



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 12:30 AM UTC

PDB ID : 4V60 / pdb_00004v60
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

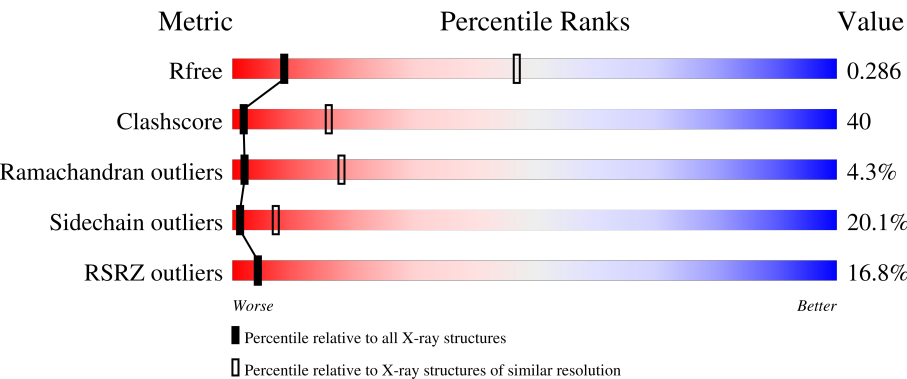
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	15% 40%42%12%• 6%
1	B	861	15% 41%41%11%• 6%
1	C	861	14% 41%40%12%• 6%
1	D	861	13% 38%42%12%• 6%
1	E	861	16% 39%43%12%• 6%

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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	15% 38% 41% 13% • 6%
1	f	861	16% 38% 42% 13% • 6%
1	g	861	18% 38% 41% 14% • 6%
1	h	861	22% 39% 42% 12% • 6%
1	i	861	20% 42% 39% 13% • 6%
1	j	861	16% 38% 42% 13% • 6%
1	k	861	14% 39% 41% 12% • 6%
1	l	861	14% 40% 40% 13% • 6%
1	m	861	15% 43% 39% 12% • 6%

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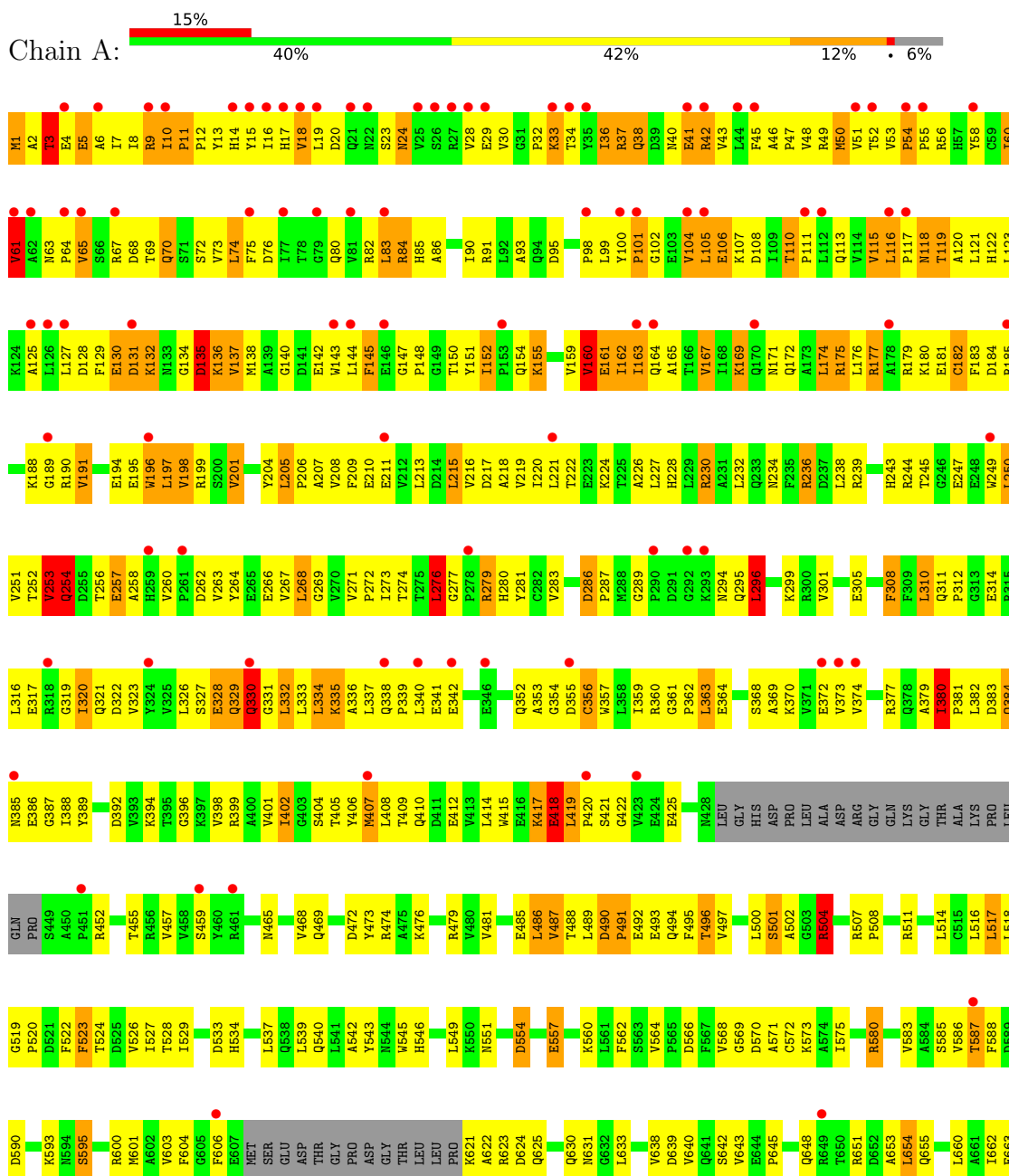
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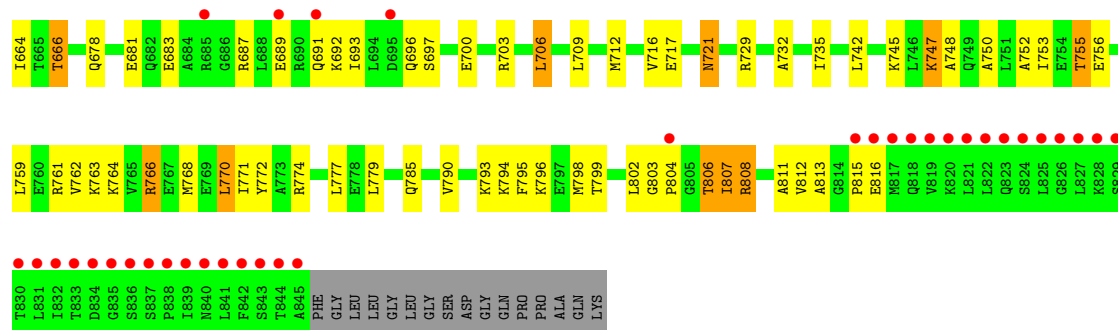
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	l	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	m	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			

3 Residue-property plots

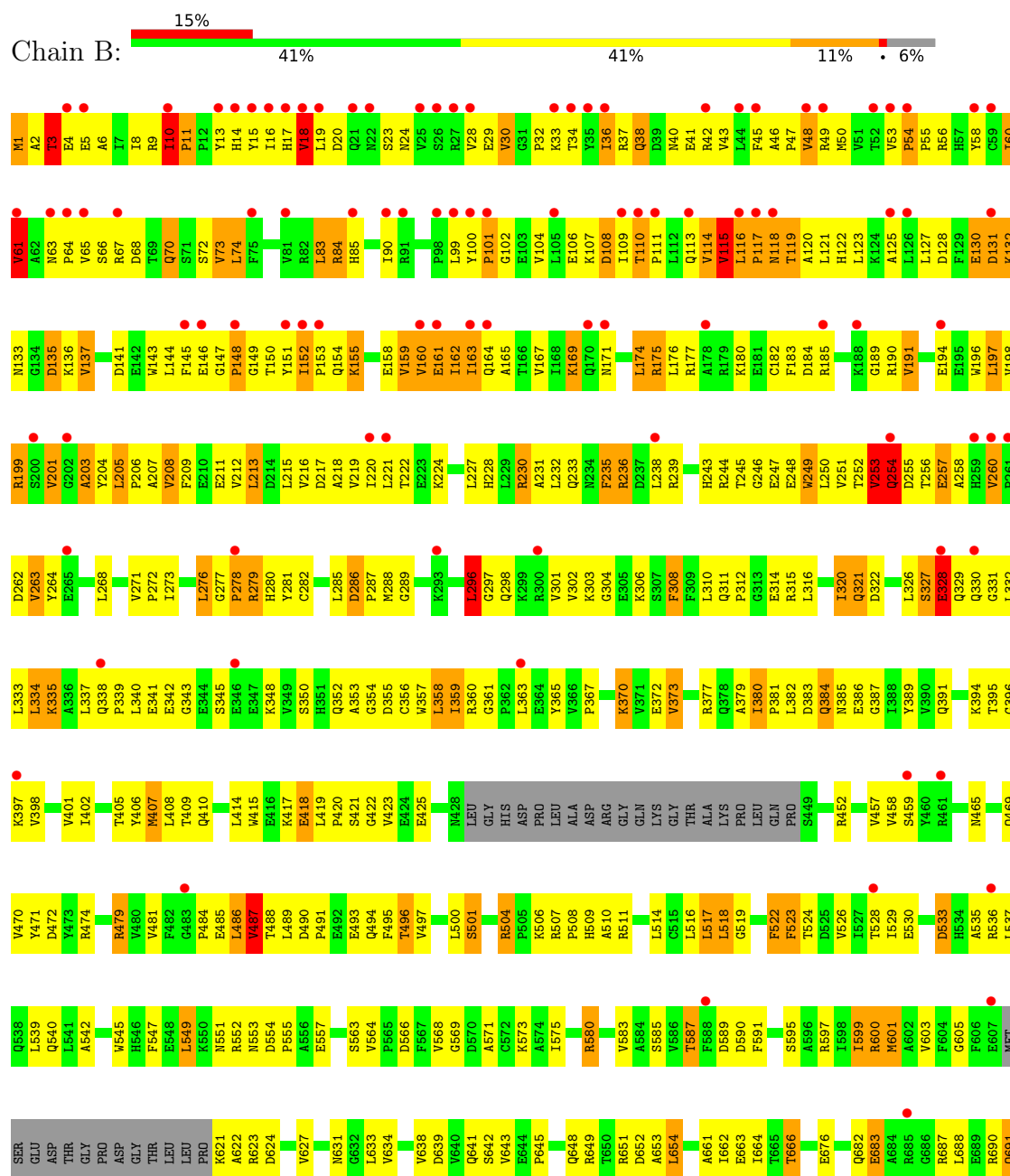
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

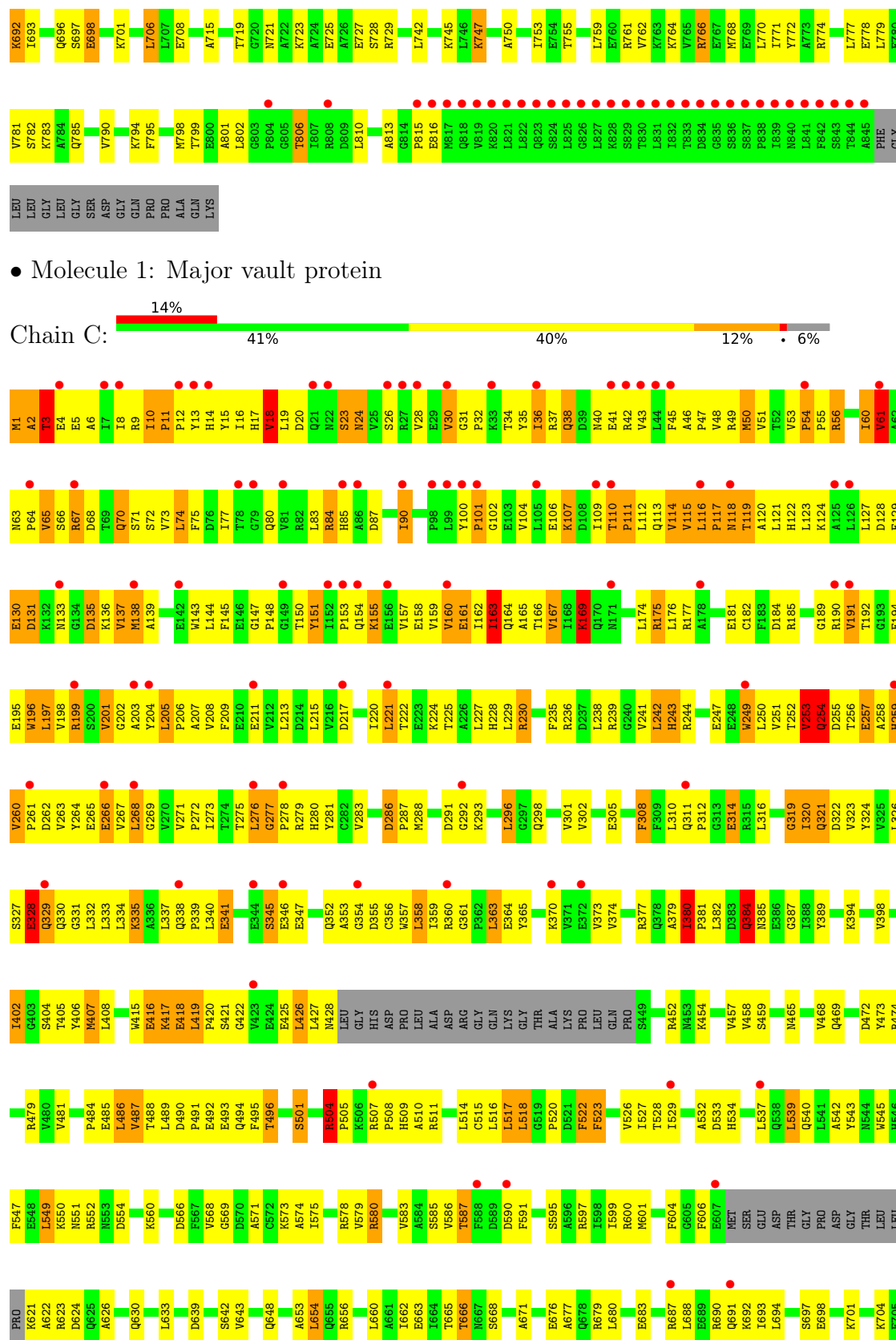
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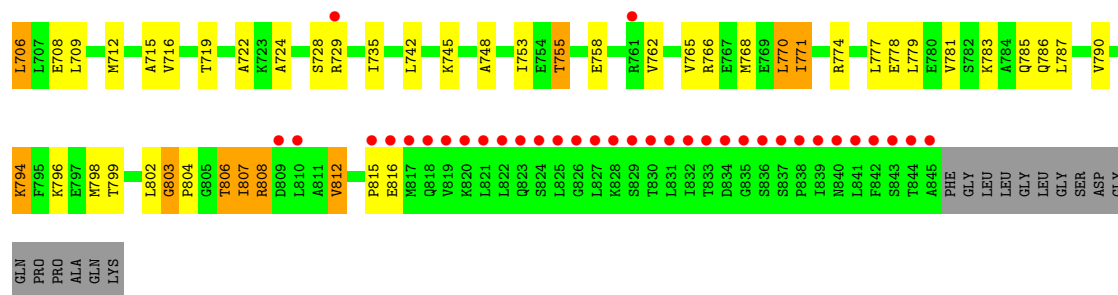




