wwPDB EM Validation Summary Report (i)

Mar 13, 2026 – 01:47 AM UTC

PDB ID	:	9R87 / pdb_00009r87
EMDB ID	:	EMD-53806
Title	:	Cap of the vault protein from Human Brain
Authors	:	Lovestam, S.L.; Scheres, S.H.W.
Deposited on	:	2025-05-15
Resolution	:	3.60 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 (i) 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 (i)) were used in the production of this report:

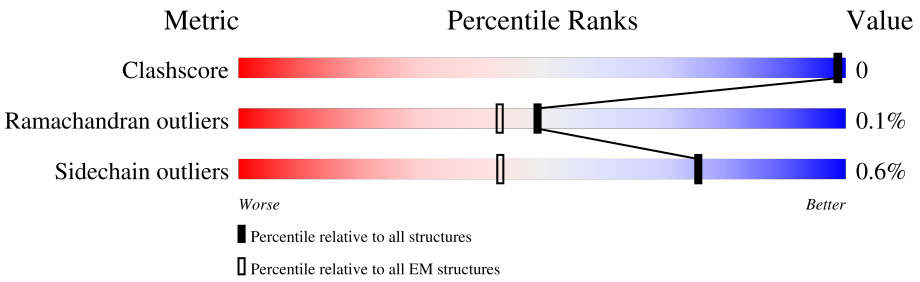
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

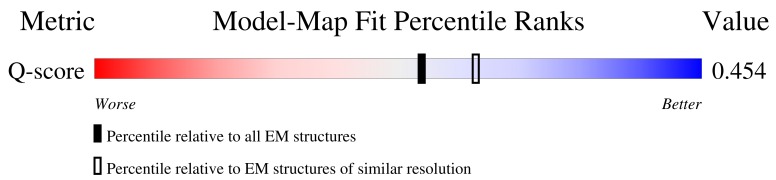
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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	9% 91%
1	A1	893	7% 93%
1	A2	893	7% 93%
1	A3	893	7% 93%

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Mol	Chain	Length	Quality of chain
1	A4	893	7% 93%
1	Ar	893	7% 93%
1	As	893	7% 93%
1	At	893	7% 93%
1	Au	893	7% 93%
1	Av	893	7% 93%
1	Aw	893	7% 93%
1	Ax	893	7% 93%
1	Ay	893	7% 93%
1	Az	893	7% 93%
1	B	893	6% 94%
1	C	893	9% 91%
1	D	893	6% 94%
1	E	893	9% 91%
1	F	893	6% 94%
1	G	893	9% 91%
1	H	893	6% 94%
1	I	893	9% 91%
1	J	893	6% 94%
1	K	893	9% 91%
1	L	893	6% 94%
1	M	893	9% 91%
1	N	893	6% 94%
1	O	893	9% 91%
1	P	893	6% 94%

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Mol	Chain	Length	Quality of chain
1	Q	893	9% 91%
1	R	893	6% 94%
1	S	893	9% 91%
1	T	893	6% 94%
1	U	893	9% 91%
1	V	893	6% 94%
1	W	893	9% 91%
1	X	893	6% 94%
1	Y	893	9% 91%
1	Z	893	6% 94%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 42419 atoms, of which 21814 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Major vault protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	84	1297	404	665	104	122	2	0	0
			Total	C	H	N	O	S		
1	A1	66	1048	322	541	84	99	2	0	0
			Total	C	H	N	O	S		
1	A2	66	1048	322	541	84	99	2	0	0
			Total	C	H	N	O	S		
1	A3	66	1048	322	541	84	99	2	0	0
			Total	C	H	N	O	S		
1	A4	66	1048	322	541	84	99	2	0	0
			Total	C	H	N	O	S		
1	Ar	66	1048	322	541	84	99	2	0	0
			Total	C	H	N	O	S		
1	As	66	1048	322	541	84	99	2	0	0
			Total	C	H	N	O	S		
1	At	66	1048	322	541	84	99	2	0	0
			Total	C	H	N	O	S		
1	Au	66	1048	322	541	84	99	2	0	0
			Total	C	H	N	O	S		
1	Av	66	1048	322	541	84	99	2	0	0
			Total	C	H	N	O	S		
1	Aw	66	1048	322	541	84	99	2	0	0
			Total	C	H	N	O	S		
1	Ax	66	1048	322	541	84	99	2	0	0
			Total	C	H	N	O	S		
1	Ay	66	1048	322	541	84	99	2	0	0
			Total	C	H	N	O	S		
1	Az	66	1048	322	541	84	99	2	0	0
			Total	C	H	N	O	S		
1	B	58	918	283	472	75	86	2	0	0
			Total	C	H	N	O	S		
1	C	84	1297	404	665	104	122	2	0	0
			Total	C	H	N	O	S		
1	D	58	918	283	472	75	86	2	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	E	84	1297	404	665	104	122	2	0	0
			Total	C	H	N	O	S		
1	F	58	918	283	472	75	86	2	0	0
			Total	C	H	N	O	S		
1	G	84	1297	404	665	104	122	2	0	0
			Total	C	H	N	O	S		
1	H	58	918	283	472	75	86	2	0	0
			Total	C	H	N	O	S		
1	I	84	1297	404	665	104	122	2	0	0
			Total	C	H	N	O	S		
1	J	58	918	283	472	75	86	2	0	0
			Total	C	H	N	O	S		
1	K	84	1297	404	665	104	122	2	0	0
			Total	C	H	N	O	S		
1	L	58	918	283	472	75	86	2	0	0
			Total	C	H	N	O	S		
1	M	84	1297	404	665	104	122	2	0	0
			Total	C	H	N	O	S		
1	N	58	918	283	472	75	86	2	0	0
			Total	C	H	N	O	S		
1	O	84	1297	404	665	104	122	2	0	0
			Total	C	H	N	O	S		
1	P	58	918	283	472	75	86	2	0	0
			Total	C	H	N	O	S		
1	Q	84	1297	404	665	104	122	2	0	0
			Total	C	H	N	O	S		
1	R	58	918	283	472	75	86	2	0	0
			Total	C	H	N	O	S		
1	S	84	1297	404	665	104	122	2	0	0
			Total	C	H	N	O	S		
1	T	58	918	283	472	75	86	2	0	0
			Total	C	H	N	O	S		
1	U	84	1297	404	665	104	122	2	0	0
			Total	C	H	N	O	S		
1	V	58	918	283	472	75	86	2	0	0
			Total	C	H	N	O	S		
1	W	84	1297	404	665	104	122	2	0	0
			Total	C	H	N	O	S		
1	X	58	918	283	472	75	86	2	0	0
			Total	C	H	N	O	S		
1	Y	84	1297	404	665	104	122	2	0	0

