



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2022 – 07:53 am GMT

PDB ID : 7PKR
EMDB ID : EMD-13478
Title : Vault structure in primmed conformation
Authors : Guerra, P.; Gonzalez-Alamos, M.; Llauro, A.; Casanas, A.; Querol-Audi, J.; de Pablo, P.; Verdaguer, N.
Deposited on : 2021-08-26
Resolution : 3.80 Å(reported)
Based on initial model : 4HL8

This is a wwPDB EM 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/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

EMDB validation analysis : 0.0.0.dev97
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

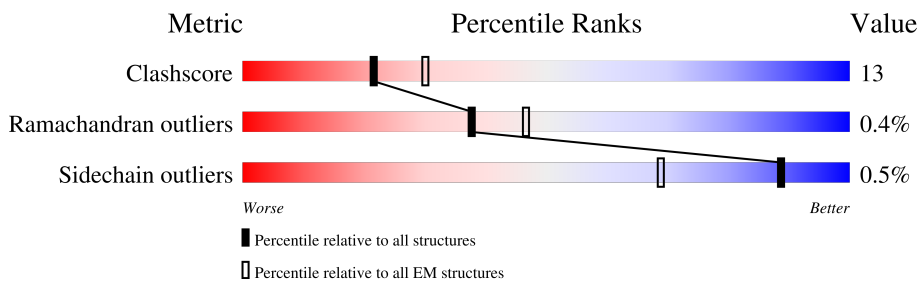
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	861	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">11%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 11%, orange 11%, green 61%, yellow 30%, grey 9%);"></div> <div style="text-align: left;">61% 30% 9%</div> </div>
1	AA	861	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">11%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 11%, orange 11%, green 64%, yellow 26%, grey 9%);"></div> <div style="text-align: left;">64% 26% 9%</div> </div>
1	AB	861	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">11%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 11%, orange 11%, green 63%, yellow 27%, grey 9%);"></div> <div style="text-align: left;">63% 27% 9%</div> </div>
1	AC	861	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">13%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 13%, orange 13%, green 62%, yellow 28%, grey 9%);"></div> <div style="text-align: left;">62% 28% 9%</div> </div>
1	B	861	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">12%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 12%, orange 12%, green 63%, yellow 28%, grey 9%);"></div> <div style="text-align: left;">63% 28% 9%</div> </div>
1	BA	861	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">13%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 13%, orange 13%, green 63%, yellow 27%, grey 9%);"></div> <div style="text-align: left;">63% 27% 9%</div> </div>
1	BB	861	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">13%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 13%, orange 13%, green 62%, yellow 28%, grey 9%);"></div> <div style="text-align: left;">62% 28% 9%</div> </div>
1	C	861	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">13%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 13%, orange 13%, green 61%, yellow 29%, grey 9%);"></div> <div style="text-align: left;">61% 29% 9%</div> </div>

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Mol	Chain	Length	Quality of chain			
1	CA	861	12%	64%	26%	• 9%
1	CB	861	13%	62%	28%	• 9%
1	D	861	13%	63%	27%	• 9%
1	DA	861	13%	64%	27%	• 9%
1	DB	861	11%	63%	27%	• 9%
1	E	861	14%	62%	28%	• 9%
1	EA	861	11%	64%	26%	• 9%
1	EB	861	12%	62%	29%	• 9%
1	F	861	12%	63%	28%	• 9%
1	FA	861	14%	64%	26%	• 9%
1	FB	861	11%	62%	28%	• 9%
1	G	861	13%	62%	28%	• 9%
1	GA	861	12%	63%	27%	• 9%
1	GB	861	13%	63%	27%	• 9%
1	H	861	12%	60%	30%	• 9%
1	HA	861	13%	64%	27%	• 9%
1	HB	861	13%	62%	28%	• 9%
1	I	861	13%	63%	28%	• 9%
1	IA	861	13%	63%	27%	• 9%
1	IB	861	13%	60%	30%	• 9%
1	J	861	11%	61%	30%	• 9%
1	JA	861	12%	64%	26%	• 9%
1	JB	861	14%	61%	29%	• 9%
1	K	861	13%	63%	28%	• 9%
1	KA	861	13%	62%	29%	• 9%

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Mol	Chain	Length	Quality of chain			
1	KB	861	13%	63%	27%	9%
1	L	861	11%	64%	27%	9%
1	LA	861	12%	63%	27%	9%
1	LB	861	13%	61%	29%	9%
1	M	861	13%	63%	27%	9%
1	MA	861	13%	62%	29%	9%
1	MB	861	11%	60%	30%	9%
1	N	861	11%	64%	27%	9%
1	NA	861	12%	63%	27%	9%
1	NB	861	11%	62%	28%	9%
1	O	861	12%	62%	28%	9%
1	OA	861	12%	64%	27%	9%
1	OB	861	11%	63%	27%	9%
1	P	861	11%	62%	28%	9%
1	PA	861	12%	64%	26%	9%
1	PB	861	11%	62%	28%	9%
1	Q	861	12%	62%	29%	9%
1	QA	861	12%	63%	27%	9%
1	QB	861	12%	62%	28%	9%
1	R	861	12%	62%	28%	9%
1	RA	861	12%	64%	26%	9%
1	RB	861	12%	63%	27%	9%
1	S	861	10%	64%	26%	9%
1	SA	861	13%	63%	27%	9%
1	SB	861	12%	64%	26%	9%

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Mol	Chain	Length	Quality of chain			
1	T	861	13%	64%	26%	• 9%
1	TA	861	13%	63%	27%	• 9%
1	TB	861	14%	64%	26%	• 9%
1	UA	861	13%	62%	28%	• 9%
1	UB	861	13%	60%	30%	• 9%
1	V	861	11%	62%	28%	• 9%
1	VA	861	12%	64%	26%	• 9%
1	VB	861	14%	59%	31%	• 9%
1	W	861	13%	64%	26%	• 9%
1	WA	861	13%	63%	27%	• 9%
1	WB	861	11%	62%	28%	• 9%
1	X	861	12%	62%	29%	• 9%
1	XA	861	12%	64%	26%	• 9%
1	XB	861	11%	63%	27%	• 9%
1	Y	861	12%	64%	26%	• 9%
1	YA	861	12%	63%	27%	• 9%
1	YB	861	11%	62%	28%	• 9%
1	Z	861	13%	62%	28%	• 9%
1	ZA	861	13%	64%	26%	• 9%
1	ZB	861	12%	61%	29%	• 9%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 479700 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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					AltConf	Trace
			Total	C	N	O	S		
1	A	782	6150	3871	1100	1164	15	0	0
1	B	782	6150	3871	1100	1164	15	0	0
1	C	782	6150	3871	1100	1164	15	0	0
1	D	782	6150	3871	1100	1164	15	0	0
1	E	782	6150	3871	1100	1164	15	0	0
1	F	782	6150	3871	1100	1164	15	0	0
1	G	782	6150	3871	1100	1164	15	0	0
1	H	782	6150	3871	1100	1164	15	0	0
1	I	782	6150	3871	1100	1164	15	0	0
1	J	782	6150	3871	1100	1164	15	0	0
1	K	782	6150	3871	1100	1164	15	0	0
1	L	782	6150	3871	1100	1164	15	0	0
1	M	782	6150	3871	1100	1164	15	0	0
1	N	782	6150	3871	1100	1164	15	0	0
1	O	782	6150	3871	1100	1164	15	0	0
1	P	782	6150	3871	1100	1164	15	0	0
1	Q	782	6150	3871	1100	1164	15	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	S	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	T	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	V	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	W	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	X	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	Y	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	Z	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	AA	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	BA	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	CA	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	DA	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	EA	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	FA	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	GA	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	HA	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	IA	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	JA	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	KA	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	LA	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	MA	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	NA	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	OA	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	PA	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	QA	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	RA	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	SA	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	TA	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	UA	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	VA	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	WA	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	XA	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	YA	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	ZA	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	AB	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	BB	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	CB	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	DB	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	EB	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	FB	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	GB	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0
1	HB	782	Total 6150	C 3871	N 1100	O 1164	S 15	0	0

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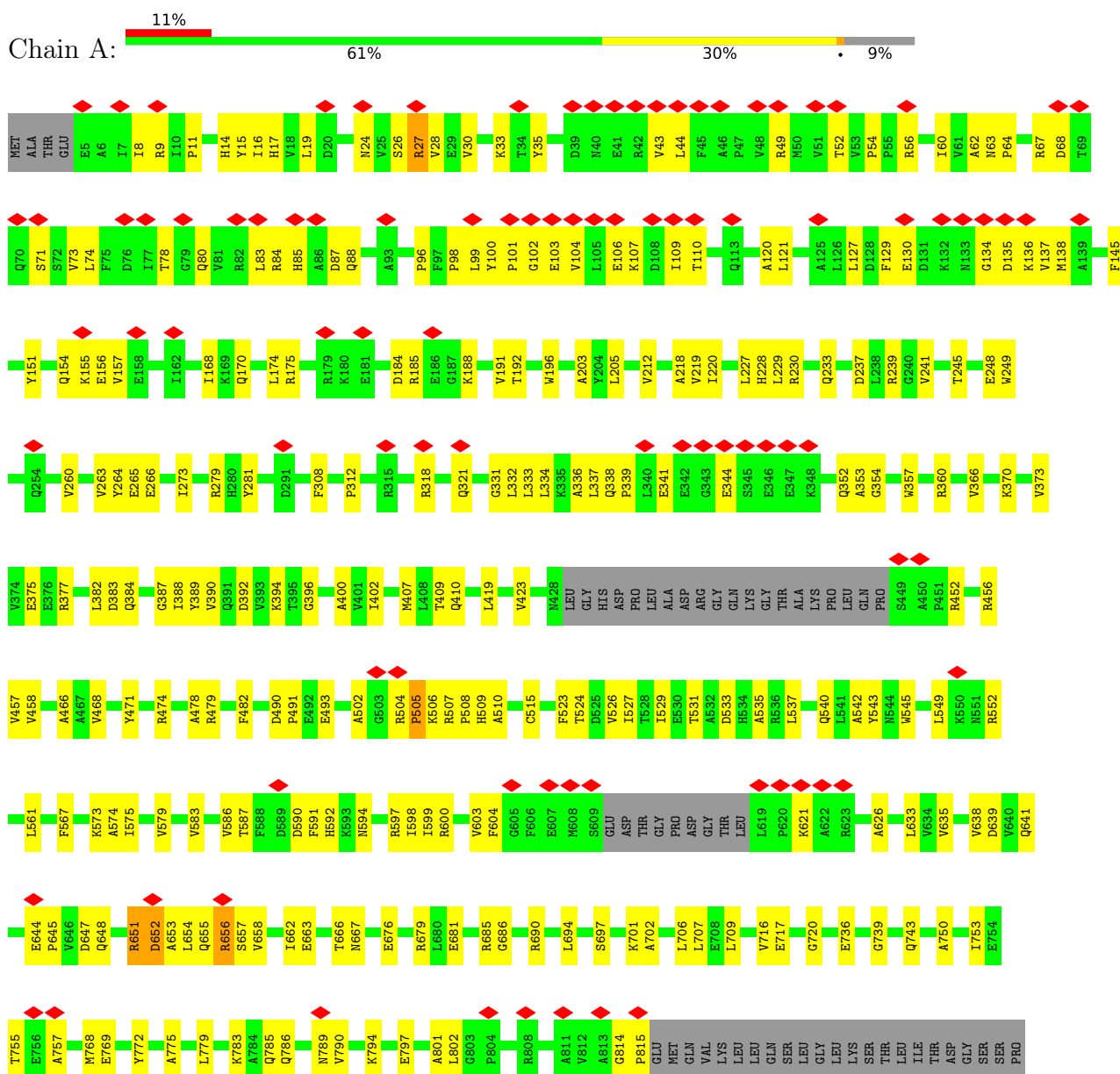
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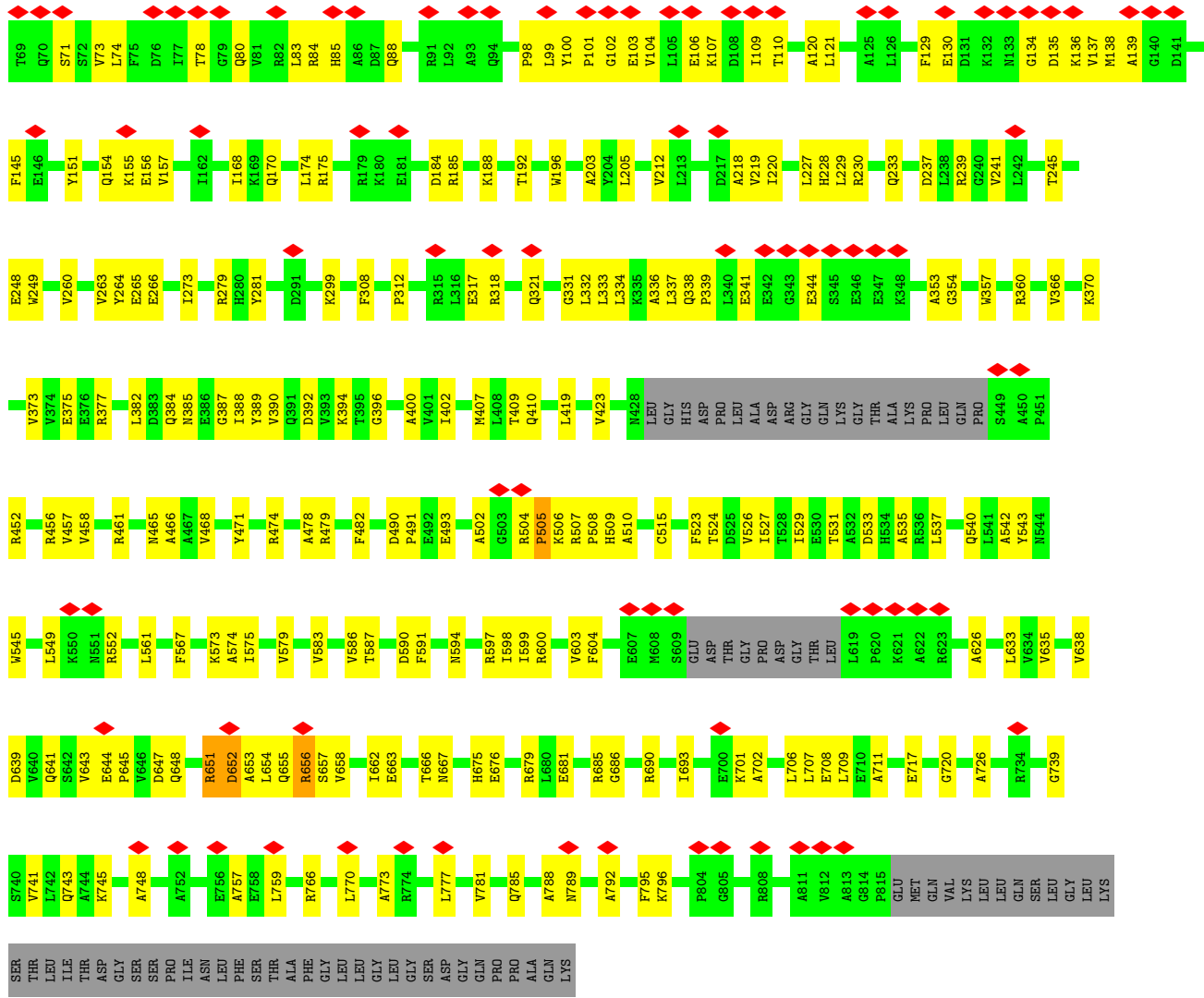
Mol	Chain	Residues	Atoms					AltConf	Trace
1	IB	782	Total	C	N	O	S	0	0
			6150	3871	1100	1164	15		
1	JB	782	Total	C	N	O	S	0	0
			6150	3871	1100	1164	15		
1	KB	782	Total	C	N	O	S	0	0
			6150	3871	1100	1164	15		
1	LB	782	Total	C	N	O	S	0	0
			6150	3871	1100	1164	15		
1	MB	782	Total	C	N	O	S	0	0
			6150	3871	1100	1164	15		
1	NB	782	Total	C	N	O	S	0	0
			6150	3871	1100	1164	15		
1	OB	782	Total	C	N	O	S	0	0
			6150	3871	1100	1164	15		
1	PB	782	Total	C	N	O	S	0	0
			6150	3871	1100	1164	15		
1	QB	782	Total	C	N	O	S	0	0
			6150	3871	1100	1164	15		
1	RB	782	Total	C	N	O	S	0	0
			6150	3871	1100	1164	15		
1	SB	782	Total	C	N	O	S	0	0
			6150	3871	1100	1164	15		
1	TB	782	Total	C	N	O	S	0	0
			6150	3871	1100	1164	15		
1	UB	782	Total	C	N	O	S	0	0
			6150	3871	1100	1164	15		
1	VB	782	Total	C	N	O	S	0	0
			6150	3871	1100	1164	15		
1	WB	782	Total	C	N	O	S	0	0
			6150	3871	1100	1164	15		
1	XB	782	Total	C	N	O	S	0	0
			6150	3871	1100	1164	15		
1	YB	782	Total	C	N	O	S	0	0
			6150	3871	1100	1164	15		
1	ZB	782	Total	C	N	O	S	0	0
			6150	3871	1100	1164	15		
1	AC	782	Total	C	N	O	S	0	0
			6150	3871	1100	1164	15		

3 Residue-property plots

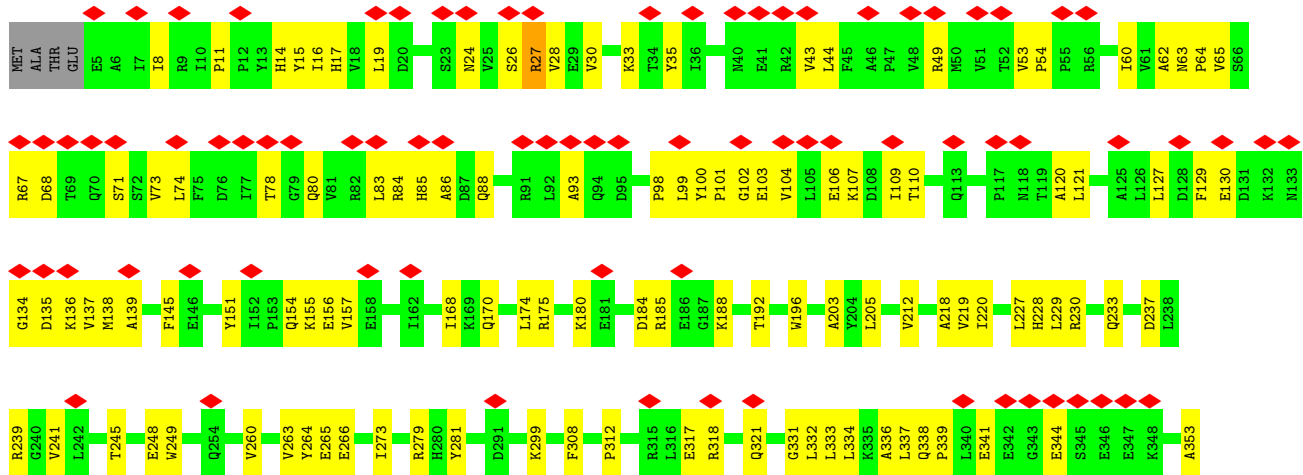
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

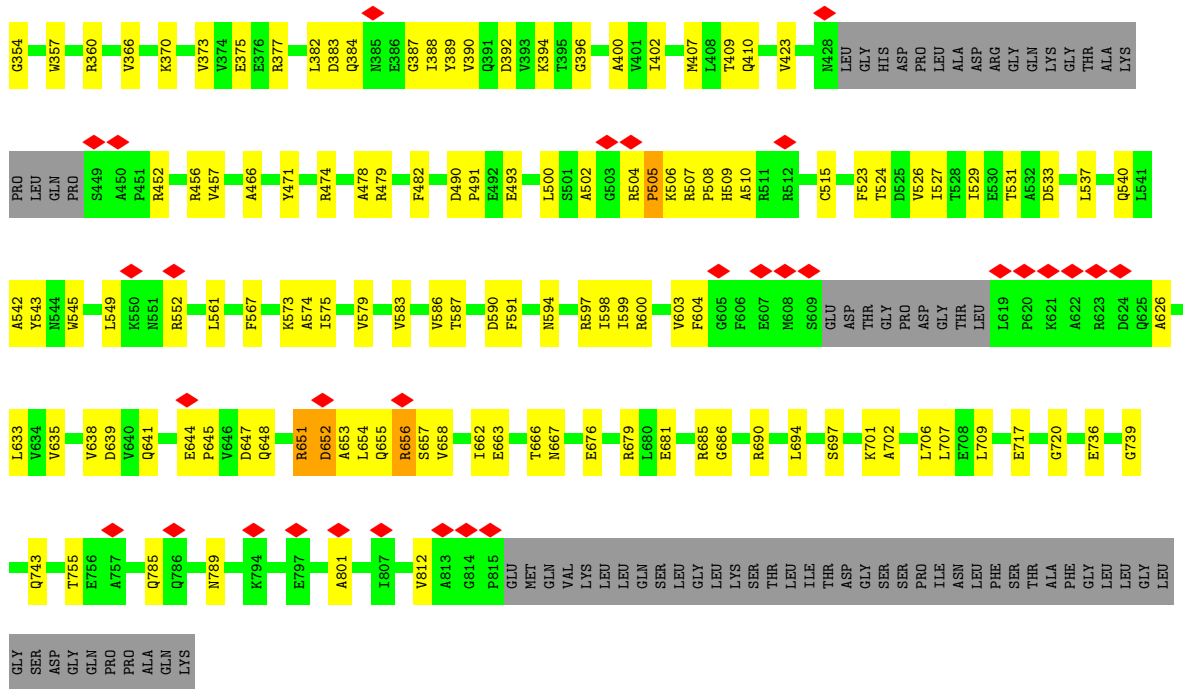
• Molecule 1: Major vault protein



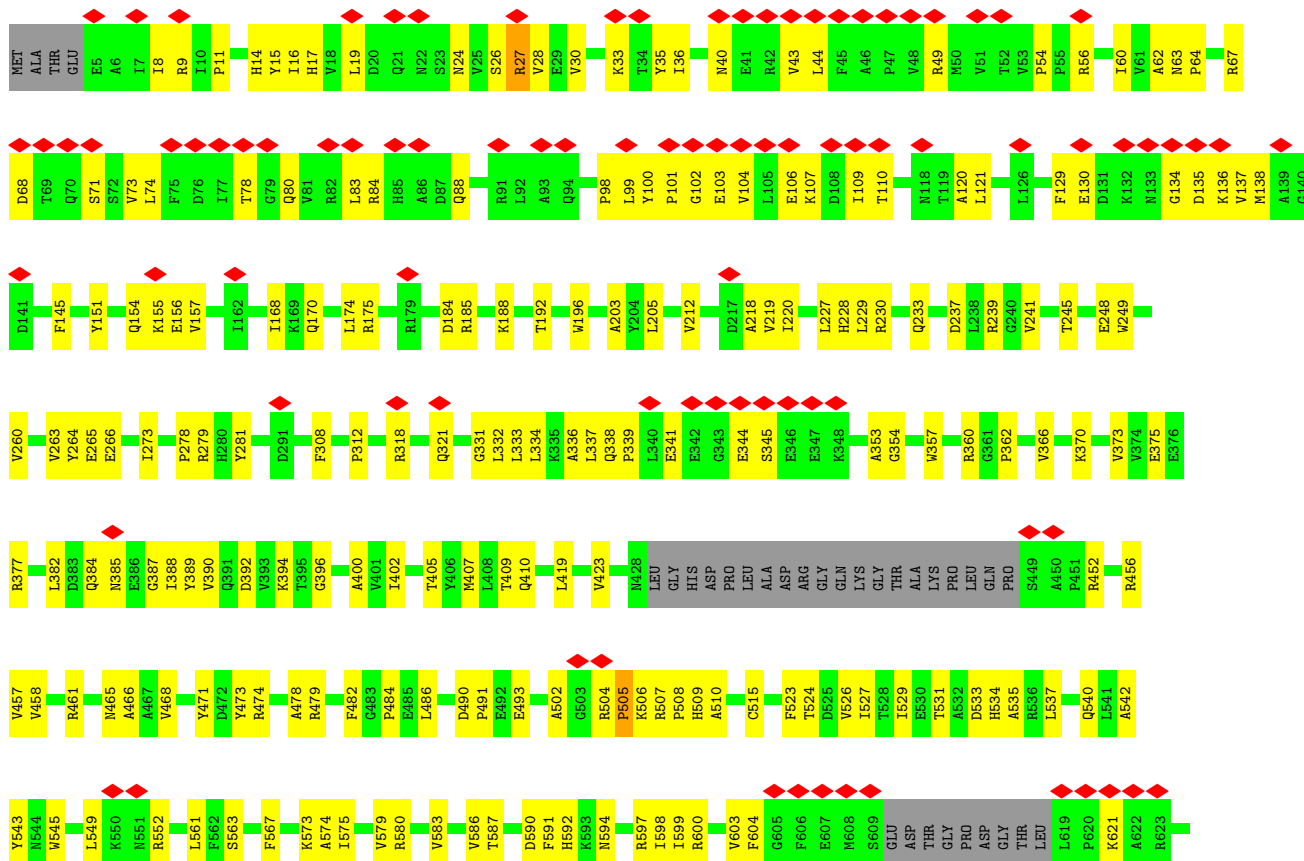


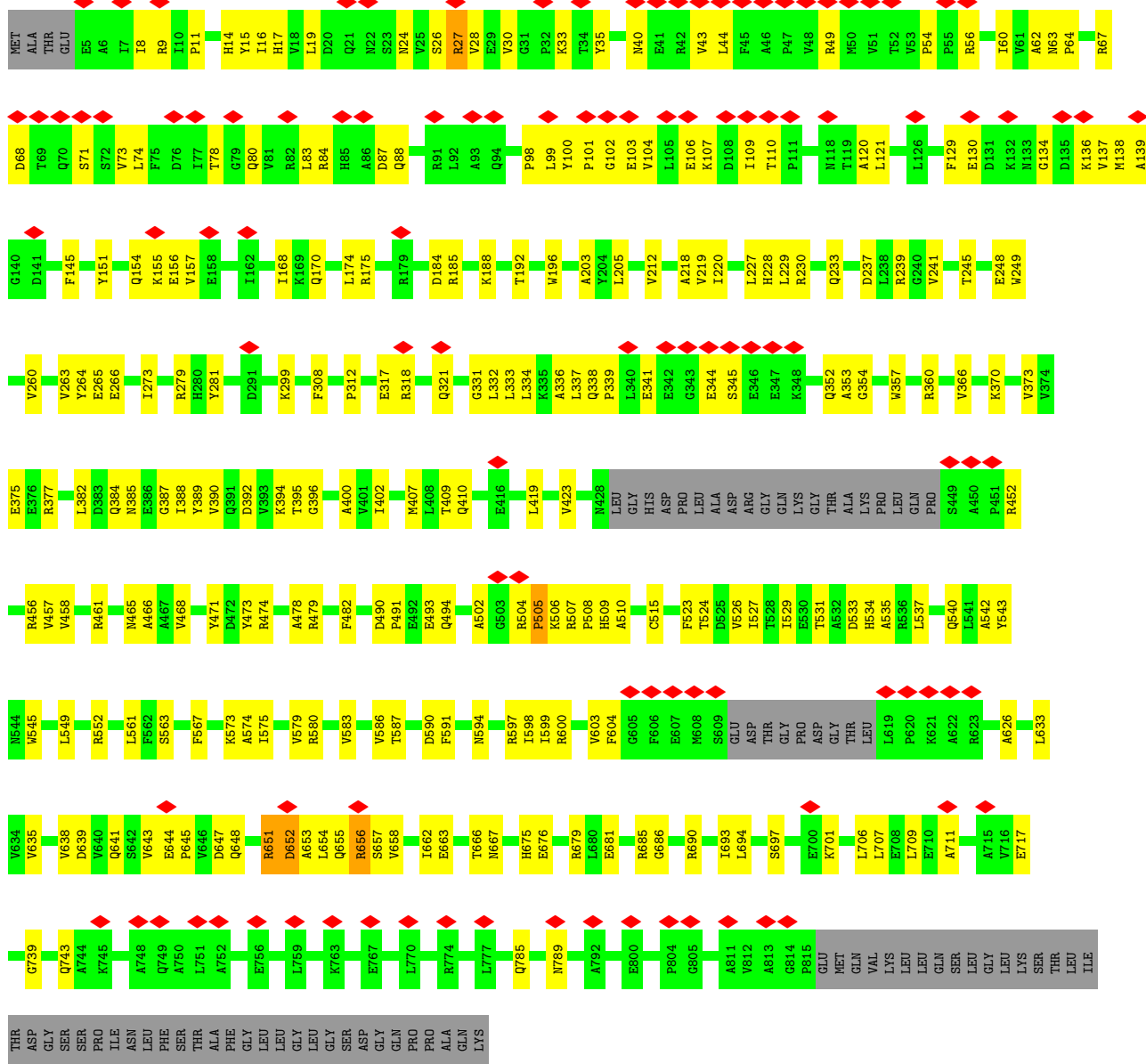
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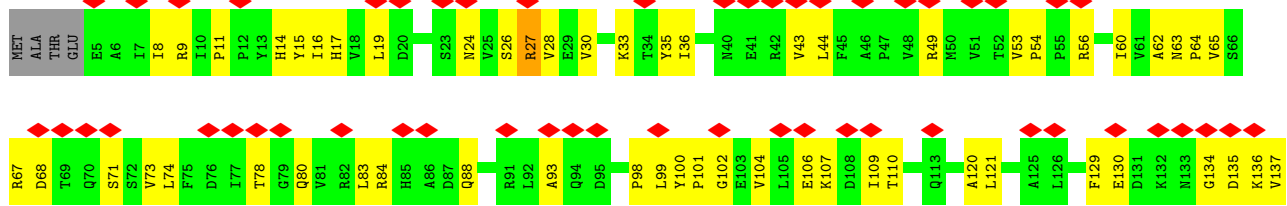


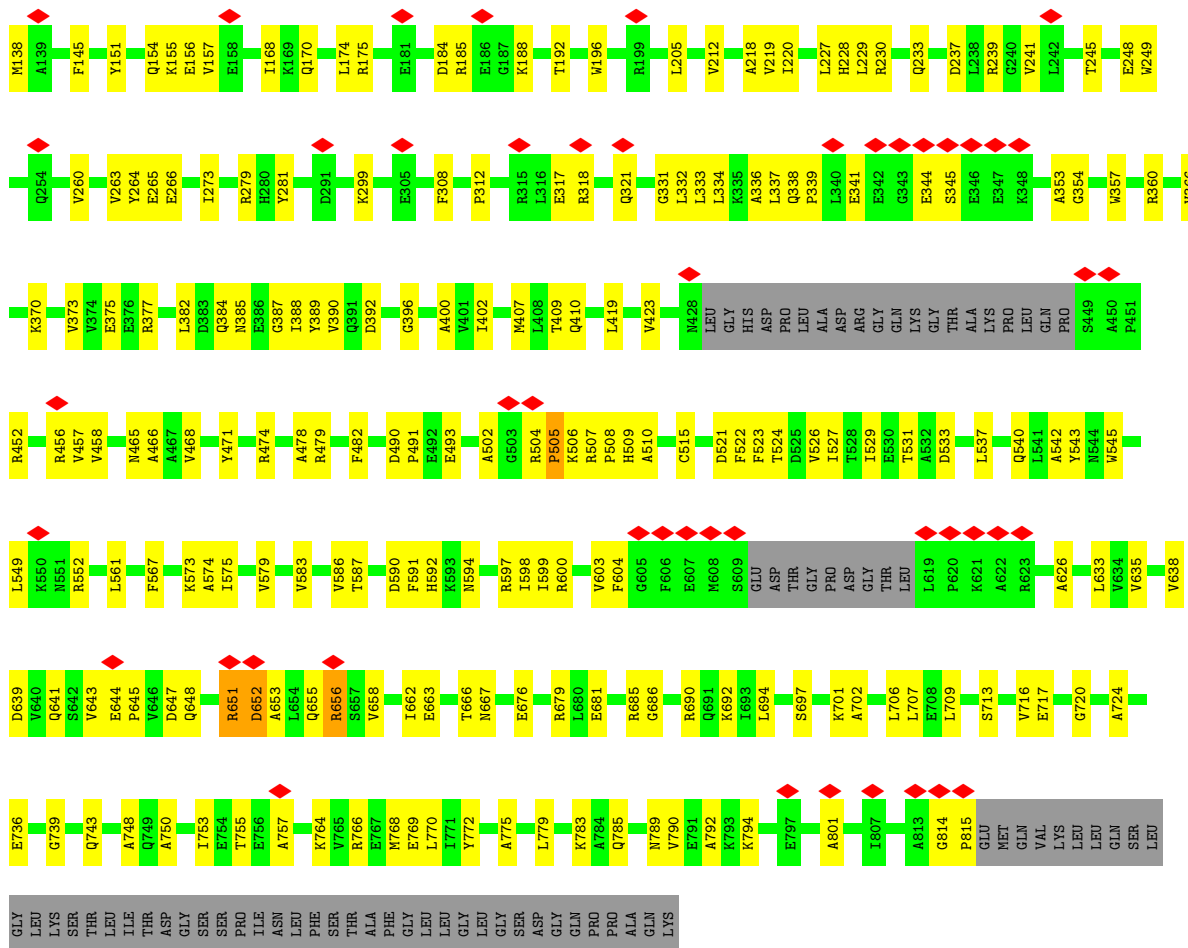
- Molecule 1: Major vault protein



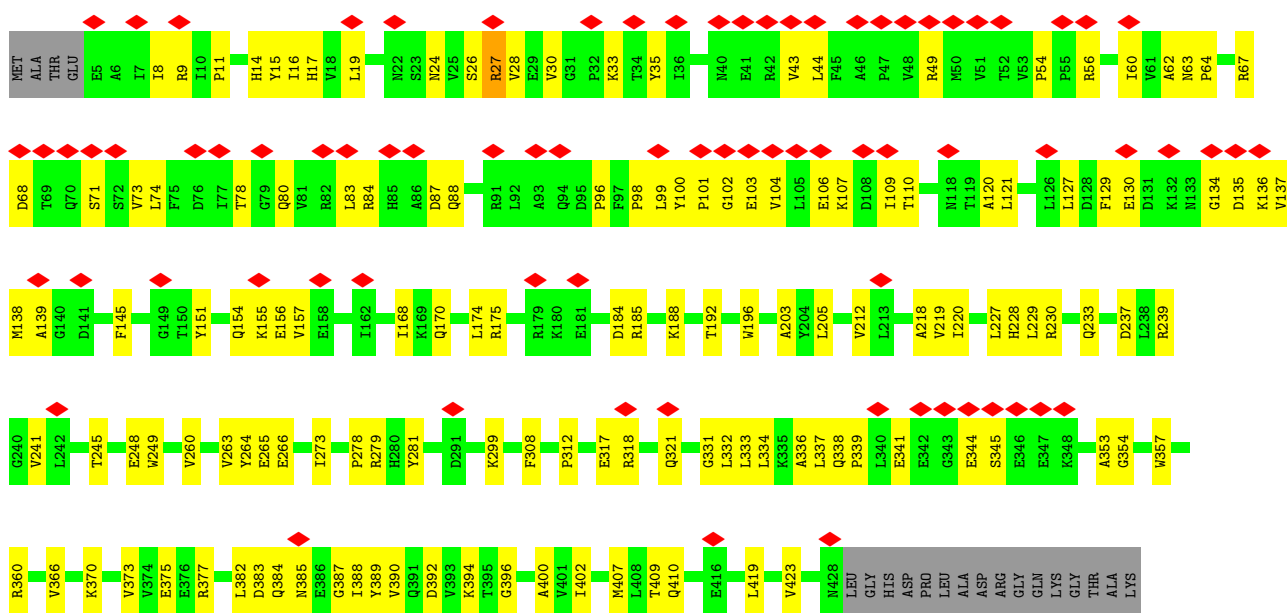


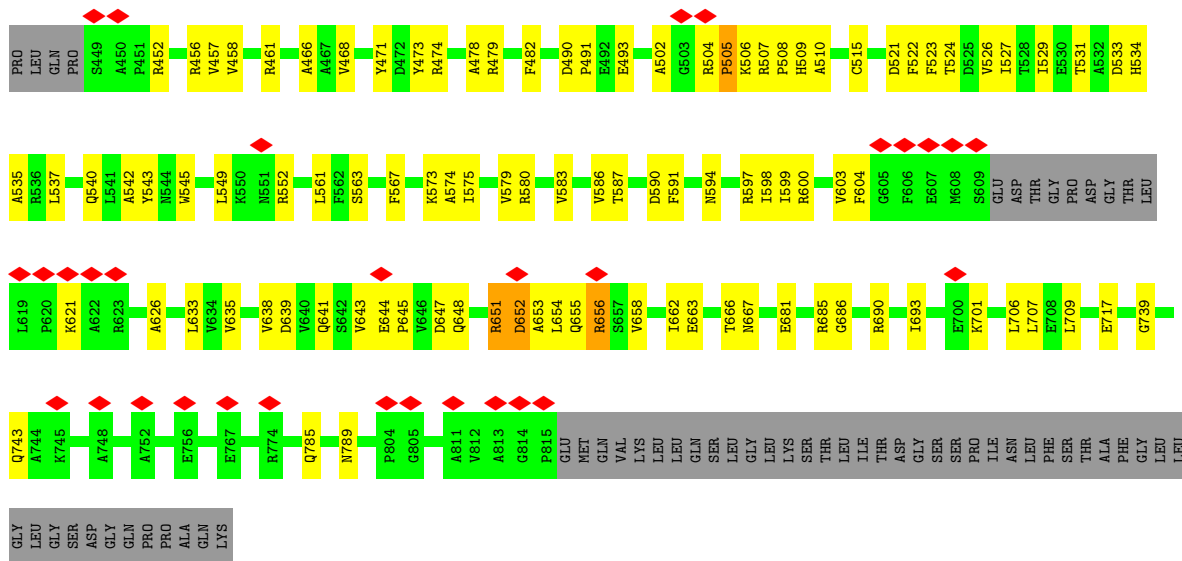
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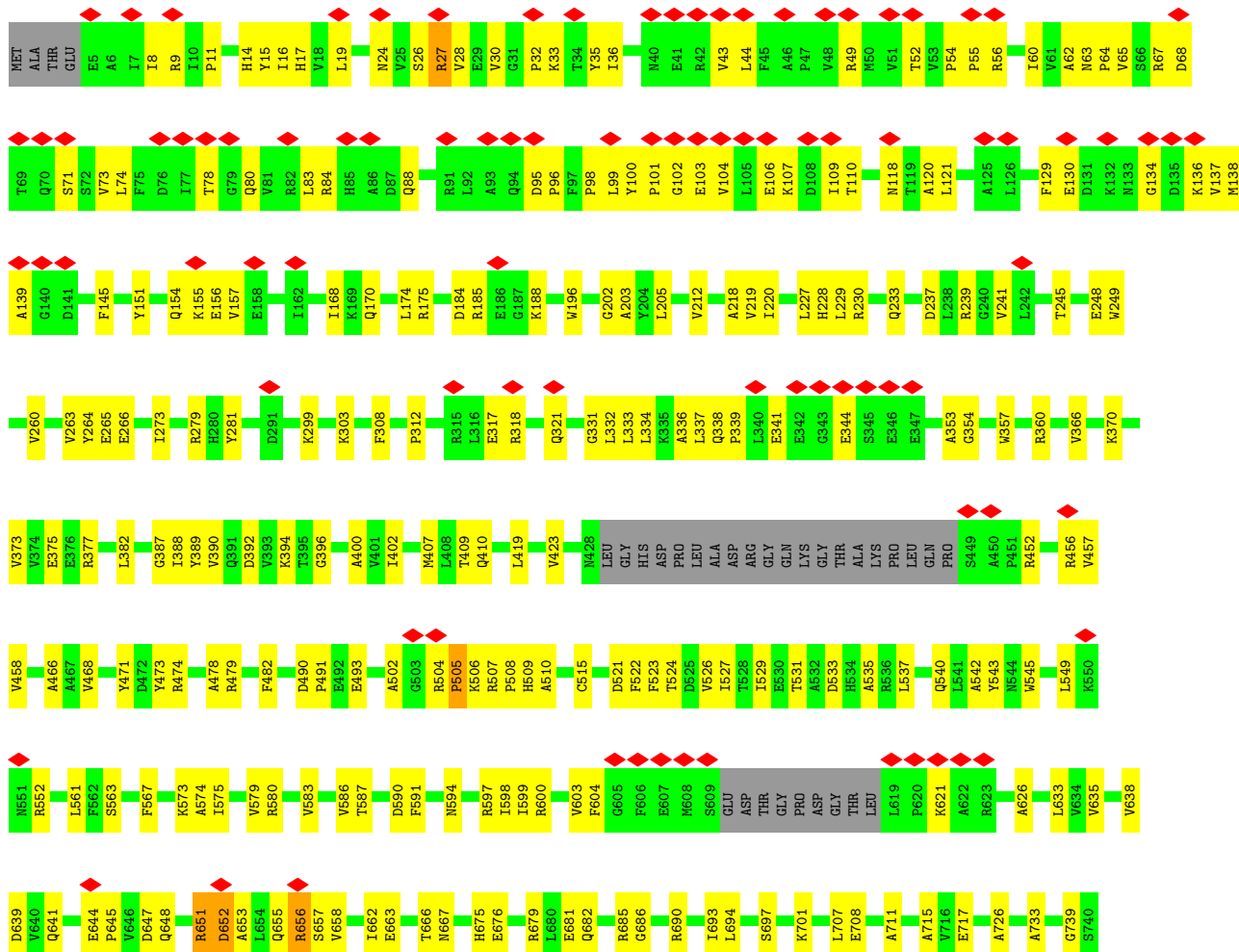


