



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:33 PM GMT

PDB ID : 4V60  
Title : The structure of rat liver vault at 3.5 angstrom resolution  
Authors : Kato, K.; Zhou, Y.; Tanaka, H.; Yao, M.; Yamashita, E.; Yoshimura, M.;  
Tsukihara, T.  
Deposited on : 2008-10-24  
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

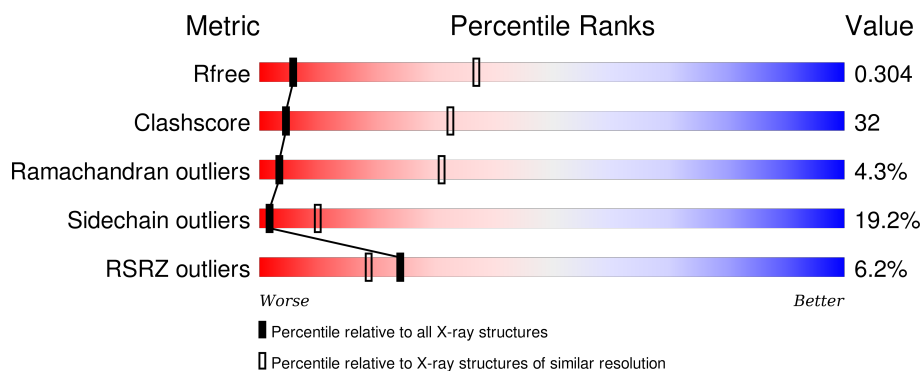
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	861	<div> <div>5%</div> <div>33% 46% 14% • 6%</div> </div>
1	B	861	<div> <div>5%</div> <div>33% 49% 11% • 6%</div> </div>
1	C	861	<div> <div>5%</div> <div>31% 51% 11% • 6%</div> </div>
1	D	861	<div> <div>6%</div> <div>31% 51% 12% • 6%</div> </div>
1	E	861	<div> <div>8%</div> <div>32% 50% 12% • 6%</div> </div>




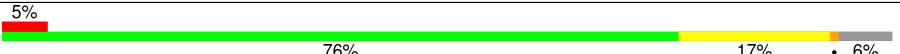
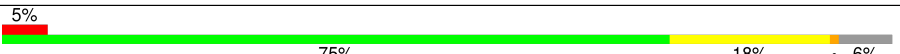
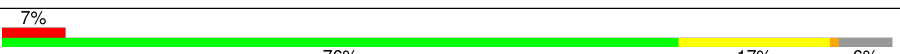
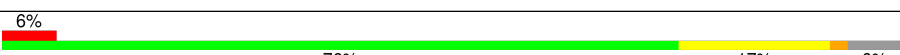
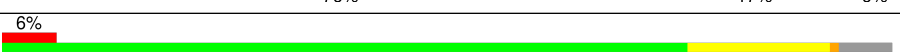

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Mol	Chain	Length	Quality of chain
1	F	861	
1	G	861	
1	H	861	
1	I	861	
1	J	861	
1	K	861	
1	L	861	
1	M	861	
1	N	861	
1	O	861	
1	P	861	
1	Q	861	
1	R	861	
1	S	861	
1	T	861	
1	U	861	
1	V	861	
1	W	861	
1	X	861	
1	Y	861	
1	Z	861	
1	a	861	
1	b	861	
1	c	861	
1	d	861	

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Mol	Chain	Length	Quality of chain
1	e	861	
1	f	861	
1	g	861	
1	h	861	
1	i	861	
1	j	861	
1	k	861	
1	l	861	
1	m	861	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 241956 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Major vault protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	B	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	C	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	D	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	E	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	F	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	G	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	H	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	I	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	J	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	K	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	L	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	M	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	N	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	O	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	P	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	R	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	S	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	T	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	U	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	V	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	W	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	X	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	Y	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	Z	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	a	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	b	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	c	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	d	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	e	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	f	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	g	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	h	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	i	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	j	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	k	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30

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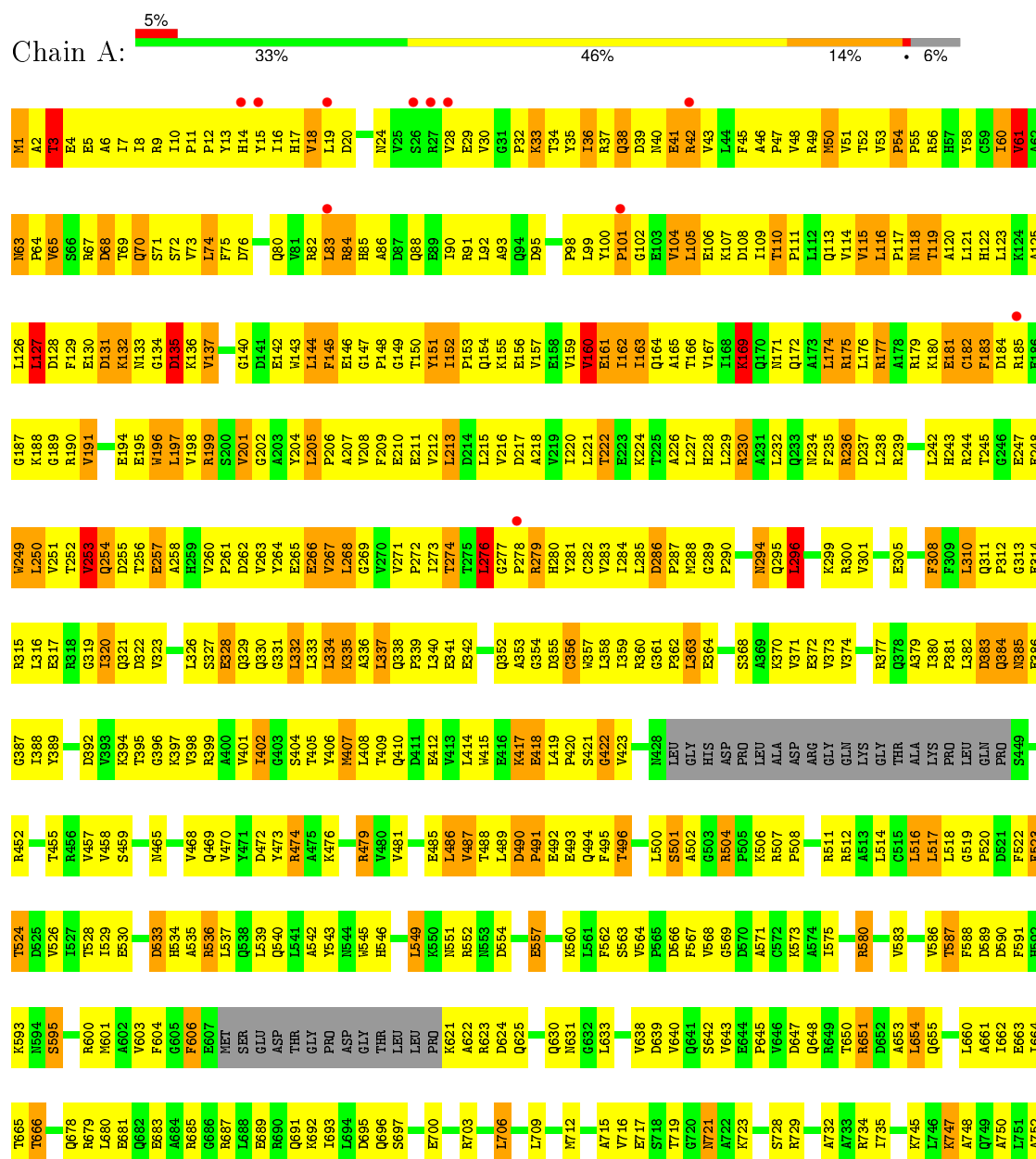
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	l	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	m	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			

### 3 Residue-property plots

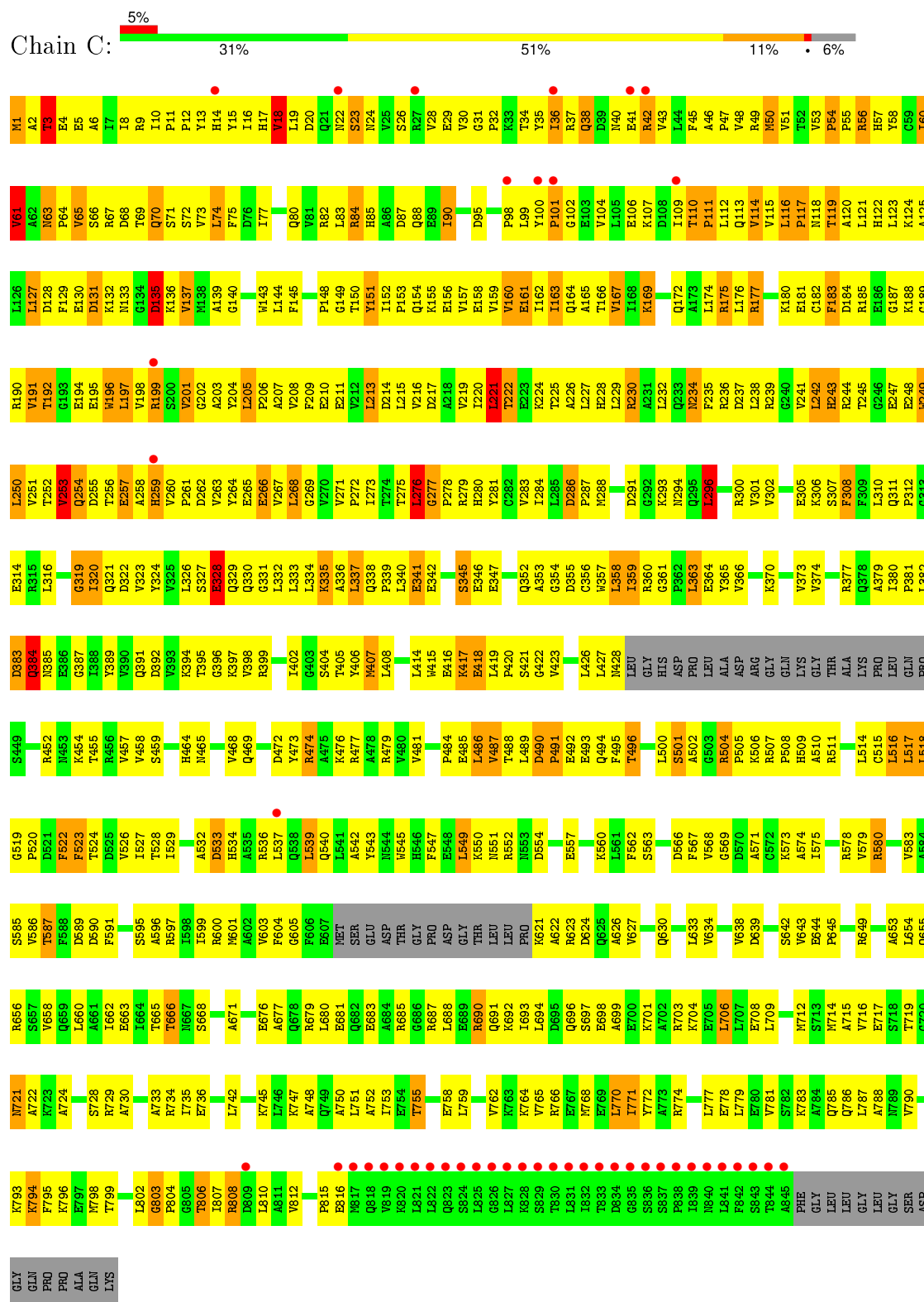
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