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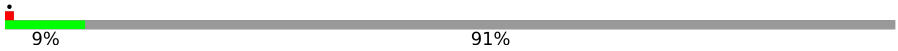
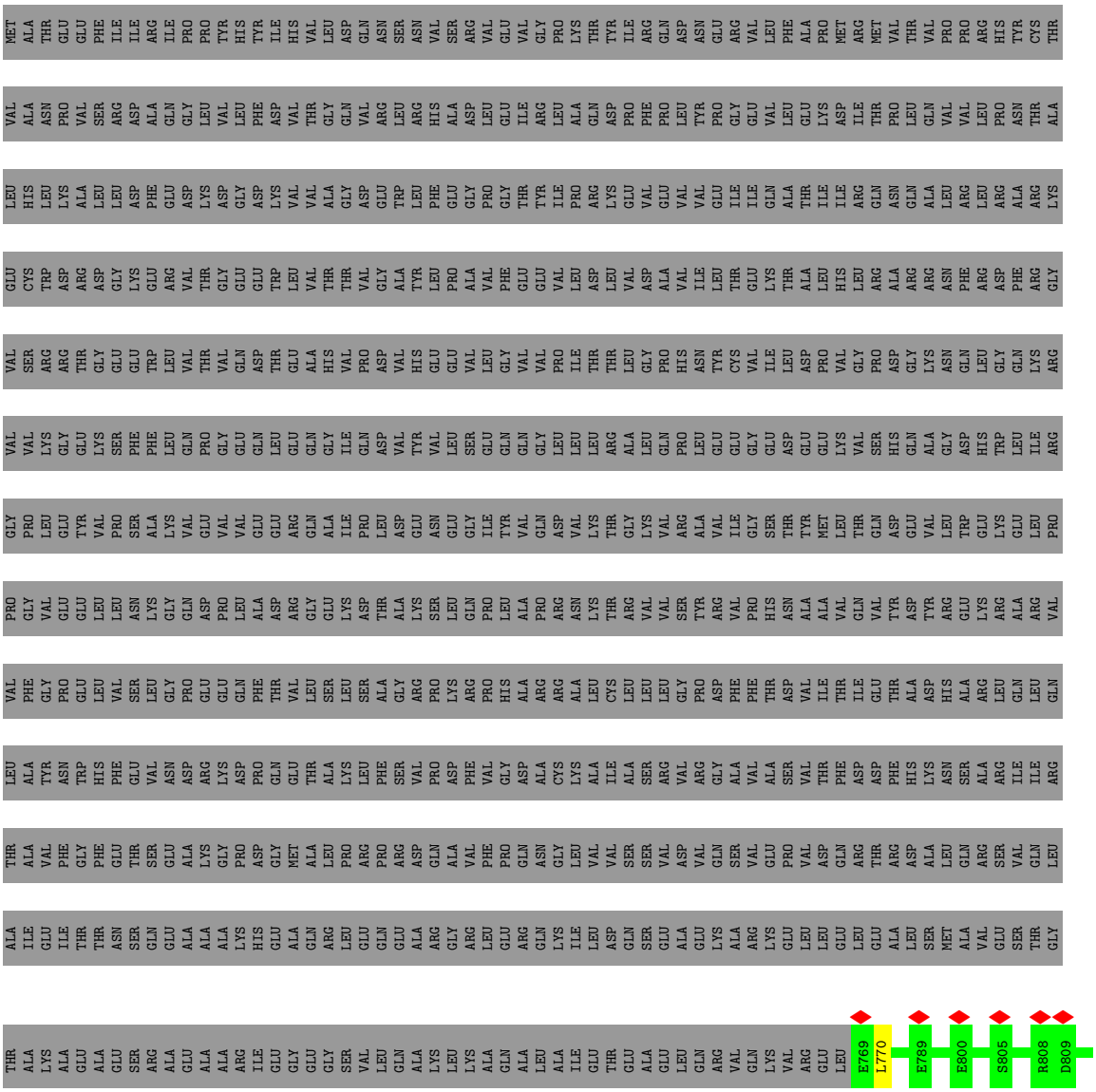
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	Z	58	918	283	472	75	86	2	0	0

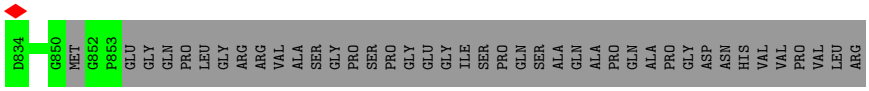
3 Residue-property plots (i)

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

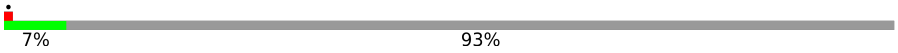
Chain A: 