• Molecule 1: Major vault protein



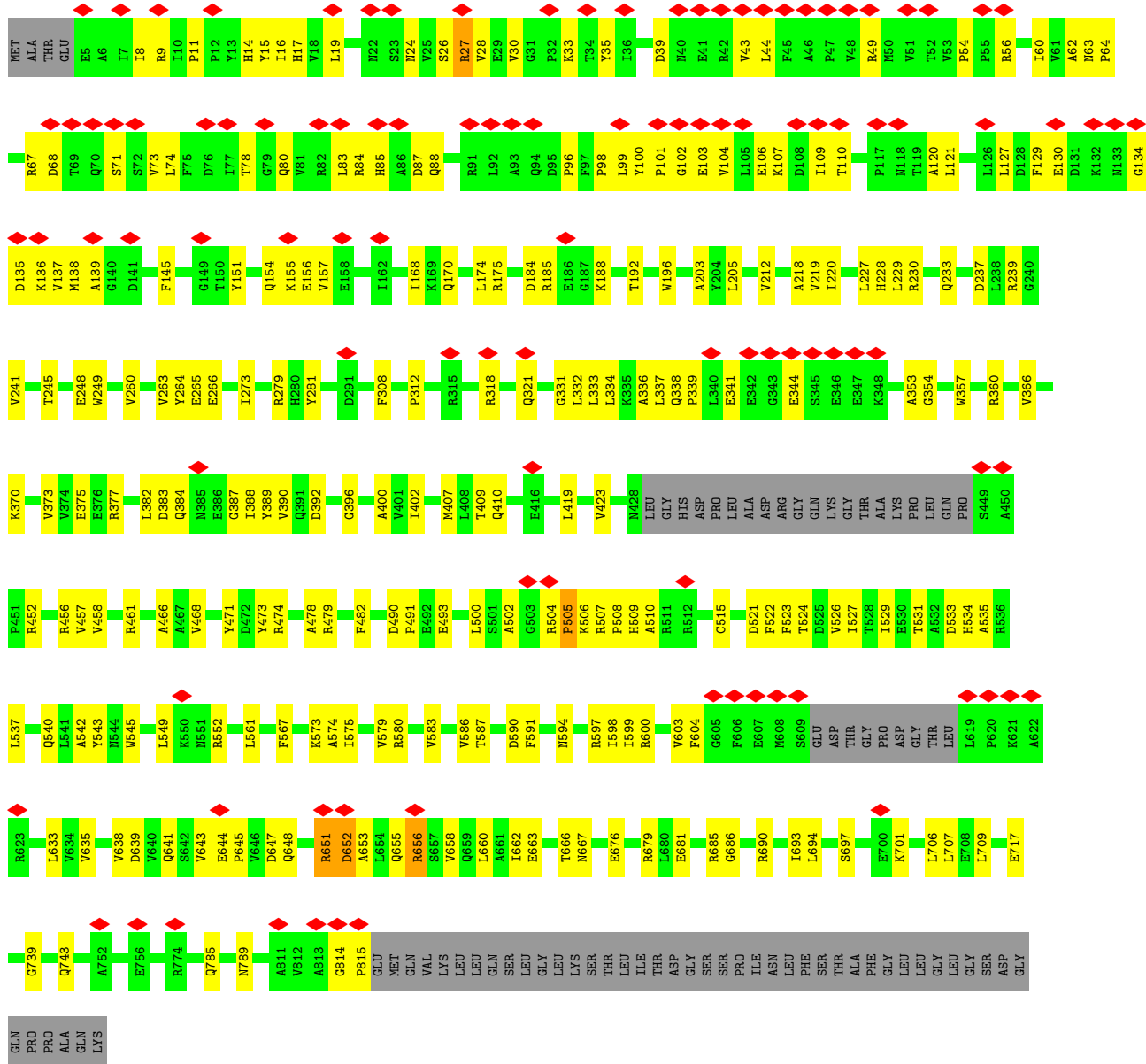


• Molecule 1: Major vault protein



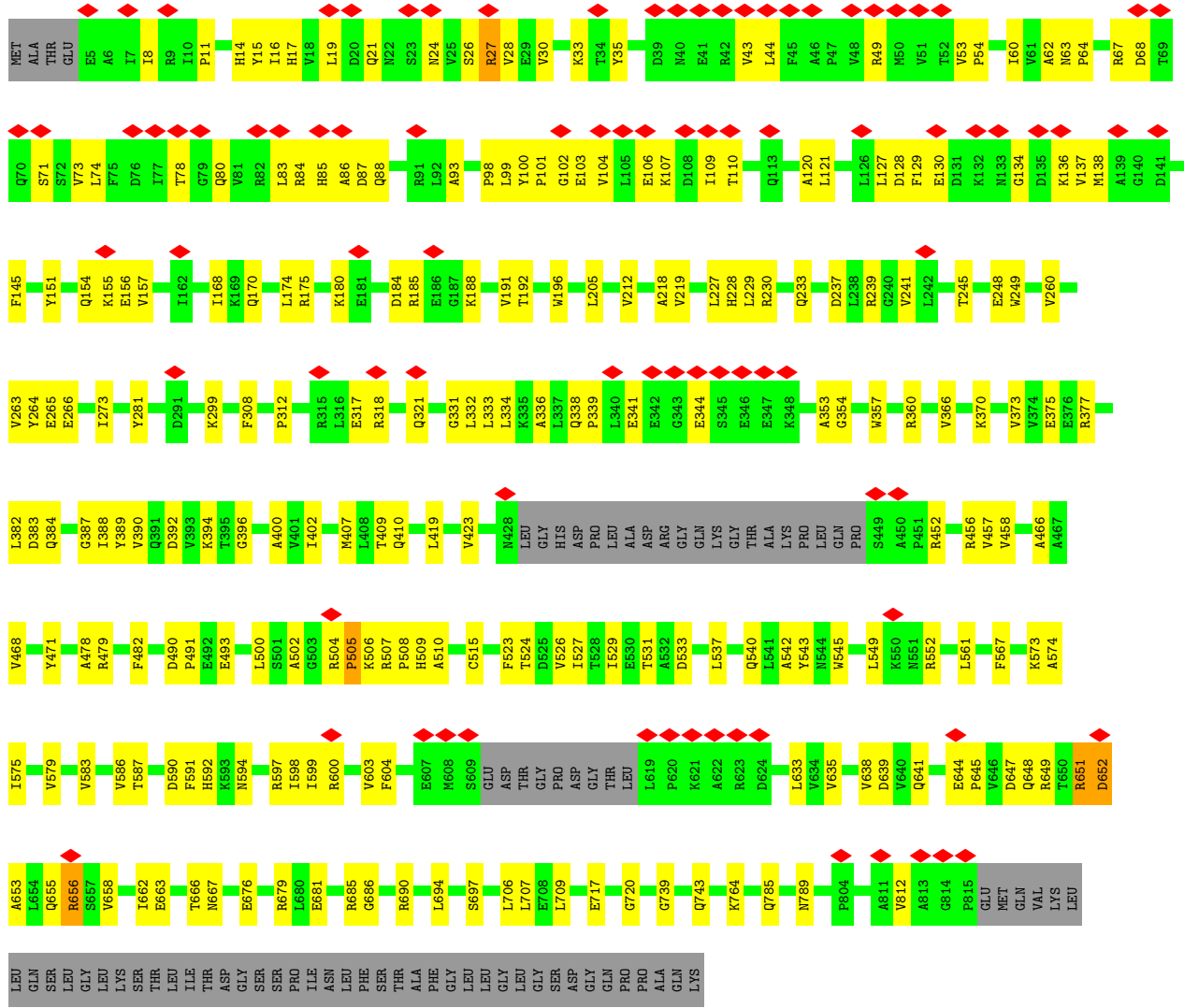


• Molecule 1: Major vault protein

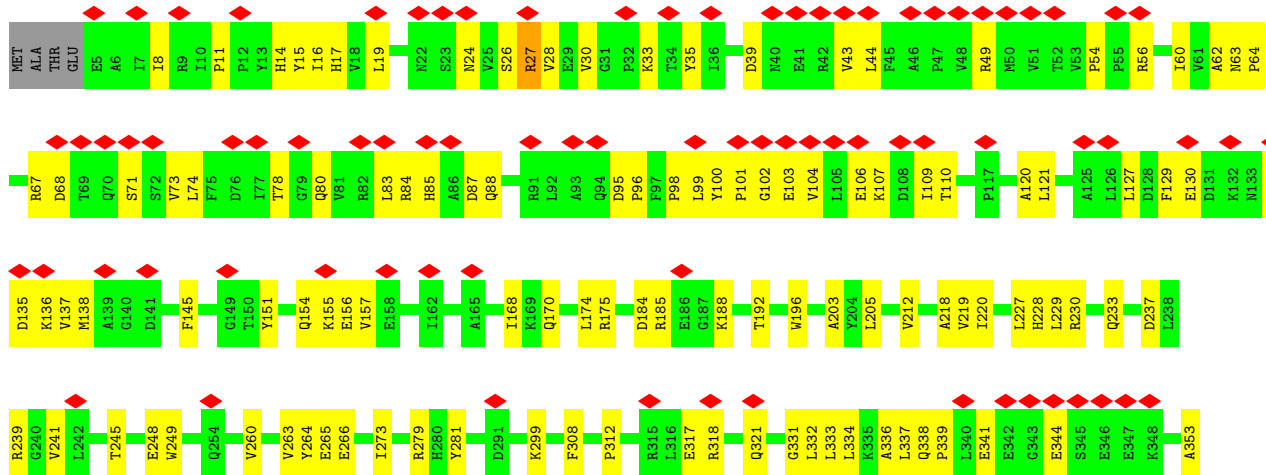


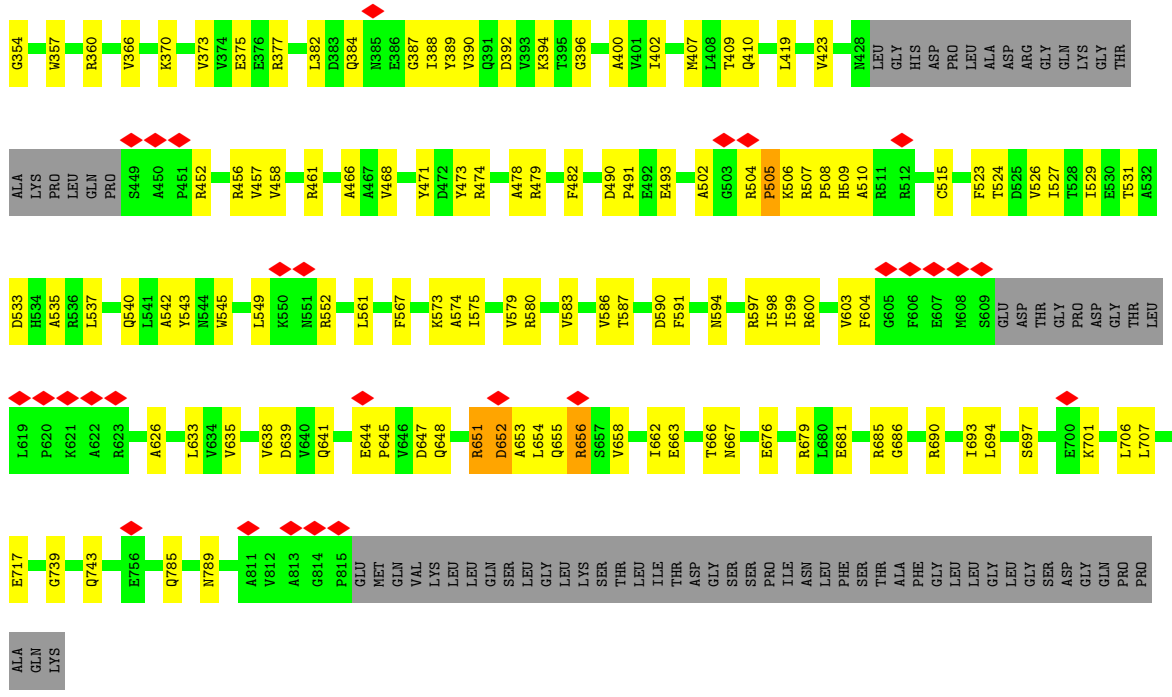
• Molecule 1: Major vault protein



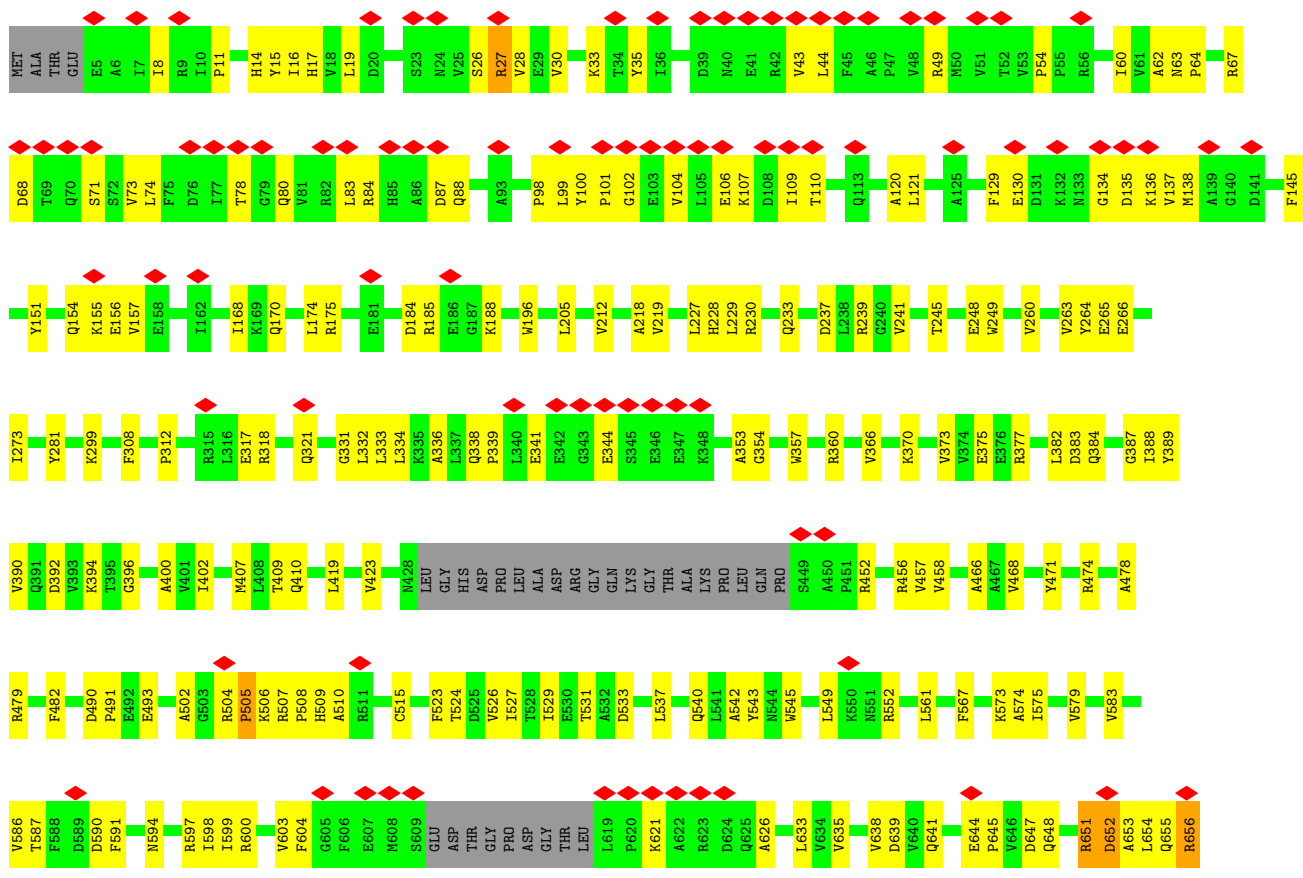


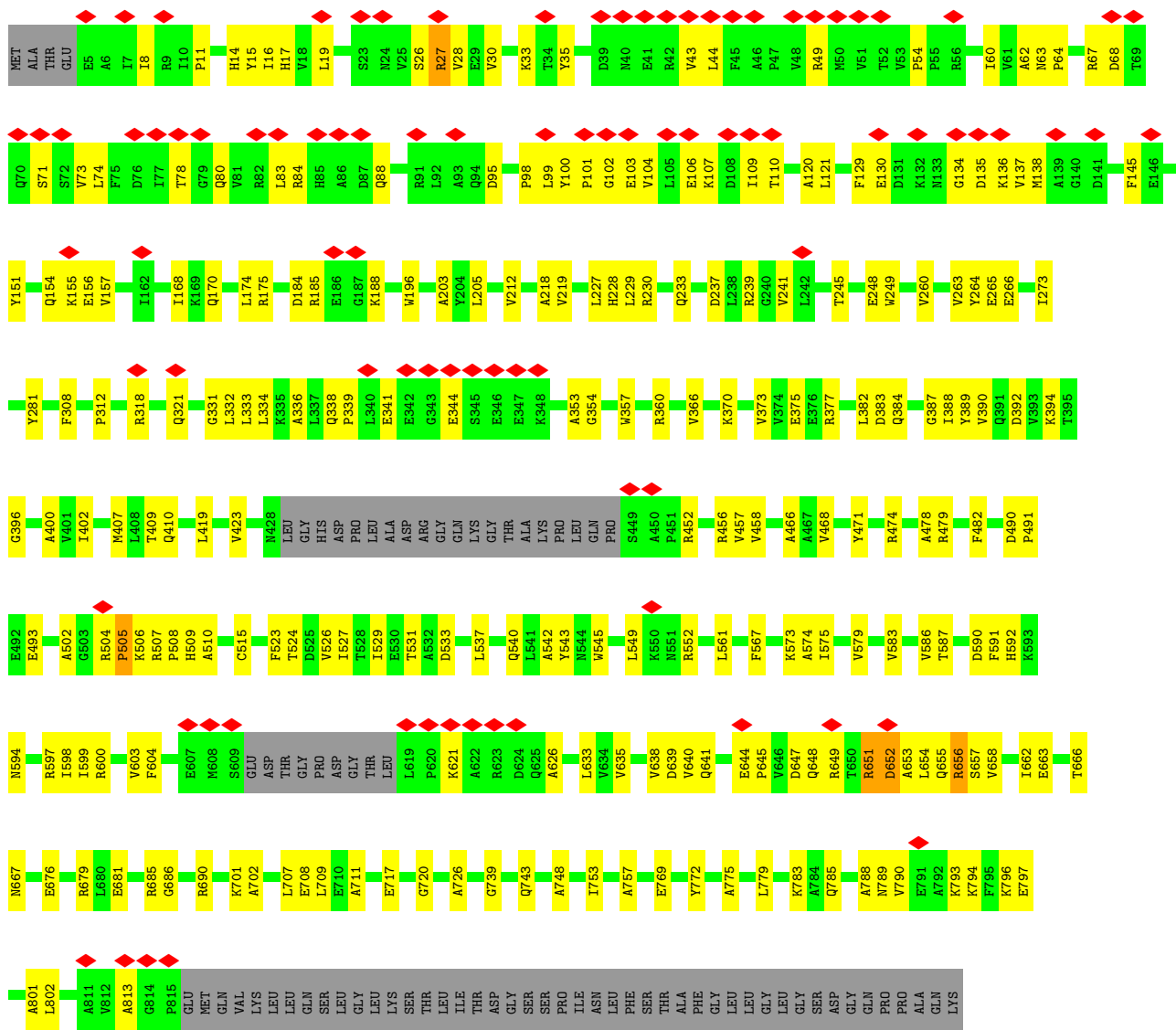
• Molecule 1: Major vault protein



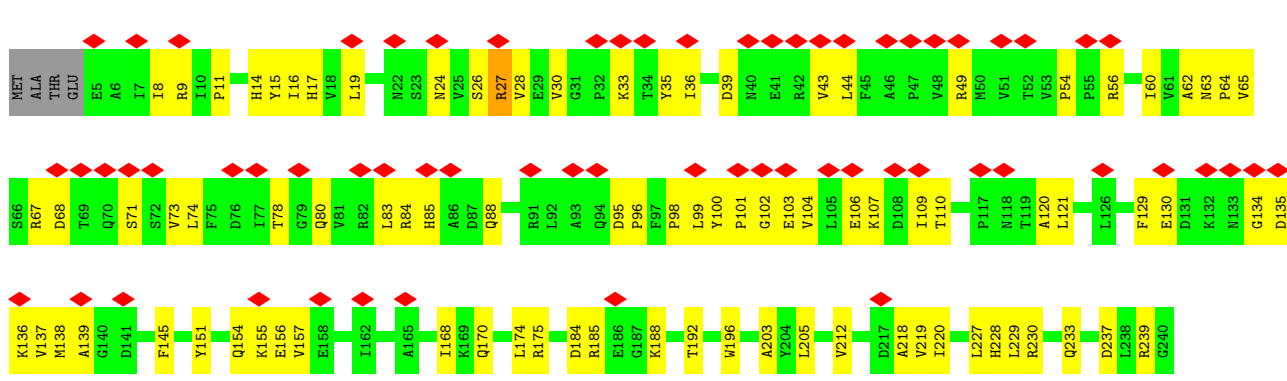


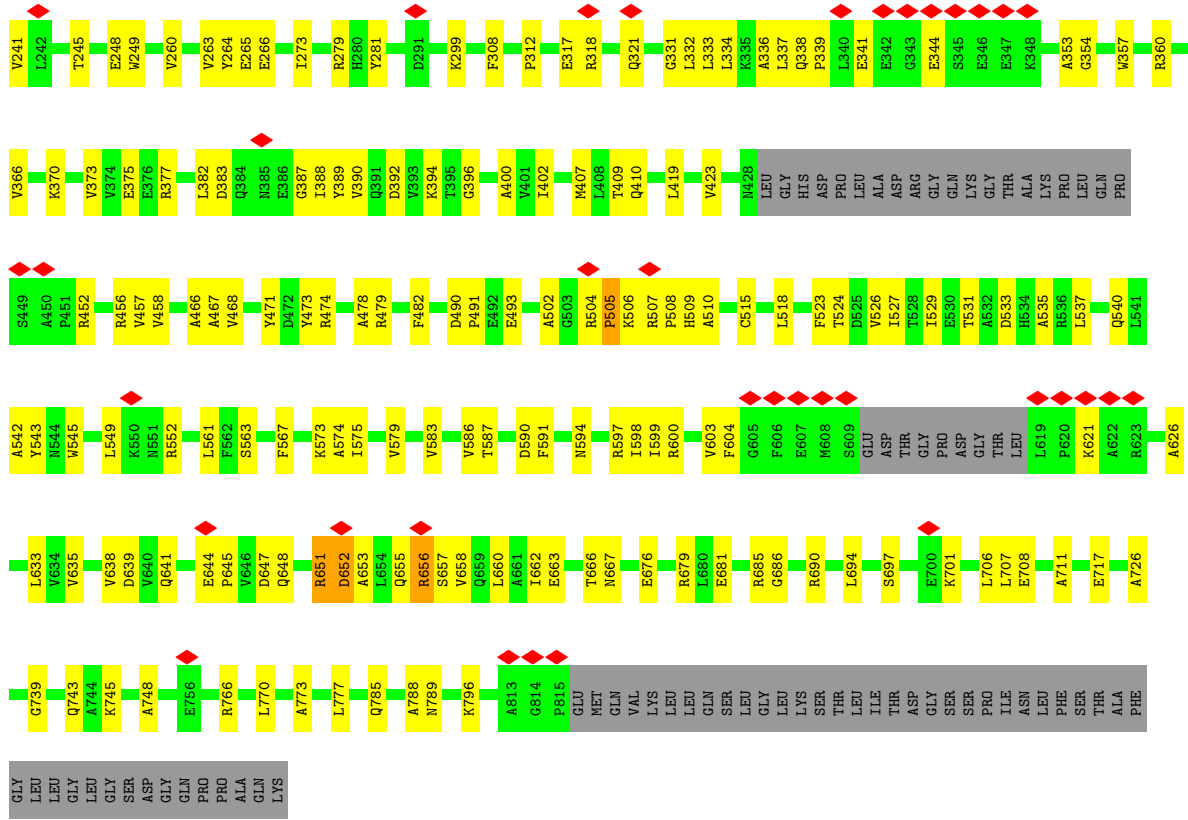
• Molecule 1: Major vault protein



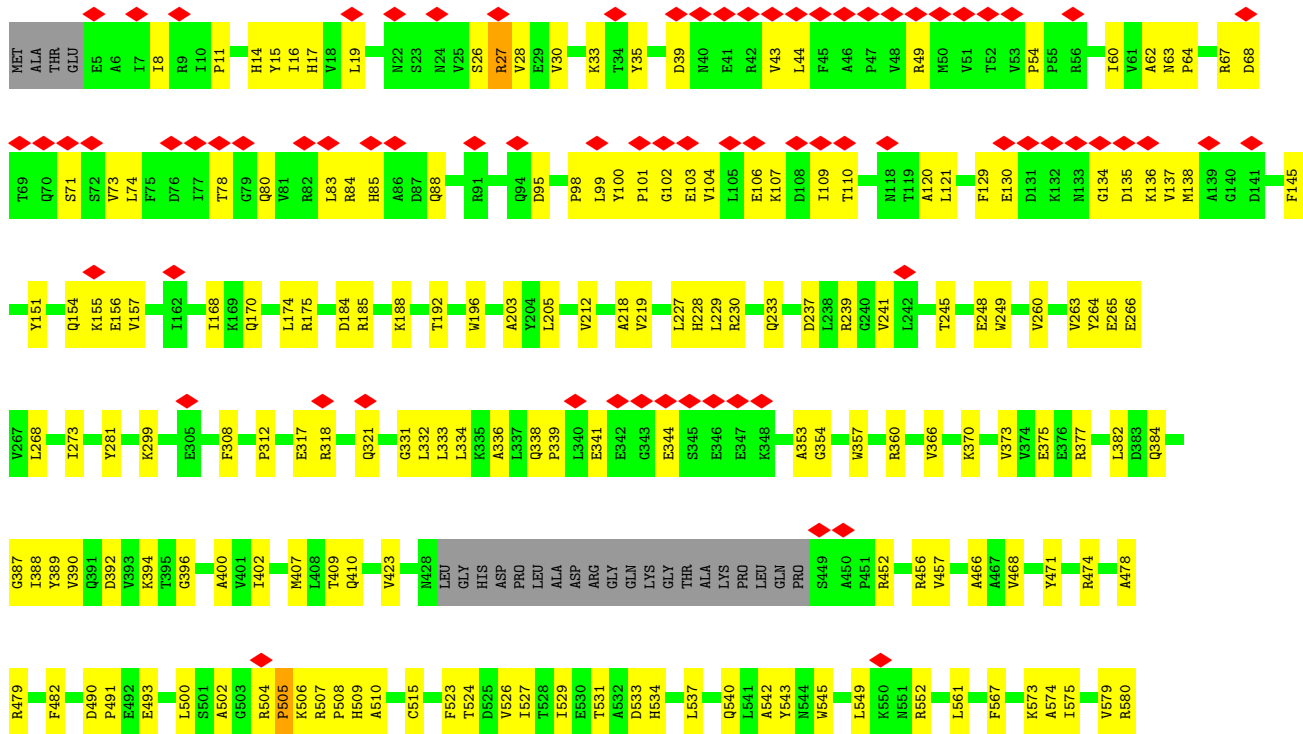


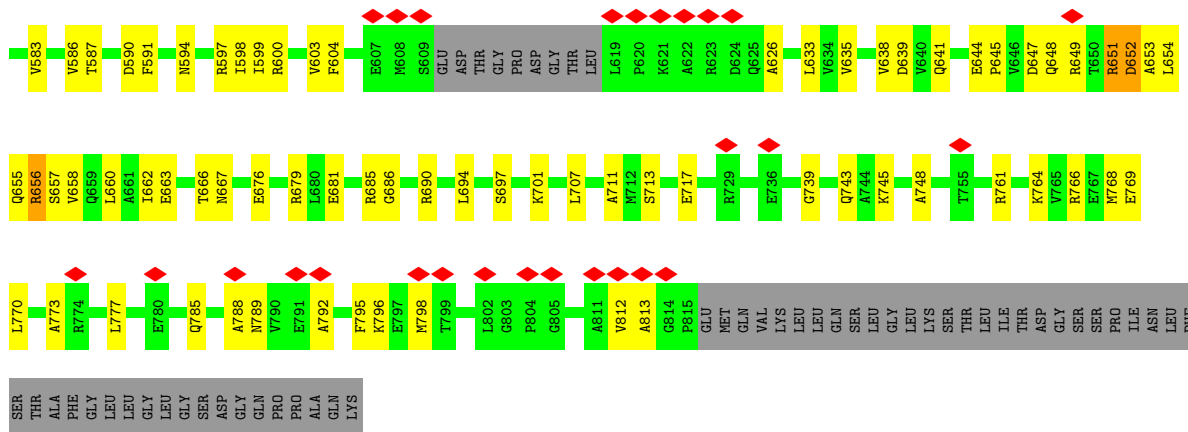
• Molecule 1: Major vault protein



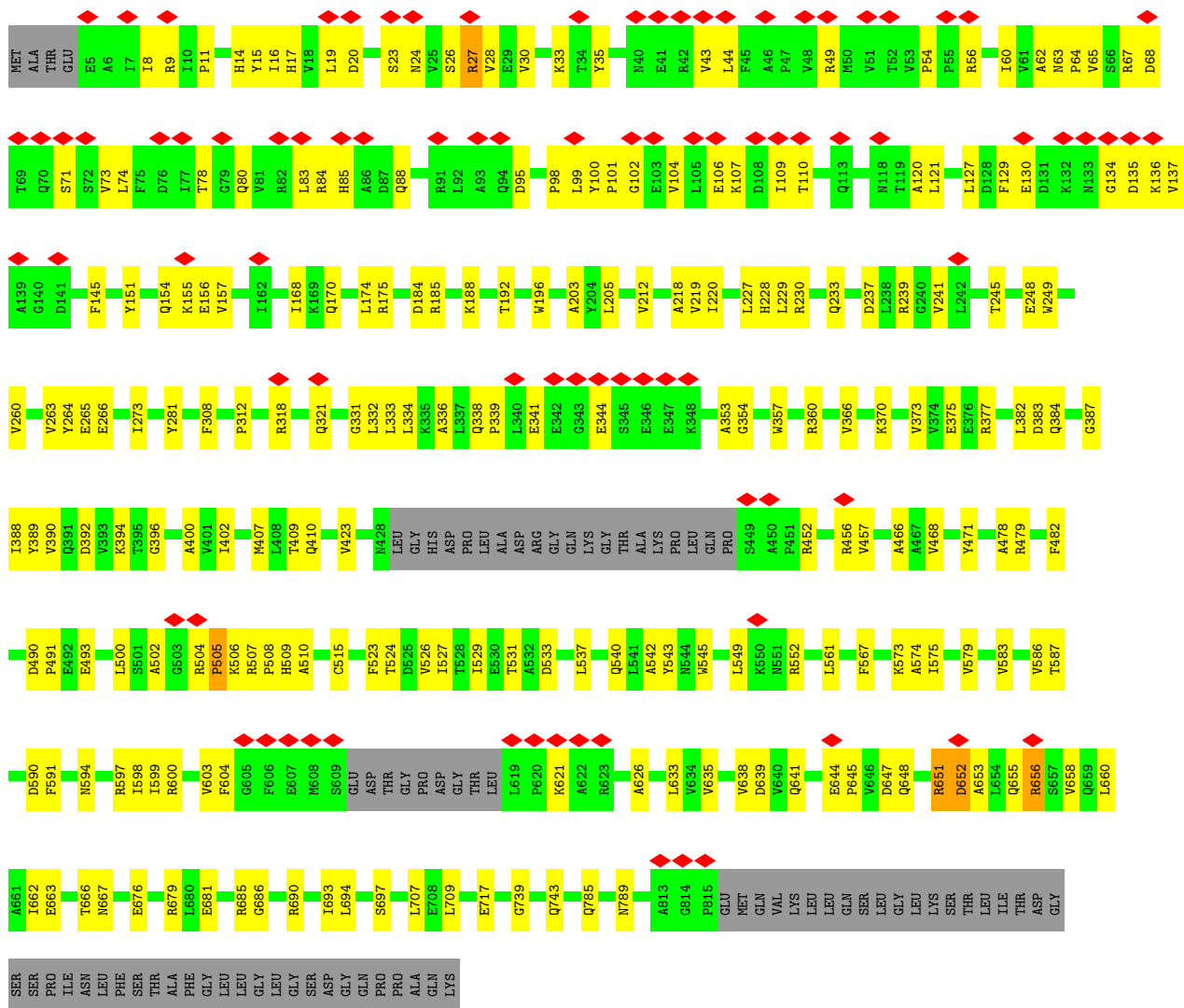


• Molecule 1: Major vault protein

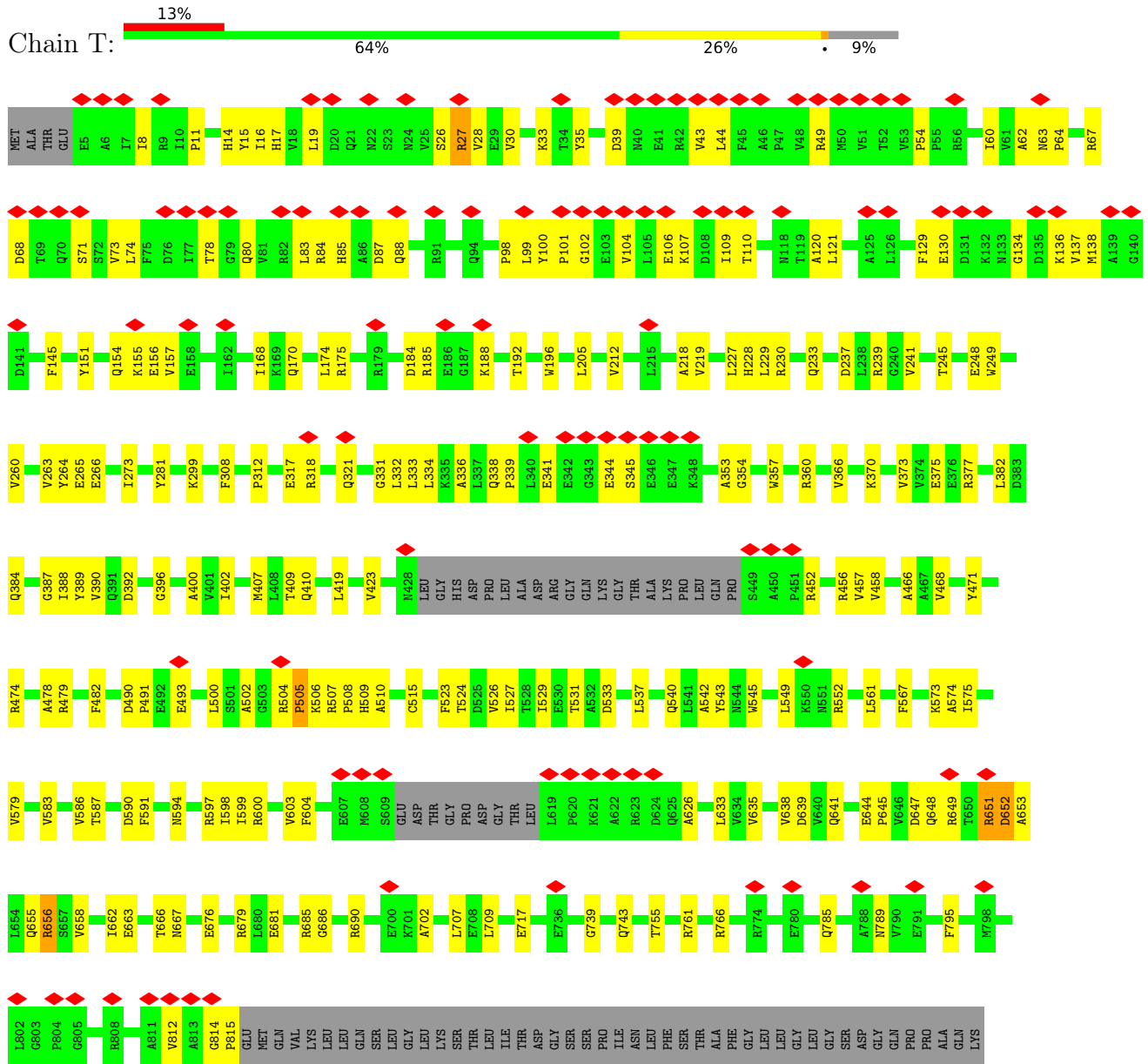




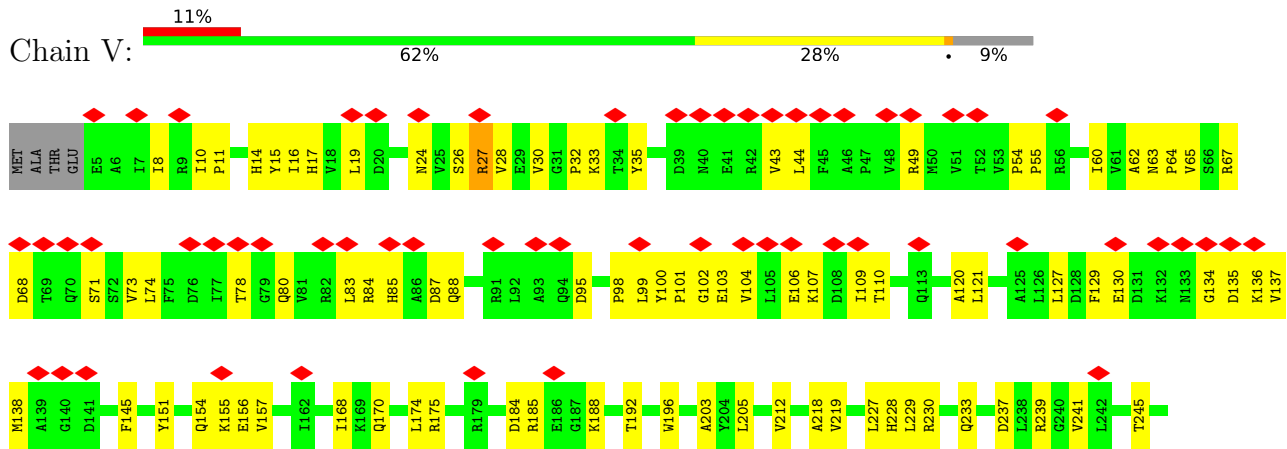
• Molecule 1: Major vault protein

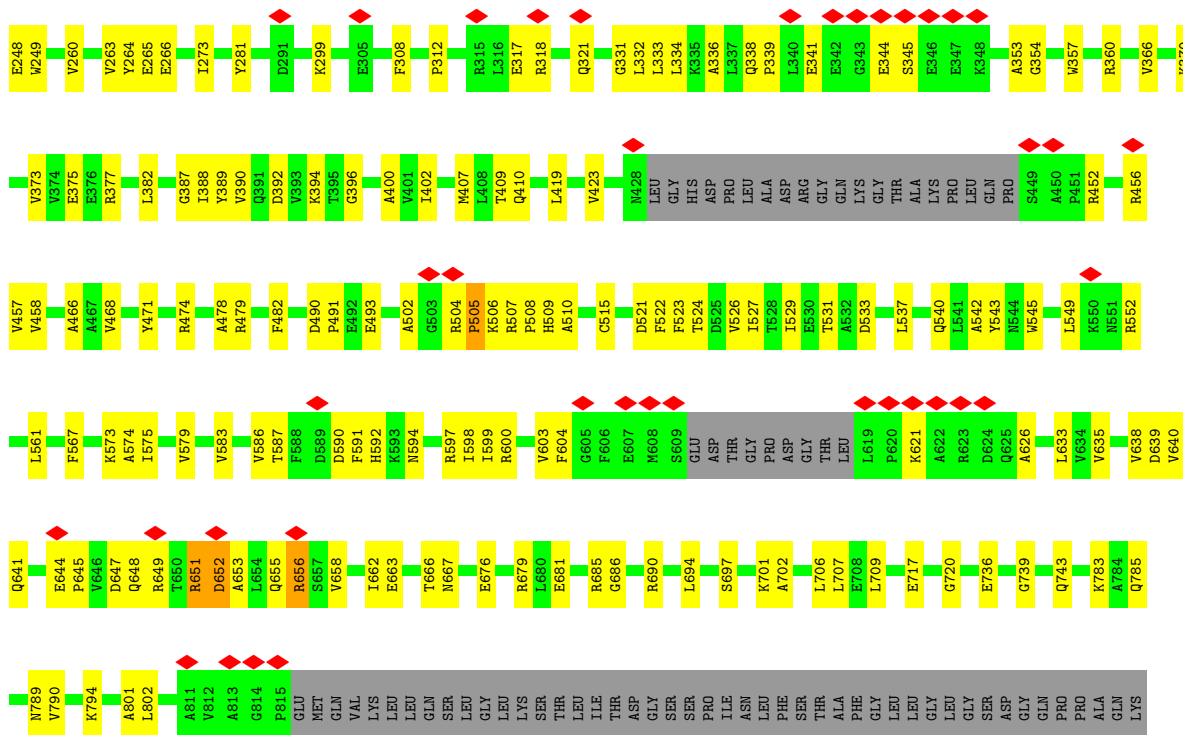


• Molecule 1: Major vault protein

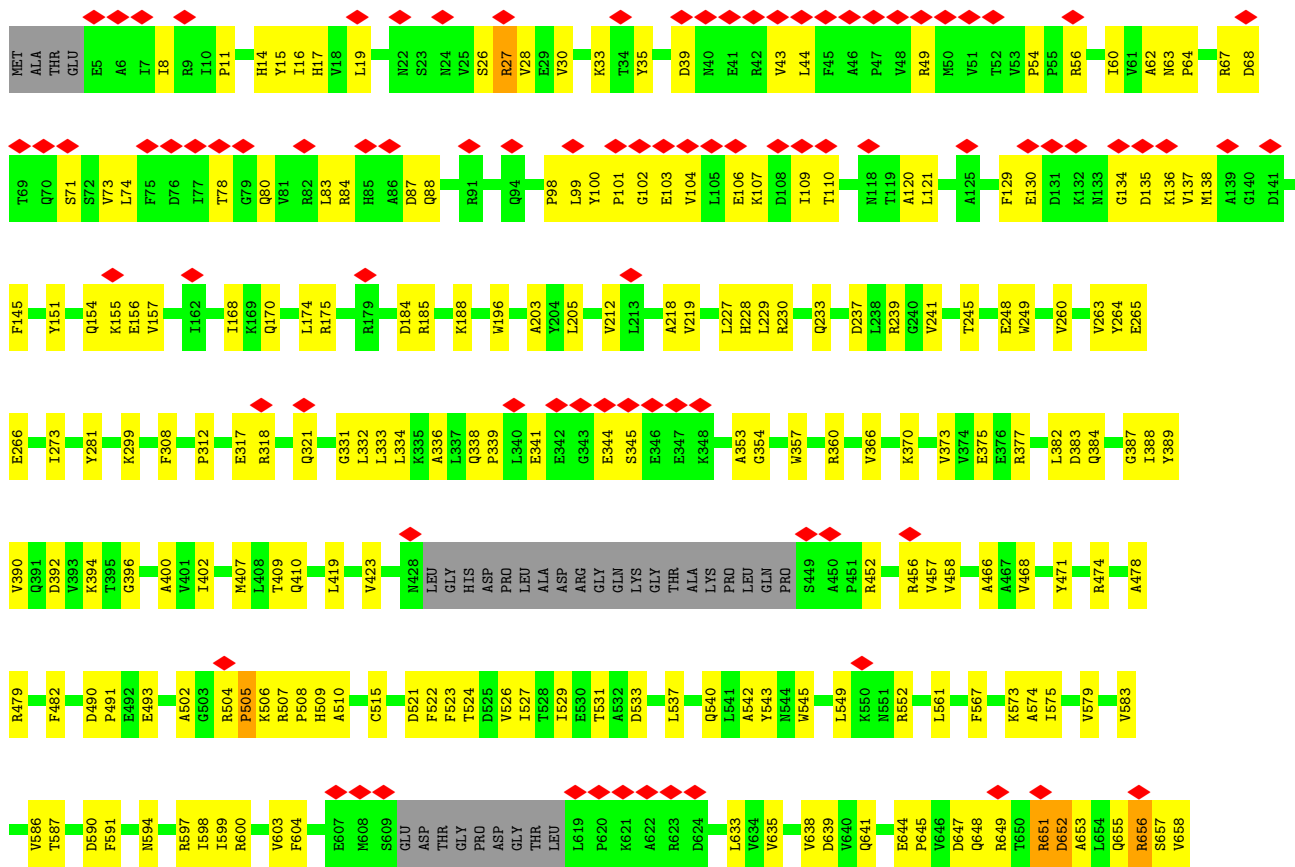


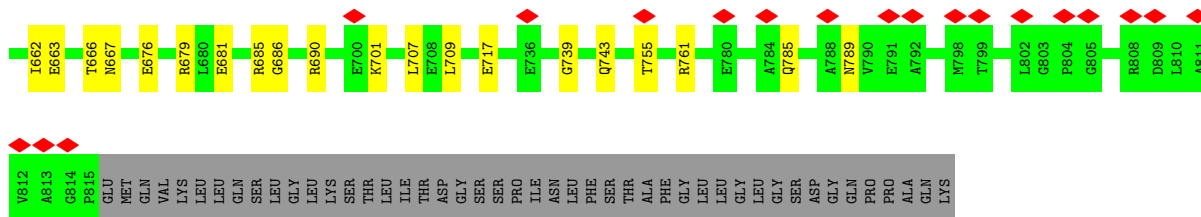