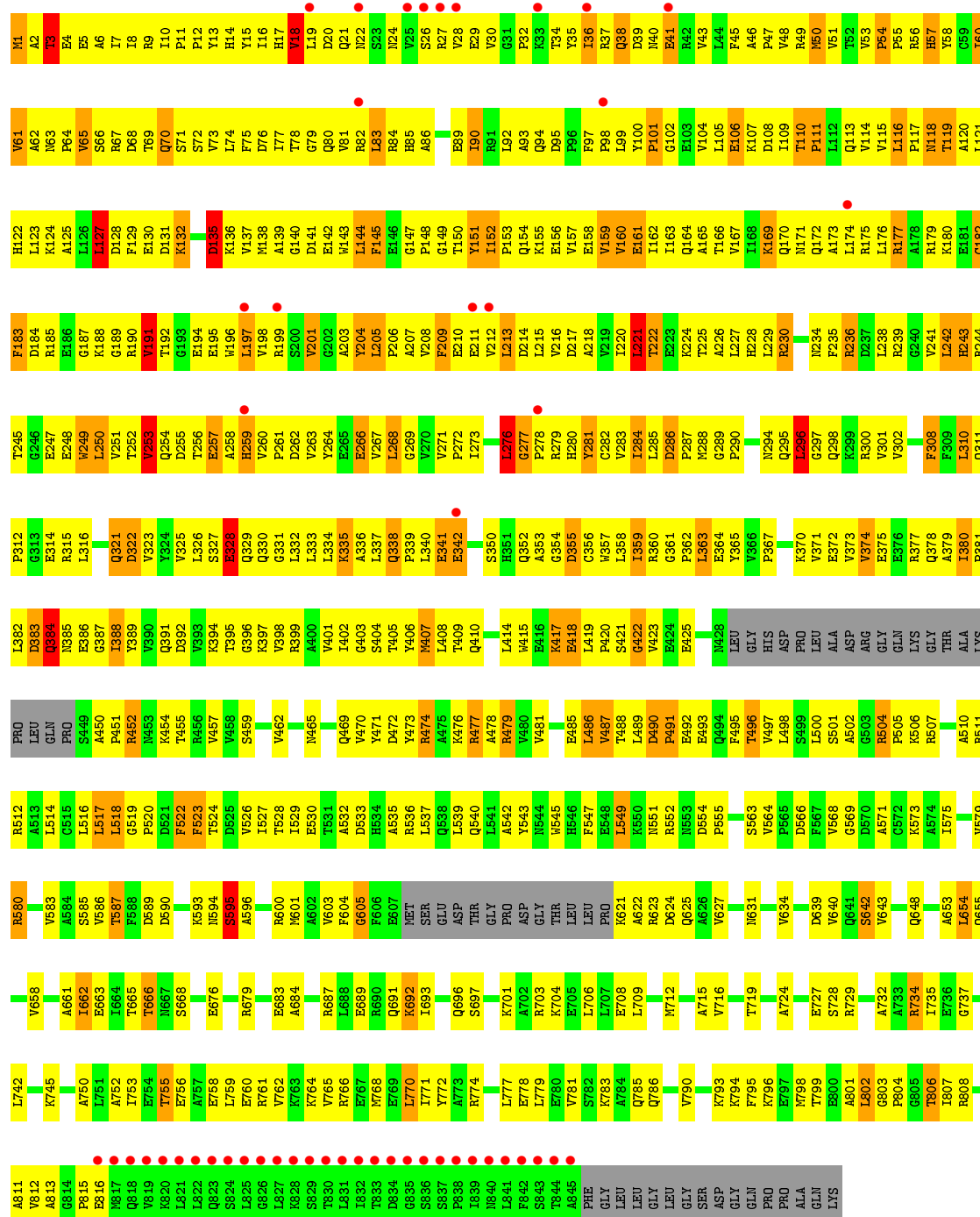
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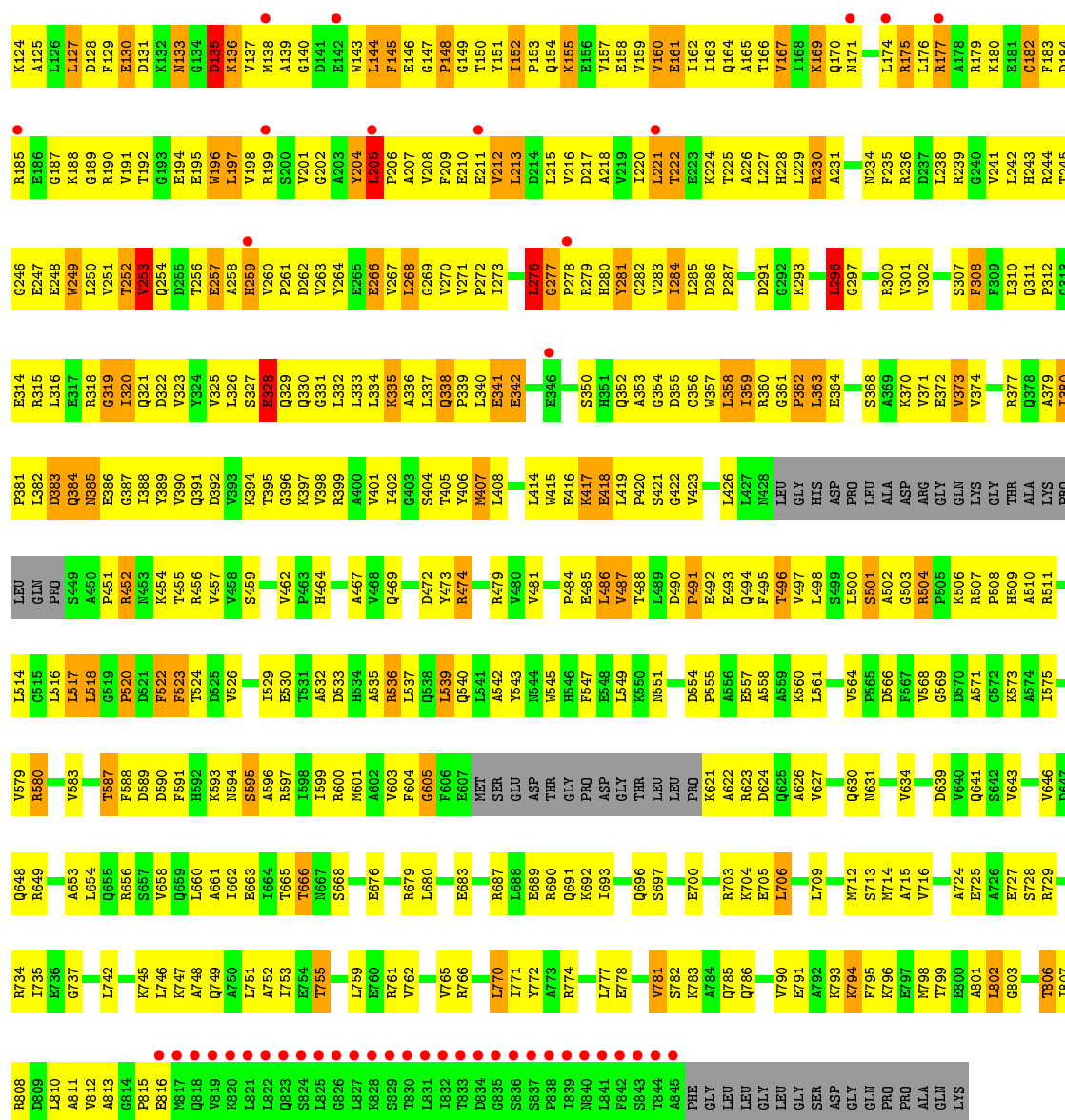


