



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 29, 2020 – 05:36 PM BST

PDB ID : 4V60
Title : The structure of rat liver vault at 3.5 angstrom resolution
Authors : Kato, K.; Zhou, Y.; Tanaka, H.; Yao, M.; Yamashita, E.; Yoshimura, M.;
Tsukihara, T.
Deposited on : 2008-10-24
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : **FAILED**
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) : 2.13

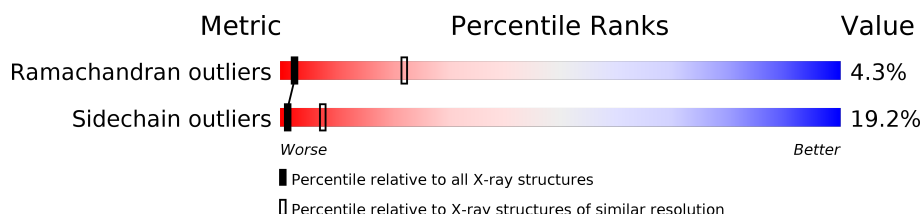
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)


























The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	861	77% 17% • 6%
1	B	861	79% 15% • 6%
1	C	861	77% 16% • 6%
1	D	861	78% 15% • 6%
1	E	861	78% 15% • 6%
1	F	861	78% 16% • 6%
1	G	861	77% 17% • 6%
1	H	861	77% 17% • 6%
1	I	861	77% 16% • 6%

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Mol	Chain	Length	Quality of chain
1	J	861	
1	K	861	
1	L	861	
1	M	861	
1	N	861	
1	O	861	
1	P	861	
1	Q	861	
1	R	861	
1	S	861	
1	T	861	
1	U	861	
1	V	861	
1	W	861	
1	X	861	
1	Y	861	
1	Z	861	
1	a	861	
1	b	861	
1	c	861	
1	d	861	
1	e	861	
1	f	861	
1	g	861	
1	h	861	

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Mol	Chain	Length	Quality of chain
1	i	861	<div><div></div><div>75%18%6%</div></div>
1	j	861	<div><div></div><div>76%17%6%</div></div>
1	k	861	<div><div></div><div>76%17%6%</div></div>
1	l	861	<div><div></div><div>77%16%6%</div></div>
1	m	861	<div><div></div><div>77%16%6%</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 241956 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Major vault protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	B	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	C	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	D	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	E	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	F	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	G	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	H	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	I	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	J	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	K	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	L	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	M	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	N	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	O	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	P	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	R	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	S	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	T	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	U	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	V	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	W	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	X	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	Y	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	Z	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	a	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	b	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	c	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	d	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	e	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	f	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	g	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	h	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	i	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	j	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30
1	k	812	Total 6204	C 3915	N 1101	O 1172	S 16	0	0	30

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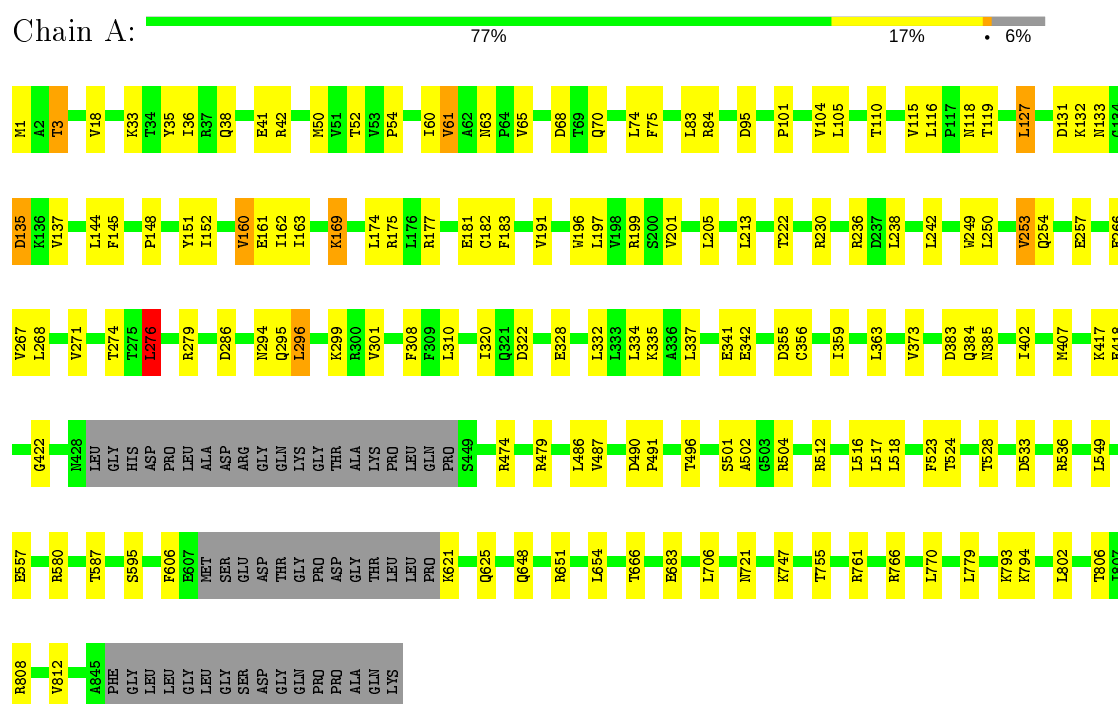
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	l	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			
1	m	812	Total	C	N	O	S	0	0	30
			6204	3915	1101	1172	16			

3 Residue-property plots

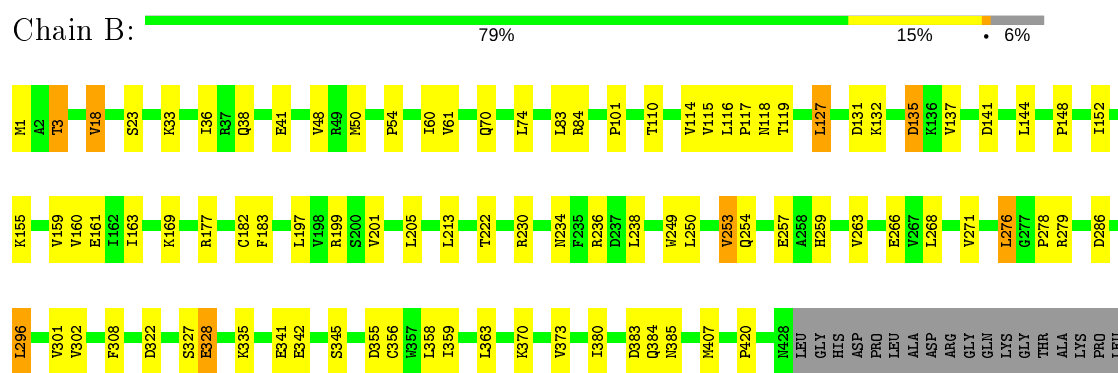
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

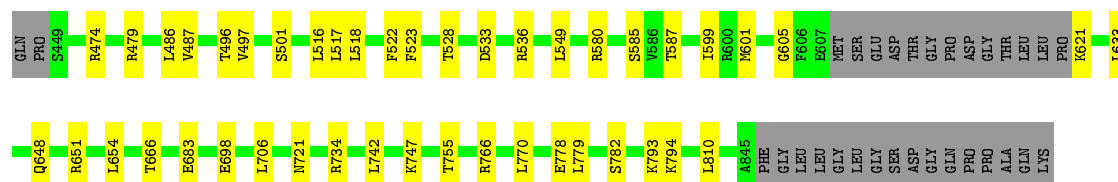
Note EDS failed to run properly.