• Molecule 1: Major vault protein



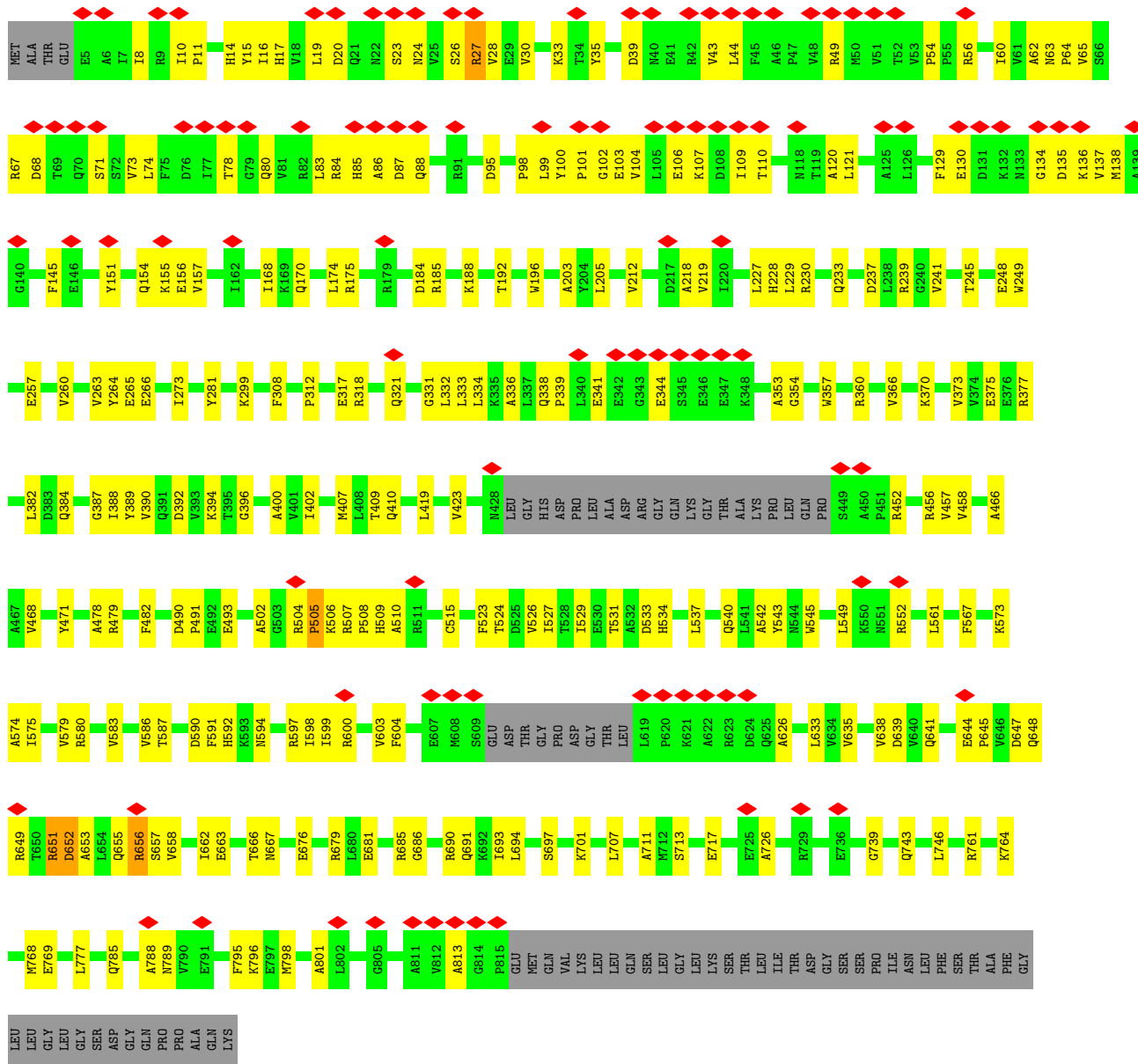


• Molecule 1: Major vault protein



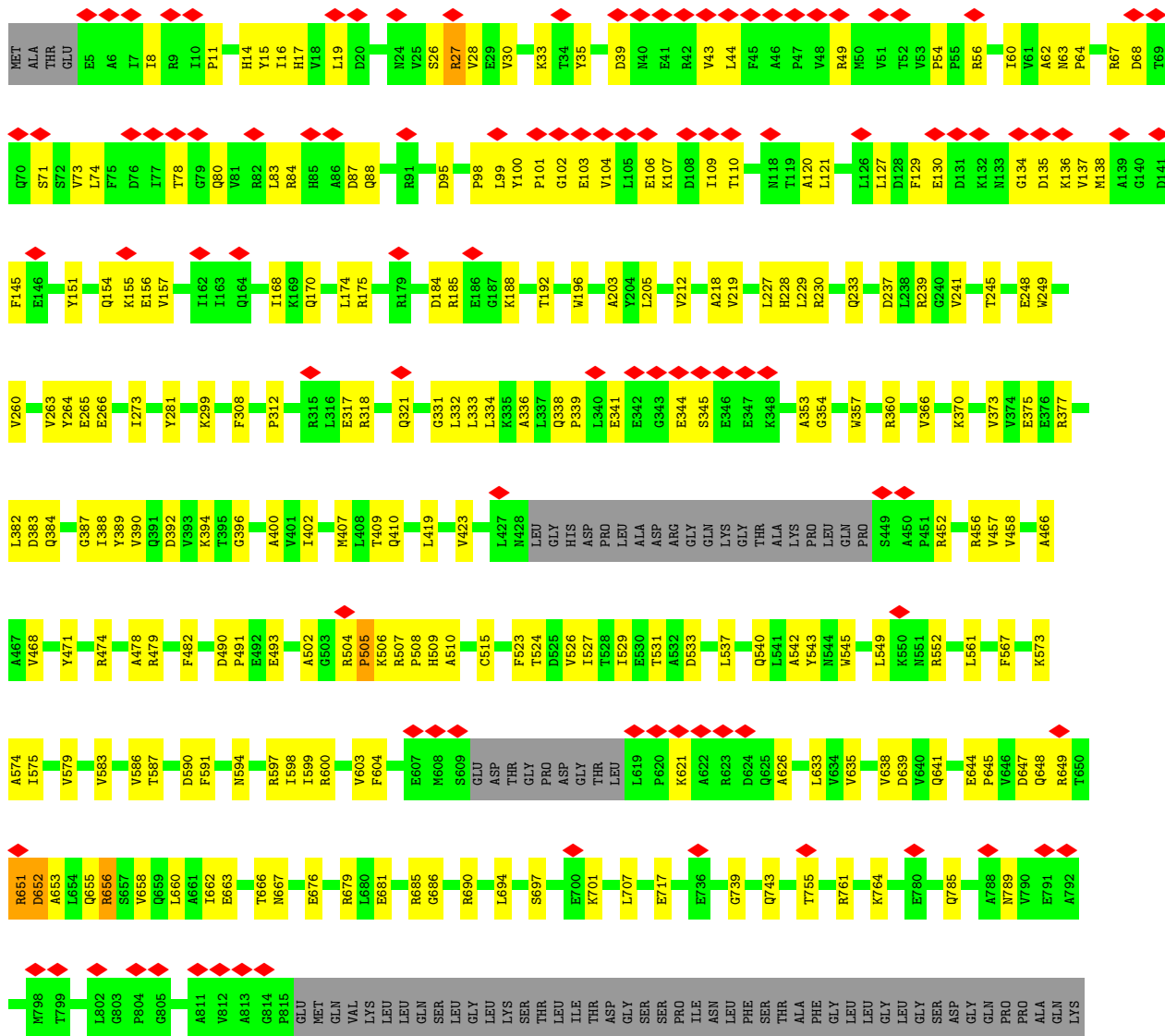


• Molecule 1: Major vault protein

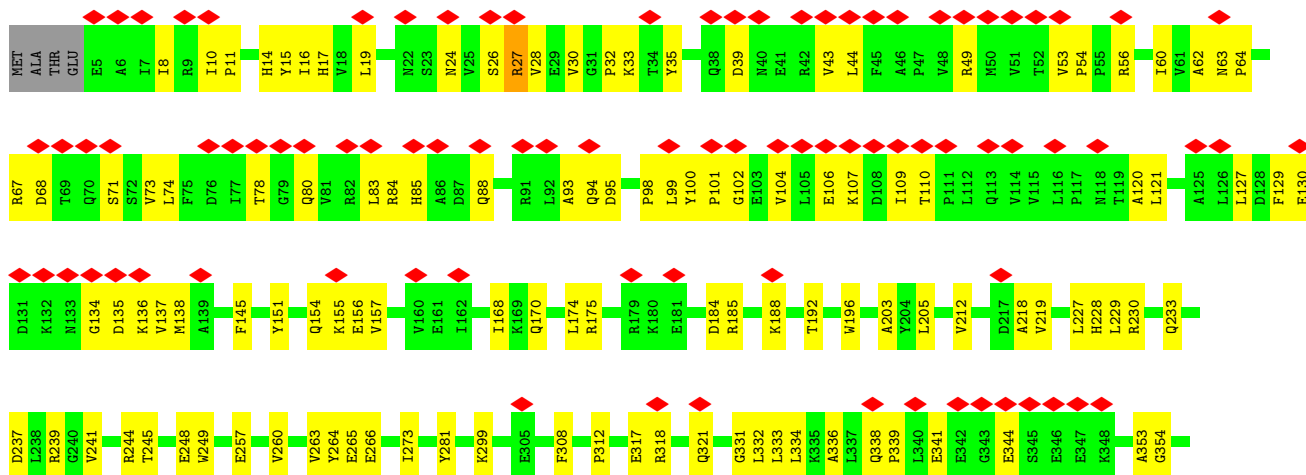


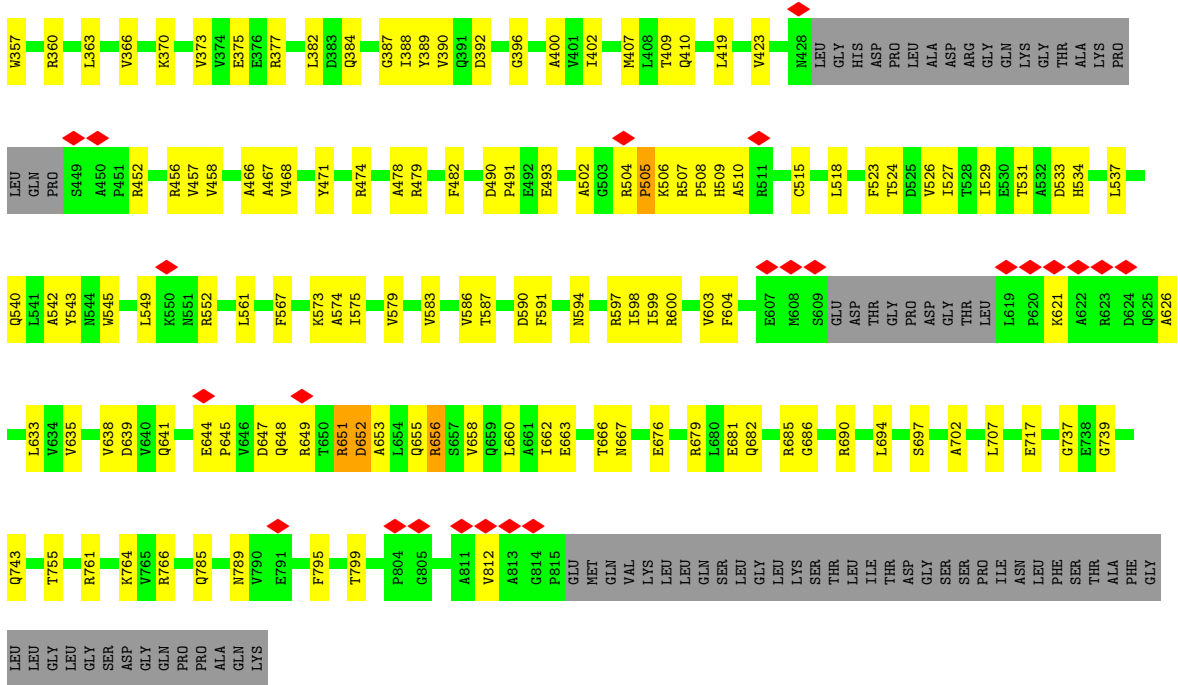
• Molecule 1: Major vault protein



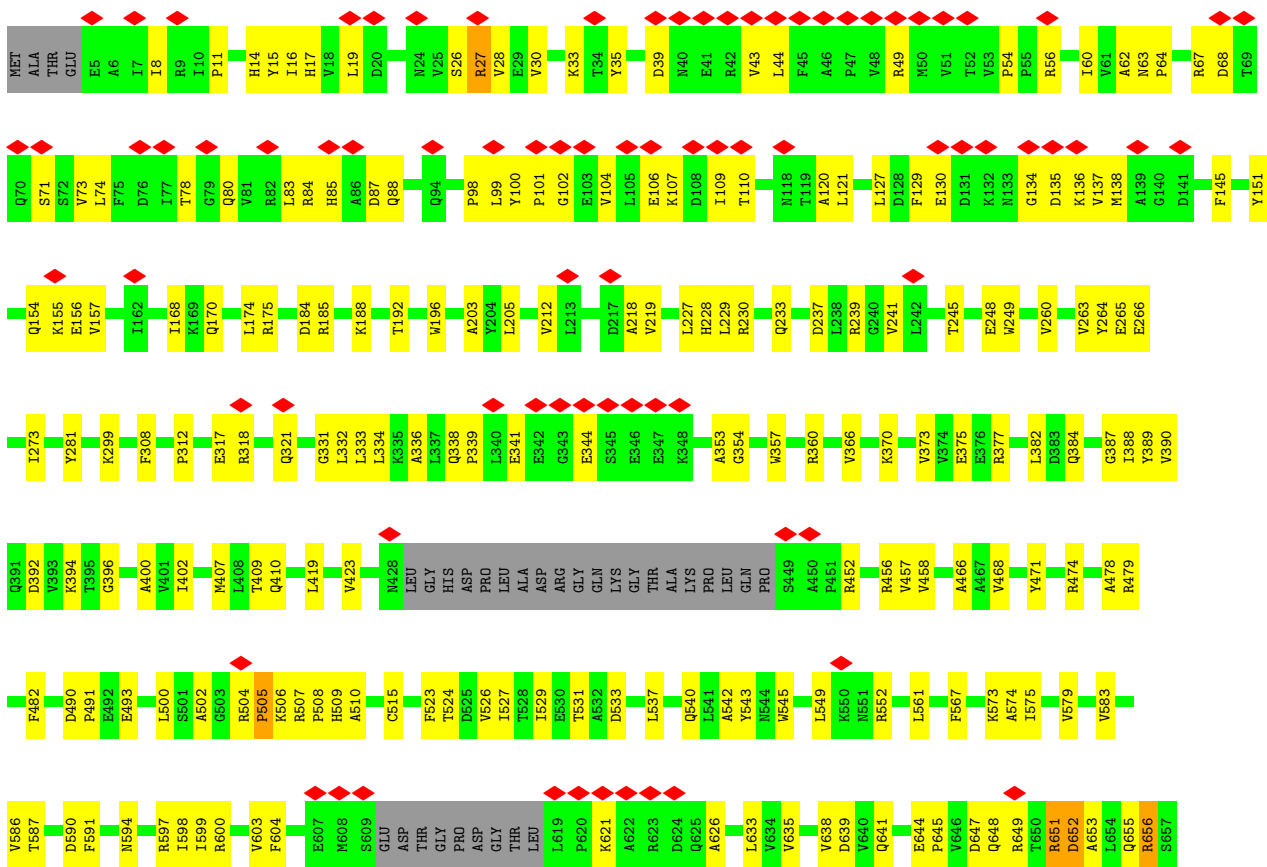


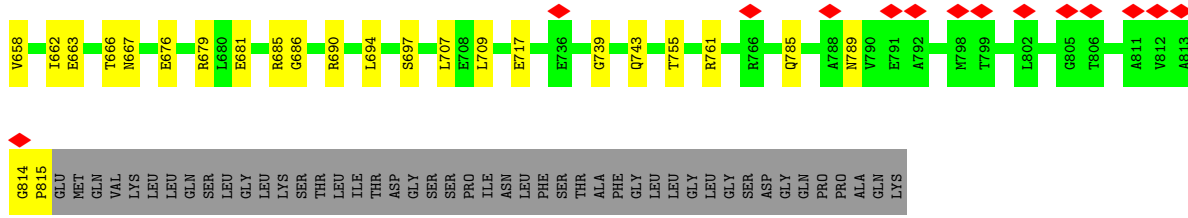
• Molecule 1: Major vault protein



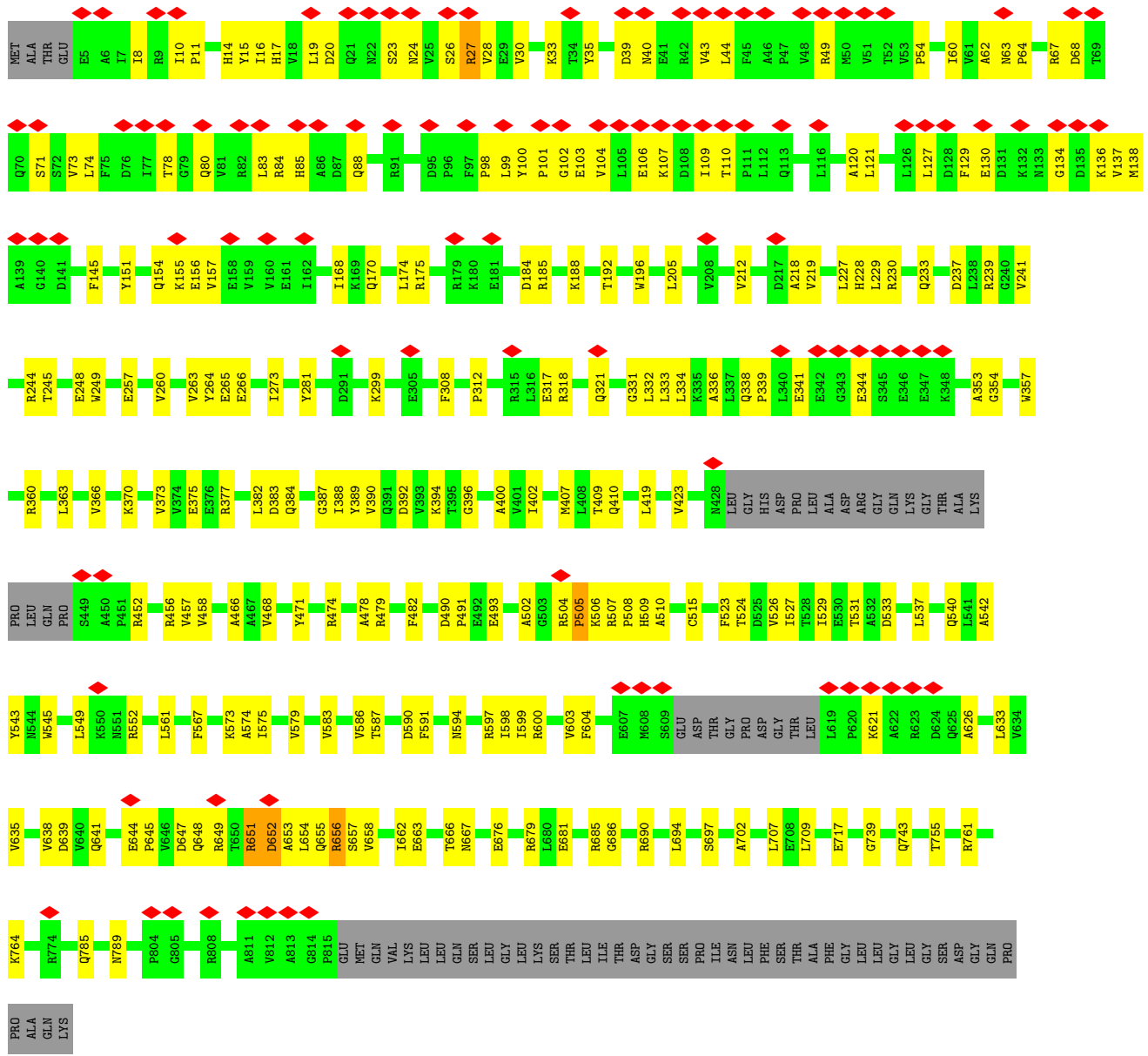


● Molecule 1: Major vault protein



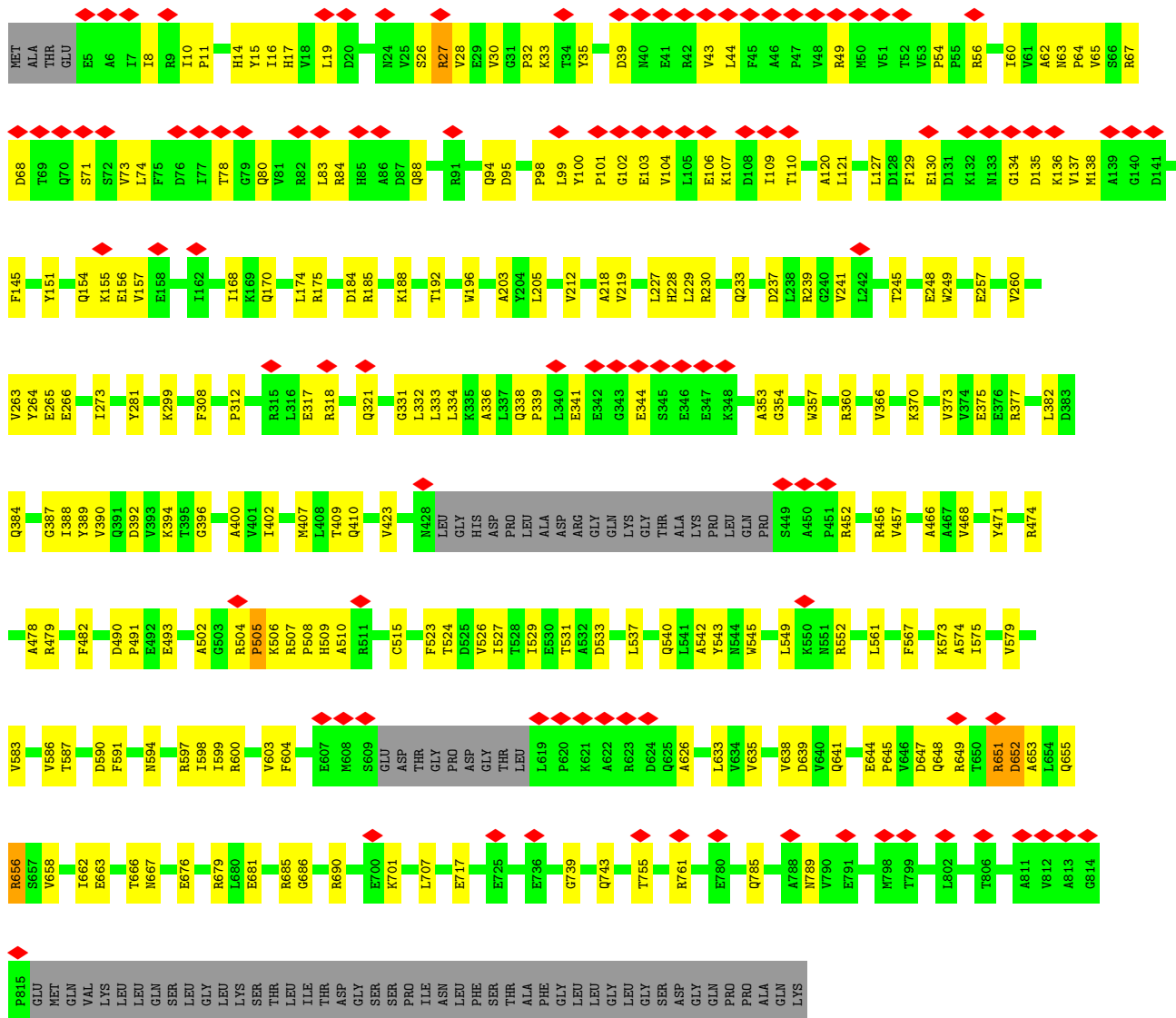


• Molecule 1: Major vault protein

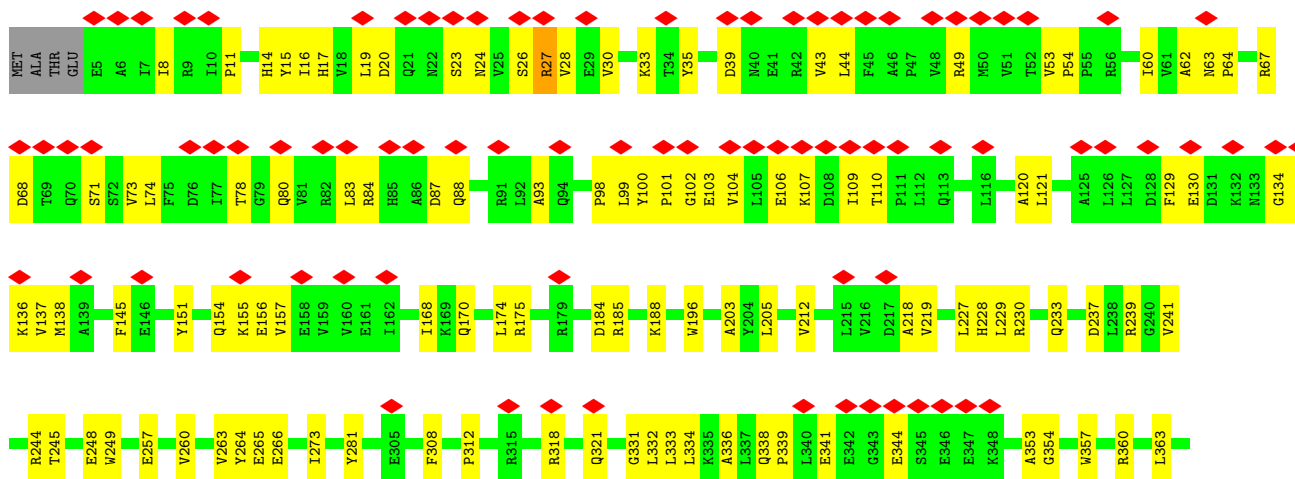


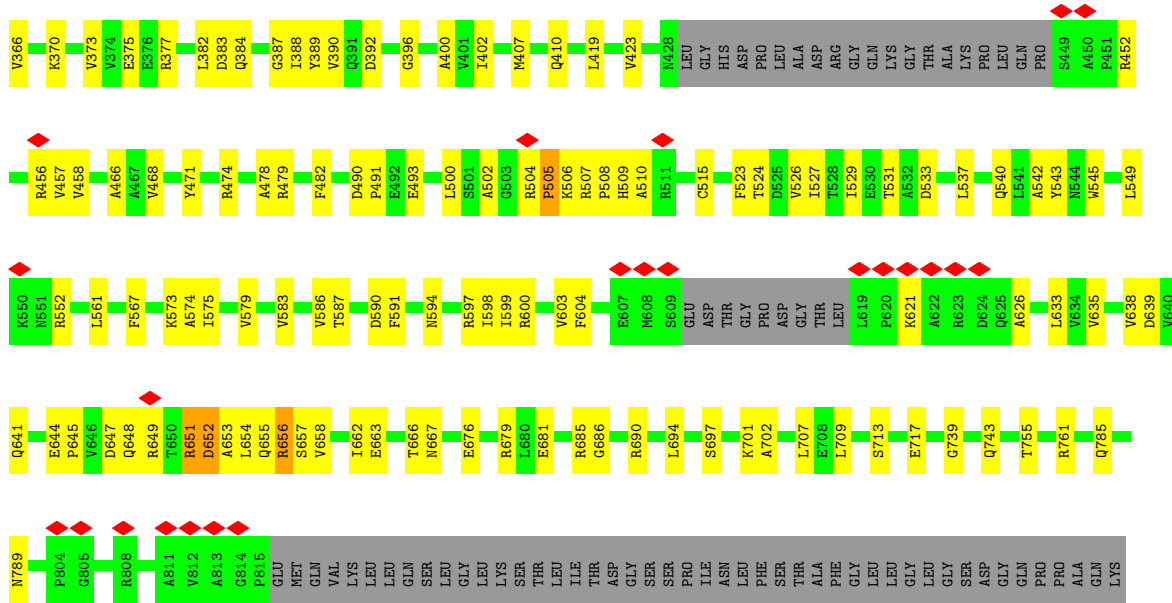
• Molecule 1: Major vault protein



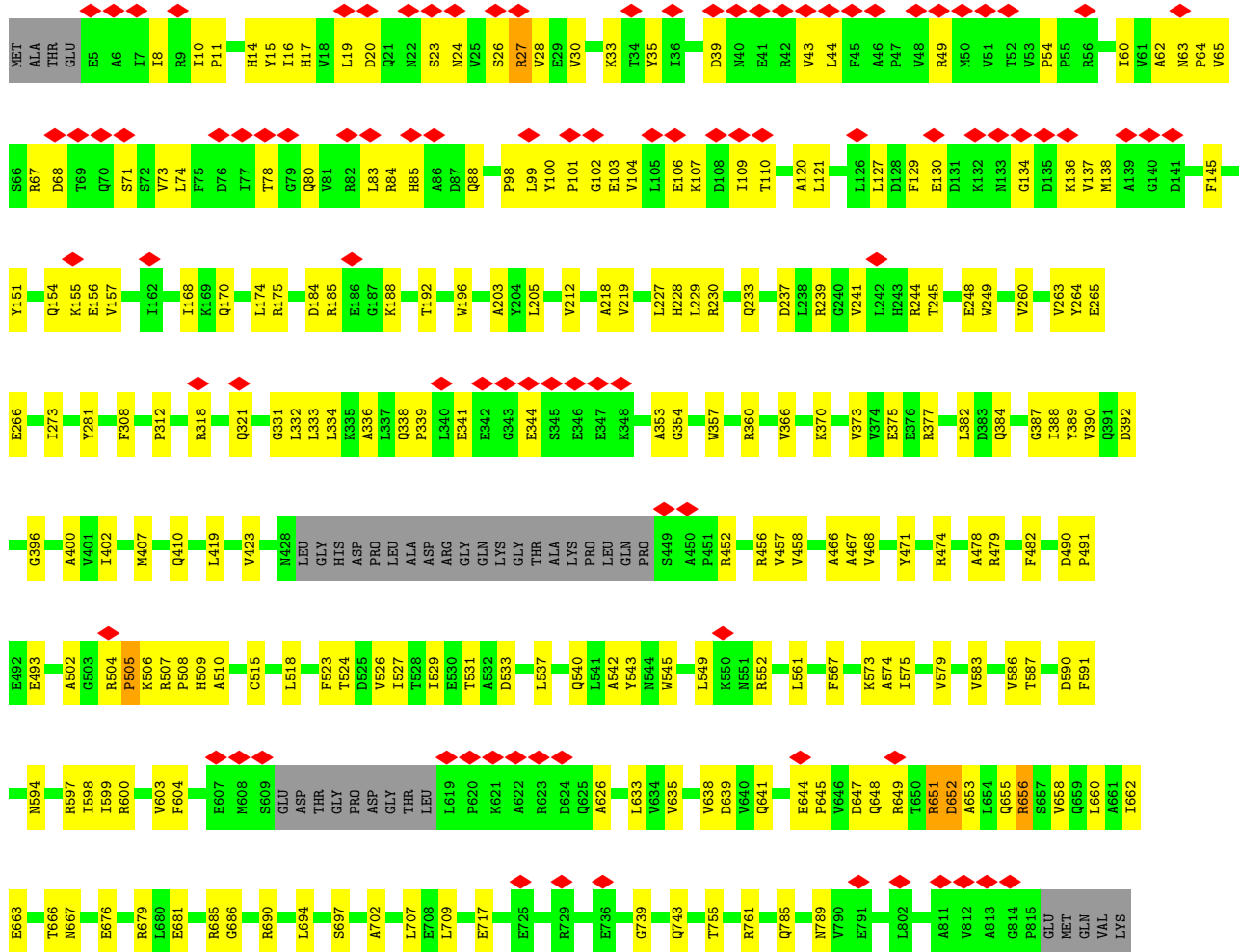


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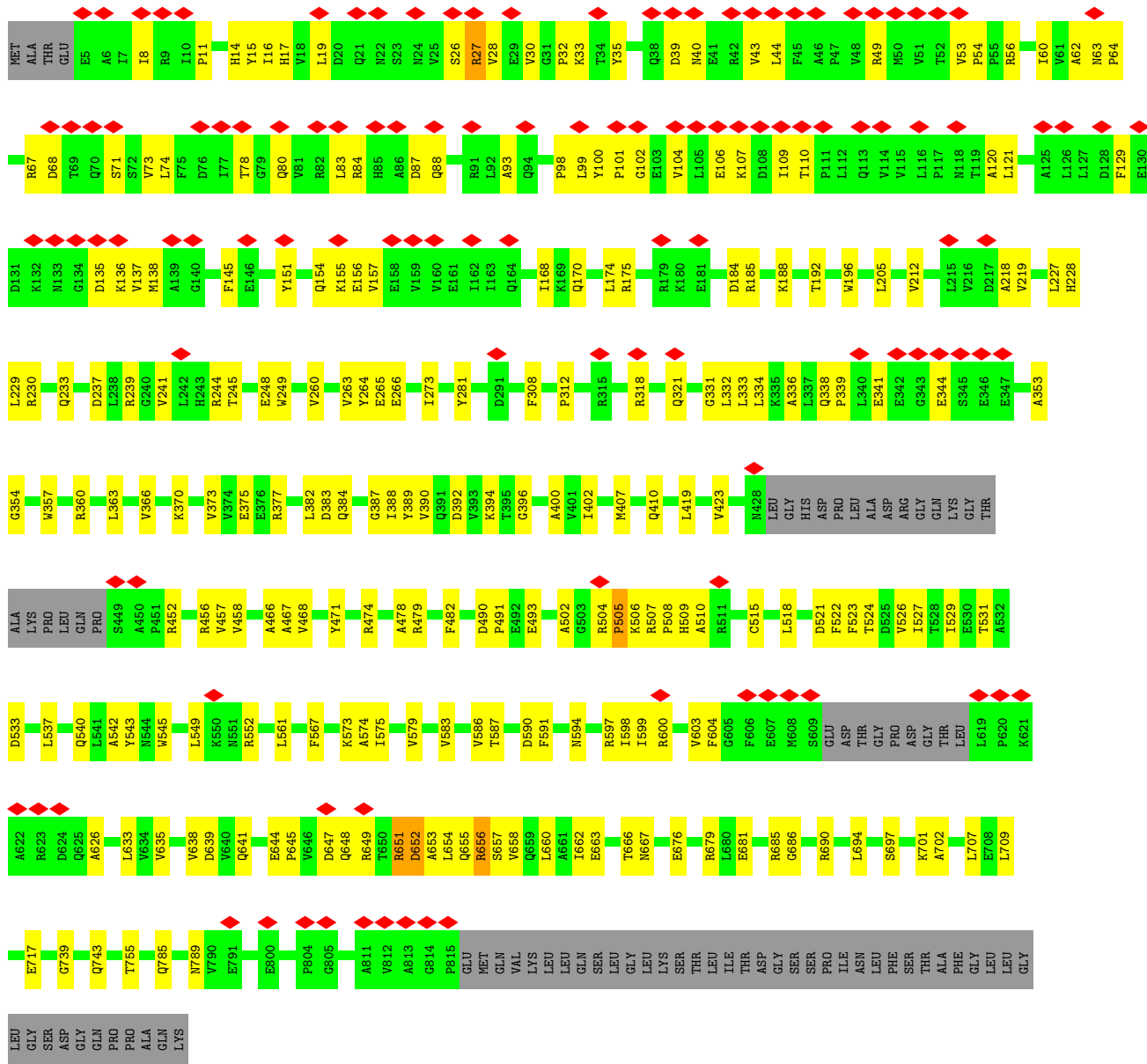


• Molecule 1: Major vault protein

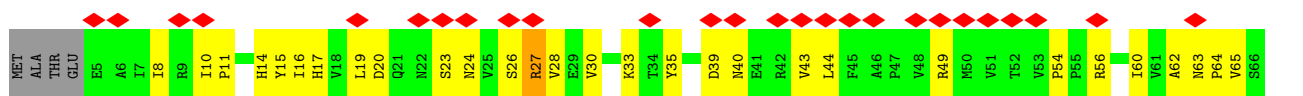


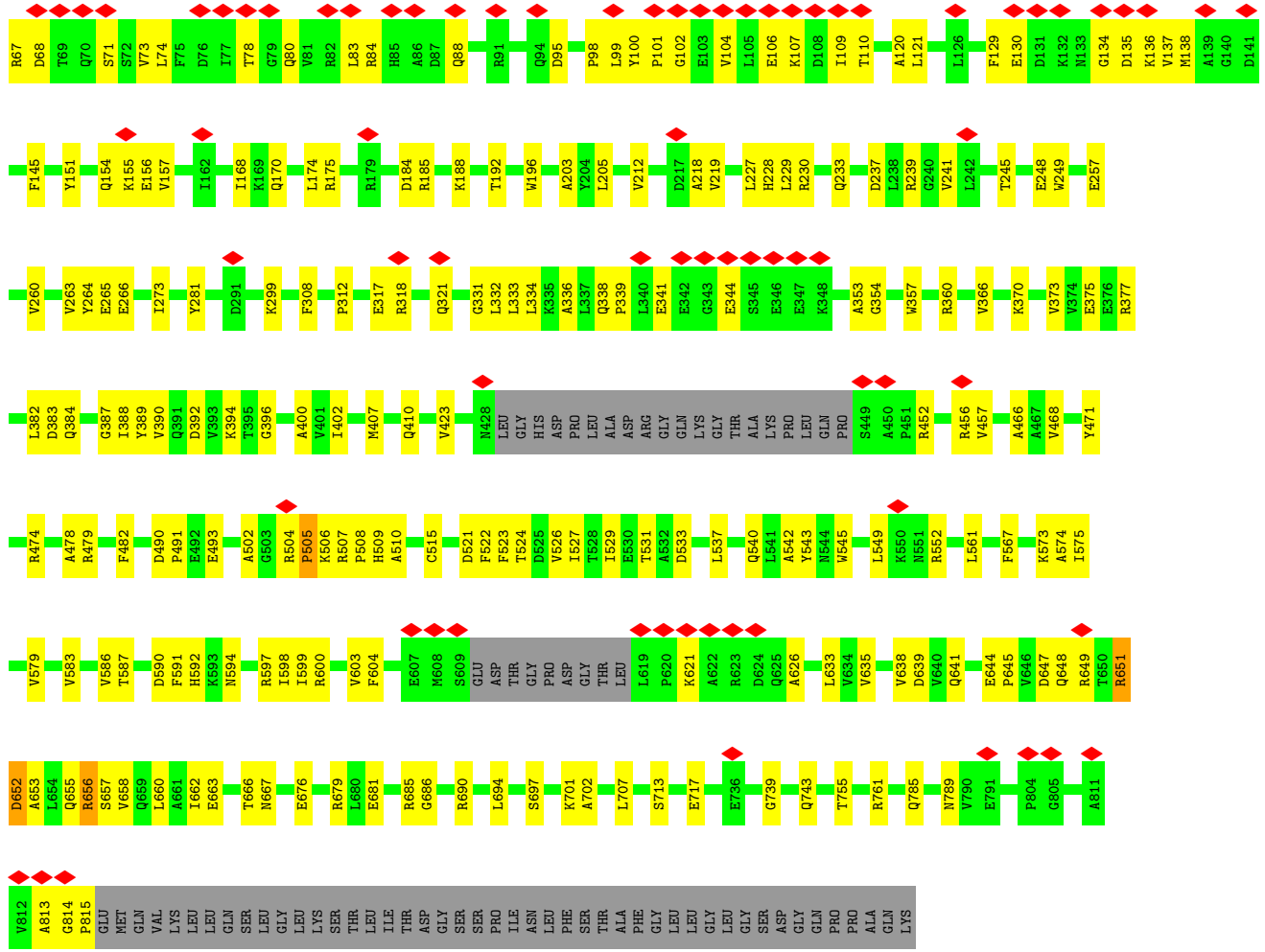
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• Molecule 1: Major vault protein

