wwPDB EM Validation Summary Report

Jul 11, 2026 – 01:42 pm BST

PDB ID	:	9QWQ / pdb_00009qwq
EMDB ID	:	EMD-53423
Title	:	Human vault protein - committed conformation
Authors	:	Lapenta, F.; Marechal, N.; Durand, A.; Aupic, J.; Cassetta, A.
Deposited on	:	2025-04-15
Resolution	:	4.45 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

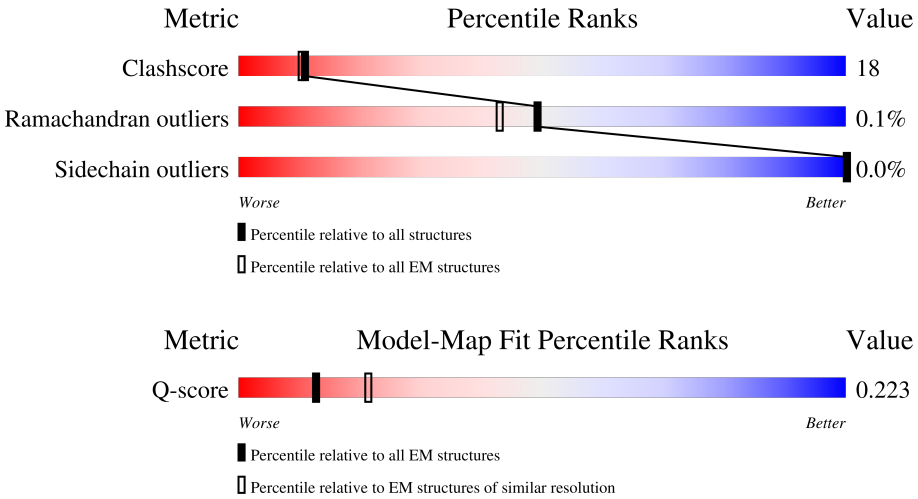
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.45 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3027 (3.95 - 4.95)

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	893	58% 30% 13%
1	AA	893	58% 29% 13%
1	AB	893	57% 30% 13%
1	AC	893	57% 30% 13%

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Mol	Chain	Length	Quality of chain
1	B	893	57% 30% 13%
1	BA	893	55% 32% 13%
1	BB	893	58% 30% 13%
1	C	893	57% 30% 13%
1	CA	893	56% 31% 13%
1	CB	893	58% 29% 13%
1	D	893	56% 31% 13%
1	DA	893	52% 36% 13%
1	DB	893	61% 26% 13%
1	E	893	56% 31% 13%
1	EA	893	55% 32% 13%
1	EB	893	58% 29% 13%
1	F	893	56% 31% 13%
1	FA	893	55% 32% 13%
1	FB	893	55% 32% 13%
1	G	893	59% 28% 13%
1	GA	893	56% 31% 13%
1	GB	893	56% 31% 13%
1	H	893	55% 32% 13%
1	HA	893	58% 29% 13%
1	HB	893	58% 30% 13%
1	I	893	54% 33% 13%
1	IA	893	57% 30% 13%
1	IB	893	55% 33% 13%
1	J	893	56% 32% 13%

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Mol	Chain	Length	Quality of chain
1	JA	893	56% 31% 13%
1	JB	893	52% 35% 13%
1	K	893	57% 30% 13%
1	KA	893	57% 30% 13%
1	KB	893	55% 32% 13%
1	L	893	59% 28% 13%
1	LA	893	56% 31% 13%
1	LB	893	55% 32% 13%
1	M	893	59% 28% 13%
1	MA	893	55% 33% 13%
1	MB	893	55% 32% 13%
1	N	893	58% 29% 13%
1	NA	893	55% 32% 13%
1	NB	893	55% 32% 13%
1	O	893	56% 32% 13%
1	OA	893	56% 31% 13%
1	OB	893	55% 33% 13%
1	P	893	59% 28% 13%
1	PA	893	55% 33% 13%
1	PB	893	55% 32% 13%
1	Q	893	59% 28% 13%
1	QA	893	54% 33% 13%
1	QB	893	57% 30% 13%
1	R	893	64% 24% 13%
1	RA	893	60% 28% 13%

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Mol	Chain	Length	Quality of chain
1	RB	893	53% 34% 13%
1	S	893	8% 65% 22% 13%
1	SA	893	63% 24% 13%
1	SB	893	56% 31% 13%
1	T	893	64% 23% 13%
1	TA	893	5% 61% 26% 13%
1	TB	893	55% 32% 13%
1	UA	893	15% 64% 23% 13%
1	UB	893	55% 32% 13%
1	V	893	64% 23% 13%
1	VA	893	10% 61% 26% 13%
1	VB	893	53% 34% 13%
1	W	893	60% 27% 13%
1	WA	893	61% 26% 13%
1	WB	893	53% 34% 13%
1	X	893	60% 27% 13%
1	XA	893	57% 30% 13%
1	XB	893	53% 34% 13%
1	Y	893	58% 29% 13%
1	YA	893	57% 30% 13%
1	YB	893	53% 34% 13%
1	Z	893	57% 30% 13%
1	ZA	893	58% 29% 13%
1	ZB	893	56% 31% 13%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 482118 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	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	AA	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	AB	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	AC	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	B	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	BA	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	BB	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	C	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	CA	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	CB	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	D	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	DA	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	DB	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	E	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	EA	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	EB	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	F	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	FA	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	FB	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	G	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	GA	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	GB	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	H	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	HA	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	HB	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	I	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	IA	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	IB	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	J	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	JA	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	JB	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	K	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	KA	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	KB	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	L	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	LA	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	LB	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	M	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	MA	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	MB	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	N	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	NA	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	NB	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	O	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	OA	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	OB	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	P	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	PA	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	PB	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	Q	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	QA	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	QB	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	R	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	RA	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	RB	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	S	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	SA	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	SB	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		
1	T	779	Total	C	N	O	S	0	0
			6181	3890	1105	1176	10		

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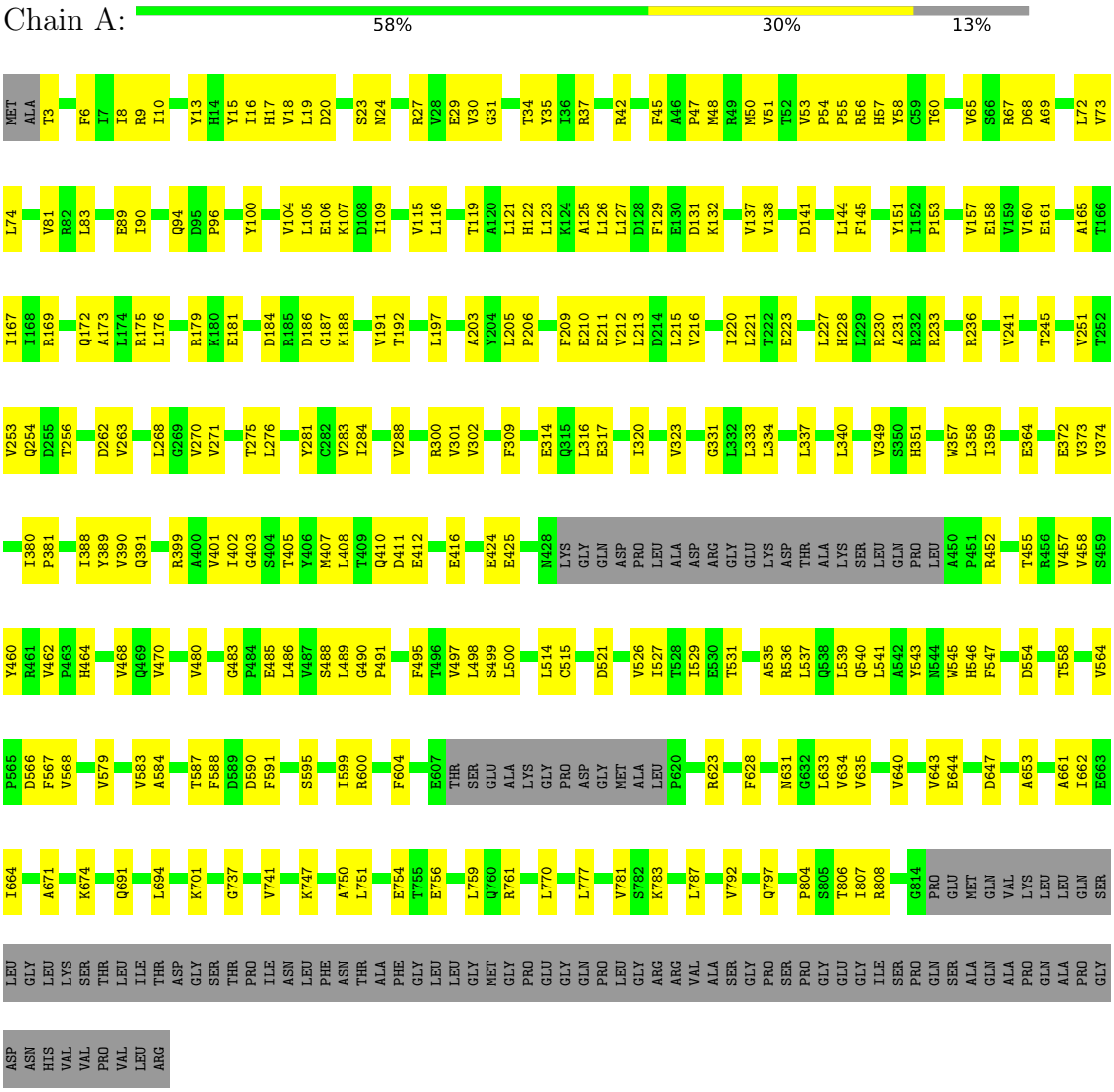
Mol	Chain	Residues	Atoms					AltConf	Trace
1	TA	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	TB	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	UA	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	UB	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	V	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	VA	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	VB	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	W	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	WA	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	WB	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	X	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	XA	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	XB	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	Y	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	YA	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	YB	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	Z	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	ZA	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0
1	ZB	779	Total 6181	C 3890	N 1105	O 1176	S 10	0	0

3 Residue-property plots (i)

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.

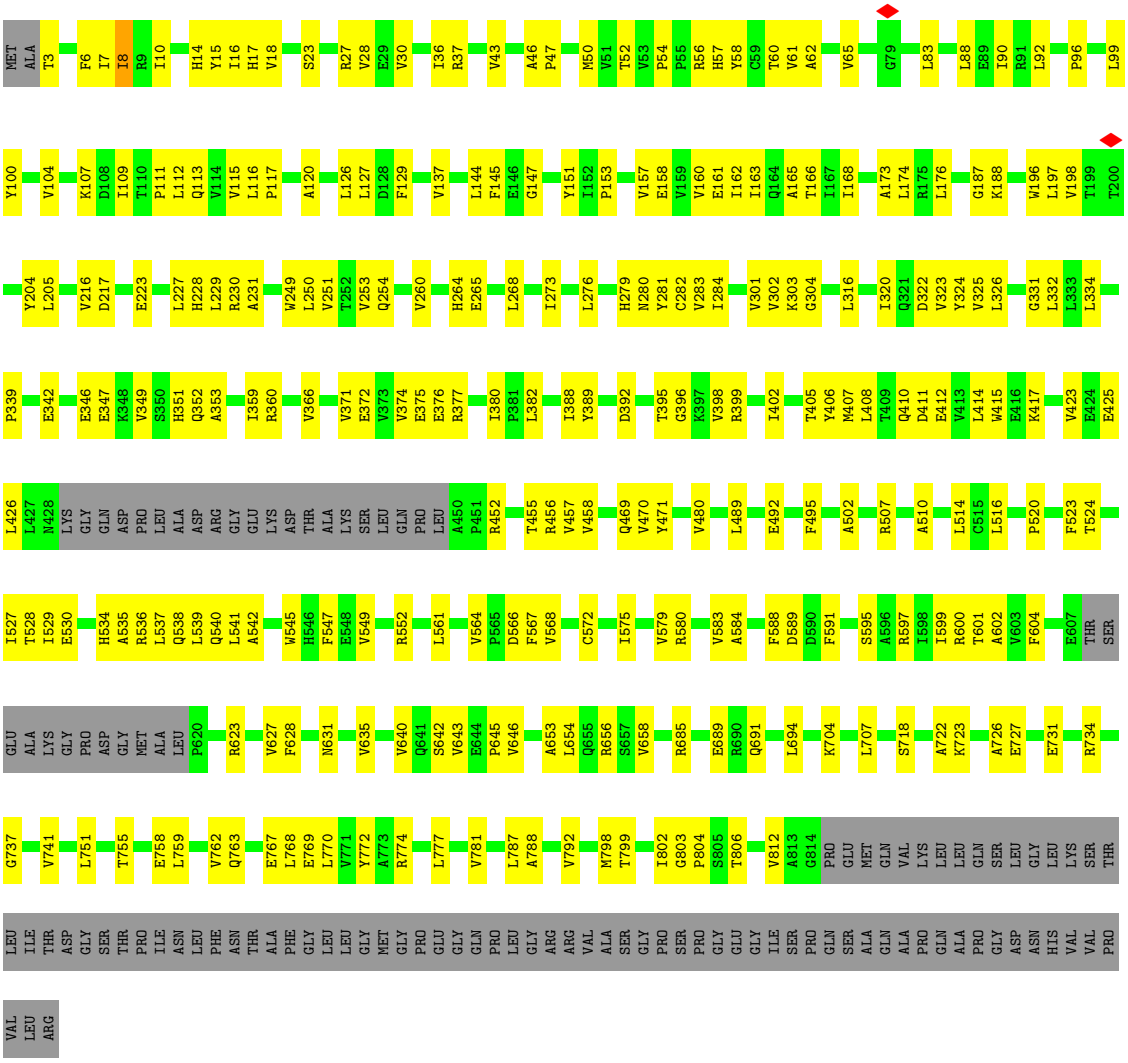
• Molecule 1: Major vault protein

Chain A:



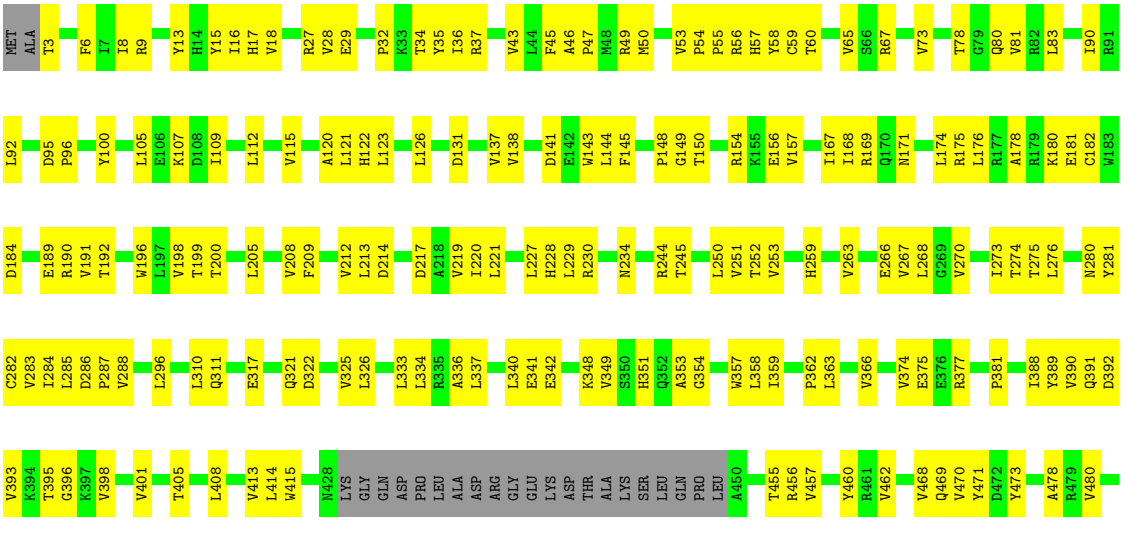
• Molecule 1: Major vault protein

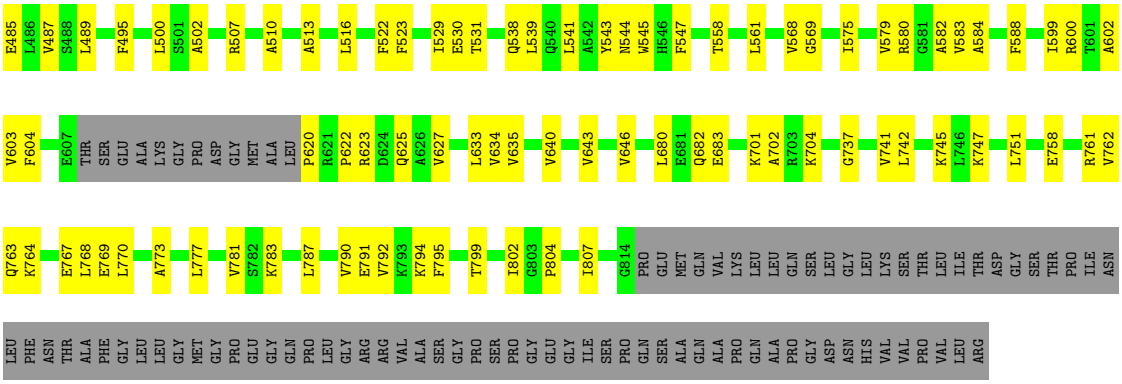
Chain AA:



• Molecule 1: Major vault protein

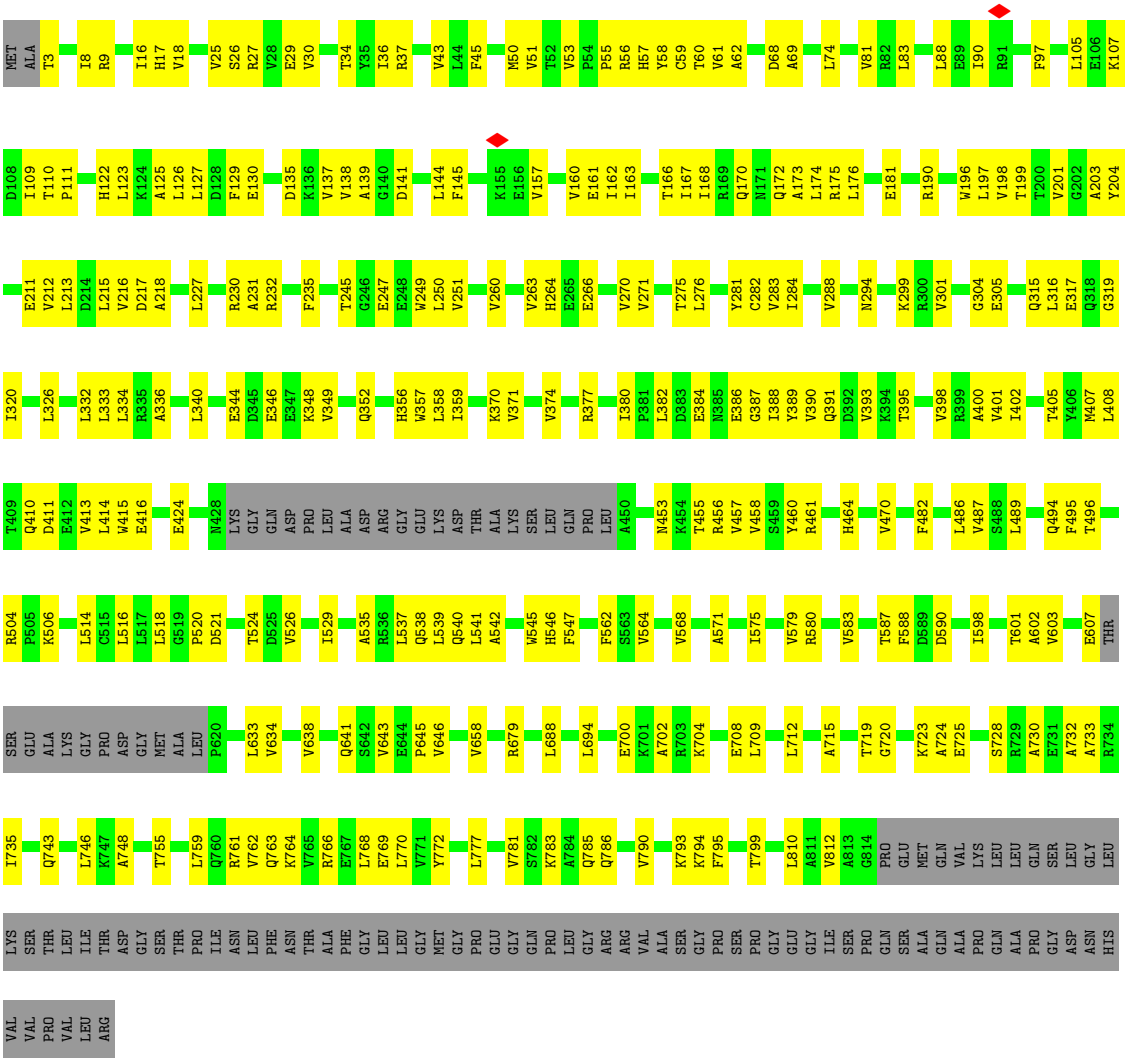
Chain AB:





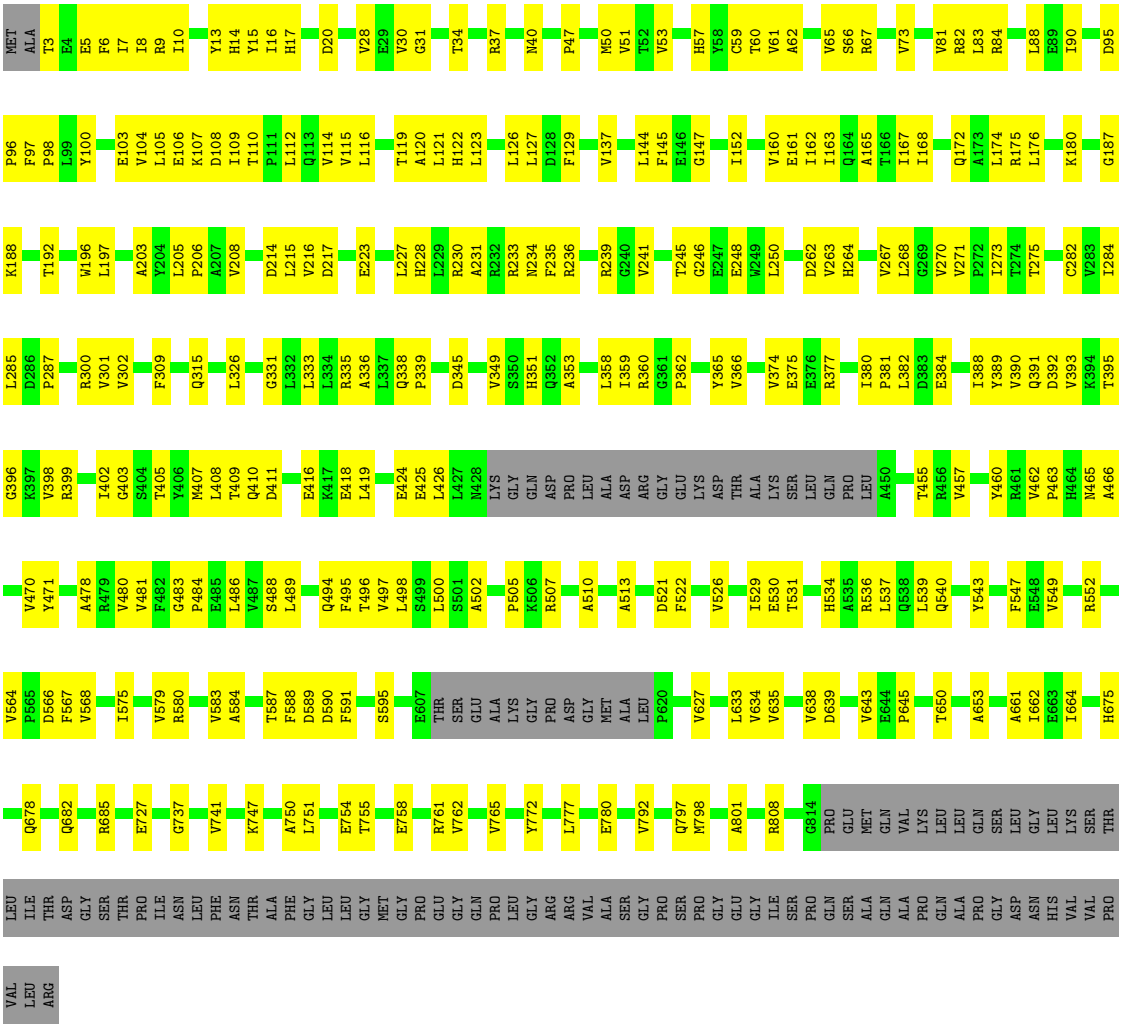
• Molecule 1: Major vault protein

Chain AC:



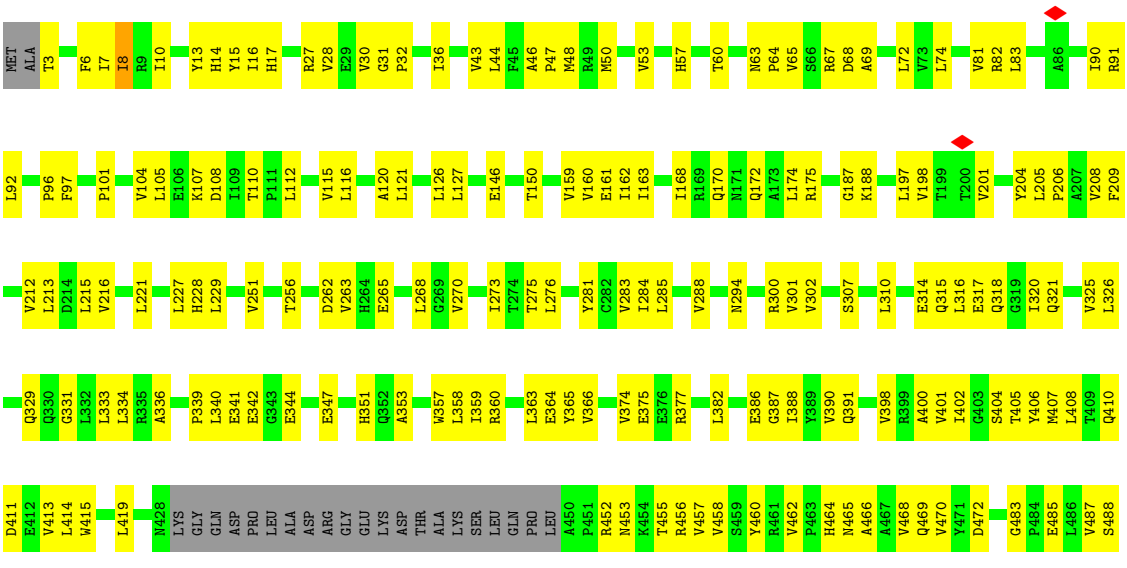
• Molecule 1: Major vault protein

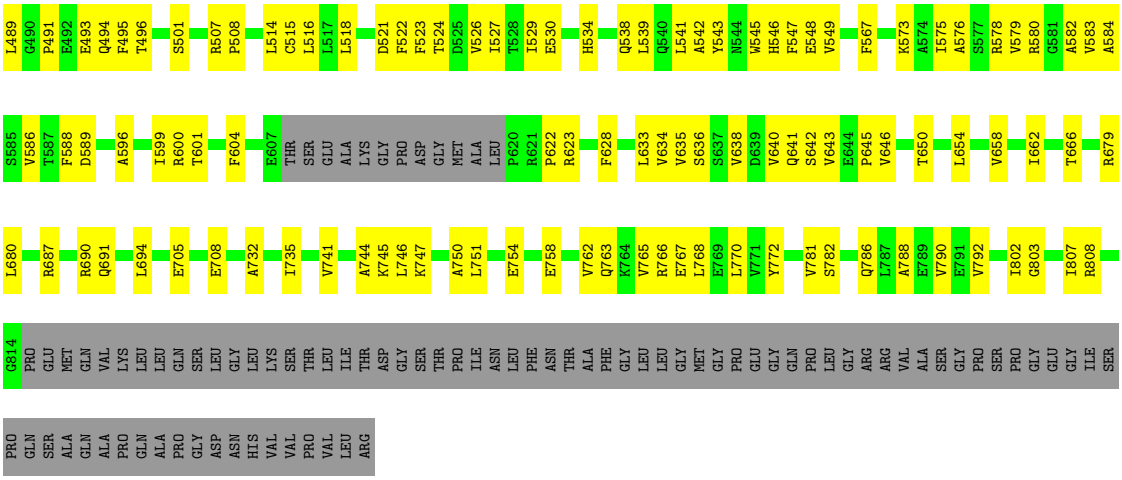
Chain B:



• Molecule 1: Major vault protein

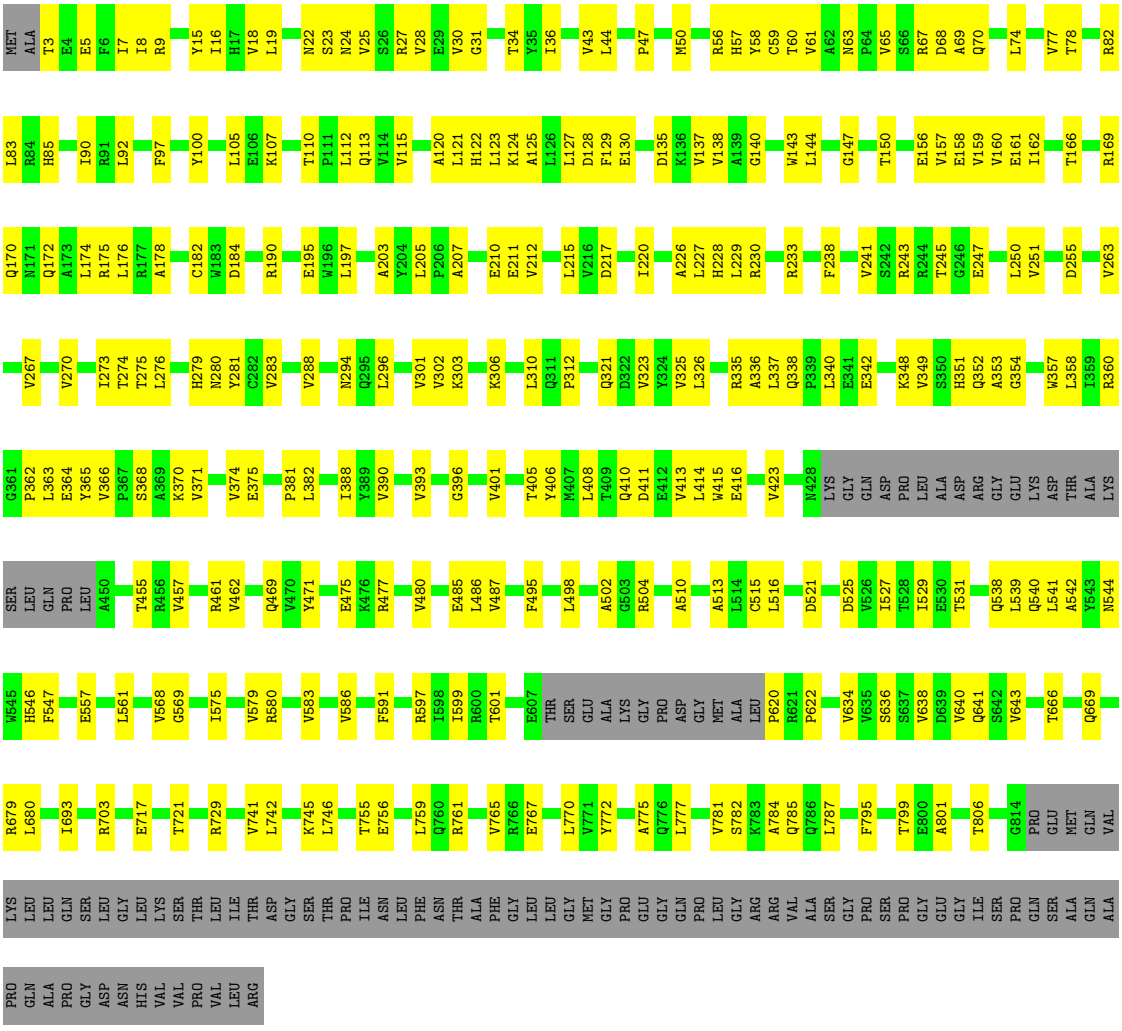
Chain BA:





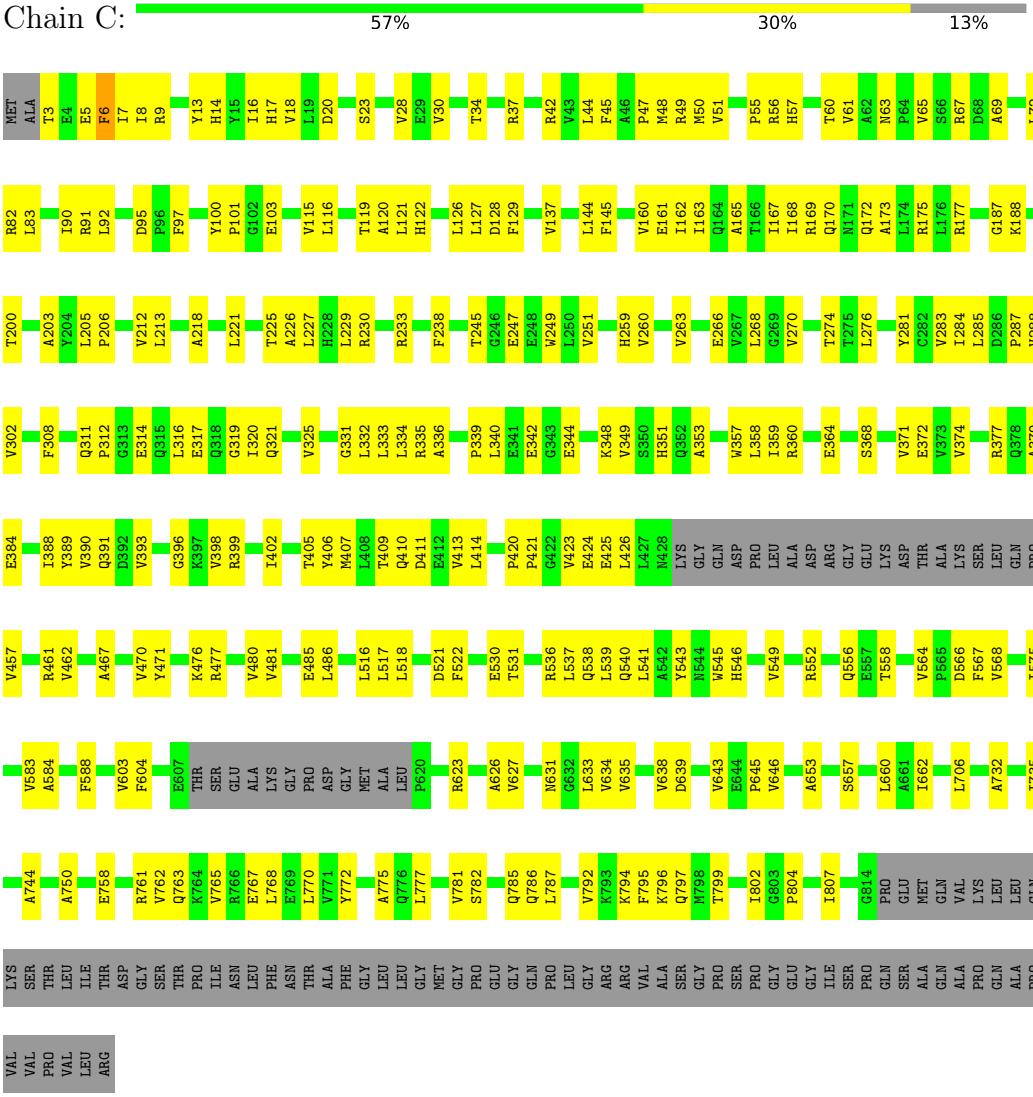
• Molecule 1: Major vault protein

Chain BB:



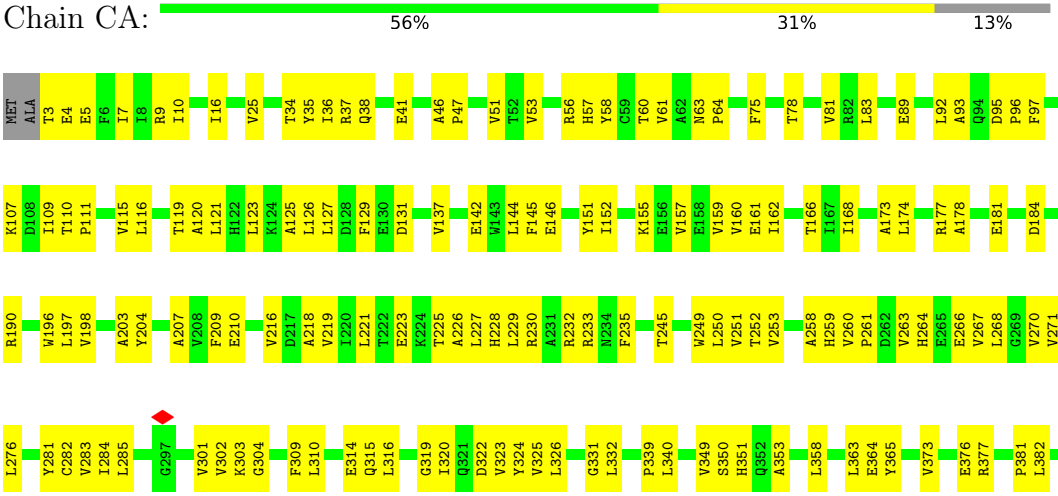
• Molecule 1: Major vault protein

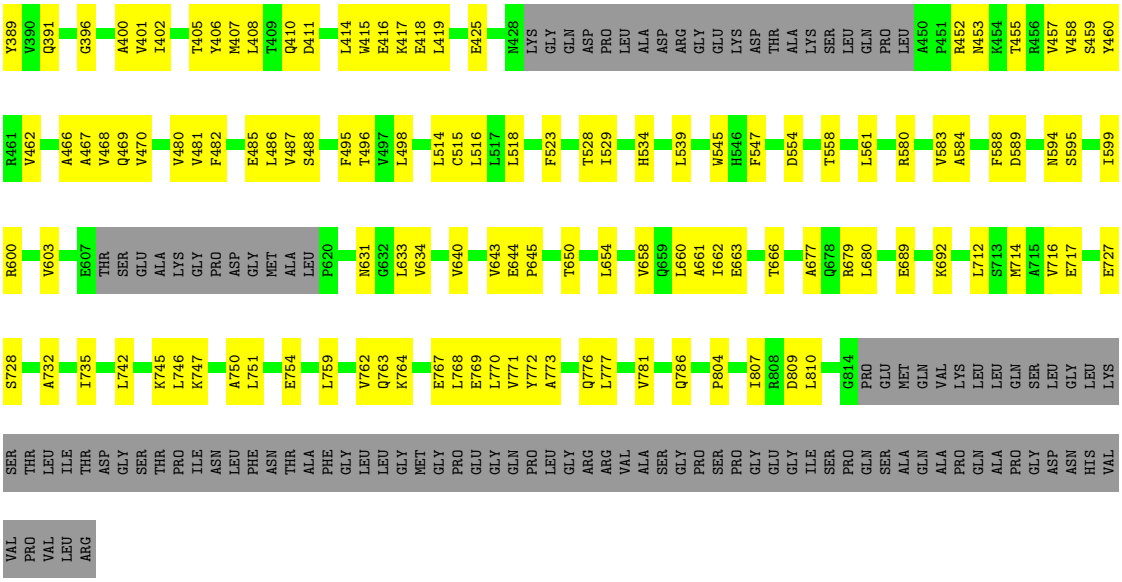
Chain C:



• Molecule 1: Major vault protein

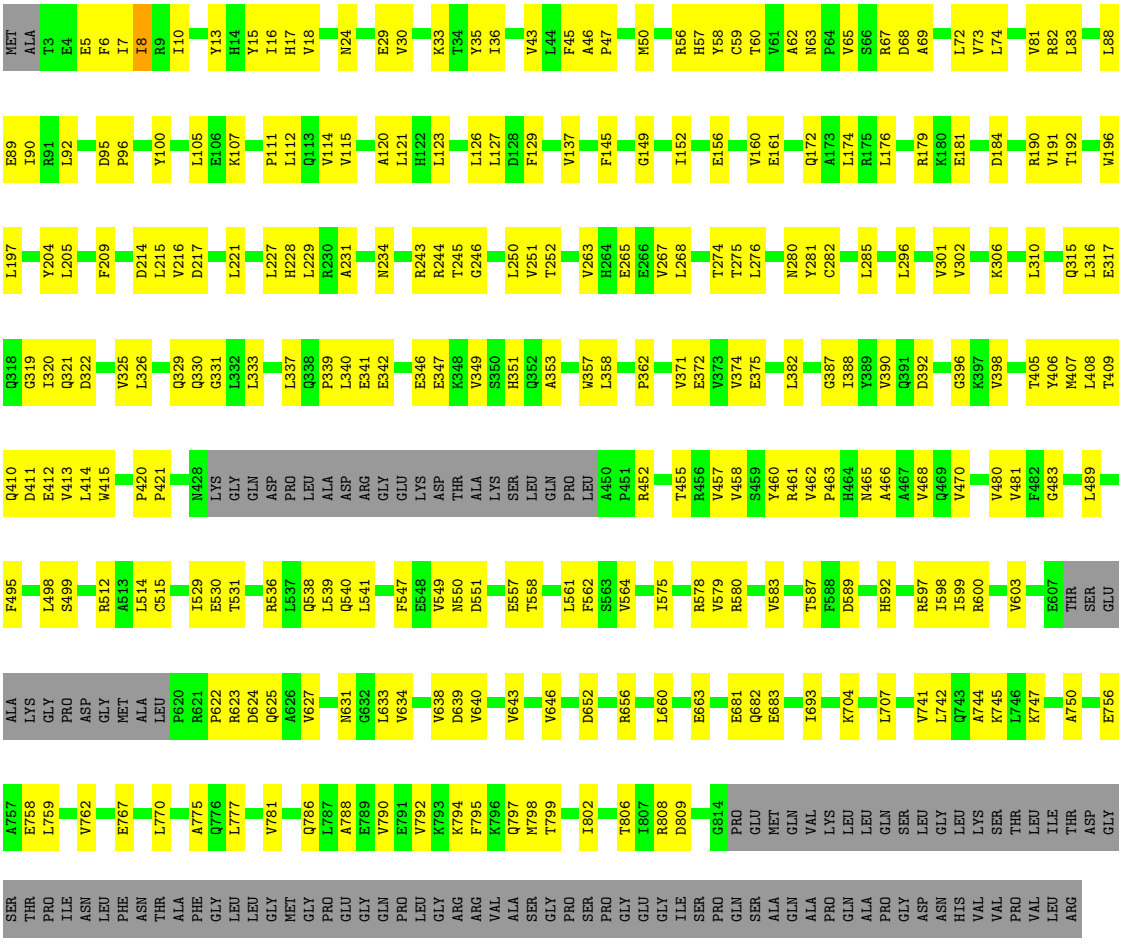
Chain CA:





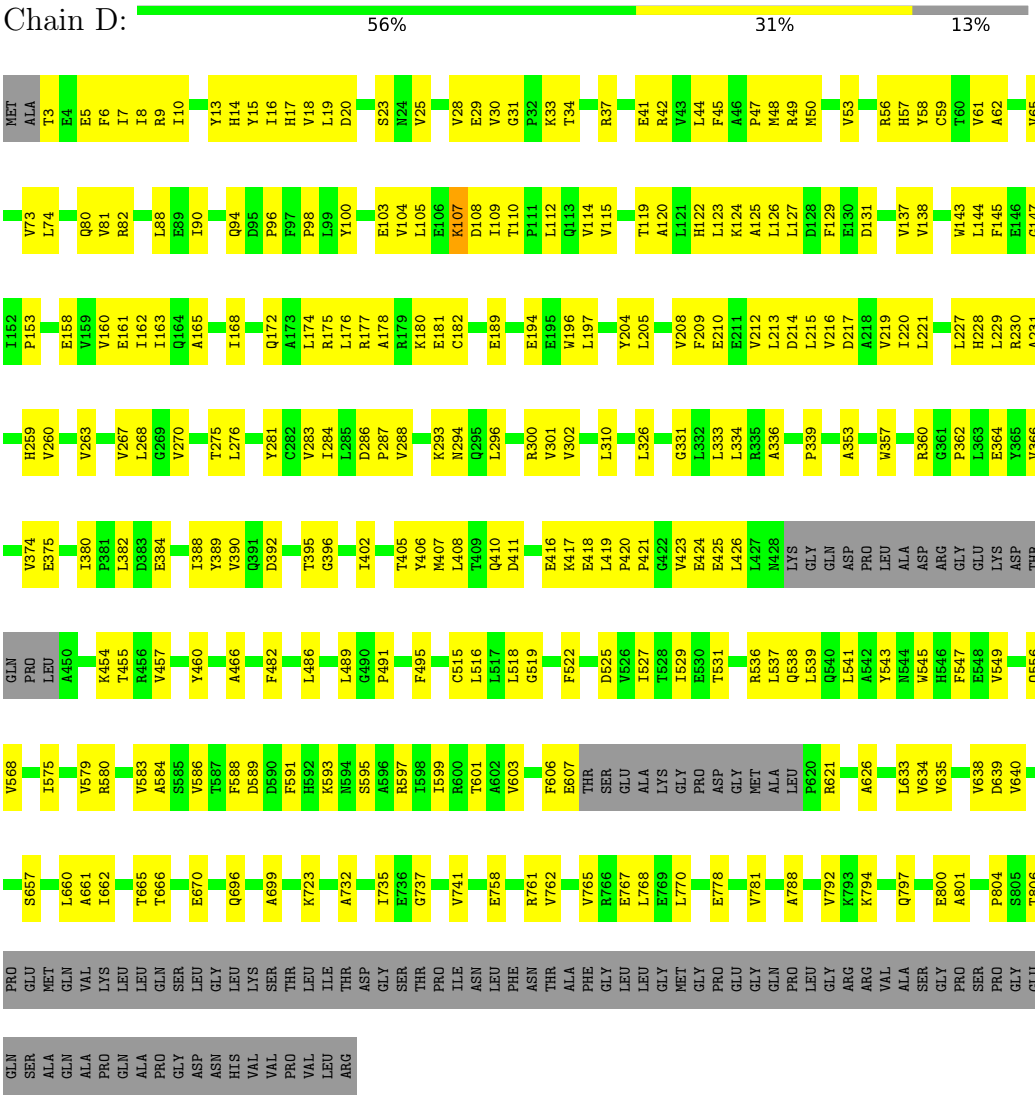
• Molecule 1: Major vault protein

Chain CB:



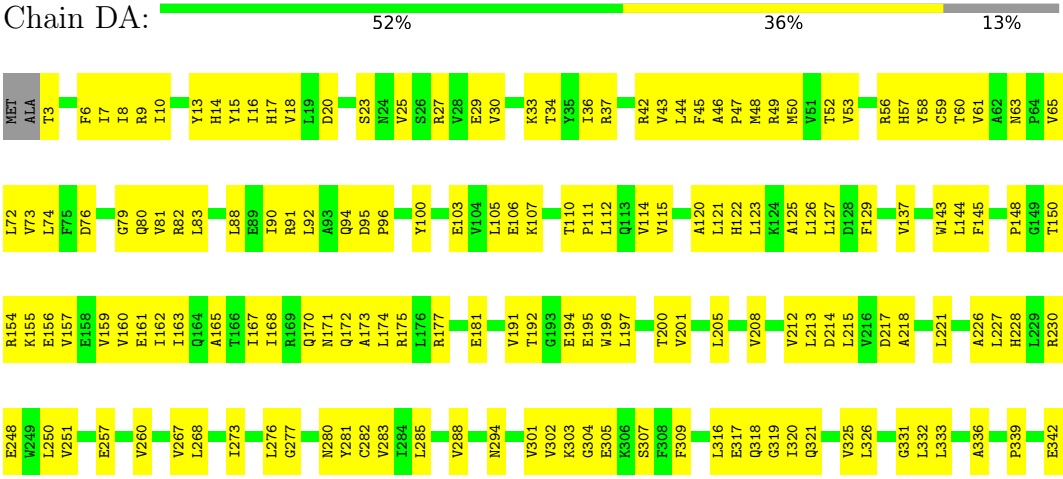
• Molecule 1: Major vault protein

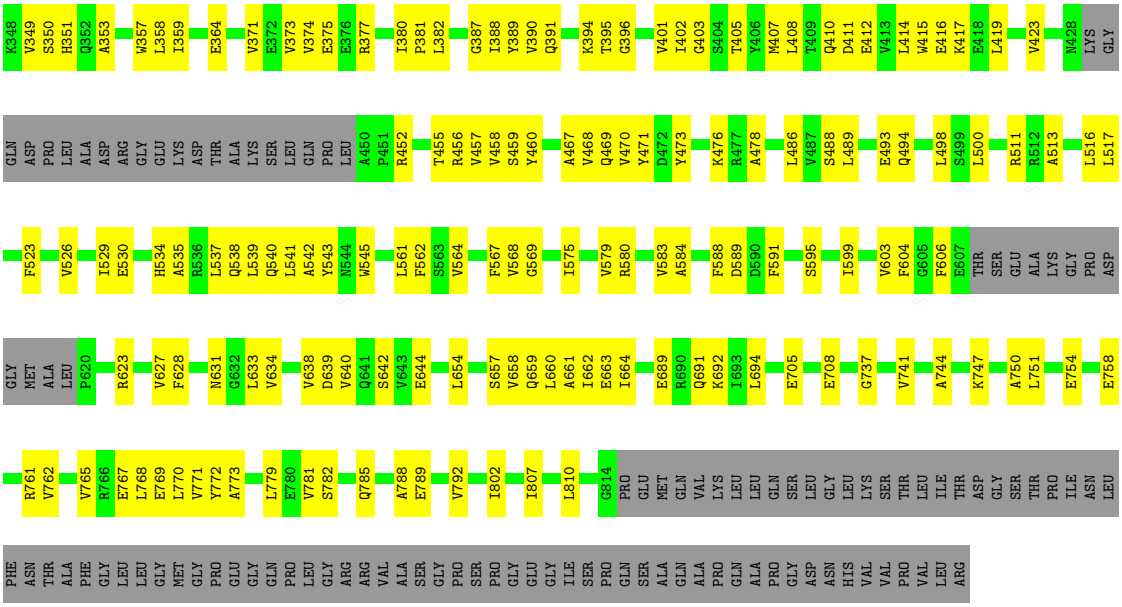
Chain D:



• Molecule 1: Major vault protein

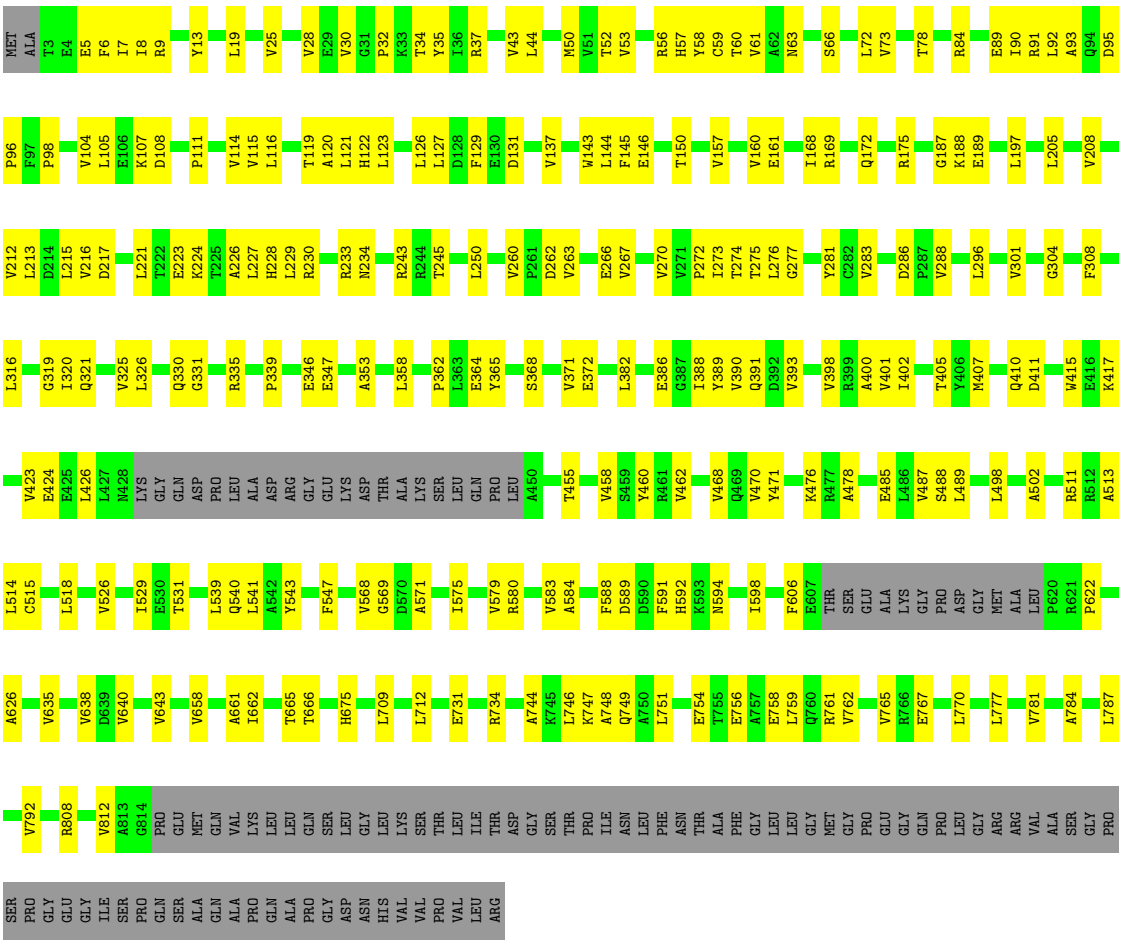
Chain DA:





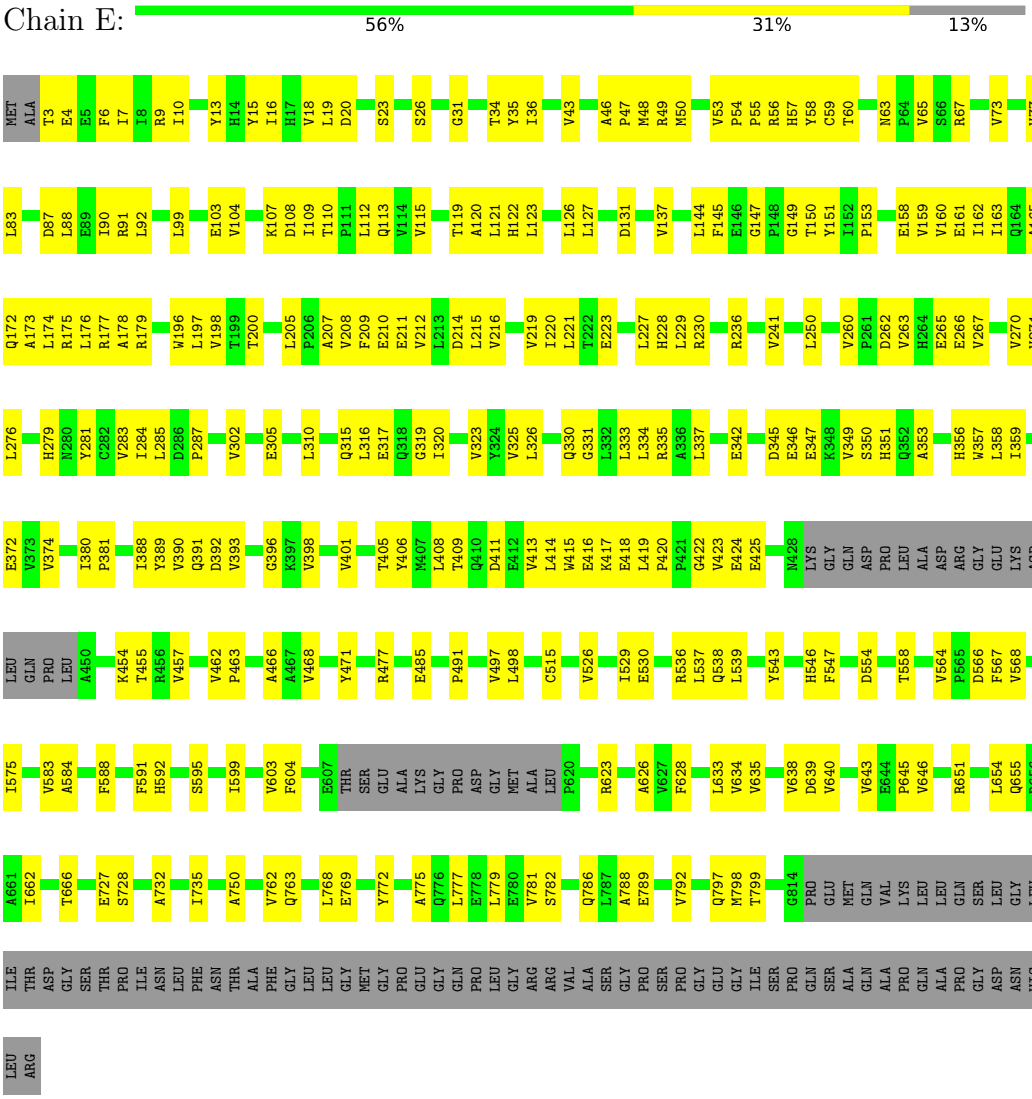
• Molecule 1: Major vault protein

Chain DB:



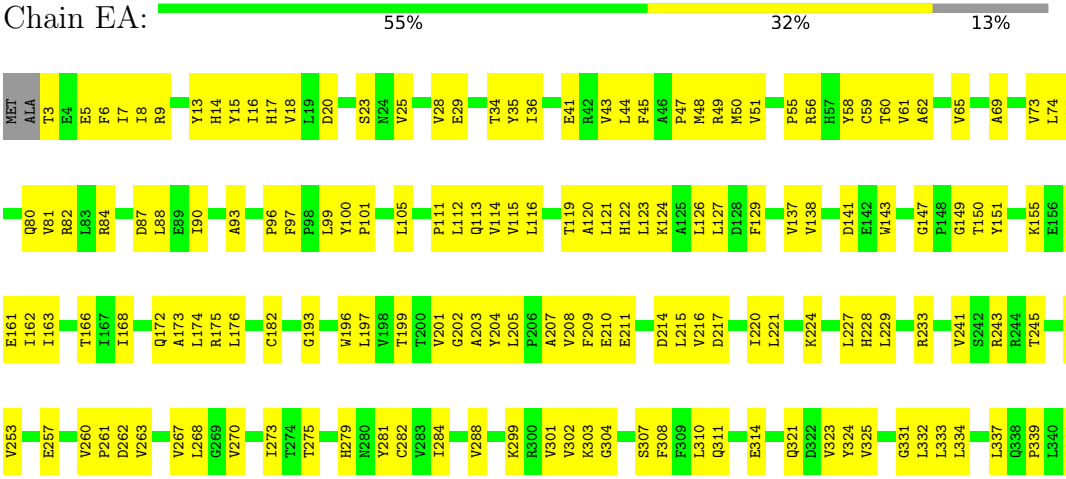
• Molecule 1: Major vault protein

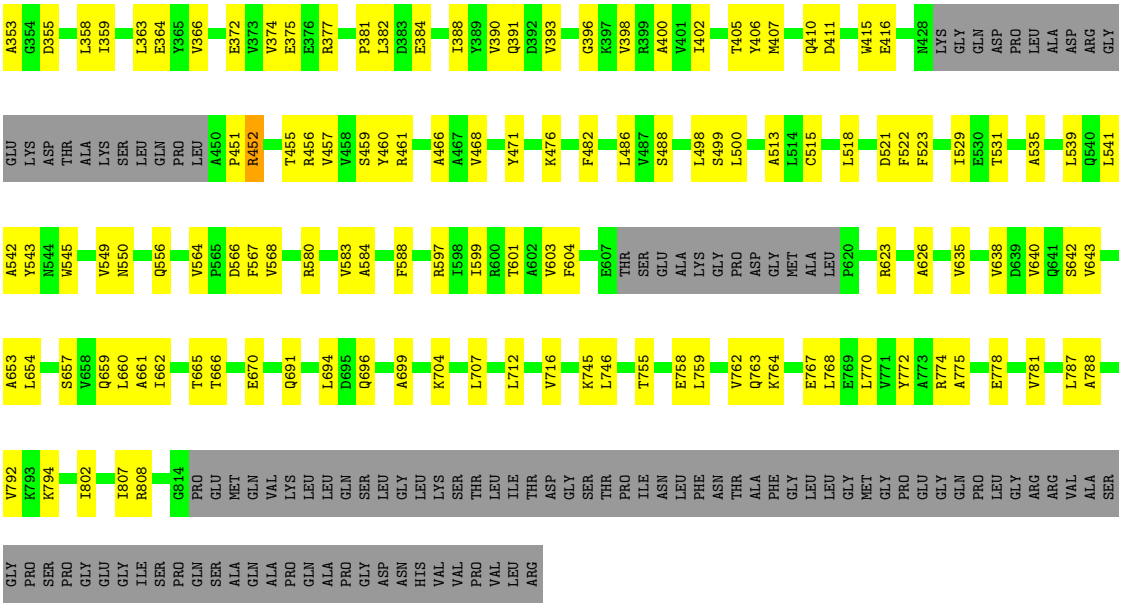
Chain E:



• Molecule 1: Major vault protein

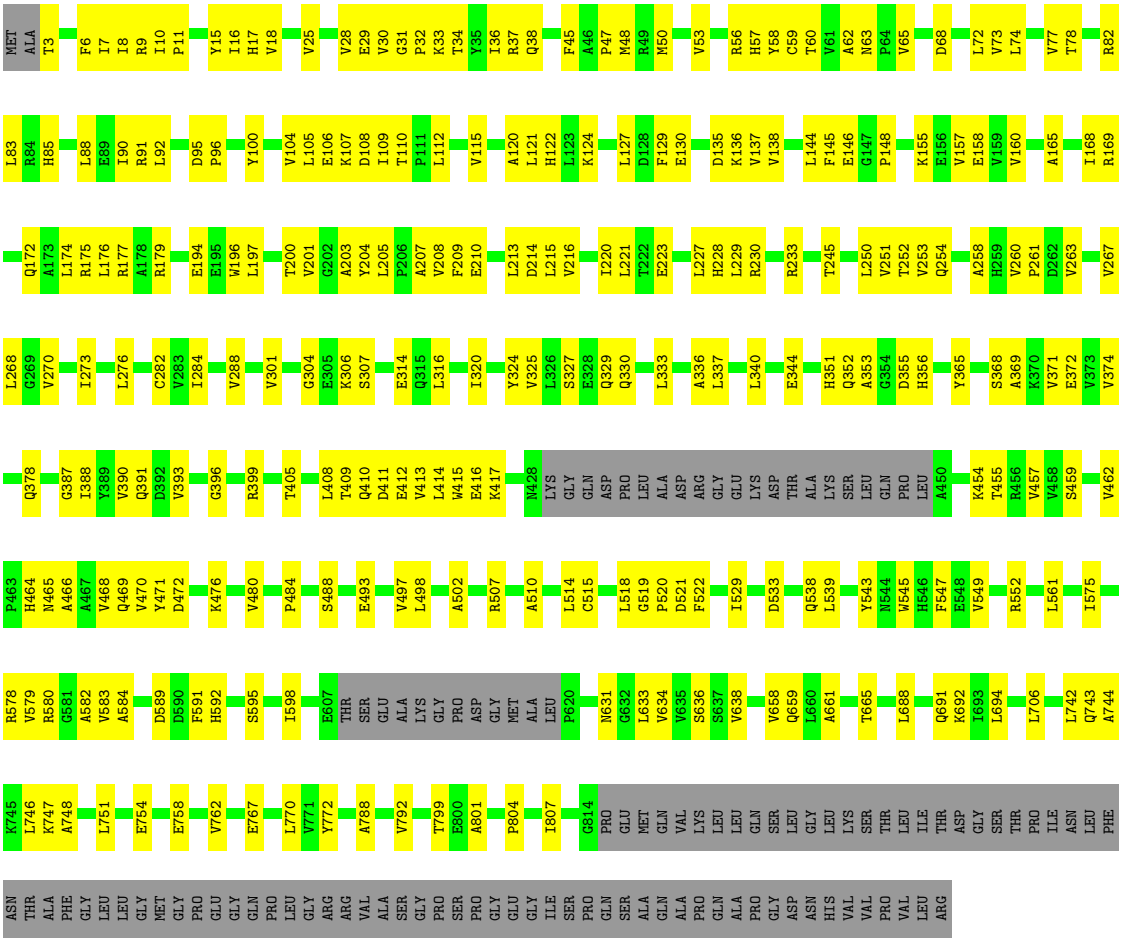
Chain EA:





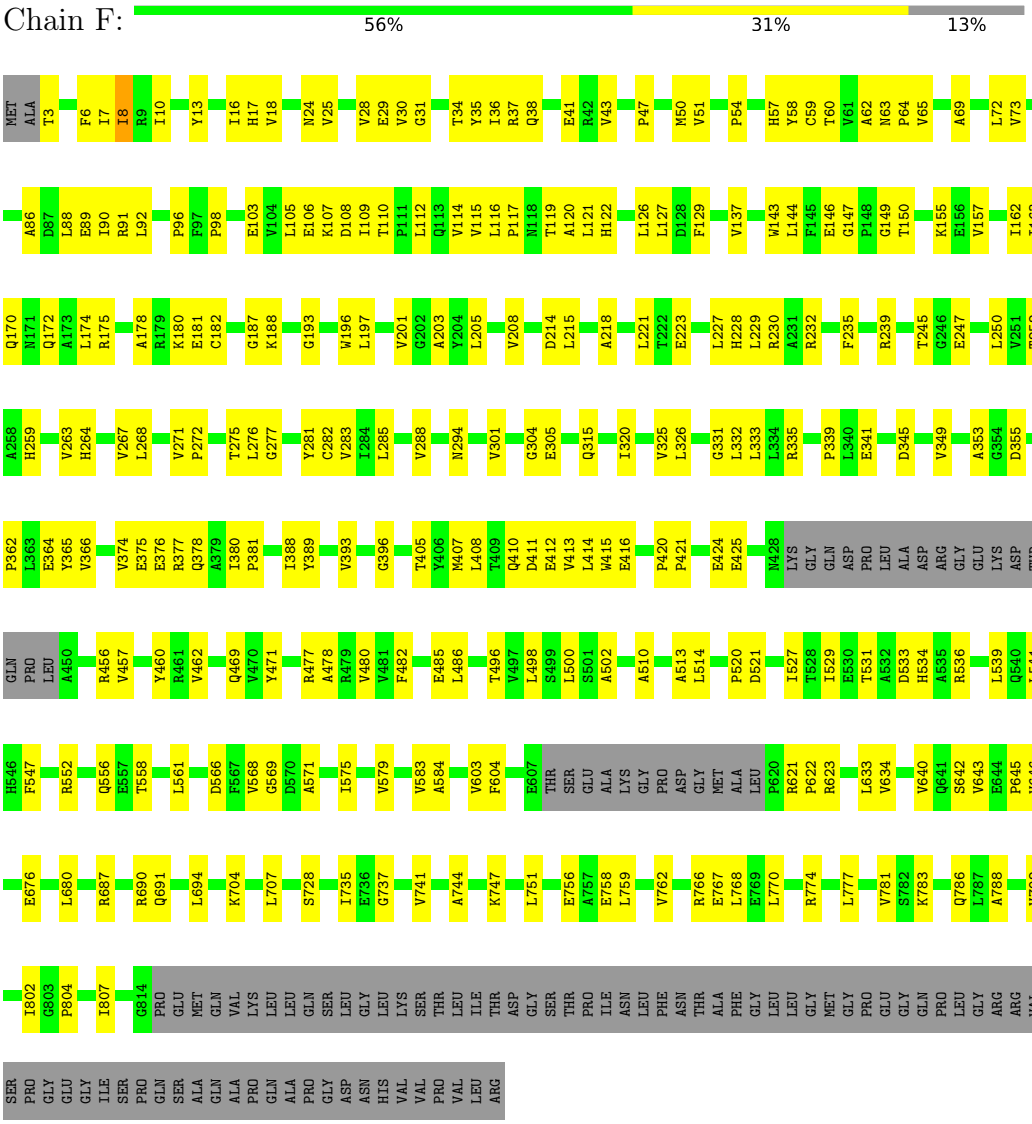
• Molecule 1: Major vault protein

Chain EB:



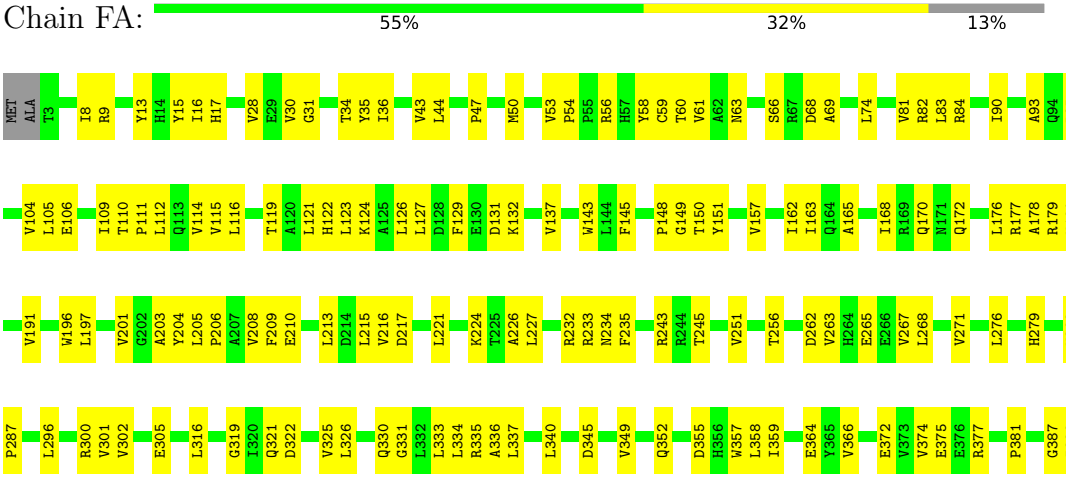
• Molecule 1: Major vault protein

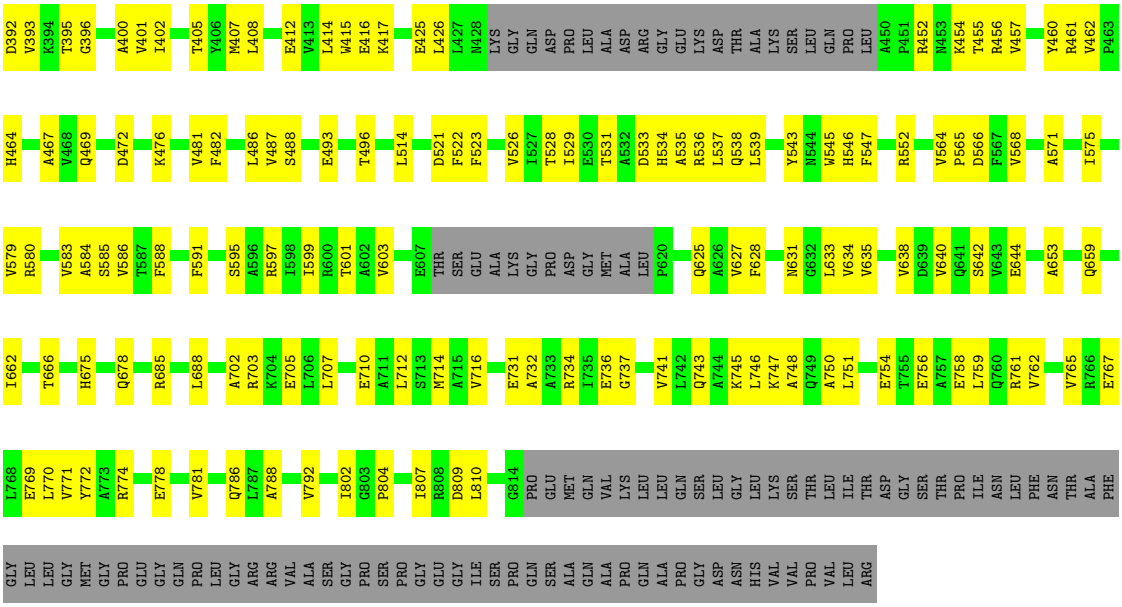
Chain F:



• Molecule 1: Major vault protein

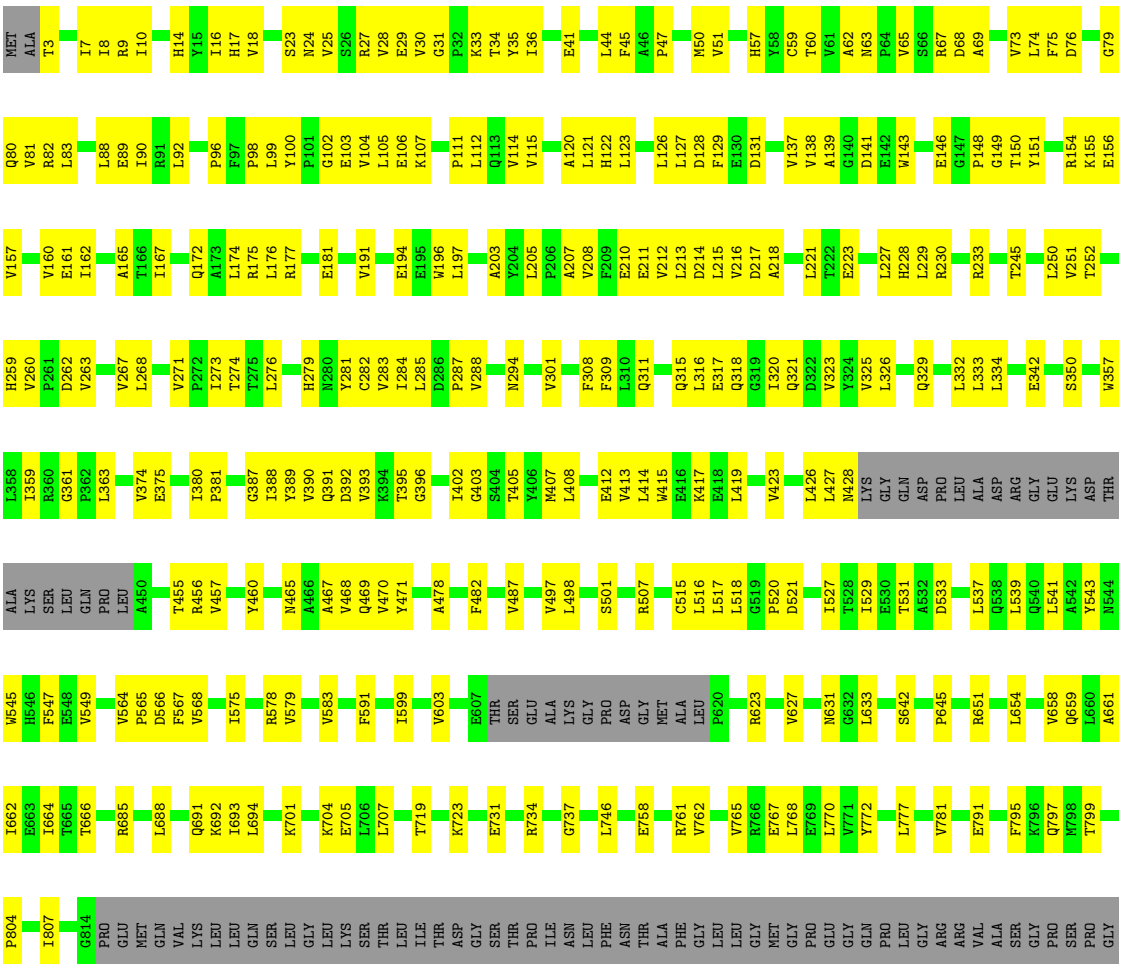
Chain FA:





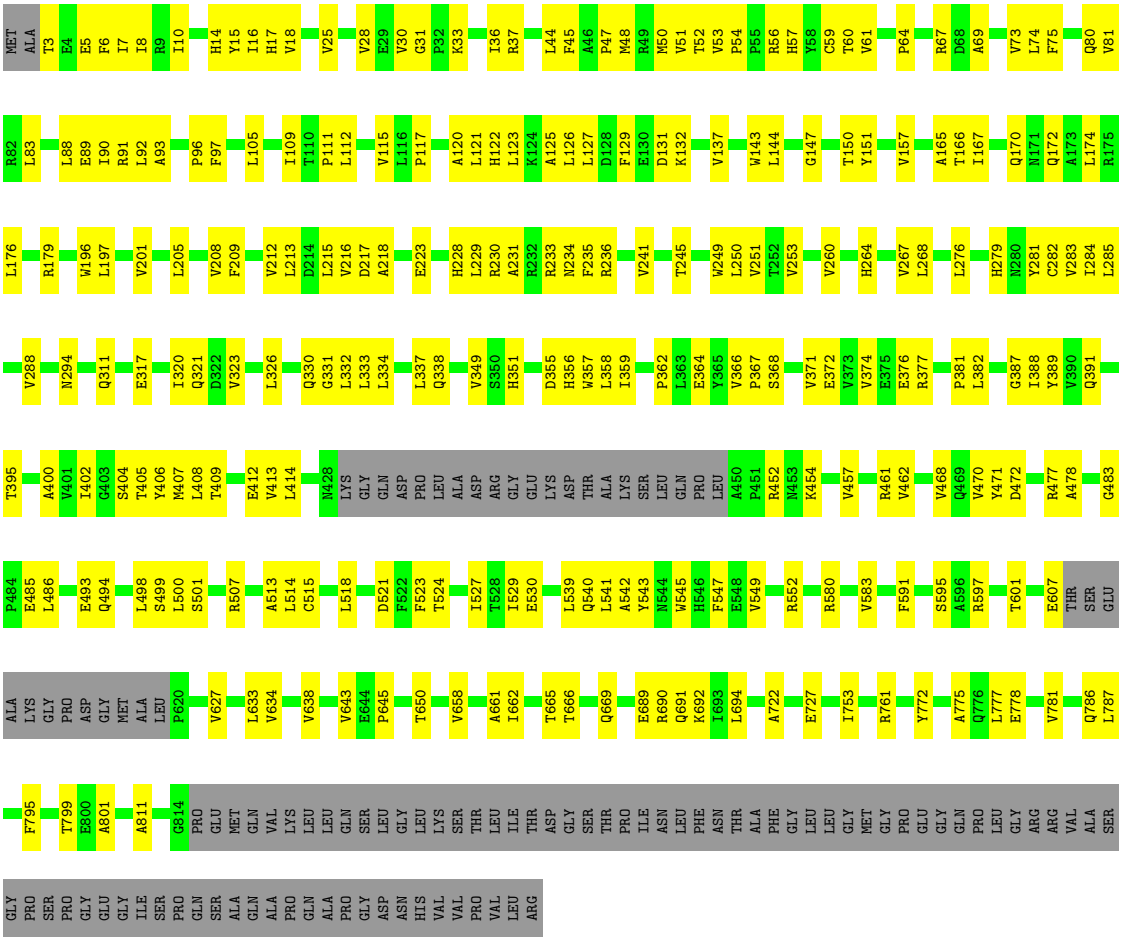
• Molecule 1: Major vault protein

Chain FB:



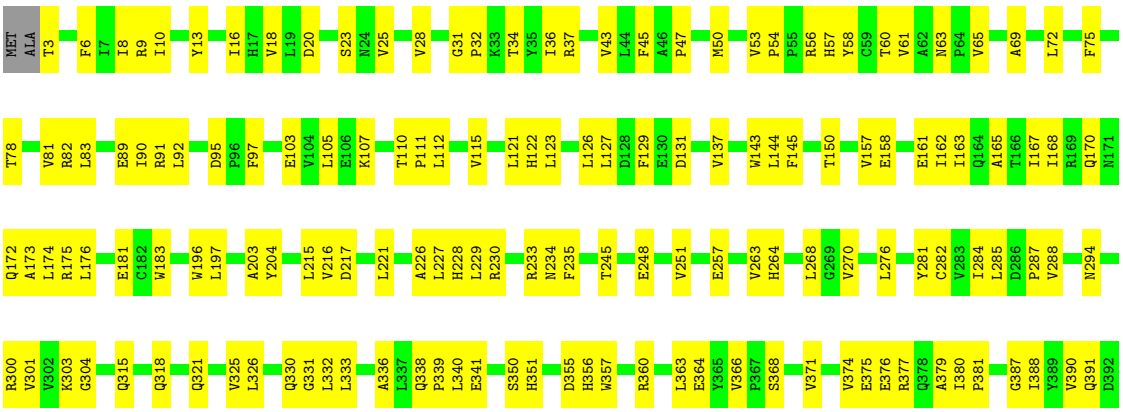
• Molecule 1: Major vault protein

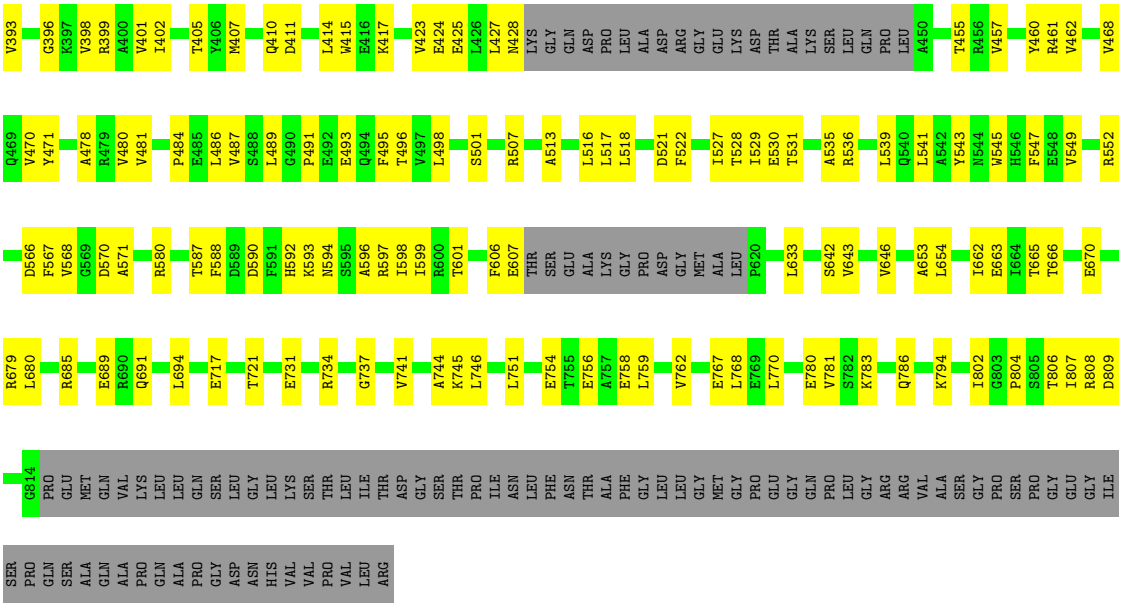
Chain G:



• Molecule 1: Major vault protein

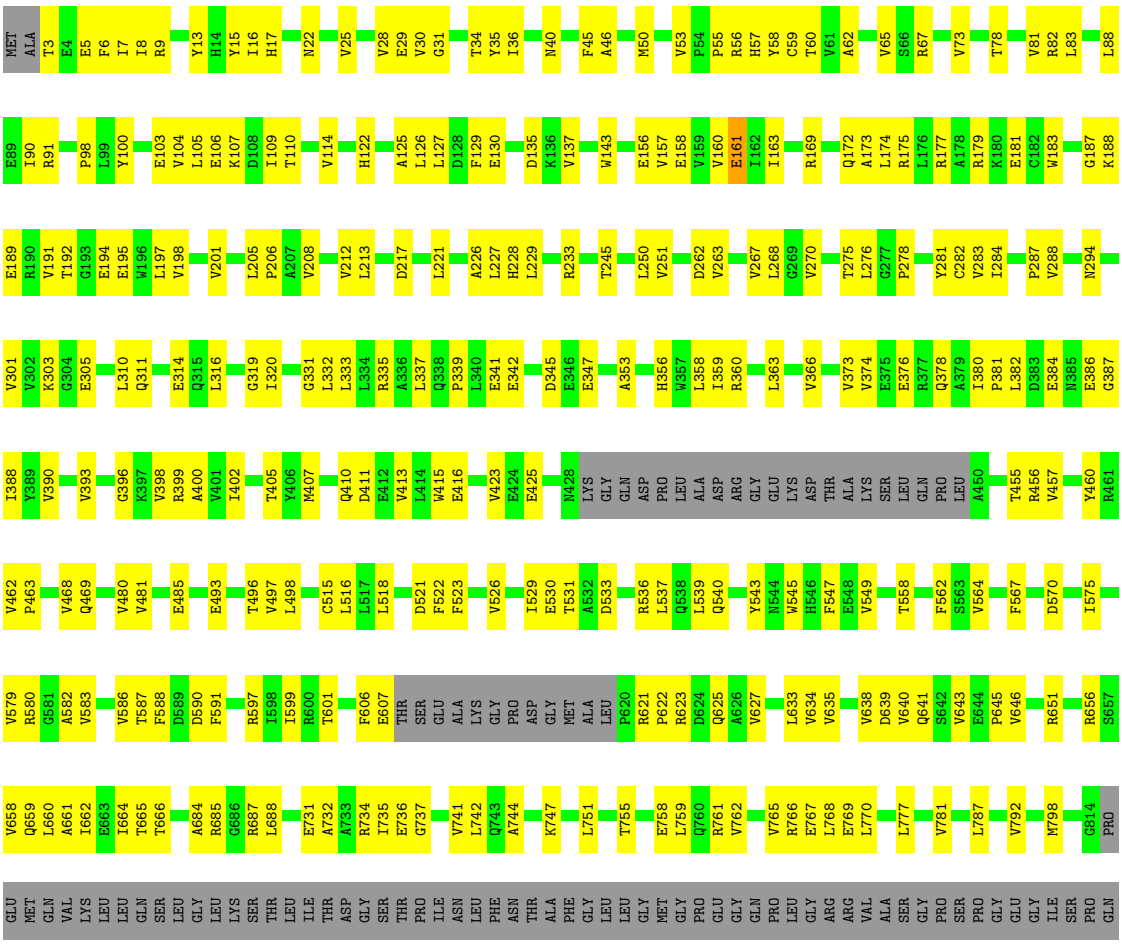
Chain GA:





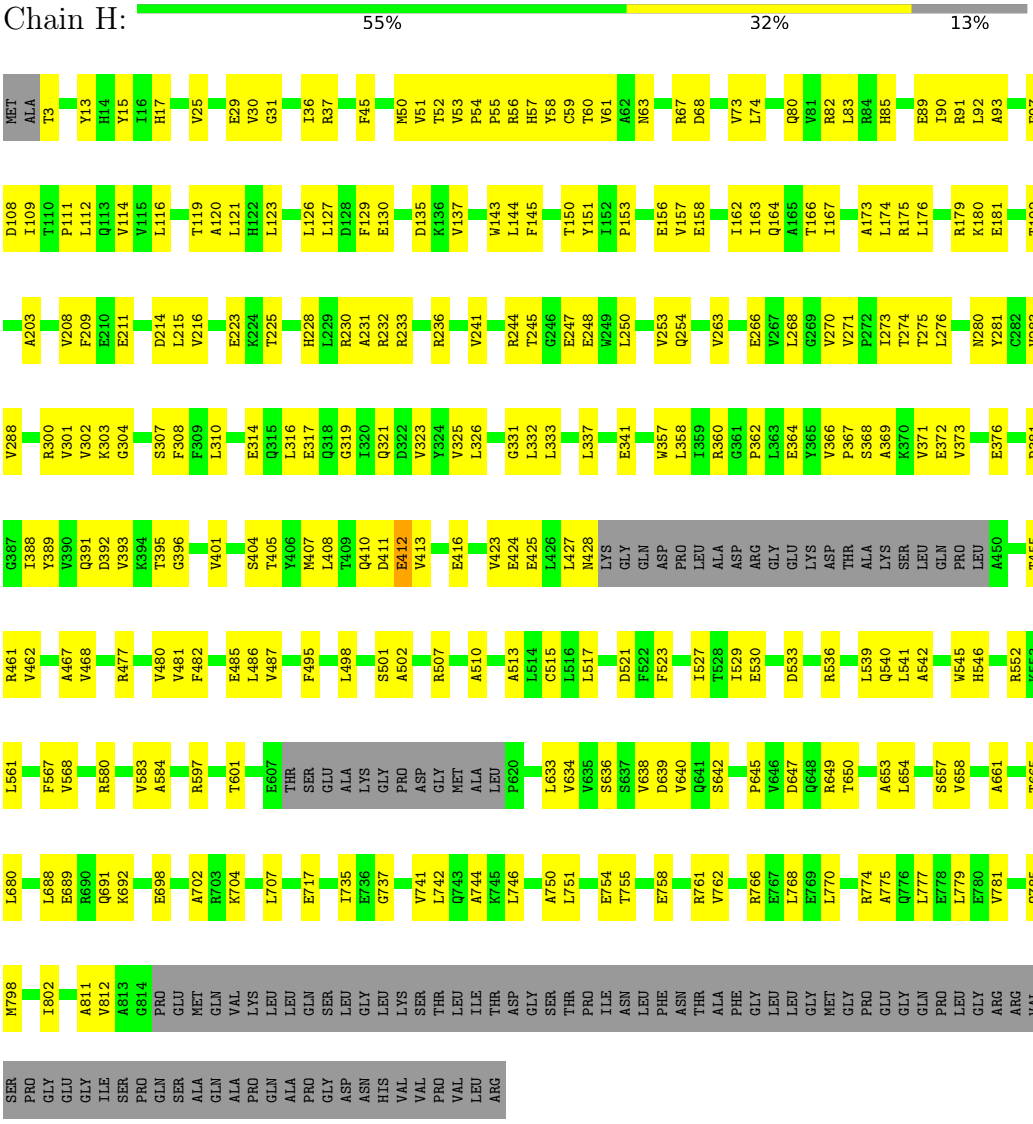
• Molecule 1: Major vault protein

Chain GB:



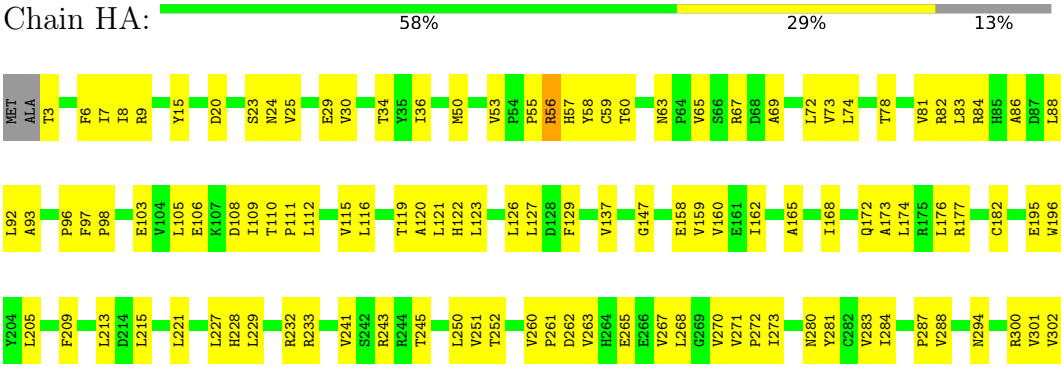
• Molecule 1: Major vault protein

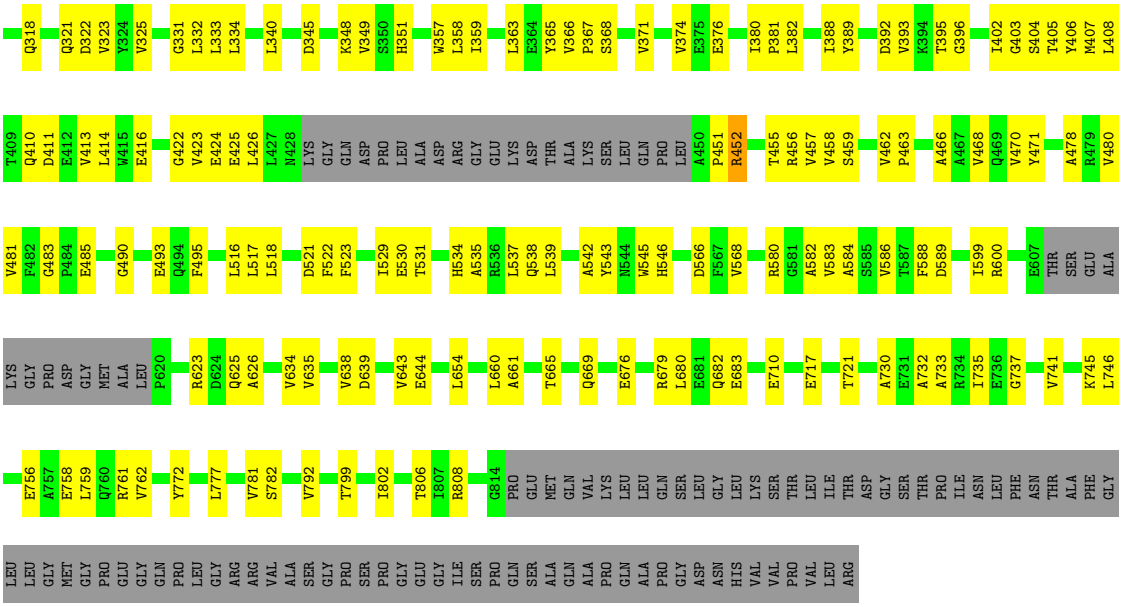
Chain H:



• Molecule 1: Major vault protein

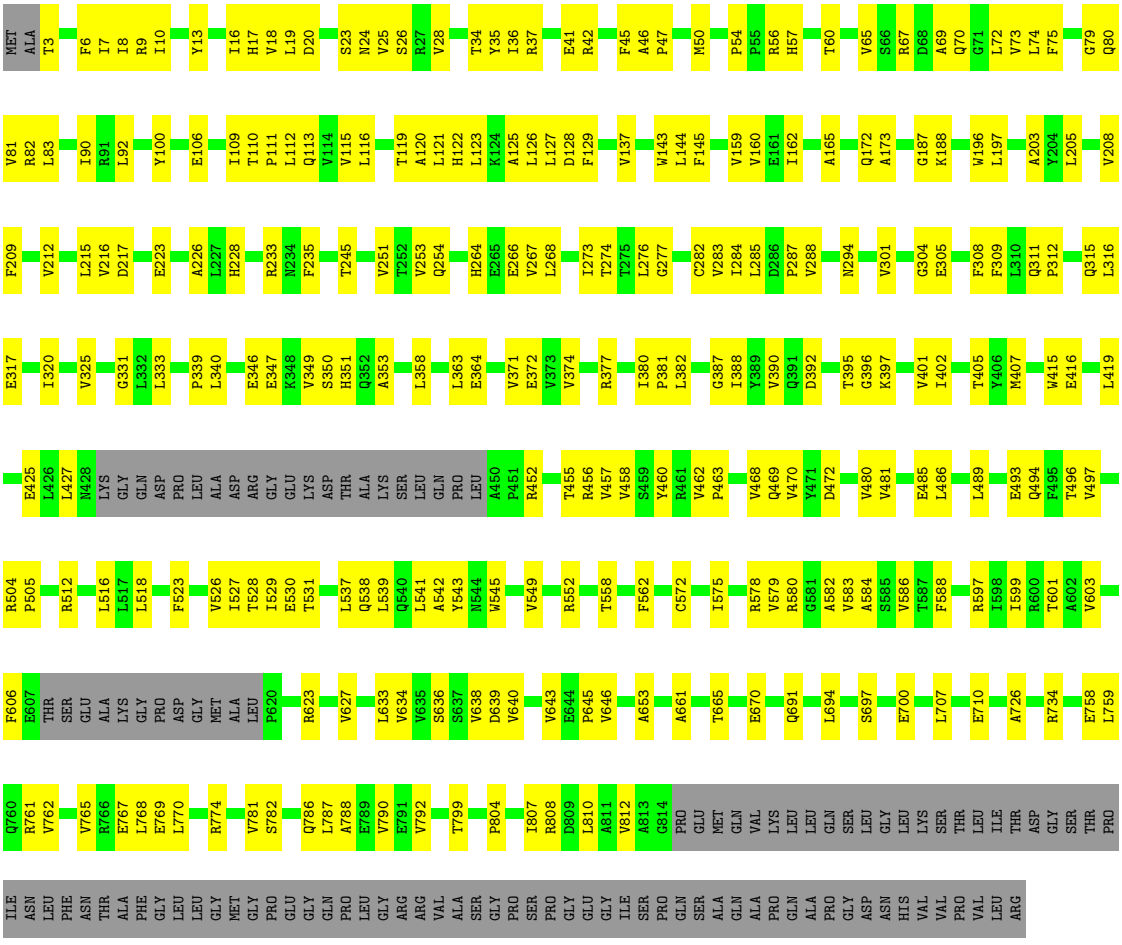
Chain HA:





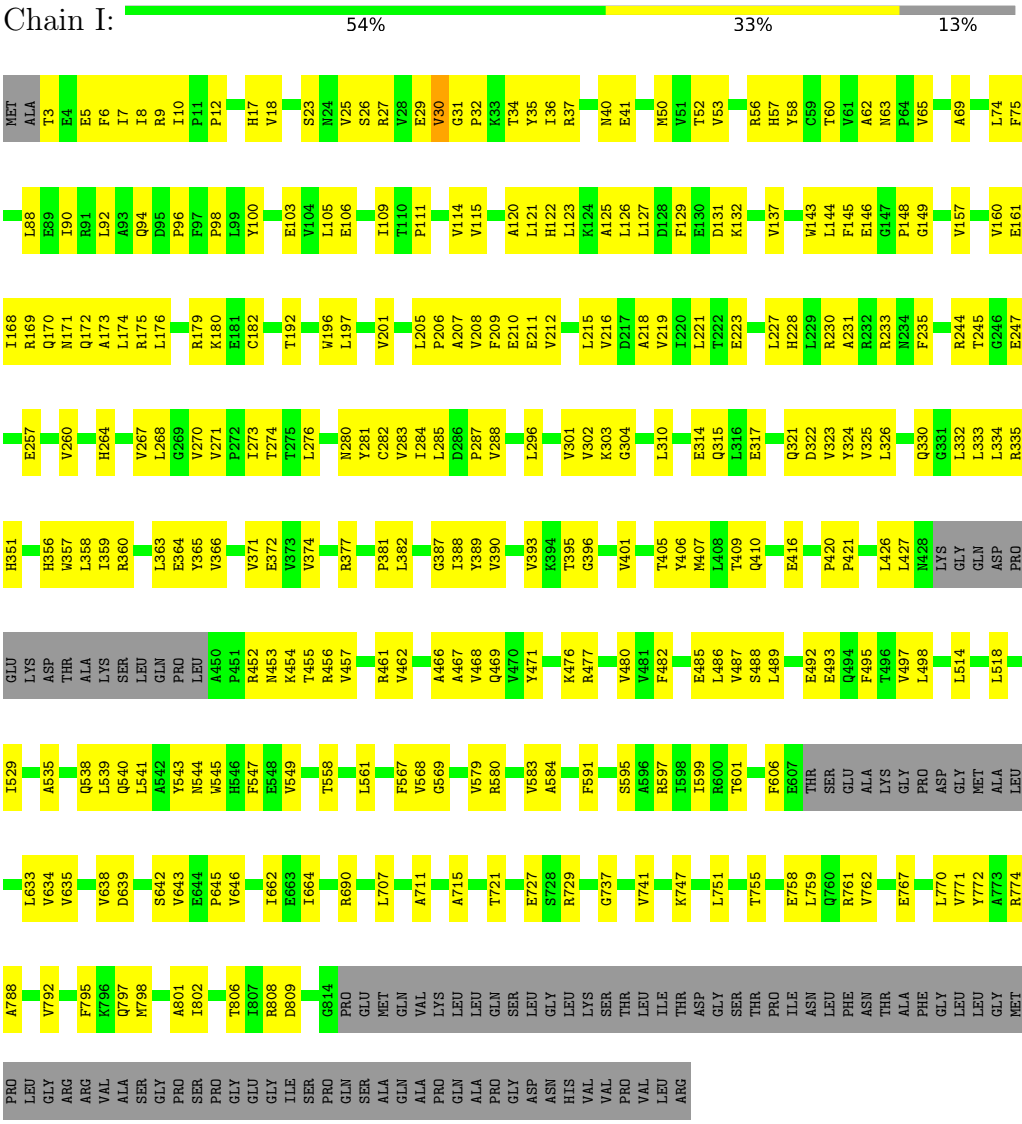
• Molecule 1: Major vault protein

Chain HB:



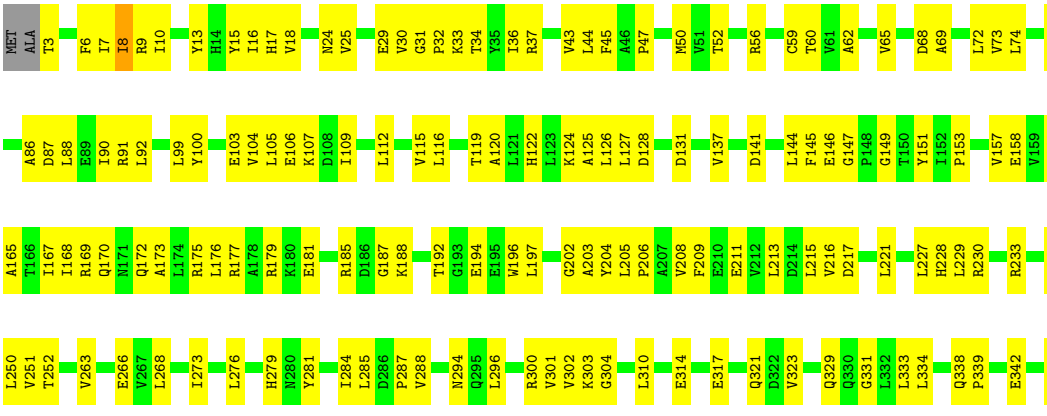
• Molecule 1: Major vault protein

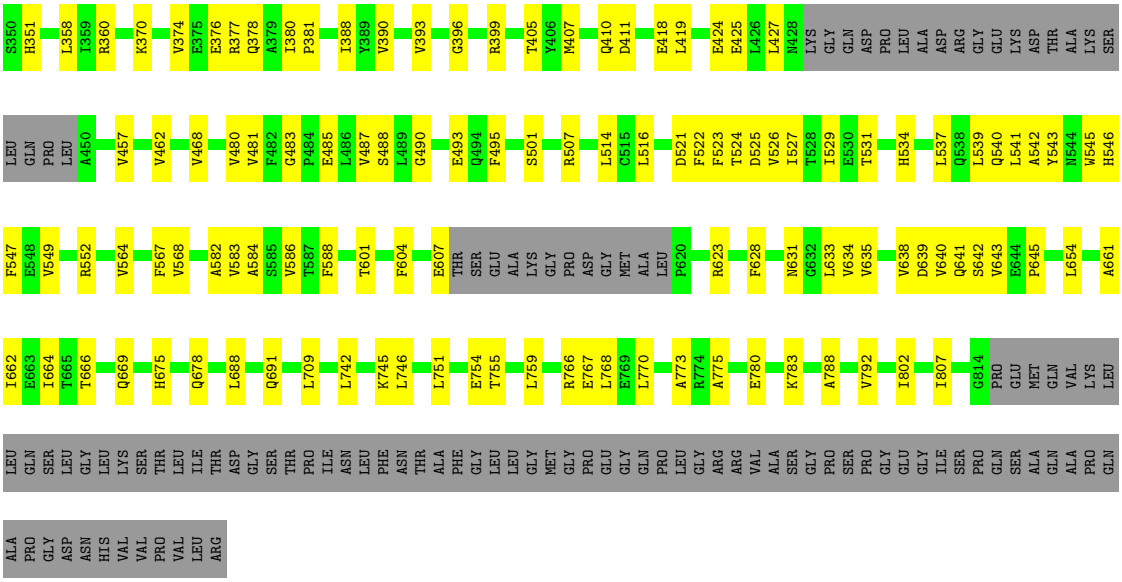
Chain I:



• Molecule 1: Major vault protein

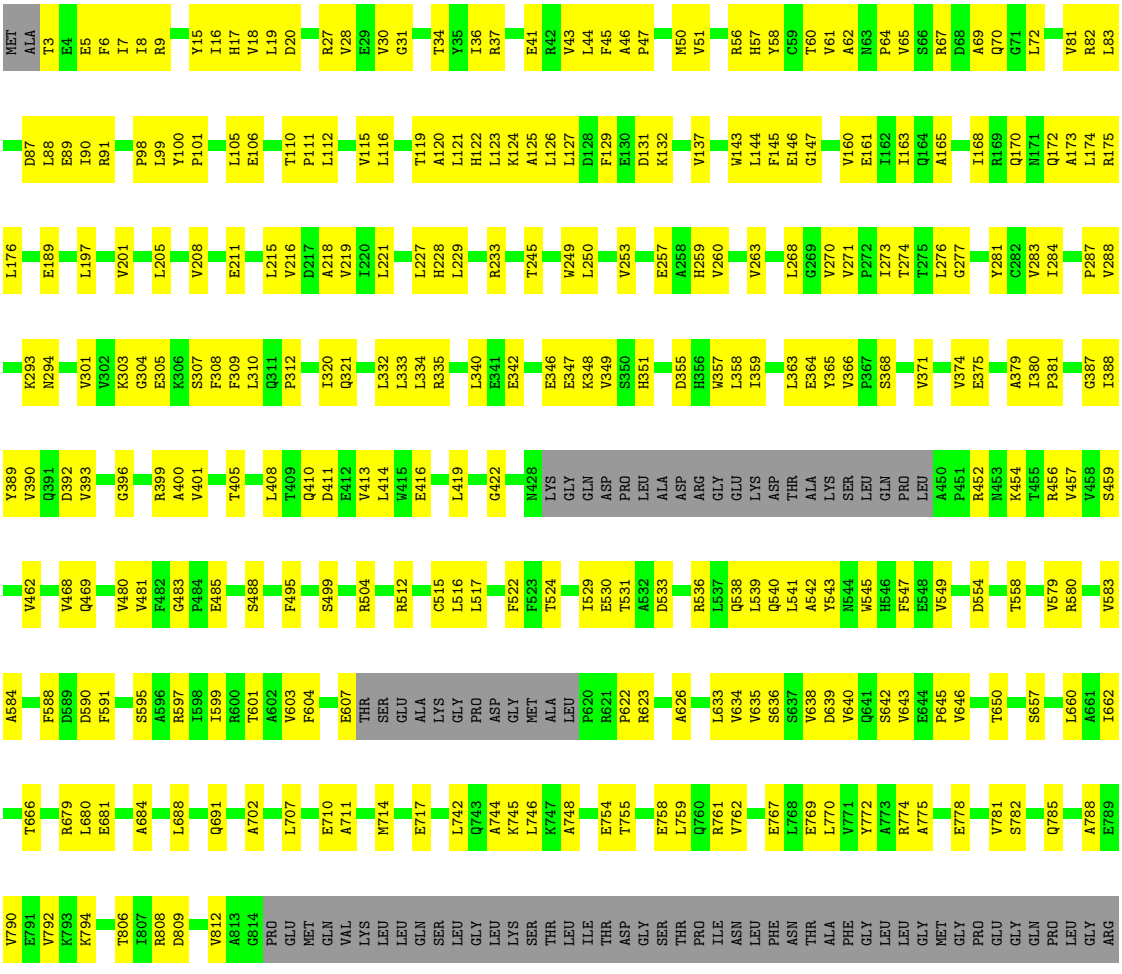
Chain IA:

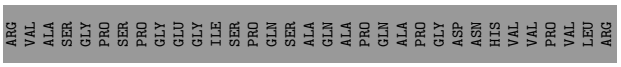




• Molecule 1: Major vault protein

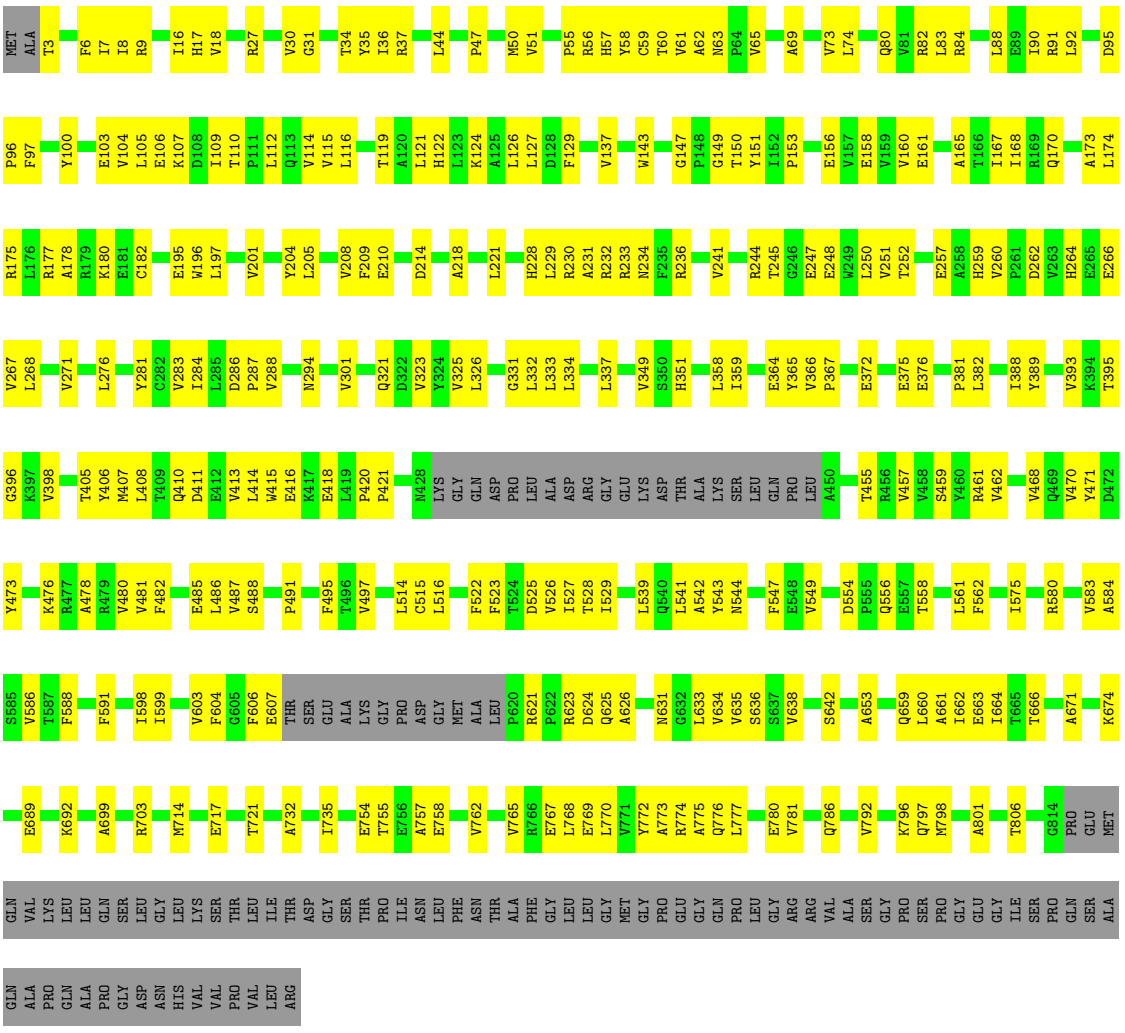
Chain IB:





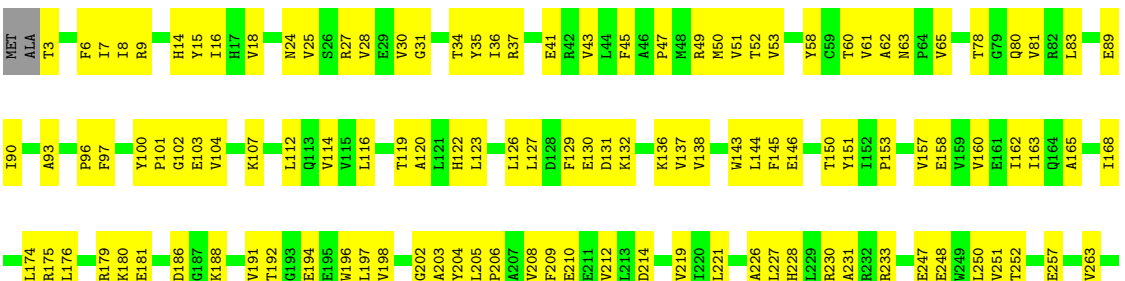
• Molecule 1: Major vault protein

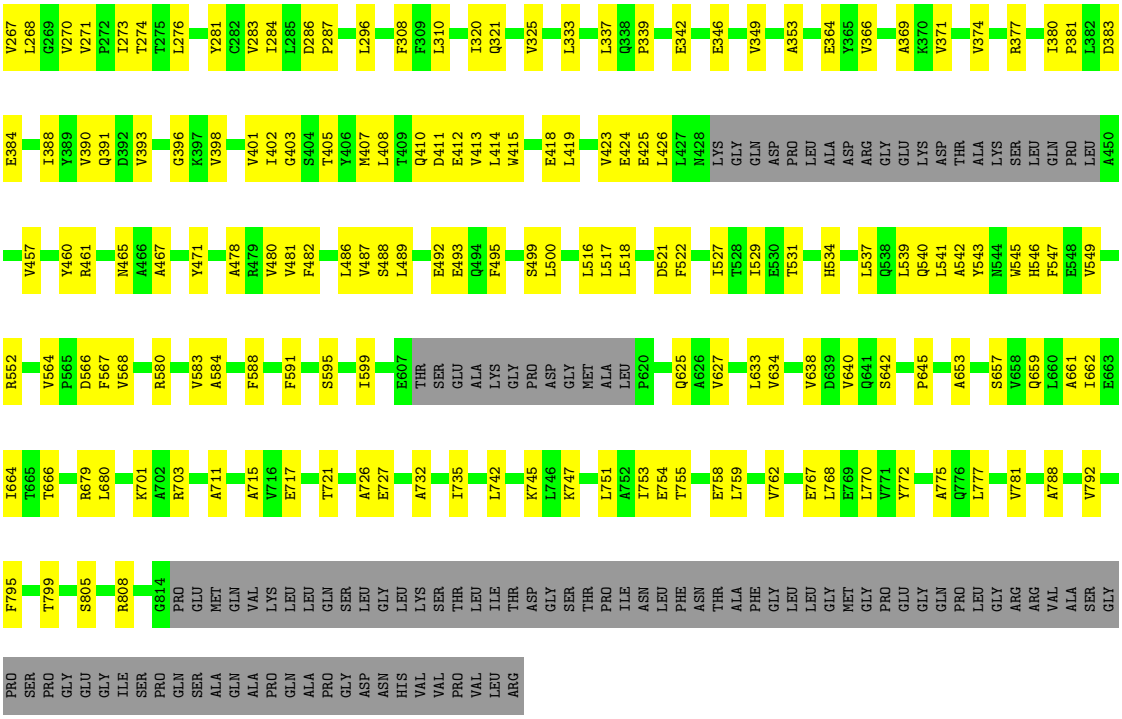
Chain J:



• Molecule 1: Major vault protein

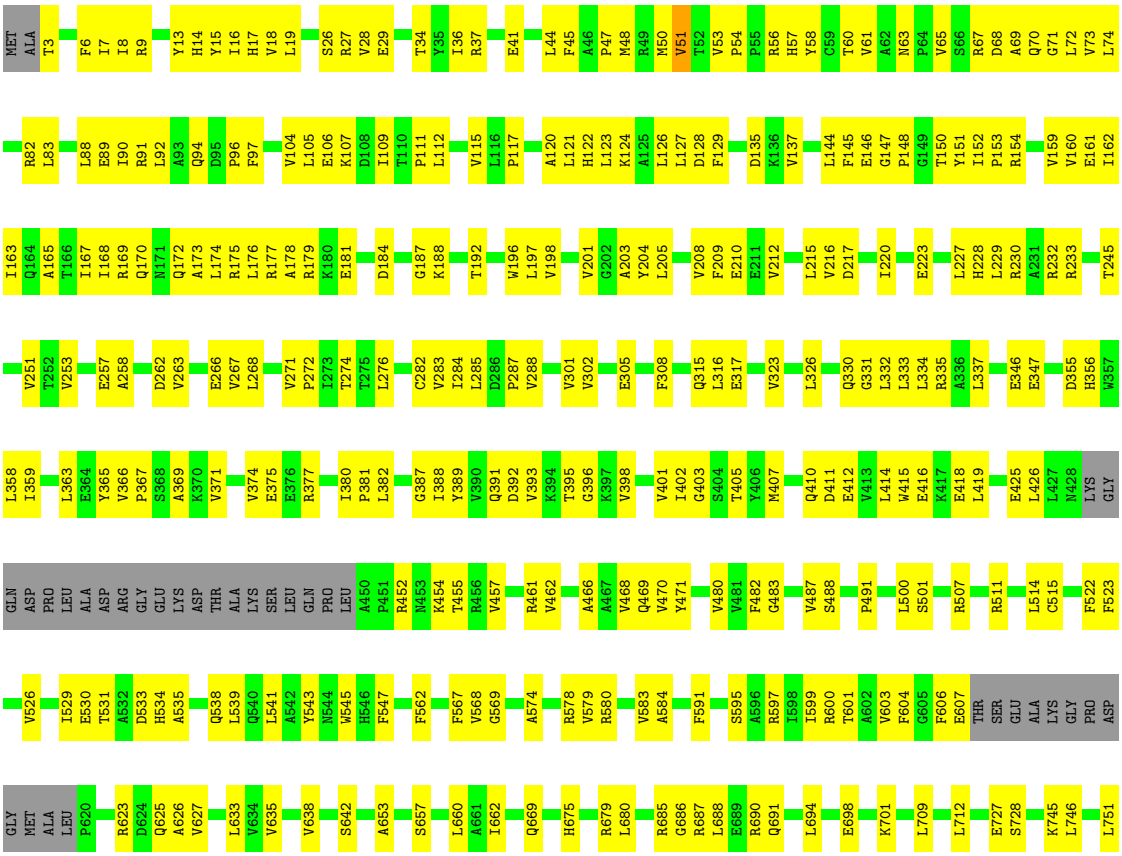
Chain JA:

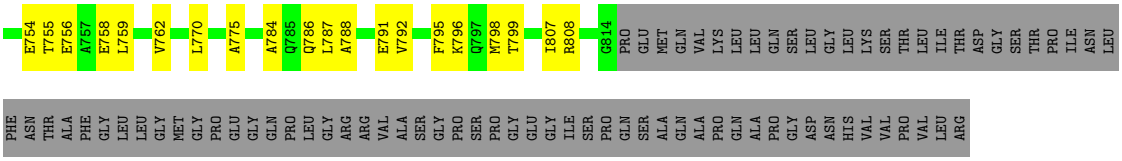




• Molecule 1: Major vault protein

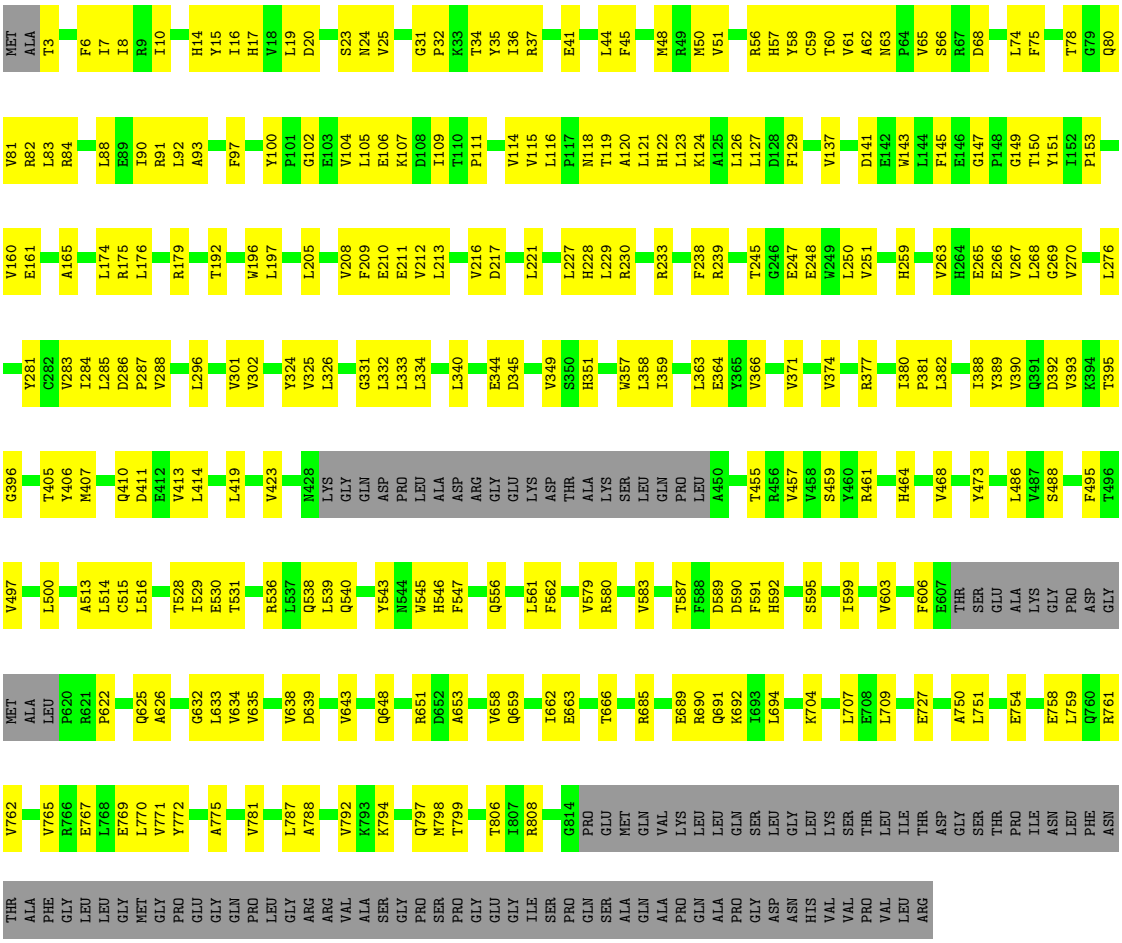
Chain JB:





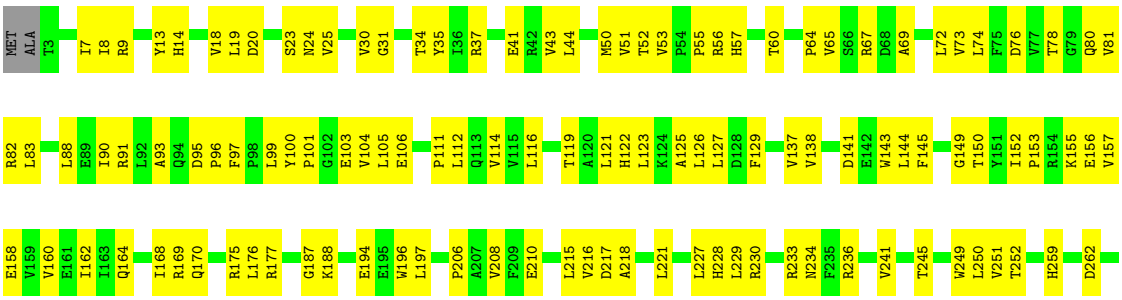
• Molecule 1: Major vault protein

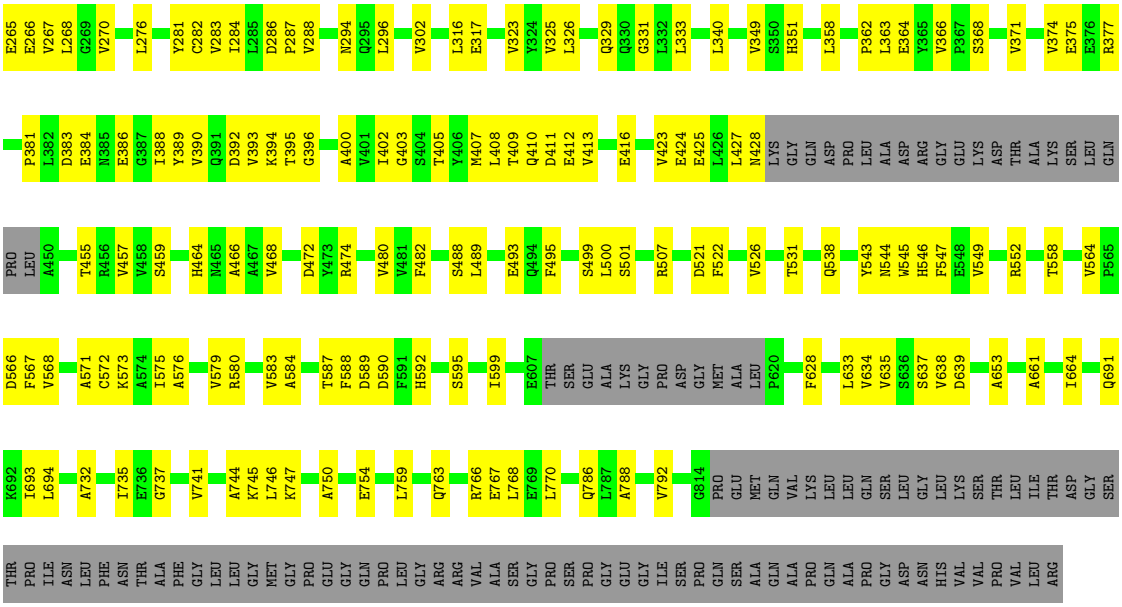
Chain K:



• Molecule 1: Major vault protein

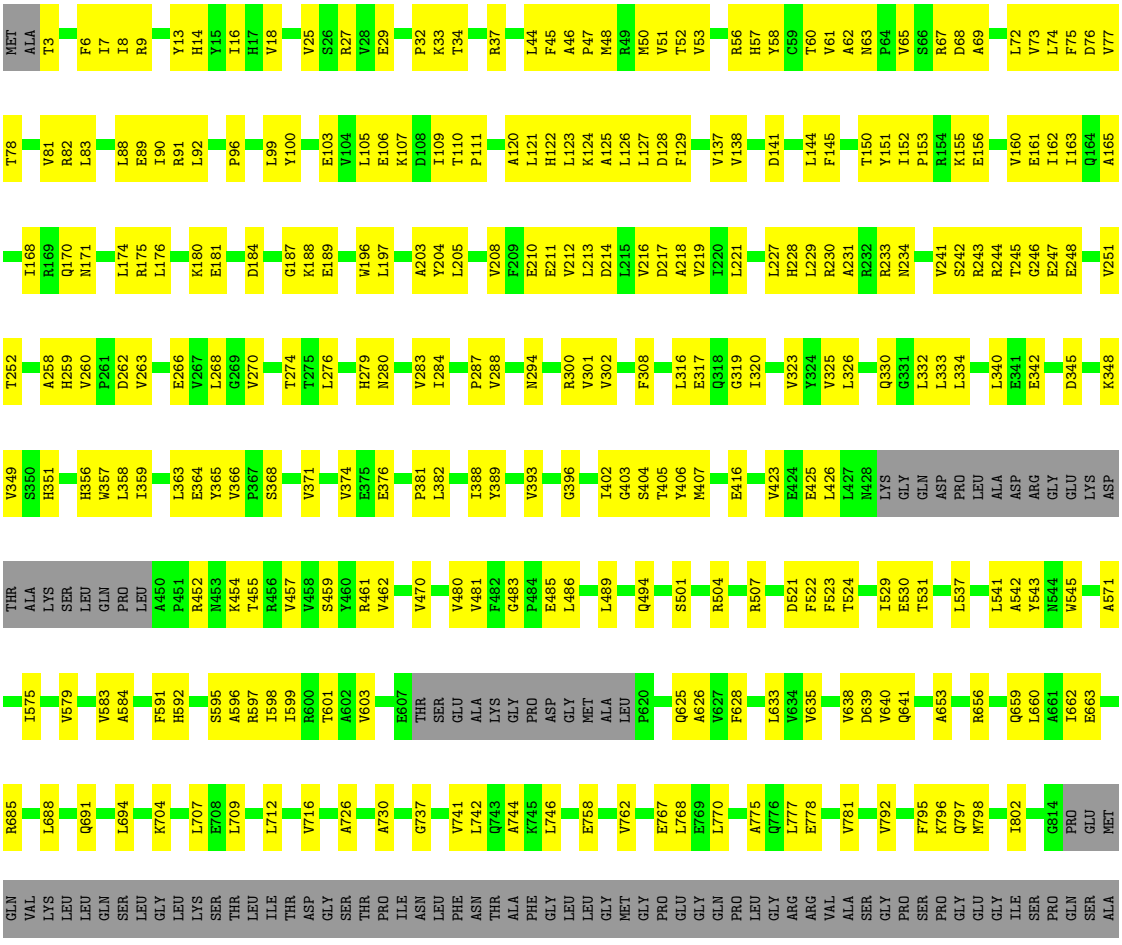
Chain KA:





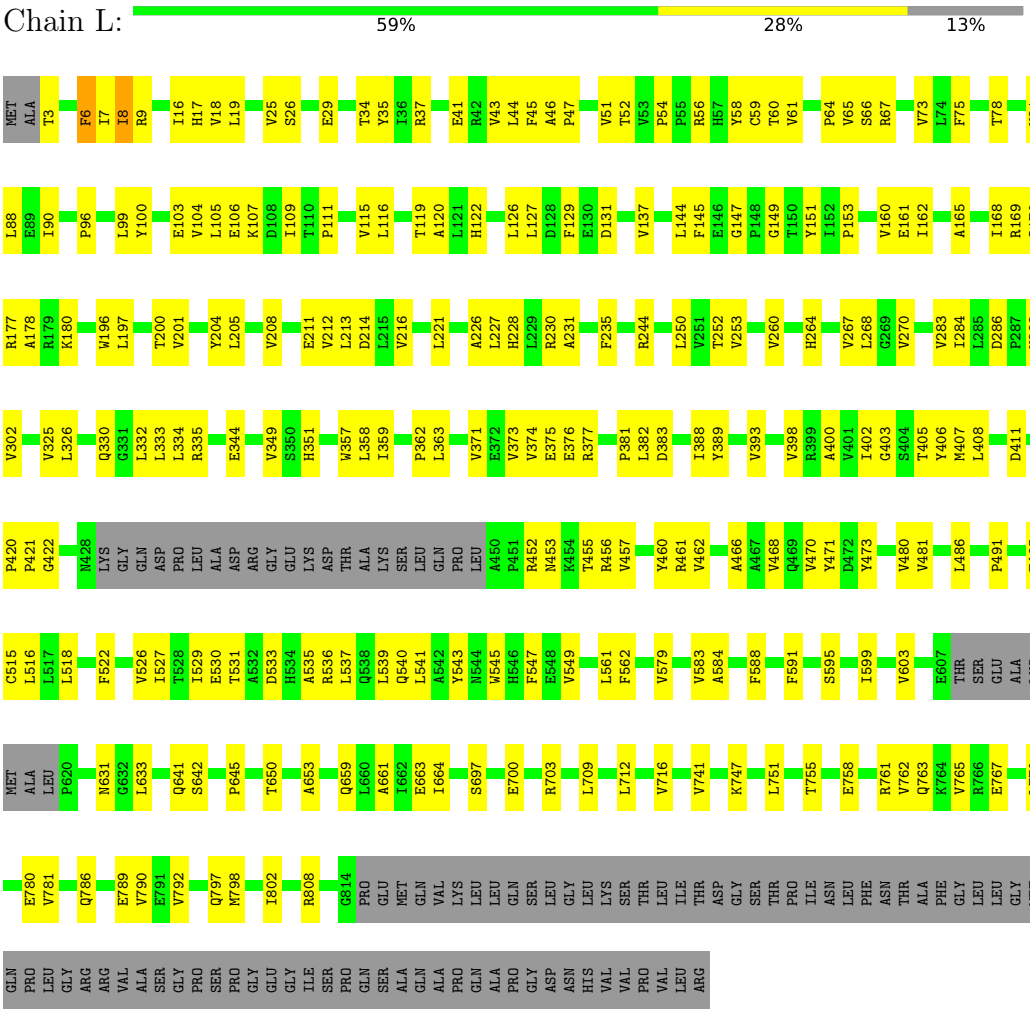
• Molecule 1: Major vault protein

Chain KB:



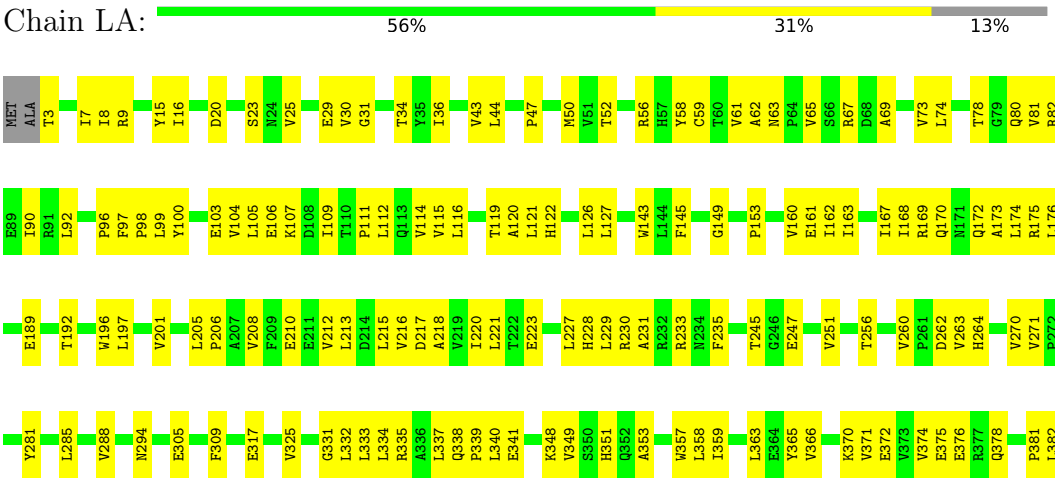
• Molecule 1: Major vault protein

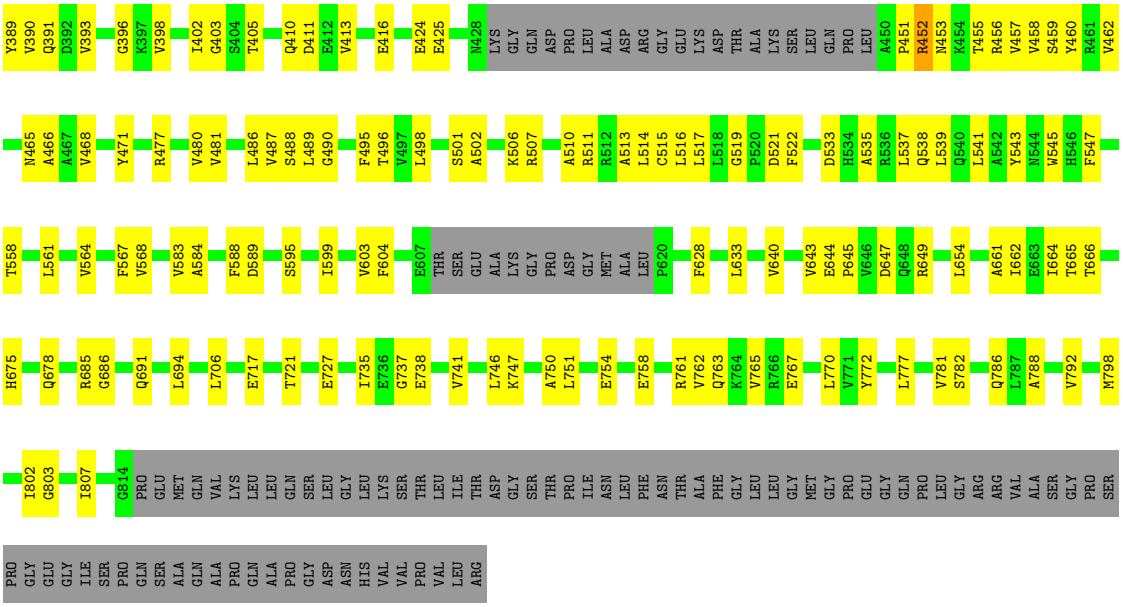
Chain L:



• Molecule 1: Major vault protein

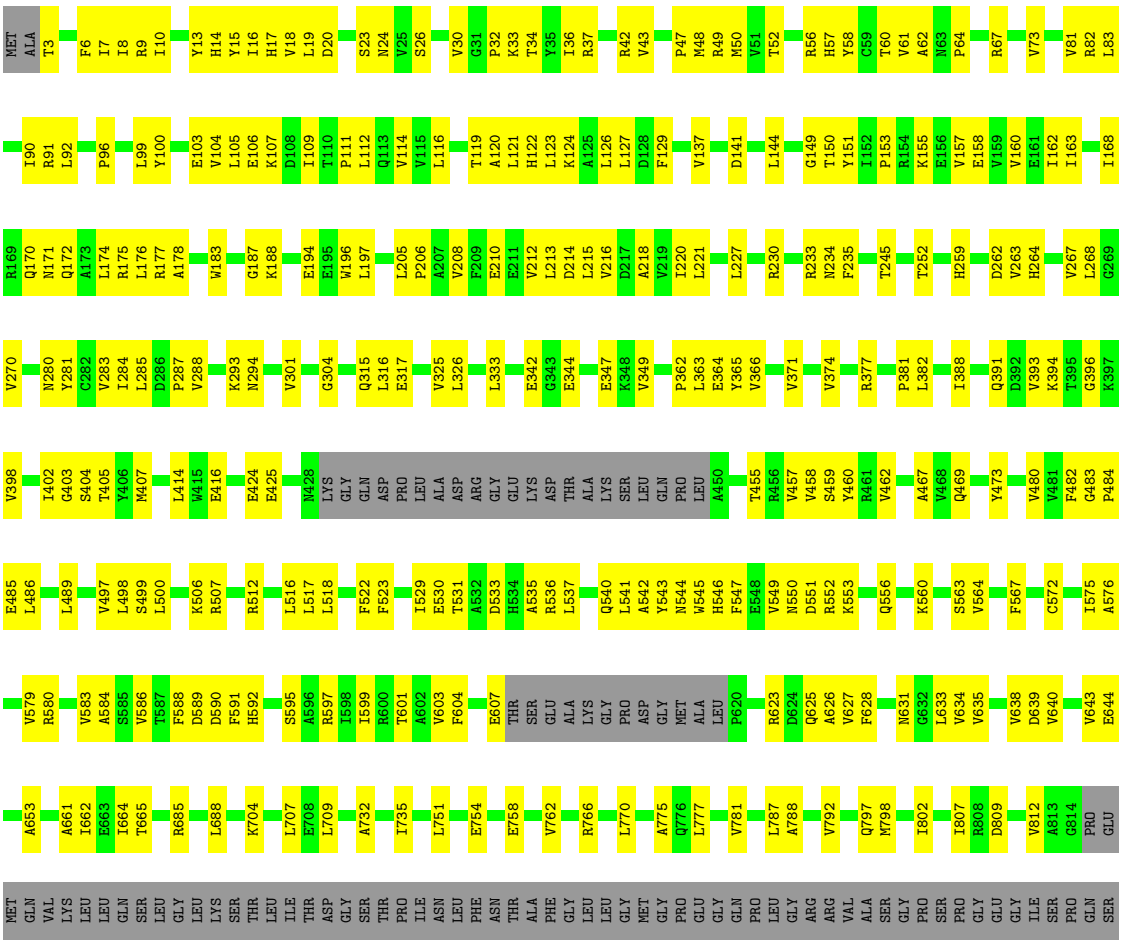
Chain LA:





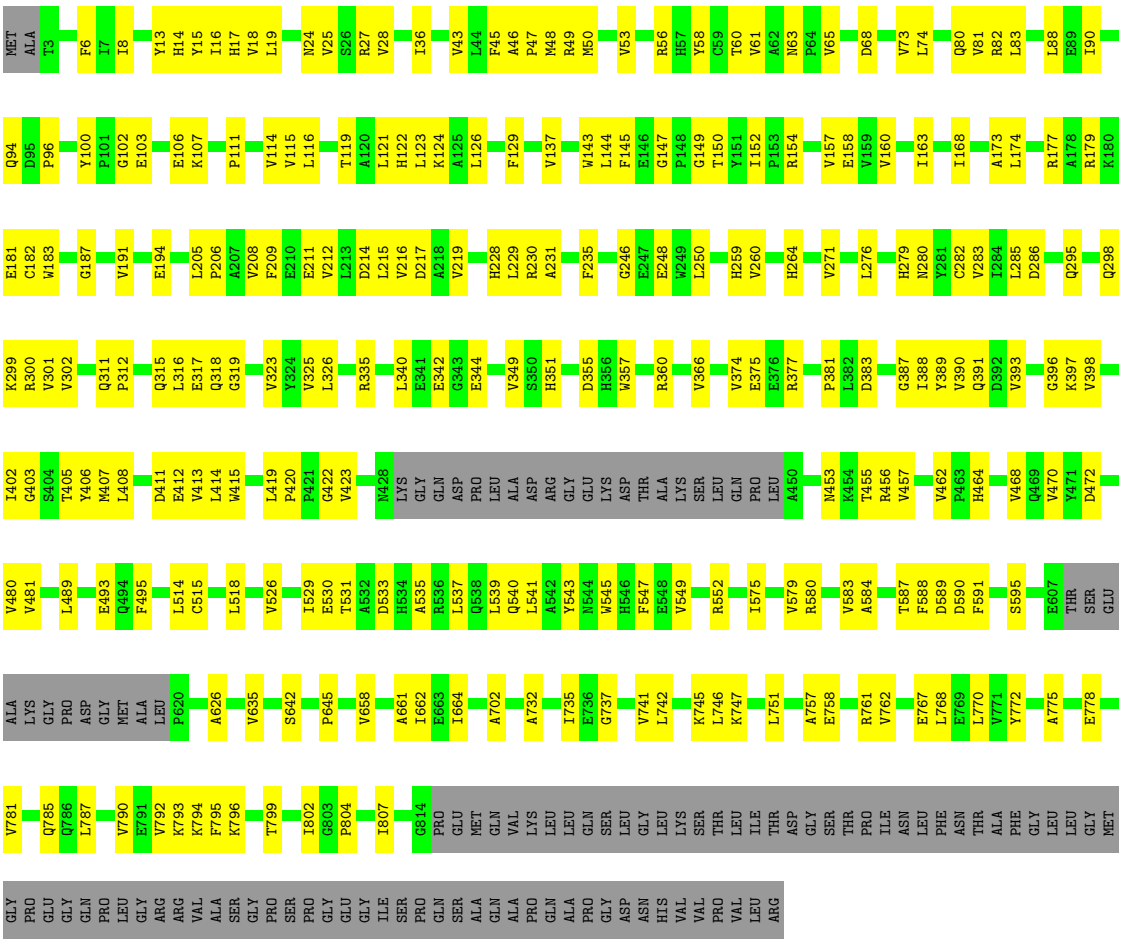
• Molecule 1: Major vault protein

Chain LB:



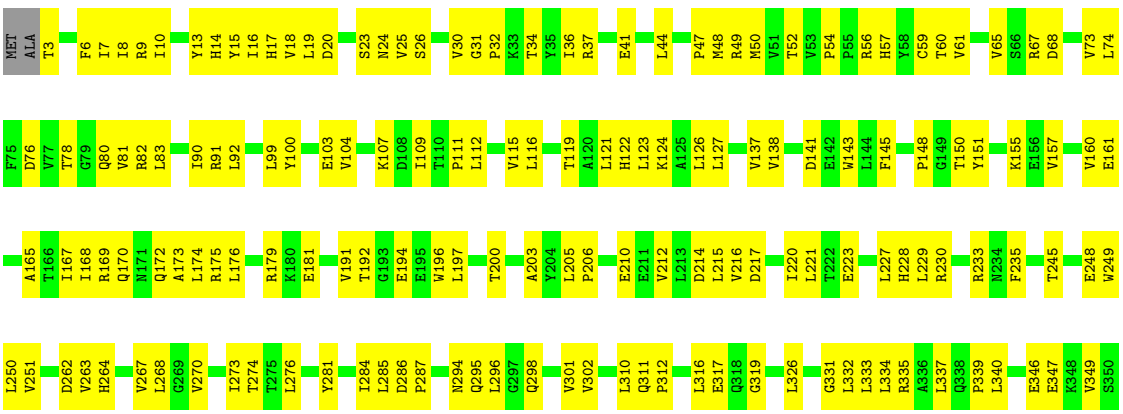
• Molecule 1: Major vault protein

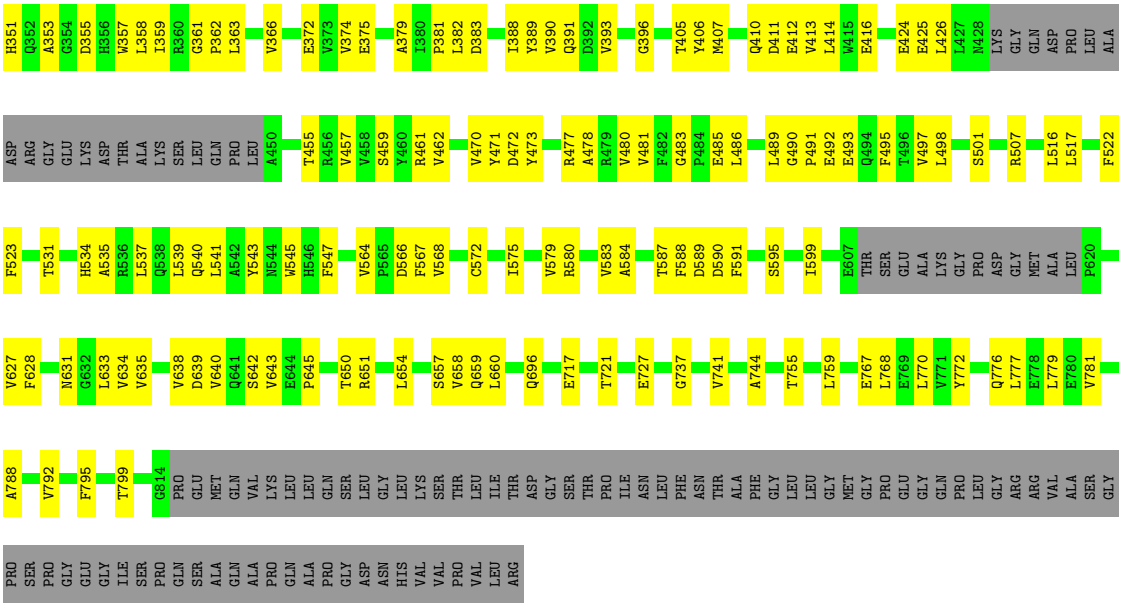
Chain M:



• Molecule 1: Major vault protein

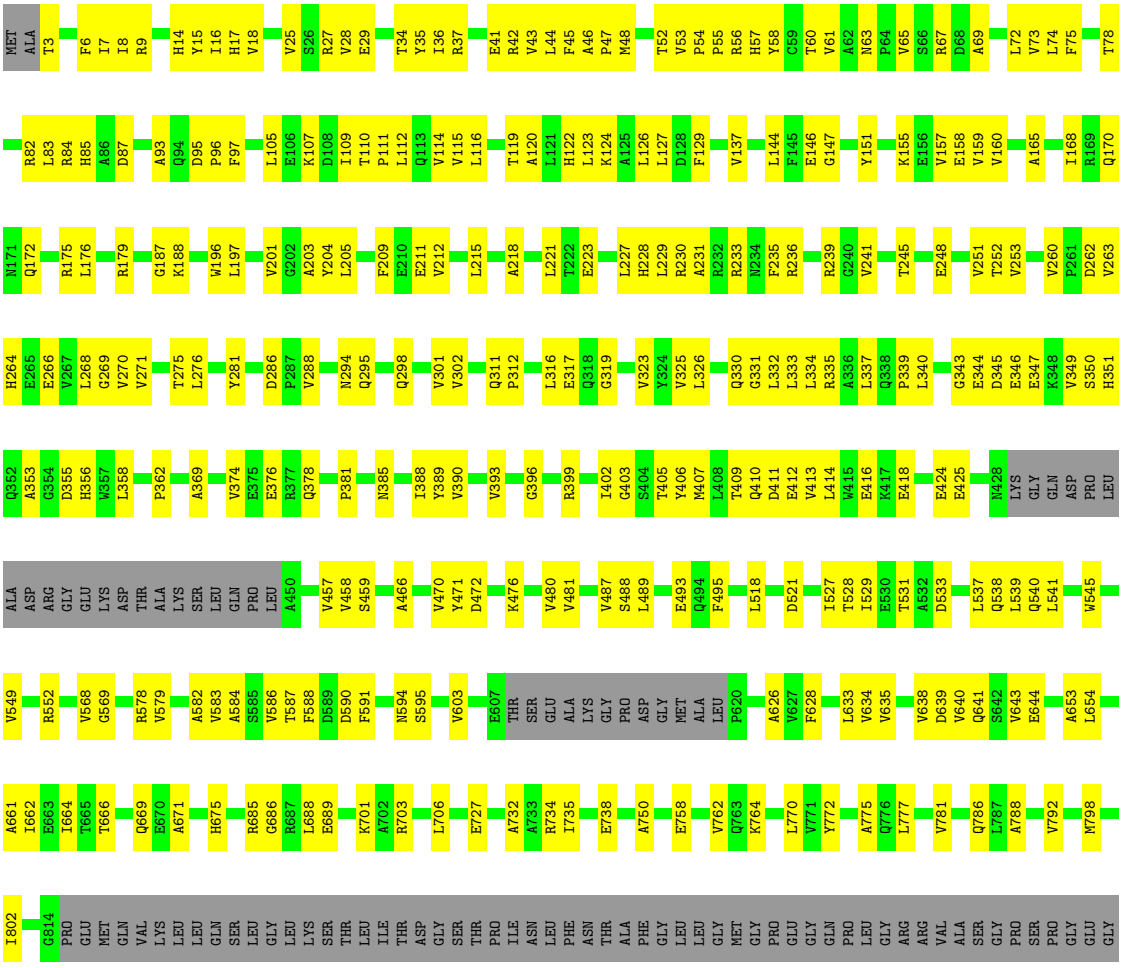
Chain MA:





• Molecule 1: Major vault protein

Chain MB:



• Molecule 1: Major vault protein

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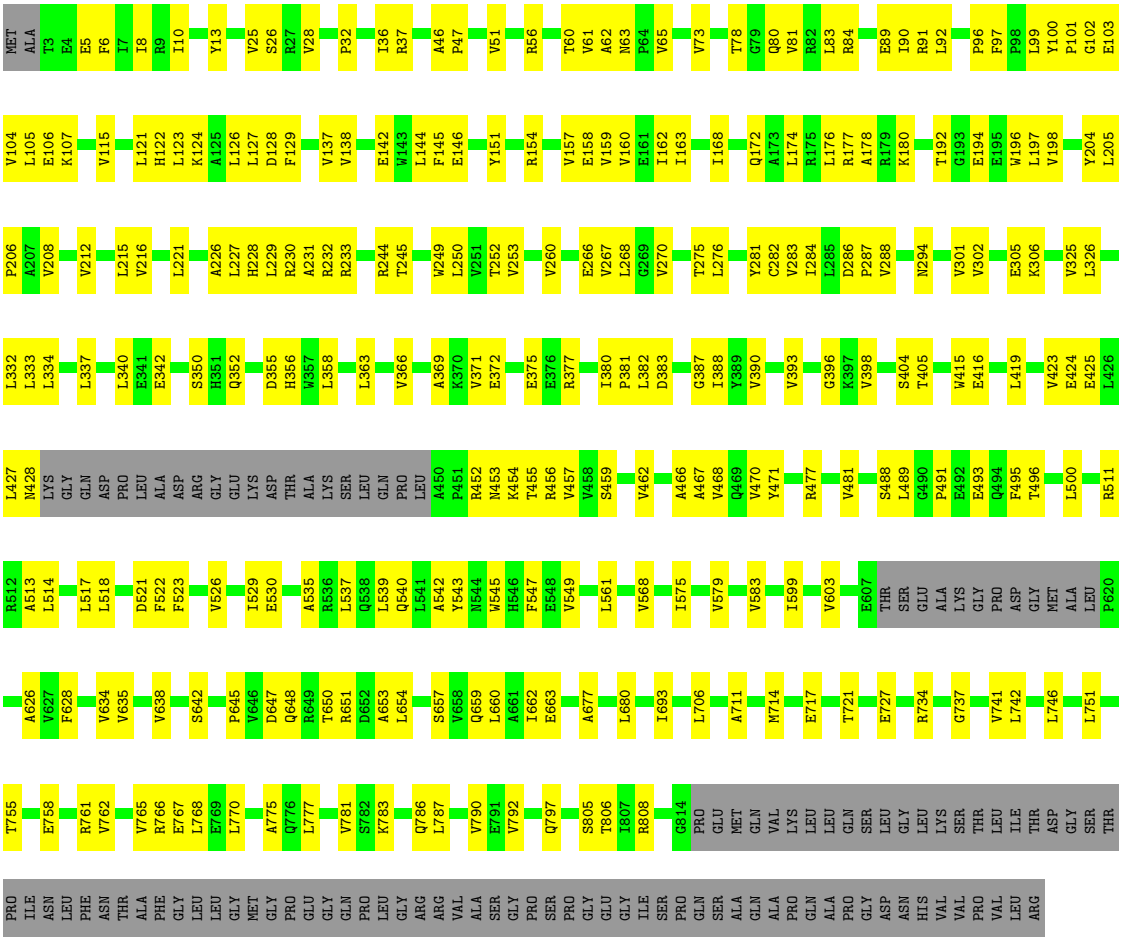
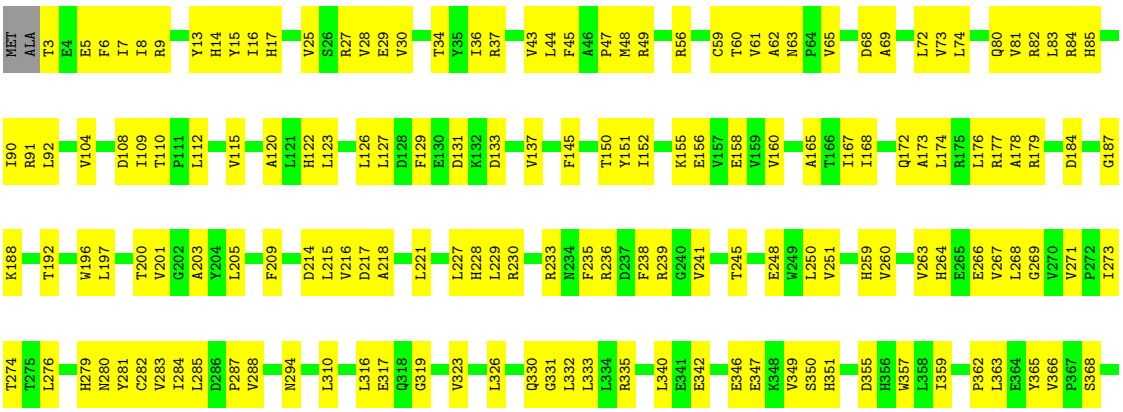
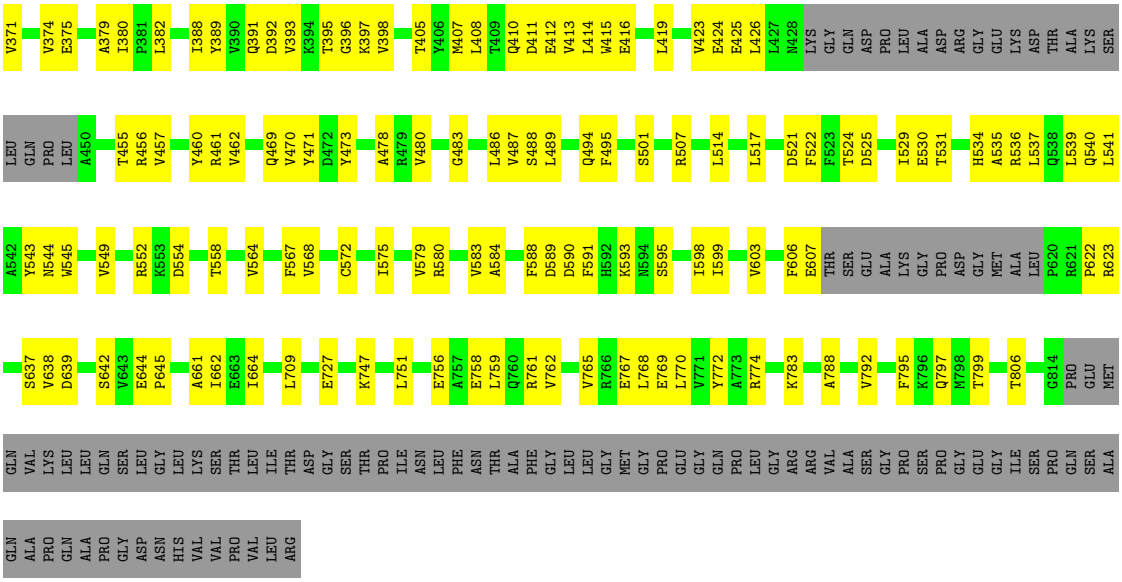


• Molecule 1: Major vault protein

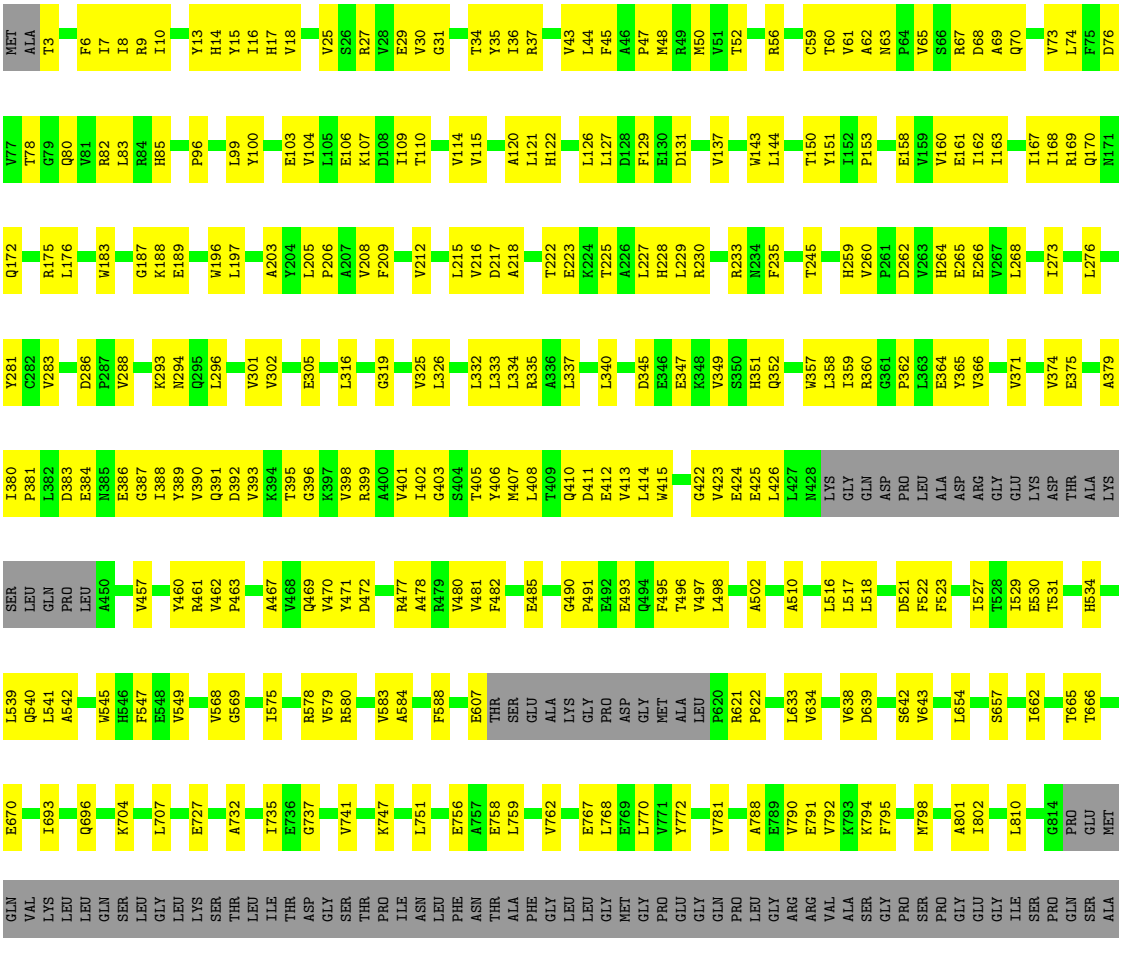
Chain NA:





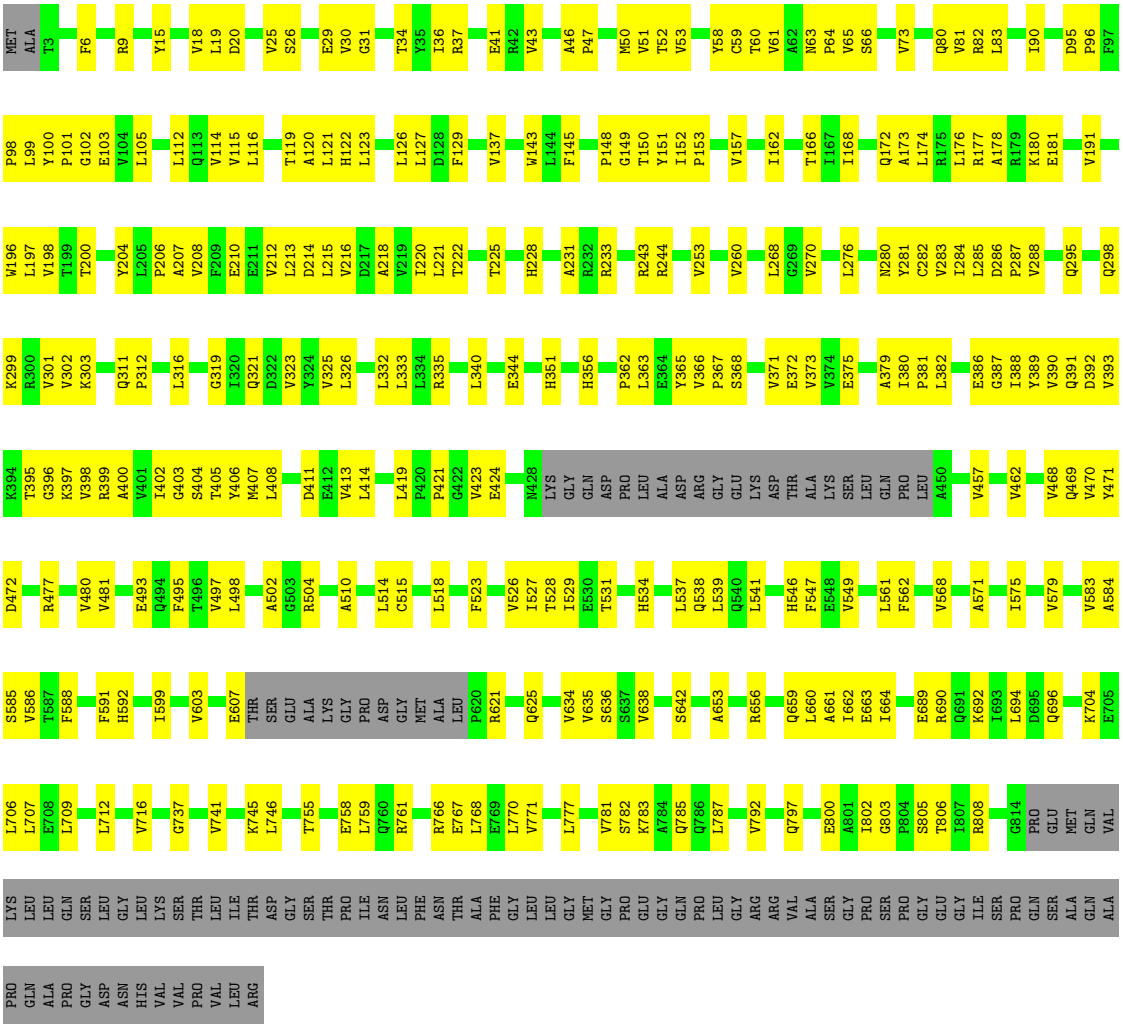
• Molecule 1: Major vault protein

Chain NB:



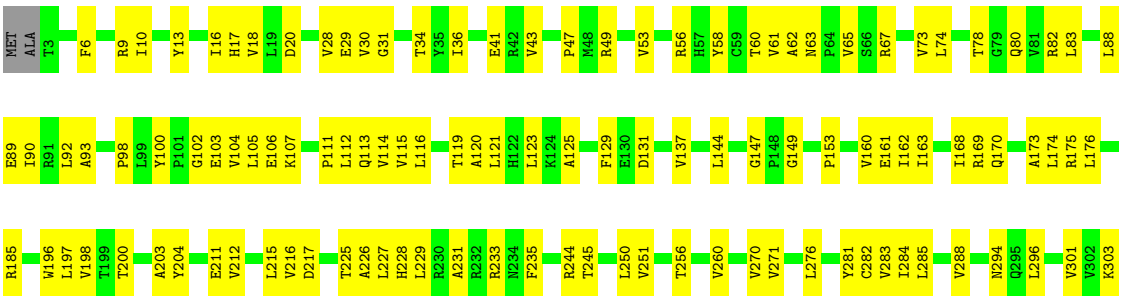
• Molecule 1: Major vault protein

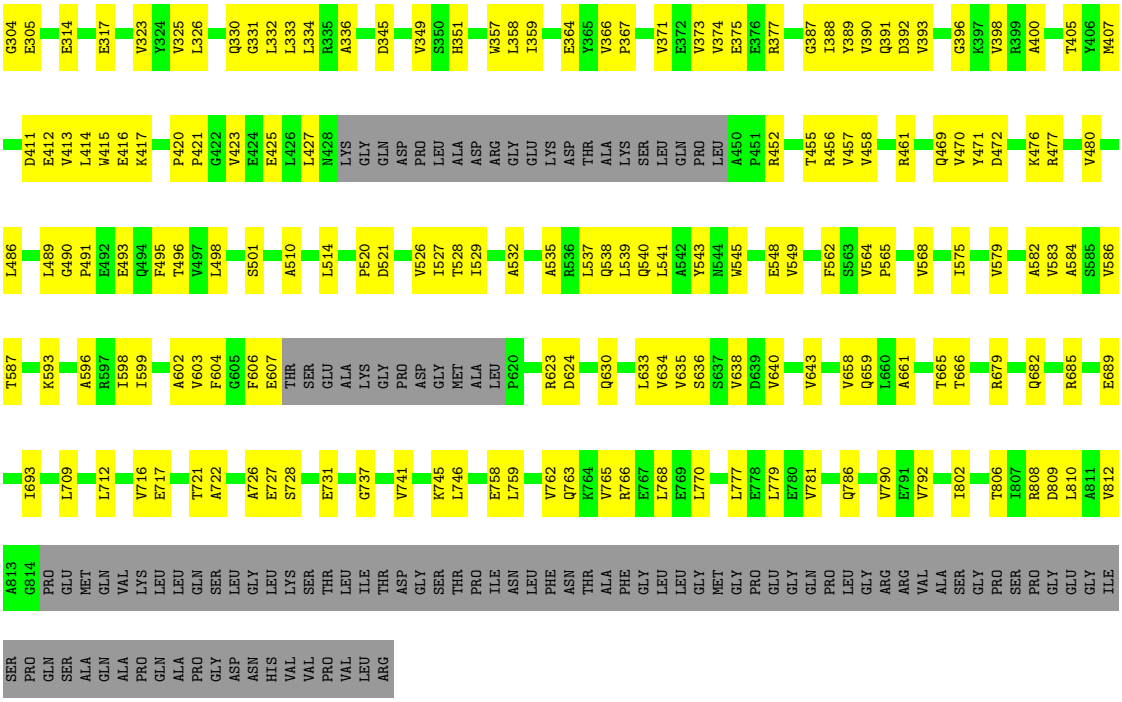
Chain O:



• Molecule 1: Major vault protein

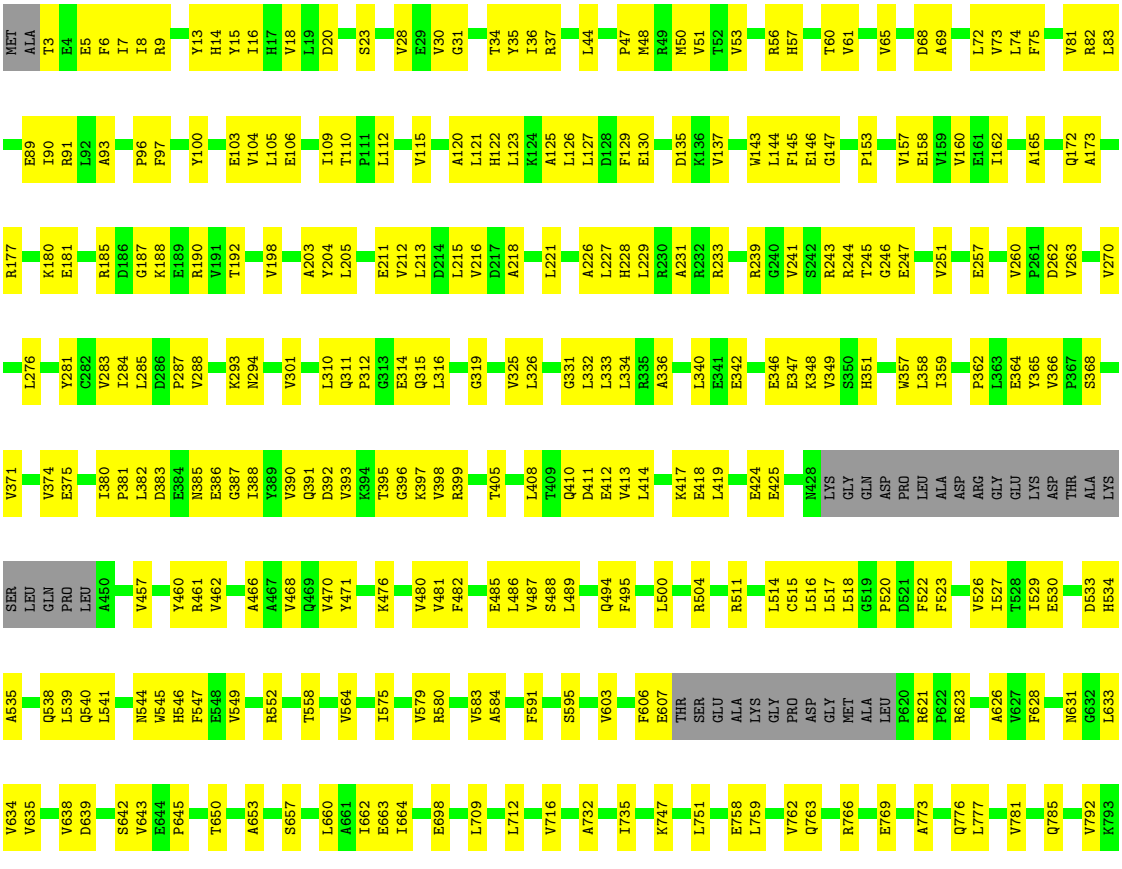
Chain OA:

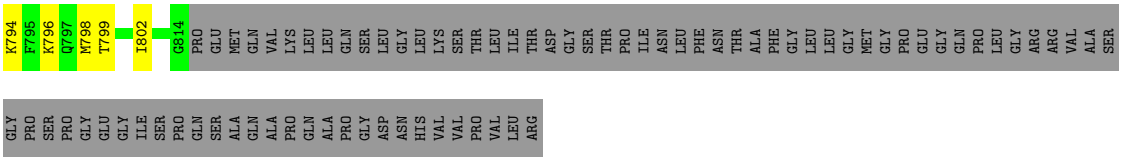




• Molecule 1: Major vault protein

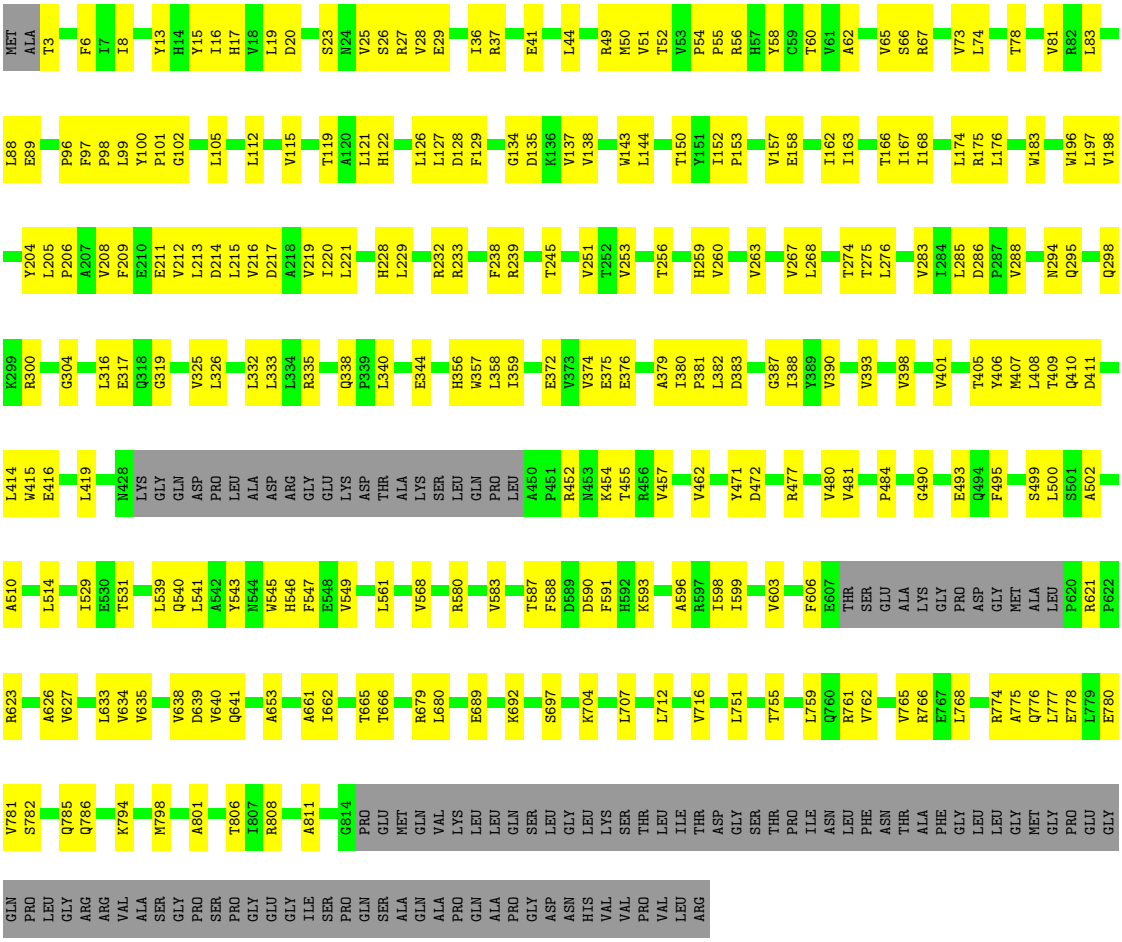
Chain OB:





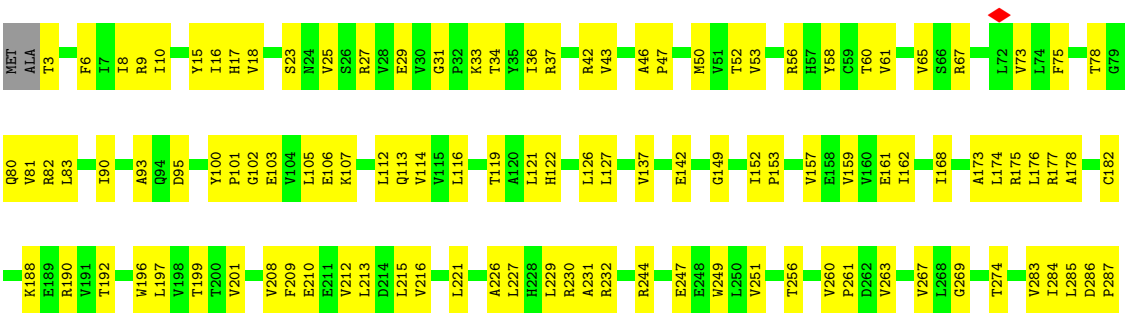
• Molecule 1: Major vault protein

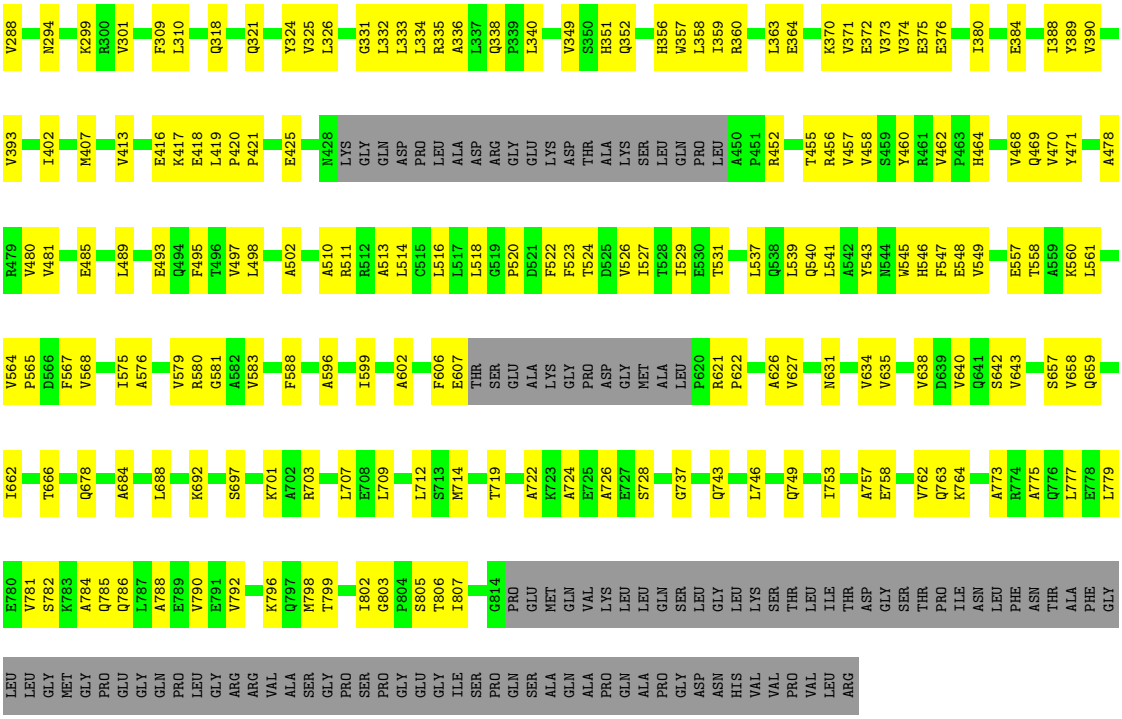
Chain P:



• Molecule 1: Major vault protein

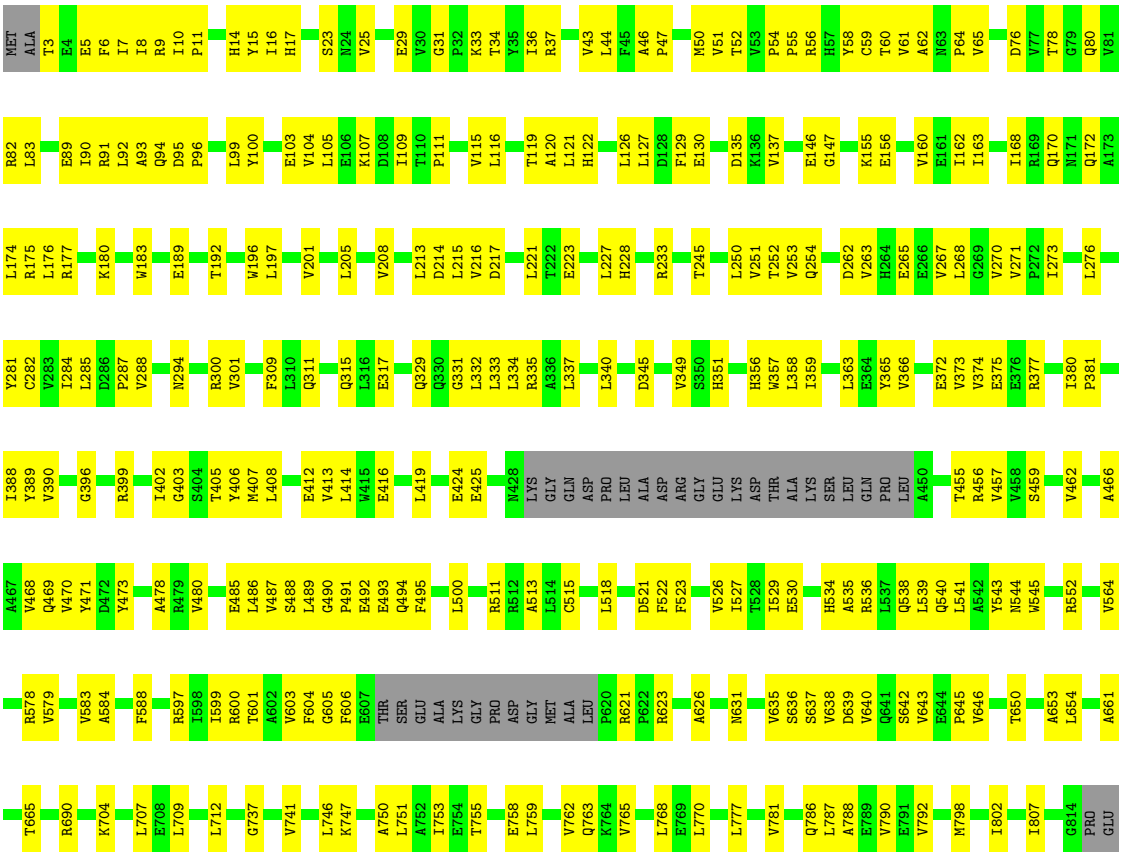
Chain PA:

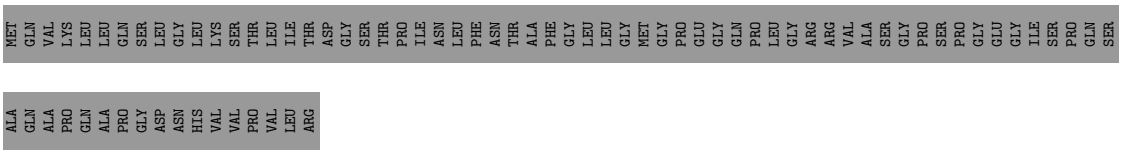




• Molecule 1: Major vault protein

Chain PB:





• Molecule 1: Major vault protein

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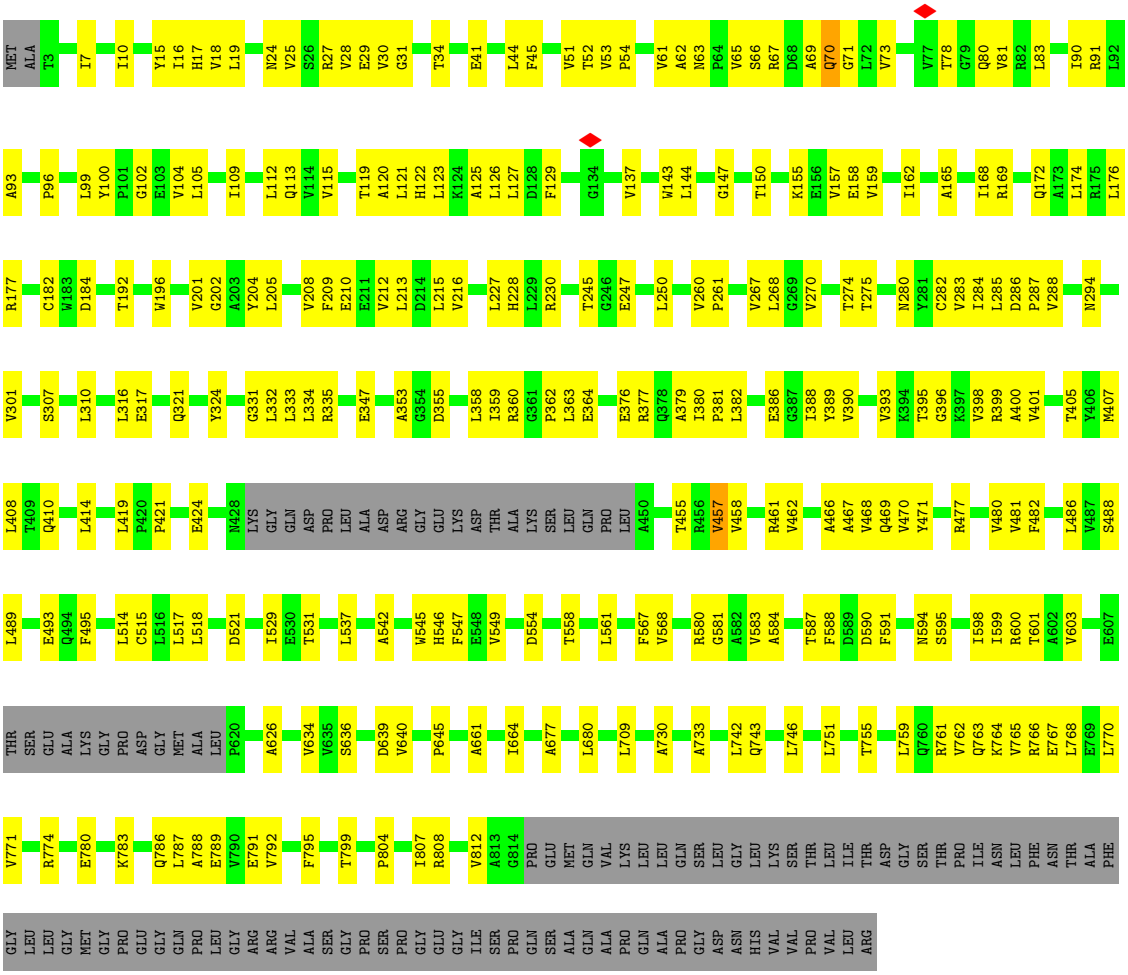
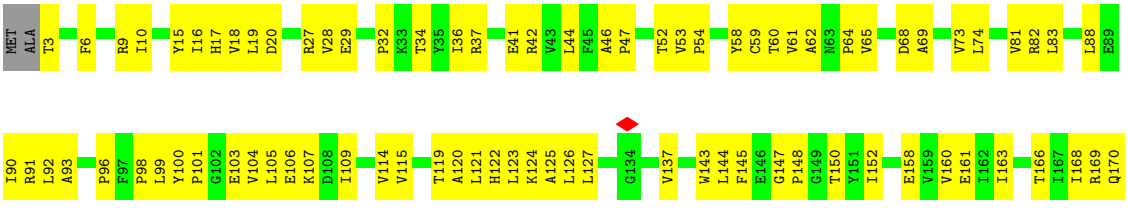
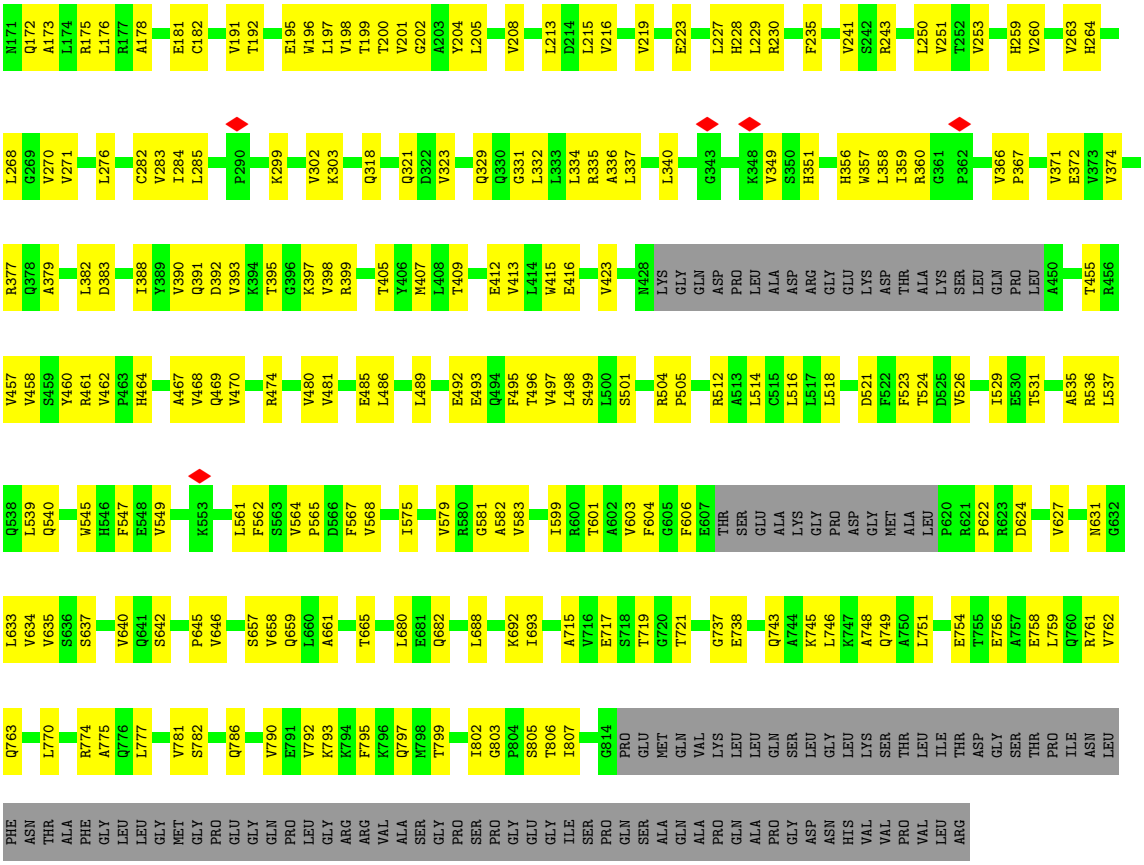


• Molecule 1: Major vault protein

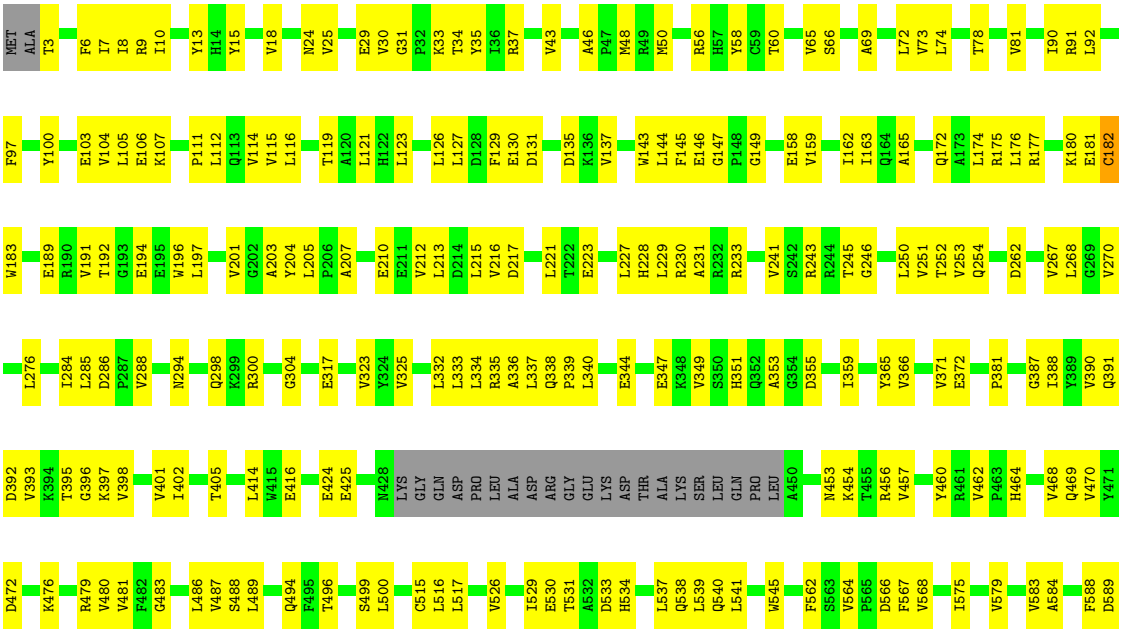
Chain QA:

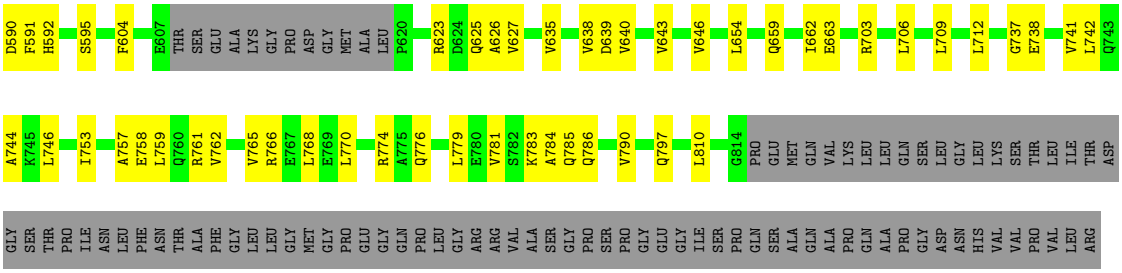




• Molecule 1: Major vault protein

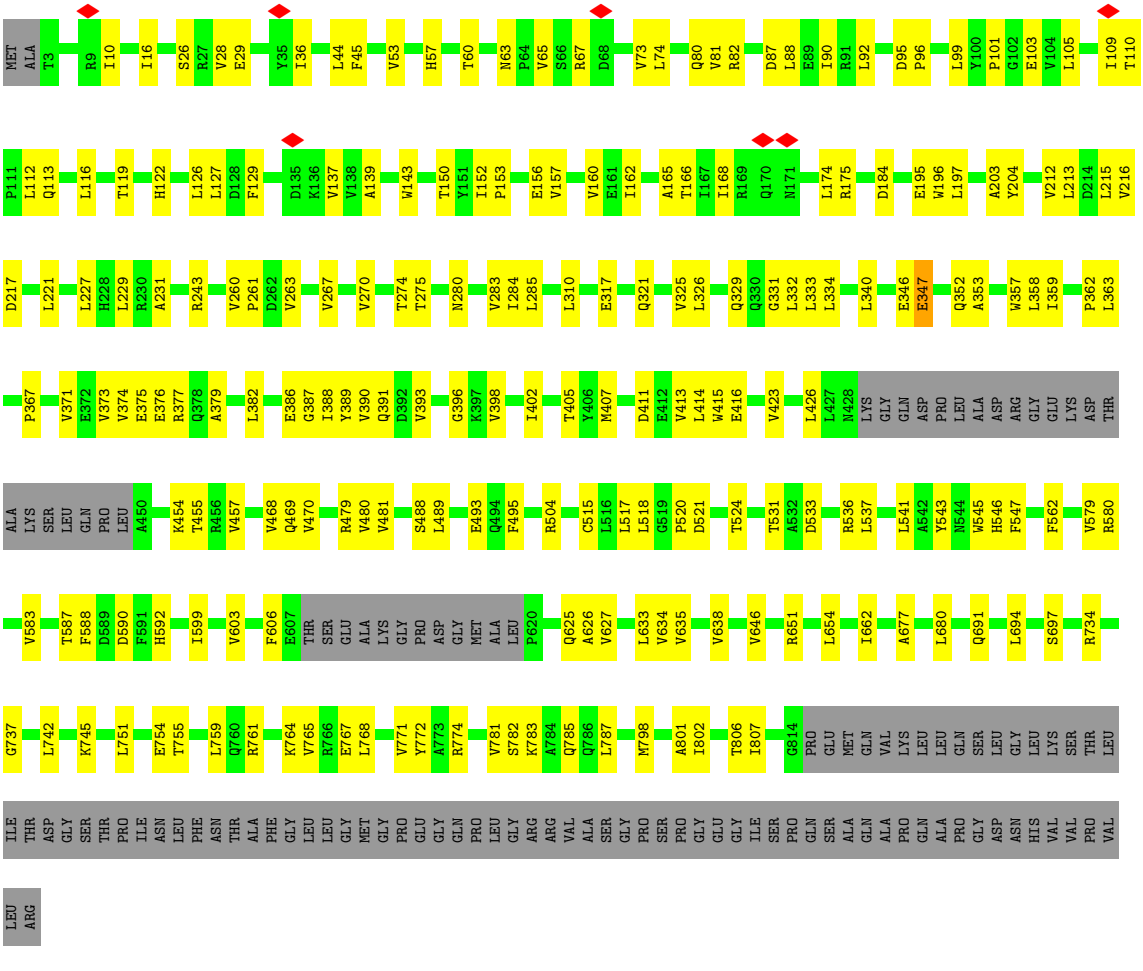
Chain QB:





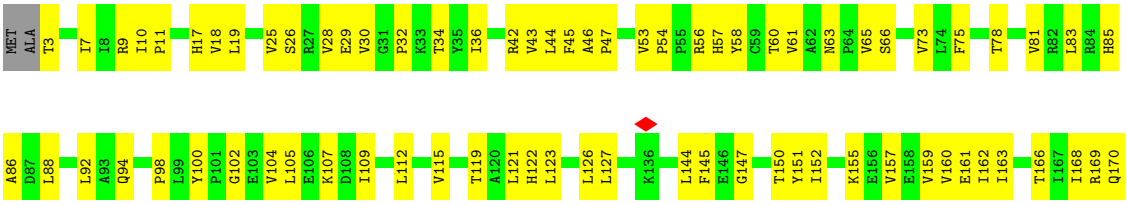
• Molecule 1: Major vault protein

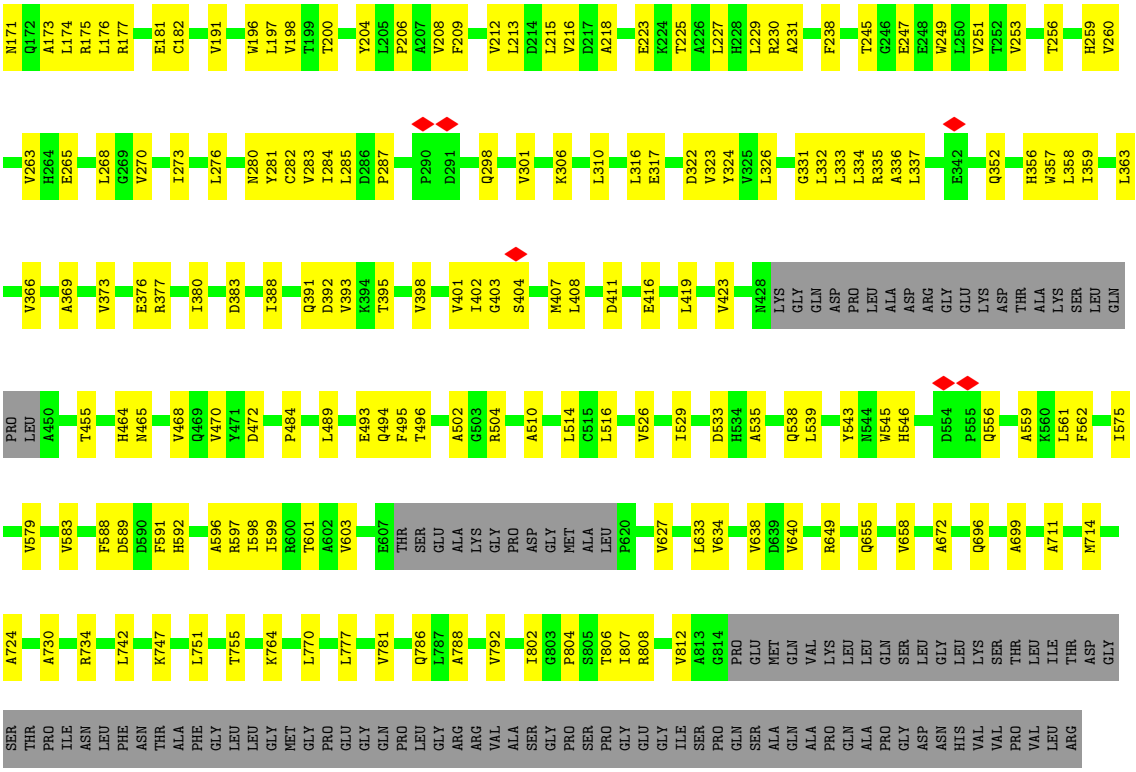
Chain R:



• Molecule 1: Major vault protein

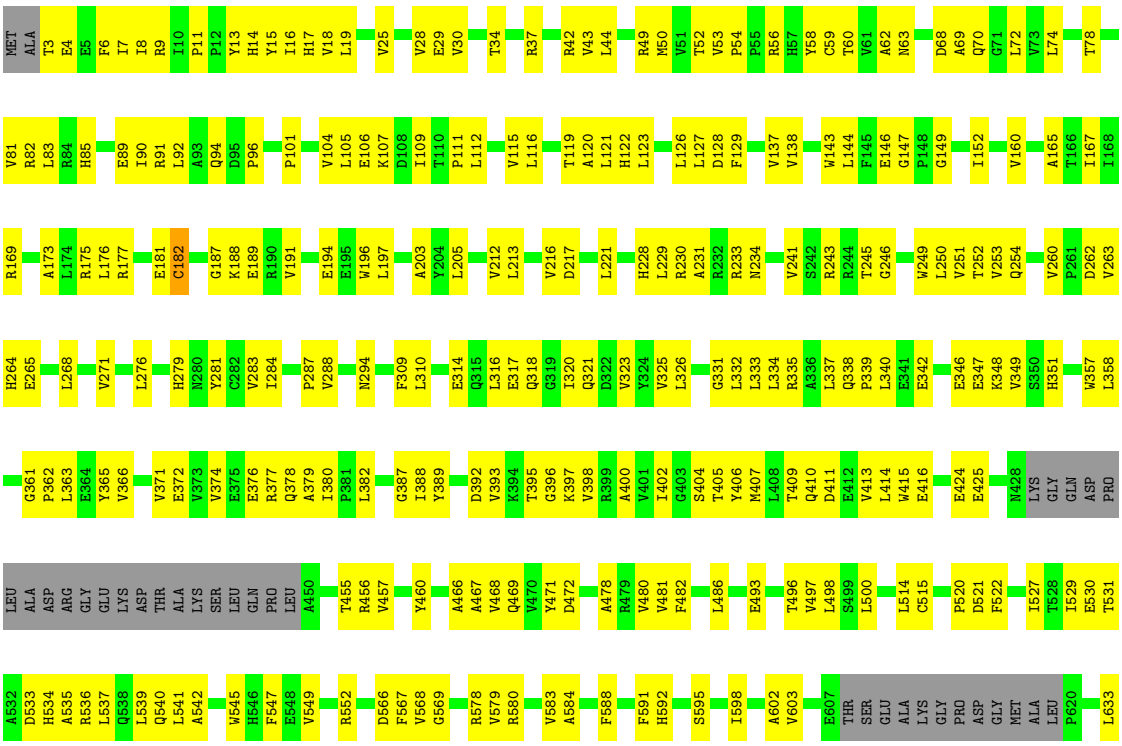
Chain RA:

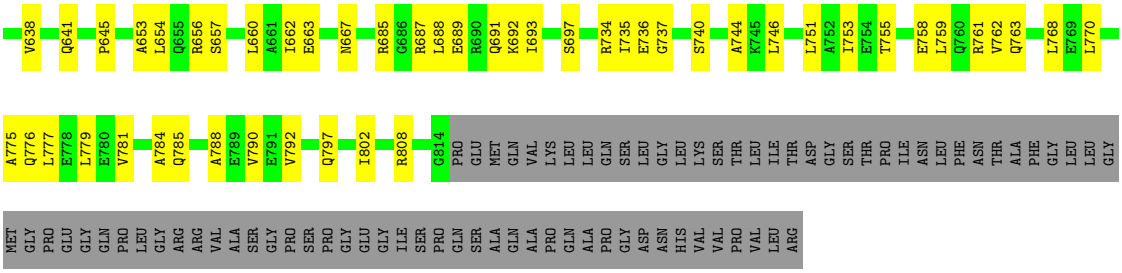




• Molecule 1: Major vault protein

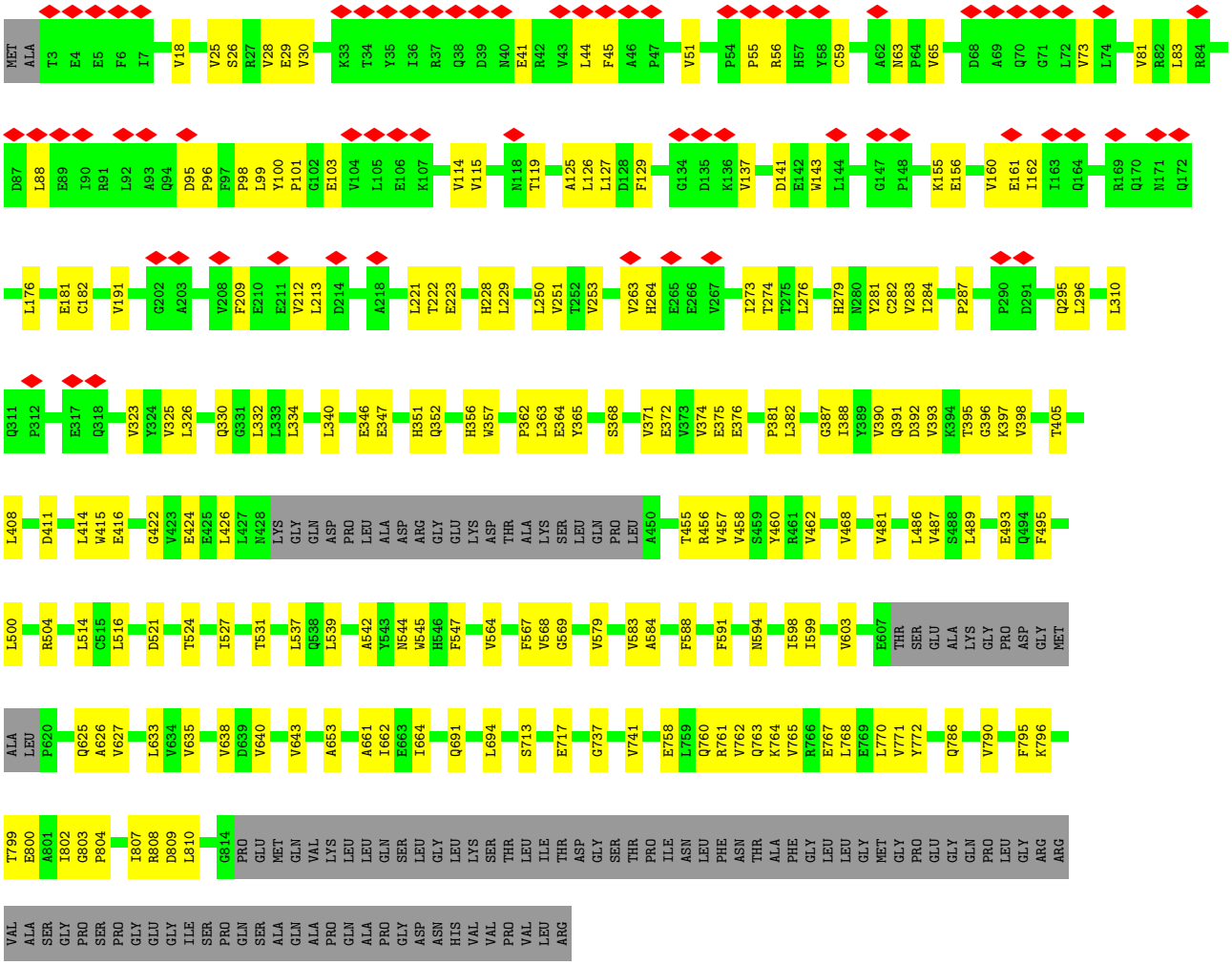
Chain RB:





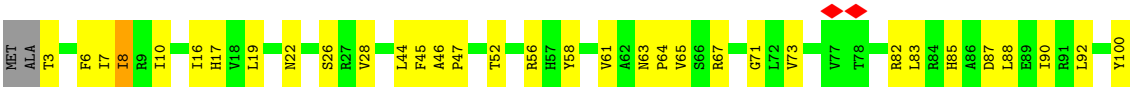
• Molecule 1: Major vault protein

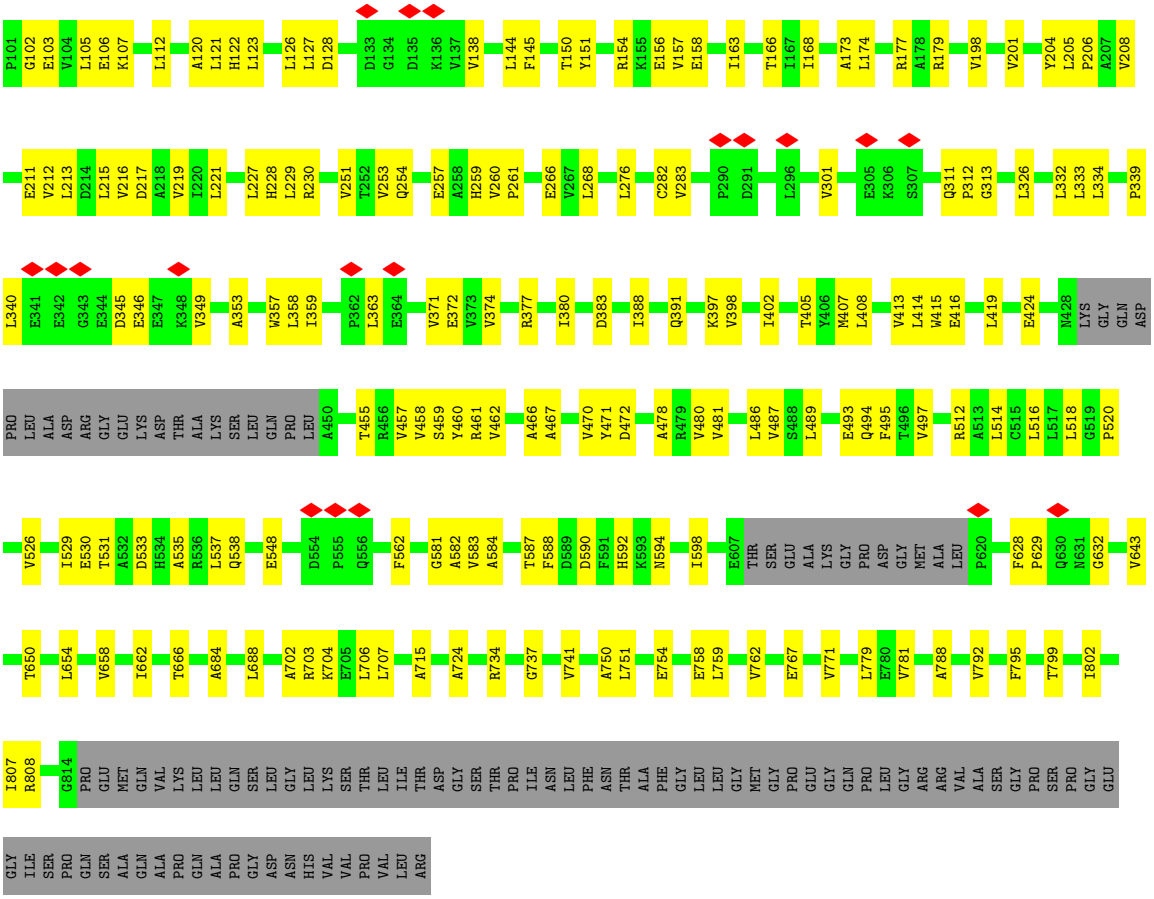
Chain S:



• Molecule 1: Major vault protein

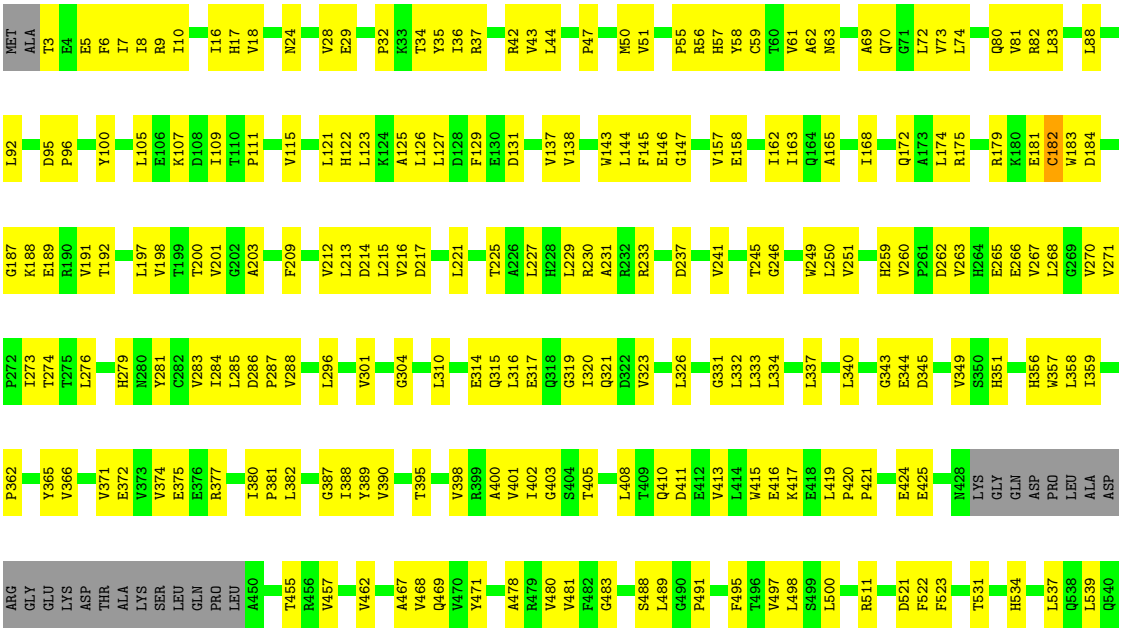
Chain SA:

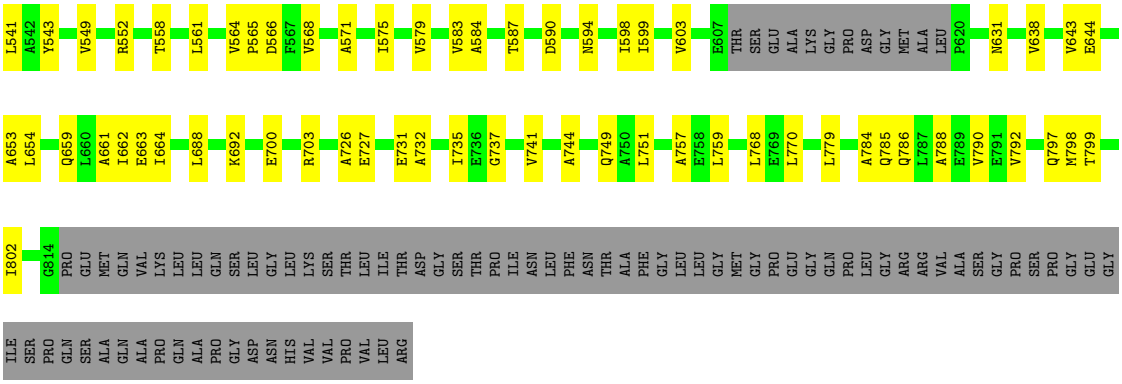




• Molecule 1: Major vault protein

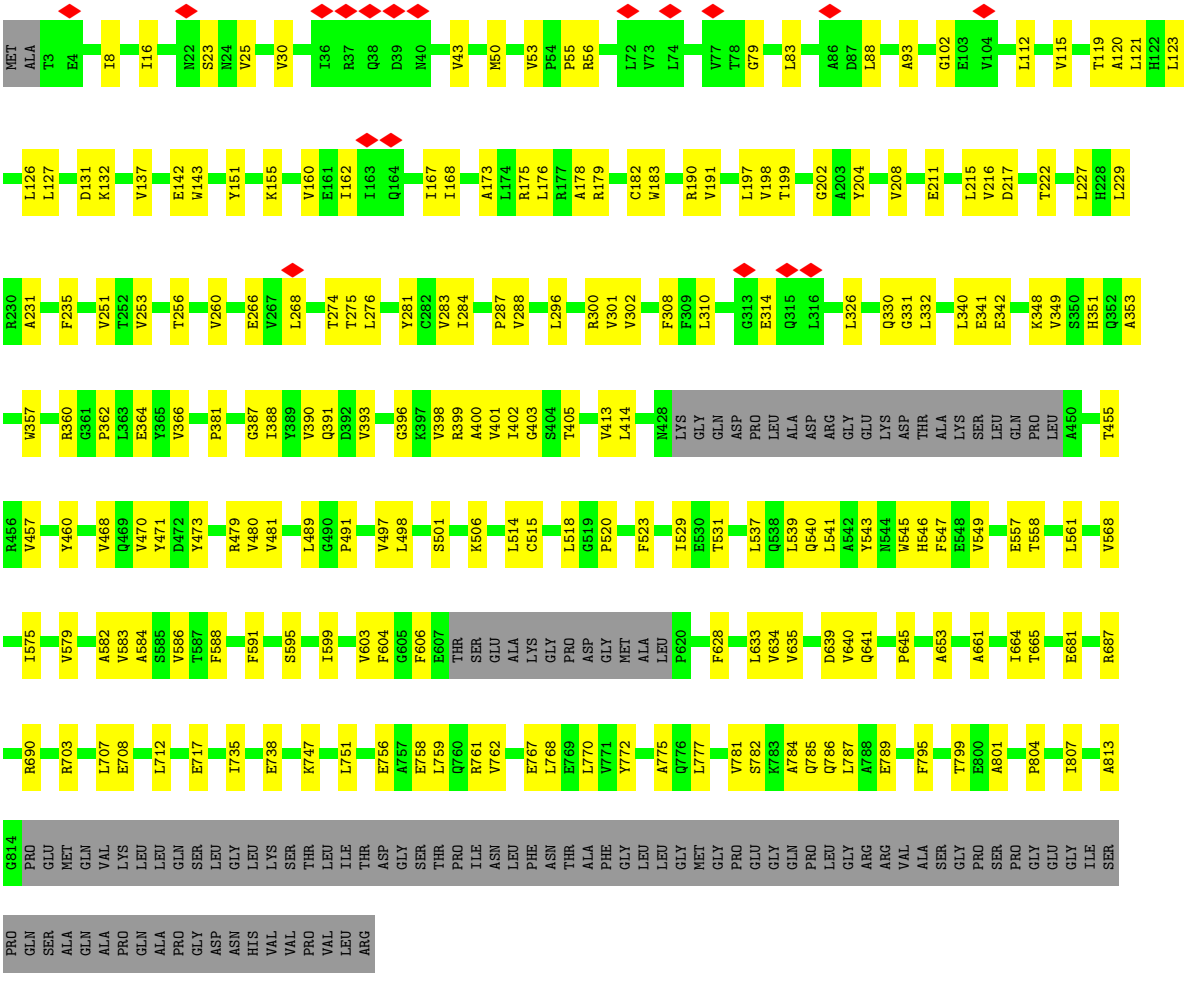
Chain SB:





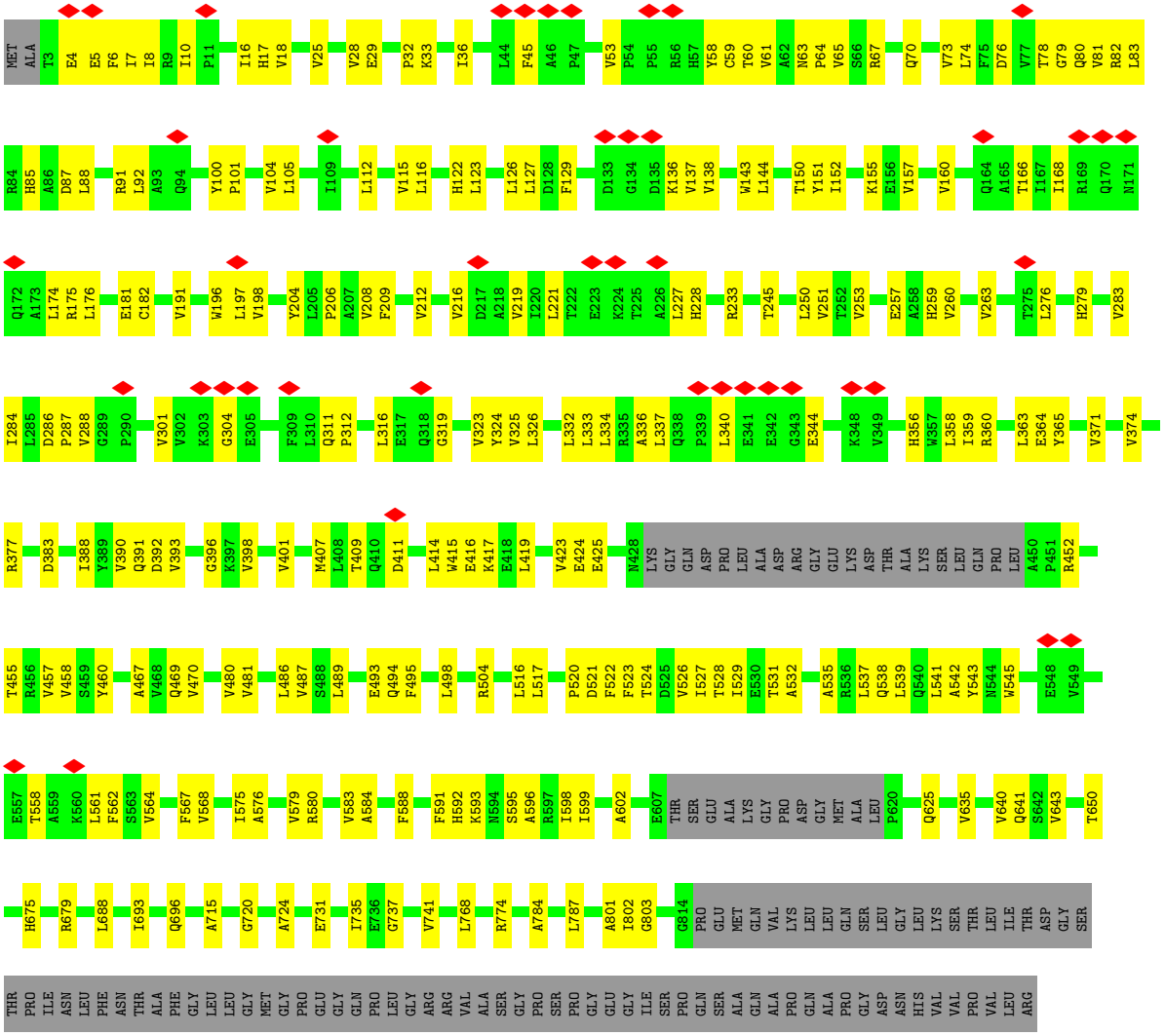
• Molecule 1: Major vault protein

Chain T:



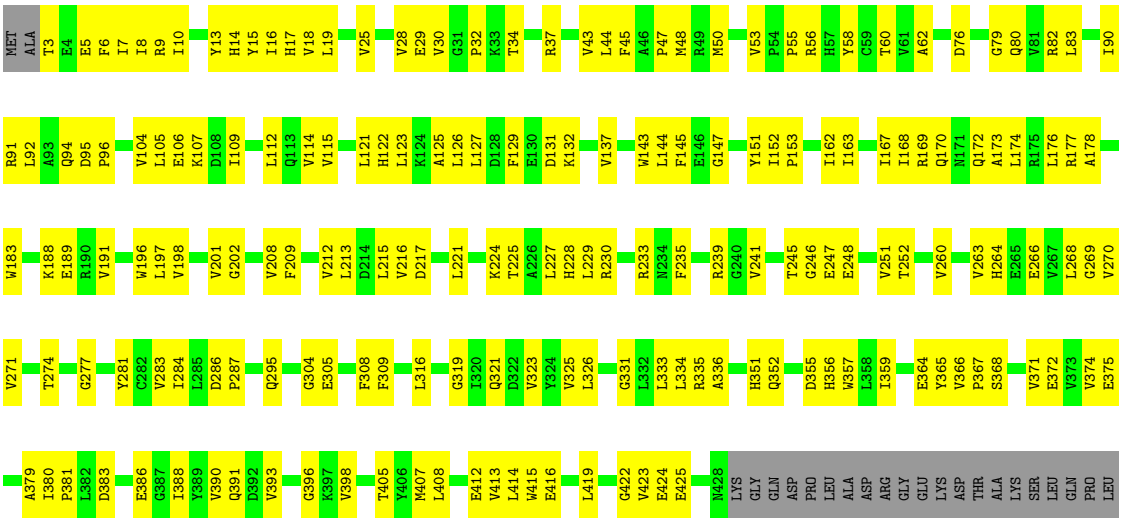
• Molecule 1: Major vault protein

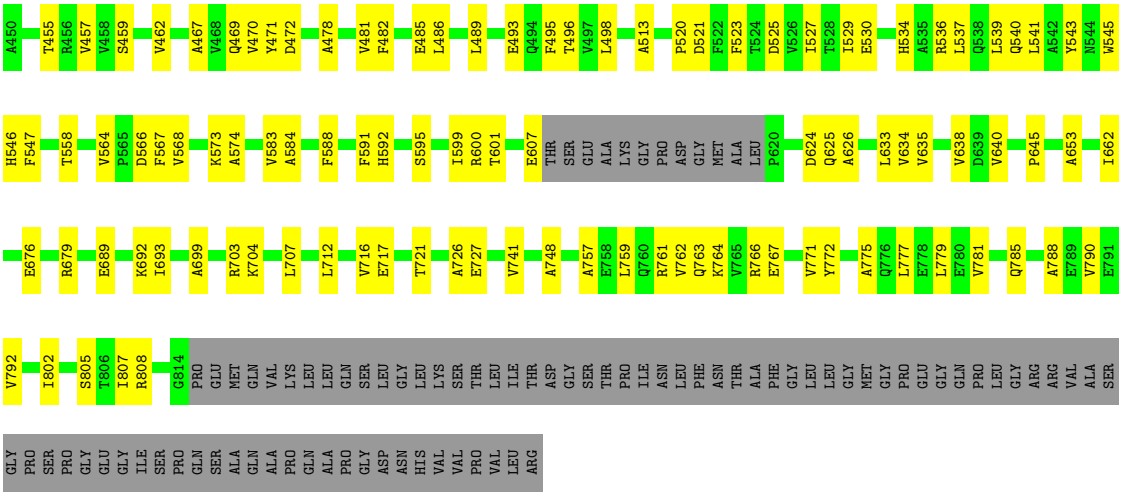
Chain TA:



• Molecule 1: Major vault protein

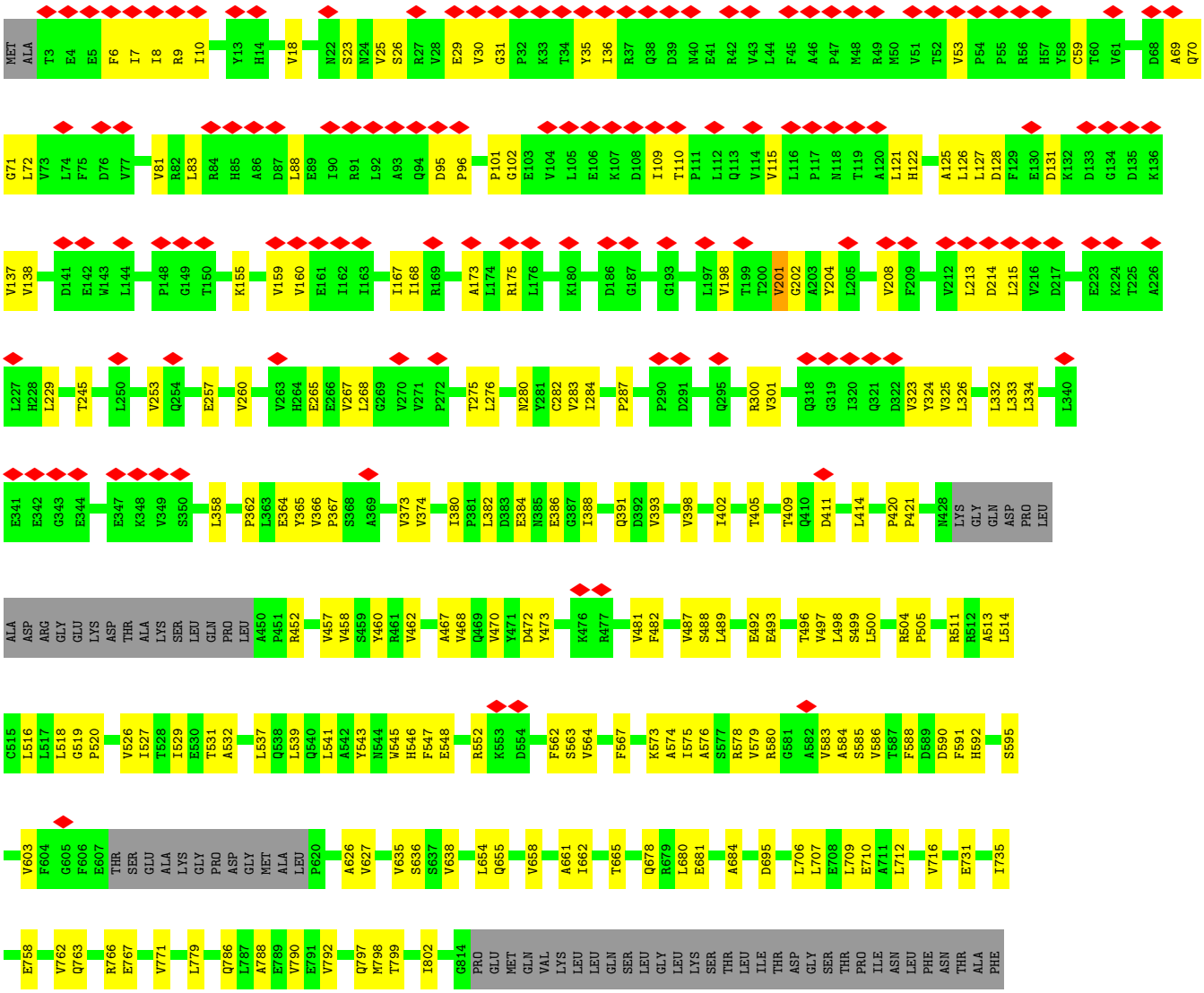
Chain TB:

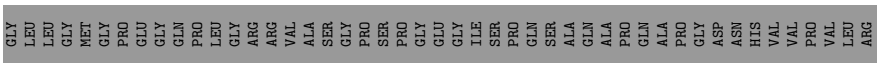




• Molecule 1: Major vault protein

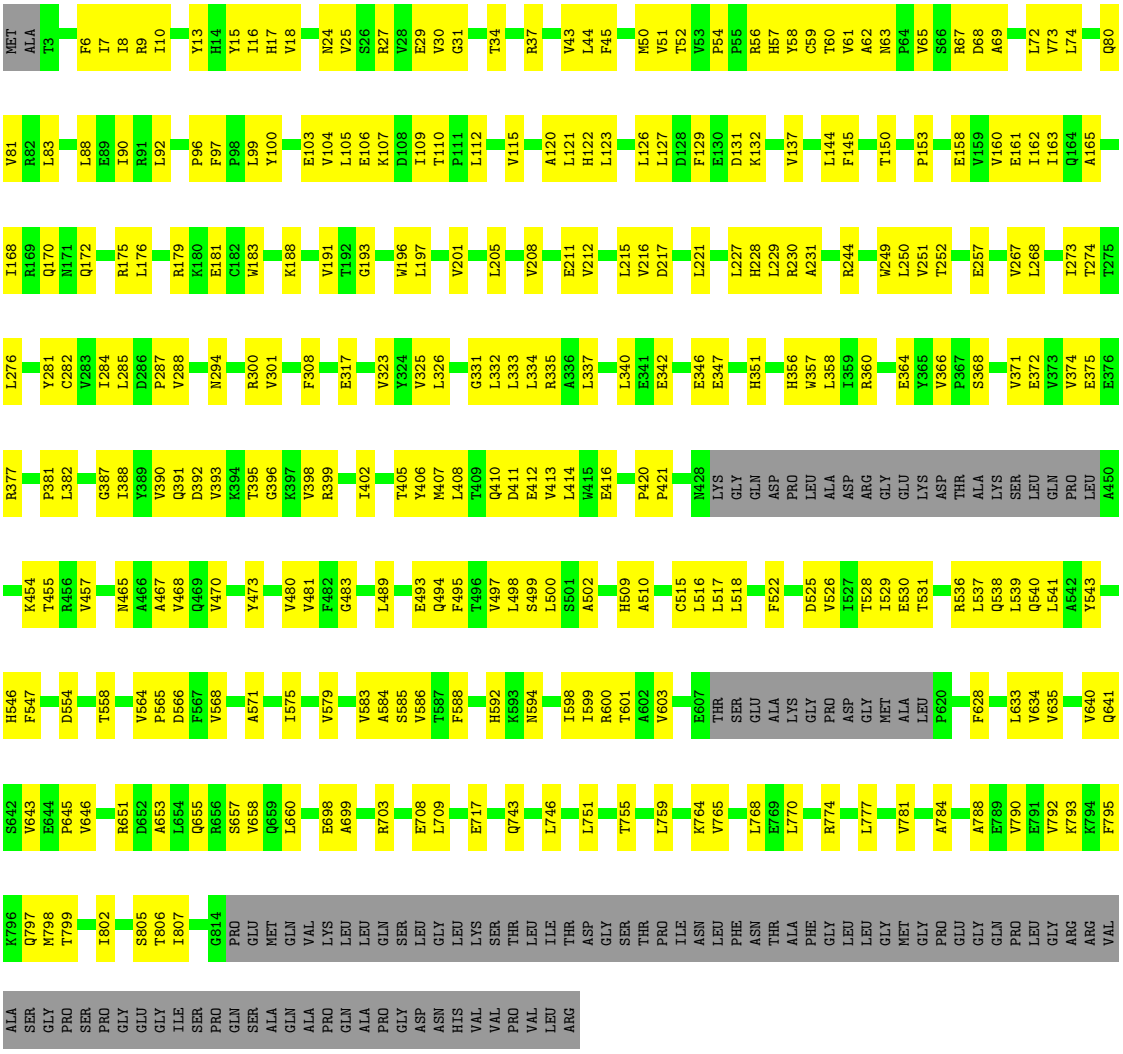
Chain UA:





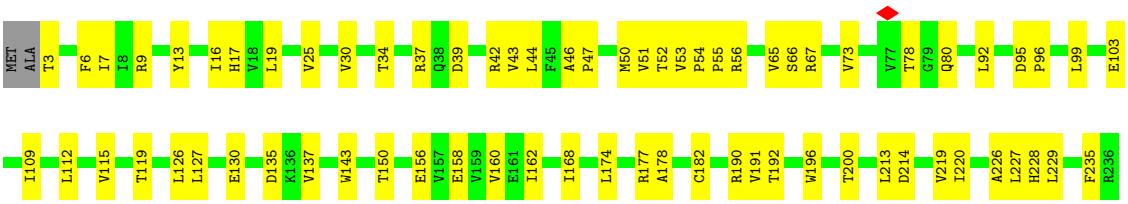
• Molecule 1: Major vault protein

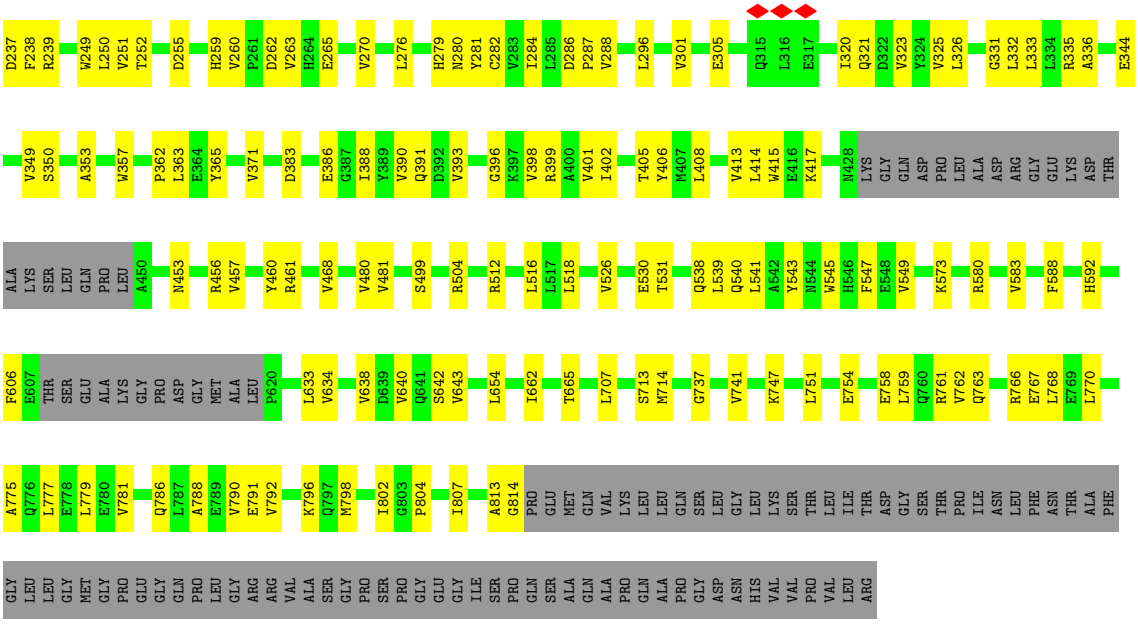
Chain UB:



• Molecule 1: Major vault protein

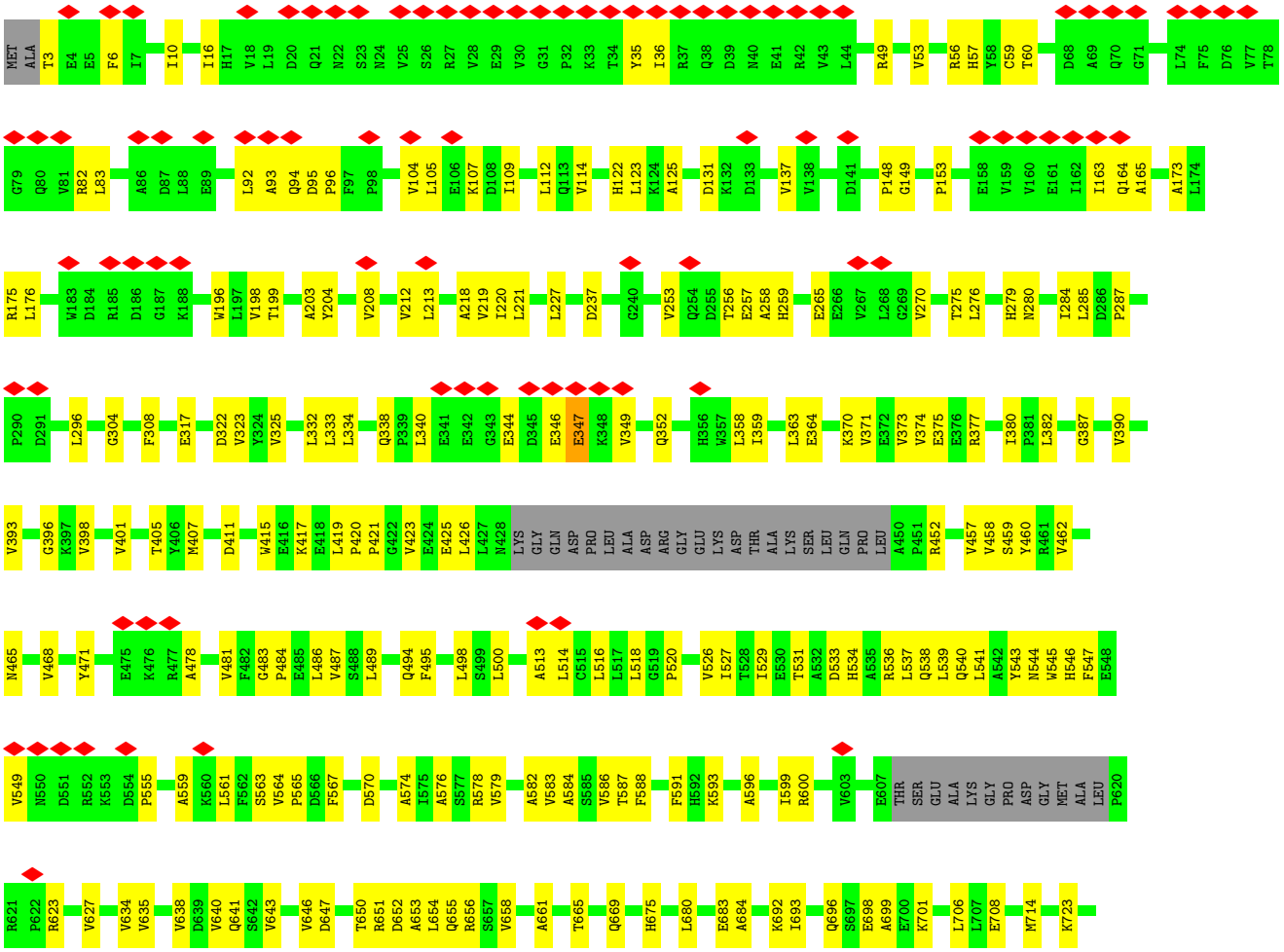
Chain V:

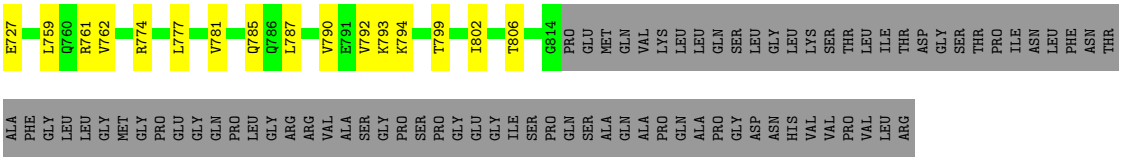




• Molecule 1: Major vault protein

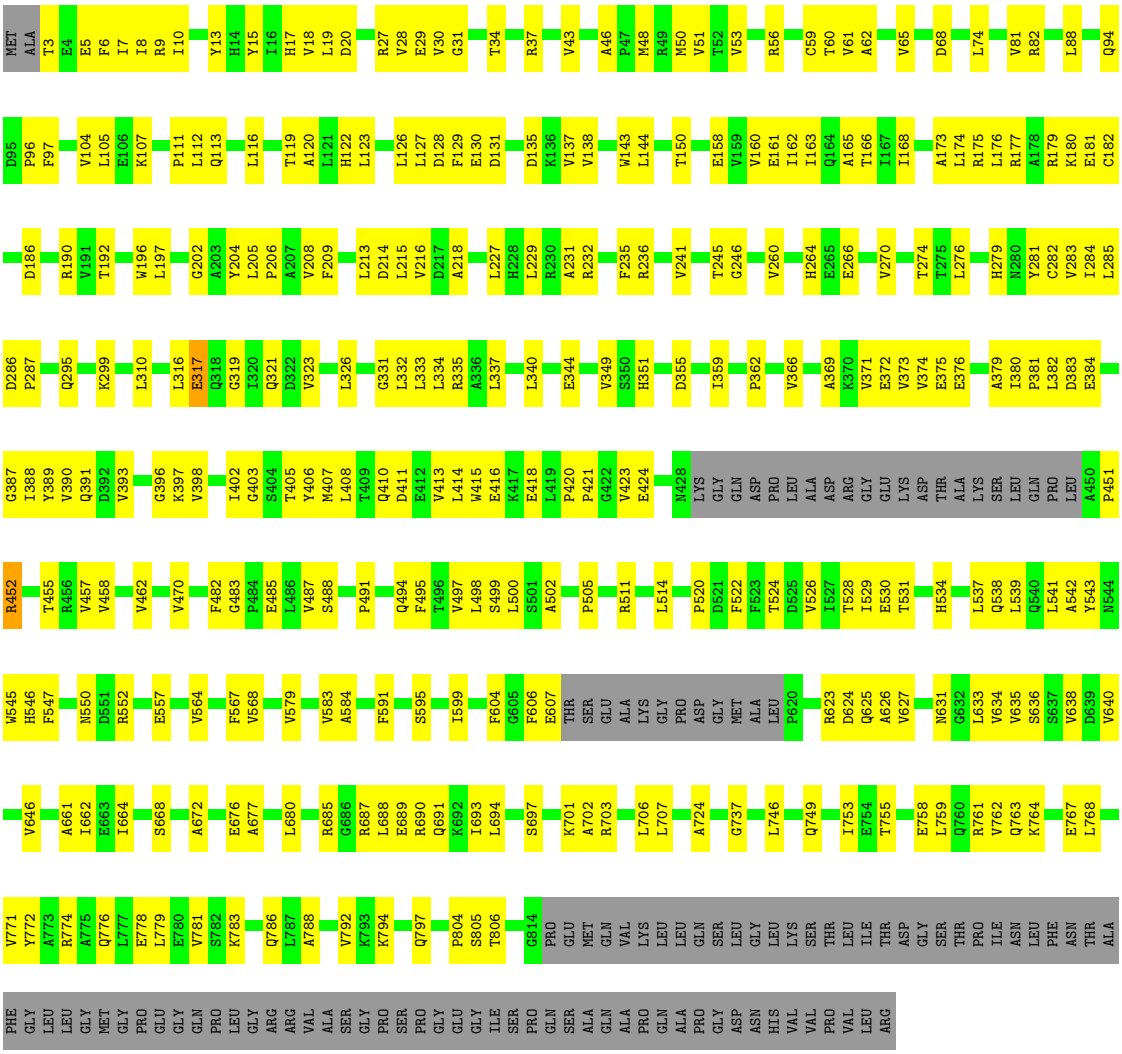
Chain VA:





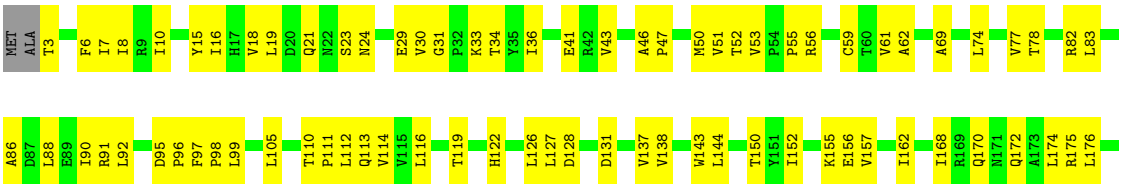
• Molecule 1: Major vault protein

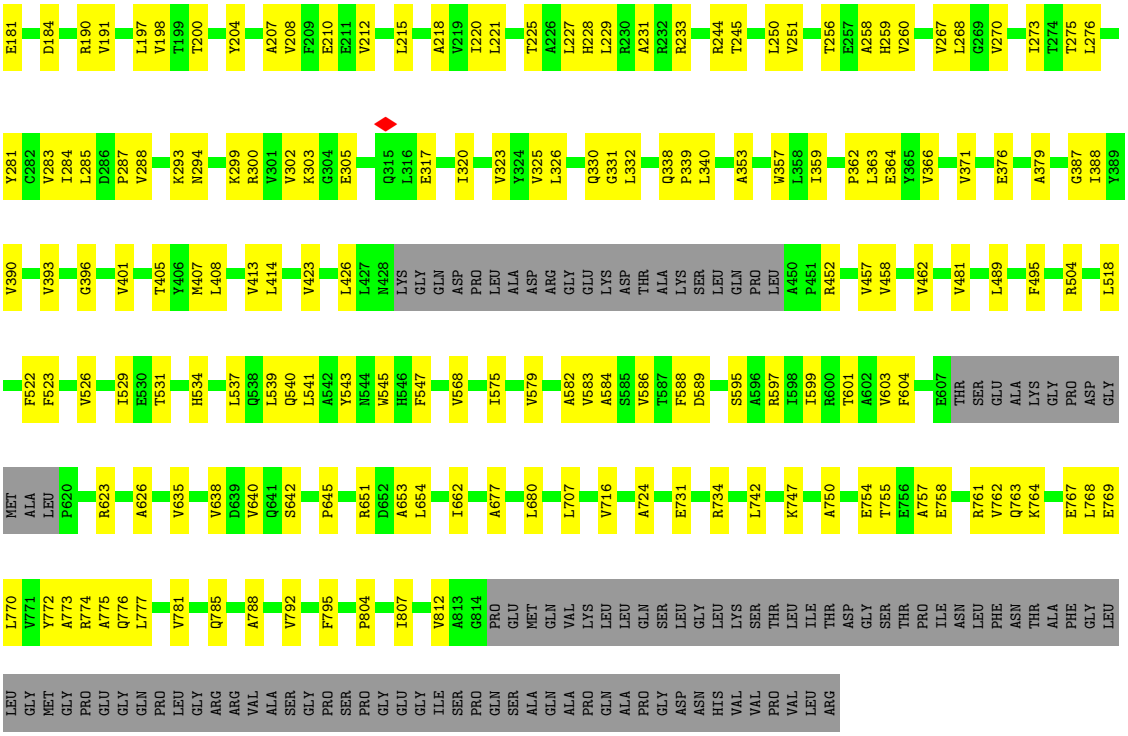
Chain VB:



• Molecule 1: Major vault protein

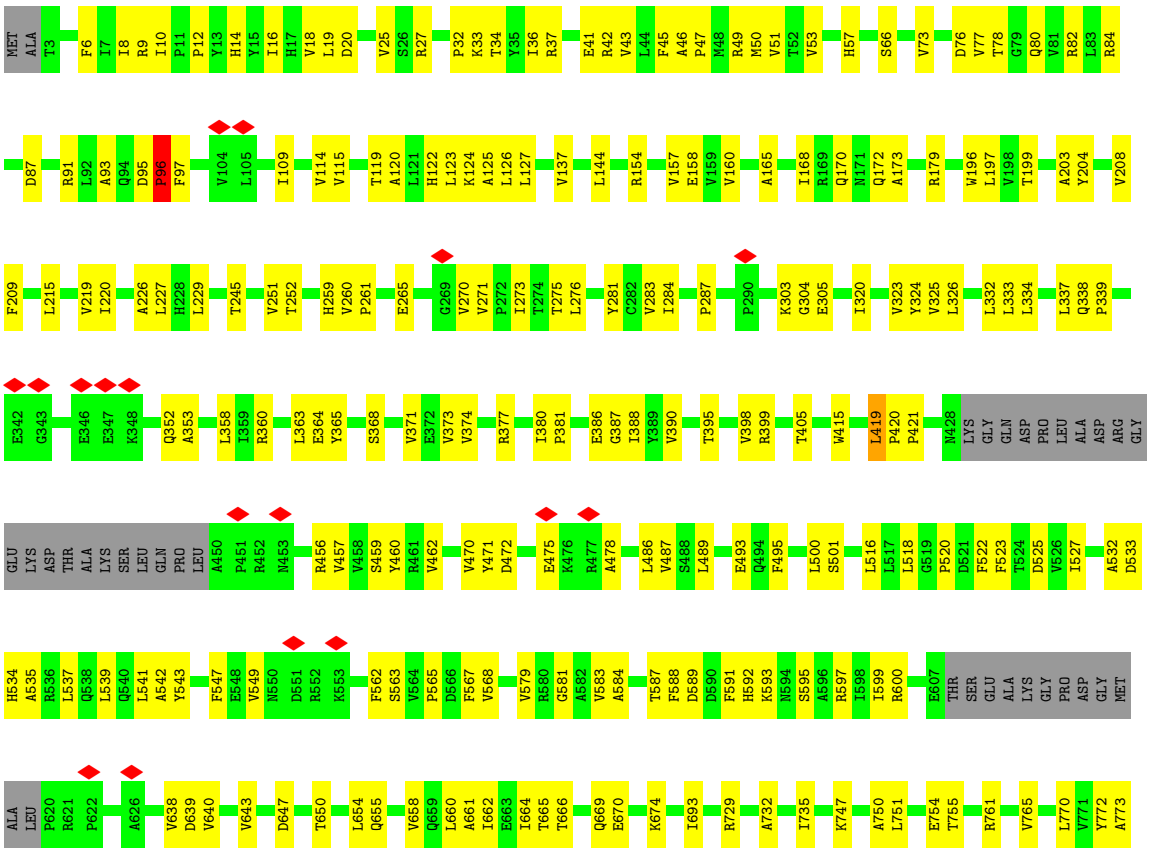
Chain W:

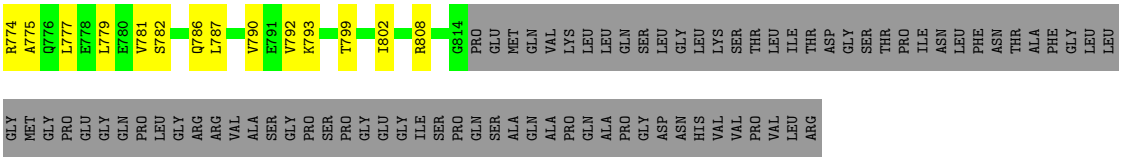




• Molecule 1: Major vault protein

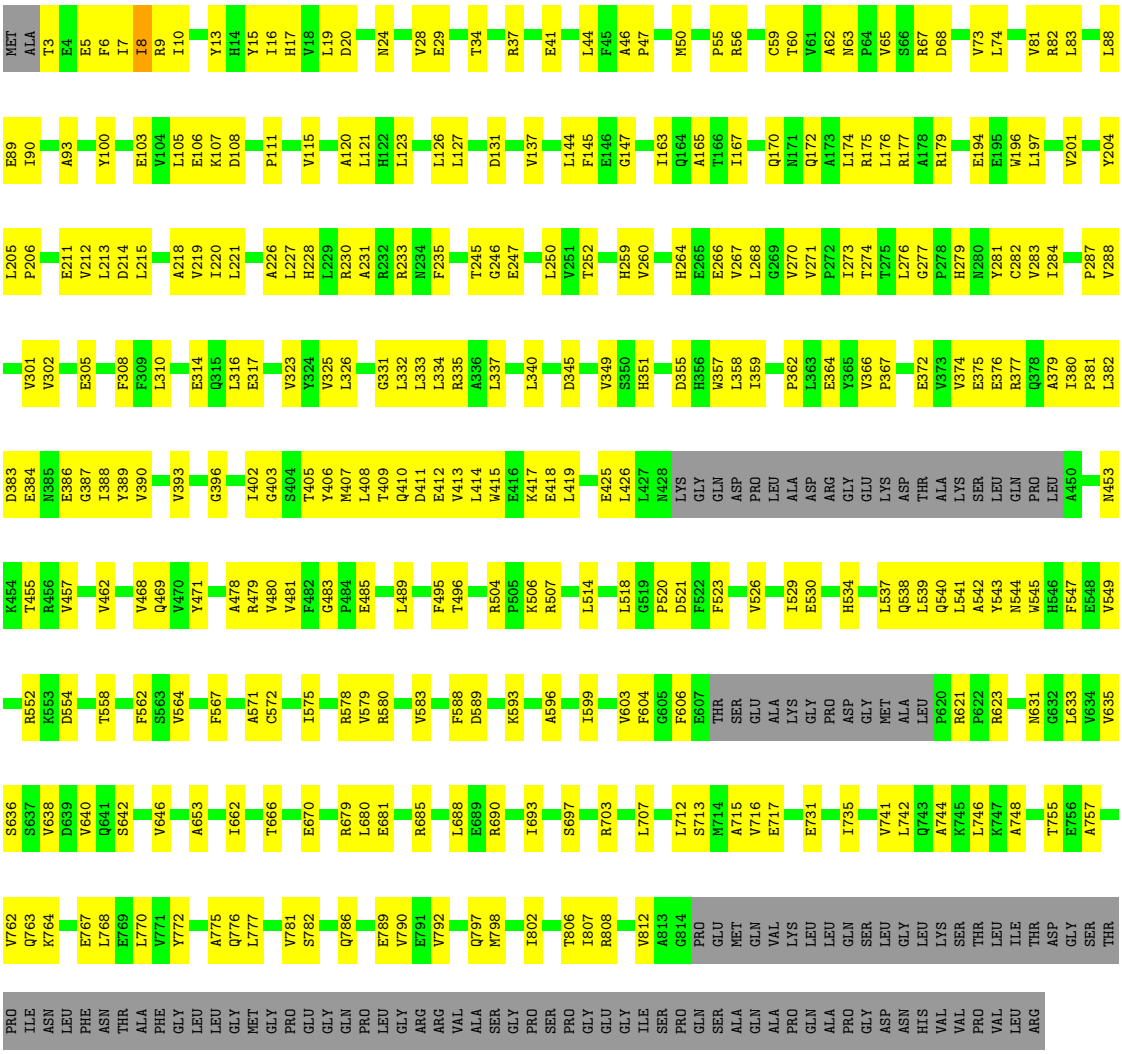
Chain WA:





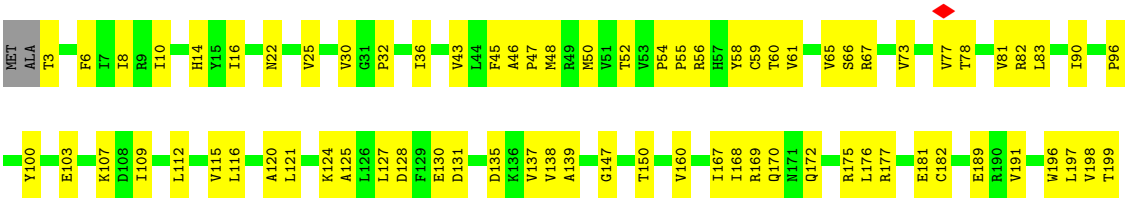
• Molecule 1: Major vault protein

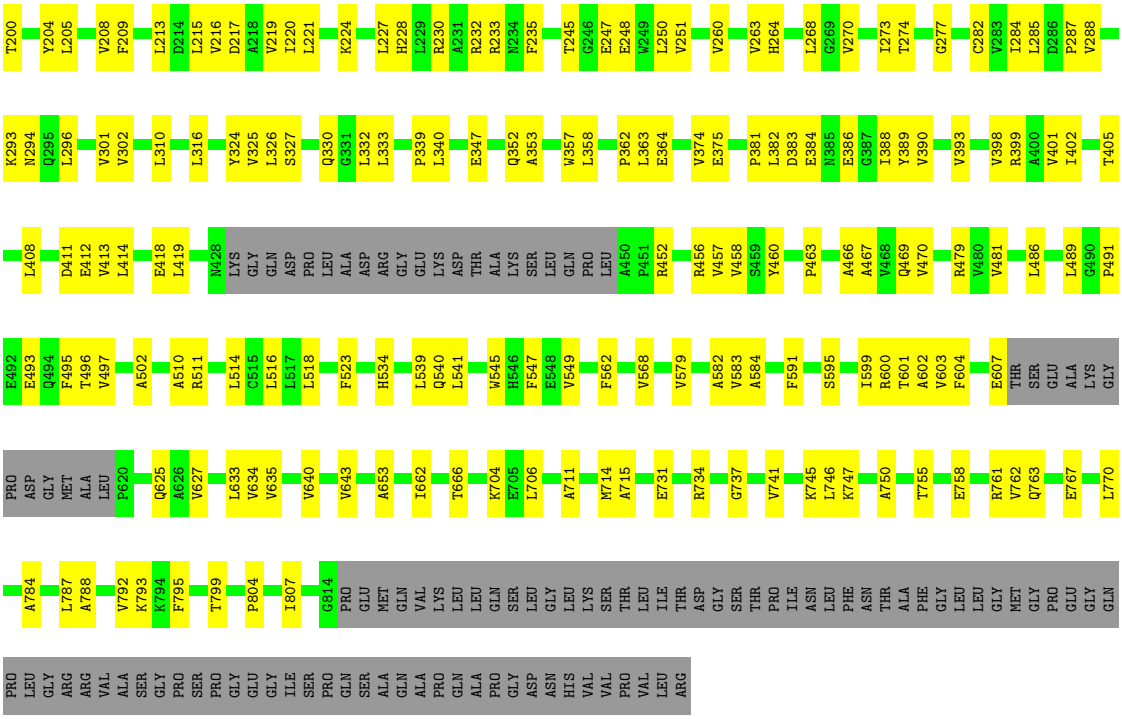
Chain WB:



• Molecule 1: Major vault protein

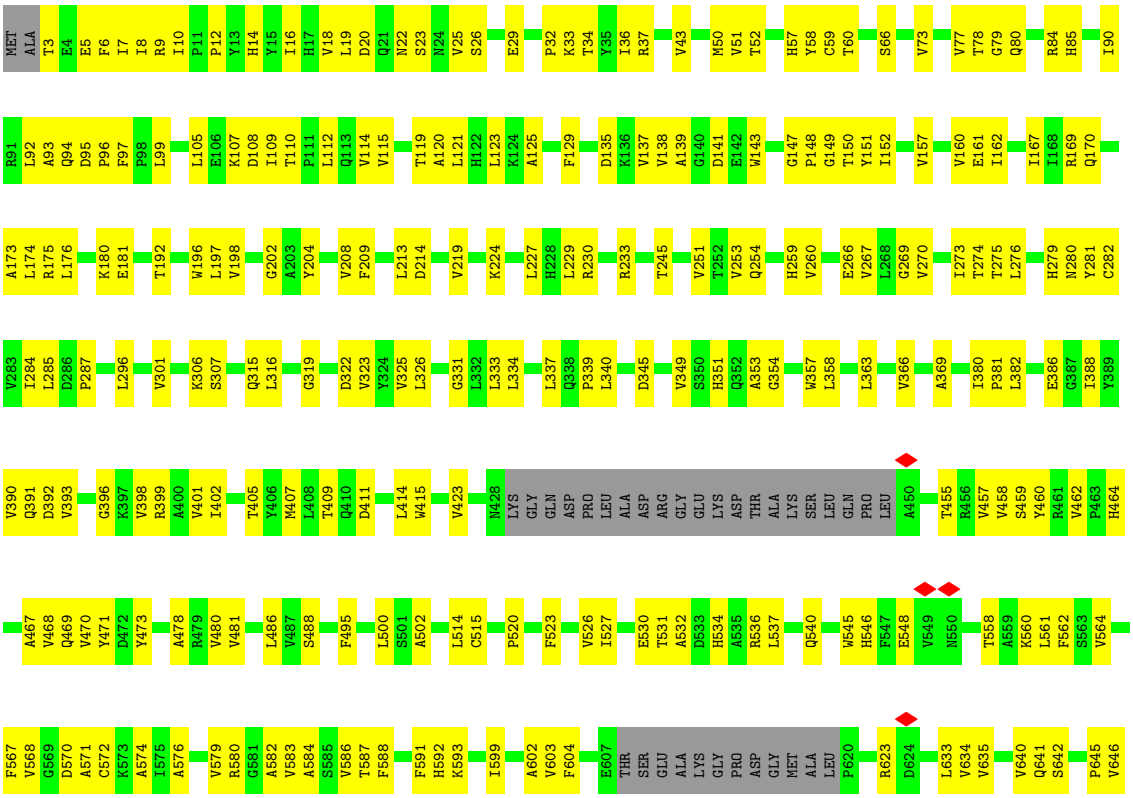
Chain X:

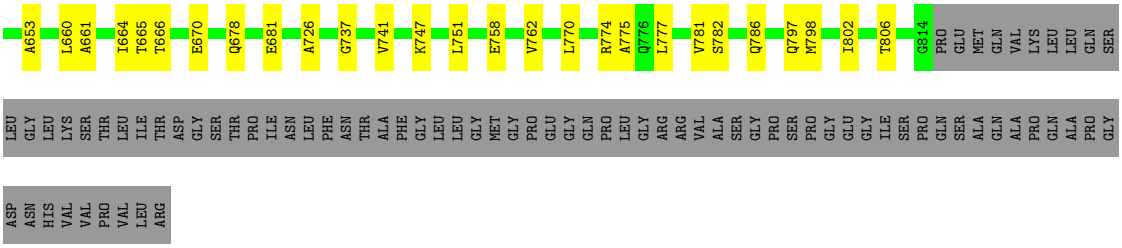




• Molecule 1: Major vault protein

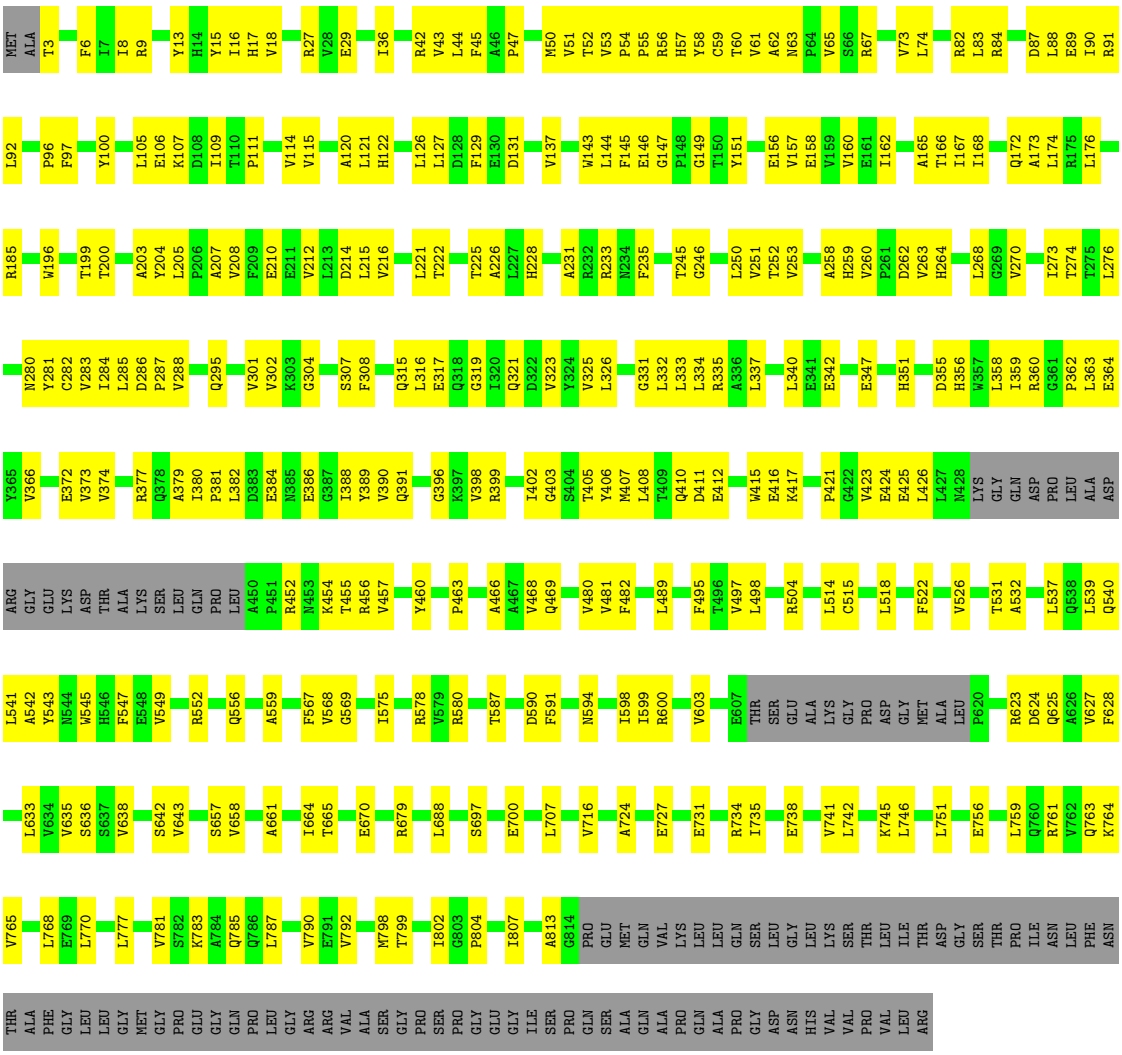
Chain XA: 57% 30% 13%





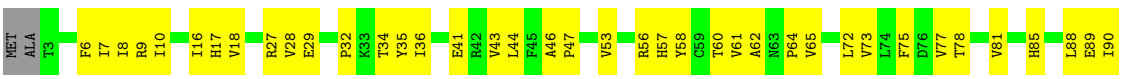
• Molecule 1: Major vault protein

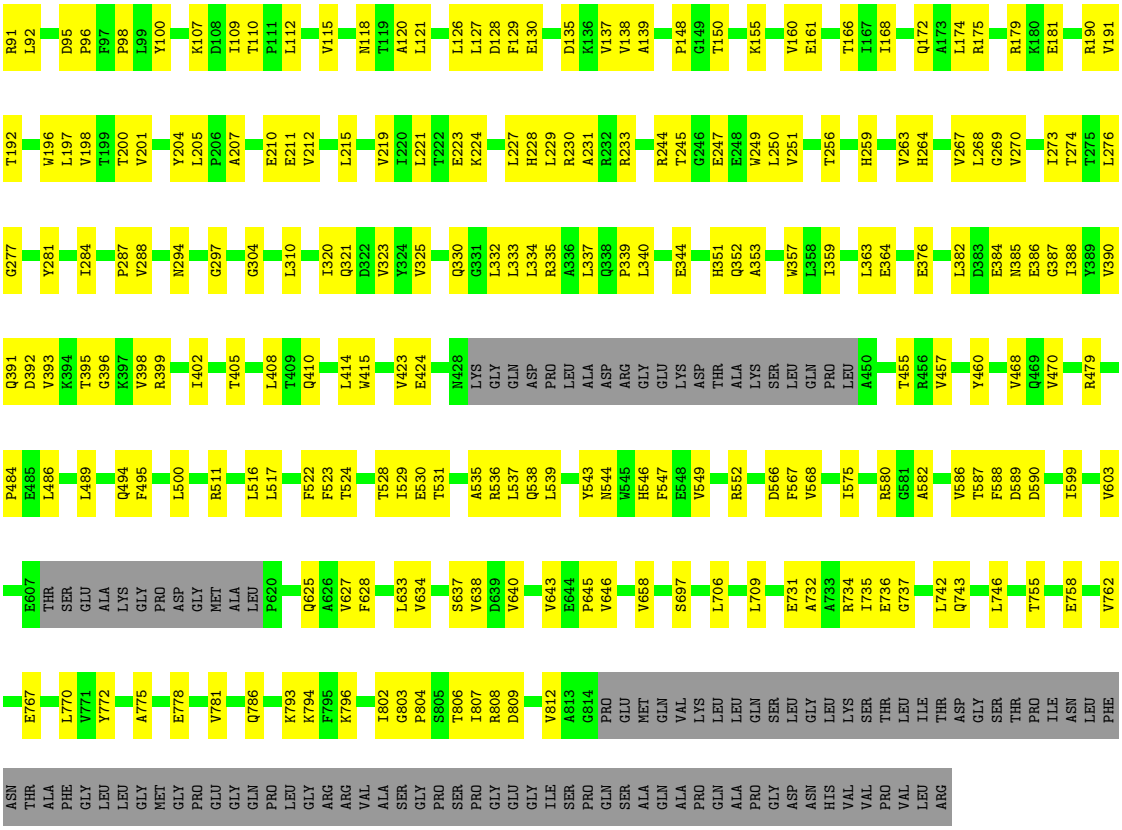
Chain XB:



• Molecule 1: Major vault protein

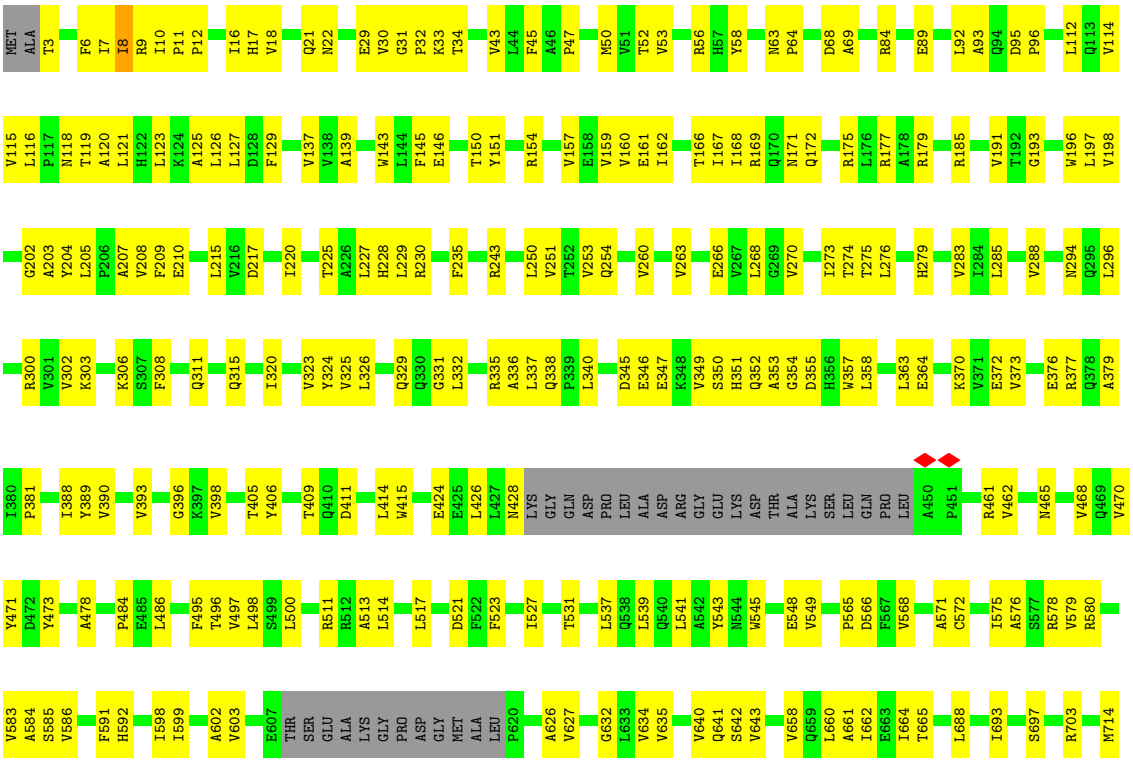
Chain Y:

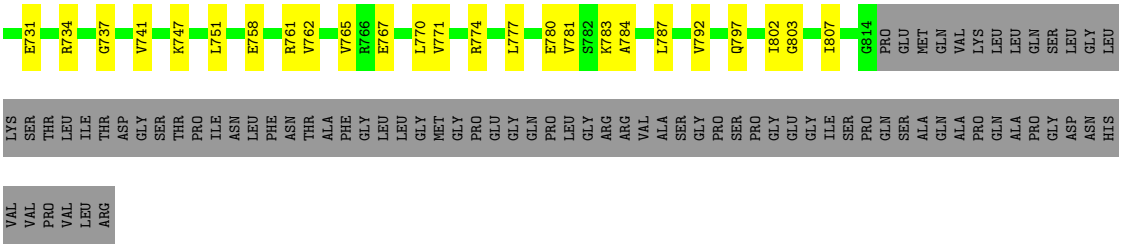




• Molecule 1: Major vault protein

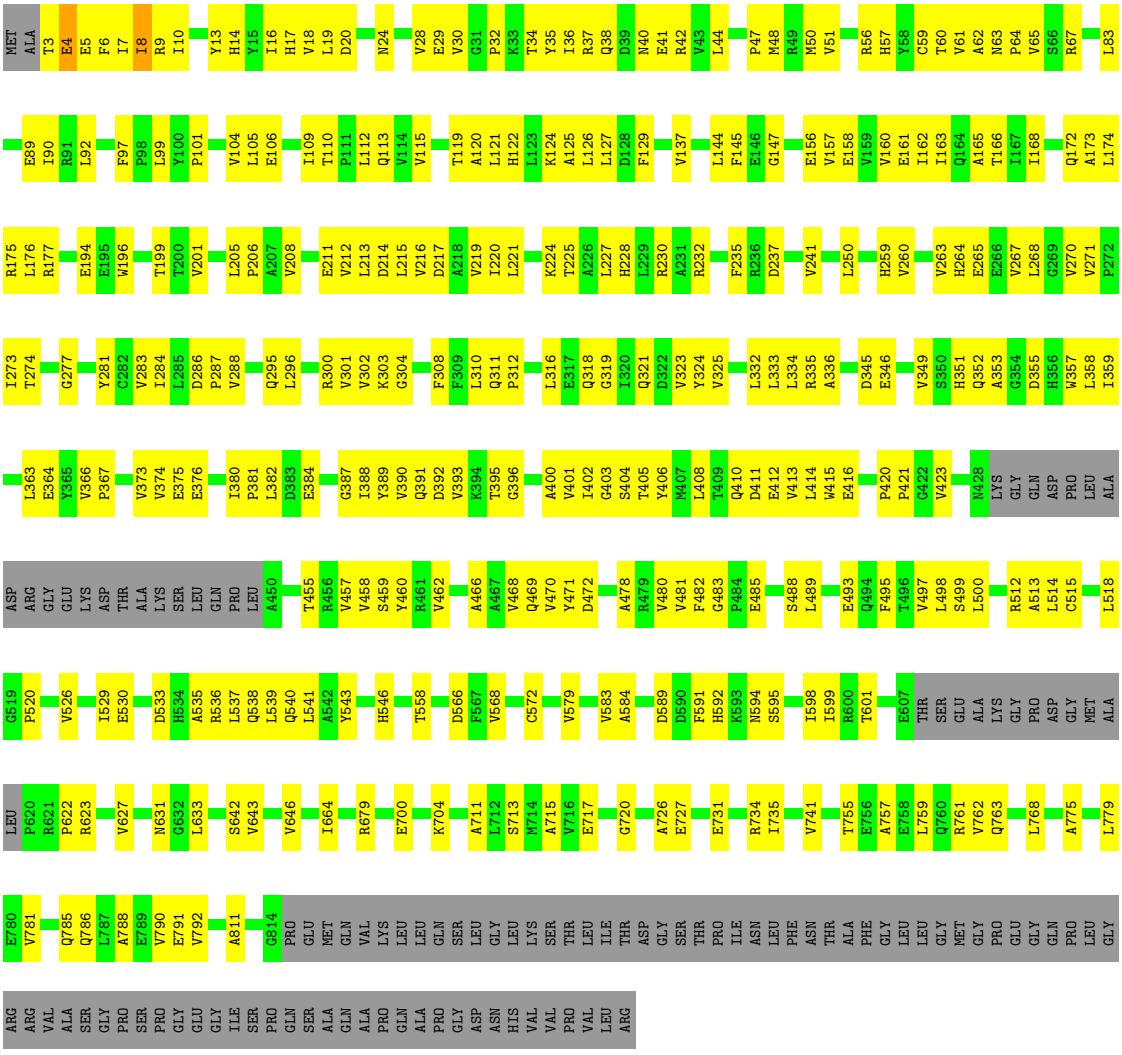
Chain YA:





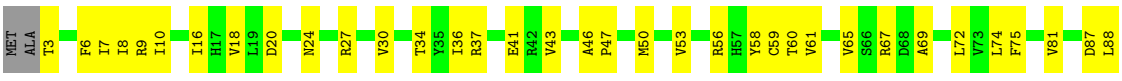
• Molecule 1: Major vault protein

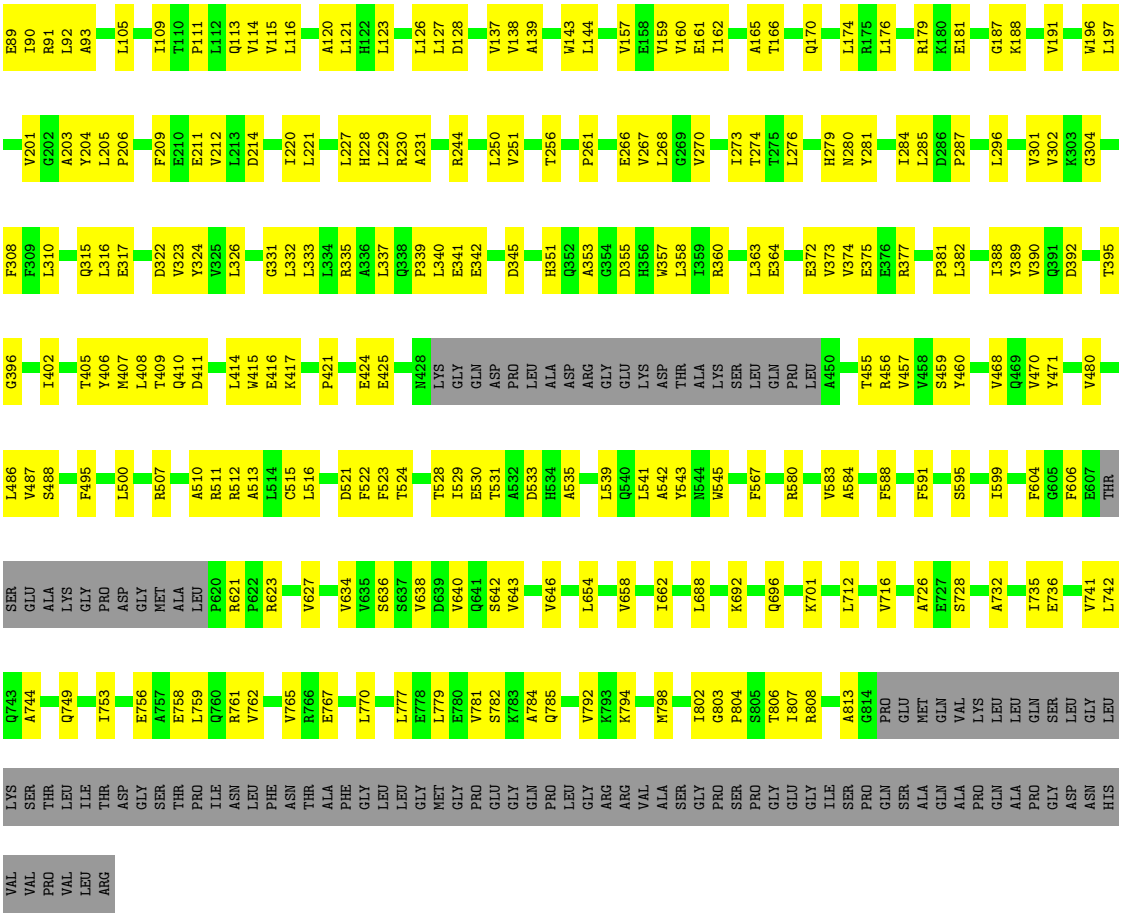
Chain YB:



• Molecule 1: Major vault protein

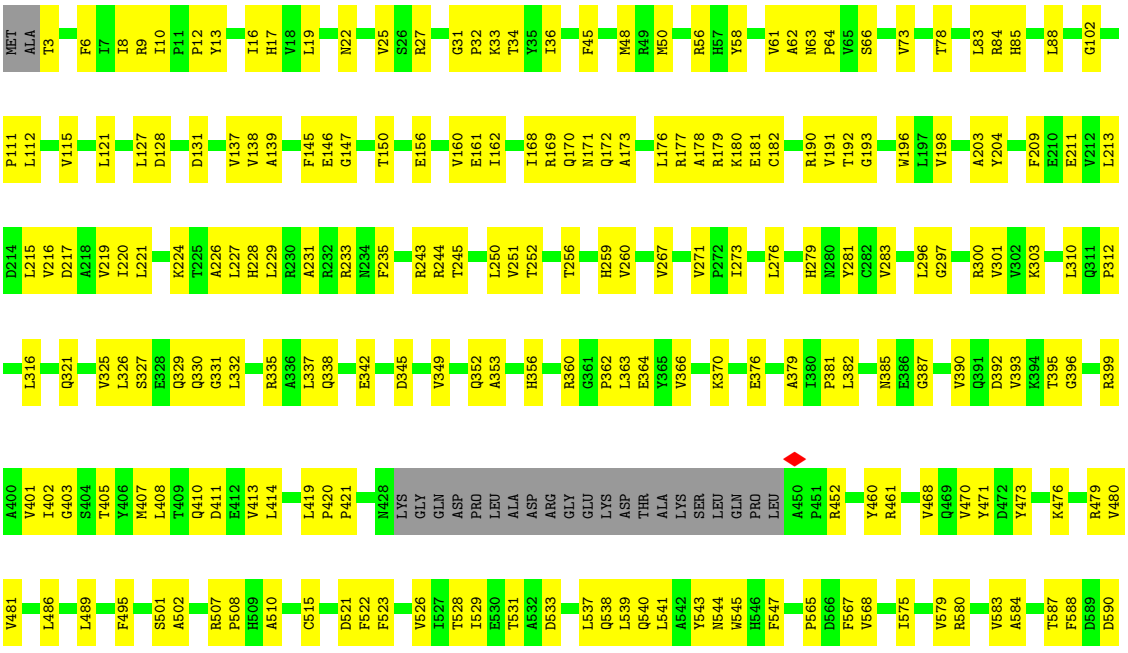
Chain Z:

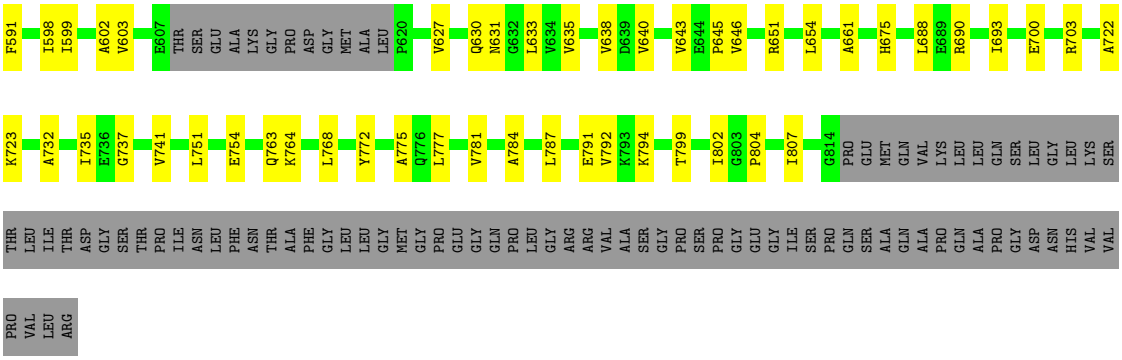




• Molecule 1: Major vault protein

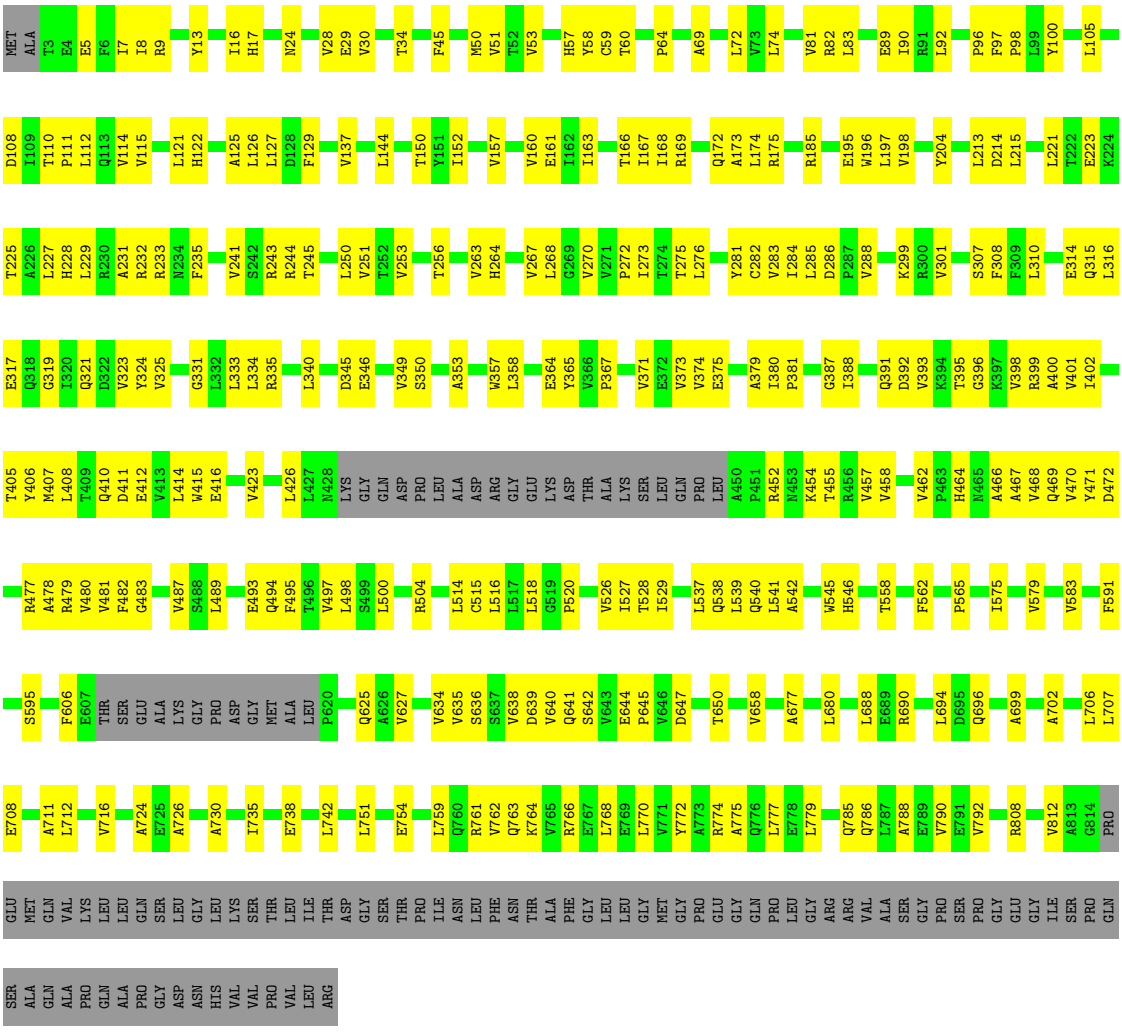
Chain ZA:





• Molecule 1: Major vault protein

Chain ZB:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23998	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.15	Depositor
Minimum defocus (nm)	551	Depositor
Maximum defocus (nm)	2330	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.709	Depositor
Minimum map value	-0.418	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.095	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	861.7984, 861.7984, 861.7984	wwPDB
Map dimensions	1024, 1024, 1024	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8416, 0.8416, 0.8416	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	0.24	0/6291	0.45	0/8533
1	AA	0.19	0/6291	0.44	0/8533
1	AB	0.17	0/6291	0.45	0/8533
1	AC	0.17	0/6291	0.45	0/8533
1	B	0.23	0/6291	0.45	0/8533
1	BA	0.20	0/6291	0.45	0/8533
1	BB	0.17	0/6291	0.43	0/8533
1	C	0.24	0/6291	0.46	0/8533
1	CA	0.20	0/6291	0.46	0/8533
1	CB	0.18	0/6291	0.43	0/8533
1	D	0.24	0/6291	0.45	0/8533
1	DA	0.21	0/6291	0.46	0/8533
1	DB	0.19	0/6291	0.44	0/8533
1	E	0.24	0/6291	0.46	0/8533
1	EA	0.22	0/6291	0.45	0/8533
1	EB	0.20	0/6291	0.45	0/8533
1	F	0.23	0/6291	0.46	0/8533
1	FA	0.23	0/6291	0.45	0/8533
1	FB	0.20	0/6291	0.44	0/8533
1	G	0.22	0/6291	0.45	0/8533
1	GA	0.22	0/6291	0.45	0/8533
1	GB	0.21	0/6291	0.45	0/8533
1	H	0.24	0/6291	0.46	1/8533 (0.0%)
1	HA	0.23	0/6291	0.45	0/8533
1	HB	0.21	0/6291	0.44	0/8533
1	I	0.23	0/6291	0.48	2/8533 (0.0%)
1	IA	0.23	0/6291	0.45	0/8533
1	IB	0.22	0/6291	0.46	0/8533
1	J	0.21	0/6291	0.45	0/8533
1	JA	0.23	0/6291	0.45	0/8533
1	JB	0.22	0/6291	0.46	0/8533
1	K	0.20	0/6291	0.44	0/8533
1	KA	0.23	0/6291	0.45	0/8533
1	KB	0.22	0/6291	0.45	0/8533

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	L	0.20	0/6291	0.44	0/8533
1	LA	0.23	0/6291	0.45	0/8533
1	LB	0.23	0/6291	0.46	0/8533
1	M	0.19	0/6291	0.44	0/8533
1	MA	0.24	0/6291	0.46	0/8533
1	MB	0.22	0/6291	0.45	0/8533
1	N	0.19	0/6291	0.44	0/8533
1	NA	0.24	0/6291	0.45	0/8533
1	NB	0.23	0/6291	0.45	0/8533
1	O	0.18	0/6291	0.44	0/8533
1	OA	0.16	0/6291	0.44	0/8533
1	OB	0.22	0/6291	0.44	0/8533
1	P	0.18	0/6291	0.43	0/8533
1	PA	0.16	0/6291	0.44	0/8533
1	PB	0.22	0/6291	0.45	0/8533
1	Q	0.19	0/6291	0.45	0/8533
1	QA	0.16	0/6291	0.45	0/8533
1	QB	0.22	0/6291	0.45	0/8533
1	R	0.16	0/6291	0.43	0/8533
1	RA	0.15	0/6291	0.43	0/8533
1	RB	0.21	0/6291	0.44	0/8533
1	S	0.16	0/6291	0.41	0/8533
1	SA	0.17	0/6291	0.43	0/8533
1	SB	0.22	0/6291	0.45	0/8533
1	T	0.16	0/6291	0.42	0/8533
1	TA	0.14	0/6291	0.41	0/8533
1	TB	0.21	0/6291	0.45	0/8533
1	UA	0.14	0/6291	0.41	0/8533
1	UB	0.21	0/6291	0.45	0/8533
1	V	0.17	0/6291	0.43	0/8533
1	VA	0.14	0/6291	0.43	0/8533
1	VB	0.21	0/6291	0.45	0/8533
1	W	0.17	0/6291	0.44	0/8533
1	WA	0.17	0/6291	0.46	0/8533
1	WB	0.20	0/6291	0.45	0/8533
1	X	0.17	0/6291	0.43	0/8533
1	XA	0.16	0/6291	0.44	0/8533
1	XB	0.19	0/6291	0.46	0/8533
1	Y	0.18	0/6291	0.43	0/8533
1	YA	0.16	0/6291	0.45	0/8533
1	YB	0.18	0/6291	0.45	0/8533
1	Z	0.19	0/6291	0.44	0/8533
1	ZA	0.16	0/6291	0.44	0/8533

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	ZB	0.17	0/6291	0.44	0/8533
All	All	0.20	0/490698	0.45	3/665574 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	84	ARG	N-CA-C	-6.73	102.17	110.65
1	H	411	ASP	CA-CB-CG	5.23	117.83	112.60
1	I	83	LEU	N-CA-CB	-5.22	102.05	110.81

There are no chirality outliers.

There are no planarity outliers.

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	6181	0	6203	231	0
1	AA	6181	0	6203	249	0
1	AB	6181	0	6203	261	0
1	AC	6181	0	6203	261	0
1	B	6181	0	6203	236	0
1	BA	6181	0	6203	270	0
1	BB	6181	0	6203	230	0
1	C	6181	0	6203	247	0
1	CA	6181	0	6203	258	0
1	CB	6181	0	6203	237	0
1	D	6181	0	6203	266	0
1	DA	6181	0	6203	299	0
1	DB	6181	0	6203	203	0
1	E	6181	0	6203	250	0
1	EA	6181	0	6203	241	0
1	EB	6181	0	6203	217	0
1	F	6181	0	6203	238	0
1	FA	6181	0	6203	248	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	FB	6181	0	6203	234	0
1	G	6181	0	6203	236	0
1	GA	6181	0	6203	229	0
1	GB	6181	0	6203	250	0
1	H	6181	0	6203	266	0
1	HA	6181	0	6203	229	0
1	HB	6181	0	6203	220	0
1	I	6181	0	6203	279	0
1	IA	6181	0	6203	242	0
1	IB	6181	0	6203	264	0
1	J	6181	0	6203	259	0
1	JA	6181	0	6203	229	0
1	JB	6181	0	6203	291	0
1	K	6181	0	6203	269	0
1	KA	6181	0	6203	224	0
1	KB	6181	0	6203	262	0
1	L	6181	0	6203	210	0
1	LA	6181	0	6203	253	0
1	LB	6181	0	6203	248	0
1	M	6181	0	6203	222	0
1	MA	6181	0	6203	262	0
1	MB	6181	0	6203	255	0
1	N	6181	0	6203	232	0
1	NA	6181	0	6203	255	0
1	NB	6181	0	6203	259	0
1	O	6181	0	6203	259	0
1	OA	6181	0	6203	317	0
1	OB	6181	0	6203	259	0
1	P	6181	0	6203	236	0
1	PA	6181	0	6203	288	0
1	PB	6181	0	6203	259	0
1	Q	6181	0	6203	228	0
1	QA	6181	0	6203	289	0
1	QB	6181	0	6203	232	0
1	R	6181	0	6203	180	0
1	RA	6181	0	6203	241	0
1	RB	6181	0	6203	262	0
1	S	6181	0	6203	174	0
1	SA	6181	0	6203	182	0
1	SB	6181	0	6203	241	0
1	T	6181	0	6203	176	0
1	TA	6181	0	6203	212	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	TB	6181	0	6203	264	0
1	UA	6181	0	6203	191	0
1	UB	6181	0	6203	276	0
1	V	6181	0	6203	201	0
1	VA	6181	0	6203	220	0
1	VB	6181	0	6203	277	0
1	W	6181	0	6203	256	0
1	WA	6181	0	6203	244	0
1	WB	6181	0	6203	298	0
1	X	6181	0	6203	229	0
1	XA	6181	0	6203	267	0
1	XB	6181	0	6203	303	0
1	Y	6181	0	6203	235	0
1	YA	6181	0	6203	253	0
1	YB	6181	0	6203	326	0
1	Z	6181	0	6203	244	0
1	ZA	6181	0	6203	244	0
1	ZB	6181	0	6203	267	0
All	All	482118	0	483834	17748	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 18.

The worst 5 of 17748 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QB:18:VAL:HG12	1:QB:43:VAL:HG12	1.29	1.14
1:C:81:VAL:HG13	1:C:83:LEU:HD11	1.33	1.07
1:P:215:LEU:O	1:P:215:LEU:HD12	1.54	1.07
1:UA:470:VAL:HG13	1:UA:481:VAL:HG21	1.35	1.01
1:D:529:ILE:HD12	1:D:583:VAL:HG21	1.39	1.00

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	773/893 (87%)	646 (84%)	126 (16%)	1 (0%)	48	83
1	AA	773/893 (87%)	637 (82%)	135 (18%)	1 (0%)	48	83
1	AB	773/893 (87%)	650 (84%)	123 (16%)	0	100	100
1	AC	773/893 (87%)	647 (84%)	126 (16%)	0	100	100
1	B	773/893 (87%)	659 (85%)	114 (15%)	0	100	100
1	BA	773/893 (87%)	638 (82%)	134 (17%)	1 (0%)	48	83
1	BB	773/893 (87%)	672 (87%)	101 (13%)	0	100	100
1	C	773/893 (87%)	644 (83%)	128 (17%)	1 (0%)	48	83
1	CA	773/893 (87%)	631 (82%)	142 (18%)	0	100	100
1	CB	773/893 (87%)	640 (83%)	132 (17%)	1 (0%)	48	83
1	D	773/893 (87%)	664 (86%)	108 (14%)	1 (0%)	48	83
1	DA	773/893 (87%)	634 (82%)	139 (18%)	0	100	100
1	DB	773/893 (87%)	654 (85%)	119 (15%)	0	100	100
1	E	773/893 (87%)	650 (84%)	123 (16%)	0	100	100
1	EA	773/893 (87%)	642 (83%)	130 (17%)	1 (0%)	48	83
1	EB	773/893 (87%)	649 (84%)	124 (16%)	0	100	100
1	F	773/893 (87%)	659 (85%)	113 (15%)	1 (0%)	48	83
1	FA	773/893 (87%)	629 (81%)	144 (19%)	0	100	100
1	FB	773/893 (87%)	648 (84%)	125 (16%)	0	100	100
1	G	773/893 (87%)	640 (83%)	133 (17%)	0	100	100
1	GA	773/893 (87%)	646 (84%)	127 (16%)	0	100	100
1	GB	773/893 (87%)	640 (83%)	132 (17%)	1 (0%)	48	83
1	H	773/893 (87%)	655 (85%)	118 (15%)	0	100	100
1	HA	773/893 (87%)	642 (83%)	129 (17%)	2 (0%)	36	71
1	HB	773/893 (87%)	655 (85%)	118 (15%)	0	100	100
1	I	773/893 (87%)	657 (85%)	115 (15%)	1 (0%)	48	83
1	IA	773/893 (87%)	648 (84%)	124 (16%)	1 (0%)	48	83
1	IB	773/893 (87%)	649 (84%)	122 (16%)	2 (0%)	36	71
1	J	773/893 (87%)	649 (84%)	124 (16%)	0	100	100
1	JA	773/893 (87%)	641 (83%)	132 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	JB	773/893 (87%)	647 (84%)	125 (16%)	1 (0%)	48 83
1	K	773/893 (87%)	651 (84%)	122 (16%)	0	100 100
1	KA	773/893 (87%)	643 (83%)	130 (17%)	0	100 100
1	KB	773/893 (87%)	666 (86%)	107 (14%)	0	100 100
1	L	773/893 (87%)	652 (84%)	119 (15%)	2 (0%)	36 71
1	LA	773/893 (87%)	655 (85%)	117 (15%)	1 (0%)	48 83
1	LB	773/893 (87%)	658 (85%)	115 (15%)	0	100 100
1	M	773/893 (87%)	655 (85%)	118 (15%)	0	100 100
1	MA	773/893 (87%)	638 (82%)	135 (18%)	0	100 100
1	MB	773/893 (87%)	656 (85%)	117 (15%)	0	100 100
1	N	773/893 (87%)	657 (85%)	116 (15%)	0	100 100
1	NA	773/893 (87%)	646 (84%)	127 (16%)	0	100 100
1	NB	773/893 (87%)	653 (84%)	119 (15%)	1 (0%)	48 83
1	O	773/893 (87%)	652 (84%)	121 (16%)	0	100 100
1	OA	773/893 (87%)	661 (86%)	112 (14%)	0	100 100
1	OB	773/893 (87%)	655 (85%)	118 (15%)	0	100 100
1	P	773/893 (87%)	668 (86%)	105 (14%)	0	100 100
1	PA	773/893 (87%)	646 (84%)	127 (16%)	0	100 100
1	PB	773/893 (87%)	654 (85%)	119 (15%)	0	100 100
1	Q	773/893 (87%)	654 (85%)	118 (15%)	1 (0%)	48 83
1	QA	773/893 (87%)	640 (83%)	133 (17%)	0	100 100
1	QB	773/893 (87%)	664 (86%)	107 (14%)	2 (0%)	36 71
1	R	773/893 (87%)	654 (85%)	118 (15%)	1 (0%)	48 83
1	RA	773/893 (87%)	655 (85%)	118 (15%)	0	100 100
1	RB	773/893 (87%)	671 (87%)	100 (13%)	2 (0%)	36 71
1	S	773/893 (87%)	677 (88%)	96 (12%)	0	100 100
1	SA	773/893 (87%)	681 (88%)	90 (12%)	2 (0%)	36 71
1	SB	773/893 (87%)	643 (83%)	128 (17%)	2 (0%)	36 71
1	T	773/893 (87%)	665 (86%)	107 (14%)	1 (0%)	48 83
1	TA	773/893 (87%)	679 (88%)	93 (12%)	1 (0%)	48 83
1	TB	773/893 (87%)	654 (85%)	119 (15%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	UA	773/893 (87%)	662 (86%)	108 (14%)	3 (0%)	30 67
1	UB	773/893 (87%)	665 (86%)	108 (14%)	0	100 100
1	V	773/893 (87%)	665 (86%)	108 (14%)	0	100 100
1	VA	773/893 (87%)	652 (84%)	120 (16%)	1 (0%)	48 83
1	VB	773/893 (87%)	654 (85%)	117 (15%)	2 (0%)	36 71
1	W	773/893 (87%)	647 (84%)	126 (16%)	0	100 100
1	WA	773/893 (87%)	662 (86%)	109 (14%)	2 (0%)	36 71
1	WB	773/893 (87%)	666 (86%)	106 (14%)	1 (0%)	48 83
1	X	773/893 (87%)	656 (85%)	116 (15%)	1 (0%)	48 83
1	XA	773/893 (87%)	669 (86%)	104 (14%)	0	100 100
1	XB	773/893 (87%)	643 (83%)	130 (17%)	0	100 100
1	Y	773/893 (87%)	650 (84%)	123 (16%)	0	100 100
1	YA	773/893 (87%)	654 (85%)	118 (15%)	1 (0%)	48 83
1	YB	773/893 (87%)	666 (86%)	104 (14%)	3 (0%)	30 67
1	Z	773/893 (87%)	645 (83%)	128 (17%)	0	100 100
1	ZA	773/893 (87%)	668 (86%)	105 (14%)	0	100 100
1	ZB	773/893 (87%)	660 (85%)	113 (15%)	0	100 100
All	All	60294/69654 (87%)	50949 (84%)	9299 (15%)	46 (0%)	49 83

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	6	PHE
1	CB	8	ILE
1	EA	452	ARG
1	GB	161	GLU
1	HA	452	ARG

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	666/755 (88%)	666 (100%)	0	100	100
1	AA	666/755 (88%)	666 (100%)	0	100	100
1	AB	666/755 (88%)	666 (100%)	0	100	100
1	AC	666/755 (88%)	666 (100%)	0	100	100
1	B	666/755 (88%)	666 (100%)	0	100	100
1	BA	666/755 (88%)	666 (100%)	0	100	100
1	BB	666/755 (88%)	666 (100%)	0	100	100
1	C	666/755 (88%)	666 (100%)	0	100	100
1	CA	666/755 (88%)	666 (100%)	0	100	100
1	CB	666/755 (88%)	666 (100%)	0	100	100
1	D	666/755 (88%)	666 (100%)	0	100	100
1	DA	666/755 (88%)	666 (100%)	0	100	100
1	DB	666/755 (88%)	666 (100%)	0	100	100
1	E	666/755 (88%)	666 (100%)	0	100	100
1	EA	666/755 (88%)	666 (100%)	0	100	100
1	EB	666/755 (88%)	666 (100%)	0	100	100
1	F	666/755 (88%)	666 (100%)	0	100	100
1	FA	666/755 (88%)	666 (100%)	0	100	100
1	FB	666/755 (88%)	666 (100%)	0	100	100
1	G	666/755 (88%)	666 (100%)	0	100	100
1	GA	666/755 (88%)	666 (100%)	0	100	100
1	GB	666/755 (88%)	666 (100%)	0	100	100
1	H	666/755 (88%)	665 (100%)	1 (0%)	87	85
1	HA	666/755 (88%)	666 (100%)	0	100	100
1	HB	666/755 (88%)	666 (100%)	0	100	100
1	I	666/755 (88%)	665 (100%)	1 (0%)	87	85
1	IA	666/755 (88%)	666 (100%)	0	100	100
1	IB	666/755 (88%)	666 (100%)	0	100	100
1	J	666/755 (88%)	666 (100%)	0	100	100
1	JA	666/755 (88%)	666 (100%)	0	100	100
1	JB	666/755 (88%)	666 (100%)	0	100	100
1	K	666/755 (88%)	666 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	KA	666/755 (88%)	666 (100%)	0	100	100
1	KB	666/755 (88%)	666 (100%)	0	100	100
1	L	666/755 (88%)	666 (100%)	0	100	100
1	LA	666/755 (88%)	666 (100%)	0	100	100
1	LB	666/755 (88%)	666 (100%)	0	100	100
1	M	666/755 (88%)	666 (100%)	0	100	100
1	MA	666/755 (88%)	666 (100%)	0	100	100
1	MB	666/755 (88%)	666 (100%)	0	100	100
1	N	666/755 (88%)	666 (100%)	0	100	100
1	NA	666/755 (88%)	666 (100%)	0	100	100
1	NB	666/755 (88%)	666 (100%)	0	100	100
1	O	666/755 (88%)	666 (100%)	0	100	100
1	OA	666/755 (88%)	666 (100%)	0	100	100
1	OB	666/755 (88%)	666 (100%)	0	100	100
1	P	666/755 (88%)	666 (100%)	0	100	100
1	PA	666/755 (88%)	666 (100%)	0	100	100
1	PB	666/755 (88%)	666 (100%)	0	100	100
1	Q	666/755 (88%)	665 (100%)	1 (0%)	87	85
1	QA	666/755 (88%)	666 (100%)	0	100	100
1	QB	666/755 (88%)	666 (100%)	0	100	100
1	R	666/755 (88%)	666 (100%)	0	100	100
1	RA	666/755 (88%)	666 (100%)	0	100	100
1	RB	666/755 (88%)	666 (100%)	0	100	100
1	S	666/755 (88%)	666 (100%)	0	100	100
1	SA	666/755 (88%)	666 (100%)	0	100	100
1	SB	666/755 (88%)	666 (100%)	0	100	100
1	T	666/755 (88%)	666 (100%)	0	100	100
1	TA	666/755 (88%)	666 (100%)	0	100	100
1	TB	666/755 (88%)	666 (100%)	0	100	100
1	UA	666/755 (88%)	666 (100%)	0	100	100
1	UB	666/755 (88%)	666 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	V	666/755 (88%)	666 (100%)	0	100	100
1	VA	666/755 (88%)	666 (100%)	0	100	100
1	VB	666/755 (88%)	666 (100%)	0	100	100
1	W	666/755 (88%)	666 (100%)	0	100	100
1	WA	666/755 (88%)	665 (100%)	1 (0%)	87	85
1	WB	666/755 (88%)	666 (100%)	0	100	100
1	X	666/755 (88%)	666 (100%)	0	100	100
1	XA	666/755 (88%)	666 (100%)	0	100	100
1	XB	666/755 (88%)	666 (100%)	0	100	100
1	Y	666/755 (88%)	666 (100%)	0	100	100
1	YA	666/755 (88%)	666 (100%)	0	100	100
1	YB	666/755 (88%)	666 (100%)	0	100	100
1	Z	666/755 (88%)	666 (100%)	0	100	100
1	ZA	666/755 (88%)	666 (100%)	0	100	100
1	ZB	666/755 (88%)	666 (100%)	0	100	100
All	All	51948/58890 (88%)	51944 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	412	GLU
1	I	83	LEU
1	Q	457	VAL
1	WA	96	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 422 such sidechains are listed below:

Mol	Chain	Res	Type
1	NA	550	ASN
1	R	63	ASN
1	YB	17	HIS
1	O	295	GLN
1	P	294	ASN

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 oligosaccharides 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.