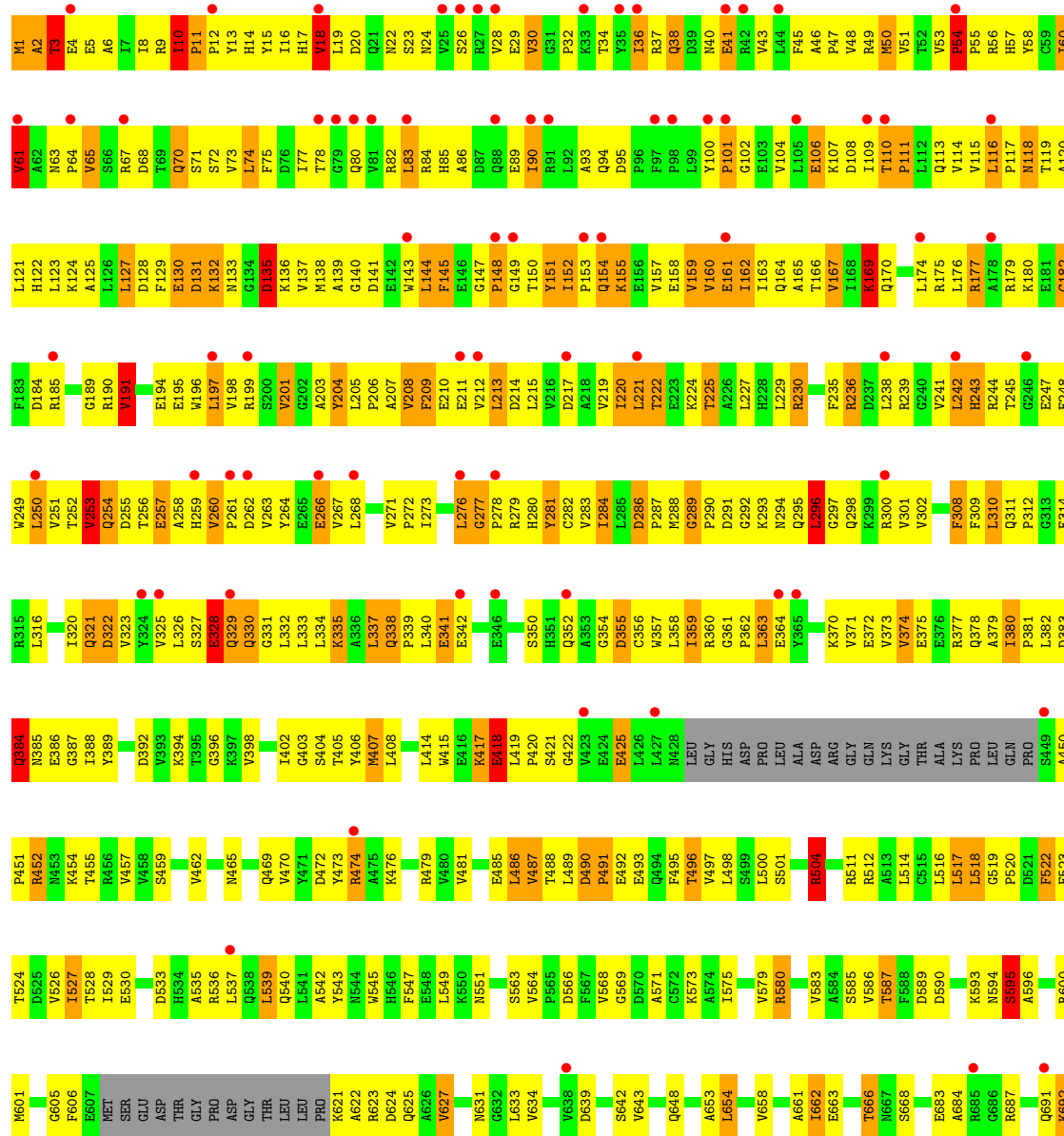
• Molecule 1: Major vault protein

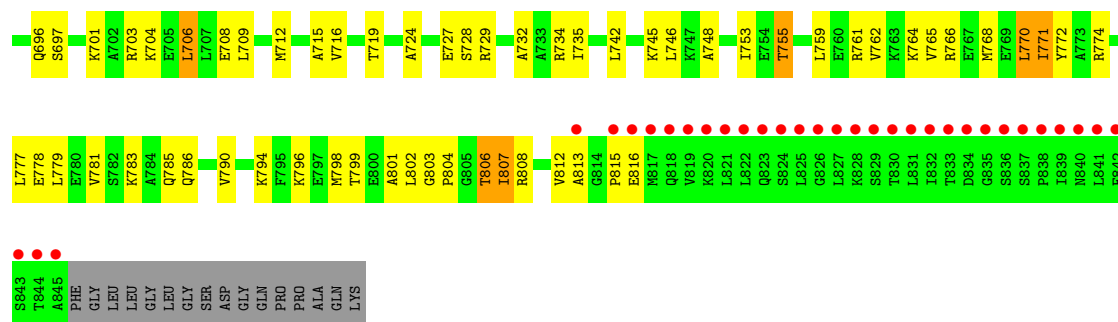




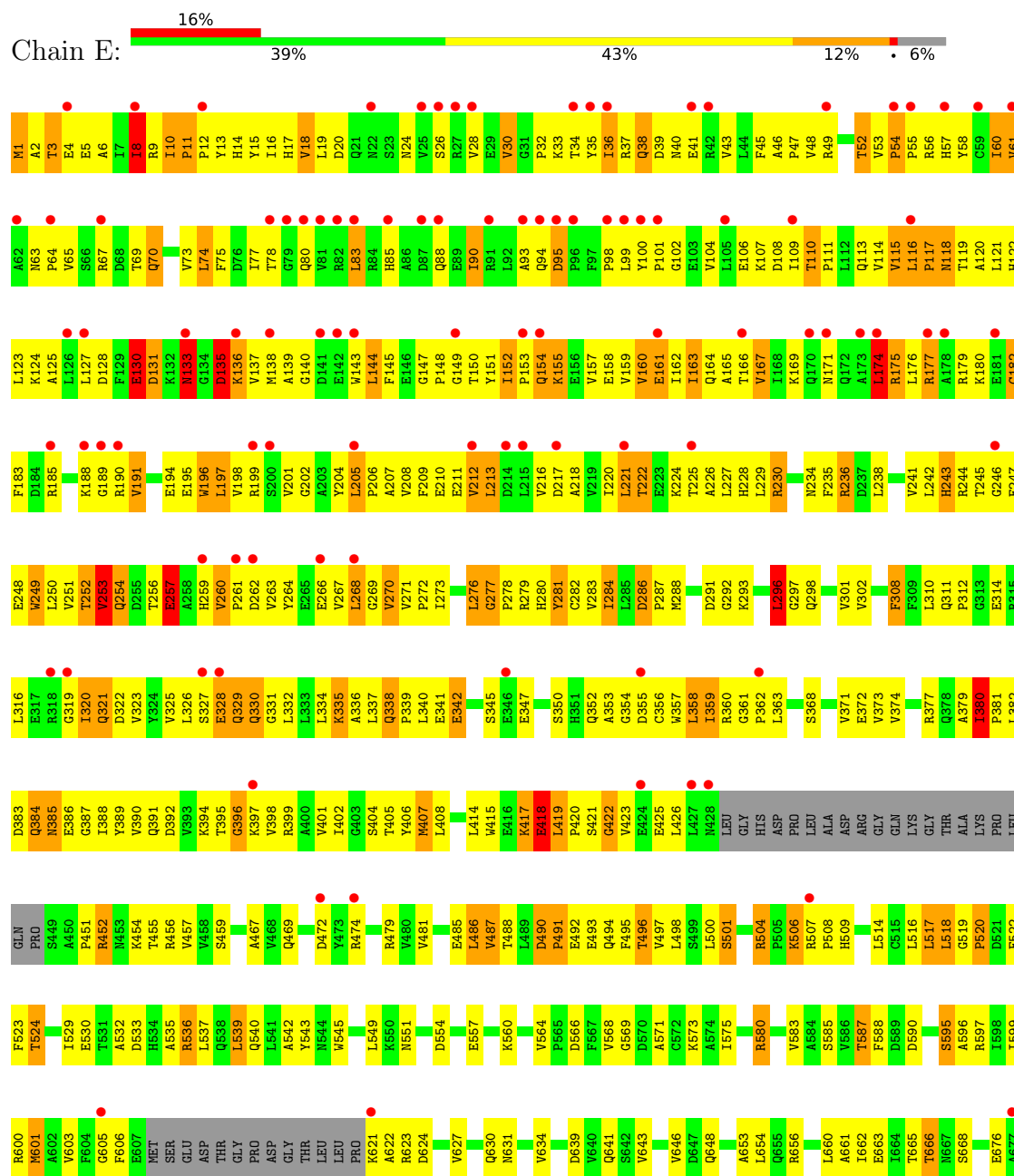


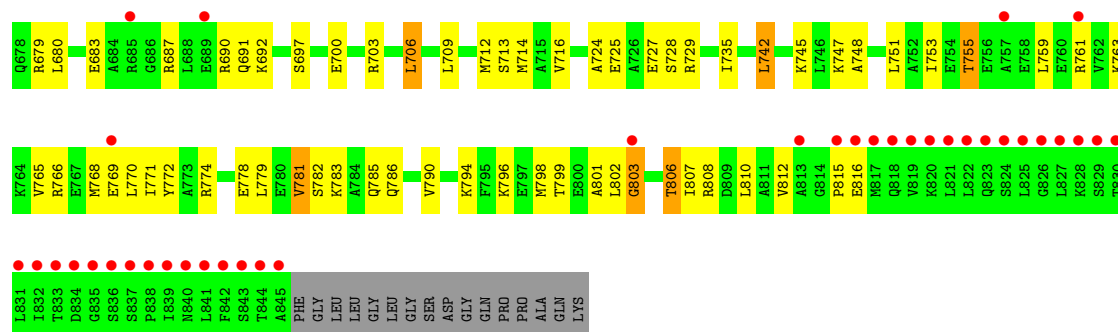
• Molecule 1: Major vault protein



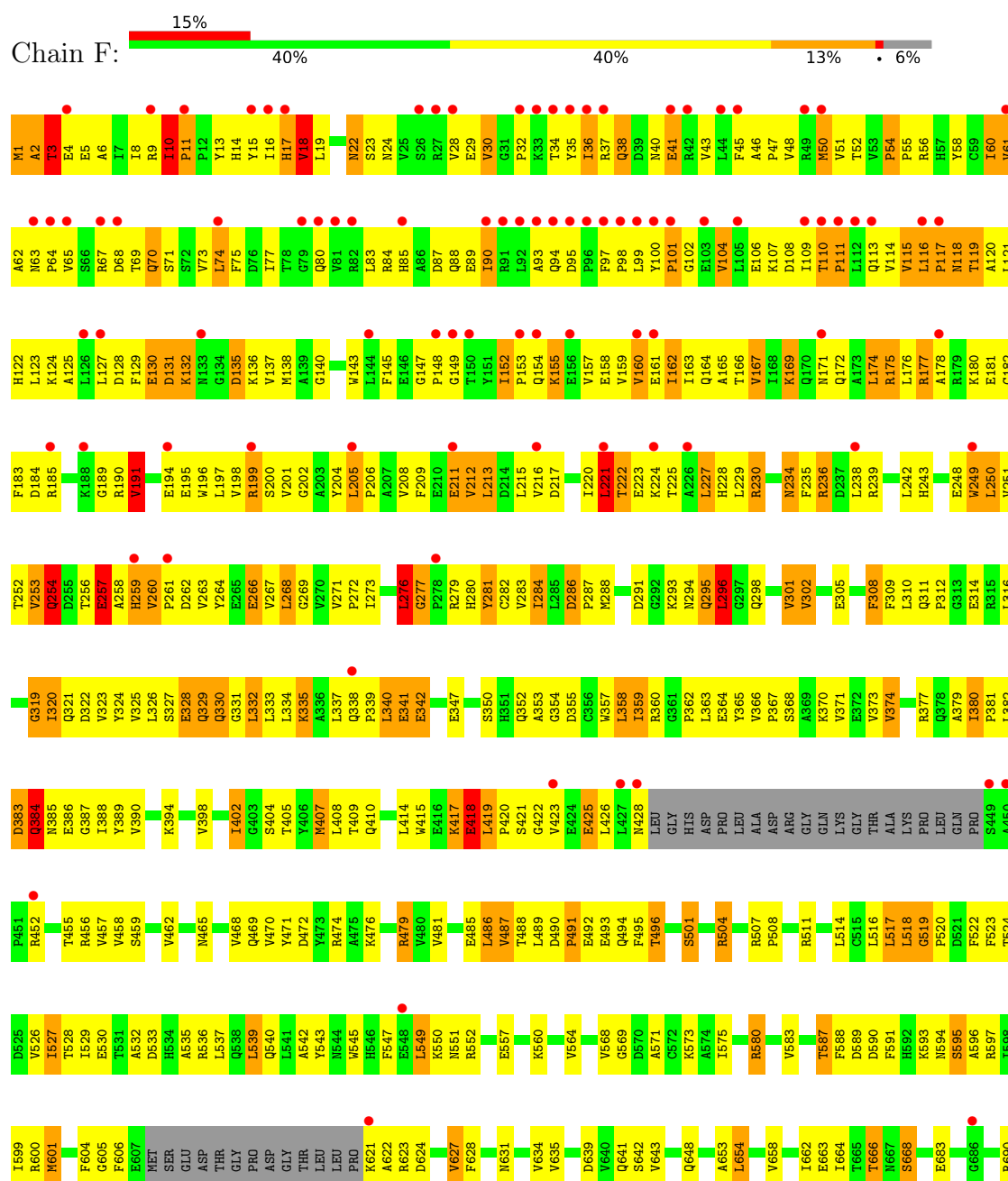


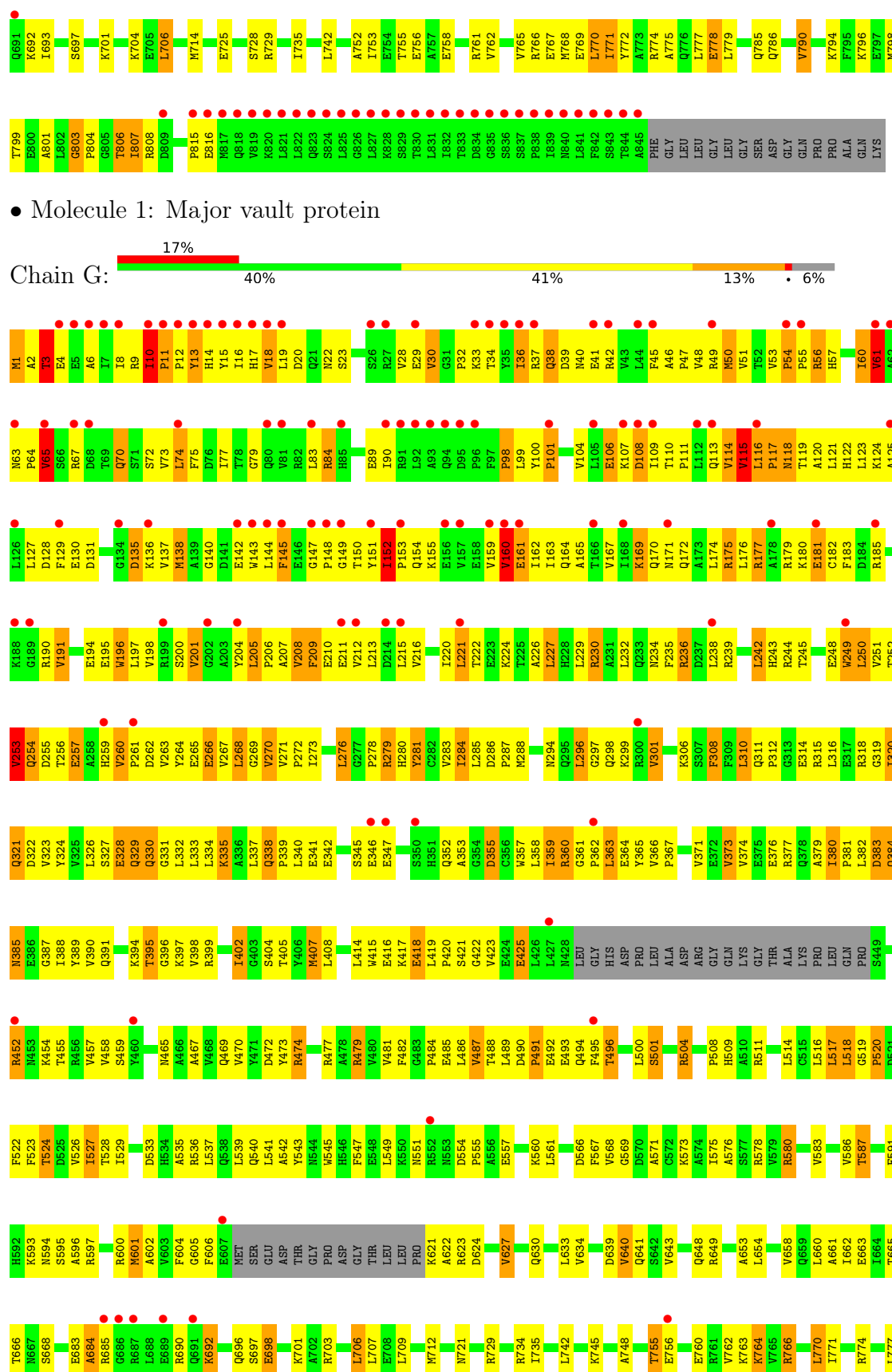
● Molecule 1: Major vault protein

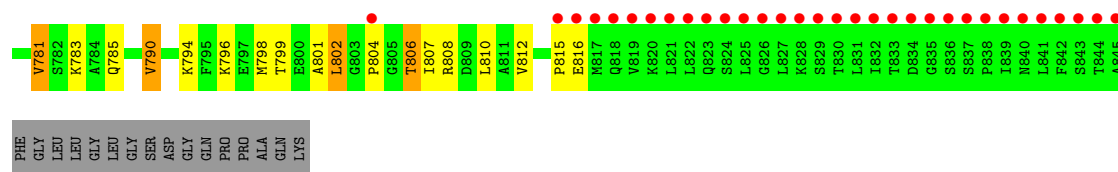




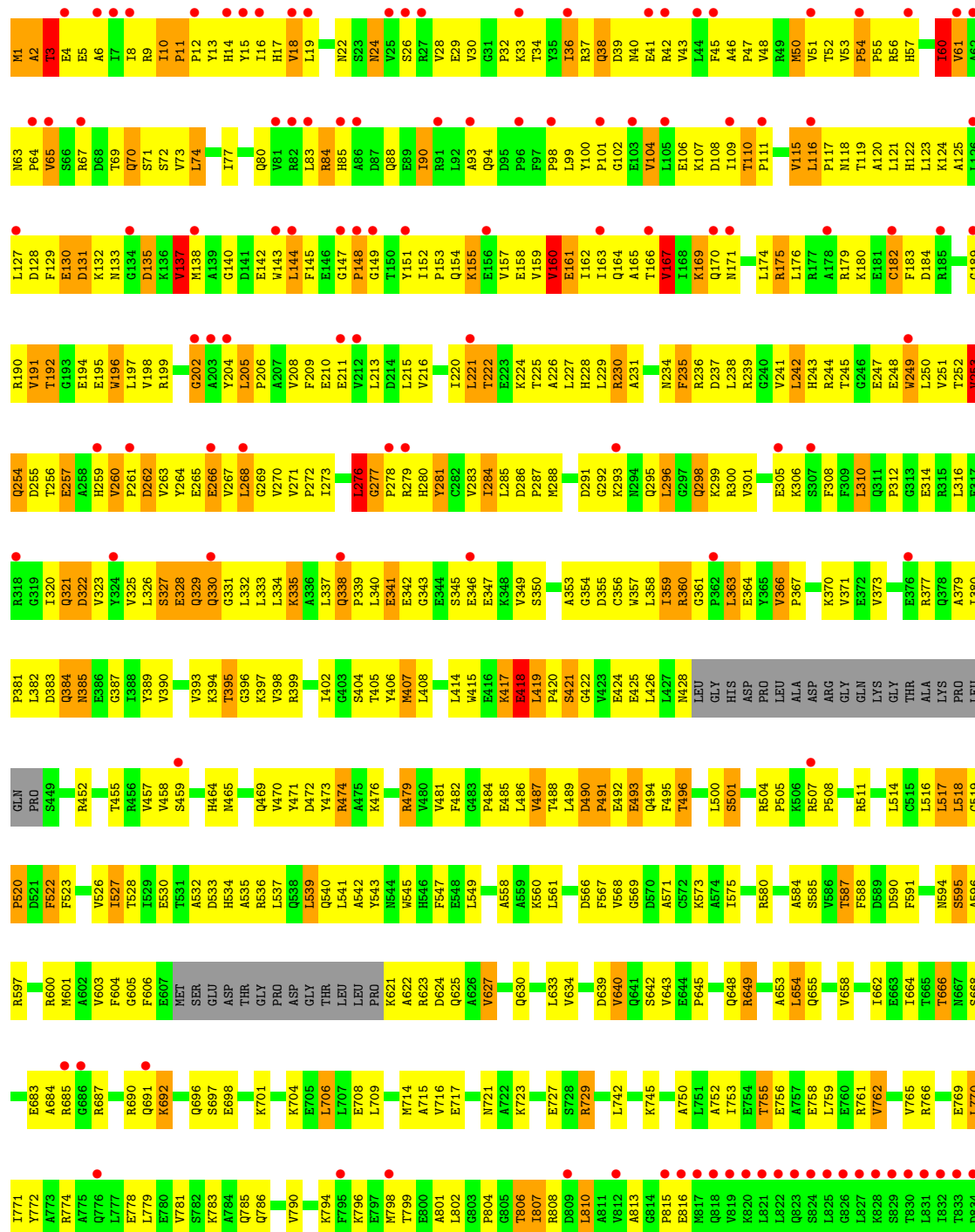
• Molecule 1: Major vault protein