- Molecule 1: Major vault protein



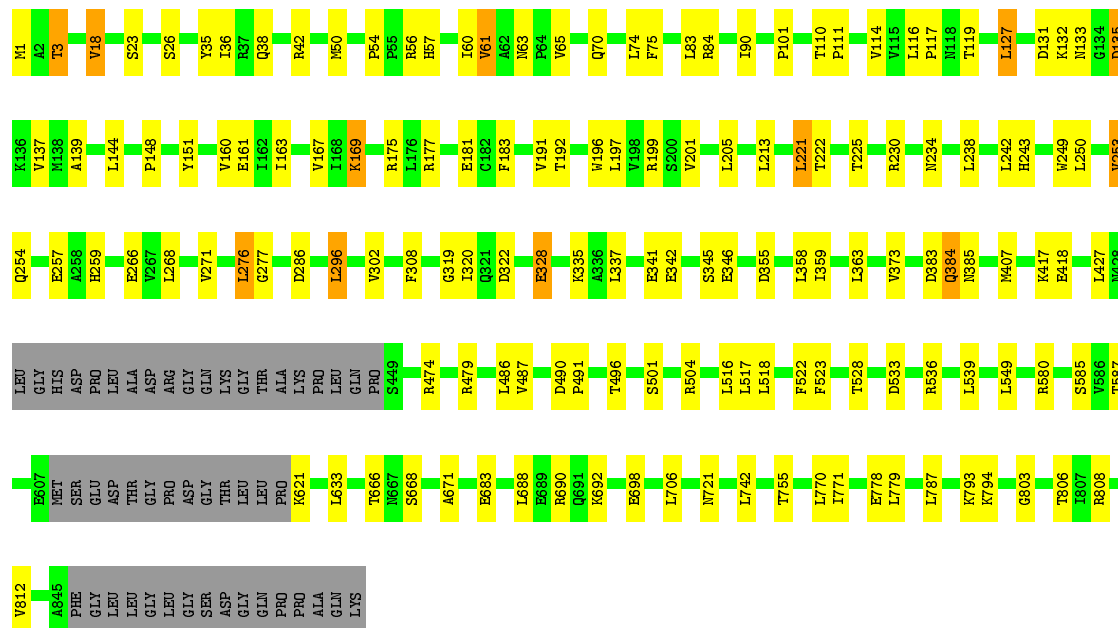
- Molecule 1: Major vault protein





- Molecule 1: Major vault protein

Chain C: 77% 16% 6%

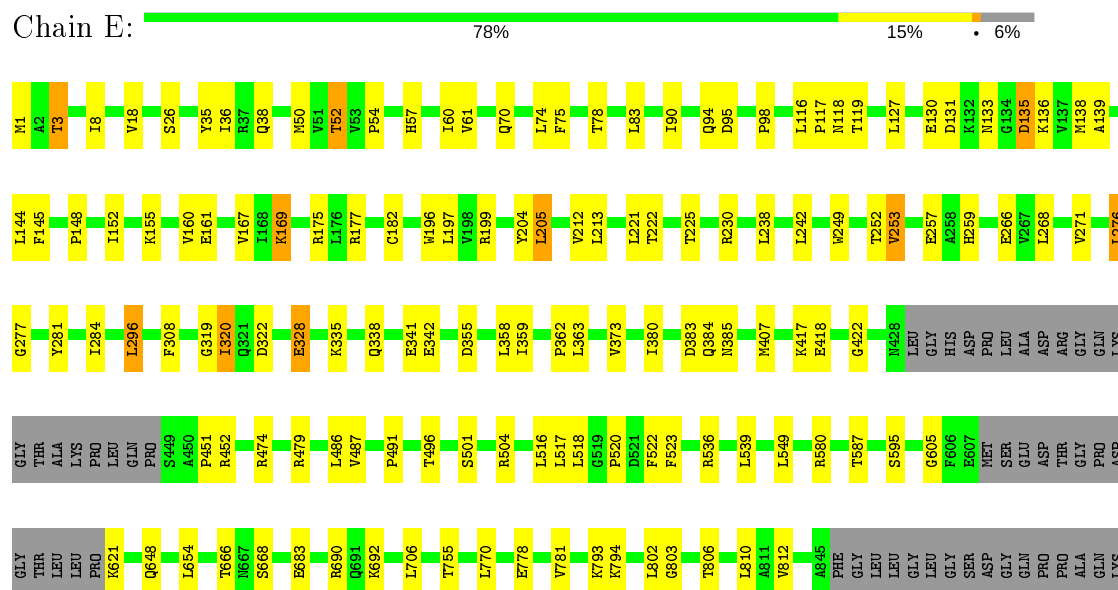


- Molecule 1: Major vault protein

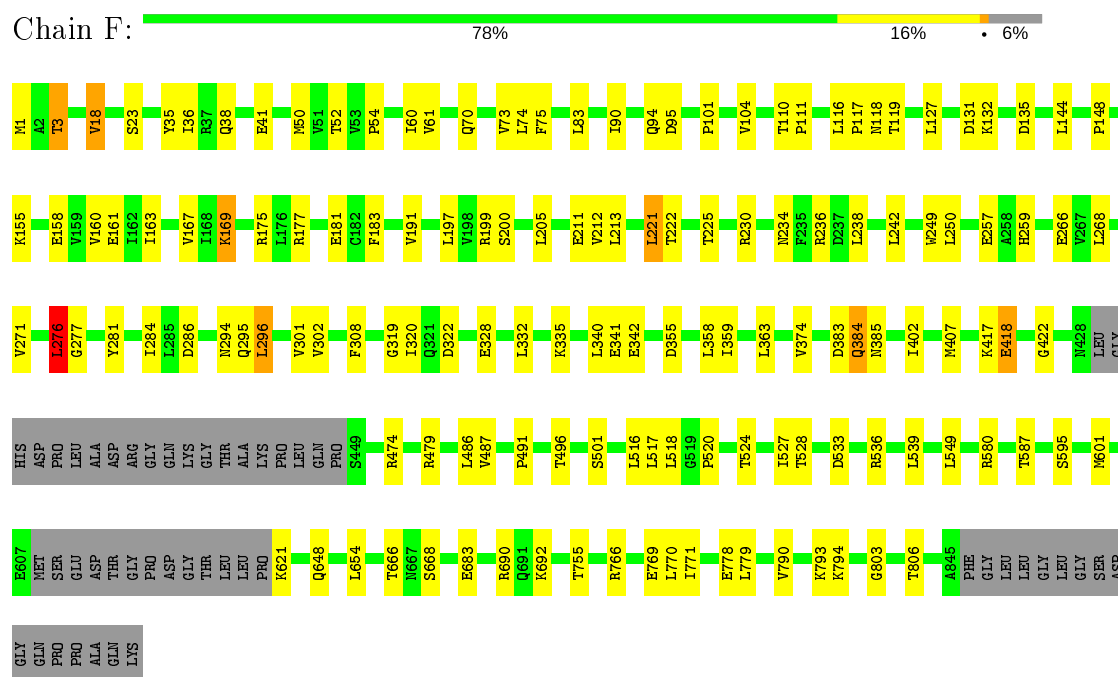
Chain D: 78% 15% 6%



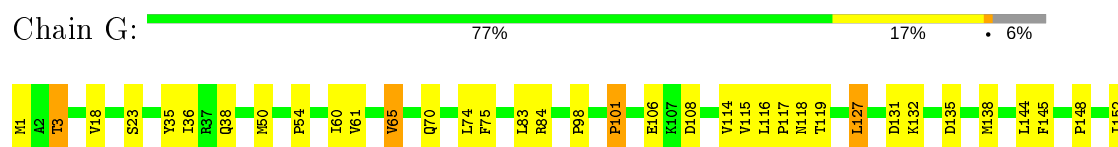
- Molecule 1: Major vault protein

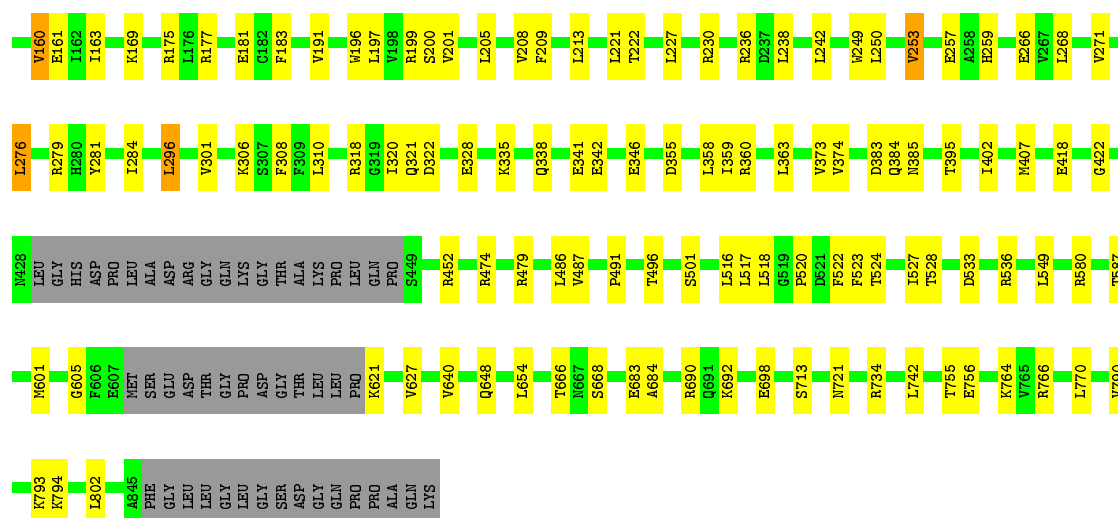


- Molecule 1: Major vault protein



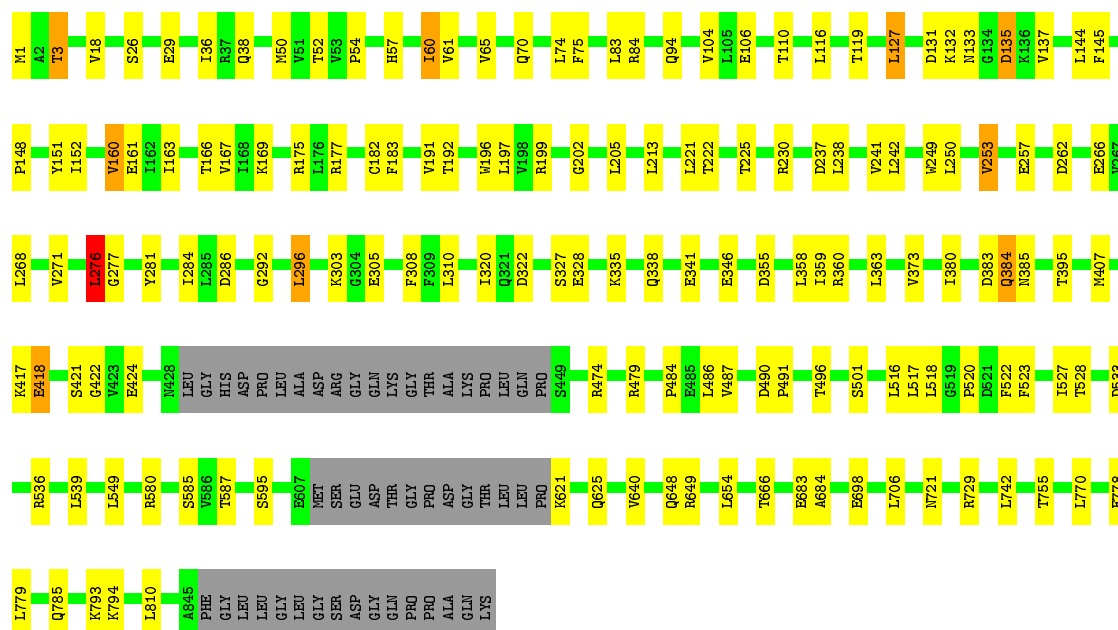
- Molecule 1: Major vault protein





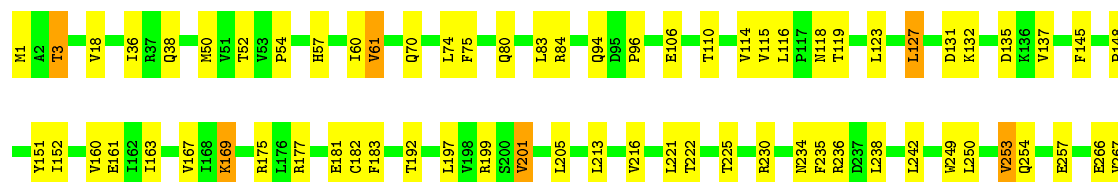
