wwPDB EM Validation Summary Report (i)

Mar 10, 2022 – 08:04 pm GMT

PDB ID	:	7PKZ
EMDB ID	:	EMD-13483
Title	:	Vault structure in committed conformation
Authors	:	Guerra, P.; Gonzalez-Alamos, M.; Llauro, A.; Casanas, A.; Querol-Audi, J.; de Pablo, P.; Verdaguer, N.
Deposited on	:	2021-08-27
Resolution	:	9.80 Å(reported)
Based on initial model	:	4HL8

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

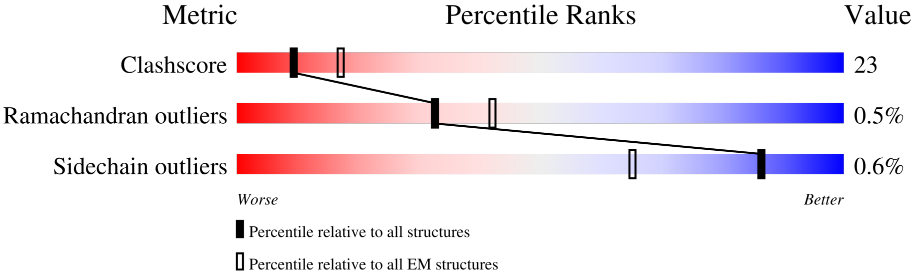
EMDB validation analysis	:	0.0.0.dev97
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

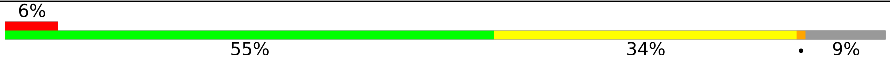
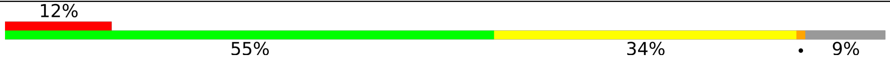
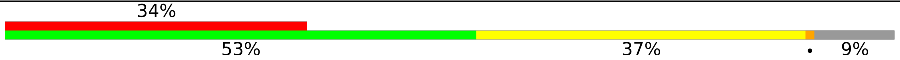
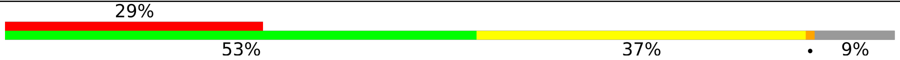
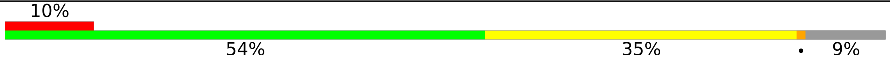
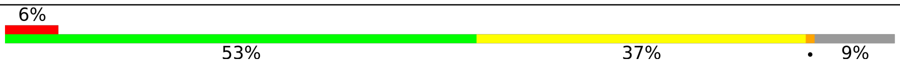
The reported resolution of this entry is 9.80 Å.

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 <=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	
1	AA	861	
1	AB	861	
1	AC	861	
1	B	861	
1	BA	861	
1	BB	861	
1	C	861	

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Mol	Chain	Length	Quality of chain
1	CA	861	7% 55% 34% • 9%
1	CB	861	7% 54% 36% • 9%
1	D	861	33% 48% 42% • 9%
1	DA	861	9% 55% 34% • 9%
1	DB	861	5% 53% 36% • 9%
1	E	861	9% 51% 39% • 9%
1	EA	861	7% 55% 35% • 9%
1	EB	861	7% 53% 36% • 9%
1	F	861	29% 49% 41% • 9%
1	FA	861	8% 54% 35% • 9%
1	FB	861	5% 51% 39% • 9%
1	G	861	8% 52% 37% • 9%
1	GA	861	6% 55% 35% • 9%
1	GB	861	11% 52% 38% • 9%
1	H	861	25% 54% 36% • 9%
1	HA	861	7% 54% 36% • 9%
1	HB	861	16% 54% 35% • 9%
1	I	861	7% 53% 36% • 9%
1	IA	861	6% 52% 37% • 9%
1	IB	861	20% 55% 35% • 9%
1	J	861	22% 54% 36% • 9%
1	JA	861	5% 54% 36% • 9%
1	JB	861	22% 54% 35% • 9%
1	K	861	8% 54% 36% • 9%
1	KA	861	7% 53% 37% • 9%

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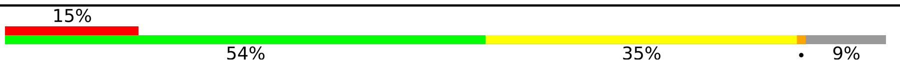
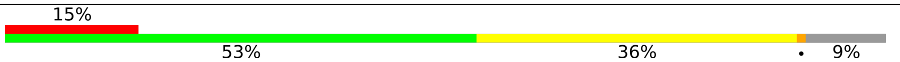
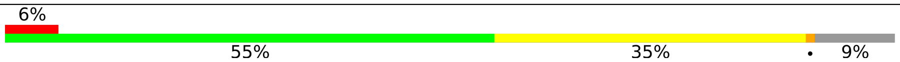
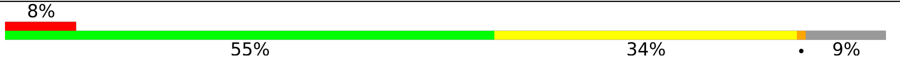
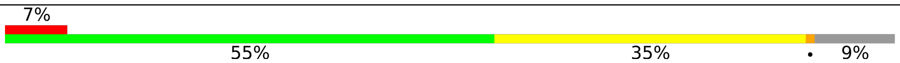
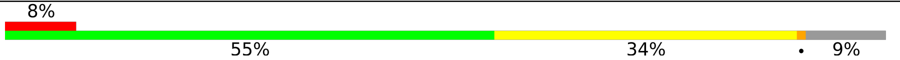
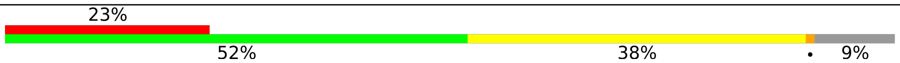
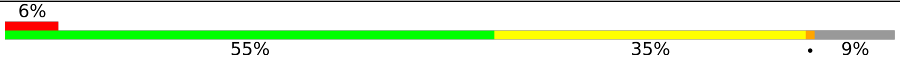
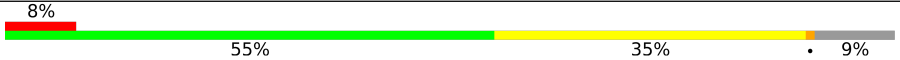
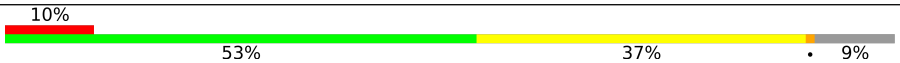
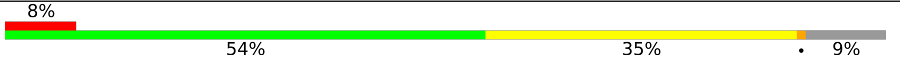
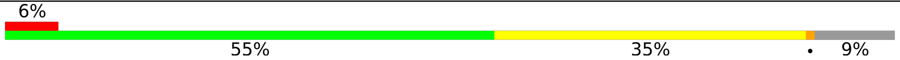
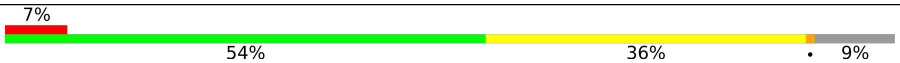
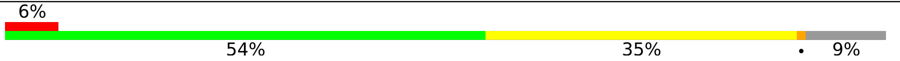
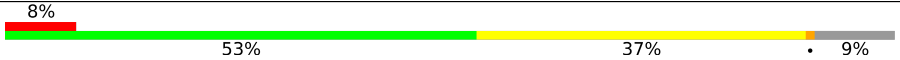
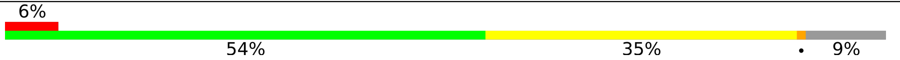
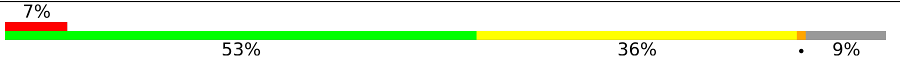
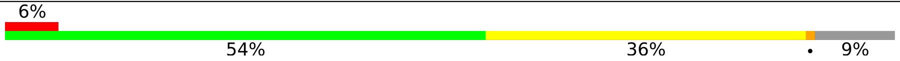
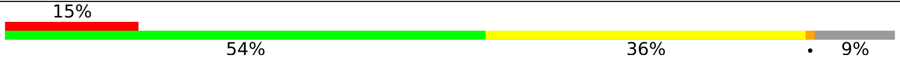
Mol	Chain	Length	Quality of chain
1	KB	861	
1	L	861	
1	LA	861	
1	LB	861	
1	M	861	
1	MA	861	
1	MB	861	
1	N	861	
1	NA	861	
1	NB	861	
1	O	861	
1	OA	861	
1	OB	861	
1	P	861	
1	PA	861	
1	PB	861	
1	Q	861	
1	QA	861	
1	QB	861	
1	R	861	
1	RA	861	
1	RB	861	
1	S	861	
1	SA	861	
1	SB	861	

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Mol	Chain	Length	Quality of chain
1	T	861	7% 53% 36% • 9%
1	TA	861	7% 54% 36% • 9%
1	TB	861	9% 53% 37% • 9%
1	UA	861	18% 55% 35% • 9%
1	UB	861	19% 52% 37% • 9%
1	V	861	7% 54% 35% • 9%
1	VA	861	7% 55% 35% • 9%
1	VB	861	14% 51% 38% • 9%
1	W	861	7% 54% 35% • 9%
1	WA	861	18% 55% 35% • 9%
1	WB	861	17% 52% 37% • 9%
1	X	861	8% 54% 36% • 9%
1	XA	861	7% 53% 37% • 9%
1	XB	861	16% 53% 36% • 9%
1	Y	861	7% 55% 35% • 9%
1	YA	861	15% 55% 34% • 9%
1	YB	861	20% 54% 36% • 9%
1	Z	861	9% 55% 34% • 9%
1	ZA	861	6% 53% 37% • 9%
1	ZB	861	32% 54% 36% • 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
1	A	782	Total C N O S 6150 3869 1101 1165 15	0	0
1	B	782	Total C N O S 6150 3869 1101 1165 15	0	0
1	C	782	Total C N O S 6150 3869 1101 1165 15	0	0
1	D	782	Total C N O S 6150 3869 1101 1165 15	0	0
1	E	782	Total C N O S 6150 3869 1101 1165 15	0	0
1	F	782	Total C N O S 6150 3869 1101 1165 15	0	0
1	G	782	Total C N O S 6150 3869 1101 1165 15	0	0
1	H	782	Total C N O S 6150 3869 1101 1165 15	0	0
1	I	782	Total C N O S 6150 3869 1101 1165 15	0	0
1	J	782	Total C N O S 6150 3869 1101 1165 15	0	0
1	K	782	Total C N O S 6150 3869 1101 1165 15	0	0
1	L	782	Total C N O S 6150 3869 1101 1165 15	0	0
1	M	782	Total C N O S 6150 3869 1101 1165 15	0	0
1	N	782	Total C N O S 6150 3869 1101 1165 15	0	0
1	O	782	Total C N O S 6150 3869 1101 1165 15	0	0
1	P	782	Total C N O S 6150 3869 1101 1165 15	0	0
1	Q	782	Total C N O S 6150 3869 1101 1165 15	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	S	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	T	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	V	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	W	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	X	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	Y	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	Z	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	AA	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	BA	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	CA	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	DA	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	EA	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	FA	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	GA	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	HA	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	IA	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	JA	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	KA	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	LA	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	MA	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	NA	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	OA	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	PA	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	QA	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	RA	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	SA	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	TA	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	UA	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	VA	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	WA	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	XA	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	YA	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	ZA	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	AB	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	BB	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	CB	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	DB	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	EB	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	FB	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	GB	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	HB	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	IB	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	JB	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	KB	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	LB	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	MB	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	NB	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	OB	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	PB	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	QB	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	RB	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	SB	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	TB	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	UB	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	VB	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	WB	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	XB	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	YB	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	ZB	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0
1	AC	782	Total 6150	C 3869	N 1101	O 1165	S 15	0	0

There are 624 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	ALA	THR	conflict	UNP Q62667

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Chain	Residue	Modelled	Actual	Comment	Reference
A	77	VAL	ILE	conflict	UNP Q62667
A	104	LEU	VAL	conflict	UNP Q62667
A	186	ASP	GLU	conflict	UNP Q62667
A	189	GLU	GLY	conflict	UNP Q62667
A	232	ARG	LEU	conflict	UNP Q62667
A	236	LYS	ARG	conflict	UNP Q62667
A	242	ALA	LEU	conflict	UNP Q62667
B	69	ALA	THR	conflict	UNP Q62667
B	77	VAL	ILE	conflict	UNP Q62667
B	104	LEU	VAL	conflict	UNP Q62667
B	186	ASP	GLU	conflict	UNP Q62667
B	189	GLU	GLY	conflict	UNP Q62667
B	232	ARG	LEU	conflict	UNP Q62667
B	236	LYS	ARG	conflict	UNP Q62667
B	242	ALA	LEU	conflict	UNP Q62667
C	69	ALA	THR	conflict	UNP Q62667
C	77	VAL	ILE	conflict	UNP Q62667
C	104	LEU	VAL	conflict	UNP Q62667
C	186	ASP	GLU	conflict	UNP Q62667
C	189	GLU	GLY	conflict	UNP Q62667
C	232	ARG	LEU	conflict	UNP Q62667
C	236	LYS	ARG	conflict	UNP Q62667
C	242	ALA	LEU	conflict	UNP Q62667
D	69	ALA	THR	conflict	UNP Q62667
D	77	VAL	ILE	conflict	UNP Q62667
D	104	LEU	VAL	conflict	UNP Q62667
D	186	ASP	GLU	conflict	UNP Q62667
D	189	GLU	GLY	conflict	UNP Q62667
D	232	ARG	LEU	conflict	UNP Q62667
D	236	LYS	ARG	conflict	UNP Q62667
D	242	ALA	LEU	conflict	UNP Q62667
E	69	ALA	THR	conflict	UNP Q62667
E	77	VAL	ILE	conflict	UNP Q62667
E	104	LEU	VAL	conflict	UNP Q62667
E	186	ASP	GLU	conflict	UNP Q62667
E	189	GLU	GLY	conflict	UNP Q62667
E	232	ARG	LEU	conflict	UNP Q62667
E	236	LYS	ARG	conflict	UNP Q62667
E	242	ALA	LEU	conflict	UNP Q62667
F	69	ALA	THR	conflict	UNP Q62667
F	77	VAL	ILE	conflict	UNP Q62667
F	104	LEU	VAL	conflict	UNP Q62667

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Chain	Residue	Modelled	Actual	Comment	Reference
F	186	ASP	GLU	conflict	UNP Q62667
F	189	GLU	GLY	conflict	UNP Q62667
F	232	ARG	LEU	conflict	UNP Q62667
F	236	LYS	ARG	conflict	UNP Q62667
F	242	ALA	LEU	conflict	UNP Q62667
G	69	ALA	THR	conflict	UNP Q62667
G	77	VAL	ILE	conflict	UNP Q62667
G	104	LEU	VAL	conflict	UNP Q62667
G	186	ASP	GLU	conflict	UNP Q62667
G	189	GLU	GLY	conflict	UNP Q62667
G	232	ARG	LEU	conflict	UNP Q62667
G	236	LYS	ARG	conflict	UNP Q62667
G	242	ALA	LEU	conflict	UNP Q62667
H	69	ALA	THR	conflict	UNP Q62667
H	77	VAL	ILE	conflict	UNP Q62667
H	104	LEU	VAL	conflict	UNP Q62667
H	186	ASP	GLU	conflict	UNP Q62667
H	189	GLU	GLY	conflict	UNP Q62667
H	232	ARG	LEU	conflict	UNP Q62667
H	236	LYS	ARG	conflict	UNP Q62667
H	242	ALA	LEU	conflict	UNP Q62667
I	69	ALA	THR	conflict	UNP Q62667
I	77	VAL	ILE	conflict	UNP Q62667
I	104	LEU	VAL	conflict	UNP Q62667
I	186	ASP	GLU	conflict	UNP Q62667
I	189	GLU	GLY	conflict	UNP Q62667
I	232	ARG	LEU	conflict	UNP Q62667
I	236	LYS	ARG	conflict	UNP Q62667
I	242	ALA	LEU	conflict	UNP Q62667
J	69	ALA	THR	conflict	UNP Q62667
J	77	VAL	ILE	conflict	UNP Q62667
J	104	LEU	VAL	conflict	UNP Q62667
J	186	ASP	GLU	conflict	UNP Q62667
J	189	GLU	GLY	conflict	UNP Q62667
J	232	ARG	LEU	conflict	UNP Q62667
J	236	LYS	ARG	conflict	UNP Q62667
J	242	ALA	LEU	conflict	UNP Q62667
K	69	ALA	THR	conflict	UNP Q62667
K	77	VAL	ILE	conflict	UNP Q62667
K	104	LEU	VAL	conflict	UNP Q62667
K	186	ASP	GLU	conflict	UNP Q62667
K	189	GLU	GLY	conflict	UNP Q62667

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Chain	Residue	Modelled	Actual	Comment	Reference
K	232	ARG	LEU	conflict	UNP Q62667
K	236	LYS	ARG	conflict	UNP Q62667
K	242	ALA	LEU	conflict	UNP Q62667
L	69	ALA	THR	conflict	UNP Q62667
L	77	VAL	ILE	conflict	UNP Q62667
L	104	LEU	VAL	conflict	UNP Q62667
L	186	ASP	GLU	conflict	UNP Q62667
L	189	GLU	GLY	conflict	UNP Q62667
L	232	ARG	LEU	conflict	UNP Q62667
L	236	LYS	ARG	conflict	UNP Q62667
L	242	ALA	LEU	conflict	UNP Q62667
M	69	ALA	THR	conflict	UNP Q62667
M	77	VAL	ILE	conflict	UNP Q62667
M	104	LEU	VAL	conflict	UNP Q62667
M	186	ASP	GLU	conflict	UNP Q62667
M	189	GLU	GLY	conflict	UNP Q62667
M	232	ARG	LEU	conflict	UNP Q62667
M	236	LYS	ARG	conflict	UNP Q62667
M	242	ALA	LEU	conflict	UNP Q62667
N	69	ALA	THR	conflict	UNP Q62667
N	77	VAL	ILE	conflict	UNP Q62667
N	104	LEU	VAL	conflict	UNP Q62667
N	186	ASP	GLU	conflict	UNP Q62667
N	189	GLU	GLY	conflict	UNP Q62667
N	232	ARG	LEU	conflict	UNP Q62667
N	236	LYS	ARG	conflict	UNP Q62667
N	242	ALA	LEU	conflict	UNP Q62667
O	69	ALA	THR	conflict	UNP Q62667
O	77	VAL	ILE	conflict	UNP Q62667
O	104	LEU	VAL	conflict	UNP Q62667
O	186	ASP	GLU	conflict	UNP Q62667
O	189	GLU	GLY	conflict	UNP Q62667
O	232	ARG	LEU	conflict	UNP Q62667
O	236	LYS	ARG	conflict	UNP Q62667
O	242	ALA	LEU	conflict	UNP Q62667
P	69	ALA	THR	conflict	UNP Q62667
P	77	VAL	ILE	conflict	UNP Q62667
P	104	LEU	VAL	conflict	UNP Q62667
P	186	ASP	GLU	conflict	UNP Q62667
P	189	GLU	GLY	conflict	UNP Q62667
P	232	ARG	LEU	conflict	UNP Q62667
P	236	LYS	ARG	conflict	UNP Q62667

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Chain	Residue	Modelled	Actual	Comment	Reference
P	242	ALA	LEU	conflict	UNP Q62667
Q	69	ALA	THR	conflict	UNP Q62667
Q	77	VAL	ILE	conflict	UNP Q62667
Q	104	LEU	VAL	conflict	UNP Q62667
Q	186	ASP	GLU	conflict	UNP Q62667
Q	189	GLU	GLY	conflict	UNP Q62667
Q	232	ARG	LEU	conflict	UNP Q62667
Q	236	LYS	ARG	conflict	UNP Q62667
Q	242	ALA	LEU	conflict	UNP Q62667
R	69	ALA	THR	conflict	UNP Q62667
R	77	VAL	ILE	conflict	UNP Q62667
R	104	LEU	VAL	conflict	UNP Q62667
R	186	ASP	GLU	conflict	UNP Q62667
R	189	GLU	GLY	conflict	UNP Q62667
R	232	ARG	LEU	conflict	UNP Q62667
R	236	LYS	ARG	conflict	UNP Q62667
R	242	ALA	LEU	conflict	UNP Q62667
S	69	ALA	THR	conflict	UNP Q62667
S	77	VAL	ILE	conflict	UNP Q62667
S	104	LEU	VAL	conflict	UNP Q62667
S	186	ASP	GLU	conflict	UNP Q62667
S	189	GLU	GLY	conflict	UNP Q62667
S	232	ARG	LEU	conflict	UNP Q62667
S	236	LYS	ARG	conflict	UNP Q62667
S	242	ALA	LEU	conflict	UNP Q62667
T	69	ALA	THR	conflict	UNP Q62667
T	77	VAL	ILE	conflict	UNP Q62667
T	104	LEU	VAL	conflict	UNP Q62667
T	186	ASP	GLU	conflict	UNP Q62667
T	189	GLU	GLY	conflict	UNP Q62667
T	232	ARG	LEU	conflict	UNP Q62667
T	236	LYS	ARG	conflict	UNP Q62667
T	242	ALA	LEU	conflict	UNP Q62667
V	69	ALA	THR	conflict	UNP Q62667
V	77	VAL	ILE	conflict	UNP Q62667
V	104	LEU	VAL	conflict	UNP Q62667
V	186	ASP	GLU	conflict	UNP Q62667
V	189	GLU	GLY	conflict	UNP Q62667
V	232	ARG	LEU	conflict	UNP Q62667
V	236	LYS	ARG	conflict	UNP Q62667
V	242	ALA	LEU	conflict	UNP Q62667
W	69	ALA	THR	conflict	UNP Q62667

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Chain	Residue	Modelled	Actual	Comment	Reference
W	77	VAL	ILE	conflict	UNP Q62667
W	104	LEU	VAL	conflict	UNP Q62667
W	186	ASP	GLU	conflict	UNP Q62667
W	189	GLU	GLY	conflict	UNP Q62667
W	232	ARG	LEU	conflict	UNP Q62667
W	236	LYS	ARG	conflict	UNP Q62667
W	242	ALA	LEU	conflict	UNP Q62667
X	69	ALA	THR	conflict	UNP Q62667
X	77	VAL	ILE	conflict	UNP Q62667
X	104	LEU	VAL	conflict	UNP Q62667
X	186	ASP	GLU	conflict	UNP Q62667
X	189	GLU	GLY	conflict	UNP Q62667
X	232	ARG	LEU	conflict	UNP Q62667
X	236	LYS	ARG	conflict	UNP Q62667
X	242	ALA	LEU	conflict	UNP Q62667
Y	69	ALA	THR	conflict	UNP Q62667
Y	77	VAL	ILE	conflict	UNP Q62667
Y	104	LEU	VAL	conflict	UNP Q62667
Y	186	ASP	GLU	conflict	UNP Q62667
Y	189	GLU	GLY	conflict	UNP Q62667
Y	232	ARG	LEU	conflict	UNP Q62667
Y	236	LYS	ARG	conflict	UNP Q62667
Y	242	ALA	LEU	conflict	UNP Q62667
Z	69	ALA	THR	conflict	UNP Q62667
Z	77	VAL	ILE	conflict	UNP Q62667
Z	104	LEU	VAL	conflict	UNP Q62667
Z	186	ASP	GLU	conflict	UNP Q62667
Z	189	GLU	GLY	conflict	UNP Q62667
Z	232	ARG	LEU	conflict	UNP Q62667
Z	236	LYS	ARG	conflict	UNP Q62667
Z	242	ALA	LEU	conflict	UNP Q62667
AA	69	ALA	THR	conflict	UNP Q62667
AA	77	VAL	ILE	conflict	UNP Q62667
AA	104	LEU	VAL	conflict	UNP Q62667
AA	186	ASP	GLU	conflict	UNP Q62667
AA	189	GLU	GLY	conflict	UNP Q62667
AA	232	ARG	LEU	conflict	UNP Q62667
AA	236	LYS	ARG	conflict	UNP Q62667
AA	242	ALA	LEU	conflict	UNP Q62667
BA	69	ALA	THR	conflict	UNP Q62667
BA	77	VAL	ILE	conflict	UNP Q62667
BA	104	LEU	VAL	conflict	UNP Q62667

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Chain	Residue	Modelled	Actual	Comment	Reference
BA	186	ASP	GLU	conflict	UNP Q62667
BA	189	GLU	GLY	conflict	UNP Q62667
BA	232	ARG	LEU	conflict	UNP Q62667
BA	236	LYS	ARG	conflict	UNP Q62667
BA	242	ALA	LEU	conflict	UNP Q62667
CA	69	ALA	THR	conflict	UNP Q62667
CA	77	VAL	ILE	conflict	UNP Q62667
CA	104	LEU	VAL	conflict	UNP Q62667
CA	186	ASP	GLU	conflict	UNP Q62667
CA	189	GLU	GLY	conflict	UNP Q62667
CA	232	ARG	LEU	conflict	UNP Q62667
CA	236	LYS	ARG	conflict	UNP Q62667
CA	242	ALA	LEU	conflict	UNP Q62667
DA	69	ALA	THR	conflict	UNP Q62667
DA	77	VAL	ILE	conflict	UNP Q62667
DA	104	LEU	VAL	conflict	UNP Q62667
DA	186	ASP	GLU	conflict	UNP Q62667
DA	189	GLU	GLY	conflict	UNP Q62667
DA	232	ARG	LEU	conflict	UNP Q62667
DA	236	LYS	ARG	conflict	UNP Q62667
DA	242	ALA	LEU	conflict	UNP Q62667
EA	69	ALA	THR	conflict	UNP Q62667
EA	77	VAL	ILE	conflict	UNP Q62667
EA	104	LEU	VAL	conflict	UNP Q62667
EA	186	ASP	GLU	conflict	UNP Q62667
EA	189	GLU	GLY	conflict	UNP Q62667
EA	232	ARG	LEU	conflict	UNP Q62667
EA	236	LYS	ARG	conflict	UNP Q62667
EA	242	ALA	LEU	conflict	UNP Q62667
FA	69	ALA	THR	conflict	UNP Q62667
FA	77	VAL	ILE	conflict	UNP Q62667
FA	104	LEU	VAL	conflict	UNP Q62667
FA	186	ASP	GLU	conflict	UNP Q62667
FA	189	GLU	GLY	conflict	UNP Q62667
FA	232	ARG	LEU	conflict	UNP Q62667
FA	236	LYS	ARG	conflict	UNP Q62667
FA	242	ALA	LEU	conflict	UNP Q62667
GA	69	ALA	THR	conflict	UNP Q62667
GA	77	VAL	ILE	conflict	UNP Q62667
GA	104	LEU	VAL	conflict	UNP Q62667
GA	186	ASP	GLU	conflict	UNP Q62667
GA	189	GLU	GLY	conflict	UNP Q62667

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Chain	Residue	Modelled	Actual	Comment	Reference
GA	232	ARG	LEU	conflict	UNP Q62667
GA	236	LYS	ARG	conflict	UNP Q62667
GA	242	ALA	LEU	conflict	UNP Q62667
HA	69	ALA	THR	conflict	UNP Q62667
HA	77	VAL	ILE	conflict	UNP Q62667
HA	104	LEU	VAL	conflict	UNP Q62667
HA	186	ASP	GLU	conflict	UNP Q62667
HA	189	GLU	GLY	conflict	UNP Q62667
HA	232	ARG	LEU	conflict	UNP Q62667
HA	236	LYS	ARG	conflict	UNP Q62667
HA	242	ALA	LEU	conflict	UNP Q62667
IA	69	ALA	THR	conflict	UNP Q62667
IA	77	VAL	ILE	conflict	UNP Q62667
IA	104	LEU	VAL	conflict	UNP Q62667
IA	186	ASP	GLU	conflict	UNP Q62667
IA	189	GLU	GLY	conflict	UNP Q62667
IA	232	ARG	LEU	conflict	UNP Q62667
IA	236	LYS	ARG	conflict	UNP Q62667
IA	242	ALA	LEU	conflict	UNP Q62667
JA	69	ALA	THR	conflict	UNP Q62667
JA	77	VAL	ILE	conflict	UNP Q62667
JA	104	LEU	VAL	conflict	UNP Q62667
JA	186	ASP	GLU	conflict	UNP Q62667
JA	189	GLU	GLY	conflict	UNP Q62667
JA	232	ARG	LEU	conflict	UNP Q62667
JA	236	LYS	ARG	conflict	UNP Q62667
JA	242	ALA	LEU	conflict	UNP Q62667
KA	69	ALA	THR	conflict	UNP Q62667
KA	77	VAL	ILE	conflict	UNP Q62667
KA	104	LEU	VAL	conflict	UNP Q62667
KA	186	ASP	GLU	conflict	UNP Q62667
KA	189	GLU	GLY	conflict	UNP Q62667
KA	232	ARG	LEU	conflict	UNP Q62667
KA	236	LYS	ARG	conflict	UNP Q62667
KA	242	ALA	LEU	conflict	UNP Q62667
LA	69	ALA	THR	conflict	UNP Q62667
LA	77	VAL	ILE	conflict	UNP Q62667
LA	104	LEU	VAL	conflict	UNP Q62667
LA	186	ASP	GLU	conflict	UNP Q62667
LA	189	GLU	GLY	conflict	UNP Q62667
LA	232	ARG	LEU	conflict	UNP Q62667
LA	236	LYS	ARG	conflict	UNP Q62667

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Chain	Residue	Modelled	Actual	Comment	Reference
LA	242	ALA	LEU	conflict	UNP Q62667
MA	69	ALA	THR	conflict	UNP Q62667
MA	77	VAL	ILE	conflict	UNP Q62667
MA	104	LEU	VAL	conflict	UNP Q62667
MA	186	ASP	GLU	conflict	UNP Q62667
MA	189	GLU	GLY	conflict	UNP Q62667
MA	232	ARG	LEU	conflict	UNP Q62667
MA	236	LYS	ARG	conflict	UNP Q62667
MA	242	ALA	LEU	conflict	UNP Q62667
NA	69	ALA	THR	conflict	UNP Q62667
NA	77	VAL	ILE	conflict	UNP Q62667
NA	104	LEU	VAL	conflict	UNP Q62667
NA	186	ASP	GLU	conflict	UNP Q62667
NA	189	GLU	GLY	conflict	UNP Q62667
NA	232	ARG	LEU	conflict	UNP Q62667
NA	236	LYS	ARG	conflict	UNP Q62667
NA	242	ALA	LEU	conflict	UNP Q62667
OA	69	ALA	THR	conflict	UNP Q62667
OA	77	VAL	ILE	conflict	UNP Q62667
OA	104	LEU	VAL	conflict	UNP Q62667
OA	186	ASP	GLU	conflict	UNP Q62667
OA	189	GLU	GLY	conflict	UNP Q62667
OA	232	ARG	LEU	conflict	UNP Q62667
OA	236	LYS	ARG	conflict	UNP Q62667
OA	242	ALA	LEU	conflict	UNP Q62667
PA	69	ALA	THR	conflict	UNP Q62667
PA	77	VAL	ILE	conflict	UNP Q62667
PA	104	LEU	VAL	conflict	UNP Q62667
PA	186	ASP	GLU	conflict	UNP Q62667
PA	189	GLU	GLY	conflict	UNP Q62667
PA	232	ARG	LEU	conflict	UNP Q62667
PA	236	LYS	ARG	conflict	UNP Q62667
PA	242	ALA	LEU	conflict	UNP Q62667
QA	69	ALA	THR	conflict	UNP Q62667
QA	77	VAL	ILE	conflict	UNP Q62667
QA	104	LEU	VAL	conflict	UNP Q62667
QA	186	ASP	GLU	conflict	UNP Q62667
QA	189	GLU	GLY	conflict	UNP Q62667
QA	232	ARG	LEU	conflict	UNP Q62667
QA	236	LYS	ARG	conflict	UNP Q62667
QA	242	ALA	LEU	conflict	UNP Q62667
RA	69	ALA	THR	conflict	UNP Q62667

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Chain	Residue	Modelled	Actual	Comment	Reference
RA	77	VAL	ILE	conflict	UNP Q62667
RA	104	LEU	VAL	conflict	UNP Q62667
RA	186	ASP	GLU	conflict	UNP Q62667
RA	189	GLU	GLY	conflict	UNP Q62667
RA	232	ARG	LEU	conflict	UNP Q62667
RA	236	LYS	ARG	conflict	UNP Q62667
RA	242	ALA	LEU	conflict	UNP Q62667
SA	69	ALA	THR	conflict	UNP Q62667
SA	77	VAL	ILE	conflict	UNP Q62667
SA	104	LEU	VAL	conflict	UNP Q62667
SA	186	ASP	GLU	conflict	UNP Q62667
SA	189	GLU	GLY	conflict	UNP Q62667
SA	232	ARG	LEU	conflict	UNP Q62667
SA	236	LYS	ARG	conflict	UNP Q62667
SA	242	ALA	LEU	conflict	UNP Q62667
TA	69	ALA	THR	conflict	UNP Q62667
TA	77	VAL	ILE	conflict	UNP Q62667
TA	104	LEU	VAL	conflict	UNP Q62667
TA	186	ASP	GLU	conflict	UNP Q62667
TA	189	GLU	GLY	conflict	UNP Q62667
TA	232	ARG	LEU	conflict	UNP Q62667
TA	236	LYS	ARG	conflict	UNP Q62667
TA	242	ALA	LEU	conflict	UNP Q62667
UA	69	ALA	THR	conflict	UNP Q62667
UA	77	VAL	ILE	conflict	UNP Q62667
UA	104	LEU	VAL	conflict	UNP Q62667
UA	186	ASP	GLU	conflict	UNP Q62667
UA	189	GLU	GLY	conflict	UNP Q62667
UA	232	ARG	LEU	conflict	UNP Q62667
UA	236	LYS	ARG	conflict	UNP Q62667
UA	242	ALA	LEU	conflict	UNP Q62667
VA	69	ALA	THR	conflict	UNP Q62667
VA	77	VAL	ILE	conflict	UNP Q62667
VA	104	LEU	VAL	conflict	UNP Q62667
VA	186	ASP	GLU	conflict	UNP Q62667
VA	189	GLU	GLY	conflict	UNP Q62667
VA	232	ARG	LEU	conflict	UNP Q62667
VA	236	LYS	ARG	conflict	UNP Q62667
VA	242	ALA	LEU	conflict	UNP Q62667
WA	69	ALA	THR	conflict	UNP Q62667
WA	77	VAL	ILE	conflict	UNP Q62667
WA	104	LEU	VAL	conflict	UNP Q62667

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Chain	Residue	Modelled	Actual	Comment	Reference
WA	186	ASP	GLU	conflict	UNP Q62667
WA	189	GLU	GLY	conflict	UNP Q62667
WA	232	ARG	LEU	conflict	UNP Q62667
WA	236	LYS	ARG	conflict	UNP Q62667
WA	242	ALA	LEU	conflict	UNP Q62667
XA	69	ALA	THR	conflict	UNP Q62667
XA	77	VAL	ILE	conflict	UNP Q62667
XA	104	LEU	VAL	conflict	UNP Q62667
XA	186	ASP	GLU	conflict	UNP Q62667
XA	189	GLU	GLY	conflict	UNP Q62667
XA	232	ARG	LEU	conflict	UNP Q62667
XA	236	LYS	ARG	conflict	UNP Q62667
XA	242	ALA	LEU	conflict	UNP Q62667
YA	69	ALA	THR	conflict	UNP Q62667
YA	77	VAL	ILE	conflict	UNP Q62667
YA	104	LEU	VAL	conflict	UNP Q62667
YA	186	ASP	GLU	conflict	UNP Q62667
YA	189	GLU	GLY	conflict	UNP Q62667
YA	232	ARG	LEU	conflict	UNP Q62667
YA	236	LYS	ARG	conflict	UNP Q62667
YA	242	ALA	LEU	conflict	UNP Q62667
ZA	69	ALA	THR	conflict	UNP Q62667
ZA	77	VAL	ILE	conflict	UNP Q62667
ZA	104	LEU	VAL	conflict	UNP Q62667
ZA	186	ASP	GLU	conflict	UNP Q62667
ZA	189	GLU	GLY	conflict	UNP Q62667
ZA	232	ARG	LEU	conflict	UNP Q62667
ZA	236	LYS	ARG	conflict	UNP Q62667
ZA	242	ALA	LEU	conflict	UNP Q62667
AB	69	ALA	THR	conflict	UNP Q62667
AB	77	VAL	ILE	conflict	UNP Q62667
AB	104	LEU	VAL	conflict	UNP Q62667
AB	186	ASP	GLU	conflict	UNP Q62667
AB	189	GLU	GLY	conflict	UNP Q62667
AB	232	ARG	LEU	conflict	UNP Q62667
AB	236	LYS	ARG	conflict	UNP Q62667
AB	242	ALA	LEU	conflict	UNP Q62667
BB	69	ALA	THR	conflict	UNP Q62667
BB	77	VAL	ILE	conflict	UNP Q62667
BB	104	LEU	VAL	conflict	UNP Q62667
BB	186	ASP	GLU	conflict	UNP Q62667
BB	189	GLU	GLY	conflict	UNP Q62667

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Chain	Residue	Modelled	Actual	Comment	Reference
BB	232	ARG	LEU	conflict	UNP Q62667
BB	236	LYS	ARG	conflict	UNP Q62667
BB	242	ALA	LEU	conflict	UNP Q62667
CB	69	ALA	THR	conflict	UNP Q62667
CB	77	VAL	ILE	conflict	UNP Q62667
CB	104	LEU	VAL	conflict	UNP Q62667
CB	186	ASP	GLU	conflict	UNP Q62667
CB	189	GLU	GLY	conflict	UNP Q62667
CB	232	ARG	LEU	conflict	UNP Q62667
CB	236	LYS	ARG	conflict	UNP Q62667
CB	242	ALA	LEU	conflict	UNP Q62667
DB	69	ALA	THR	conflict	UNP Q62667
DB	77	VAL	ILE	conflict	UNP Q62667
DB	104	LEU	VAL	conflict	UNP Q62667
DB	186	ASP	GLU	conflict	UNP Q62667
DB	189	GLU	GLY	conflict	UNP Q62667
DB	232	ARG	LEU	conflict	UNP Q62667
DB	236	LYS	ARG	conflict	UNP Q62667
DB	242	ALA	LEU	conflict	UNP Q62667
EB	69	ALA	THR	conflict	UNP Q62667
EB	77	VAL	ILE	conflict	UNP Q62667
EB	104	LEU	VAL	conflict	UNP Q62667
EB	186	ASP	GLU	conflict	UNP Q62667
EB	189	GLU	GLY	conflict	UNP Q62667
EB	232	ARG	LEU	conflict	UNP Q62667
EB	236	LYS	ARG	conflict	UNP Q62667
EB	242	ALA	LEU	conflict	UNP Q62667
FB	69	ALA	THR	conflict	UNP Q62667
FB	77	VAL	ILE	conflict	UNP Q62667
FB	104	LEU	VAL	conflict	UNP Q62667
FB	186	ASP	GLU	conflict	UNP Q62667
FB	189	GLU	GLY	conflict	UNP Q62667
FB	232	ARG	LEU	conflict	UNP Q62667
FB	236	LYS	ARG	conflict	UNP Q62667
FB	242	ALA	LEU	conflict	UNP Q62667
GB	69	ALA	THR	conflict	UNP Q62667
GB	77	VAL	ILE	conflict	UNP Q62667
GB	104	LEU	VAL	conflict	UNP Q62667
GB	186	ASP	GLU	conflict	UNP Q62667
GB	189	GLU	GLY	conflict	UNP Q62667
GB	232	ARG	LEU	conflict	UNP Q62667
GB	236	LYS	ARG	conflict	UNP Q62667

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Chain	Residue	Modelled	Actual	Comment	Reference
GB	242	ALA	LEU	conflict	UNP Q62667
HB	69	ALA	THR	conflict	UNP Q62667
HB	77	VAL	ILE	conflict	UNP Q62667
HB	104	LEU	VAL	conflict	UNP Q62667
HB	186	ASP	GLU	conflict	UNP Q62667
HB	189	GLU	GLY	conflict	UNP Q62667
HB	232	ARG	LEU	conflict	UNP Q62667
HB	236	LYS	ARG	conflict	UNP Q62667
HB	242	ALA	LEU	conflict	UNP Q62667
IB	69	ALA	THR	conflict	UNP Q62667
IB	77	VAL	ILE	conflict	UNP Q62667
IB	104	LEU	VAL	conflict	UNP Q62667
IB	186	ASP	GLU	conflict	UNP Q62667
IB	189	GLU	GLY	conflict	UNP Q62667
IB	232	ARG	LEU	conflict	UNP Q62667
IB	236	LYS	ARG	conflict	UNP Q62667
IB	242	ALA	LEU	conflict	UNP Q62667
JB	69	ALA	THR	conflict	UNP Q62667
JB	77	VAL	ILE	conflict	UNP Q62667
JB	104	LEU	VAL	conflict	UNP Q62667
JB	186	ASP	GLU	conflict	UNP Q62667
JB	189	GLU	GLY	conflict	UNP Q62667
JB	232	ARG	LEU	conflict	UNP Q62667
JB	236	LYS	ARG	conflict	UNP Q62667
JB	242	ALA	LEU	conflict	UNP Q62667
KB	69	ALA	THR	conflict	UNP Q62667
KB	77	VAL	ILE	conflict	UNP Q62667
KB	104	LEU	VAL	conflict	UNP Q62667
KB	186	ASP	GLU	conflict	UNP Q62667
KB	189	GLU	GLY	conflict	UNP Q62667
KB	232	ARG	LEU	conflict	UNP Q62667
KB	236	LYS	ARG	conflict	UNP Q62667
KB	242	ALA	LEU	conflict	UNP Q62667
LB	69	ALA	THR	conflict	UNP Q62667
LB	77	VAL	ILE	conflict	UNP Q62667
LB	104	LEU	VAL	conflict	UNP Q62667
LB	186	ASP	GLU	conflict	UNP Q62667
LB	189	GLU	GLY	conflict	UNP Q62667
LB	232	ARG	LEU	conflict	UNP Q62667
LB	236	LYS	ARG	conflict	UNP Q62667
LB	242	ALA	LEU	conflict	UNP Q62667
MB	69	ALA	THR	conflict	UNP Q62667

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Chain	Residue	Modelled	Actual	Comment	Reference
MB	77	VAL	ILE	conflict	UNP Q62667
MB	104	LEU	VAL	conflict	UNP Q62667
MB	186	ASP	GLU	conflict	UNP Q62667
MB	189	GLU	GLY	conflict	UNP Q62667
MB	232	ARG	LEU	conflict	UNP Q62667
MB	236	LYS	ARG	conflict	UNP Q62667
MB	242	ALA	LEU	conflict	UNP Q62667
NB	69	ALA	THR	conflict	UNP Q62667
NB	77	VAL	ILE	conflict	UNP Q62667
NB	104	LEU	VAL	conflict	UNP Q62667
NB	186	ASP	GLU	conflict	UNP Q62667
NB	189	GLU	GLY	conflict	UNP Q62667
NB	232	ARG	LEU	conflict	UNP Q62667
NB	236	LYS	ARG	conflict	UNP Q62667
NB	242	ALA	LEU	conflict	UNP Q62667
OB	69	ALA	THR	conflict	UNP Q62667
OB	77	VAL	ILE	conflict	UNP Q62667
OB	104	LEU	VAL	conflict	UNP Q62667
OB	186	ASP	GLU	conflict	UNP Q62667
OB	189	GLU	GLY	conflict	UNP Q62667
OB	232	ARG	LEU	conflict	UNP Q62667
OB	236	LYS	ARG	conflict	UNP Q62667
OB	242	ALA	LEU	conflict	UNP Q62667
PB	69	ALA	THR	conflict	UNP Q62667
PB	77	VAL	ILE	conflict	UNP Q62667
PB	104	LEU	VAL	conflict	UNP Q62667
PB	186	ASP	GLU	conflict	UNP Q62667
PB	189	GLU	GLY	conflict	UNP Q62667
PB	232	ARG	LEU	conflict	UNP Q62667
PB	236	LYS	ARG	conflict	UNP Q62667
PB	242	ALA	LEU	conflict	UNP Q62667
QB	69	ALA	THR	conflict	UNP Q62667
QB	77	VAL	ILE	conflict	UNP Q62667
QB	104	LEU	VAL	conflict	UNP Q62667
QB	186	ASP	GLU	conflict	UNP Q62667
QB	189	GLU	GLY	conflict	UNP Q62667
QB	232	ARG	LEU	conflict	UNP Q62667
QB	236	LYS	ARG	conflict	UNP Q62667
QB	242	ALA	LEU	conflict	UNP Q62667
RB	69	ALA	THR	conflict	UNP Q62667
RB	77	VAL	ILE	conflict	UNP Q62667
RB	104	LEU	VAL	conflict	UNP Q62667

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Chain	Residue	Modelled	Actual	Comment	Reference
RB	186	ASP	GLU	conflict	UNP Q62667
RB	189	GLU	GLY	conflict	UNP Q62667
RB	232	ARG	LEU	conflict	UNP Q62667
RB	236	LYS	ARG	conflict	UNP Q62667
RB	242	ALA	LEU	conflict	UNP Q62667
SB	69	ALA	THR	conflict	UNP Q62667
SB	77	VAL	ILE	conflict	UNP Q62667
SB	104	LEU	VAL	conflict	UNP Q62667
SB	186	ASP	GLU	conflict	UNP Q62667
SB	189	GLU	GLY	conflict	UNP Q62667
SB	232	ARG	LEU	conflict	UNP Q62667
SB	236	LYS	ARG	conflict	UNP Q62667
SB	242	ALA	LEU	conflict	UNP Q62667
TB	69	ALA	THR	conflict	UNP Q62667
TB	77	VAL	ILE	conflict	UNP Q62667
TB	104	LEU	VAL	conflict	UNP Q62667
TB	186	ASP	GLU	conflict	UNP Q62667
TB	189	GLU	GLY	conflict	UNP Q62667
TB	232	ARG	LEU	conflict	UNP Q62667
TB	236	LYS	ARG	conflict	UNP Q62667
TB	242	ALA	LEU	conflict	UNP Q62667
UB	69	ALA	THR	conflict	UNP Q62667
UB	77	VAL	ILE	conflict	UNP Q62667
UB	104	LEU	VAL	conflict	UNP Q62667
UB	186	ASP	GLU	conflict	UNP Q62667
UB	189	GLU	GLY	conflict	UNP Q62667
UB	232	ARG	LEU	conflict	UNP Q62667
UB	236	LYS	ARG	conflict	UNP Q62667
UB	242	ALA	LEU	conflict	UNP Q62667
VB	69	ALA	THR	conflict	UNP Q62667
VB	77	VAL	ILE	conflict	UNP Q62667
VB	104	LEU	VAL	conflict	UNP Q62667
VB	186	ASP	GLU	conflict	UNP Q62667
VB	189	GLU	GLY	conflict	UNP Q62667
VB	232	ARG	LEU	conflict	UNP Q62667
VB	236	LYS	ARG	conflict	UNP Q62667
VB	242	ALA	LEU	conflict	UNP Q62667
WB	69	ALA	THR	conflict	UNP Q62667
WB	77	VAL	ILE	conflict	UNP Q62667
WB	104	LEU	VAL	conflict	UNP Q62667
WB	186	ASP	GLU	conflict	UNP Q62667
WB	189	GLU	GLY	conflict	UNP Q62667

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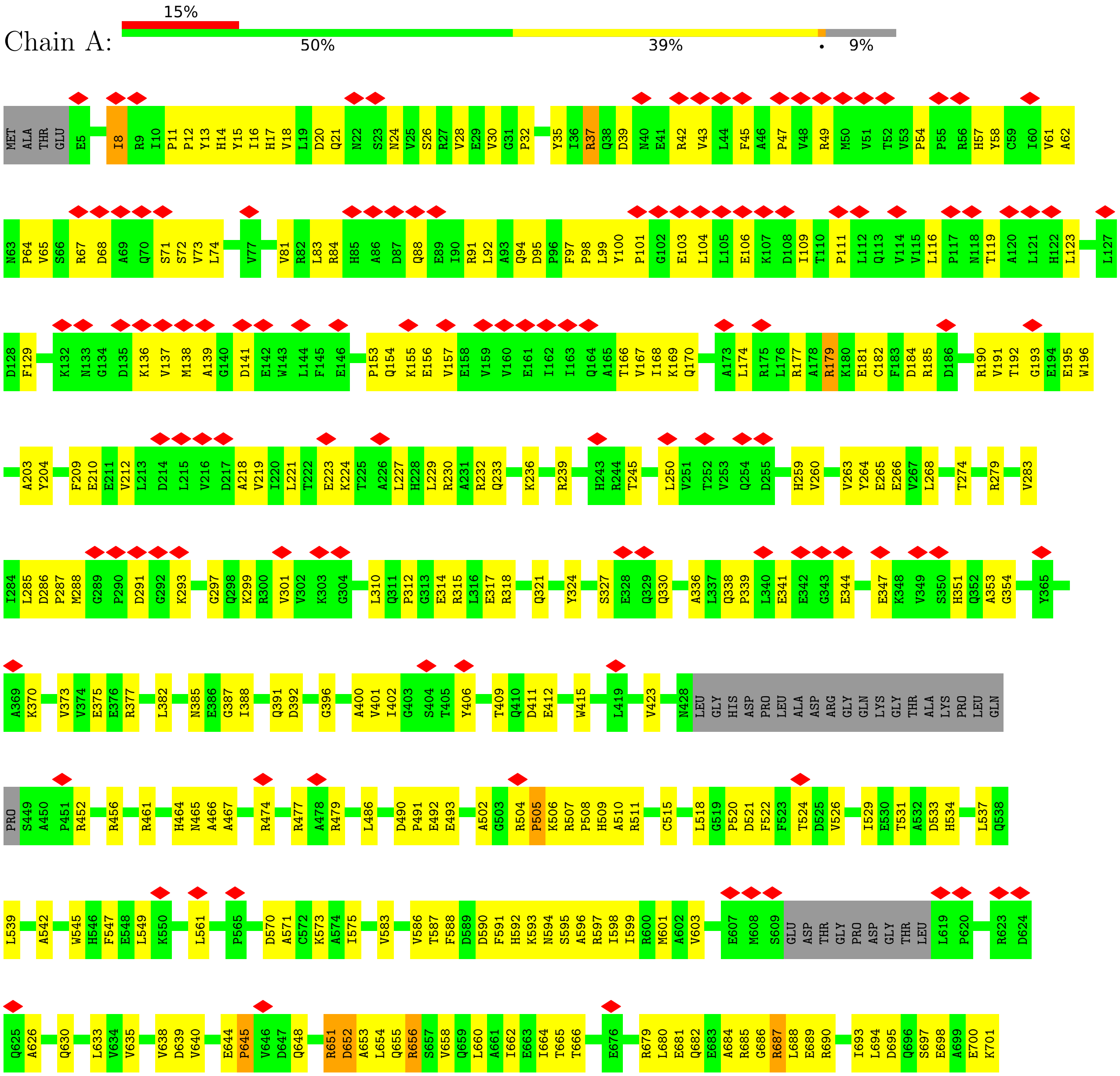
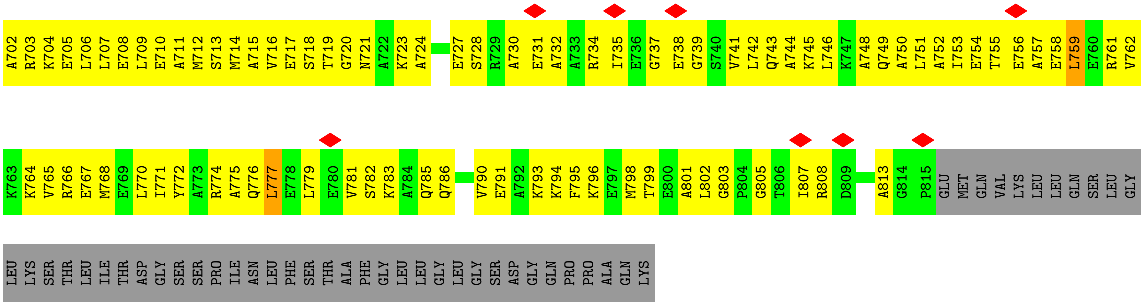
Chain	Residue	Modelled	Actual	Comment	Reference
WB	232	ARG	LEU	conflict	UNP Q62667
WB	236	LYS	ARG	conflict	UNP Q62667
WB	242	ALA	LEU	conflict	UNP Q62667
XB	69	ALA	THR	conflict	UNP Q62667
XB	77	VAL	ILE	conflict	UNP Q62667
XB	104	LEU	VAL	conflict	UNP Q62667
XB	186	ASP	GLU	conflict	UNP Q62667
XB	189	GLU	GLY	conflict	UNP Q62667
XB	232	ARG	LEU	conflict	UNP Q62667
XB	236	LYS	ARG	conflict	UNP Q62667
XB	242	ALA	LEU	conflict	UNP Q62667
YB	69	ALA	THR	conflict	UNP Q62667
YB	77	VAL	ILE	conflict	UNP Q62667
YB	104	LEU	VAL	conflict	UNP Q62667
YB	186	ASP	GLU	conflict	UNP Q62667
YB	189	GLU	GLY	conflict	UNP Q62667
YB	232	ARG	LEU	conflict	UNP Q62667
YB	236	LYS	ARG	conflict	UNP Q62667
YB	242	ALA	LEU	conflict	UNP Q62667
ZB	69	ALA	THR	conflict	UNP Q62667
ZB	77	VAL	ILE	conflict	UNP Q62667
ZB	104	LEU	VAL	conflict	UNP Q62667
ZB	186	ASP	GLU	conflict	UNP Q62667
ZB	189	GLU	GLY	conflict	UNP Q62667
ZB	232	ARG	LEU	conflict	UNP Q62667
ZB	236	LYS	ARG	conflict	UNP Q62667
ZB	242	ALA	LEU	conflict	UNP Q62667
AC	69	ALA	THR	conflict	UNP Q62667
AC	77	VAL	ILE	conflict	UNP Q62667
AC	104	LEU	VAL	conflict	UNP Q62667
AC	186	ASP	GLU	conflict	UNP Q62667
AC	189	GLU	GLY	conflict	UNP Q62667
AC	232	ARG	LEU	conflict	UNP Q62667
AC	236	LYS	ARG	conflict	UNP Q62667
AC	242	ALA	LEU	conflict	UNP Q62667