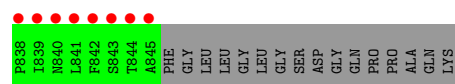




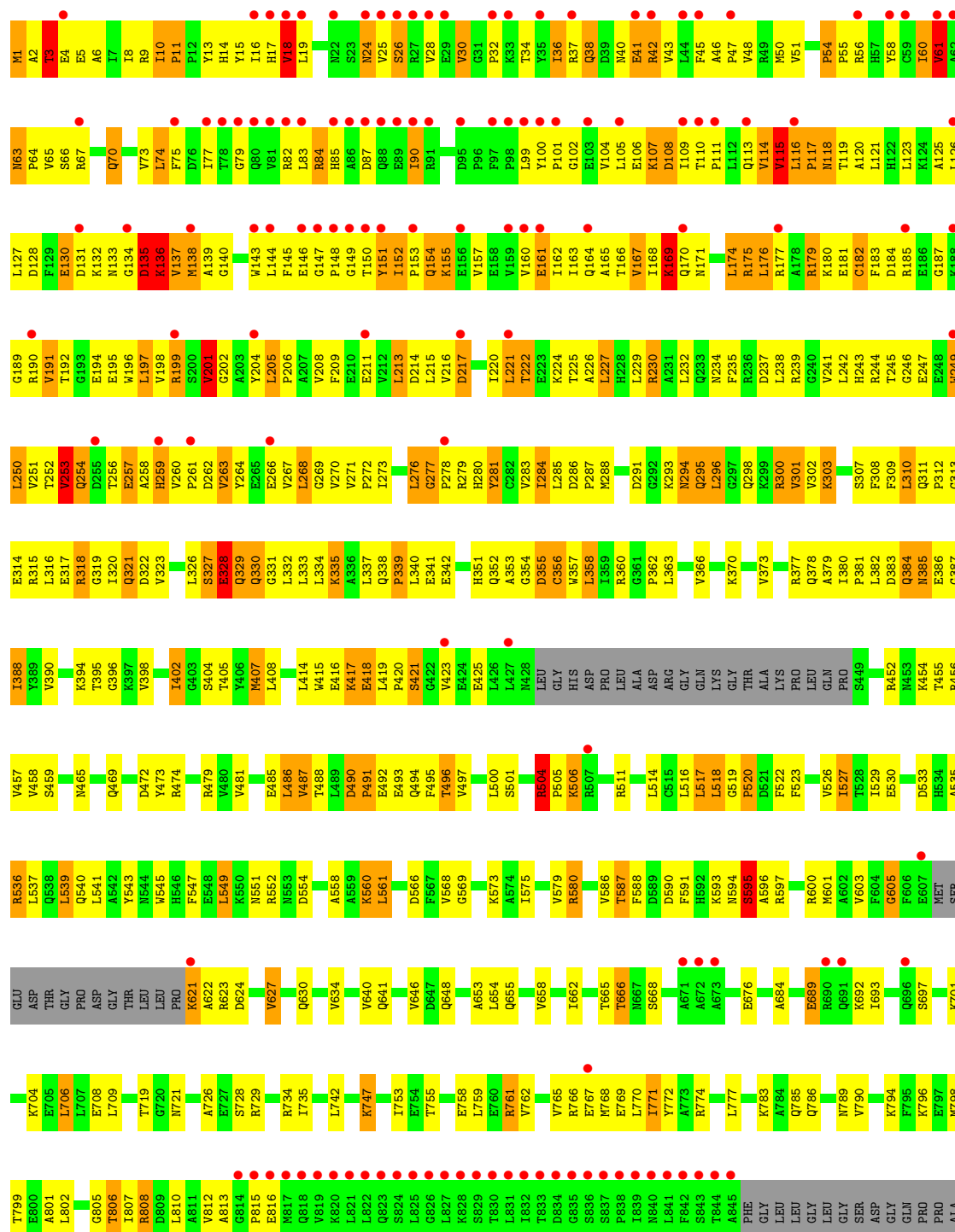
● Molecule 1: Major vault protein





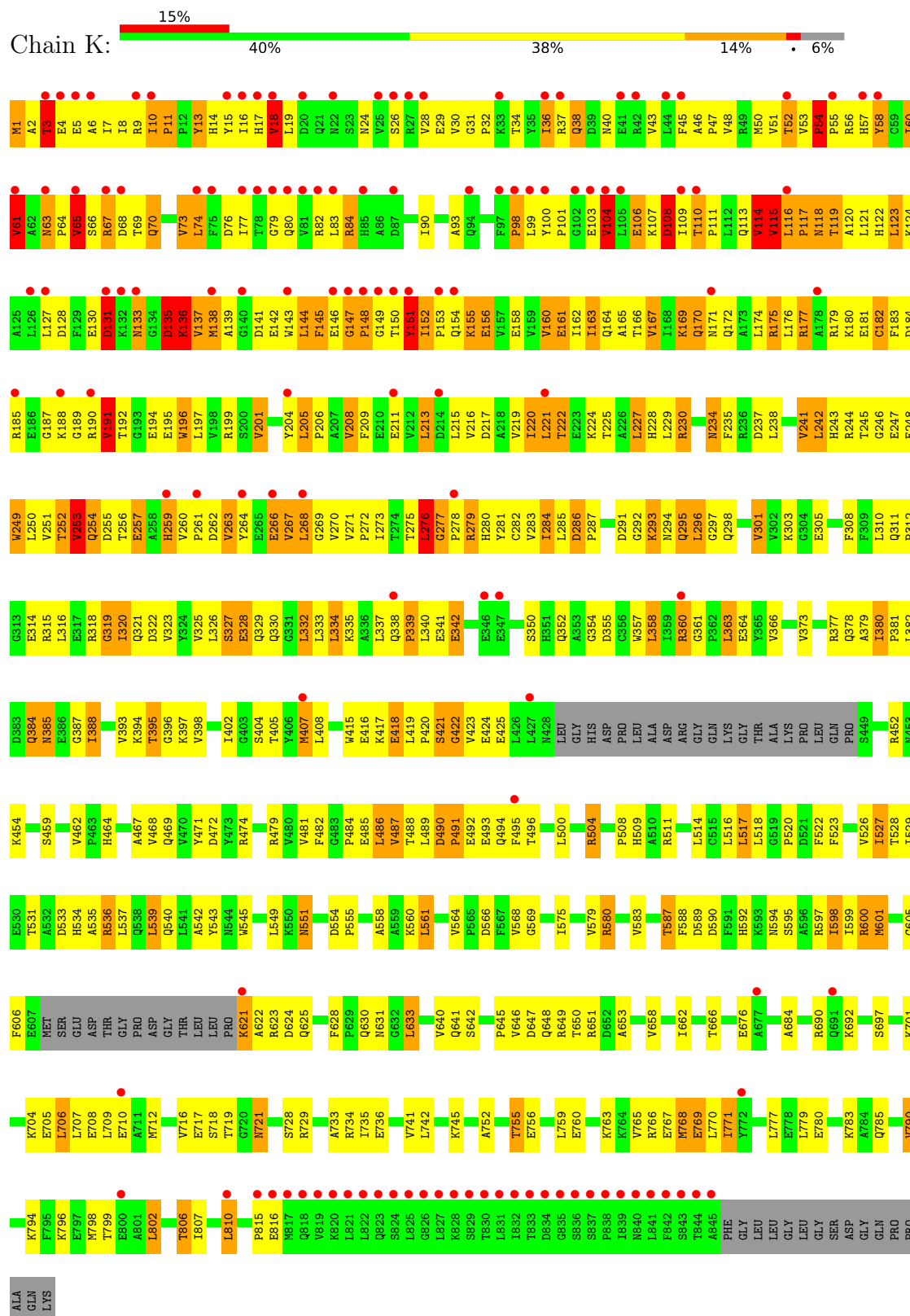


• Molecule 1: Major vault protein

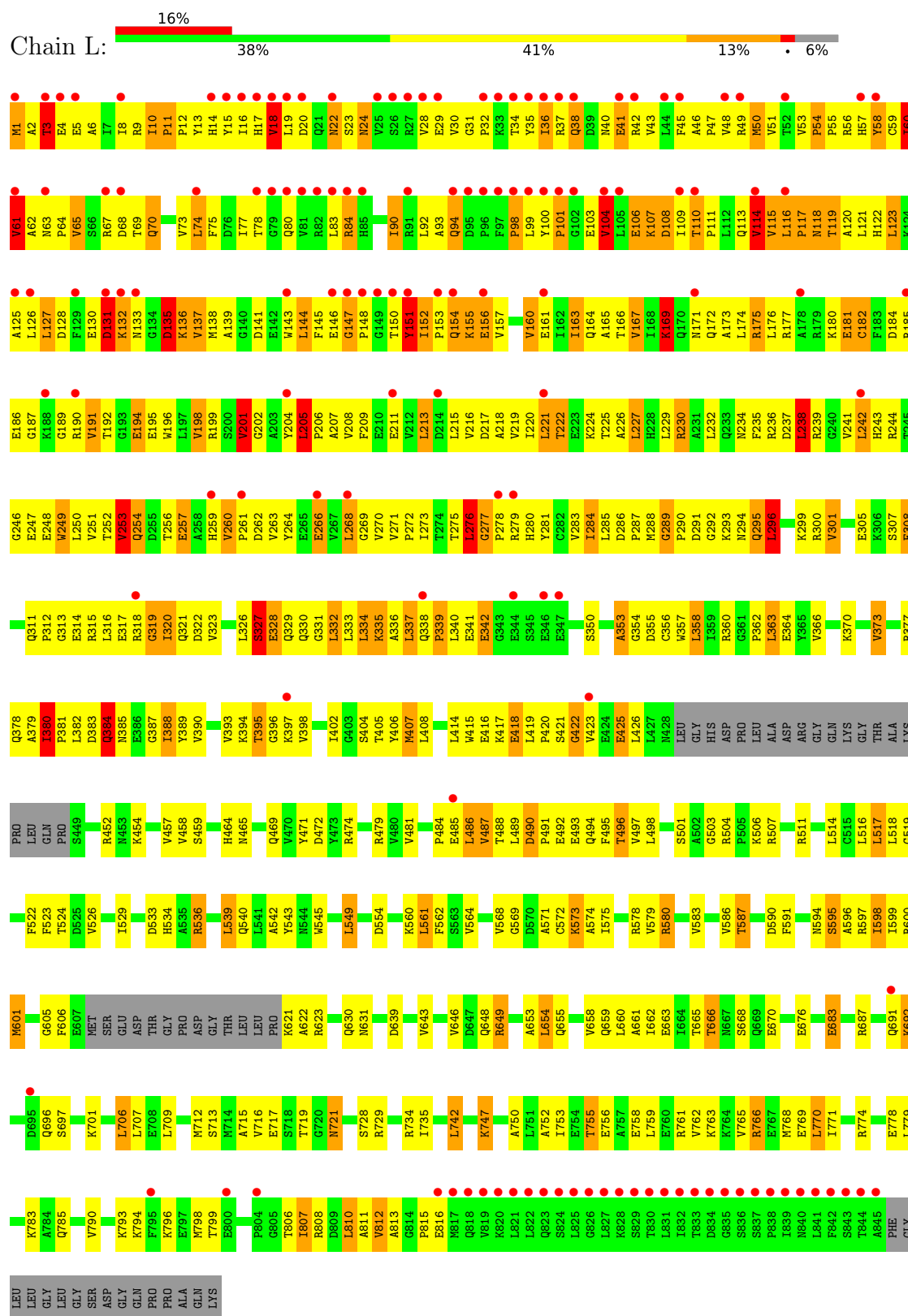


GLN
LYS

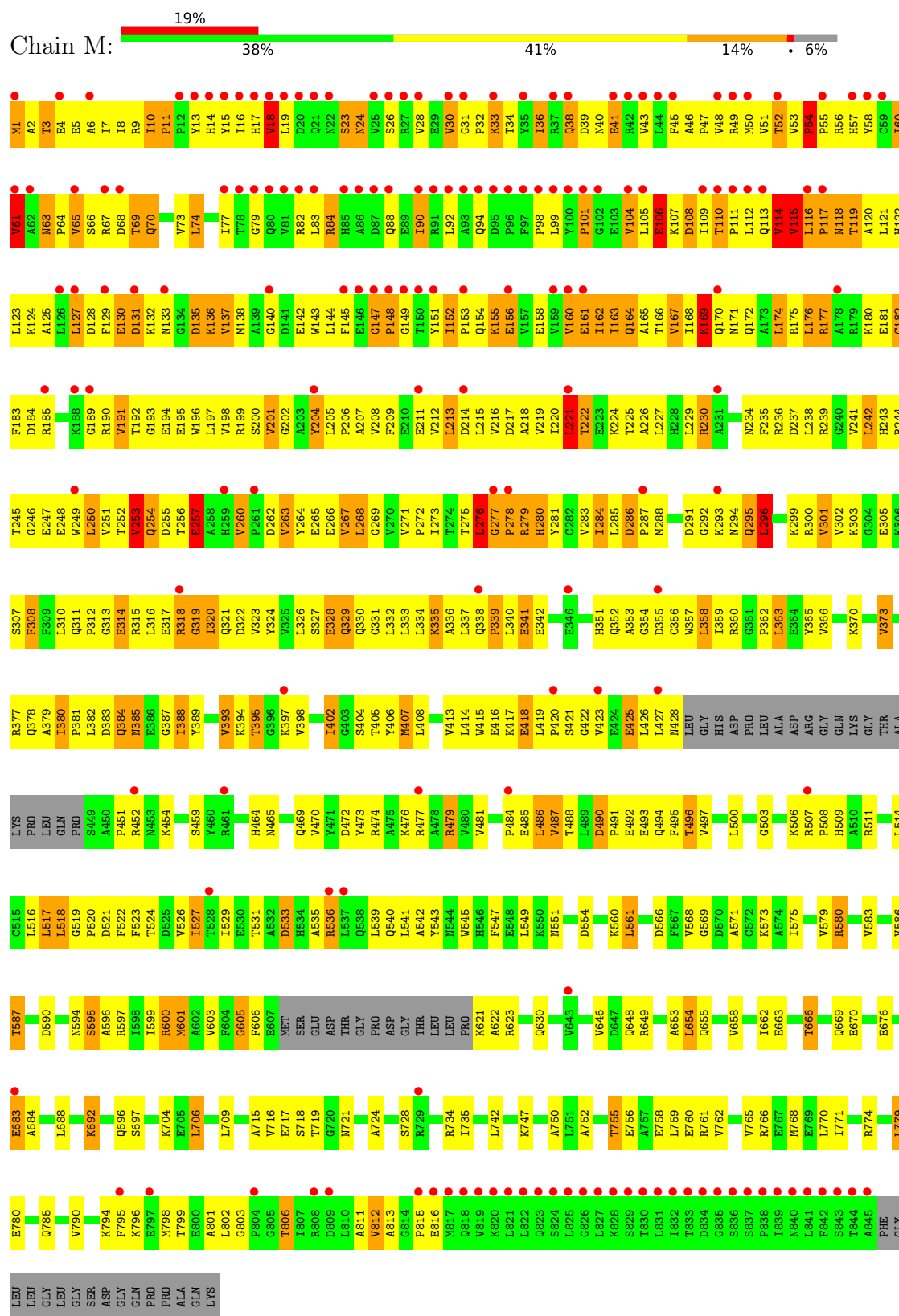
• Molecule 1: Major vault protein



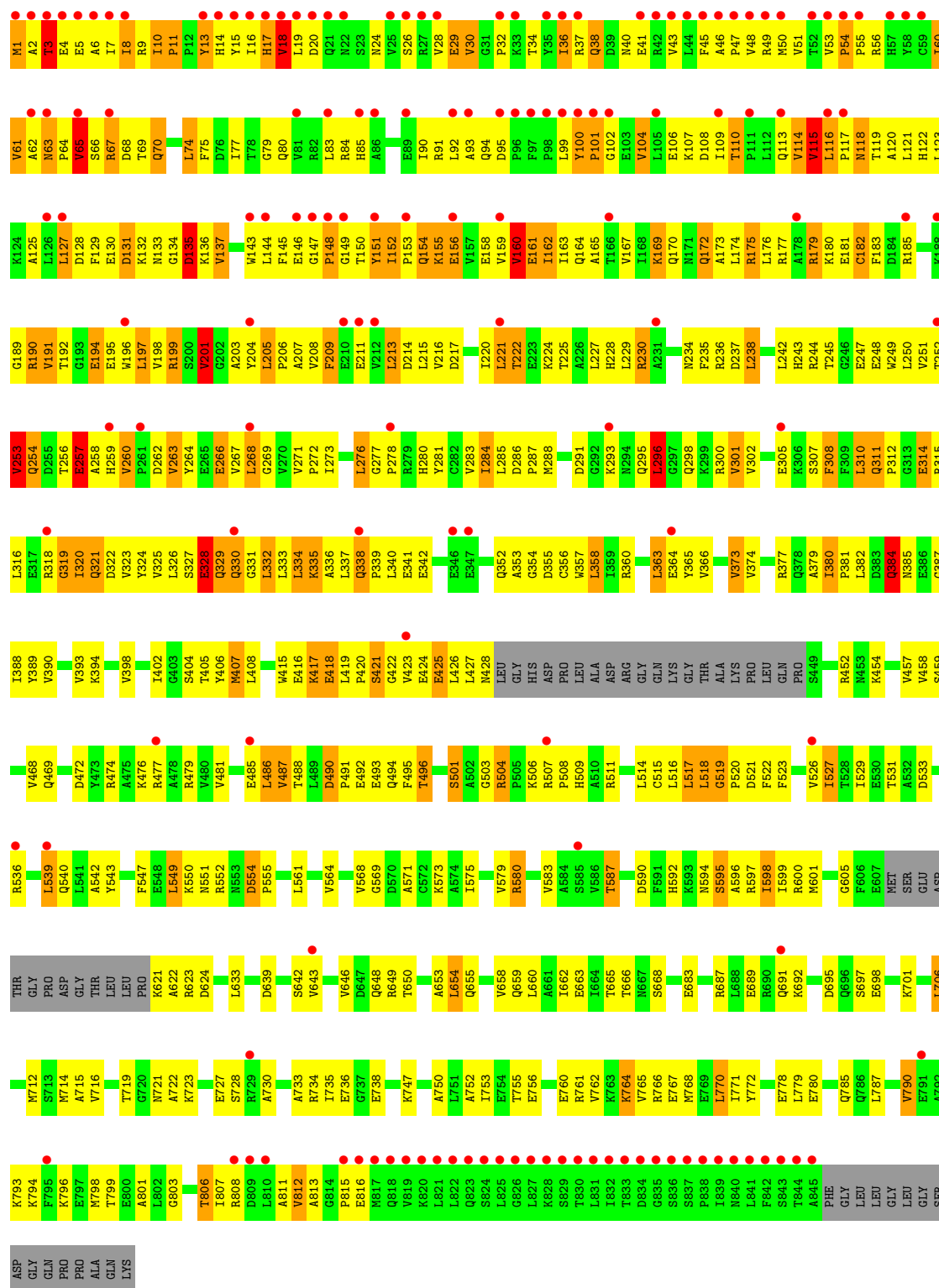
• Molecule 1: Major vault protein



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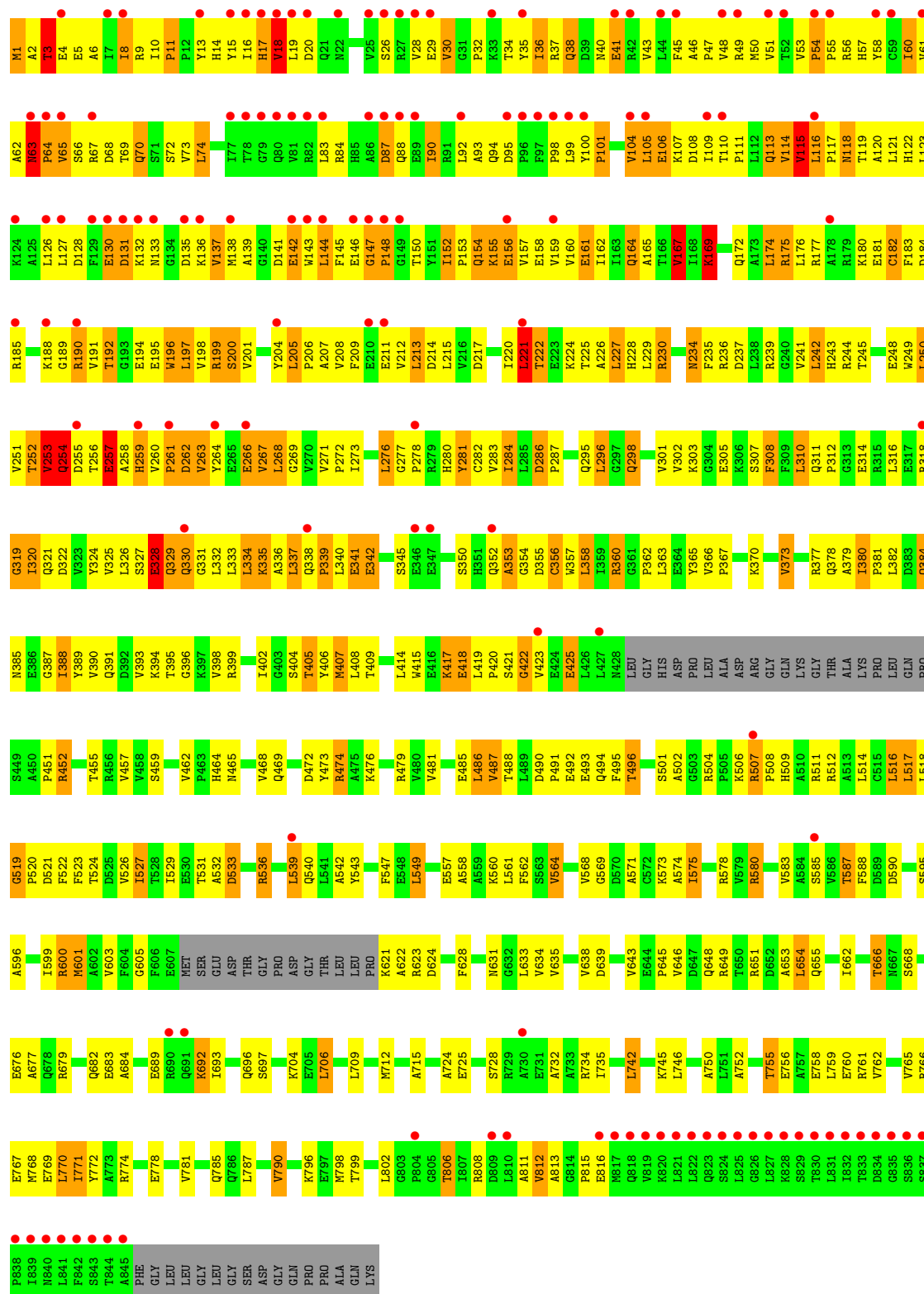