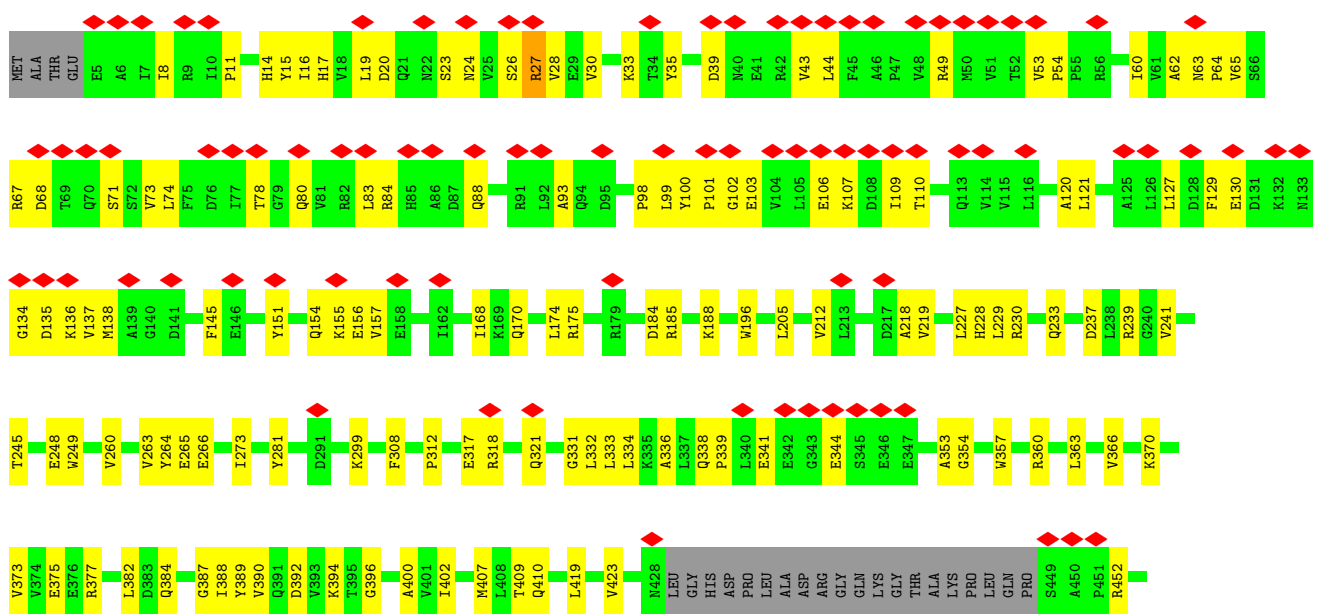


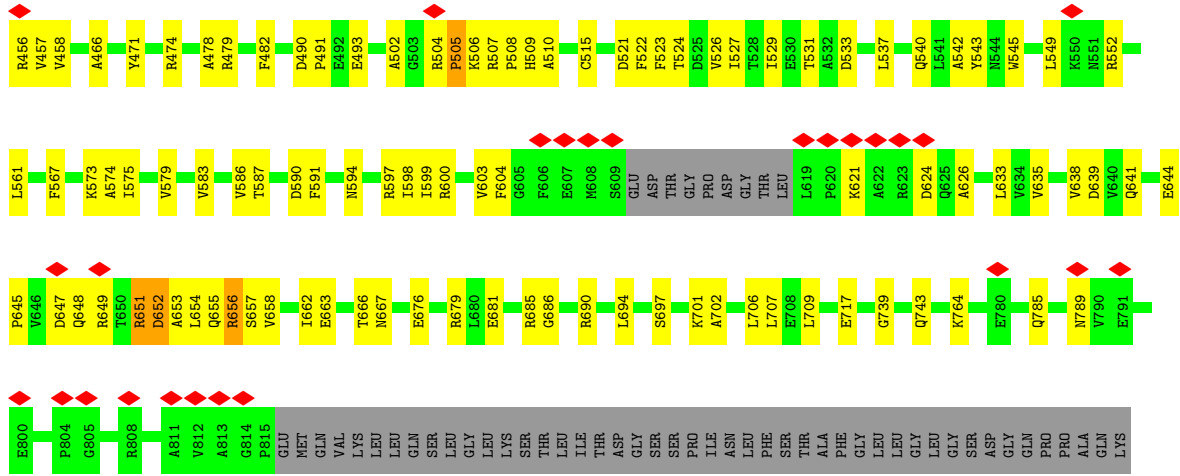
• Molecule 1: Major vault protein



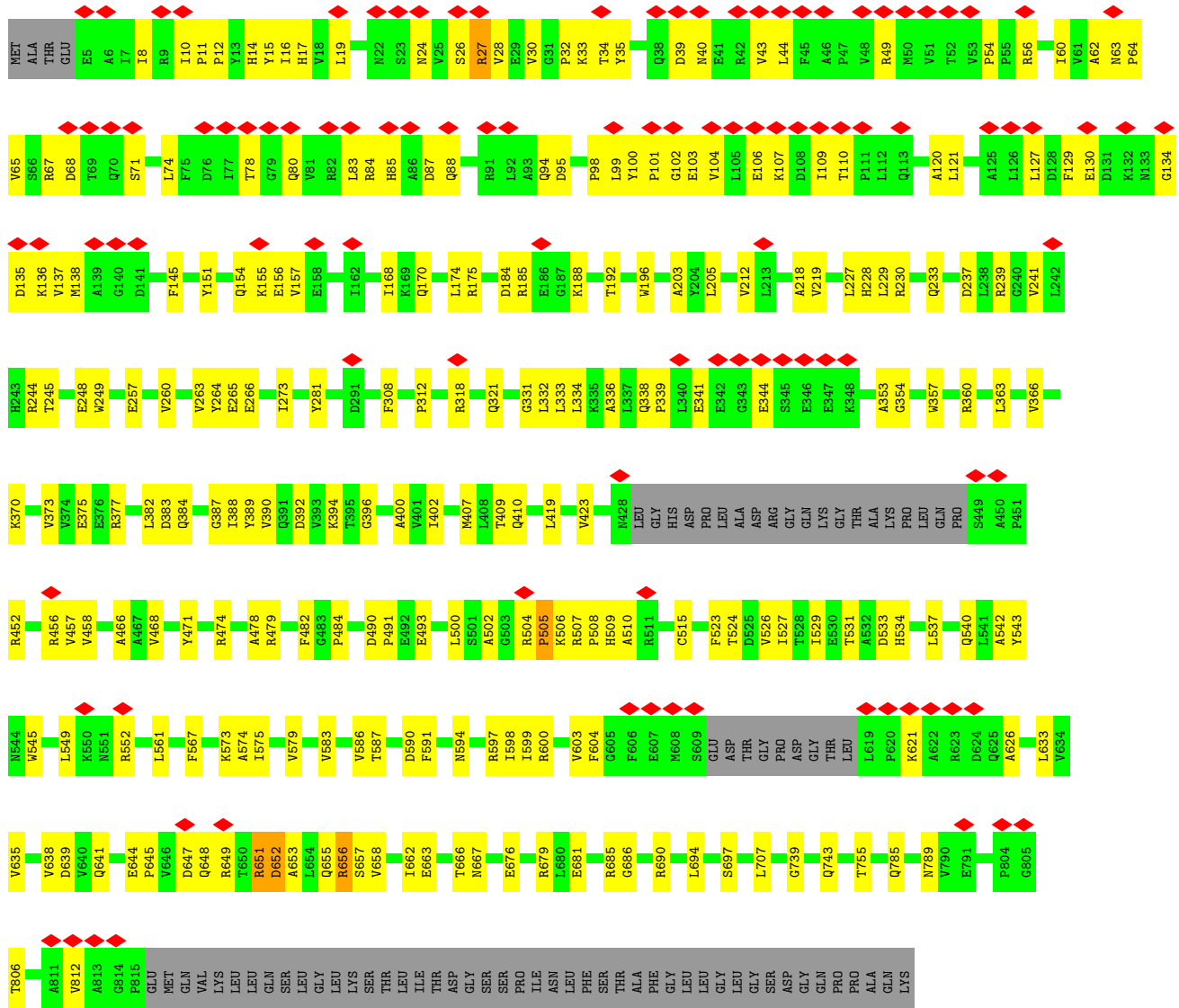


• Molecule 1: Major vault protein

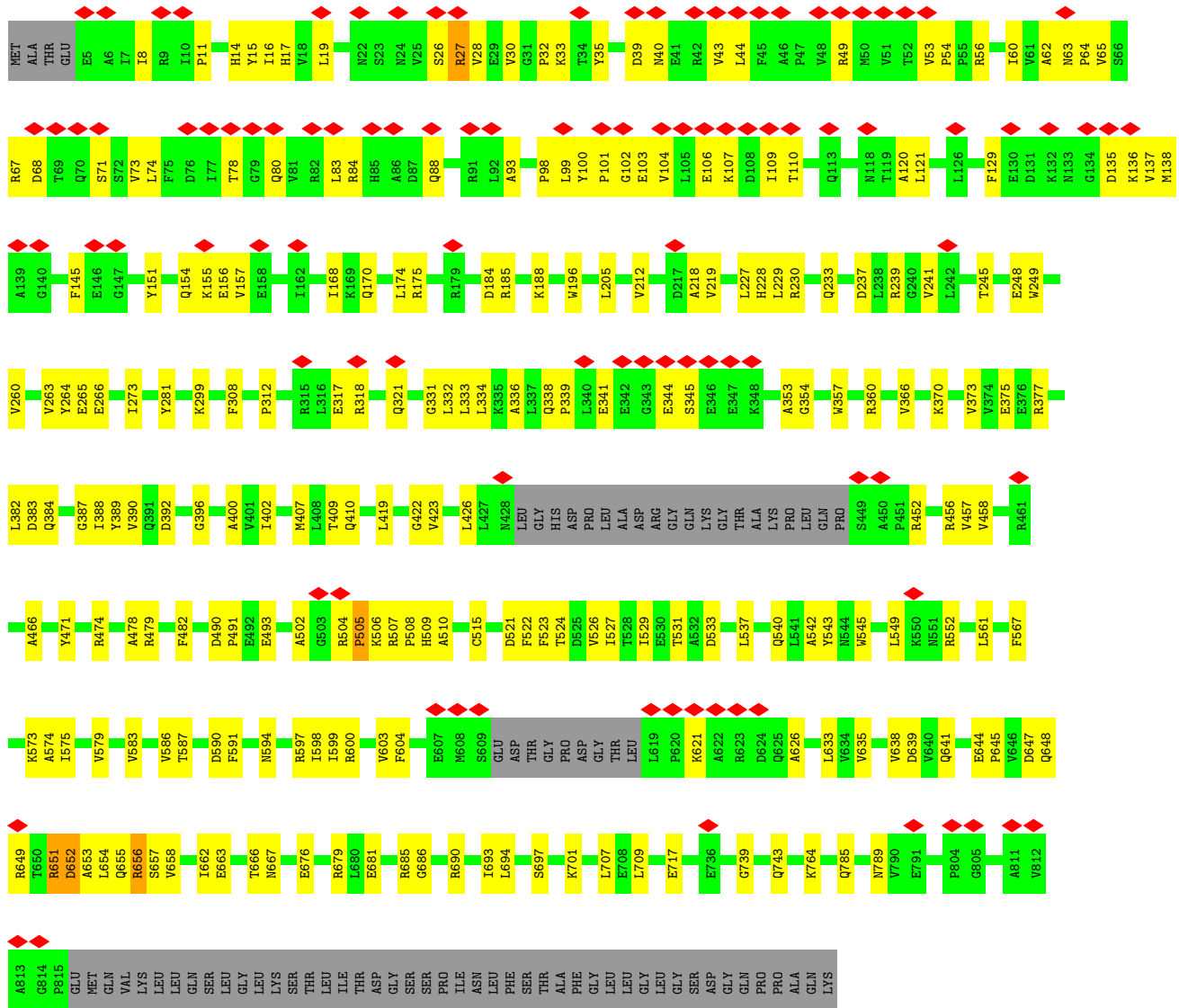




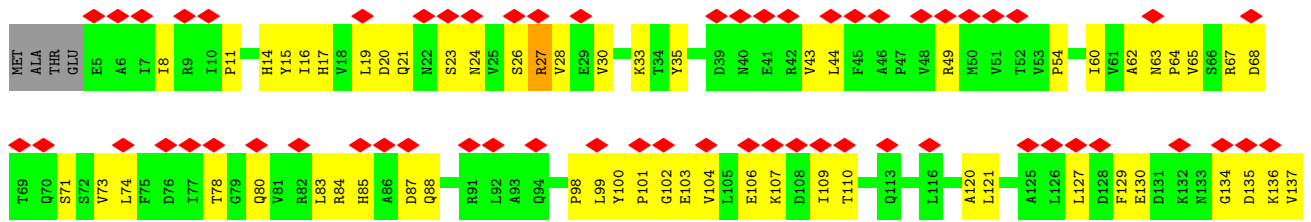
• Molecule 1: Major vault protein

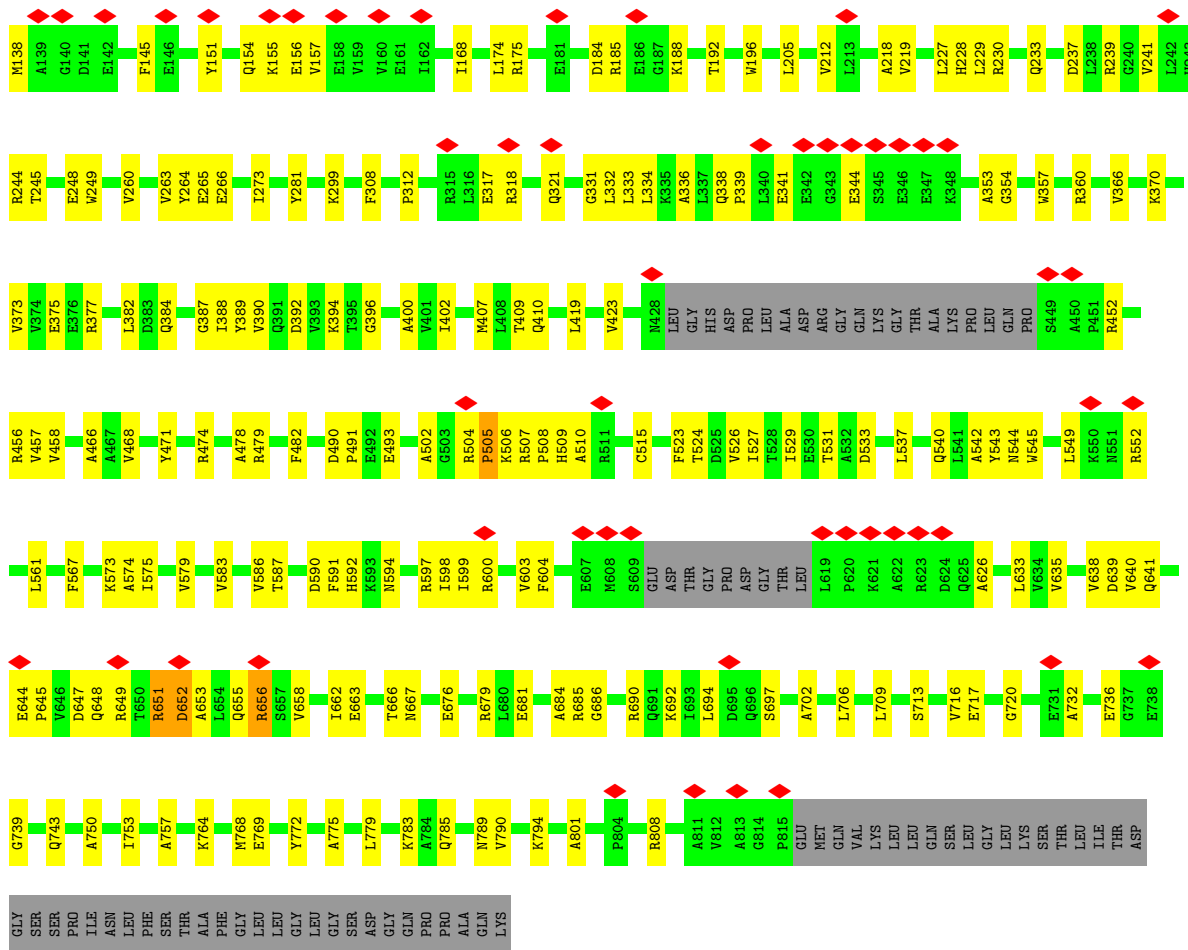


• Molecule 1: Major vault protein

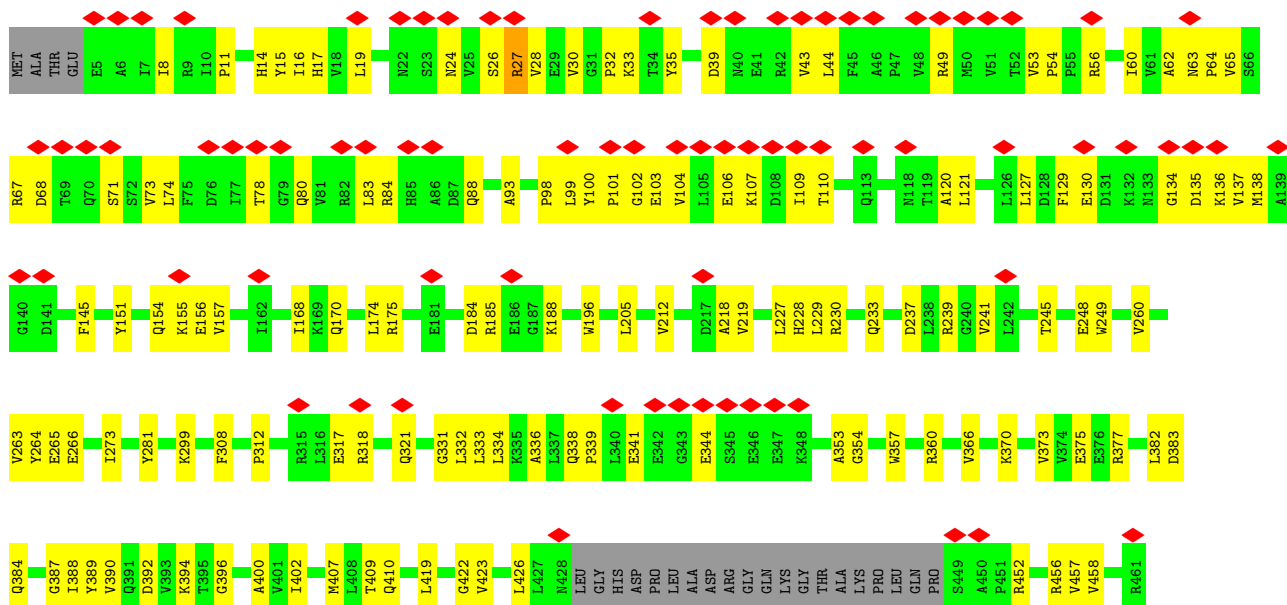


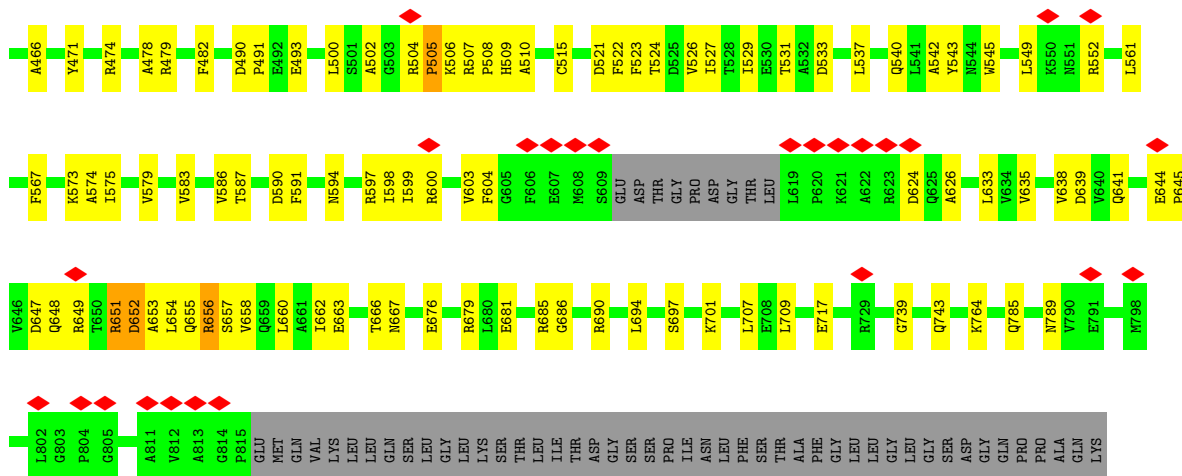
• Molecule 1: Major vault protein



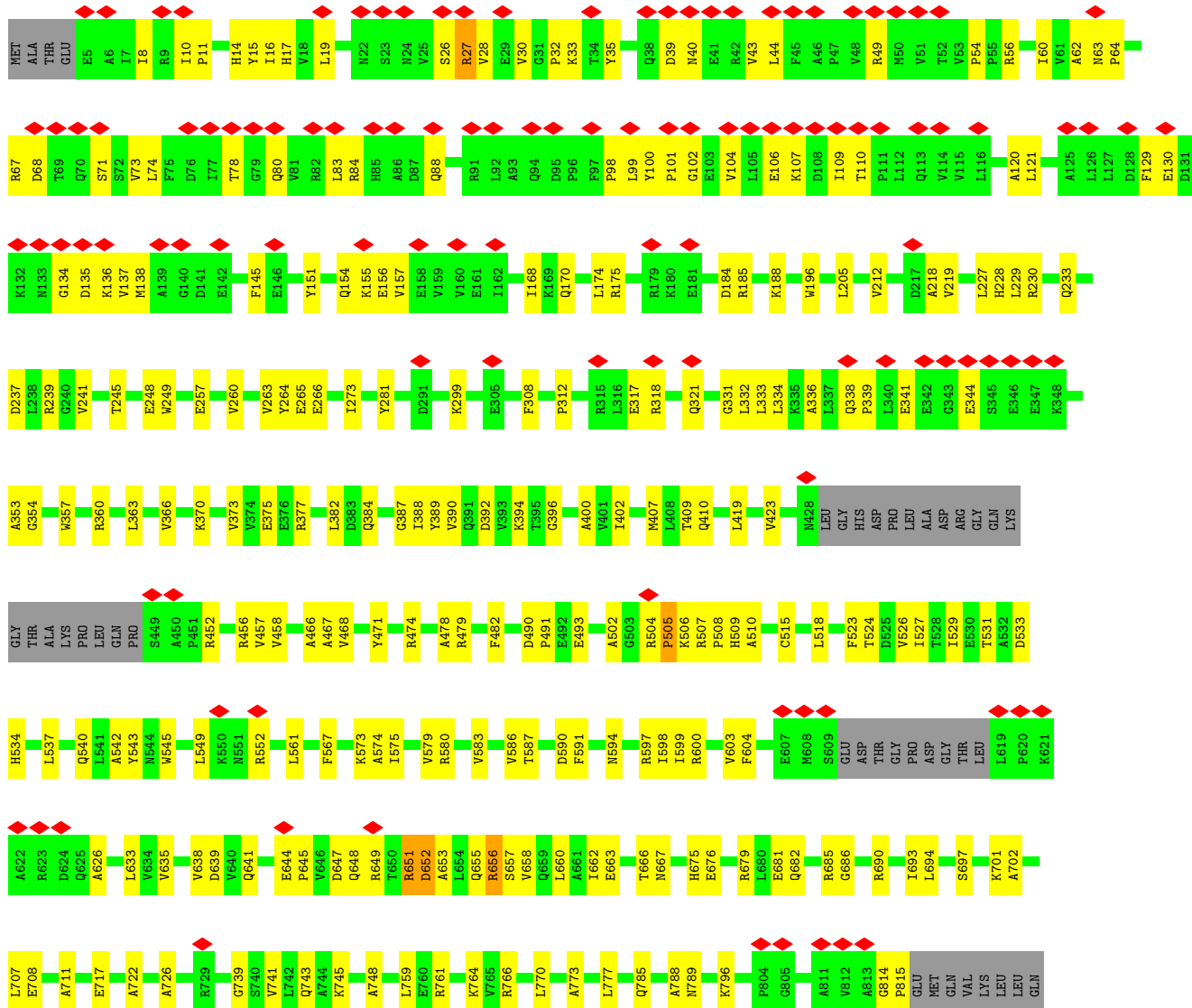


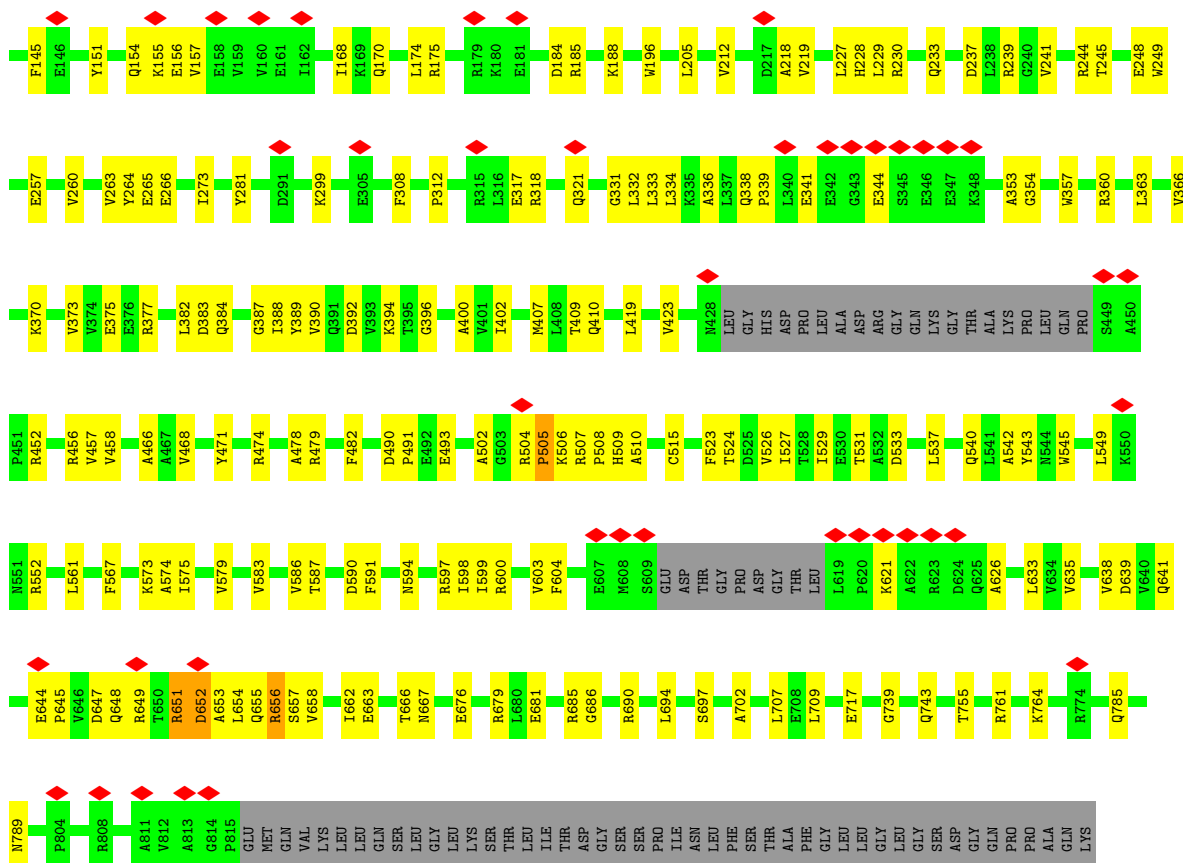
• Molecule 1: Major vault protein



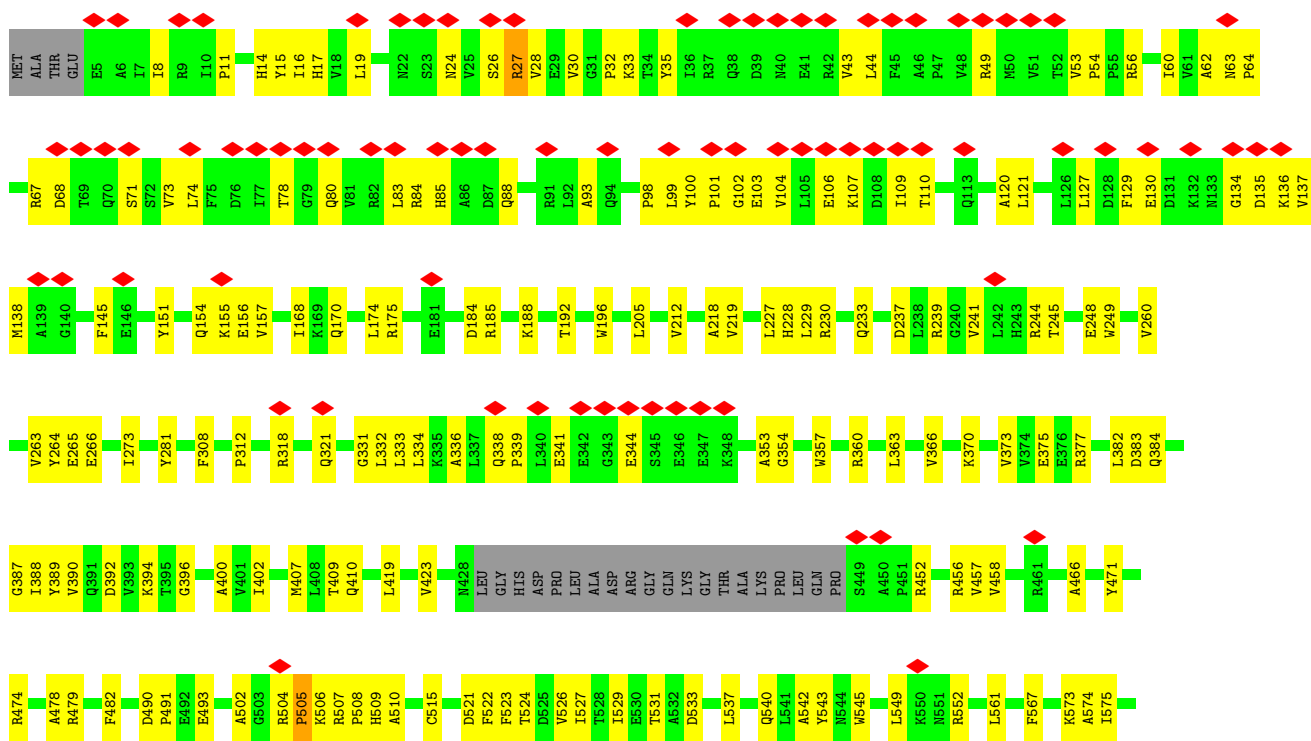


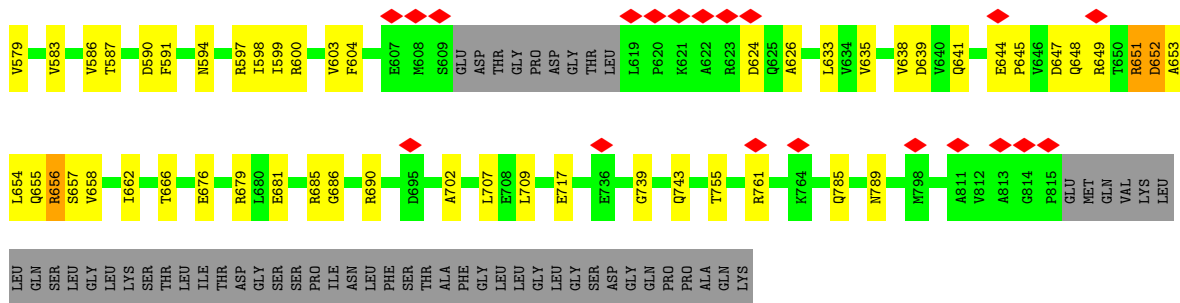
• Molecule 1: Major vault protein



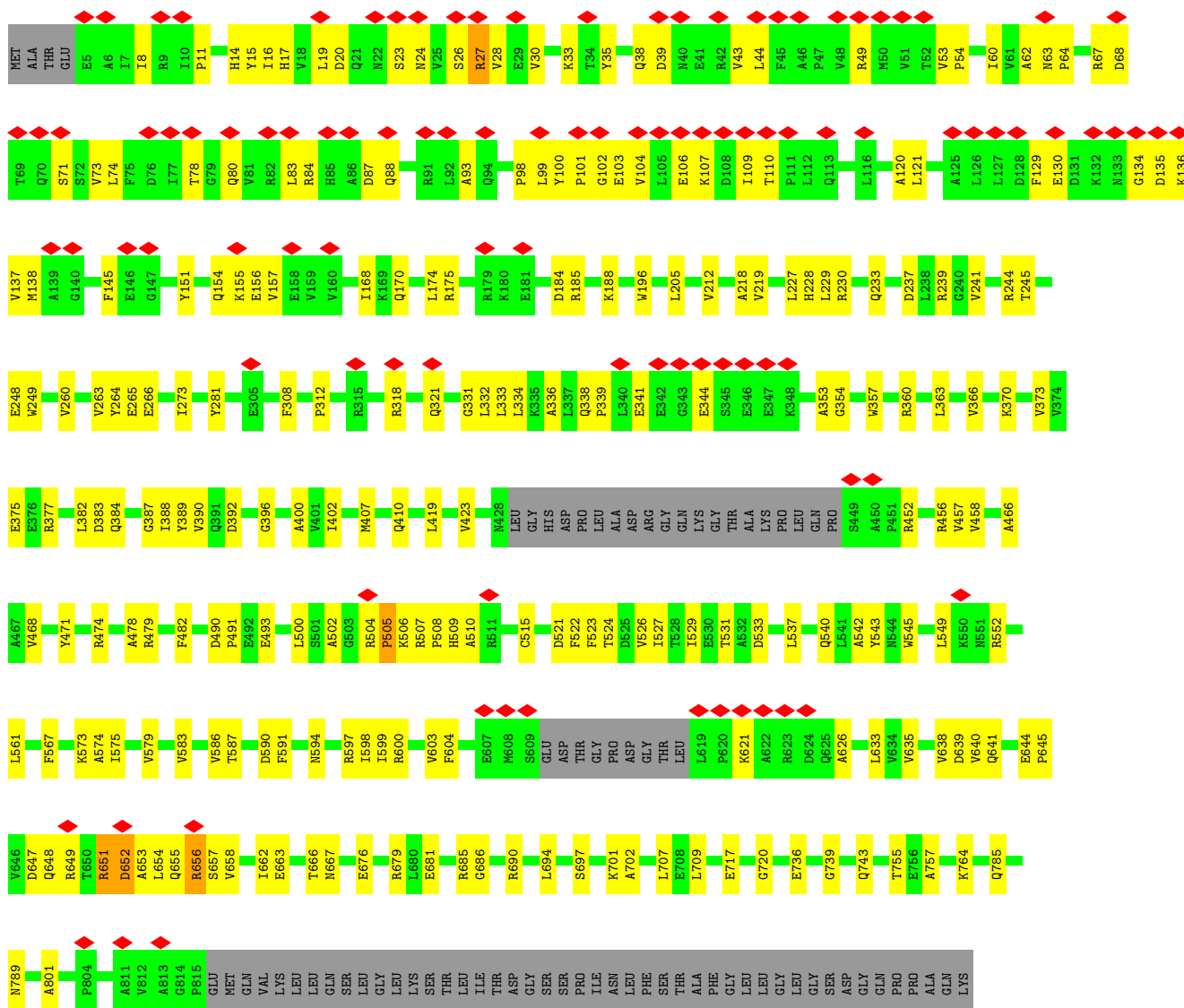


• Molecule 1: Major vault protein



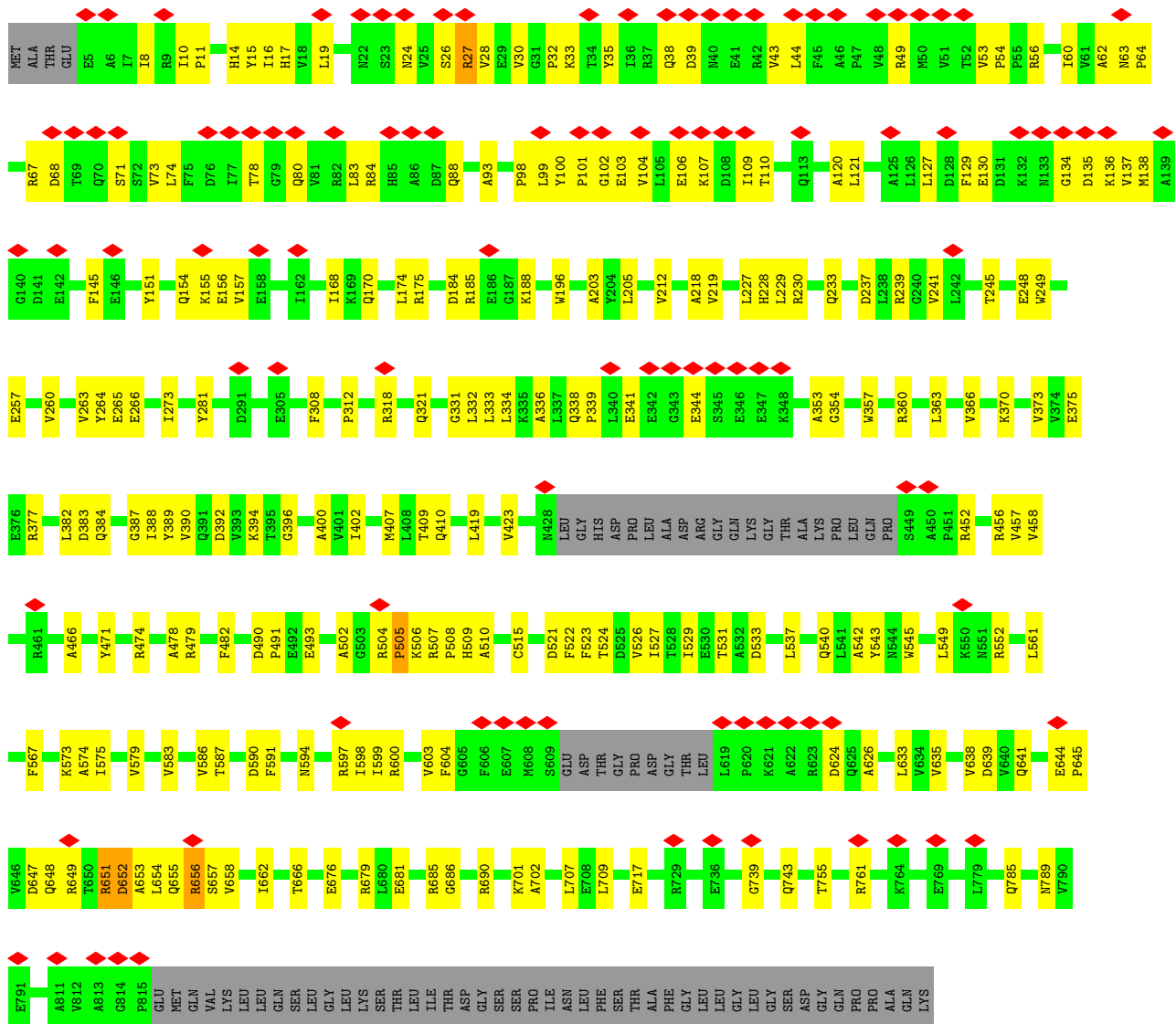


• Molecule 1: Major vault protein

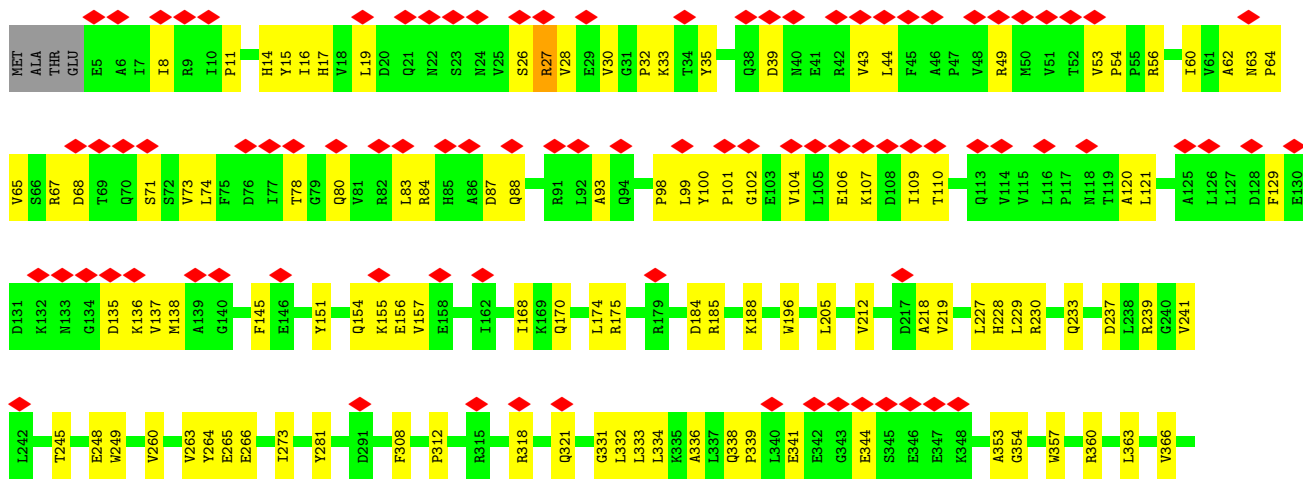


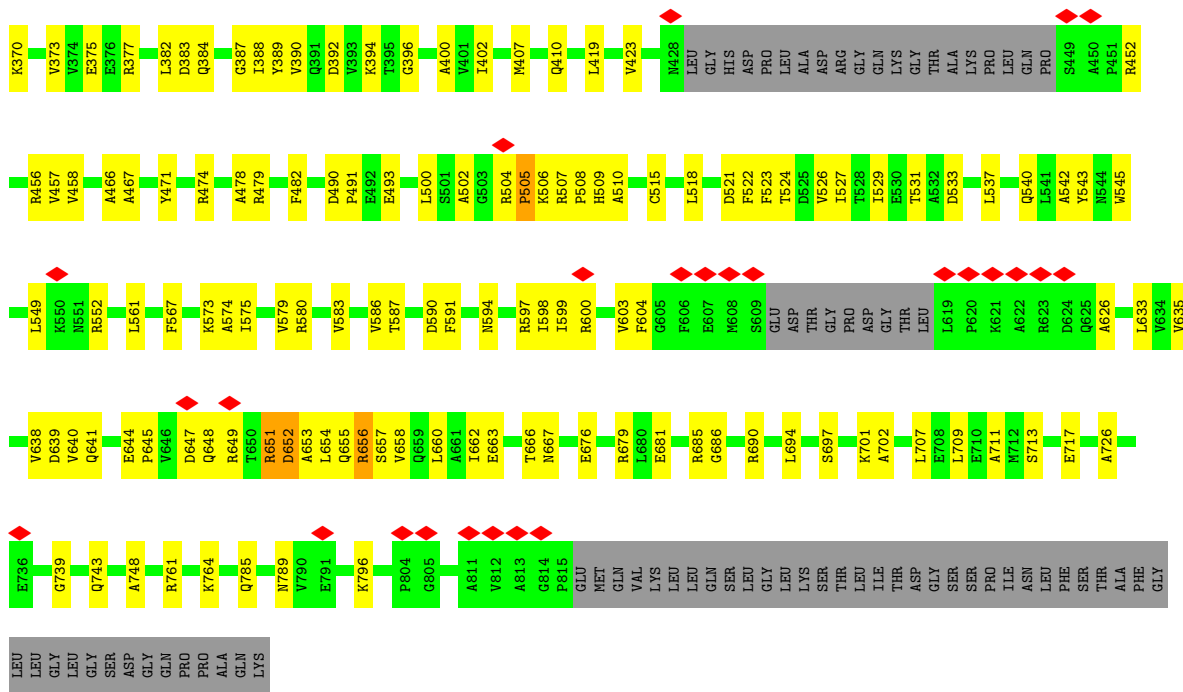
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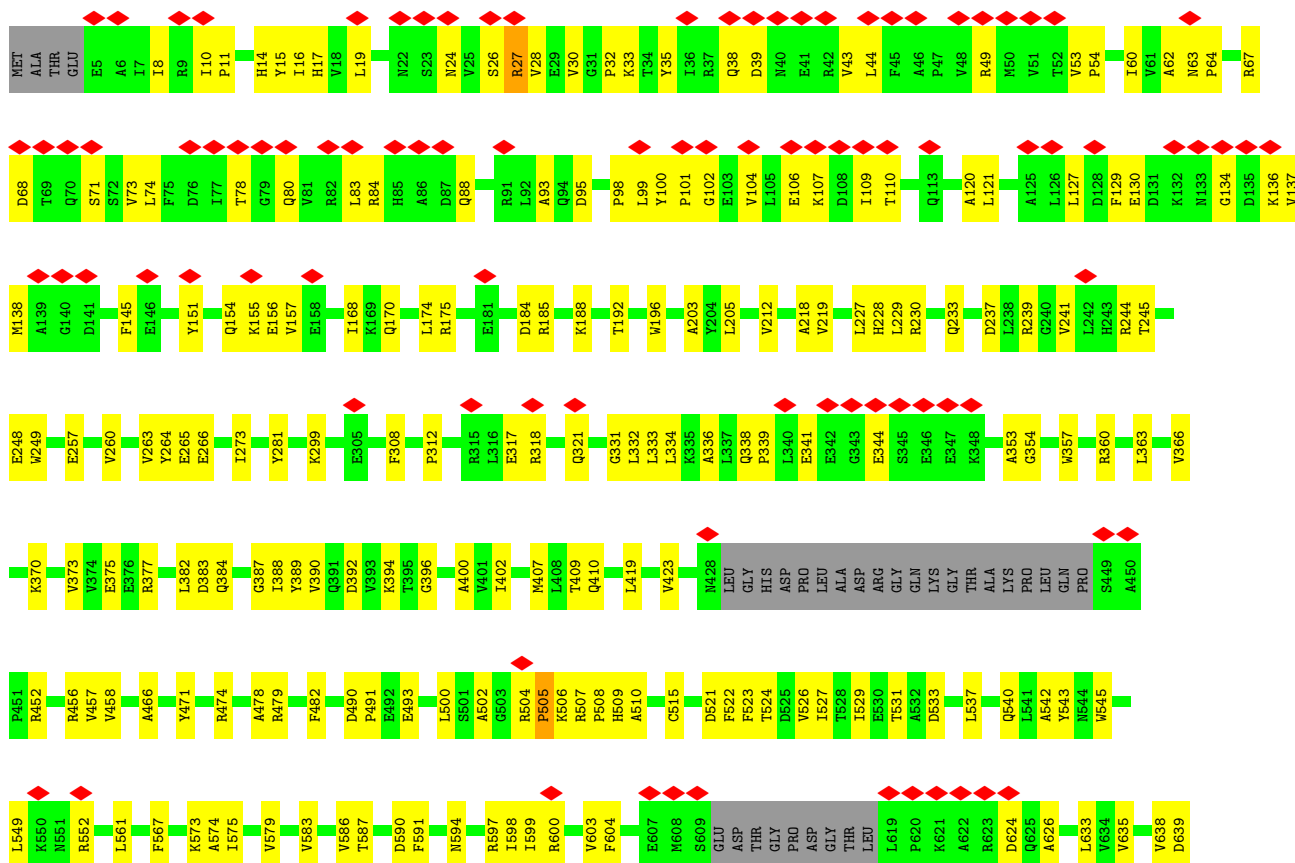