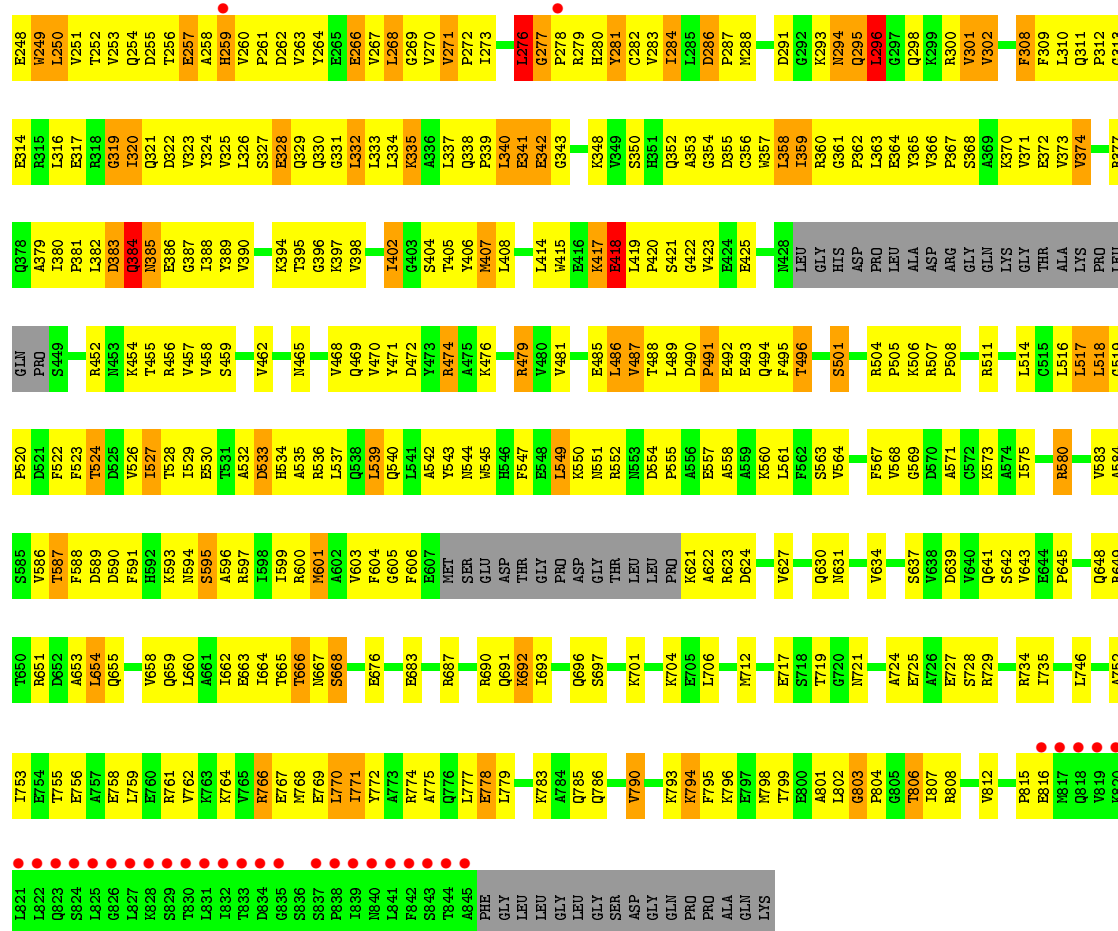


• Molecule 1: Major vault protein

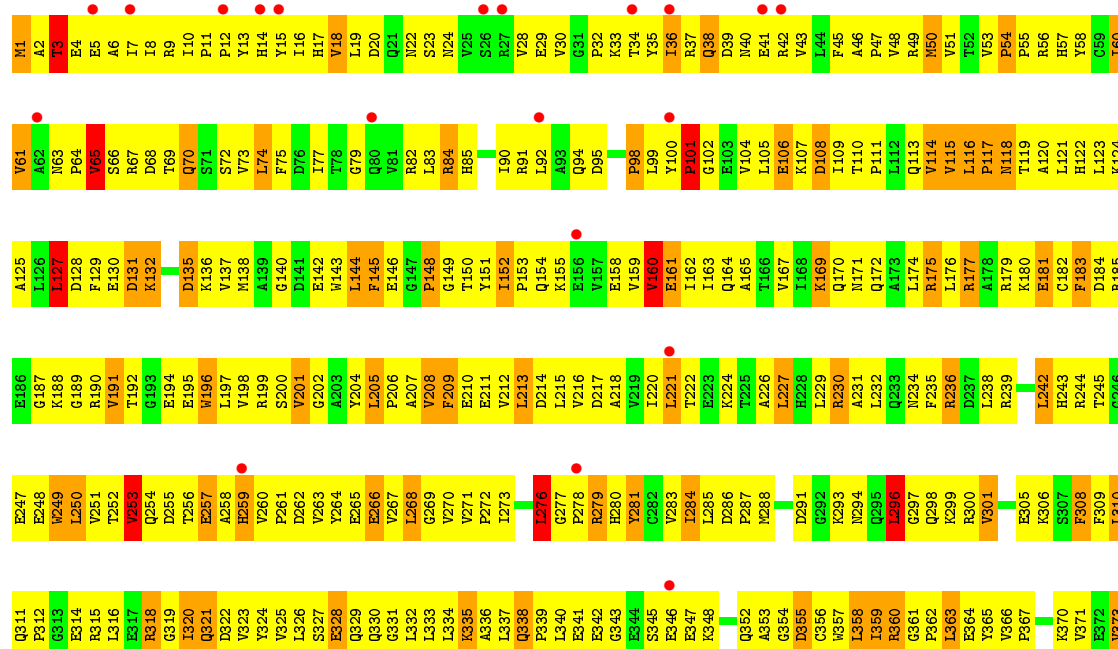




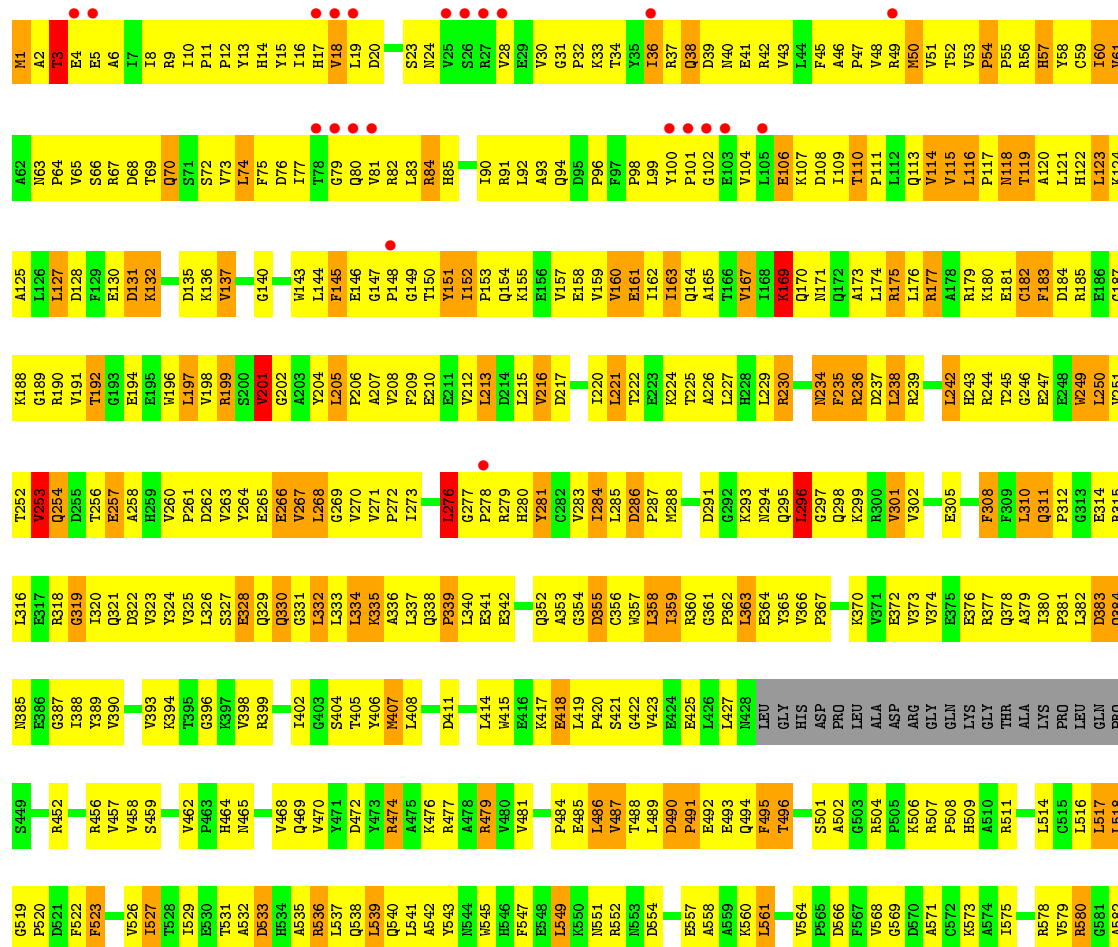


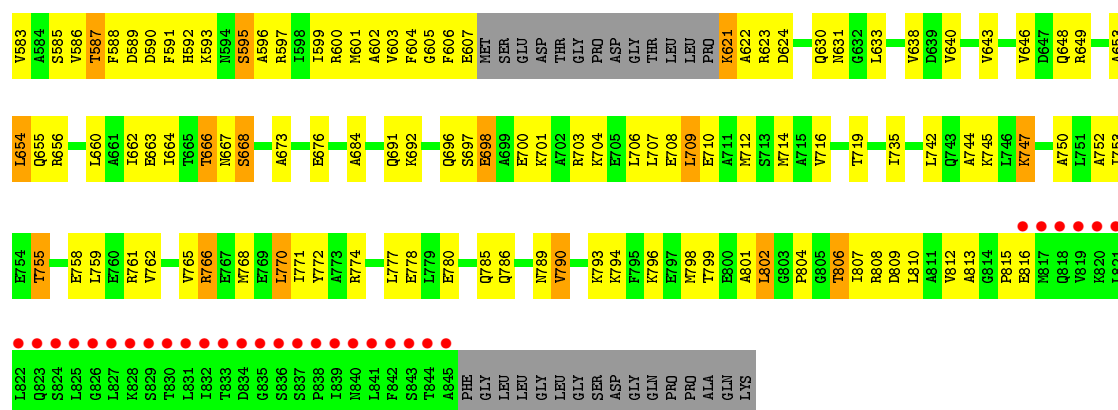


• Molecule 1: Major vault protein

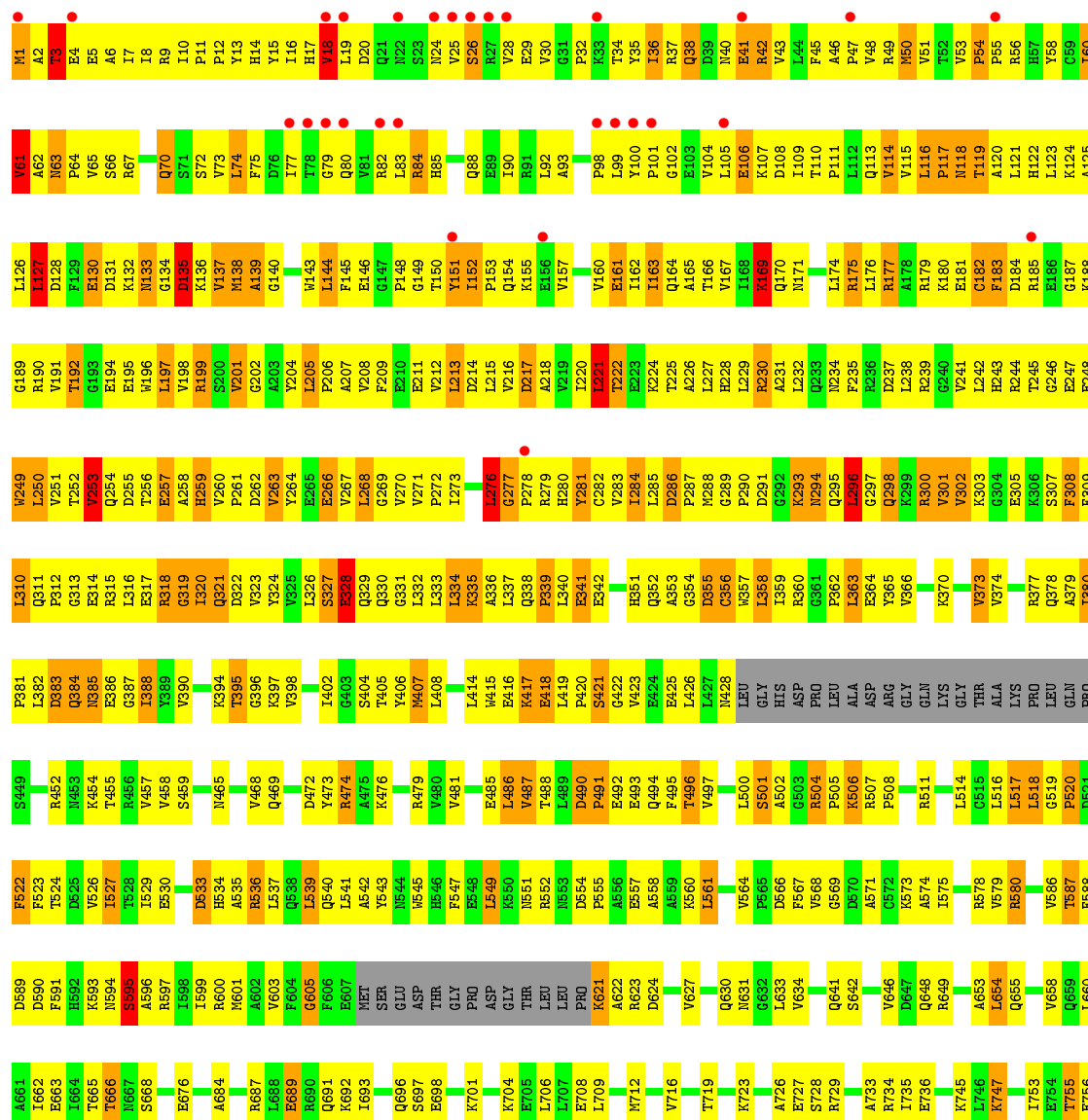


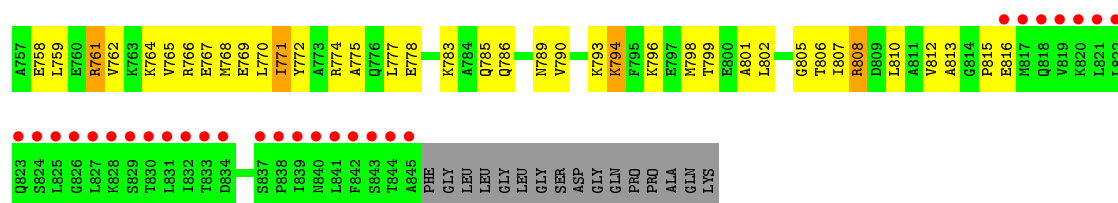




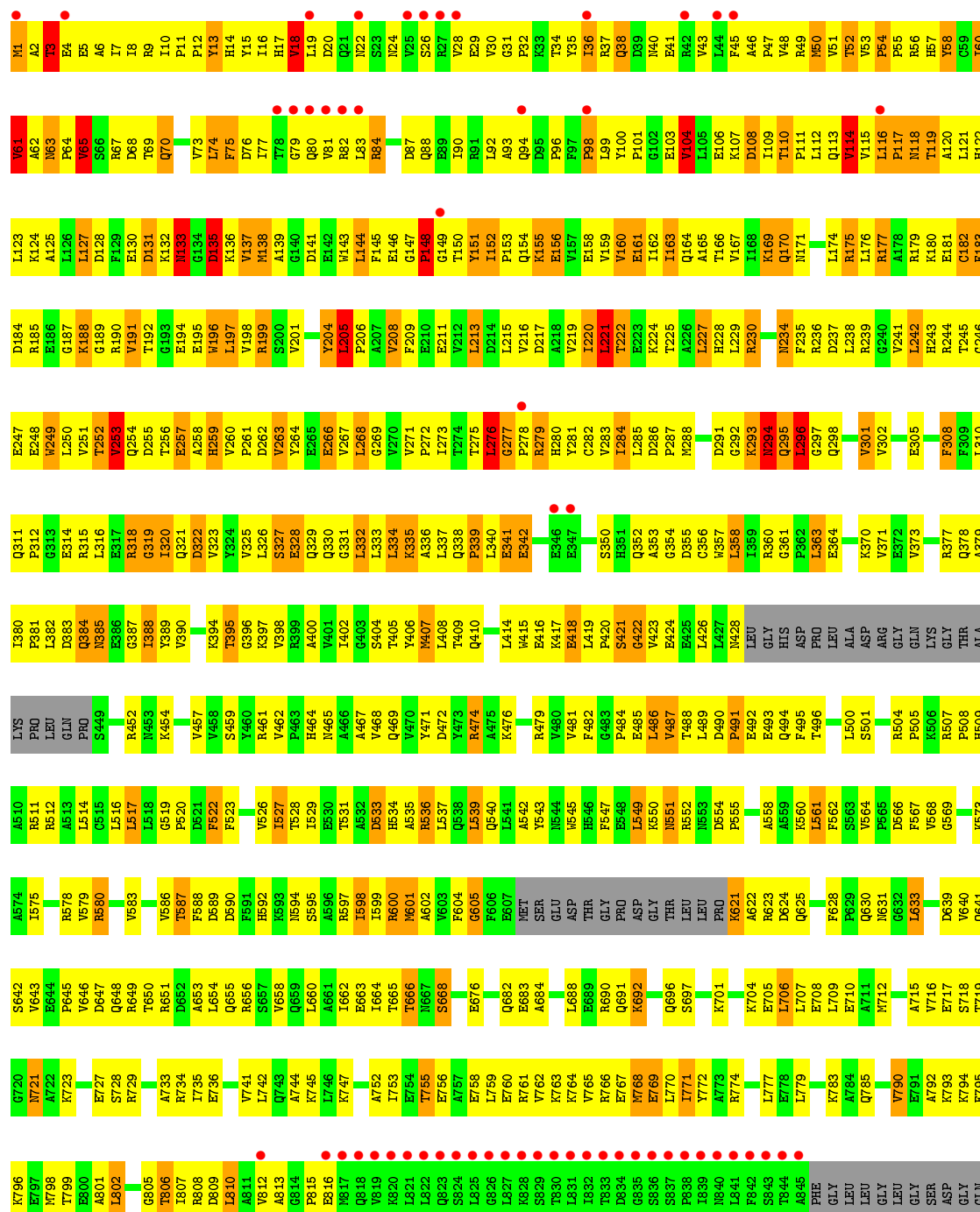


# Molecule 1: Major vault protein



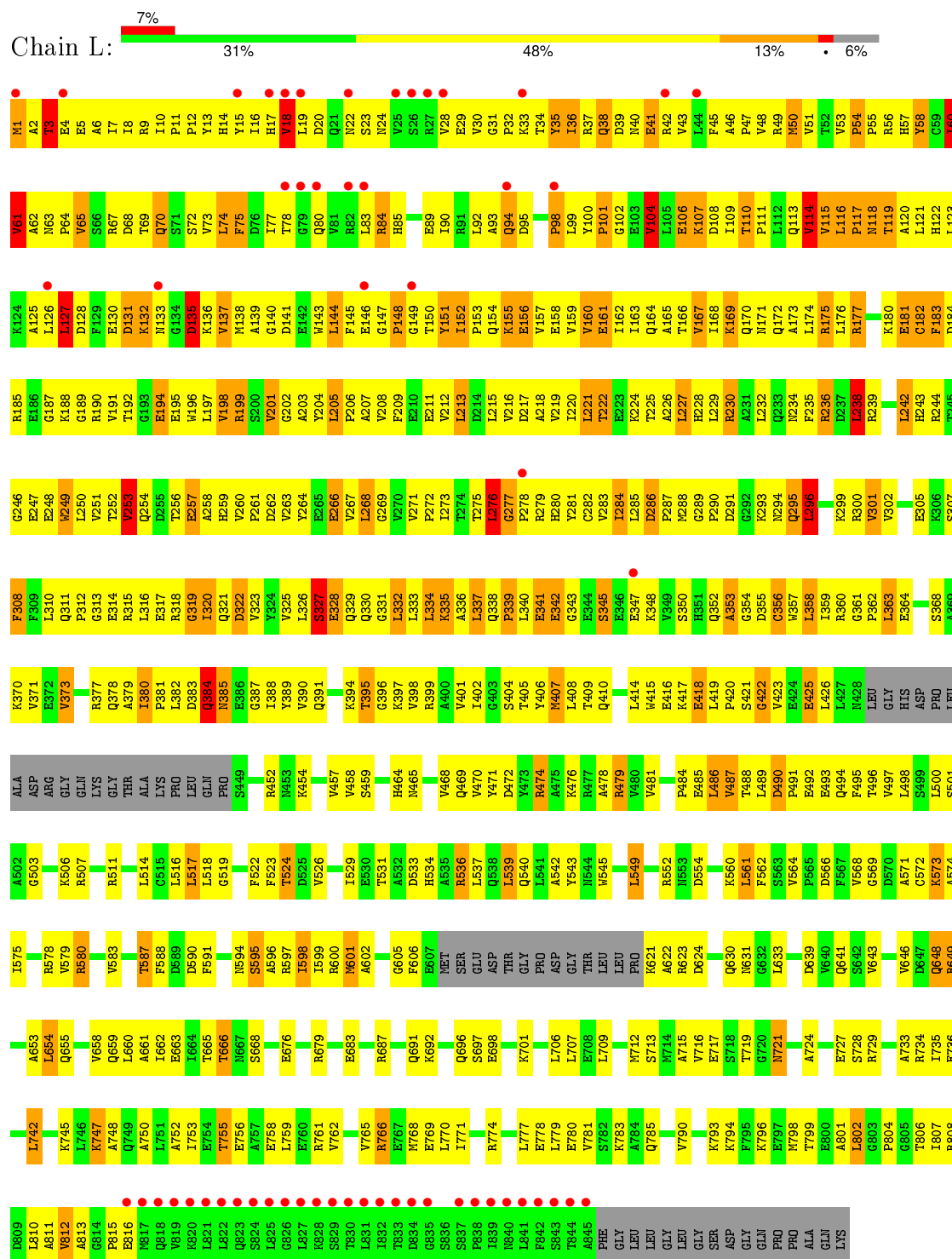