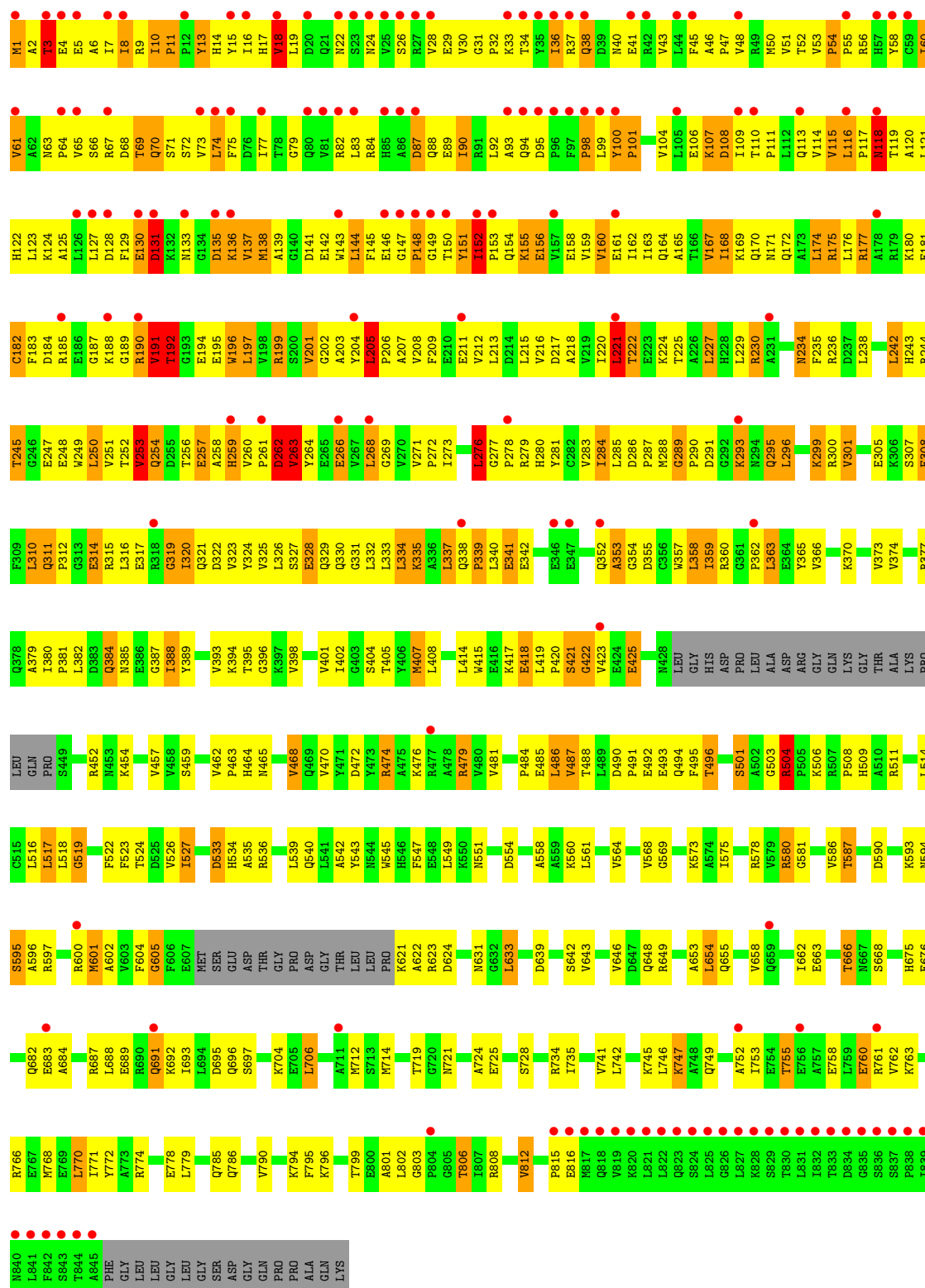


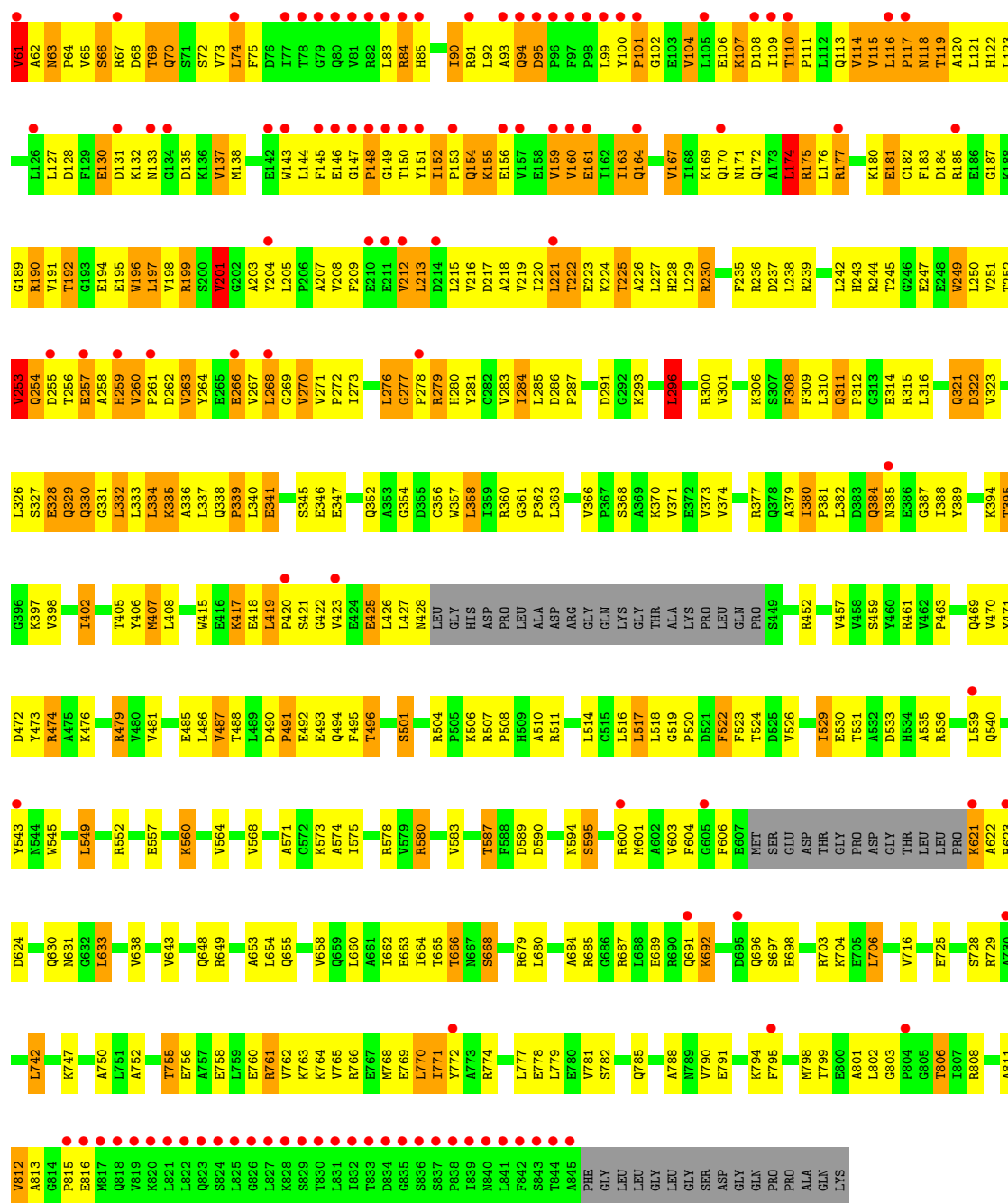


• Molecule 1: Major vault protein



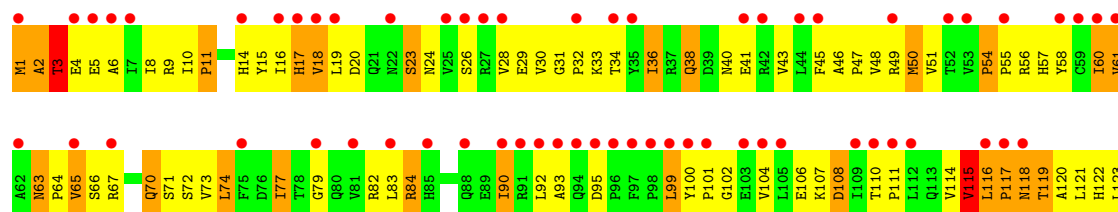


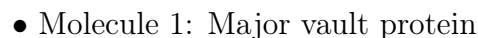




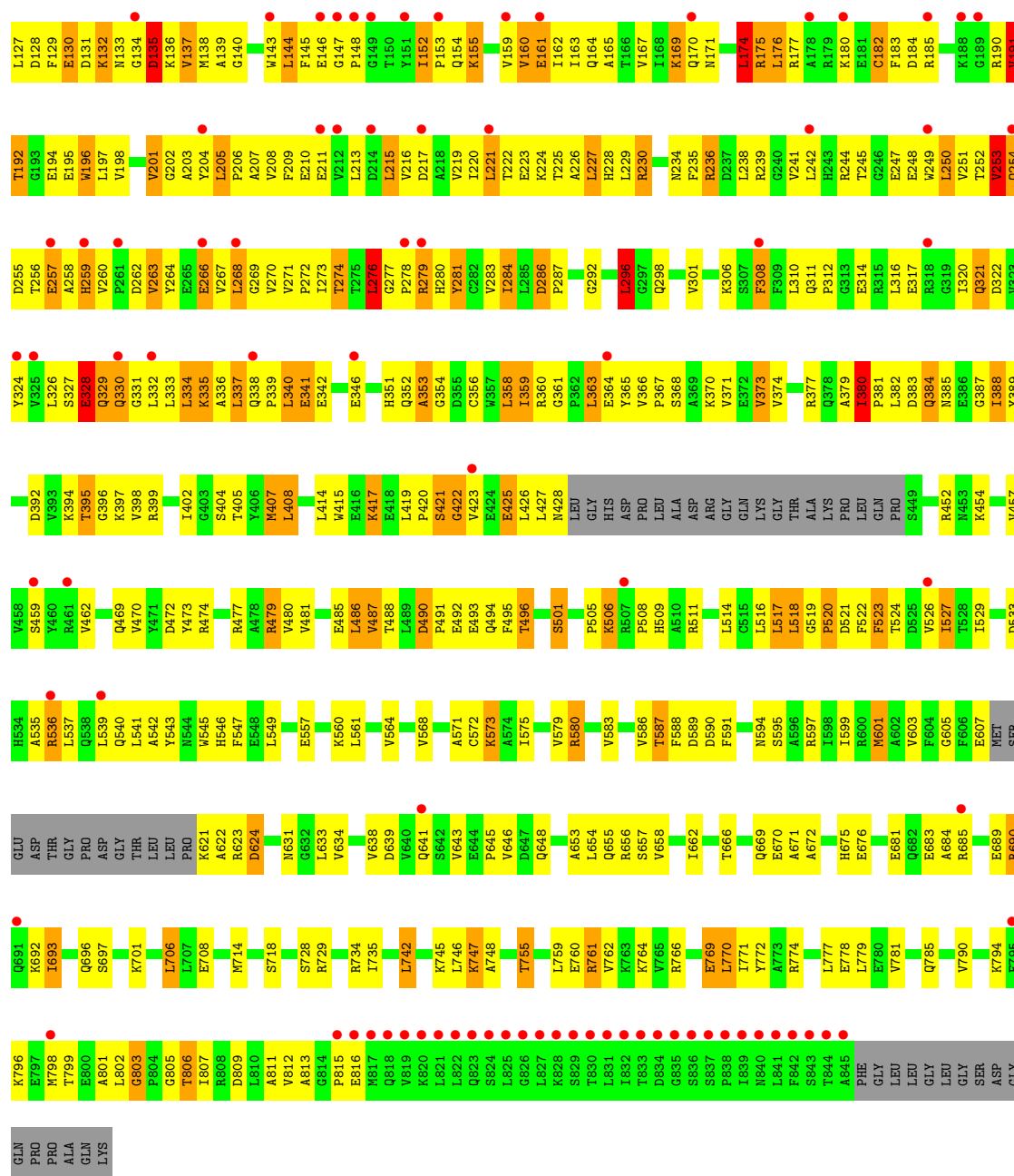
• Molecule 1: Major vault protein

Chain T: 17% 41% 42% 11% 6%

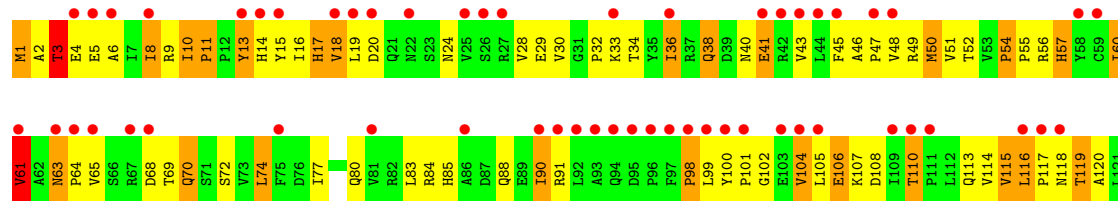


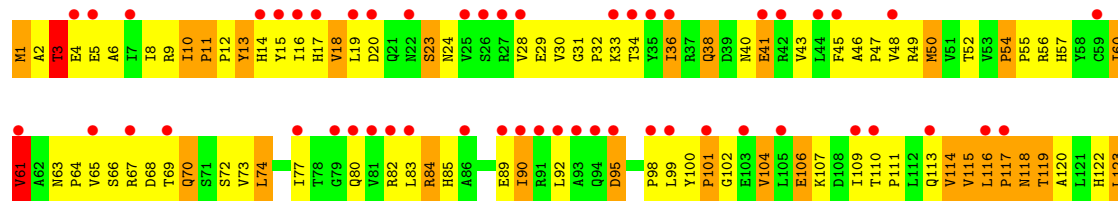


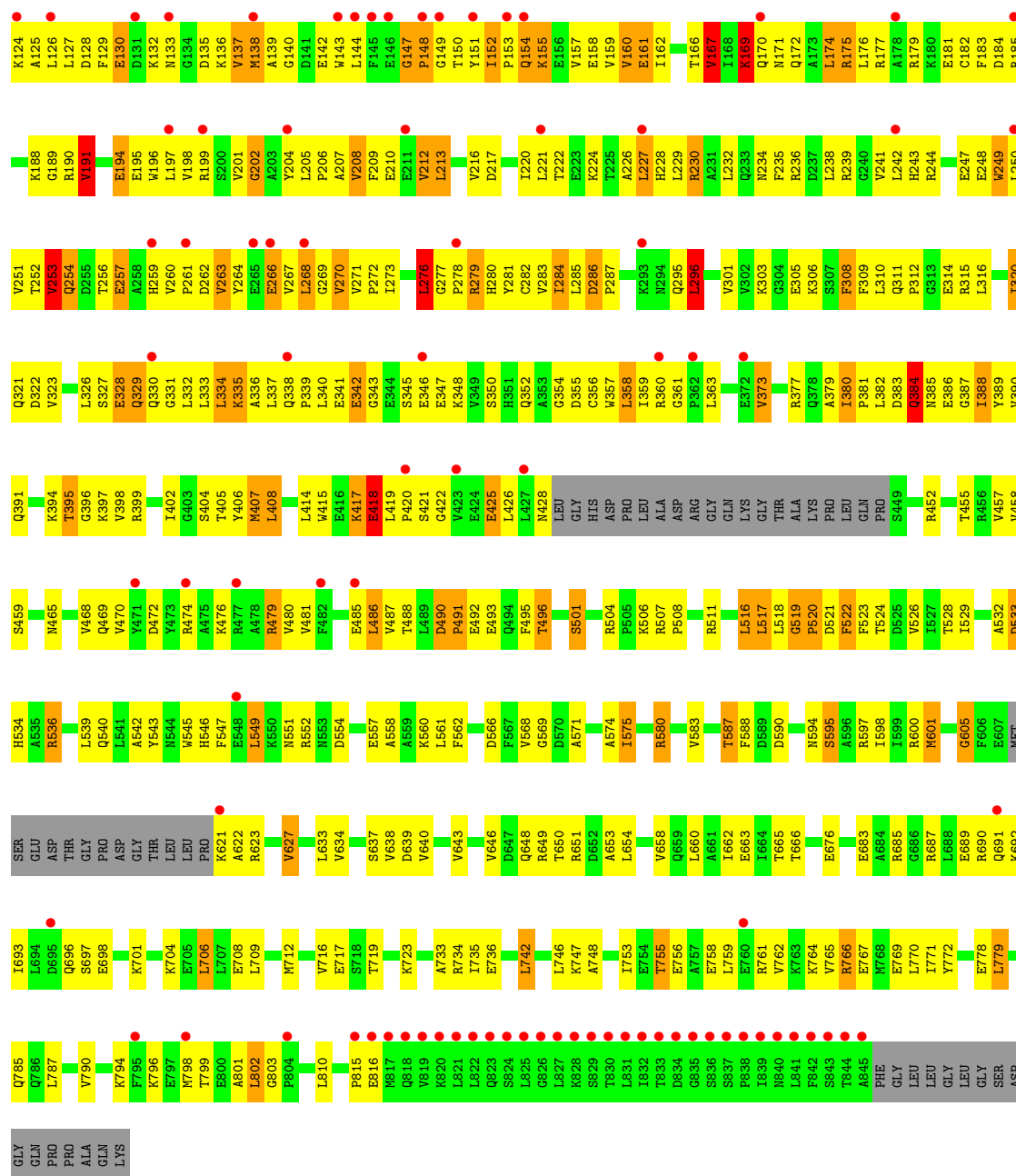
A62	A63	A64	A65	A66	A67	A68	A69	A70	A71	A72	A73	A74	A75	A76	A77	A78	A79	A80	A81	A82	A83	A84	A85	A86	A87	A88	A89	A90	A91	A92	A93	A94	A95	A96	A97	A98	A99	A100	A101	A102	A103	A104	A105	A106	A107	A108	A109	A110	A111	A112	A113	A114	A115	A116	A117	A118	A119	A120	A121	A122	A123	A124	A125	A126	A127	A128	A129	A130	A131	A132	A133	A134	A135	A136	A137	A138	A139	A140	A141	A142	A143	A144	A145	A146	A147	A148	A149	A150	A151	A152	A153	A154	A155	A156	A157	A158	A159	A160	A161	A162	A163	A164	A165	A166	A167	A168	A169	A170	A171	A172	A173	A174	A175	A176	A177	A178	A179	A180	A181	A182	A183	A184	A185	A186	A187	A188	A189	A190	A191	A192	A193	A194	A195	A196	A197	A198	A199	A200	A201	A202	A203	A204	A205	A206	A207	A208	A209	A210	A211	A212	A213	A214	A215	A216	A217	A218	A219	A220	A221	A222	A223	A224	A225	A226	A227	A228	A229	A230	A231	A232	A233	A234	A235	A236	A237	A238	A239	A240	A241	A242	A243	A244	A245	A246	A247	A248	A249	A250	A251	A252	A253	A254	A255	A256	A257	A258	A259	A260	A261	A262	A263	A264	A265	A266	A267	A268	A269	A270	A271	A272	A273	A274	A275	A276	A277	A278	A279	A280	A281	A282	A283	A284	A285	A286	A287	A288	A289	A290	A291	A292	A293	A294	A295	A296	A297	A298	A299	A300	A301	A302	A303	A304	A305	A306	A307	A308	A309	A310	A311	A312	A313	A314	A315	A316	A317	A318	A319	A320	A321	A322	A323	A324	A325	A326	A327	A328	A329	A330	A331	A332	A333	A334	A335	A336	A337	A338	A339	A340	A341	A342	A343	A344	A345	A346	A347	A348	A349	A350	A351	A352	A353	A354	A355	A356	A357	A358	A359	A360	A361	A362	A363	A364	A365	A366	A367	A368	A369	A370	A371	A372	A373	A374	A375	A376	A377	A378	A379	A380	A381	A382	A383	A384	A385	A386	A387	A388	A389	A390	A391	A392	A393	A394	A395	A396	A397	A398	A399	A400	A401	A402	A403	A404	A405	A406	A407	A408	A409	A410	A411	A412	A413	A414	A415	A416	A417	A418	A419	A420	A421	A422	A423	A424	A425	A426	A427	A428	A429	A430	A431	A432	A433	A434	A435	A436	A437	A438	A439	A440	A441	A442	A443	A444	A445	A446	A447	A448	A449	A450	A451	A452	A453	A454	A455	A456	A457	A458	A459	A460	A461	A462	A463	A464	A465	A466	A467	A468	A469	A470	A471	A472	A473	A474	A475	A476	A477	A478	A479	A480	A481	A482	A483	A484	A485	A486	A487	A488	A489	A490	A491	A492	A493	A494	A495	A496	A497	A498	A499	A500	A501	A502	A503	A504	A505	A506	A507	A508	A509	A510	A511	A512	A513	A514	A515	A516	A517	A518	A519	A520	A521	A522	A523	A524	A525	A526	A527	A528	A529	A530	A531	A532	A533	A534	A535	A536	A537	A538	A539	A540	A541	A542	A543	A544	A545	A546	A547	A548	A549	A550	A551	A552	A553	A554	A555	A556	A557	A558	A559	A560	A561	A562	A563	A564	A565	A566	A567	A568	A569	A570	A571	A572	A573	A574	A575	A576	A577	A
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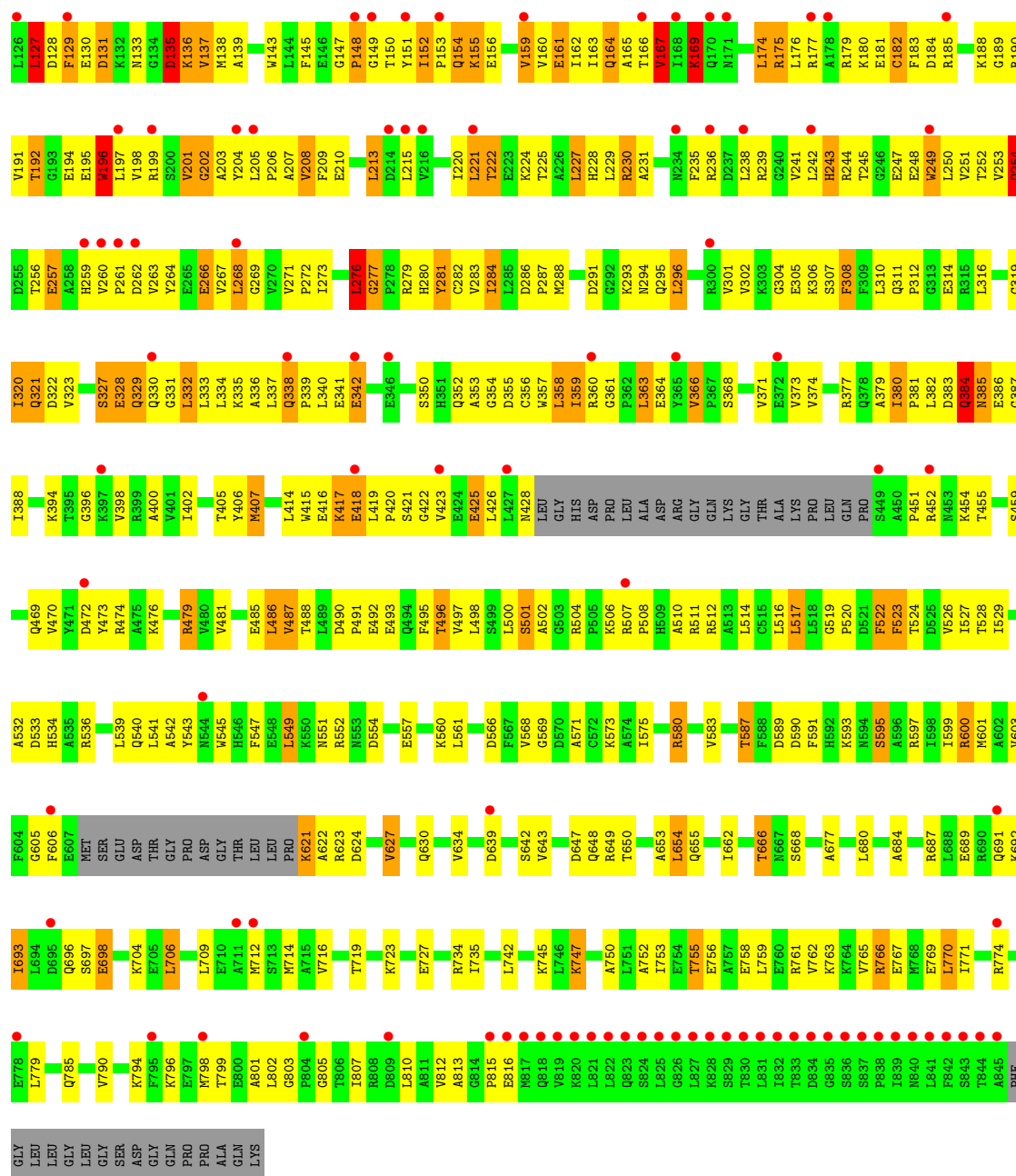


