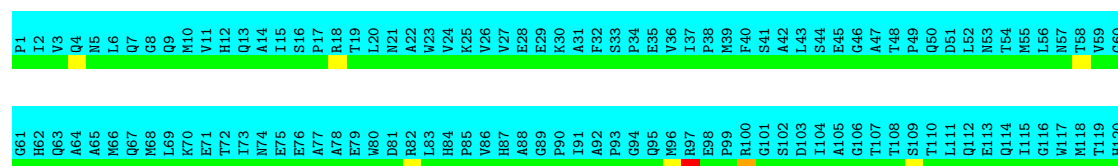
• Molecule 1: HIV-1 capsid protein

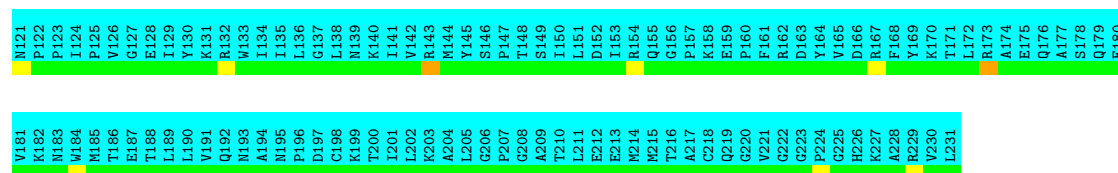
Chain GE: 100%



• Molecule 1: HIV-1 capsid protein

Chain HE: 100%

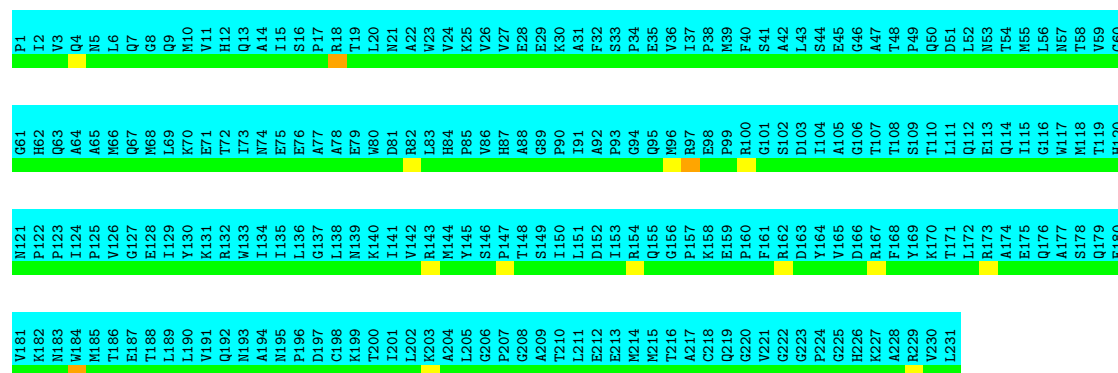




• Molecule 1: HIV-1 capsid protein

Chain IE:

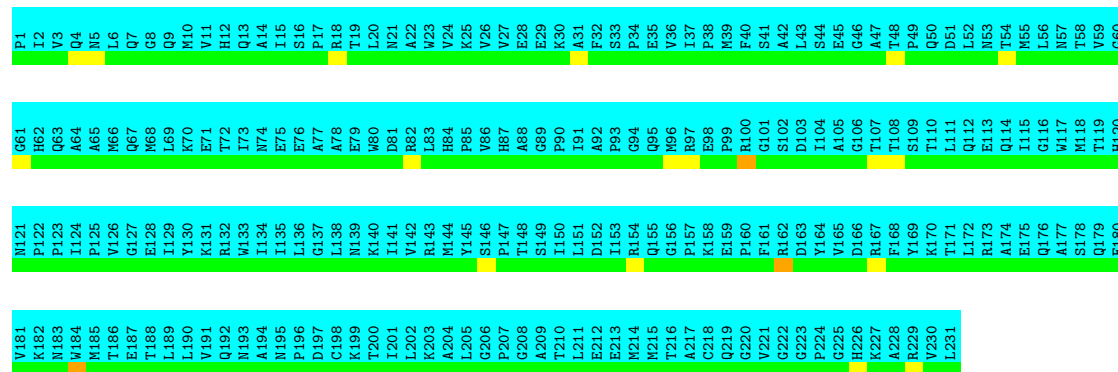
100%



• Molecule 1: HIV-1 capsid protein

Chain JE:

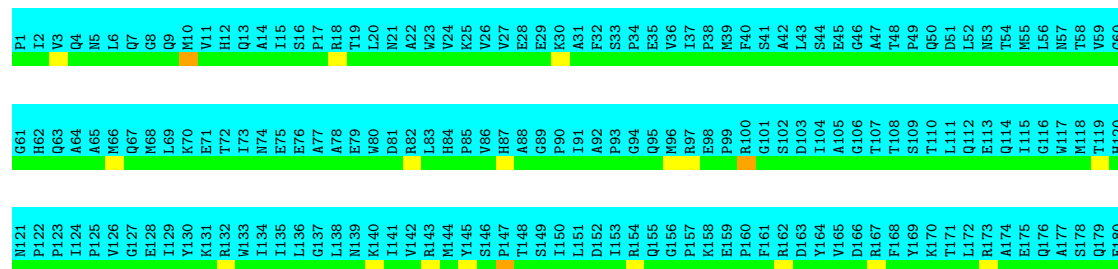
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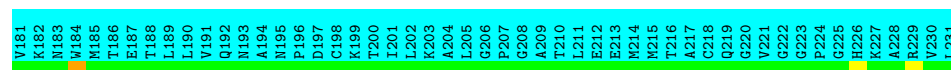


• Molecule 1: HIV-1 capsid protein

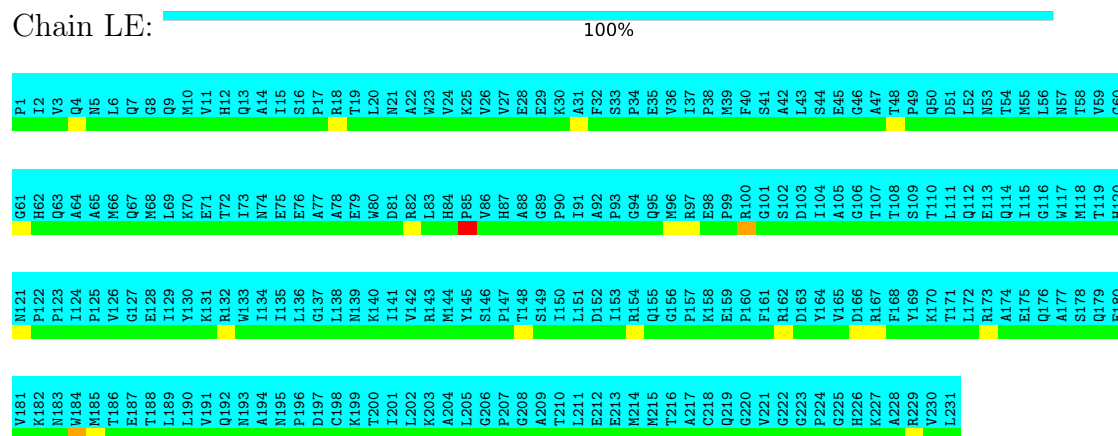
Chain KE:

100%

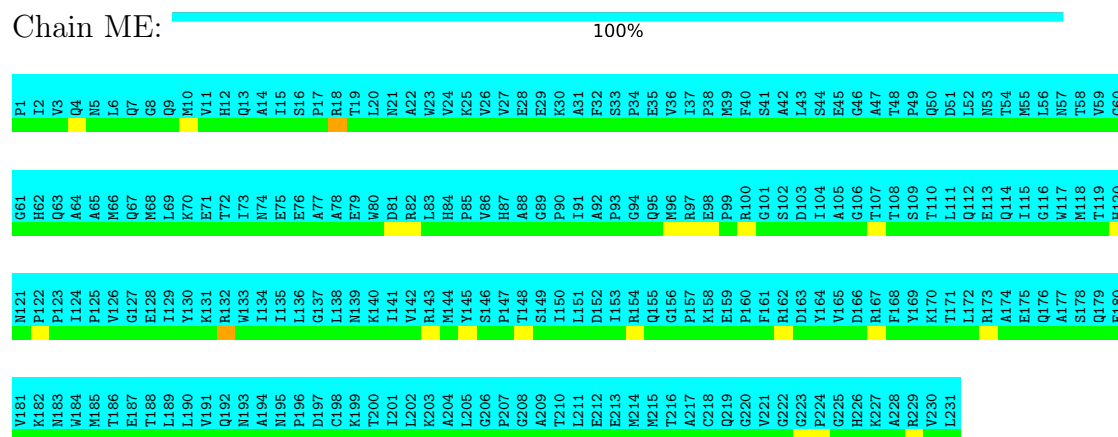




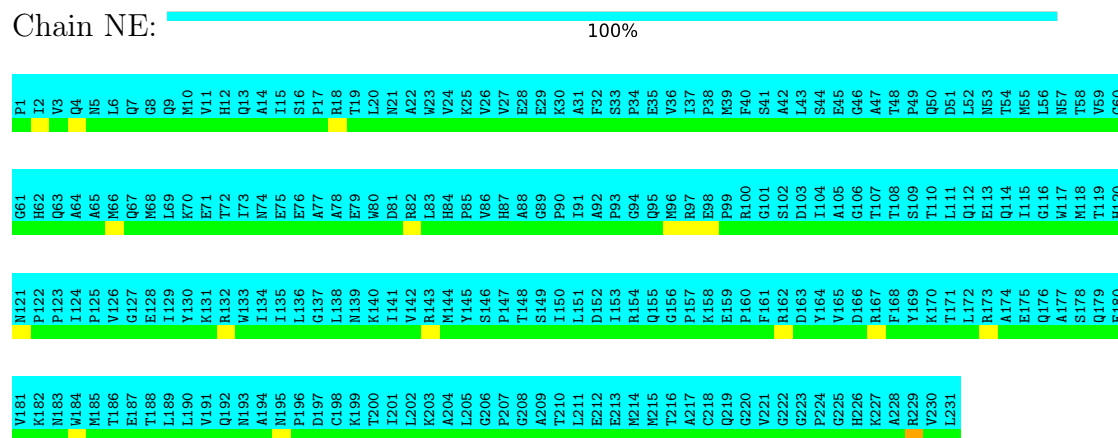
- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein



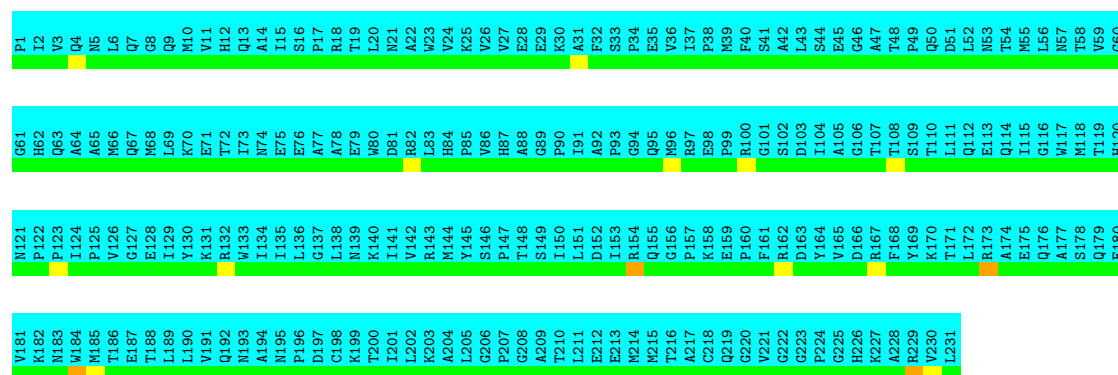
- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein

Chain OE:

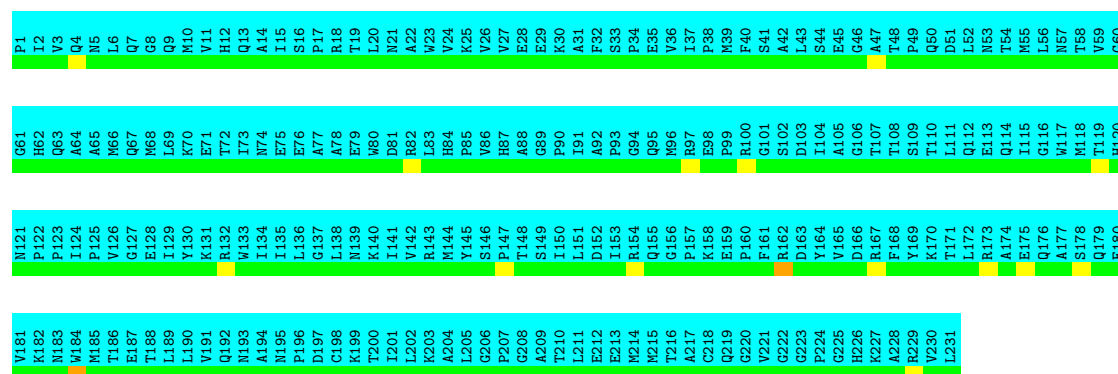
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• Molecule 1: HIV-1 capsid protein

