



wwPDB X-ray Structure Validation Summary Report

Jul 23, 2014 – 02:07 PM EDT

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 validation summary report for a publicly released PDB entry.

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

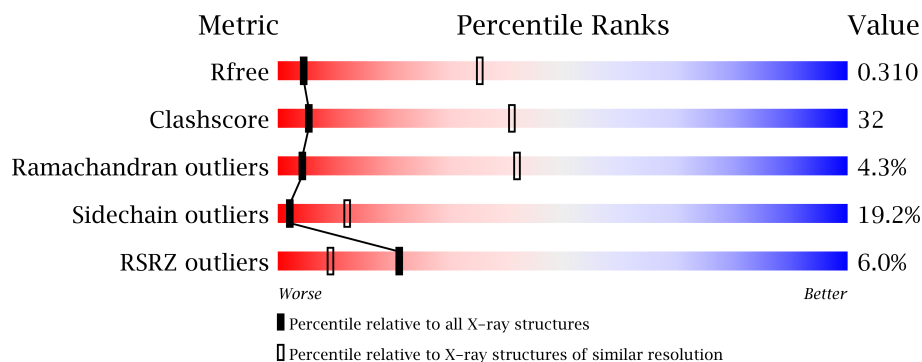
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : **FAILED**
EDS : stable23489
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

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}	66092	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	861	
1	B	861	
1	C	861	
1	D	861	
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	
1	N	861	

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Mol	Chain	Length	Quality of chain
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	
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 hydrogen and 0 are deuterium.

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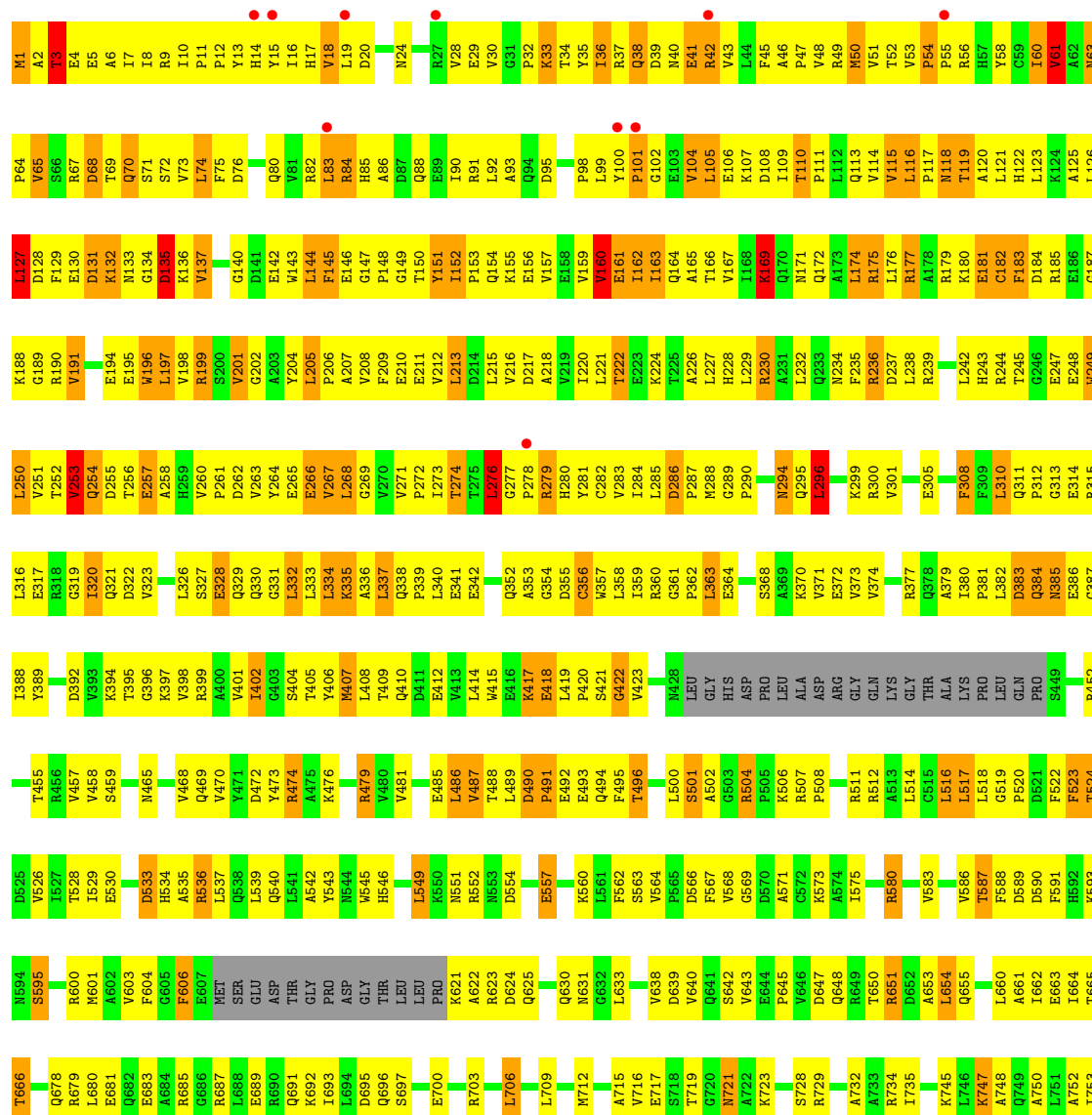
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	l	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	m	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			

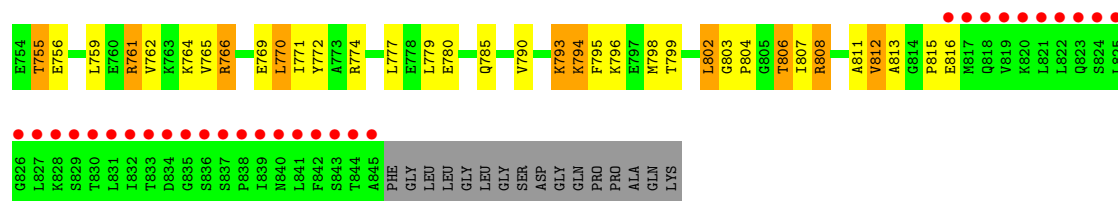
3 Residue-property plots

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 ($RSRZ > 2$). 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.

• Molecule 1: Major vault protein

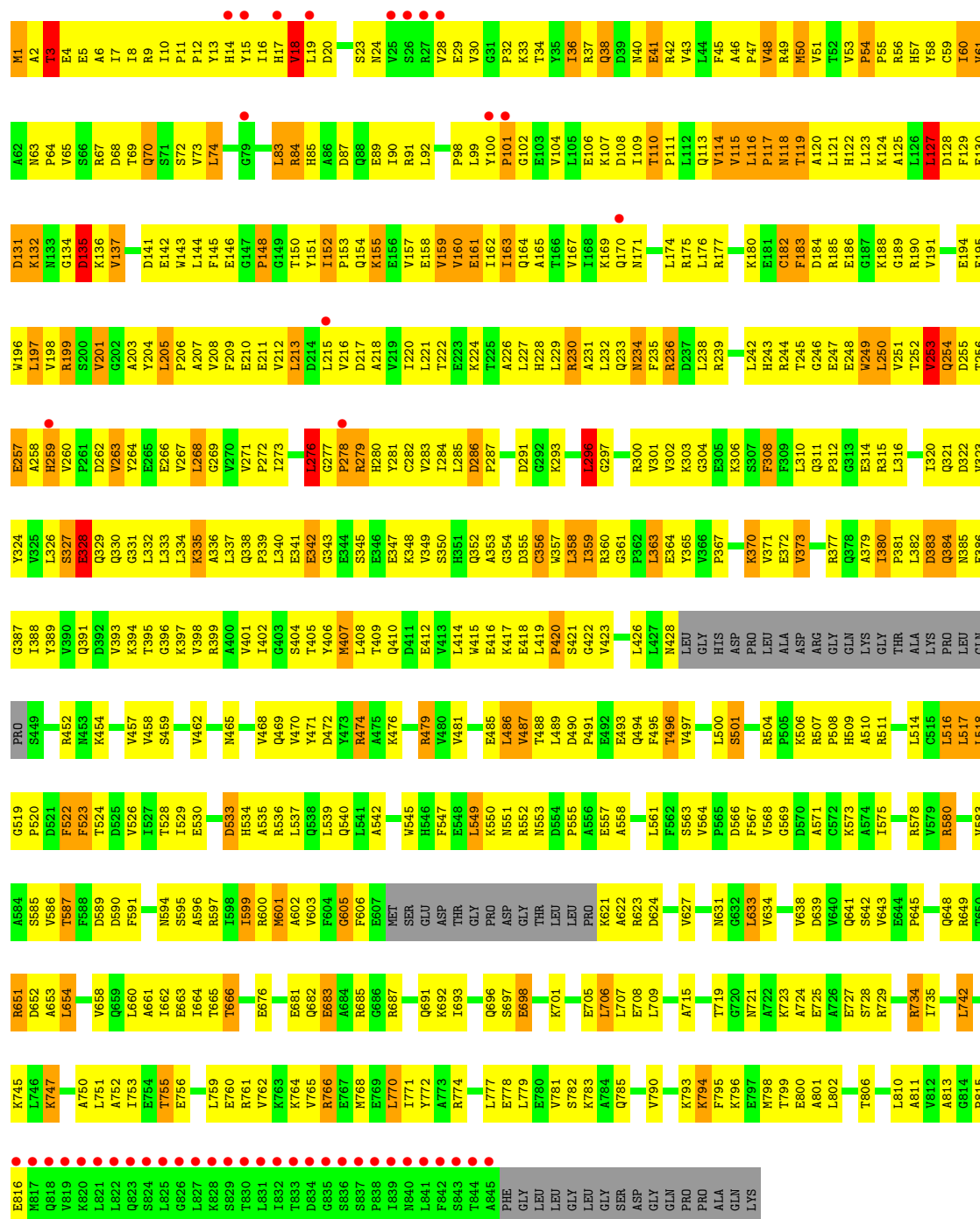
Chain A: 





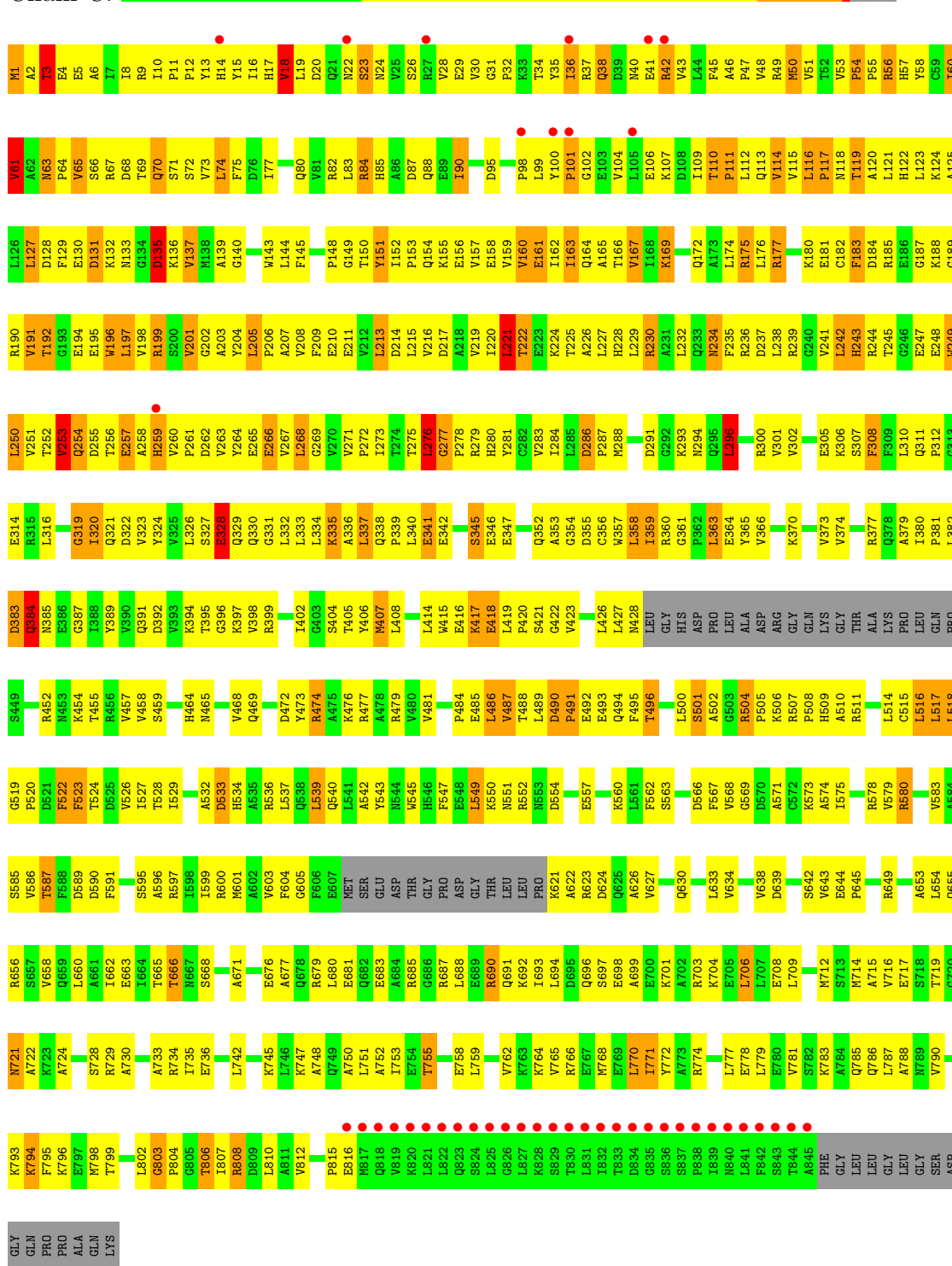
Molecule 1: Major vault protein

Chain B:



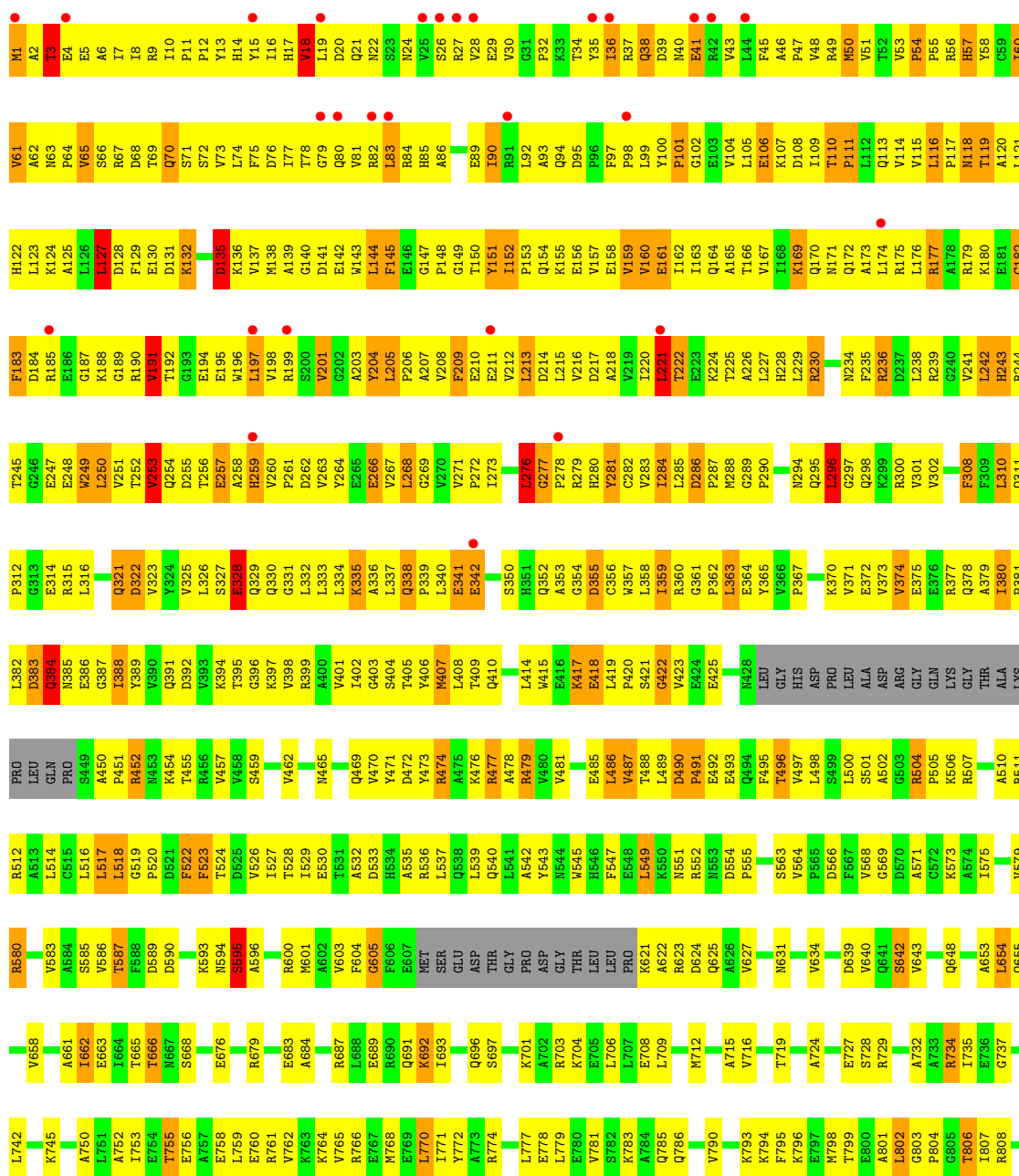
● Molecule 1: Major vault protein

Chain C:



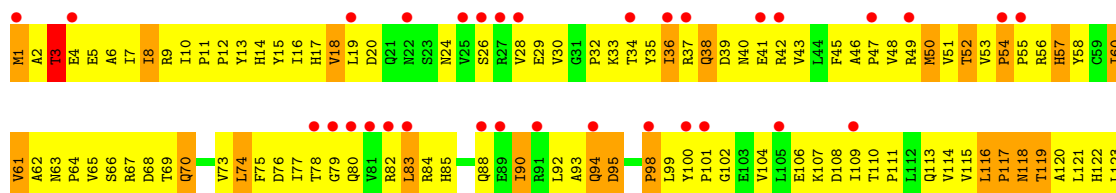
● Molecule 1: Major vault protein

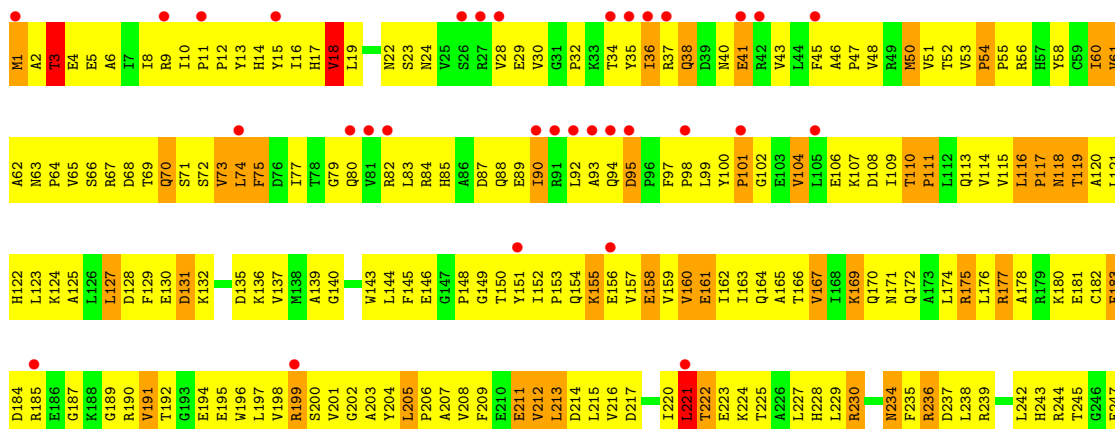
Chain D:

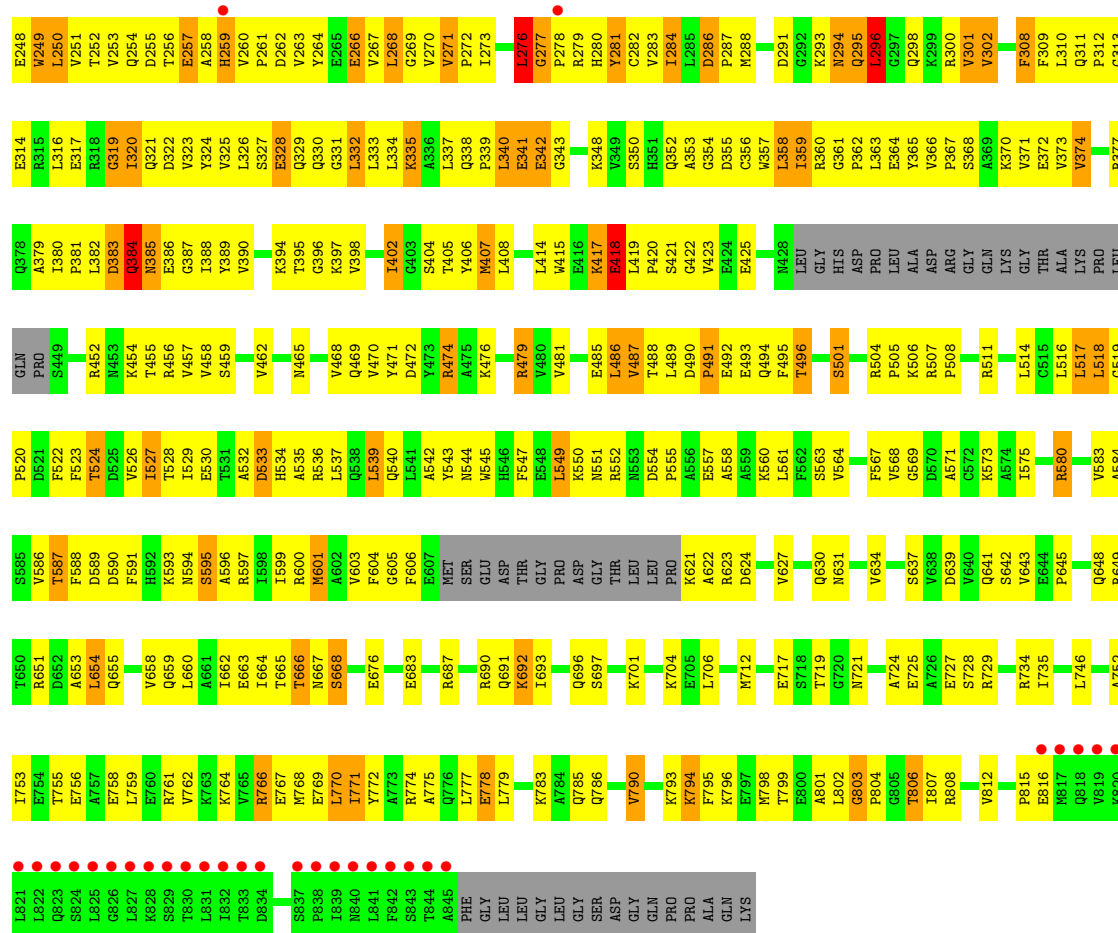


• Molecule 1: Major vault protein

Chain E:

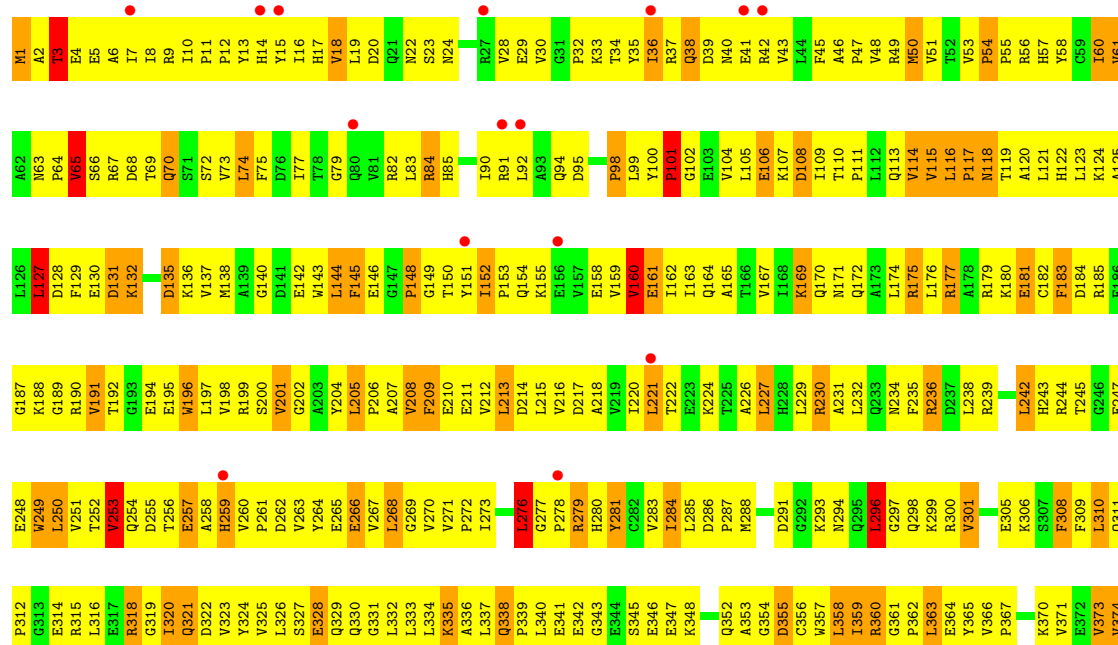






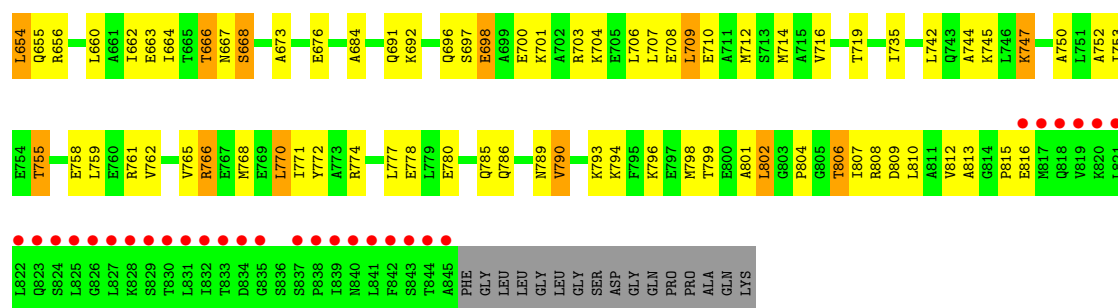
• Molecule 1: Major vault protein

Chain G:



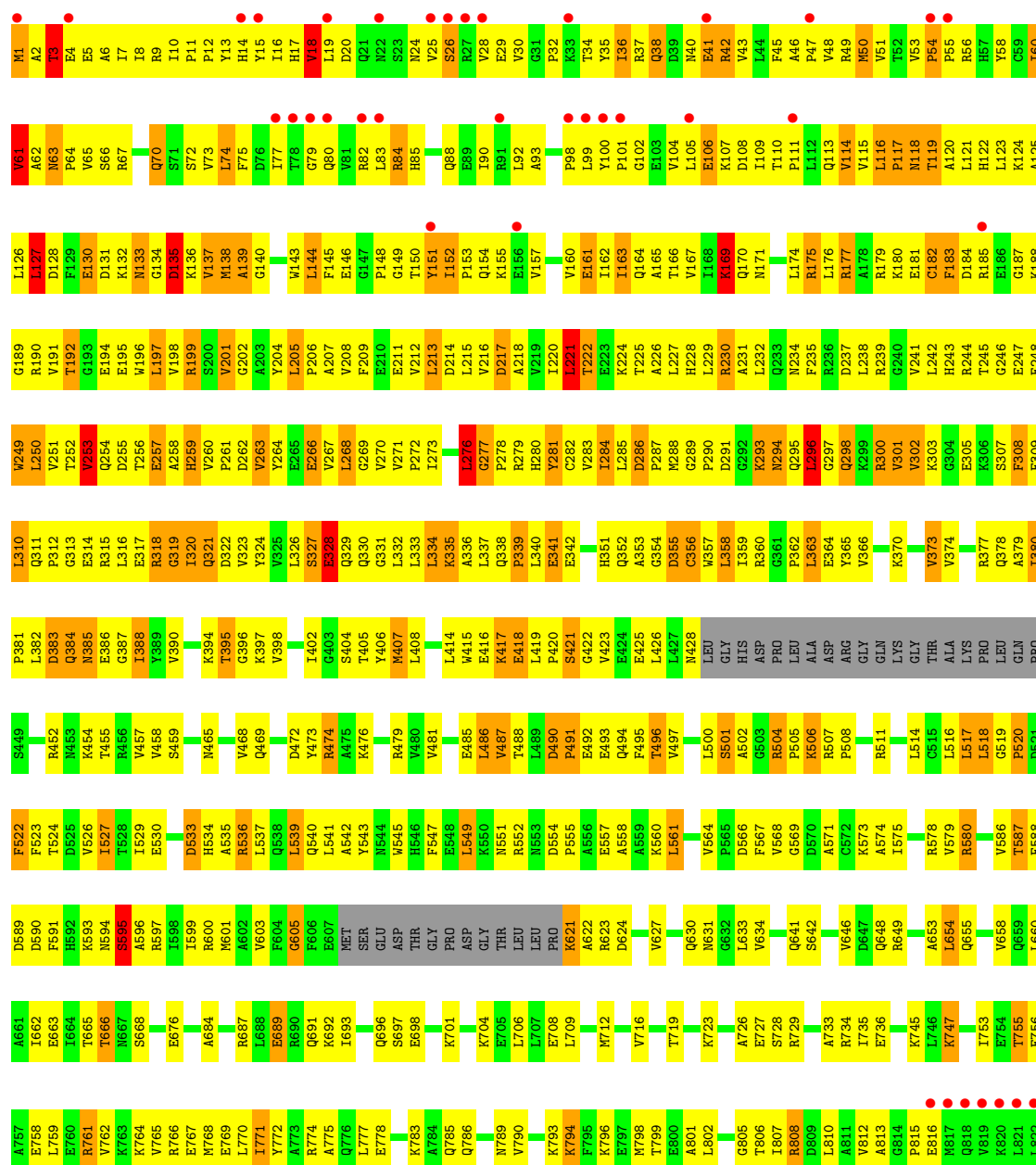


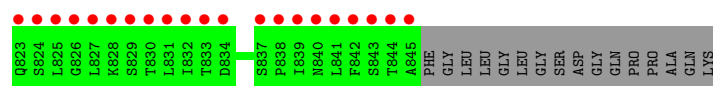




• Molecule 1: Major vault protein

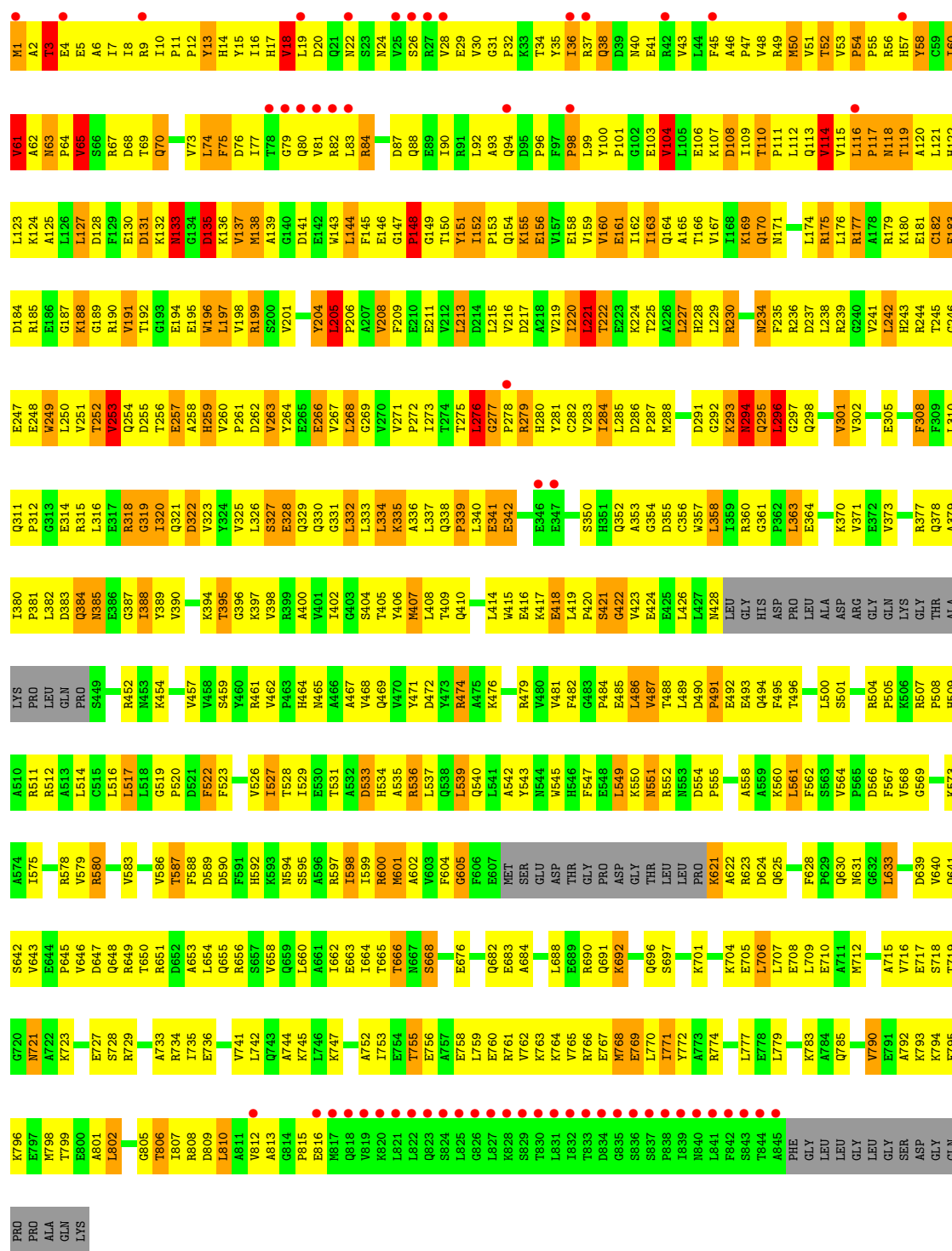
Chain J:





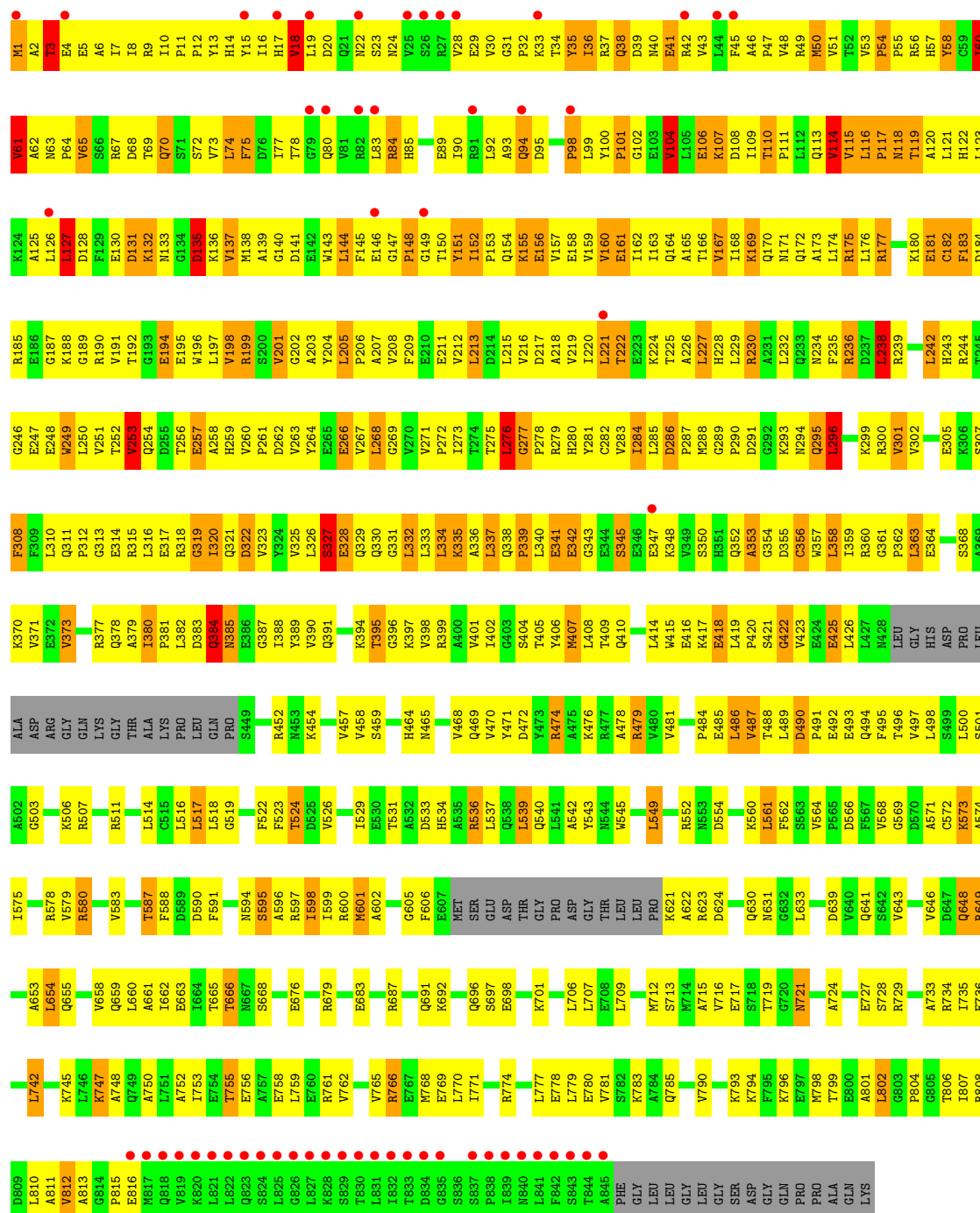
• Molecule 1: Major vault protein

Chain K:



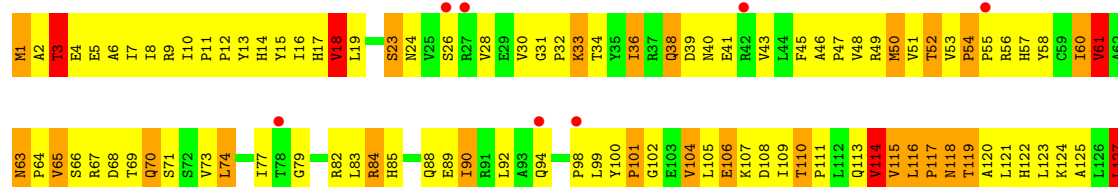
• Molecule 1: Major vault protein

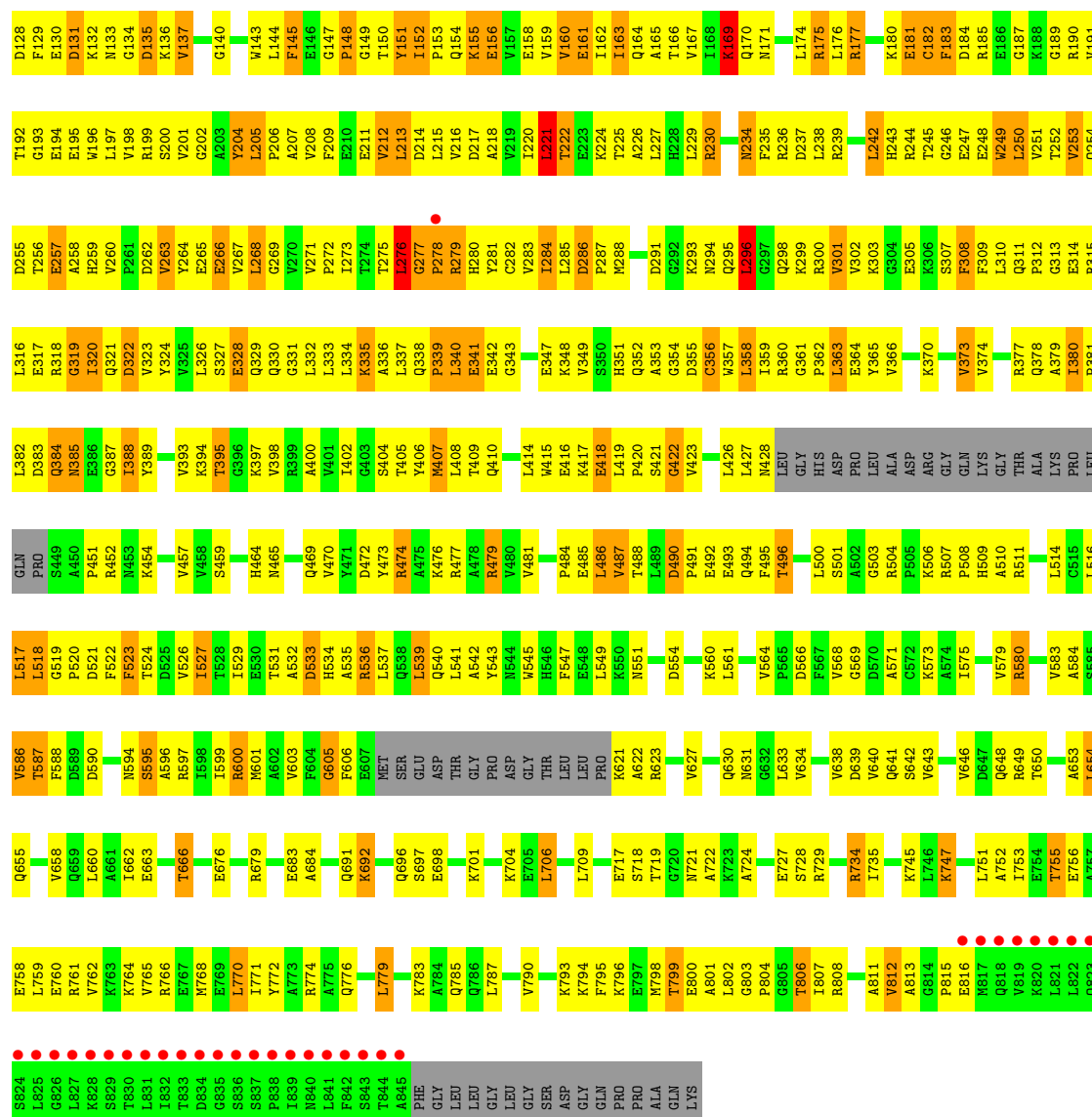
Chain L:



- Molecule 1: Major vault protein

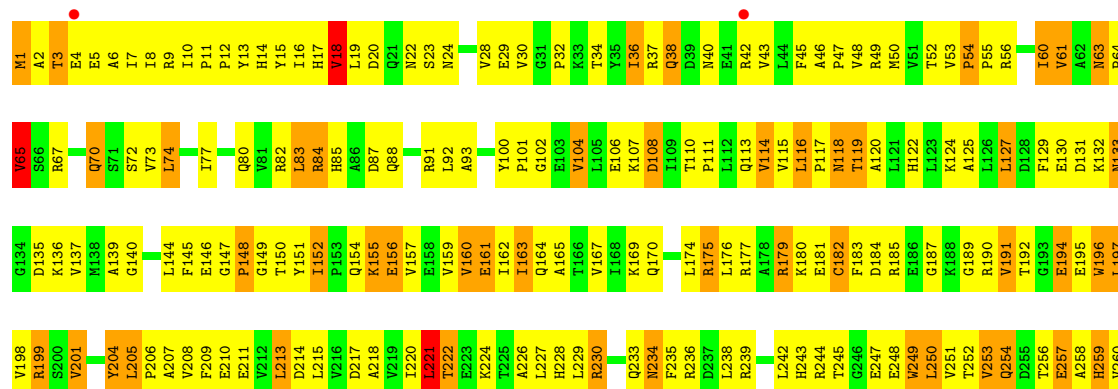
Chain M:

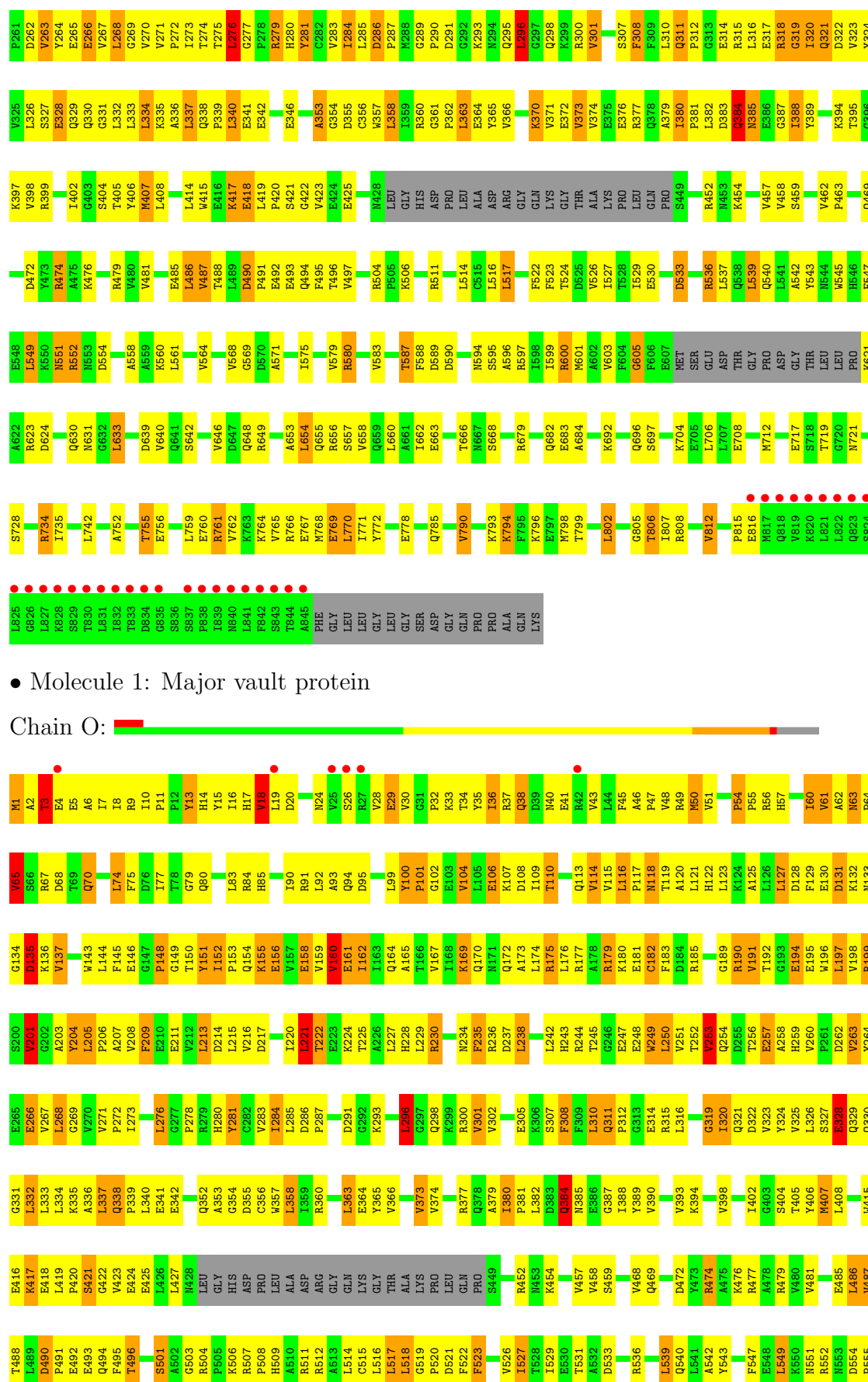


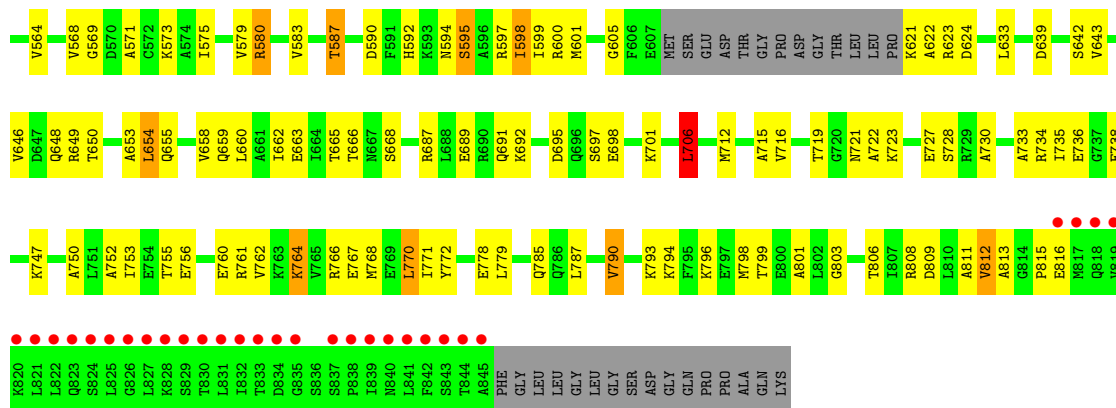


• Molecule 1: Major vault protein

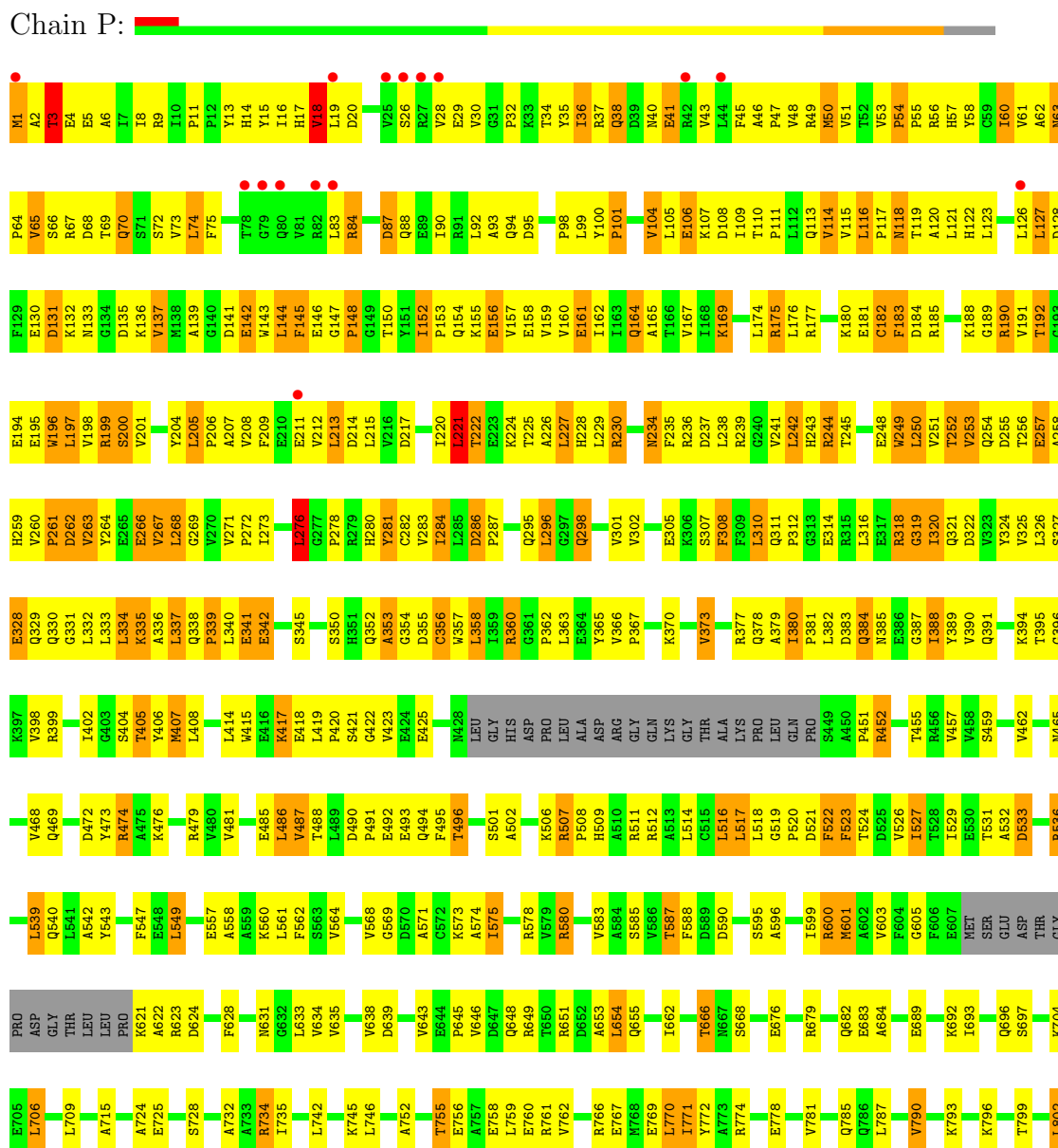
Chain N:

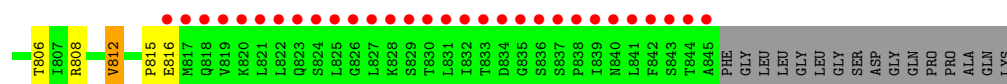






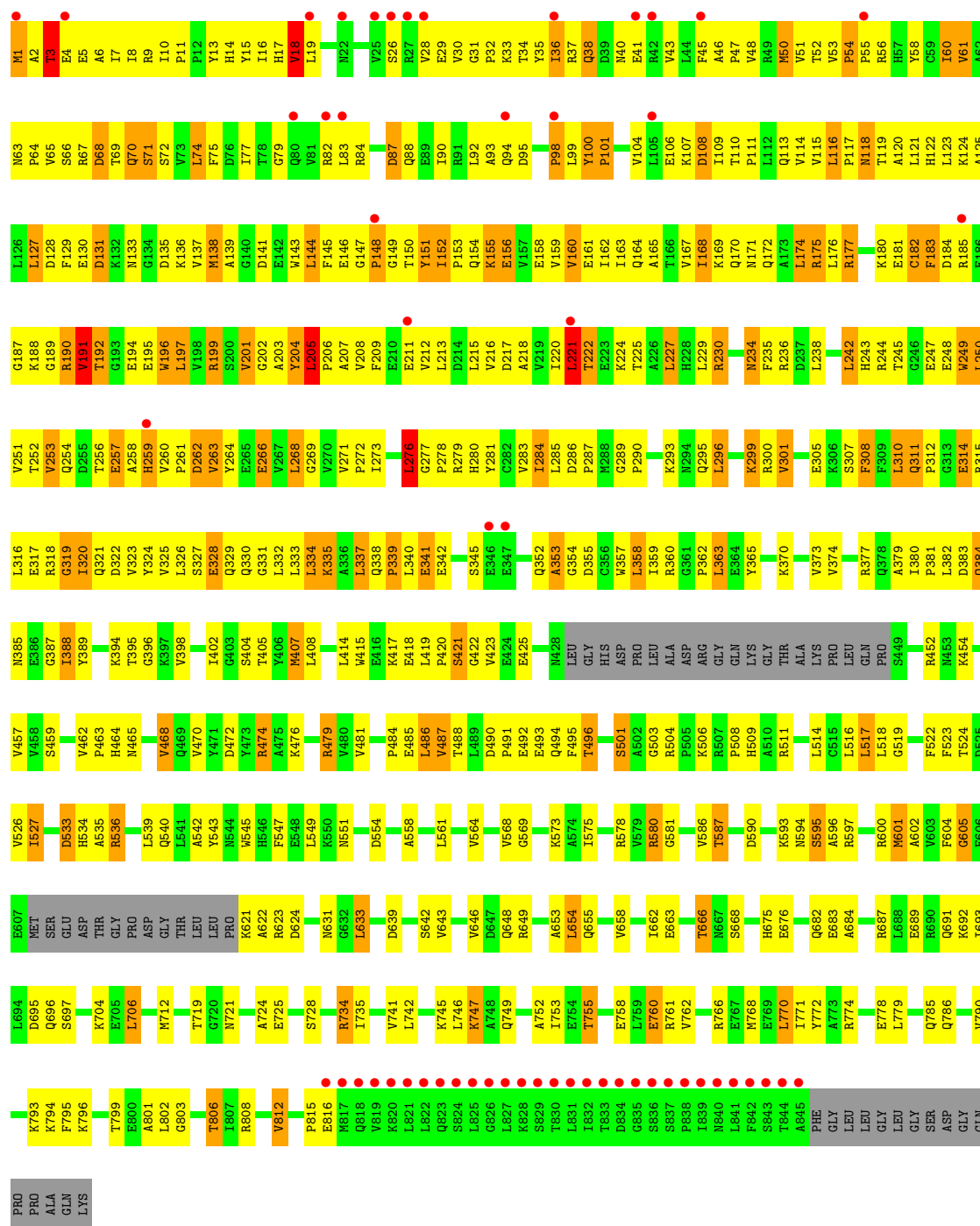
• Molecule 1: Major vault protein





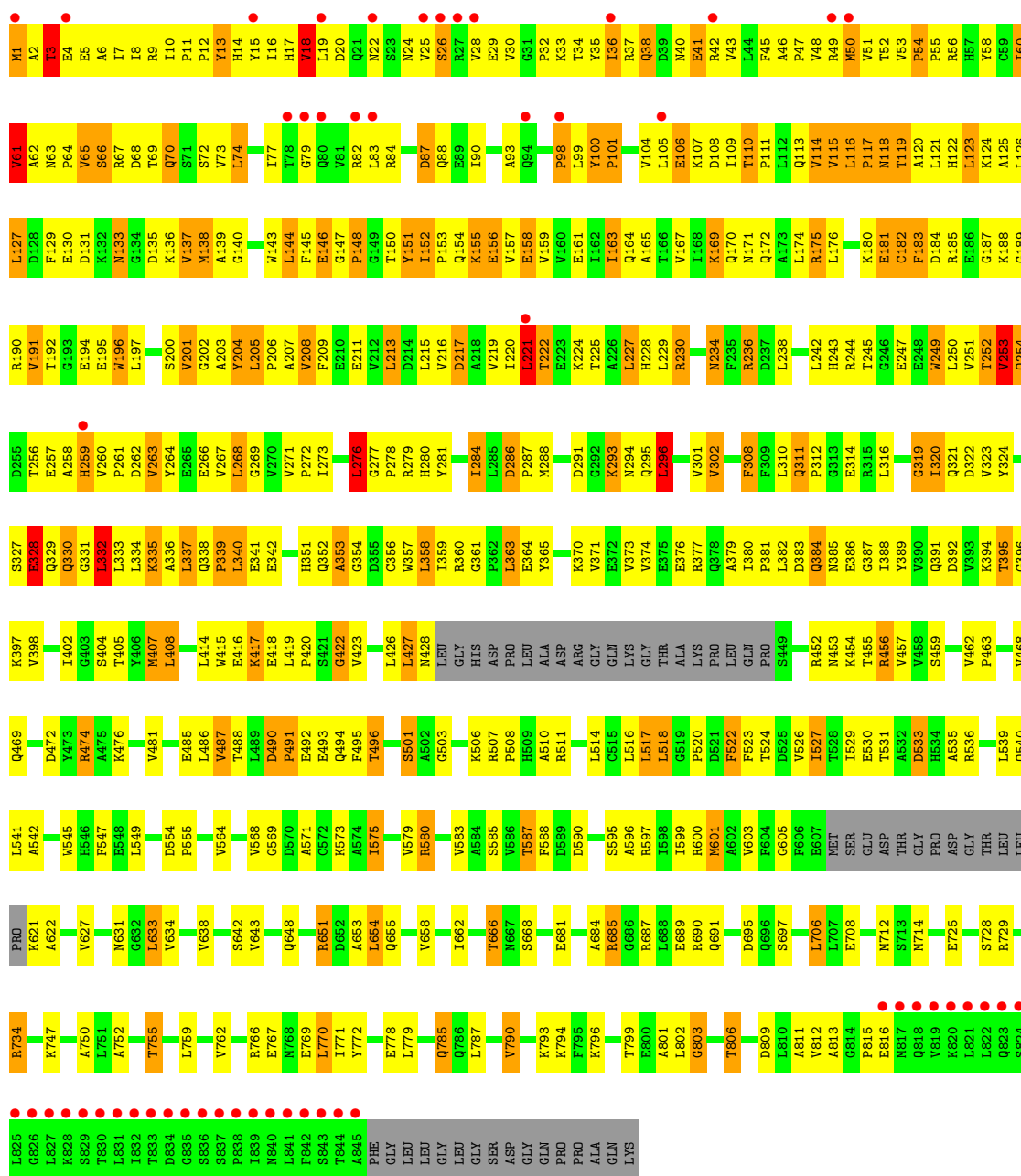
• Molecule 1: Major vault protein

Chain Q:



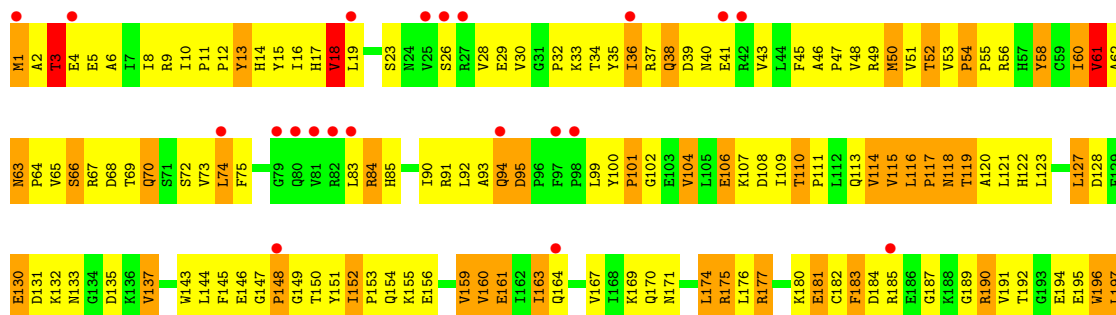
• Molecule 1: Major vault protein

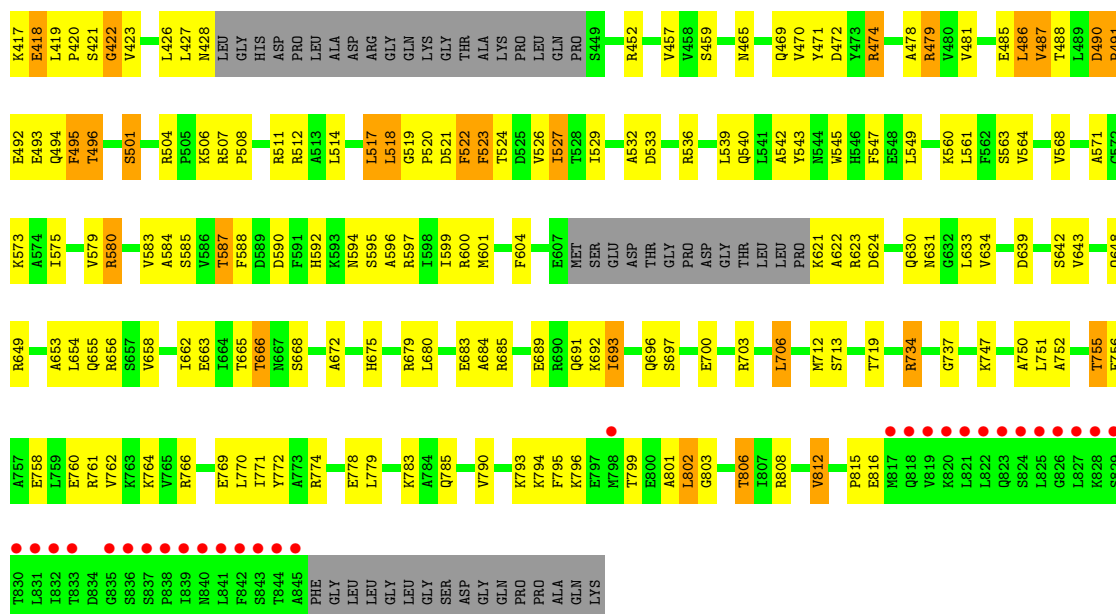
Chain R:



• Molecule 1: Major vault protein

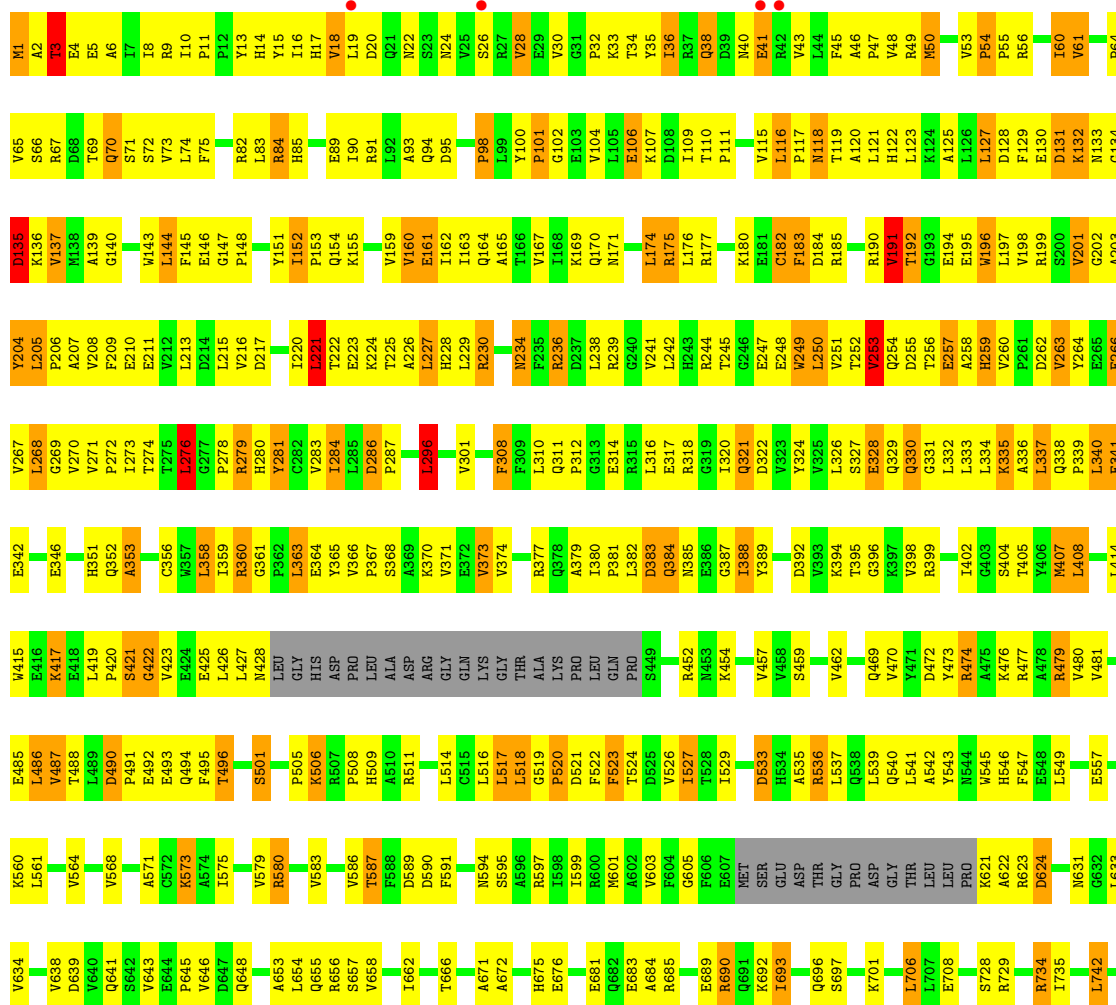
Chain S:

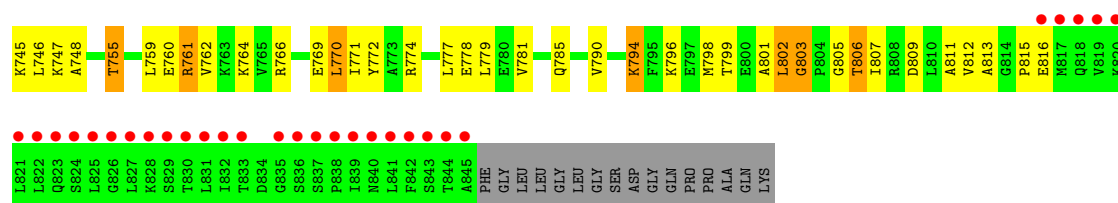




• Molecule 1: Major vault protein

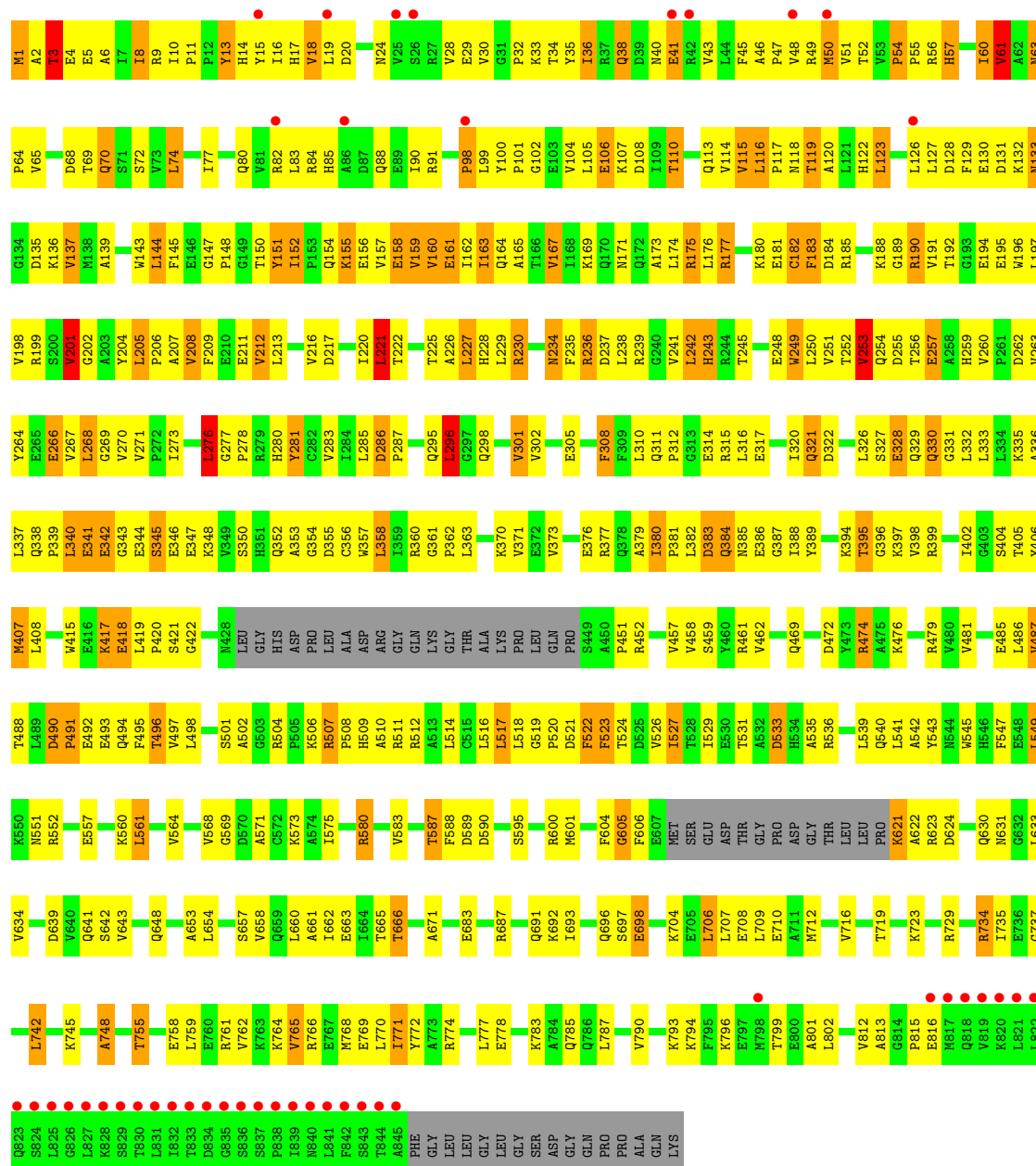
Chain U:





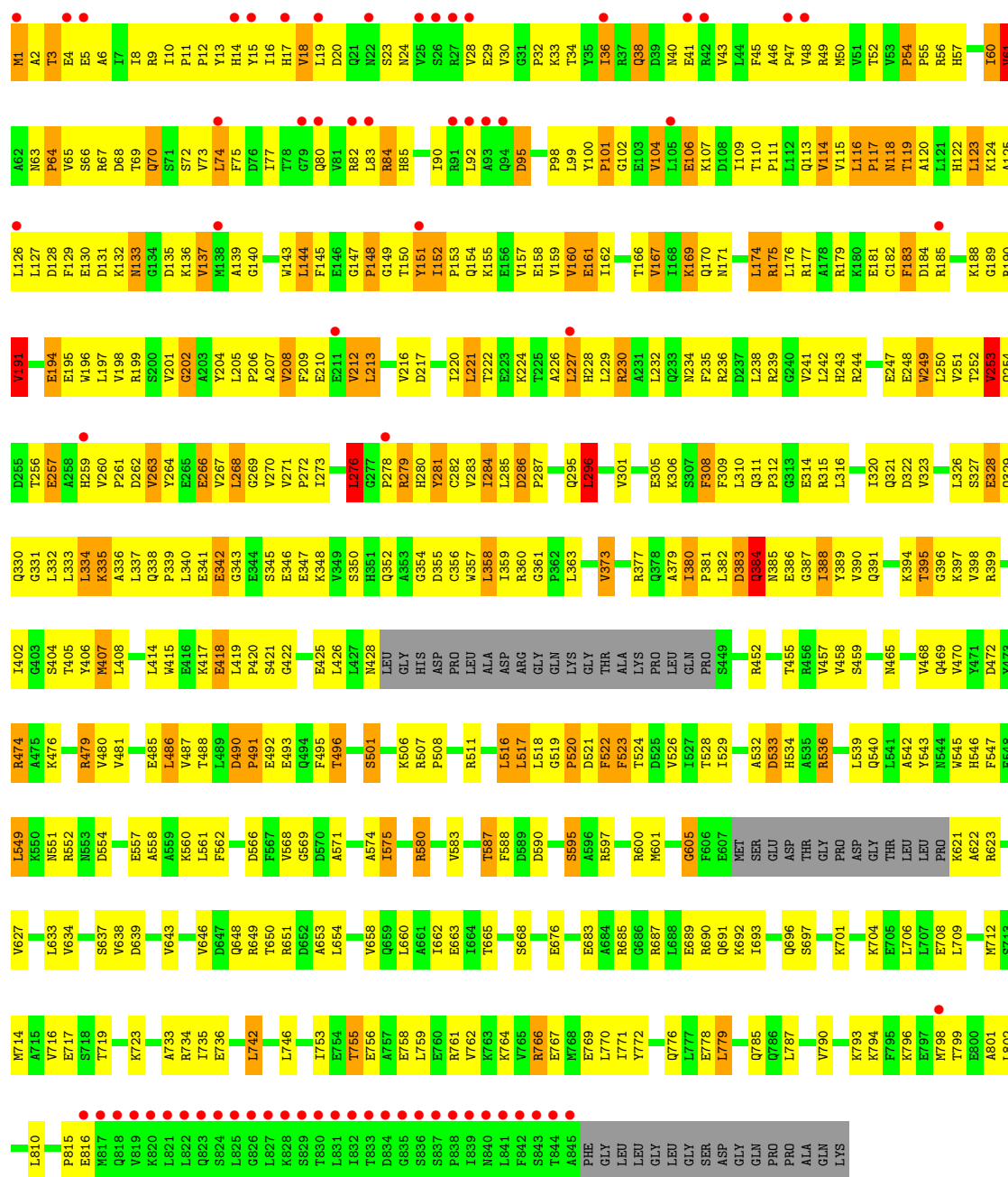
• Molecule 1: Major vault protein

Chain V:



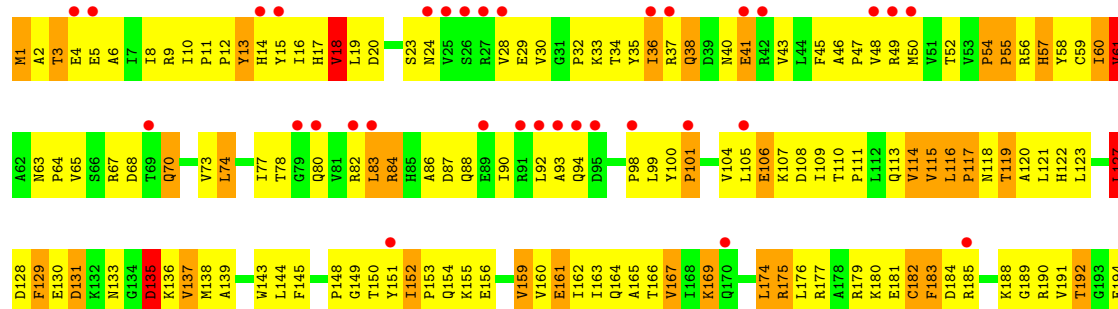
• Molecule 1: Major vault protein

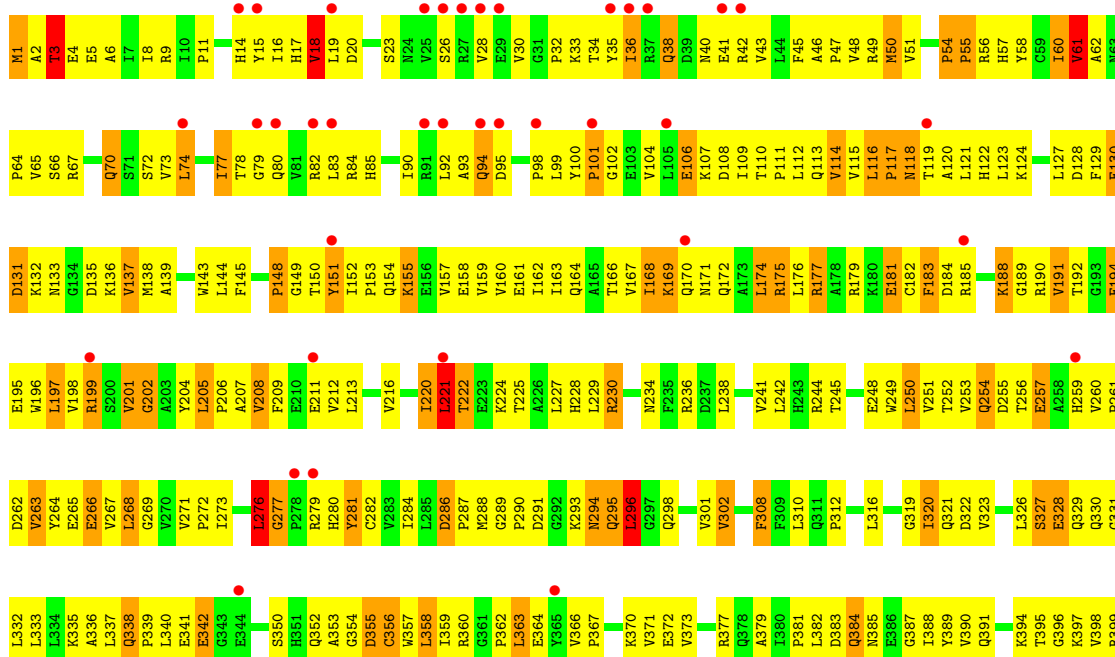
Chain W:

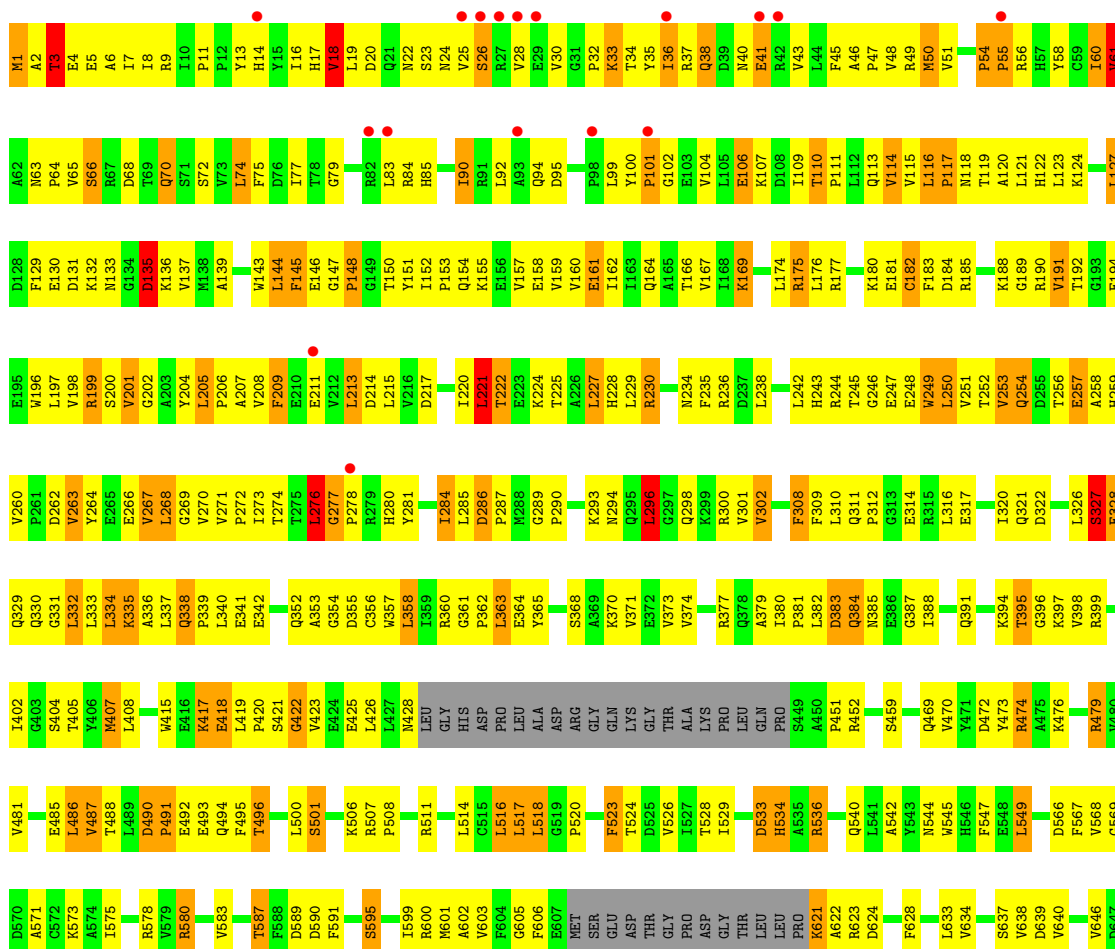


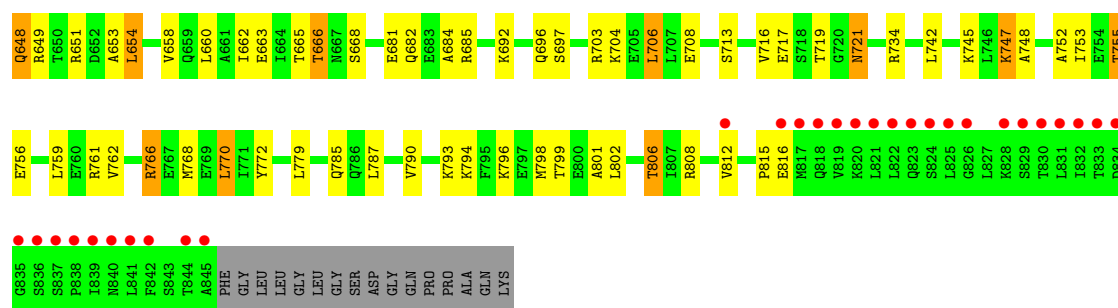
• Molecule 1: Major vault protein

Chain X:



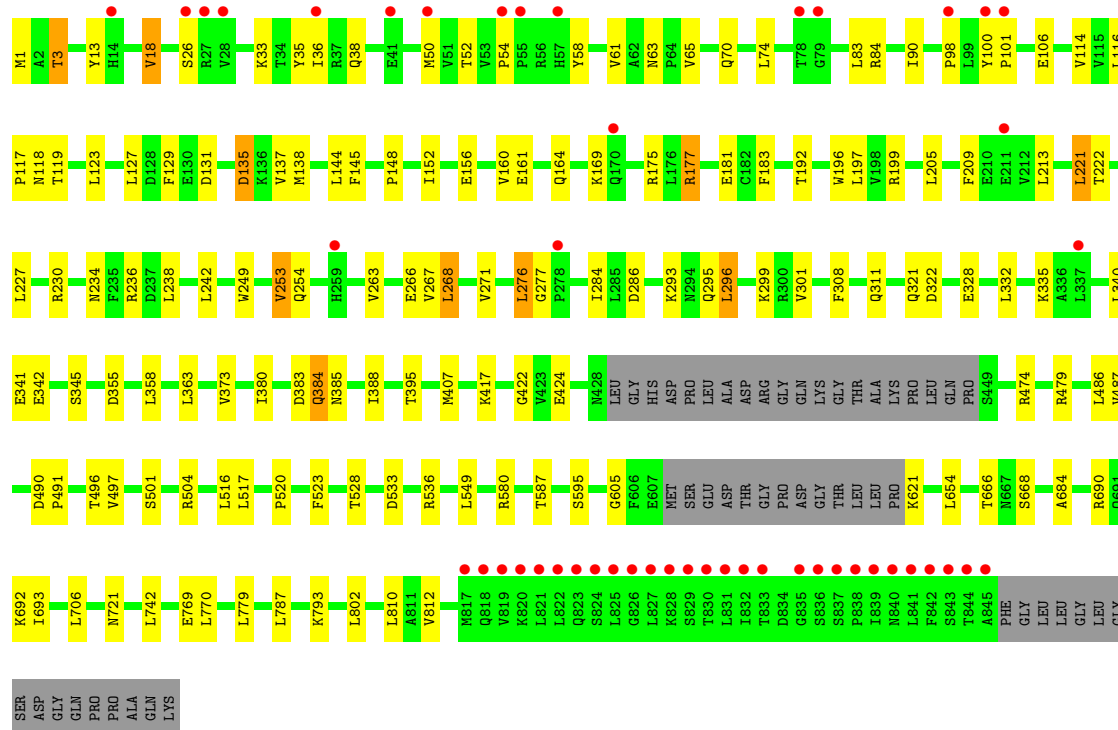






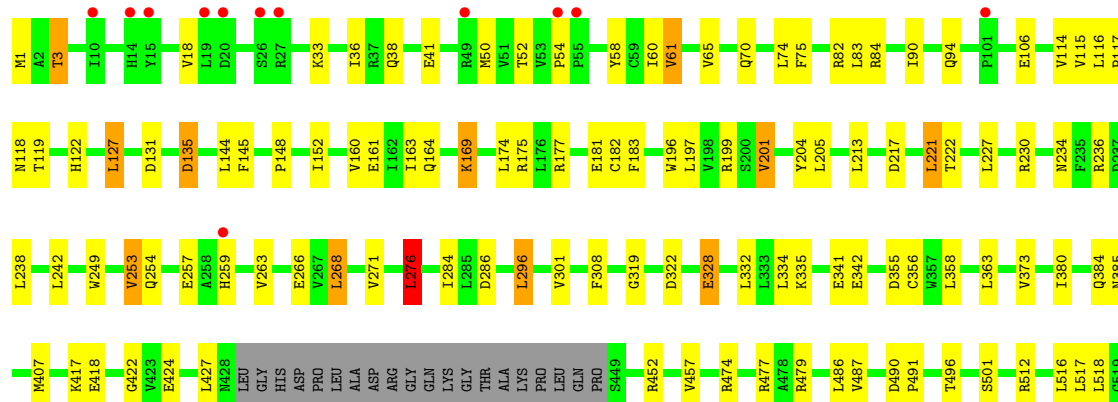
• Molecule 1: Major vault protein

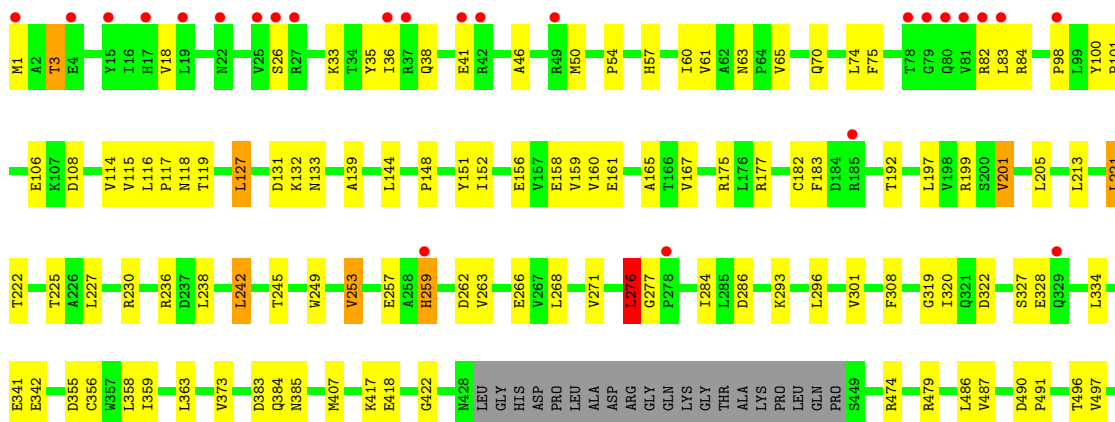
Chain a:

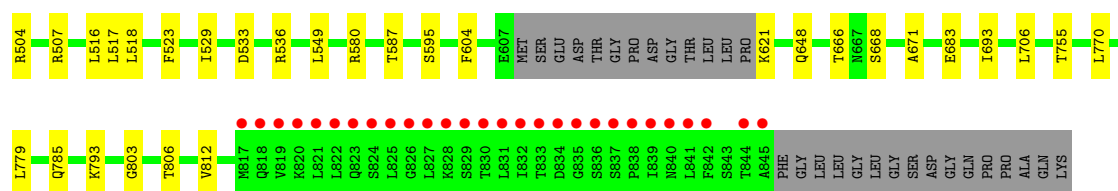


• Molecule 1: Major vault protein

Chain b:

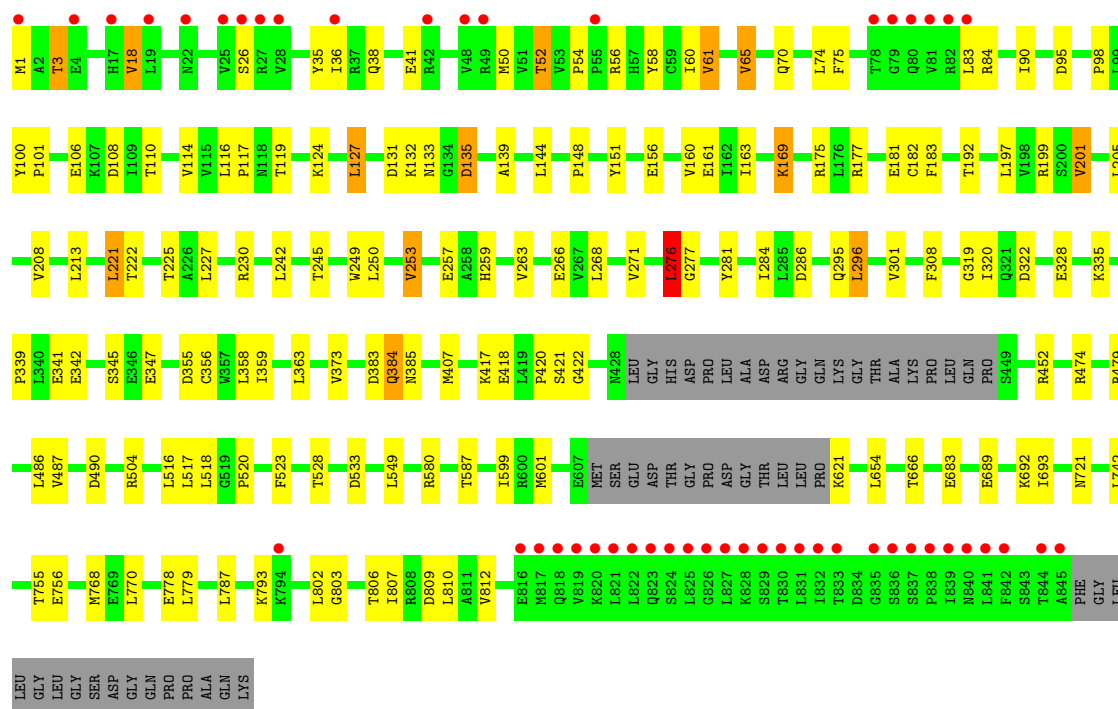






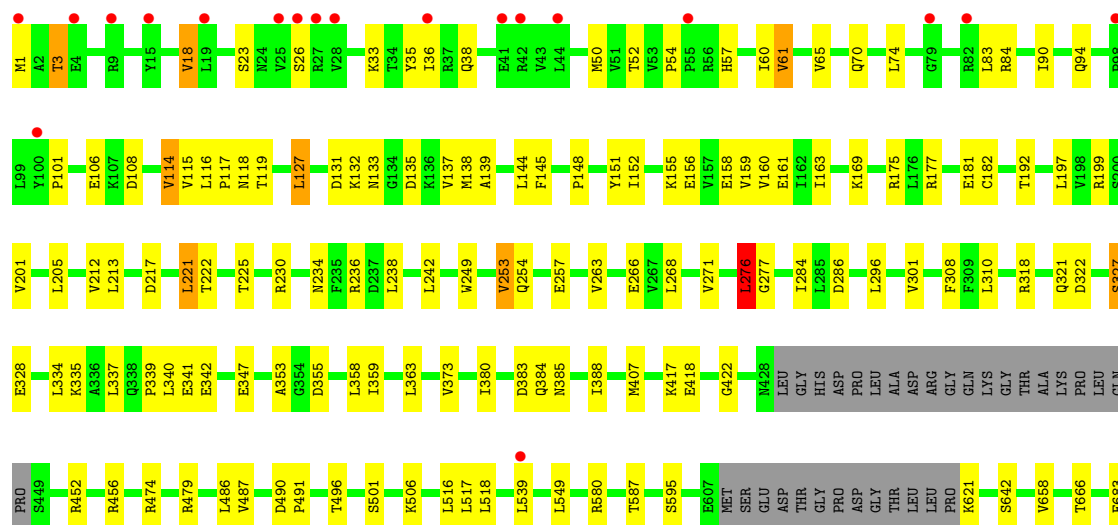
• Molecule 1: Major vault protein

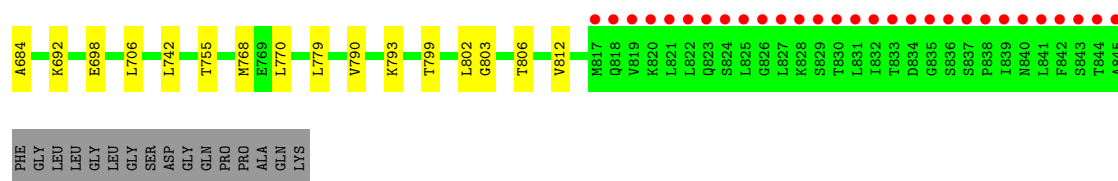
Chain e:



• Molecule 1: Major vault protein

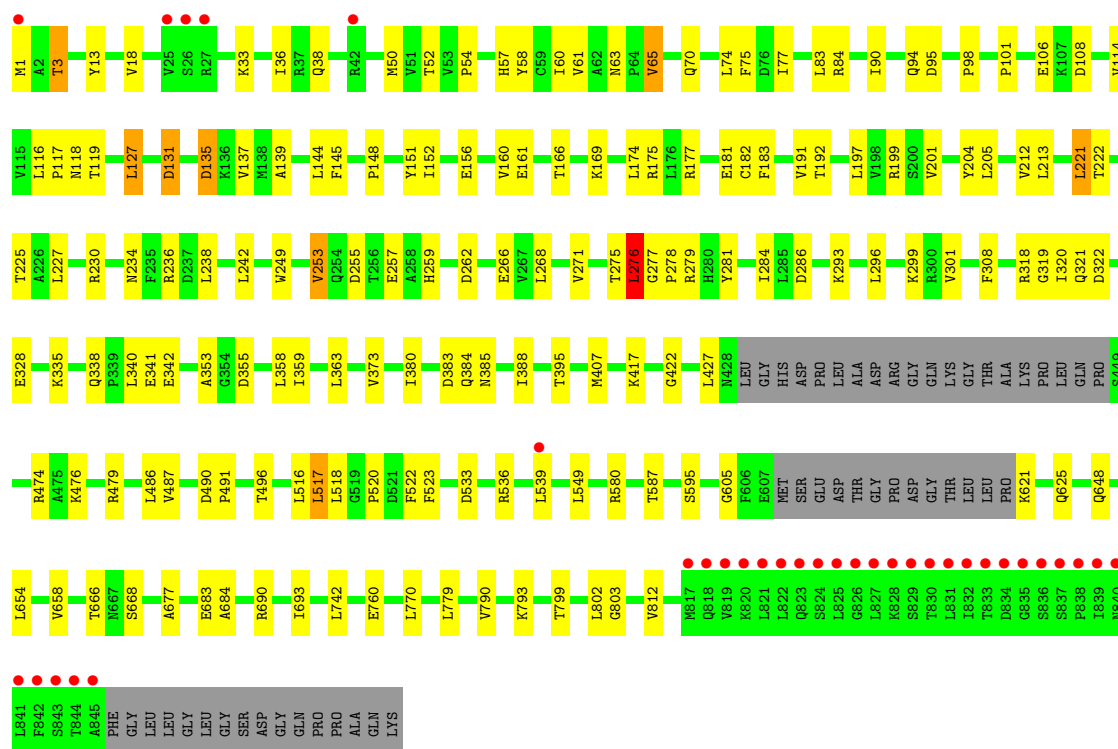
Chain f:





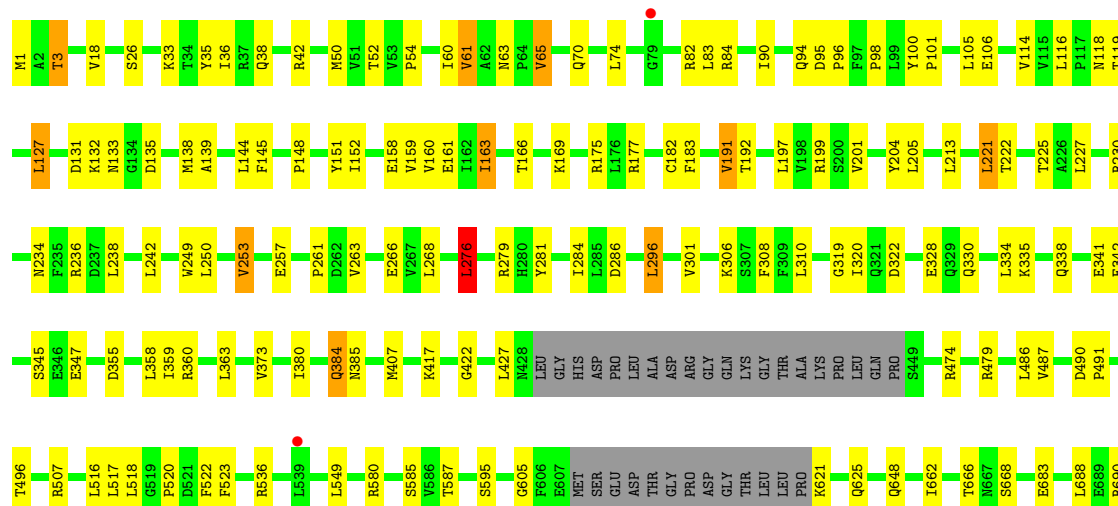
• Molecule 1: Major vault protein

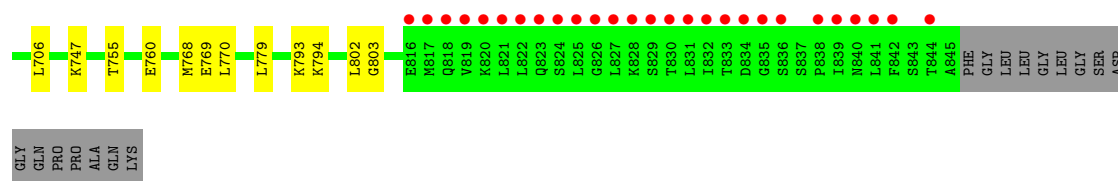
Chain g:



• Molecule 1: Major vault protein

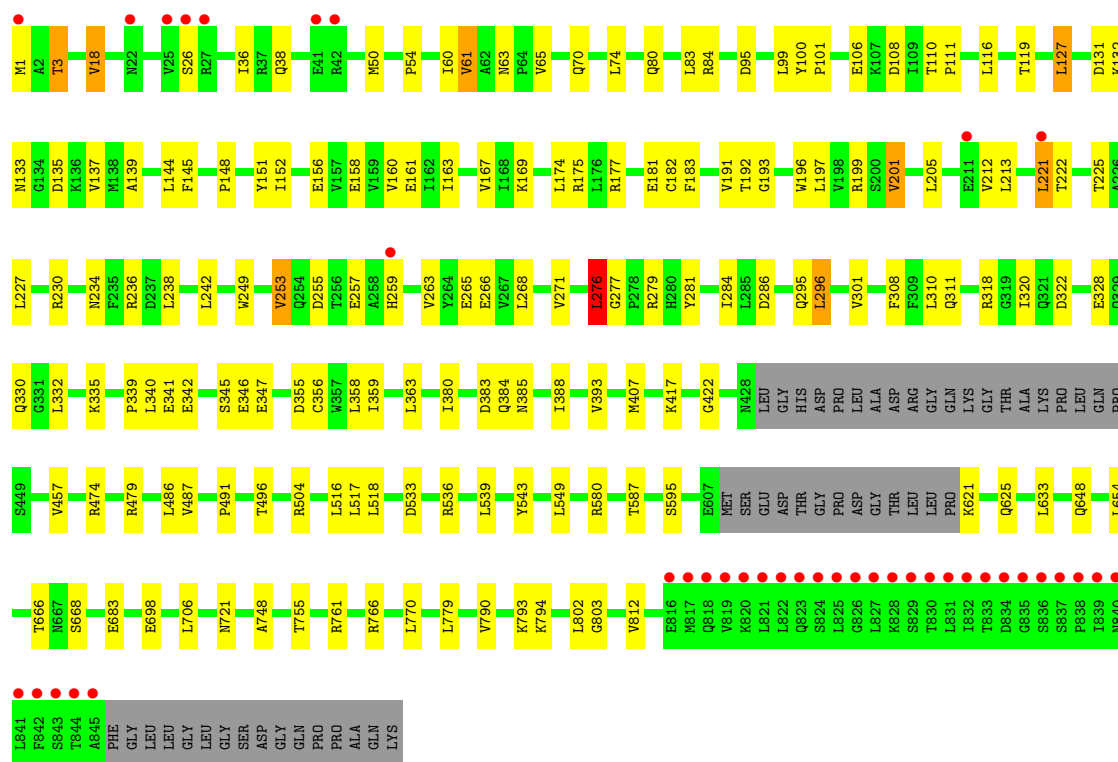
Chain h:





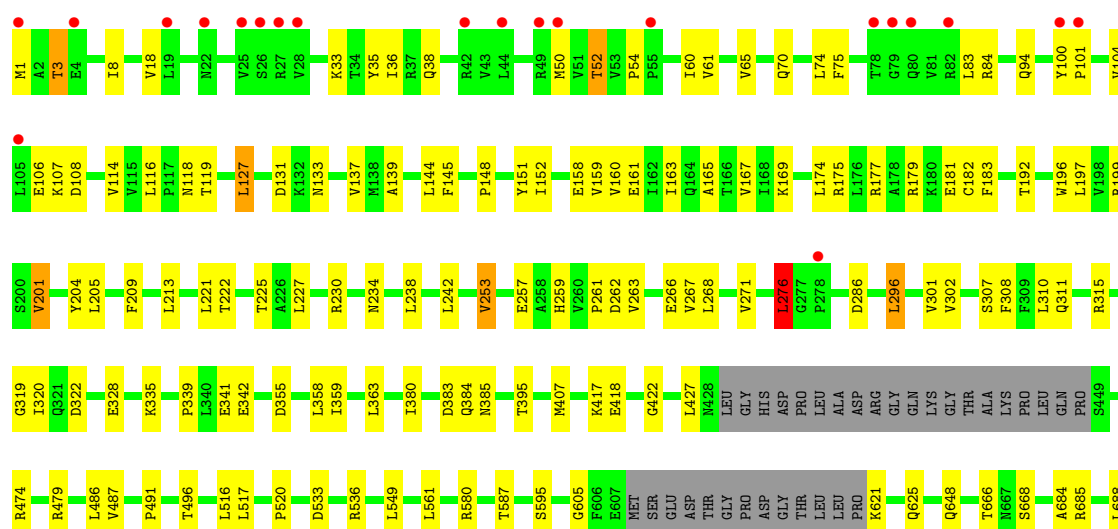
• Molecule 1: Major vault protein

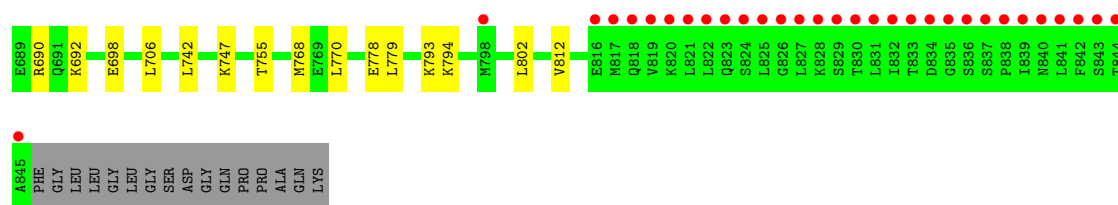
Chain i:



• Molecule 1: Major vault protein

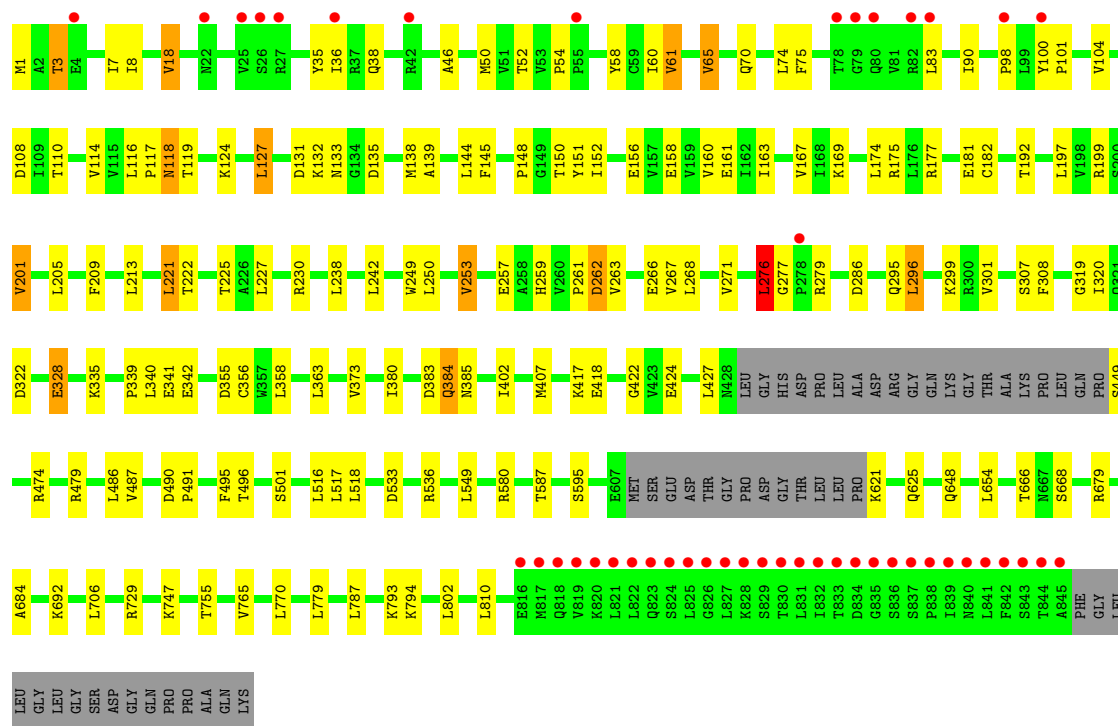
Chain j:





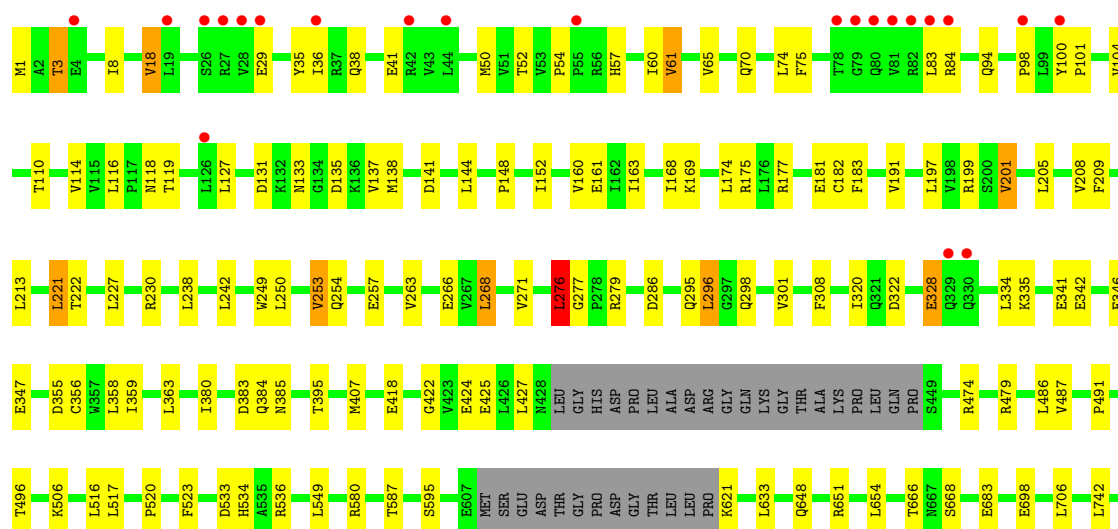
• Molecule 1: Major vault protein

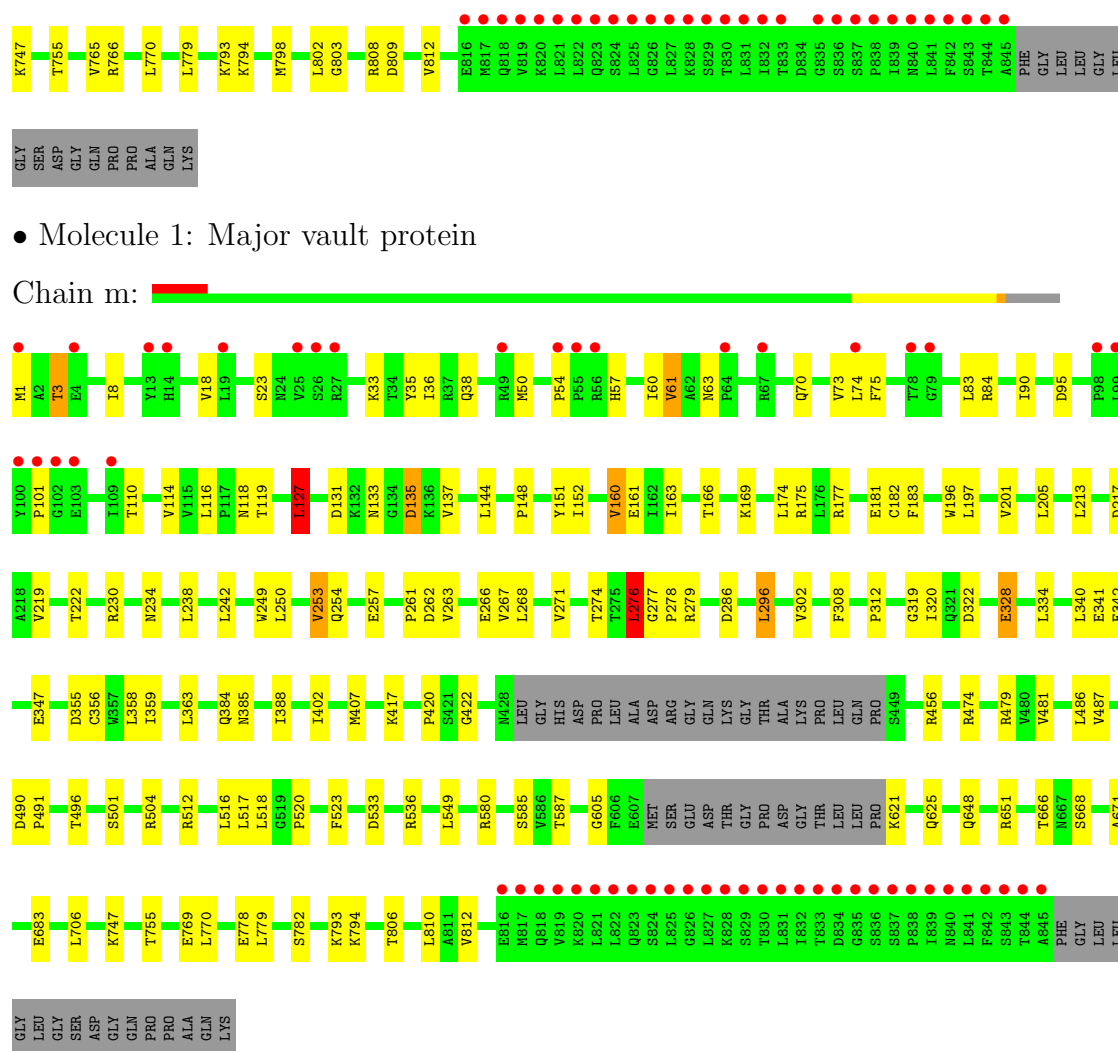
Chain k:



• Molecule 1: Major vault protein

Chain l:





4 Data and refinement statistics

Xtriage (Phenix) failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
Refinement program	CNS	Depositor
R, R_{free}	0.311 , 0.330 0.310 , 0.310	Depositor DCC
R_{free} test set	76647 reflections (5.27%)	DCC
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 72.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	241956	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 32.

The worst 5 of 15693 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

5.3.1 Protein backbone ⓘ

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%)	7	53
1	B	776/861 (90%)	640 (82%)	114 (15%)	22 (3%)	8	55
1	C	776/861 (90%)	639 (82%)	109 (14%)	28 (4%)	5	49
1	D	776/861 (90%)	635 (82%)	108 (14%)	33 (4%)	4	42
1	E	776/861 (90%)	637 (82%)	107 (14%)	32 (4%)	4	44
1	F	776/861 (90%)	627 (81%)	118 (15%)	31 (4%)	5	44
1	G	776/861 (90%)	648 (84%)	101 (13%)	27 (4%)	6	50
1	H	776/861 (90%)	636 (82%)	109 (14%)	31 (4%)	5	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles		
1	I	776/861 (90%)	650 (84%)	98 (13%)	28 (4%)	5	49	
1	J	776/861 (90%)	637 (82%)	109 (14%)	30 (4%)	5	45	
1	K	776/861 (90%)	631 (81%)	104 (13%)	41 (5%)	3	35	
1	L	776/861 (90%)	637 (82%)	103 (13%)	36 (5%)	4	39	
1	M	776/861 (90%)	633 (82%)	107 (14%)	36 (5%)	4	39	
1	N	776/861 (90%)	639 (82%)	102 (13%)	35 (4%)	4	40	
1	O	776/861 (90%)	637 (82%)	102 (13%)	37 (5%)	4	38	
1	P	776/861 (90%)	627 (81%)	117 (15%)	32 (4%)	4	44	
1	Q	776/861 (90%)	633 (82%)	104 (13%)	39 (5%)	3	37	
1	R	776/861 (90%)	627 (81%)	109 (14%)	40 (5%)	3	35	
1	S	776/861 (90%)	624 (80%)	115 (15%)	37 (5%)	4	38	
1	T	776/861 (90%)	631 (81%)	113 (15%)	32 (4%)	4	44	
1	U	776/861 (90%)	642 (83%)	100 (13%)	34 (4%)	4	41	
1	V	776/861 (90%)	639 (82%)	110 (14%)	27 (4%)	6	50	
1	W	776/861 (90%)	647 (83%)	96 (12%)	33 (4%)	4	42	
1	X	776/861 (90%)	648 (84%)	97 (12%)	31 (4%)	5	44	
1	Y	776/861 (90%)	644 (83%)	98 (13%)	34 (4%)	4	41	
1	Z	776/861 (90%)	649 (84%)	97 (12%)	30 (4%)	5	45	
1	a	776/861 (90%)	639 (82%)	108 (14%)	29 (4%)	5	48	
1	b	776/861 (90%)	635 (82%)	112 (14%)	29 (4%)	5	48	
1	c	776/861 (90%)	642 (83%)	101 (13%)	33 (4%)	4	42	
1	d	776/861 (90%)	630 (81%)	118 (15%)	28 (4%)	5	49	
1	e	776/861 (90%)	629 (81%)	113 (15%)	34 (4%)	4	41	
1	f	776/861 (90%)	642 (83%)	99 (13%)	35 (4%)	4	40	
1	g	776/861 (90%)	637 (82%)	98 (13%)	41 (5%)	3	35	
1	h	776/861 (90%)	639 (82%)	97 (12%)	40 (5%)	3	35	
1	i	776/861 (90%)	634 (82%)	104 (13%)	38 (5%)	3	37	
1	j	776/861 (90%)	634 (82%)	107 (14%)	35 (4%)	4	40	
1	k	776/861 (90%)	633 (82%)	105 (14%)	38 (5%)	3	37	
1	l	776/861 (90%)	632 (81%)	107 (14%)	37 (5%)	4	38	
1	m	776/861 (90%)	634 (82%)	108 (14%)	34 (4%)	4	41	

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	30264/33579 (90%)	24831 (82%)	4143 (14%)	1290 (4%)	4 42

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%)	2 10
1	B	663/727 (91%)	545 (82%)	118 (18%)	2 16
1	C	663/727 (91%)	536 (81%)	127 (19%)	2 12
1	D	663/727 (91%)	543 (82%)	120 (18%)	2 15
1	E	663/727 (91%)	550 (83%)	113 (17%)	3 18
1	F	663/727 (91%)	543 (82%)	120 (18%)	2 15
1	G	663/727 (91%)	533 (80%)	130 (20%)	2 11
1	H	663/727 (91%)	533 (80%)	130 (20%)	2 11
1	I	663/727 (91%)	537 (81%)	126 (19%)	2 13
1	J	663/727 (91%)	532 (80%)	131 (20%)	2 11
1	K	663/727 (91%)	519 (78%)	144 (22%)	1 9
1	L	663/727 (91%)	536 (81%)	127 (19%)	2 12
1	M	663/727 (91%)	537 (81%)	126 (19%)	2 13
1	N	663/727 (91%)	535 (81%)	128 (19%)	2 12
1	O	663/727 (91%)	528 (80%)	135 (20%)	2 10
1	P	663/727 (91%)	527 (80%)	136 (20%)	2 10
1	Q	663/727 (91%)	528 (80%)	135 (20%)	2 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R	663/727 (91%)	521 (79%)	142 (21%)	1	9
1	S	663/727 (91%)	539 (81%)	124 (19%)	2	13
1	T	663/727 (91%)	540 (81%)	123 (19%)	2	13
1	U	663/727 (91%)	532 (80%)	131 (20%)	2	11
1	V	663/727 (91%)	530 (80%)	133 (20%)	2	11
1	W	663/727 (91%)	545 (82%)	118 (18%)	2	16
1	X	663/727 (91%)	534 (80%)	129 (20%)	2	12
1	Y	663/727 (91%)	547 (82%)	116 (18%)	3	17
1	Z	663/727 (91%)	535 (81%)	128 (19%)	2	12
1	a	663/727 (91%)	538 (81%)	125 (19%)	2	13
1	b	663/727 (91%)	534 (80%)	129 (20%)	2	12
1	c	663/727 (91%)	531 (80%)	132 (20%)	2	11
1	d	663/727 (91%)	542 (82%)	121 (18%)	2	14
1	e	663/727 (91%)	534 (80%)	129 (20%)	2	12
1	f	663/727 (91%)	536 (81%)	127 (19%)	2	12
1	g	663/727 (91%)	533 (80%)	130 (20%)	2	11
1	h	663/727 (91%)	535 (81%)	128 (19%)	2	12
1	i	663/727 (91%)	533 (80%)	130 (20%)	2	11
1	j	663/727 (91%)	540 (81%)	123 (19%)	2	13
1	k	663/727 (91%)	531 (80%)	132 (20%)	2	11
1	l	663/727 (91%)	541 (82%)	122 (18%)	2	14
1	m	663/727 (91%)	541 (82%)	122 (18%)	2	14
All	All	25857/28353 (91%)	20881 (81%)	4976 (19%)	2	12

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 ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th 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 ²)	Q<0.9
1	A	812/861 (94%)	0.26	40 (4%) 28 12	46, 106, 218, 285	0
1	B	812/861 (94%)	0.30	45 (5%) 24 10	30, 112, 219, 284	0
1	C	812/861 (94%)	0.32	41 (5%) 28 12	54, 113, 221, 291	0
1	D	812/861 (94%)	0.45	57 (7%) 16 7	43, 113, 218, 277	0
1	E	812/861 (94%)	0.54	74 (9%) 9 5	53, 112, 222, 283	0
1	F	812/861 (94%)	0.40	62 (7%) 14 7	46, 114, 223, 278	0
1	G	812/861 (94%)	0.29	45 (5%) 24 10	55, 113, 223, 258	0
1	H	812/861 (94%)	0.18	37 (4%) 31 14	50, 112, 221, 281	0
1	I	812/861 (94%)	0.31	47 (5%) 22 9	56, 108, 215, 266	0
1	J	812/861 (94%)	0.42	59 (7%) 15 7	44, 105, 215, 277	0
1	K	812/861 (94%)	0.41	57 (7%) 16 7	32, 98, 207, 278	0
1	L	812/861 (94%)	0.37	55 (6%) 17 8	33, 99, 210, 277	0
1	M	812/861 (94%)	0.21	38 (4%) 30 13	45, 103, 207, 293	0
1	N	812/861 (94%)	0.12	31 (3%) 38 17	40, 104, 210, 249	0
1	O	812/861 (94%)	0.13	35 (4%) 34 14	33, 103, 214, 272	0
1	P	812/861 (94%)	0.25	45 (5%) 24 10	35, 103, 211, 294	0
1	Q	812/861 (94%)	0.39	56 (6%) 17 7	35, 101, 215, 277	0
1	R	812/861 (94%)	0.36	53 (6%) 18 8	37, 101, 217, 298	0
1	S	812/861 (94%)	0.34	53 (6%) 18 8	48, 106, 212, 284	0
1	T	812/861 (94%)	0.26	44 (5%) 25 10	52, 114, 220, 288	0
1	U	812/861 (94%)	0.15	33 (4%) 35 15	53, 113, 221, 282	0
1	V	812/861 (94%)	0.23	43 (5%) 25 10	57, 114, 220, 287	0
1	W	812/861 (94%)	0.44	66 (8%) 12 6	48, 116, 223, 288	0
1	X	812/861 (94%)	0.48	71 (8%) 10 6	47, 117, 220, 300	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Y	812/861 (94%)	0.42	67 (8%) 11 6	43, 117, 218, 278	0
1	Z	812/861 (94%)	0.28	46 (5%) 23 10	51, 114, 219, 263	0
1	a	812/861 (94%)	0.26	48 (5%) 22 9	50, 113, 216, 300	0
1	b	812/861 (94%)	0.25	42 (5%) 26 11	28, 110, 217, 281	0
1	c	812/861 (94%)	0.35	56 (6%) 17 7	26, 109, 218, 277	0
1	d	812/861 (94%)	0.31	53 (6%) 18 8	49, 106, 213, 274	0
1	e	812/861 (94%)	0.28	49 (6%) 21 9	47, 105, 210, 284	0
1	f	812/861 (94%)	0.27	48 (5%) 22 9	43, 106, 214, 266	0
1	g	812/861 (94%)	0.17	35 (4%) 34 14	50, 109, 213, 285	0
1	h	812/861 (94%)	0.12	29 (3%) 41 18	54, 110, 210, 277	0
1	i	812/861 (94%)	0.19	40 (4%) 28 12	48, 108, 215, 271	0
1	j	812/861 (94%)	0.29	52 (6%) 19 8	50, 105, 216, 267	0
1	k	812/861 (94%)	0.29	46 (5%) 23 10	41, 104, 210, 261	0
1	l	812/861 (94%)	0.34	51 (6%) 19 8	46, 105, 213, 300	0
1	m	812/861 (94%)	0.37	54 (6%) 17 8	40, 106, 219, 276	0
All	All	31668/33579 (94%)	0.30	1903 (6%) 21 9	26, 108, 217, 300	0

The worst 5 of 1903 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Y	27	ARG	16.0
1	R	26	SER	13.8
1	l	27	ARG	12.8
1	W	27	ARG	12.5
1	d	82	ARG	12.0

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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.