• Molecule 1: Major vault protein

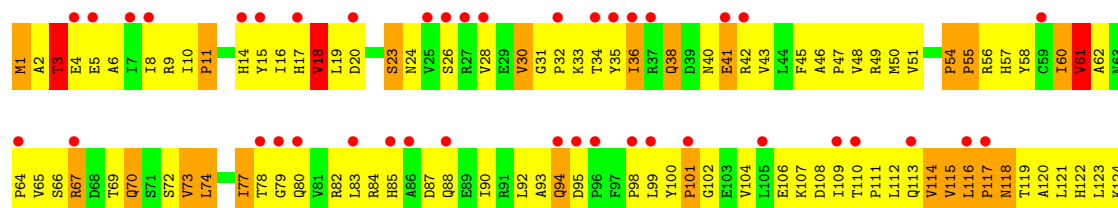


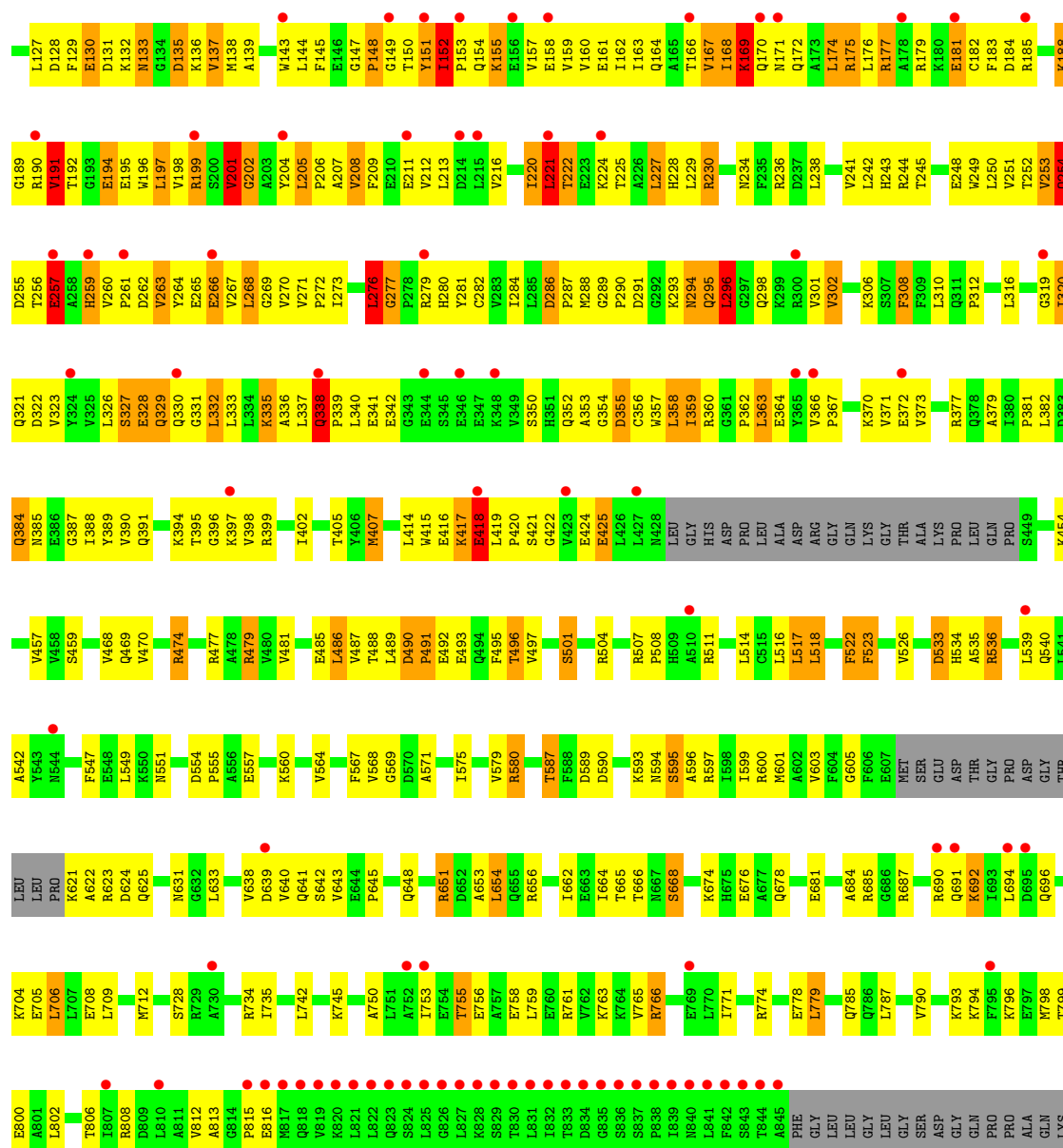


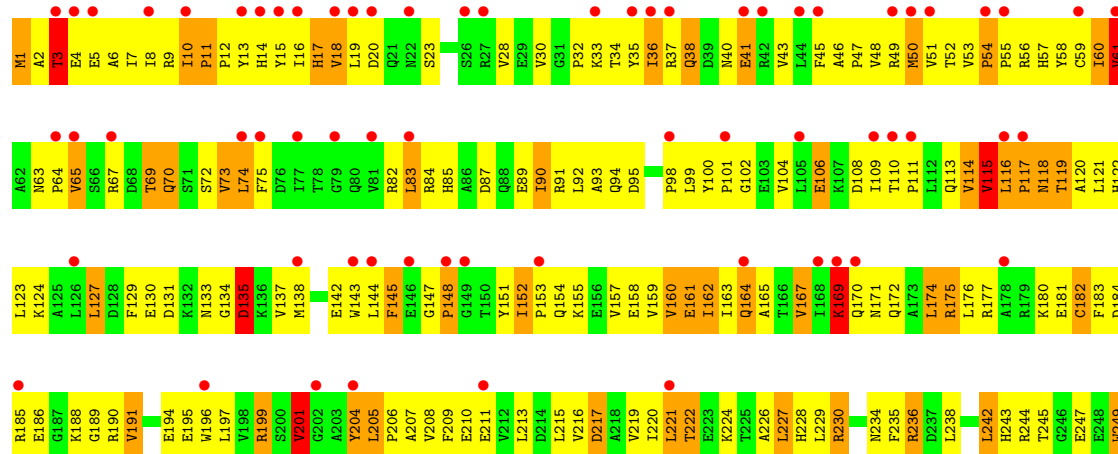


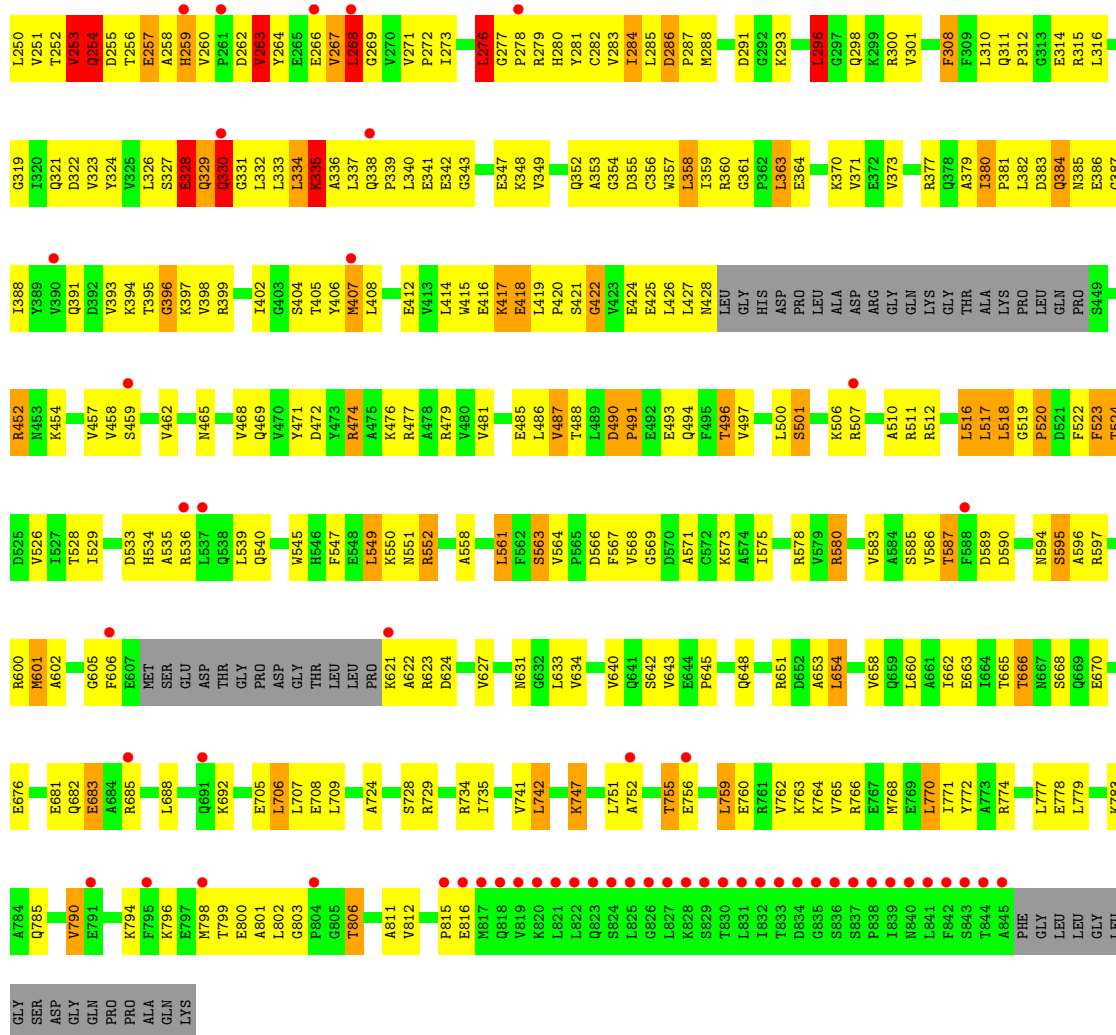


• Molecule 1: Major vault protein

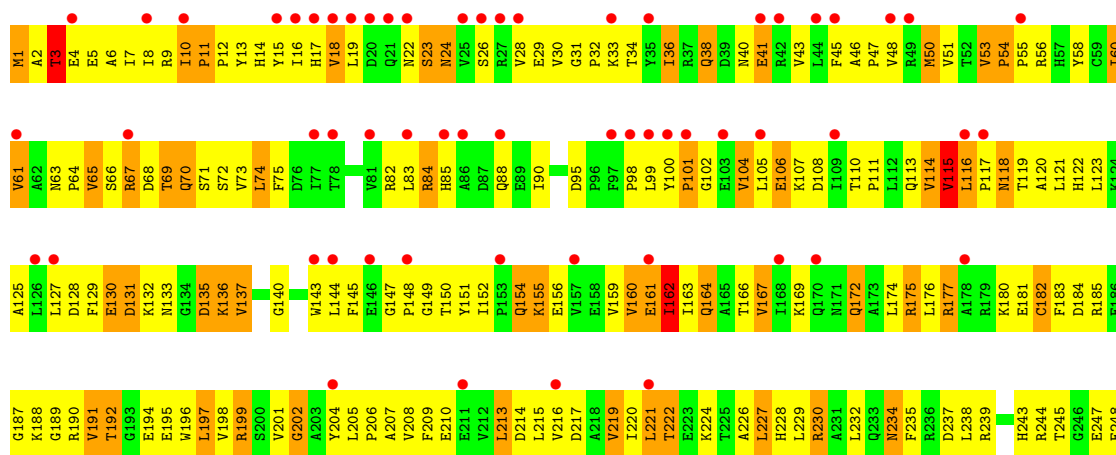


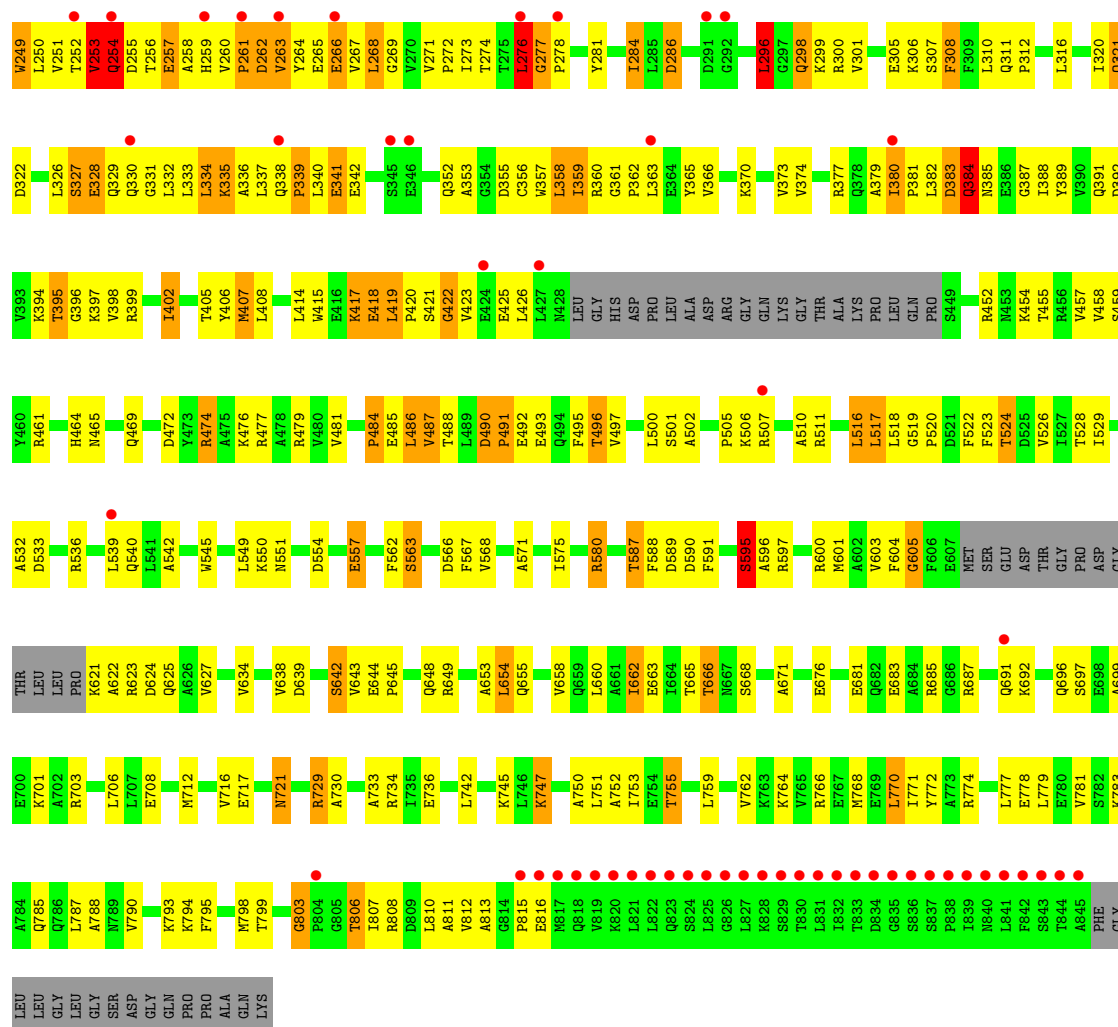




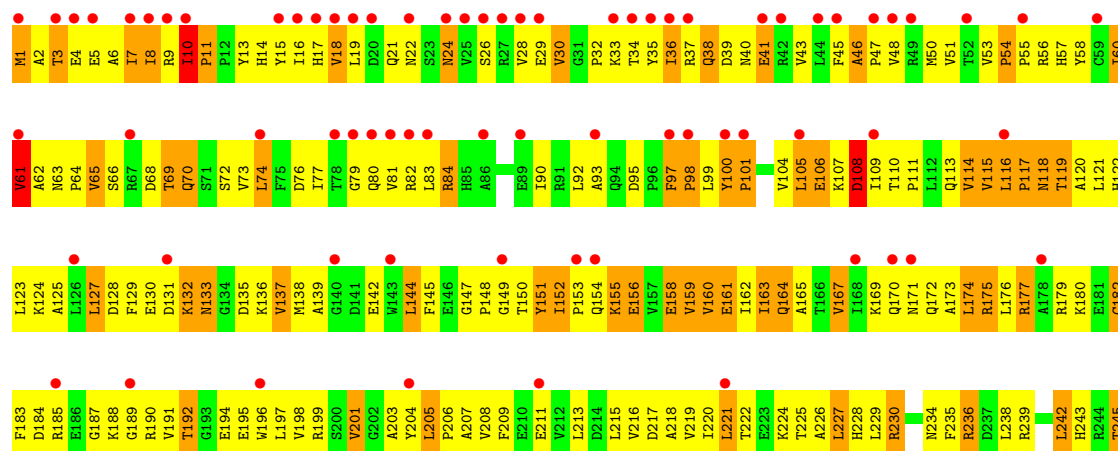
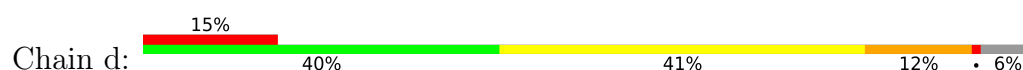