Chain PE:

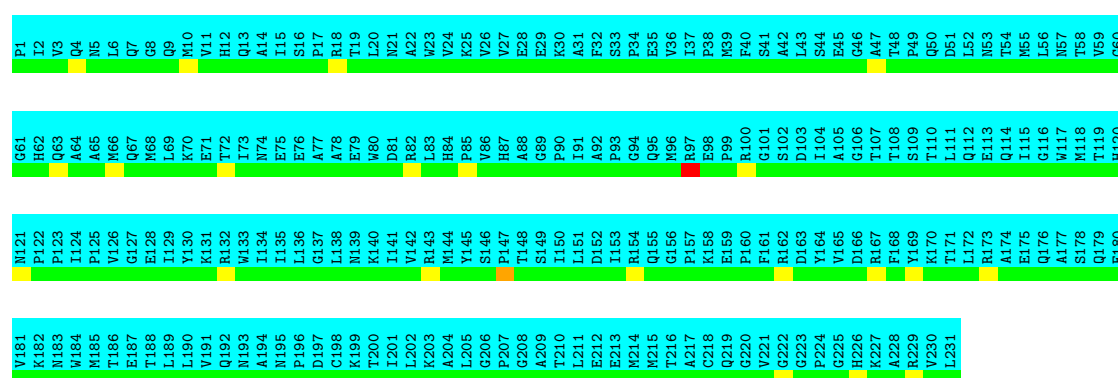
100%



• Molecule 1: HIV-1 capsid protein

Chain QE:

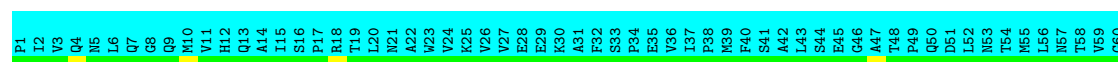
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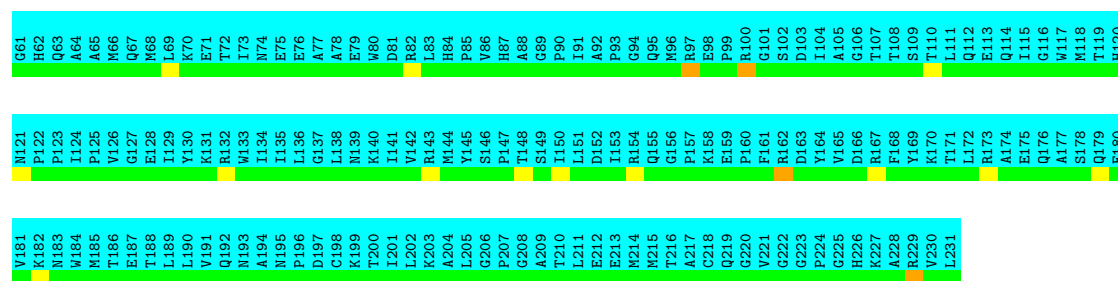


• Molecule 1: HIV-1 capsid protein

Chain RE:

100%

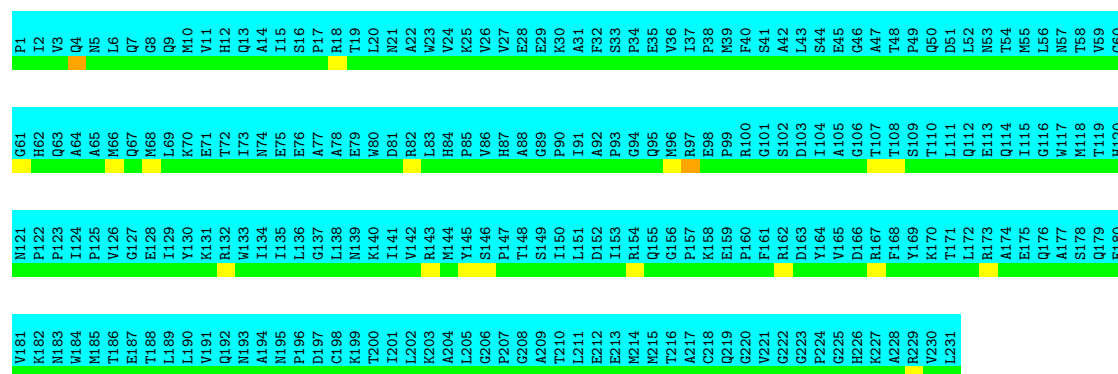




- Molecule 1: HIV-1 capsid protein

Chain SE:

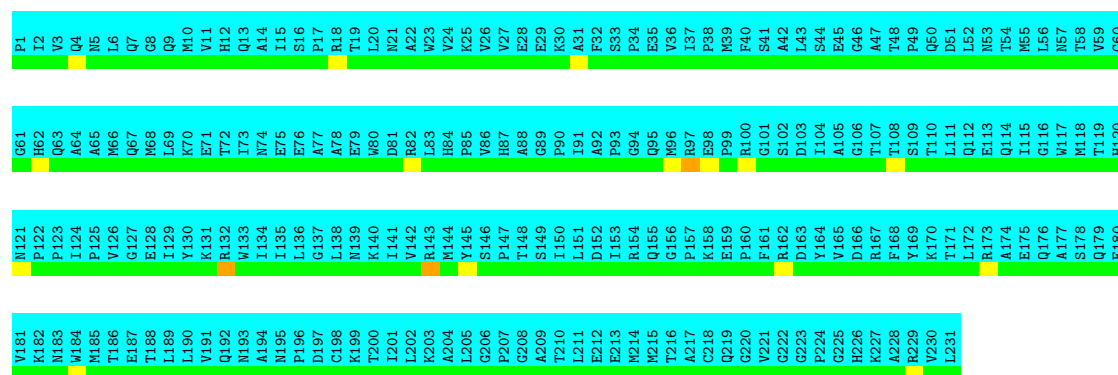
100%



- Molecule 1: HIV-1 capsid protein

Chain TE:

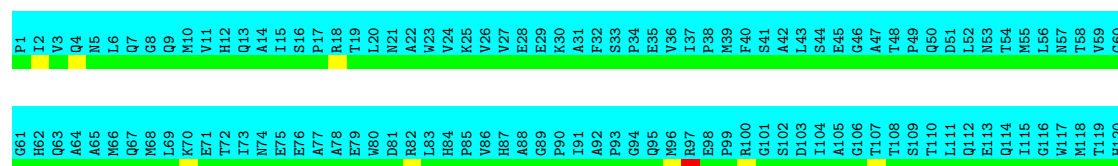
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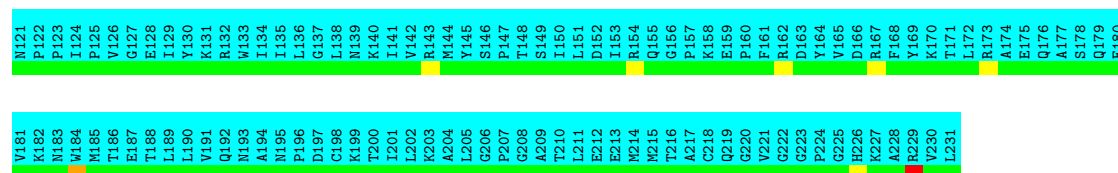


- Molecule 1: HIV-1 capsid protein

Chain UE:

100%

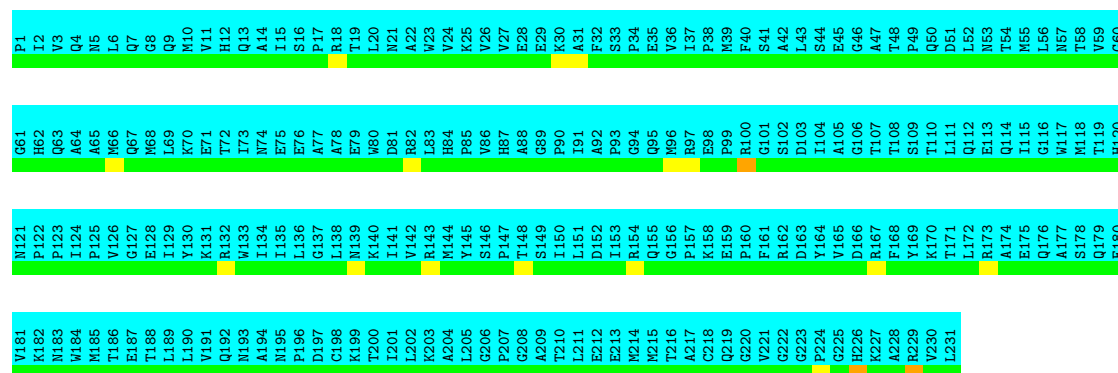




• Molecule 1: HIV-1 capsid protein

Chain VE:

100%



• Molecule 1: HIV-1 capsid protein

Chain WE:

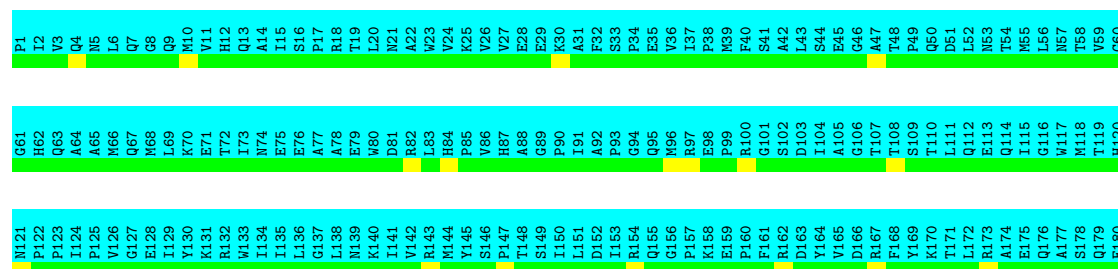
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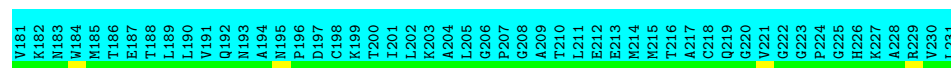


• Molecule 1: HIV-1 capsid protein

Chain XE:

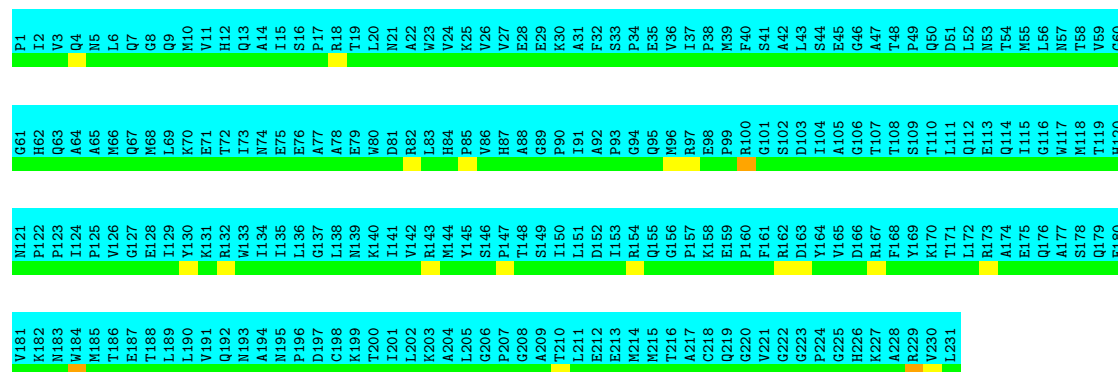
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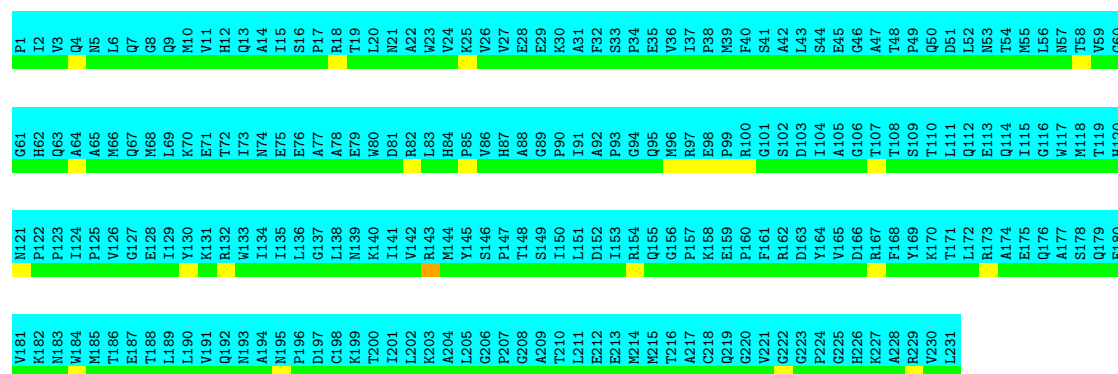
- Molecule 1: HIV-1 capsid protein