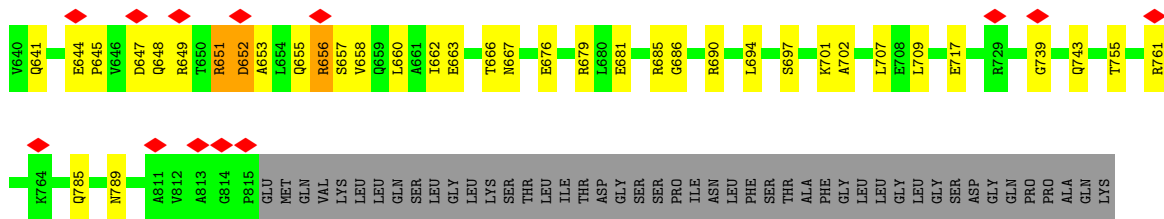
• Molecule 1: Major vault protein



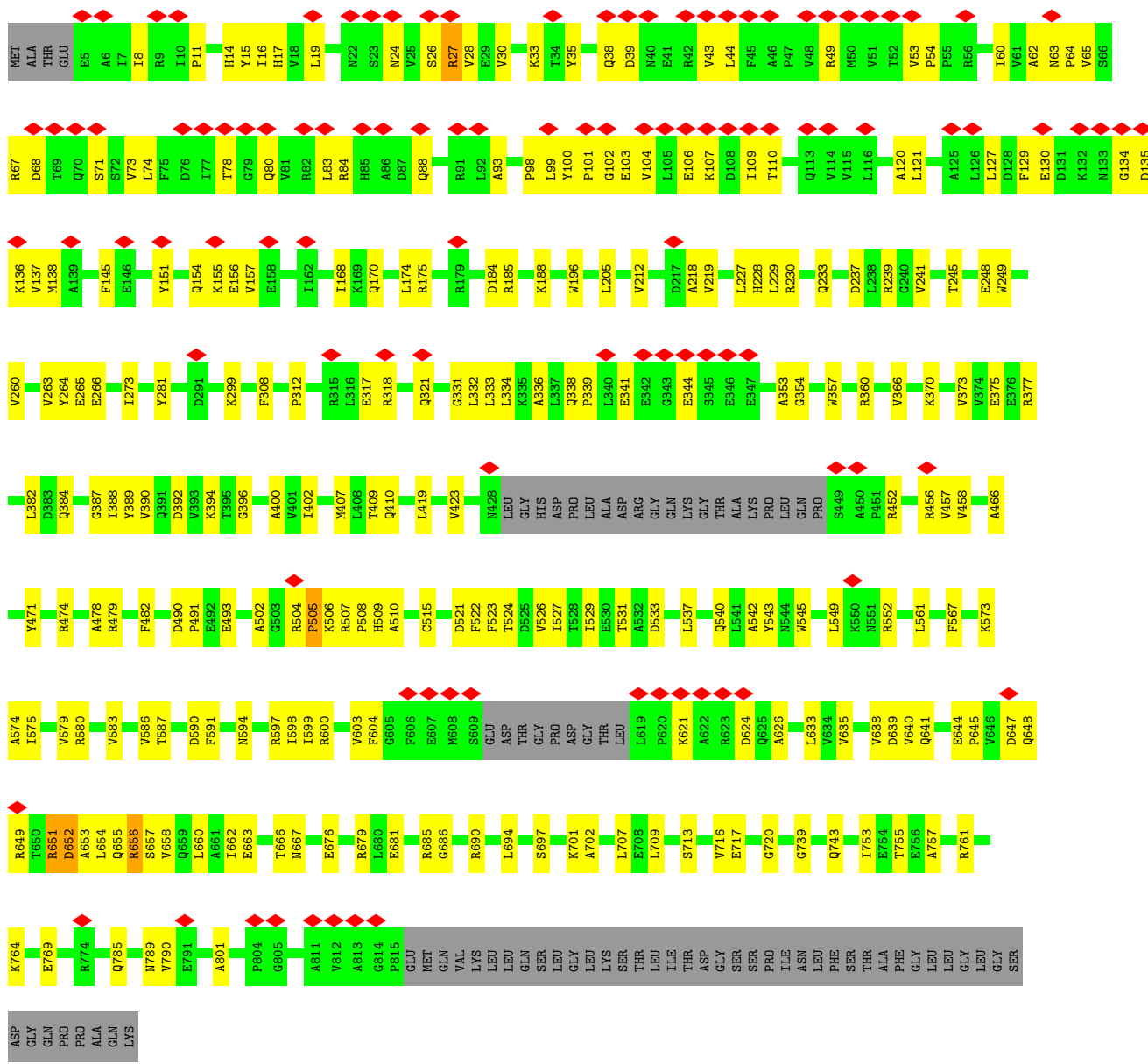


• Molecule 1: Major vault protein



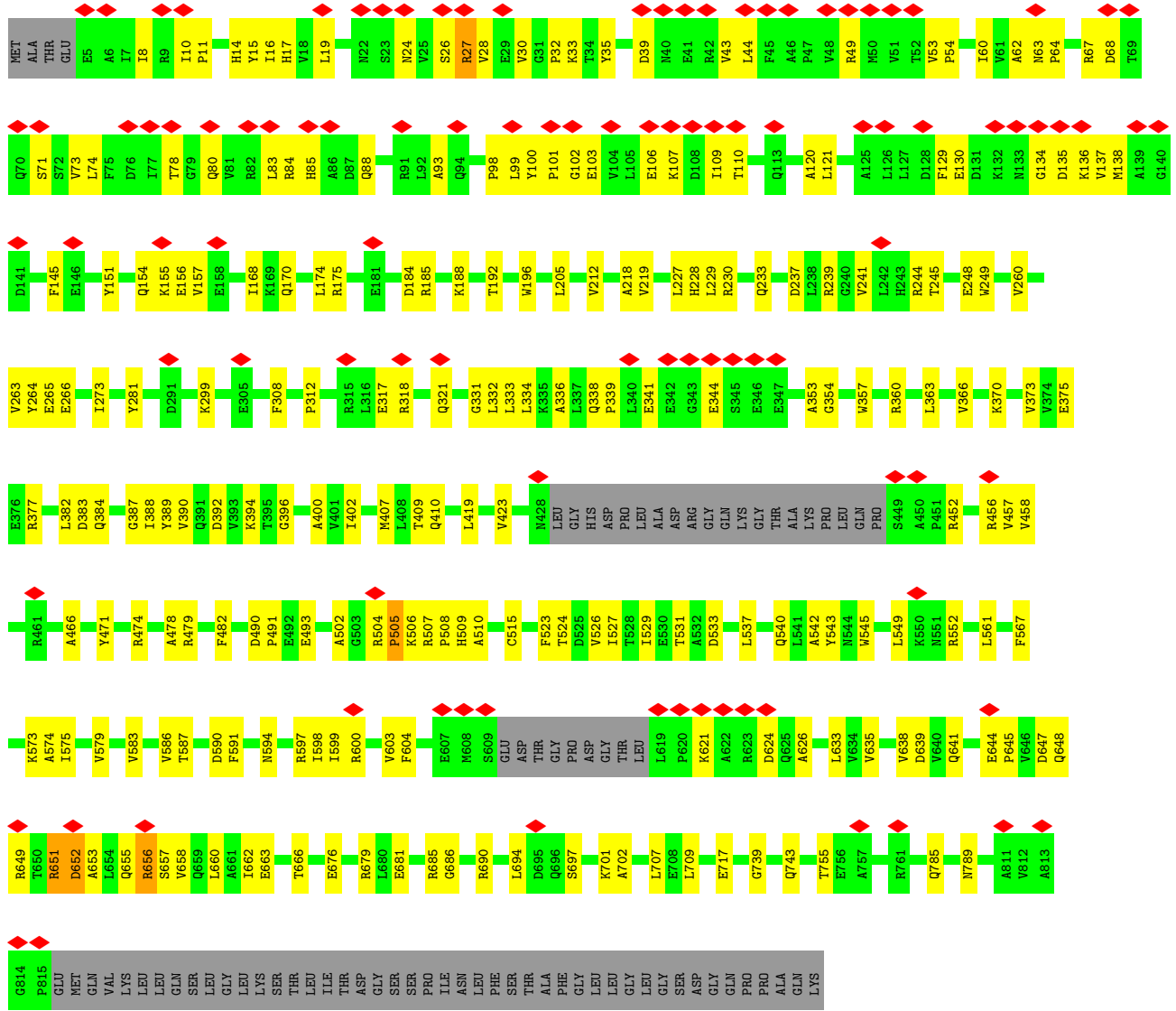


• Molecule 1: Major vault protein

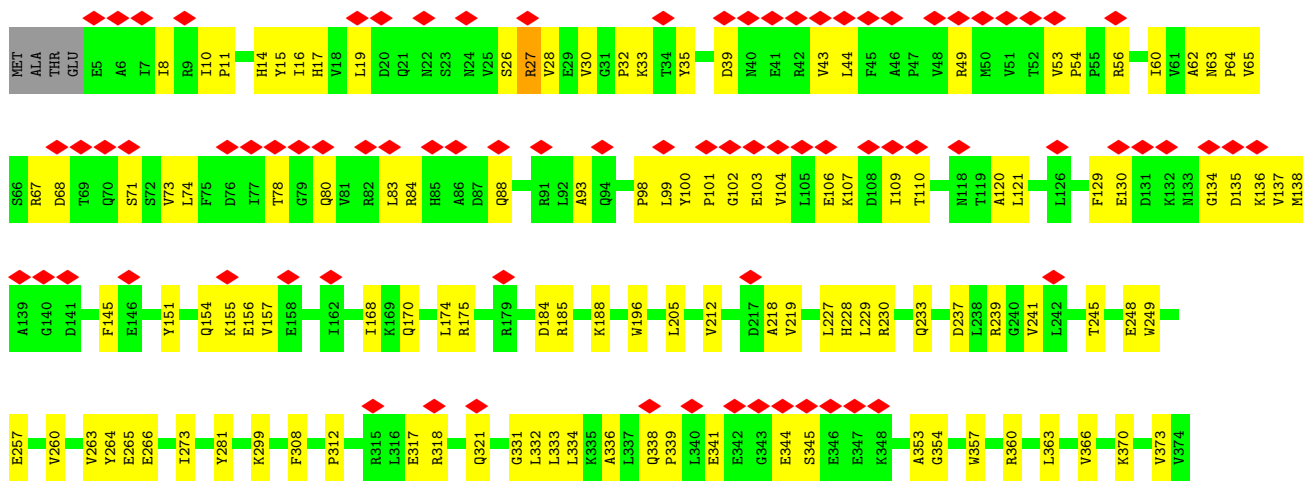


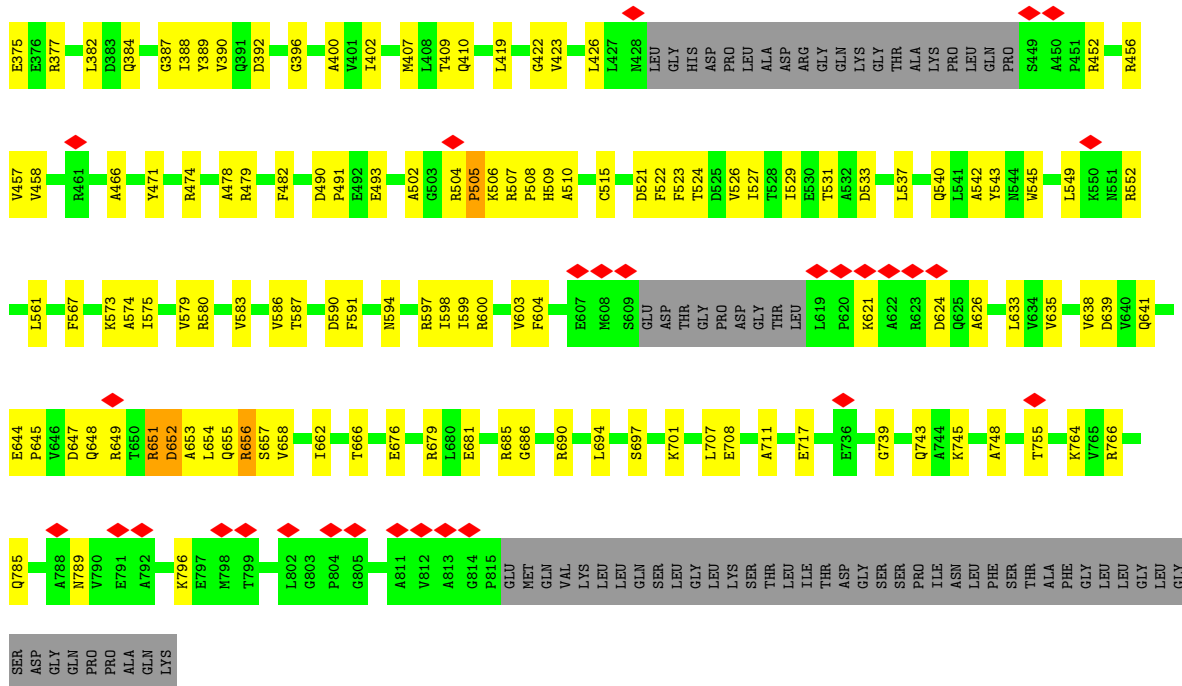
• Molecule 1: Major vault protein



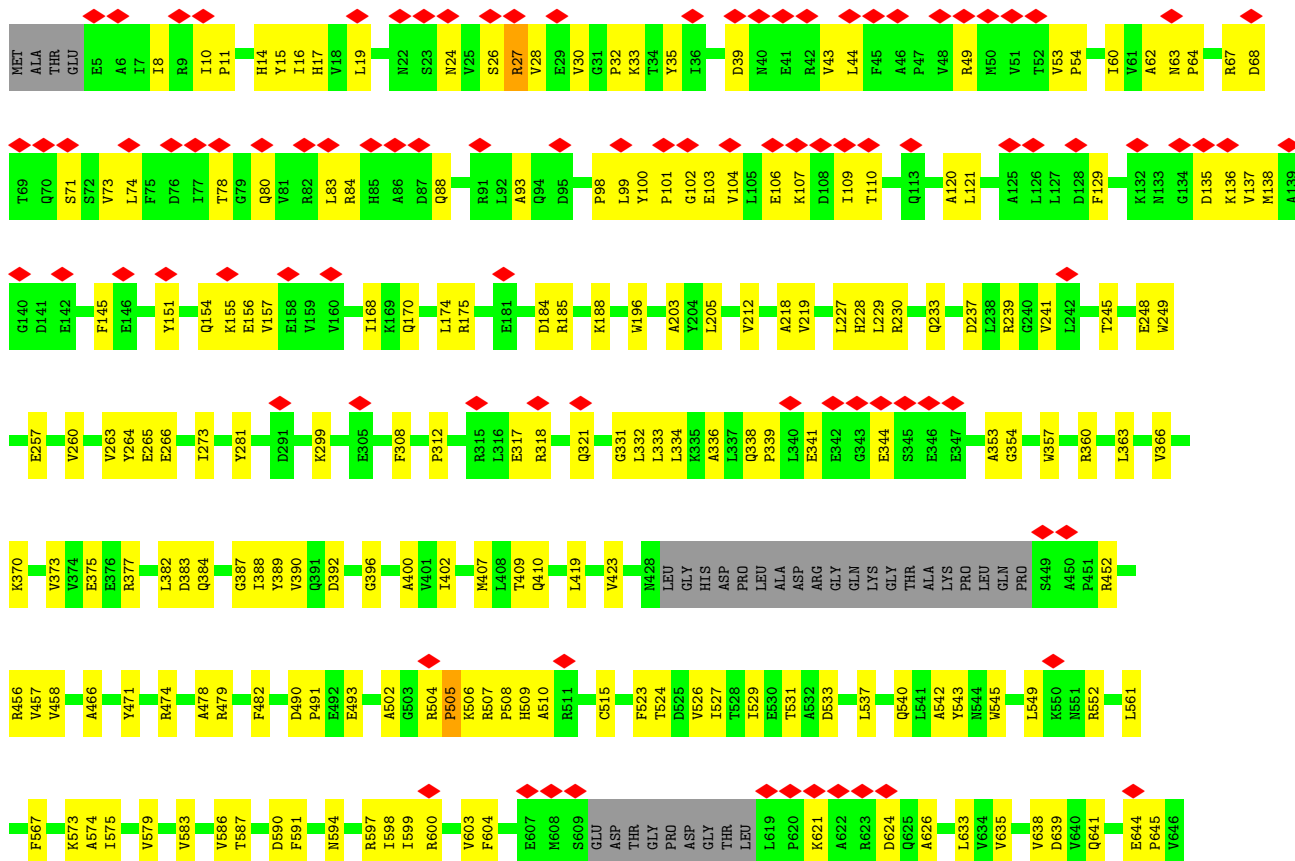


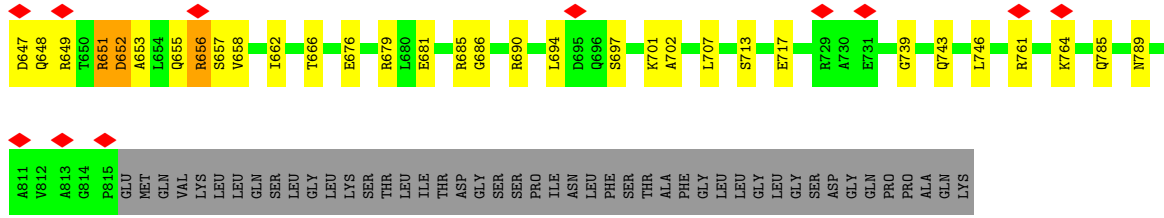
• Molecule 1: Major vault protein



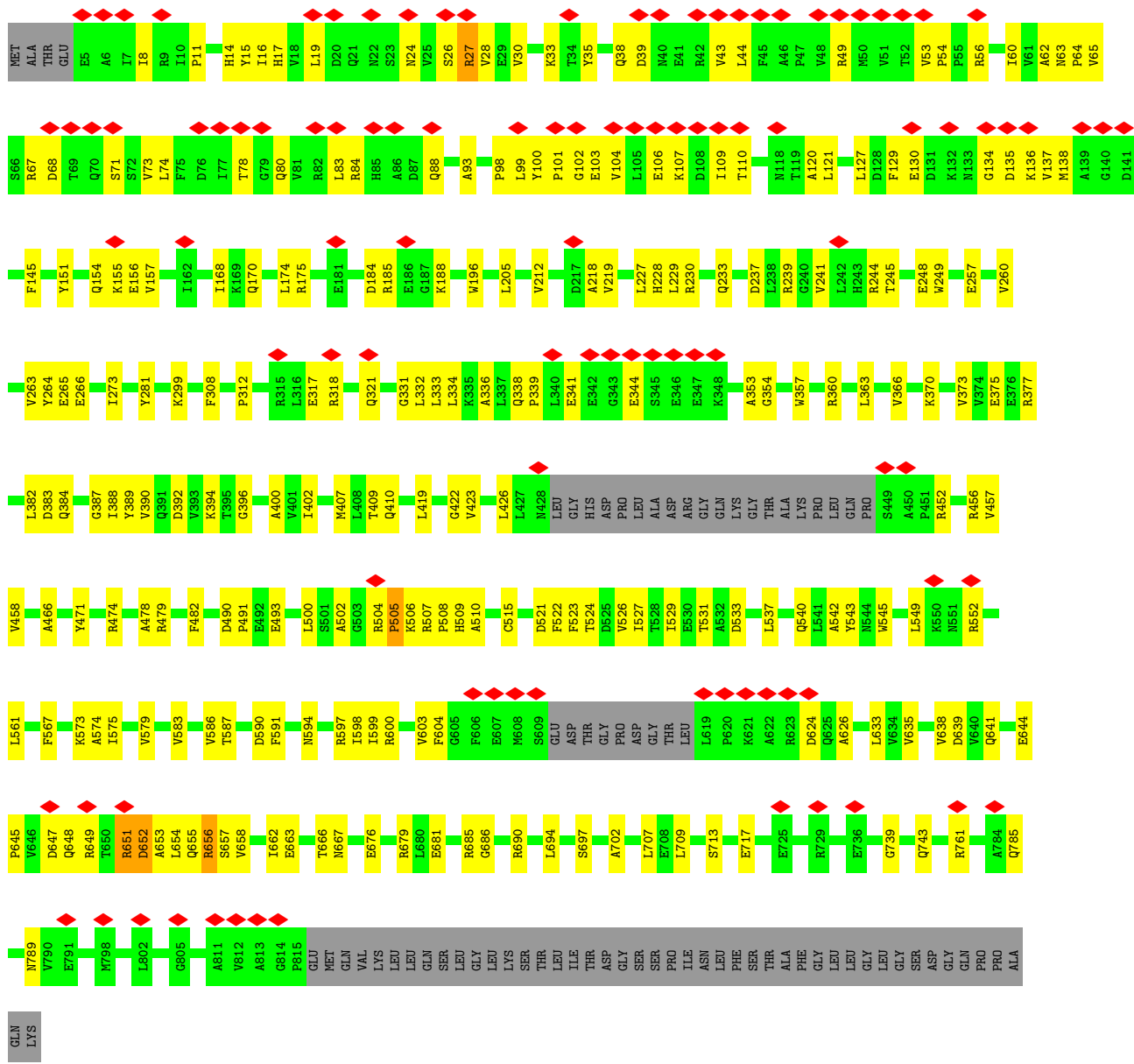


• Molecule 1: Major vault protein



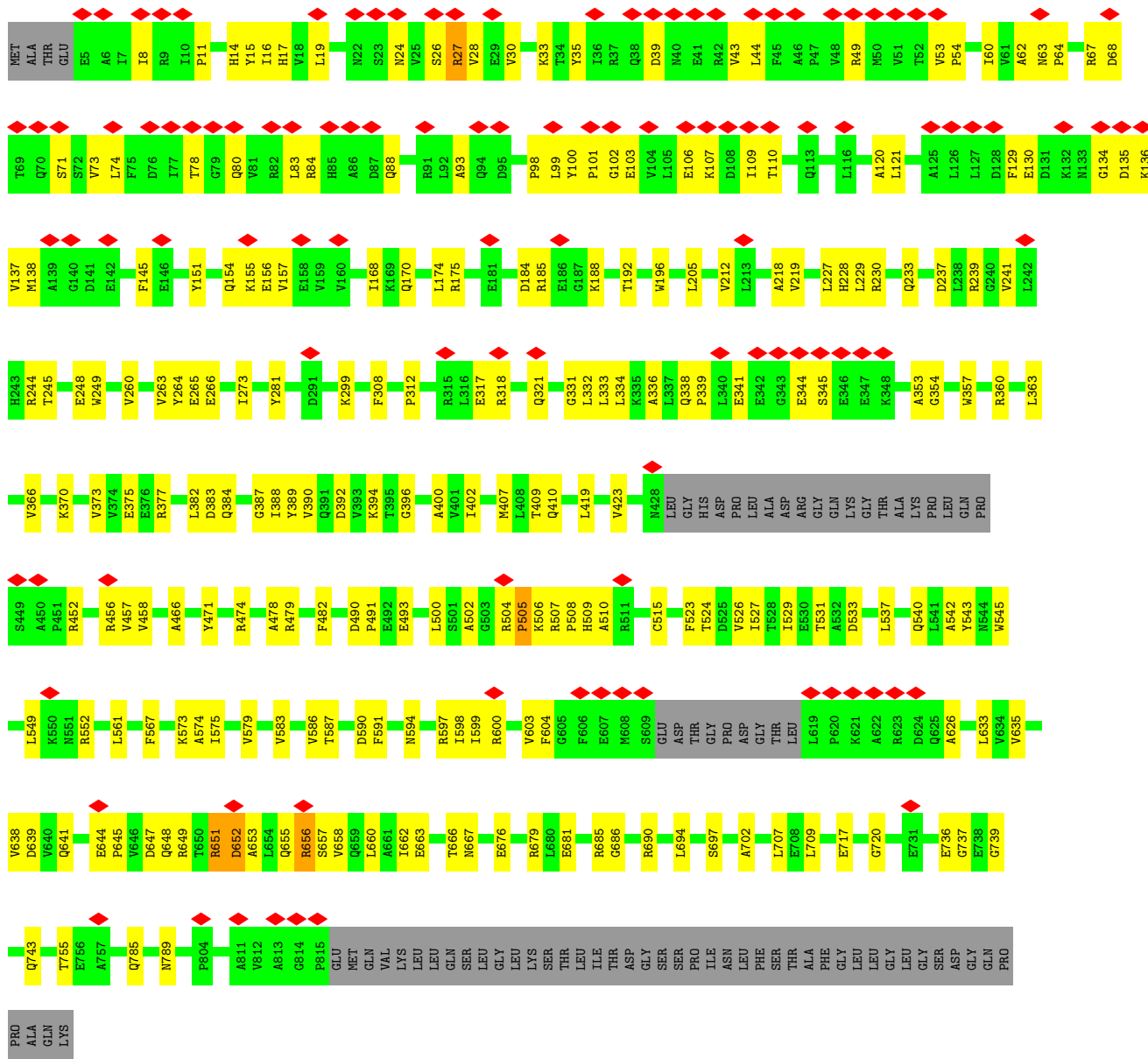


● Molecule 1: Major vault protein

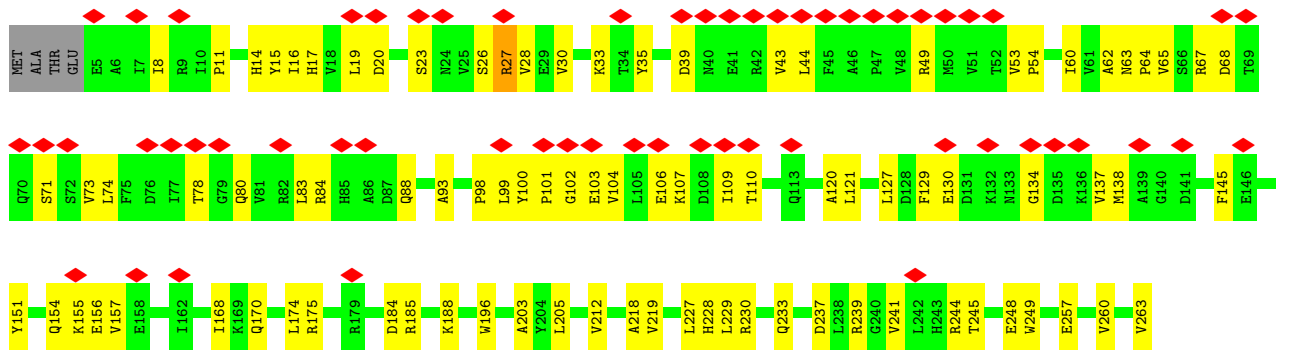


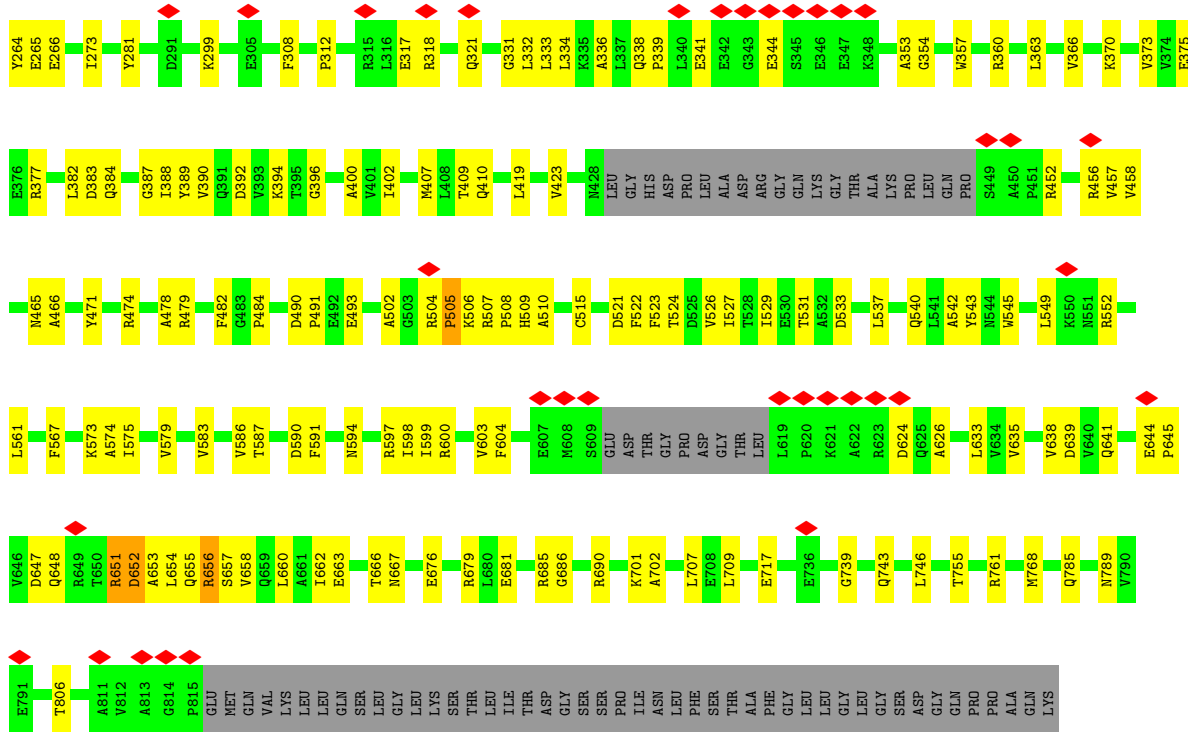
● Molecule 1: Major vault protein



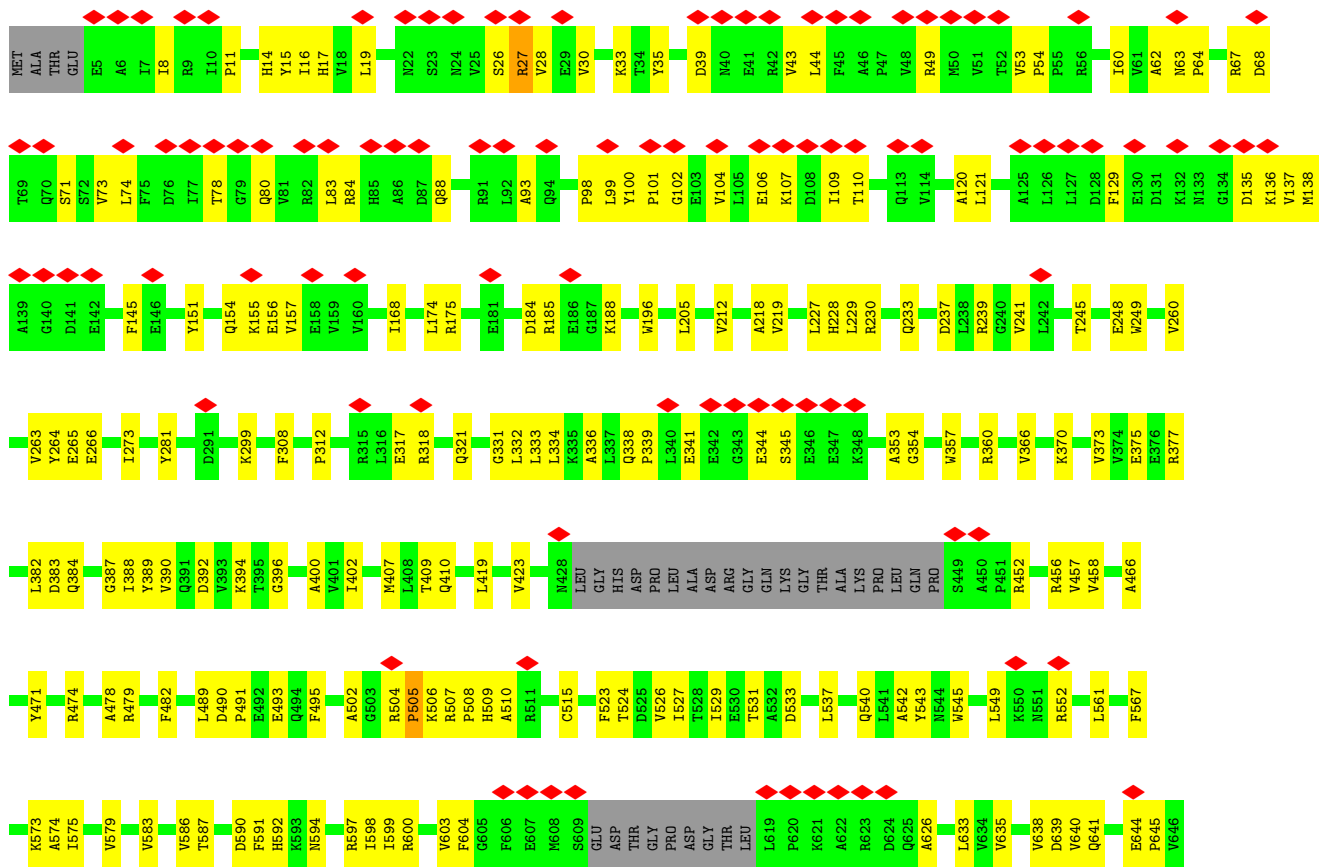


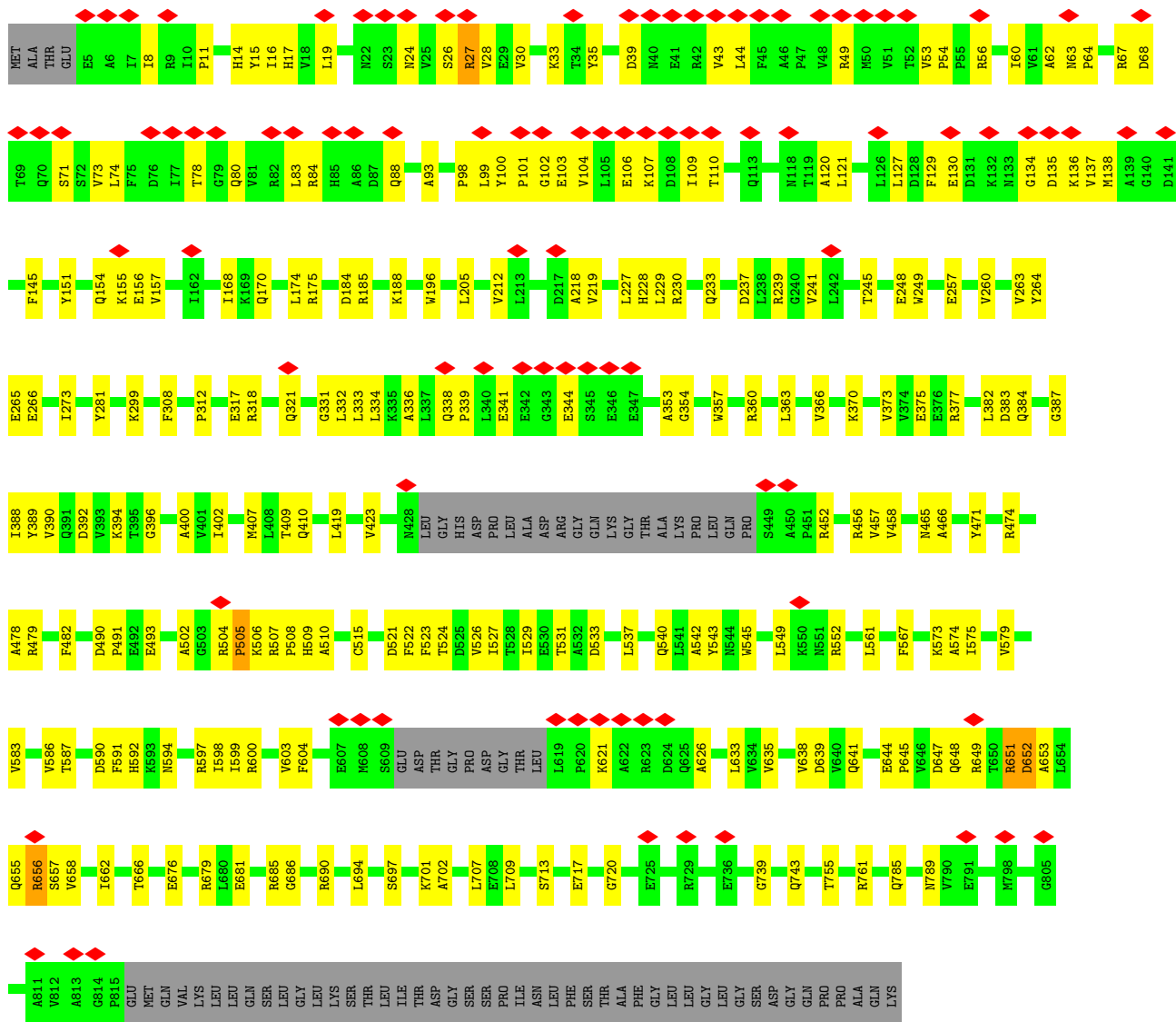
• Molecule 1: Major vault protein



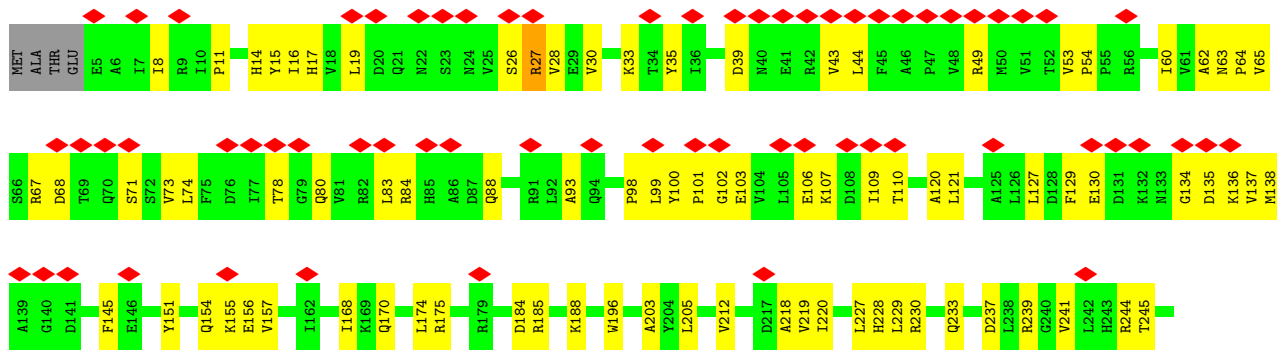


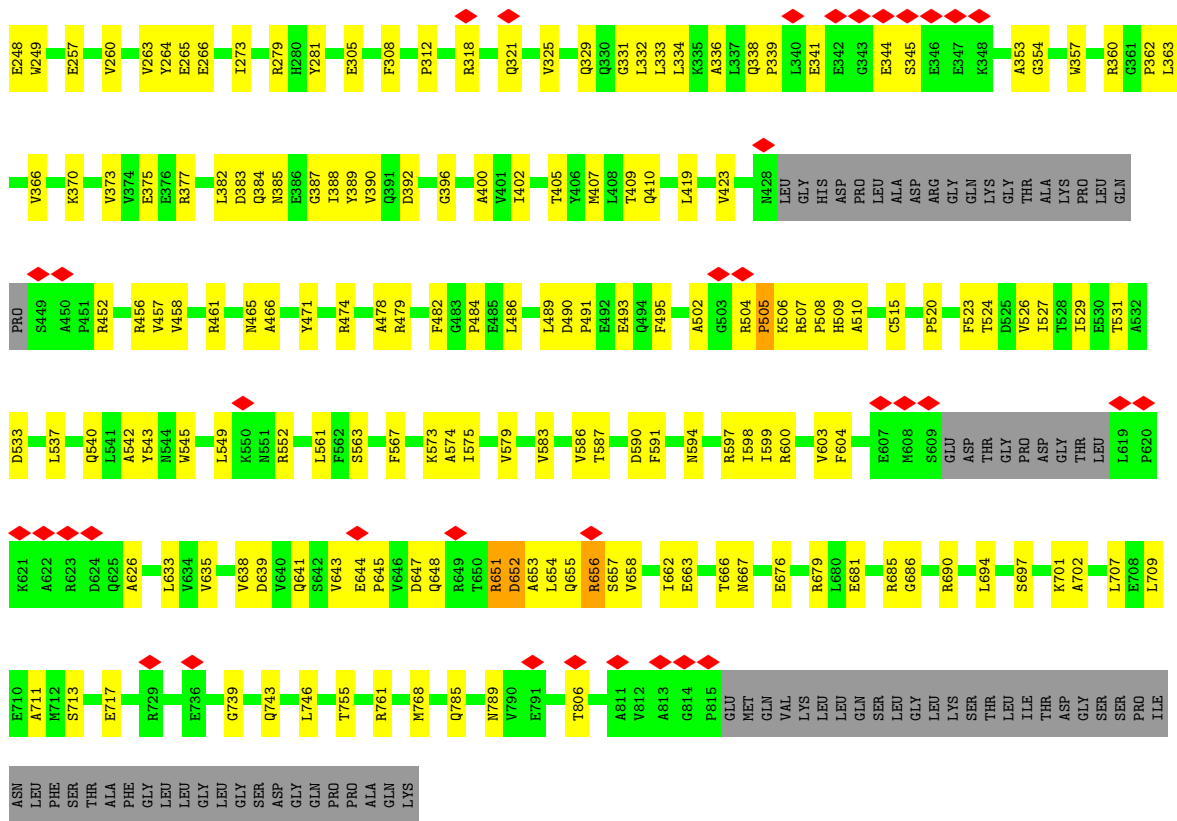
• Molecule 1: Major vault protein



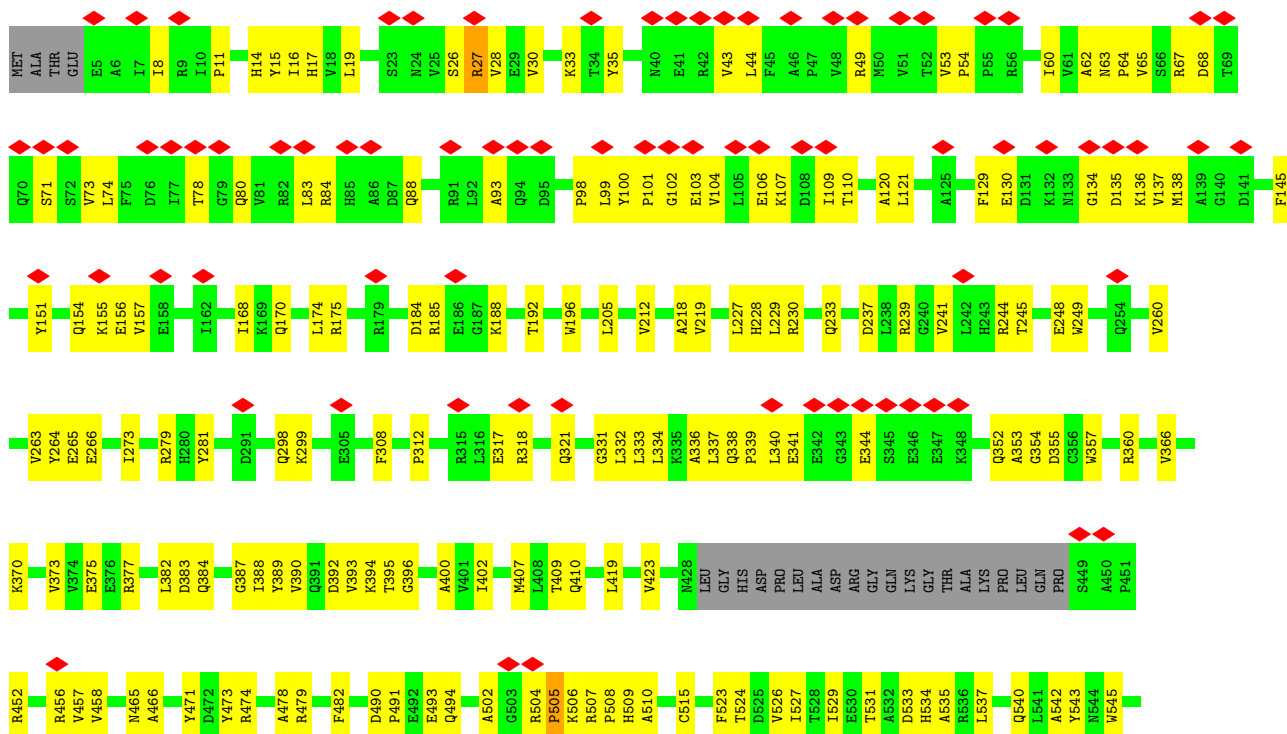