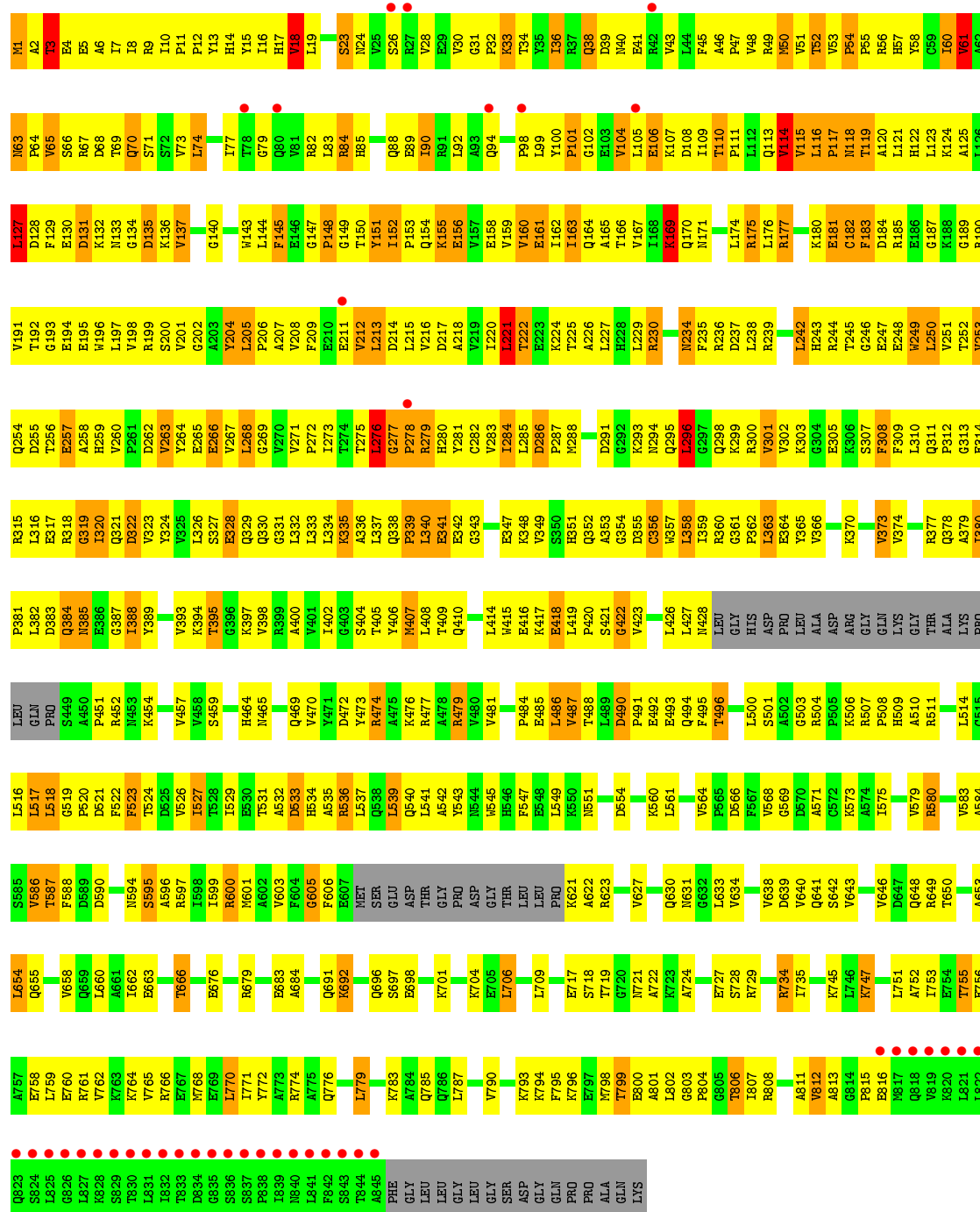
# Molecule 1: Major vault protein



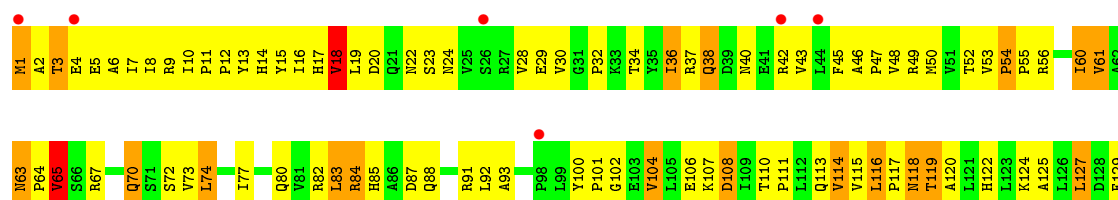
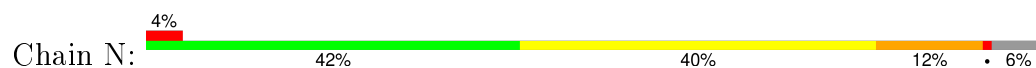
PRO  
PRO  
ALA  
GLN  
LYS

• Molecule 1: Major vault protein

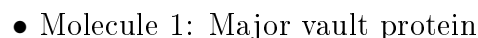




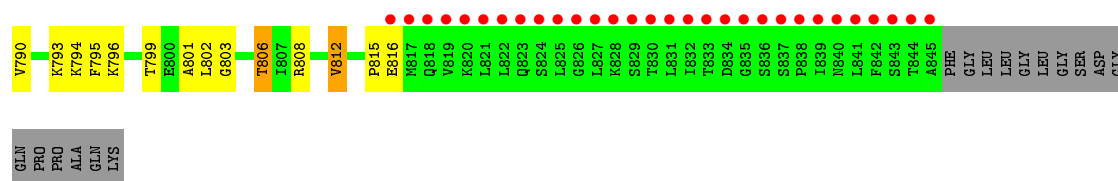
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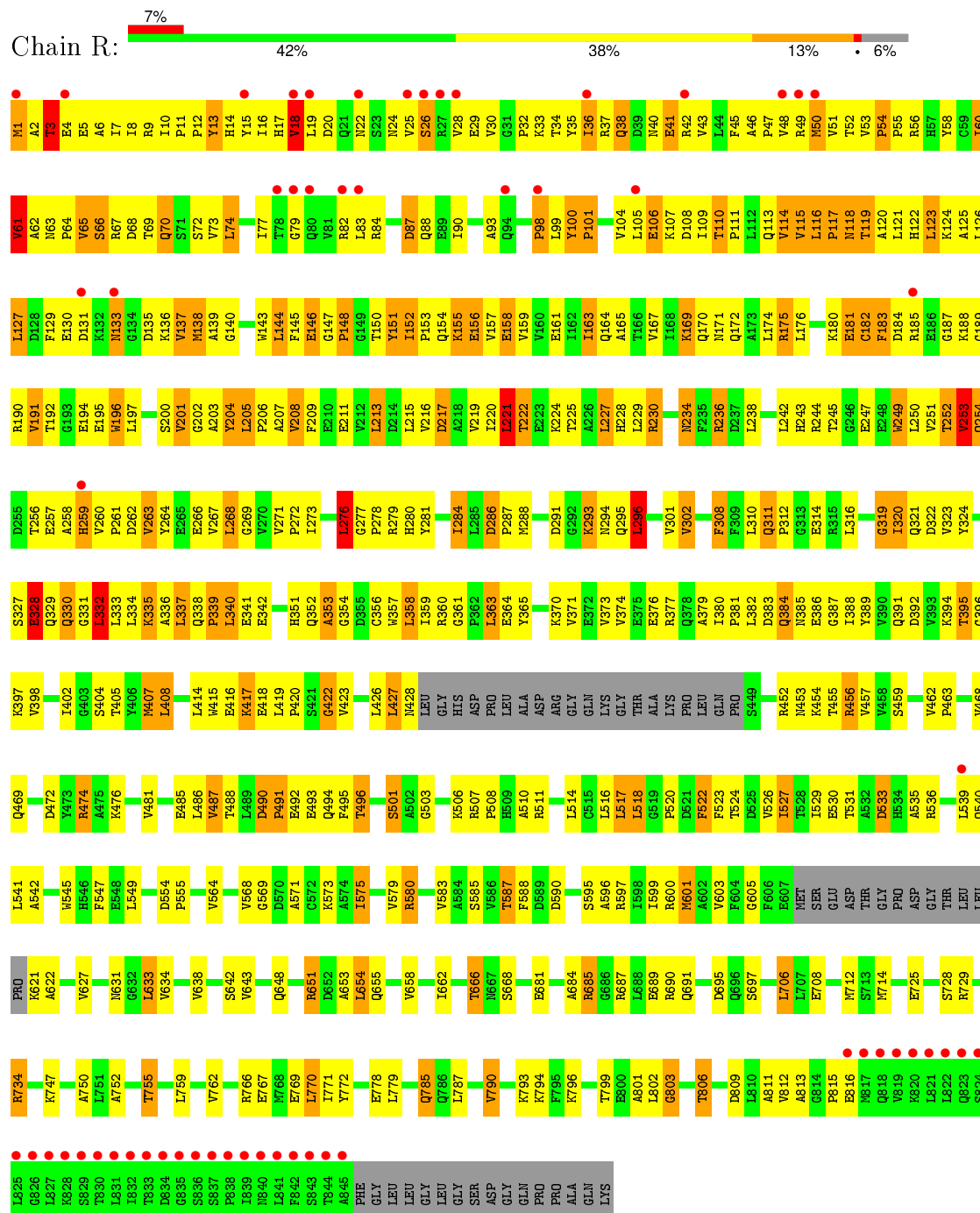