Chain YE: 100%



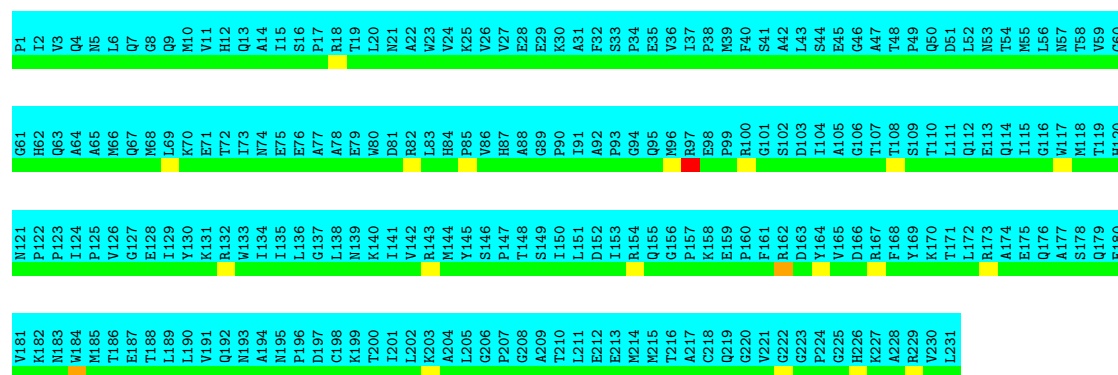
- Molecule 1: HIV-1 capsid protein

Chain ZE: 100%



- Molecule 1: HIV-1 capsid protein

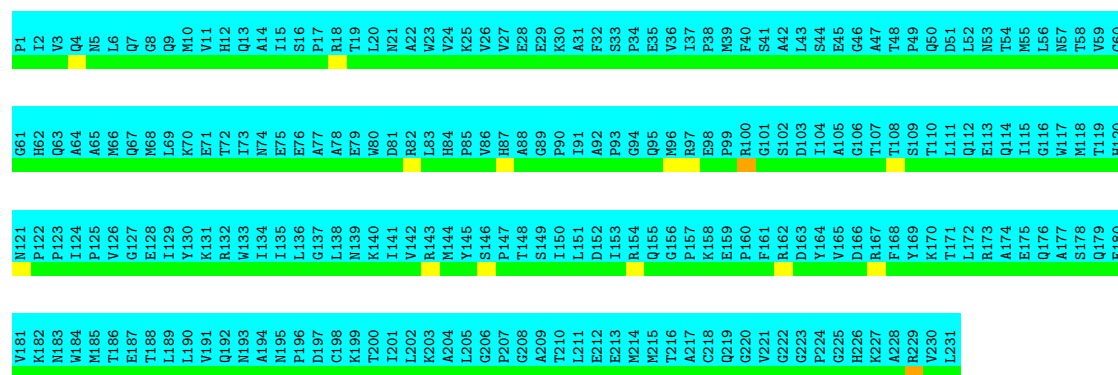
Chain aE: 100%



- Molecule 1: HIV-1 capsid protein

Chain bE:

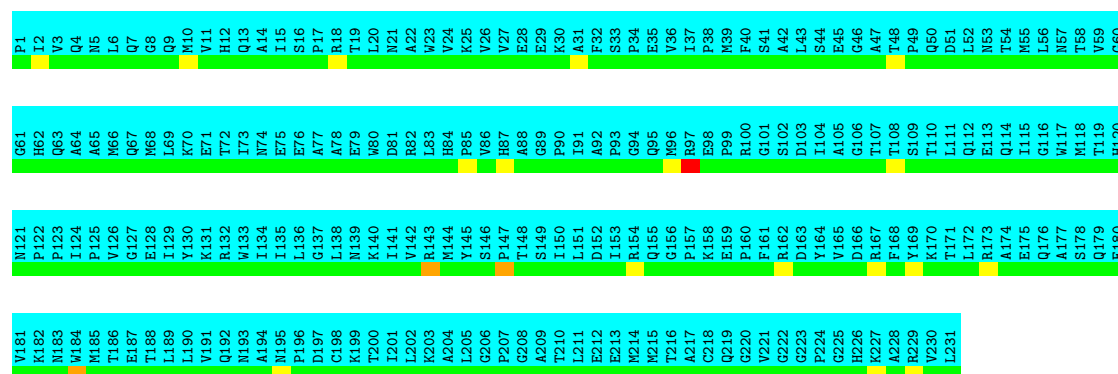
100%



• Molecule 1: HIV-1 capsid protein

Chain cE:

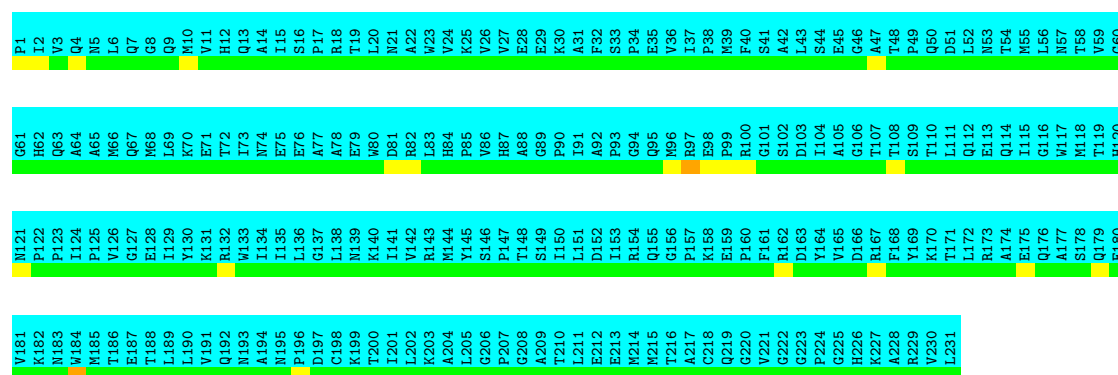
100%



• Molecule 1: HIV-1 capsid protein

Chain dE:

100%

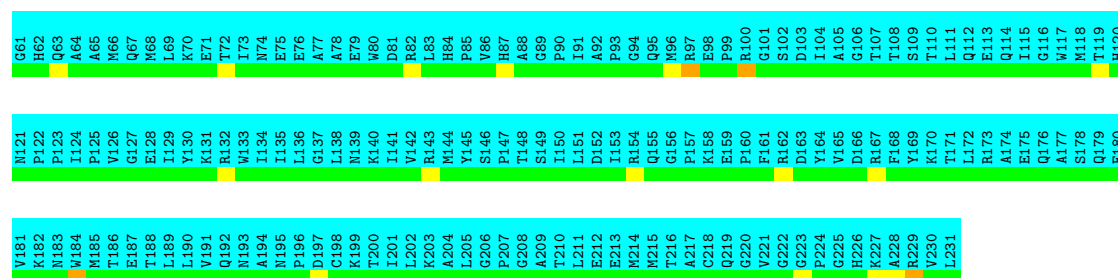


• Molecule 1: HIV-1 capsid protein

Chain eE:

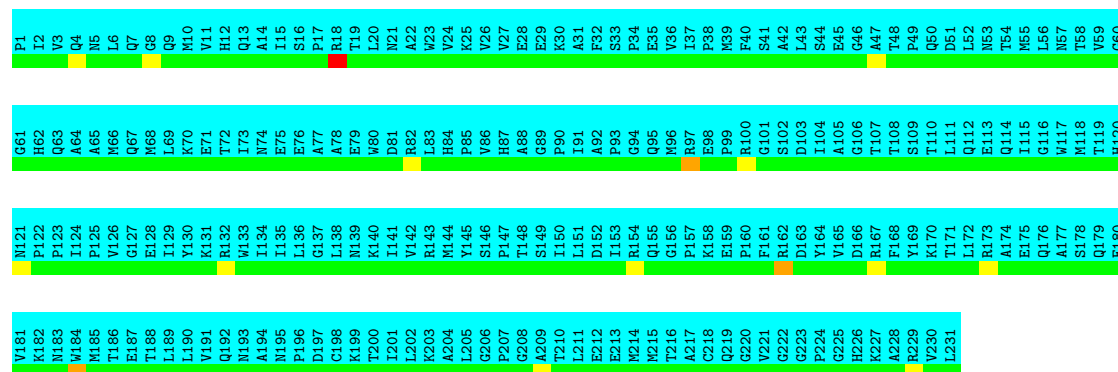
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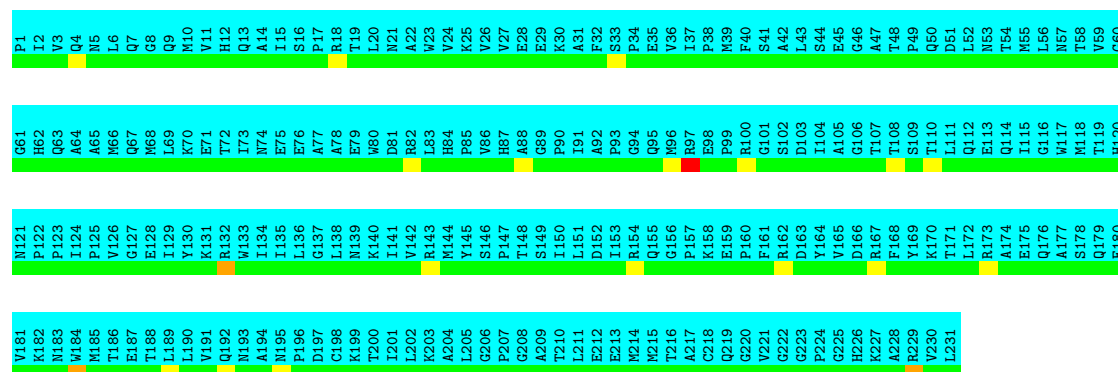
- Molecule 1: HIV-1 capsid protein

Chain fE:



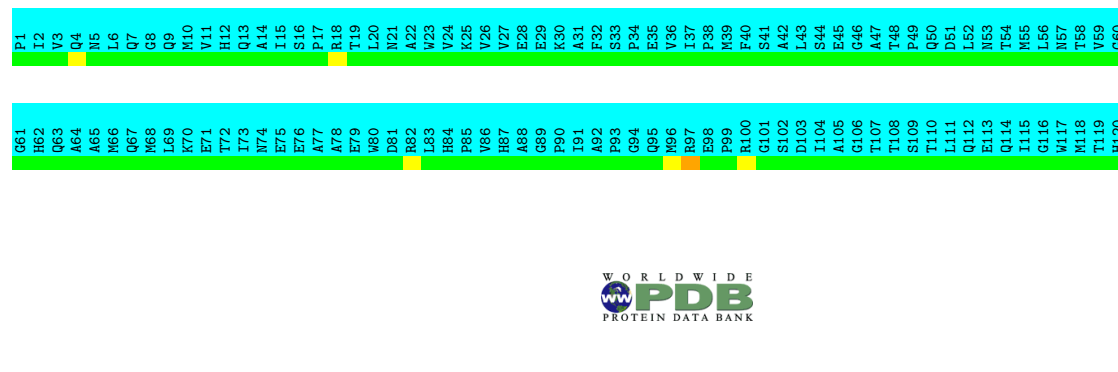
- Molecule 1: HIV-1 capsid protein

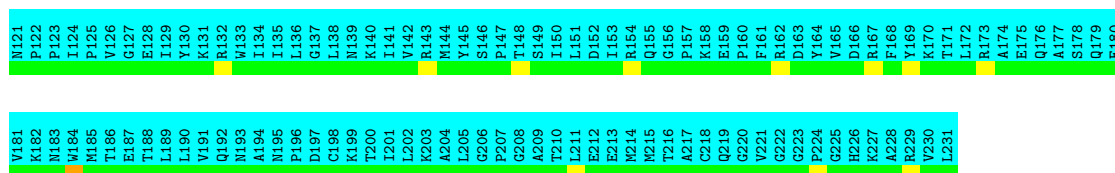
Chain gE:



- Molecule 1: HIV-1 capsid protein

Chain hE:

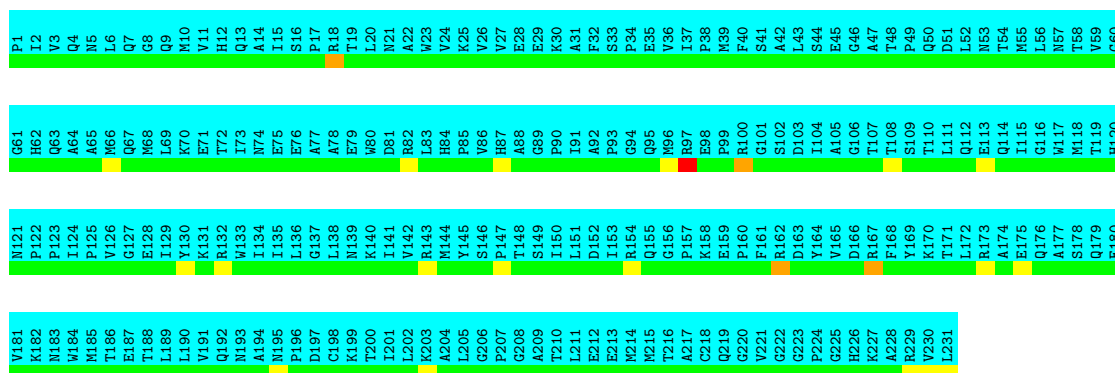




• Molecule 1: HIV-1 capsid protein

Chain iE:

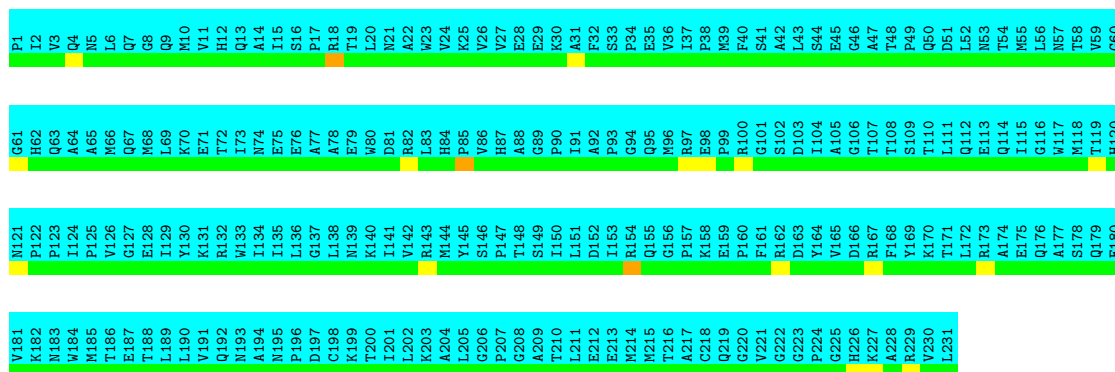
100%



• Molecule 1: HIV-1 capsid protein

Chain jE:

100%



• Molecule 1: HIV-1 capsid protein

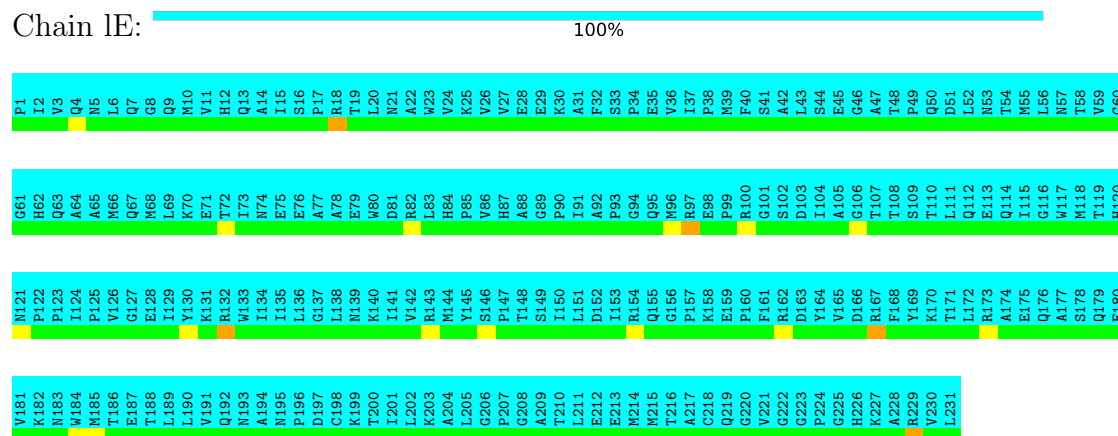
Chain kE:

100%

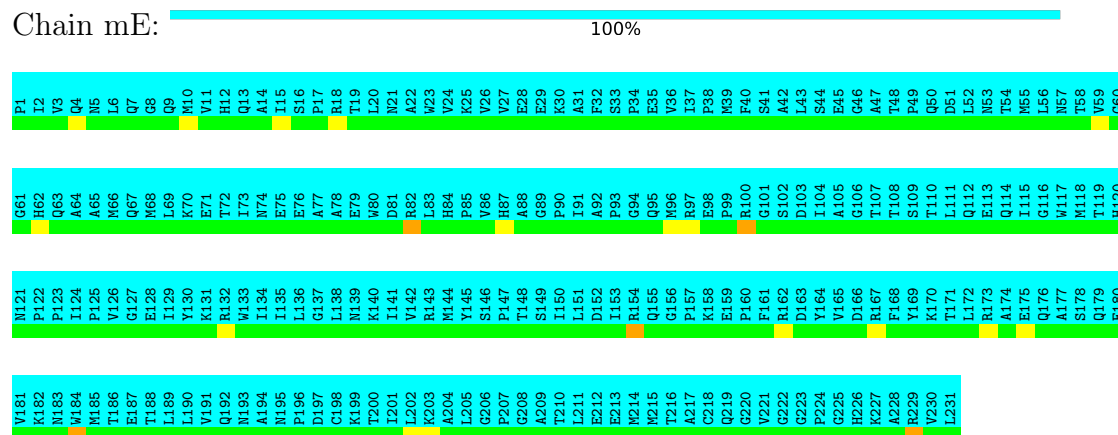




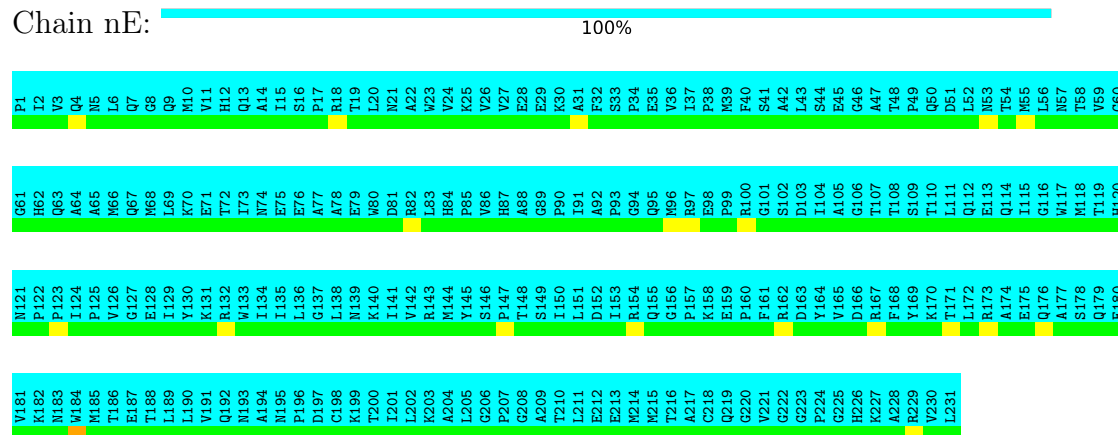
- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein



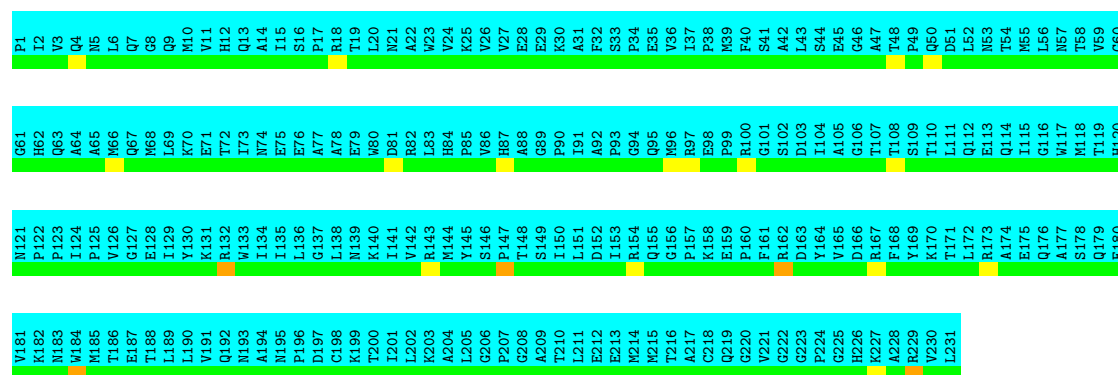
- Molecule 1: HIV-1 capsid protein



- Molecule 1: HIV-1 capsid protein

Chain oE:

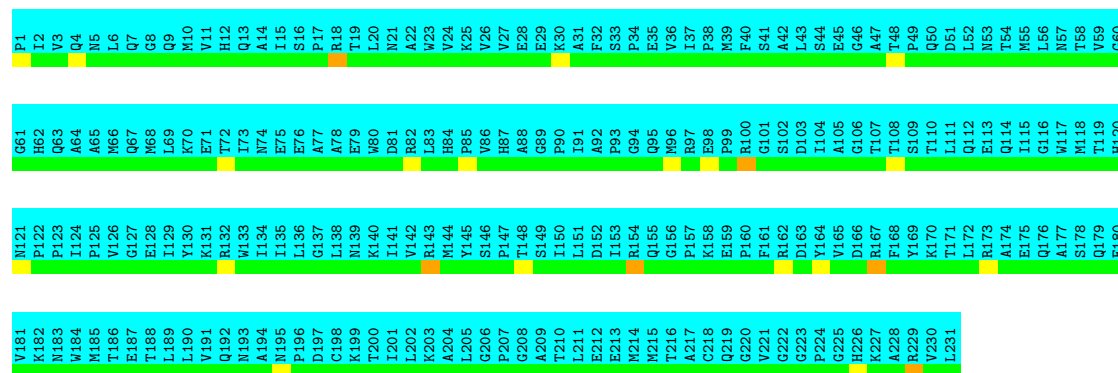
100%



- Molecule 1: HIV-1 capsid protein

Chain pE:

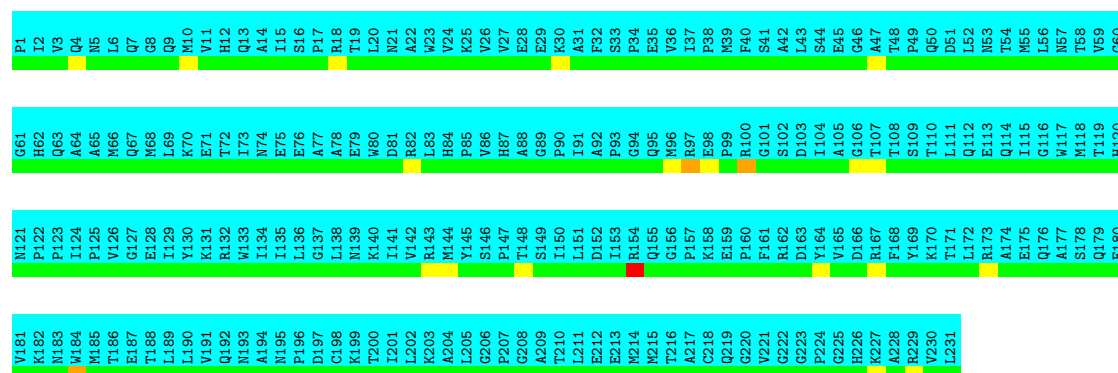
100%



- Molecule 1: HIV-1 capsid protein

Chain qE:

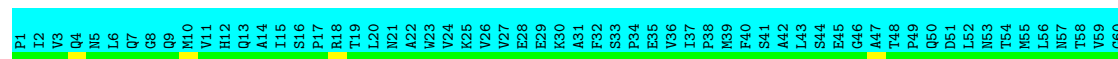
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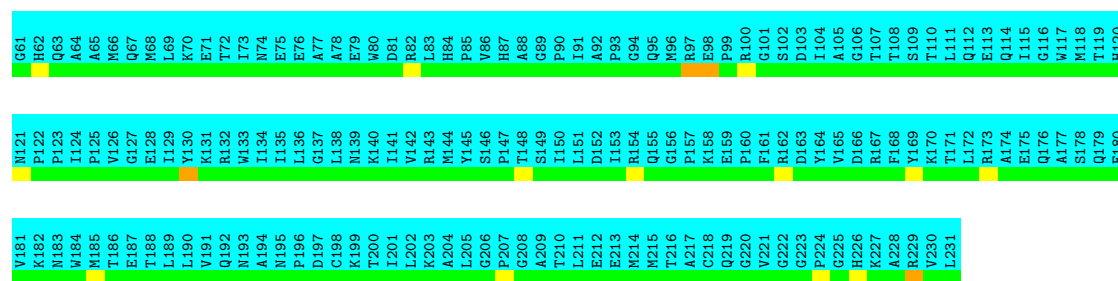


- Molecule 1: HIV-1 capsid protein

Chain rE:

100%

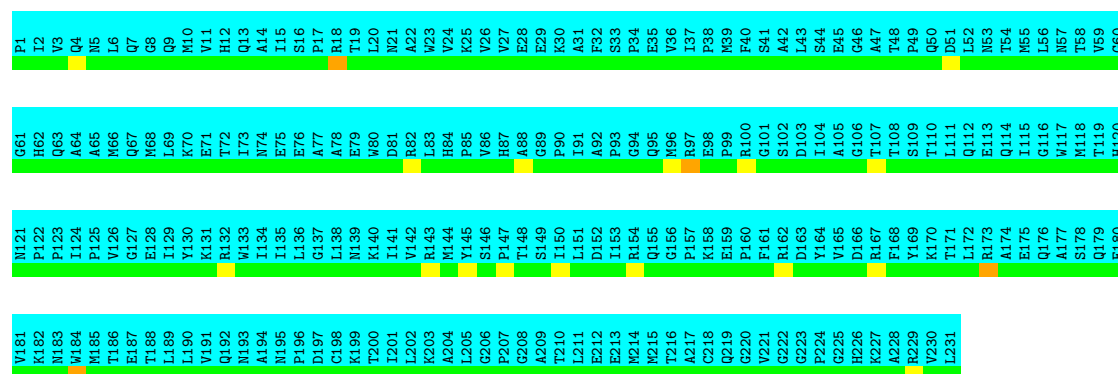




- Molecule 1: HIV-1 capsid protein

Chain sE:

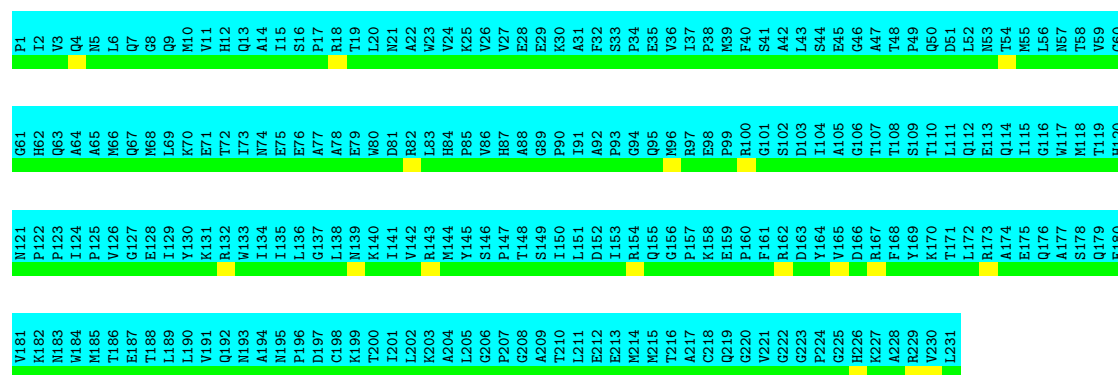
100%



- Molecule 1: HIV-1 capsid protein

Chain tE:

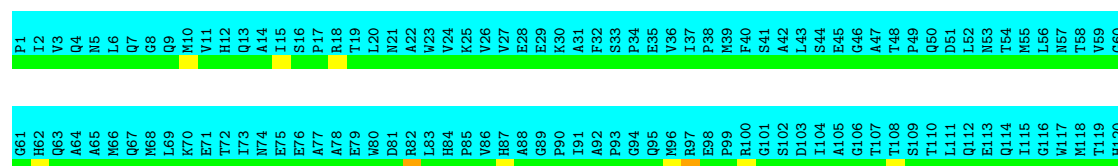
100%



- Molecule 1: HIV-1 capsid protein

Chain uE:

100%

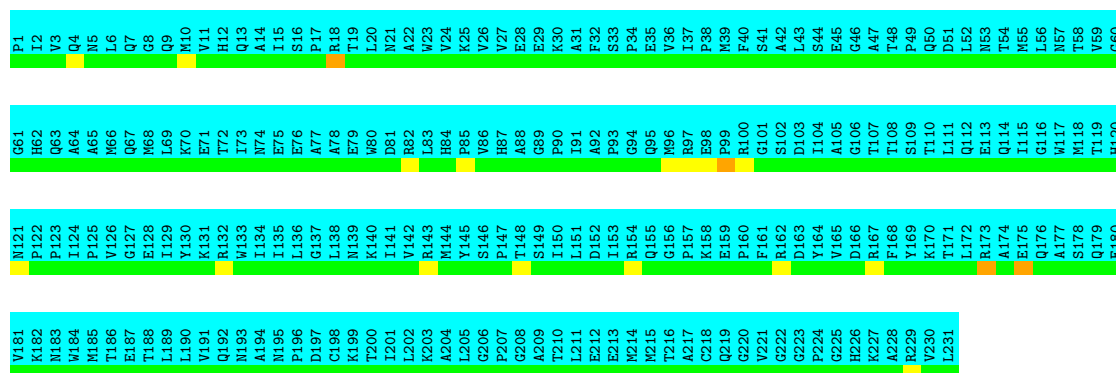




• Molecule 1: HIV-1 capsid protein

Chain vE:

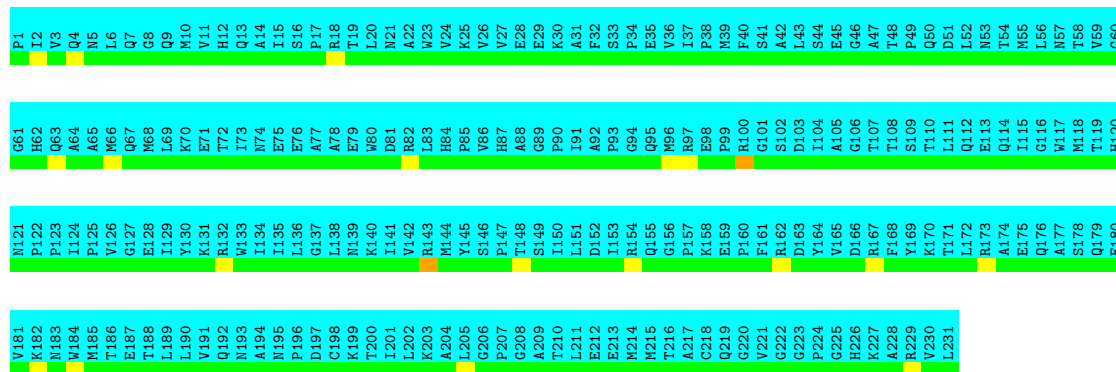
100%



• Molecule 1: HIV-1 capsid protein

Chain wE:

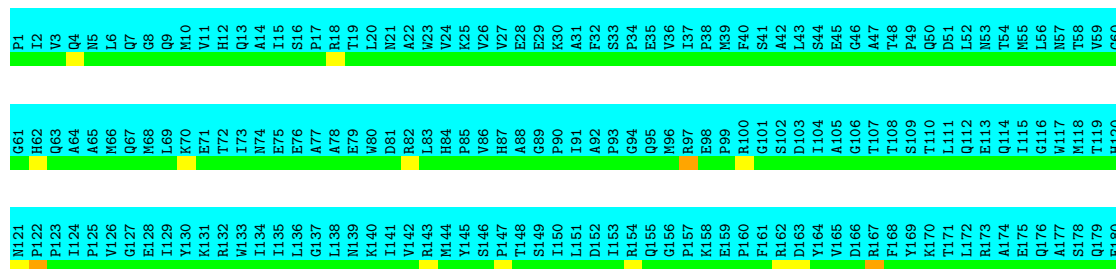
100%



• Molecule 1: HIV-1 capsid protein

Chain xE:

100%



V181	K182	M183	M184	M185	T186	E187	T188	L189	L190	V191	Q192	N193	A194	P195	P196	D197	C198	C199	T200	L201	L202	K203	A204	L205	G206	P207	G208	A209	T210	L211	E212	E213	M214	M215	T216	A217	C218	Q219	G220	V221	G222	G223	P224	G225	H226	K227	A228	R229	V230	L231
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• Molecule 1: HIV-1 capsid protein

Chain yE:

100%

P1	I2	Q3	Q4	N5	L6	Q7	Q8	Q9	M10	V11	H12	I13	A14	I15	E16	S16	P17	A18	T19	L20	N21	A22	W23	V24	K25	V26	V27	E28	G29	P30	K31	A32	F33	S34	E35	Q36	V37	I38	P39	R40	G41	S42	A43	D44	I45	A46	G47	T48	P49	S50	D51	L52	N53	T54	M55	I56	N57	M58	V59	G60
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G61	H62	Q63	A64	A65	M66	Q67	M68	L69	K70	E71	T72	I73	N74	E75	E76	A77	A78	E79	W80	D81	R82	L83	H84	P85	V86	H87	V88	A89	G90	P91	I92	A93	P94	Q95	Q96	M97	R98	E99	R100	G101	S102	A103	I104	A105	G106	T107	A108	S109	P110	T111	L112	E113	Q114	I115	G116	A117	M118	T119	V120
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N121	P122	P123	I124	P125	V126	G127	E128	L129	V130	K131	R132	W133	I134	I135	L136	G137	L138	N139	K140	I141	A142	R143	V144	Y145	S146	P147	T148	S149	T150	I151	D152	I153	R154	Q155	G156	P157	K158	E159	P160	F161	R162	D163	I164	V165	D166	K167	F168	R169	K170	T171	L172	R173	A174	I175	Q176	A177	S178	Q179	E180
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V181	K182	M183	M184	M185	T186	E187	T188	L189	L190	V191	Q192	N193	A194	P195	P196	D197	C198	C199	T200	L201	L202	K203	A204	L205	G206	P207	G208	A209	T210	L211	E212	E213	M214	M215	T216	A217	C218	Q219	G220	V221	G222	G223	P224	G225	H226	K227	A228	R229	V230	L231
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• Molecule 1: HIV-1 capsid protein

Chain zE:

100%

P1	I2	Q3	Q4	N5	L6	Q7	Q8	Q9	M10	V11	H12	I13	A14	I15	E16	S16	P17	A18	T19	L20	N21	A22	W23	V24	K25	V26	V27	E28	G29	P30	K31	A32	F33	S34	E35	Q36	V37	I38	P39	R40	G41	S42	A43	D44	I45	A46	G47	T48	P49	S50	D51	L52	N53	T54	M55	I56	N57	M58	V59	G60
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G61	H62	Q63	A64	A65	M66	Q67	M68	L69	K70	E71	T72	I73	N74	E75	E76	A77	A78	E79	W80	D81	R82	L83	H84	P85	V86	H87	V88	A89	G90	P91	I92	A93	P94	Q95	Q96	M97	R98	E99	R100	G101	S102	A103	I104	A105	G106	T107	A108	S109	P110	T111	L112	E113	Q114	I115	G116	A117	M118	T119	V120
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N121	P122	P123	I124	P125	V126	G127	E128	L129	V130	K131	R132	W133	I134	I135	L136	G137	L138	N139	K140	I141	A142	R143	V144	Y145	S146	P147	T148	S149	T150	I151	D152	I153	R154	Q155	G156	P157	K158	E159	P160	F161	R162	D163	I164	V165	D166	K167	F168	R169	K170	T171	L172	R173	A174	I175	Q176	A177	S178	Q179	E180
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V181	K182	M183	M184	M185	T186	E187	T188	L189	L190	V191	Q192	N193	A194	P195	P196	D197	C198	C199	T200	L201	L202	K203	A204	L205	G206	P207	G208	A209	T210	L211	E212	E213	M214	M215	T216	A217	C218	Q219	G220	V221	G222	G223	P224	G225	H226	K227	A228	R229	V230	L231
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• Molecule 1: HIV-1 capsid protein

Chain 0E:

100%

P1	I2	Q3	Q4	N5	L6	Q7	Q8	Q9	M10	V11	H12	I13	A14	I15	E16	S16	P17	A18	T19	L20	N21	A22	W23	V24	K25	V26	V27	E28	G29	P30	K31	A32	F33	S34	E35	Q36	V37	I38	P39	R40	G41	S42	A43	D44	I45	A46	G47	T48	P49	S50	D51	L52	N53	T54	M55	I56	N57	M58	V59	G60
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G61	H62	Q63	A64	A65	M66	Q67	M68	L69	K70	E71	T72	I73	N74	E75	E76	A77	A78	E79	W80	D81	R82	L83	H84	P85	V86	H87	V88	A89	G90	P91	I92	A93	P94	Q95	Q96	M97	R98	E99	R100	G101	S102	A103	I104	A105	G106	T107	A108	S109	P110	T111	L112	E113	Q114	I115	G116	A117	M118	T119	V120
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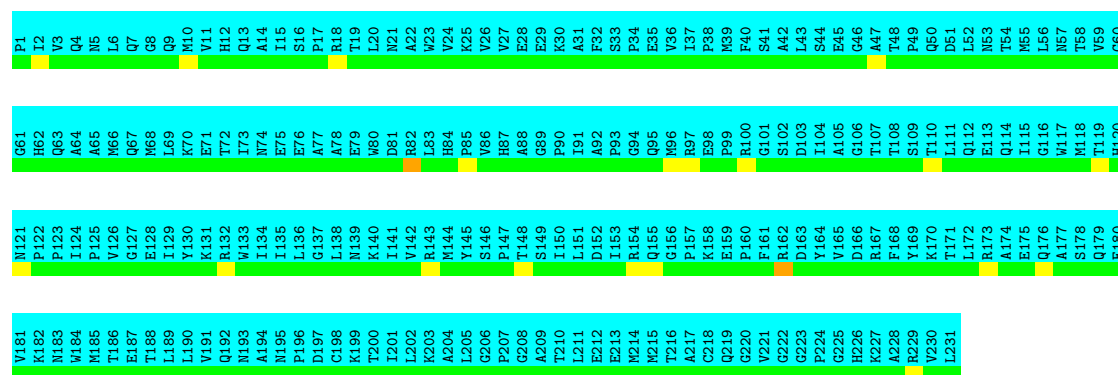
N121	P122	P123	I124	P125	V126	G127	E128	L129	V130	K131	R132	W133	I134	I135	L136	G137	L138	N139	K140	I141	A142	R143	V144	Y145	S146	P147	T148	S149	T150	I151	D152	I153	R154	Q155	G156	P157	K158	E159	P160	F161	R162	D163	I164	V165	D166	K167	F168	R169	K170	T171	L172	R173	A174	I175	Q176	A177	S178	Q179	E180
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V181	K182	M183	M184	M185	T186	E187	T188	L189	L190	V191	Q192	N193	A194	P195	P196	D197	C198	C199	T200	L201	L202	K203	A204	L205	G206	P207	G208	A209	T210	L211	E212	E213	M214	M215	T216	A217	C218	Q219	G220	V221	G222	G223	P224	G225	H226	K227	A228	R229	V230	L231
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• Molecule 1: HIV-1 capsid protein