• Molecule 1: Major vault protein

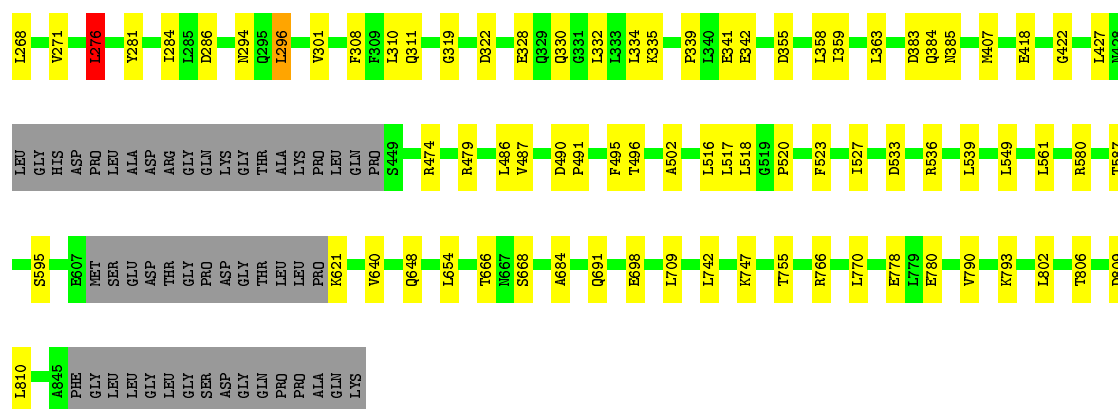
Chain H: 77% 17% 6%



• Molecule 1: Major vault protein

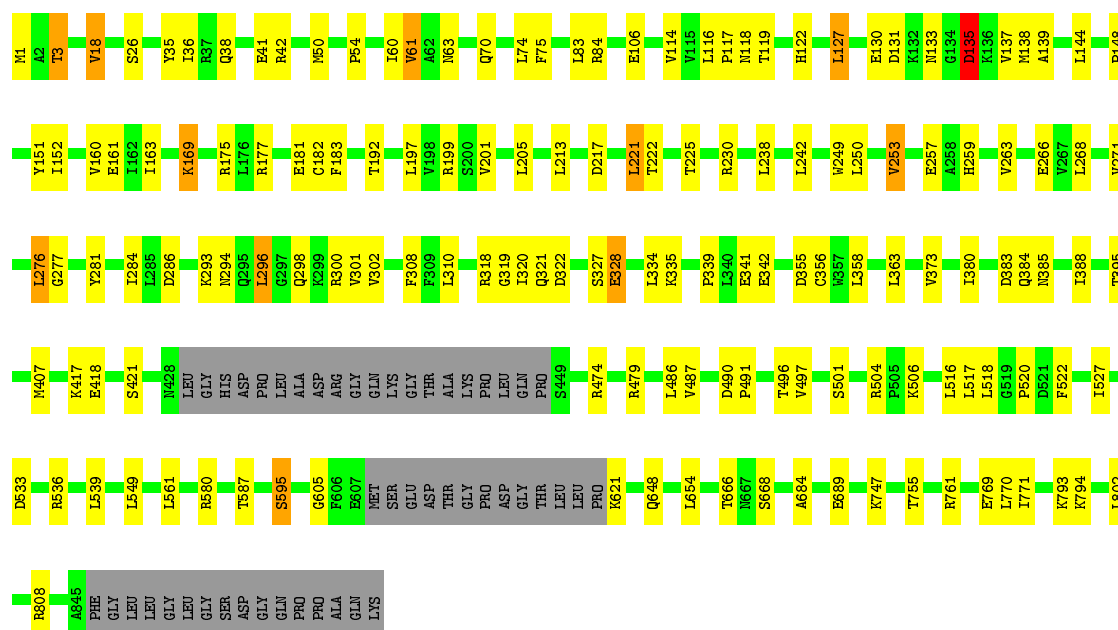
Chain I: 77% 16% 6%





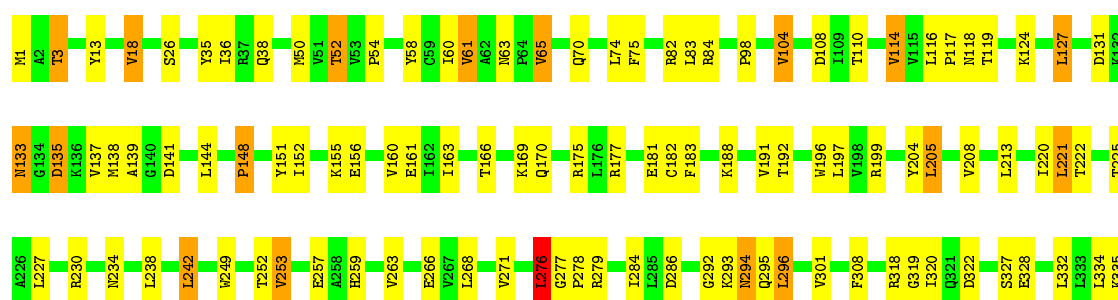
• Molecule 1: Major vault protein

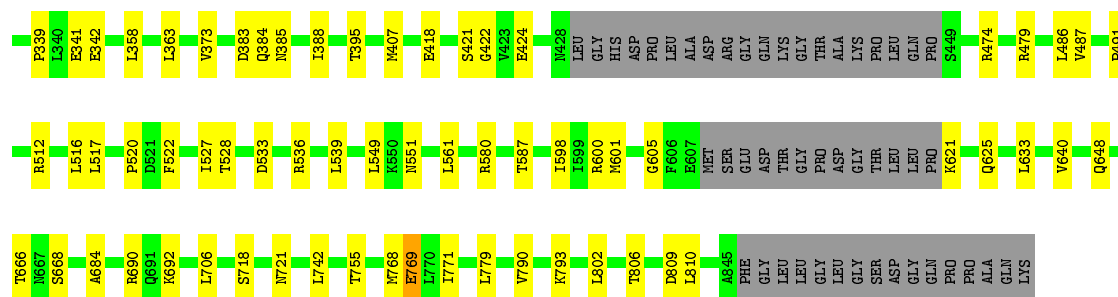
Chain J: 77% 16% 6%



• Molecule 1: Major vault protein

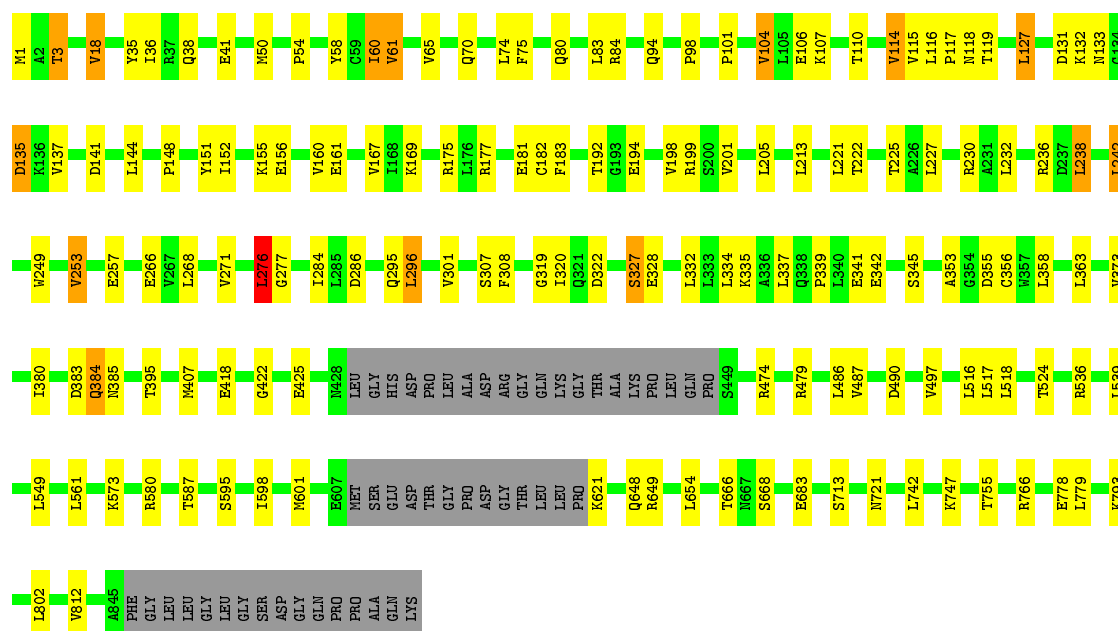
Chain K: 74% 18% 6%





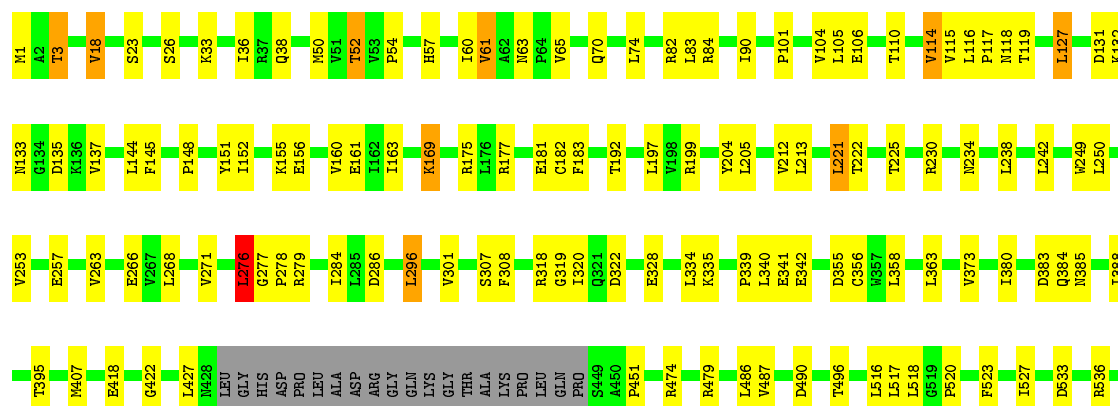
• Molecule 1: Major vault protein

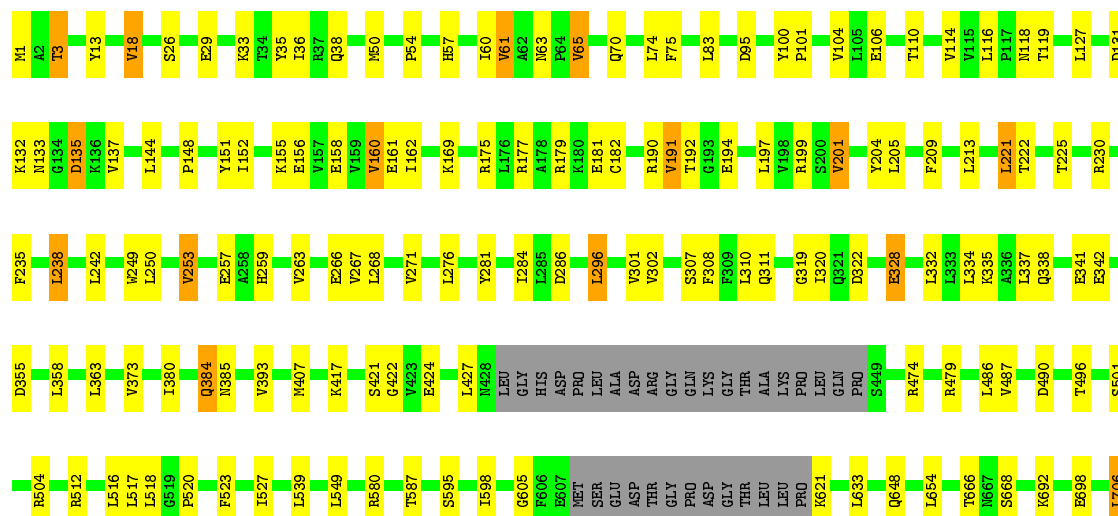
Chain L: 77% 16% 6%



• Molecule 1: Major vault protein