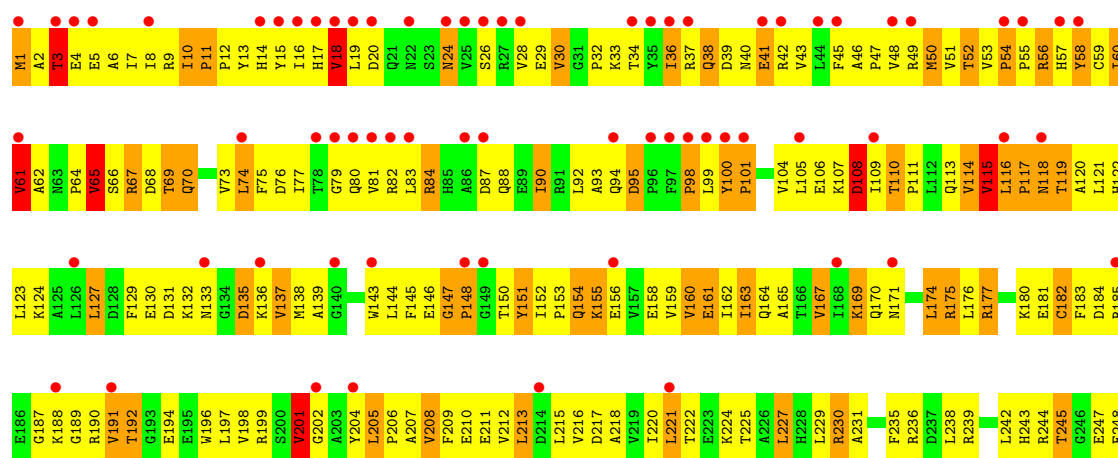
• Molecule 1: Major vault protein

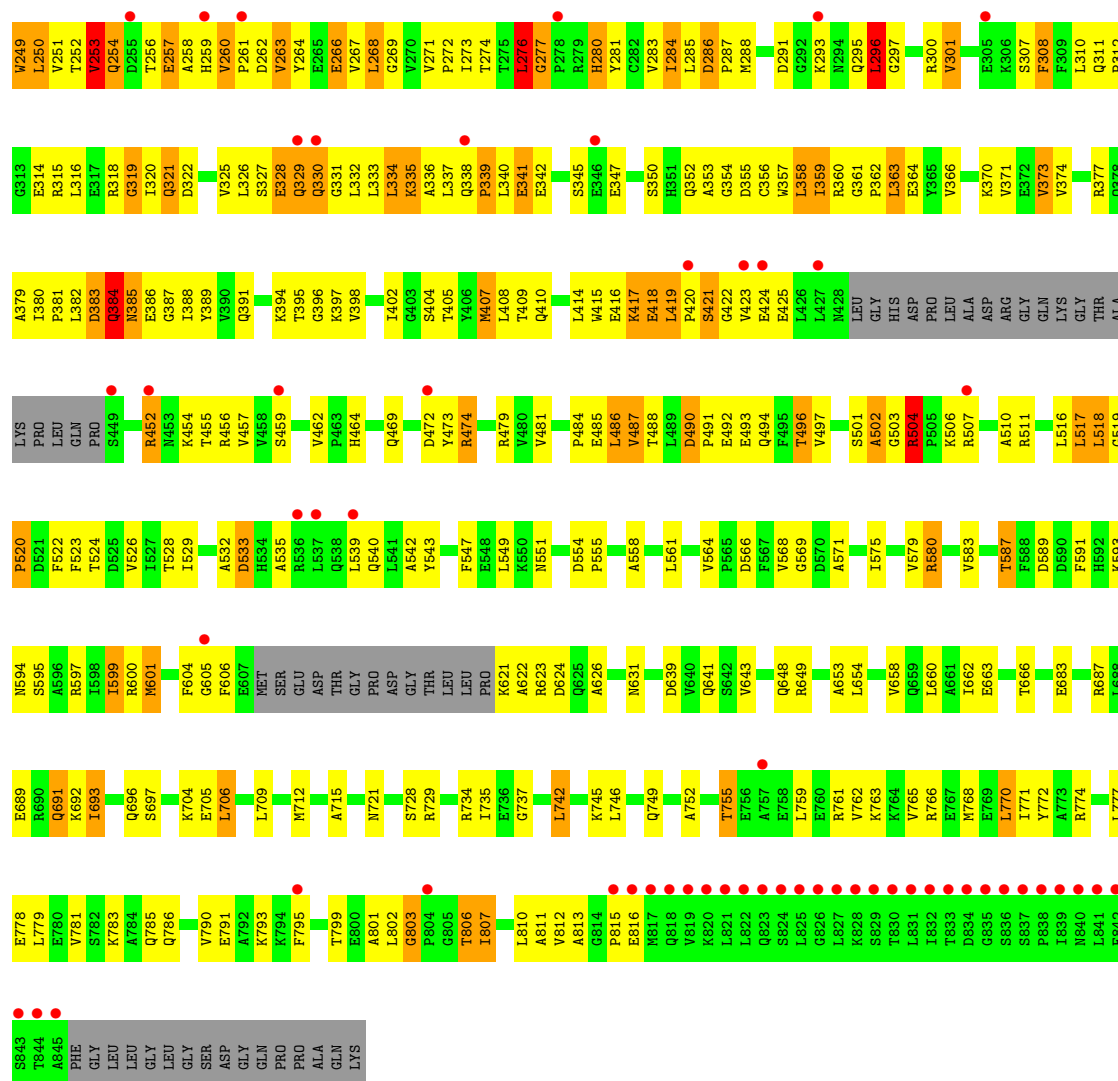




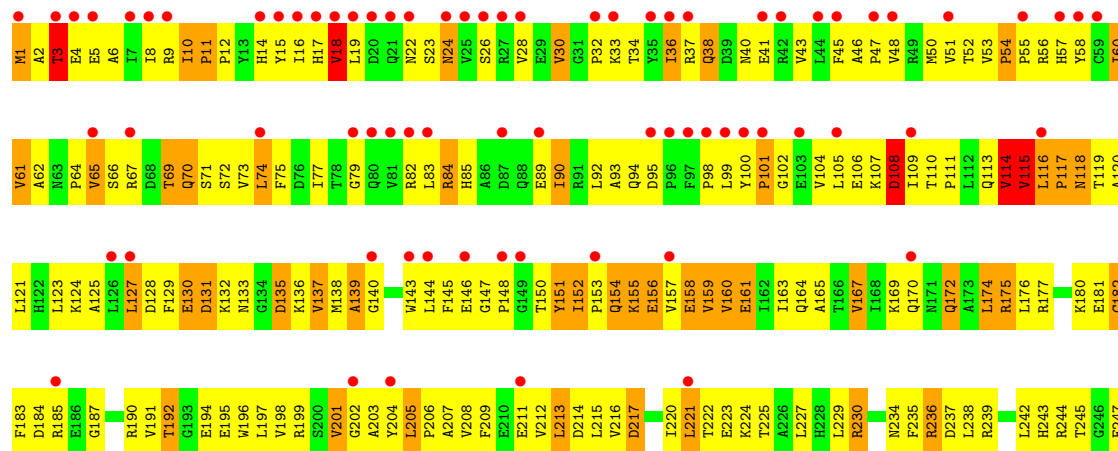
• Molecule 1: Major vault protein

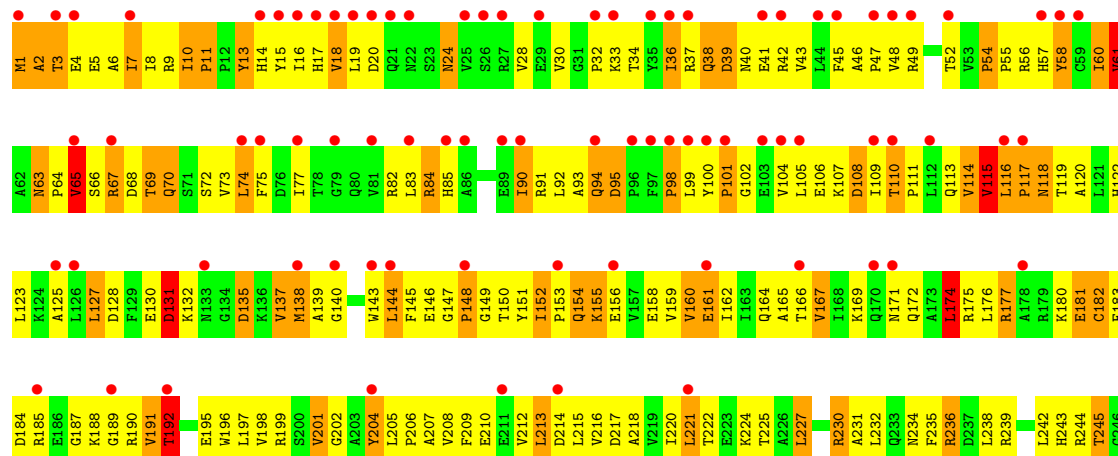


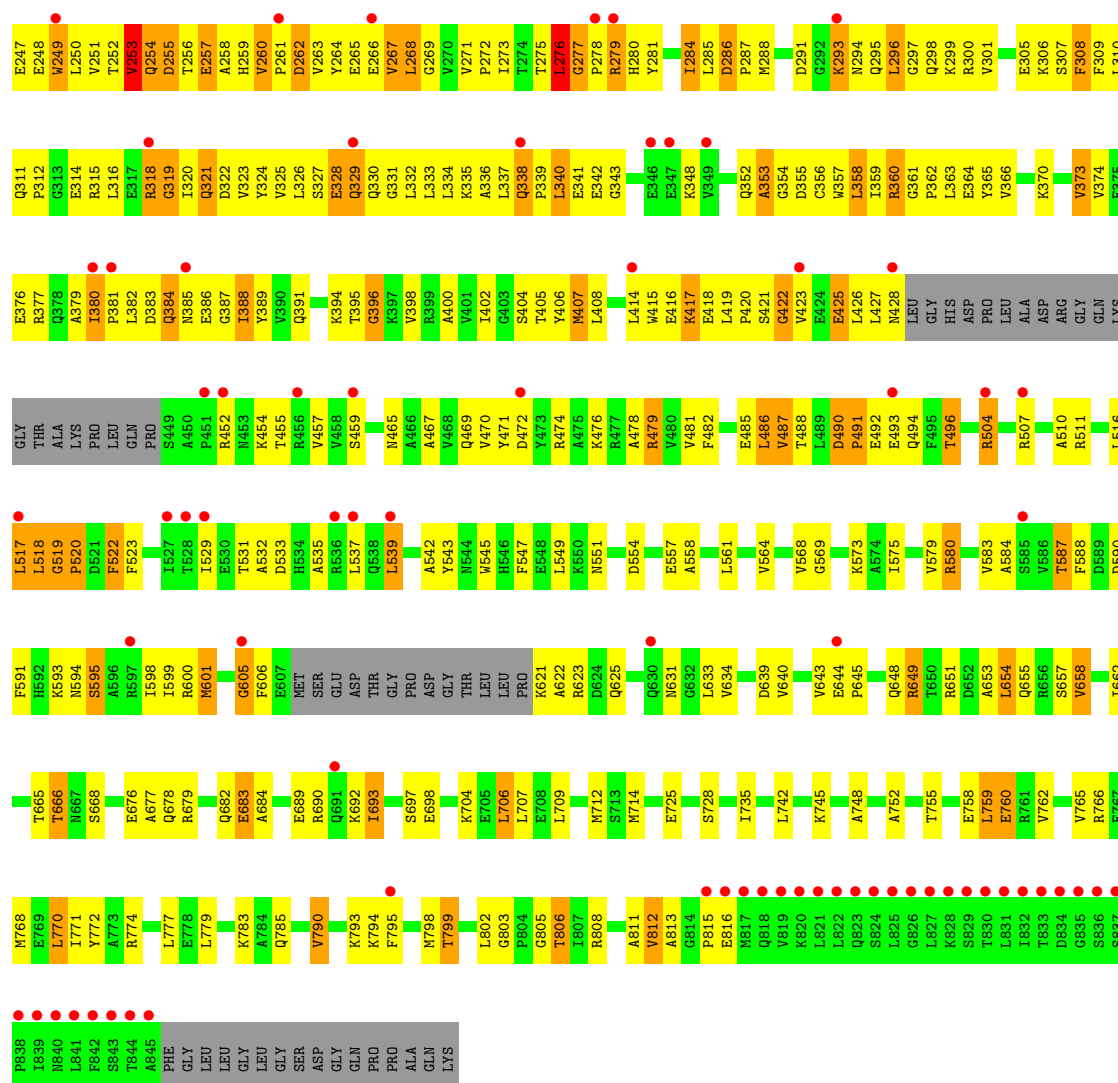




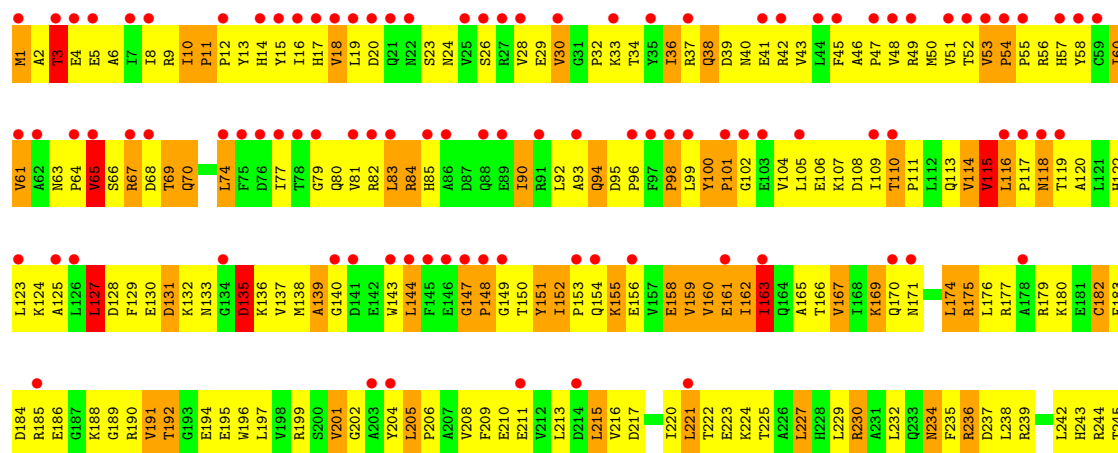
• Molecule 1: Major vault protein

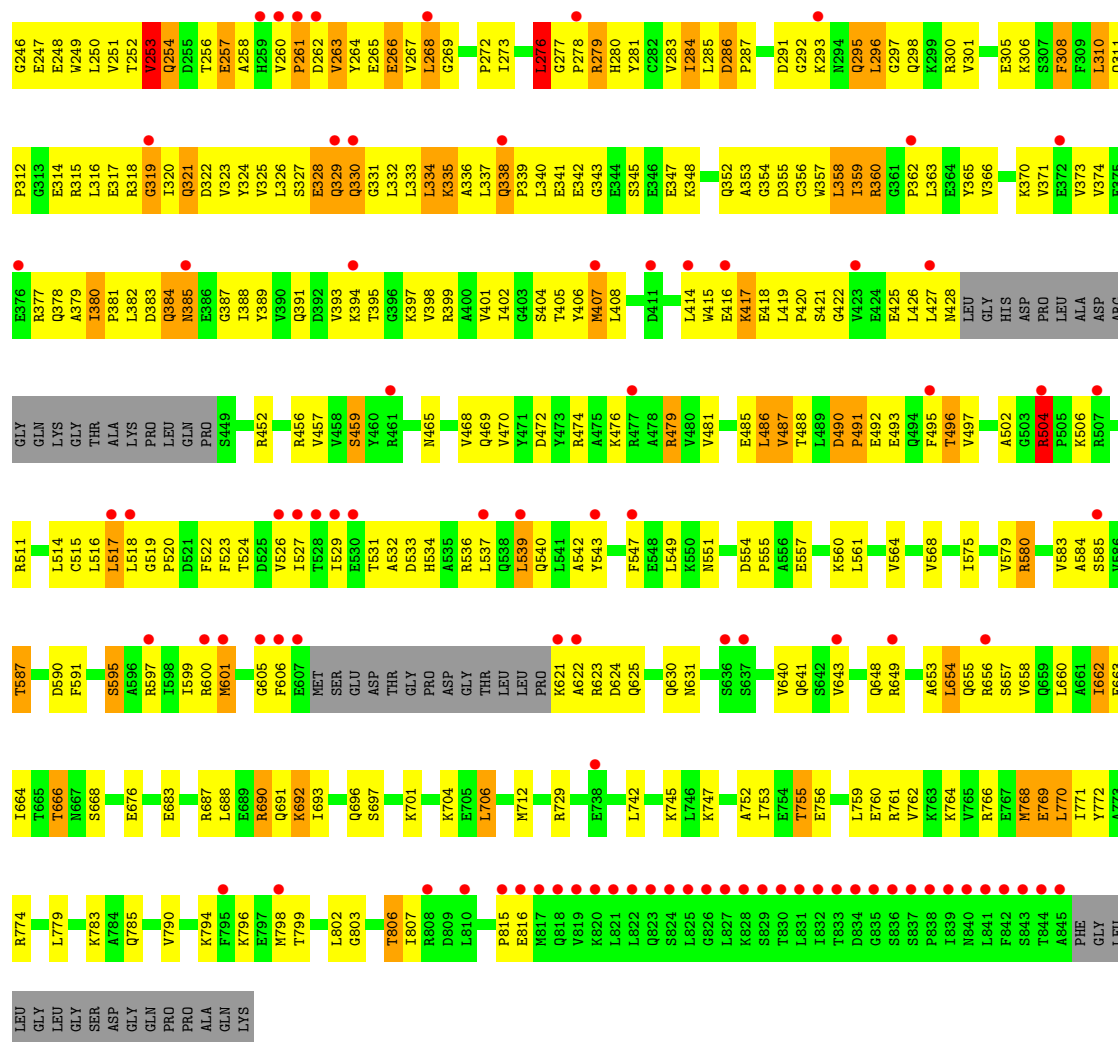




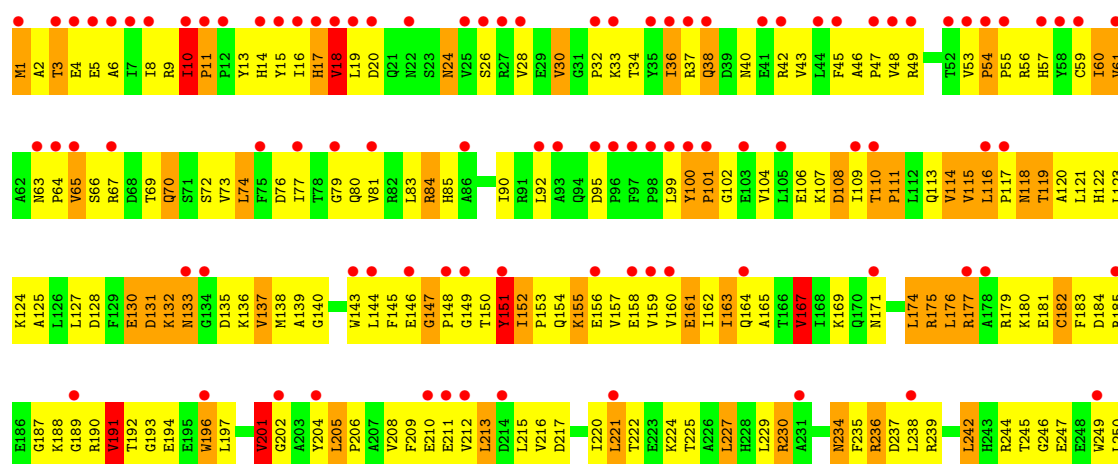


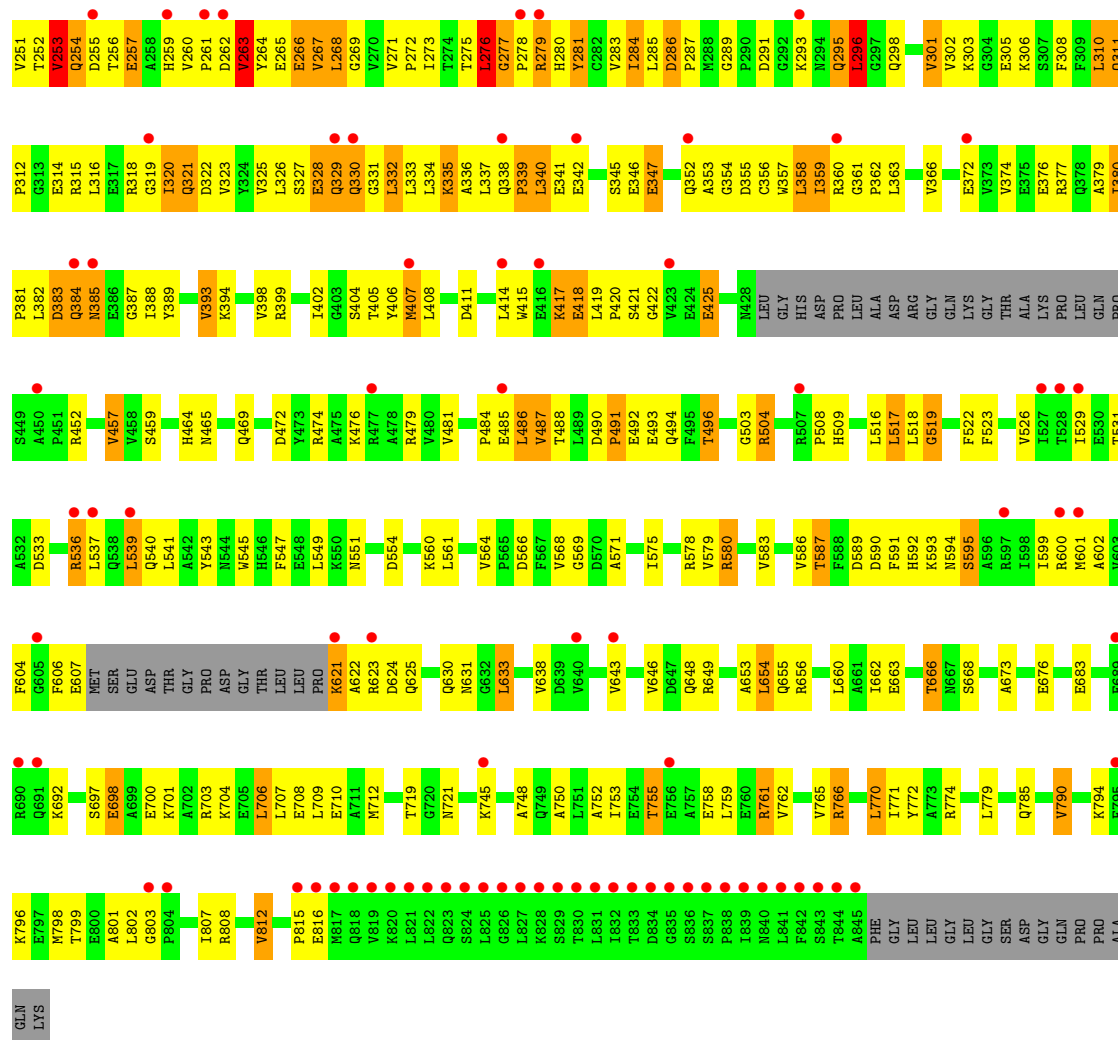
• Molecule 1: Major vault protein



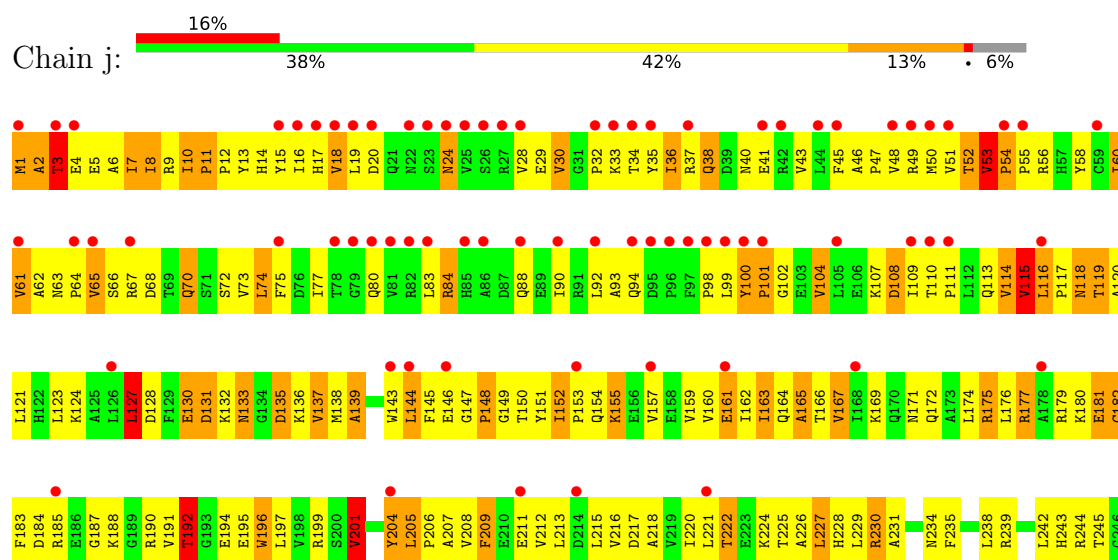


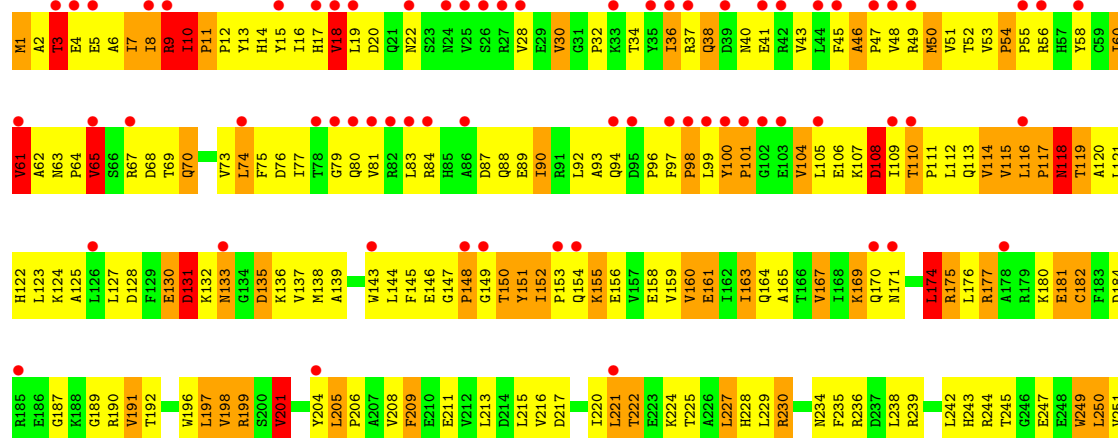
• Molecule 1: Major vault protein

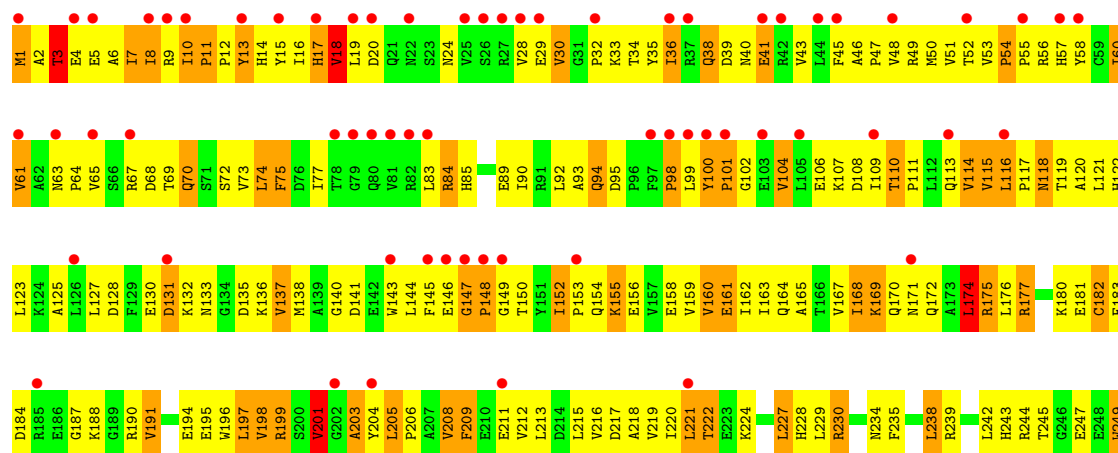


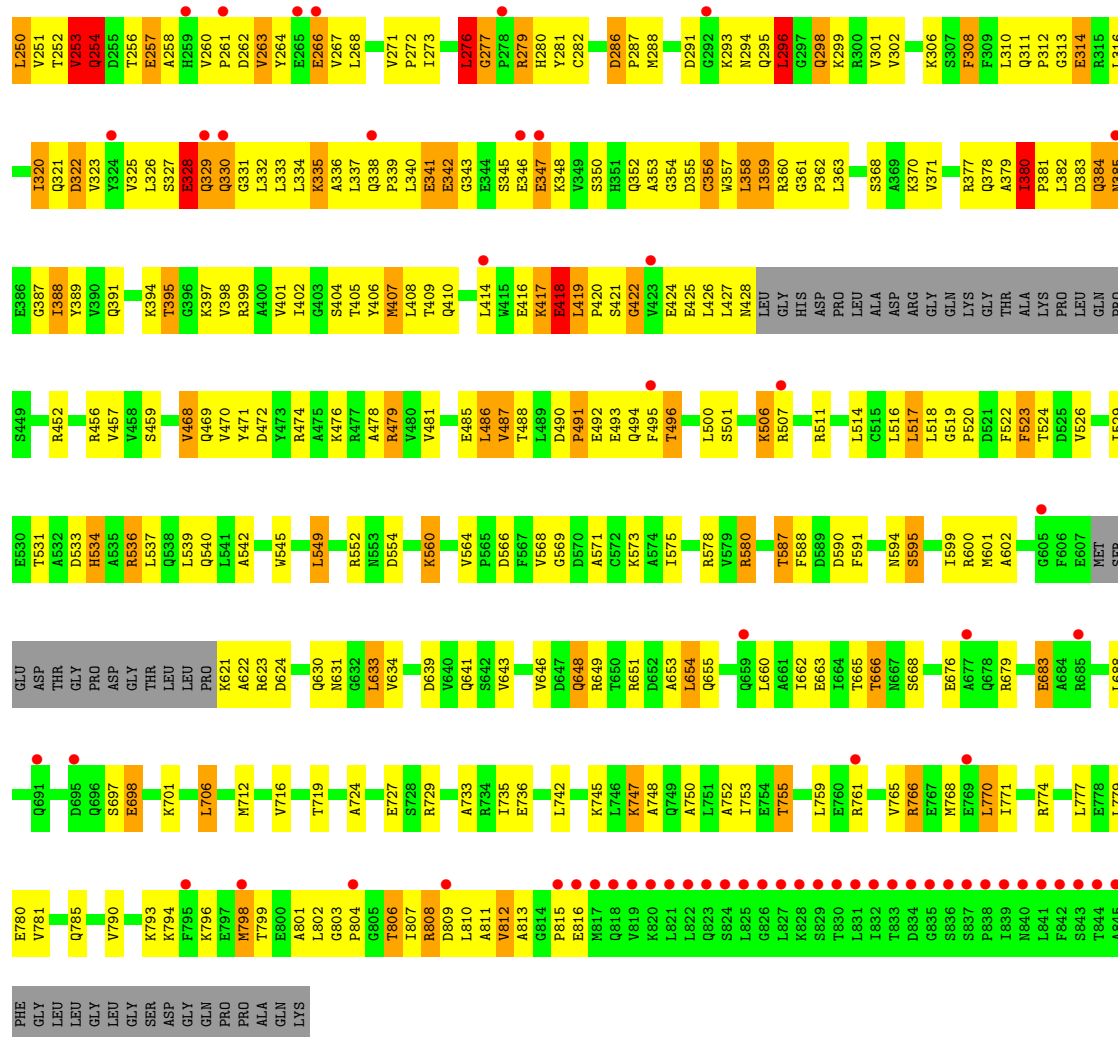


• Molecule 1: Major vault protein

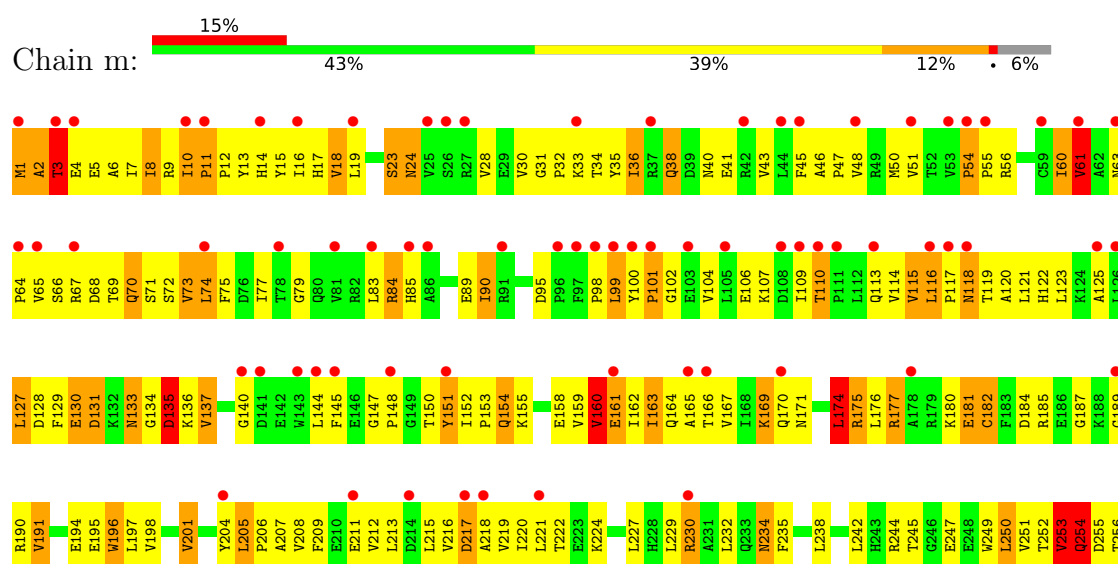


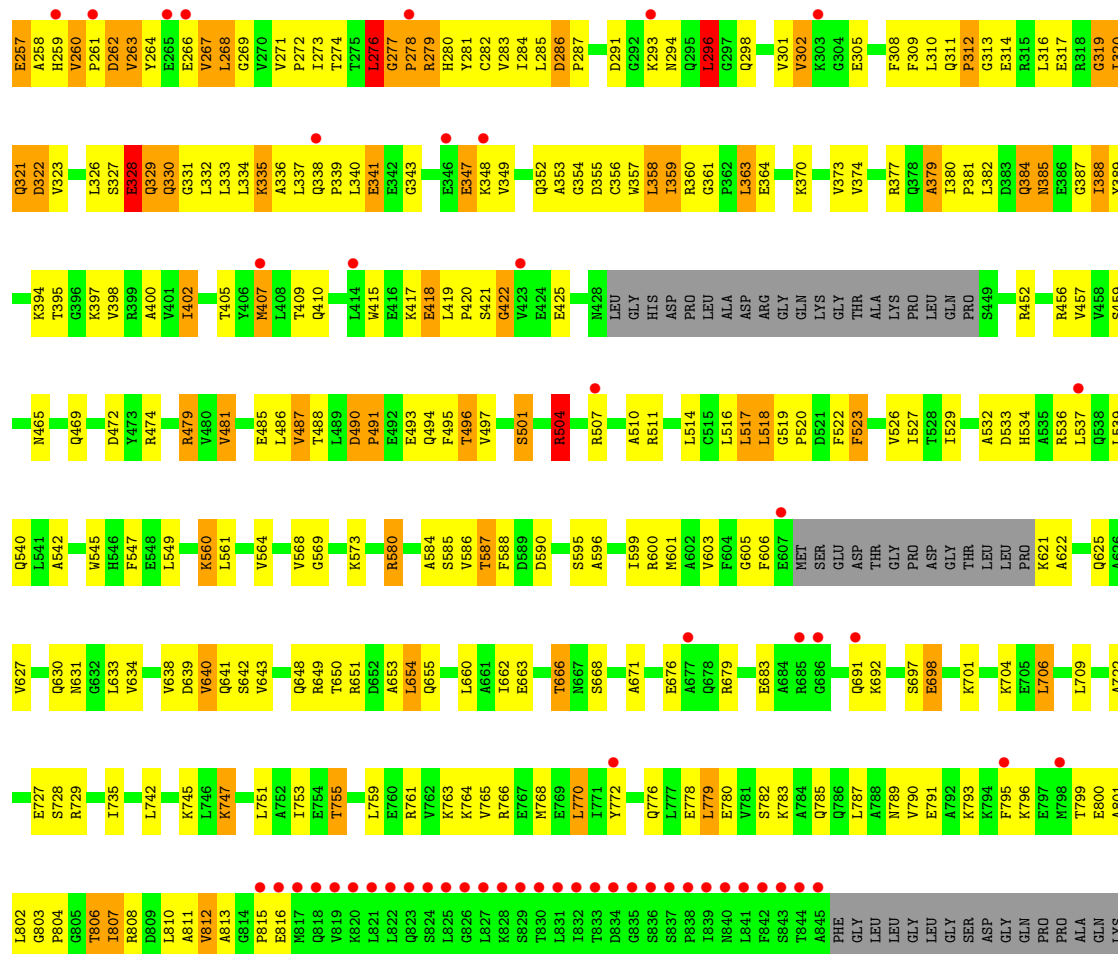






• Molecule 1: Major vault protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	702.25Å 383.80Å 598.48Å 90.00° 124.69° 90.00°	Depositor
Resolution (Å)	204.00 – 3.50 204.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	92.7 (204.00-3.50) 92.7 (204.00-3.50)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	0.21	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 3.49Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.311 , 0.330 0.286 , 0.286	Depositor DCC
R_{free} test set	76647 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	104.6	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 162.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.099 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	241956	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.68	1/6279 (0.0%)	1.02	26/8506 (0.3%)
1	B	0.68	3/6279 (0.0%)	1.01	26/8506 (0.3%)
1	C	0.68	3/6279 (0.0%)	1.02	22/8506 (0.3%)
1	D	0.68	3/6279 (0.0%)	1.02	22/8506 (0.3%)
1	E	0.69	4/6279 (0.1%)	1.03	30/8506 (0.4%)
1	F	0.68	2/6279 (0.0%)	1.01	25/8506 (0.3%)
1	G	0.68	2/6279 (0.0%)	0.99	19/8506 (0.2%)
1	H	0.68	3/6279 (0.0%)	1.01	24/8506 (0.3%)
1	I	0.69	2/6279 (0.0%)	1.00	19/8506 (0.2%)
1	J	0.70	2/6279 (0.0%)	1.03	21/8506 (0.2%)
1	K	0.70	2/6279 (0.0%)	1.05	31/8506 (0.4%)
1	L	0.71	2/6279 (0.0%)	1.04	30/8506 (0.4%)
1	M	0.71	3/6279 (0.0%)	1.03	26/8506 (0.3%)
1	N	0.69	2/6279 (0.0%)	1.02	25/8506 (0.3%)
1	O	0.71	3/6279 (0.0%)	1.03	23/8506 (0.3%)
1	P	0.71	2/6279 (0.0%)	1.06	34/8506 (0.4%)
1	Q	0.71	3/6279 (0.0%)	1.04	29/8506 (0.3%)
1	R	0.72	4/6279 (0.1%)	1.07	32/8506 (0.4%)
1	S	0.68	2/6279 (0.0%)	1.02	22/8506 (0.3%)
1	T	0.68	1/6279 (0.0%)	1.02	29/8506 (0.3%)
1	U	0.66	0/6279	1.00	14/8506 (0.2%)
1	V	0.67	0/6279	0.98	15/8506 (0.2%)
1	W	0.68	2/6279 (0.0%)	1.00	22/8506 (0.3%)
1	X	0.68	1/6279 (0.0%)	1.02	27/8506 (0.3%)
1	Y	0.68	1/6279 (0.0%)	1.02	25/8506 (0.3%)
1	Z	0.67	3/6279 (0.0%)	1.01	18/8506 (0.2%)
1	a	0.67	2/6279 (0.0%)	1.01	29/8506 (0.3%)
1	b	0.69	1/6279 (0.0%)	1.03	21/8506 (0.2%)
1	c	0.69	3/6279 (0.0%)	1.03	24/8506 (0.3%)
1	d	0.68	2/6279 (0.0%)	1.04	24/8506 (0.3%)
1	e	0.69	2/6279 (0.0%)	1.05	30/8506 (0.4%)
1	f	0.69	1/6279 (0.0%)	1.03	31/8506 (0.4%)
1	g	0.68	3/6279 (0.0%)	1.03	21/8506 (0.2%)
1	h	0.67	0/6279	1.02	20/8506 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	i	0.69	1/6279 (0.0%)	1.03	27/8506 (0.3%)
1	j	0.68	1/6279 (0.0%)	1.03	28/8506 (0.3%)
1	k	0.68	0/6279	1.03	33/8506 (0.4%)
1	l	0.67	0/6279	1.00	19/8506 (0.2%)
1	m	0.69	4/6279 (0.1%)	1.02	21/8506 (0.2%)
All	All	0.69	76/244881 (0.0%)	1.02	964/331734 (0.3%)

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

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	154	GLN	CA-C	7.93	1.56	1.52
1	e	154	GLN	CA-C	7.25	1.56	1.52
1	O	154	GLN	CA-C	7.21	1.56	1.52
1	E	154	GLN	CA-C	7.09	1.55	1.52
1	W	154	GLN	CA-C	6.97	1.55	1.52

The worst 5 of 964 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	252	THR	CB-CA-C	-14.21	92.81	111.42
1	O	254	GLN	N-CA-C	-12.50	98.18	114.31
1	R	254	GLN	N-CA-C	-11.88	97.60	114.12
1	D	254	GLN	N-CA-C	-11.35	98.34	114.12
1	Q	254	GLN	N-CA-C	-11.17	98.20	114.39

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	511	0
1	B	6204	0	6224	522	0
1	C	6204	0	6224	529	0
1	D	6204	0	6224	549	0