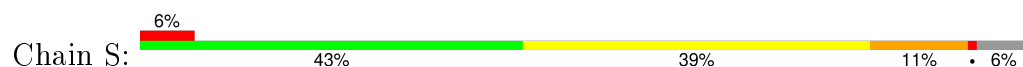


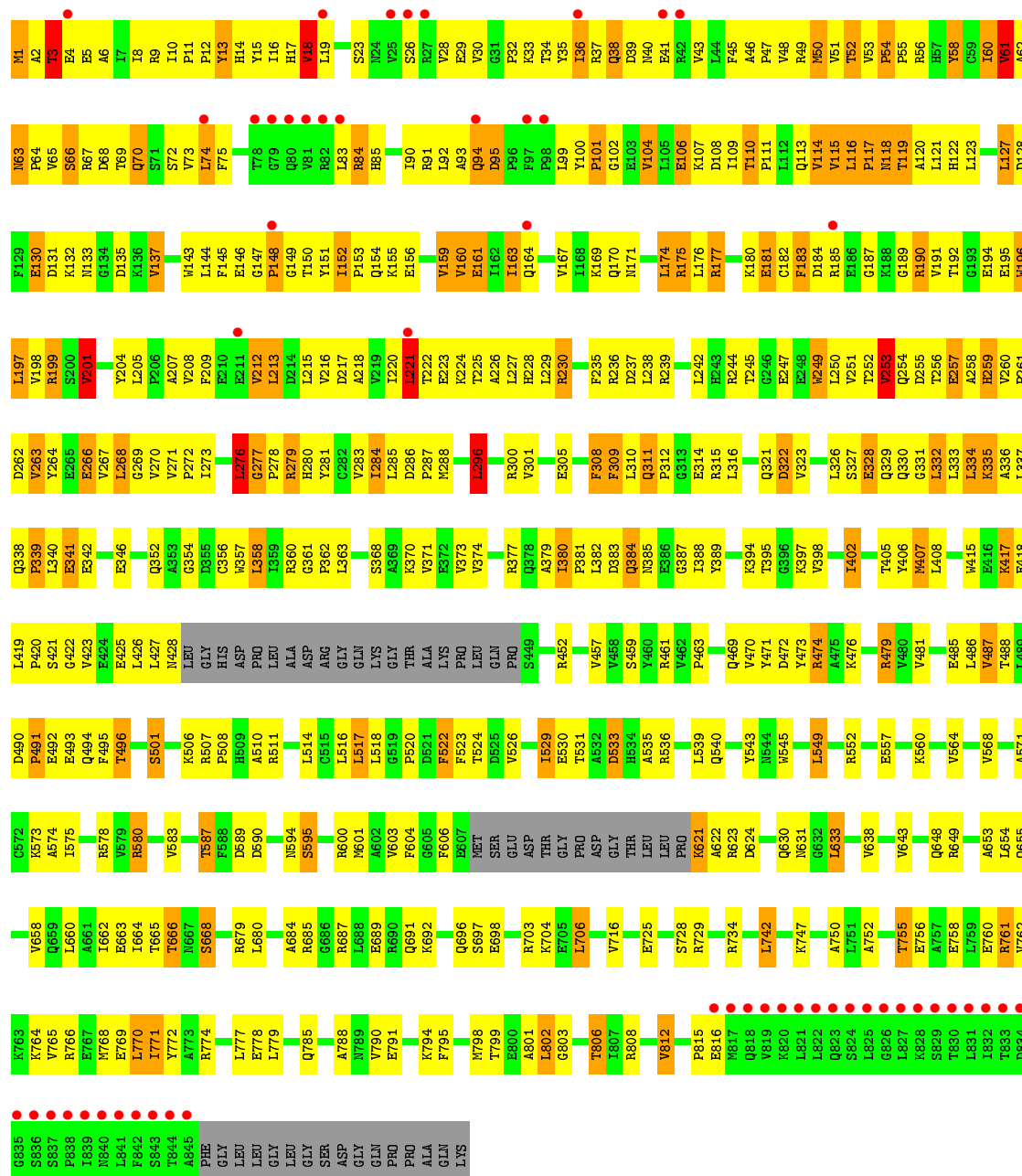


• Molecule 1: Major vault protein

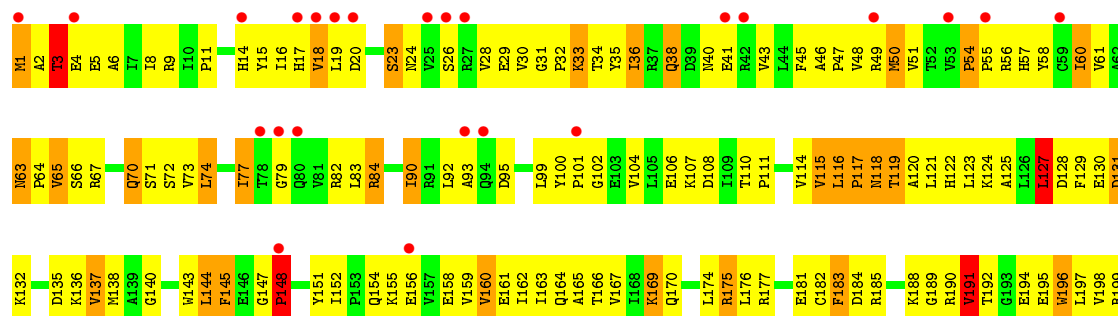


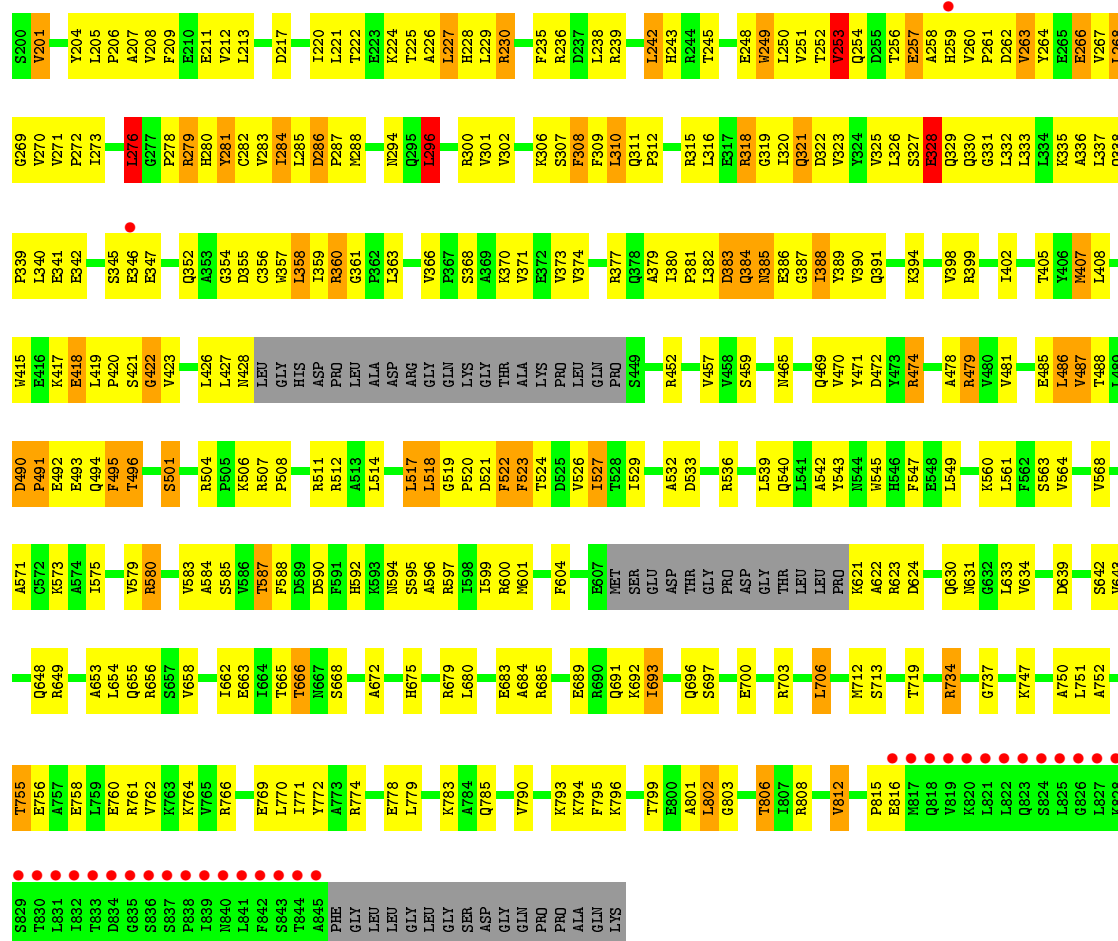
• Molecule 1: Major vault protein



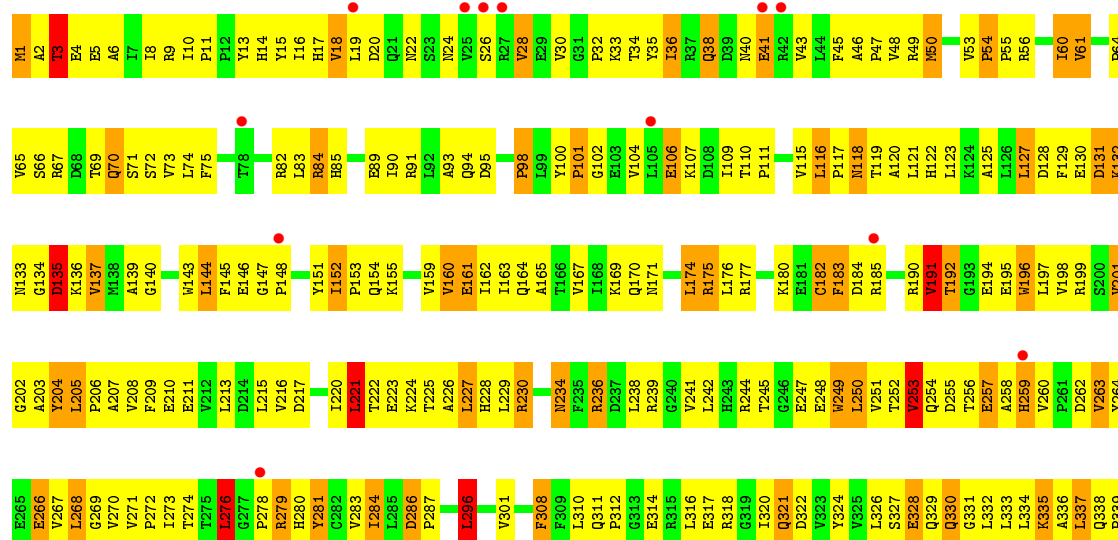


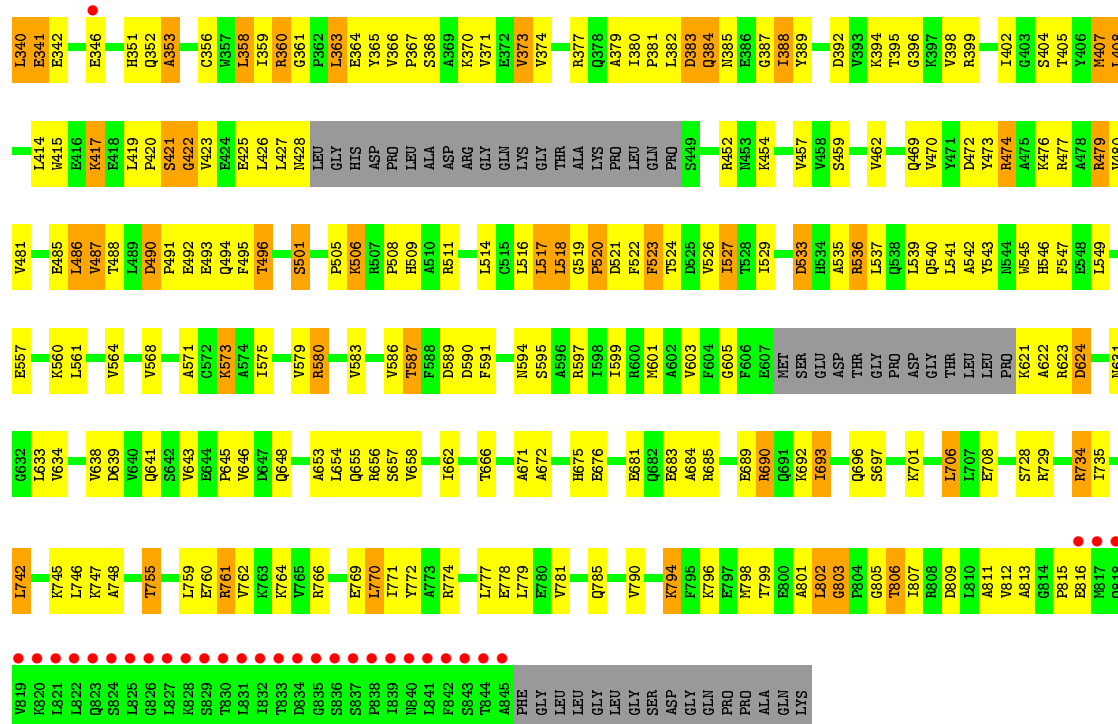
● Molecule 1: Major vault protein



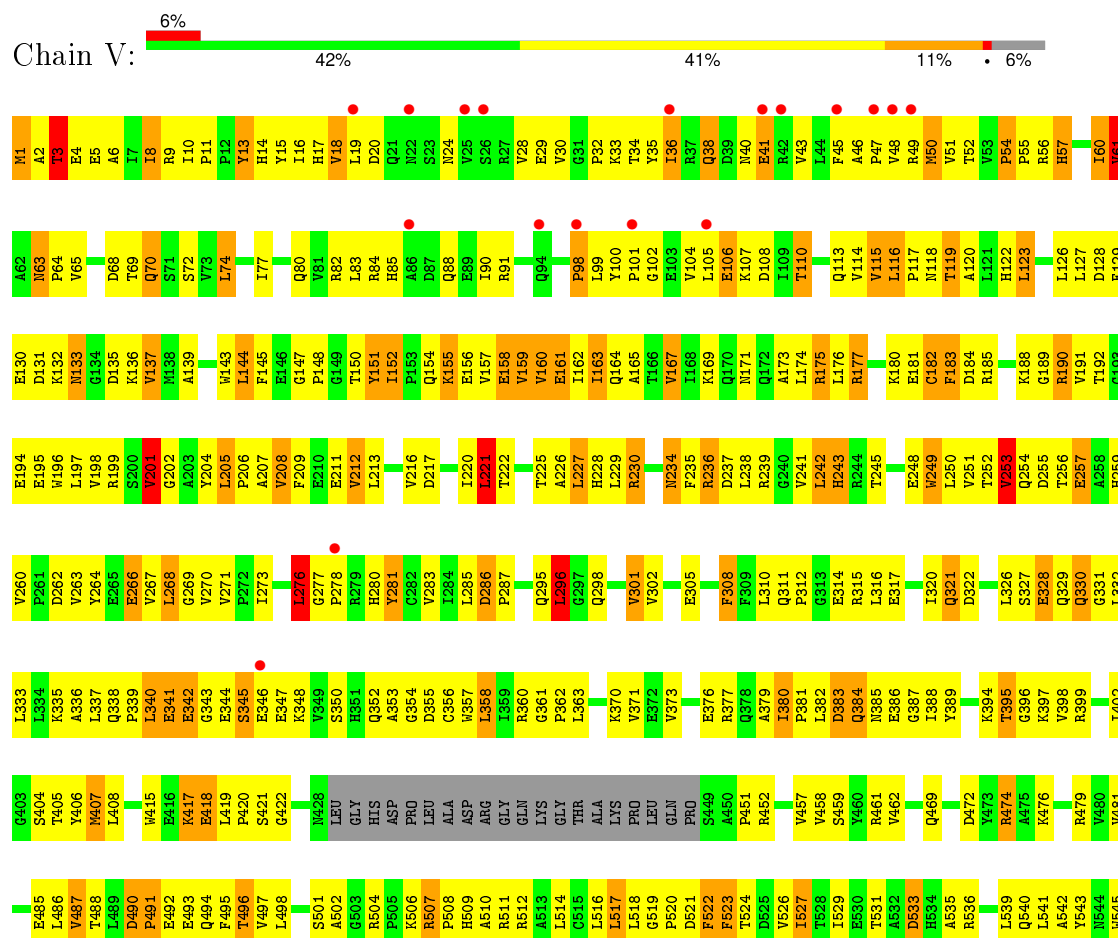


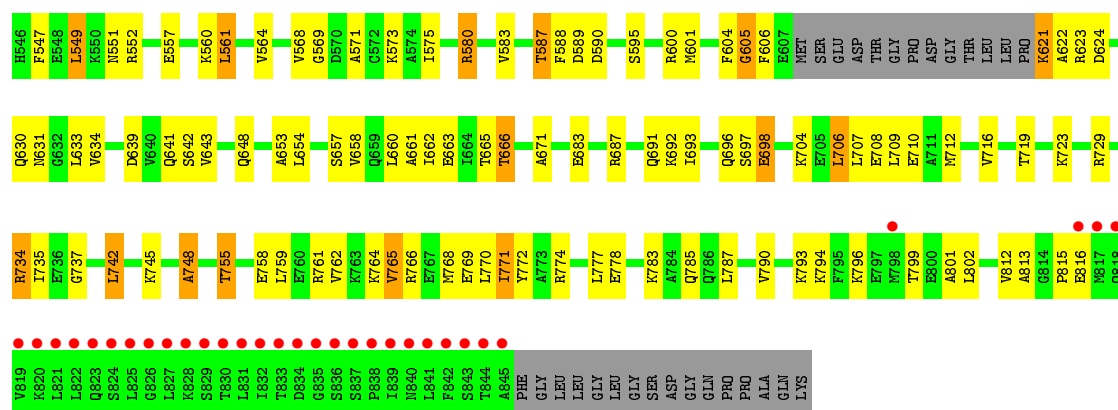
• Molecule 1: Major vault protein



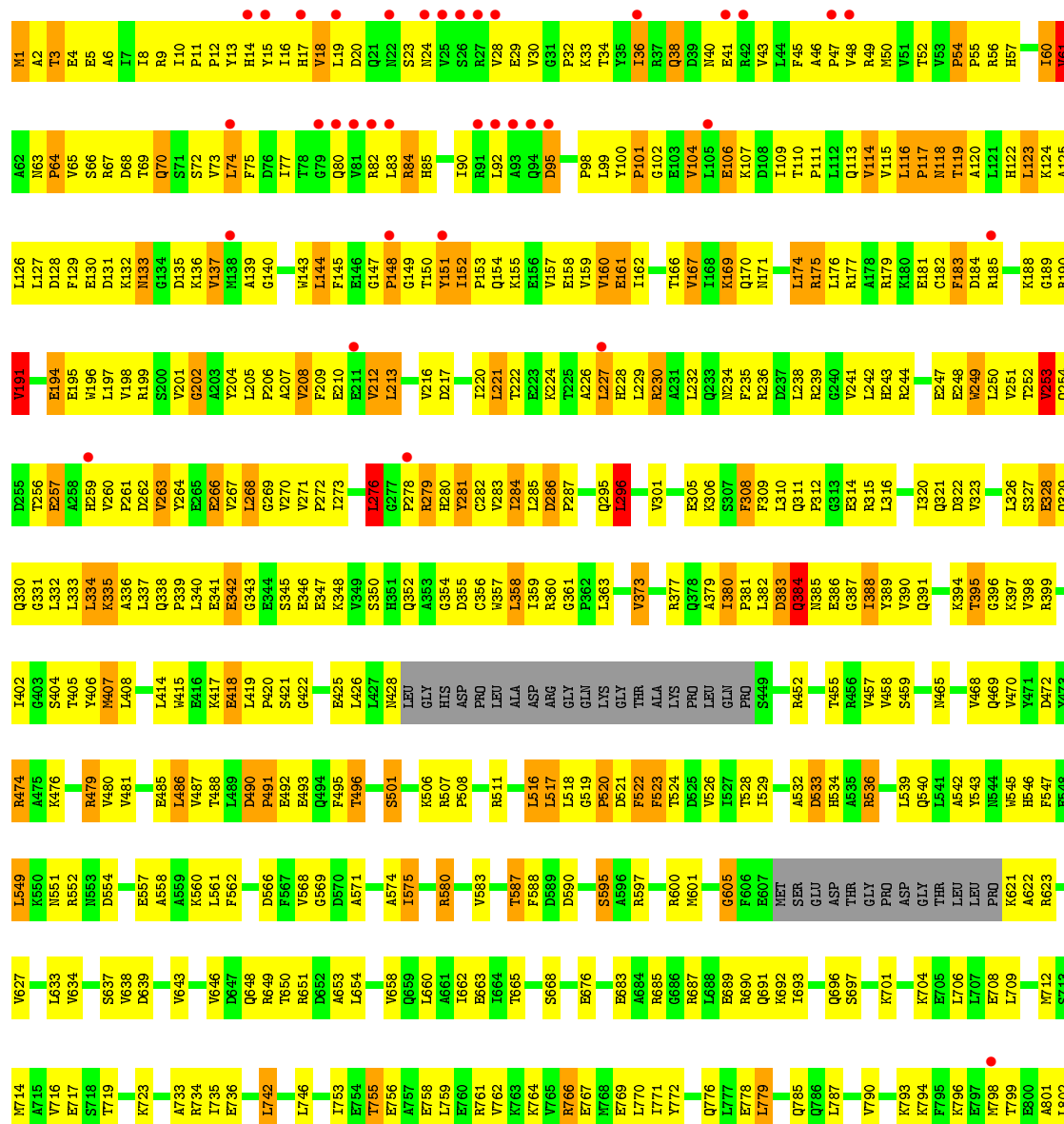
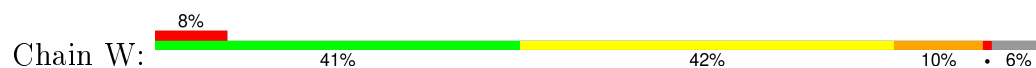