Chain M: 76% 17% 6%

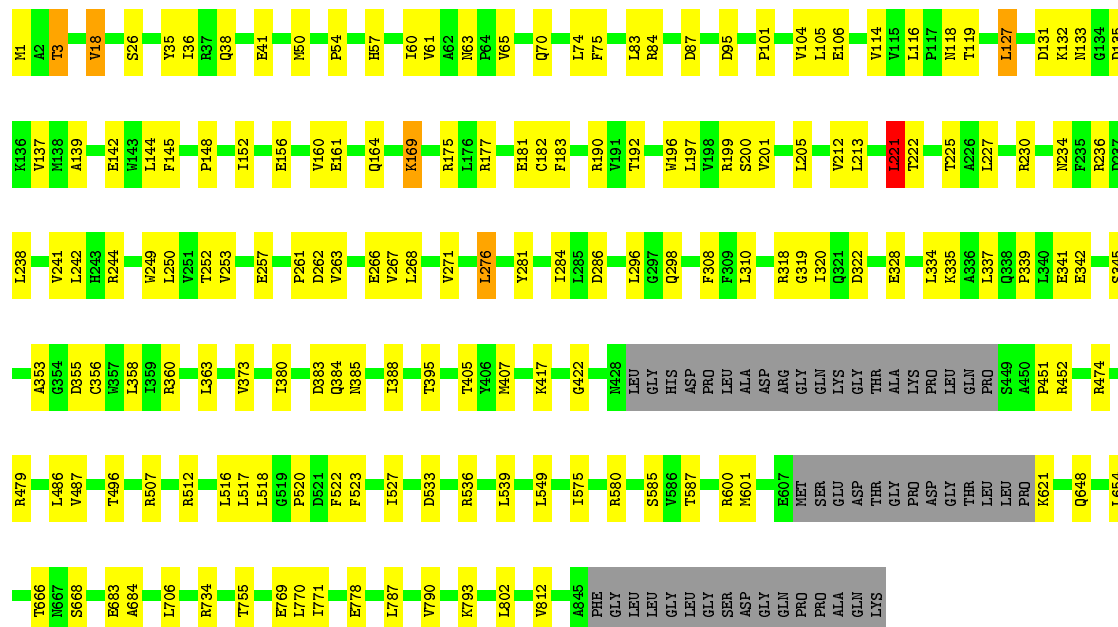






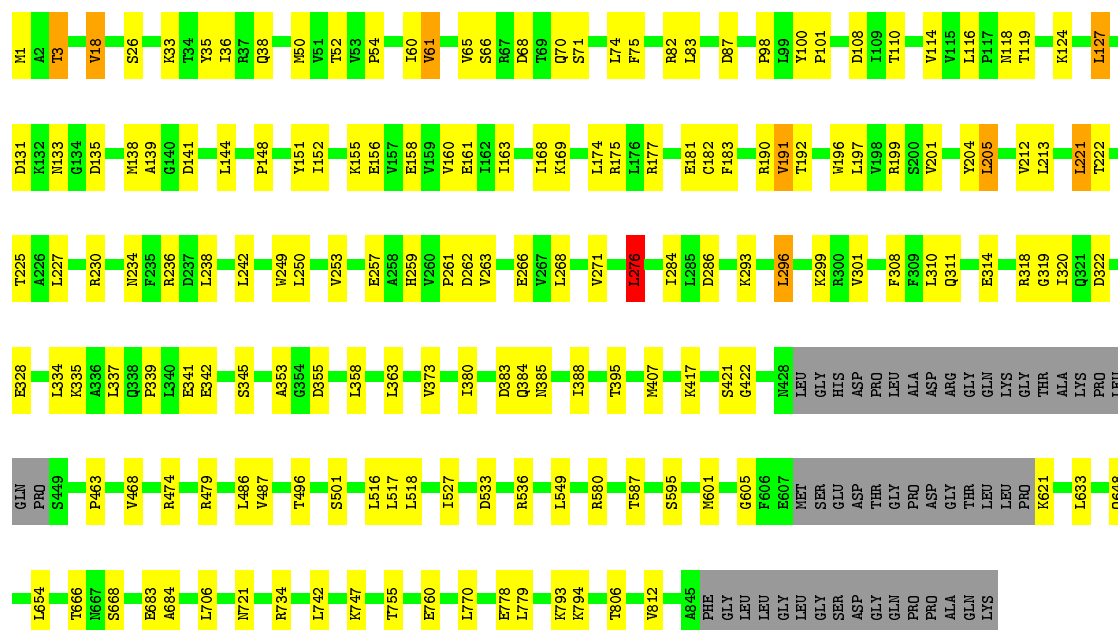
• Molecule 1: Major vault protein

Chain P: 75% 19% 6%



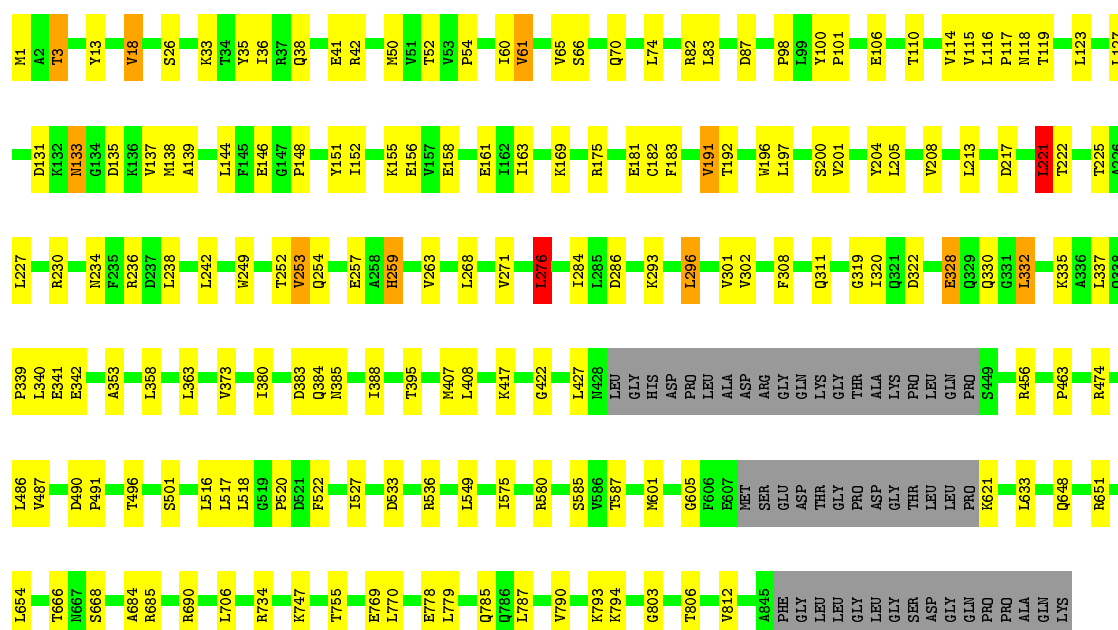
• Molecule 1: Major vault protein

Chain Q: 75% 19% 6%



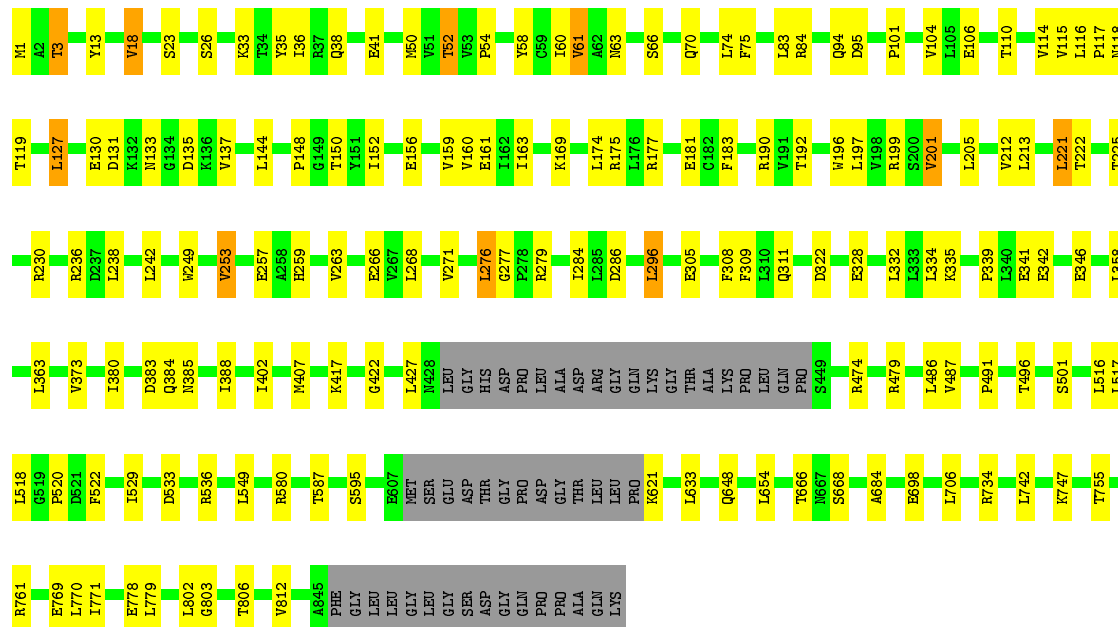
• Molecule 1: Major vault protein

Chain R:  74% 19% 6%




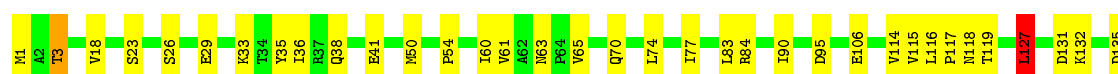
• Molecule 1: Major vault protein

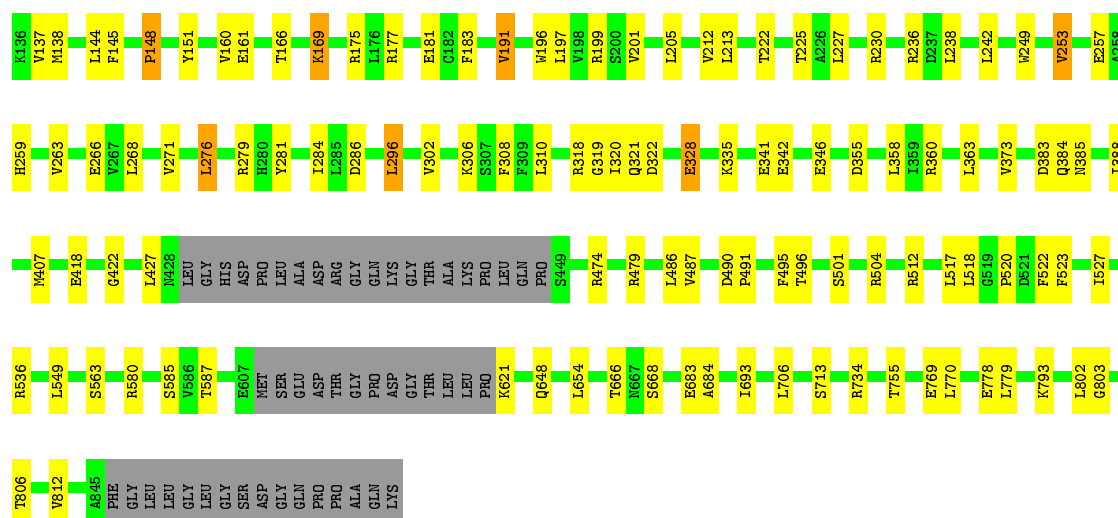
Chain S:  76% 17% 6%



• Molecule 1: Major vault protein

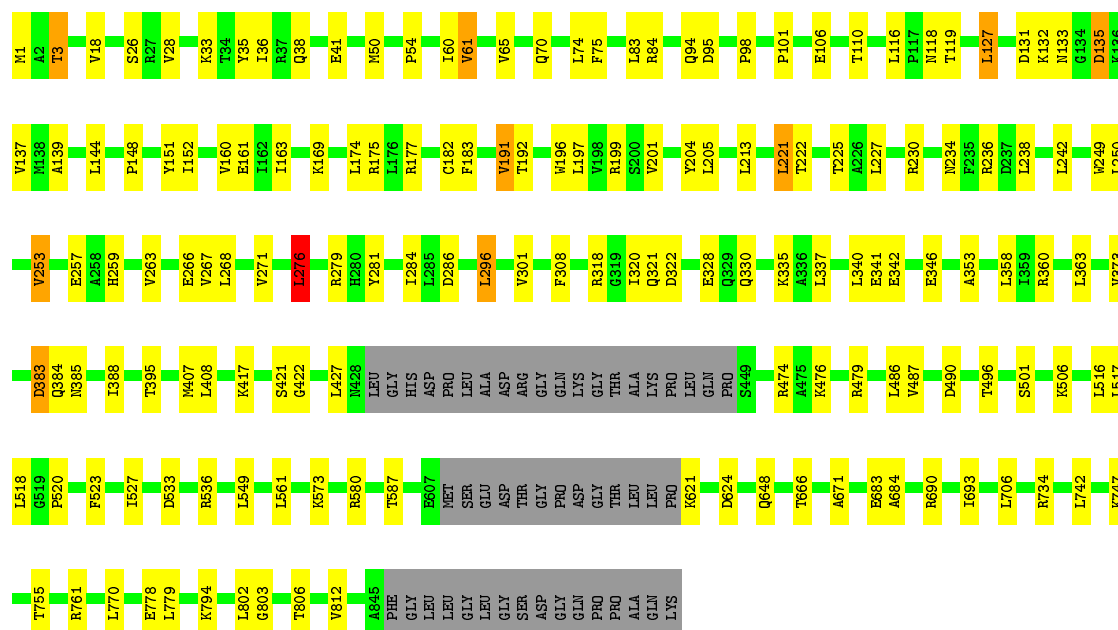
Chain T:  77% 16% 6%