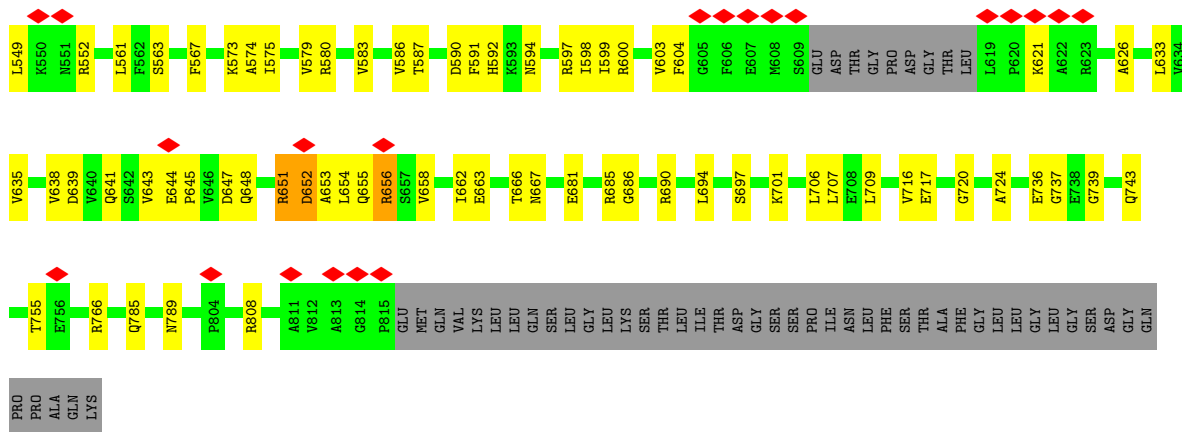
• Molecule 1: Major vault protein



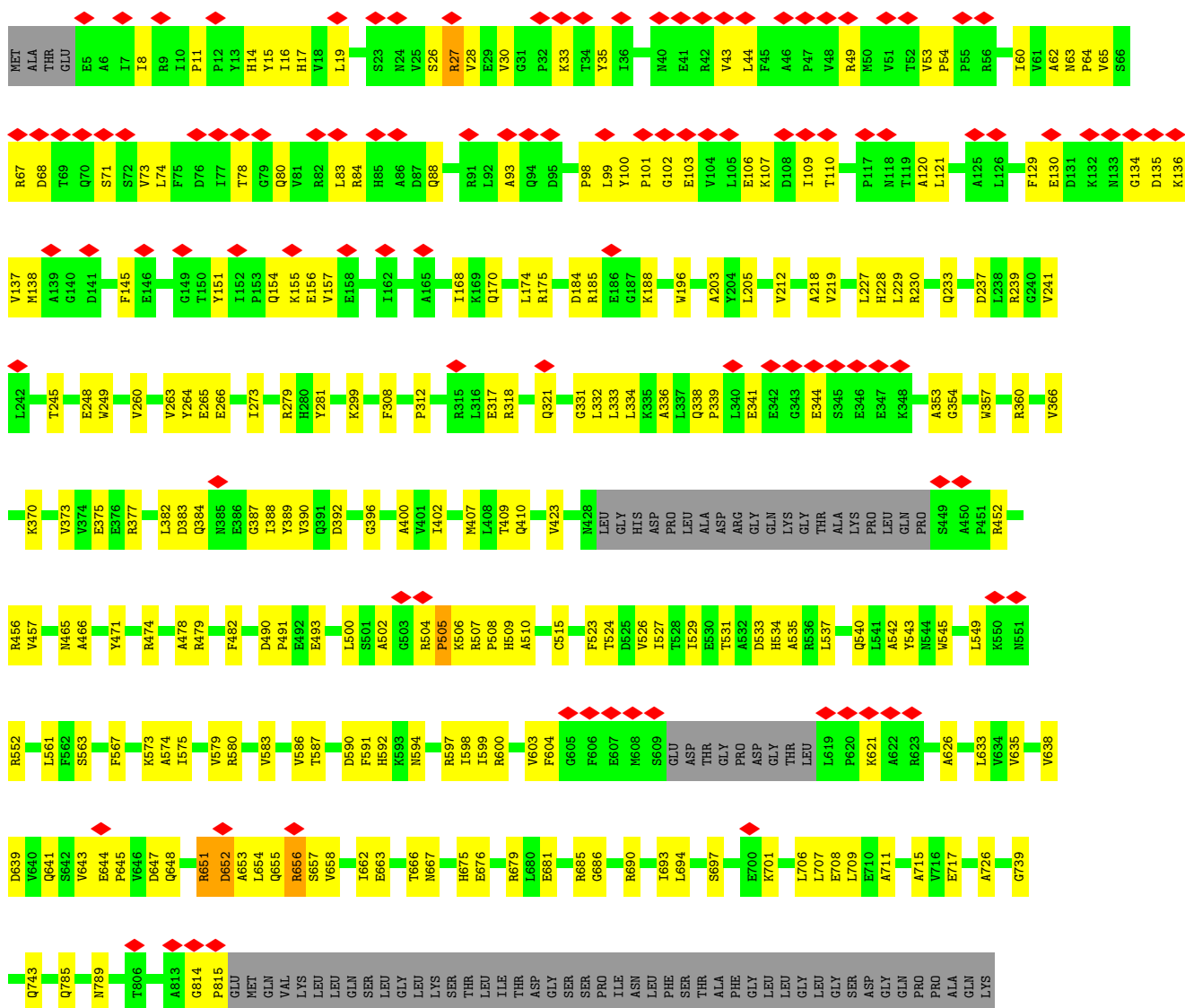


• Molecule 1: Major vault protein

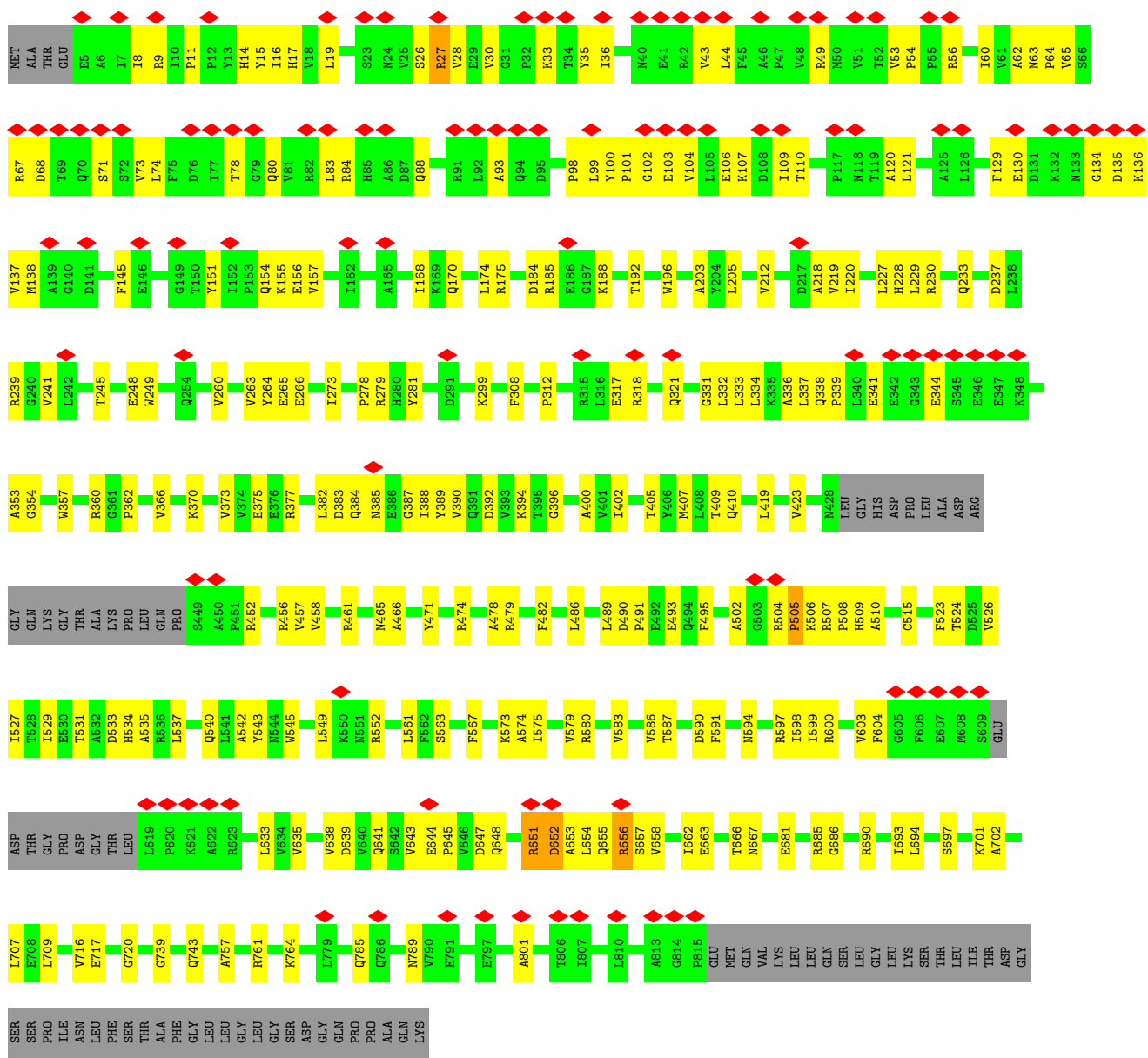




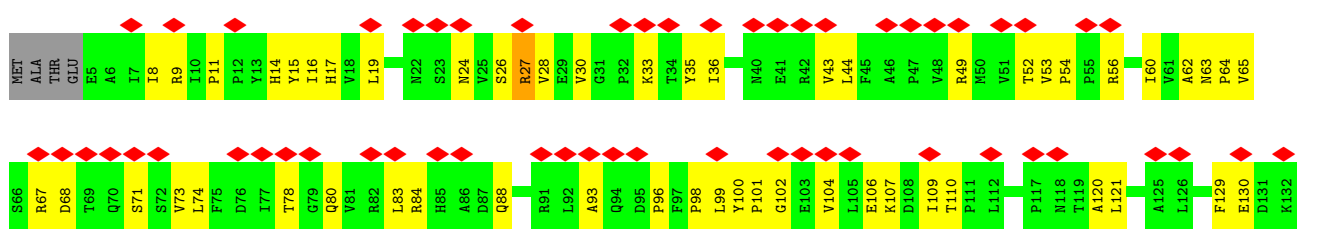
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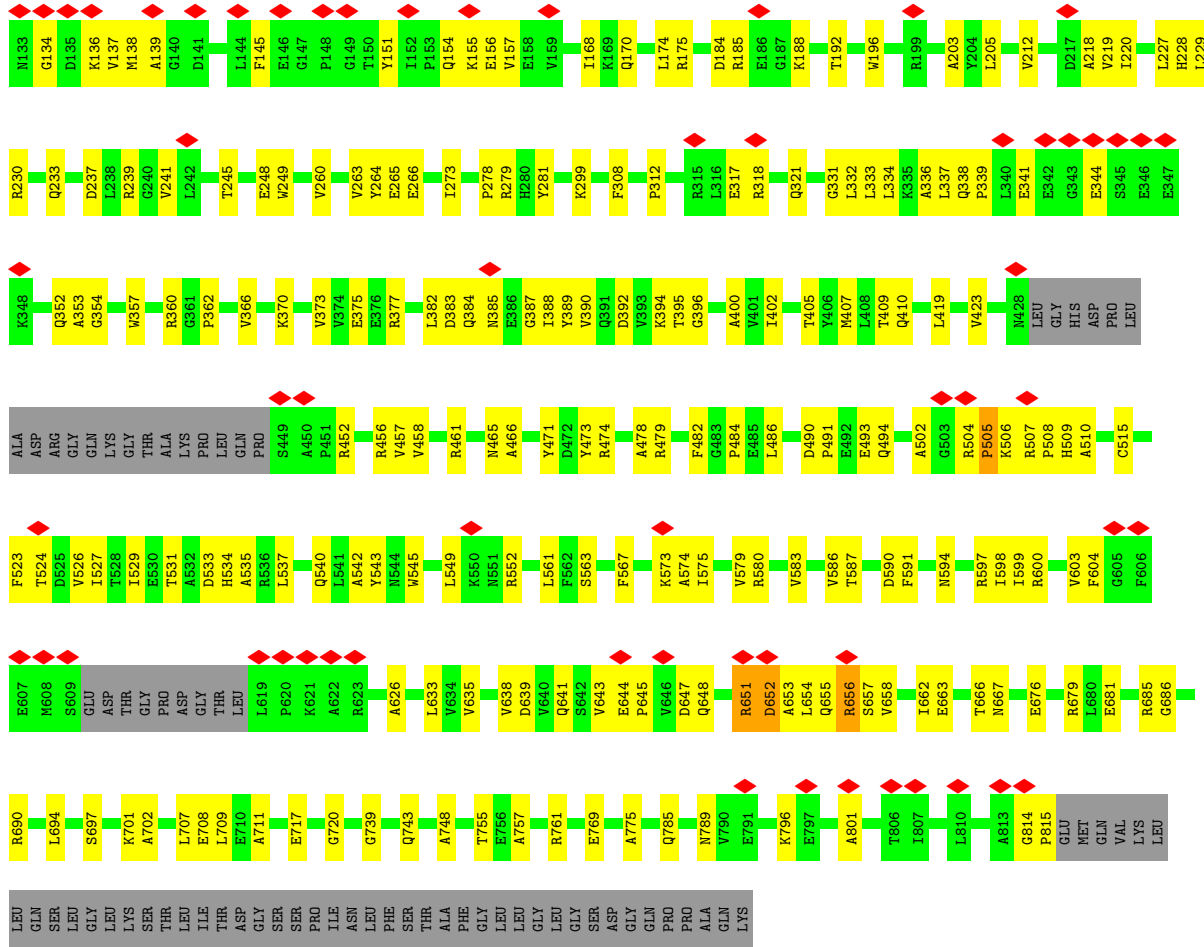


• Molecule 1: Major vault protein

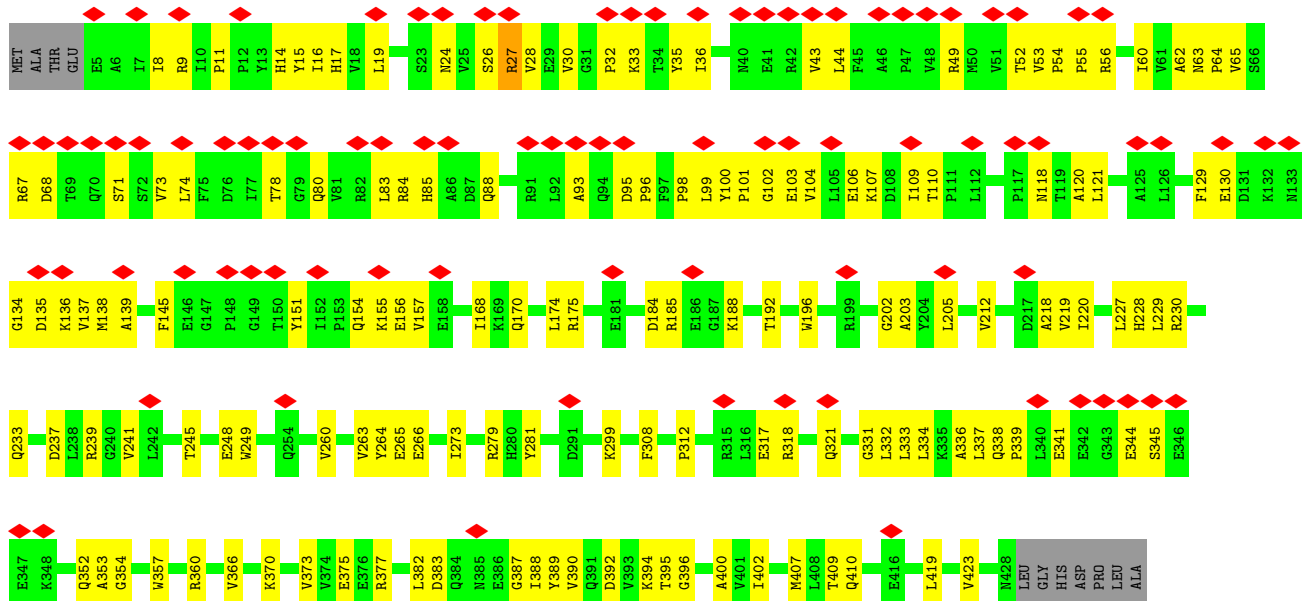


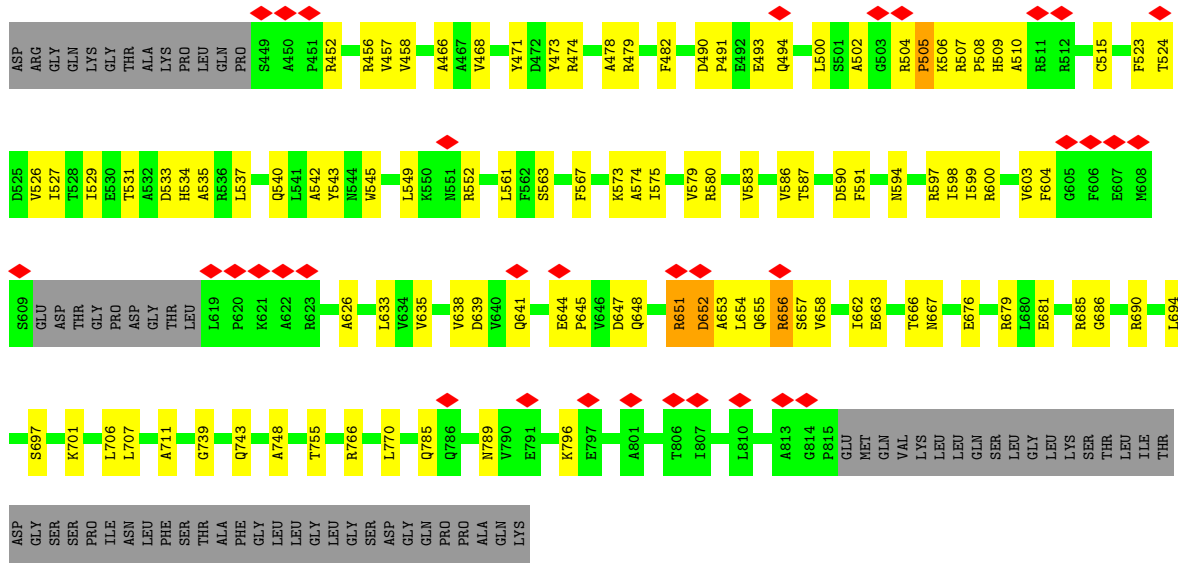
• Molecule 1: Major vault protein



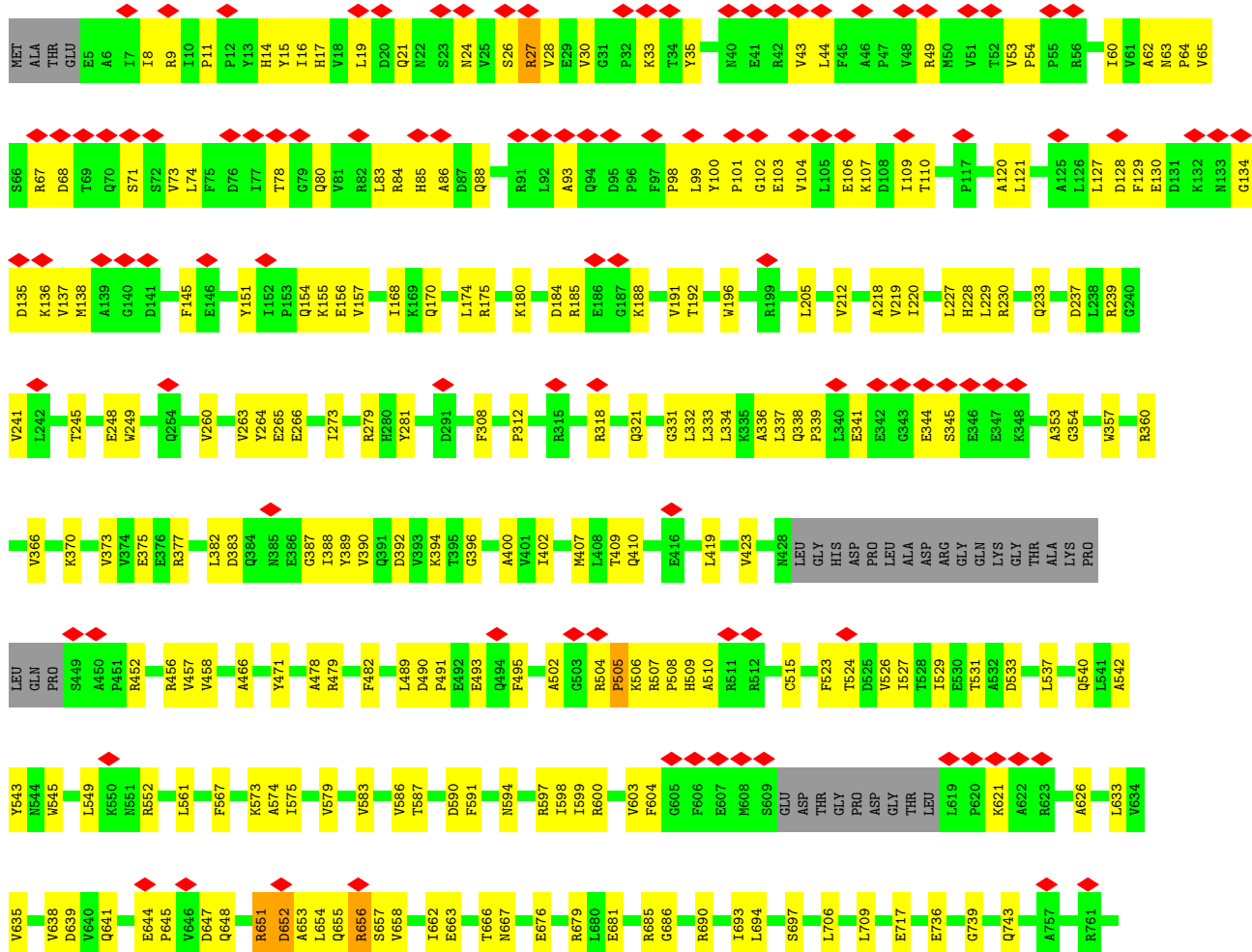


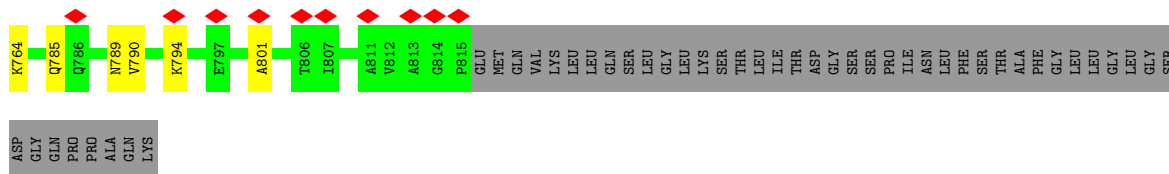
• Molecule 1: Major vault protein



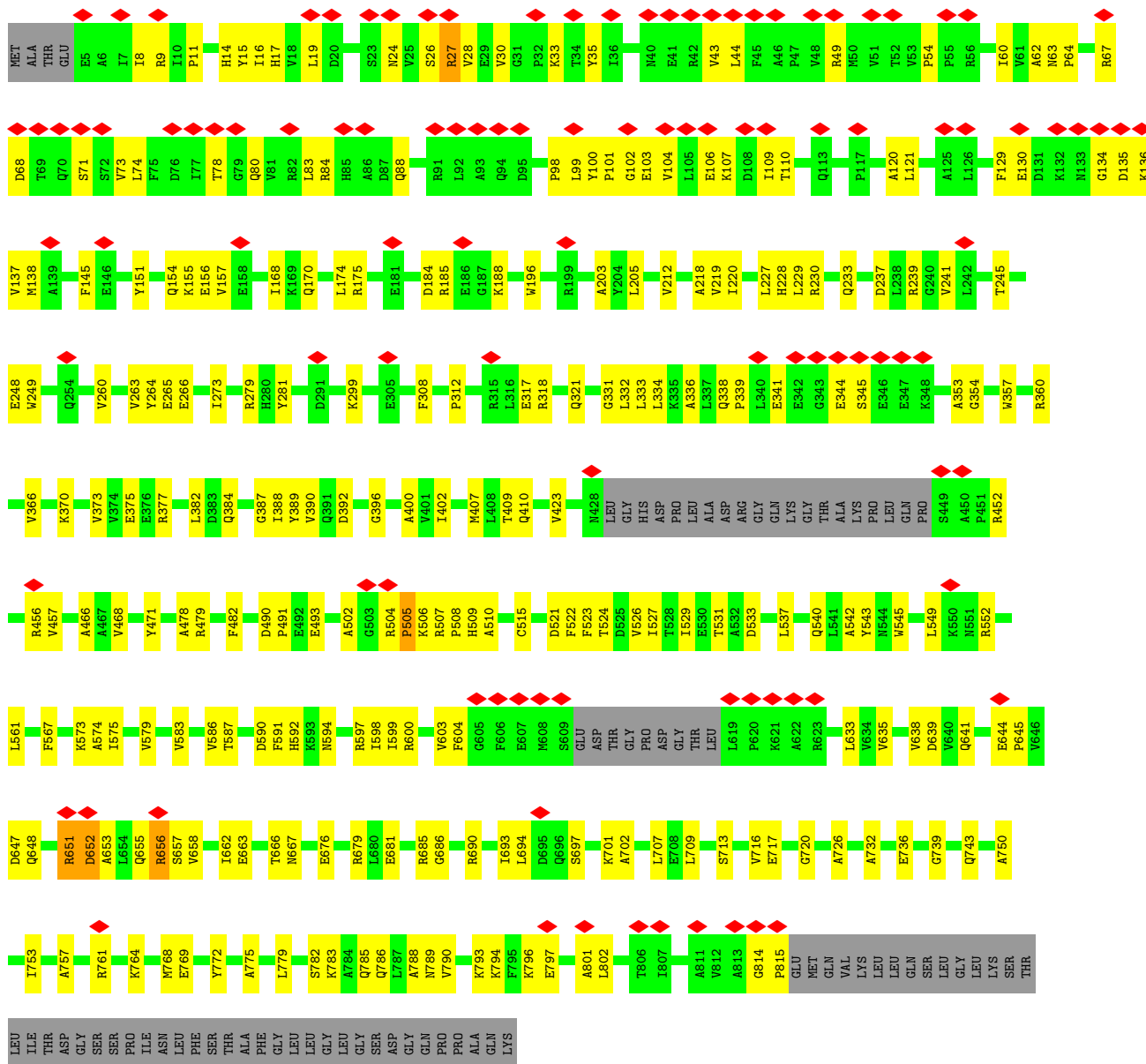


- Molecule 1: Major vault protein



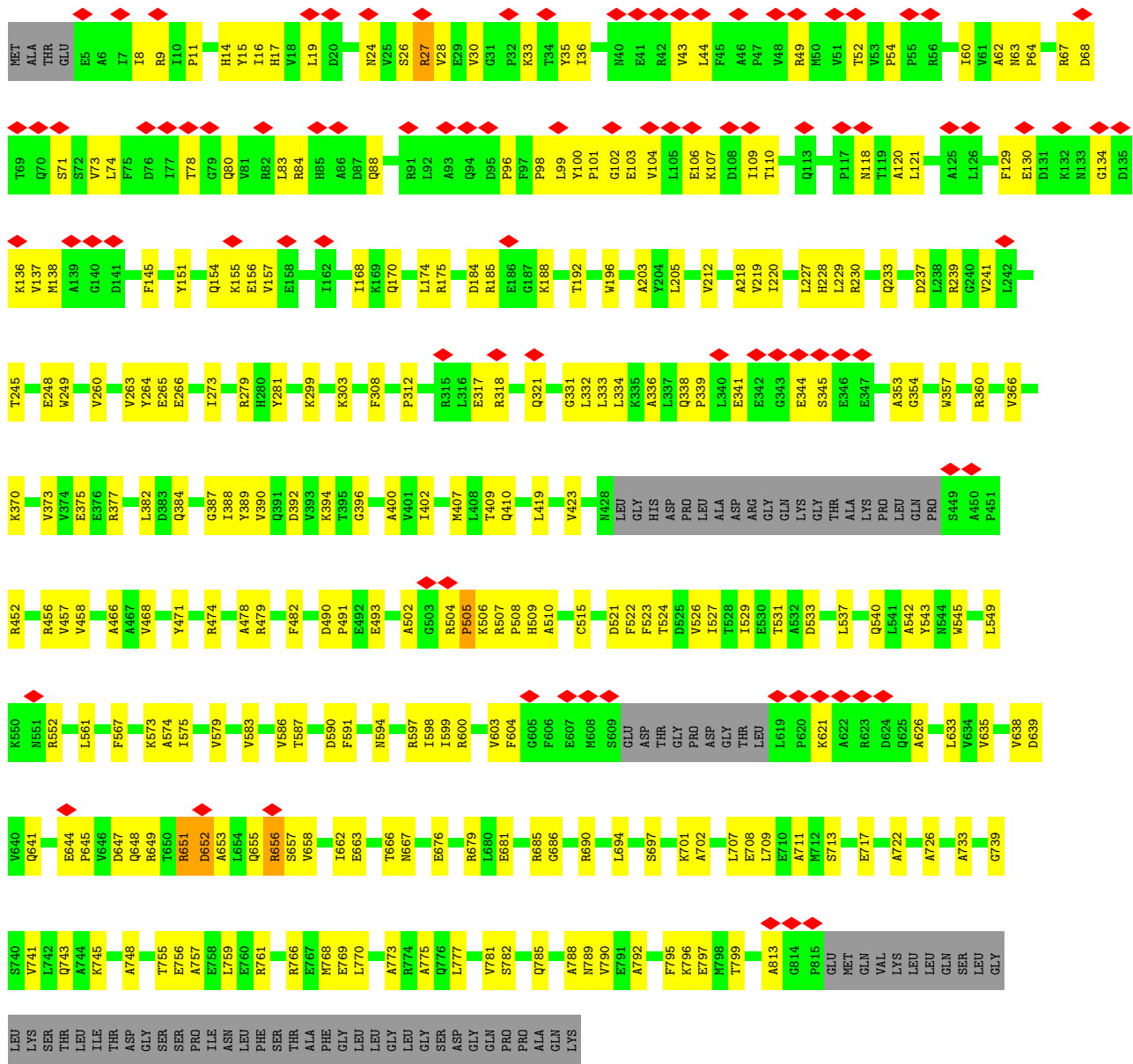


• Molecule 1: Major vault protein

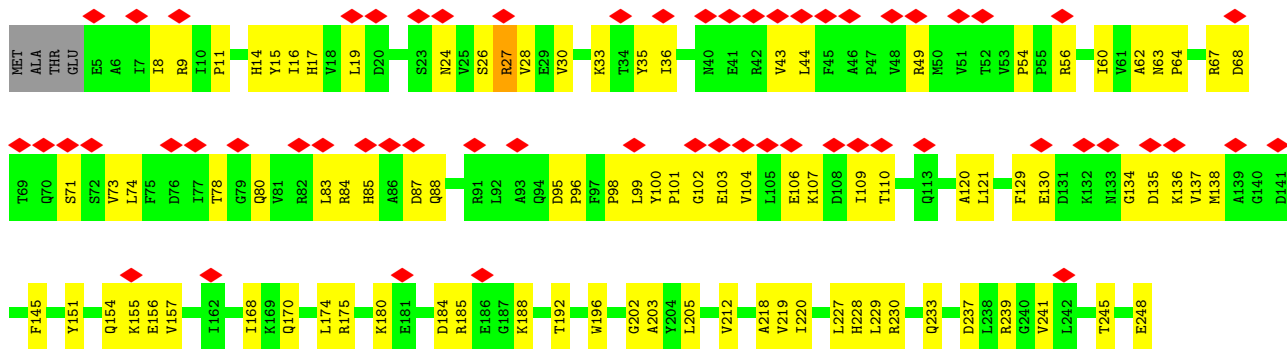


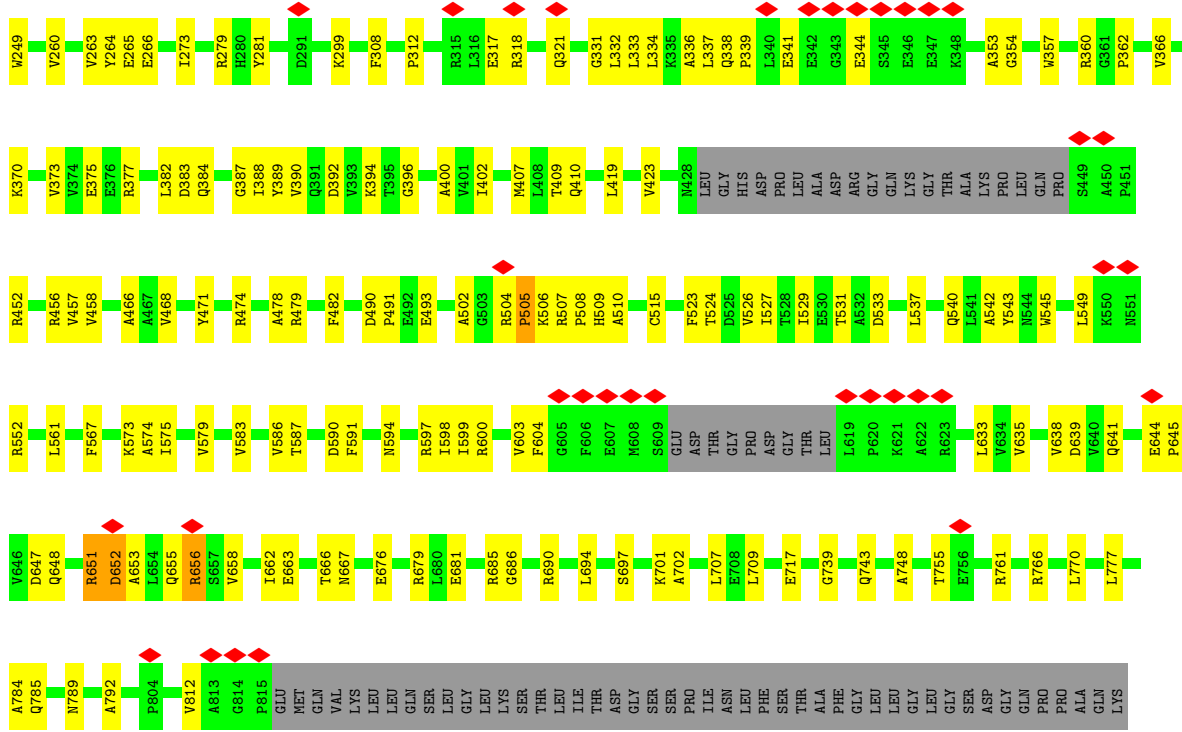
• Molecule 1: Major vault protein



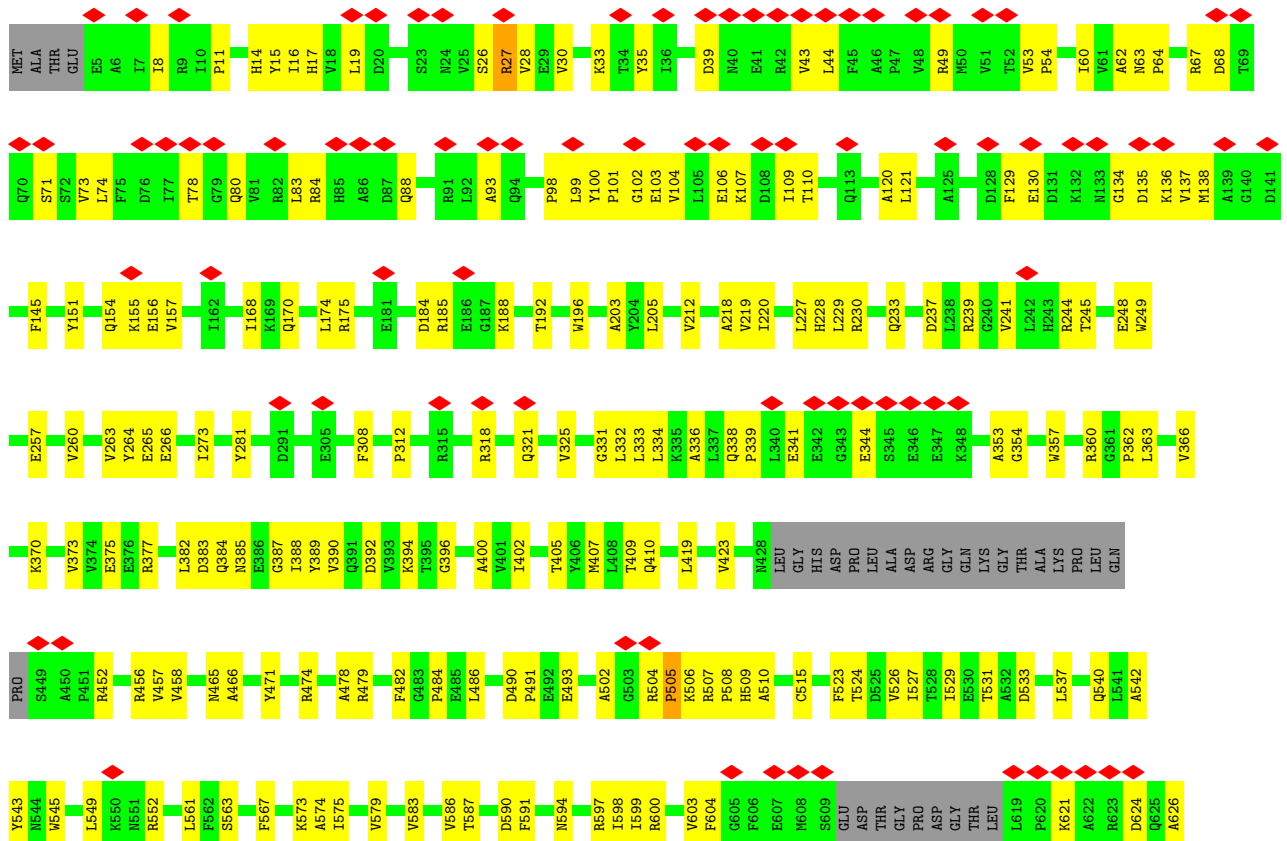


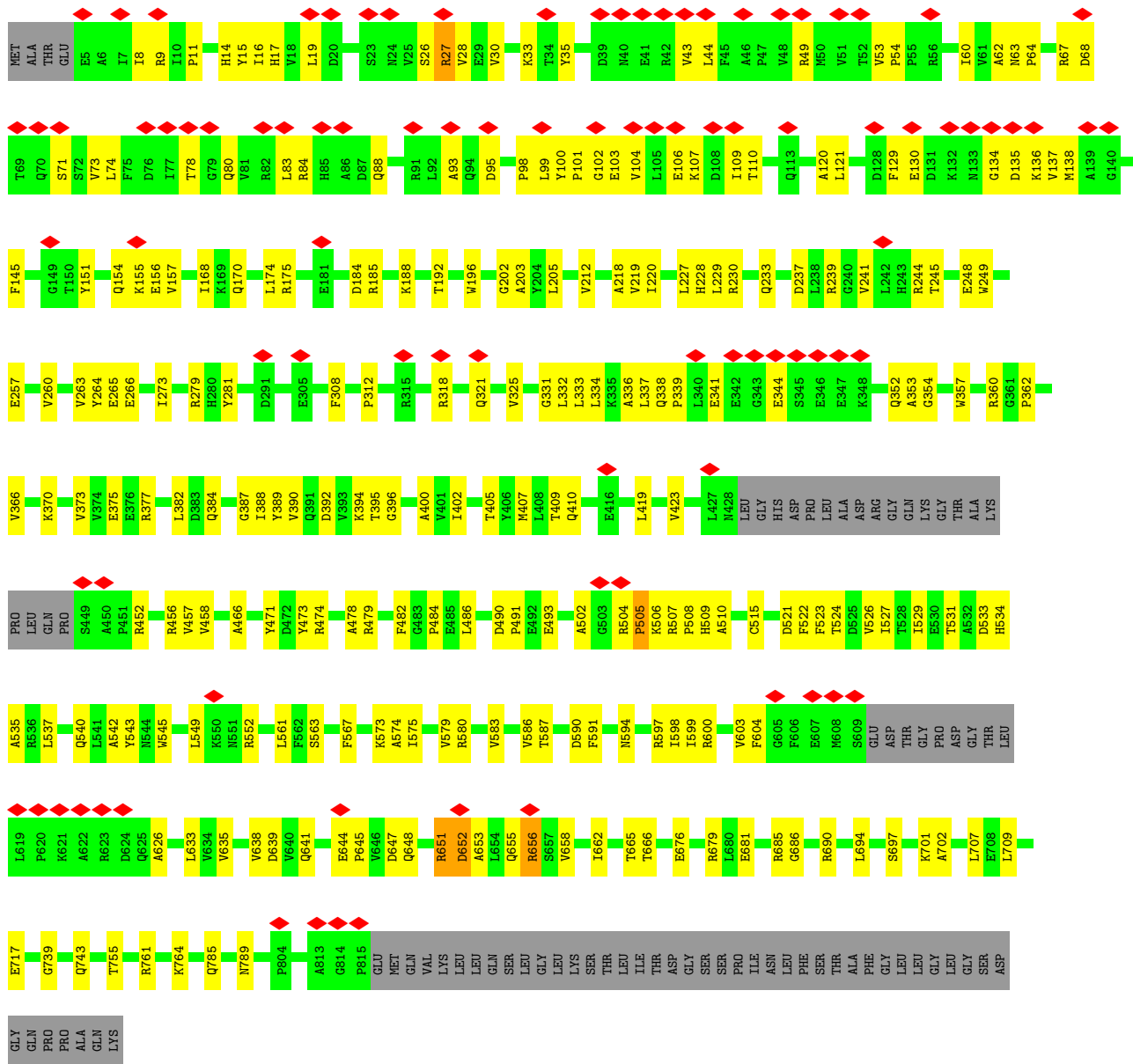
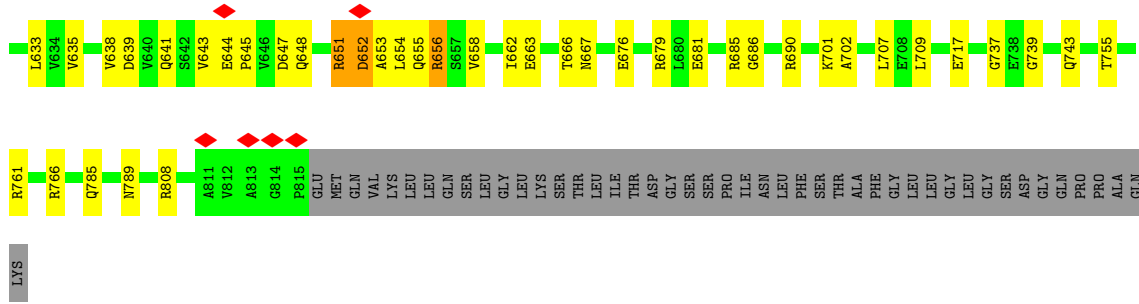
• Molecule 1: Major vault protein