1	E	6204	0	6224	531	0
1	F	6204	0	6224	503	0
1	G	6204	0	6224	502	0
1	H	6204	0	6224	518	0
1	I	6204	0	6224	522	0
1	J	6204	0	6224	541	0
1	K	6204	0	6224	568	0
1	L	6204	0	6224	610	0
1	M	6204	0	6224	579	0
1	N	6204	0	6224	536	0
1	O	6204	0	6224	528	0
1	P	6204	0	6224	567	0
1	Q	6204	0	6224	593	0
1	R	6204	0	6224	599	0
1	S	6204	0	6224	535	0
1	T	6204	0	6224	512	0
1	U	6204	0	6224	497	0
1	V	6204	0	6224	491	0
1	W	6204	0	6224	505	0
1	X	6204	0	6224	497	0
1	Y	6204	0	6224	496	0
1	Z	6204	0	6224	469	0
1	a	6204	0	6224	557	0
1	b	6204	0	6224	543	0
1	c	6204	0	6224	522	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	d	6204	0	6224	532	0
1	e	6204	0	6224	567	0
1	f	6204	0	6224	516	0
1	g	6204	0	6224	580	0
1	h	6204	0	6224	545	0
1	i	6204	0	6224	507	0
1	j	6204	0	6224	565	0
1	k	6204	0	6224	566	0
1	l	6204	0	6224	558	0
1	m	6204	0	6224	510	0
All	All	241956	0	242736	19150	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 40.

The worst 5 of 19150 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	1.45	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	1.46	1.31
1:i:653:ALA:HB1	1:j:662:ILE:CD1	1.61	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%)	3	25
1	B	776/861 (90%)	640 (82%)	114 (15%)	22 (3%)	4	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	776/861 (90%)	639 (82%)	109 (14%)	28 (4%)	2	22
1	D	776/861 (90%)	635 (82%)	108 (14%)	33 (4%)	2	18
1	E	776/861 (90%)	637 (82%)	107 (14%)	32 (4%)	2	19
1	F	776/861 (90%)	627 (81%)	118 (15%)	31 (4%)	2	19
1	G	776/861 (90%)	648 (84%)	101 (13%)	27 (4%)	3	23
1	H	776/861 (90%)	636 (82%)	109 (14%)	31 (4%)	2	19
1	I	776/861 (90%)	650 (84%)	98 (13%)	28 (4%)	2	22
1	J	776/861 (90%)	637 (82%)	109 (14%)	30 (4%)	2	20
1	K	776/861 (90%)	631 (81%)	104 (13%)	41 (5%)	1	14
1	L	776/861 (90%)	637 (82%)	103 (13%)	36 (5%)	2	17
1	M	776/861 (90%)	633 (82%)	107 (14%)	36 (5%)	2	17
1	N	776/861 (90%)	639 (82%)	102 (13%)	35 (4%)	2	17
1	O	776/861 (90%)	637 (82%)	102 (13%)	37 (5%)	2	16
1	P	776/861 (90%)	627 (81%)	117 (15%)	32 (4%)	2	19
1	Q	776/861 (90%)	633 (82%)	104 (13%)	39 (5%)	1	15
1	R	776/861 (90%)	627 (81%)	109 (14%)	40 (5%)	1	14
1	S	776/861 (90%)	624 (80%)	115 (15%)	37 (5%)	2	16
1	T	776/861 (90%)	631 (81%)	113 (15%)	32 (4%)	2	19
1	U	776/861 (90%)	642 (83%)	100 (13%)	34 (4%)	2	17
1	V	776/861 (90%)	639 (82%)	110 (14%)	27 (4%)	3	23
1	W	776/861 (90%)	647 (83%)	96 (12%)	33 (4%)	2	18
1	X	776/861 (90%)	648 (84%)	97 (12%)	31 (4%)	2	19
1	Y	776/861 (90%)	644 (83%)	98 (13%)	34 (4%)	2	17
1	Z	776/861 (90%)	649 (84%)	97 (12%)	30 (4%)	2	20
1	a	776/861 (90%)	639 (82%)	108 (14%)	29 (4%)	2	21
1	b	776/861 (90%)	635 (82%)	112 (14%)	29 (4%)	2	21
1	c	776/861 (90%)	642 (83%)	101 (13%)	33 (4%)	2	18
1	d	776/861 (90%)	630 (81%)	118 (15%)	28 (4%)	2	22
1	e	776/861 (90%)	629 (81%)	113 (15%)	34 (4%)	2	17
1	f	776/861 (90%)	642 (83%)	99 (13%)	35 (4%)	2	17
1	g	776/861 (90%)	637 (82%)	98 (13%)	41 (5%)	1	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	h	776/861 (90%)	639 (82%)	97 (12%)	40 (5%)	1	14
1	i	776/861 (90%)	634 (82%)	104 (13%)	38 (5%)	1	16
1	j	776/861 (90%)	634 (82%)	107 (14%)	35 (4%)	2	17
1	k	776/861 (90%)	633 (82%)	105 (14%)	38 (5%)	1	16
1	l	748/861 (87%)	616 (82%)	97 (13%)	35 (5%)	2	17
1	m	776/861 (90%)	634 (82%)	108 (14%)	34 (4%)	2	17
All	All	30236/33579 (90%)	24815 (82%)	4133 (14%)	1288 (4%)	2	18

5 of 1288 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%)	530 (80%)	133 (20%)	1	7
1	B	663/727 (91%)	542 (82%)	121 (18%)	2	10
1	C	663/727 (91%)	533 (80%)	130 (20%)	1	8
1	D	663/727 (91%)	528 (80%)	135 (20%)	1	7
1	E	663/727 (91%)	542 (82%)	121 (18%)	2	10
1	F	663/727 (91%)	531 (80%)	132 (20%)	1	7
1	G	663/727 (91%)	529 (80%)	134 (20%)	1	7
1	H	663/727 (91%)	529 (80%)	134 (20%)	1	7
1	I	663/727 (91%)	520 (78%)	143 (22%)	1	6
1	J	663/727 (91%)	521 (79%)	142 (21%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	663/727 (91%)	520 (78%)	143 (22%)	1	6
1	L	663/727 (91%)	525 (79%)	138 (21%)	1	6
1	M	663/727 (91%)	527 (80%)	136 (20%)	1	7
1	N	663/727 (91%)	532 (80%)	131 (20%)	1	7
1	O	663/727 (91%)	527 (80%)	136 (20%)	1	7
1	P	663/727 (91%)	522 (79%)	141 (21%)	1	6
1	Q	663/727 (91%)	521 (79%)	142 (21%)	1	6