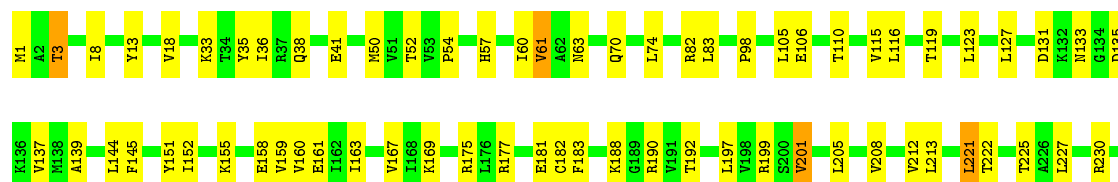
• Molecule 1: Major vault protein

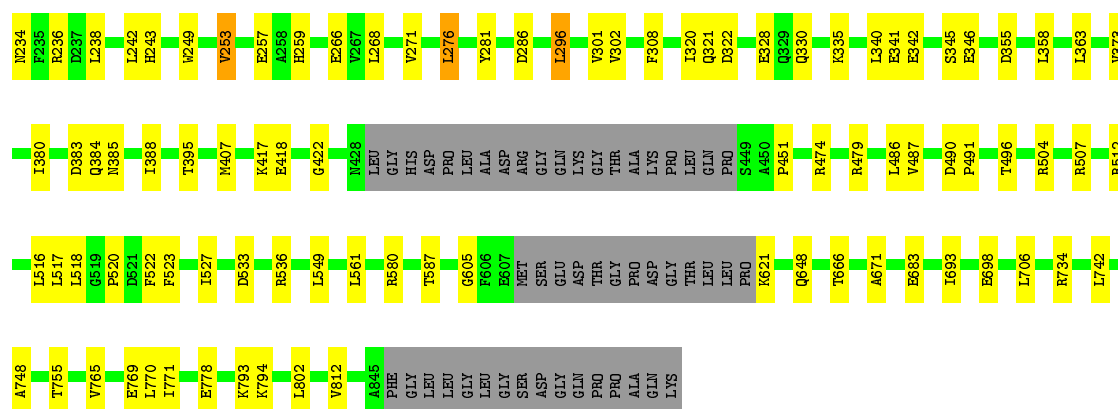
Chain U: 76% 17% 6%



• Molecule 1: Major vault protein

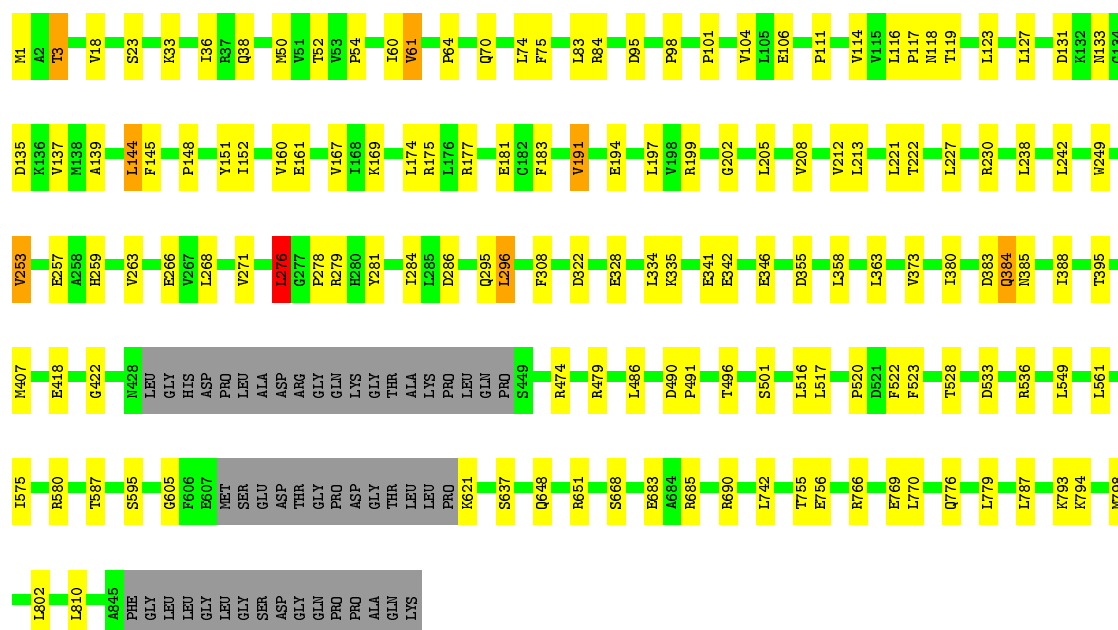
Chain V: 76% 17% 6%





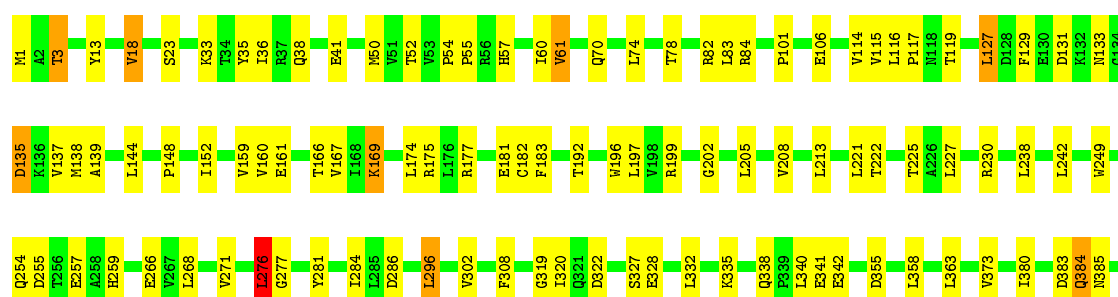
• Molecule 1: Major vault protein

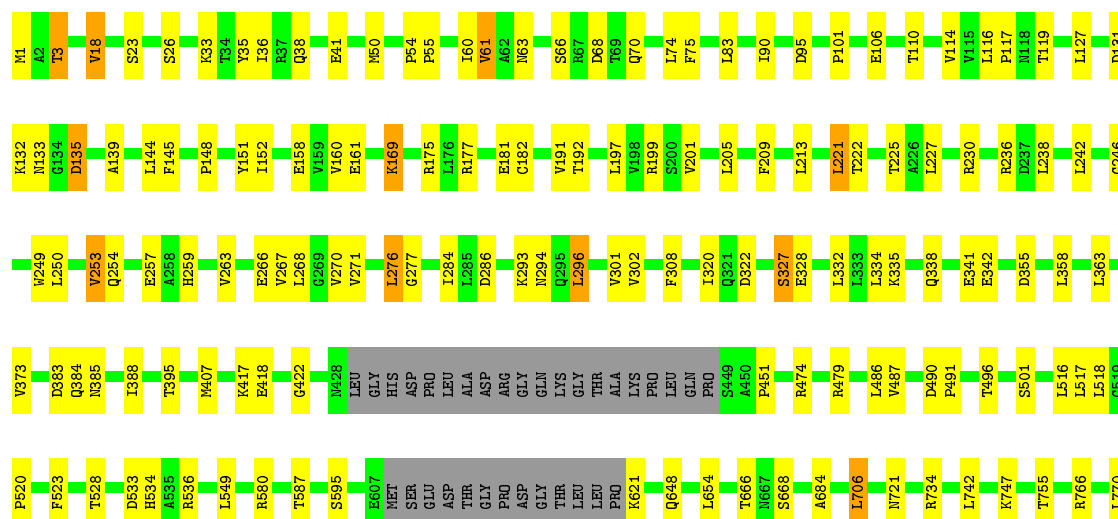
Chain W: 77% 16% • 6%

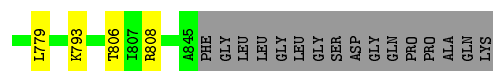


• Molecule 1: Major vault protein

Chain X: 77% 17% • 6%

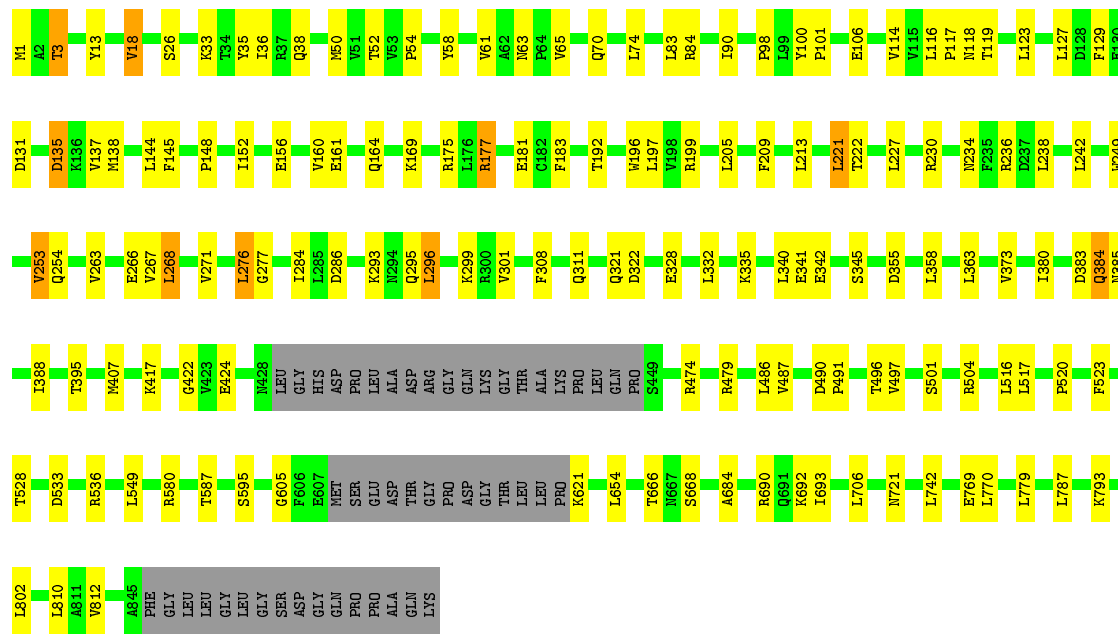






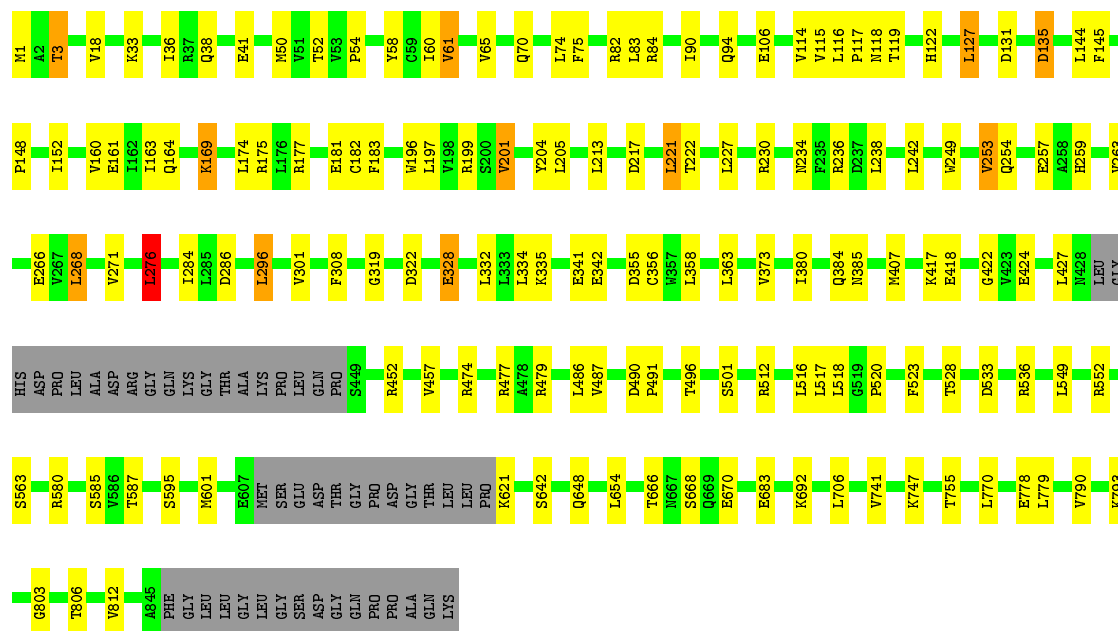
- Molecule 1: Major vault protein