Chain 1E:

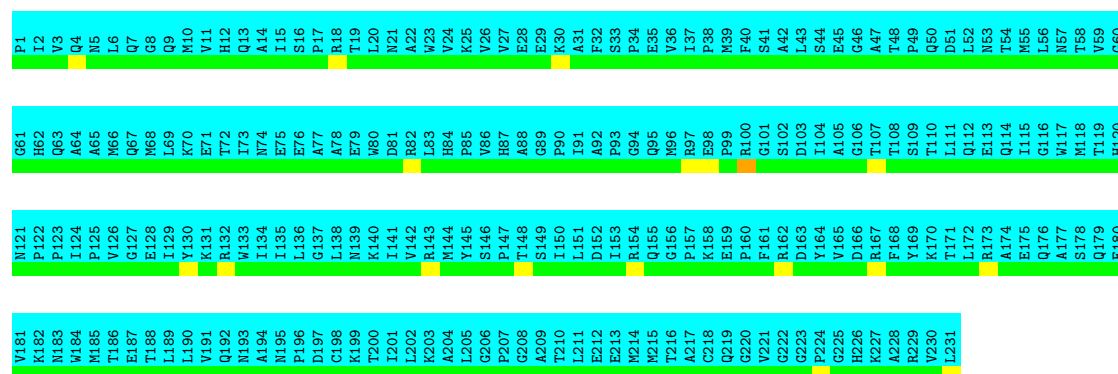
100%



- Molecule 1: HIV-1 capsid protein

Chain 2E:

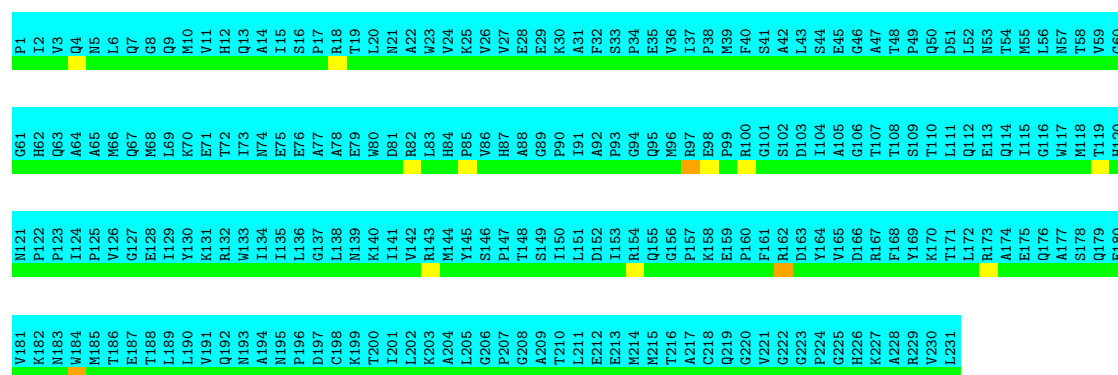
100%



- Molecule 1: HIV-1 capsid protein

Chain 3E:

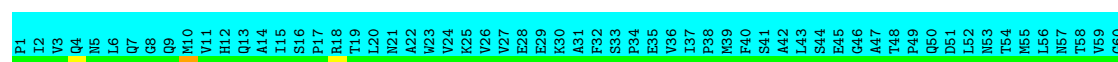
100%



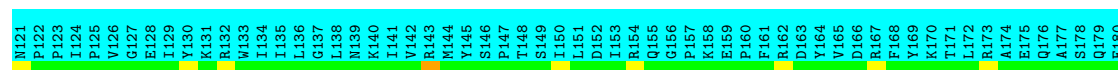
- Molecule 1: HIV-1 capsid protein

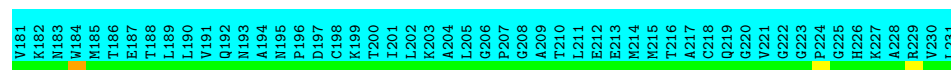
Chain 4E:

100%





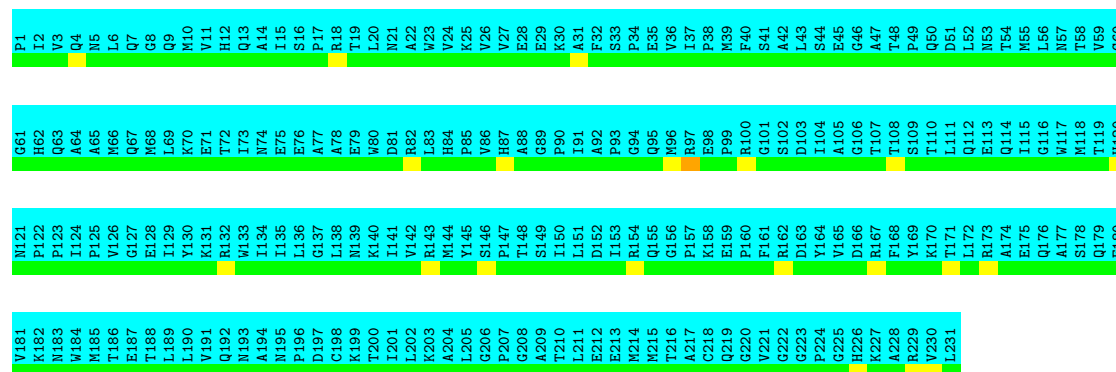




- Molecule 1: HIV-1 capsid protein

Chain BF:

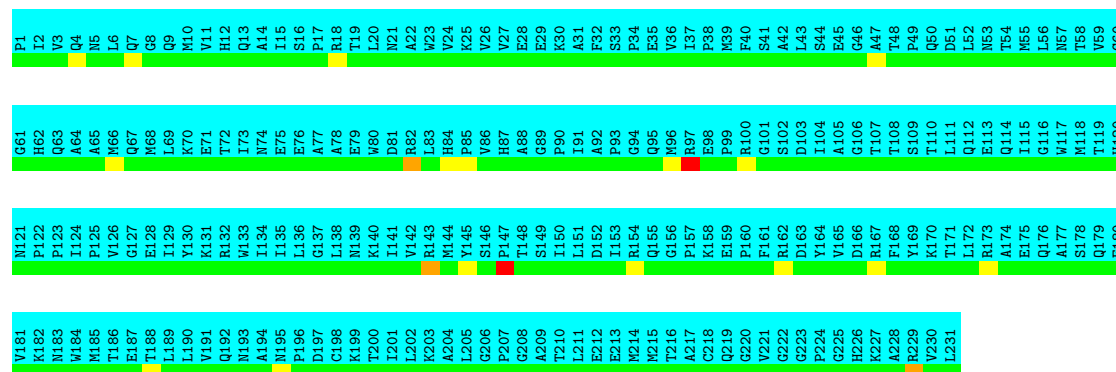
100%



- Molecule 1: HIV-1 capsid protein

Chain CF:

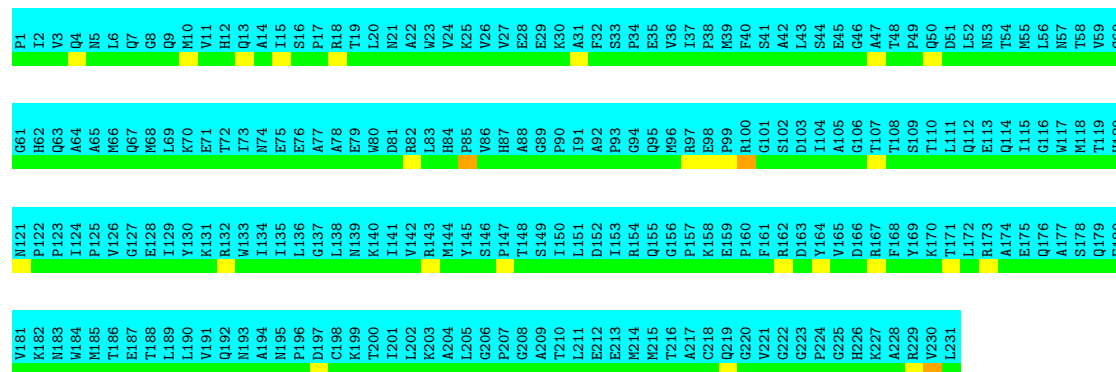
100%



- Molecule 1: HIV-1 capsid protein

Chain DF:

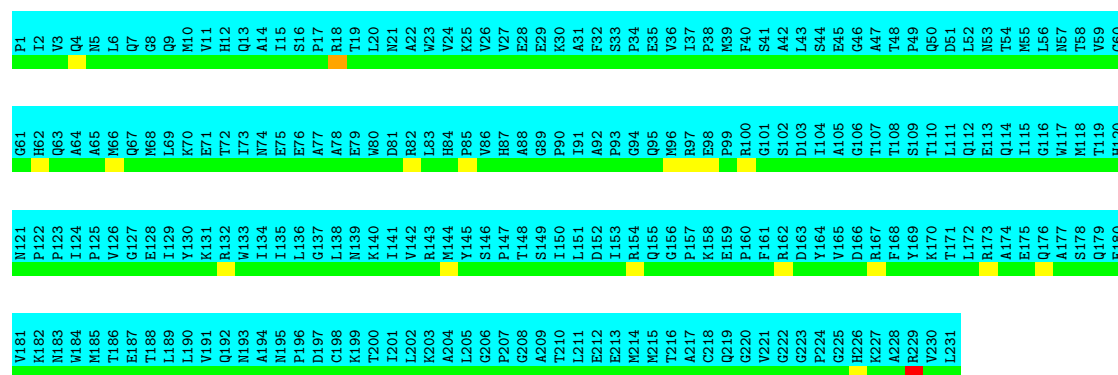
100%



- Molecule 1: HIV-1 capsid protein

Chain EF:

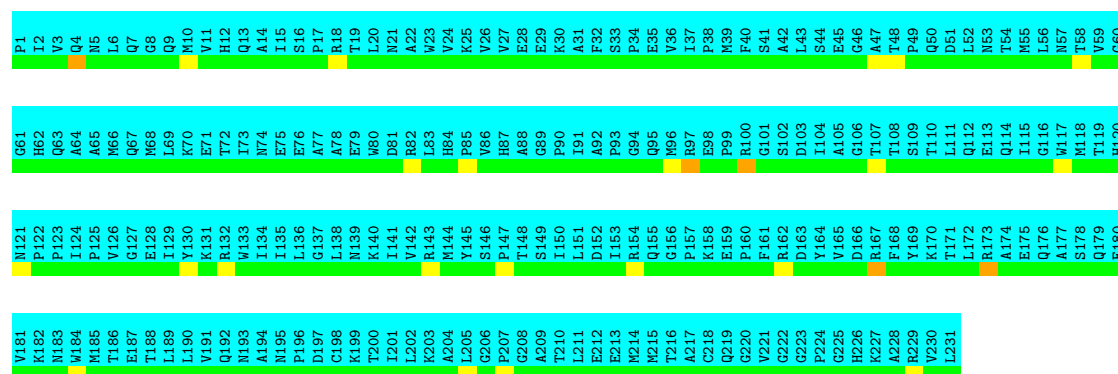
100%



• Molecule 1: HIV-1 capsid protein

Chain FF:

100%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *data-guided molecular dynamics*.

Of the 87 calculated structures, 1 were deposited, based on the following criterion: *inner turns of helical assembly*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
TALOS	structure calculation	
X-PLOR NIH	structure calculation	
X-PLOR NIH	refinement	
NAMD	structure calculation	2.13

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1126
Number of shifts mapped to atoms	1126
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	0	0	0	-

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is -.

There are no clashes.