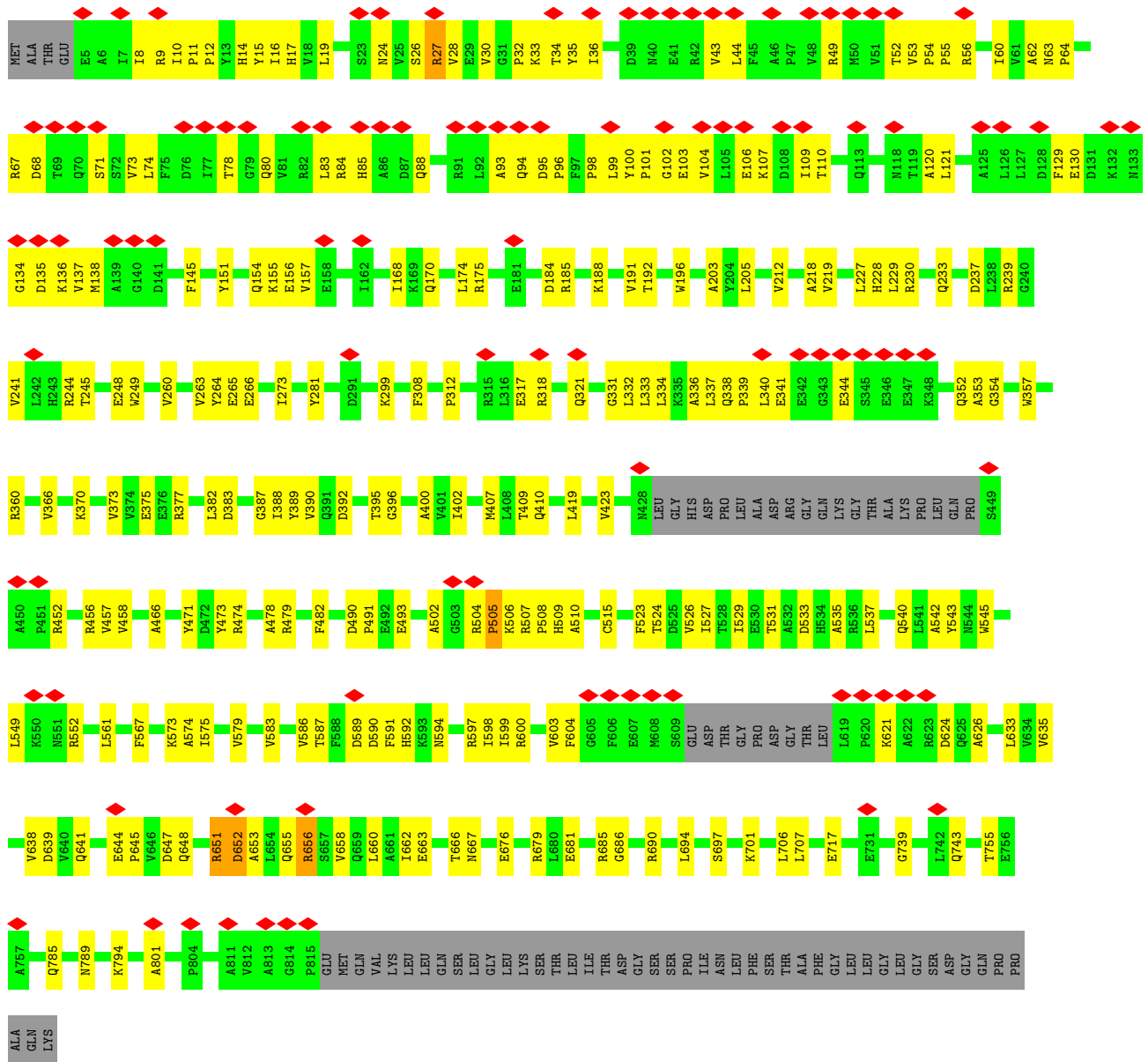


• Molecule 1: Major vault protein

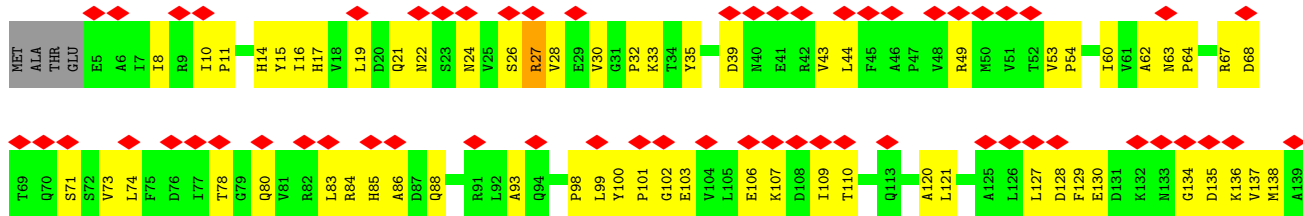


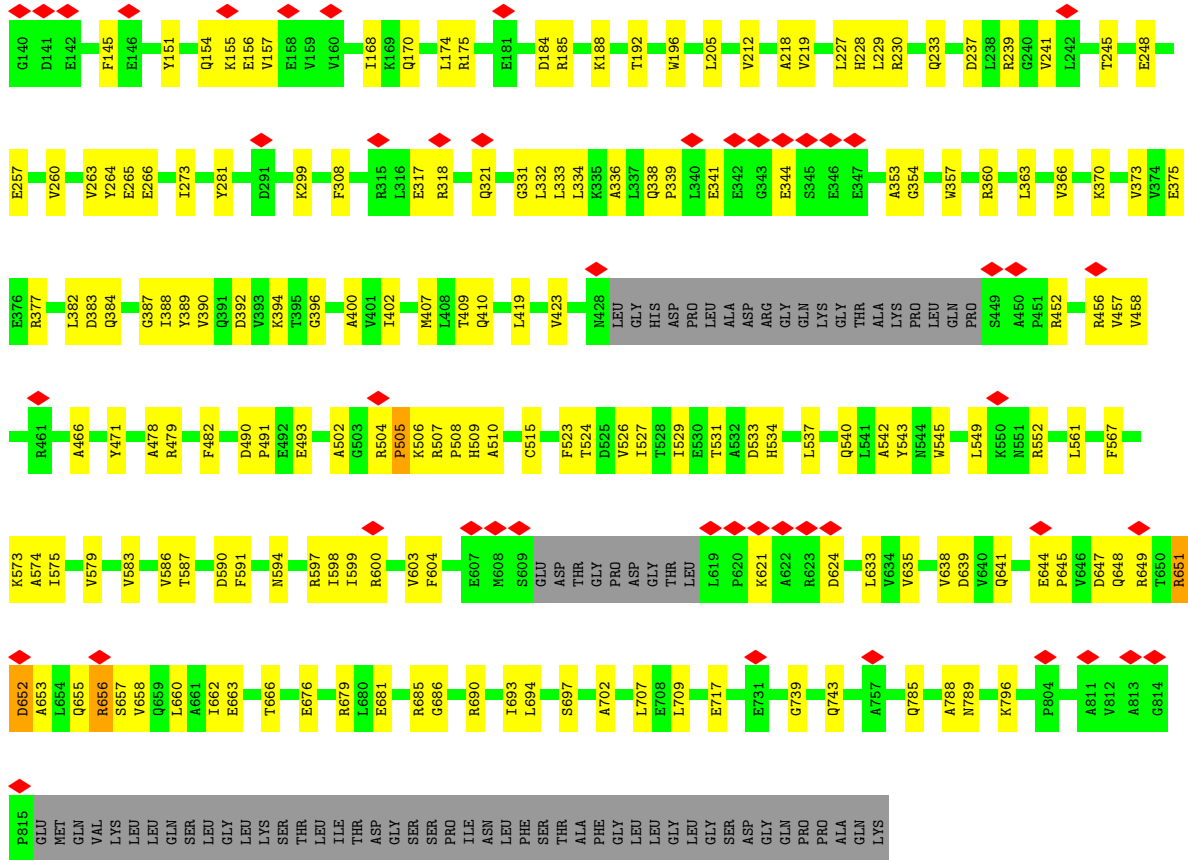


• Molecule 1: Major vault protein

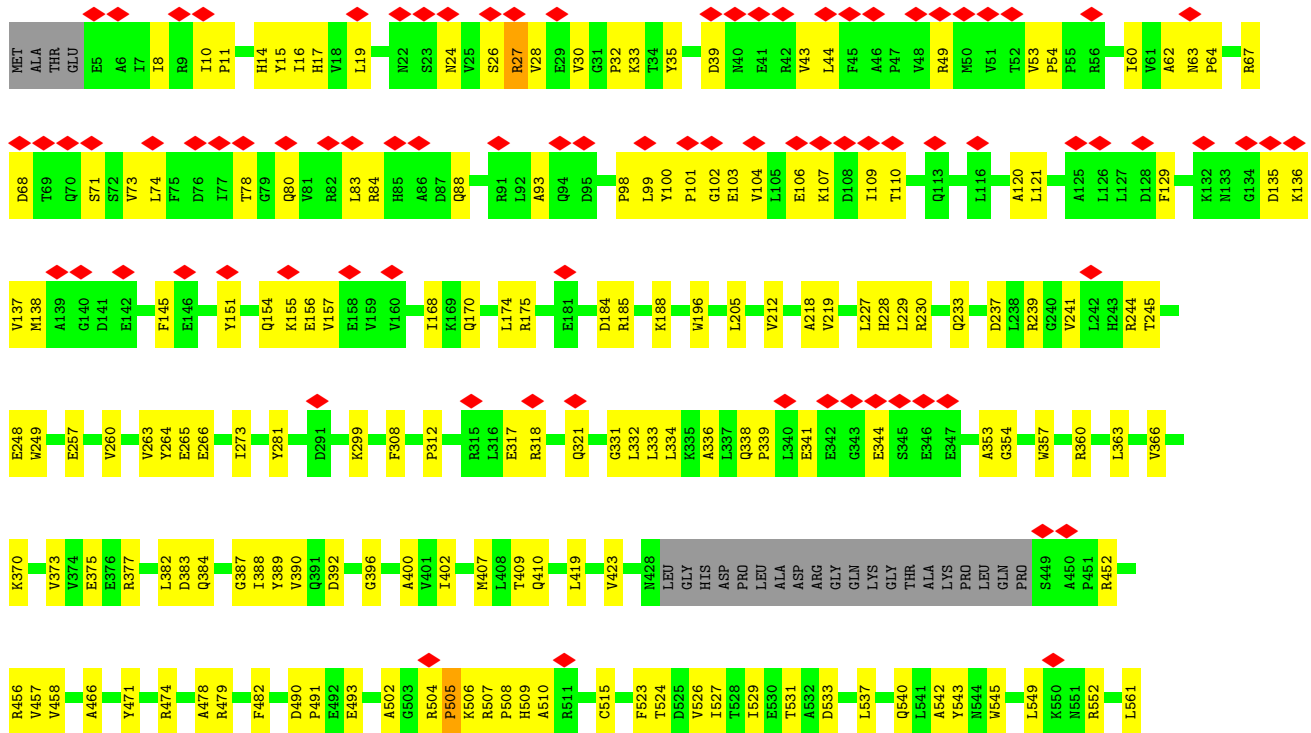


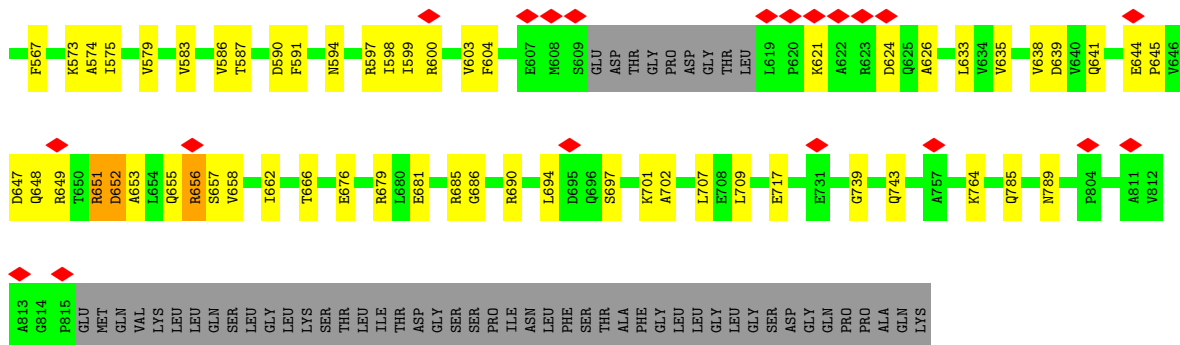
• Molecule 1: Major vault protein



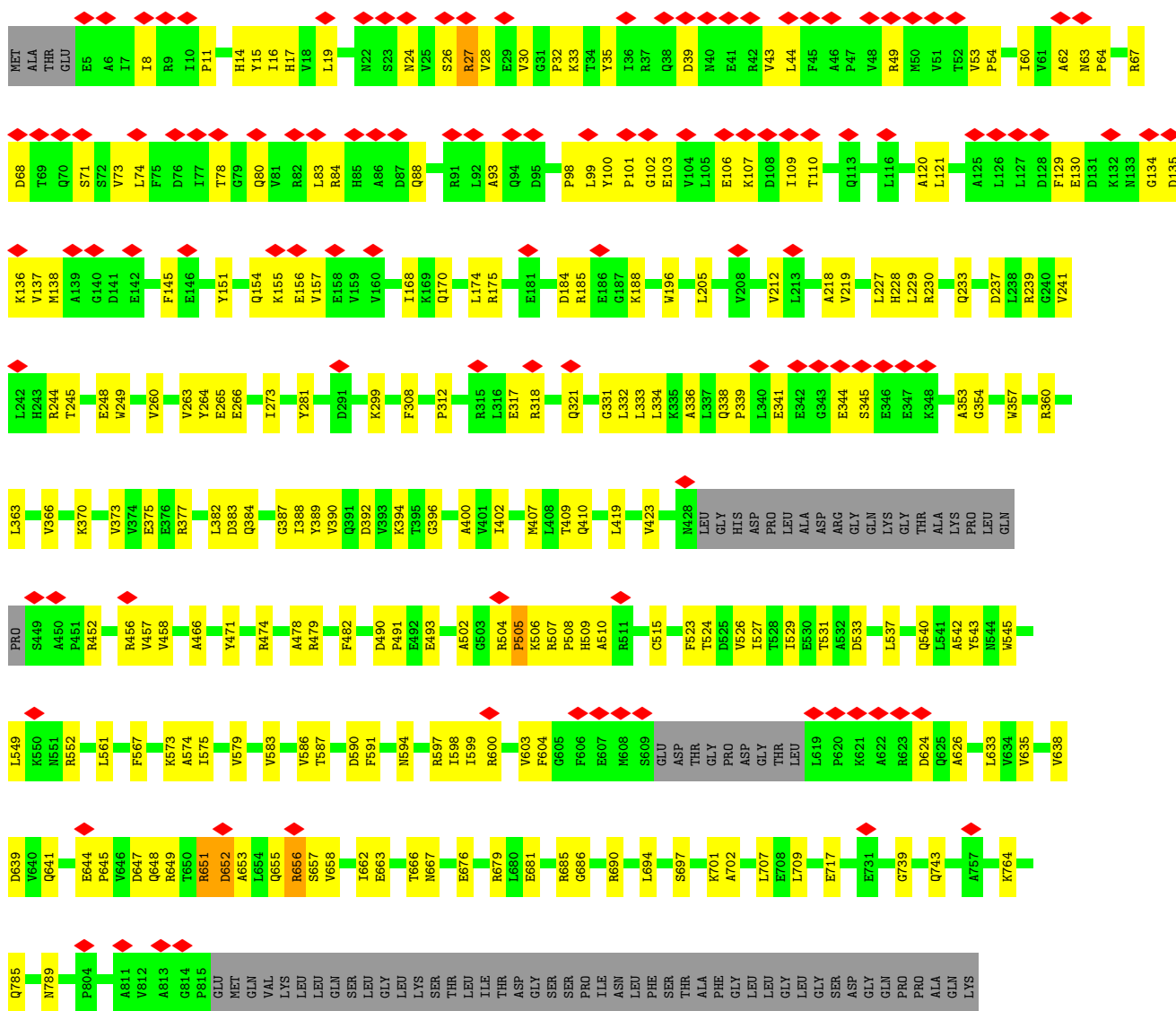


Molecule 1: Major vault protein

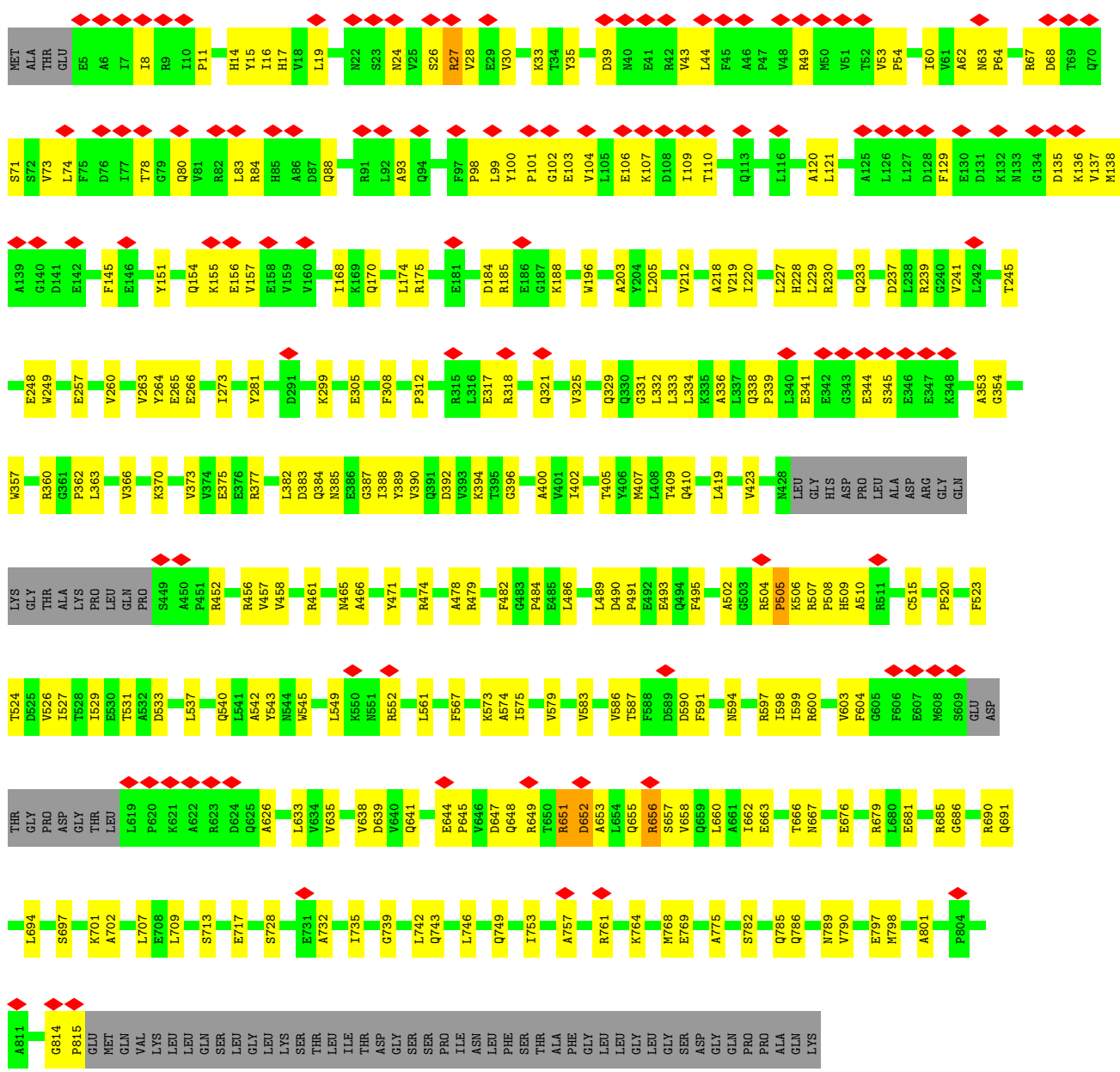




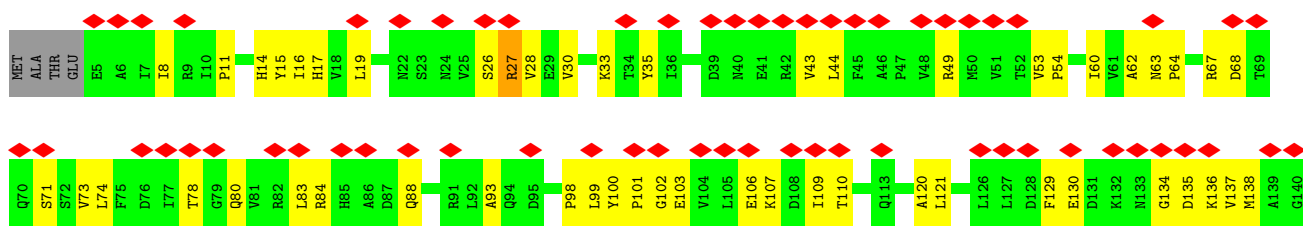
• Molecule 1: Major vault protein

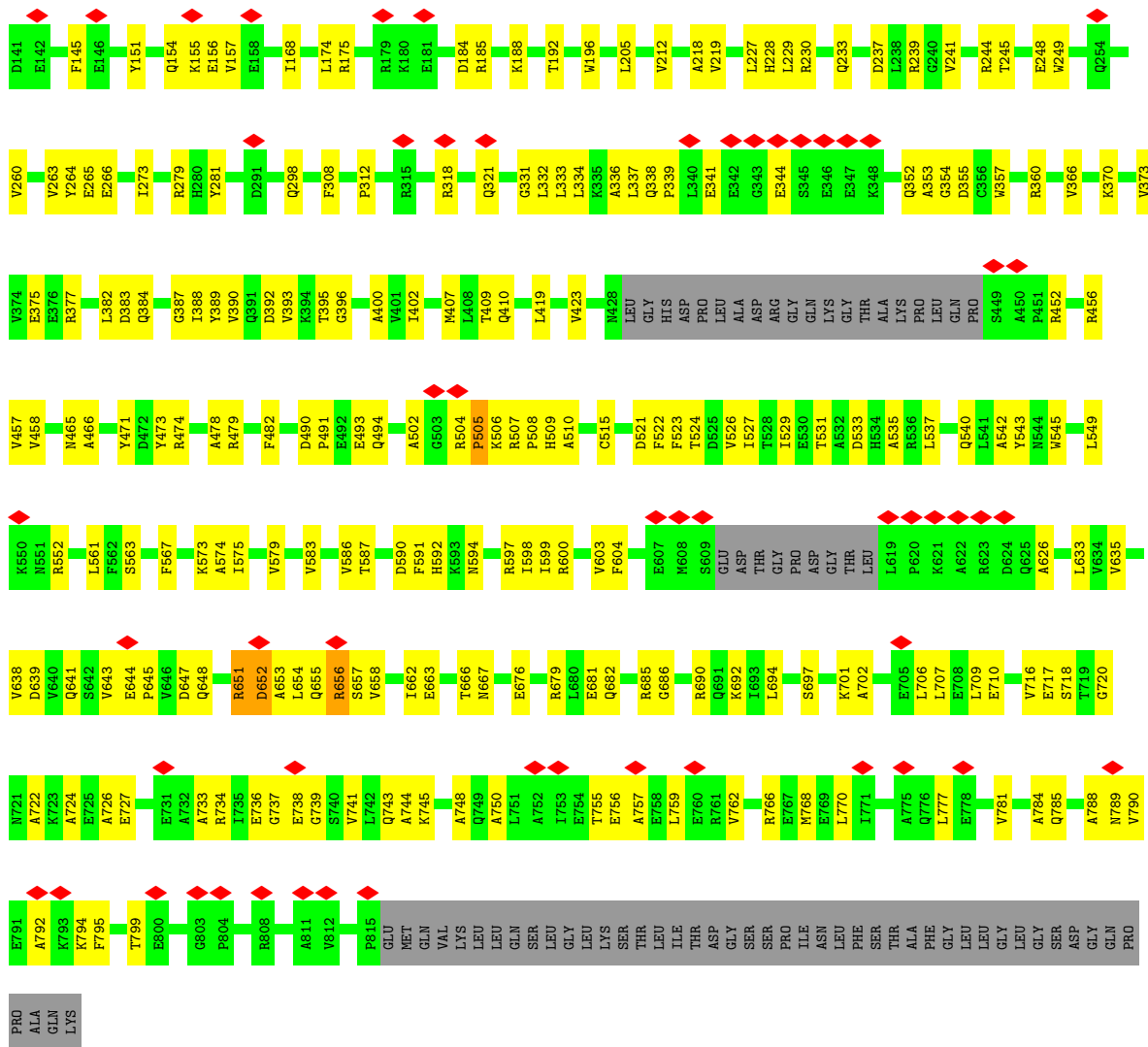


• Molecule 1: Major vault protein

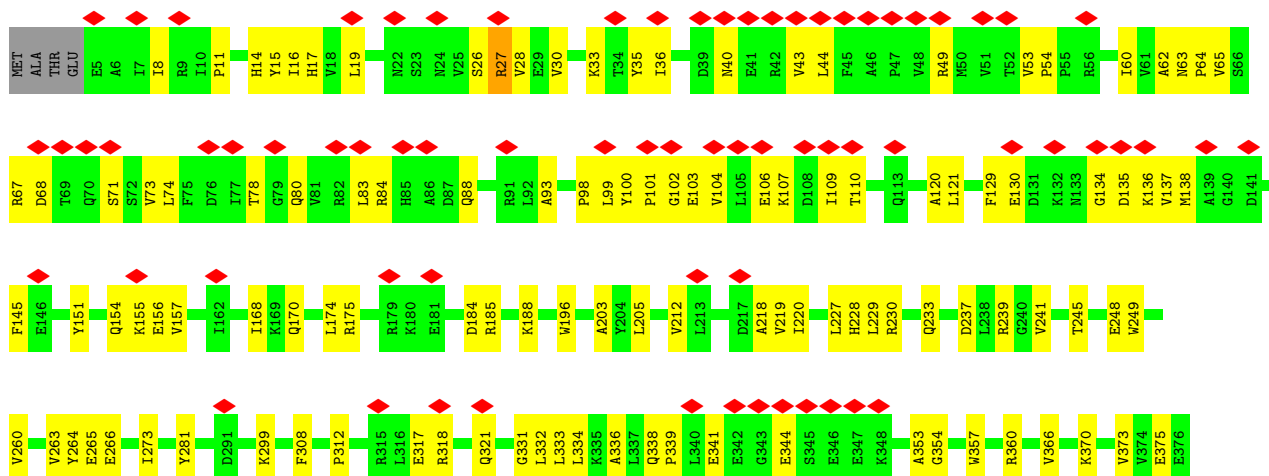


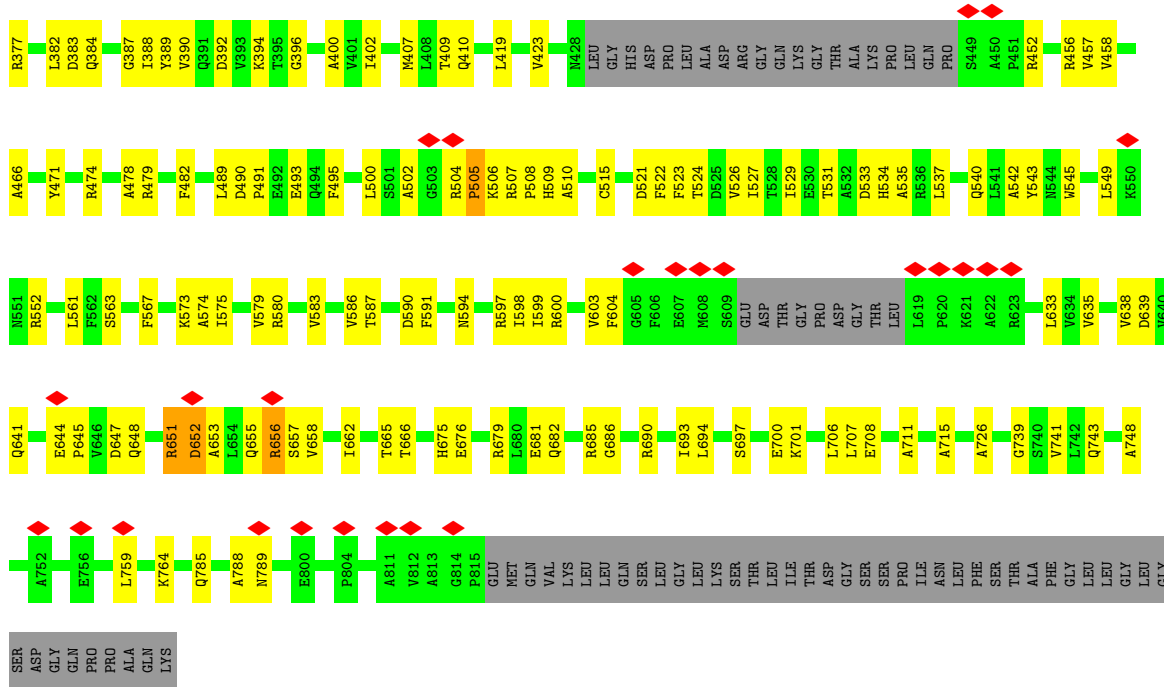
• Molecule 1: Major vault protein



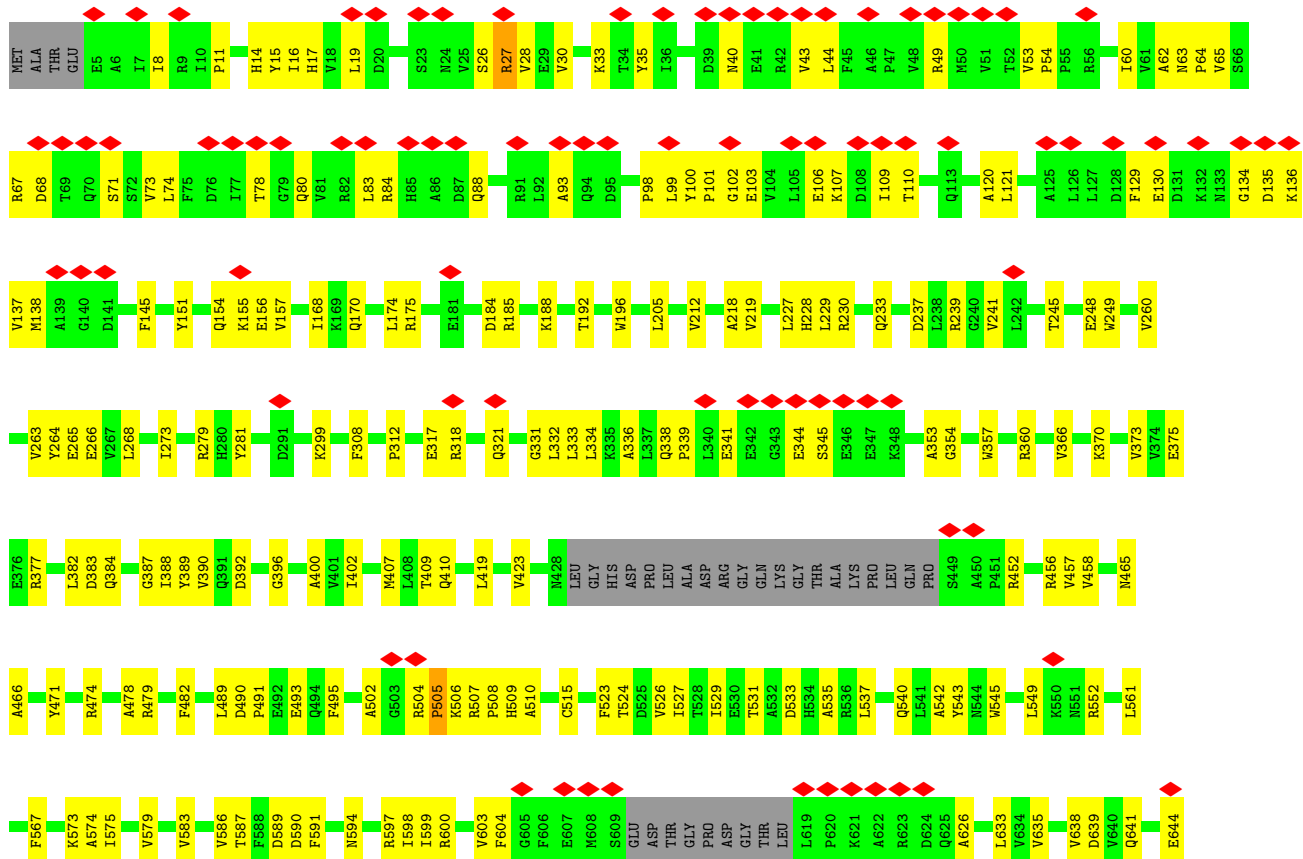


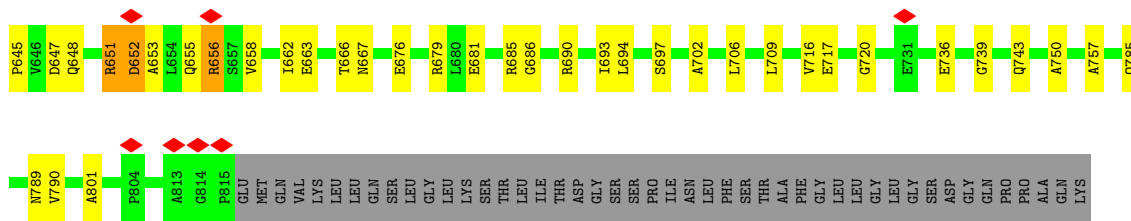
• Molecule 1: Major vault protein



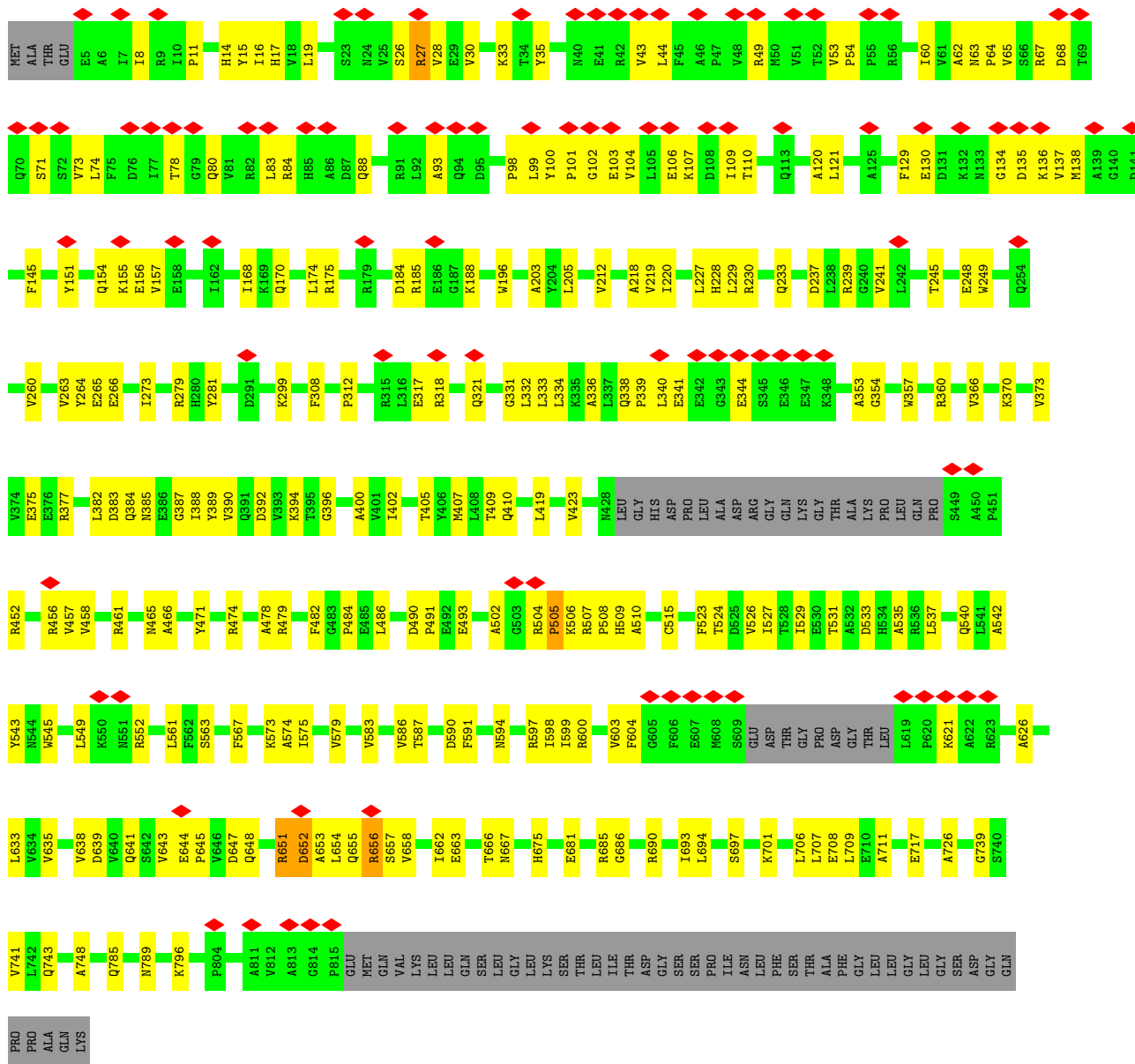


• Molecule 1: Major vault protein



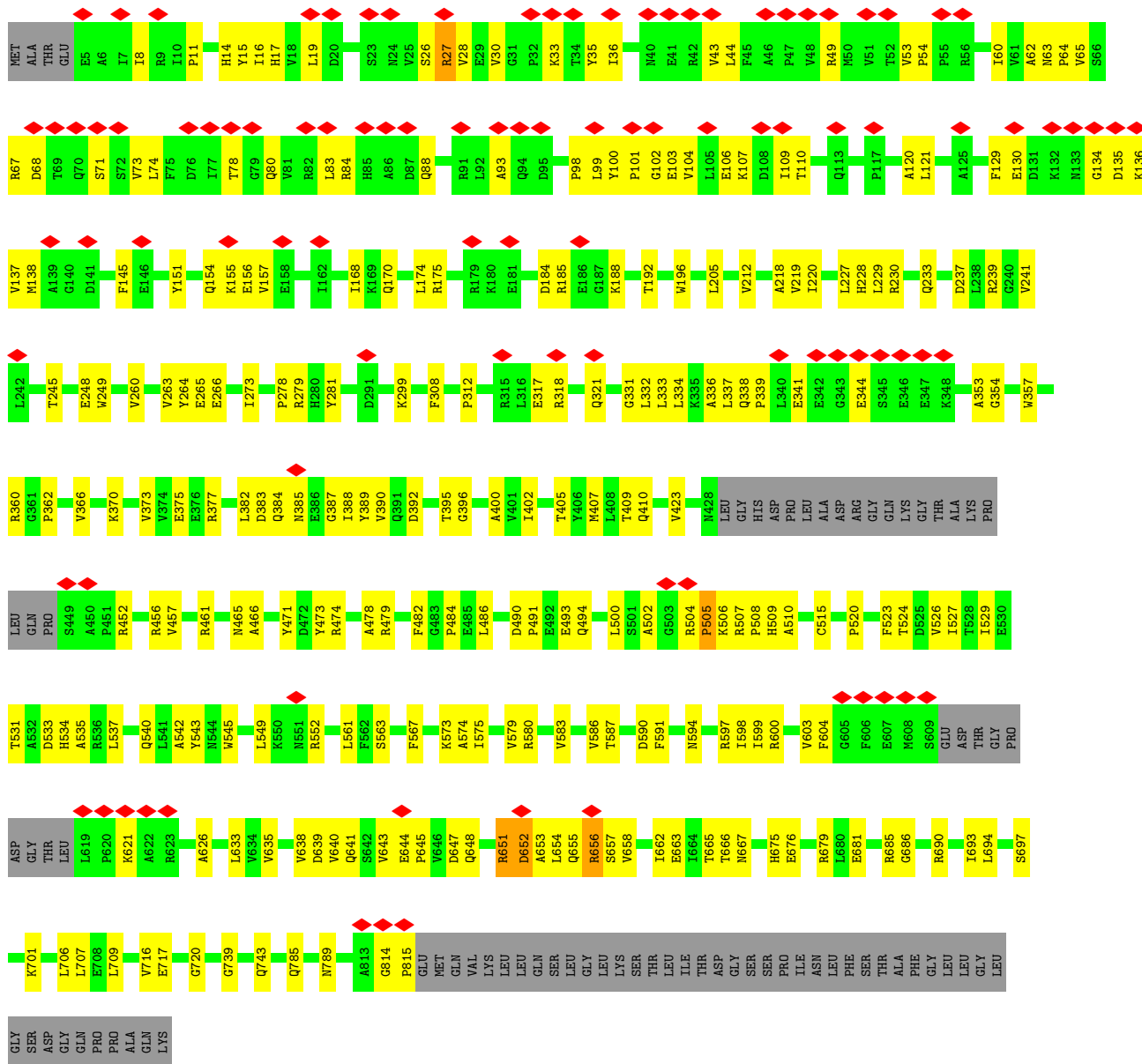


• Molecule 1: Major vault protein

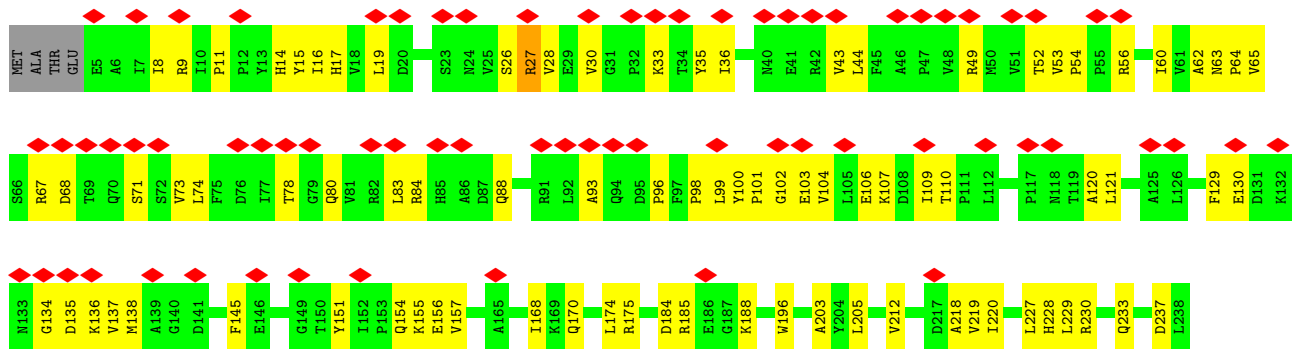
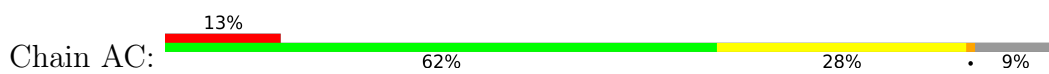