Chain a: 77% 16% 6%

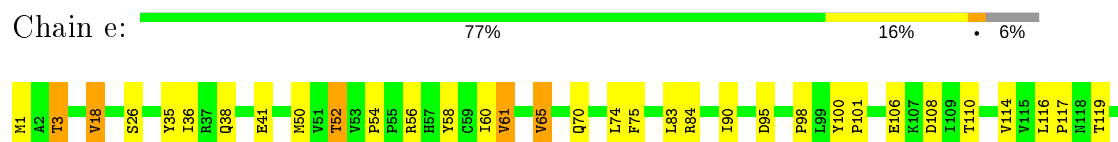


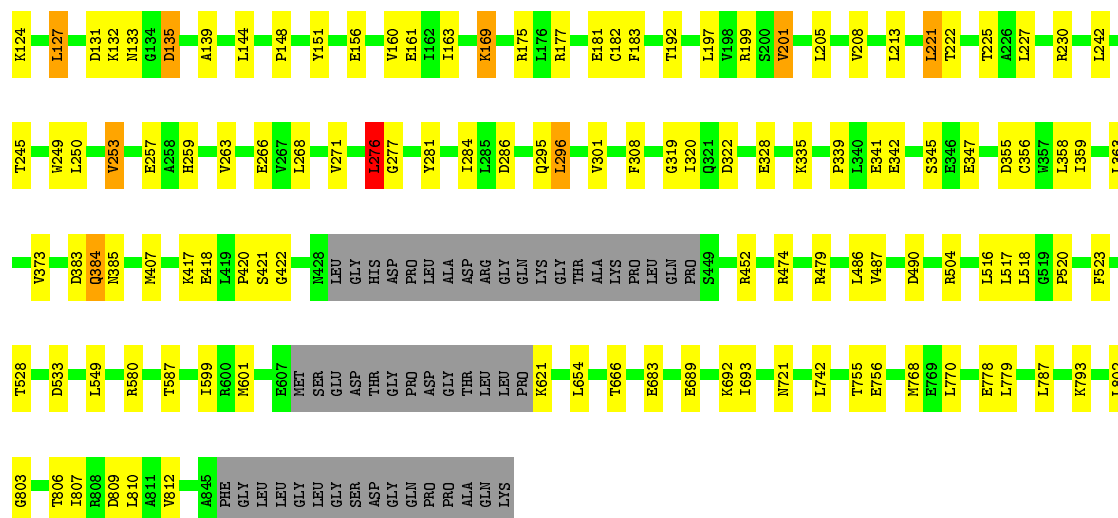
- Molecule 1: Major vault protein

Chain b: 77% 16% 6%



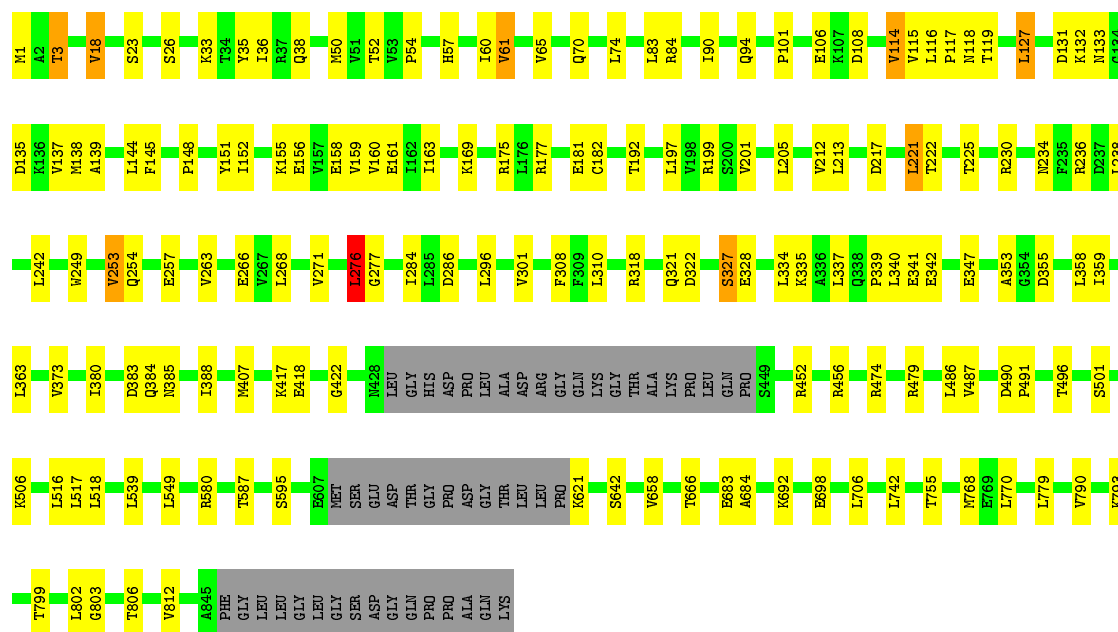
- Molecule 1: Major vault protein





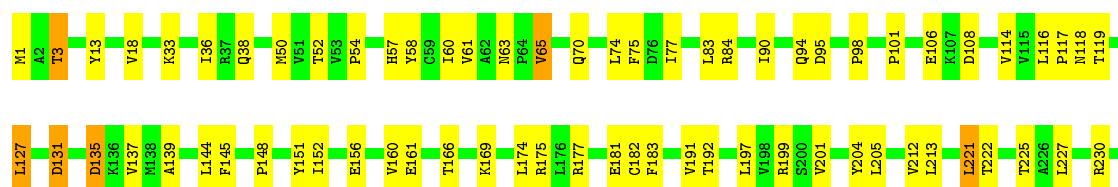
• Molecule 1: Major vault protein

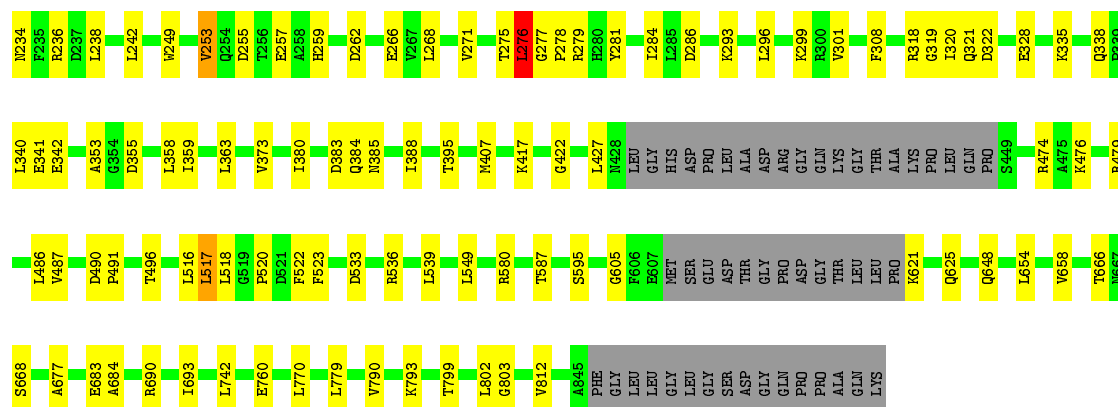
Chain f: 76% 17% 6%



• Molecule 1: Major vault protein

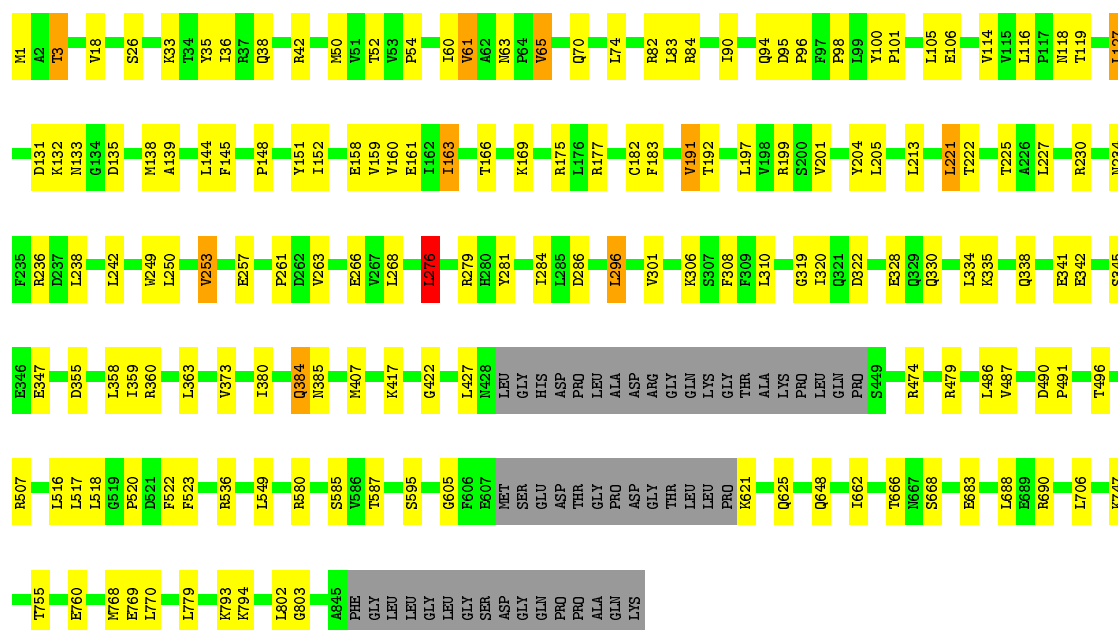
Chain g: 75% 18% 6%





• Molecule 1: Major vault protein

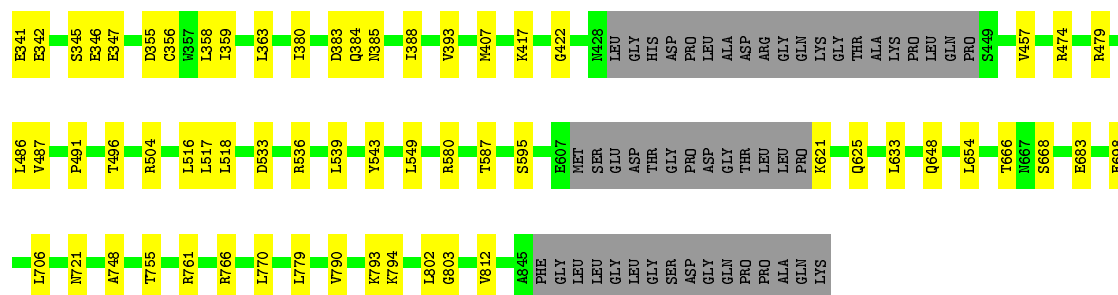
Chain h: 76% 17% 6%