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	0	0	-	-	-	-
1	0A	0	-	-	-	-
1	0B	0	-	-	-	-
1	0C	0	-	-	-	-
1	0D	0	-	-	-	-
1	0E	0	-	-	-	-

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1	0	-	-	-	-
1	1A	0	-	-	-	-
1	1B	0	-	-	-	-
1	1C	0	-	-	-	-
1	1D	0	-	-	-	-
1	1E	0	-	-	-	-
1	2	0	-	-	-	-
1	2A	0	-	-	-	-
1	2B	0	-	-	-	-
1	2C	0	-	-	-	-
1	2D	0	-	-	-	-
1	2E	0	-	-	-	-
1	3	0	-	-	-	-
1	3A	0	-	-	-	-
1	3B	0	-	-	-	-
1	3C	0	-	-	-	-
1	3D	0	-	-	-	-
1	3E	0	-	-	-	-
1	4	0	-	-	-	-
1	4A	0	-	-	-	-
1	4B	0	-	-	-	-
1	4C	0	-	-	-	-
1	4D	0	-	-	-	-
1	4E	0	-	-	-	-
1	5	0	-	-	-	-
1	5A	0	-	-	-	-
1	5B	0	-	-	-	-
1	5C	0	-	-	-	-
1	5D	0	-	-	-	-
1	5E	0	-	-	-	-
1	6	0	-	-	-	-
1	6A	0	-	-	-	-
1	6B	0	-	-	-	-
1	6C	0	-	-	-	-
1	6D	0	-	-	-	-
1	6E	0	-	-	-	-
1	7	0	-	-	-	-
1	7A	0	-	-	-	-
1	7B	0	-	-	-	-
1	7C	0	-	-	-	-
1	7D	0	-	-	-	-
1	7E	0	-	-	-	-

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	8	0	-	-	-	-
1	8A	0	-	-	-	-
1	8B	0	-	-	-	-
1	8C	0	-	-	-	-
1	8D	0	-	-	-	-
1	8E	0	-	-	-	-
1	9	0	-	-	-	-
1	9A	0	-	-	-	-
1	9B	0	-	-	-	-
1	9C	0	-	-	-	-
1	9D	0	-	-	-	-
1	9E	0	-	-	-	-
1	A	0	-	-	-	-
1	AA	0	-	-	-	-
1	AB	0	-	-	-	-
1	AC	0	-	-	-	-
1	AD	0	-	-	-	-
1	AE	0	-	-	-	-
1	AF	0	-	-	-	-
1	B	0	-	-	-	-
1	BA	0	-	-	-	-
1	BB	0	-	-	-	-
1	BC	0	-	-	-	-
1	BD	0	-	-	-	-
1	BE	0	-	-	-	-
1	BF	0	-	-	-	-
1	C	0	-	-	-	-
1	CA	0	-	-	-	-
1	CB	0	-	-	-	-
1	CC	0	-	-	-	-
1	CD	0	-	-	-	-
1	CE	0	-	-	-	-
1	CF	0	-	-	-	-
1	D	0	-	-	-	-
1	DA	0	-	-	-	-
1	DB	0	-	-	-	-
1	DC	0	-	-	-	-
1	DD	0	-	-	-	-
1	DE	0	-	-	-	-
1	DF	0	-	-	-	-
1	E	0	-	-	-	-
1	EA	0	-	-	-	-

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	EB	0	-	-	-	-
1	EC	0	-	-	-	-
1	ED	0	-	-	-	-
1	EE	0	-	-	-	-
1	EF	0	-	-	-	-
1	F	0	-	-	-	-
1	FA	0	-	-	-	-
1	FB	0	-	-	-	-
1	FC	0	-	-	-	-
1	FD	0	-	-	-	-
1	FE	0	-	-	-	-
1	FF	0	-	-	-	-
1	G	0	-	-	-	-
1	GA	0	-	-	-	-
1	GB	0	-	-	-	-
1	GC	0	-	-	-	-
1	GD	0	-	-	-	-
1	GE	0	-	-	-	-
1	H	0	-	-	-	-
1	HA	0	-	-	-	-
1	HB	0	-	-	-	-
1	HC	0	-	-	-	-
1	HD	0	-	-	-	-
1	HE	0	-	-	-	-
1	I	0	-	-	-	-
1	IA	0	-	-	-	-
1	IB	0	-	-	-	-
1	IC	0	-	-	-	-
1	ID	0	-	-	-	-
1	IE	0	-	-	-	-
1	J	0	-	-	-	-
1	JA	0	-	-	-	-
1	JB	0	-	-	-	-
1	JC	0	-	-	-	-
1	JD	0	-	-	-	-
1	JE	0	-	-	-	-
1	K	0	-	-	-	-
1	KA	0	-	-	-	-
1	KB	0	-	-	-	-
1	KC	0	-	-	-	-
1	KD	0	-	-	-	-
1	KE	0	-	-	-	-

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	L	0	-	-	-	-
1	LA	0	-	-	-	-
1	LB	0	-	-	-	-
1	LC	0	-	-	-	-
1	LD	0	-	-	-	-
1	LE	0	-	-	-	-
1	M	0	-	-	-	-
1	MA	0	-	-	-	-
1	MB	0	-	-	-	-
1	MC	0	-	-	-	-
1	MD	0	-	-	-	-
1	ME	0	-	-	-	-
1	N	0	-	-	-	-
1	NA	0	-	-	-	-
1	NB	0	-	-	-	-
1	NC	0	-	-	-	-
1	ND	0	-	-	-	-
1	NE	0	-	-	-	-
1	O	0	-	-	-	-
1	OA	0	-	-	-	-
1	OB	0	-	-	-	-
1	OC	0	-	-	-	-
1	OD	0	-	-	-	-
1	OE	0	-	-	-	-
1	P	0	-	-	-	-
1	PA	0	-	-	-	-
1	PB	0	-	-	-	-
1	PC	0	-	-	-	-
1	PD	0	-	-	-	-
1	PE	0	-	-	-	-
1	Q	0	-	-	-	-
1	QA	0	-	-	-	-
1	QB	0	-	-	-	-
1	QC	0	-	-	-	-
1	QD	0	-	-	-	-
1	QE	0	-	-	-	-
1	R	0	-	-	-	-
1	RA	0	-	-	-	-
1	RB	0	-	-	-	-
1	RC	0	-	-	-	-
1	RD	0	-	-	-	-
1	RE	0	-	-	-	-

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	S	0	-	-	-	-
1	SA	0	-	-	-	-
1	SB	0	-	-	-	-
1	SC	0	-	-	-	-
1	SD	0	-	-	-	-
1	SE	0	-	-	-	-
1	T	0	-	-	-	-
1	TA	0	-	-	-	-
1	TB	0	-	-	-	-
1	TC	0	-	-	-	-
1	TD	0	-	-	-	-
1	TE	0	-	-	-	-
1	U	0	-	-	-	-
1	UA	0	-	-	-	-
1	UB	0	-	-	-	-
1	UC	0	-	-	-	-
1	UD	0	-	-	-	-
1	UE	0	-	-	-	-
1	V	0	-	-	-	-
1	VA	0	-	-	-	-
1	VB	0	-	-	-	-
1	VC	0	-	-	-	-
1	VD	0	-	-	-	-
1	VE	0	-	-	-	-
1	W	0	-	-	-	-
1	WA	0	-	-	-	-
1	WB	0	-	-	-	-
1	WC	0	-	-	-	-
1	WD	0	-	-	-	-
1	WE	0	-	-	-	-
1	X	0	-	-	-	-
1	XA	0	-	-	-	-
1	XB	0	-	-	-	-
1	XC	0	-	-	-	-
1	XD	0	-	-	-	-
1	XE	0	-	-	-	-
1	Y	0	-	-	-	-
1	YA	0	-	-	-	-
1	YB	0	-	-	-	-
1	YC	0	-	-	-	-
1	YD	0	-	-	-	-
1	YE	0	-	-	-	-

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	Z	0	-	-	-	-
1	ZA	0	-	-	-	-
1	ZB	0	-	-	-	-
1	ZC	0	-	-	-	-
1	ZD	0	-	-	-	-
1	ZE	0	-	-	-	-
1	a	0	-	-	-	-
1	aA	0	-	-	-	-
1	aB	0	-	-	-	-
1	aC	0	-	-	-	-
1	aD	0	-	-	-	-
1	aE	0	-	-	-	-
1	b	0	-	-	-	-
1	bA	0	-	-	-	-
1	bB	0	-	-	-	-
1	bC	0	-	-	-	-
1	bD	0	-	-	-	-
1	bE	0	-	-	-	-
1	c	0	-	-	-	-
1	cA	0	-	-	-	-
1	cB	0	-	-	-	-
1	cC	0	-	-	-	-
1	cD	0	-	-	-	-
1	cE	0	-	-	-	-
1	d	0	-	-	-	-
1	dA	0	-	-	-	-
1	dB	0	-	-	-	-
1	dC	0	-	-	-	-
1	dD	0	-	-	-	-
1	dE	0	-	-	-	-
1	e	0	-	-	-	-
1	eA	0	-	-	-	-
1	eB	0	-	-	-	-
1	eC	0	-	-	-	-
1	eD	0	-	-	-	-
1	eE	0	-	-	-	-
1	f	0	-	-	-	-
1	fA	0	-	-	-	-
1	fB	0	-	-	-	-
1	fC	0	-	-	-	-
1	fD	0	-	-	-	-
1	fE	0	-	-	-	-

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	g	0	-	-	-	-
1	gA	0	-	-	-	-
1	gB	0	-	-	-	-
1	gC	0	-	-	-	-
1	gD	0	-	-	-	-
1	gE	0	-	-	-	-
1	h	0	-	-	-	-
1	hA	0	-	-	-	-
1	hB	0	-	-	-	-
1	hC	0	-	-	-	-
1	hD	0	-	-	-	-
1	hE	0	-	-	-	-
1	i	0	-	-	-	-
1	iA	0	-	-	-	-
1	iB	0	-	-	-	-
1	iC	0	-	-	-	-
1	iD	0	-	-	-	-
1	iE	0	-	-	-	-
1	j	0	-	-	-	-
1	jA	0	-	-	-	-
1	jB	0	-	-	-	-
1	jC	0	-	-	-	-
1	jD	0	-	-	-	-
1	jE	0	-	-	-	-
1	k	0	-	-	-	-
1	kA	0	-	-	-	-
1	kB	0	-	-	-	-
1	kC	0	-	-	-	-
1	kD	0	-	-	-	-
1	kE	0	-	-	-	-
1	l	0	-	-	-	-
1	lA	0	-	-	-	-
1	lB	0	-	-	-	-
1	lC	0	-	-	-	-
1	lD	0	-	-	-	-
1	lE	0	-	-	-	-
1	m	0	-	-	-	-
1	mA	0	-	-	-	-
1	mB	0	-	-	-	-
1	mC	0	-	-	-	-
1	mD	0	-	-	-	-
1	mE	0	-	-	-	-

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	n	0	-	-	-	-
1	nA	0	-	-	-	-
1	nB	0	-	-	-	-
1	nC	0	-	-	-	-
1	nD	0	-	-	-	-
1	nE	0	-	-	-	-
1	o	0	-	-	-	-
1	oA	0	-	-	-	-
1	oB	0	-	-	-	-
1	oC	0	-	-	-	-
1	oD	0	-	-	-	-
1	oE	0	-	-	-	-
1	p	0	-	-	-	-
1	pA	0	-	-	-	-
1	pB	0	-	-	-	-
1	pC	0	-	-	-	-
1	pD	0	-	-	-	-
1	pE	0	-	-	-	-
1	q	0	-	-	-	-
1	qA	0	-	-	-	-
1	qB	0	-	-	-	-
1	qC	0	-	-	-	-
1	qD	0	-	-	-	-
1	qE	0	-	-	-	-
1	r	0	-	-	-	-
1	rA	0	-	-	-	-
1	rB	0	-	-	-	-
1	rC	0	-	-	-	-
1	rD	0	-	-	-	-
1	rE	0	-	-	-	-
1	s	0	-	-	-	-
1	sA	0	-	-	-	-
1	sB	0	-	-	-	-
1	sC	0	-	-	-	-
1	sD	0	-	-	-	-
1	sE	0	-	-	-	-
1	t	0	-	-	-	-
1	tA	0	-	-	-	-
1	tB	0	-	-	-	-
1	tC	0	-	-	-	-
1	tD	0	-	-	-	-
1	tE	0	-	-	-	-

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	u	0	-	-	-	-
1	uA	0	-	-	-	-
1	uB	0	-	-	-	-
1	uC	0	-	-	-	-
1	uD	0	-	-	-	-
1	uE	0	-	-	-	-
1	v	0	-	-	-	-
1	vA	0	-	-	-	-
1	vB	0	-	-	-	-
1	vC	0	-	-	-	-
1	vD	0	-	-	-	-
1	vE	0	-	-	-	-
1	w	0	-	-	-	-
1	wA	0	-	-	-	-
1	wB	0	-	-	-	-
1	wC	0	-	-	-	-
1	wD	0	-	-	-	-
1	wE	0	-	-	-	-
1	x	0	-	-	-	-
1	xA	0	-	-	-	-
1	xB	0	-	-	-	-
1	xC	0	-	-	-	-
1	xD	0	-	-	-	-
1	xE	0	-	-	-	-
1	y	0	-	-	-	-
1	yA	0	-	-	-	-
1	yB	0	-	-	-	-
1	yC	0	-	-	-	-
1	yD	0	-	-	-	-
1	yE	0	-	-	-	-
1	z	0	-	-	-	-
1	zA	0	-	-	-	-
1	zB	0	-	-	-	-
1	zC	0	-	-	-	-
1	zD	0	-	-	-	-
1	zE	0	-	-	-	-
All	All	0	-	-	-	-

There are no Ramachandran outliers.