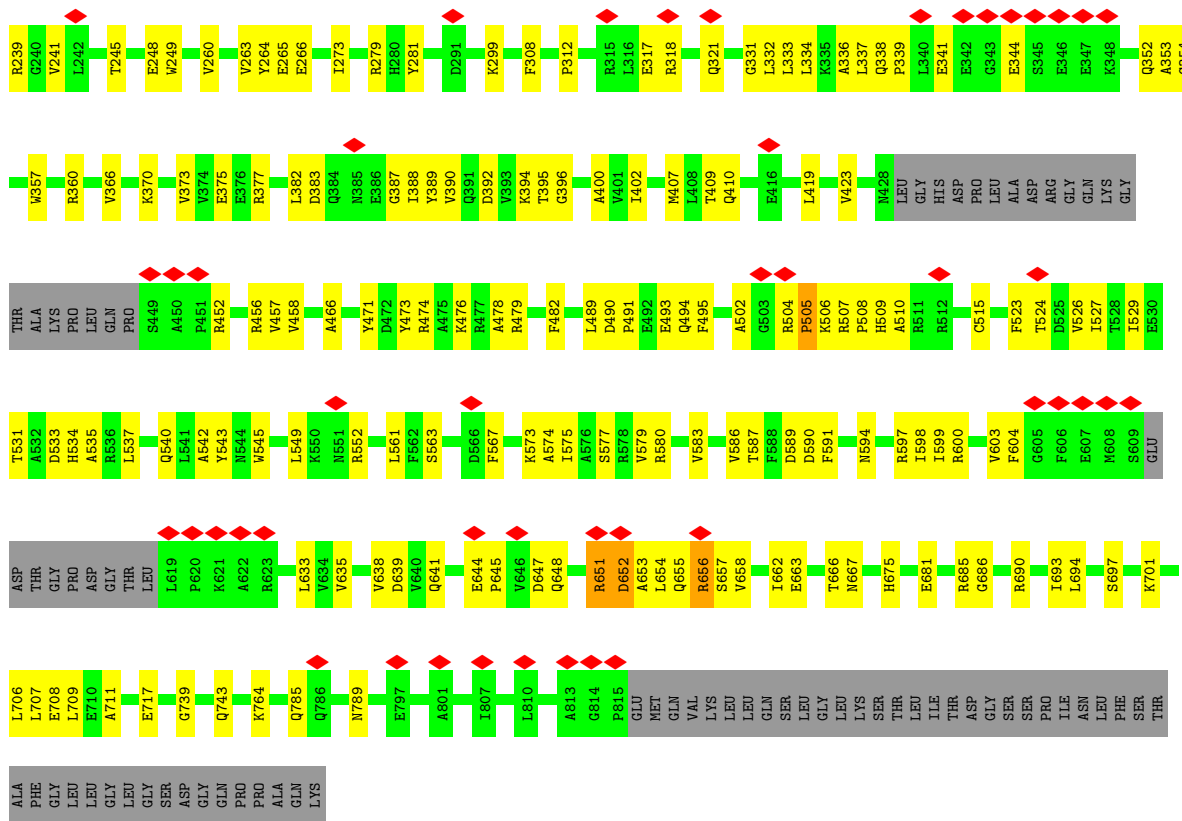
• Molecule 1: Major vault protein





• Molecule 1: Major vault protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9793	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.180	Depositor
Minimum map value	-0.144	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	676.0, 676.0, 676.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.69, 1.69, 1.69	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.25	0/6255	0.53	0/8475
1	AA	0.25	0/6255	0.53	0/8475
1	AB	0.25	0/6255	0.53	0/8475
1	AC	0.25	0/6255	0.53	0/8475
1	B	0.25	0/6255	0.53	0/8475
1	BA	0.25	0/6255	0.53	0/8475
1	BB	0.25	0/6255	0.53	0/8475
1	C	0.25	0/6255	0.53	0/8475
1	CA	0.25	0/6255	0.53	0/8475
1	CB	0.25	0/6255	0.53	0/8475
1	D	0.25	0/6255	0.53	0/8475
1	DA	0.25	0/6255	0.53	0/8475
1	DB	0.25	0/6255	0.53	0/8475
1	E	0.25	0/6255	0.53	0/8475
1	EA	0.25	0/6255	0.53	0/8475
1	EB	0.25	0/6255	0.53	0/8475
1	F	0.25	0/6255	0.53	0/8475
1	FA	0.25	0/6255	0.53	0/8475
1	FB	0.25	0/6255	0.53	0/8475
1	G	0.25	0/6255	0.53	0/8475
1	GA	0.25	0/6255	0.53	0/8475
1	GB	0.25	0/6255	0.53	0/8475
1	H	0.25	0/6255	0.53	0/8475
1	HA	0.25	0/6255	0.53	0/8475
1	HB	0.25	0/6255	0.53	0/8475
1	I	0.25	0/6255	0.53	0/8475
1	IA	0.25	0/6255	0.53	0/8475
1	IB	0.25	0/6255	0.53	0/8475
1	J	0.25	0/6255	0.53	0/8475
1	JA	0.25	0/6255	0.53	0/8475
1	JB	0.25	0/6255	0.53	0/8475
1	K	0.25	0/6255	0.53	0/8475
1	KA	0.25	0/6255	0.53	0/8475
1	KB	0.25	0/6255	0.53	0/8475

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	L	0.25	0/6255	0.53	0/8475
1	LA	0.25	0/6255	0.53	0/8475
1	LB	0.25	0/6255	0.53	0/8475
1	M	0.25	0/6255	0.53	0/8475
1	MA	0.25	0/6255	0.53	0/8475
1	MB	0.25	0/6255	0.53	0/8475
1	N	0.25	0/6255	0.53	0/8475
1	NA	0.25	0/6255	0.53	0/8475
1	NB	0.25	0/6255	0.53	0/8475
1	O	0.25	0/6255	0.53	0/8475
1	OA	0.25	0/6255	0.53	0/8475
1	OB	0.25	0/6255	0.53	0/8475
1	P	0.25	0/6255	0.53	0/8475
1	PA	0.25	0/6255	0.53	0/8475
1	PB	0.25	0/6255	0.53	0/8475
1	Q	0.25	0/6255	0.53	0/8475
1	QA	0.25	0/6255	0.53	0/8475
1	QB	0.25	0/6255	0.53	0/8475
1	R	0.25	0/6255	0.53	0/8475
1	RA	0.25	0/6255	0.53	0/8475
1	RB	0.25	0/6255	0.53	0/8475
1	S	0.25	0/6255	0.53	0/8475
1	SA	0.25	0/6255	0.53	0/8475
1	SB	0.25	0/6255	0.53	0/8475
1	T	0.25	0/6255	0.53	0/8475
1	TA	0.25	0/6255	0.53	0/8475
1	TB	0.25	0/6255	0.53	0/8475
1	UA	0.25	0/6255	0.53	0/8475
1	UB	0.25	0/6255	0.53	0/8475
1	V	0.25	0/6255	0.53	0/8475
1	VA	0.25	0/6255	0.53	0/8475
1	VB	0.25	0/6255	0.53	0/8475
1	W	0.25	0/6255	0.53	0/8475
1	WA	0.25	0/6255	0.53	0/8475
1	WB	0.25	0/6255	0.53	0/8475
1	X	0.25	0/6255	0.53	0/8475
1	XA	0.25	0/6255	0.53	0/8475
1	XB	0.25	0/6255	0.53	0/8475
1	Y	0.25	0/6255	0.53	0/8475
1	YA	0.25	0/6255	0.53	0/8475
1	YB	0.25	0/6255	0.53	0/8475
1	Z	0.25	0/6255	0.53	0/8475
1	ZA	0.25	0/6255	0.53	0/8475

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	ZB	0.25	0/6255	0.53	0/8475
All	All	0.25	0/487890	0.53	0/661050

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	0	2
1	AA	0	2
1	AB	0	2
1	AC	0	2
1	B	0	2
1	BA	0	2
1	BB	0	2
1	C	0	2
1	CA	0	2
1	CB	0	2
1	D	0	2
1	DA	0	2
1	DB	0	2
1	E	0	2
1	EA	0	2
1	EB	0	2
1	F	0	2
1	FA	0	2
1	FB	0	2
1	G	0	2
1	GA	0	2
1	GB	0	2
1	H	0	2
1	HA	0	2
1	HB	0	2
1	I	0	2
1	IA	0	2
1	IB	0	2
1	J	0	2
1	JA	0	2
1	JB	0	2
1	K	0	2
1	KA	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	KB	0	2
1	L	0	2
1	LA	0	2
1	LB	0	2
1	M	0	2
1	MA	0	2
1	MB	0	2
1	N	0	2
1	NA	0	2
1	NB	0	2
1	O	0	2
1	OA	0	2
1	OB	0	2
1	P	0	2
1	PA	0	2
1	PB	0	2
1	Q	0	2
1	QA	0	2
1	QB	0	2
1	R	0	2
1	RA	0	2
1	RB	0	2
1	S	0	2
1	SA	0	2
1	SB	0	2
1	T	0	2
1	TA	0	2
1	TB	0	2
1	UA	0	2
1	UB	0	2
1	V	0	2
1	VA	0	2
1	VB	0	2
1	W	0	2
1	WA	0	2
1	WB	0	2
1	X	0	2
1	XA	0	2
1	XB	0	2
1	Y	0	2
1	YA	0	2
1	YB	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	Z	0	2
1	ZA	0	2
1	ZB	0	2
All	All	0	156

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 156 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	644	GLU	Peptide
1	A	651	ARG	Peptide
1	B	644	GLU	Peptide
1	B	651	ARG	Peptide
1	C	644	GLU	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in 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	6150	0	6175	211	0
1	AA	6150	0	6175	155	0
1	AB	6150	0	6175	166	0
1	AC	6150	0	6175	192	0
1	B	6150	0	6175	177	0
1	BA	6150	0	6175	172	0
1	BB	6150	0	6175	196	0
1	C	6150	0	6175	210	0
1	CA	6150	0	6175	158	0
1	CB	6150	0	6175	188	0
1	D	6150	0	6175	177	0
1	DA	6150	0	6175	164	0
1	DB	6150	0	6175	165	0
1	E	6150	0	6175	189	0
1	EA	6150	0	6175	159	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	EB	6150	0	6175	194	0
1	F	6150	0	6175	169	0
1	FA	6150	0	6175	165	0
1	FB	6150	0	6175	199	0
1	G	6150	0	6175	185	0
1	GA	6150	0	6175	167	0
1	GB	6150	0	6175	175	0
1	H	6150	0	6175	211	0
1	HA	6150	0	6175	163	0
1	HB	6150	0	6175	183	0
1	I	6150	0	6175	178	0
1	IA	6150	0	6175	184	0
1	IB	6150	0	6175	204	0
1	J	6150	0	6175	222	0
1	JA	6150	0	6175	162	0
1	JB	6150	0	6175	209	0
1	K	6150	0	6175	176	0
1	KA	6150	0	6175	210	0
1	KB	6150	0	6175	182	0
1	L	6150	0	6175	170	0
1	LA	6150	0	6175	159	0
1	LB	6150	0	6175	213	0
1	M	6150	0	6175	167	0
1	MA	6150	0	6175	197	0
1	MB	6150	0	6175	234	0
1	N	6150	0	6175	161	0
1	NA	6150	0	6175	165	0
1	NB	6150	0	6175	181	0
1	O	6150	0	6175	193	0
1	OA	6150	0	6175	165	0
1	OB	6150	0	6175	179	0
1	P	6150	0	6175	187	0
1	PA	6150	0	6175	166	0
1	PB	6150	0	6175	180	0
1	Q	6150	0	6175	198	0
1	QA	6150	0	6175	168	0
1	QB	6150	0	6175	229	0
1	R	6150	0	6175	187	0
1	RA	6150	0	6175	163	0
1	RB	6150	0	6175	213	0
1	S	6150	0	6175	159	0
1	SA	6150	0	6175	167	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	SB	6150	0	6175	162	0
1	T	6150	0	6175	156	0
1	TA	6150	0	6175	171	0
1	TB	6150	0	6175	160	0
1	UA	6150	0	6175	175	0
1	UB	6150	0	6175	272	0
1	V	6150	0	6175	181	0
1	VA	6150	0	6175	163	0
1	VB	6150	0	6175	290	0
1	W	6150	0	6175	153	0
1	WA	6150	0	6175	168	0
1	WB	6150	0	6175	191	0
1	X	6150	0	6175	191	0
1	XA	6150	0	6175	162	0
1	XB	6150	0	6175	170	0
1	Y	6150	0	6175	158	0
1	YA	6150	0	6175	165	0
1	YB	6150	0	6175	185	0
1	Z	6150	0	6175	176	0
1	ZA	6150	0	6175	165	0
1	ZB	6150	0	6175	202	0
All	All	479700	0	481650	12482	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 13.

The worst 5 of 12482 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:QB:9:ARG:HH12	1:RB:21:GLN:CA	1.60	1.15
1:QB:9:ARG:HH12	1:RB:21:GLN:HA	1.14	1.07
1:QB:32:PRO:CG	1:RB:78:THR:HG21	1.86	1.05
1:QB:32:PRO:HG3	1:RB:78:THR:HG21	1.33	1.04
1:QB:9:ARG:NH1	1:RB:21:GLN:HA	1.72	1.03

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 PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	AA	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	AB	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	AC	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	B	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	BA	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	BB	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	C	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	CA	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	CB	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	D	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	DA	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	DB	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	E	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	EA	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	EB	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	F	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	FA	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	FB	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	G	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	GA	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	GB	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	H	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	HA	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	HB	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	IA	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	IB	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	J	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	JA	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	JB	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	K	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	KA	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	KB	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	L	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	LA	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	LB	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	M	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	MA	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	MB	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	N	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	NA	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	NB	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	O	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	OA	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	OB	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	P	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	PA	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	PB	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	Q	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	QA	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	QB	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	R	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	RA	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	RB	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	S	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	SA	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	SB	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	T	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	TA	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	TB	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	UA	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	UB	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	V	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	VA	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	VB	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	W	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	WA	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	WB	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	X	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	XA	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	XB	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	Y	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	YA	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	YB	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	Z	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	ZA	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
1	ZB	776/861 (90%)	710 (92%)	63 (8%)	3 (0%)	34	70
All	All	60528/67158 (90%)	55380 (92%)	4914 (8%)	234 (0%)	38	70

5 of 234 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	652	ASP
1	B	652	ASP
1	C	652	ASP
1	D	652	ASP
1	E	652	ASP

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	AA	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	AB	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	AC	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	B	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	BA	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	BB	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	C	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	CA	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	CB	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	D	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	DA	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	DB	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	E	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	EA	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	EB	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	F	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	FA	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	FB	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	G	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	GA	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	GB	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	H	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	HA	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	HB	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	I	655/727 (90%)	652 (100%)	3 (0%)	88	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	IA	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	IB	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	J	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	JA	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	JB	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	K	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	KA	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	KB	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	L	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	LA	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	LB	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	M	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	MA	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	MB	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	N	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	NA	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	NB	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	O	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	OA	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	OB	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	P	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	PA	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	PB	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	Q	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	QA	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	QB	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	R	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	RA	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	RB	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	S	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	SA	655/727 (90%)	652 (100%)	3 (0%)	88	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	SB	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	T	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	TA	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	TB	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	UA	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	UB	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	V	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	VA	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	VB	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	W	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	WA	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	WB	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	X	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	XA	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	XB	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	Y	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	YA	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	YB	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	Z	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	ZA	655/727 (90%)	652 (100%)	3 (0%)	88	94
1	ZB	655/727 (90%)	652 (100%)	3 (0%)	88	94
All	All	51090/56706 (90%)	50856 (100%)	234 (0%)	89	94

5 of 234 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	NA	239	ARG
1	WB	656	ARG
1	WA	656	ARG
1	WB	27	ARG
1	PB	239	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

Mol	Chain	Res	Type
1	VA	228	HIS
1	IB	228	HIS
1	YB	40	ASN
1	XA	228	HIS
1	DB	228	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 monosaccharides 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.

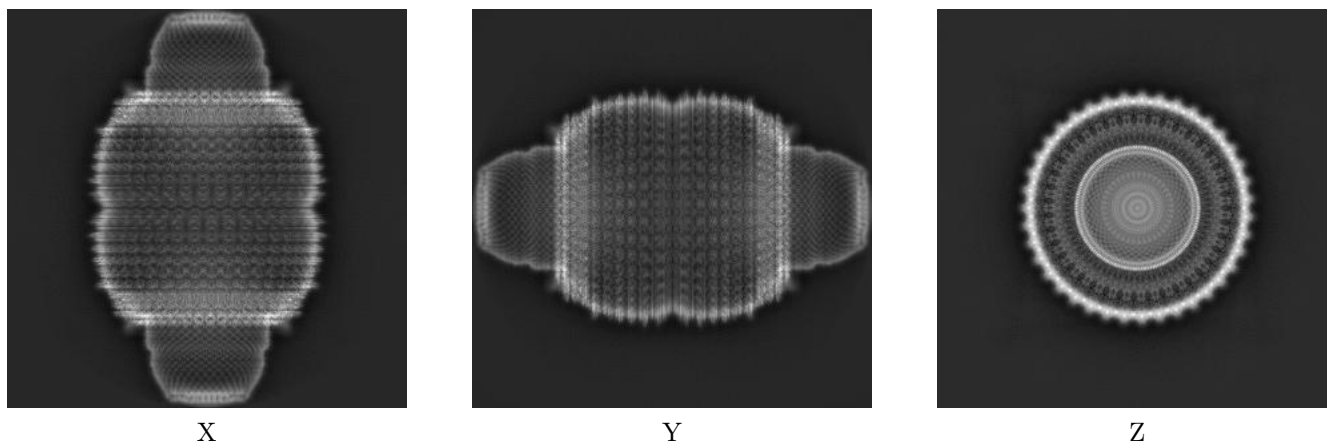
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13478. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

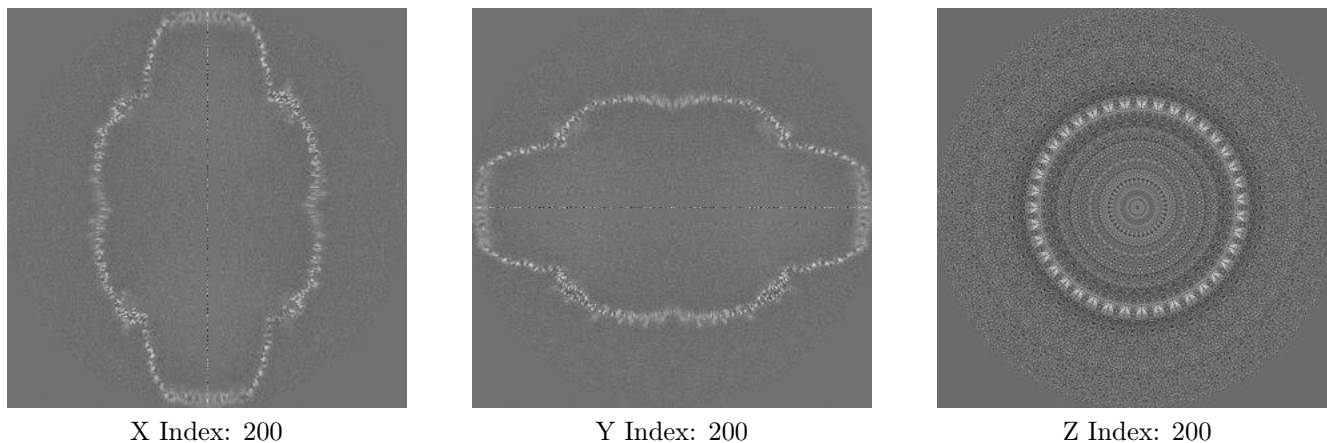
6.1.1 Primary map



The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

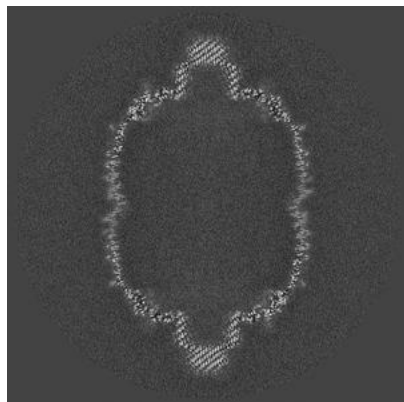
6.2.1 Primary map



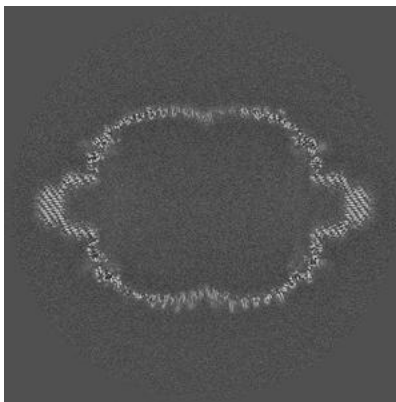
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

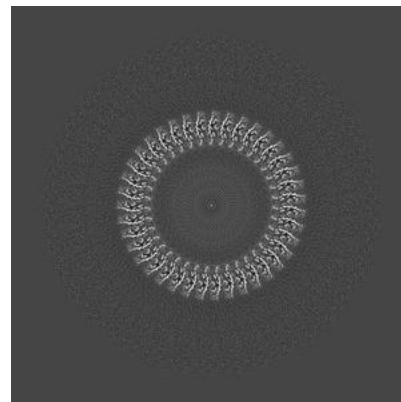
6.3.1 Primary map



X Index: 255



Y Index: 255



Z Index: 307

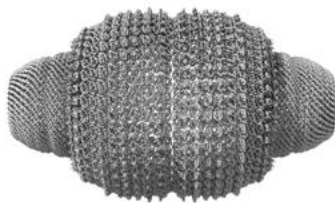
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

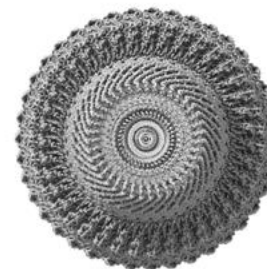
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

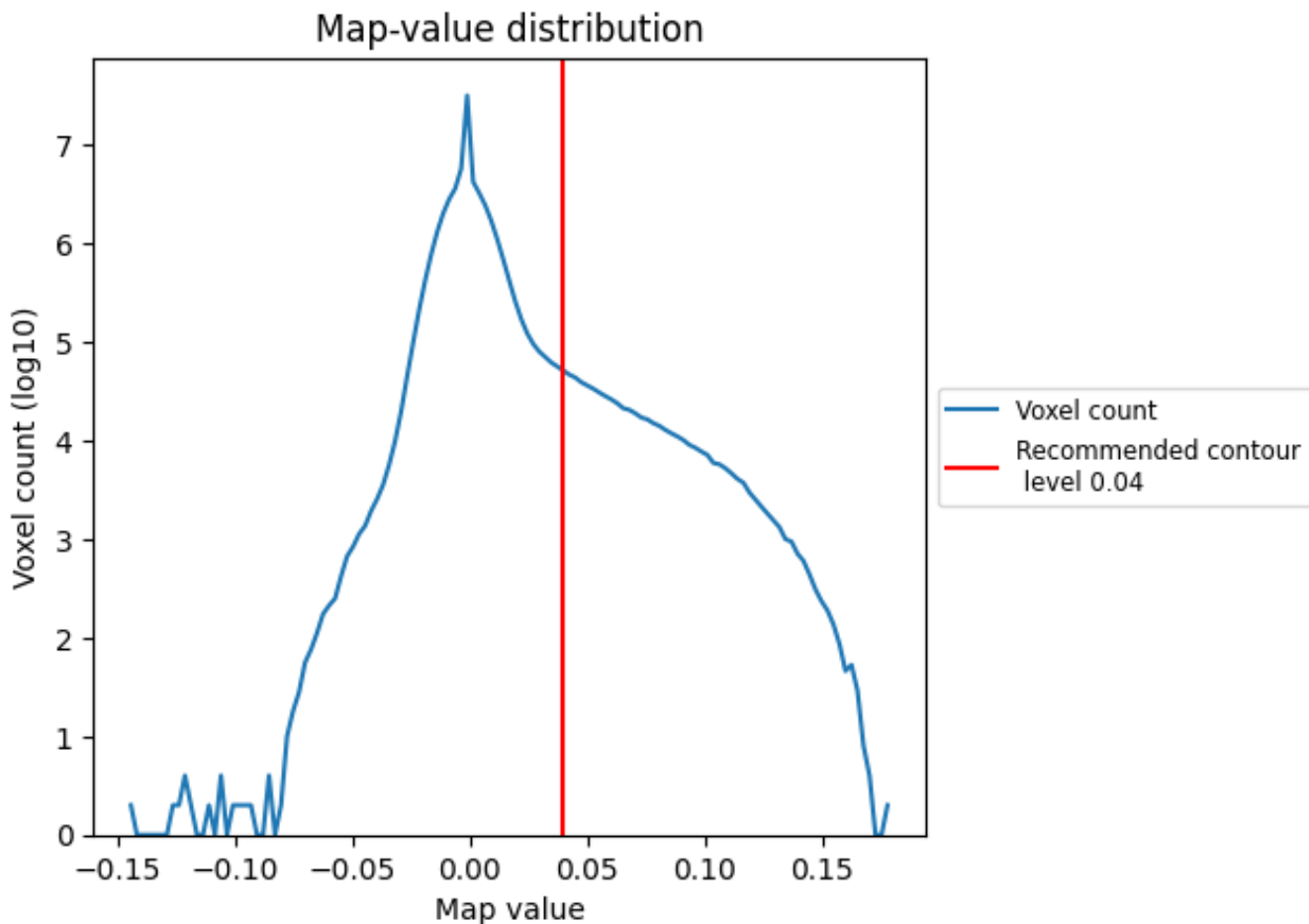
6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

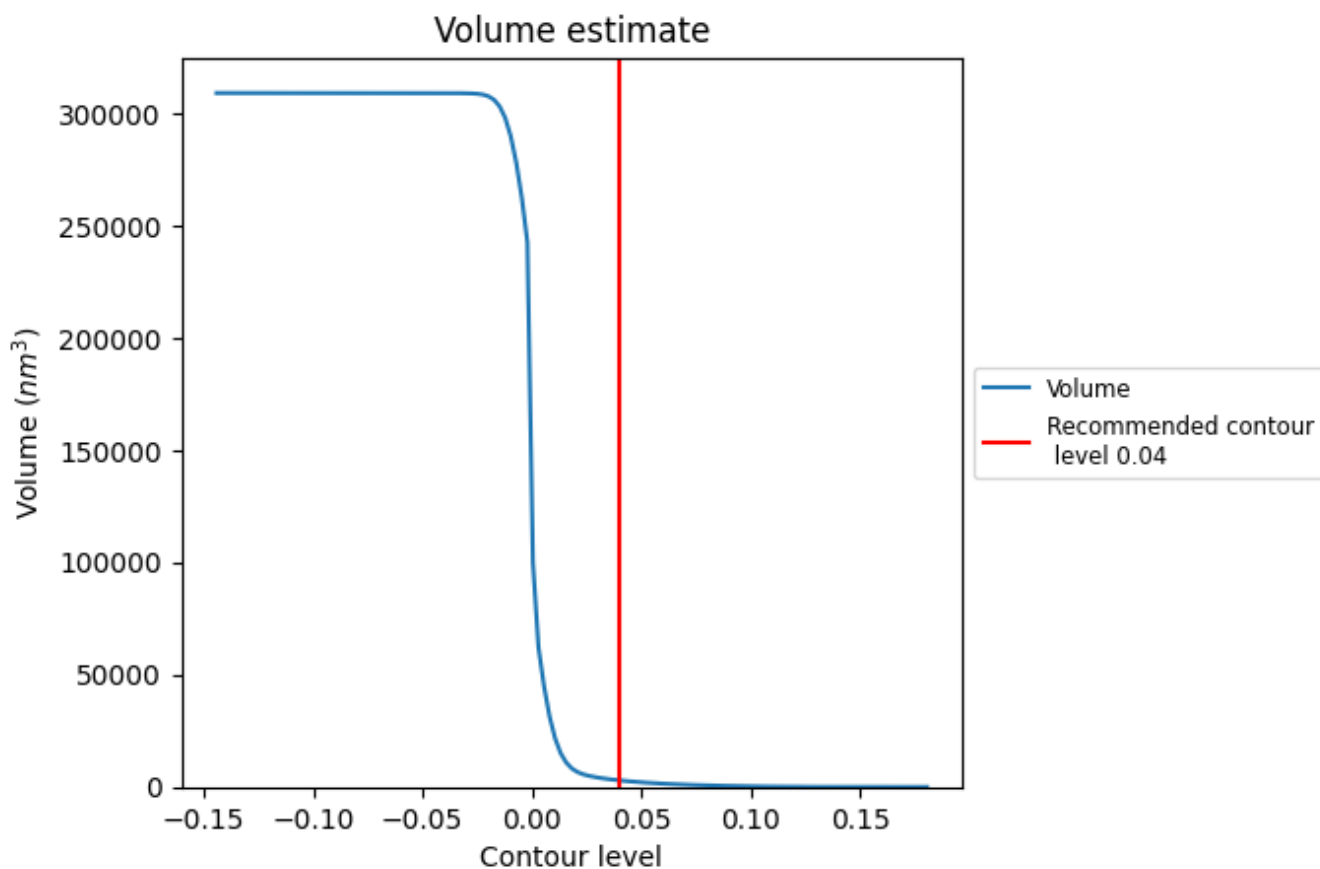
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

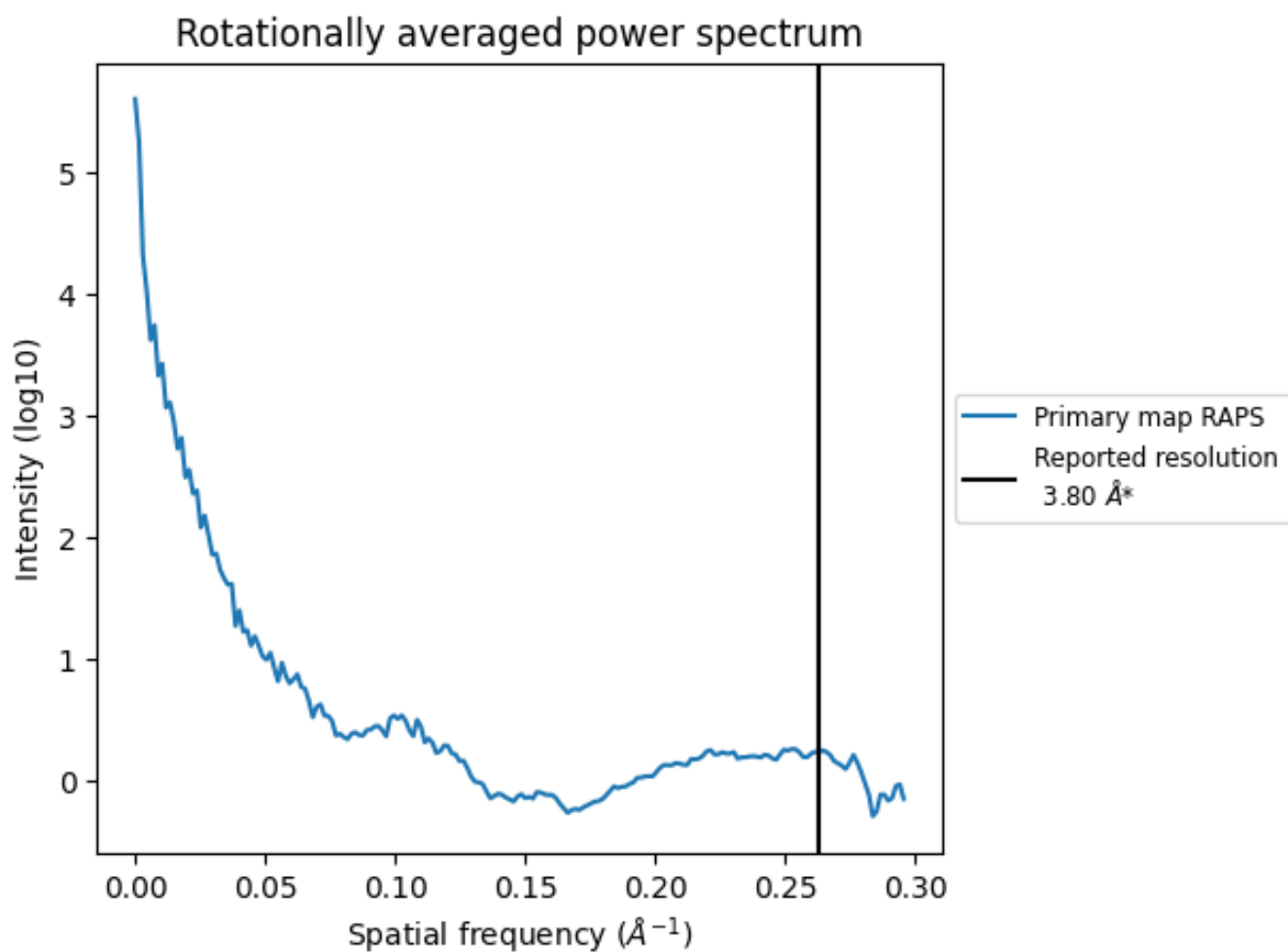
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 2923 nm³; this corresponds to an approximate mass of 2640 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

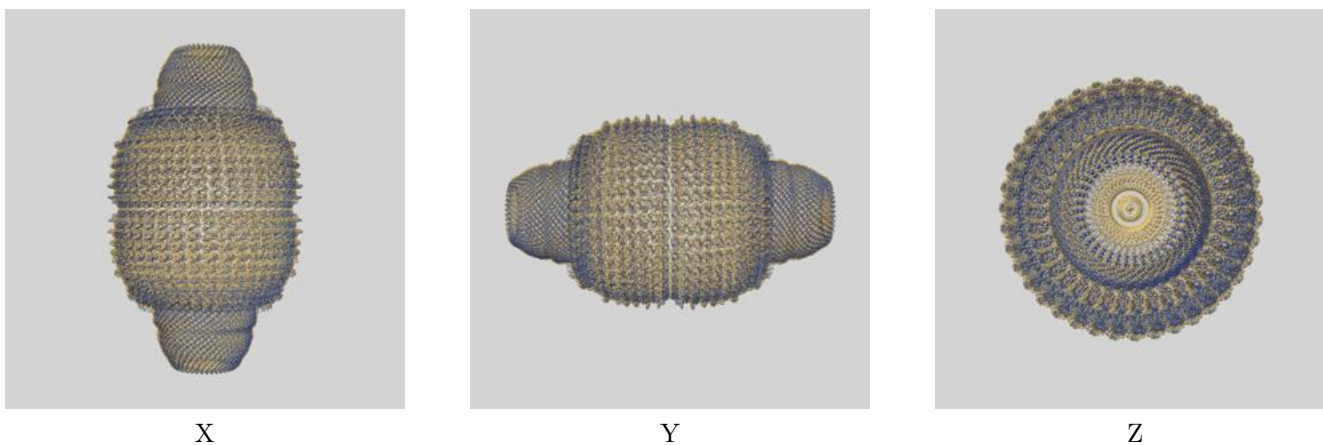
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

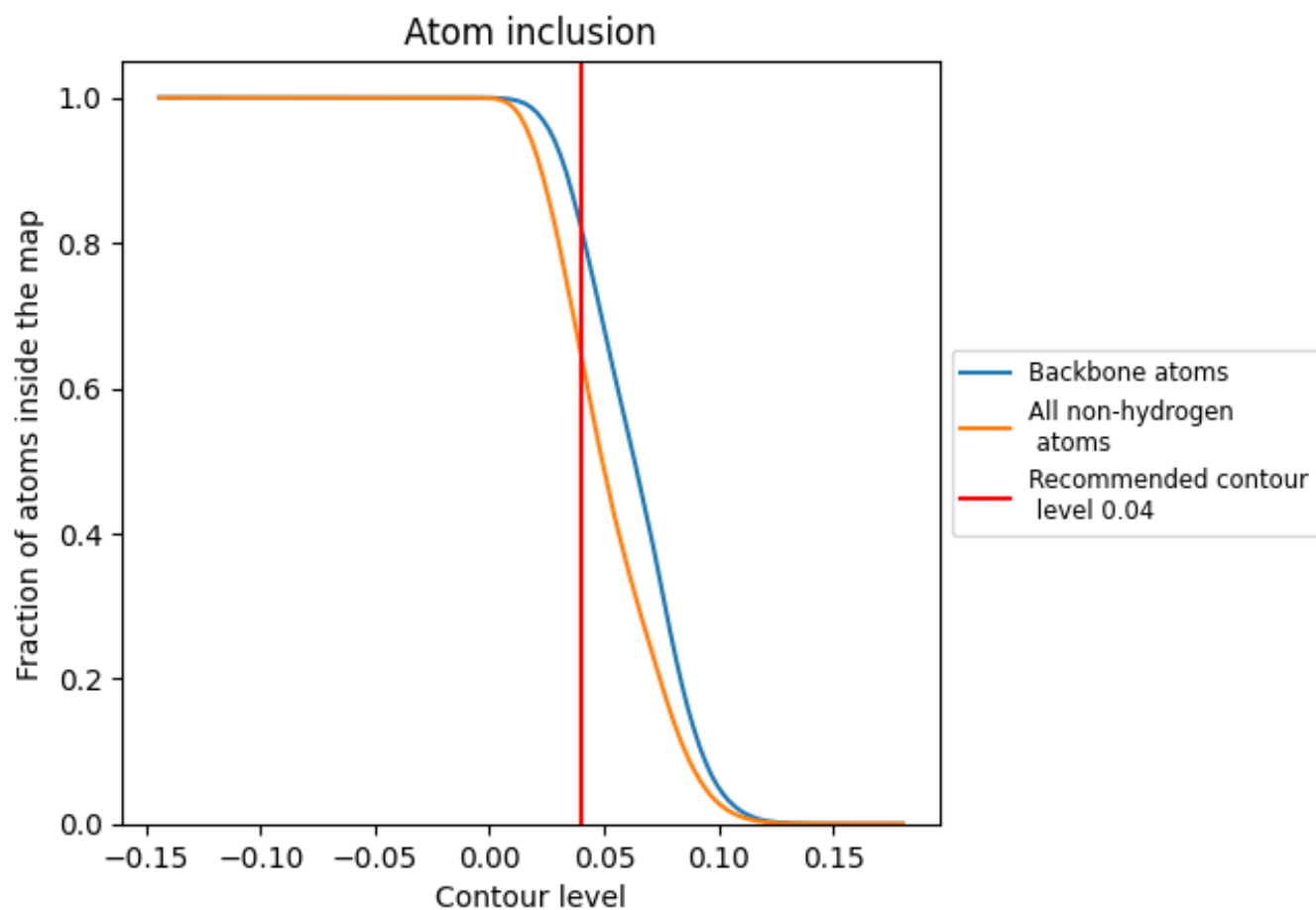
This section contains information regarding the fit between EMDB map EMD-13478 and PDB model 7PKR. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.