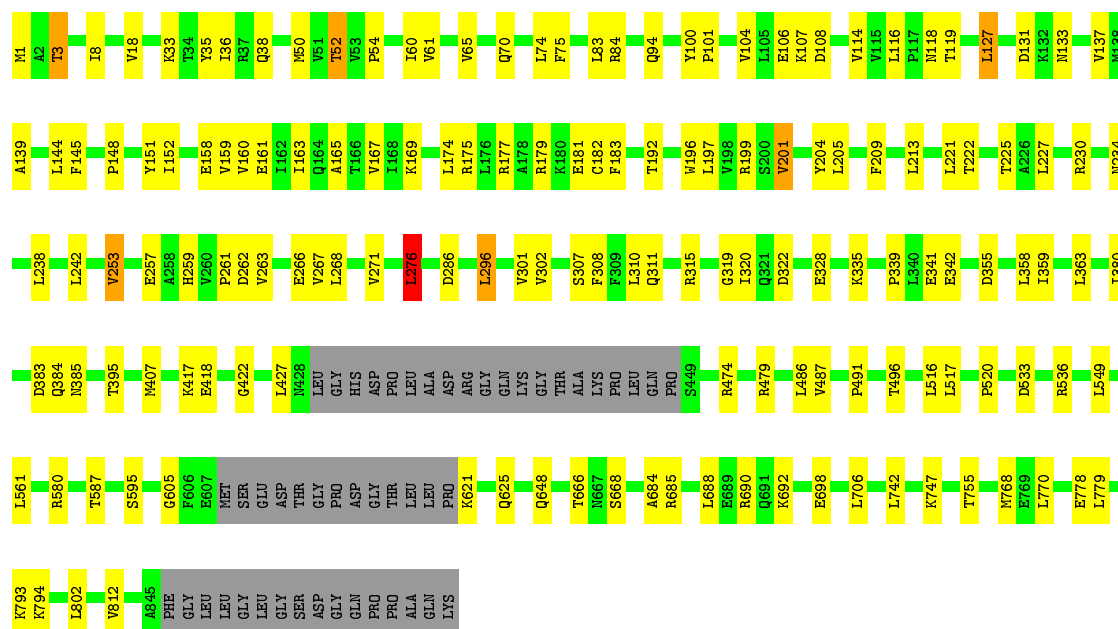
• Molecule 1: Major vault protein

Chain i: 75% 18% 6%

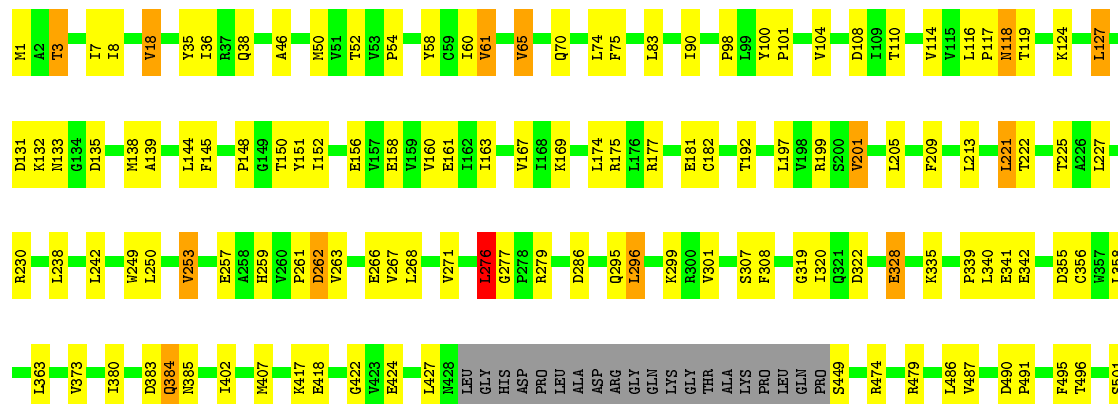
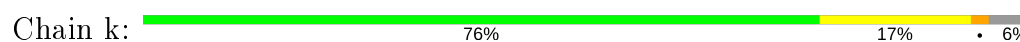


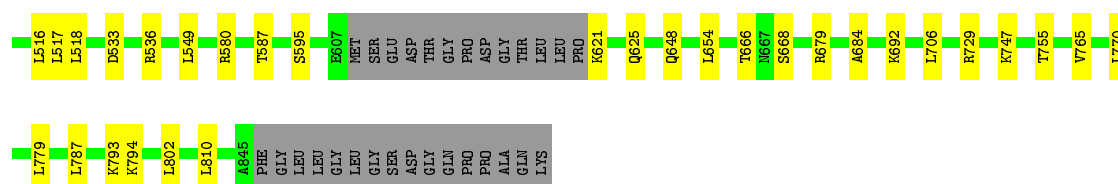


• Molecule 1: Major vault protein



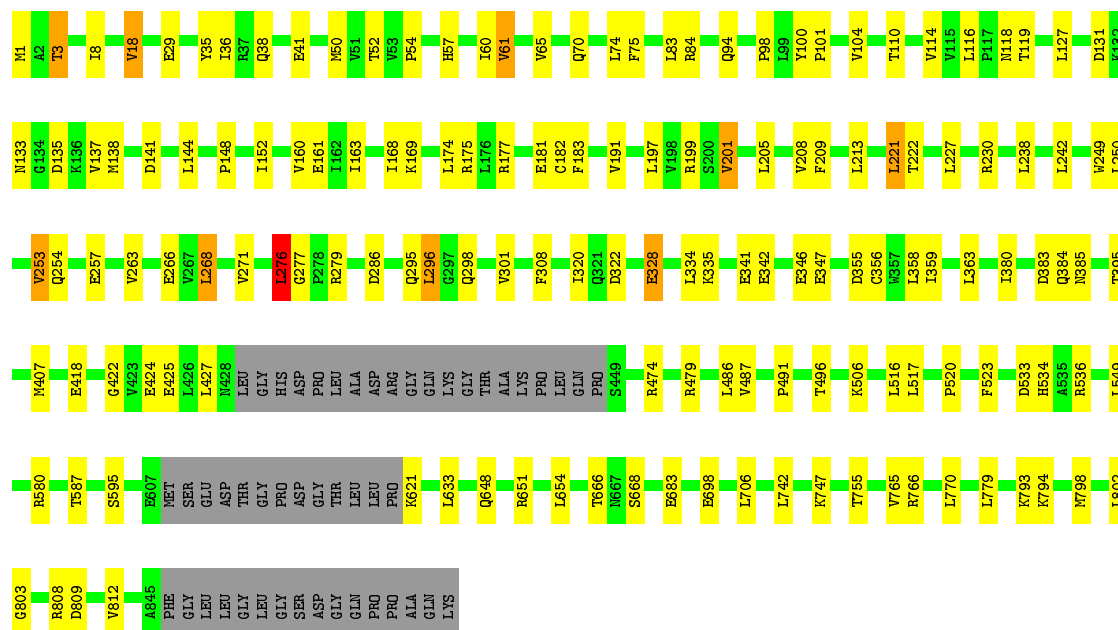
• Molecule 1: Major vault protein





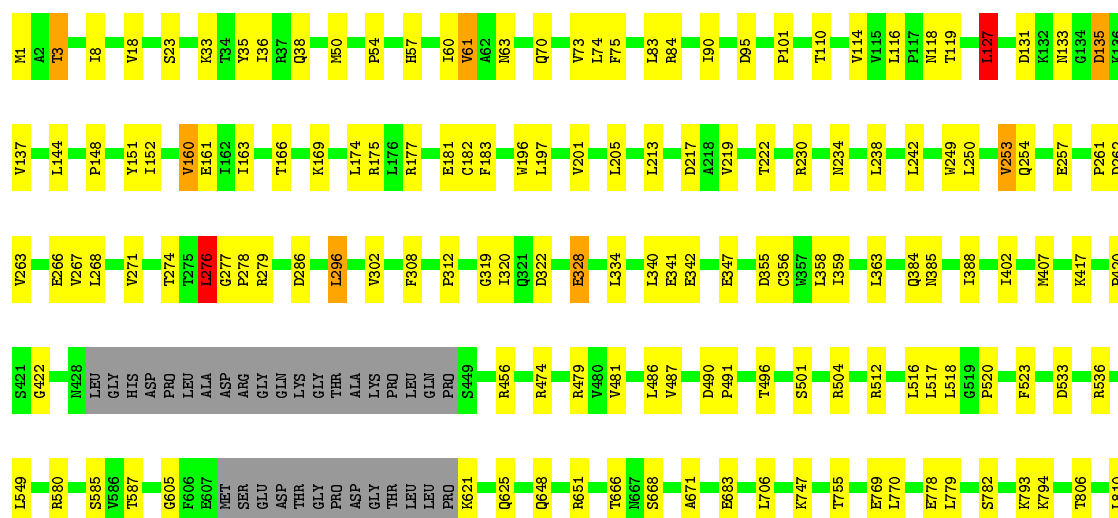
• Molecule 1: Major vault protein

Chain l: 77% 16% 6%



• Molecule 1: Major vault protein

Chain m: 77% 16% 6%



A814	V812	A845	PHE
			GLY
			LEU
			LEU
			GLY
			LEU
			GLY
			SER
			ASP
			GLY
			GLN
			PRO
			PRO
			ALA
			GLN
			LYS