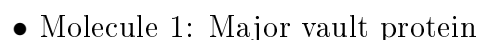
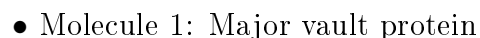
### • Molecule 1: Major vault protein

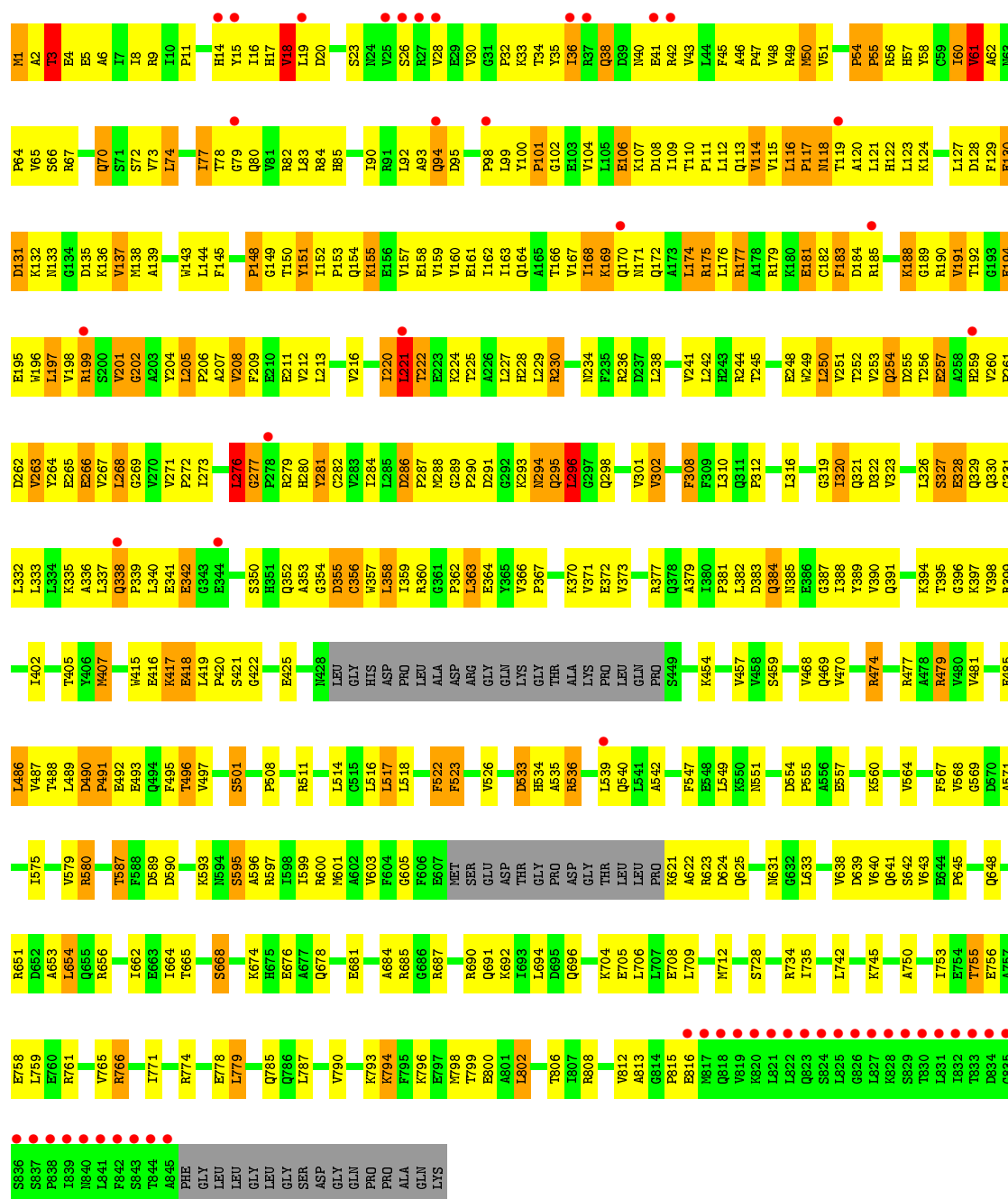




### • Molecule 1: Major vault protein

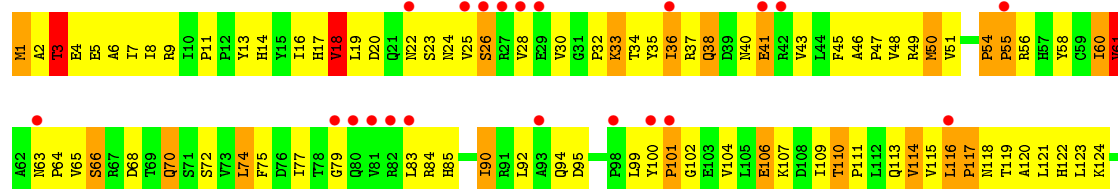




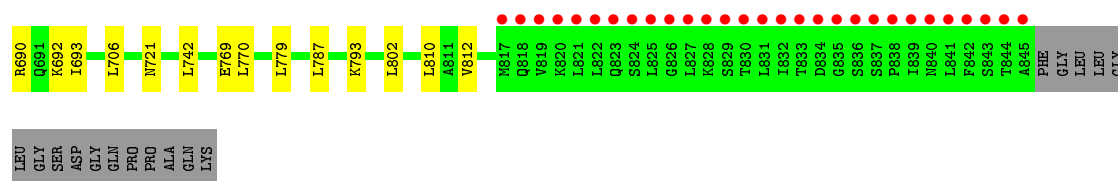


• Molecule 1: Major vault protein

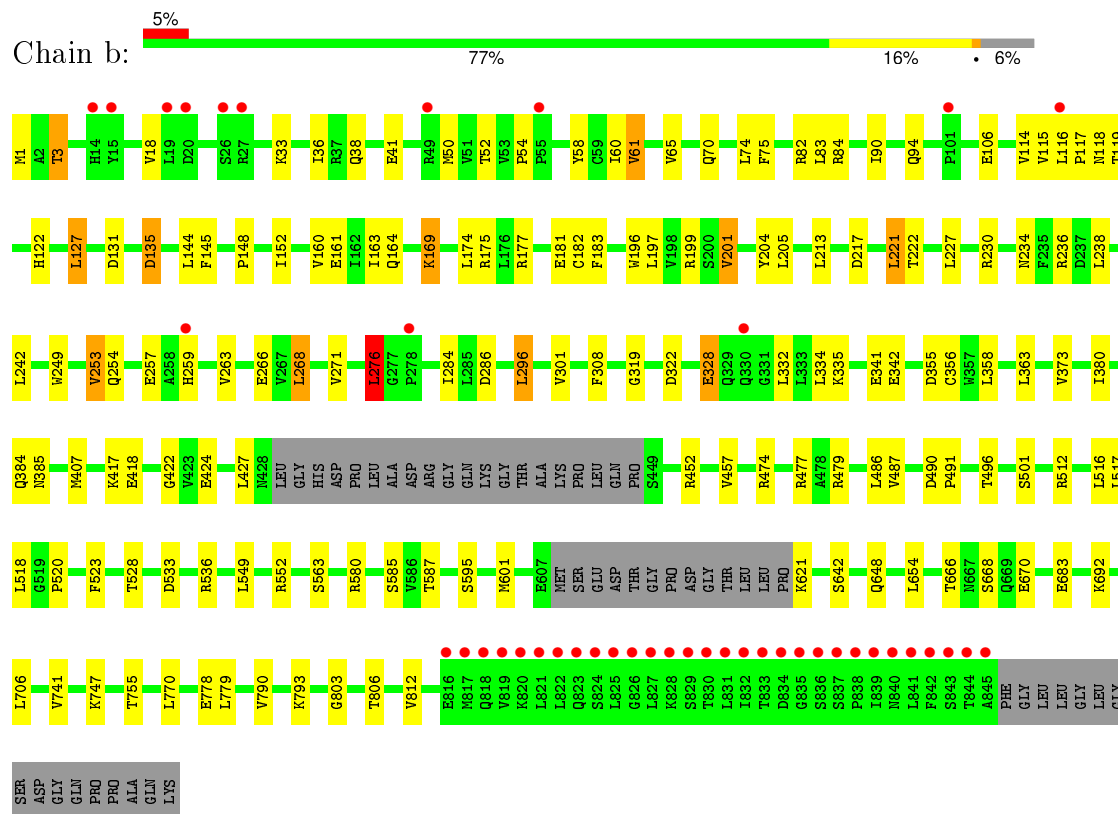
Chain Z: 7% 44% 39% 11% 6%



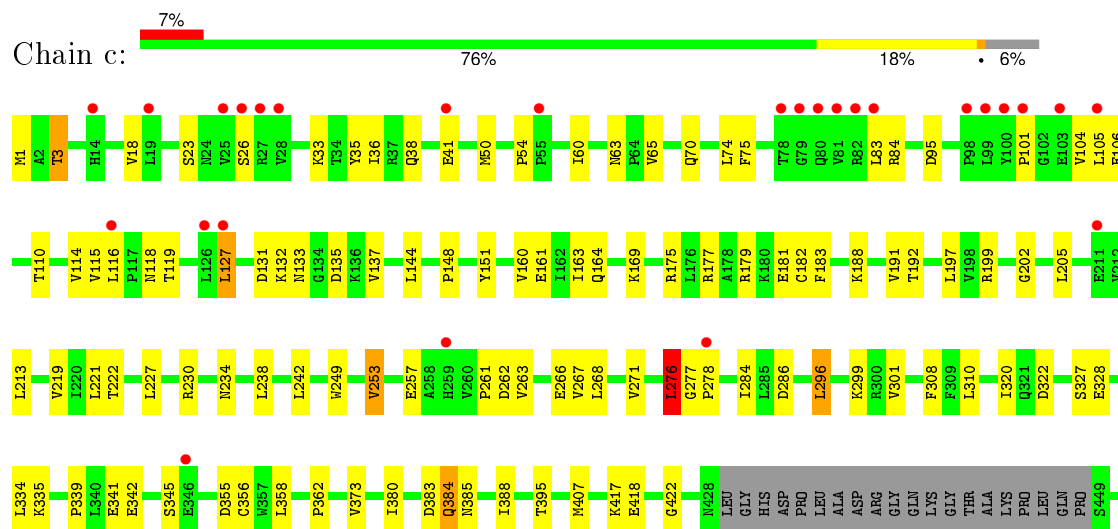


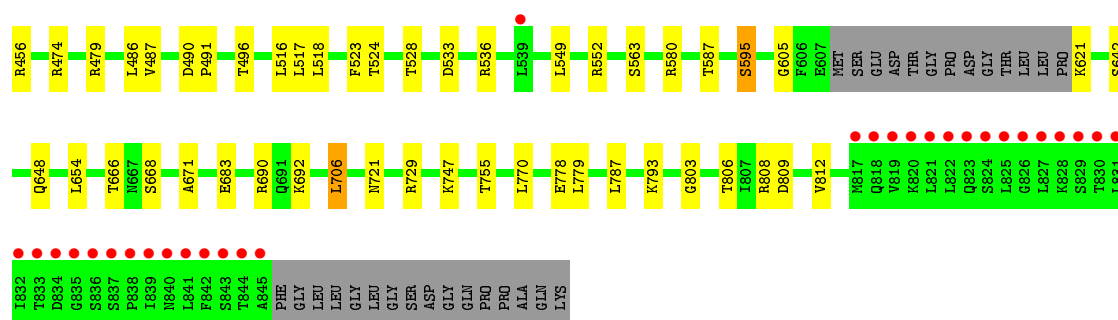


• Molecule 1: Major vault protein

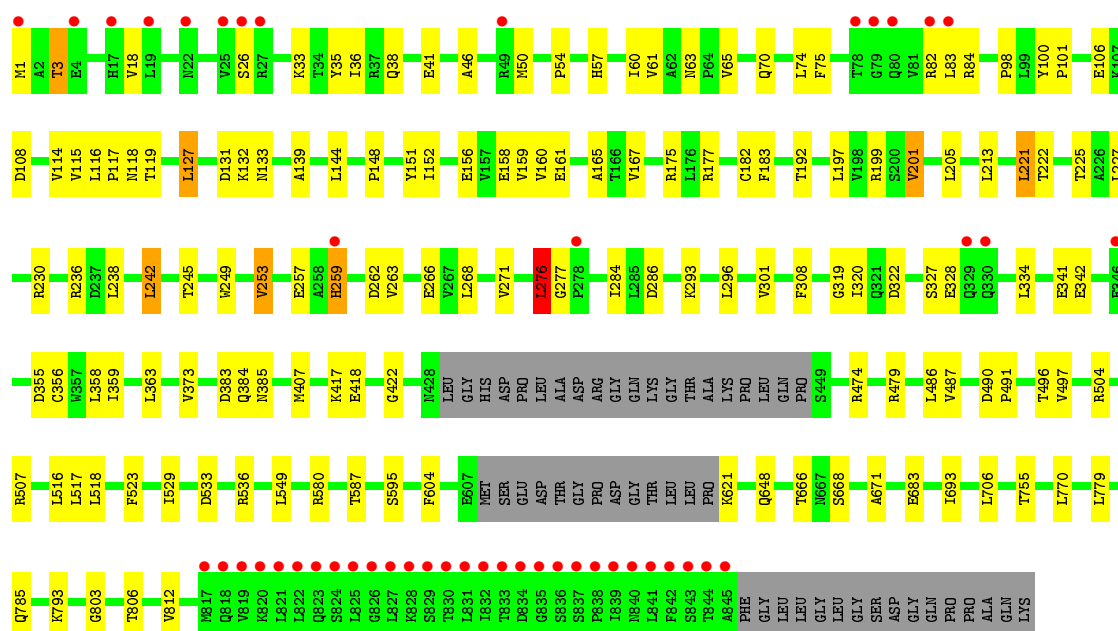
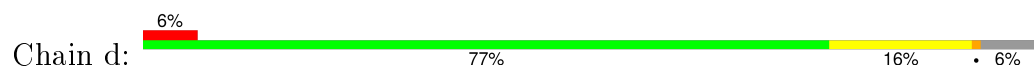