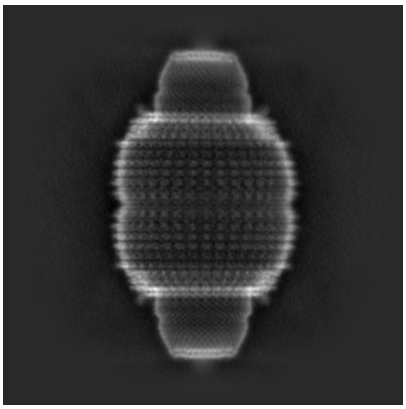
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-53423. These allow visual inspection of the internal detail of the map and identification of artifacts.

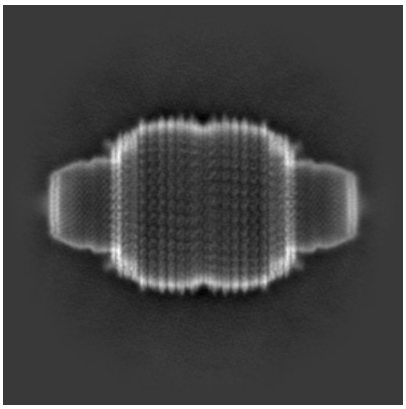
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

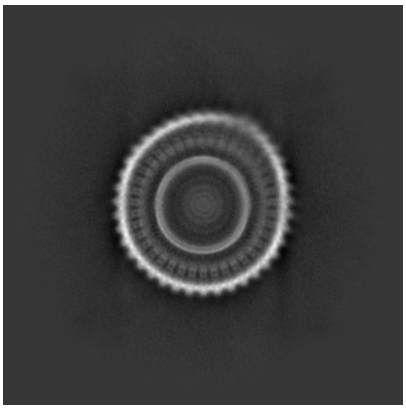
6.1.1 Primary map



X

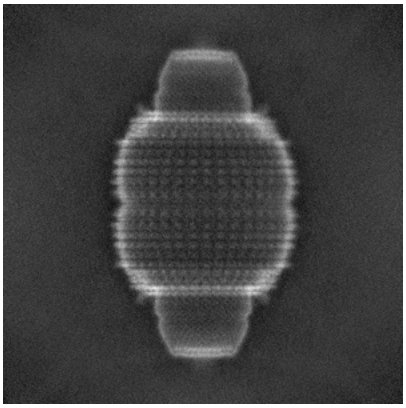


Y

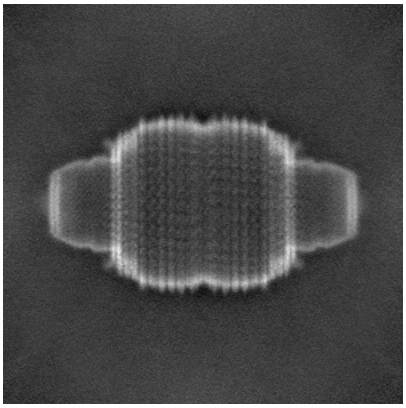


Z

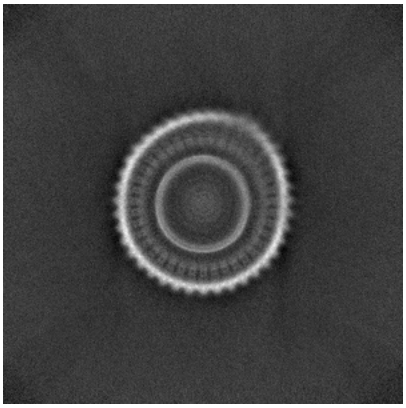
6.1.2 Raw map



X



Y

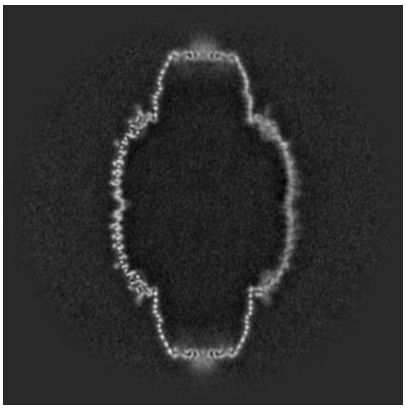


Z

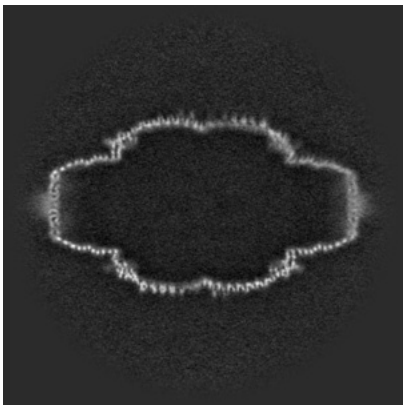
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

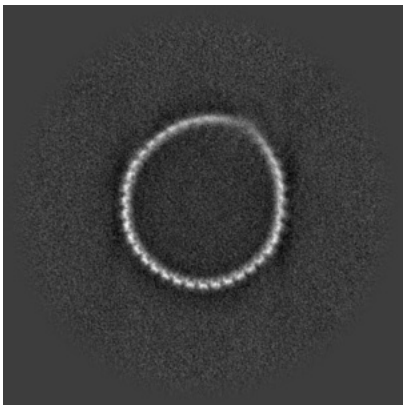
6.2.1 Primary map



X Index: 512

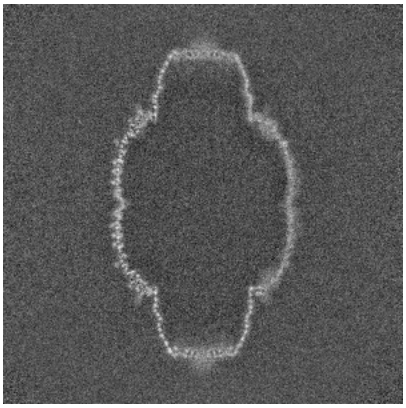


Y Index: 512

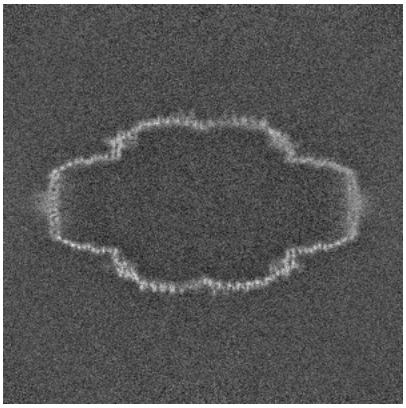


Z Index: 512

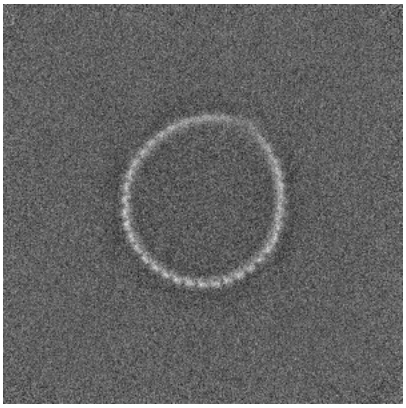
6.2.2 Raw map



X Index: 512



Y Index: 512

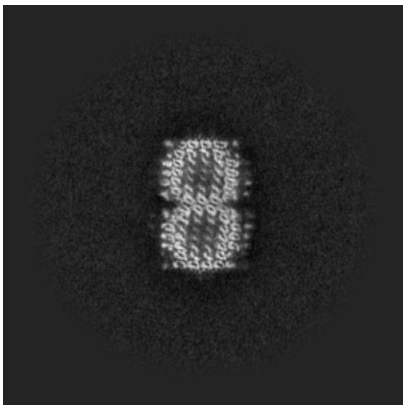


Z Index: 512

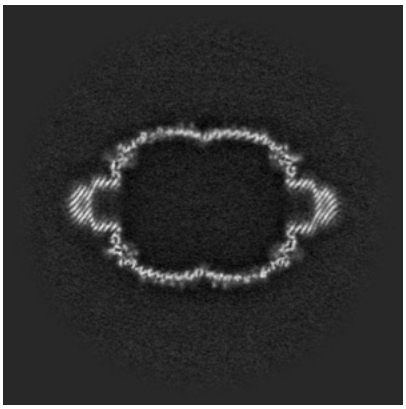
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

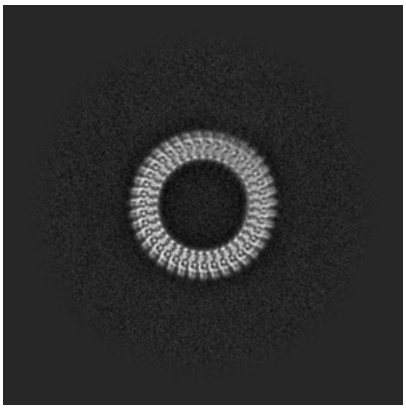
6.3.1 Primary map



X Index: 310

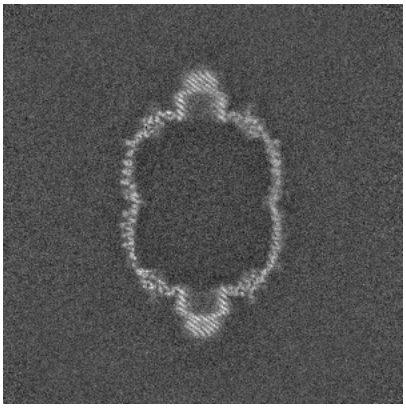


Y Index: 404

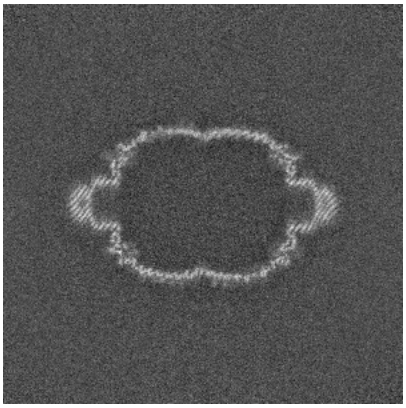


Z Index: 296

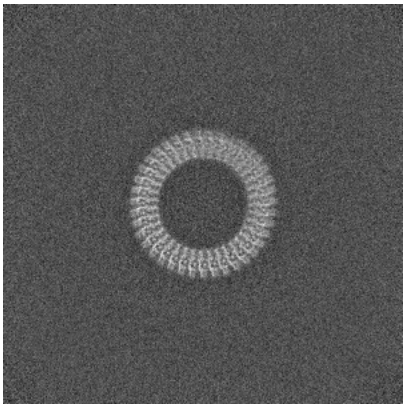
6.3.2 Raw map



X Index: 404



Y Index: 404

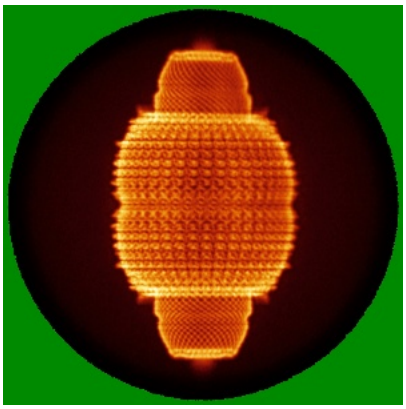


Z Index: 297

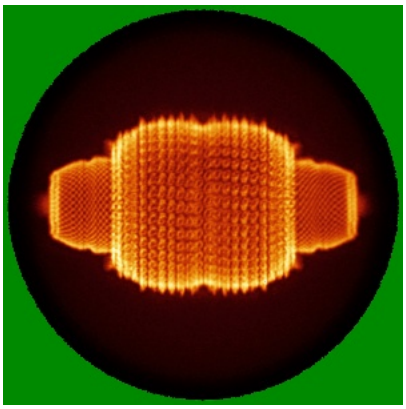
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

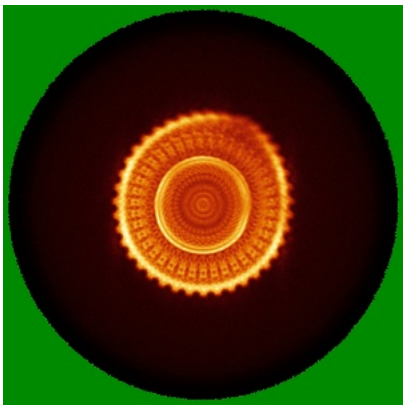
6.4.1 Primary map



X

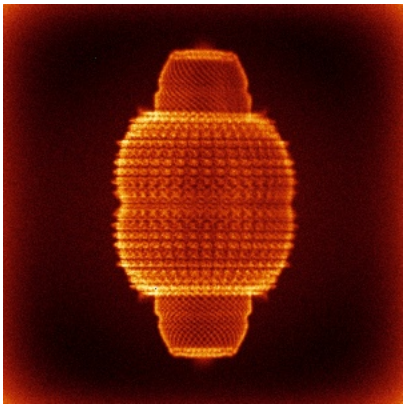


Y

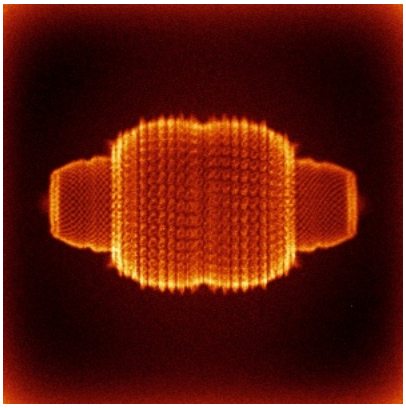


Z

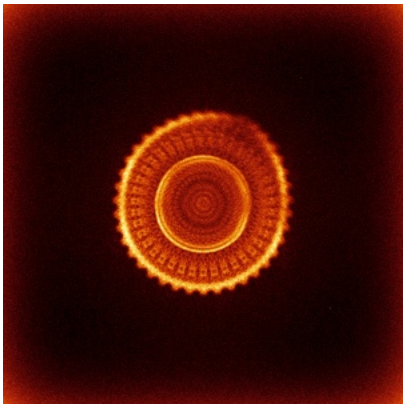
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

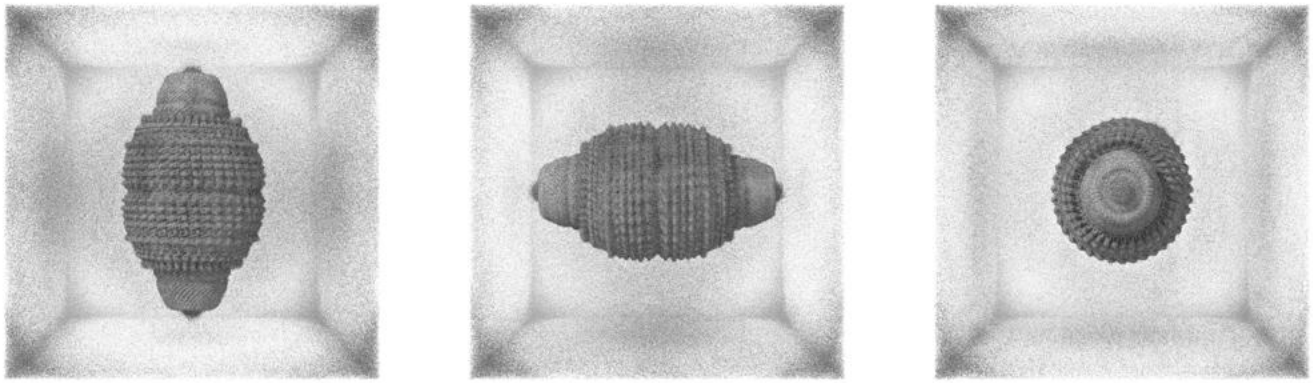
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

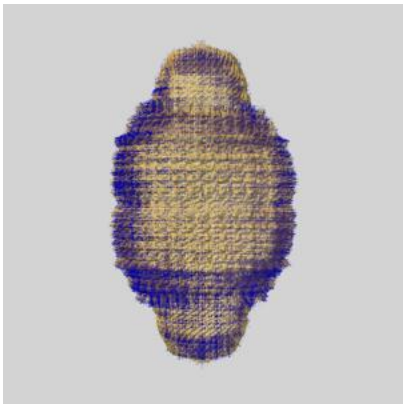
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

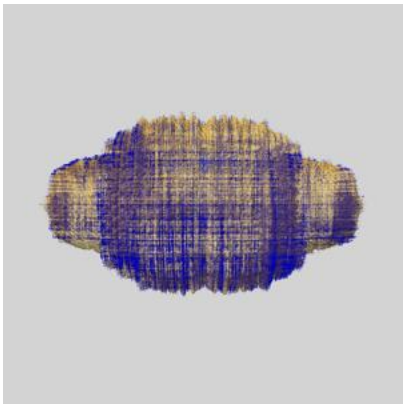
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

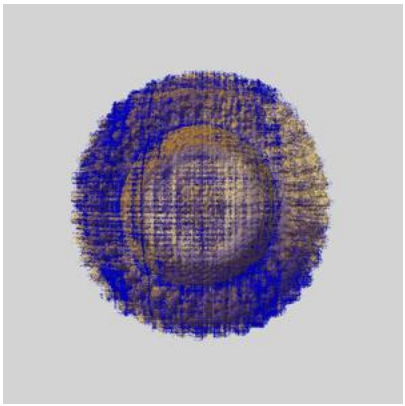
6.6.1 emd_53423_msk_1.map (i)



X



Y

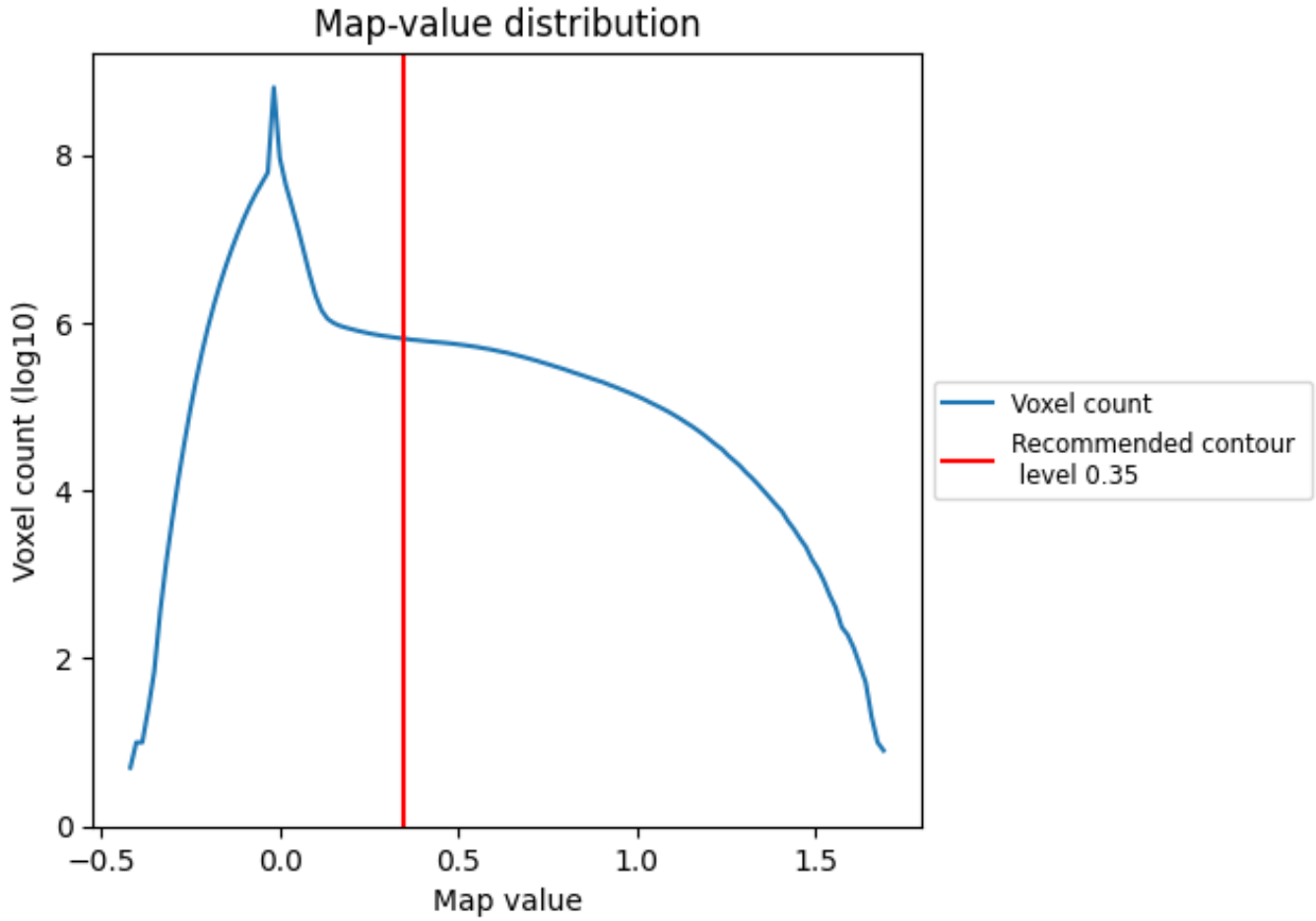


Z

7 Map analysis

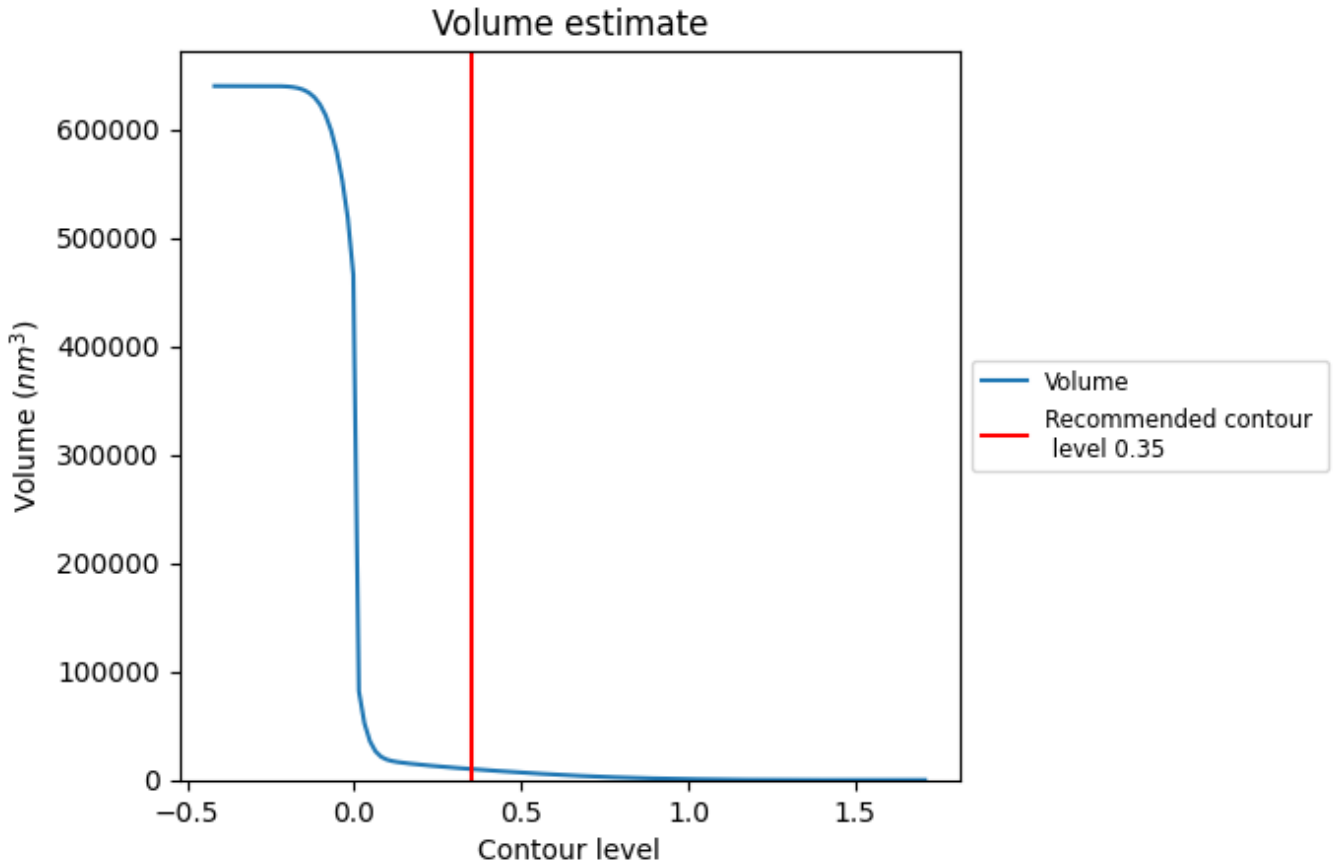
This section contains the results of statistical analysis of the map.

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.

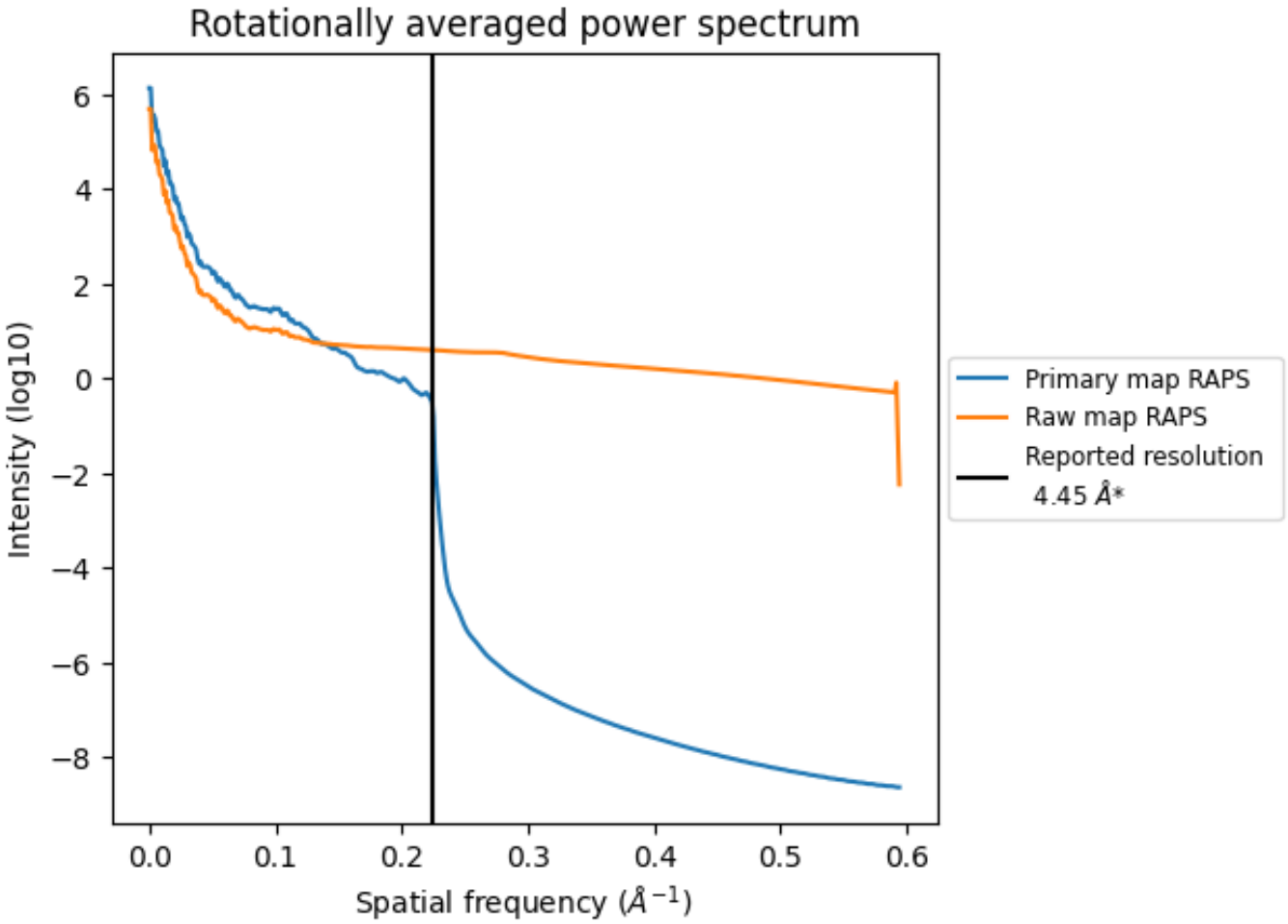
7.2 Volume estimate (i)



The volume at the recommended contour level is 10088 nm^3; this corresponds to an approximate mass of 9113 kDa.

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

7.3 Rotationally averaged power spectrum (i)

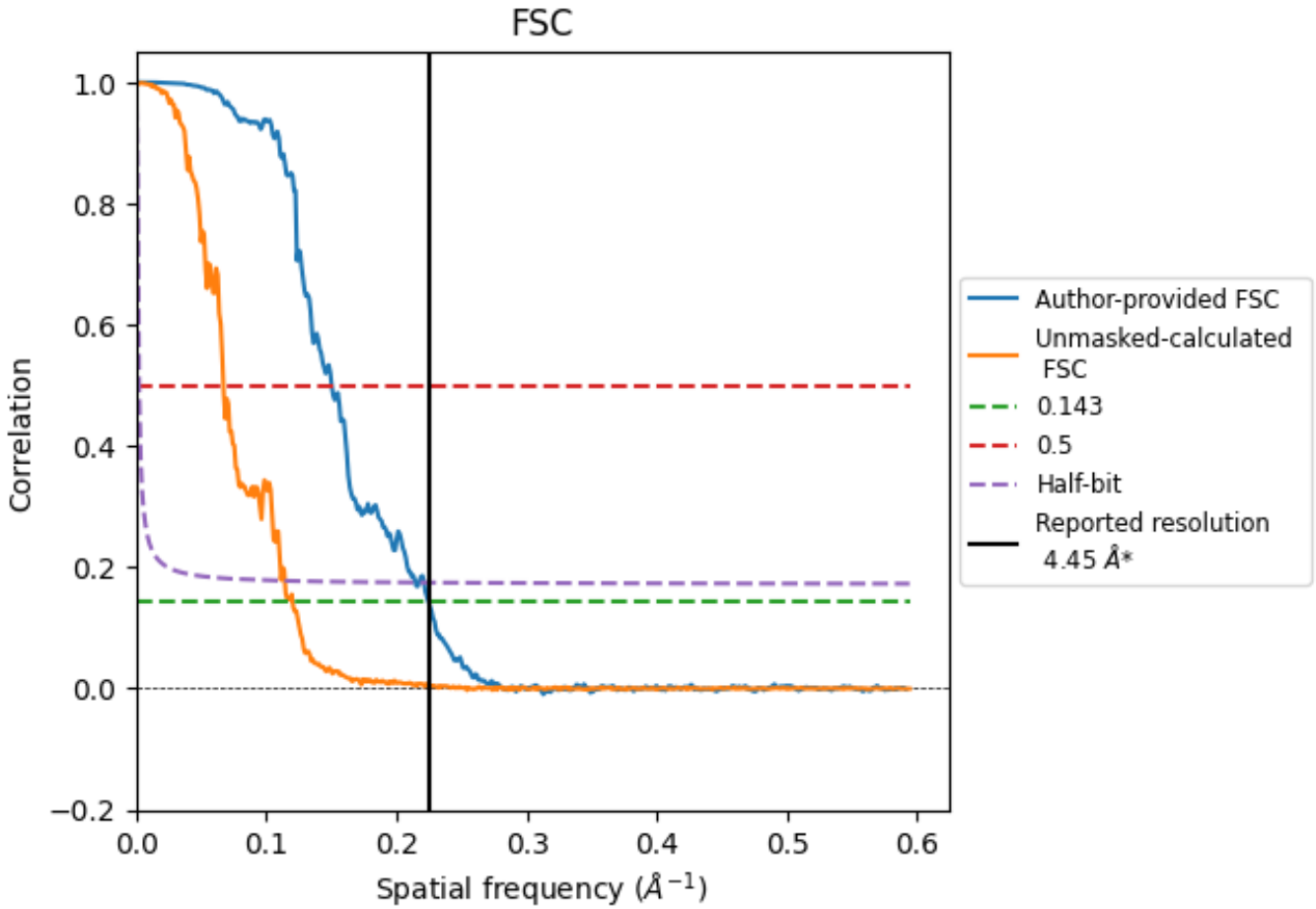


*Reported resolution corresponds to spatial frequency of 0.225 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.225 Å^{-1}

8.2 Resolution estimates (i)

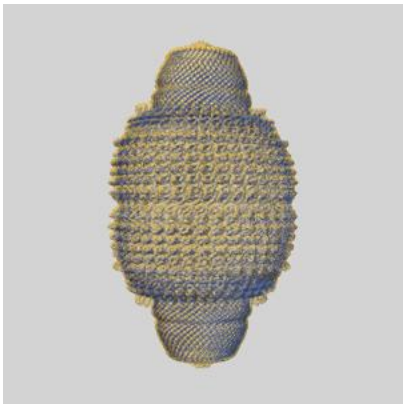
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.45	-	-
Author-provided FSC curve	4.45	6.66	4.66
Unmasked-calculated*	8.32	14.90	8.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.32 differs from the reported value 4.45 by more than 10 %

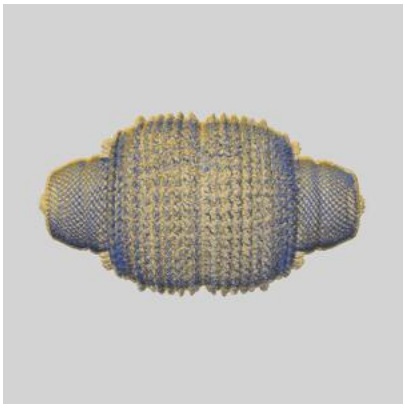
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-53423 and PDB model 9QWQ. Per-residue inclusion information can be found in section 3 on page 10.

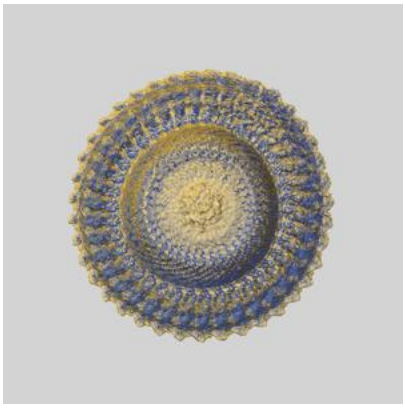
9.1 Map-model overlay



X



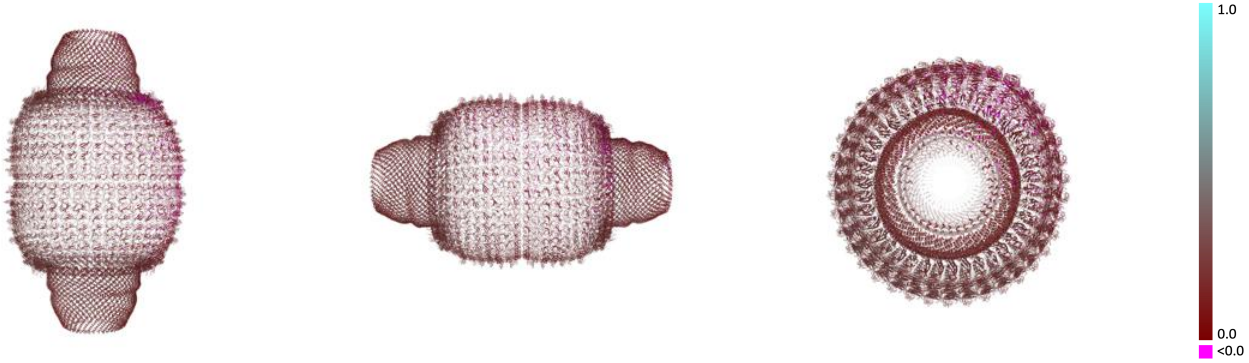
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 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.

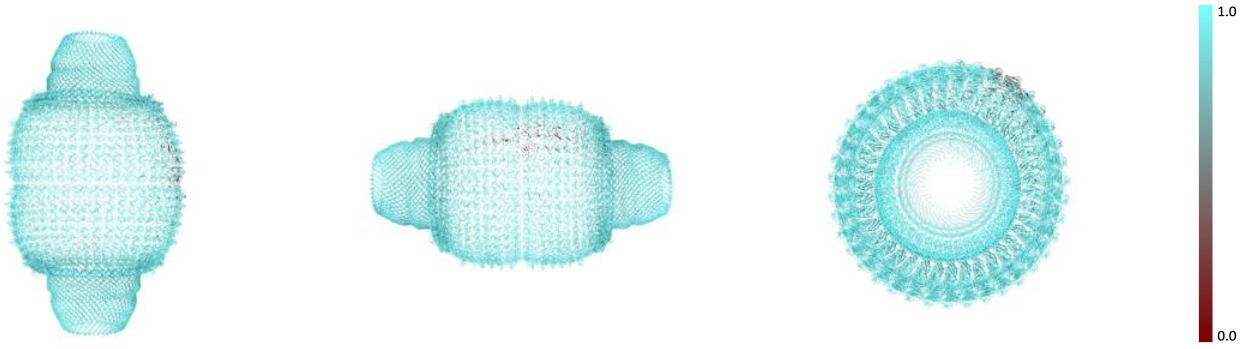
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

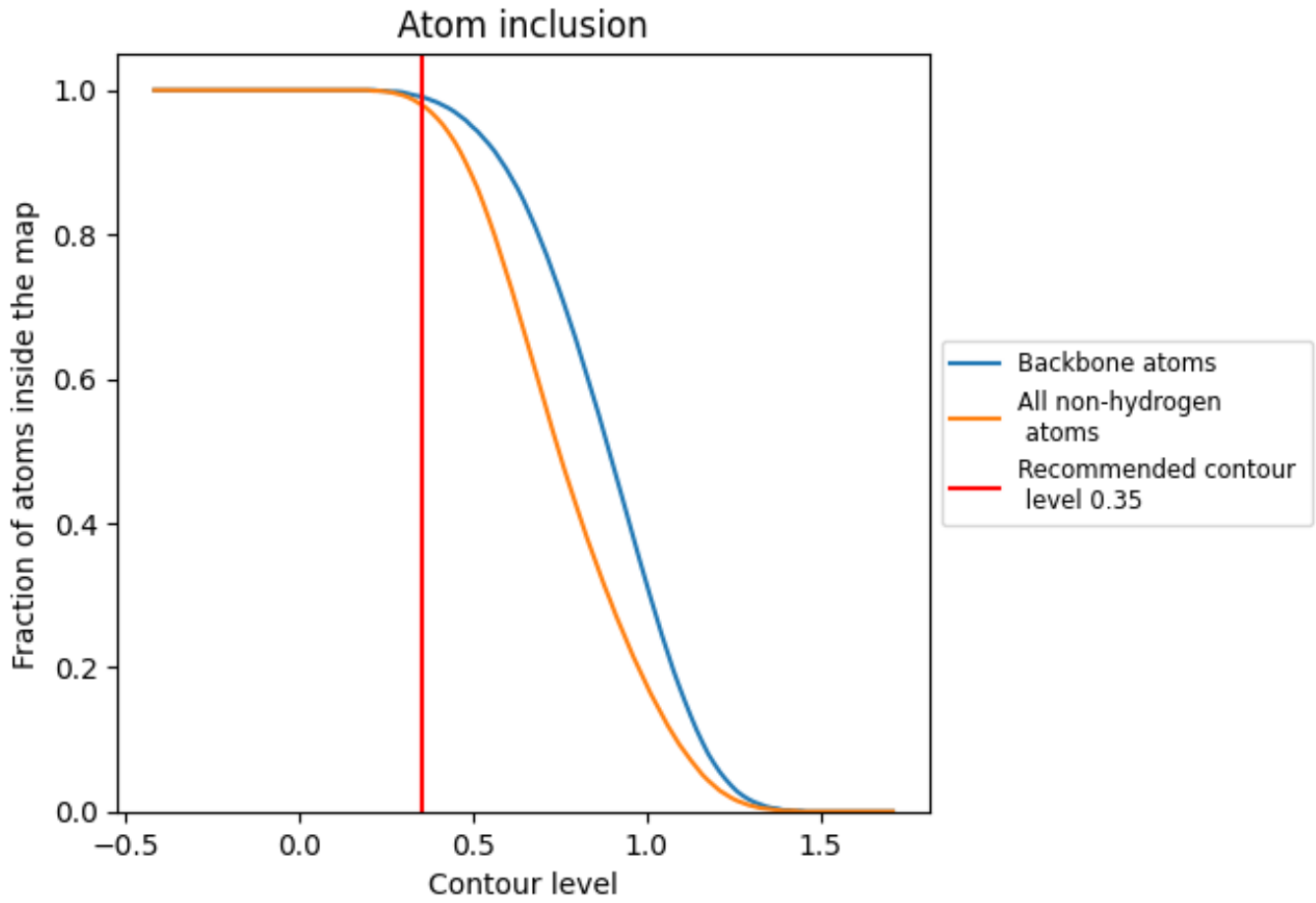
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9800	0.2230
A	0.9920	0.2640
AA	0.9800	0.2250
AB	0.9940	0.1880
AC	0.9780	0.1870
B	0.9930	0.2640
BA	0.9760	0.2270
BB	0.9940	0.2040
C	0.9920	0.2630
CA	0.9820	0.2260
CB	0.9950	0.2160
D	0.9940	0.2620
DA	0.9910	0.2320
DB	0.9940	0.2230
E	0.9950	0.2540
EA	0.9940	0.2430
EB	0.9960	0.2340
F	0.9890	0.2530
FA	0.9940	0.2480
FB	0.9940	0.2360
G	0.9910	0.2520
GA	0.9910	0.2540
GB	0.9920	0.2410
H	0.9910	0.2430
HA	0.9920	0.2590
HB	0.9890	0.2440
I	0.9930	0.2380
IA	0.9920	0.2610
IB	0.9920	0.2460
J	0.9950	0.2370
JA	0.9880	0.2620
JB	0.9930	0.2500
K	0.9920	0.2360
KA	0.9910	0.2660
KB	0.9940	0.2560

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Chain	Atom inclusion	Q-score
L	0.9910	0.2340
LA	0.9890	0.2630
LB	0.9930	0.2550
M	0.9920	0.2250
MA	0.9910	0.2640
MB	0.9910	0.2580
N	0.9930	0.2230
NA	0.9900	0.2650
NB	0.9910	0.2580
O	0.9920	0.2170
OA	0.9830	0.1810
OB	0.9910	0.2580
P	0.9910	0.2040
PA	0.9860	0.1750
PB	0.9890	0.2560
Q	0.9880	0.2020
QA	0.9780	0.1640
QB	0.9870	0.2560
R	0.9610	0.1900
RA	0.9710	0.1640
RB	0.9890	0.2510
S	0.8700	0.1770
SA	0.9420	0.1590
SB	0.9890	0.2500
T	0.9570	0.1780
TA	0.8820	0.1460
TB	0.9930	0.2500
UA	0.7690	0.1330
UB	0.9910	0.2430
V	0.9820	0.1810
VA	0.8320	0.1360
VB	0.9900	0.2370
W	0.9910	0.1900
WA	0.9540	0.1530
WB	0.9940	0.2270
X	0.9940	0.2080
XA	0.9770	0.1600
XB	0.9940	0.2160
Y	0.9930	0.2190
YA	0.9860	0.1680
YB	0.9960	0.2000
Z	0.9890	0.2210

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Chain	Atom inclusion	Q-score
ZA	0.9930	0.1880
ZB	0.9880	0.1970