4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	702.25Å 383.80Å 598.48Å 90.00° 124.69° 90.00°	Depositor
Resolution (Å)	204.00 – 3.50	Depositor
% Data completeness (in resolution range)	92.7 (204.00-3.50)	Depositor
R_{merge}	0.23	Depositor
R_{sym}	0.21	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 3.49Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.311 , 0.330	Depositor
Wilson B-factor (Å ²)	104.6	Xtriage
Anisotropy	0.212	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.099 for h,-k,-h-l	Xtriage
Total number of atoms	241956	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.50	0/6279	0.69	3/8506 (0.0%)
1	B	0.50	0/6279	0.68	4/8506 (0.0%)
1	C	0.50	0/6279	0.69	5/8506 (0.1%)
1	D	0.50	0/6279	0.69	5/8506 (0.1%)
1	E	0.51	0/6279	0.69	3/8506 (0.0%)
1	F	0.50	0/6279	0.68	2/8506 (0.0%)
1	G	0.49	0/6279	0.68	3/8506 (0.0%)
1	H	0.50	0/6279	0.68	4/8506 (0.0%)
1	I	0.51	0/6279	0.69	3/8506 (0.0%)
1	J	0.51	0/6279	0.71	4/8506 (0.0%)
1	K	0.53	0/6279	0.73	6/8506 (0.1%)
1	L	0.52	0/6279	0.72	4/8506 (0.0%)
1	M	0.52	0/6279	0.71	3/8506 (0.0%)
1	N	0.51	0/6279	0.71	3/8506 (0.0%)
1	O	0.52	0/6279	0.71	3/8506 (0.0%)
1	P	0.52	0/6279	0.73	7/8506 (0.1%)
1	Q	0.52	0/6279	0.72	6/8506 (0.1%)
1	R	0.53	0/6279	0.74	4/8506 (0.0%)
1	S	0.50	0/6279	0.70	4/8506 (0.0%)
1	T	0.50	0/6279	0.69	3/8506 (0.0%)
1	U	0.49	0/6279	0.68	5/8506 (0.1%)
1	V	0.50	0/6279	0.67	4/8506 (0.0%)
1	W	0.49	0/6279	0.68	5/8506 (0.1%)
1	X	0.49	0/6279	0.69	3/8506 (0.0%)
1	Y	0.50	0/6279	0.68	3/8506 (0.0%)
1	Z	0.50	0/6279	0.69	4/8506 (0.0%)
1	a	0.49	0/6279	0.69	3/8506 (0.0%)
1	b	0.51	0/6279	0.70	5/8506 (0.1%)
1	c	0.51	0/6279	0.70	5/8506 (0.1%)
1	d	0.50	0/6279	0.71	5/8506 (0.1%)
1	e	0.51	0/6279	0.71	4/8506 (0.0%)
1	f	0.51	0/6279	0.70	4/8506 (0.0%)
1	g	0.50	0/6279	0.70	6/8506 (0.1%)
1	h	0.49	0/6279	0.70	3/8506 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	i	0.50	0/6279	0.70	4/8506 (0.0%)
1	j	0.50	0/6279	0.71	4/8506 (0.0%)
1	k	0.51	0/6279	0.72	4/8506 (0.0%)
1	l	0.50	0/6279	0.70	4/8506 (0.0%)
1	m	0.51	0/6279	0.69	4/8506 (0.0%)
All	All	0.51	0/244881	0.70	158/331734 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	1
1	B	1	0
1	C	1	1
1	D	1	1
1	E	1	1
1	F	1	0
1	G	1	0
1	H	1	0
1	I	1	0
1	J	1	1
1	K	1	1
1	L	1	0
1	M	1	0
1	N	1	0
1	O	1	0
1	P	1	0
1	Q	1	0
1	R	1	0
1	S	1	0
1	T	1	1
1	U	1	0
1	V	1	1
1	W	1	0
1	X	1	1
1	Y	1	0
1	Z	1	1
1	a	1	1
1	b	1	0
1	c	1	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	d	1	0
1	e	1	1
1	f	1	0
1	g	1	0
1	h	1	0
1	i	1	1
1	j	1	0
1	k	1	0
1	l	1	0
1	m	1	1
All	All	39	14

There are no bond length outliers.

The worst 5 of 158 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	j	165	ALA	CB-CA-C	-7.38	99.03	110.10
1	E	276	LEU	CA-CB-CG	7.24	131.95	115.30
1	K	276	LEU	CA-CB-CG	7.10	131.64	115.30
1	l	276	LEU	CA-CB-CG	7.04	131.49	115.30
1	P	252	THR	CB-CA-C	-6.96	92.81	111.60

5 of 39 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	3	THR	CB
1	B	3	THR	CB
1	C	3	THR	CB
1	D	3	THR	CB
1	E	3	THR	CB

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	504	ARG	Peptide
1	C	504	ARG	Peptide
1	D	504	ARG	Peptide
1	E	504	ARG	Peptide
1	J	135	ASP	Peptide

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	776/861 (90%)	634 (82%)	119 (15%)	23 (3%)	4	30
1	B	776/861 (90%)	640 (82%)	114 (15%)	22 (3%)	5	32
1	C	776/861 (90%)	639 (82%)	109 (14%)	28 (4%)	3	26
1	D	776/861 (90%)	635 (82%)	108 (14%)	33 (4%)	2	22
1	E	776/861 (90%)	637 (82%)	107 (14%)	32 (4%)	3	23
1	F	776/861 (90%)	627 (81%)	118 (15%)	31 (4%)	3	24
1	G	776/861 (90%)	648 (84%)	101 (13%)	27 (4%)	3	27
1	H	776/861 (90%)	636 (82%)	109 (14%)	31 (4%)	3	24
1	I	776/861 (90%)	650 (84%)	98 (13%)	28 (4%)	3	26
1	J	776/861 (90%)	637 (82%)	109 (14%)	30 (4%)	3	25
1	K	776/861 (90%)	631 (81%)	104 (13%)	41 (5%)	2	17
1	L	776/861 (90%)	637 (82%)	103 (13%)	36 (5%)	2	21
1	M	776/861 (90%)	633 (82%)	107 (14%)	36 (5%)	2	21
1	N	776/861 (90%)	639 (82%)	102 (13%)	35 (4%)	2	21
1	O	776/861 (90%)	637 (82%)	102 (13%)	37 (5%)	2	20
1	P	776/861 (90%)	627 (81%)	117 (15%)	32 (4%)	3	23
1	Q	776/861 (90%)	633 (82%)	104 (13%)	39 (5%)	2	19
1	R	776/861 (90%)	627 (81%)	109 (14%)	40 (5%)	2	18
1	S	776/861 (90%)	624 (80%)	115 (15%)	37 (5%)	2	20
1	T	776/861 (90%)	631 (81%)	113 (15%)	32 (4%)	3	23
1	U	776/861 (90%)	642 (83%)	100 (13%)	34 (4%)	2	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	V	776/861 (90%)	639 (82%)	110 (14%)	27 (4%)	3	27
1	W	776/861 (90%)	647 (83%)	96 (12%)	33 (4%)	2	22
1	X	776/861 (90%)	648 (84%)	97 (12%)	31 (4%)	3	24
1	Y	776/861 (90%)	644 (83%)	98 (13%)	34 (4%)	2	21
1	Z	776/861 (90%)	649 (84%)	97 (12%)	30 (4%)	3	25
1	a	776/861 (90%)	639 (82%)	108 (14%)	29 (4%)	3	26
1	b	776/861 (90%)	635 (82%)	112 (14%)	29 (4%)	3	26
1	c	776/861 (90%)	642 (83%)	101 (13%)	33 (4%)	2	22
1	d	776/861 (90%)	630 (81%)	118 (15%)	28 (4%)	3	26
1	e	776/861 (90%)	629 (81%)	113 (15%)	34 (4%)	2	21
1	f	776/861 (90%)	642 (83%)	99 (13%)	35 (4%)	2	21
1	g	776/861 (90%)	637 (82%)	98 (13%)	41 (5%)	2	17
1	h	776/861 (90%)	639 (82%)	97 (12%)	40 (5%)	2	18
1	i	776/861 (90%)	634 (82%)	104 (13%)	38 (5%)	2	19
1	j	776/861 (90%)	634 (82%)	107 (14%)	35 (4%)	2	21
1	k	776/861 (90%)	633 (82%)	105 (14%)	38 (5%)	2	19
1	l	776/861 (90%)	632 (81%)	107 (14%)	37 (5%)	2	20
1	m	776/861 (90%)	634 (82%)	108 (14%)	34 (4%)	2	21
All	All	30264/33579 (90%)	24831 (82%)	4143 (14%)	1290 (4%)	2	22

5 of 1290 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	ASP
1	A	148	PRO
1	A	169	LYS
1	A	253	VAL
1	A	296	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	663/727 (91%)	527 (80%)	136 (20%)	1	6
1	B	663/727 (91%)	545 (82%)	118 (18%)	2	10
1	C	663/727 (91%)	536 (81%)	127 (19%)	1	7
1	D	663/727 (91%)	543 (82%)	120 (18%)	1	9
1	E	663/727 (91%)	550 (83%)	113 (17%)	2	12
1	F	663/727 (91%)	543 (82%)	120 (18%)	1	9
1	G	663/727 (91%)	533 (80%)	130 (20%)	1	7
1	H	663/727 (91%)	533 (80%)	130 (20%)	1	7
1	I	663/727 (91%)	537 (81%)	126 (19%)	1	8
1	J	663/727 (91%)	532 (80%)	131 (20%)	1	7
1	K	663/727 (91%)	519 (78%)	144 (22%)	1	5
1	L	663/727 (91%)	536 (81%)	127 (19%)	1	7
1	M	663/727 (91%)	537 (81%)	126 (19%)	1	8
1	N	663/727 (91%)	535 (81%)	128 (19%)	1	7
1	O	663/727 (91%)	528 (80%)	135 (20%)	1	6
1	P	663/727 (91%)	527 (80%)	136 (20%)	1	6
1	Q	663/727 (91%)	528 (80%)	135 (20%)	1	6
1	R	663/727 (91%)	521 (79%)	142 (21%)	1	5
1	S	663/727 (91%)	539 (81%)	124 (19%)	1	8
1	T	663/727 (91%)	540 (81%)	123 (19%)	1	8
1	U	663/727 (91%)	532 (80%)	131 (20%)	1	7
1	V	663/727 (91%)	530 (80%)	133 (20%)	1	6
1	W	663/727 (91%)	545 (82%)	118 (18%)	2	10
1	X	663/727 (91%)	534 (80%)	129 (20%)	1	7
1	Y	663/727 (91%)	547 (82%)	116 (18%)	2	10
1	Z	663/727 (91%)	535 (81%)	128 (19%)	1	7
1	a	663/727 (91%)	538 (81%)	125 (19%)	1	8
1	b	663/727 (91%)	534 (80%)	129 (20%)	1	7
1	c	663/727 (91%)	531 (80%)	132 (20%)	1	7
1	d	663/727 (91%)	542 (82%)	121 (18%)	1	8
1	e	663/727 (91%)	534 (80%)	129 (20%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	f	663/727 (91%)	536 (81%)	127 (19%)	1	7
1	g	663/727 (91%)	533 (80%)	130 (20%)	1	7
1	h	663/727 (91%)	535 (81%)	128 (19%)	1	7
1	i	663/727 (91%)	533 (80%)	130 (20%)	1	7
1	j	663/727 (91%)	540 (81%)	123 (19%)	1	8
1	k	663/727 (91%)	531 (80%)	132 (20%)	1	7
1	l	663/727 (91%)	541 (82%)	122 (18%)	1	8
1	m	663/727 (91%)	541 (82%)	122 (18%)	1	8
All	All	25857/28353 (91%)	20881 (81%)	4976 (19%)	1	7

5 of 4976 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	276	LEU
1	V	345	SER
1	j	794	LYS
1	R	779	LEU
1	T	363	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 645 such sidechains are listed below:

Mol	Chain	Res	Type
1	R	378	GLN
1	V	509	HIS
1	j	776	GLN
1	S	22	ASN
1	T	494	GLN

5.3.3 RNA ⓘ

There are no RNA 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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.