• Molecule 1: Major vault protein

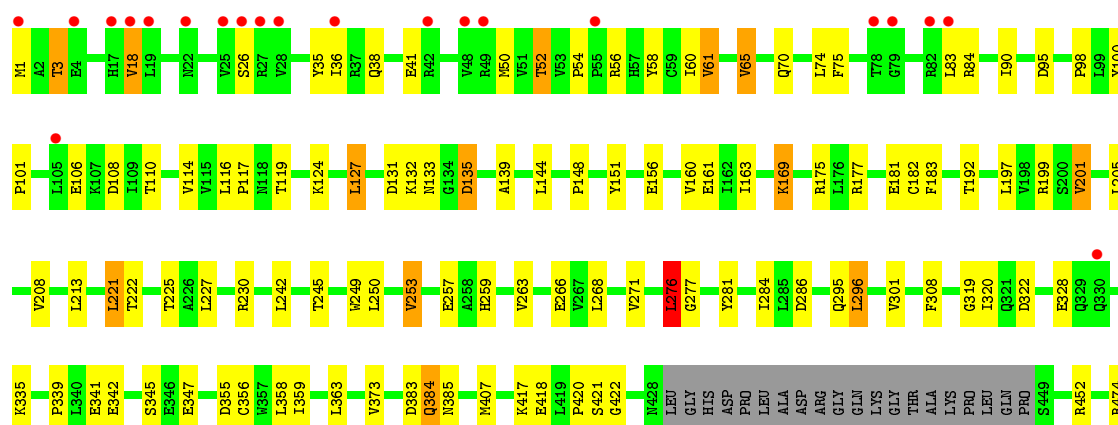
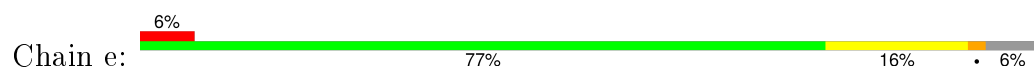


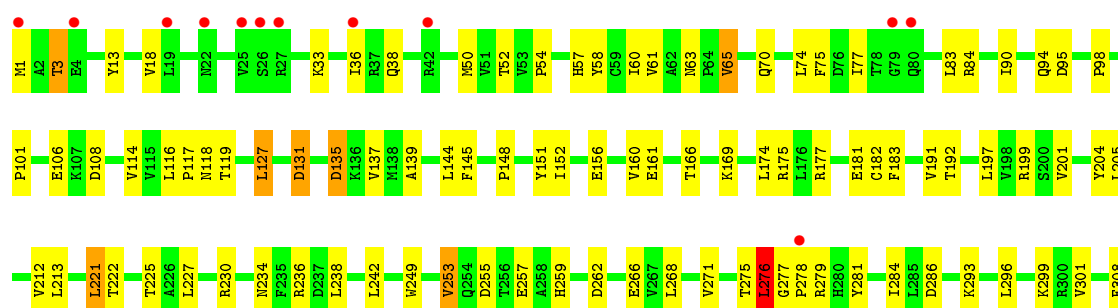


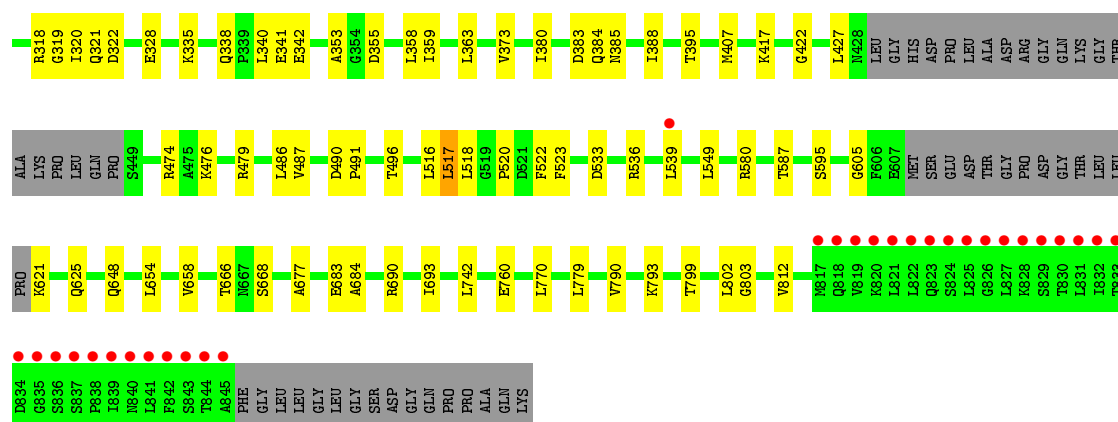
• Molecule 1: Major vault protein



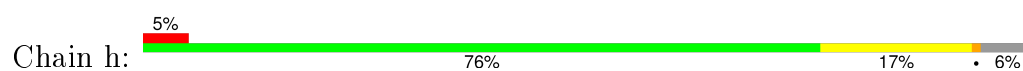
• Molecule 1: Major vault protein

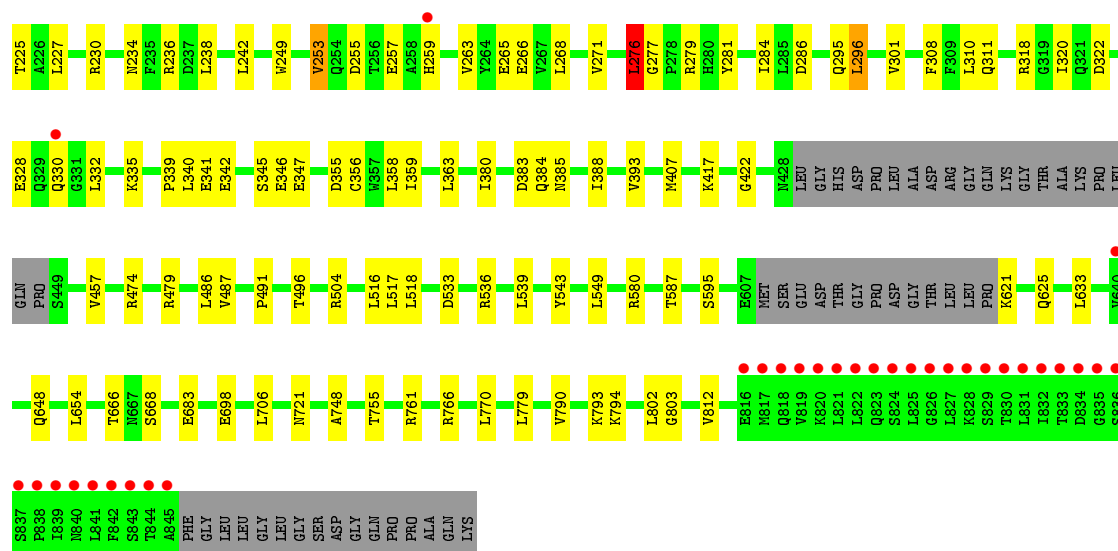




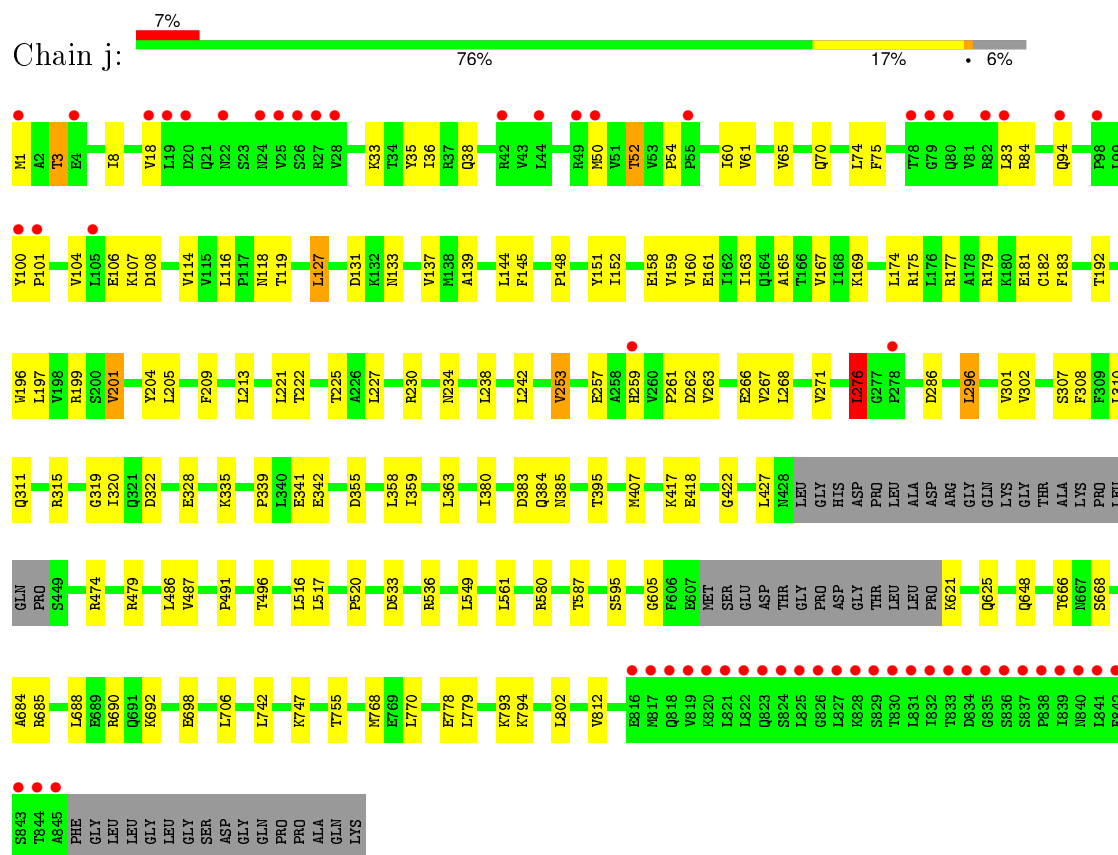


• Molecule 1: Major vault protein

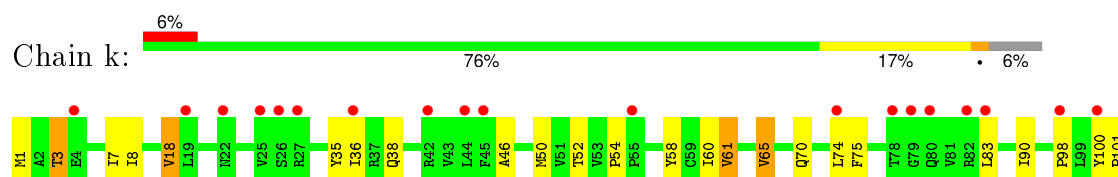




• Molecule 1: Major vault protein



• Molecule 1: Major vault protein







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	702.25Å 383.80Å 598.48Å 90.00° 124.69° 90.00°	Depositor
Resolution (Å)	204.00 – 3.50 203.54 – 3.47	Depositor EDS
% Data completeness (in resolution range)	92.7 (204.00-3.50) 91.4 (203.54-3.47)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	0.21	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 3.49Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.311 , 0.330 0.305 , 0.304	Depositor DCC
$R_{free}$ test set	75687 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	104.6	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 115.3	EDS
Estimated twinning fraction	0.099 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	46 of 1530892 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	241956	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.50	0/6279	0.69	3/8506 (0.0%)
1	B	0.50	0/6279	0.68	4/8506 (0.0%)
1	C	0.50	0/6279	0.69	5/8506 (0.1%)
1	D	0.50	0/6279	0.69	5/8506 (0.1%)
1	E	0.51	0/6279	0.69	3/8506 (0.0%)
1	F	0.50	0/6279	0.68	2/8506 (0.0%)
1	G	0.49	0/6279	0.68	3/8506 (0.0%)
1	H	0.50	0/6279	0.68	4/8506 (0.0%)
1	I	0.51	0/6279	0.69	3/8506 (0.0%)
1	J	0.51	0/6279	0.71	4/8506 (0.0%)
1	K	0.53	0/6279	0.73	6/8506 (0.1%)
1	L	0.52	0/6279	0.72	4/8506 (0.0%)
1	M	0.52	0/6279	0.71	3/8506 (0.0%)
1	N	0.51	0/6279	0.71	3/8506 (0.0%)
1	O	0.52	0/6279	0.71	3/8506 (0.0%)
1	P	0.52	0/6279	0.73	7/8506 (0.1%)
1	Q	0.52	0/6279	0.72	6/8506 (0.1%)
1	R	0.53	0/6279	0.74	4/8506 (0.0%)
1	S	0.50	0/6279	0.70	4/8506 (0.0%)
1	T	0.50	0/6279	0.69	3/8506 (0.0%)
1	U	0.49	0/6279	0.68	5/8506 (0.1%)
1	V	0.50	0/6279	0.67	4/8506 (0.0%)
1	W	0.49	0/6279	0.68	5/8506 (0.1%)
1	X	0.49	0/6279	0.69	3/8506 (0.0%)
1	Y	0.50	0/6279	0.68	3/8506 (0.0%)
1	Z	0.50	0/6279	0.69	4/8506 (0.0%)
1	a	0.49	0/6279	0.69	3/8506 (0.0%)
1	b	0.51	0/6279	0.70	5/8506 (0.1%)
1	c	0.51	0/6279	0.70	5/8506 (0.1%)
1	d	0.50	0/6279	0.71	5/8506 (0.1%)
1	e	0.51	0/6279	0.71	4/8506 (0.0%)
1	f	0.51	0/6279	0.70	4/8506 (0.0%)
1	g	0.50	0/6279	0.70	6/8506 (0.1%)
1	h	0.49	0/6279	0.70	3/8506 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	i	0.50	0/6279	0.70	4/8506 (0.0%)
1	j	0.50	0/6279	0.71	4/8506 (0.0%)
1	k	0.51	0/6279	0.72	4/8506 (0.0%)
1	l	0.50	0/6279	0.70	4/8506 (0.0%)
1	m	0.51	0/6279	0.69	4/8506 (0.0%)
All	All	0.51	0/244881	0.70	158/331734 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	1
1	B	1	0
1	C	1	1
1	D	1	1
1	E	1	1
1	F	1	0
1	G	1	0
1	H	1	0
1	I	1	0
1	J	1	1
1	K	1	1
1	L	1	0
1	M	1	0
1	N	1	0
1	O	1	0
1	P	1	0
1	Q	1	0
1	R	1	0
1	S	1	0
1	T	1	1
1	U	1	0
1	V	1	1
1	W	1	0
1	X	1	1
1	Y	1	0
1	Z	1	1
1	a	1	1
1	b	1	0
1	c	1	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	d	1	0
1	e	1	1
1	f	1	0
1	g	1	0
1	h	1	0
1	i	1	1
1	j	1	0
1	k	1	0
1	l	1	0
1	m	1	1
All	All	39	14

There are no bond length outliers.