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	0	0	-	-	-
1	0A	0	-	-	-
1	0B	0	-	-	-
1	0C	0	-	-	-
1	0D	0	-	-	-
1	0E	0	-	-	-
1	1	0	-	-	-
1	1A	0	-	-	-
1	1B	0	-	-	-
1	1C	0	-	-	-
1	1D	0	-	-	-
1	1E	0	-	-	-
1	2	0	-	-	-
1	2A	0	-	-	-
1	2B	0	-	-	-
1	2C	0	-	-	-
1	2D	0	-	-	-
1	2E	0	-	-	-
1	3	0	-	-	-
1	3A	0	-	-	-
1	3B	0	-	-	-
1	3C	0	-	-	-
1	3D	0	-	-	-
1	3E	0	-	-	-
1	4	0	-	-	-
1	4A	0	-	-	-
1	4B	0	-	-	-
1	4C	0	-	-	-
1	4D	0	-	-	-
1	4E	0	-	-	-
1	5	0	-	-	-
1	5A	0	-	-	-
1	5B	0	-	-	-
1	5C	0	-	-	-
1	5D	0	-	-	-
1	5E	0	-	-	-
1	6	0	-	-	-

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	6A	0	-	-	-
1	6B	0	-	-	-
1	6C	0	-	-	-
1	6D	0	-	-	-
1	6E	0	-	-	-
1	7	0	-	-	-
1	7A	0	-	-	-
1	7B	0	-	-	-
1	7C	0	-	-	-
1	7D	0	-	-	-
1	7E	0	-	-	-
1	8	0	-	-	-
1	8A	0	-	-	-
1	8B	0	-	-	-
1	8C	0	-	-	-
1	8D	0	-	-	-
1	8E	0	-	-	-
1	9	0	-	-	-
1	9A	0	-	-	-
1	9B	0	-	-	-
1	9C	0	-	-	-
1	9D	0	-	-	-
1	9E	0	-	-	-
1	A	0	-	-	-
1	AA	0	-	-	-
1	AB	0	-	-	-
1	AC	0	-	-	-
1	AD	0	-	-	-
1	AE	0	-	-	-
1	AF	0	-	-	-
1	B	0	-	-	-
1	BA	0	-	-	-
1	BB	0	-	-	-
1	BC	0	-	-	-
1	BD	0	-	-	-
1	BE	0	-	-	-
1	BF	0	-	-	-
1	C	0	-	-	-
1	CA	0	-	-	-
1	CB	0	-	-	-
1	CC	0	-	-	-
1	CD	0	-	-	-

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	CE	0	-	-	-
1	CF	0	-	-	-
1	D	0	-	-	-
1	DA	0	-	-	-
1	DB	0	-	-	-
1	DC	0	-	-	-
1	DD	0	-	-	-
1	DE	0	-	-	-
1	DF	0	-	-	-
1	E	0	-	-	-
1	EA	0	-	-	-
1	EB	0	-	-	-
1	EC	0	-	-	-
1	ED	0	-	-	-
1	EE	0	-	-	-
1	EF	0	-	-	-
1	F	0	-	-	-
1	FA	0	-	-	-
1	FB	0	-	-	-
1	FC	0	-	-	-
1	FD	0	-	-	-
1	FE	0	-	-	-
1	FF	0	-	-	-
1	G	0	-	-	-
1	GA	0	-	-	-
1	GB	0	-	-	-
1	GC	0	-	-	-
1	GD	0	-	-	-
1	GE	0	-	-	-
1	H	0	-	-	-
1	HA	0	-	-	-
1	HB	0	-	-	-
1	HC	0	-	-	-
1	HD	0	-	-	-
1	HE	0	-	-	-
1	I	0	-	-	-
1	IA	0	-	-	-
1	IB	0	-	-	-
1	IC	0	-	-	-
1	ID	0	-	-	-
1	IE	0	-	-	-
1	J	0	-	-	-

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	JA	0	-	-	-
1	JB	0	-	-	-
1	JC	0	-	-	-
1	JD	0	-	-	-
1	JE	0	-	-	-
1	K	0	-	-	-
1	KA	0	-	-	-
1	KB	0	-	-	-
1	KC	0	-	-	-
1	KD	0	-	-	-
1	KE	0	-	-	-
1	L	0	-	-	-
1	LA	0	-	-	-
1	LB	0	-	-	-
1	LC	0	-	-	-
1	LD	0	-	-	-
1	LE	0	-	-	-
1	M	0	-	-	-
1	MA	0	-	-	-
1	MB	0	-	-	-
1	MC	0	-	-	-
1	MD	0	-	-	-
1	ME	0	-	-	-
1	N	0	-	-	-
1	NA	0	-	-	-
1	NB	0	-	-	-
1	NC	0	-	-	-
1	ND	0	-	-	-
1	NE	0	-	-	-
1	O	0	-	-	-
1	OA	0	-	-	-
1	OB	0	-	-	-
1	OC	0	-	-	-
1	OD	0	-	-	-
1	OE	0	-	-	-
1	P	0	-	-	-
1	PA	0	-	-	-
1	PB	0	-	-	-
1	PC	0	-	-	-
1	PD	0	-	-	-
1	PE	0	-	-	-
1	Q	0	-	-	-

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	QA	0	-	-	-
1	QB	0	-	-	-
1	QC	0	-	-	-
1	QD	0	-	-	-
1	QE	0	-	-	-
1	R	0	-	-	-
1	RA	0	-	-	-
1	RB	0	-	-	-
1	RC	0	-	-	-
1	RD	0	-	-	-
1	RE	0	-	-	-
1	S	0	-	-	-
1	SA	0	-	-	-
1	SB	0	-	-	-
1	SC	0	-	-	-
1	SD	0	-	-	-
1	SE	0	-	-	-
1	T	0	-	-	-
1	TA	0	-	-	-
1	TB	0	-	-	-
1	TC	0	-	-	-
1	TD	0	-	-	-
1	TE	0	-	-	-
1	U	0	-	-	-
1	UA	0	-	-	-
1	UB	0	-	-	-
1	UC	0	-	-	-
1	UD	0	-	-	-
1	UE	0	-	-	-
1	V	0	-	-	-
1	VA	0	-	-	-
1	VB	0	-	-	-
1	VC	0	-	-	-
1	VD	0	-	-	-
1	VE	0	-	-	-
1	W	0	-	-	-
1	WA	0	-	-	-
1	WB	0	-	-	-
1	WC	0	-	-	-
1	WD	0	-	-	-
1	WE	0	-	-	-
1	X	0	-	-	-

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	XA	0	-	-	-
1	XB	0	-	-	-
1	XC	0	-	-	-
1	XD	0	-	-	-
1	XE	0	-	-	-
1	Y	0	-	-	-
1	YA	0	-	-	-
1	YB	0	-	-	-
1	YC	0	-	-	-
1	YD	0	-	-	-
1	YE	0	-	-	-
1	Z	0	-	-	-
1	ZA	0	-	-	-
1	ZB	0	-	-	-
1	ZC	0	-	-	-
1	ZD	0	-	-	-
1	ZE	0	-	-	-
1	a	0	-	-	-
1	aA	0	-	-	-
1	aB	0	-	-	-
1	aC	0	-	-	-
1	aD	0	-	-	-
1	aE	0	-	-	-
1	b	0	-	-	-
1	bA	0	-	-	-
1	bB	0	-	-	-
1	bC	0	-	-	-
1	bD	0	-	-	-
1	bE	0	-	-	-
1	c	0	-	-	-
1	cA	0	-	-	-
1	cB	0	-	-	-
1	cC	0	-	-	-
1	cD	0	-	-	-
1	cE	0	-	-	-
1	d	0	-	-	-
1	dA	0	-	-	-
1	dB	0	-	-	-
1	dC	0	-	-	-
1	dD	0	-	-	-
1	dE	0	-	-	-
1	e	0	-	-	-

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	eA	0	-	-	-
1	eB	0	-	-	-
1	eC	0	-	-	-
1	eD	0	-	-	-
1	eE	0	-	-	-
1	f	0	-	-	-
1	fA	0	-	-	-
1	fB	0	-	-	-
1	fC	0	-	-	-
1	fD	0	-	-	-
1	fE	0	-	-	-
1	g	0	-	-	-
1	gA	0	-	-	-
1	gB	0	-	-	-
1	gC	0	-	-	-
1	gD	0	-	-	-
1	gE	0	-	-	-
1	h	0	-	-	-
1	hA	0	-	-	-
1	hB	0	-	-	-
1	hC	0	-	-	-
1	hD	0	-	-	-
1	hE	0	-	-	-
1	i	0	-	-	-
1	iA	0	-	-	-
1	iB	0	-	-	-
1	iC	0	-	-	-
1	iD	0	-	-	-
1	iE	0	-	-	-
1	j	0	-	-	-
1	jA	0	-	-	-
1	jB	0	-	-	-
1	jC	0	-	-	-
1	jD	0	-	-	-
1	jE	0	-	-	-
1	k	0	-	-	-
1	kA	0	-	-	-
1	kB	0	-	-	-
1	kC	0	-	-	-
1	kD	0	-	-	-
1	kE	0	-	-	-
1	l	0	-	-	-

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	lA	0	-	-	-
1	lB	0	-	-	-
1	lC	0	-	-	-
1	lD	0	-	-	-
1	lE	0	-	-	-
1	m	0	-	-	-
1	mA	0	-	-	-
1	mB	0	-	-	-
1	mC	0	-	-	-
1	mD	0	-	-	-
1	mE	0	-	-	-
1	n	0	-	-	-
1	nA	0	-	-	-
1	nB	0	-	-	-
1	nC	0	-	-	-
1	nD	0	-	-	-
1	nE	0	-	-	-
1	o	0	-	-	-
1	oA	0	-	-	-
1	oB	0	-	-	-
1	oC	0	-	-	-
1	oD	0	-	-	-
1	oE	0	-	-	-
1	p	0	-	-	-
1	pA	0	-	-	-
1	pB	0	-	-	-
1	pC	0	-	-	-
1	pD	0	-	-	-
1	pE	0	-	-	-
1	q	0	-	-	-
1	qA	0	-	-	-
1	qB	0	-	-	-
1	qC	0	-	-	-
1	qD	0	-	-	-
1	qE	0	-	-	-
1	r	0	-	-	-
1	rA	0	-	-	-
1	rB	0	-	-	-
1	rC	0	-	-	-
1	rD	0	-	-	-
1	rE	0	-	-	-
1	s	0	-	-	-

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	sA	0	-	-	-
1	sB	0	-	-	-
1	sC	0	-	-	-
1	sD	0	-	-	-
1	sE	0	-	-	-
1	t	0	-	-	-
1	tA	0	-	-	-
1	tB	0	-	-	-
1	tC	0	-	-	-
1	tD	0	-	-	-
1	tE	0	-	-	-
1	u	0	-	-	-
1	uA	0	-	-	-
1	uB	0	-	-	-
1	uC	0	-	-	-
1	uD	0	-	-	-
1	uE	0	-	-	-
1	v	0	-	-	-
1	vA	0	-	-	-
1	vB	0	-	-	-
1	vC	0	-	-	-
1	vD	0	-	-	-
1	vE	0	-	-	-
1	w	0	-	-	-
1	wA	0	-	-	-
1	wB	0	-	-	-
1	wC	0	-	-	-
1	wD	0	-	-	-
1	wE	0	-	-	-
1	x	0	-	-	-
1	xA	0	-	-	-
1	xB	0	-	-	-
1	xC	0	-	-	-
1	xD	0	-	-	-
1	xE	0	-	-	-
1	y	0	-	-	-
1	yA	0	-	-	-
1	yB	0	-	-	-
1	yC	0	-	-	-
1	yD	0	-	-	-
1	yE	0	-	-	-
1	z	0	-	-	-

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	zA	0	-	-	-
1	zB	0	-	-	-
1	zC	0	-	-	-
1	zD	0	-	-	-
1	zE	0	-	-	-
All	All	0	-	-	-

There are no protein residues with a non-rotameric sidechain to report.

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 0% for the well-defined parts and 0% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1126
Number of shifts mapped to atoms	1126
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	223	-0.48 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	205	0.47 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	190	-0.48 ± 0.14	None needed (< 0.5 ppm)
^{15}N	209	0.38 ± 0.20	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 1076 atoms were assigned a chemical shift out of a possible 1068228. 2 out of 12474 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	612/422982 (0%)	0/167832 (0%)	413/174636 (0%)	199/80514 (0%)
Sidechain	424/580986 (0%)	0/342090 (0%)	424/212814 (0%)	0/26082 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	40/64260 (0%)	0/34020 (0%)	40/26082 (0%)	0/4158 (0%)
Overall	1076/1068228 (0%)	0/543942 (0%)	877/413532 (0%)	199/110754 (0%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 1076 atoms were assigned a chemical shift out of a possible 1068228. 2 out of 12474 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	612/422982 (0%)	0/167832 (0%)	413/174636 (0%)	199/80514 (0%)
Sidechain	424/580986 (0%)	0/342090 (0%)	424/212814 (0%)	0/26082 (0%)
Aromatic	40/64260 (0%)	0/34020 (0%)	40/26082 (0%)	0/4158 (0%)
Overall	1076/1068228 (0%)	0/543942 (0%)	877/413532 (0%)	199/110754 (0%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots ⓘ

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list) due to size of model.