3 Residue-property plots ⓘ

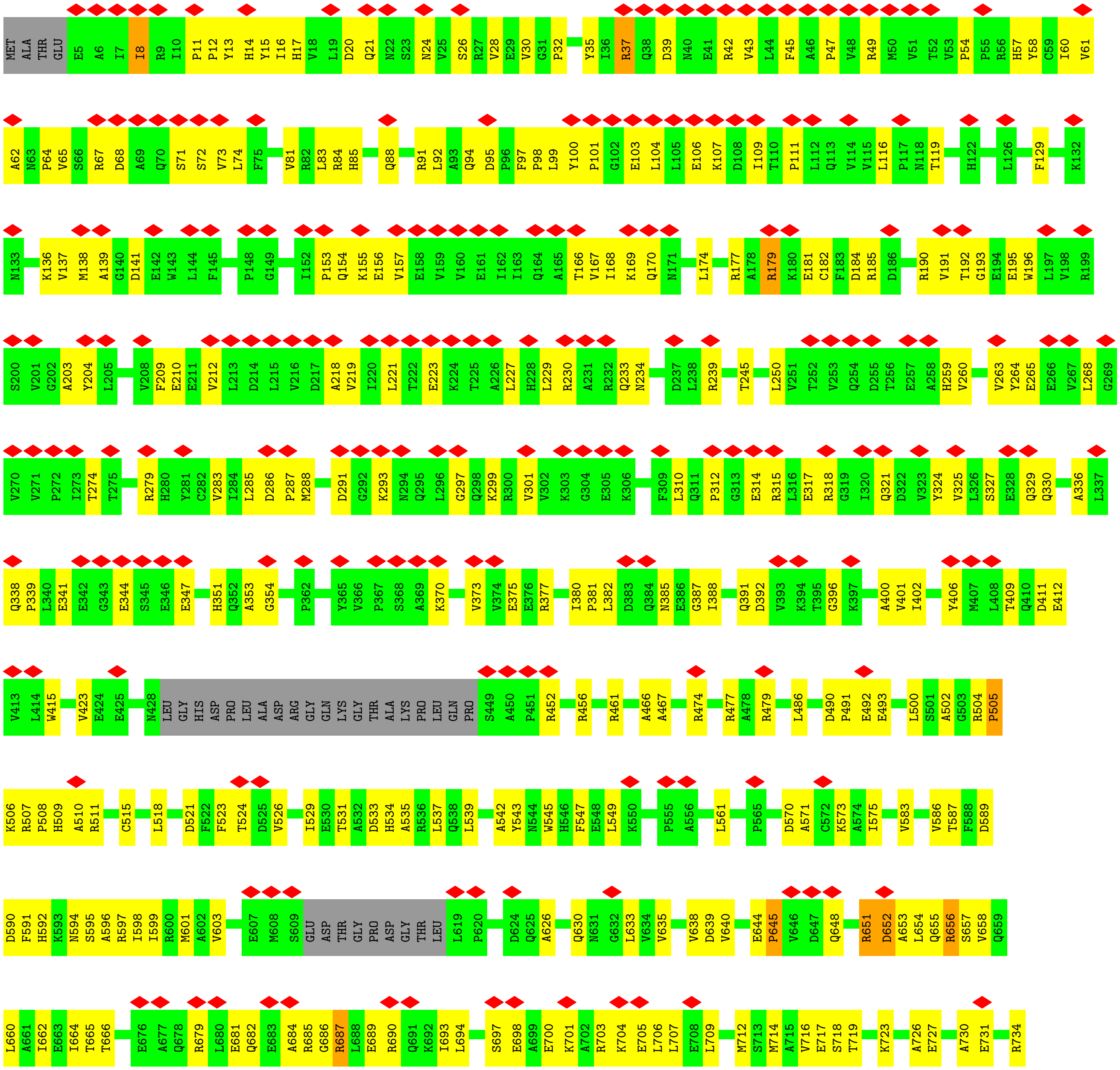
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

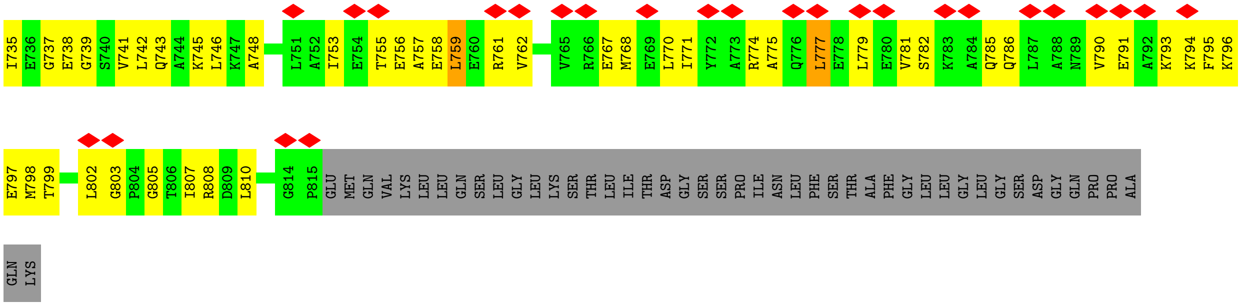
- Molecule 1: Major vault protein





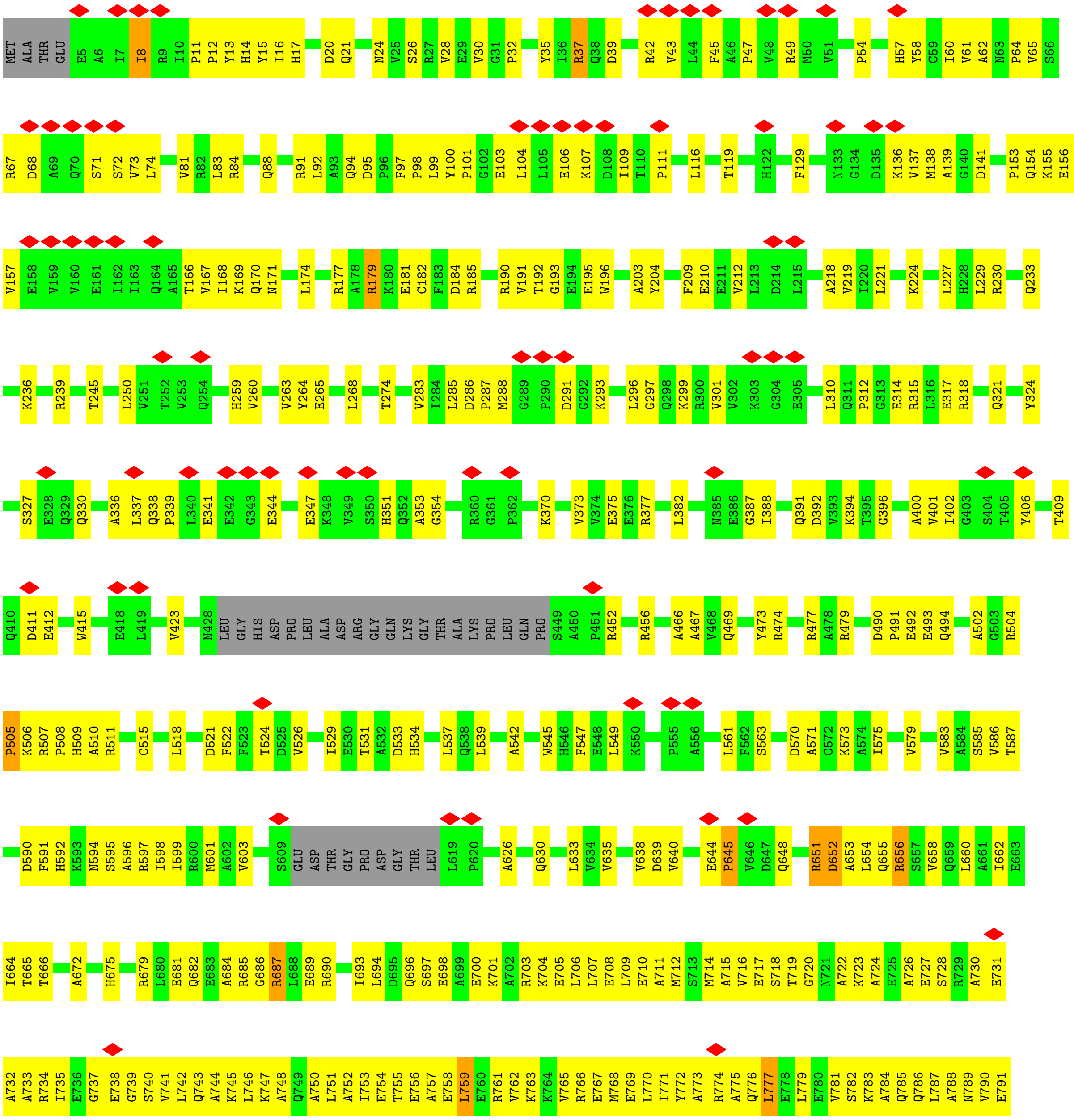
- Molecule 1: Major vault protein

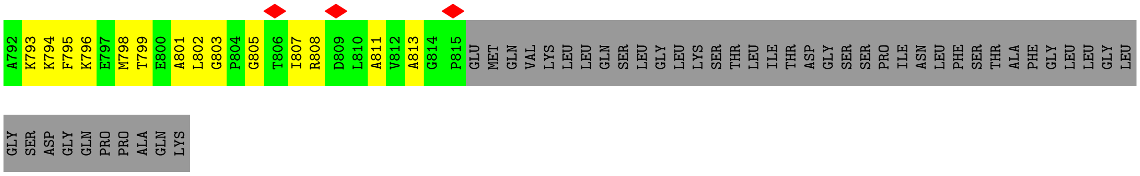




- Molecule 1: Major vault protein

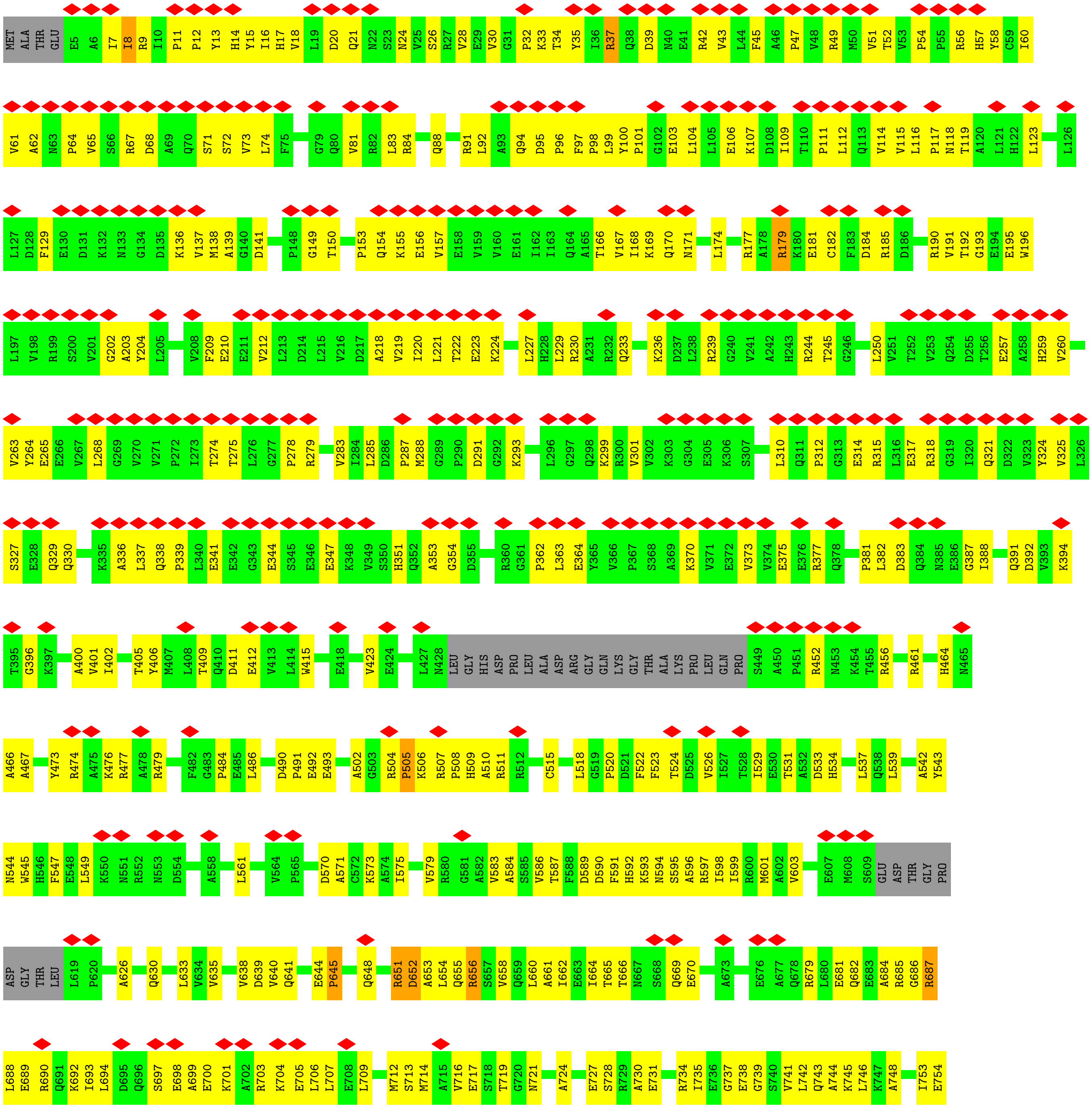
Chain C:

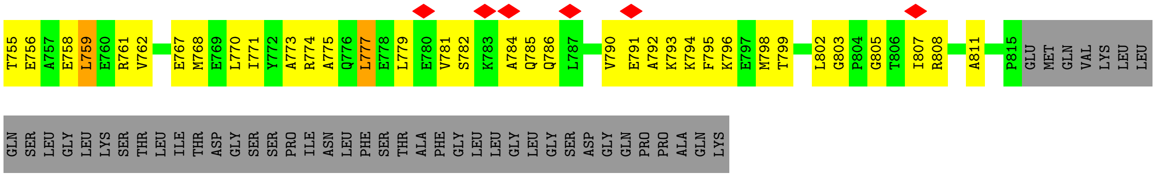





- Molecule 1: Major vault protein

Chain D:





- Molecule 1: Major vault protein

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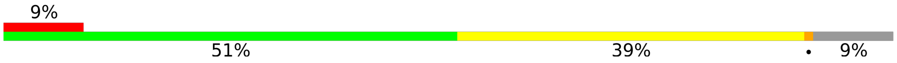
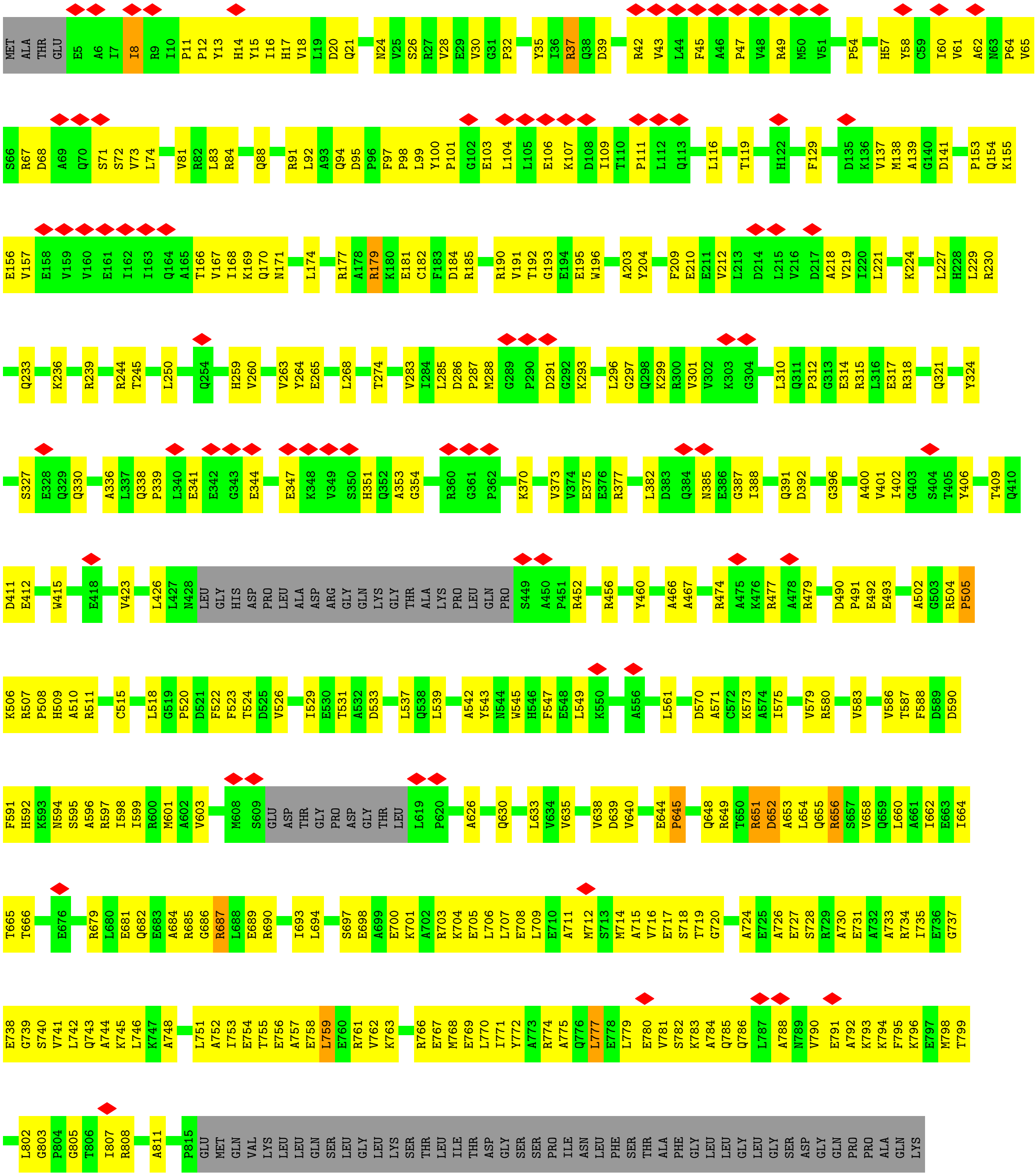
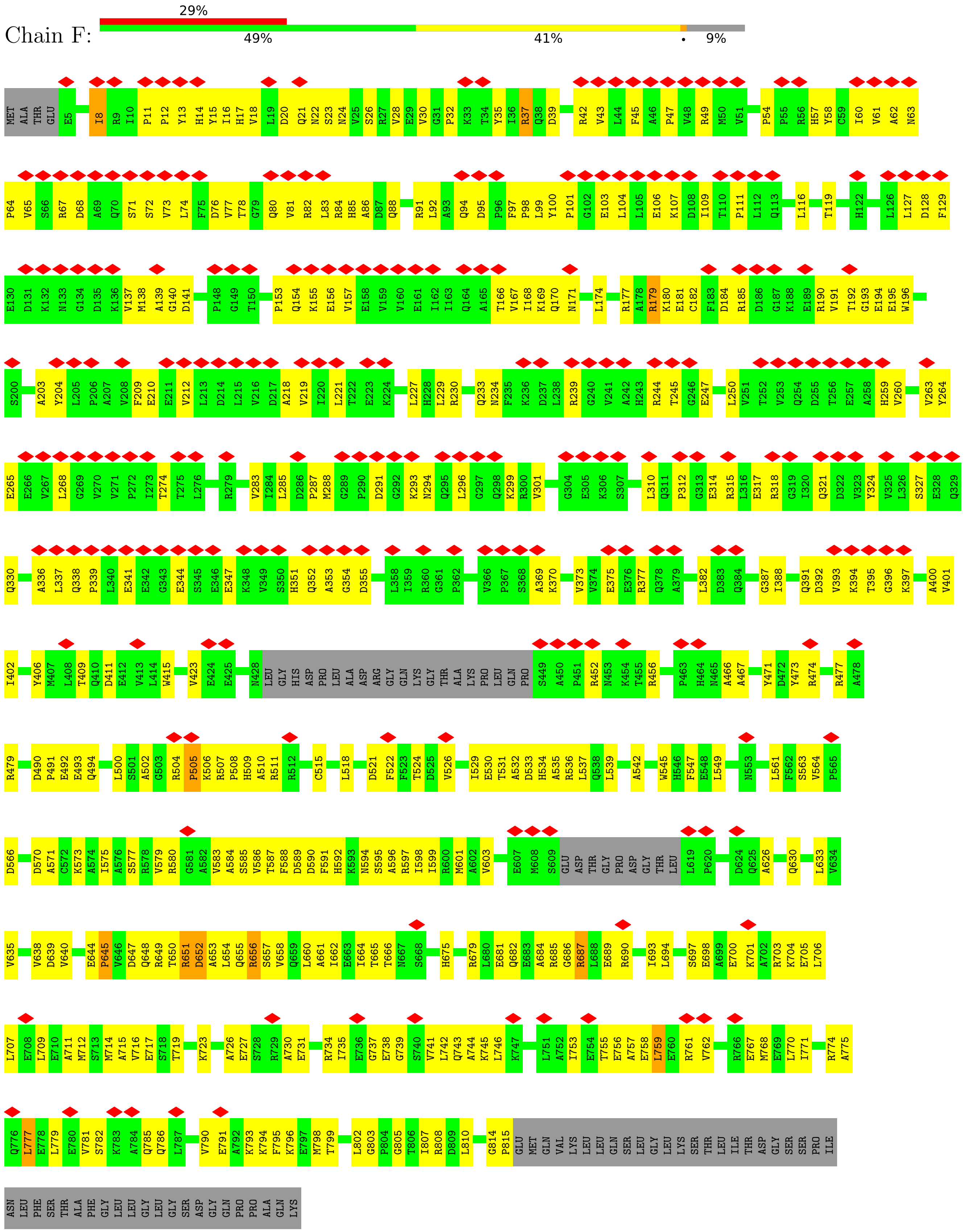


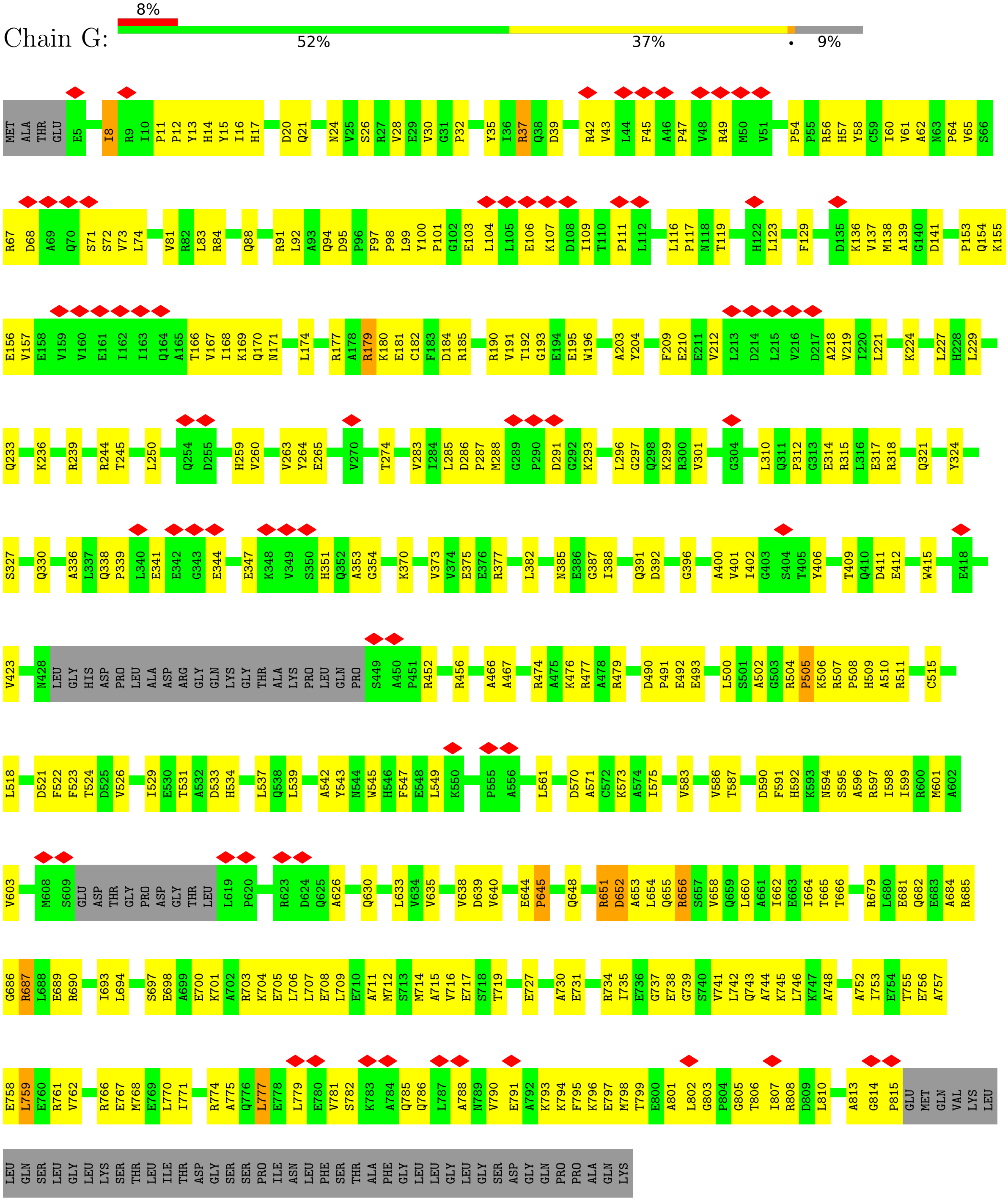


- Molecule 1: Major vault protein



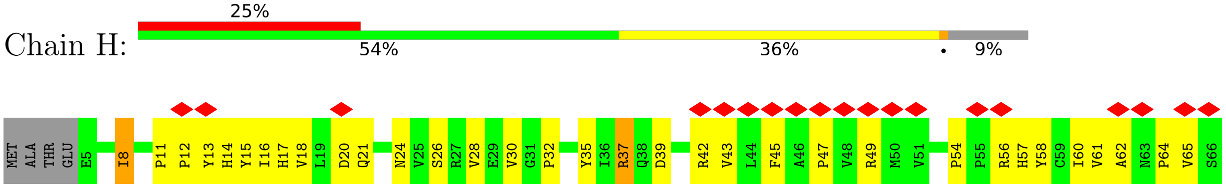
- Molecule 1: Major vault protein

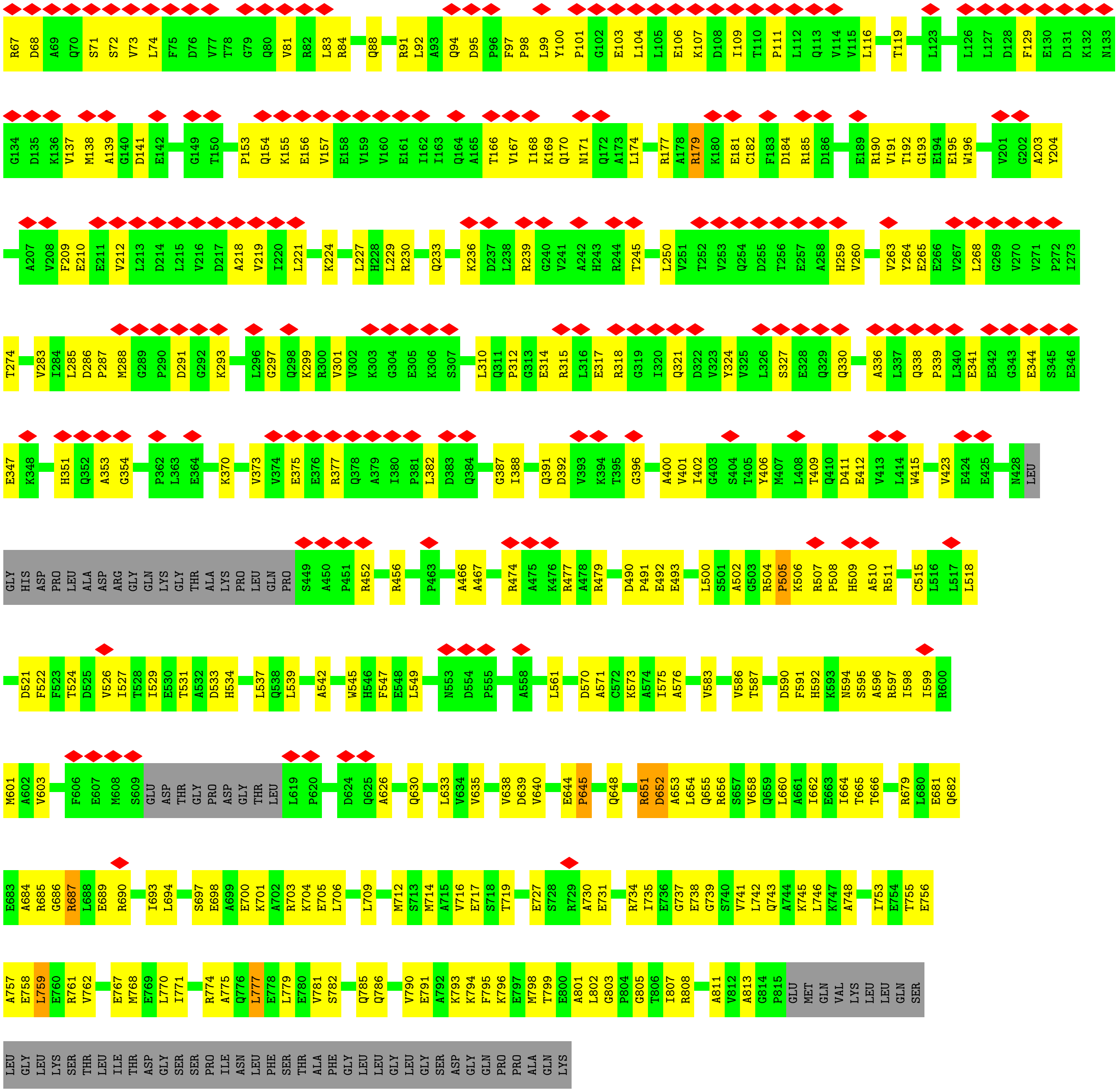
Chain G:



- Molecule 1: Major vault protein

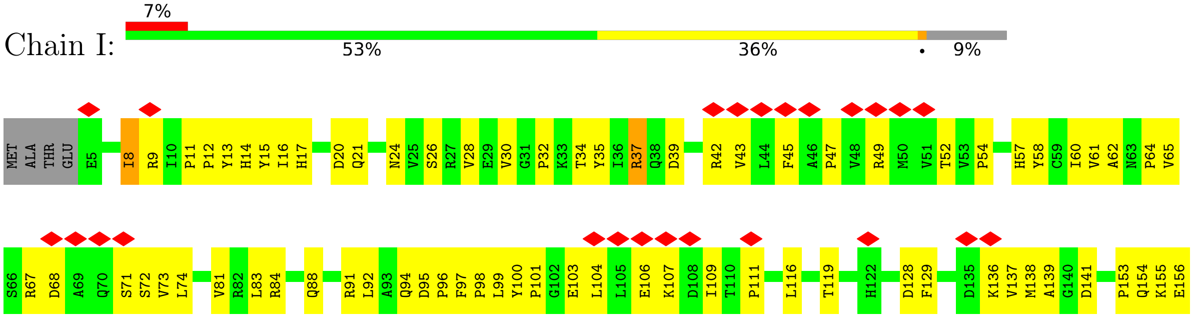
Chain H:

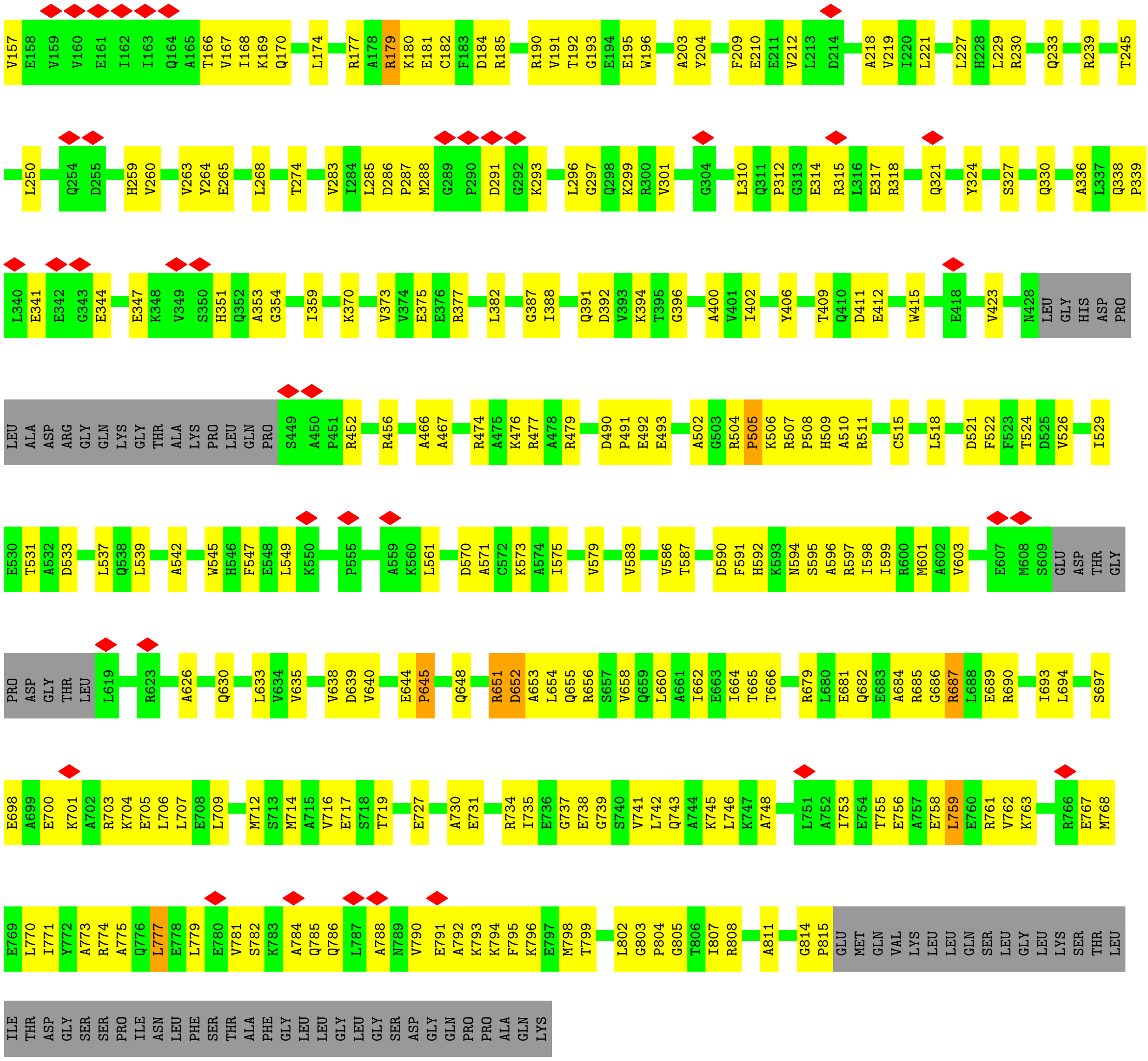




- Molecule 1: Major vault protein

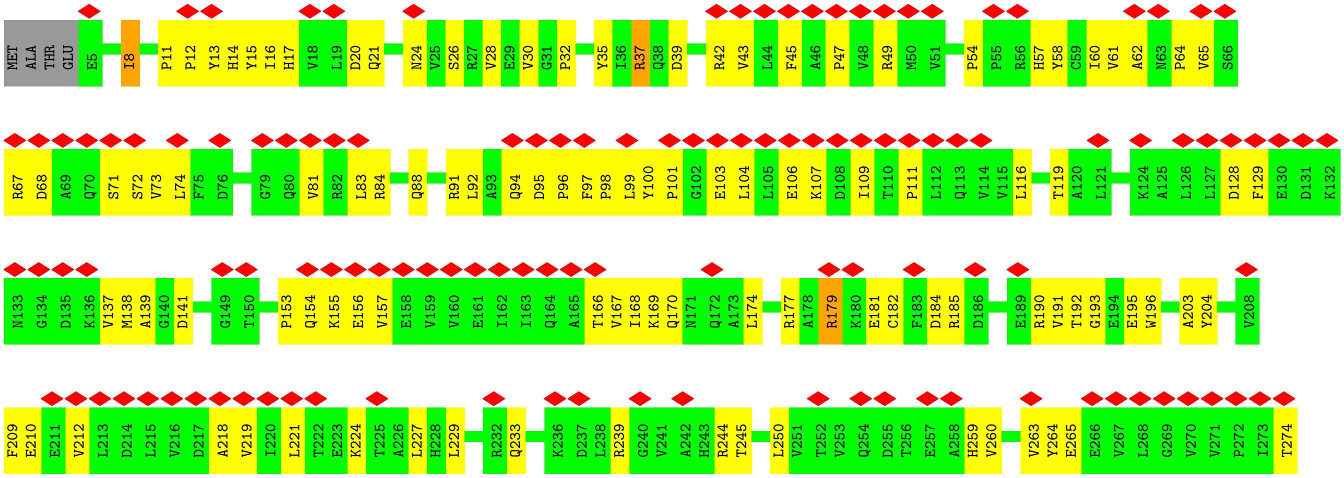
Chain I:

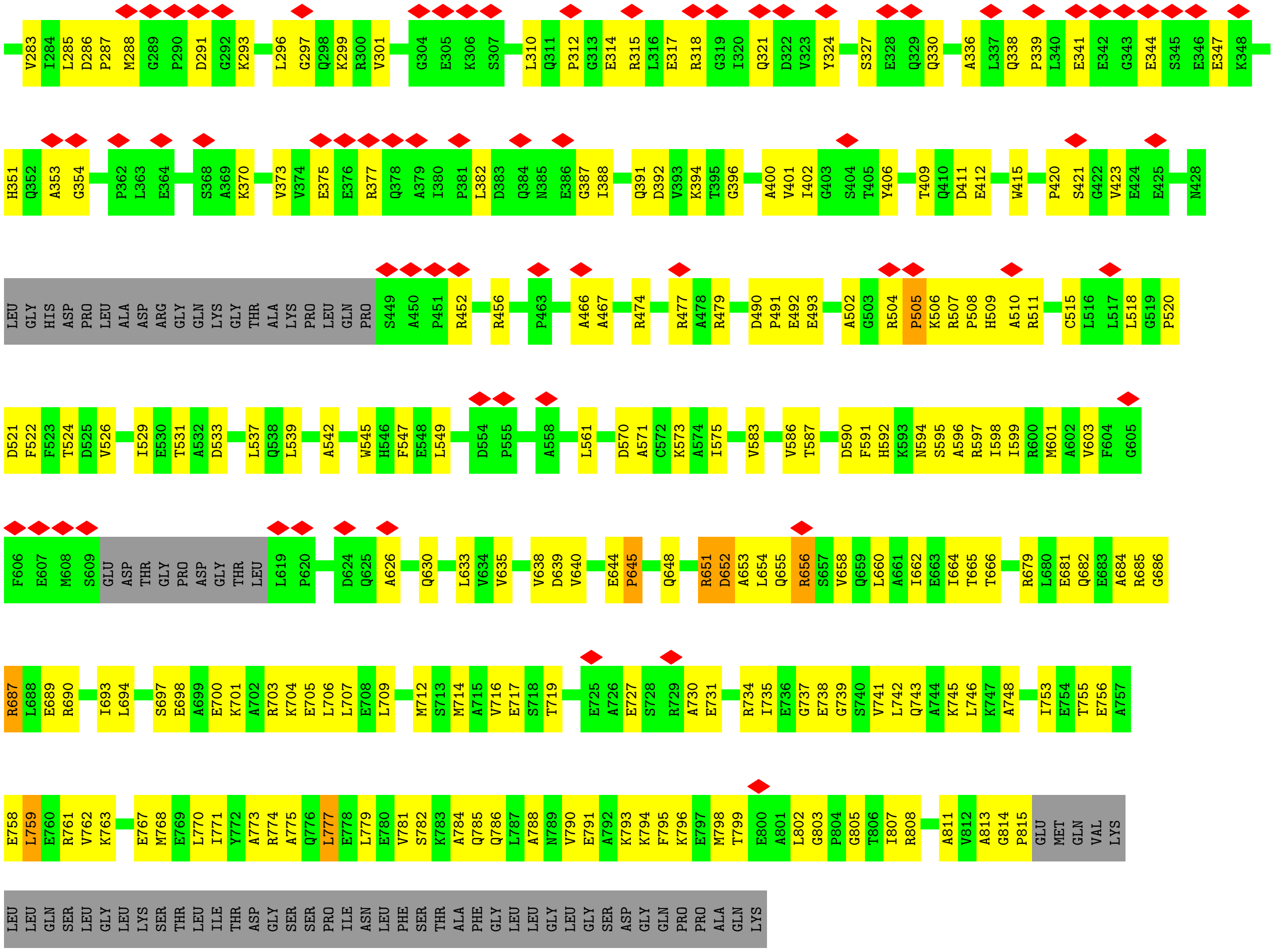




- Molecule 1: Major vault protein

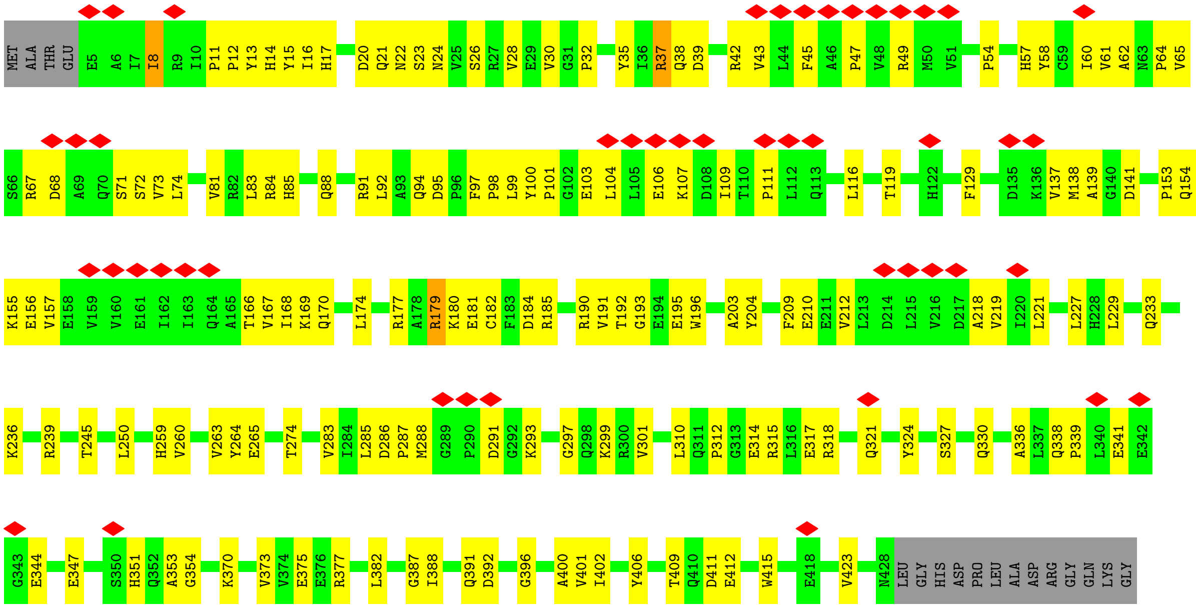
Chain J:

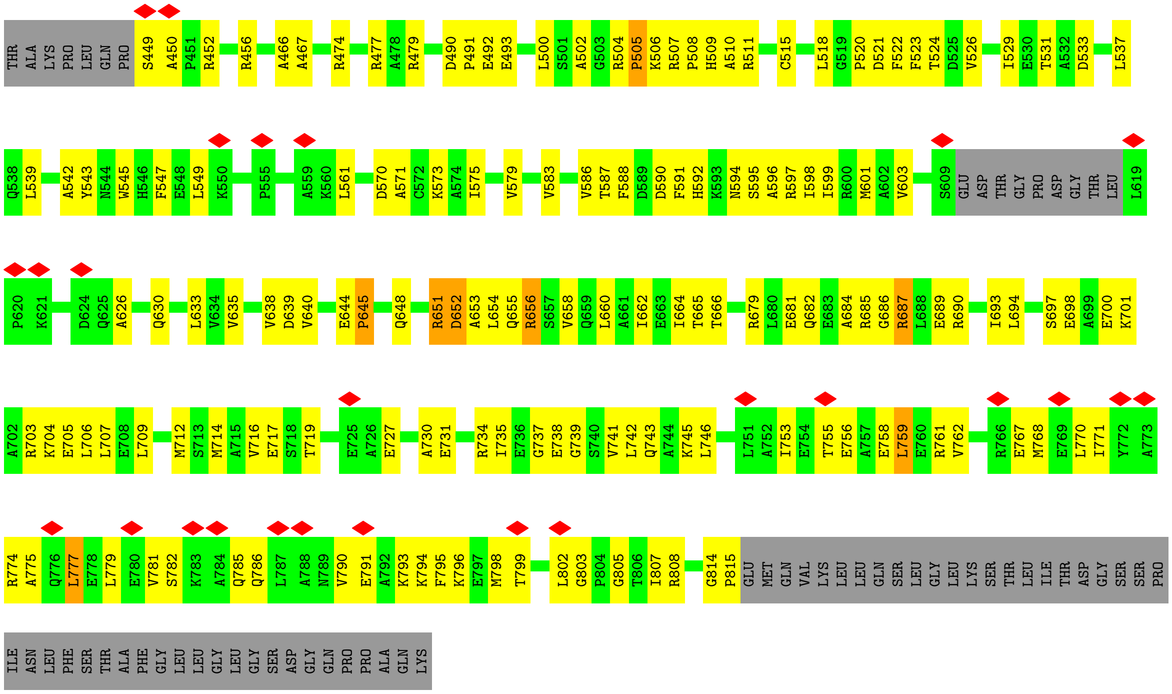




- Molecule 1: Major vault protein

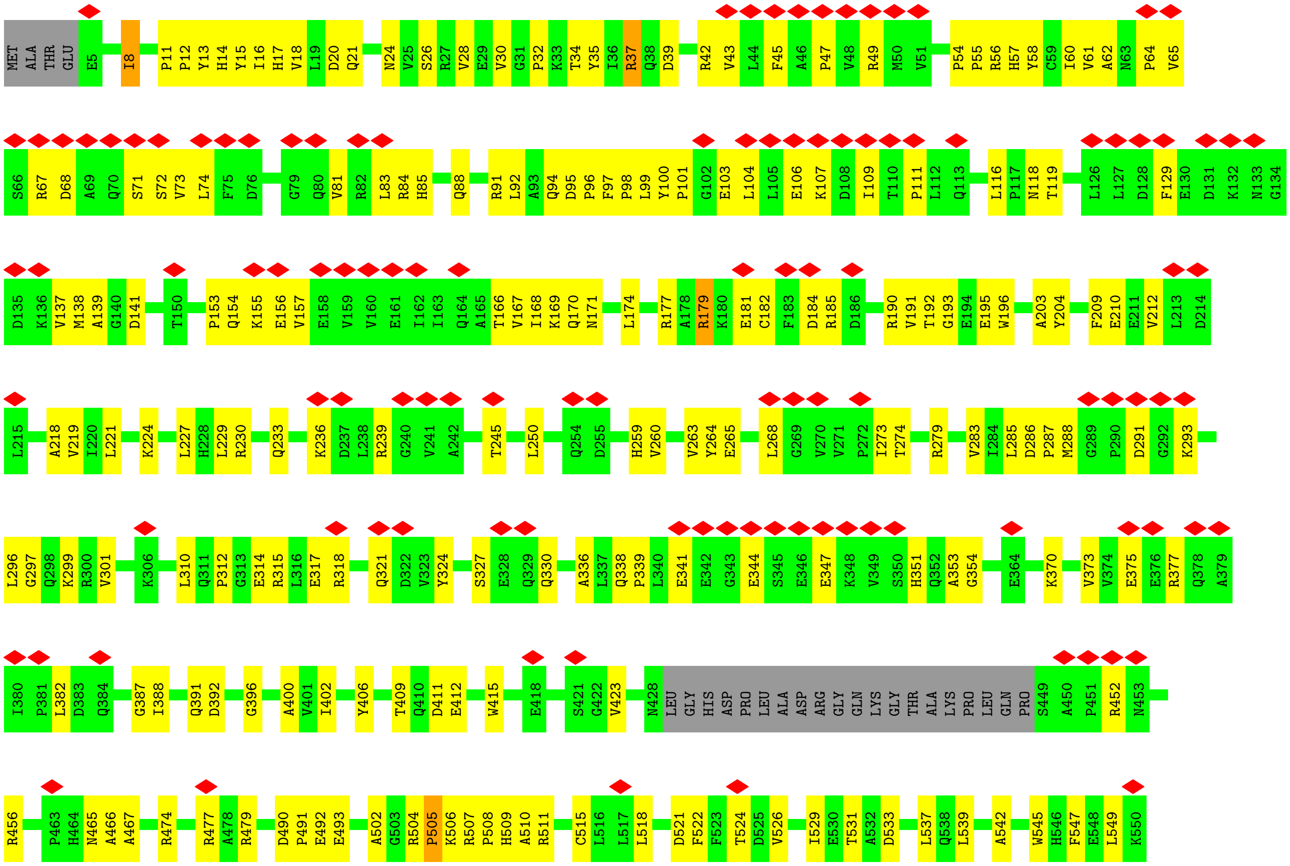
Chain K:

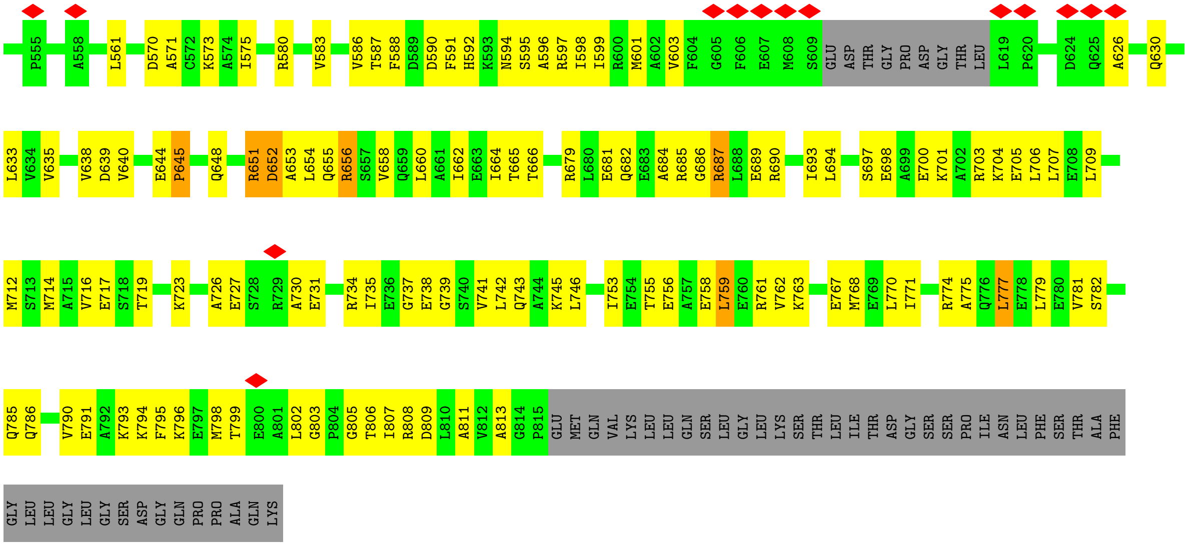




- Molecule 1: Major vault protein

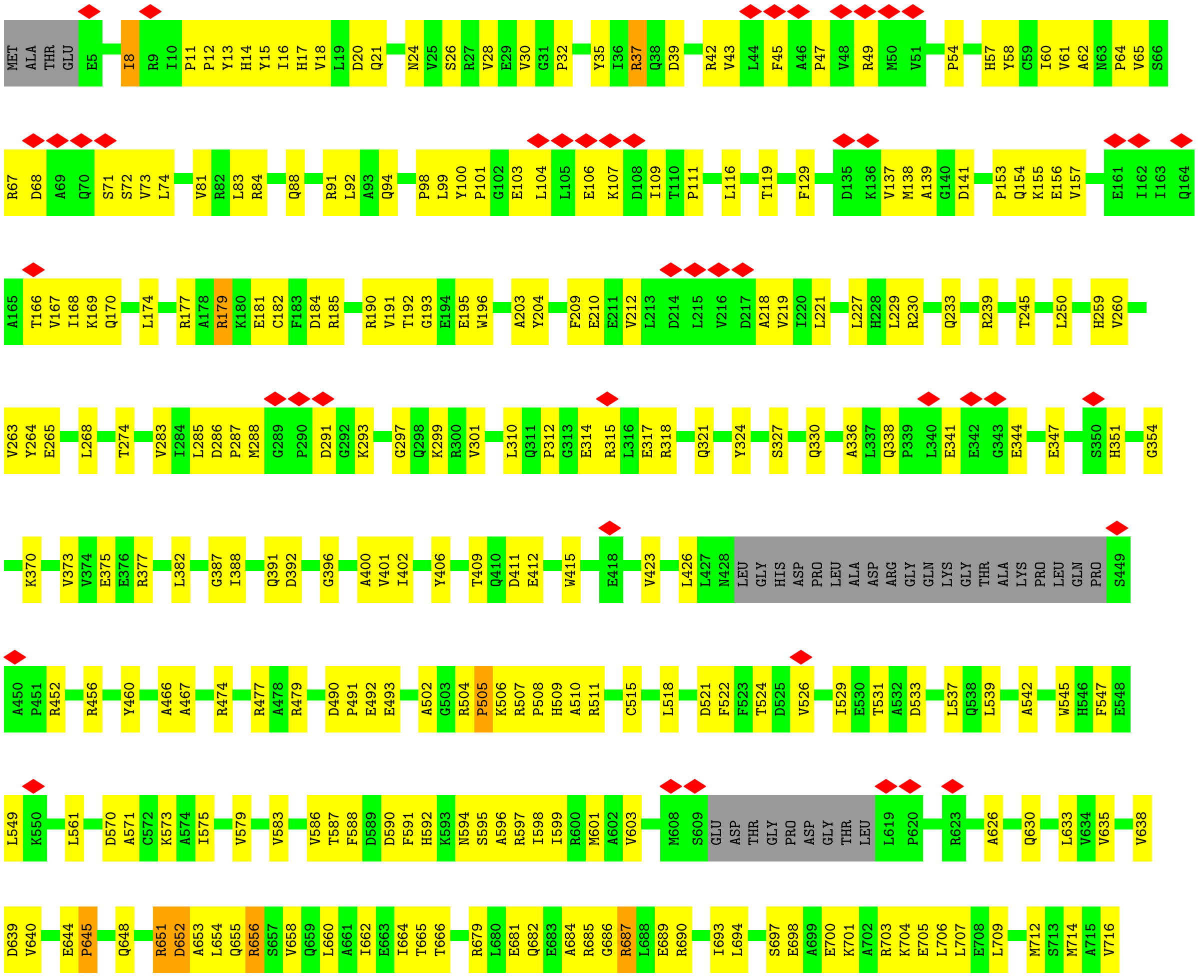
Chain L:

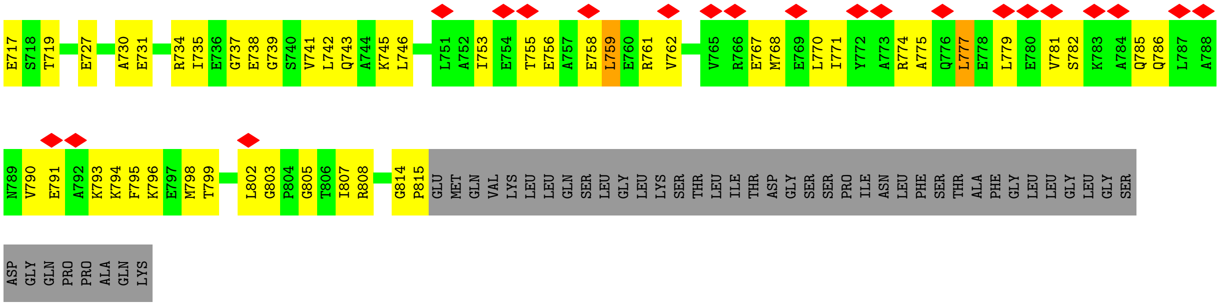




- Molecule 1: Major vault protein

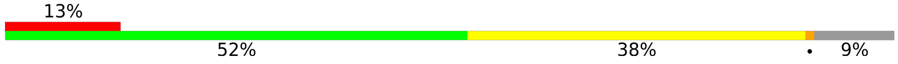
Chain M:

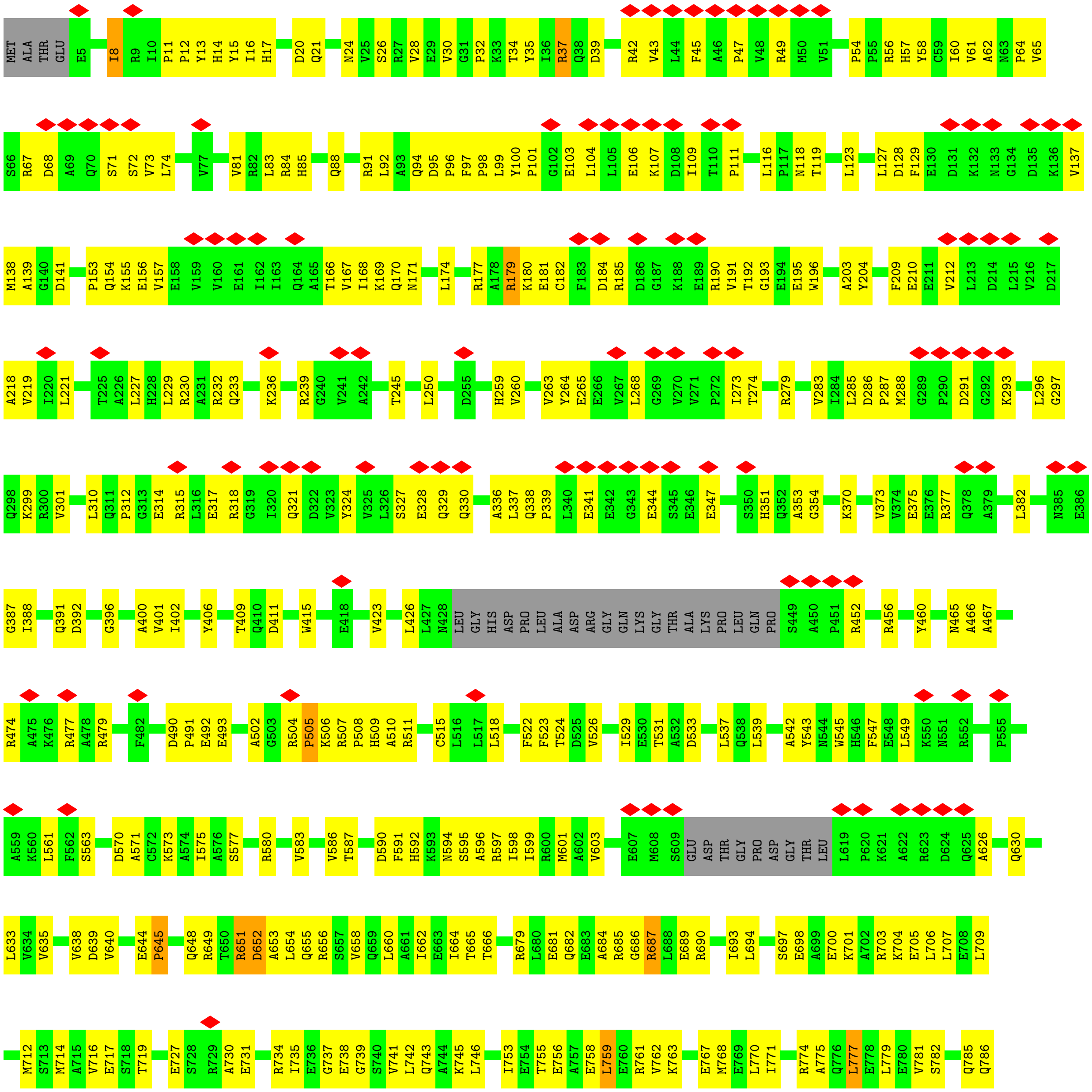


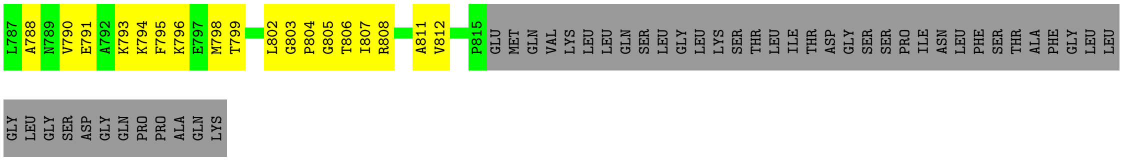


- Molecule 1: Major vault protein

Chain N:

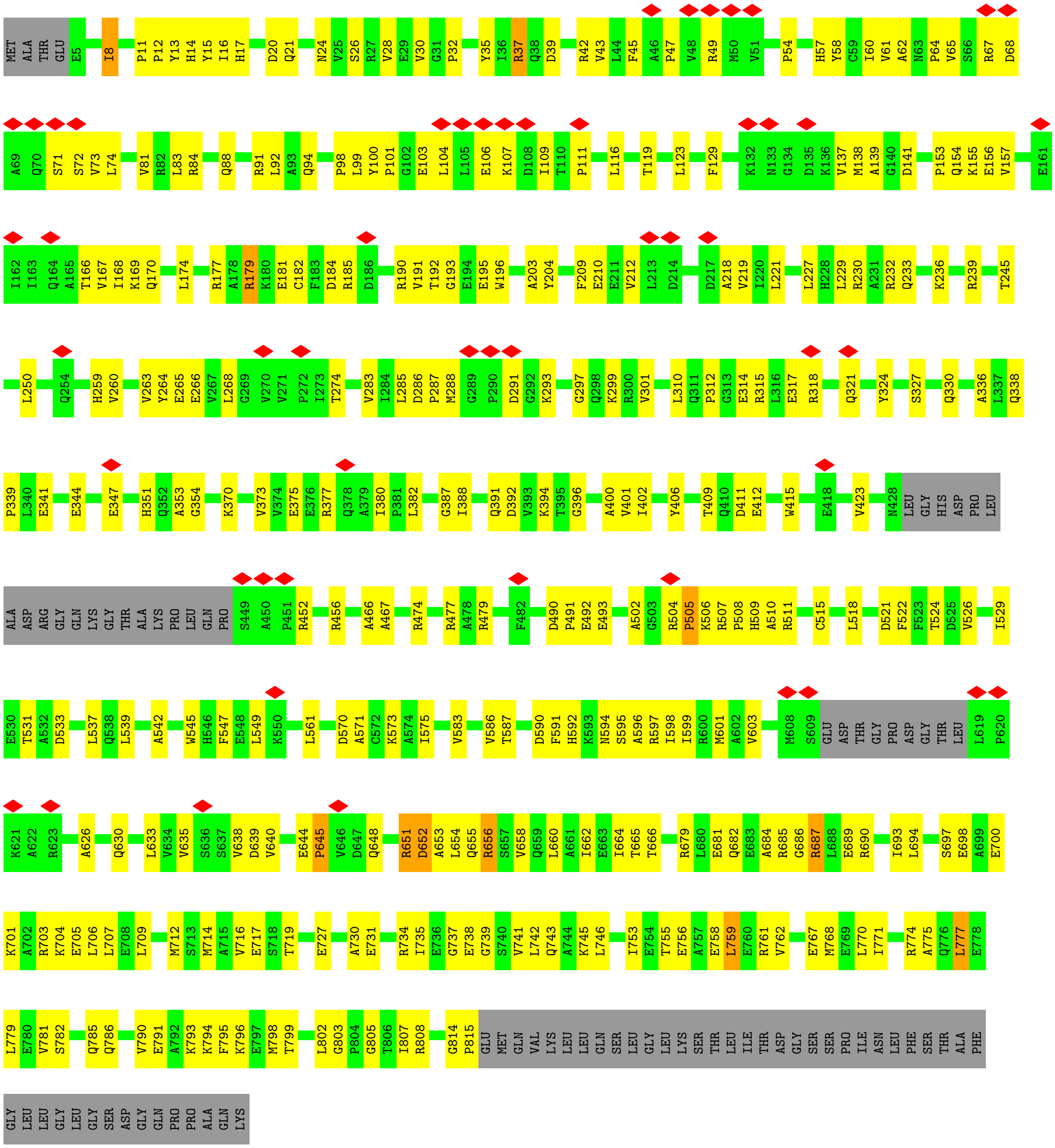






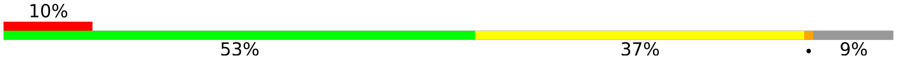
- Molecule 1: Major vault protein

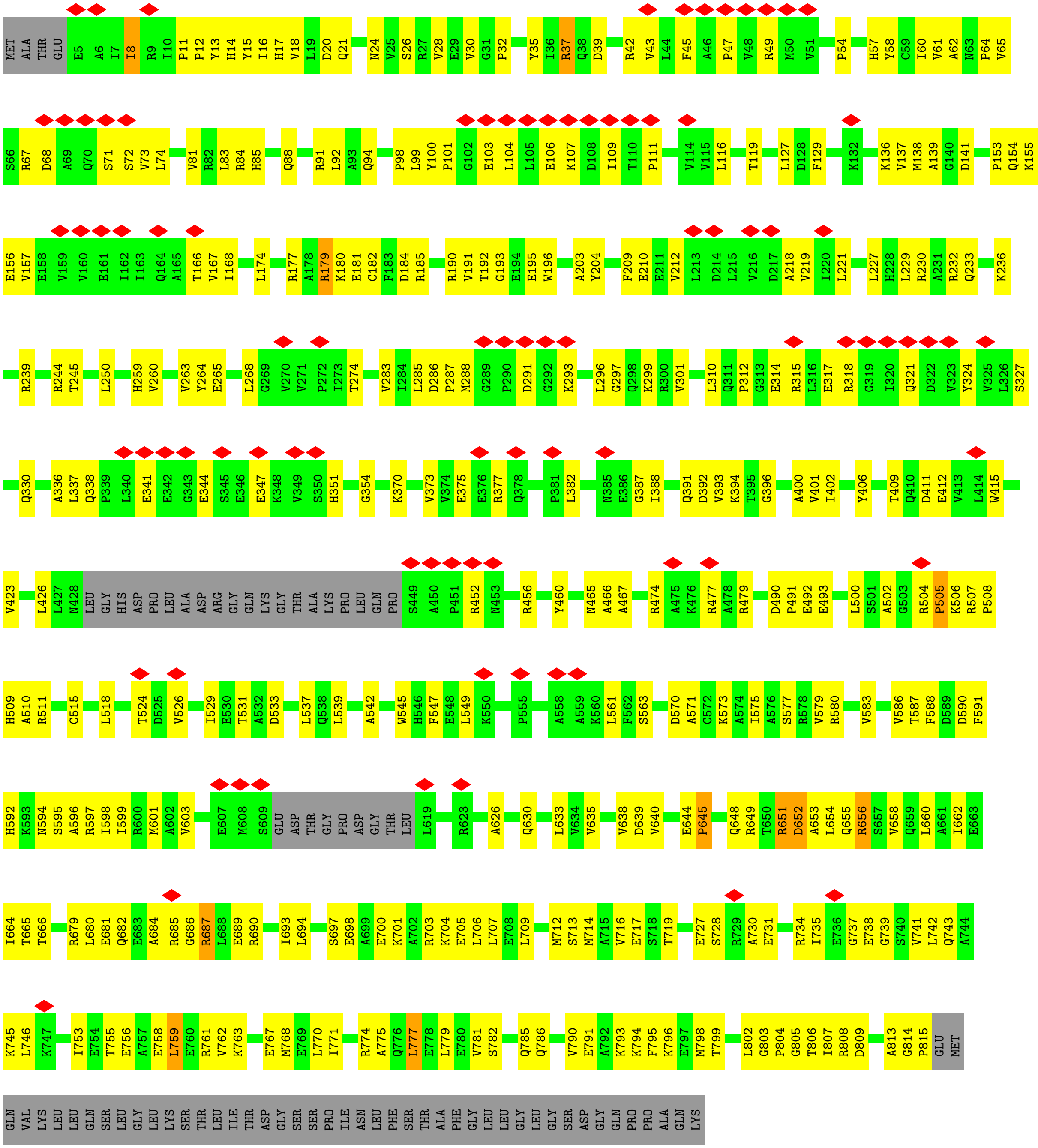
Chain O:



- Molecule 1: Major vault protein

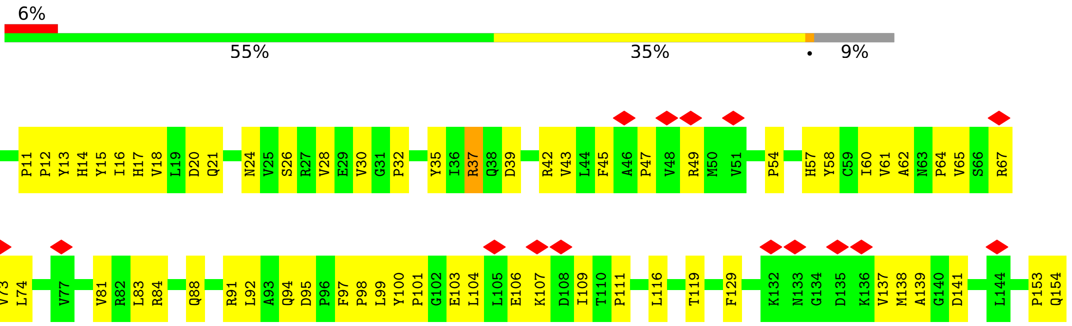
Chain P:

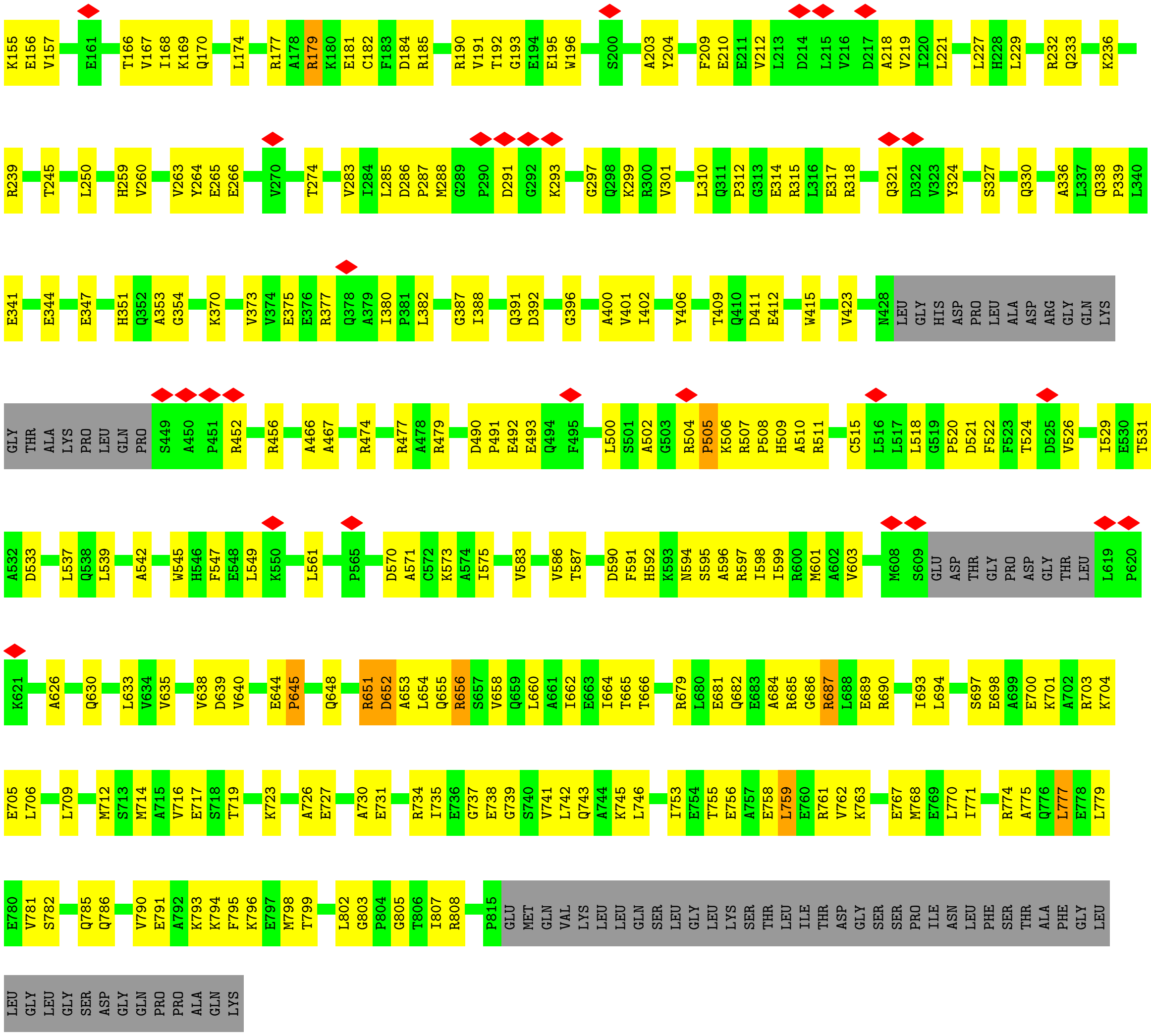




- Molecule 1: Major vault protein

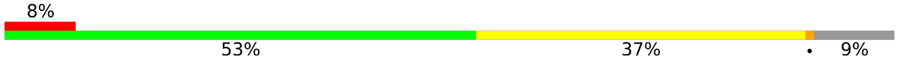
Chain Q:

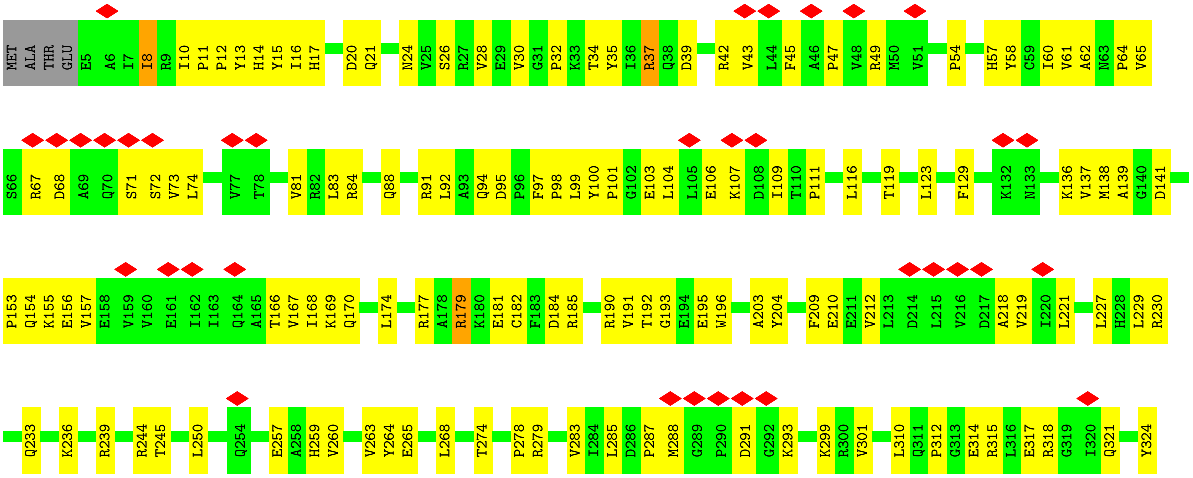


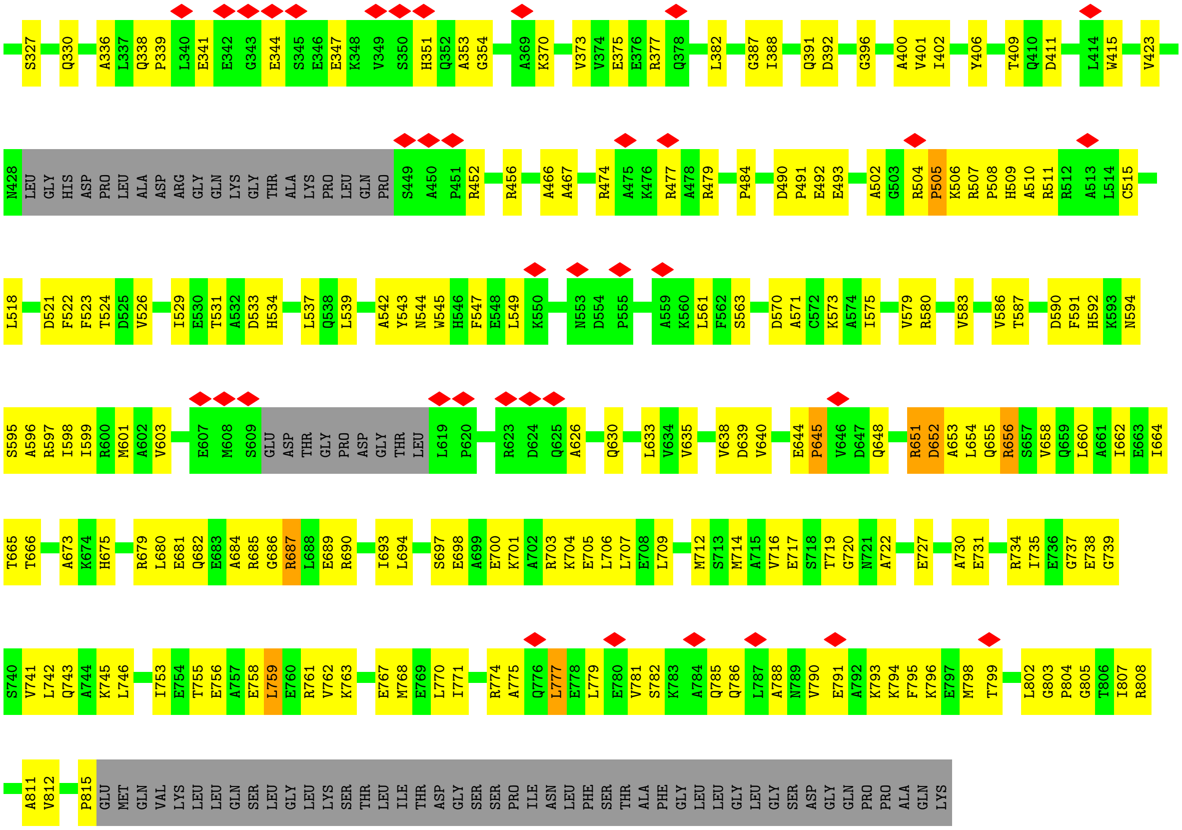


- Molecule 1: Major vault protein

Chain R:

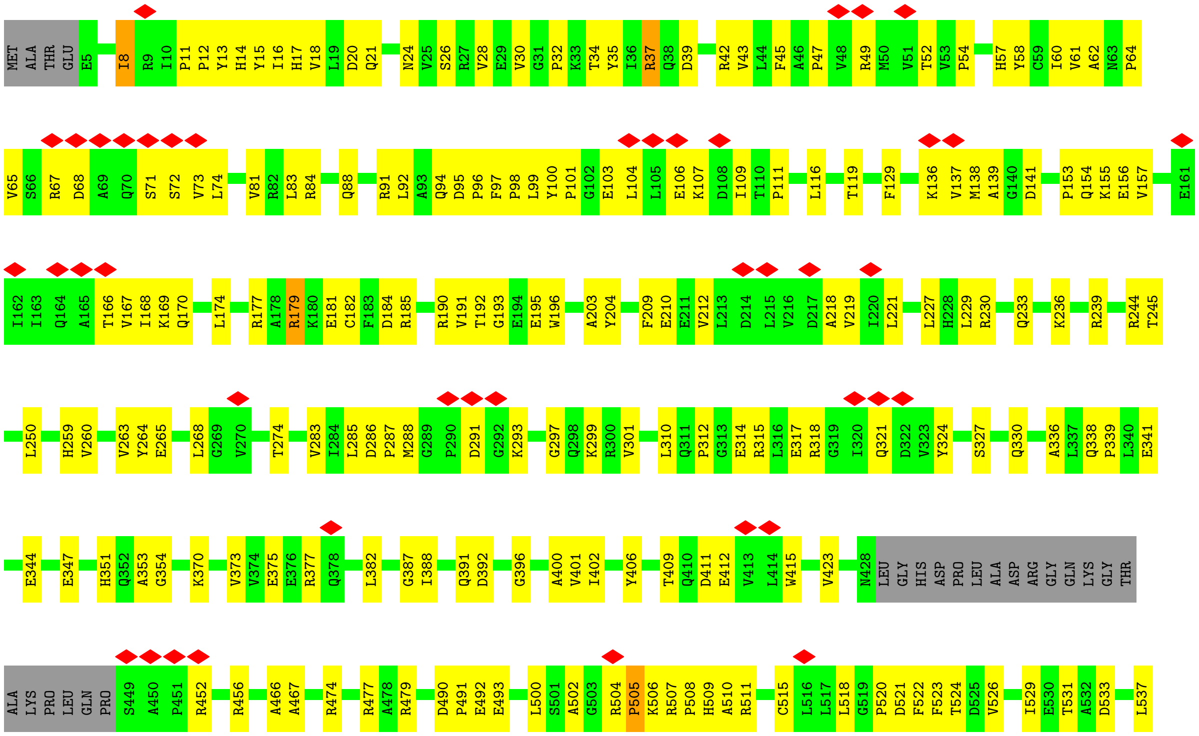


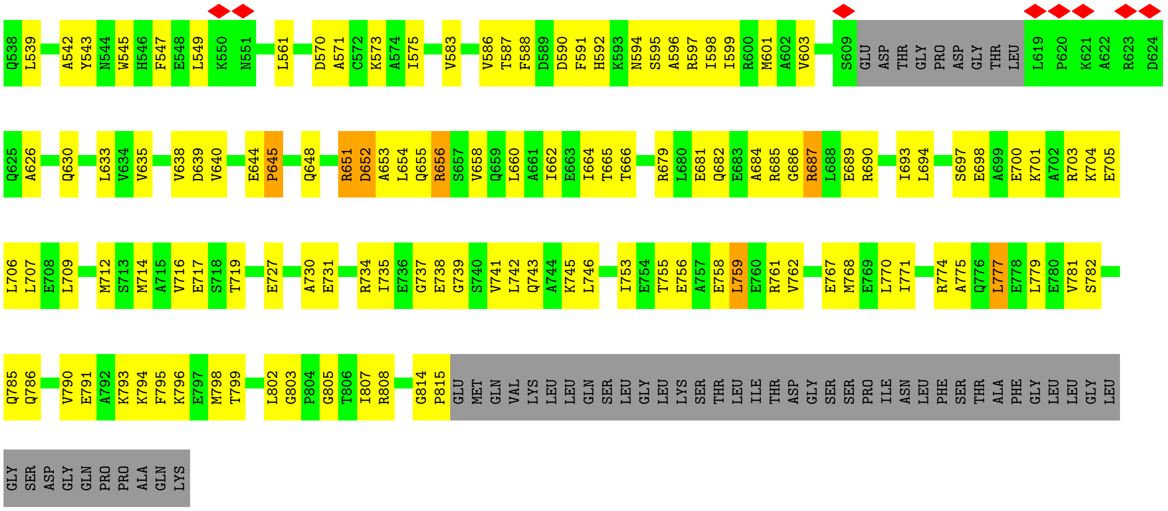




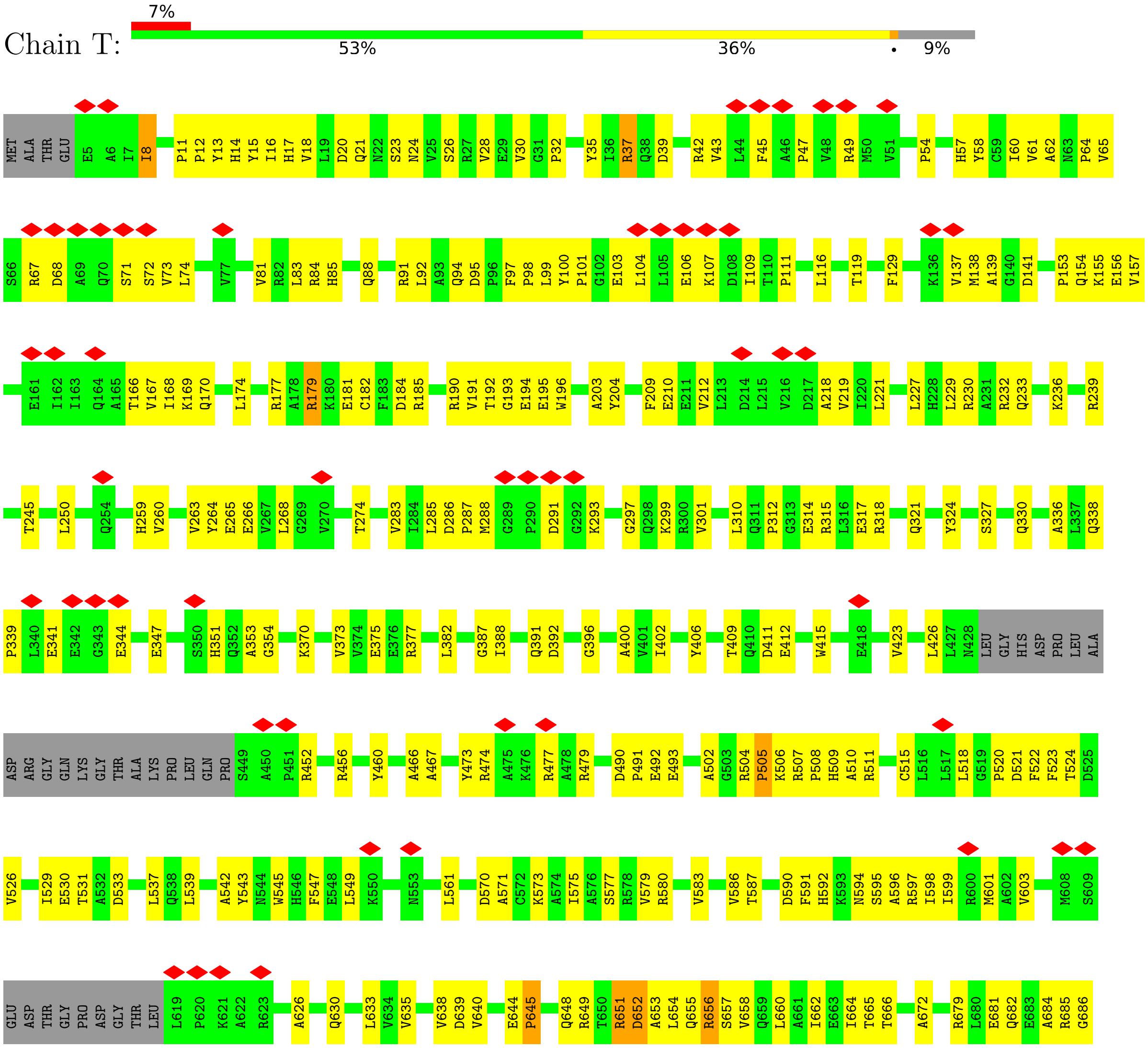
- Molecule 1: Major vault protein

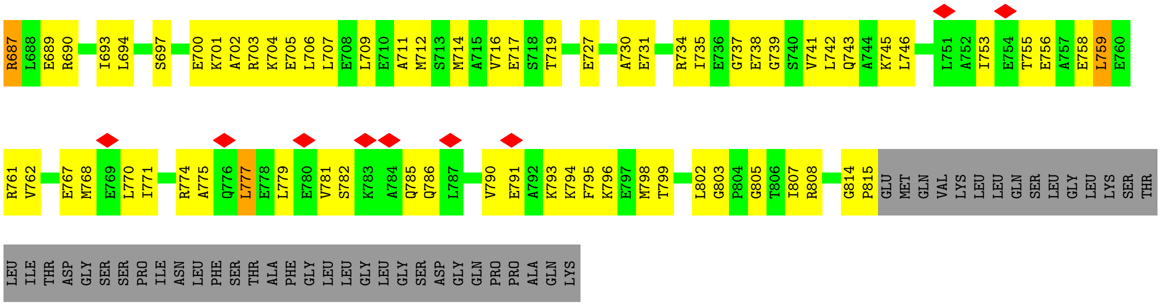
Chain S:





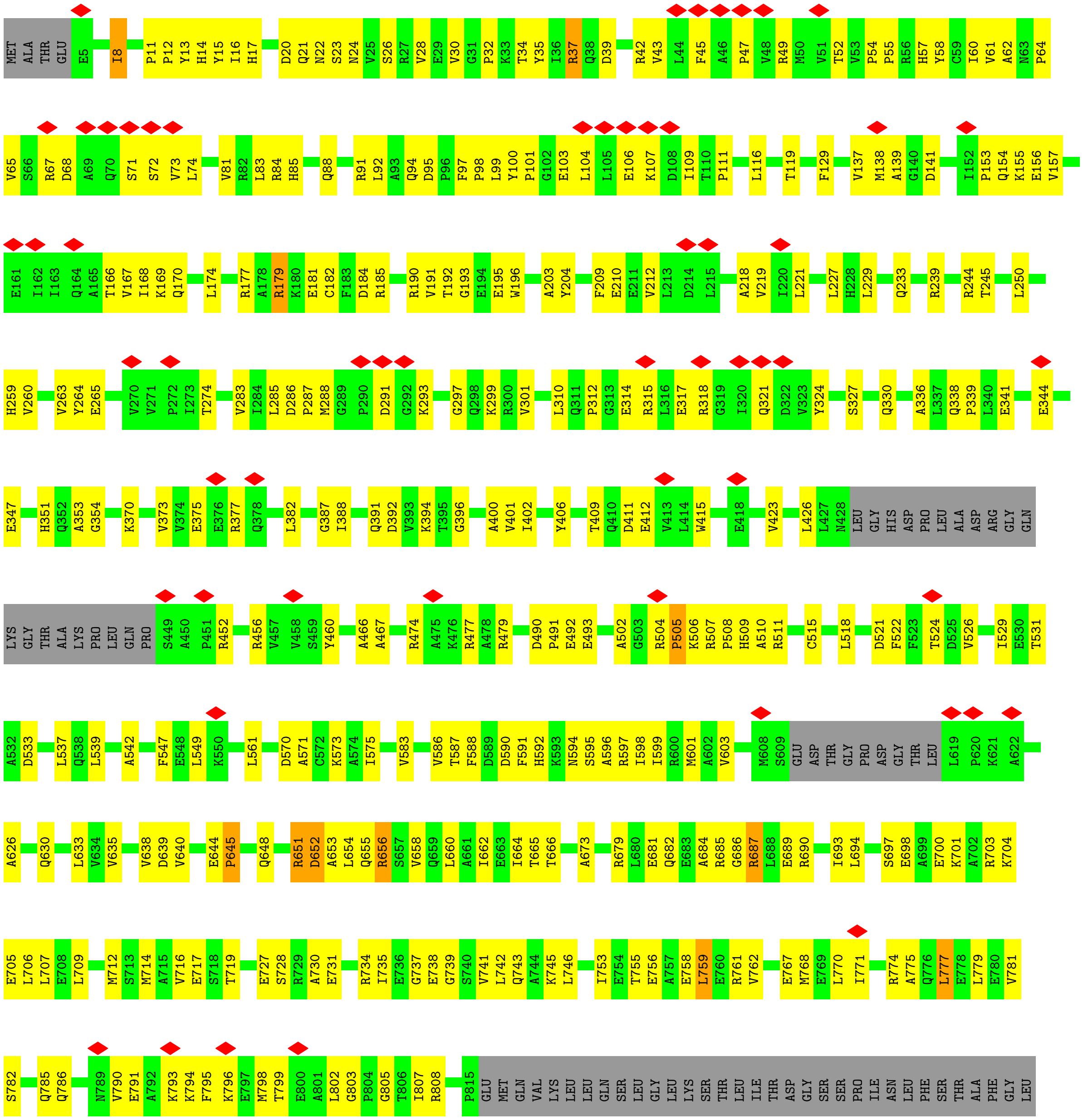
- Molecule 1: Major vault protein



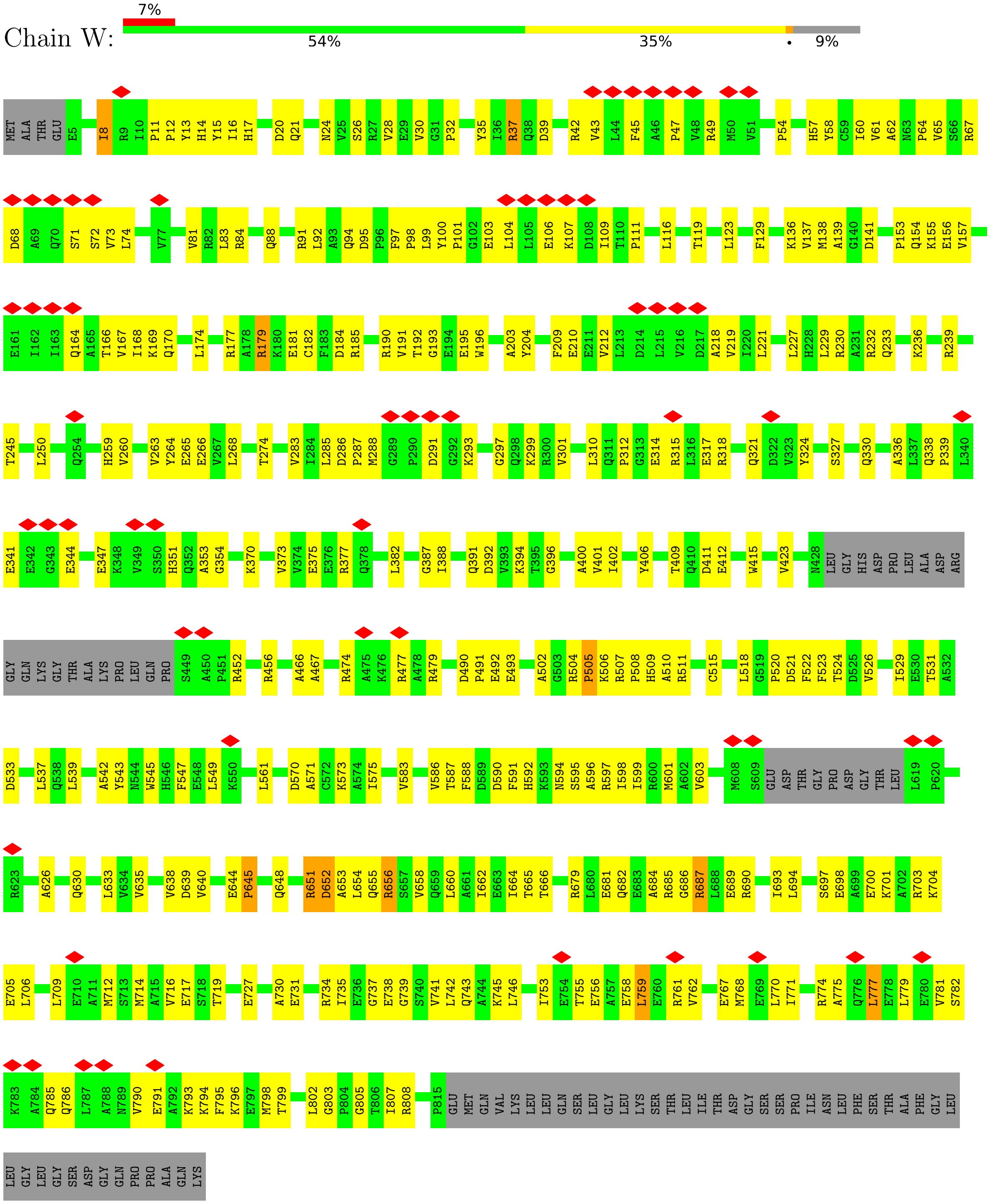


- Molecule 1: Major vault protein

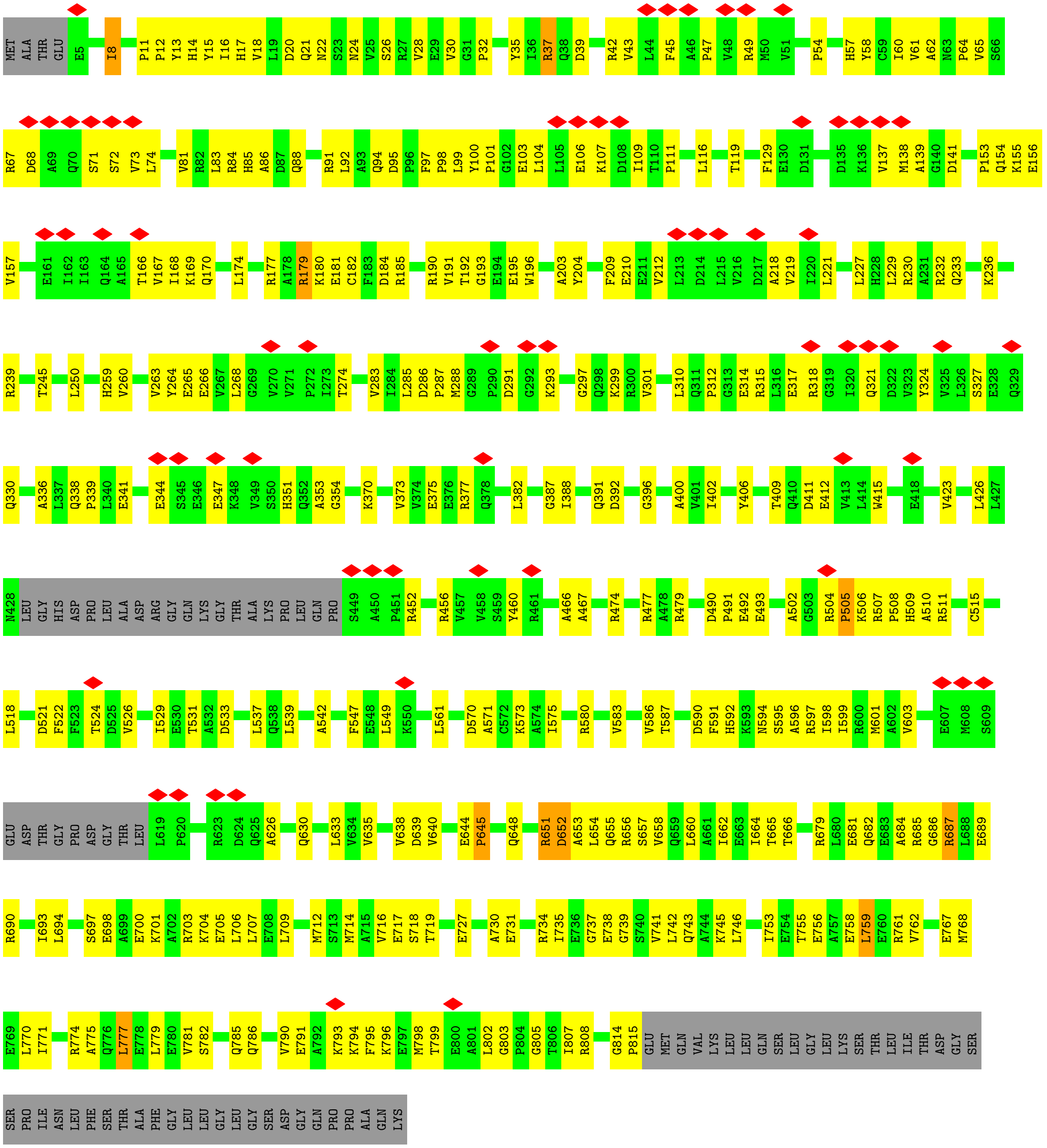
Chain V:



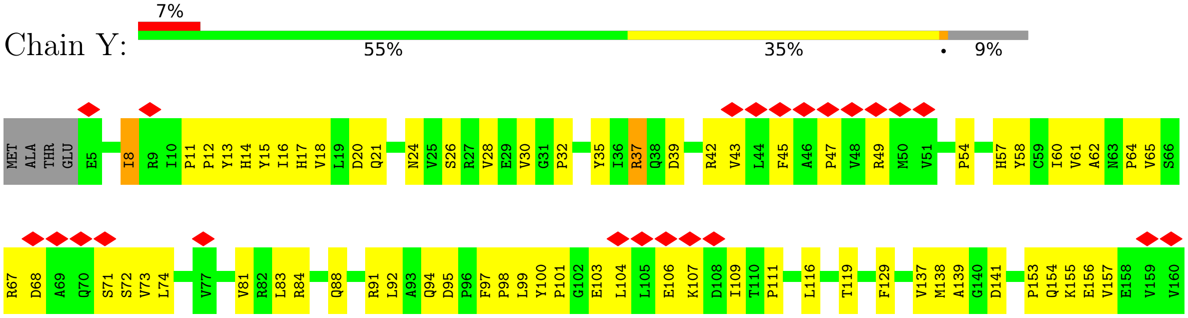
- Molecule 1: Major vault protein

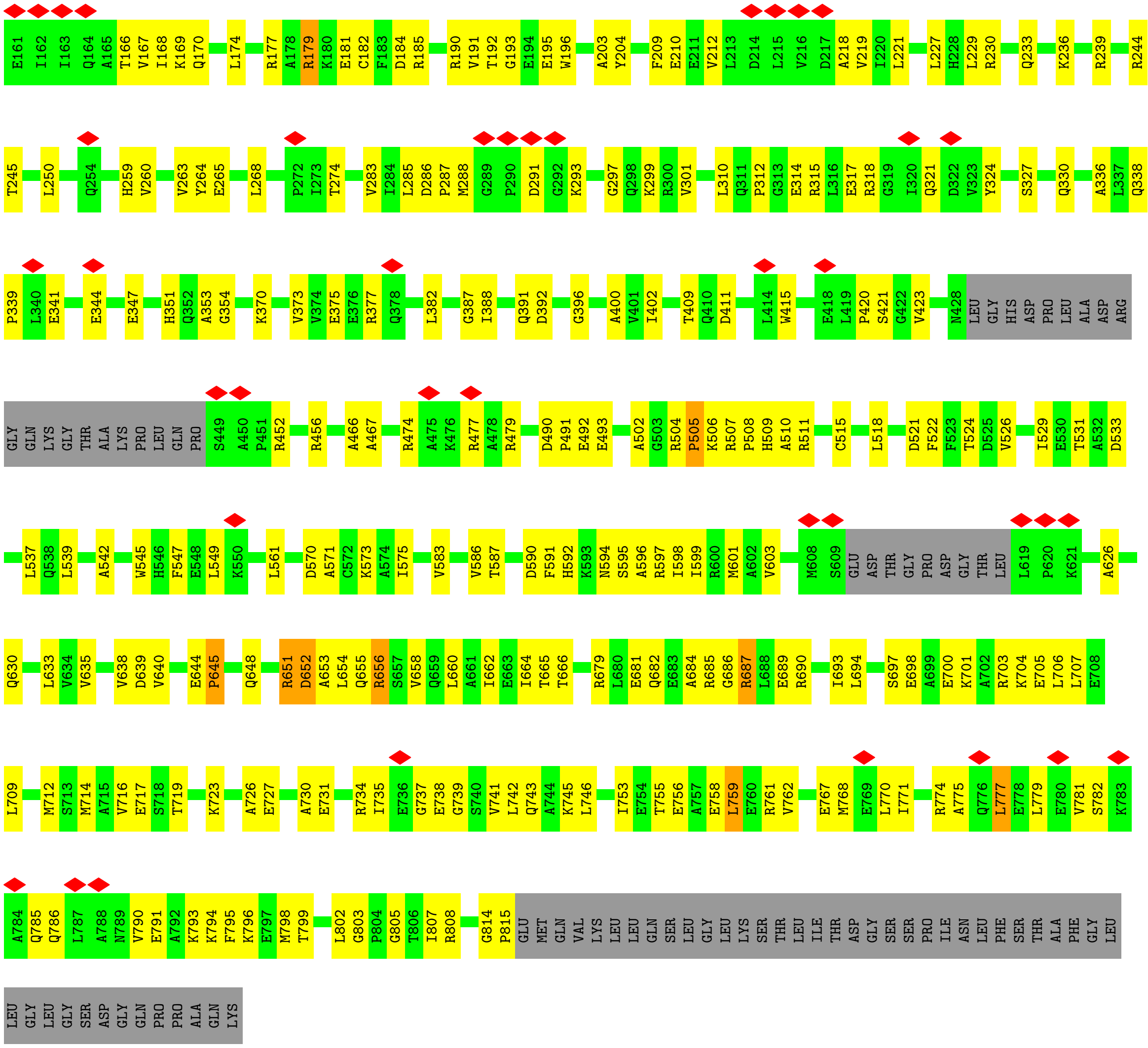


- Molecule 1: Major vault protein

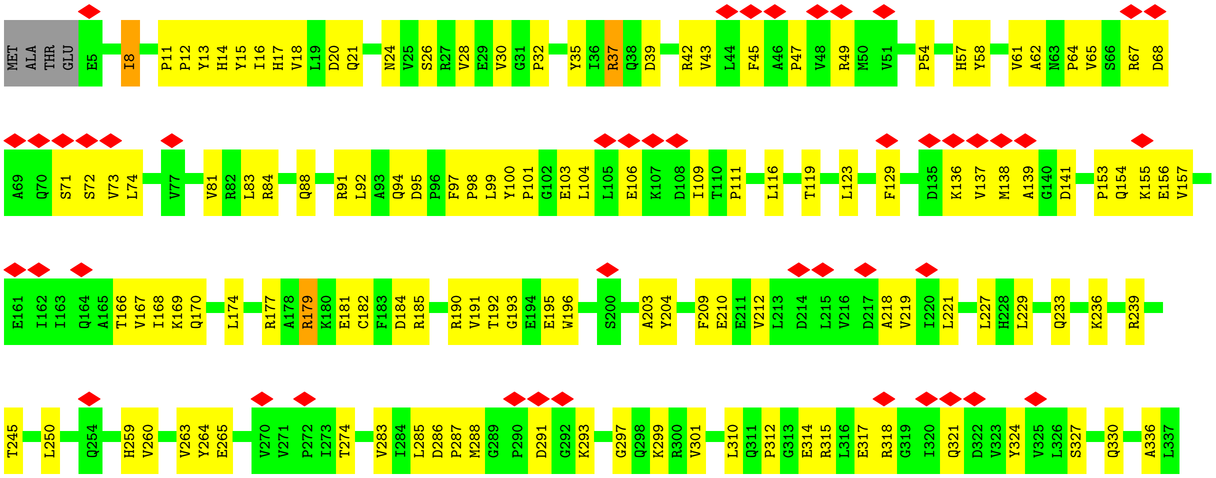


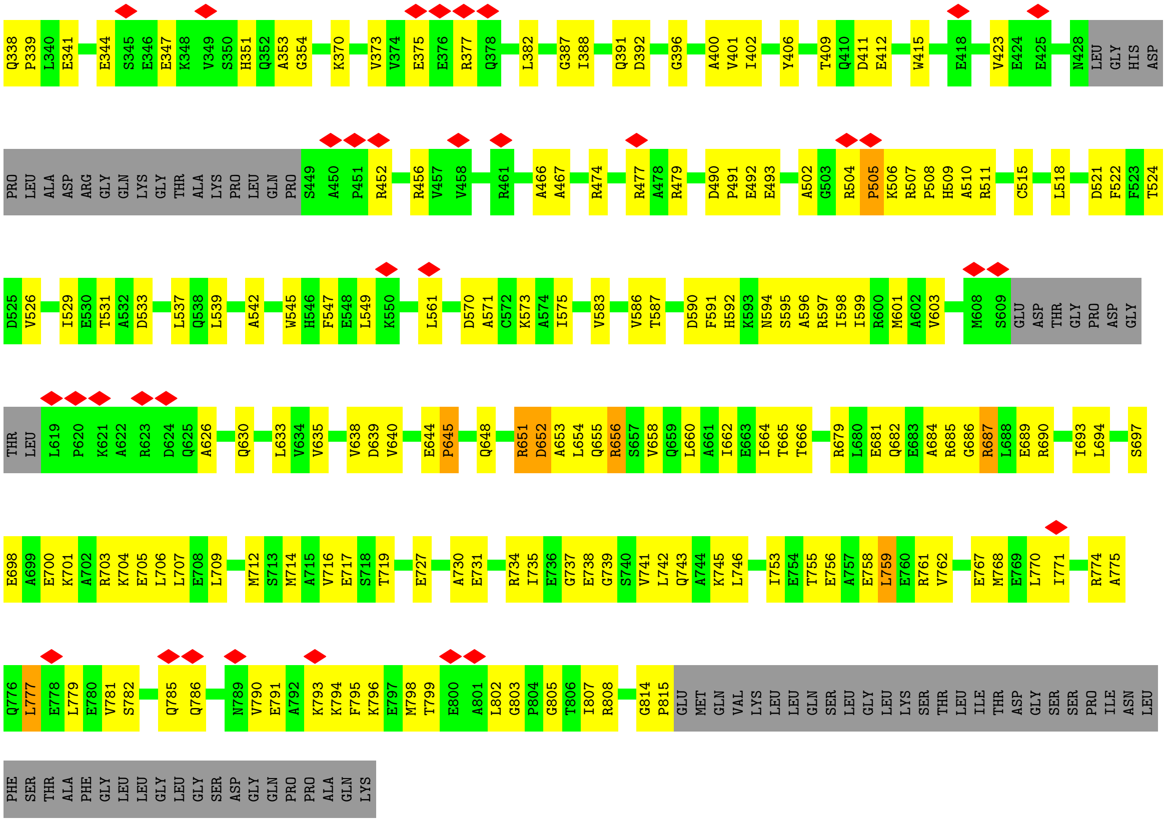
- Molecule 1: Major vault protein



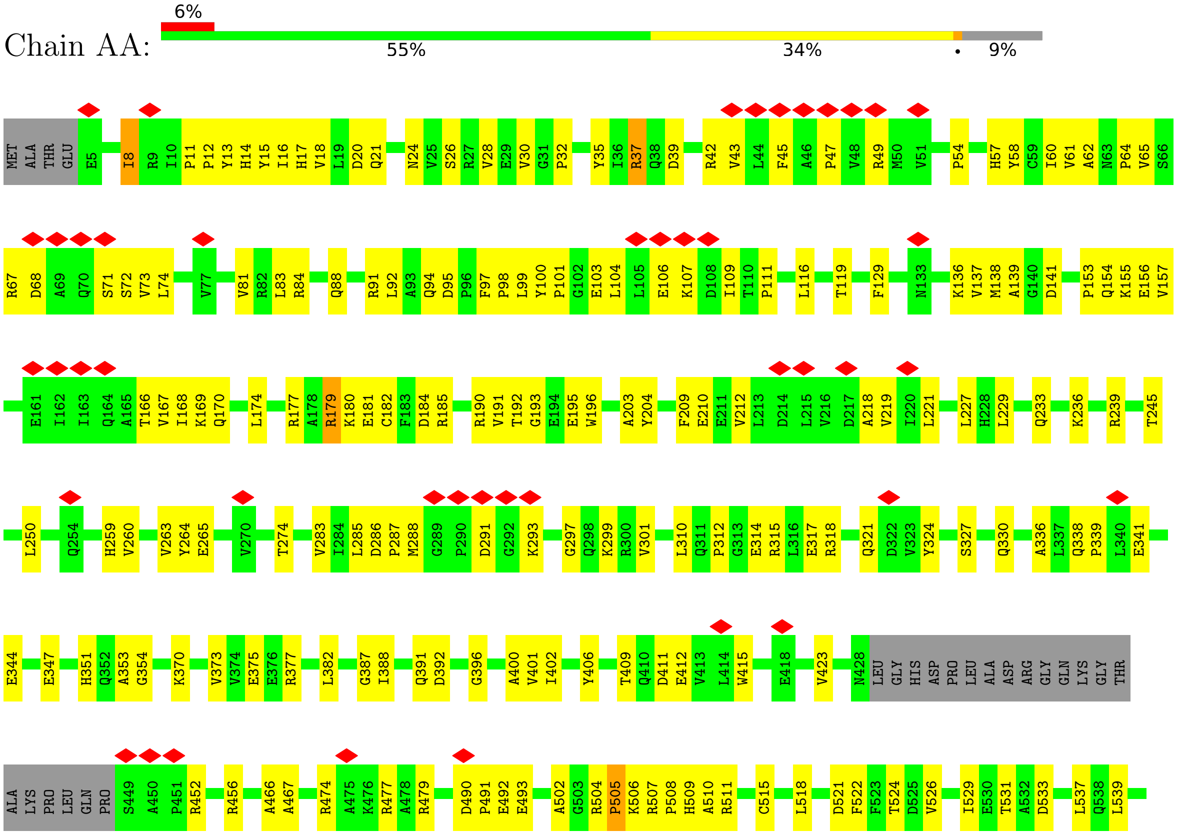


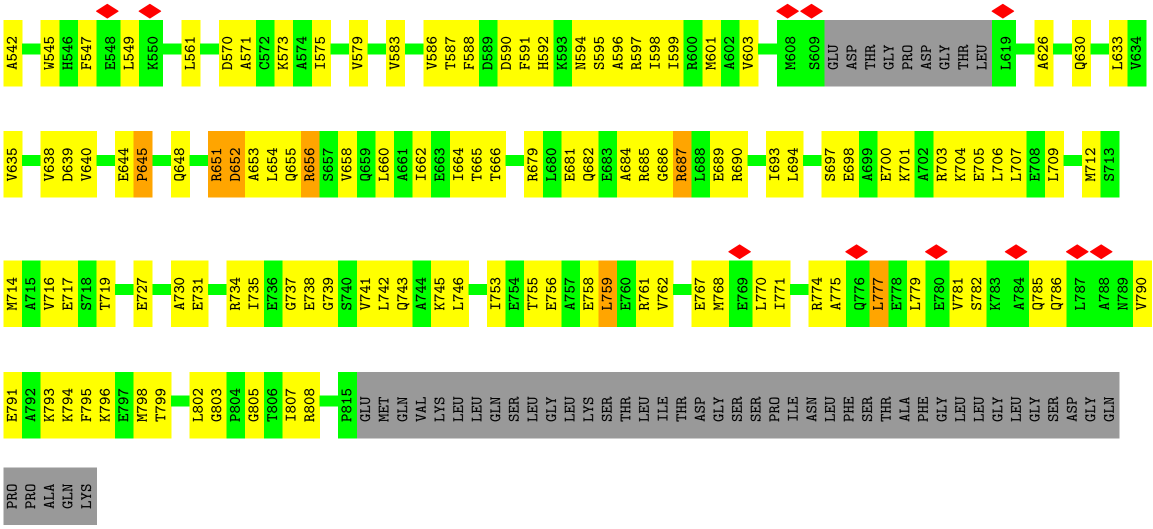
- Molecule 1: Major vault protein





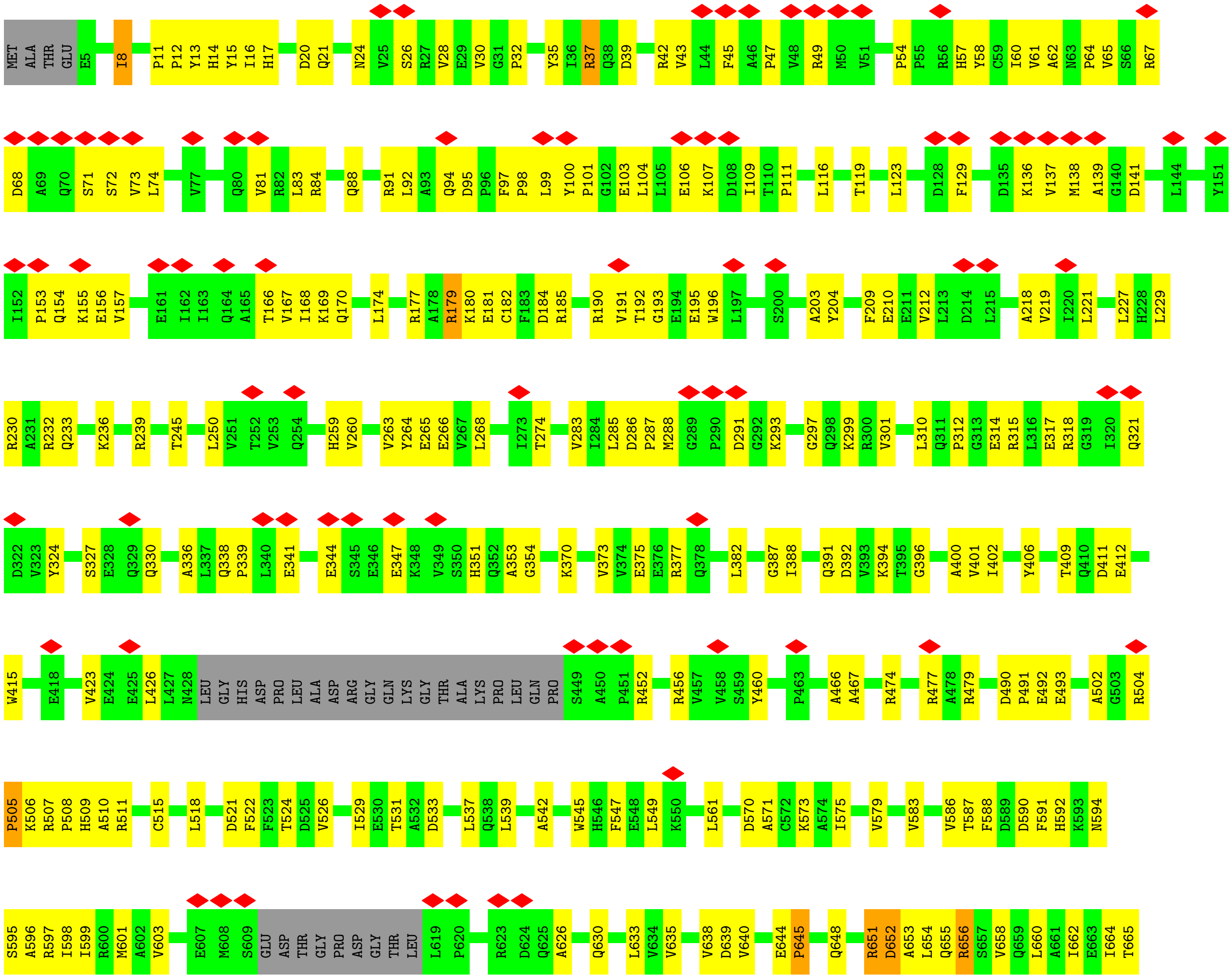
- Molecule 1: Major vault protein

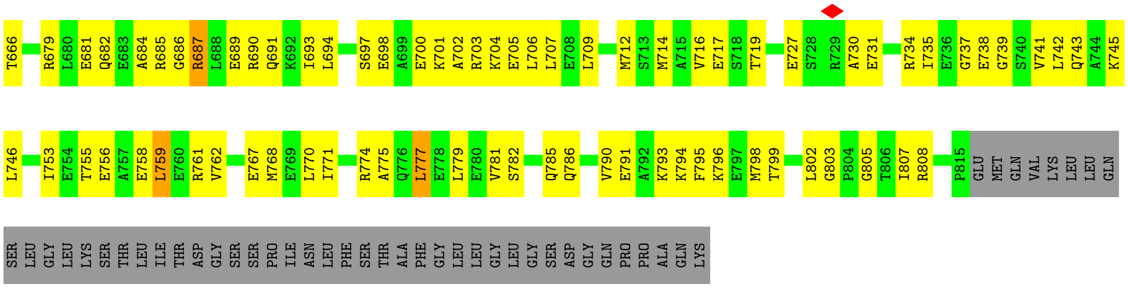




- Molecule 1: Major vault protein

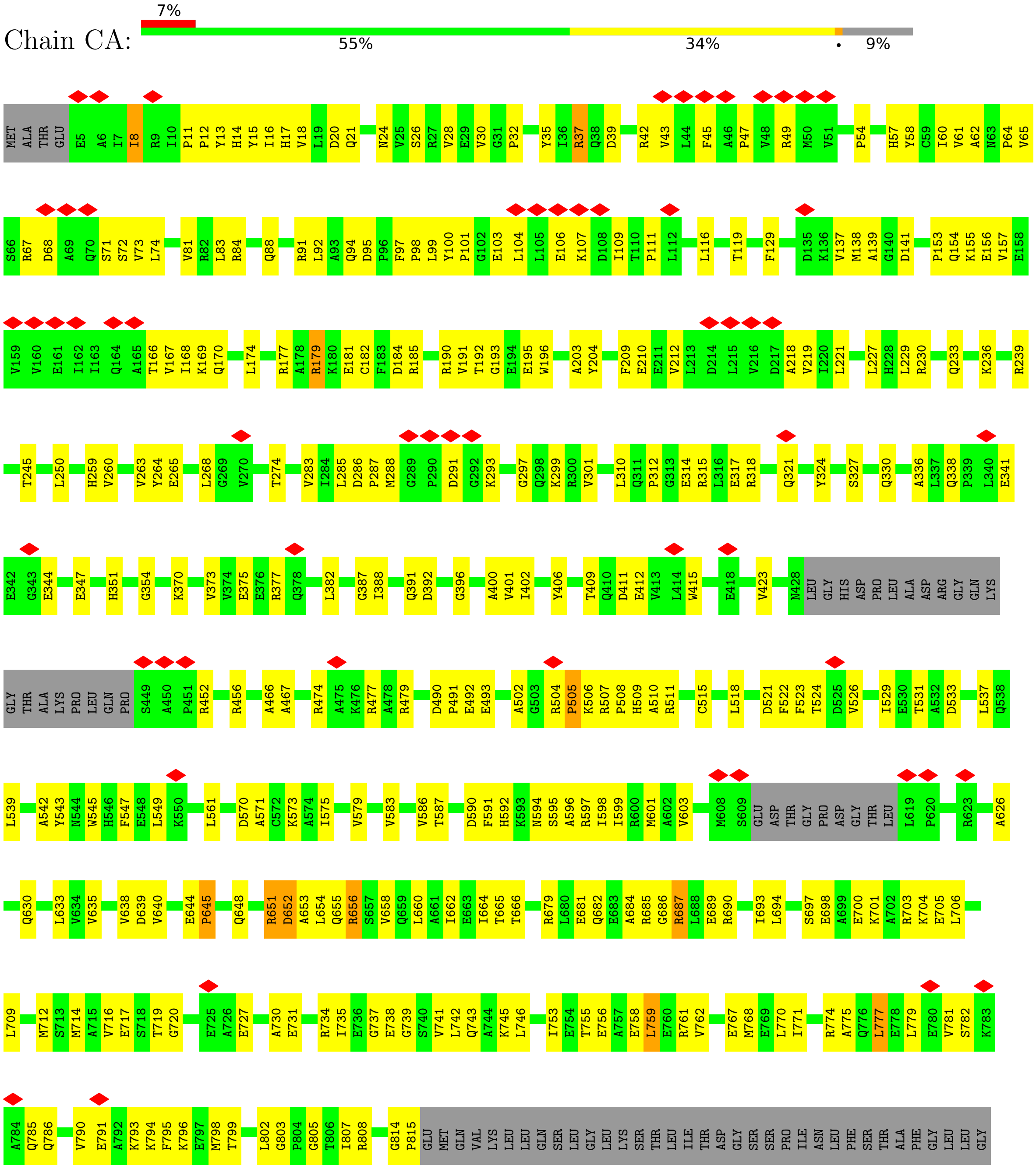
Chain BA:





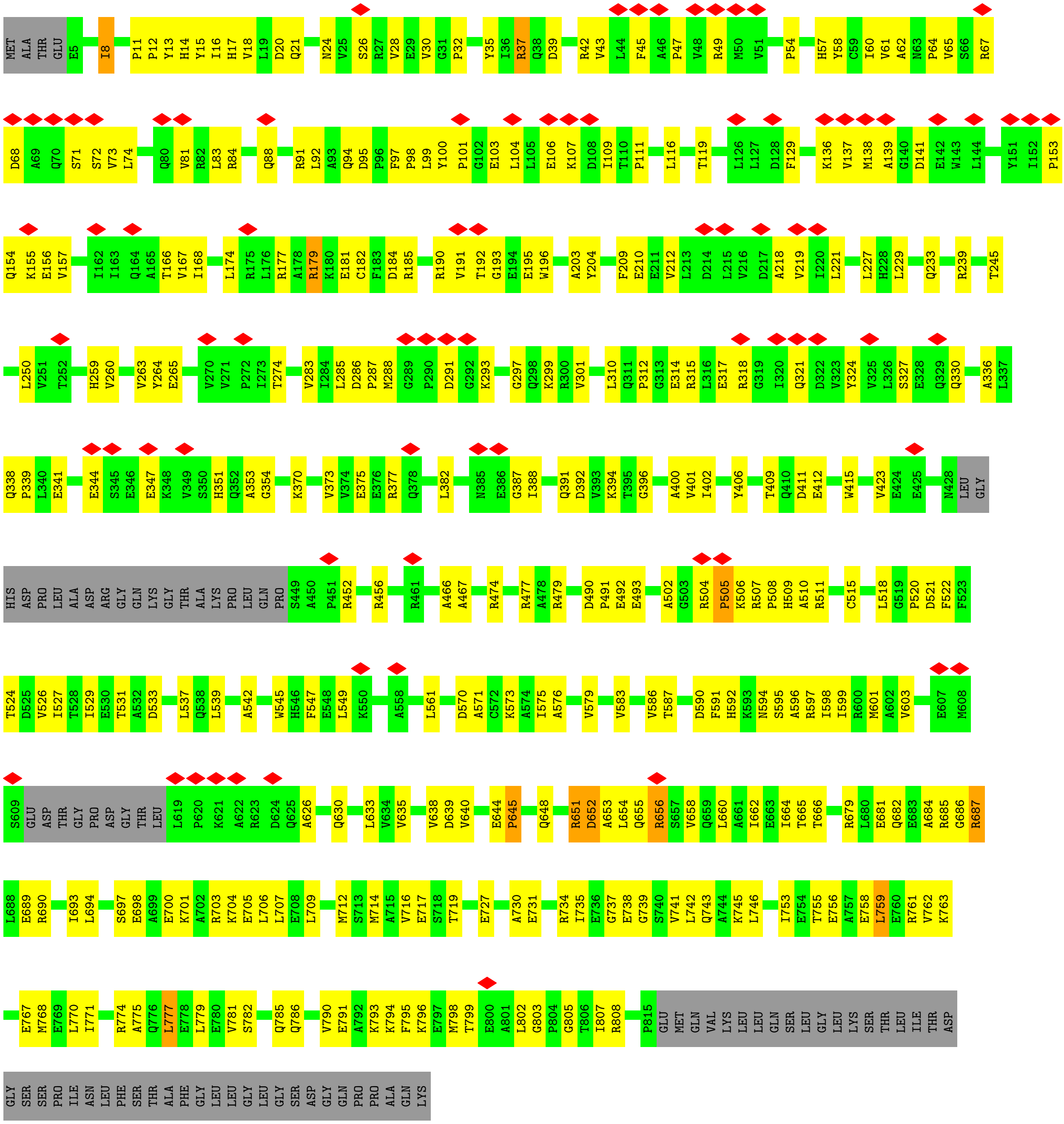
- Molecule 1: Major vault protein

Chain CA:



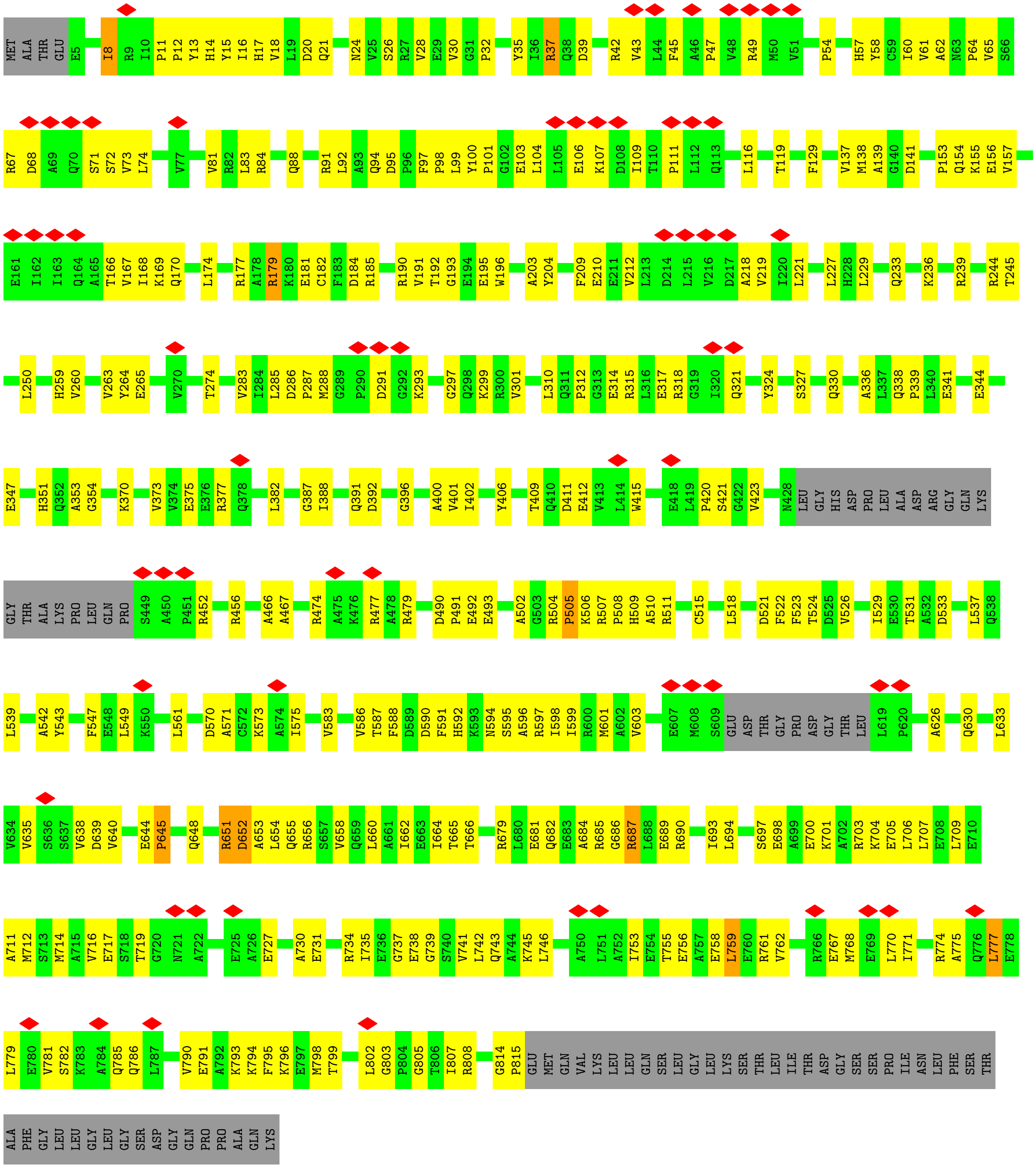
- Molecule 1: Major vault protein

Chain DA:



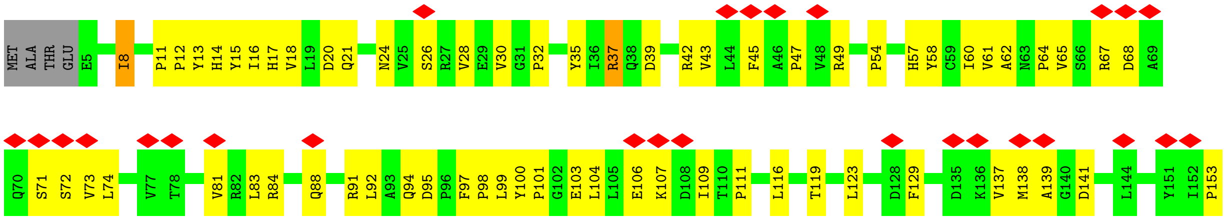
- Molecule 1: Major vault protein

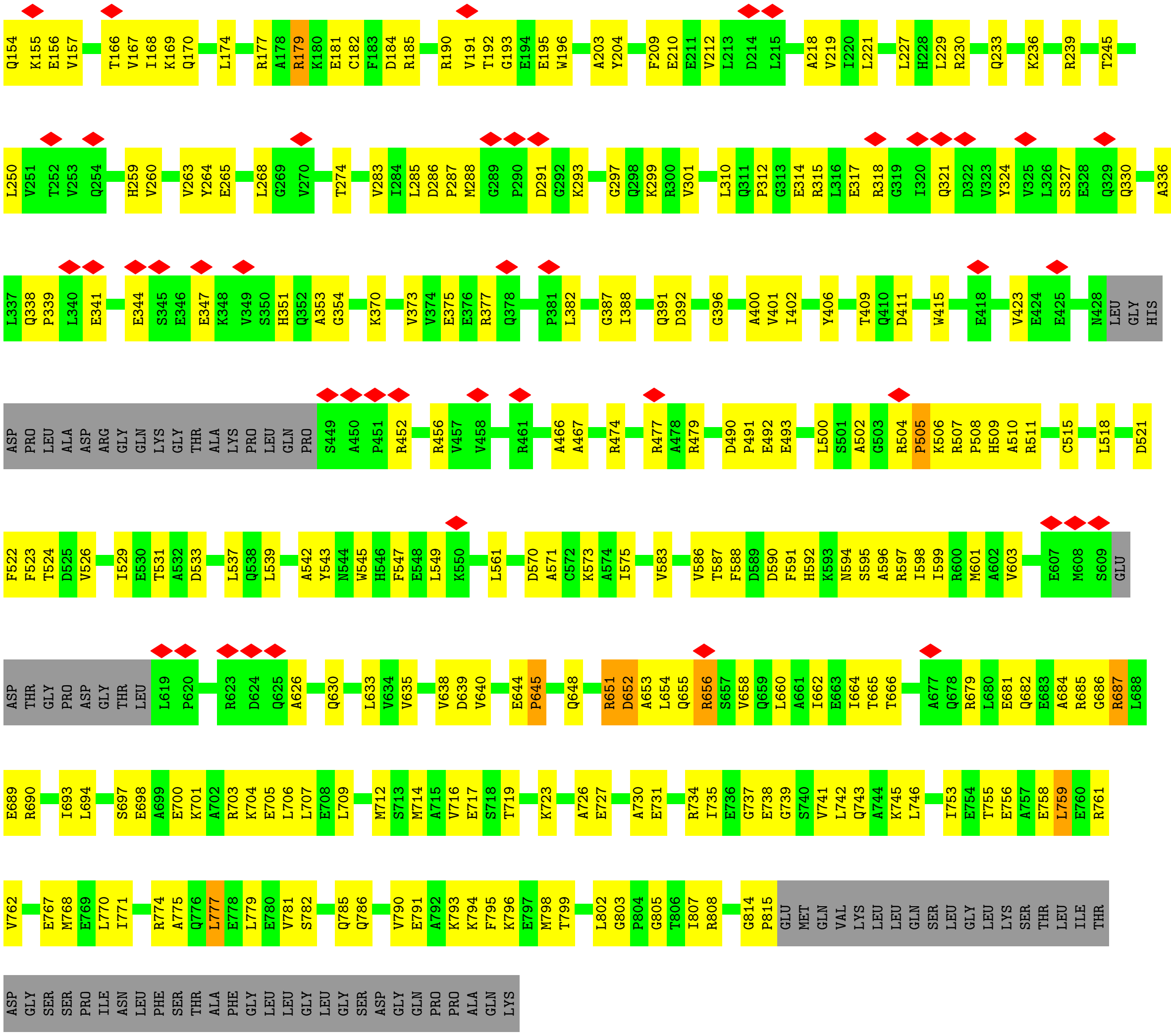
Chain EA:



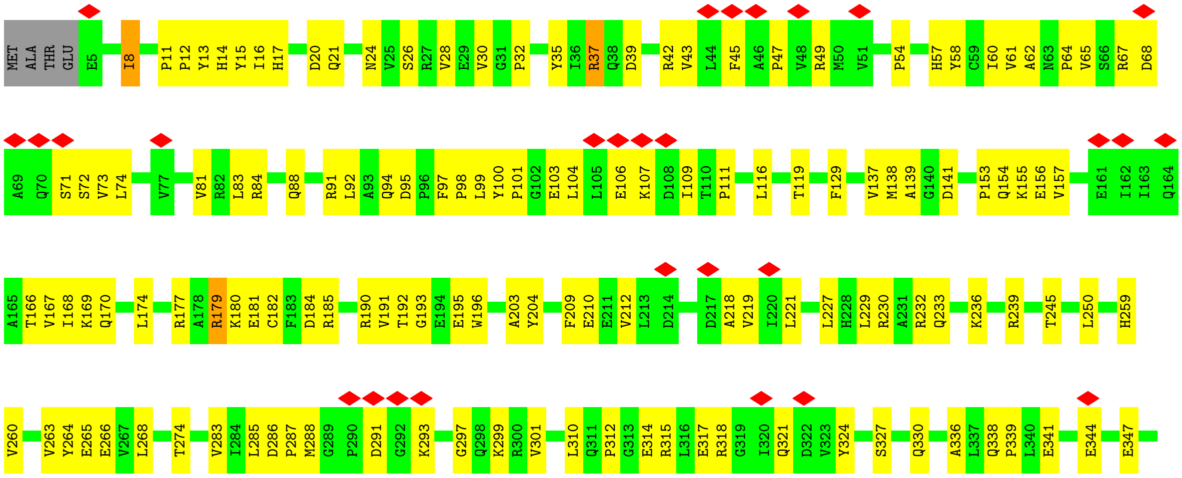
- Molecule 1: Major vault protein

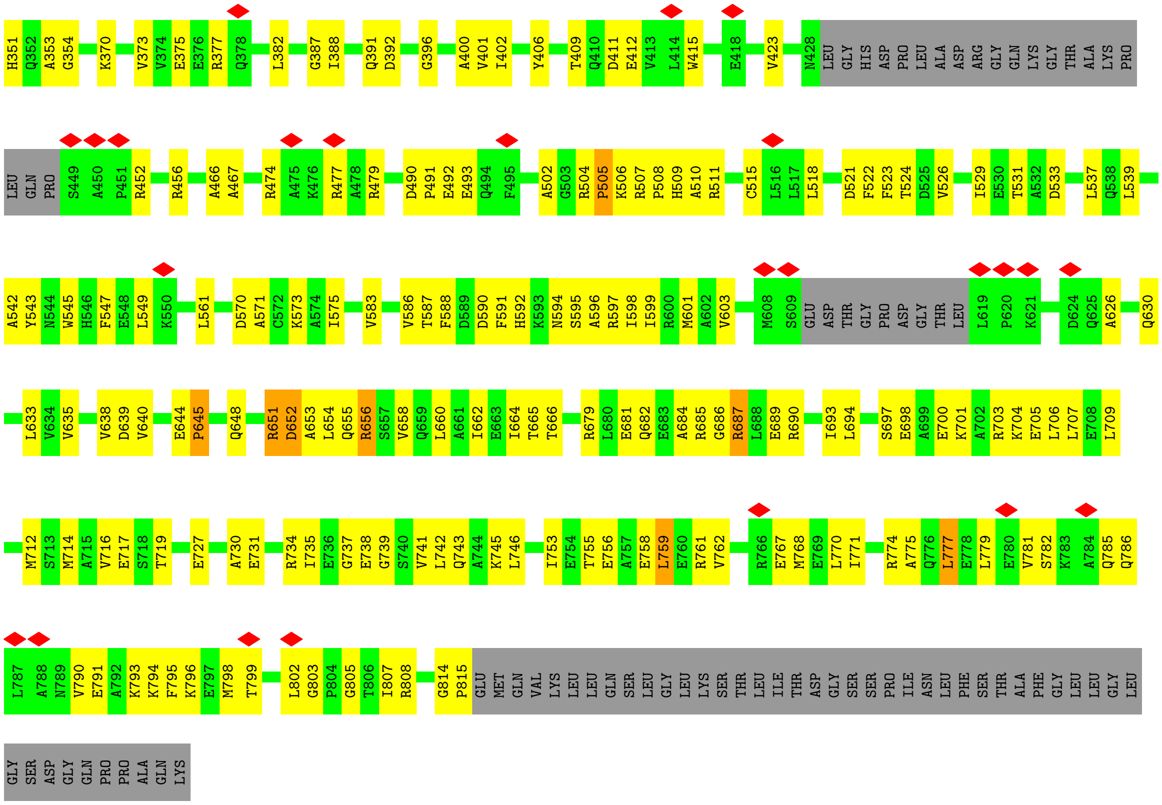
Chain FA:





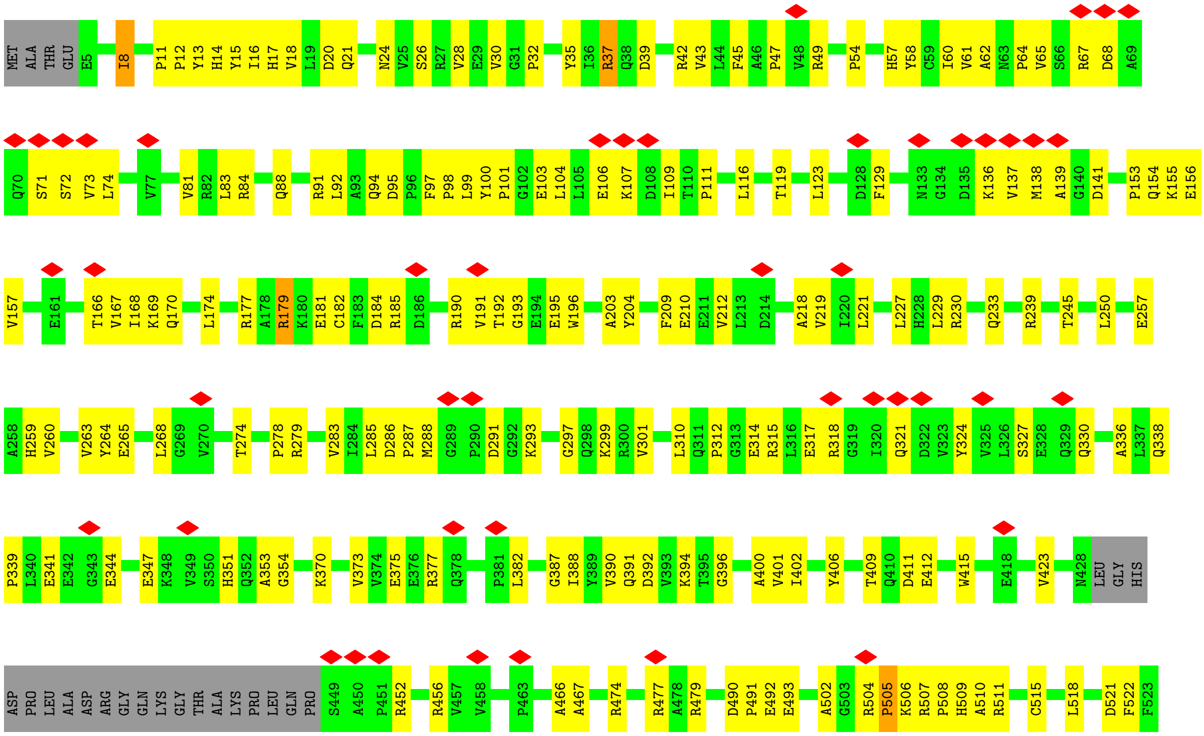
- Molecule 1: Major vault protein

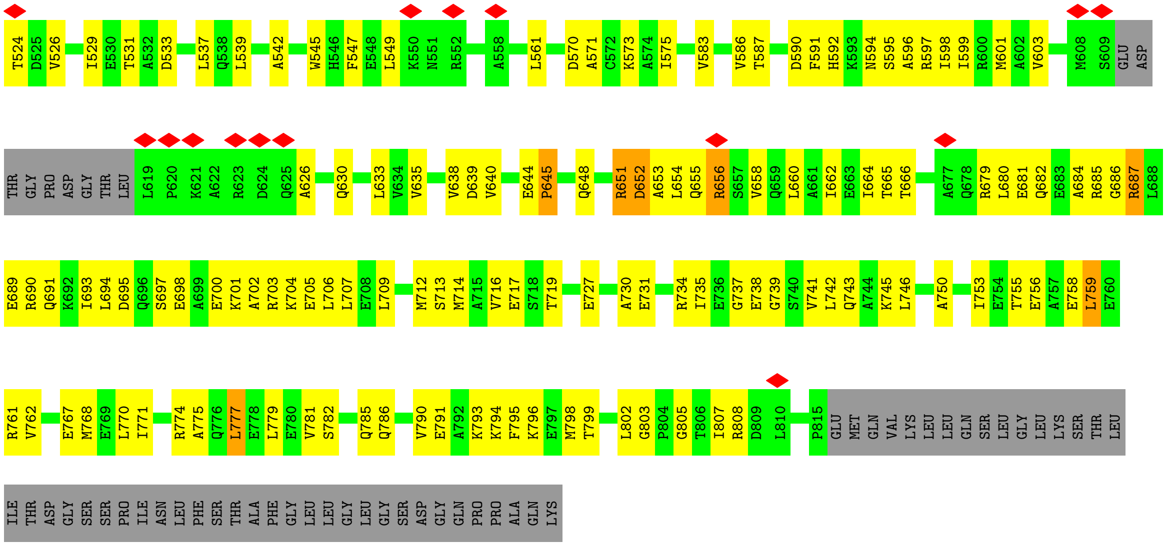




- Molecule 1: Major vault protein

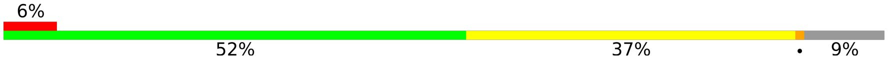
Chain HA:

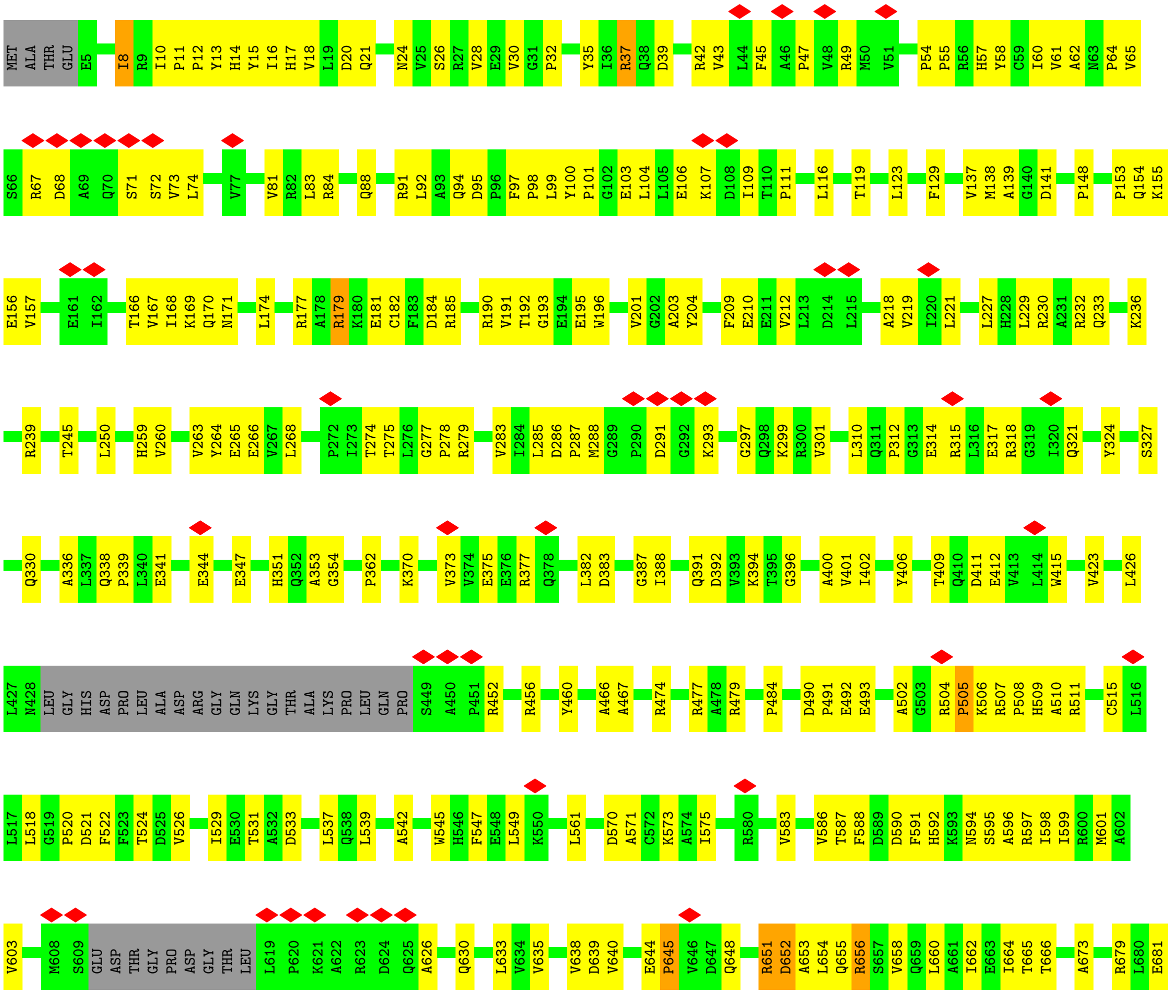


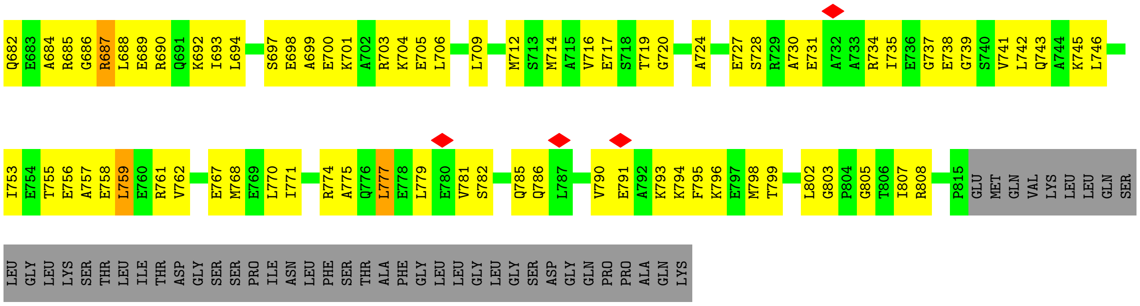


- Molecule 1: Major vault protein

Chain IA:

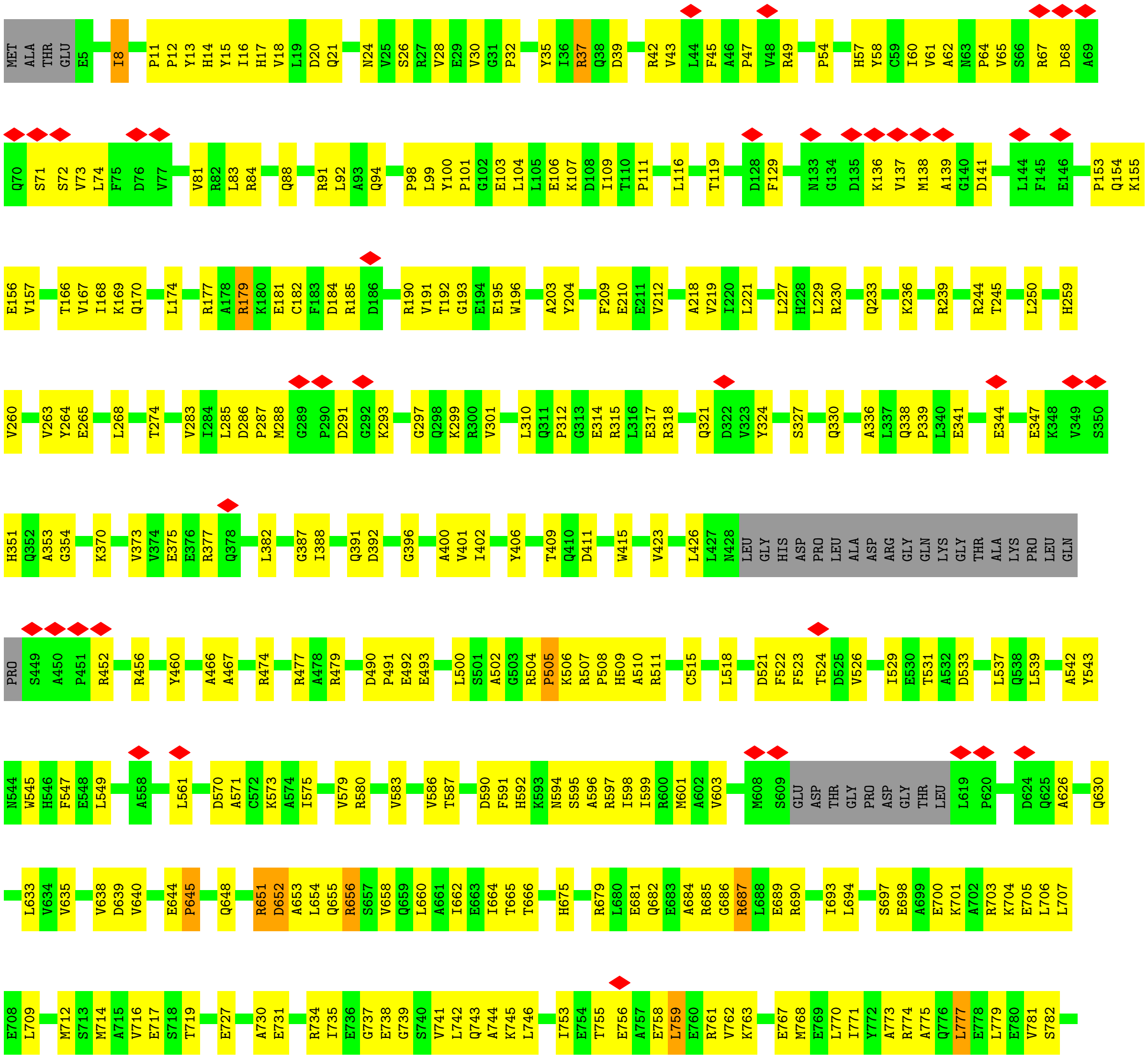






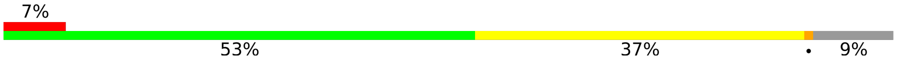
- Molecule 1: Major vault protein

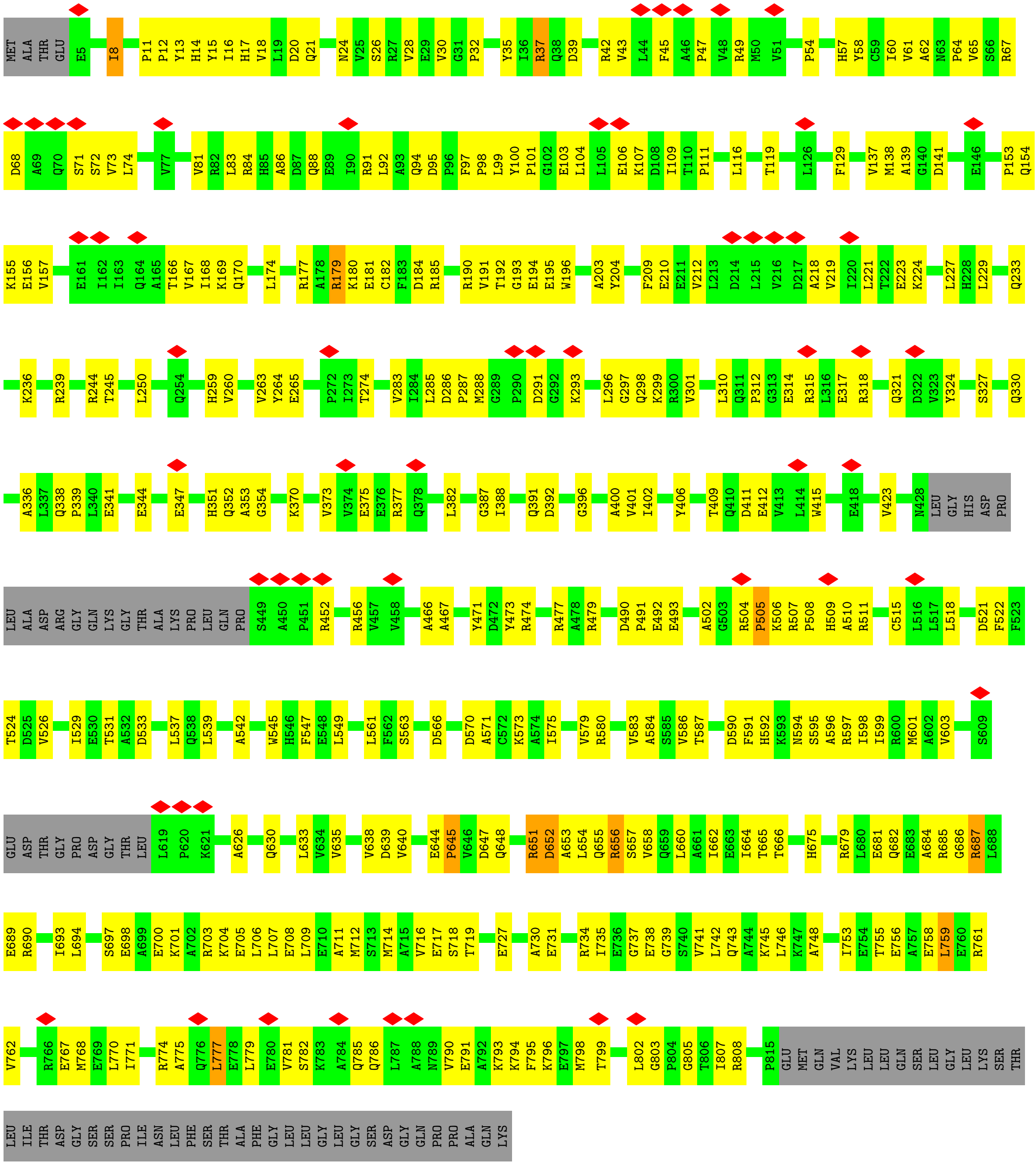
Chain JA:



• Molecule 1: Major vault protein

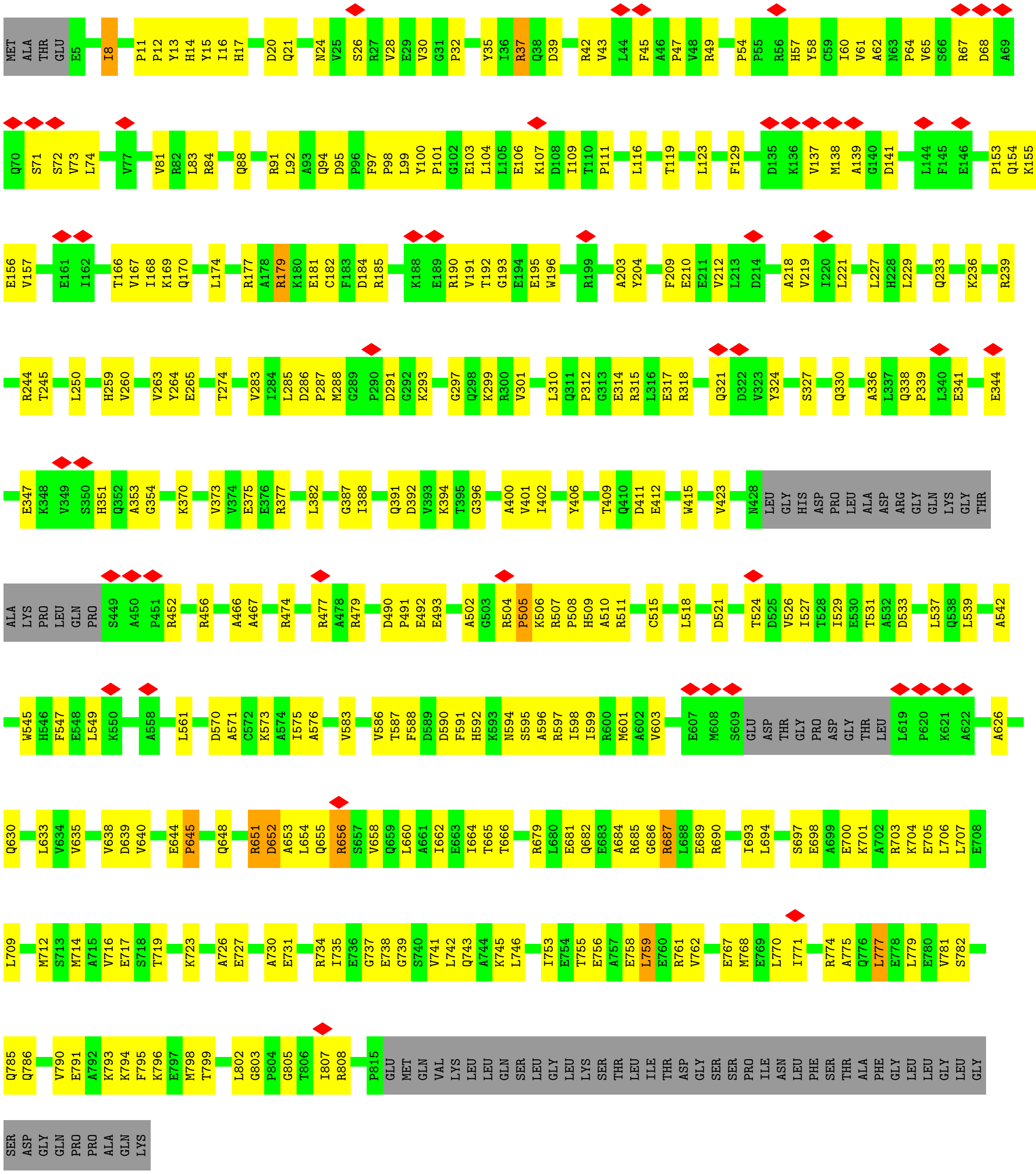
Chain KA:





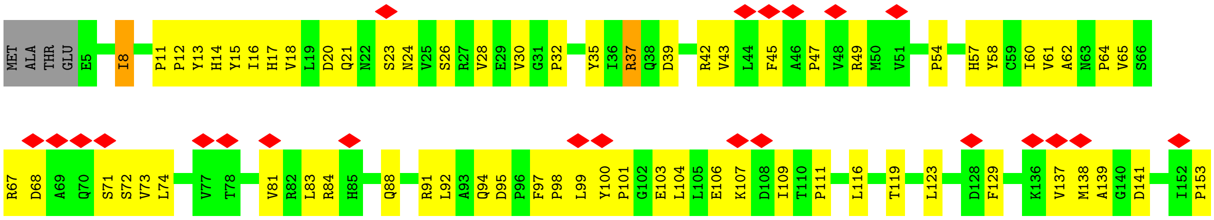
• Molecule 1: Major vault protein

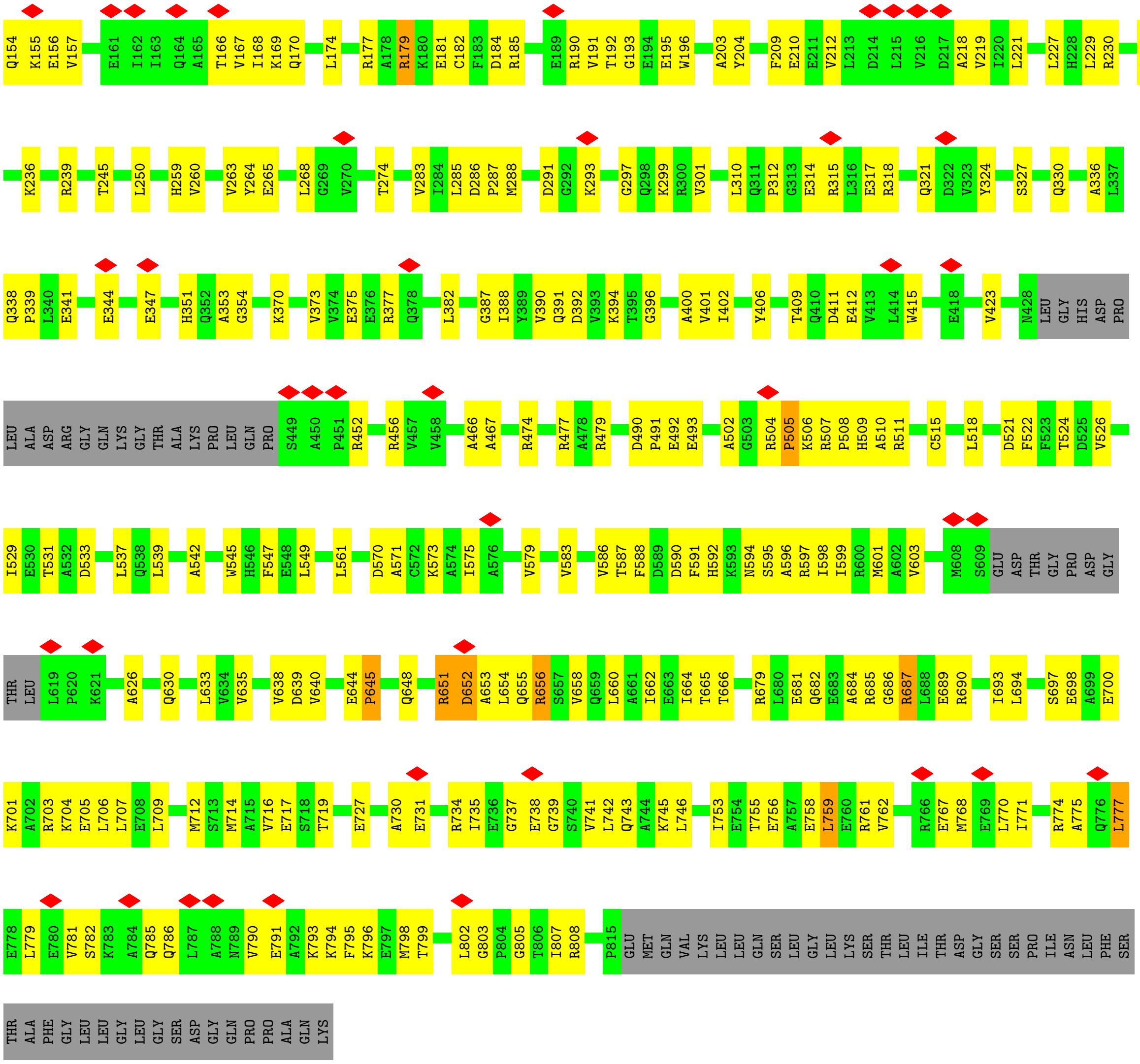
Chain LA:



- Molecule 1: Major vault protein

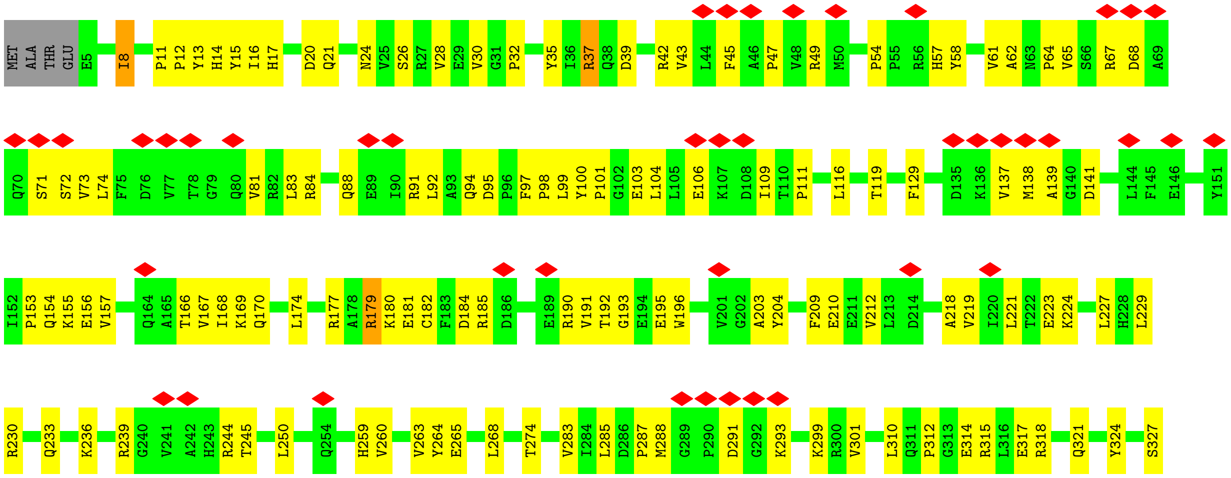
Chain MA:

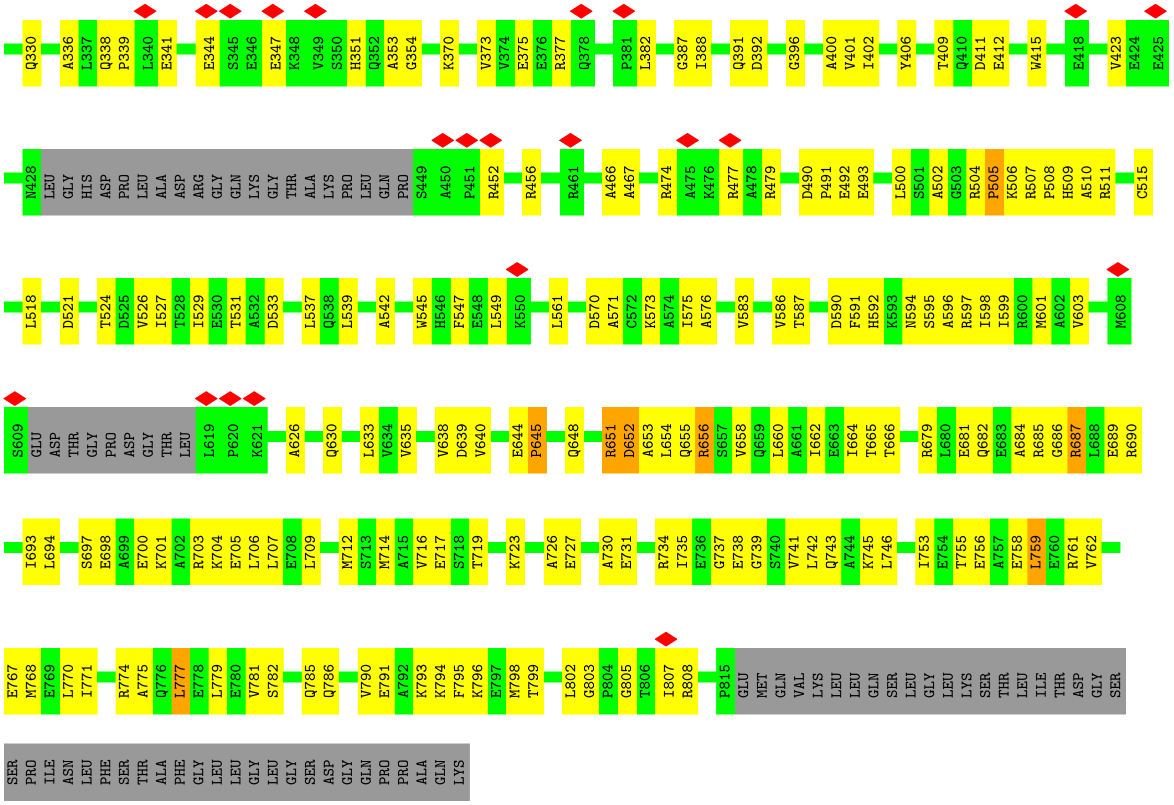




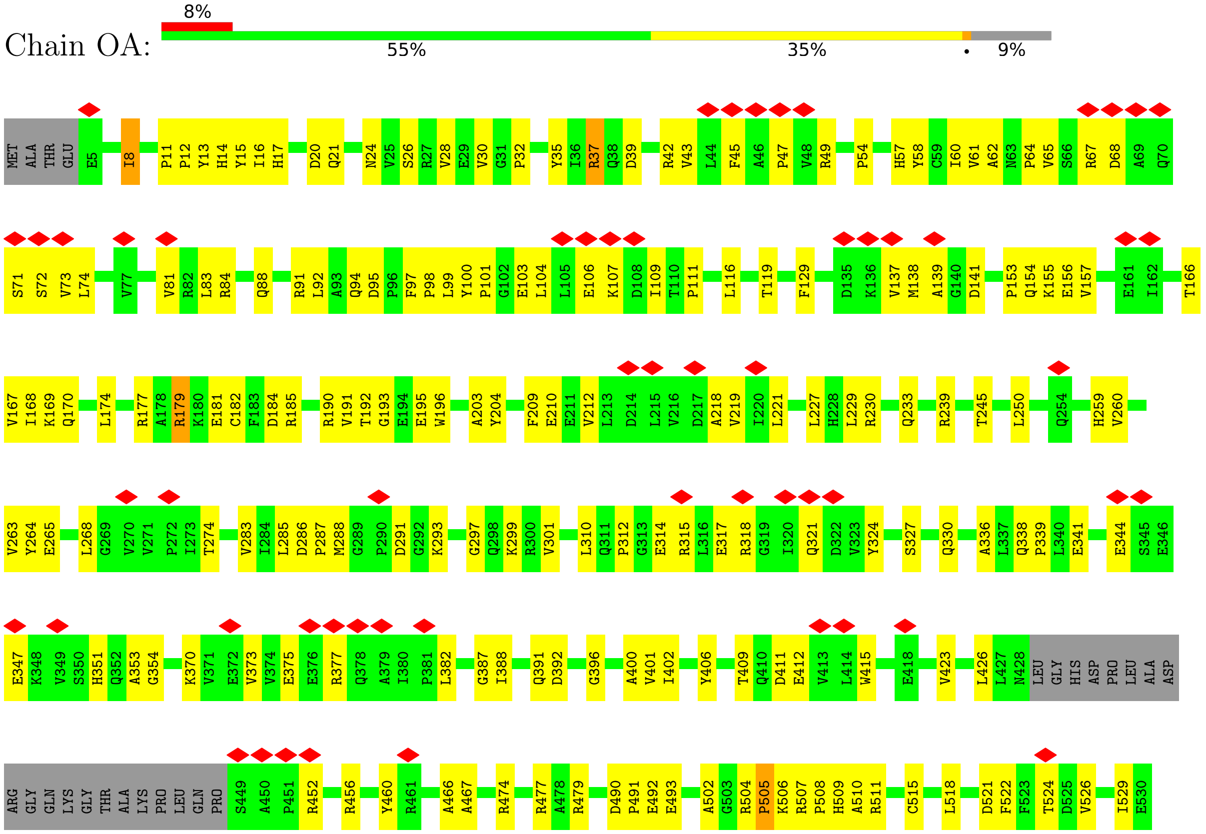
- Molecule 1: Major vault protein

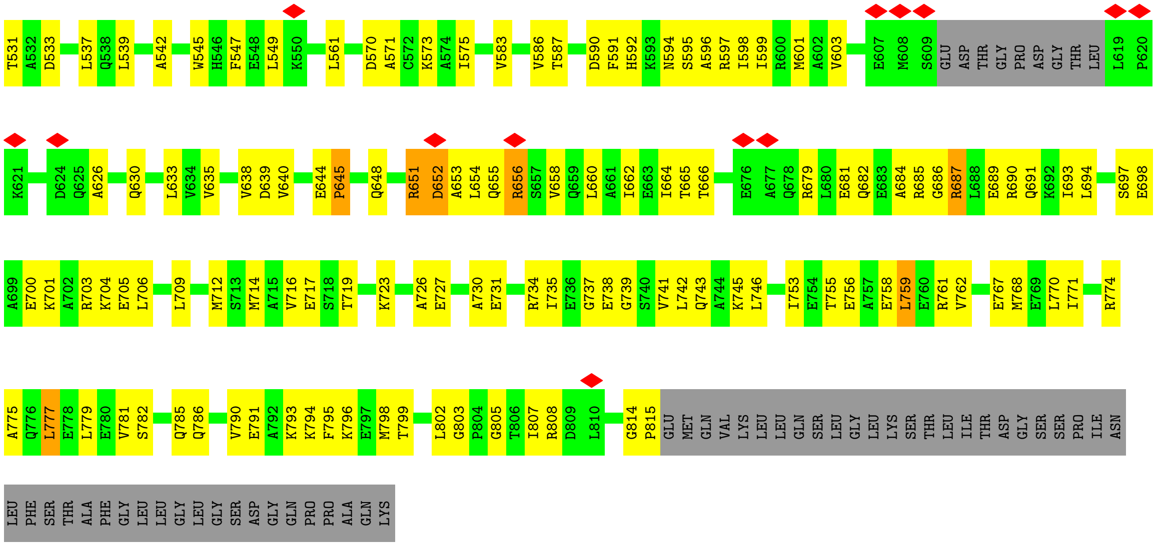
Chain NA:





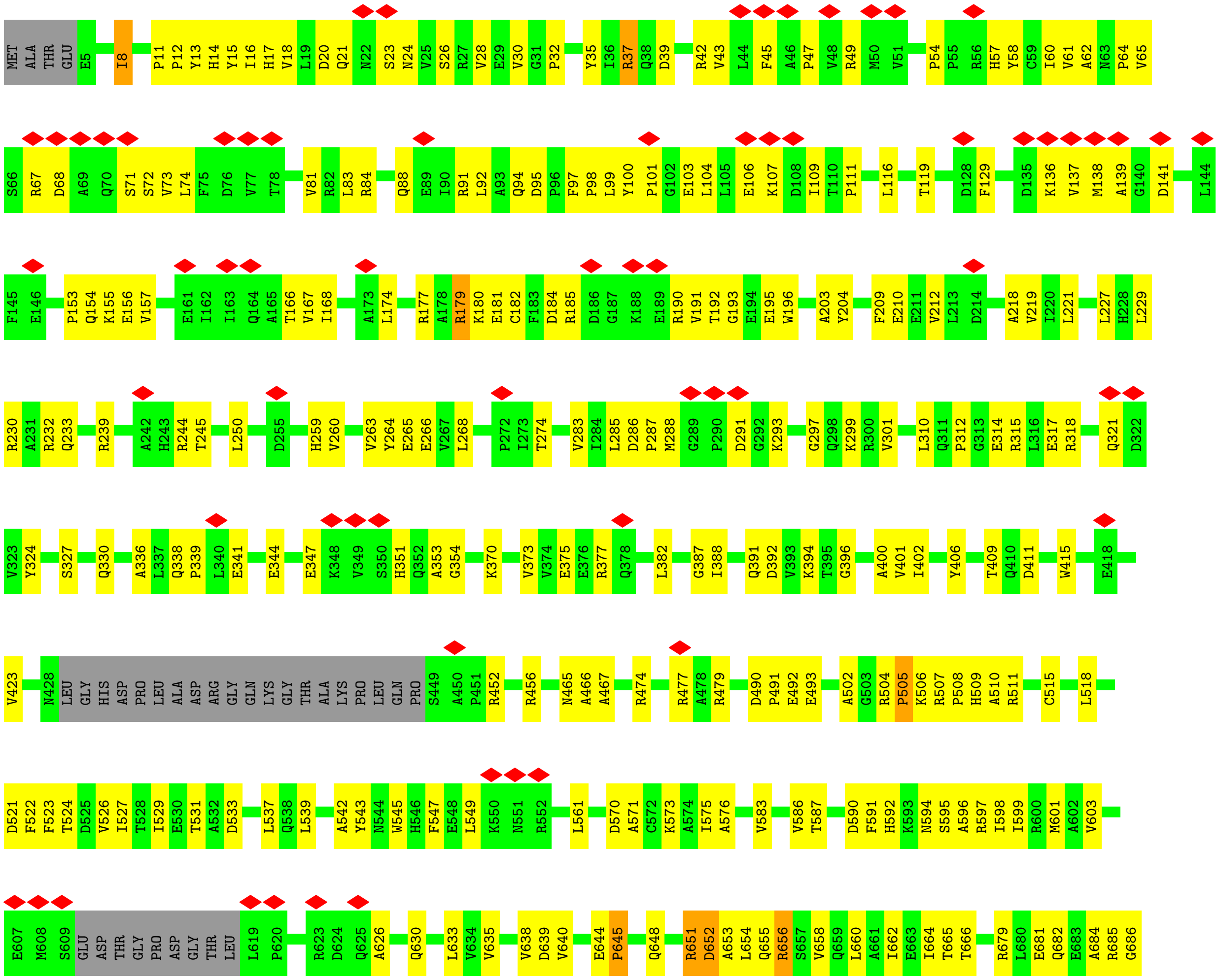
- Molecule 1: Major vault protein

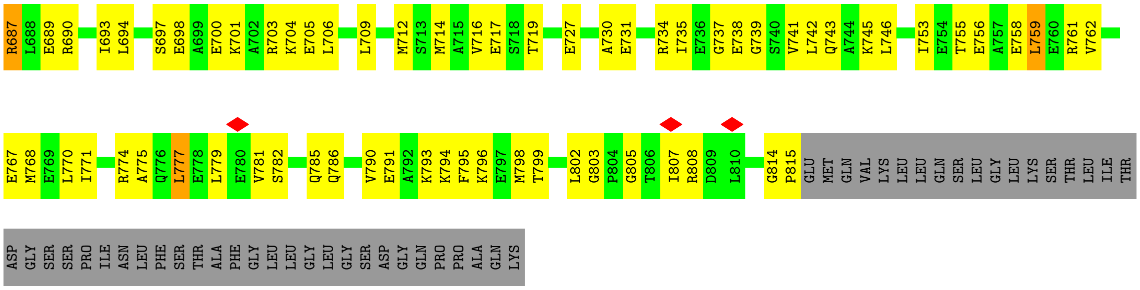




- Molecule 1: Major vault protein

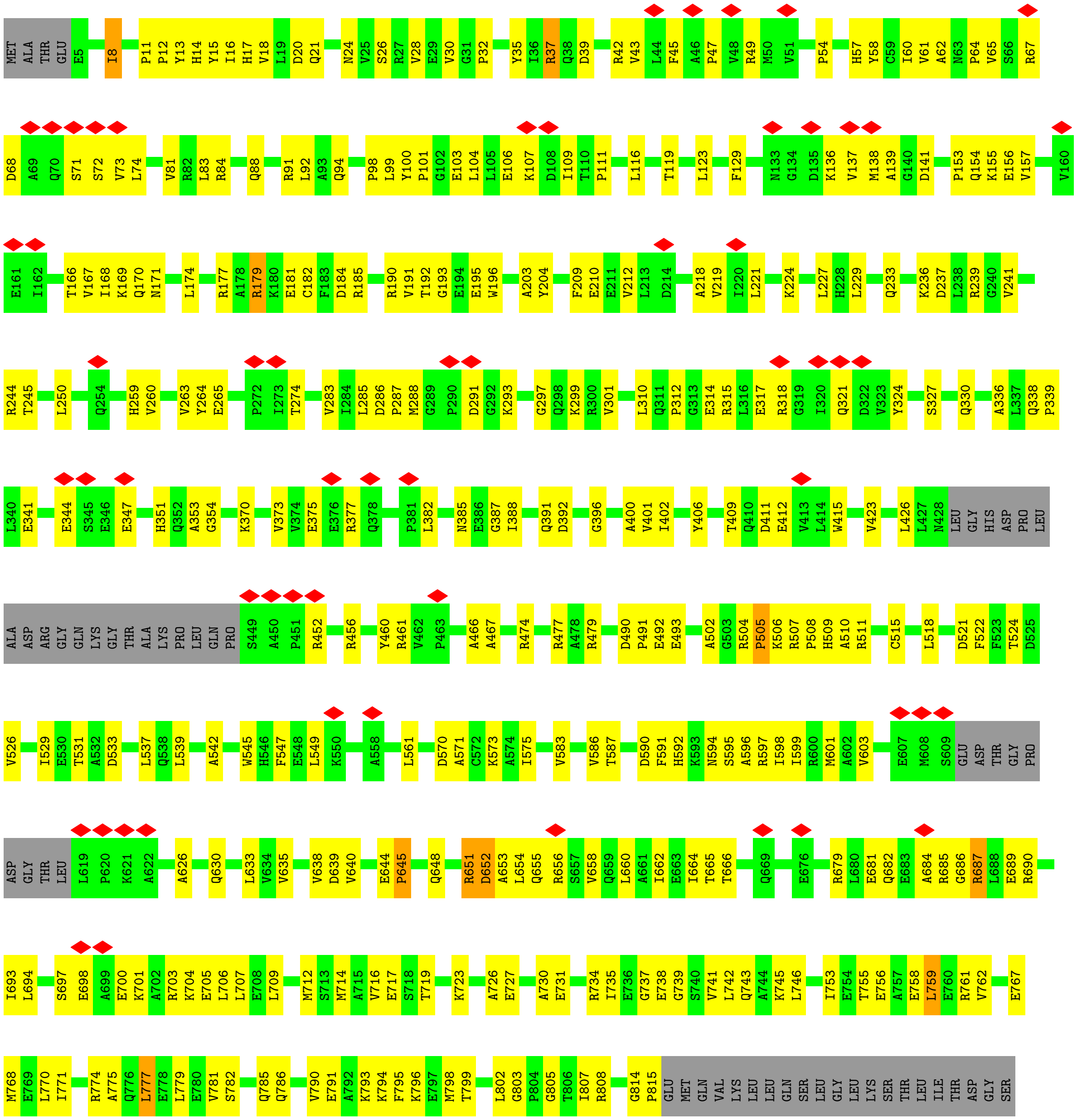
Chain PA:

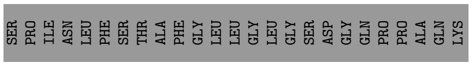




• Molecule 1: Major vault protein

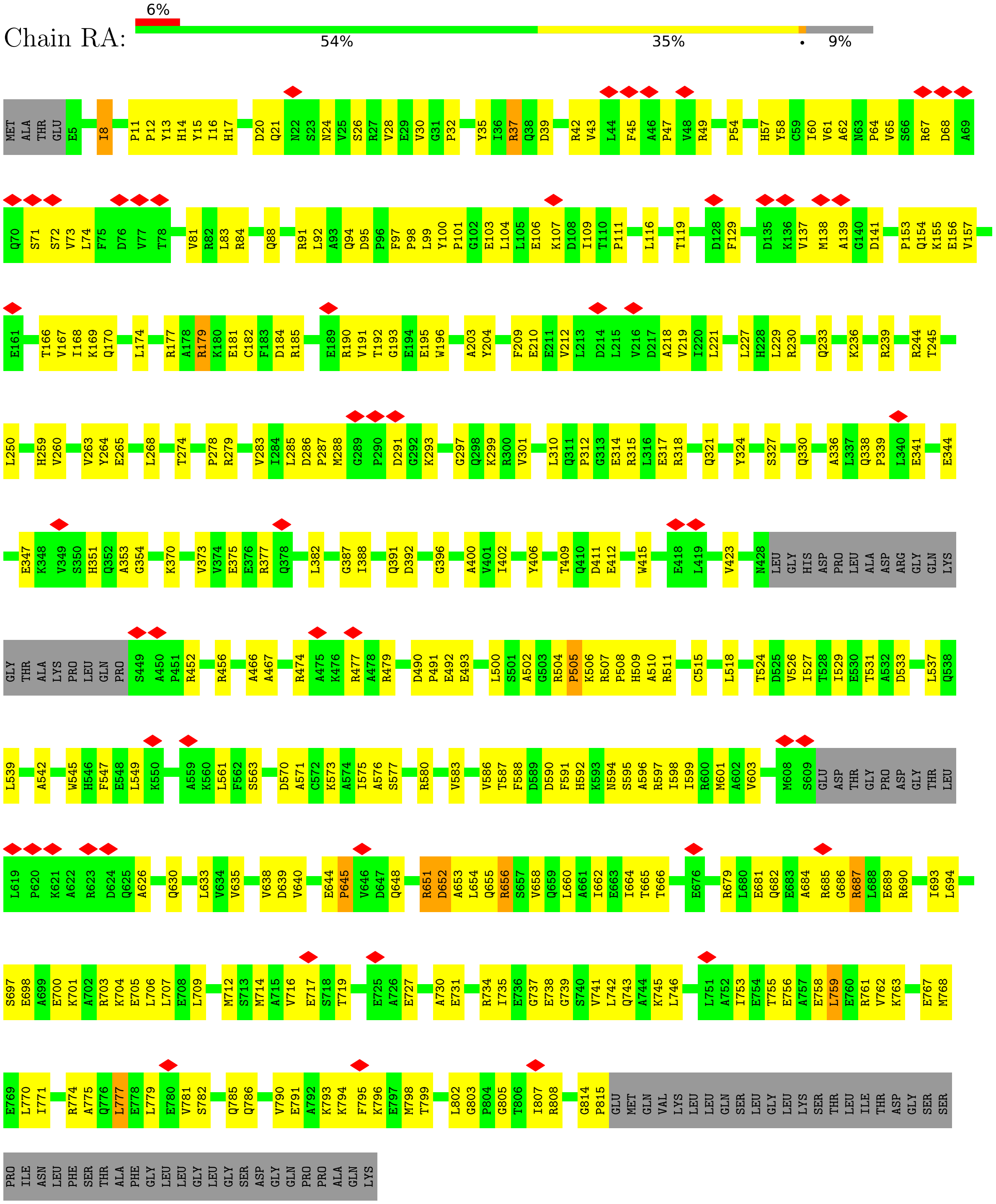
Chain QA:





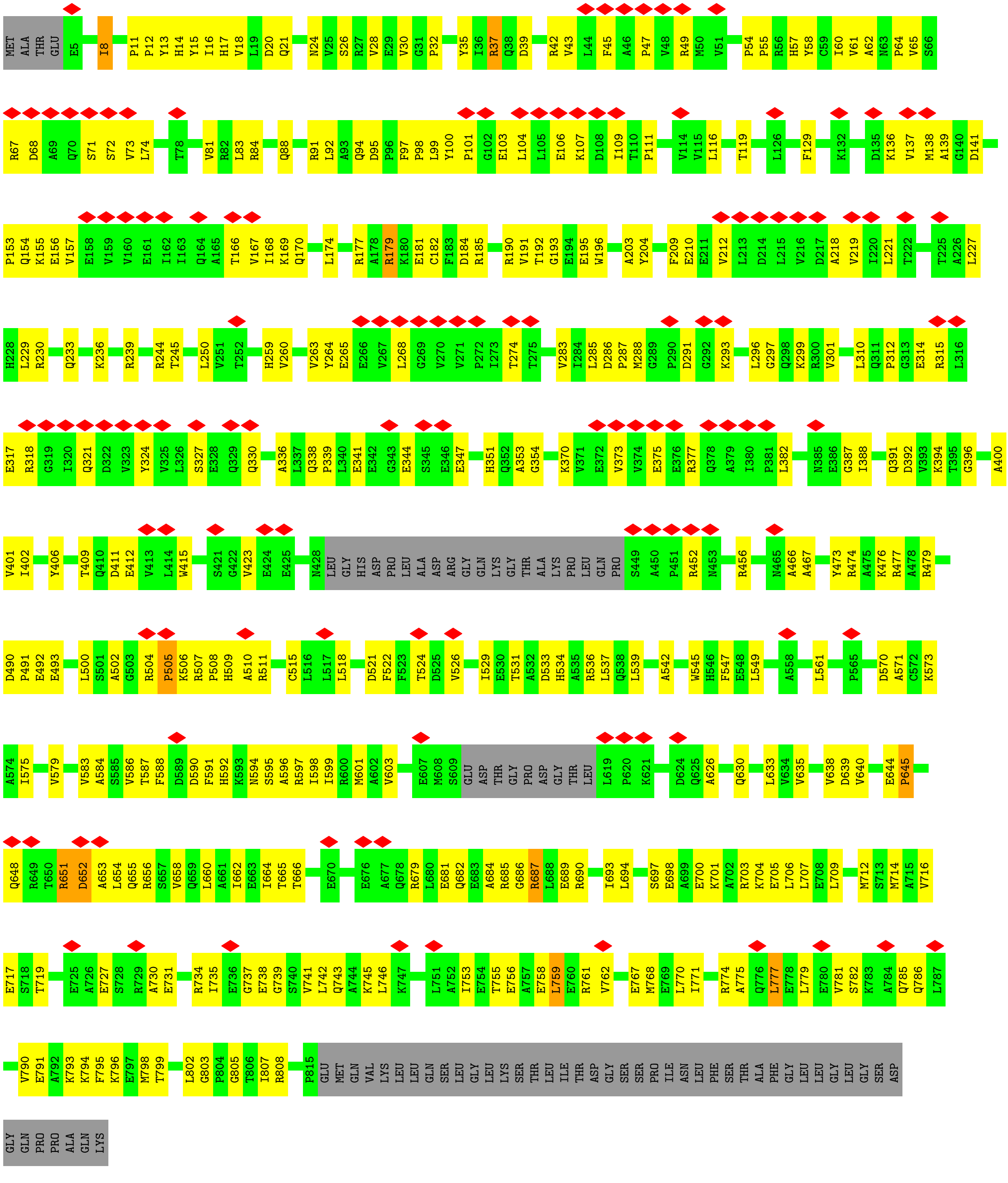
- Molecule 1: Major vault protein

Chain RA:



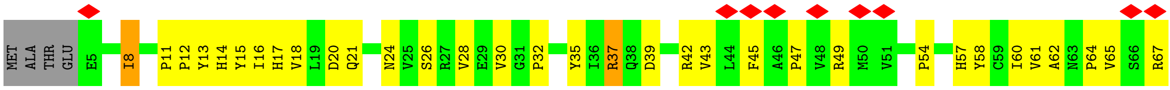
- Molecule 1: Major vault protein

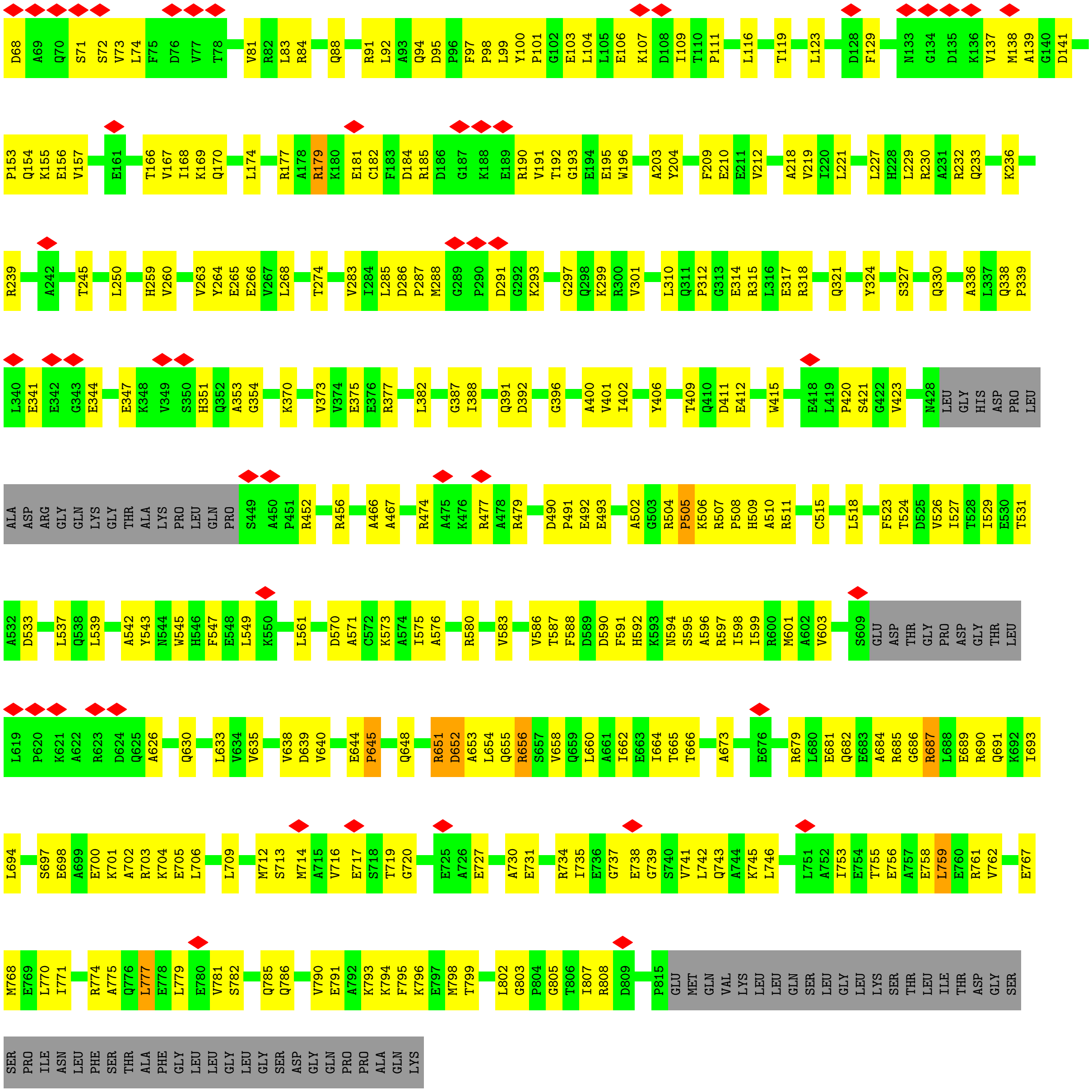
Chain SA:



• Molecule 1: Major vault protein

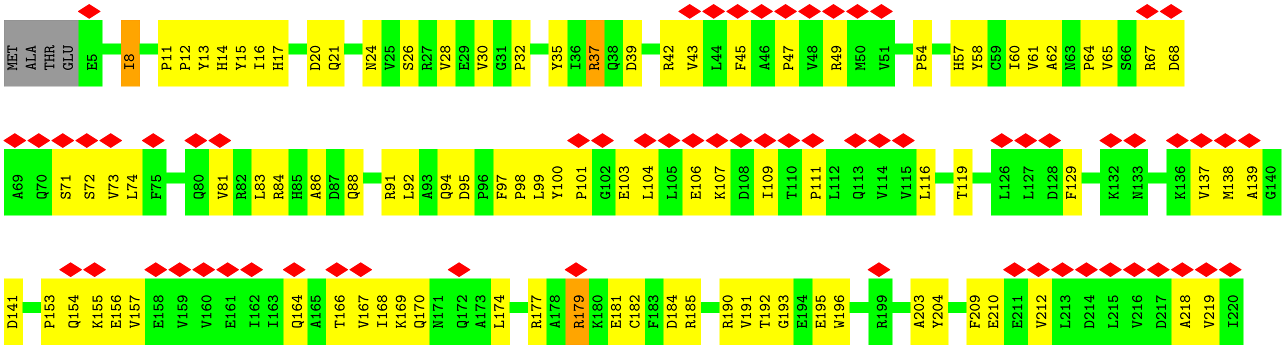
Chain TA:

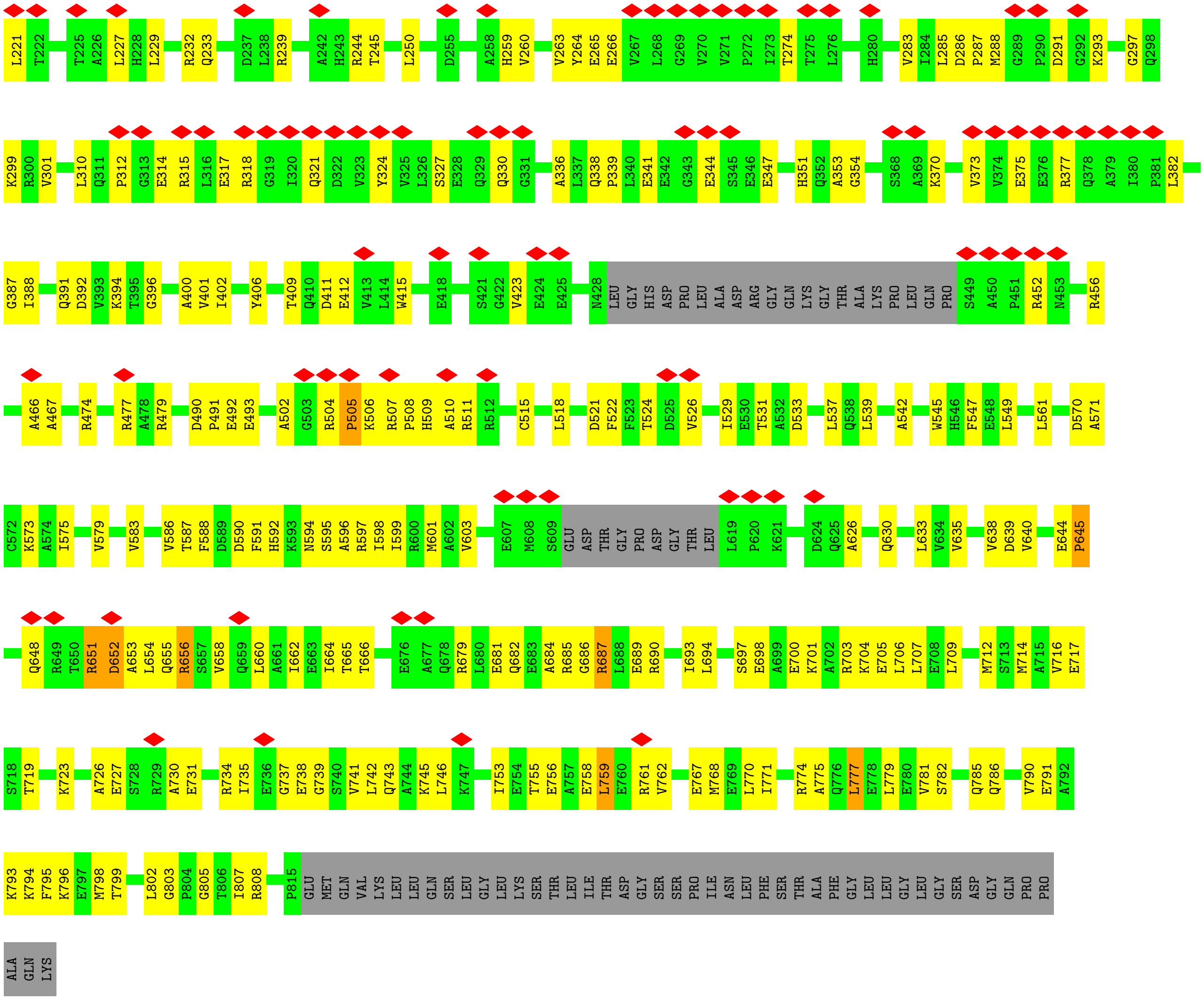




- Molecule 1: Major vault protein

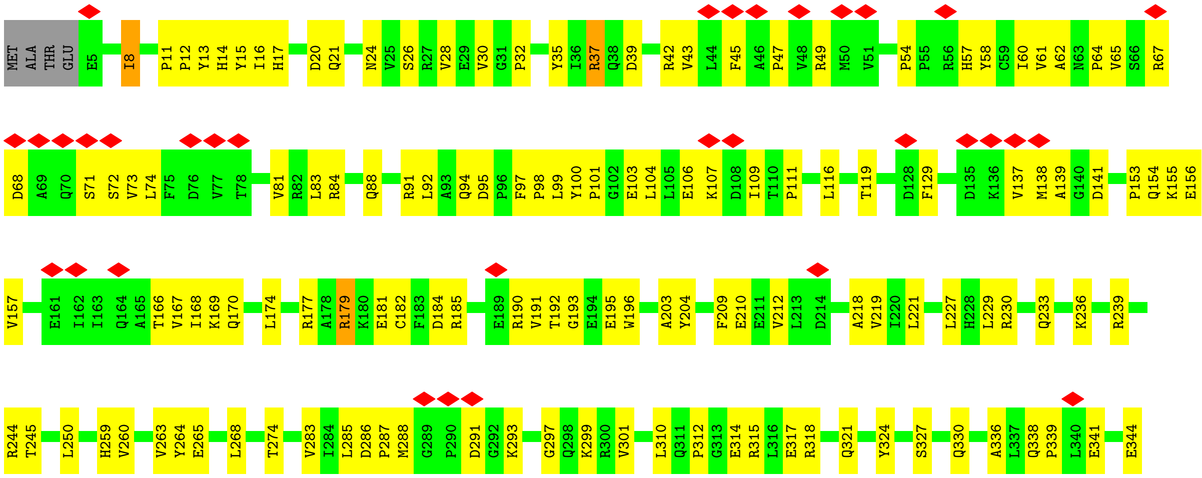
Chain UA:

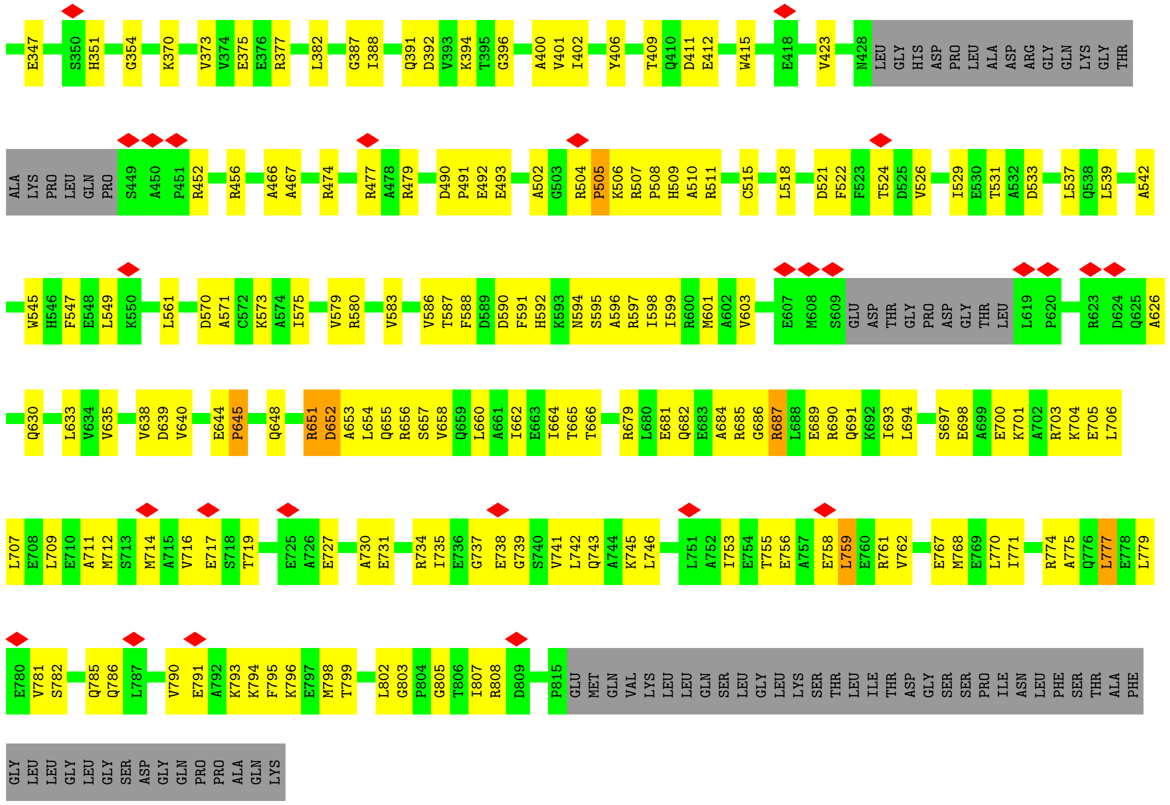




- Molecule 1: Major vault protein

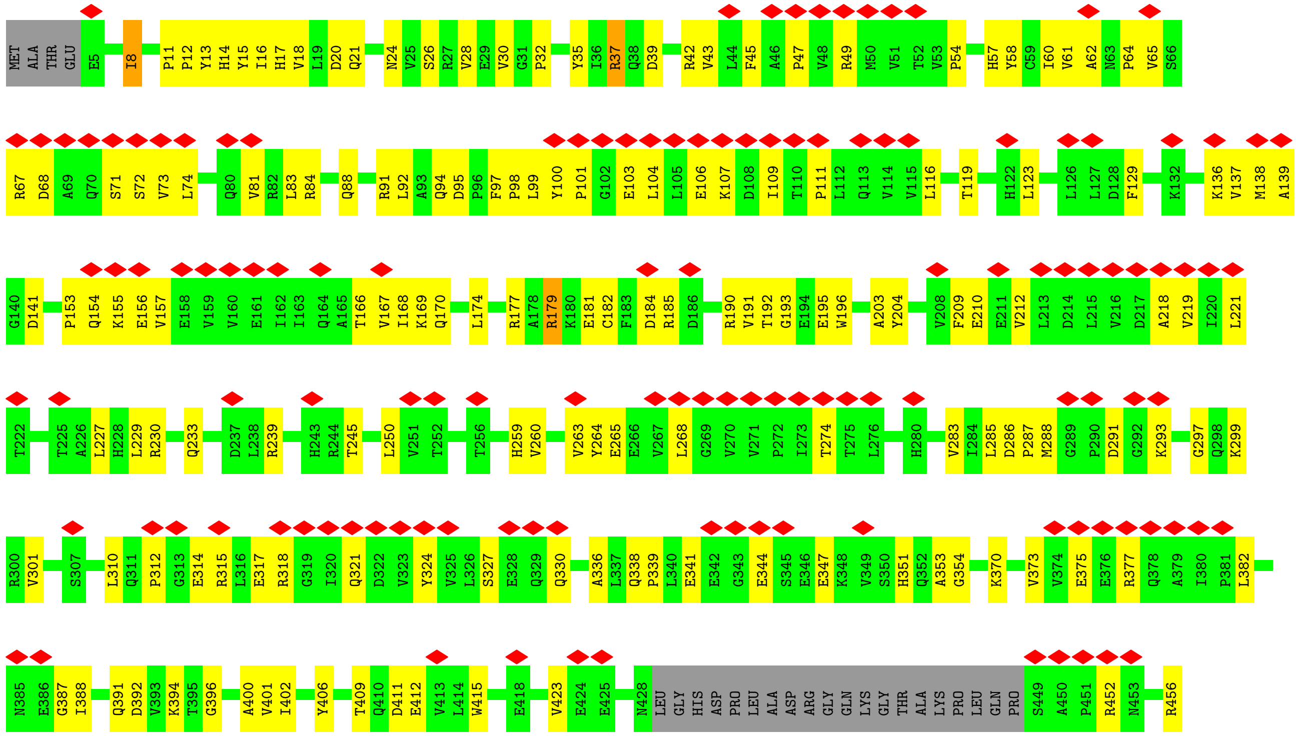
Chain VA:

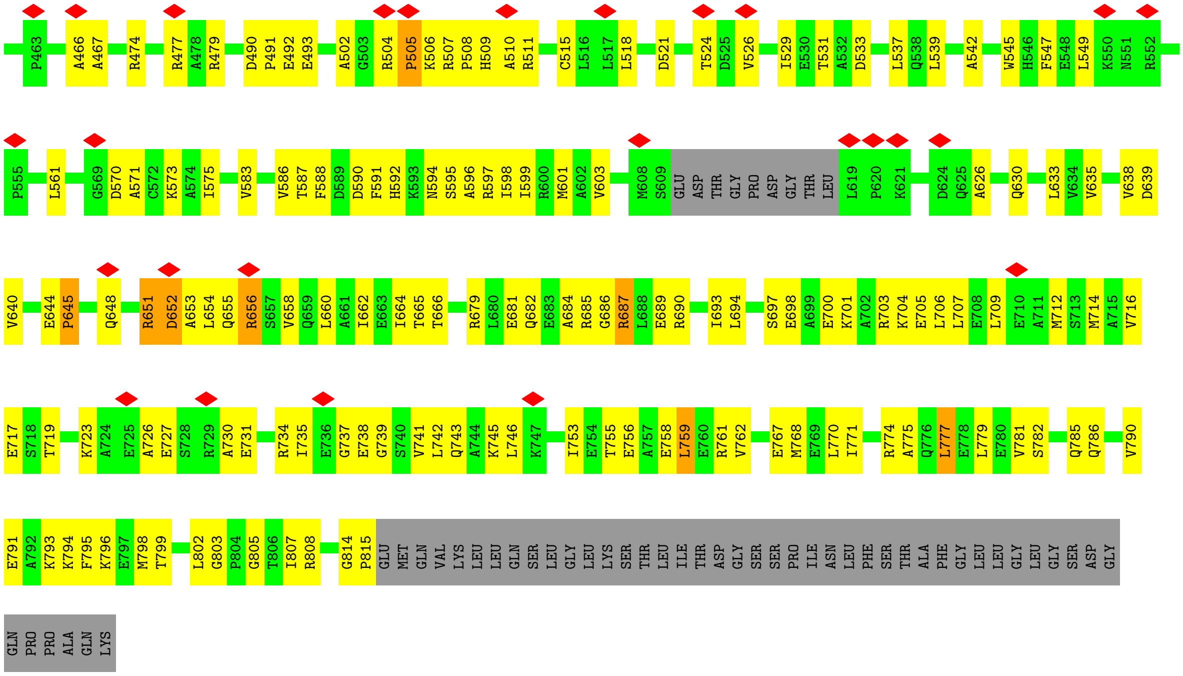




- Molecule 1: Major vault protein

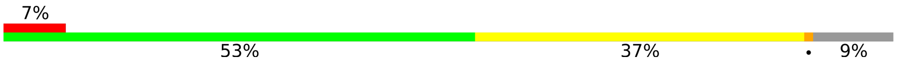
Chain WA:

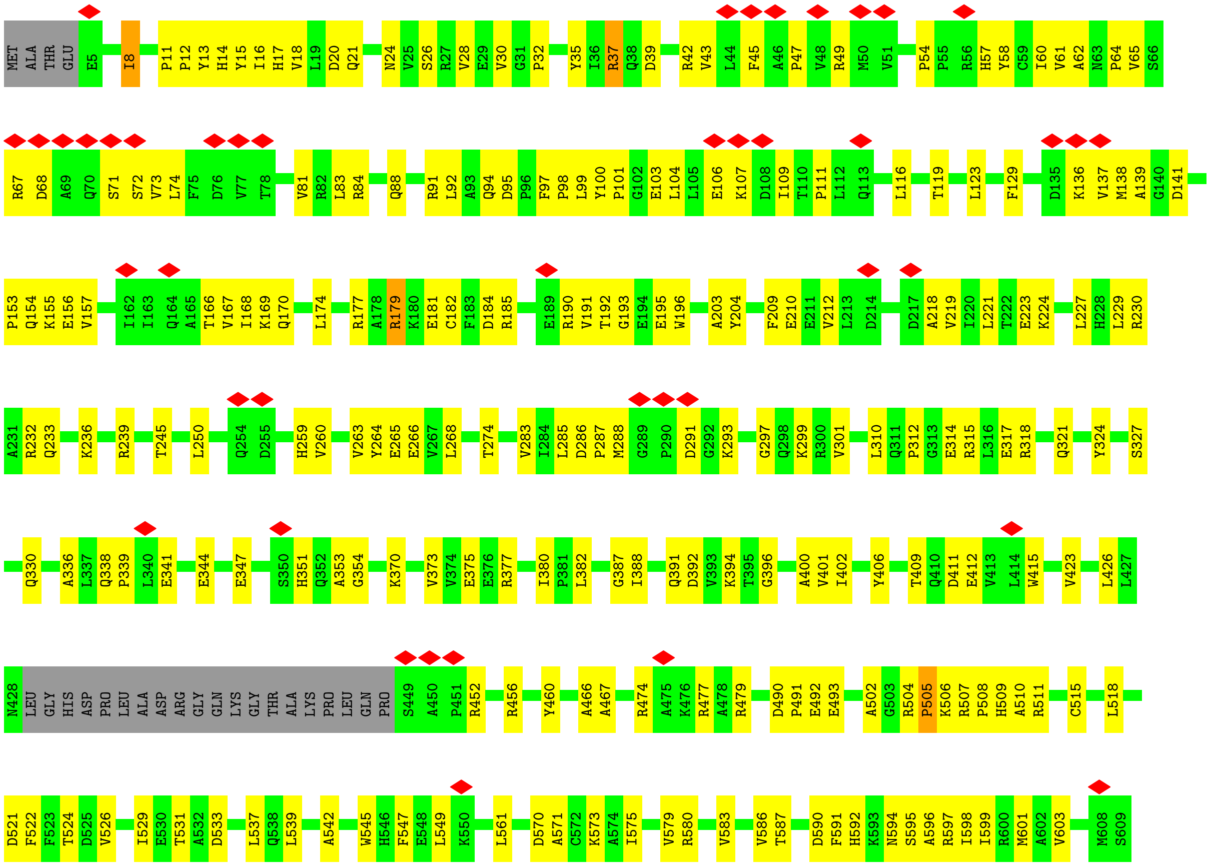


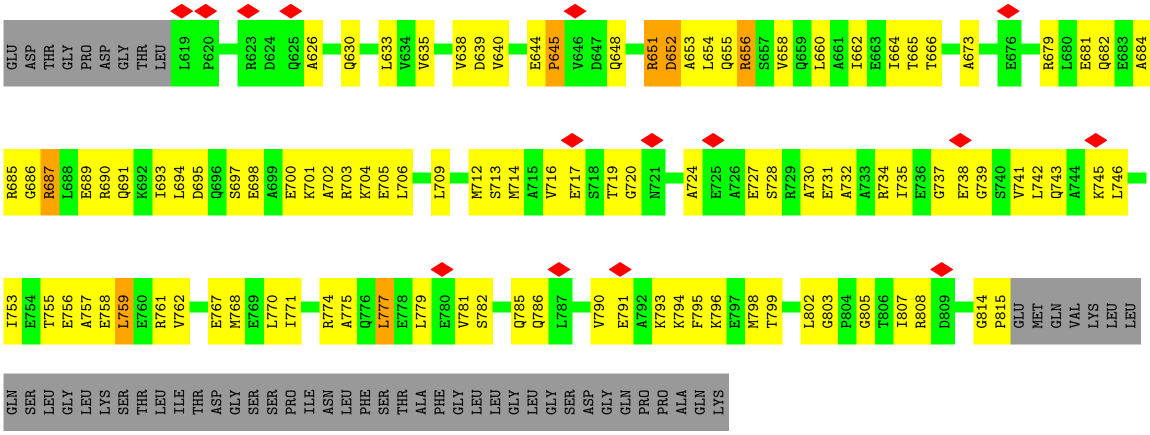


- Molecule 1: Major vault protein

Chain XA:

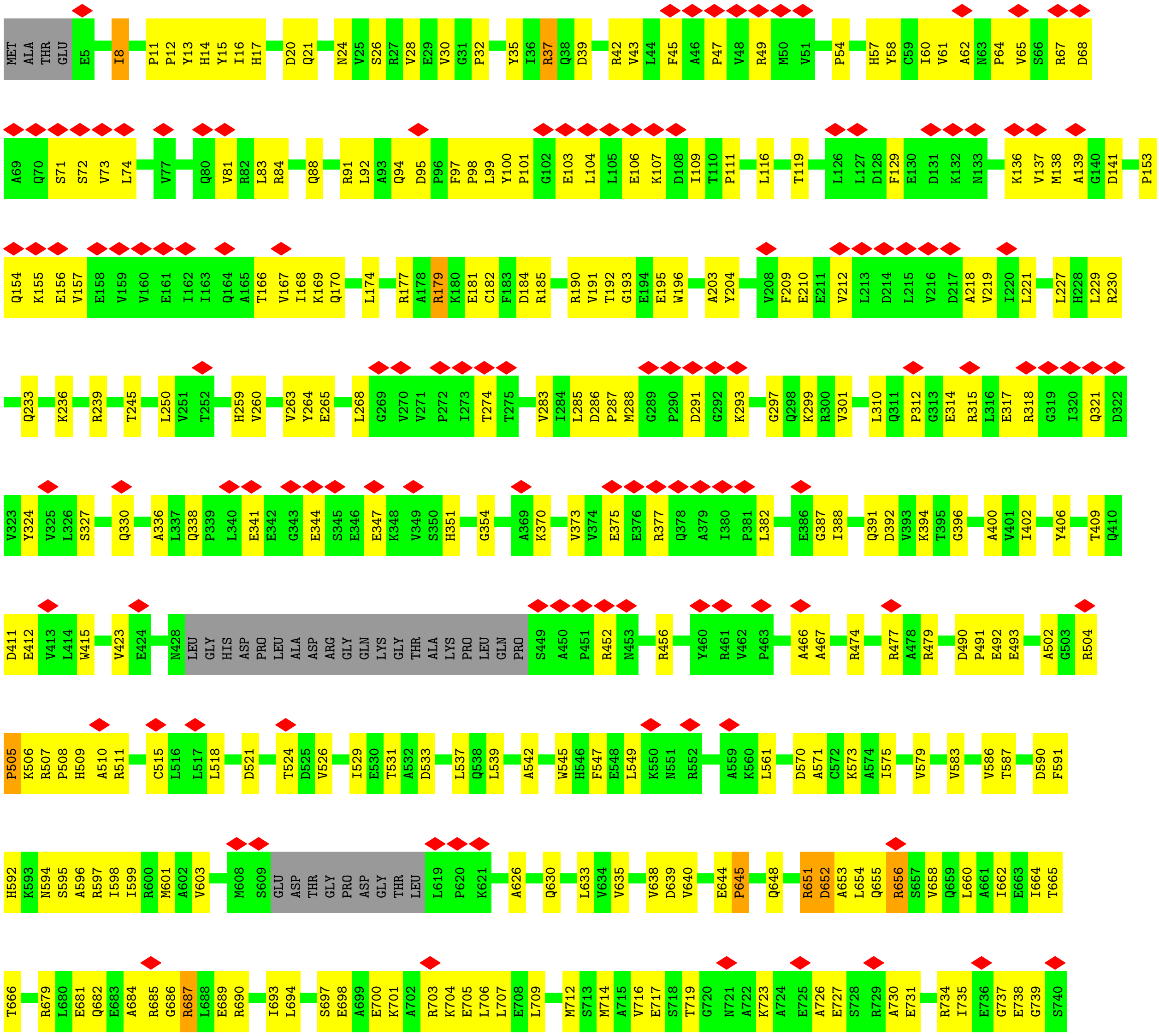


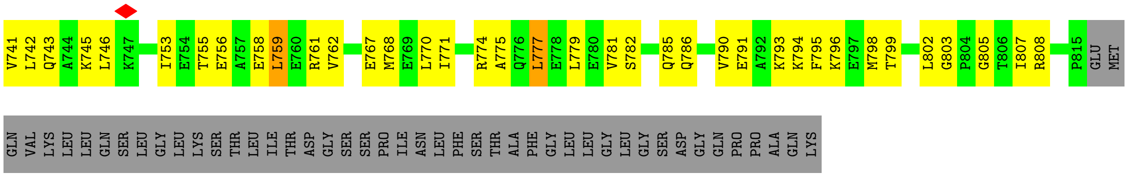




- Molecule 1: Major vault protein

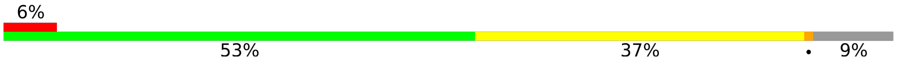
Chain YA:

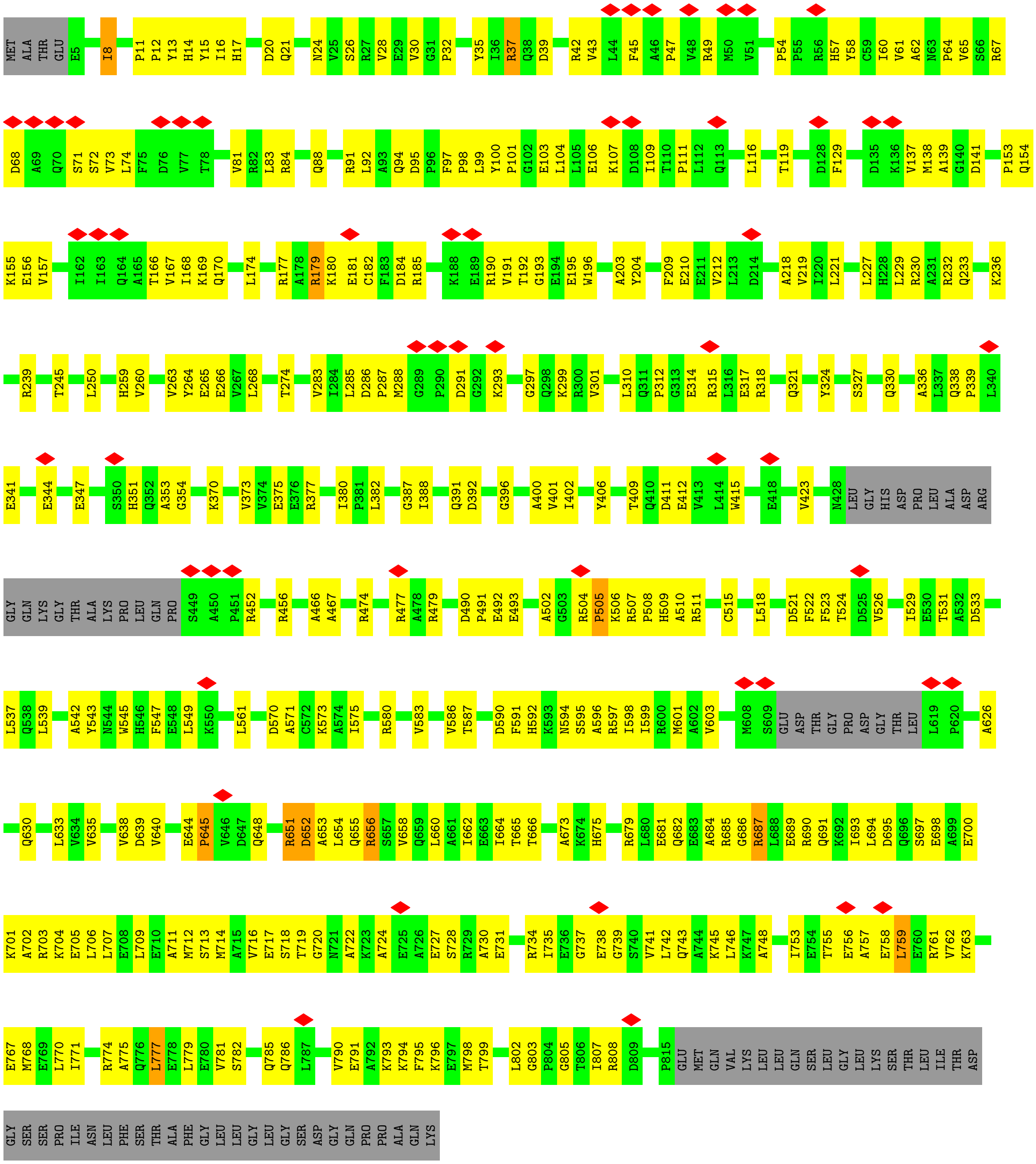




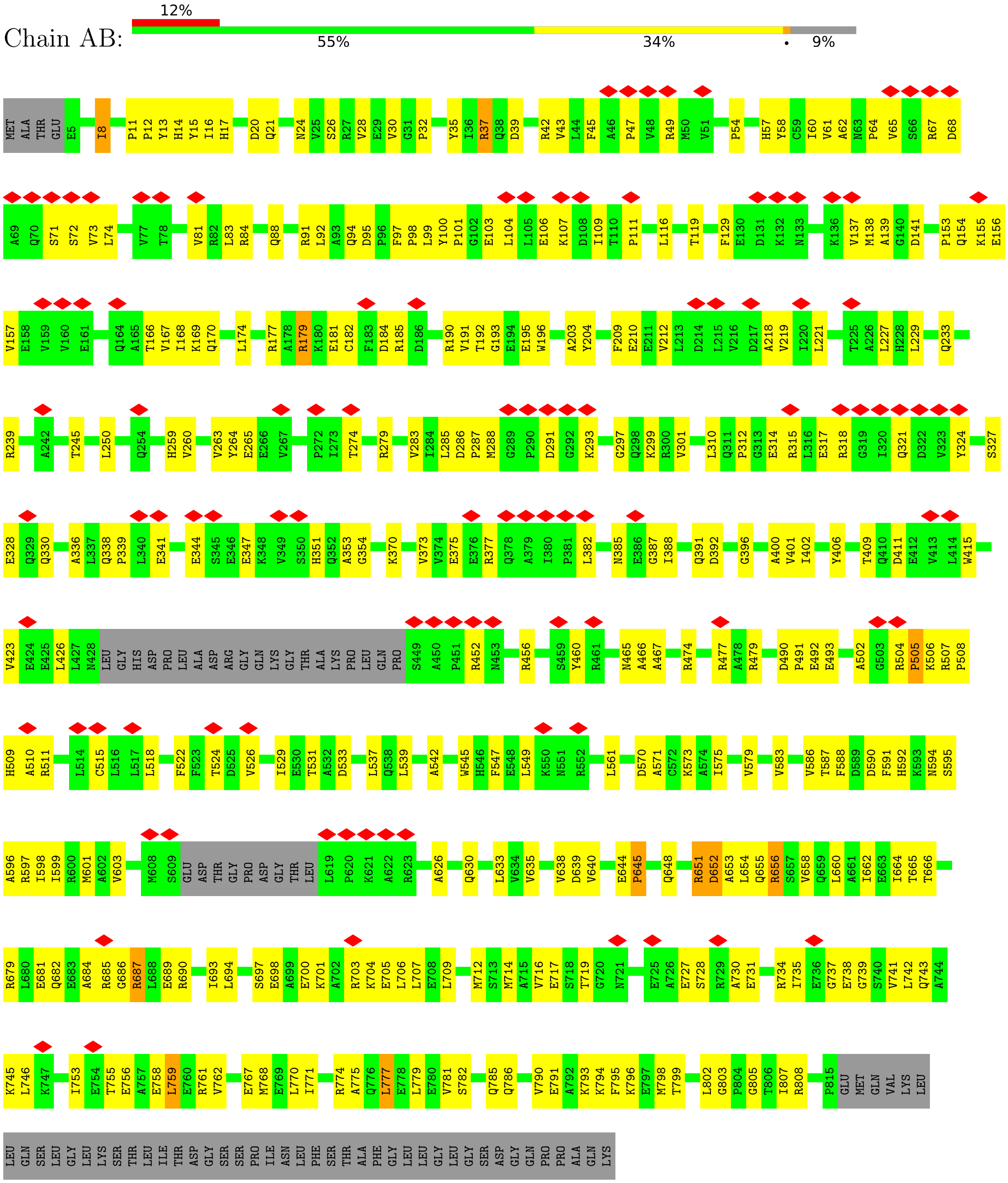
- Molecule 1: Major vault protein

Chain ZA:

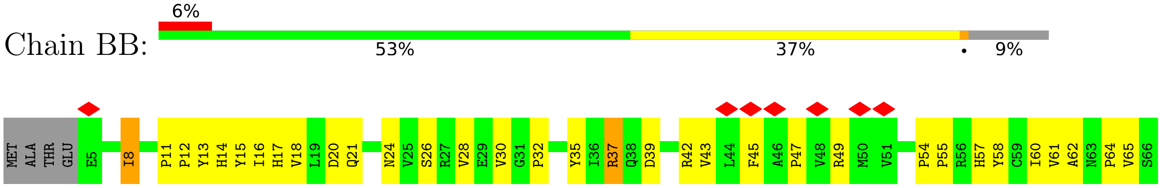


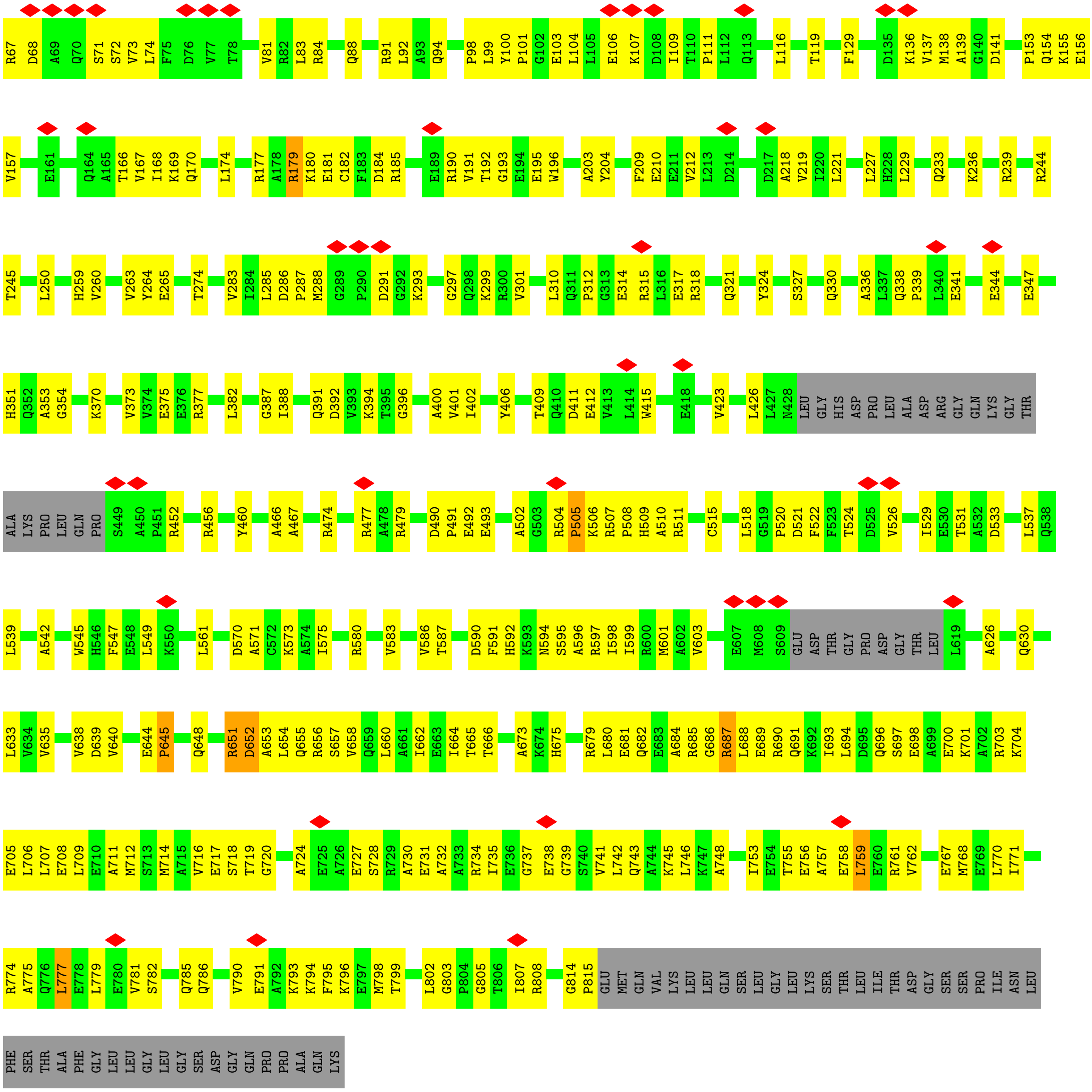


- Molecule 1: Major vault protein



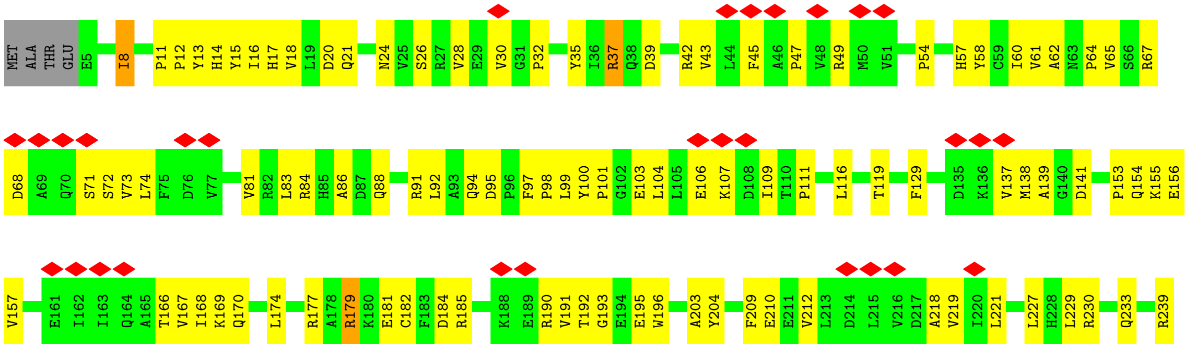
- Molecule 1: Major vault protein

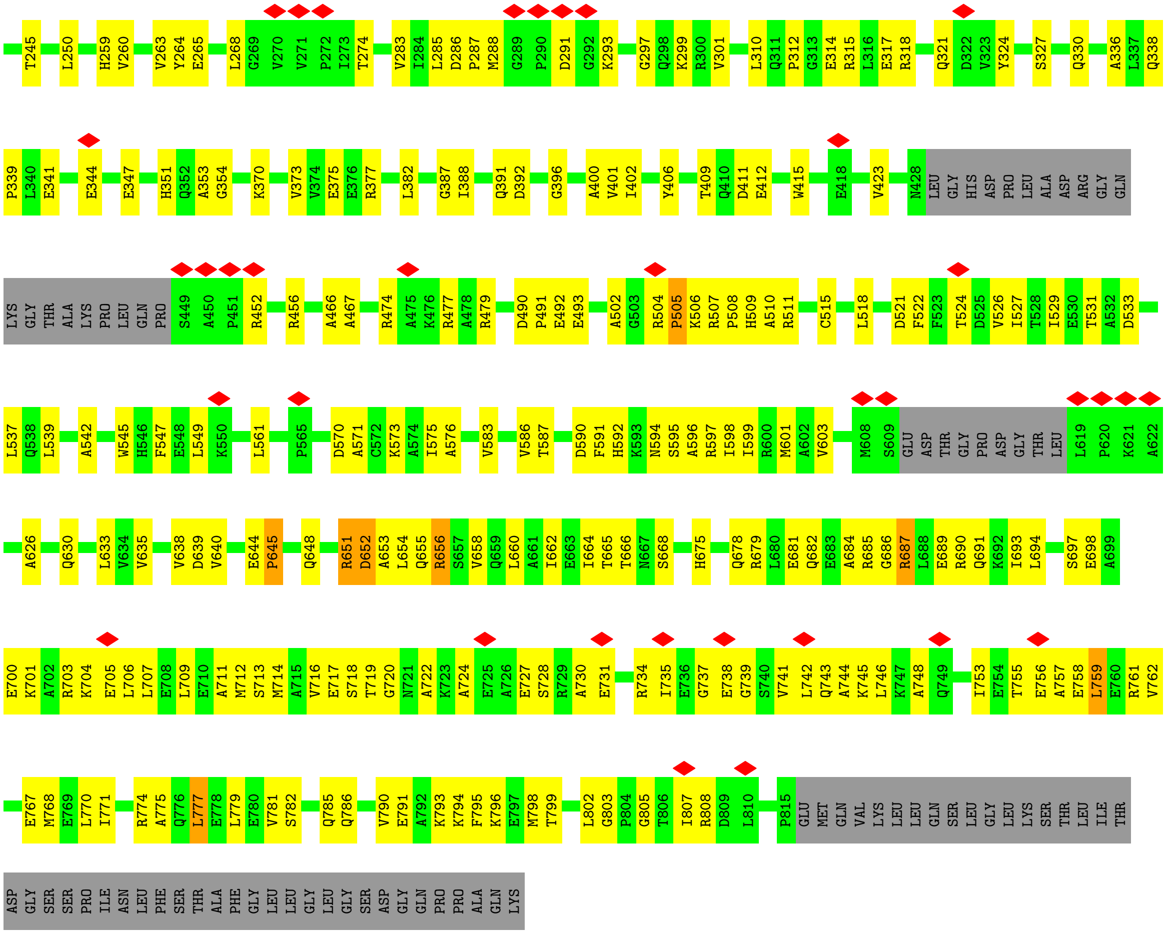




- Molecule 1: Major vault protein

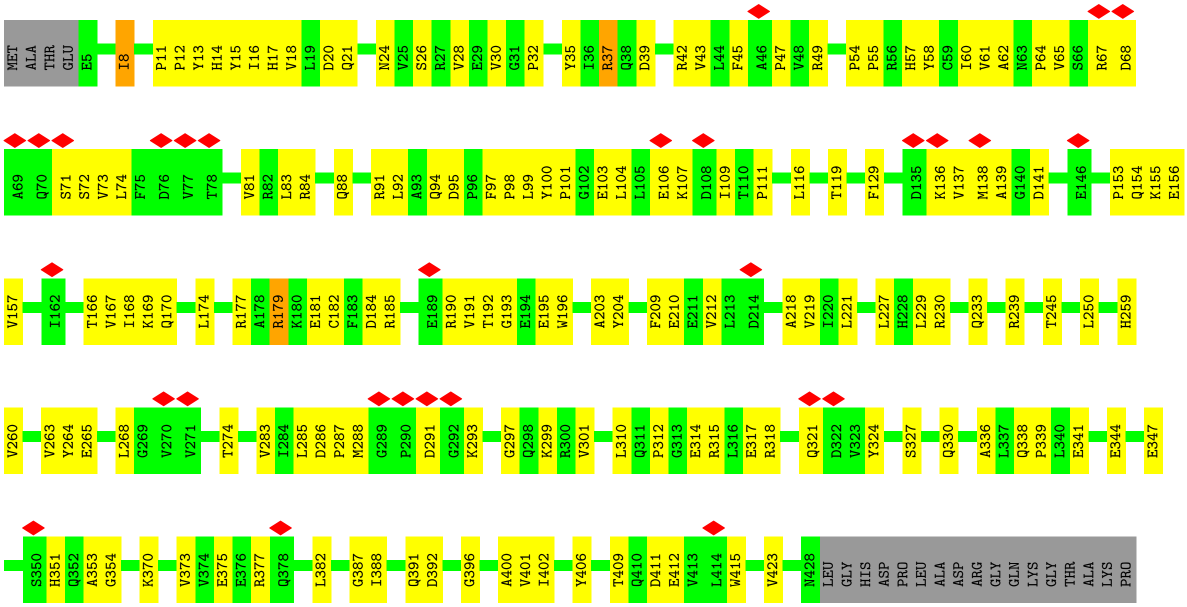
Chain CB:

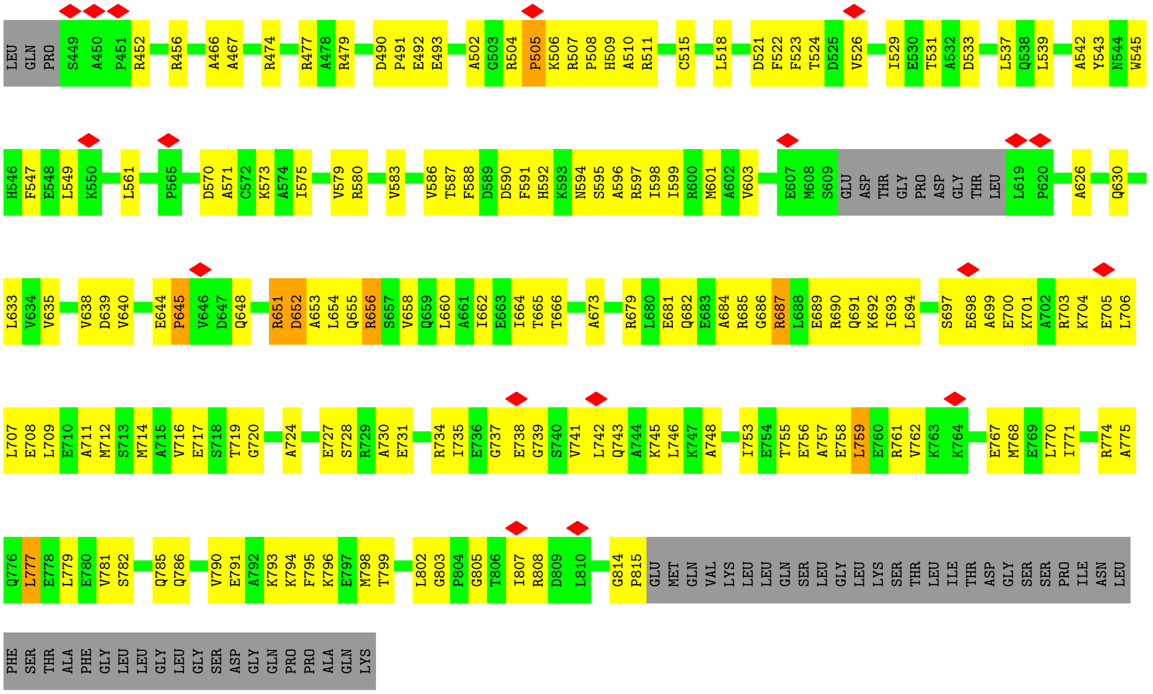




- Molecule 1: Major vault protein

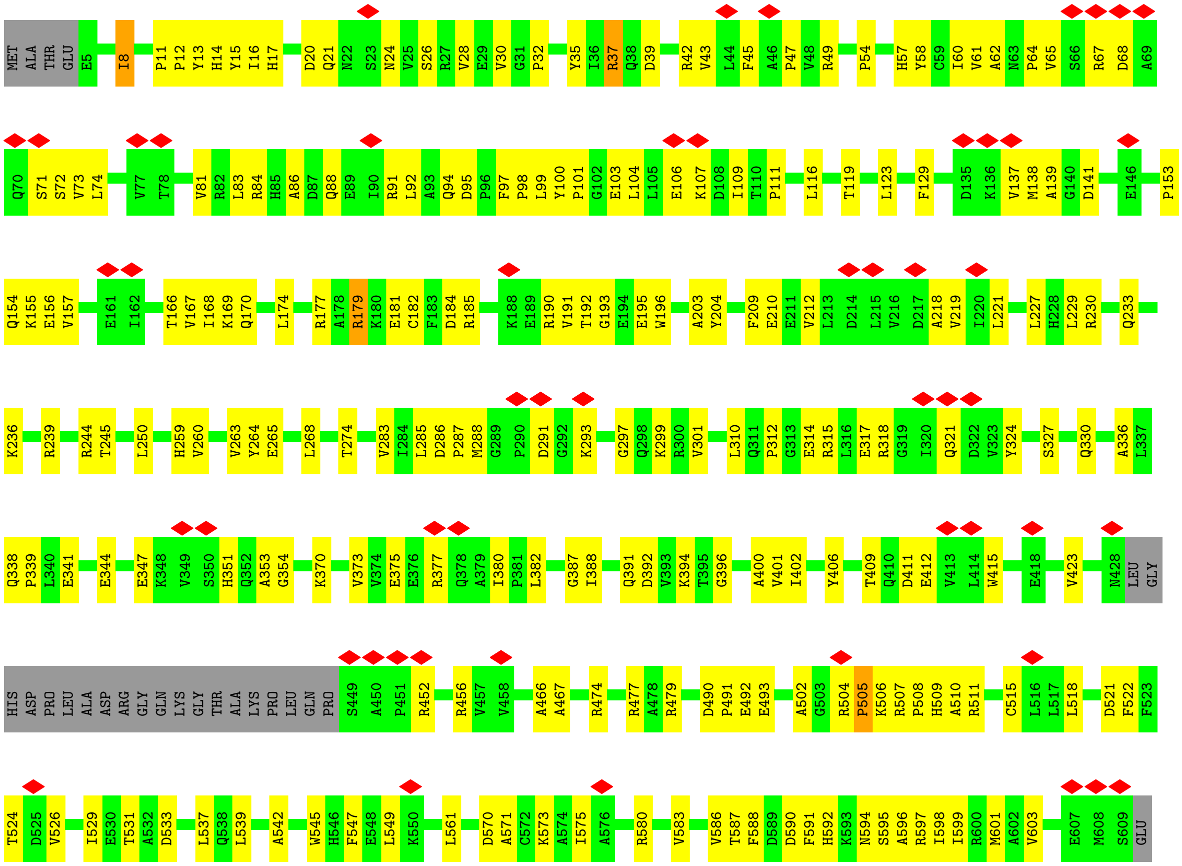
Chain DB:

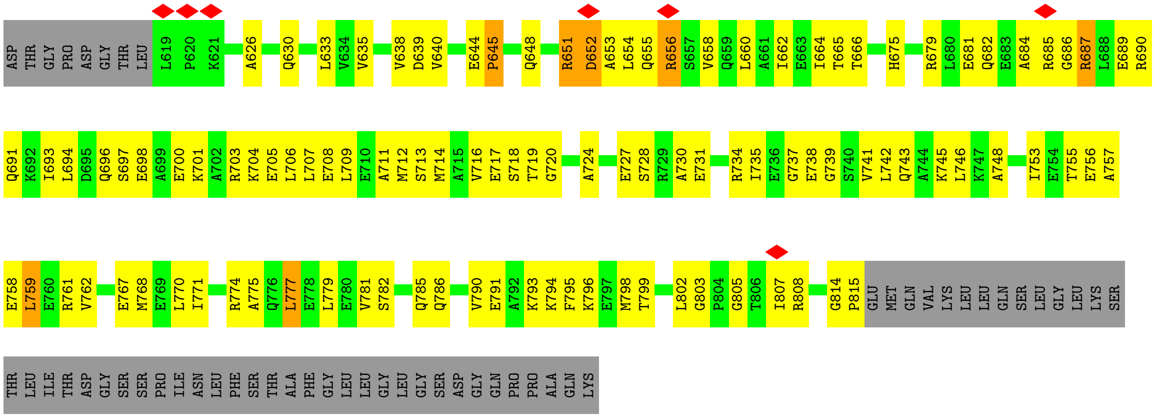




- Molecule 1: Major vault protein

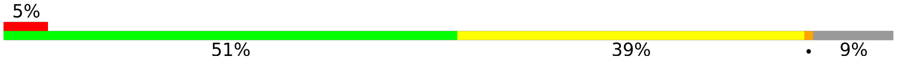
Chain EB:

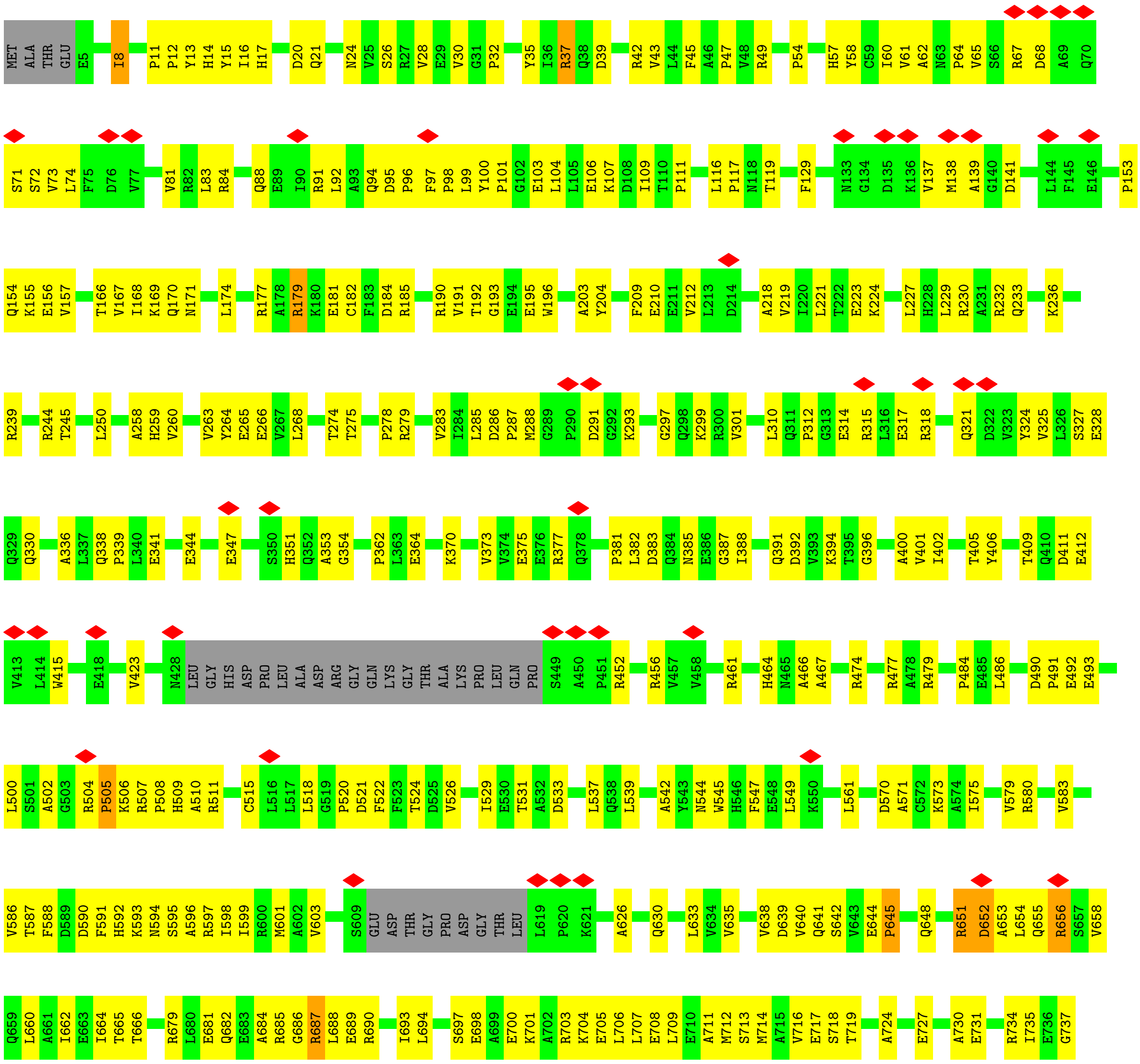


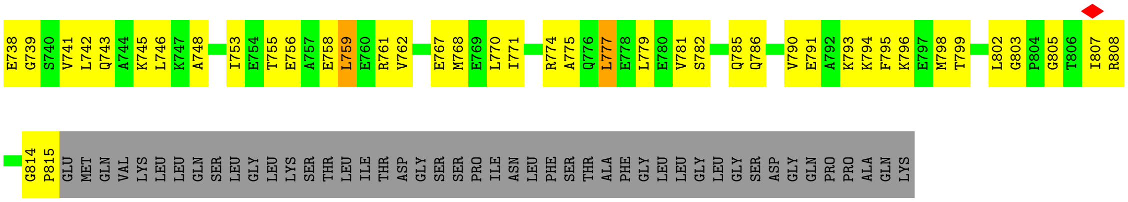


- Molecule 1: Major vault protein

Chain FB:

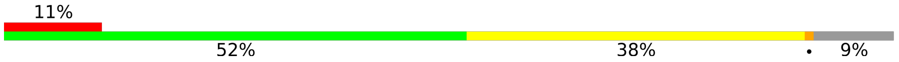


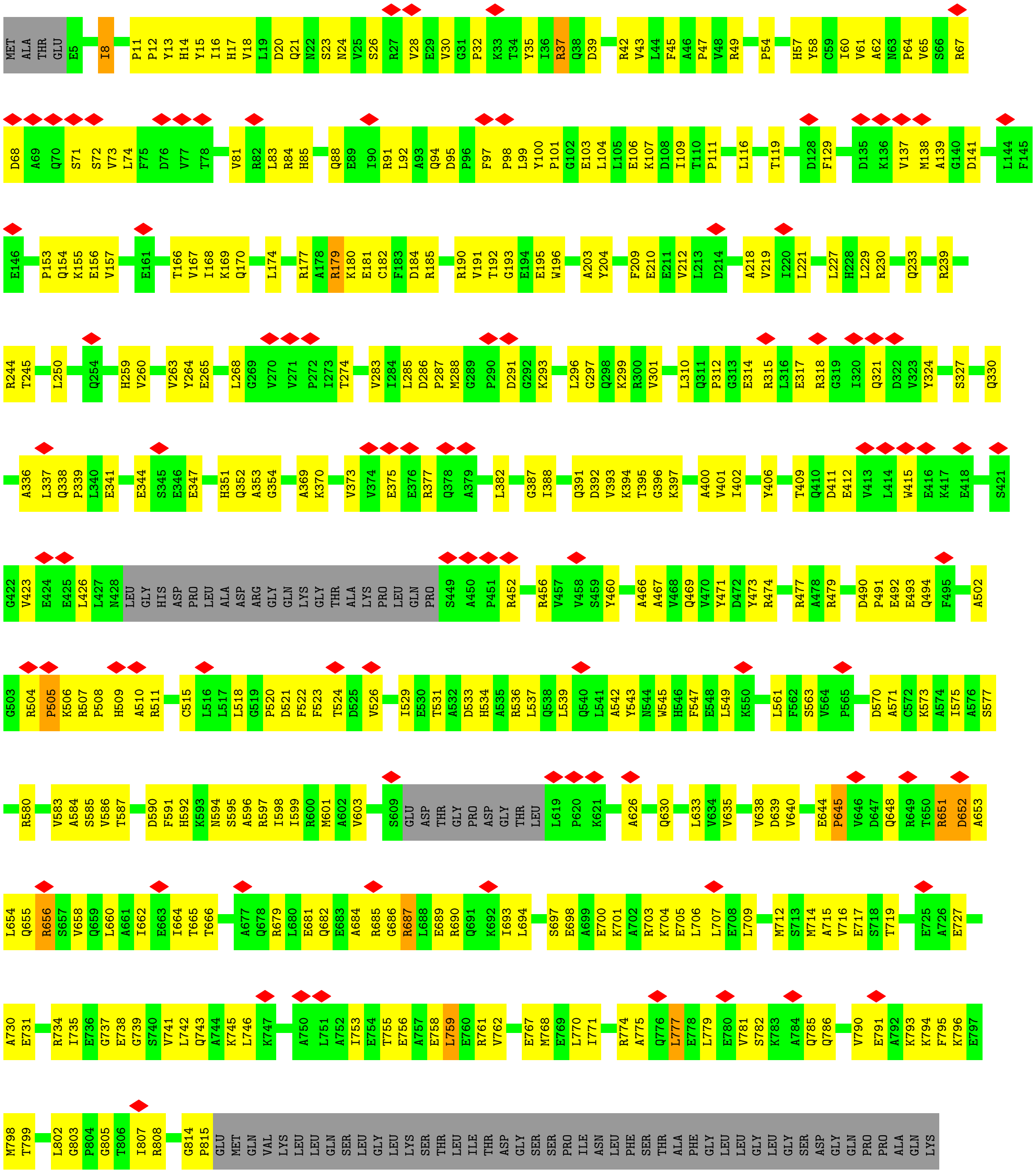




- Molecule 1: Major vault protein

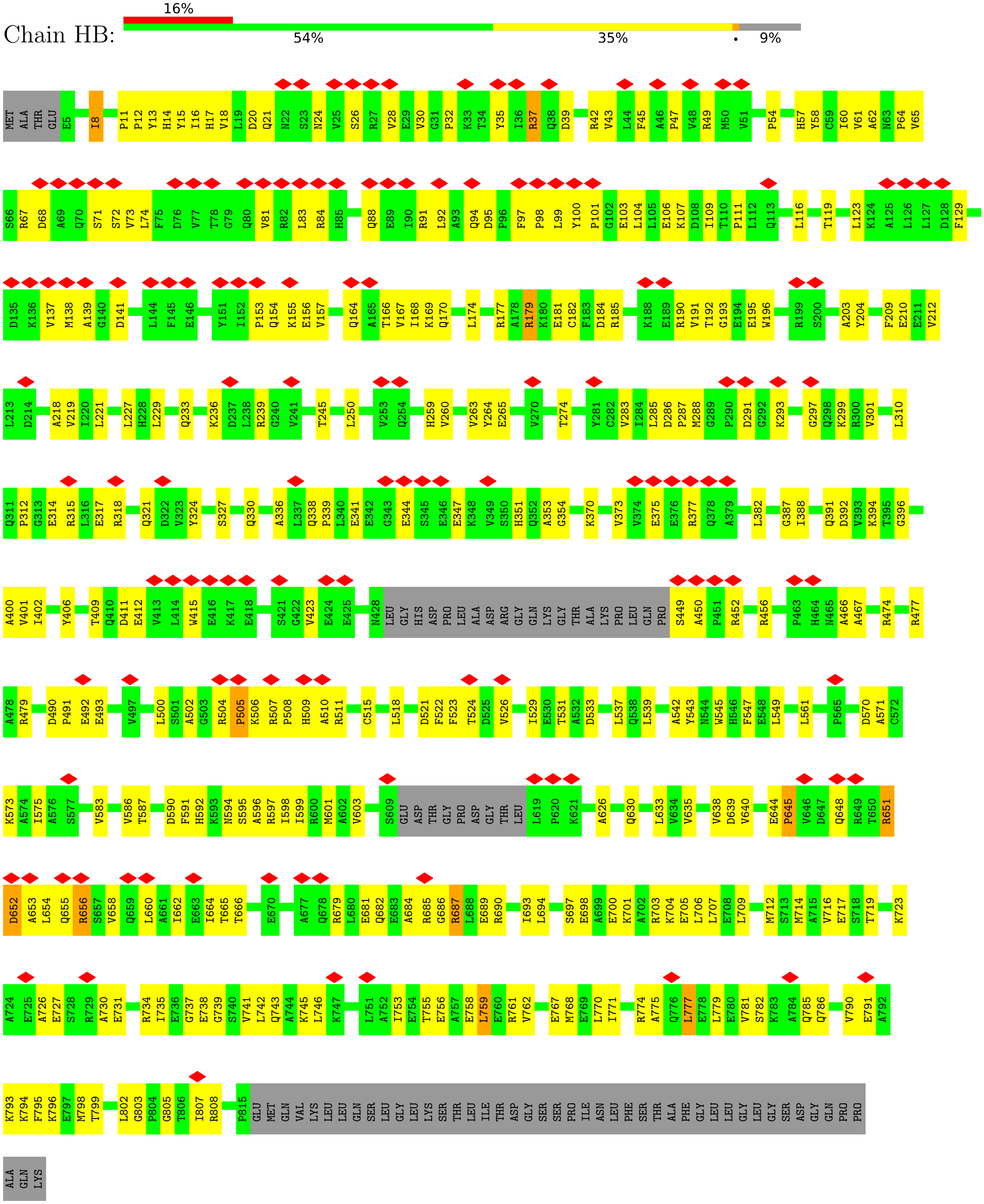
Chain GB:





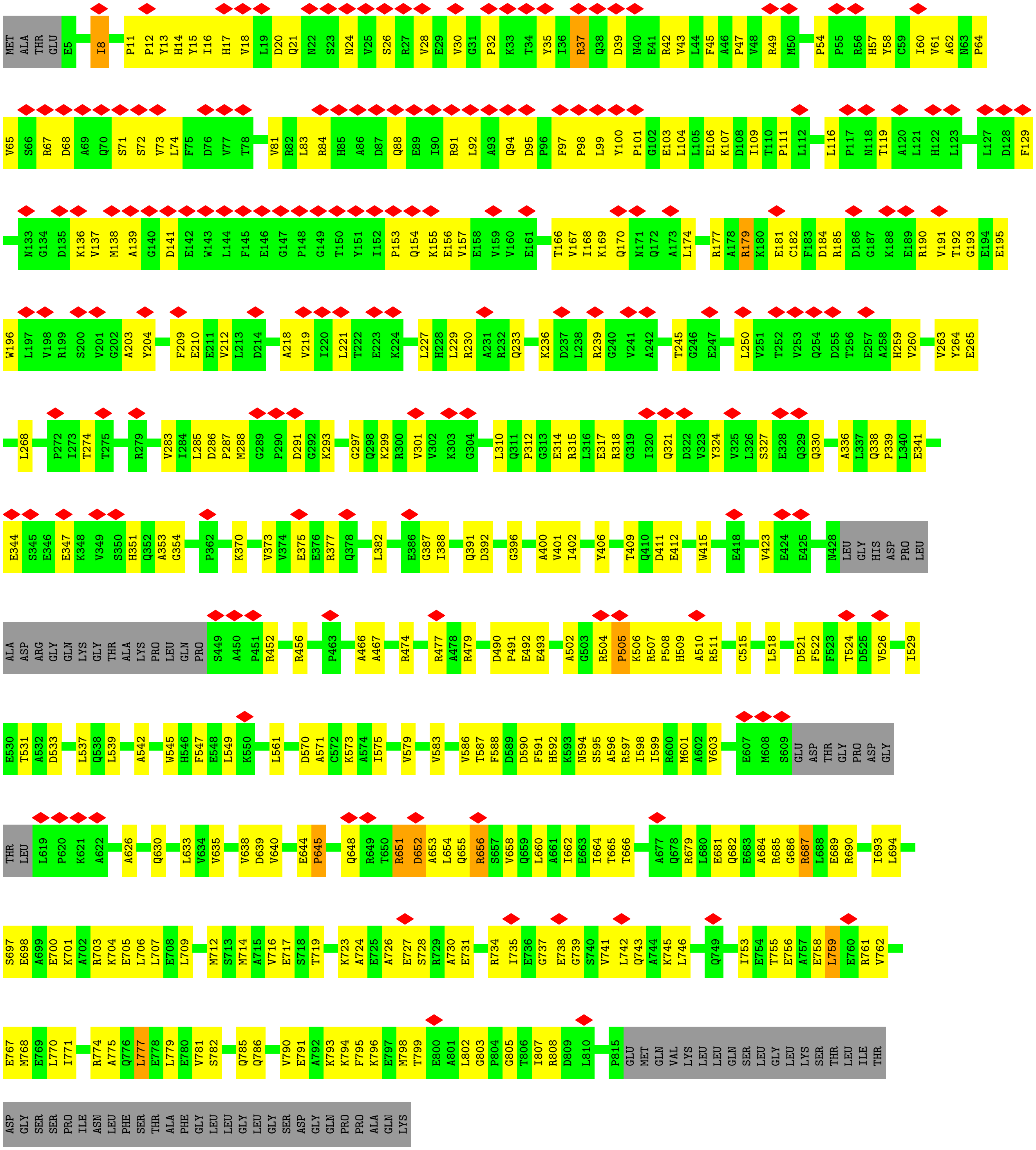
- Molecule 1: Major vault protein

Chain HB:



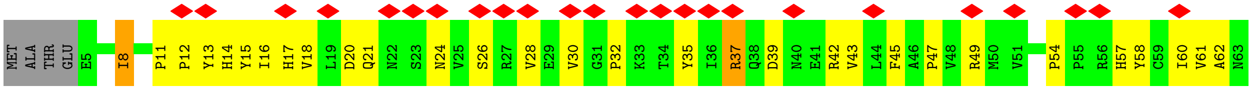
- Molecule 1: Major vault protein

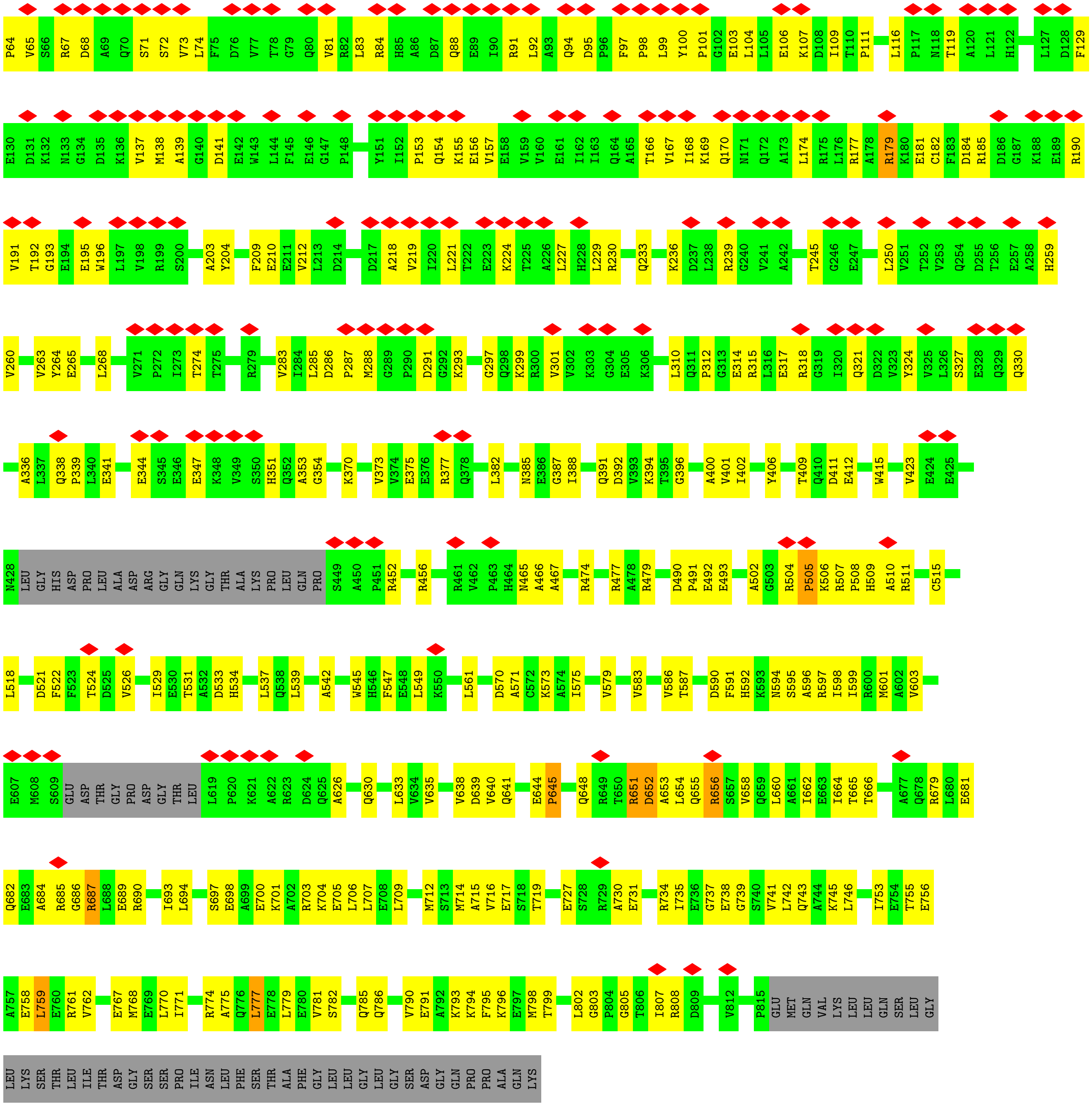
Chain IB:



- Molecule 1: Major vault protein

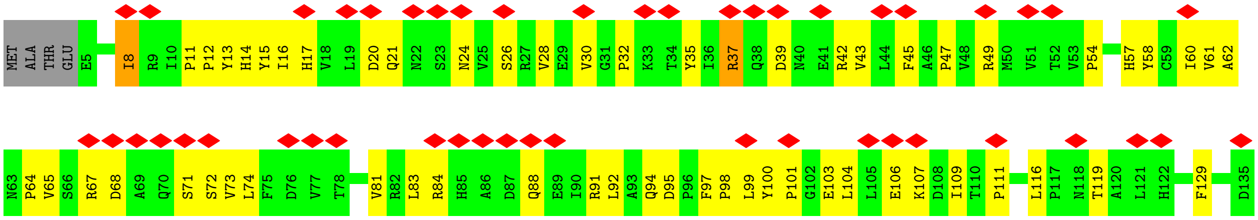
Chain JB:

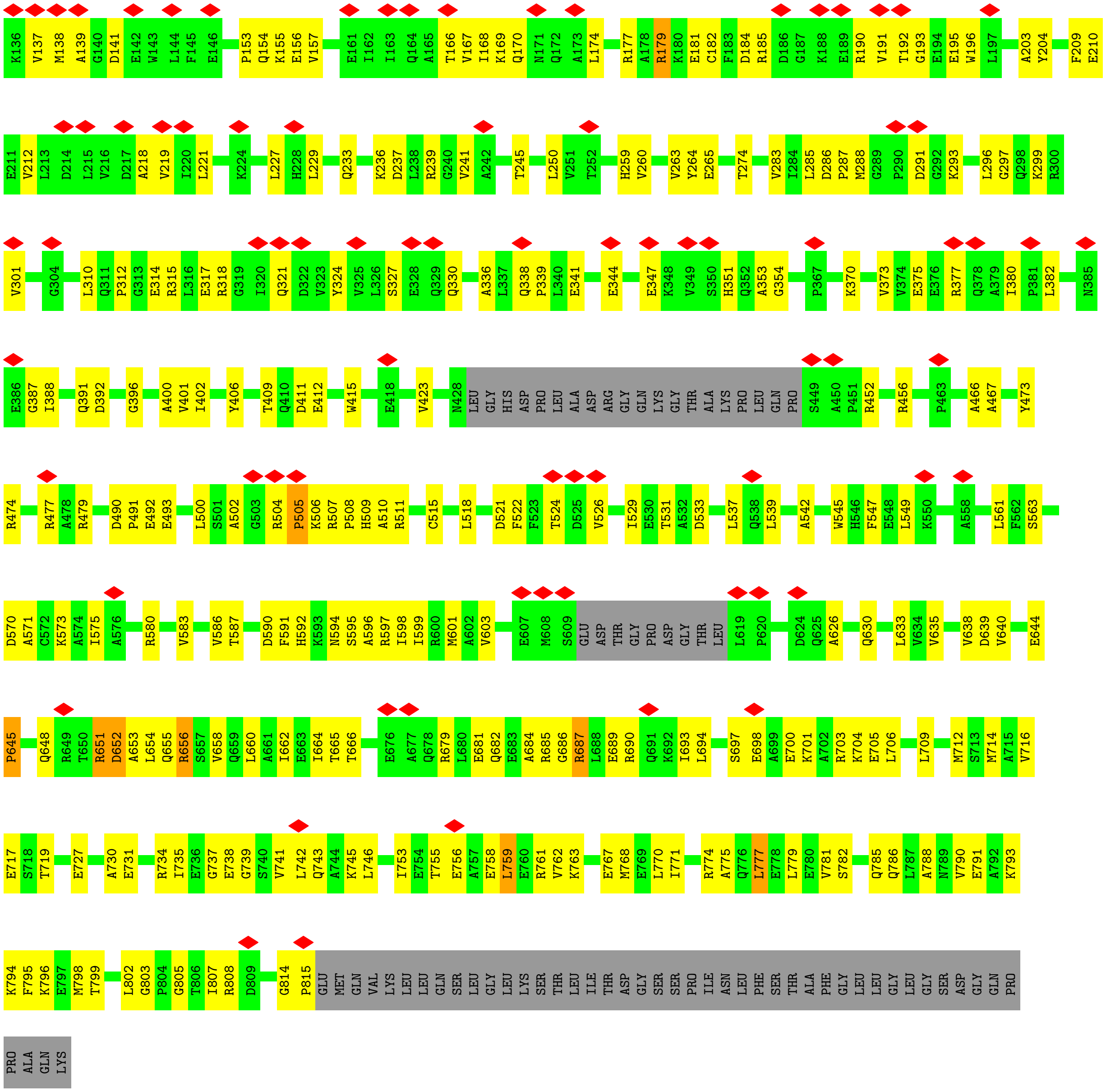




- Molecule 1: Major vault protein

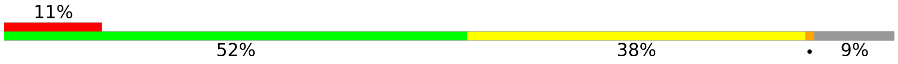
Chain KB:

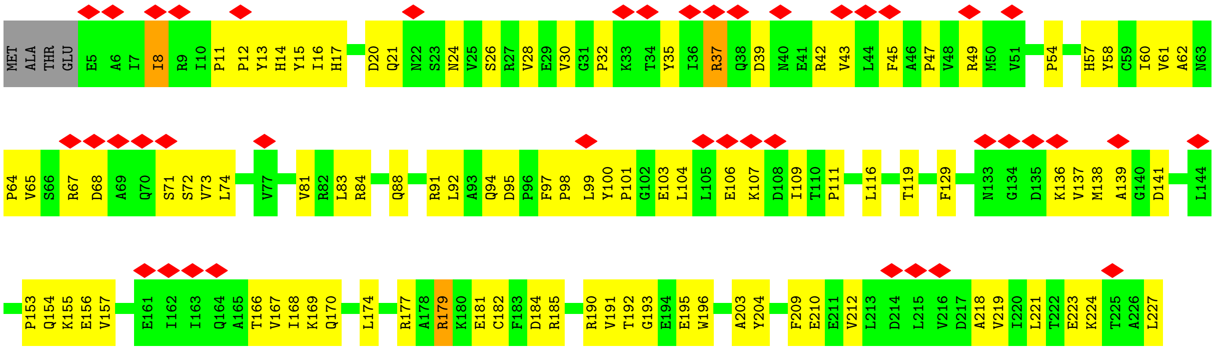


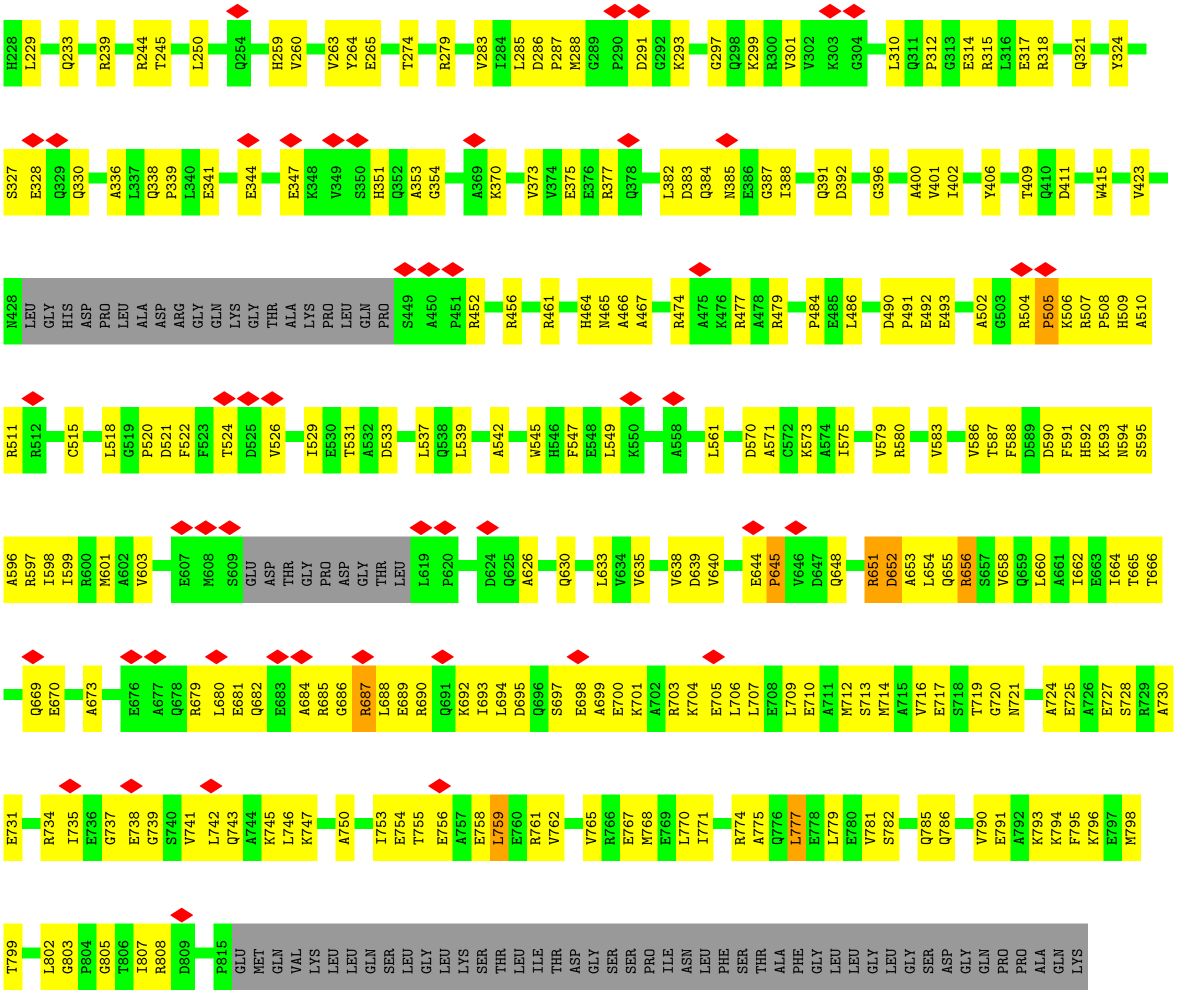


- Molecule 1: Major vault protein

Chain LB:

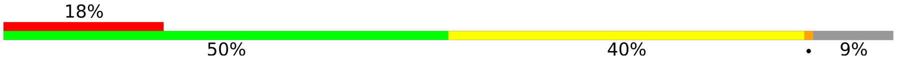


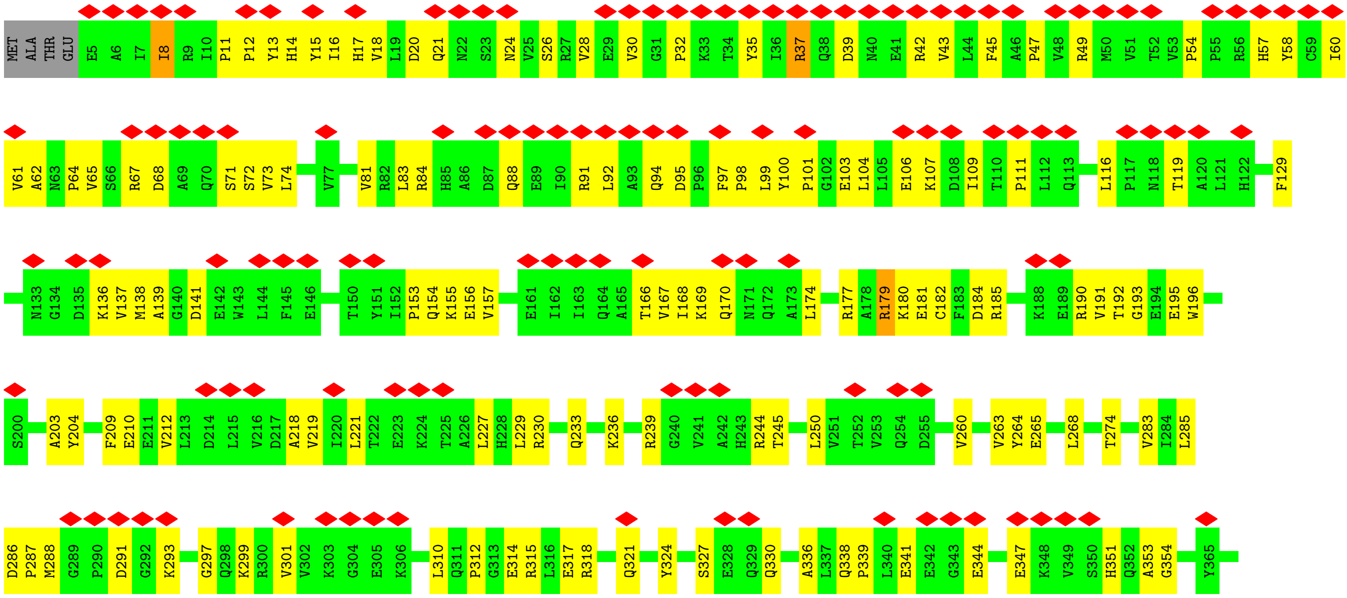


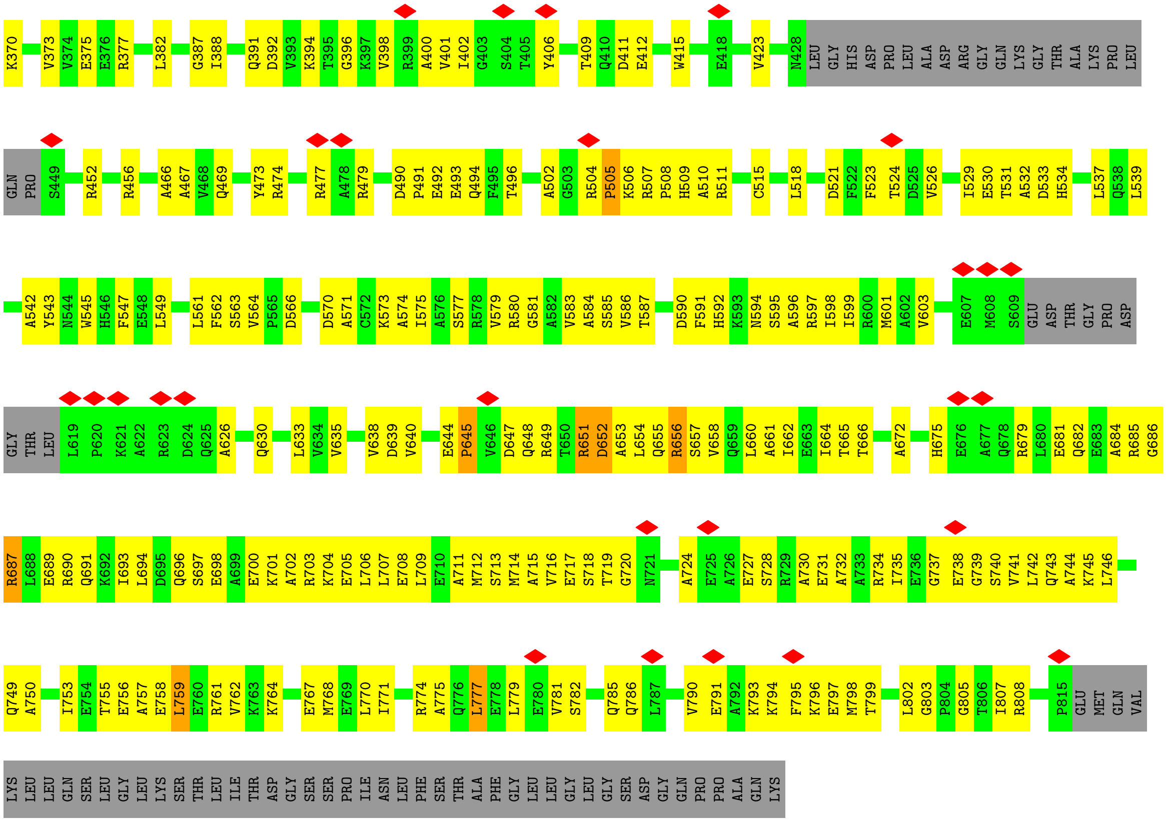


- Molecule 1: Major vault protein

Chain MB:

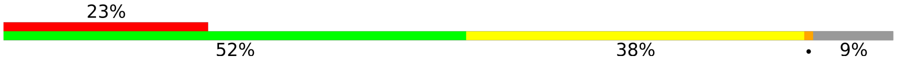


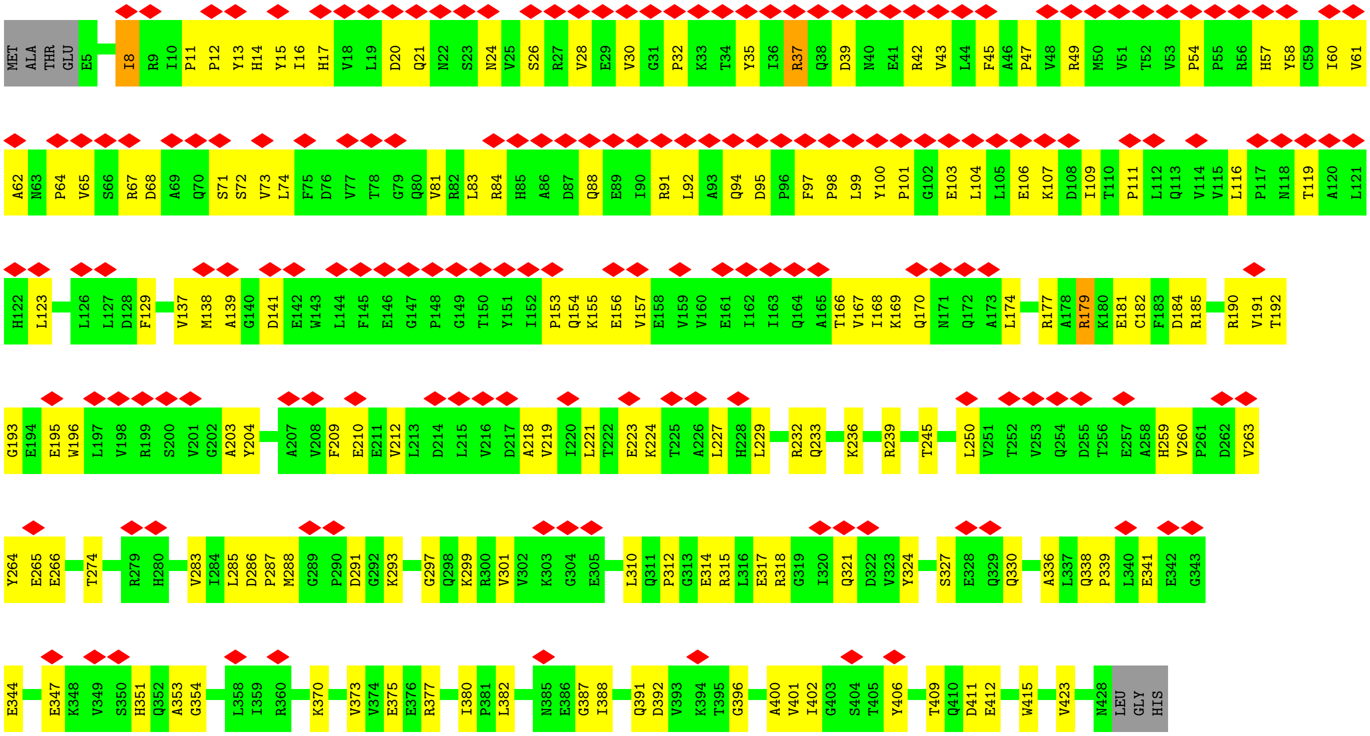


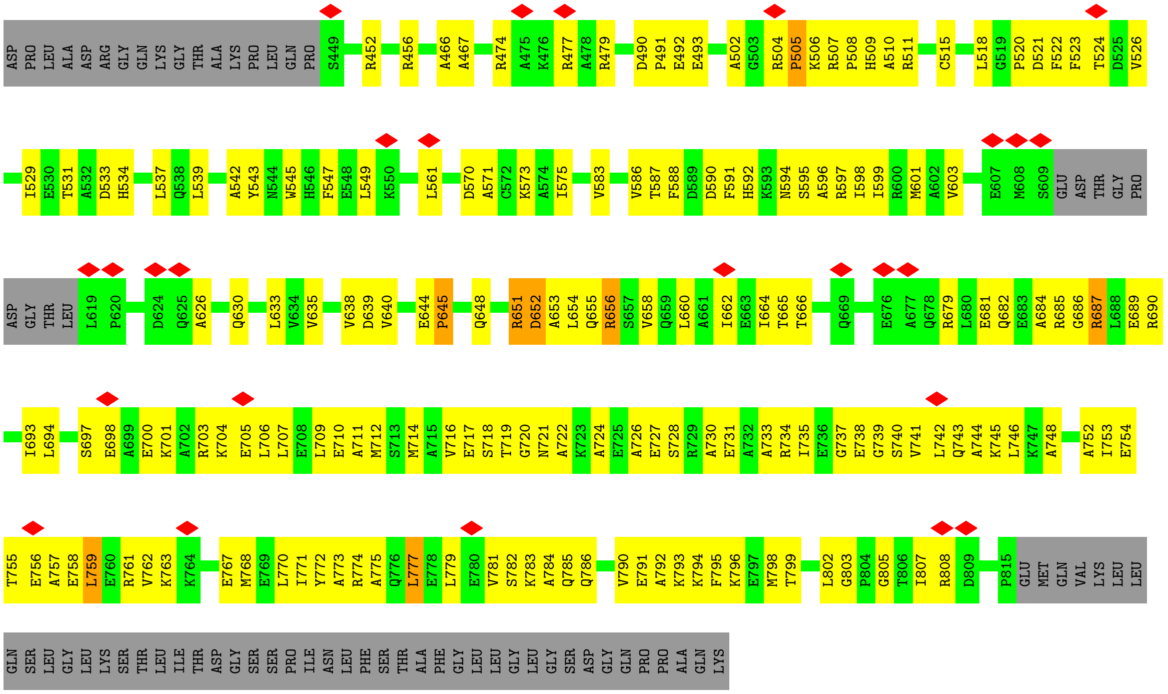


- Molecule 1: Major vault protein

Chain NB:

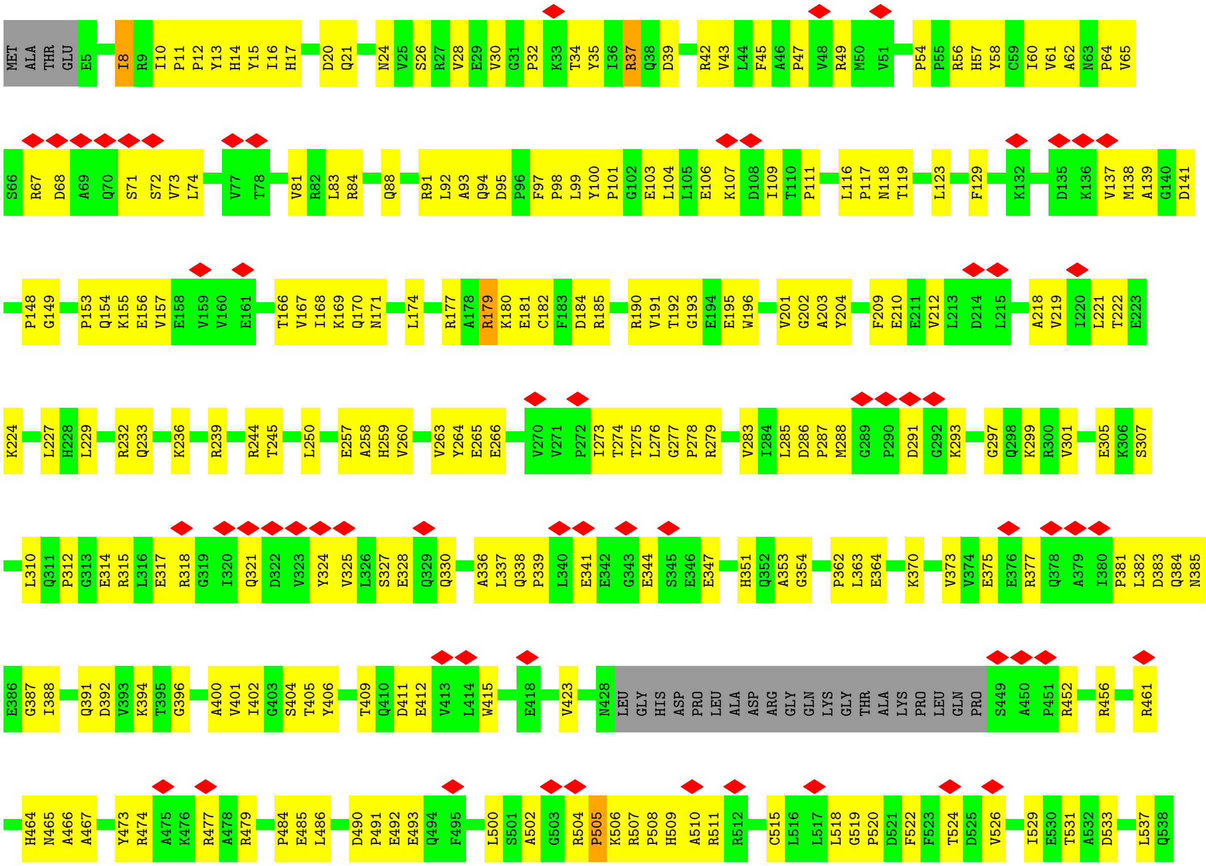


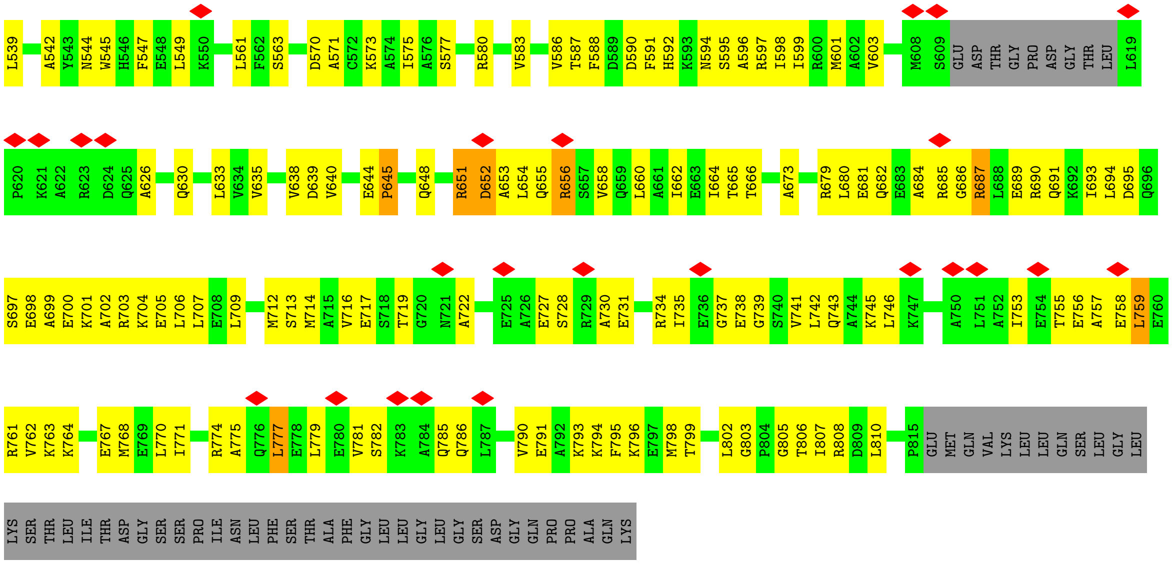




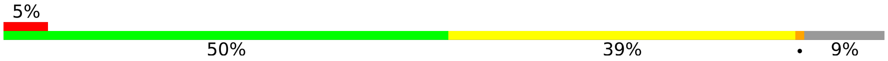
- Molecule 1: Major vault protein

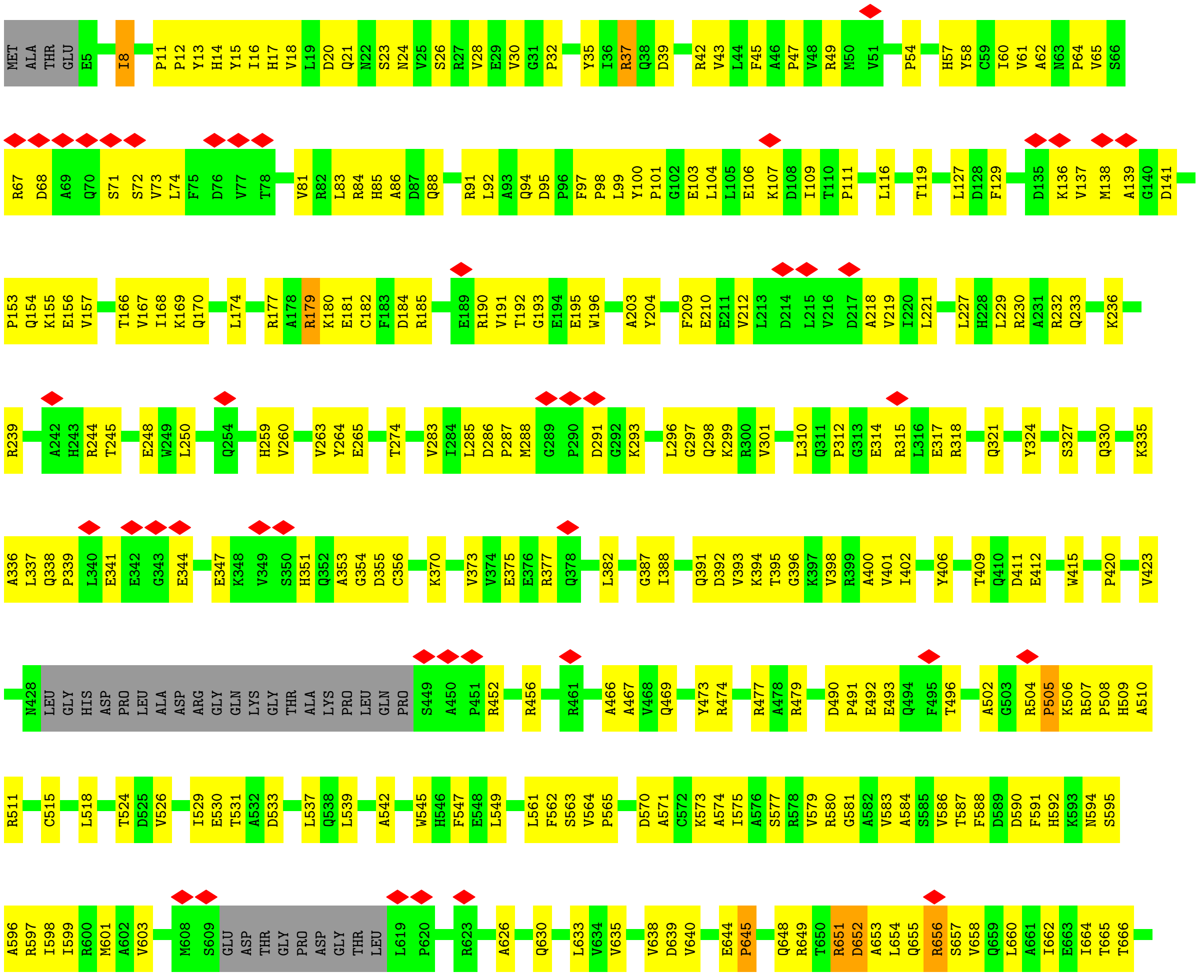
Chain OB:

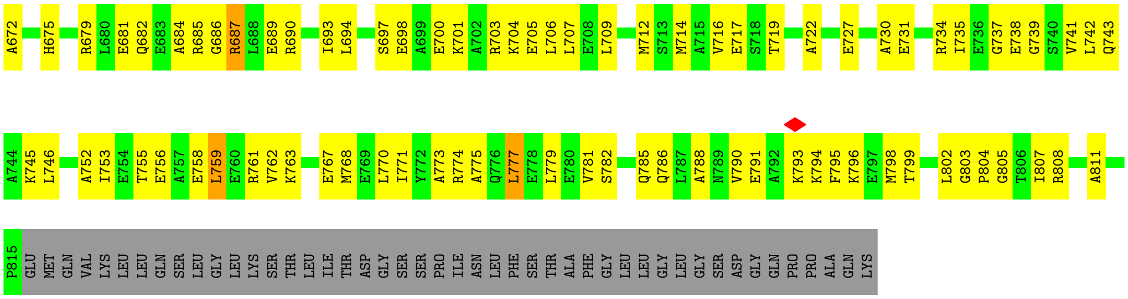




- Molecule 1: Major vault protein

Chain PB:




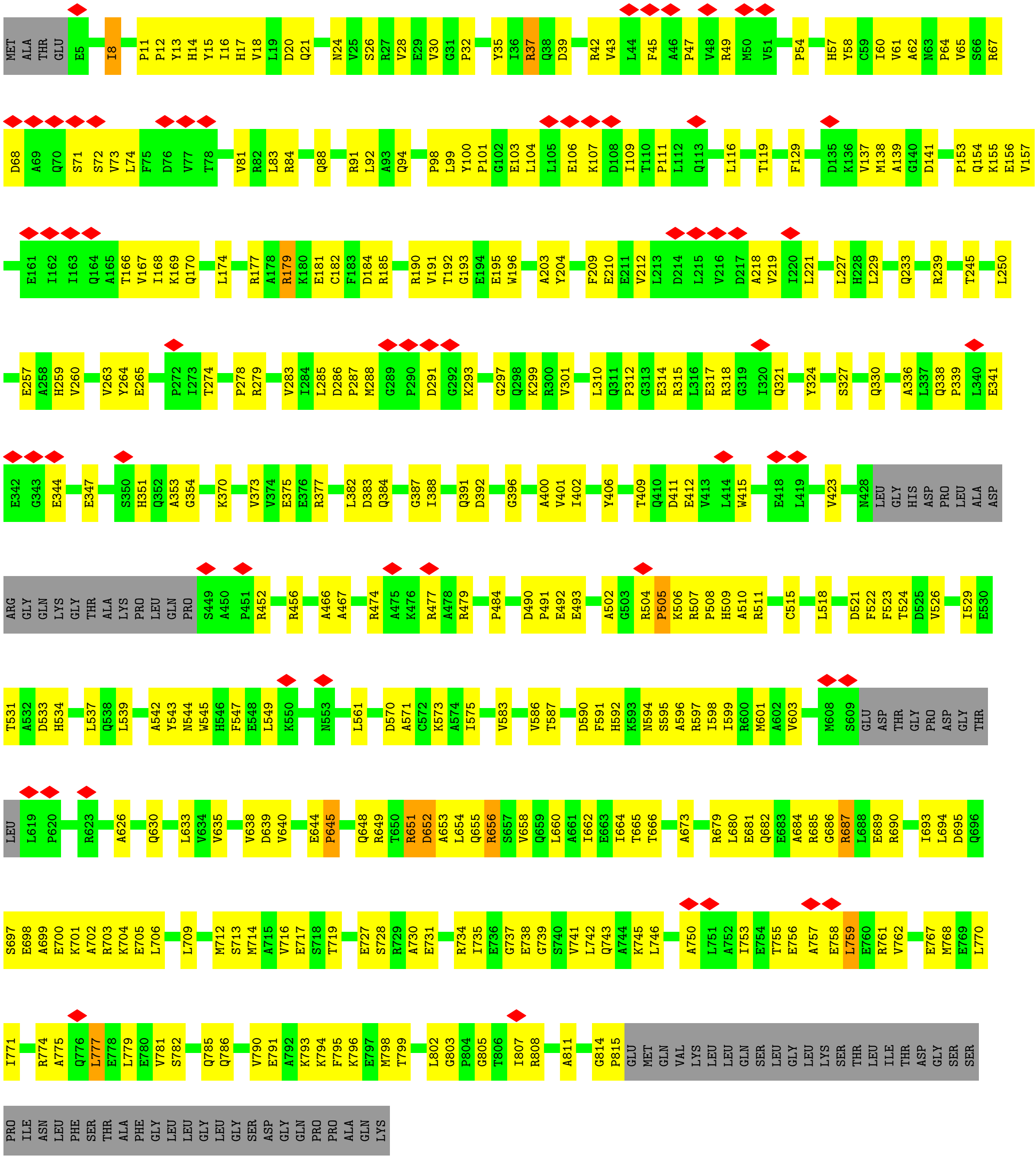


- Molecule 1: Major vault protein

Chain QB:

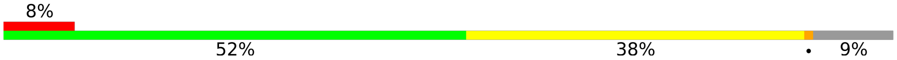

- Molecule 1: Major vault protein

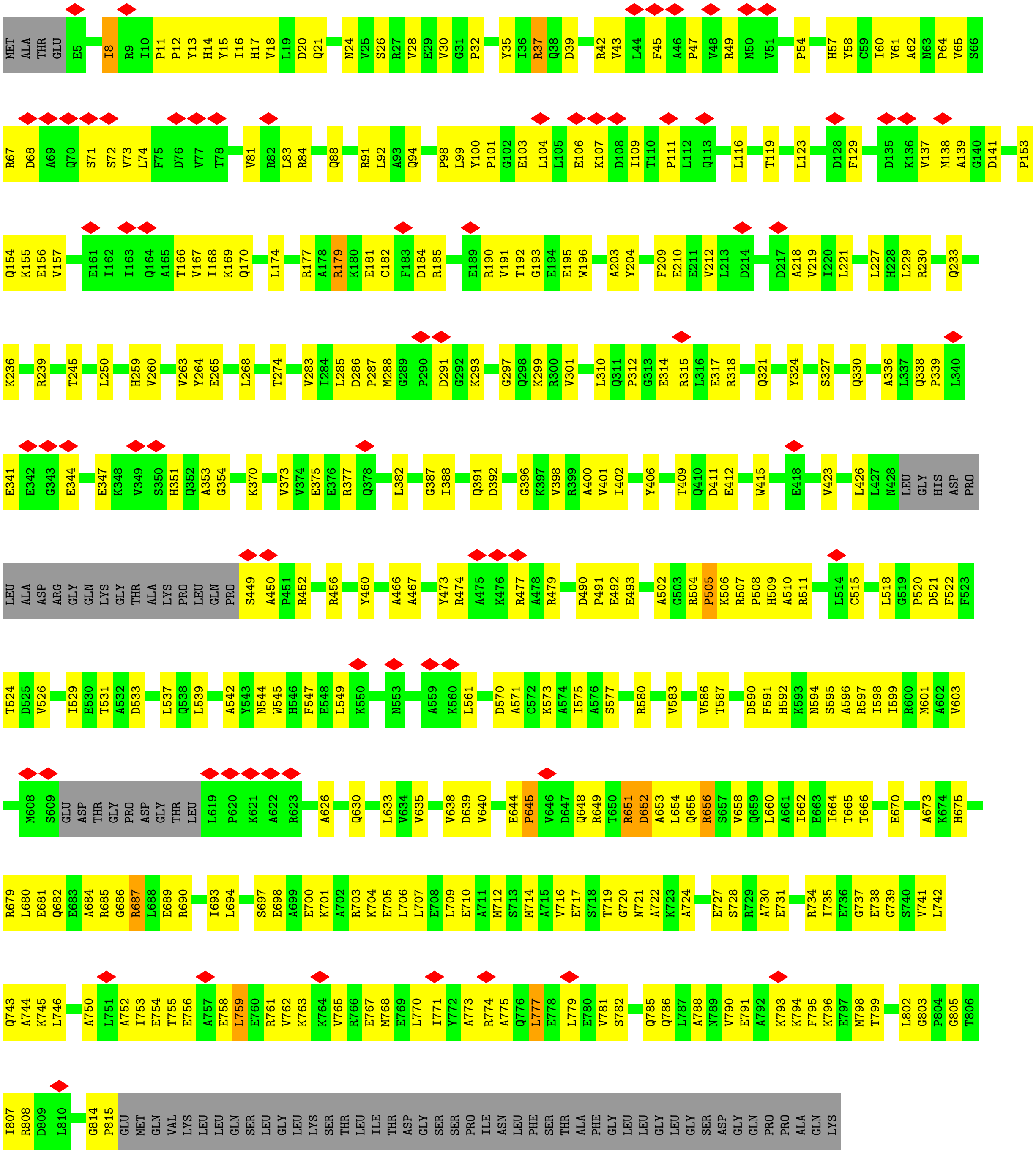
Chain RB:



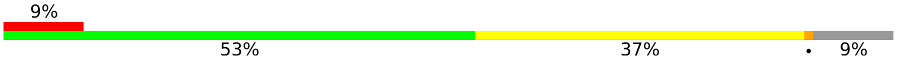
- Molecule 1: Major vault protein

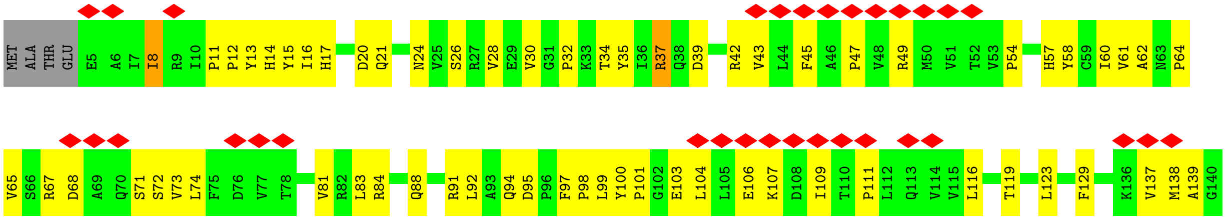
Chain SB:

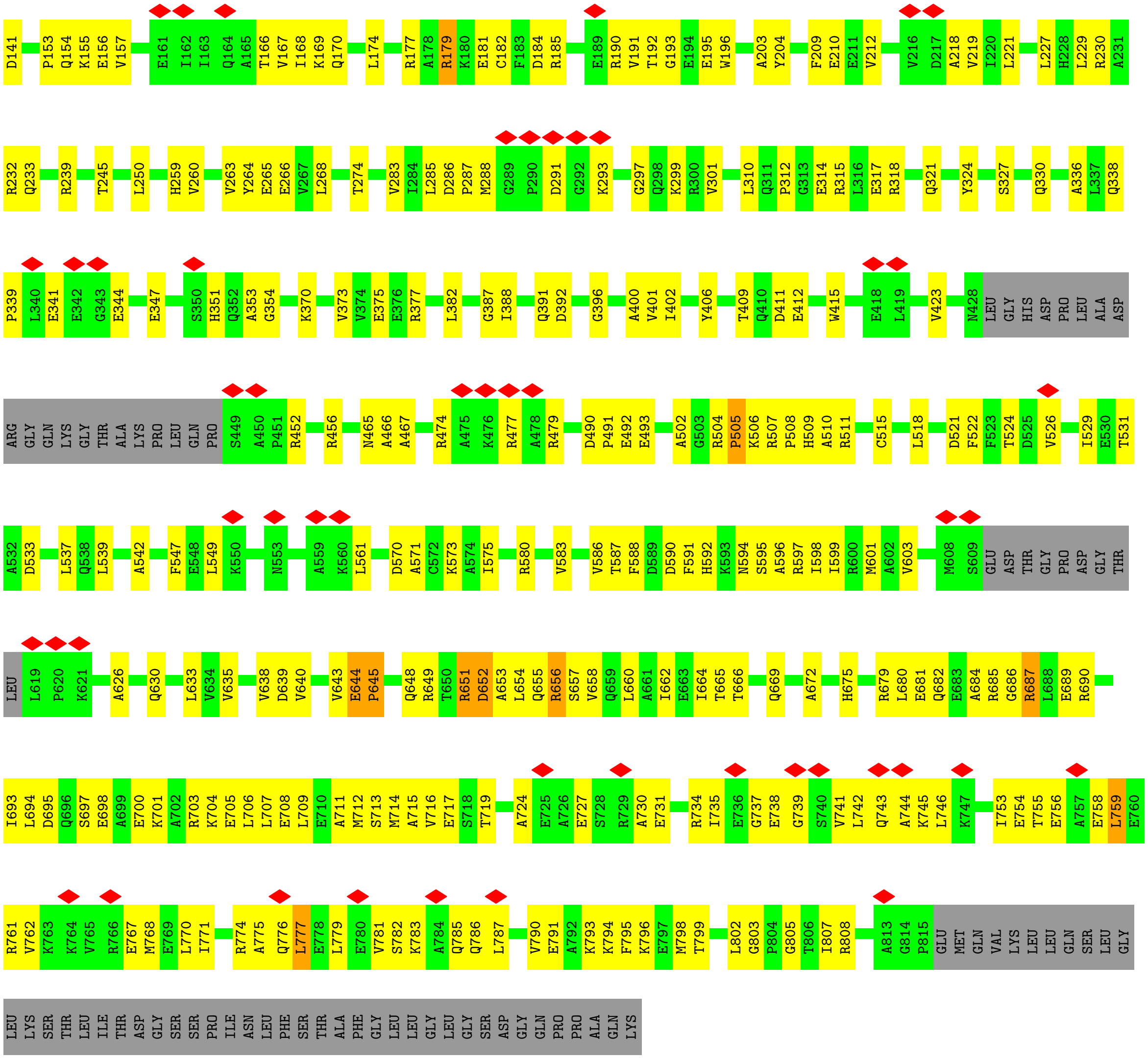




- Molecule 1: Major vault protein

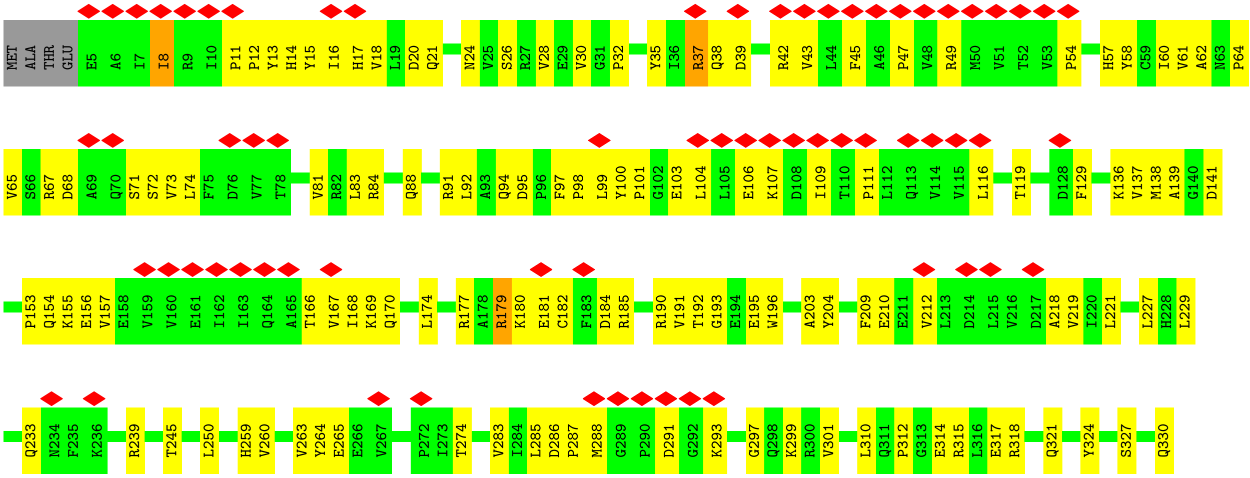
Chain TB:


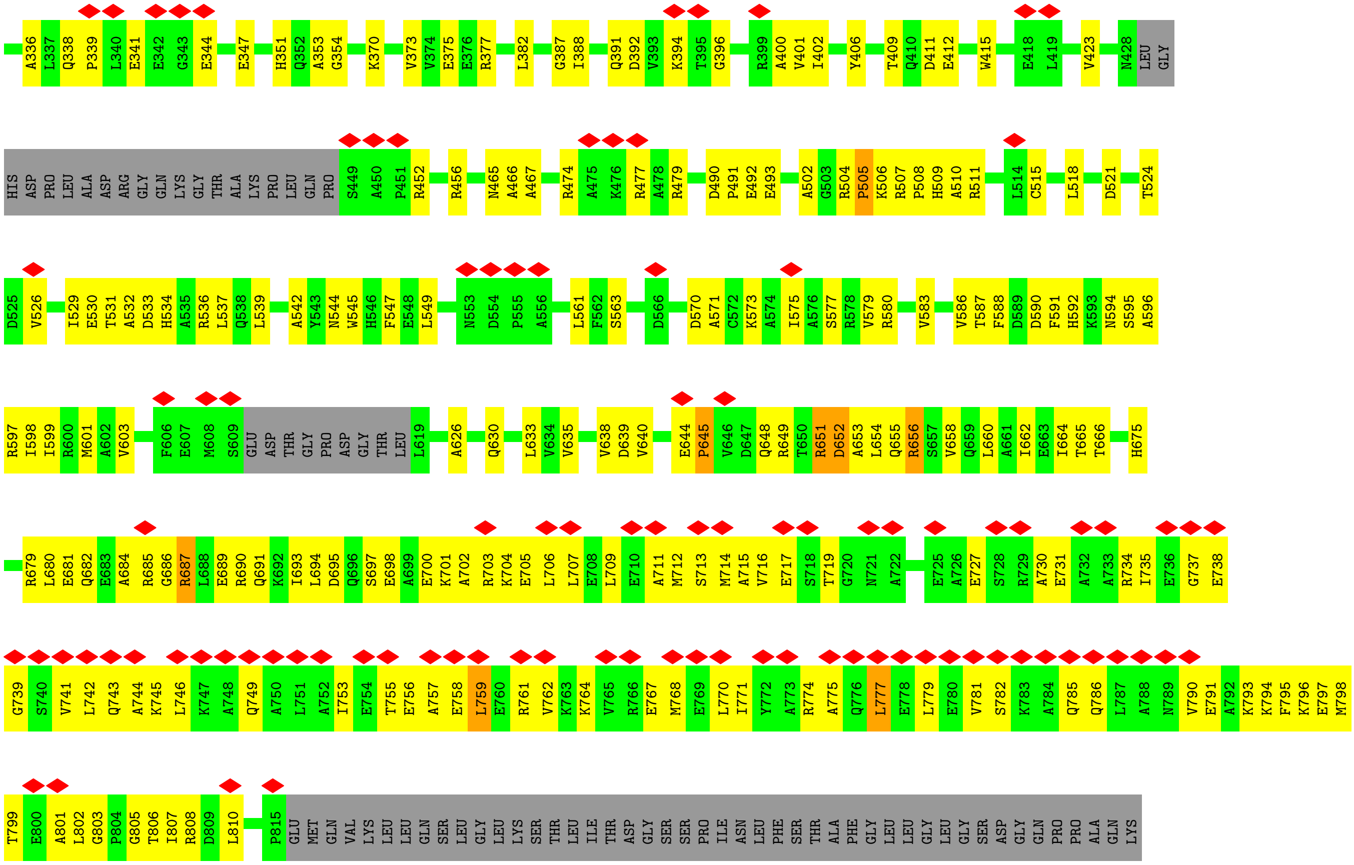




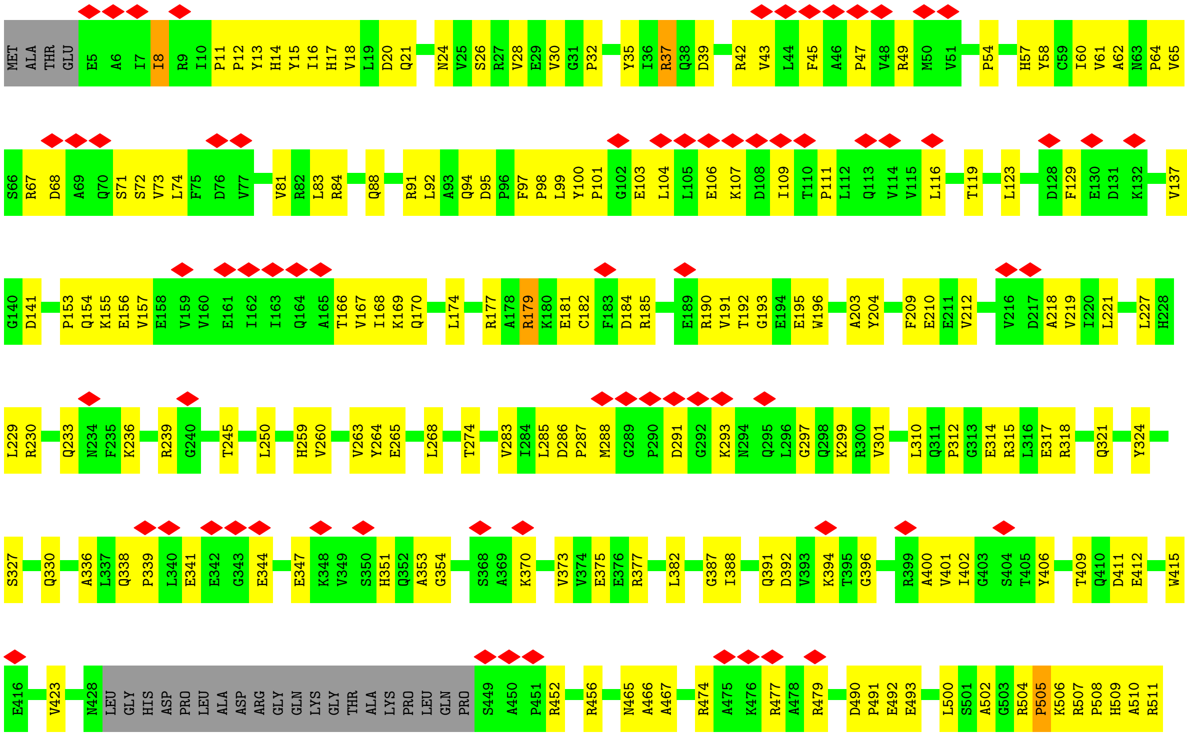
- Molecule 1: Major vault protein

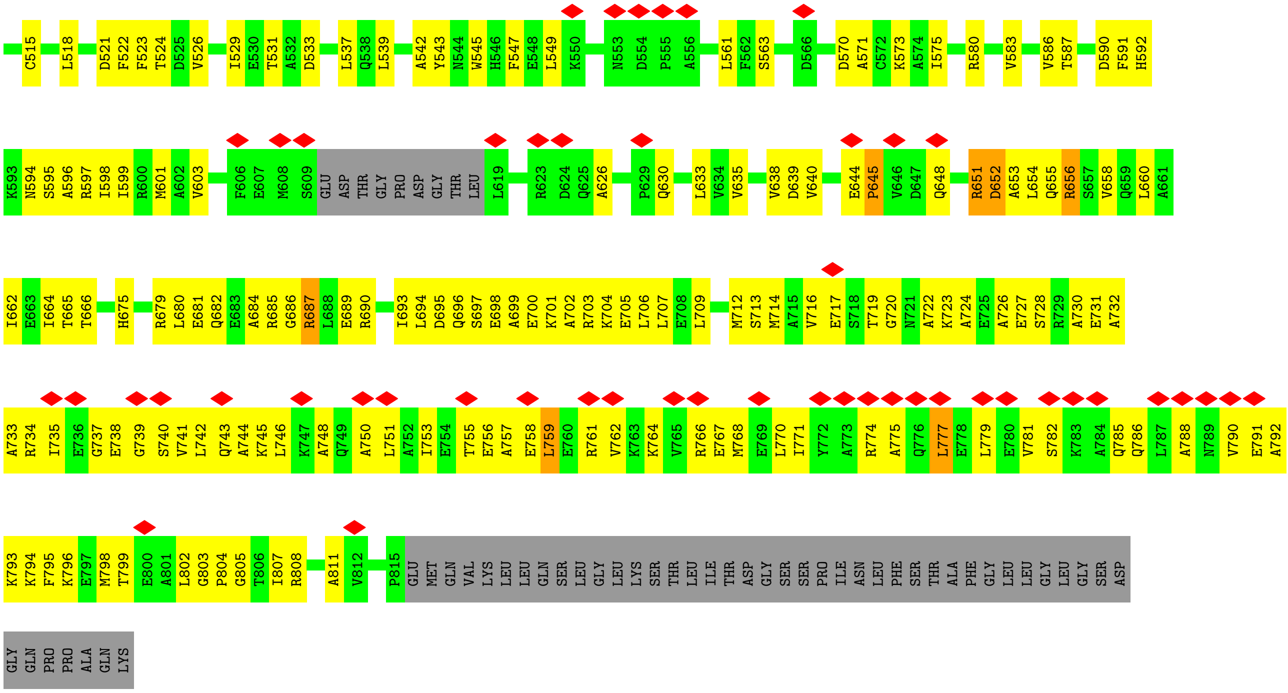
Chain UB:



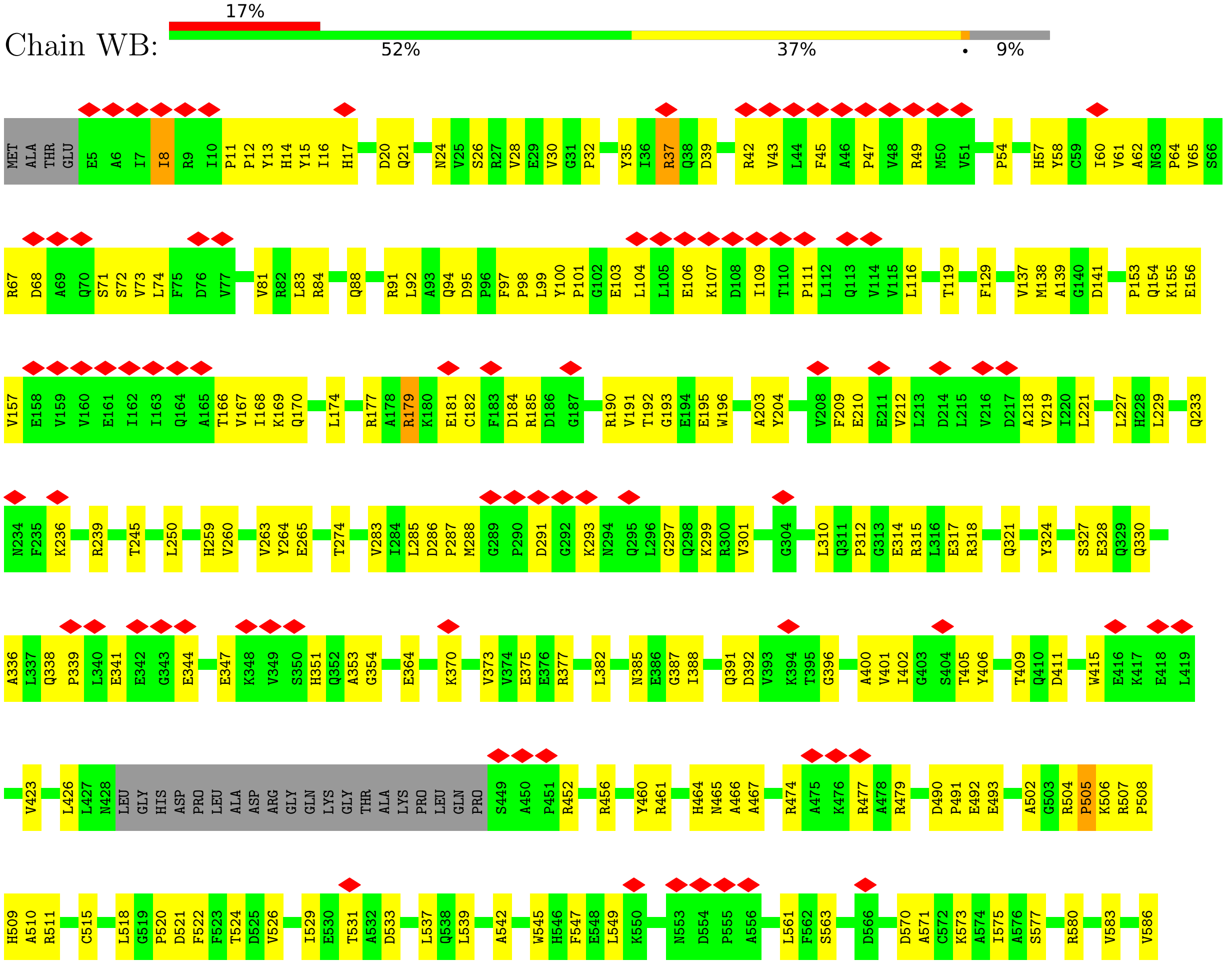


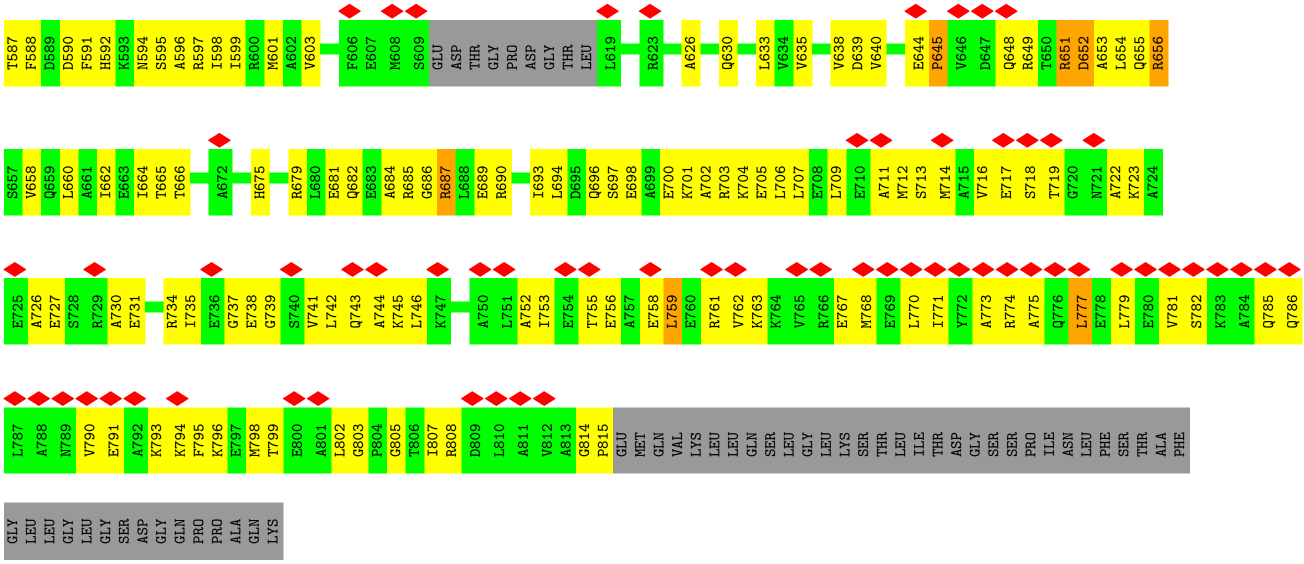
- Molecule 1: Major vault protein





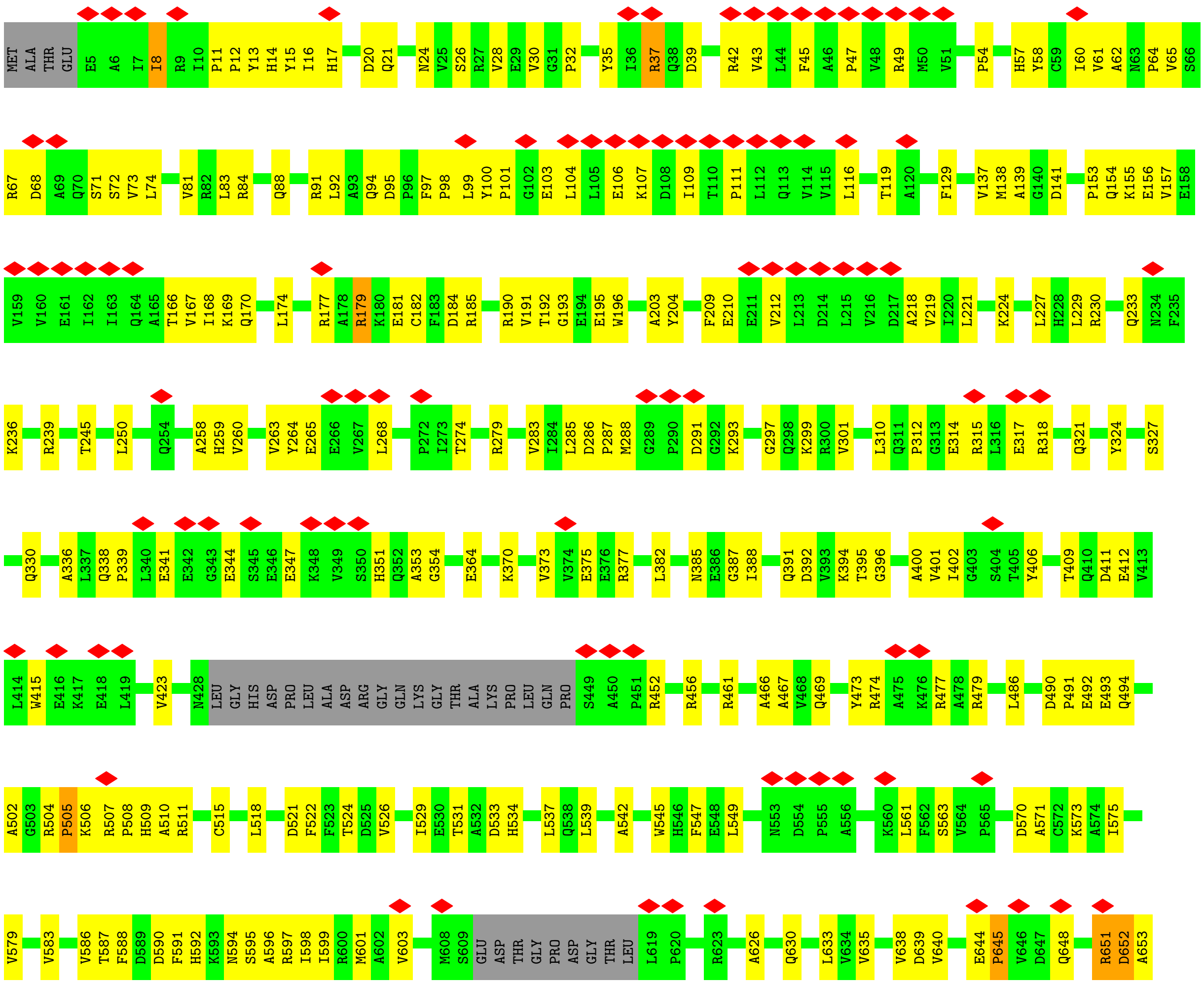
- Molecule 1: Major vault protein

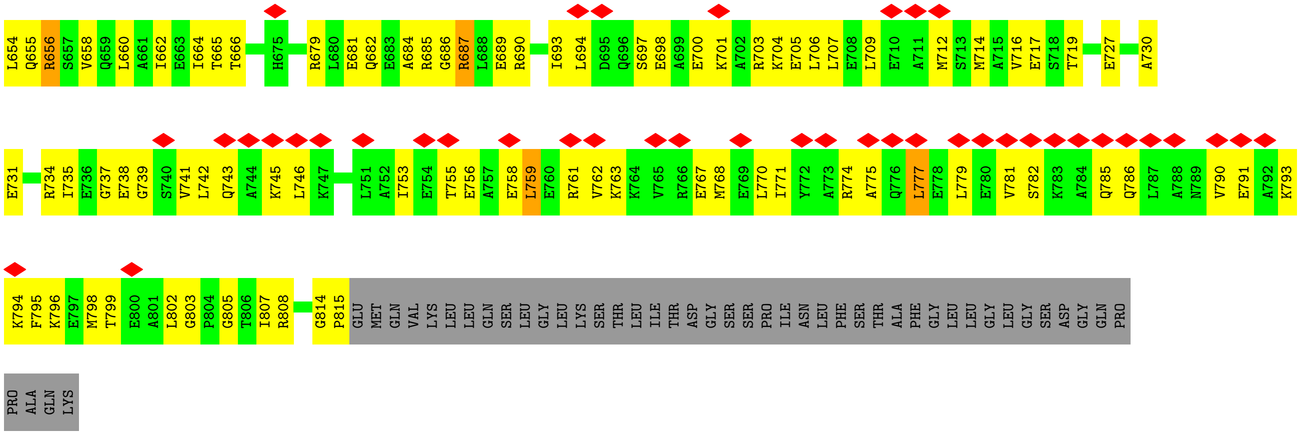




- Molecule 1: Major vault protein

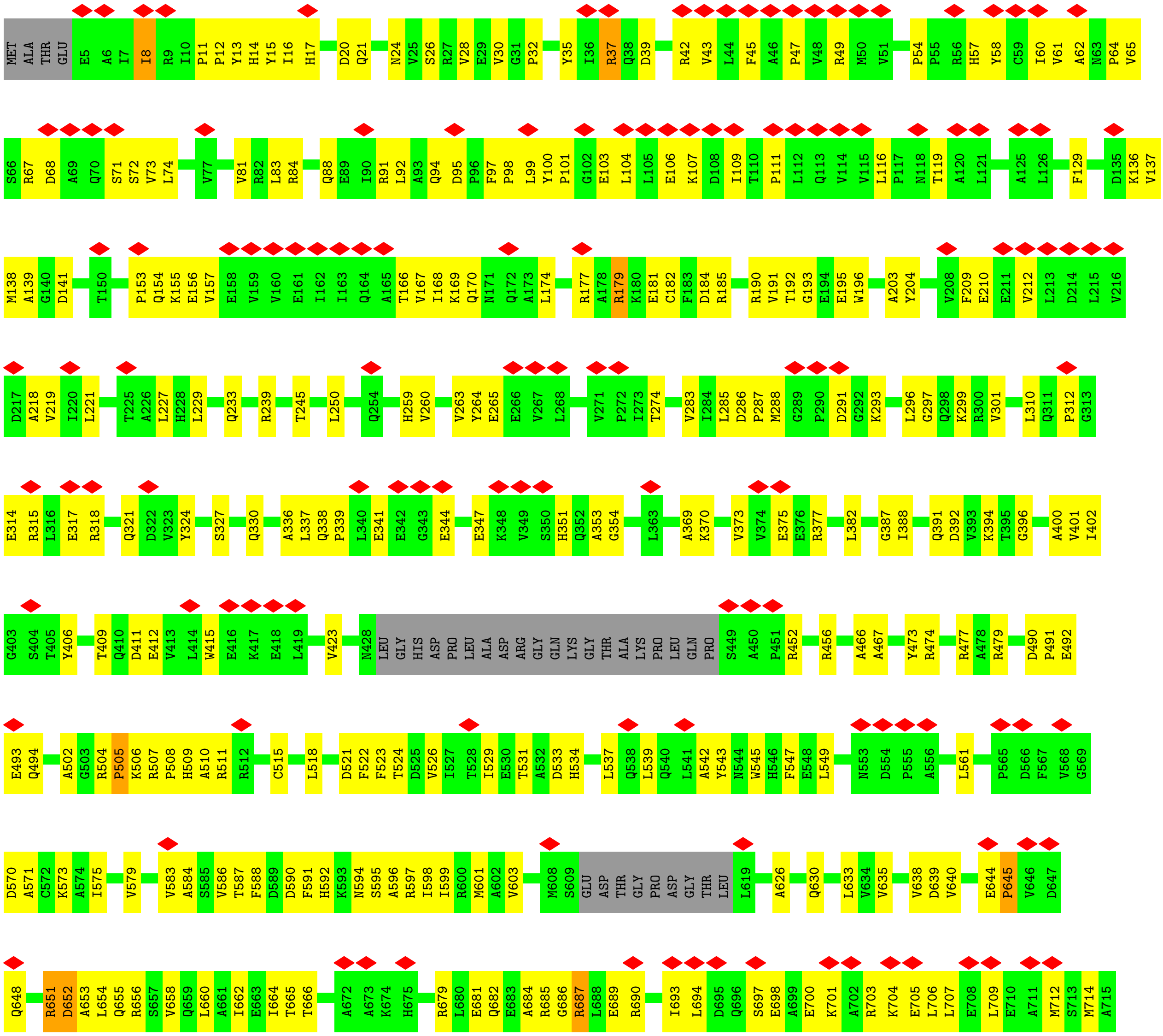
Chain XB:

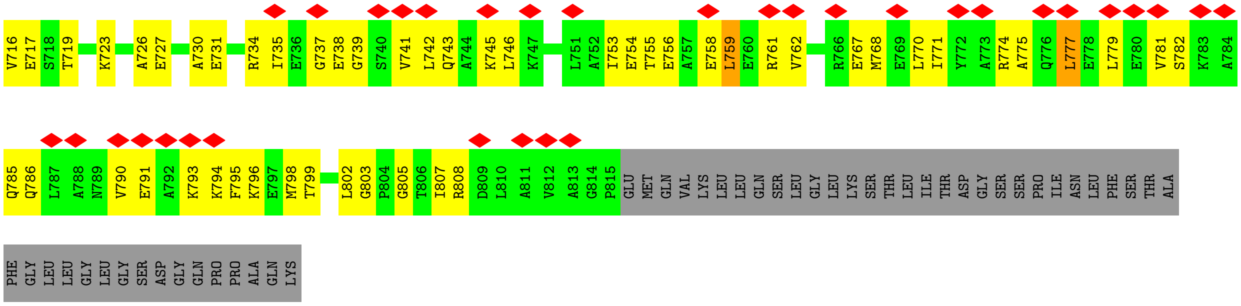




- Molecule 1: Major vault protein

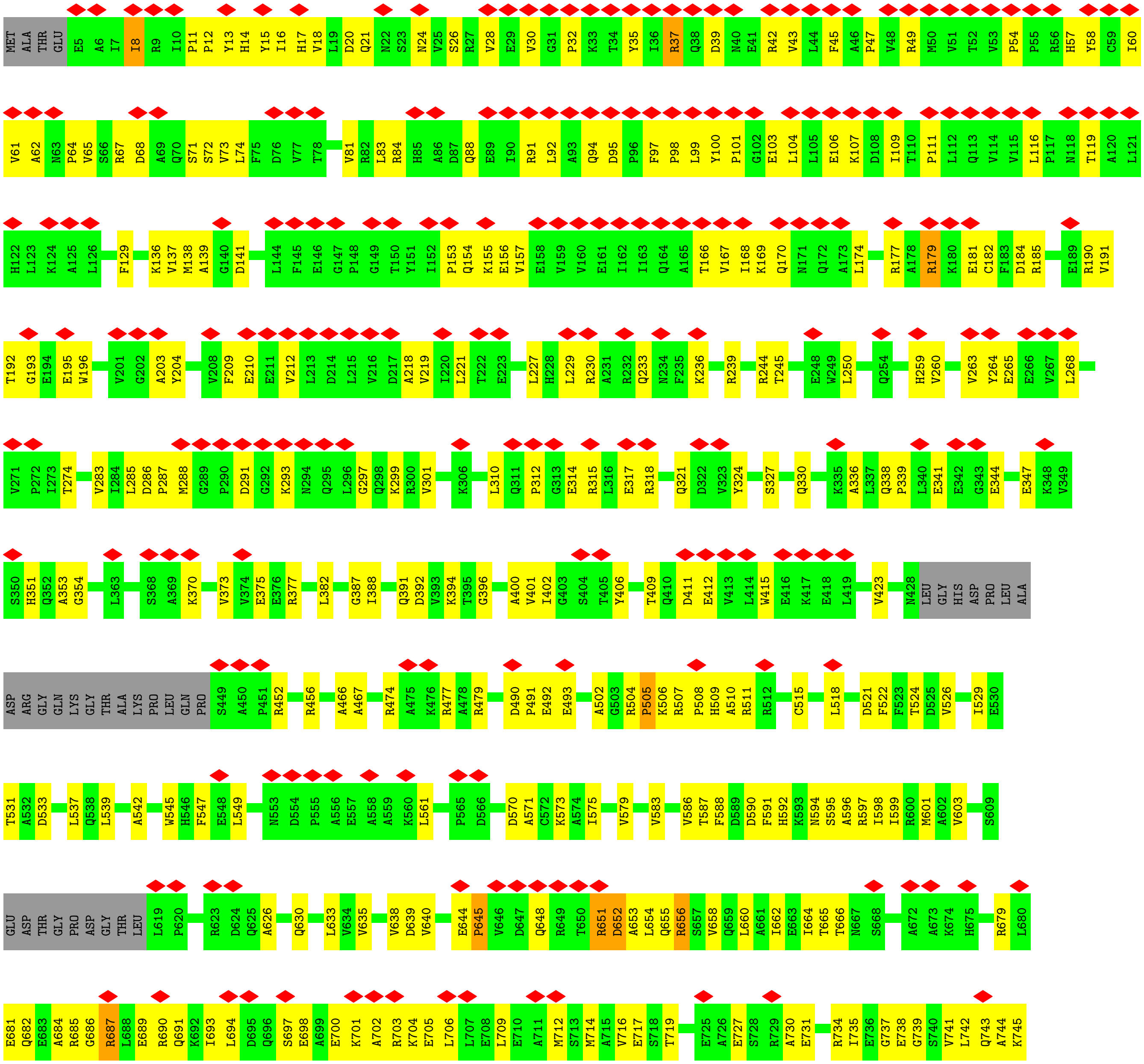
Chain YB:

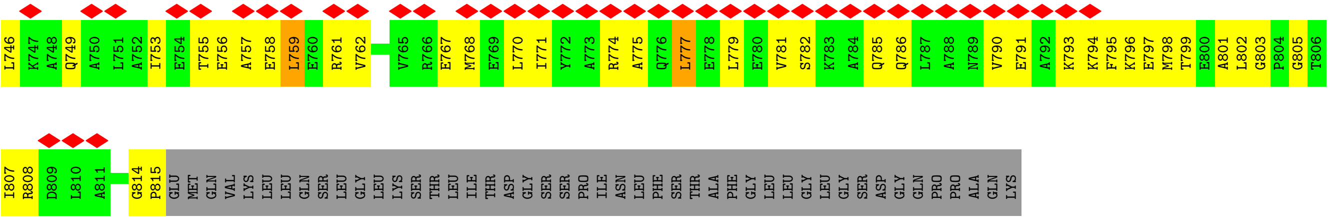




- Molecule 1: Major vault protein

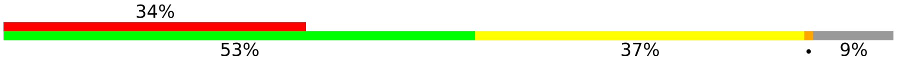
Chain ZB:

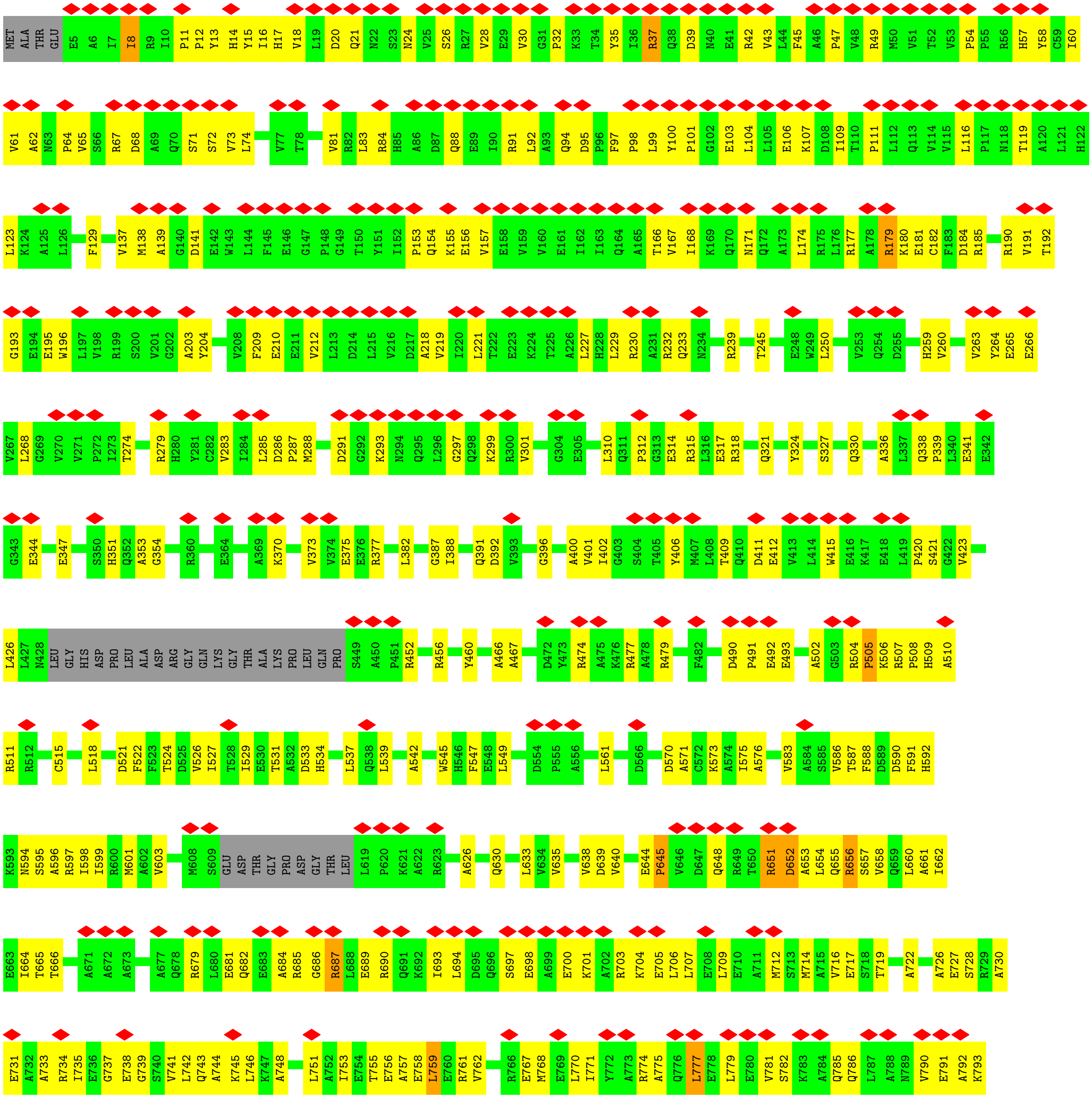


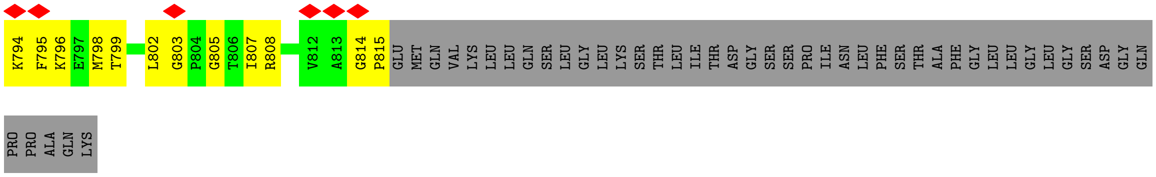


- Molecule 1: Major vault protein

Chain AC:






K794
F795
K796
E797
M798
T799
L802
G803
P804
G805
T806
I807
R808
V812
A813
G814
P815
GLU
MET
GLN
VAL
LYS
LEU
LEU
GLN
SER
LEU
GLY
LEU
LYS
SER
THR
LEU
ILE
THR
ASP
GLY
SER
SER
PRO
ILE
ASN
LEU
PHE
SER
THR
ALA
PHE
GLY
LEU
LEU
GLY
LEU
GLY
SER
ASP
GLY
GLN
PRO
PRO
ALA
GLN
LYS

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20864	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 ($e^-/\text{Å}^2$)	41.9	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	0.322	Depositor
Minimum map value	-0.098	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	735.0, 735.0, 735.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	3.675, 3.675, 3.675	Depositor

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	0.27	0/6255	0.58	3/8474 (0.0%)
1	AA	0.27	0/6255	0.58	3/8474 (0.0%)
1	AB	0.27	0/6255	0.58	3/8474 (0.0%)
1	AC	0.27	0/6255	0.58	3/8474 (0.0%)
1	B	0.27	0/6255	0.58	3/8474 (0.0%)
1	BA	0.27	0/6255	0.59	3/8474 (0.0%)
1	BB	0.27	0/6255	0.58	3/8474 (0.0%)
1	C	0.27	0/6255	0.58	3/8474 (0.0%)
1	CA	0.27	0/6255	0.58	3/8474 (0.0%)
1	CB	0.27	0/6255	0.58	3/8474 (0.0%)
1	D	0.27	0/6255	0.58	3/8474 (0.0%)
1	DA	0.27	0/6255	0.58	3/8474 (0.0%)
1	DB	0.27	0/6255	0.59	3/8474 (0.0%)
1	E	0.27	0/6255	0.58	3/8474 (0.0%)
1	EA	0.27	0/6255	0.59	3/8474 (0.0%)
1	EB	0.27	0/6255	0.58	3/8474 (0.0%)
1	F	0.27	0/6255	0.58	3/8474 (0.0%)
1	FA	0.27	0/6255	0.59	3/8474 (0.0%)
1	FB	0.27	0/6255	0.58	3/8474 (0.0%)
1	G	0.27	0/6255	0.58	3/8474 (0.0%)
1	GA	0.27	0/6255	0.58	3/8474 (0.0%)
1	GB	0.27	0/6255	0.58	3/8474 (0.0%)
1	H	0.27	0/6255	0.58	3/8474 (0.0%)
1	HA	0.27	0/6255	0.59	3/8474 (0.0%)
1	HB	0.27	0/6255	0.59	2/8474 (0.0%)
1	I	0.27	0/6255	0.58	3/8474 (0.0%)
1	IA	0.27	0/6255	0.59	3/8474 (0.0%)
1	IB	0.27	0/6255	0.58	2/8474 (0.0%)
1	J	0.27	0/6255	0.58	3/8474 (0.0%)
1	JA	0.27	0/6255	0.58	3/8474 (0.0%)
1	JB	0.27	0/6255	0.58	3/8474 (0.0%)
1	K	0.27	0/6255	0.58	3/8474 (0.0%)
1	KA	0.27	0/6255	0.58	3/8474 (0.0%)
1	KB	0.27	0/6255	0.58	3/8474 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	L	0.27	0/6255	0.59	3/8474 (0.0%)
1	LA	0.27	0/6255	0.58	3/8474 (0.0%)
1	LB	0.27	0/6255	0.59	3/8474 (0.0%)
1	M	0.27	0/6255	0.59	3/8474 (0.0%)
1	MA	0.27	0/6255	0.59	2/8474 (0.0%)
1	MB	0.27	0/6255	0.58	3/8474 (0.0%)
1	N	0.27	0/6255	0.58	3/8474 (0.0%)
1	NA	0.27	0/6255	0.58	3/8474 (0.0%)
1	NB	0.27	0/6255	0.58	3/8474 (0.0%)
1	O	0.27	0/6255	0.58	3/8474 (0.0%)
1	OA	0.27	0/6255	0.58	3/8474 (0.0%)
1	OB	0.27	0/6255	0.58	3/8474 (0.0%)
1	P	0.27	0/6255	0.58	3/8474 (0.0%)
1	PA	0.27	0/6255	0.58	3/8474 (0.0%)
1	PB	0.27	0/6255	0.58	3/8474 (0.0%)
1	Q	0.27	0/6255	0.58	3/8474 (0.0%)
1	QA	0.27	0/6255	0.58	3/8474 (0.0%)
1	QB	0.27	0/6255	0.58	3/8474 (0.0%)
1	R	0.27	0/6255	0.58	3/8474 (0.0%)
1	RA	0.27	0/6255	0.58	3/8474 (0.0%)
1	RB	0.27	0/6255	0.58	3/8474 (0.0%)
1	S	0.27	0/6255	0.58	3/8474 (0.0%)
1	SA	0.27	0/6255	0.58	3/8474 (0.0%)
1	SB	0.27	0/6255	0.58	3/8474 (0.0%)
1	T	0.27	0/6255	0.59	3/8474 (0.0%)
1	TA	0.27	0/6255	0.59	3/8474 (0.0%)
1	TB	0.27	0/6255	0.58	3/8474 (0.0%)
1	UA	0.27	0/6255	0.58	3/8474 (0.0%)
1	UB	0.27	0/6255	0.58	3/8474 (0.0%)
1	V	0.27	0/6255	0.58	3/8474 (0.0%)
1	VA	0.27	0/6255	0.58	3/8474 (0.0%)
1	VB	0.27	0/6255	0.58	3/8474 (0.0%)
1	W	0.27	0/6255	0.58	3/8474 (0.0%)
1	WA	0.27	0/6255	0.58	3/8474 (0.0%)
1	WB	0.27	0/6255	0.58	3/8474 (0.0%)
1	X	0.27	0/6255	0.58	3/8474 (0.0%)
1	XA	0.27	0/6255	0.59	3/8474 (0.0%)
1	XB	0.27	0/6255	0.59	3/8474 (0.0%)
1	Y	0.27	0/6255	0.59	3/8474 (0.0%)
1	YA	0.27	0/6255	0.58	3/8474 (0.0%)
1	YB	0.27	0/6255	0.58	3/8474 (0.0%)
1	Z	0.27	0/6255	0.59	3/8474 (0.0%)
1	ZA	0.27	0/6255	0.58	3/8474 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	ZB	0.27	0/6255	0.58	3/8474 (0.0%)
All	All	0.27	0/487890	0.58	231/660972 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	AA	0	3
1	AB	0	3
1	AC	0	3
1	B	0	3
1	BA	0	3
1	BB	0	3
1	C	0	3
1	CA	0	3
1	CB	0	3
1	D	0	3
1	DA	0	3
1	DB	0	3
1	E	0	3
1	EA	0	3
1	EB	0	3
1	F	0	3
1	FA	0	3
1	FB	0	3
1	G	0	3
1	GA	0	3
1	GB	0	3
1	H	0	3
1	HA	0	3
1	HB	0	3
1	I	0	3
1	IA	0	3
1	IB	0	3
1	J	0	3
1	JA	0	3
1	JB	0	3
1	K	0	3
1	KA	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	KB	0	3
1	L	0	3
1	LA	0	3
1	LB	0	3
1	M	0	3
1	MA	0	3
1	MB	0	3
1	N	0	3
1	NA	0	3
1	NB	0	3
1	O	0	3
1	OA	0	3
1	OB	0	3
1	P	0	3
1	PA	0	3
1	PB	0	3
1	Q	0	3
1	QA	0	3
1	QB	0	3
1	R	0	3
1	RA	0	3
1	RB	0	3
1	S	0	3
1	SA	0	3
1	SB	0	3
1	T	0	3
1	TA	0	3
1	TB	0	3
1	UA	0	3
1	UB	0	3
1	V	0	3
1	VA	0	3
1	VB	0	3
1	W	0	3
1	WA	0	3
1	WB	0	3
1	X	0	3
1	XA	0	3
1	XB	0	3
1	Y	0	3
1	YA	0	3
1	YB	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	Z	0	3
1	ZA	0	3
1	ZB	0	3
All	All	0	234

There are no bond length outliers.

The worst 5 of 231 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	777	LEU	CA-CB-CG	6.98	131.36	115.30
1	Z	777	LEU	CA-CB-CG	6.98	131.35	115.30
1	IA	777	LEU	CA-CB-CG	6.98	131.35	115.30
1	F	777	LEU	CA-CB-CG	6.98	131.34	115.30
1	QA	777	LEU	CA-CB-CG	6.98	131.35	115.30

There are no chirality outliers.

5 of 234 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	37	ARG	Peptide
1	A	644	GLU	Peptide
1	A	8	ILE	Peptide
1	B	37	ARG	Peptide
1	B	8	ILE	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	6169	728	0
1	AA	6150	0	6170	230	0
1	AB	6150	0	6170	245	0
1	AC	6150	0	6169	430	0
1	B	6150	0	6170	391	0
1	BA	6150	0	6170	235	0
1	BB	6150	0	6170	320	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	6150	0	6168	877	0
1	CA	6150	0	6170	226	0
1	CB	6150	0	6170	303	0
1	D	6150	0	6169	912	0
1	DA	6150	0	6170	229	0
1	DB	6150	0	6170	314	0
1	E	6150	0	6170	493	0
1	EA	6150	0	6170	226	0
1	EB	6150	0	6170	320	0
1	F	6150	0	6169	812	0
1	FA	6150	0	6170	230	0
1	FB	6150	0	6170	396	0
1	G	6150	0	6170	313	0
1	GA	6150	0	6170	229	0
1	GB	6150	0	6170	375	0
1	H	6150	0	6170	259	0
1	HA	6150	0	6170	258	0
1	HB	6150	0	6170	236	0
1	I	6150	0	6170	288	0
1	IA	6150	0	6170	360	0
1	IB	6150	0	6170	240	0
1	J	6150	0	6170	264	0
1	JA	6150	0	6170	252	0
1	JB	6150	0	6170	245	0
1	K	6150	0	6170	260	0
1	KA	6150	0	6170	360	0
1	KB	6150	0	6170	238	0
1	L	6150	0	6170	311	0
1	LA	6150	0	6170	229	0
1	LB	6150	0	6170	511	0
1	M	6150	0	6170	230	0
1	MA	6150	0	6170	239	0
1	MB	6150	0	6170	586	0
1	N	6150	0	6170	340	0
1	NA	6150	0	6170	230	0
1	NB	6150	0	6170	376	0
1	O	6150	0	6170	230	0
1	OA	6150	0	6170	231	0
1	OB	6150	0	6169	641	0
1	P	6150	0	6170	309	0
1	PA	6150	0	6170	241	0
1	PB	6150	0	6170	619	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Q	6150	0	6170	234	0
1	QA	6150	0	6170	242	0
1	QB	6150	0	6170	240	0
1	R	6150	0	6170	309	0
1	RA	6150	0	6170	240	0
1	RB	6150	0	6170	292	0
1	S	6150	0	6170	241	0
1	SA	6150	0	6170	248	0
1	SB	6150	0	6170	339	0
1	T	6150	0	6170	274	0
1	TA	6150	0	6170	247	0
1	TB	6150	0	6170	389	0
1	UA	6150	0	6170	232	0
1	UB	6150	0	6167	582	0
1	V	6150	0	6170	241	0
1	VA	6150	0	6170	242	0
1	VB	6150	0	6166	560	0
1	W	6150	0	6170	233	0
1	WA	6150	0	6170	227	0
1	WB	6150	0	6170	349	0
1	X	6150	0	6170	240	0
1	XA	6150	0	6170	263	0
1	XB	6150	0	6170	270	0
1	Y	6150	0	6170	225	0
1	YA	6150	0	6170	226	0
1	YB	6150	0	6170	247	0
1	Z	6150	0	6170	230	0
1	ZA	6150	0	6170	282	0
1	ZB	6150	0	6169	375	0
All	All	479700	0	481245	21752	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 23.

The worst 5 of 21752 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:UB:757:ALA:CB	1:VB:751:LEU:HB3	1.24	1.68
1:ZB:735:ILE:CB	1:AC:726:ALA:CB	1.77	1.62
1:C:779:LEU:CD1	1:E:770:LEU:HA	1.10	1.57
1:ZB:735:ILE:CG2	1:AC:726:ALA:HB1	1.33	1.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:MET:CE	1:C:763:LYS:HB2	1.08	1.54

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%)	673 (87%)	99 (13%)	4 (0%)	29	69
1	AA	776/861 (90%)	671 (86%)	101 (13%)	4 (0%)	29	69
1	AB	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	AC	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	B	776/861 (90%)	673 (87%)	99 (13%)	4 (0%)	29	69
1	BA	776/861 (90%)	675 (87%)	97 (12%)	4 (0%)	29	69
1	BB	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	C	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	CA	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	CB	776/861 (90%)	673 (87%)	99 (13%)	4 (0%)	29	69
1	D	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	DA	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	DB	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	E	776/861 (90%)	673 (87%)	99 (13%)	4 (0%)	29	69
1	EA	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	EB	776/861 (90%)	673 (87%)	99 (13%)	4 (0%)	29	69
1	F	776/861 (90%)	675 (87%)	97 (12%)	4 (0%)	29	69
1	FA	776/861 (90%)	675 (87%)	97 (12%)	4 (0%)	29	69
1	FB	776/861 (90%)	673 (87%)	99 (13%)	4 (0%)	29	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	776/861 (90%)	675 (87%)	97 (12%)	4 (0%)	29	69
1	GA	776/861 (90%)	675 (87%)	97 (12%)	4 (0%)	29	69
1	GB	776/861 (90%)	673 (87%)	99 (13%)	4 (0%)	29	69
1	H	776/861 (90%)	673 (87%)	99 (13%)	4 (0%)	29	69
1	HA	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	HB	776/861 (90%)	675 (87%)	97 (12%)	4 (0%)	29	69
1	I	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	IA	776/861 (90%)	675 (87%)	97 (12%)	4 (0%)	29	69
1	IB	776/861 (90%)	675 (87%)	97 (12%)	4 (0%)	29	69
1	J	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	JA	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	JB	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	K	776/861 (90%)	673 (87%)	99 (13%)	4 (0%)	29	69
1	KA	776/861 (90%)	675 (87%)	97 (12%)	4 (0%)	29	69
1	KB	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	L	776/861 (90%)	675 (87%)	97 (12%)	4 (0%)	29	69
1	LA	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	LB	776/861 (90%)	672 (87%)	100 (13%)	4 (0%)	29	69
1	M	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	MA	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	MB	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	N	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	NA	776/861 (90%)	675 (87%)	97 (12%)	4 (0%)	29	69
1	NB	776/861 (90%)	673 (87%)	99 (13%)	4 (0%)	29	69
1	O	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	OA	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	OB	776/861 (90%)	673 (87%)	99 (13%)	4 (0%)	29	69
1	P	776/861 (90%)	675 (87%)	97 (12%)	4 (0%)	29	69
1	PA	776/861 (90%)	673 (87%)	99 (13%)	4 (0%)	29	69
1	PB	776/861 (90%)	673 (87%)	99 (13%)	4 (0%)	29	69
1	Q	776/861 (90%)	675 (87%)	97 (12%)	4 (0%)	29	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	QA	776/861 (90%)	673 (87%)	99 (13%)	4 (0%)	29	69
1	QB	776/861 (90%)	675 (87%)	97 (12%)	4 (0%)	29	69
1	R	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	RA	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	RB	776/861 (90%)	675 (87%)	97 (12%)	4 (0%)	29	69
1	S	776/861 (90%)	675 (87%)	97 (12%)	4 (0%)	29	69
1	SA	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	SB	776/861 (90%)	673 (87%)	99 (13%)	4 (0%)	29	69
1	T	776/861 (90%)	673 (87%)	99 (13%)	4 (0%)	29	69
1	TA	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	TB	776/861 (90%)	675 (87%)	97 (12%)	4 (0%)	29	69
1	UA	776/861 (90%)	673 (87%)	99 (13%)	4 (0%)	29	69
1	UB	776/861 (90%)	673 (87%)	99 (13%)	4 (0%)	29	69
1	V	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	VA	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	VB	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	W	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	WA	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	WB	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	X	776/861 (90%)	673 (87%)	99 (13%)	4 (0%)	29	69
1	XA	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	XB	776/861 (90%)	675 (87%)	97 (12%)	4 (0%)	29	69
1	Y	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	YA	776/861 (90%)	673 (87%)	99 (13%)	4 (0%)	29	69
1	YB	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	Z	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	ZA	776/861 (90%)	674 (87%)	98 (13%)	4 (0%)	29	69
1	ZB	776/861 (90%)	675 (87%)	97 (12%)	4 (0%)	29	69
All	All	60528/67158 (90%)	52566 (87%)	7650 (13%)	312 (0%)	32	69

5 of 312 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	651	ARG
1	A	652	ASP
1	B	651	ARG
1	B	652	ASP
1	C	651	ARG

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 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	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	AA	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	AB	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	AC	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	B	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	BA	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	BB	654/726 (90%)	651 (100%)	3 (0%)	88	93
1	C	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	CA	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	CB	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	D	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	DA	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	DB	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	E	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	EA	654/726 (90%)	651 (100%)	3 (0%)	88	93
1	EB	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	F	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	FA	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	FB	654/726 (90%)	649 (99%)	5 (1%)	81	89
1	G	654/726 (90%)	650 (99%)	4 (1%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	GA	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	GB	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	H	654/726 (90%)	651 (100%)	3 (0%)	88	93
1	HA	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	HB	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	I	654/726 (90%)	651 (100%)	3 (0%)	88	93
1	IA	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	IB	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	J	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	JA	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	JB	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	K	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	KA	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	KB	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	L	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	LA	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	LB	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	M	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	MA	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	MB	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	N	654/726 (90%)	651 (100%)	3 (0%)	88	93
1	NA	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	NB	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	O	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	OA	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	OB	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	P	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	PA	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	PB	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	Q	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	QA	654/726 (90%)	651 (100%)	3 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	QB	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	R	654/726 (90%)	649 (99%)	5 (1%)	81	89
1	RA	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	RB	654/726 (90%)	649 (99%)	5 (1%)	81	89
1	S	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	SA	654/726 (90%)	651 (100%)	3 (0%)	88	93
1	SB	654/726 (90%)	649 (99%)	5 (1%)	81	89
1	T	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	TA	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	TB	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	UA	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	UB	654/726 (90%)	649 (99%)	5 (1%)	81	89
1	V	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	VA	654/726 (90%)	651 (100%)	3 (0%)	88	93
1	VB	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	W	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	WA	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	WB	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	X	654/726 (90%)	651 (100%)	3 (0%)	88	93
1	XA	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	XB	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	Y	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	YA	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	YB	654/726 (90%)	651 (100%)	3 (0%)	88	93
1	Z	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	ZA	654/726 (90%)	650 (99%)	4 (1%)	86	92
1	ZB	654/726 (90%)	650 (99%)	4 (1%)	86	92
All	All	51012/56628 (90%)	50705 (99%)	307 (1%)	86	92

5 of 307 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	IB	656	ARG

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Mol	Chain	Res	Type
1	VB	656	ARG
1	KB	239	ARG
1	PB	687	ARG
1	ZB	239	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 168 such sidechains are listed below:

Mol	Chain	Res	Type
1	HB	88	GLN
1	RB	88	GLN
1	JB	534	HIS
1	OB	118	ASN
1	TB	655	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

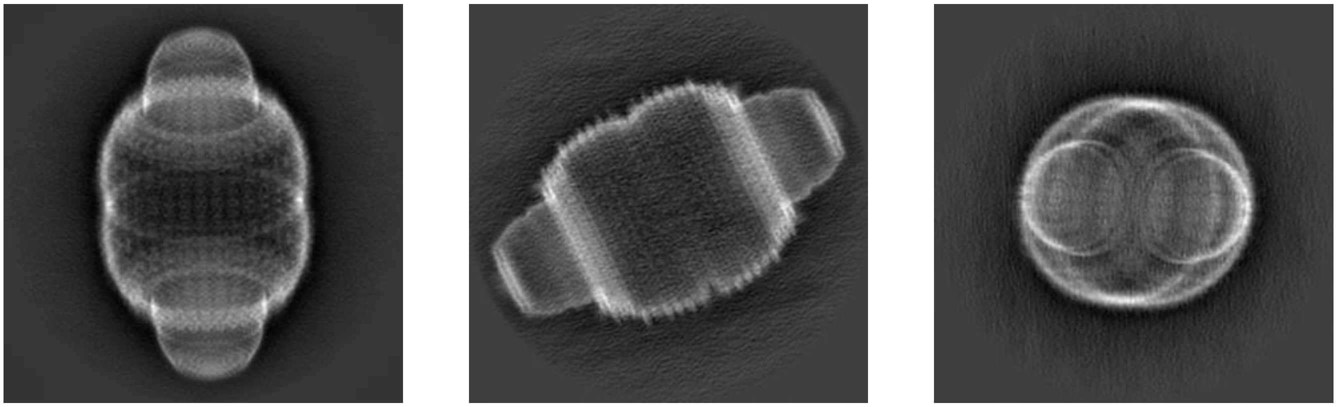
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13483. 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

6.1.1 Primary map

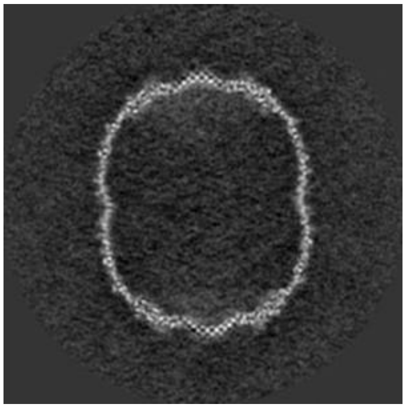


X Y Z

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

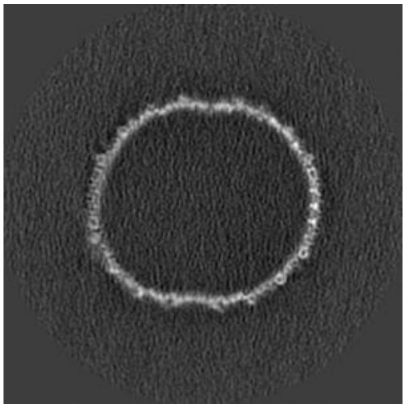
6.2 Central slices

6.2.1 Primary map



X Index: 100

Y Index: 100



Z Index: 100

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

6.3 Largest variance slices ⓘ

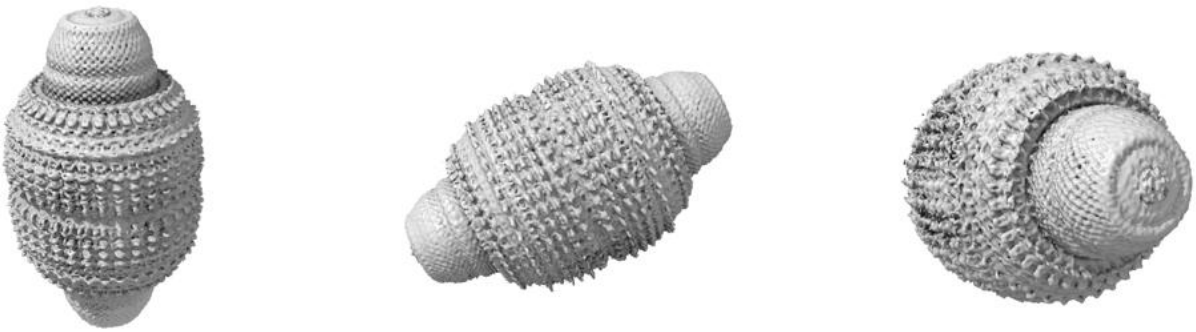
6.3.1 Primary map

X Index: 112 Y Index: 126 Z Index: 66

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

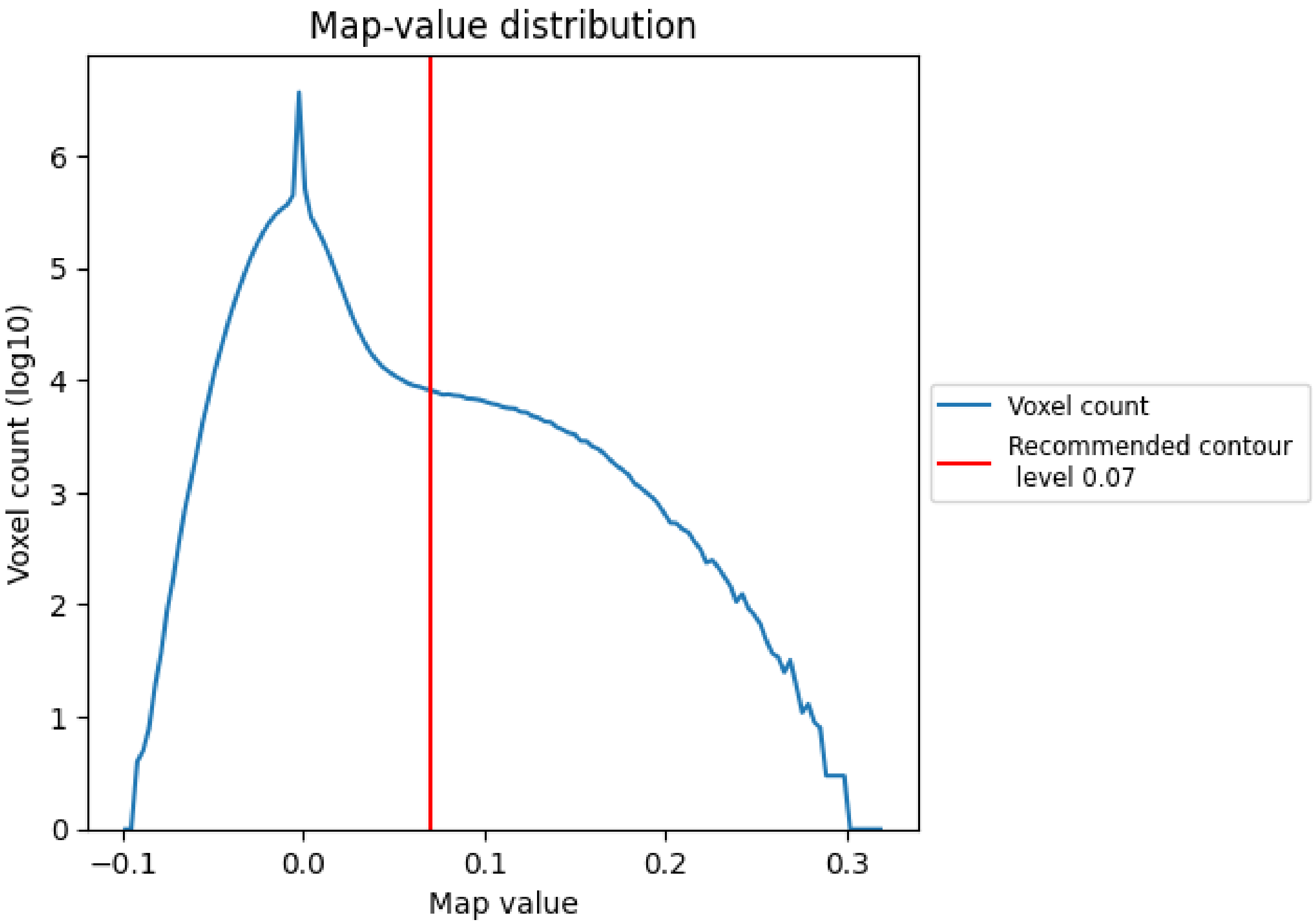
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

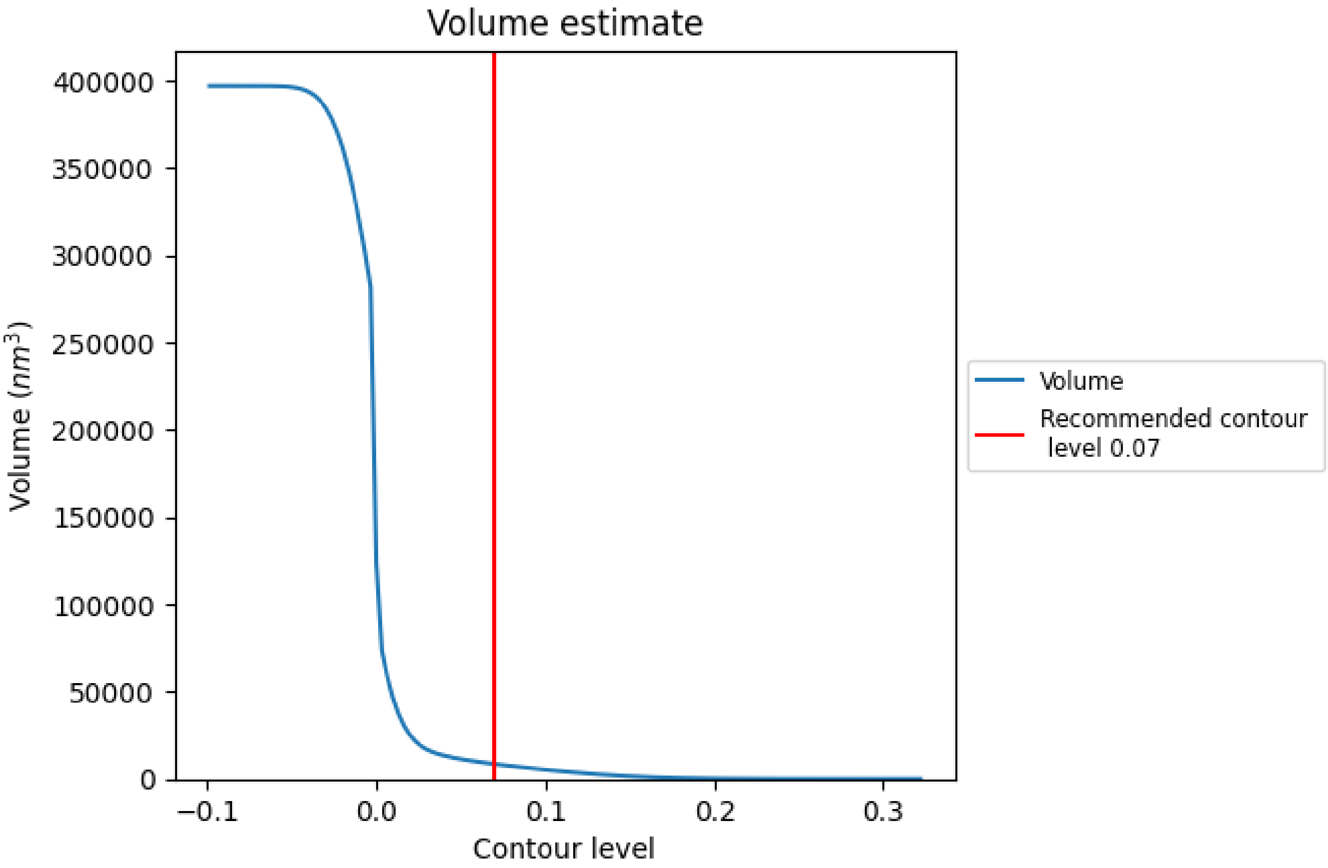
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

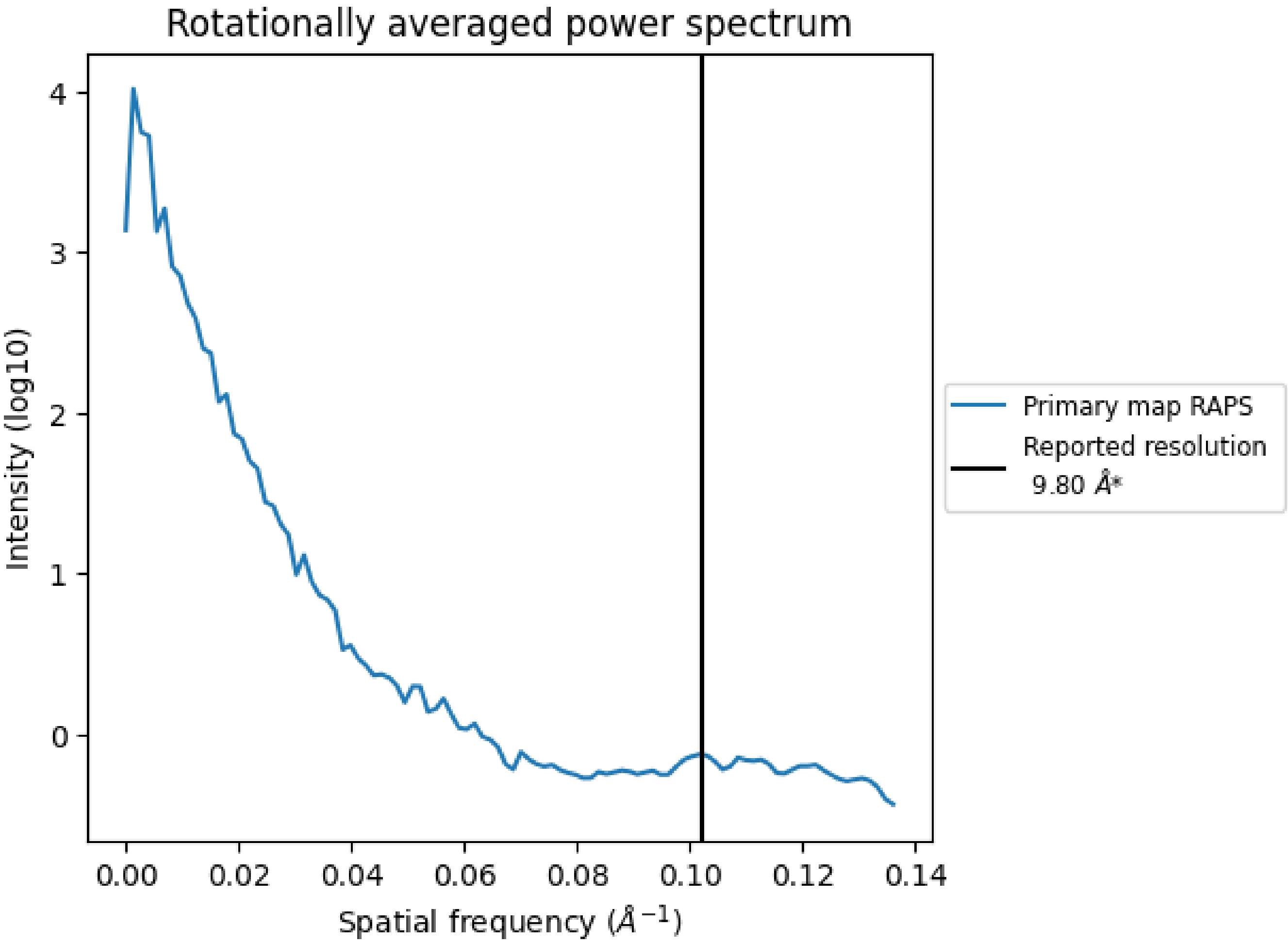
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 8639 nm^3; this corresponds to an approximate mass of 7804 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.102 $\AA^{-1}$

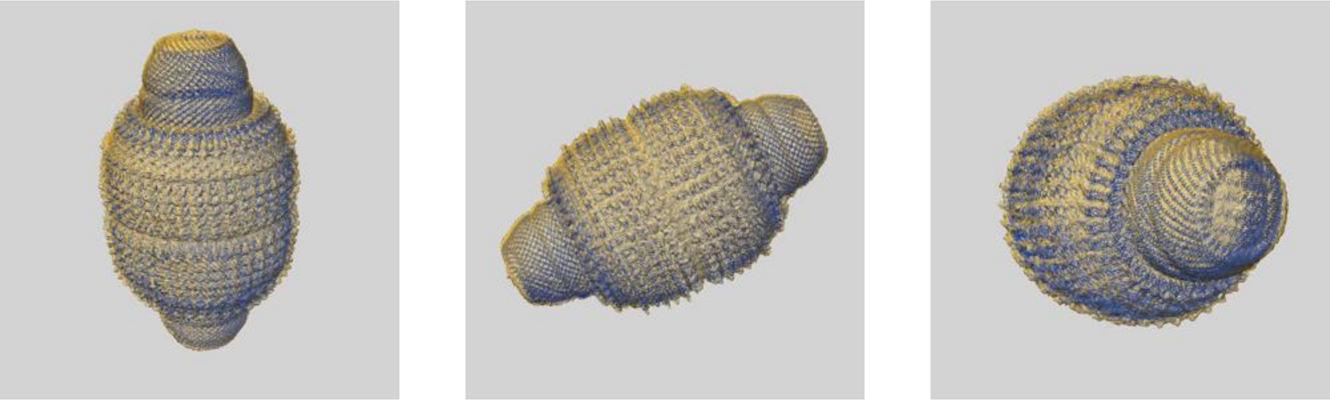
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-13483 and PDB model 7PKZ. Per-residue inclusion information can be found in section 3 on page 25.

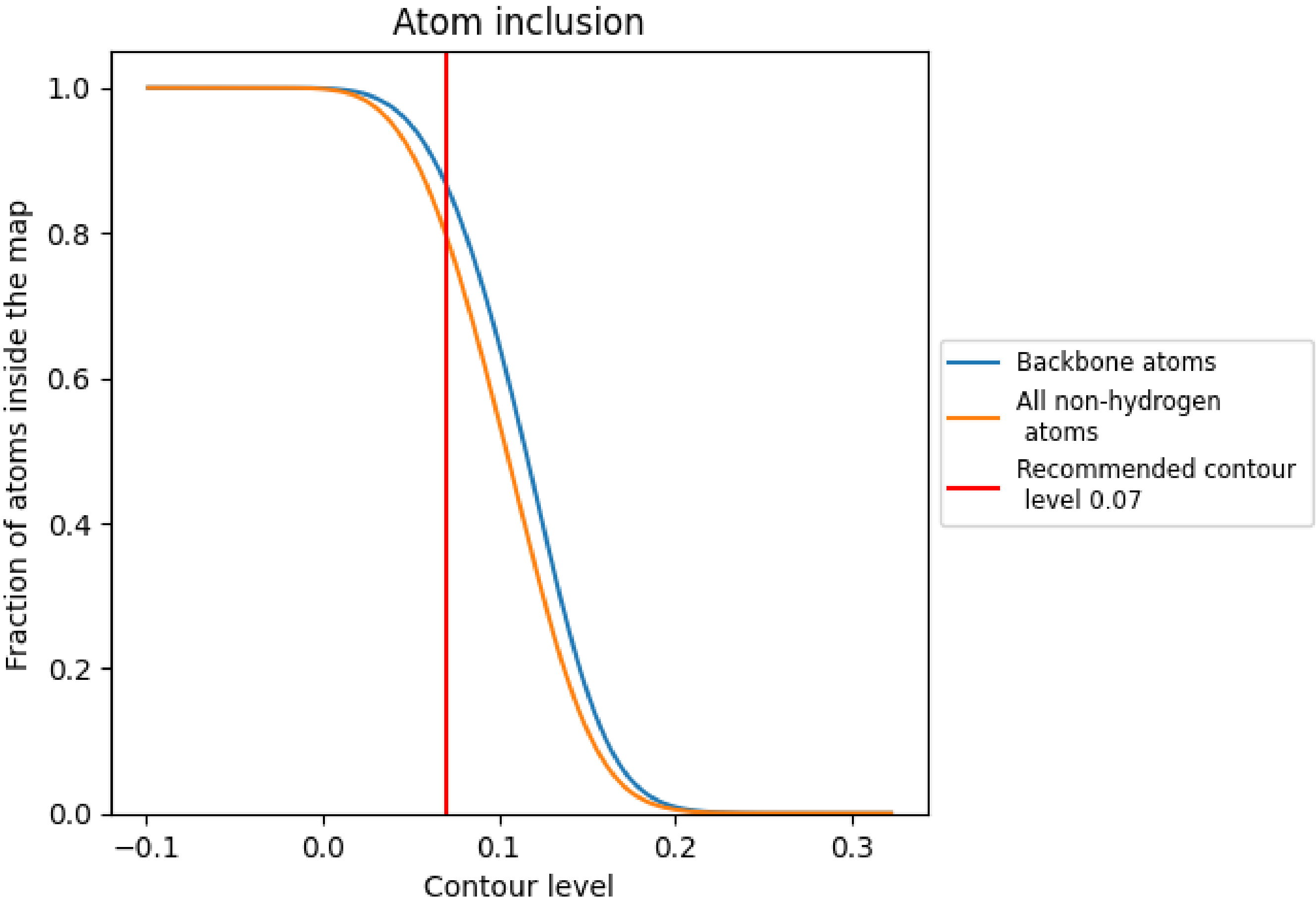
9.1 Map-model overlay ⓘ



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 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 ⓘ



At the recommended contour level, 87% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.