1	R	645/727 (89%)	504 (78%)	141 (22%)	1	5
1	S	663/727 (91%)	532 (80%)	131 (20%)	1	7
1	T	663/727 (91%)	538 (81%)	125 (19%)	1	9
1	U	663/727 (91%)	534 (80%)	129 (20%)	1	8
1	V	663/727 (91%)	535 (81%)	128 (19%)	1	8
1	W	663/727 (91%)	540 (81%)	123 (19%)	1	9
1	X	663/727 (91%)	533 (80%)	130 (20%)	1	8
1	Y	663/727 (91%)	538 (81%)	125 (19%)	1	9
1	Z	663/727 (91%)	529 (80%)	134 (20%)	1	7
1	a	663/727 (91%)	530 (80%)	133 (20%)	1	7
1	b	663/727 (91%)	521 (79%)	142 (21%)	1	6
1	c	663/727 (91%)	529 (80%)	134 (20%)	1	7
1	d	663/727 (91%)	536 (81%)	127 (19%)	1	8
1	e	663/727 (91%)	525 (79%)	138 (21%)	1	6
1	f	663/727 (91%)	537 (81%)	126 (19%)	1	8
1	g	663/727 (91%)	523 (79%)	140 (21%)	1	6
1	h	663/727 (91%)	526 (79%)	137 (21%)	1	6
1	i	663/727 (91%)	533 (80%)	130 (20%)	1	8
1	j	663/727 (91%)	527 (80%)	136 (20%)	1	7
1	k	663/727 (91%)	526 (79%)	137 (21%)	1	6
1	l	663/727 (91%)	526 (79%)	137 (21%)	1	6
1	m	663/727 (91%)	537 (81%)	126 (19%)	1	8
All	All	25839/28353 (91%)	20638 (80%)	5201 (20%)	1	7

5 of 5201 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	b	580	ARG
1	i	225	THR
1	c	373	VAL
1	b	536	ARG
1	f	152	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 816 such sidechains are listed below:

Mol	Chain	Res	Type
1	W	22	ASN
1	b	118	ASN
1	m	40	ASN
1	W	384	GLN
1	W	17	HIS

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 oligosaccharides 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, 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(Å²)	Q<0.9	
1	A	812/861 (94%)	1.37	129 (15%)	5	4	46, 106, 218, 285	0
1	B	812/861 (94%)	1.43	131 (16%)	4	4	30, 112, 219, 284	0
1	C	812/861 (94%)	1.42	120 (14%)	5	5	54, 113, 221, 291	0
1	D	812/861 (94%)	1.41	108 (13%)	7	6	43, 113, 218, 277	0
1	E	812/861 (94%)	1.52	137 (16%)	4	4	53, 112, 222, 283	0
1	F	812/861 (94%)	1.46	126 (15%)	5	5	46, 114, 223, 278	0
1	G	812/861 (94%)	1.47	144 (17%)	4	4	55, 113, 223, 258	0
1	H	812/861 (94%)	1.42	125 (15%)	5	5	50, 112, 221, 281	0
1	I	812/861 (94%)	1.37	125 (15%)	5	5	56, 108, 215, 266	0
1	J	812/861 (94%)	1.43	133 (16%)	4	4	44, 105, 215, 277	0
1	K	812/861 (94%)	1.49	131 (16%)	4	4	32, 98, 207, 278	0
1	L	812/861 (94%)	1.50	139 (17%)	4	4	33, 99, 210, 277	0
1	M	812/861 (94%)	1.54	165 (20%)	3	3	45, 103, 207, 293	0
1	N	812/861 (94%)	1.66	172 (21%)	2	3	40, 104, 210, 249	0
1	O	812/861 (94%)	1.56	152 (18%)	3	4	33, 103, 214, 272	0
1	P	812/861 (94%)	1.47	139 (17%)	4	4	35, 103, 211, 294	0
1	Q	812/861 (94%)	1.49	142 (17%)	4	4	35, 101, 215, 277	0
1	R	812/861 (94%)	1.46	140 (17%)	4	4	37, 101, 217, 298	0
1	S	812/861 (94%)	1.44	139 (17%)	4	4	48, 106, 212, 284	0
1	T	812/861 (94%)	1.44	143 (17%)	4	4	52, 114, 220, 288	0
1	U	812/861 (94%)	1.53	136 (16%)	4	4	53, 113, 221, 282	0
1	V	812/861 (94%)	1.49	137 (16%)	4	4	57, 114, 220, 287	0
1	W	812/861 (94%)	1.58	137 (16%)	4	4	48, 116, 223, 288	0
1	X	812/861 (94%)	1.57	143 (17%)	4	4	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%)	1.47	127 (15%) 5 5	43, 117, 218, 278	0
1	Z	812/861 (94%)	1.40	131 (16%) 4 4	51, 114, 219, 263	0
1	a	812/861 (94%)	1.39	133 (16%) 4 4	50, 113, 216, 300	0
1	b	812/861 (94%)	1.40	121 (14%) 5 5	28, 110, 217, 281	0
1	c	812/861 (94%)	1.38	112 (13%) 6 5	26, 109, 218, 277	0
1	d	812/861 (94%)	1.41	126 (15%) 5 5	49, 106, 213, 274	0
1	e	812/861 (94%)	1.42	127 (15%) 5 5	47, 105, 210, 284	0
1	f	812/861 (94%)	1.49	134 (16%) 4 4	43, 106, 214, 266	0
1	g	812/861 (94%)	1.58	153 (18%) 3 3	50, 109, 213, 285	0
1	h	812/861 (94%)	1.74	189 (23%) 2 2	54, 110, 210, 277	0
1	i	812/861 (94%)	1.57	174 (21%) 2 3	48, 108, 215, 271	0
1	j	812/861 (94%)	1.45	141 (17%) 4 4	50, 105, 216, 267	0
1	k	812/861 (94%)	1.41	121 (14%) 5 5	41, 104, 210, 261	0
1	l	812/861 (94%)	1.40	124 (15%) 5 5	46, 105, 213, 300	0
1	m	812/861 (94%)	1.33	126 (15%) 5 5	40, 106, 219, 276	0
All	All	31668/33579 (94%)	1.47	5332 (16%) 4 4	26, 108, 217, 300	0

The worst 5 of 5332 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	g	840	ASN	44.1
1	S	840	ASN	41.0
1	U	840	ASN	38.8
1	P	840	ASN	38.5
1	B	842	PHE	37.3

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 oligosaccharides 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.