The worst 5 of 158 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	j	165	ALA	CB-CA-C	-7.38	99.03	110.10
1	E	276	LEU	CA-CB-CG	7.24	131.95	115.30
1	K	276	LEU	CA-CB-CG	7.10	131.64	115.30
1	l	276	LEU	CA-CB-CG	7.04	131.49	115.30
1	P	252	THR	CB-CA-C	-6.96	92.81	111.60

5 of 39 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	3	THR	CB
1	B	3	THR	CB
1	C	3	THR	CB
1	D	3	THR	CB
1	E	3	THR	CB

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	504	ARG	Peptide
1	C	504	ARG	Peptide
1	D	504	ARG	Peptide
1	E	504	ARG	Peptide
1	J	135	ASP	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6204	0	6224	808	0
1	B	6204	0	6224	800	0
1	C	6204	0	6224	794	0
1	D	6204	0	6224	794	0
1	E	6204	0	6224	817	0
1	F	6204	0	6224	749	0
1	G	6204	0	6224	817	0
1	H	6204	0	6224	790	0
1	I	6204	0	6224	751	0
1	J	6204	0	6224	836	0
1	K	6204	0	6224	851	0
1	L	6204	0	6224	863	0
1	M	6204	0	6224	832	0
1	N	6204	0	6224	524	0
1	O	6204	0	6224	515	0
1	P	6204	0	6224	552	0
1	Q	6204	0	6224	581	0
1	R	6204	0	6224	588	0
1	S	6204	0	6224	522	0
1	T	6204	0	6224	500	0
1	U	6204	0	6224	481	0
1	V	6204	0	6224	477	0
1	W	6204	0	6224	494	0
1	X	6204	0	6224	484	0
1	Y	6204	0	6224	487	0
1	Z	6204	0	6224	459	0
1	a	6204	0	6224	0	0
1	b	6204	0	6224	0	0
1	c	6204	0	6224	0	0
1	d	6204	0	6224	0	0
1	e	6204	0	6224	0	0
1	f	6204	0	6224	0	0
1	g	6204	0	6224	0	0
1	h	6204	0	6224	0	0
1	i	6204	0	6224	0	0
1	j	6204	0	6224	0	0
1	k	6204	0	6224	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	l	6204	0	6224	0	0
1	m	6204	0	6224	0	0
All	All	241956	0	242736	15693	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 32.

The worst 5 of 15693 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:654:LEU:CD1	1:L:662:ILE:HD13	3.24	1.45
1:N:132:LYS:NZ	1:N:152:ILE:HD12	1.31	1.42
1:D:77:ILE:CD1	1:D:80:GLN:HB2	1.58	1.32
1:J:132:LYS:NZ	1:J:152:ILE:HD12	2.54	1.31
1:I:653:ALA:HB1	1:J:662:ILE:CD1	2.09	1.30

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	A	776/861 (90%)	634 (82%)	119 (15%)	23 (3%)	5	42
1	B	776/861 (90%)	640 (82%)	114 (15%)	22 (3%)	6	43
1	C	776/861 (90%)	639 (82%)	109 (14%)	28 (4%)	4	37
1	D	776/861 (90%)	635 (82%)	108 (14%)	33 (4%)	3	31
1	E	776/861 (90%)	637 (82%)	107 (14%)	32 (4%)	3	33
1	F	776/861 (90%)	627 (81%)	118 (15%)	31 (4%)	4	33
1	G	776/861 (90%)	648 (84%)	101 (13%)	27 (4%)	4	38
1	H	776/861 (90%)	636 (82%)	109 (14%)	31 (4%)	4	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	776/861 (90%)	650 (84%)	98 (13%)	28 (4%)	4	37
1	J	776/861 (90%)	637 (82%)	109 (14%)	30 (4%)	4	34
1	K	776/861 (90%)	631 (81%)	104 (13%)	41 (5%)	2	25
1	L	776/861 (90%)	637 (82%)	103 (13%)	36 (5%)	3	29
1	M	776/861 (90%)	633 (82%)	107 (14%)	36 (5%)	3	29
1	N	776/861 (90%)	639 (82%)	102 (13%)	35 (4%)	3	30
1	O	776/861 (90%)	637 (82%)	102 (13%)	37 (5%)	3	28
1	P	776/861 (90%)	627 (81%)	117 (15%)	32 (4%)	3	33
1	Q	776/861 (90%)	633 (82%)	104 (13%)	39 (5%)	3	27
1	R	776/861 (90%)	627 (81%)	109 (14%)	40 (5%)	2	25
1	S	776/861 (90%)	624 (80%)	115 (15%)	37 (5%)	3	28
1	T	776/861 (90%)	631 (81%)	113 (15%)	32 (4%)	3	33
1	U	776/861 (90%)	642 (83%)	100 (13%)	34 (4%)	3	30
1	V	776/861 (90%)	639 (82%)	110 (14%)	27 (4%)	4	38
1	W	776/861 (90%)	647 (83%)	96 (12%)	33 (4%)	3	31
1	X	776/861 (90%)	648 (84%)	97 (12%)	31 (4%)	4	33
1	Y	776/861 (90%)	644 (83%)	98 (13%)	34 (4%)	3	30
1	Z	776/861 (90%)	649 (84%)	97 (12%)	30 (4%)	4	34
1	a	776/861 (90%)	639 (82%)	108 (14%)	29 (4%)	4	36
1	b	776/861 (90%)	635 (82%)	112 (14%)	29 (4%)	4	36
1	c	776/861 (90%)	642 (83%)	101 (13%)	33 (4%)	3	31
1	d	776/861 (90%)	630 (81%)	118 (15%)	28 (4%)	4	37
1	e	776/861 (90%)	629 (81%)	113 (15%)	34 (4%)	3	30
1	f	776/861 (90%)	642 (83%)	99 (13%)	35 (4%)	3	30
1	g	776/861 (90%)	637 (82%)	98 (13%)	41 (5%)	2	25
1	h	776/861 (90%)	639 (82%)	97 (12%)	40 (5%)	2	25
1	i	776/861 (90%)	634 (82%)	104 (13%)	38 (5%)	3	27
1	j	776/861 (90%)	634 (82%)	107 (14%)	35 (4%)	3	30
1	k	776/861 (90%)	633 (82%)	105 (14%)	38 (5%)	3	27
1	l	776/861 (90%)	632 (81%)	107 (14%)	37 (5%)	3	28
1	m	776/861 (90%)	634 (82%)	108 (14%)	34 (4%)	3	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	30264/33579 (90%)	24831 (82%)	4143 (14%)	1290 (4%)	3	31

5 of 1290 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	ASP
1	A	148	PRO
1	A	169	LYS
1	A	253	VAL
1	A	296	LEU

### 5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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	A	663/727 (91%)	527 (80%)	136 (20%)	1	8
1	B	663/727 (91%)	545 (82%)	118 (18%)	2	13
1	C	663/727 (91%)	536 (81%)	127 (19%)	2	10
1	D	663/727 (91%)	543 (82%)	120 (18%)	2	12
1	E	663/727 (91%)	550 (83%)	113 (17%)	2	15
1	F	663/727 (91%)	543 (82%)	120 (18%)	2	12
1	G	663/727 (91%)	533 (80%)	130 (20%)	1	9
1	H	663/727 (91%)	533 (80%)	130 (20%)	1	9
1	I	663/727 (91%)	537 (81%)	126 (19%)	2	10
1	J	663/727 (91%)	532 (80%)	131 (20%)	1	9
1	K	663/727 (91%)	519 (78%)	144 (22%)	1	7
1	L	663/727 (91%)	536 (81%)	127 (19%)	2	10
1	M	663/727 (91%)	537 (81%)	126 (19%)	2	10
1	N	663/727 (91%)	535 (81%)	128 (19%)	2	10
1	O	663/727 (91%)	528 (80%)	135 (20%)	1	8
1	P	663/727 (91%)	527 (80%)	136 (20%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	663/727 (91%)	528 (80%)	135 (20%)	1	8
1	R	663/727 (91%)	521 (79%)	142 (21%)	1	7
1	S	663/727 (91%)	539 (81%)	124 (19%)	2	11
1	T	663/727 (91%)	540 (81%)	123 (19%)	2	11
1	U	663/727 (91%)	532 (80%)	131 (20%)	1	9
1	V	663/727 (91%)	530 (80%)	133 (20%)	1	9
1	W	663/727 (91%)	545 (82%)	118 (18%)	2	13
1	X	663/727 (91%)	534 (80%)	129 (20%)	2	10
1	Y	663/727 (91%)	547 (82%)	116 (18%)	2	14
1	Z	663/727 (91%)	535 (81%)	128 (19%)	2	10
1	a	663/727 (91%)	538 (81%)	125 (19%)	2	10
1	b	663/727 (91%)	534 (80%)	129 (20%)	2	10
1	c	663/727 (91%)	531 (80%)	132 (20%)	1	9
1	d	663/727 (91%)	542 (82%)	121 (18%)	2	12
1	e	663/727 (91%)	534 (80%)	129 (20%)	2	10
1	f	663/727 (91%)	536 (81%)	127 (19%)	2	10
1	g	663/727 (91%)	533 (80%)	130 (20%)	1	9
1	h	663/727 (91%)	535 (81%)	128 (19%)	2	10
1	i	663/727 (91%)	533 (80%)	130 (20%)	1	9
1	j	663/727 (91%)	540 (81%)	123 (19%)	2	11
1	k	663/727 (91%)	531 (80%)	132 (20%)	1	9
1	l	663/727 (91%)	541 (82%)	122 (18%)	2	11
1	m	663/727 (91%)	541 (82%)	122 (18%)	2	11
All	All	25857/28353 (91%)	20881 (81%)	4976 (19%)	2	10

5 of 4976 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	276	LEU
1	V	345	SER
1	j	794	LYS
1	R	779	LEU
1	T	363	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 645 such sidechains are listed below:

Mol	Chain	Res	Type
1	R	378	GLN
1	V	509	HIS
1	j	776	GLN
1	S	22	ASN
1	T	494	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	812/861 (94%)	0.15	41 (5%)	32	25	46, 106, 218, 285	0
1	B	812/861 (94%)	0.16	44 (5%)	29	23	30, 112, 219, 284	0
1	C	812/861 (94%)	0.19	44 (5%)	29	23	54, 113, 221, 291	0
1	D	812/861 (94%)	0.22	49 (6%)	25	19	43, 113, 218, 277	0
1	E	812/861 (94%)	0.39	67 (8%)	14	12	53, 112, 222, 283	0
1	F	812/861 (94%)	0.28	62 (7%)	17	14	46, 114, 223, 278	0
1	G	812/861 (94%)	0.19	50 (6%)	24	19	55, 113, 223, 258	0
1	H	812/861 (94%)	0.09	39 (4%)	34	27	50, 112, 221, 281	0
1	I	812/861 (94%)	0.18	52 (6%)	23	17	56, 108, 215, 266	0
1	J	812/861 (94%)	0.30	57 (7%)	19	15	44, 105, 215, 277	0
1	K	812/861 (94%)	0.35	56 (6%)	20	16	32, 98, 207, 278	0
1	L	812/861 (94%)	0.26	56 (6%)	20	16	33, 99, 210, 277	0
1	M	812/861 (94%)	0.06	40 (4%)	33	25	45, 103, 207, 293	0
1	N	812/861 (94%)	0.00	36 (4%)	38	29	40, 104, 210, 249	0
1	O	812/861 (94%)	0.01	38 (4%)	35	28	33, 103, 214, 272	0
1	P	812/861 (94%)	0.10	44 (5%)	29	23	35, 103, 211, 294	0
1	Q	812/861 (94%)	0.32	60 (7%)	17	14	35, 101, 215, 277	0
1	R	812/861 (94%)	0.31	58 (7%)	19	15	37, 101, 217, 298	0
1	S	812/861 (94%)	0.20	53 (6%)	22	17	48, 106, 212, 284	0
1	T	812/861 (94%)	0.13	56 (6%)	20	16	52, 114, 220, 288	0
1	U	812/861 (94%)	0.04	43 (5%)	30	23	53, 113, 221, 282	0
1	V	812/861 (94%)	0.13	49 (6%)	25	19	57, 114, 220, 287	0
1	W	812/861 (94%)	0.31	66 (8%)	15	12	48, 116, 223, 288	0
1	X	812/861 (94%)	0.28	64 (7%)	15	13	47, 117, 220, 300	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	Y	812/861 (94%)	0.18	54 (6%) 21 16	43, 117, 218, 278	0
1	Z	812/861 (94%)	0.17	56 (6%) 20 16	51, 114, 219, 263	0
1	a	812/861 (94%)	0.13	50 (6%) 24 19	50, 113, 216, 300	0
1	b	812/861 (94%)	0.12	43 (5%) 30 23	28, 110, 217, 281	0
1	c	812/861 (94%)	0.17	57 (7%) 19 15	26, 109, 218, 277	0
1	d	812/861 (94%)	0.13	48 (5%) 26 20	49, 106, 213, 274	0
1	e	812/861 (94%)	0.15	52 (6%) 23 17	47, 105, 210, 284	0
1	f	812/861 (94%)	0.17	52 (6%) 23 17	43, 106, 214, 266	0
1	g	812/861 (94%)	0.08	42 (5%) 31 24	50, 109, 213, 285	0
1	h	812/861 (94%)	0.02	40 (4%) 33 25	54, 110, 210, 277	0
1	i	812/861 (94%)	0.11	47 (5%) 26 21	48, 108, 215, 271	0
1	j	812/861 (94%)	0.19	58 (7%) 19 15	50, 105, 216, 267	0
1	k	812/861 (94%)	0.18	51 (6%) 23 18	41, 104, 210, 261	0
1	l	812/861 (94%)	0.16	52 (6%) 23 17	46, 105, 213, 300	0
1	m	812/861 (94%)	0.20	49 (6%) 25 19	40, 106, 219, 276	0
All	All	31668/33579 (94%)	0.17	1975 (6%) 24 19	26, 108, 217, 300	0

The worst 5 of 1975 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	26	SER	26.9
1	Q	26	SER	21.5
1	X	26	SER	15.8
1	K	26	SER	15.4
1	Q	25	VAL	14.9

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.