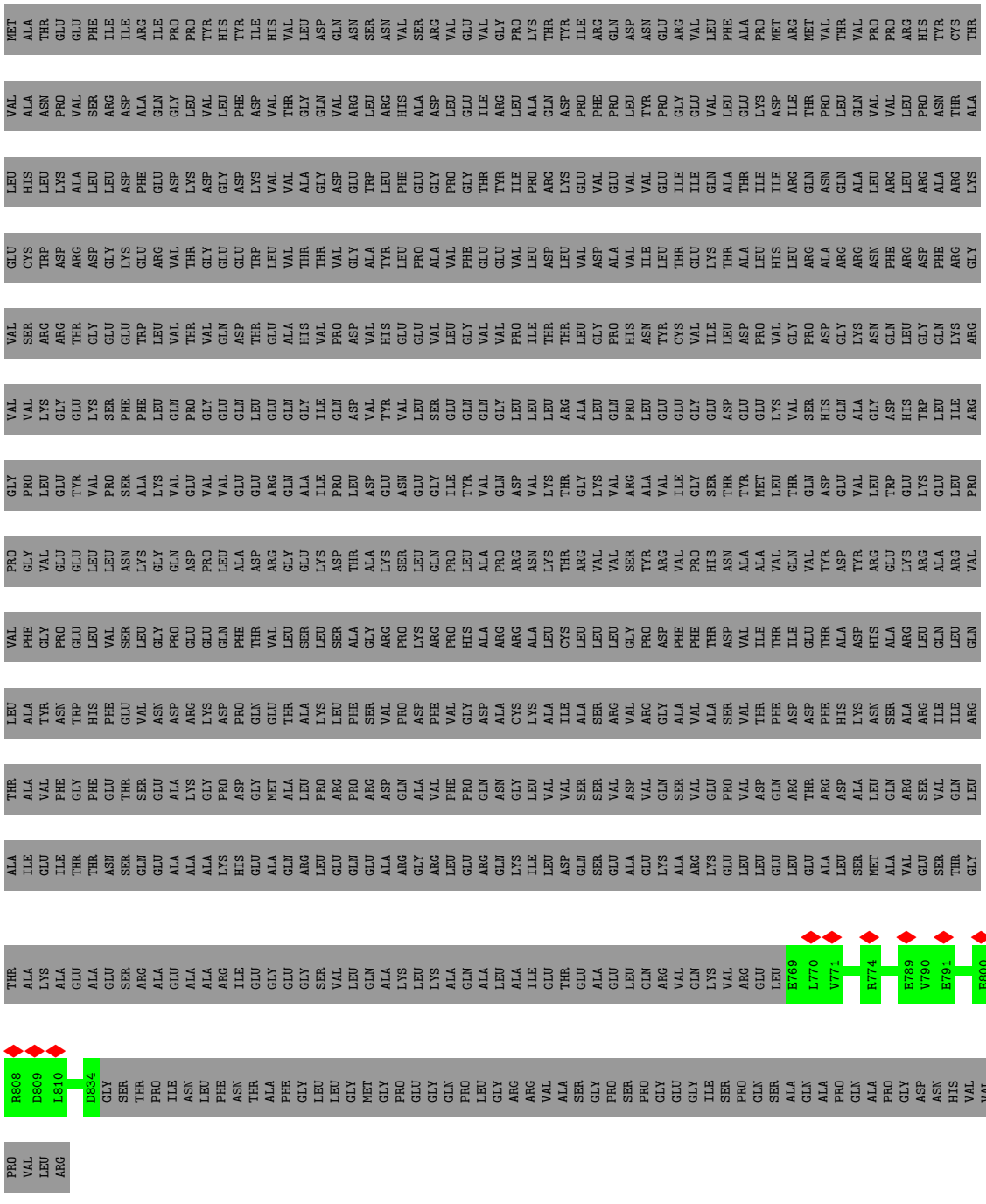




• Molecule 1: Major vault protein

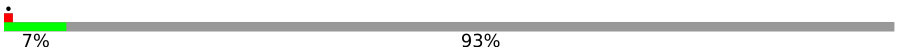
Chain A1:

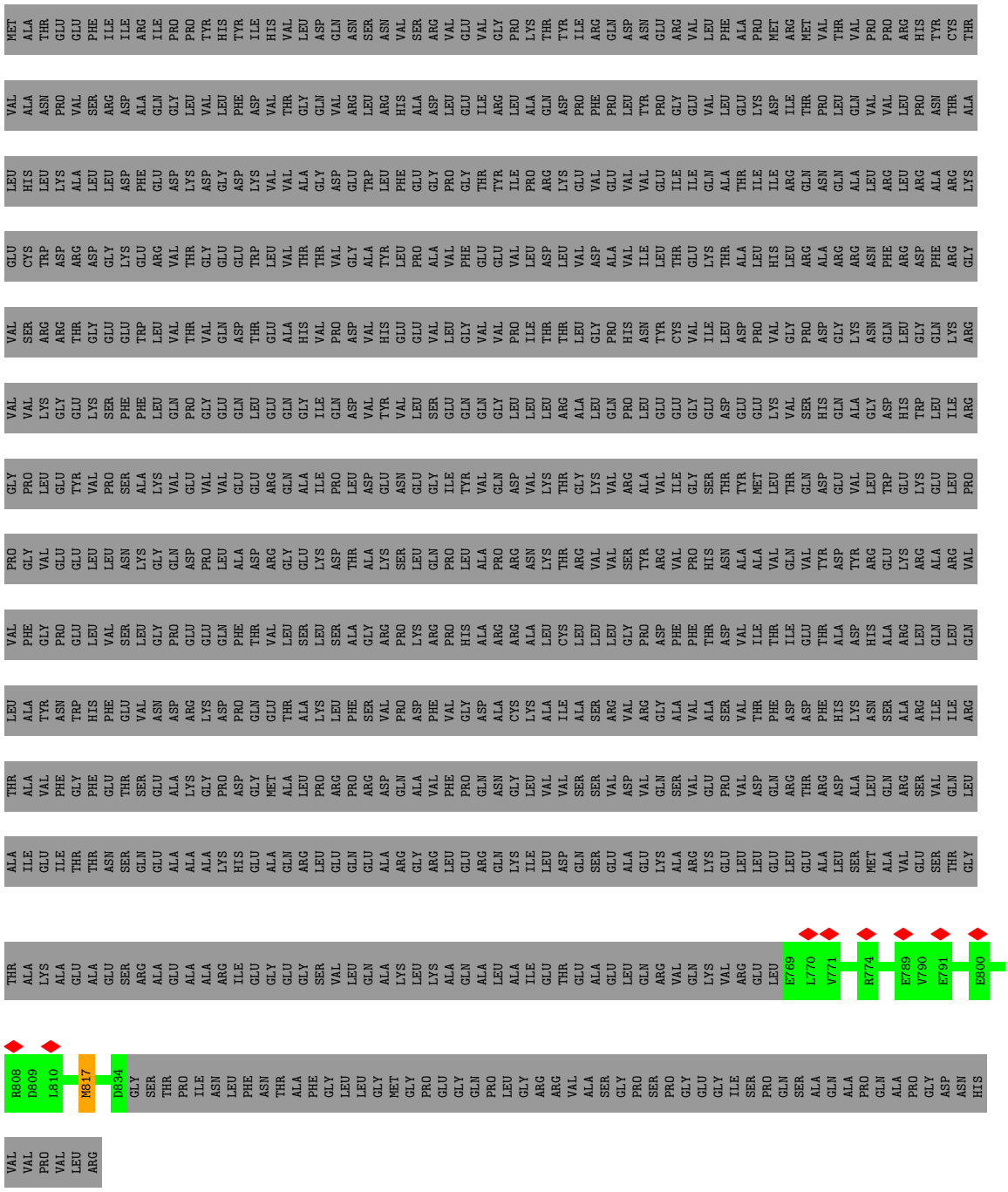




• Molecule 1: Major vault protein

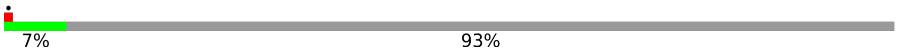
Chain A2:

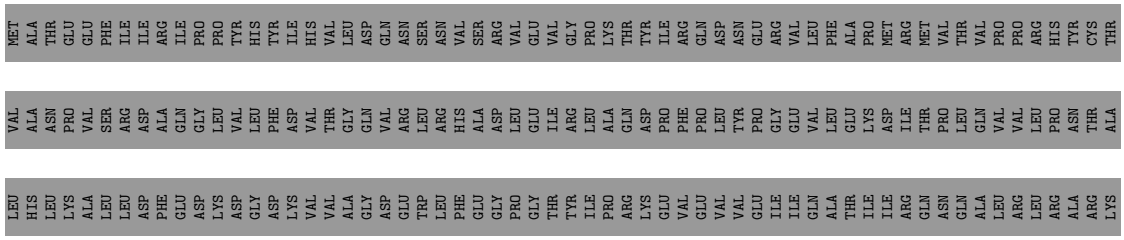


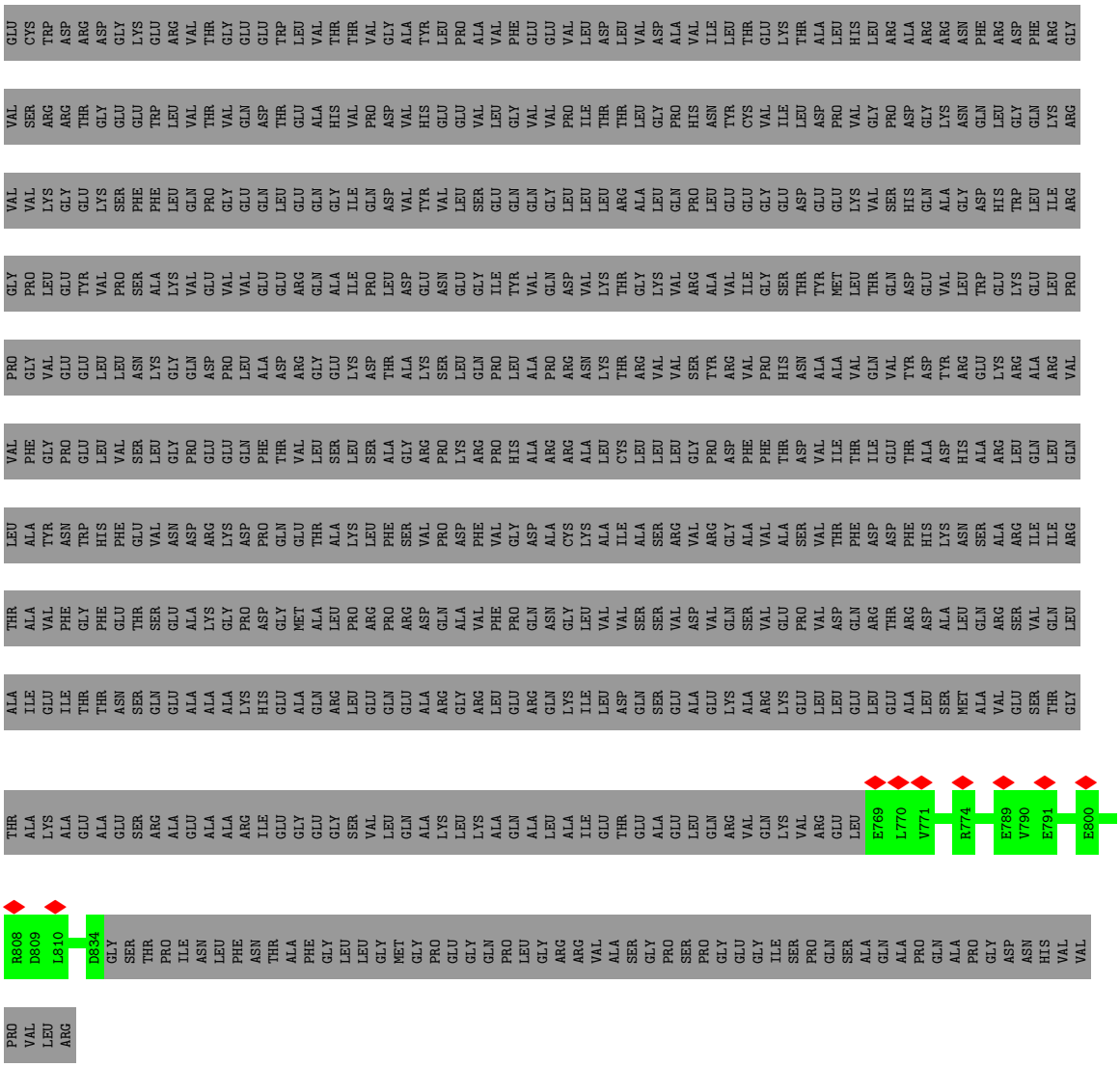


- Molecule 1: Major vault protein

Chain A3:

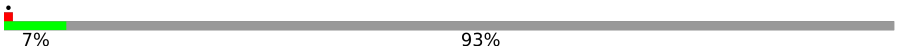


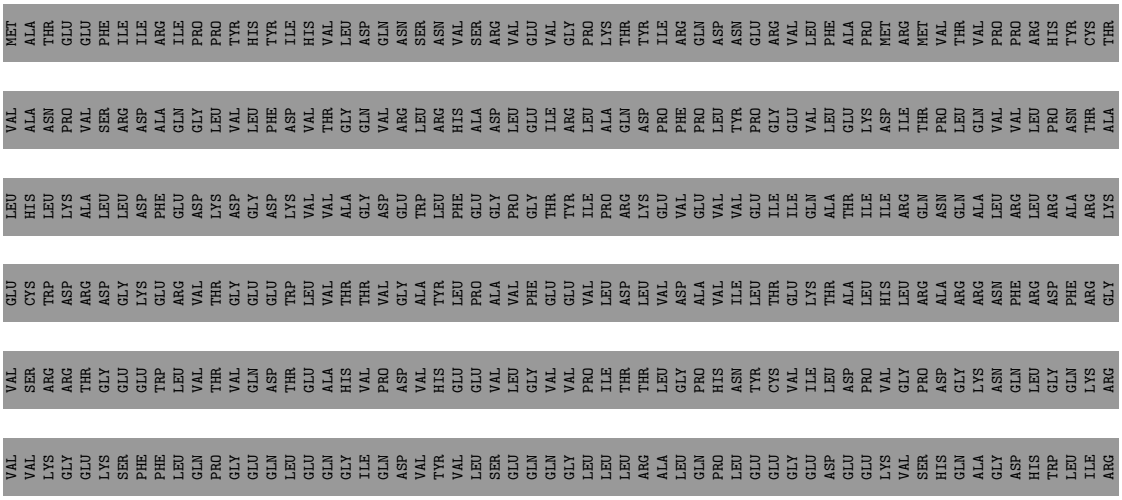


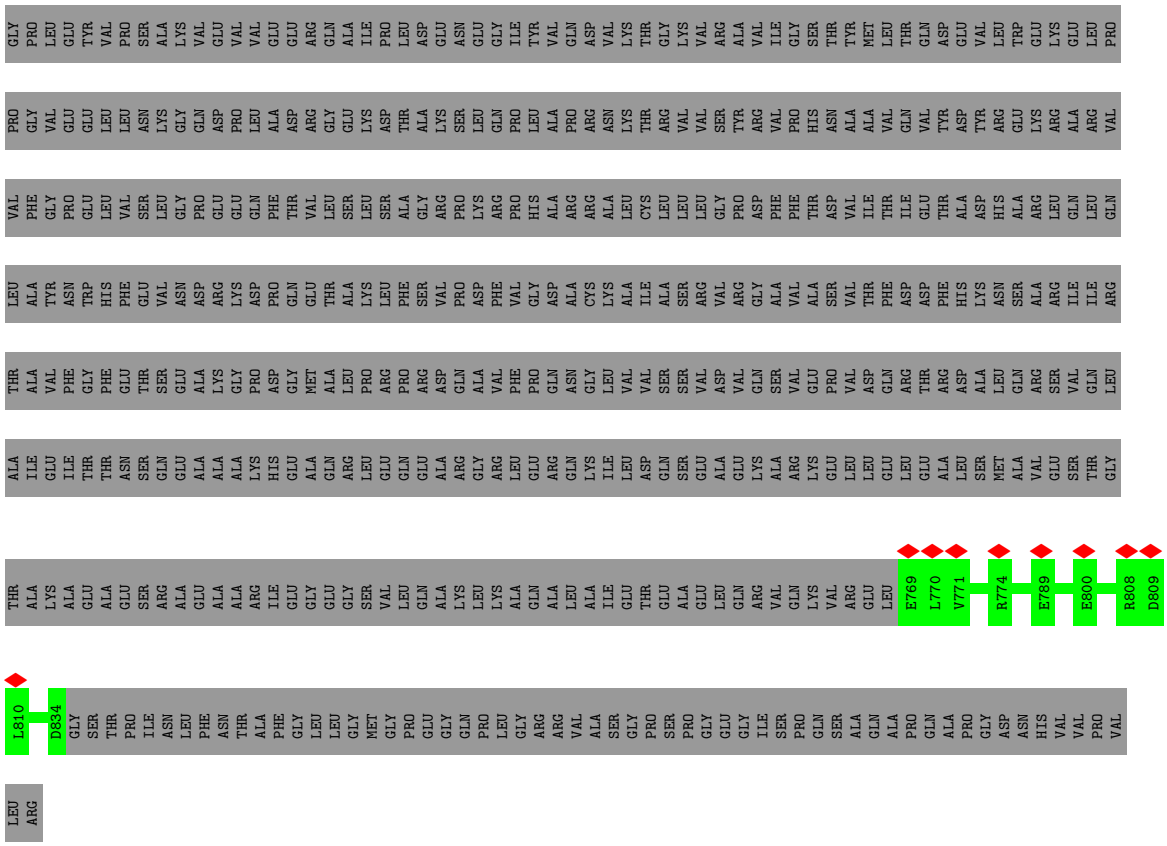


- Molecule 1: Major vault protein

Chain A4:

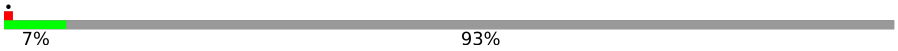


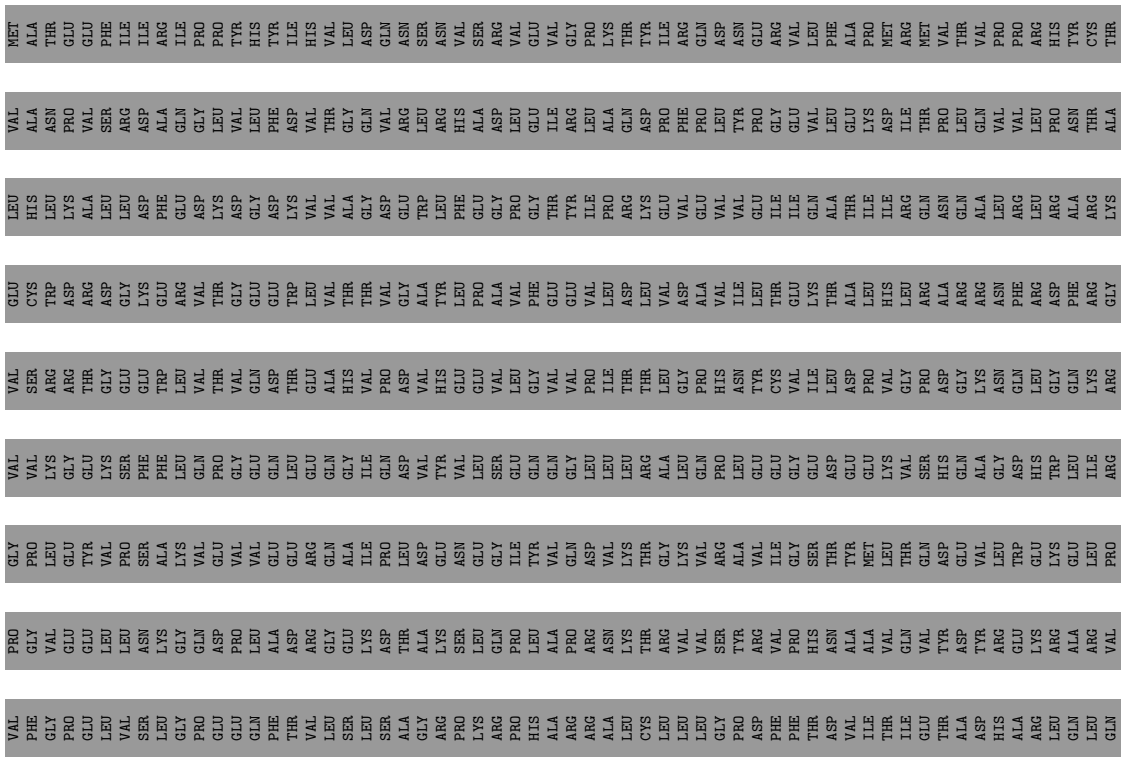




• Molecule 1: Major vault protein

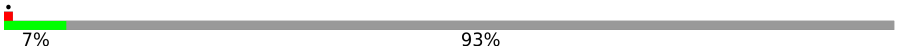
Chain Ar:

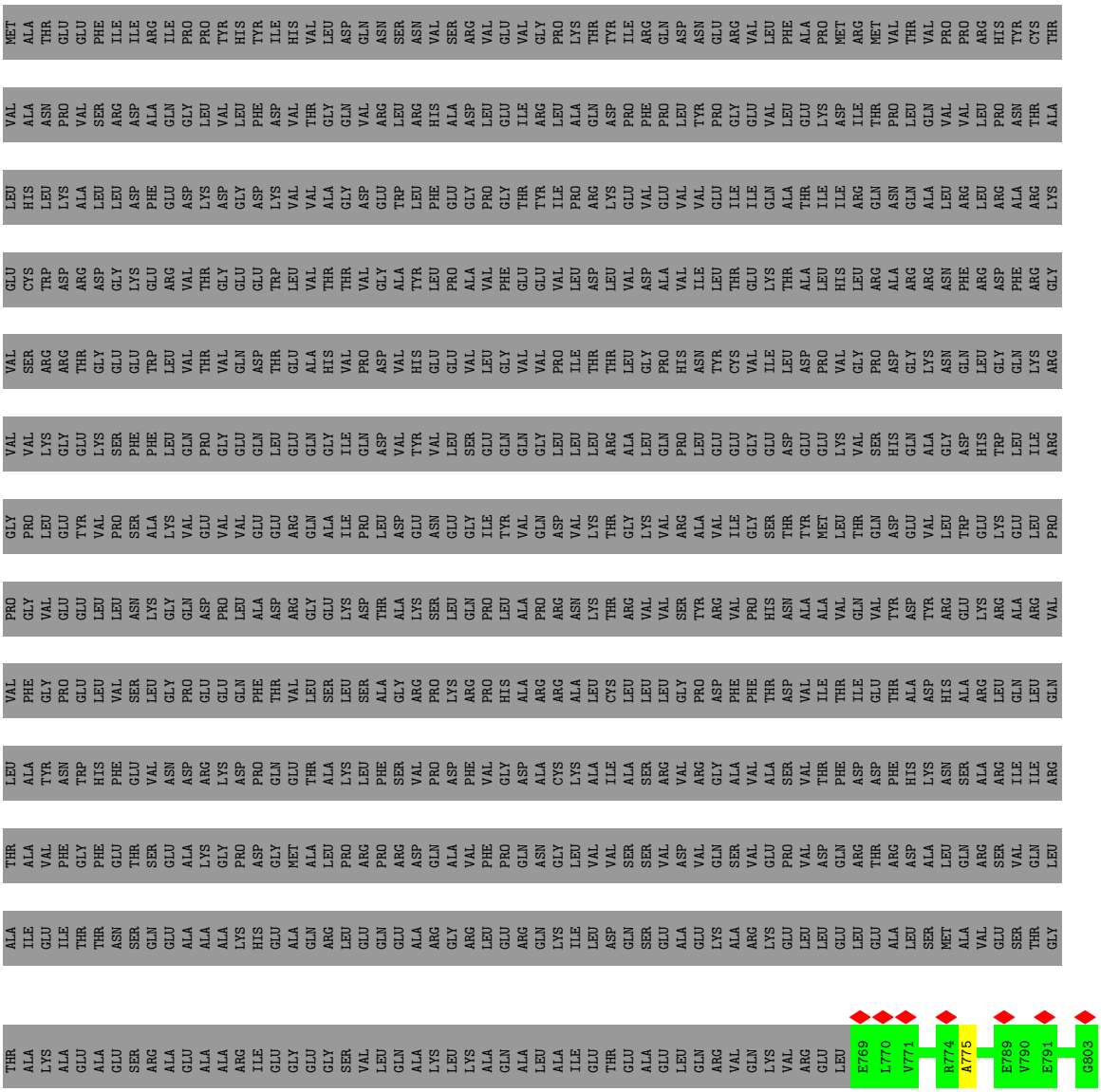


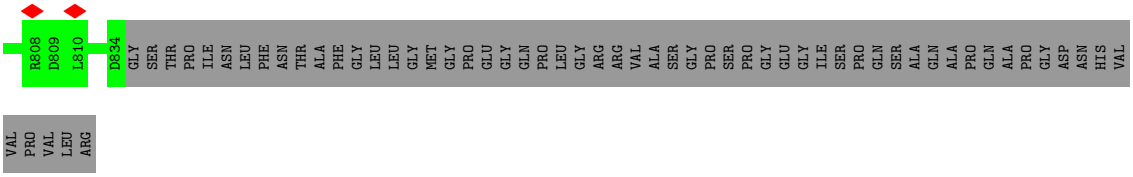


• Molecule 1: Major vault protein

Chain As:

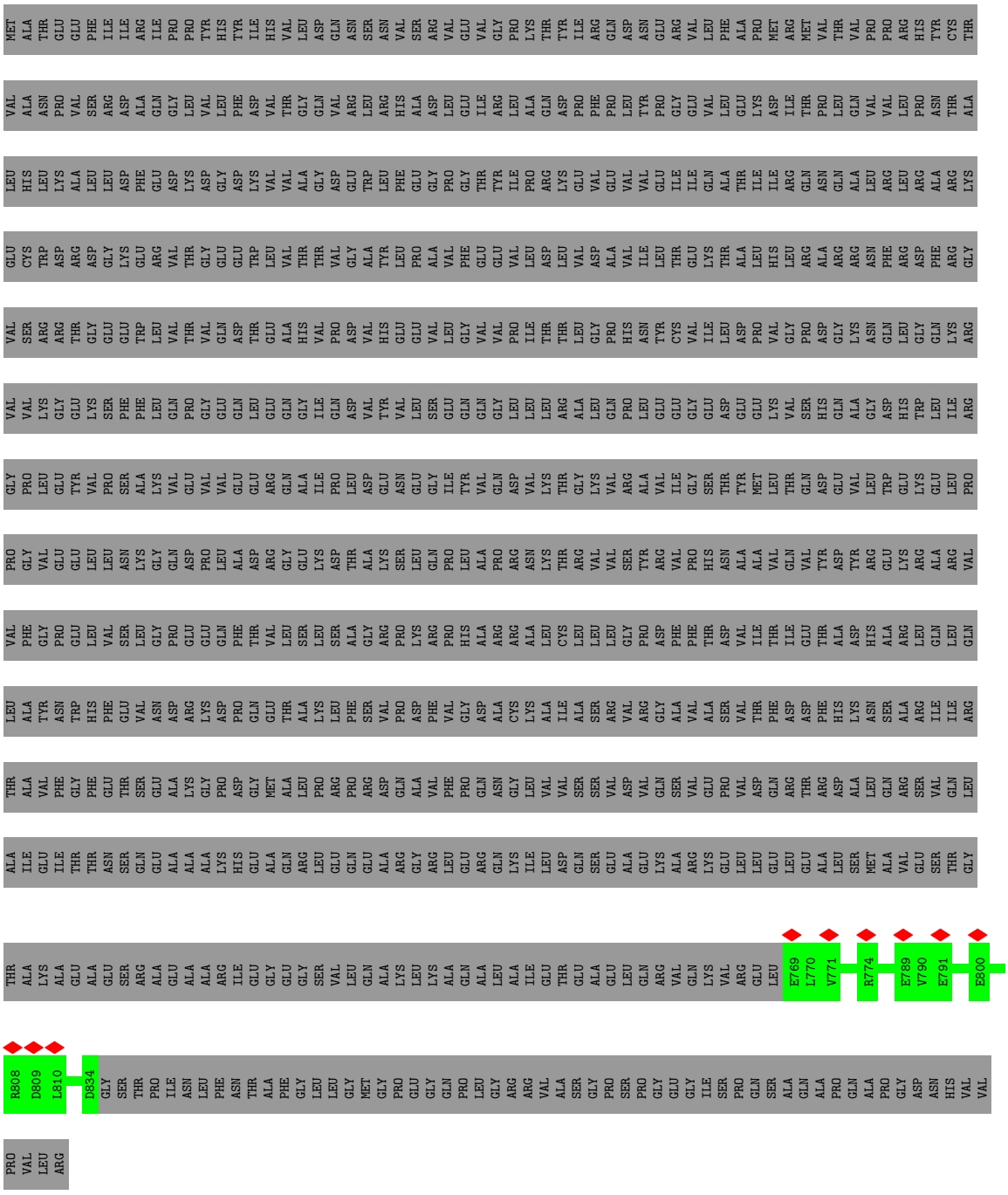






• Molecule 1: Major vault protein

Chain At: 7% 93%



• Molecule 1: Major vault protein

Chain Au: 7% 93%

MET ALA THR GLU GLU PHE ILE ILE ARG ILE PRO PRO TYR HIS TYR ILE HIS VAL LEU ASP GLN ASN SER ASN VAL SER ARG VAL GLU VAL GLY PRO LYS THR TYR ILE ARG GLN ASP ASN GLU ARG VAL LEU PHE ALA PRO MET ARG MET VAL THR VAL PRO PRO ARG HIS TYR CYS THR

VAL ALA ASN PRO VAL SER ARG ASP ALA GLN GLY LEU VAL LEU PHE ASP VAL THR GLY GLN VAL ARG LEU ARG HIS ALA ASP LEU GLU ILE ARG LEU ALA GLN ASP PRO PHE PRO LEU TYR PRO GLY GLU VAL LEU GLU LYS ASP ILE THR PRO LEU GLN VAL VAL LEU PRO ASN THR ALA

LEU HIS LEU LYS ALA LEU LEU ASP PHE GLU GLU ASP LYS ASP GLY ASP LYS VAL VAL ALA GLY ASP GLU TRP LEU PHE GLU GLY PRO GLY THR TYR ILE PRO ARG LYS GLU VAL GLU VAL VAL GLU ILE ILE GLN ALA THR ILE ILE ARG GLN ASN GLN ALA LEU ARG LEU ARG ALA ARG LYS

GLU CYS TRP ASP ARG ASP GLY LYS GLU ARG VAL THR GLY GLU GLU TRP LEU VAL THR THR VAL GLY ALA TYR LEU PRO ALA VAL PHE GLU GLU VAL LEU ASP LEU VAL ASP ALA VAL ILE LEU THR GLU LYS THR ALA HIS LEU ARG ALA ARG ARG ASN PHE ARG ASP PHE ARG GLY

VAL SER ARG ARG THR GLY GLU GLU TRP LEU VAL THR VAL GLN ASP THR GLU ALA HIS VAL PRO ASP VAL HIS GLU GLU VAL LEU GLY VAL VAL PRO ILE THR THR LEU GLY PRO HIS ASN TYR CYS VAL ILE LEU ASP PRO VAL GLY PRO ASP GLY LYS ASN GLN LEU GLY GLN LYS ARG

VAL VAL LYS GLY GLU LYS SER PHE PHE LEU GLN PRO GLY GLU GLN LEU GLU GLN GLY ILE GLN ASP VAL TYR VAL LEU SER GLU GLN GLN GLY LEU LEU LEU ARG ALA LEU GLN PRO LEU GLU GLU GLY GLU ASP GLU GLU LYS VAL SER HIS GLN ALA GLY ASP HIS TRP LEU ILE ARG

GLY PRO LEU GLU TYR VAL PRO SER ALA LYS VAL GLU VAL VAL GLU GLU ARG GLN ALA ILE PRO LEU ASP GLU ASN GLU GLY ILE TYR VAL GLN ASP VAL LYS THR GLY LYS VAL ARG ALA VAL ILE GLY SER THR TYR MET LEU THR GLN ASP GLU VAL LEU TRP GLU LYS GLU LYS PRO

PRO GLY VAL GLU GLU LEU LEU ASN LYS GLY GLN ASP PRO LEU ALA ASP ARG GLY GLU LYS ASP THR ALA LYS SER LEU GLN PRO LEU ALA PRO ARG ASN LYS THR ARG VAL VAL SER TYR ARG VAL PRO HIS ASN ALA ALA VAL GLN VAL TYR ASP TYR ARG GLU LYS ARG ALA ARG VAL

VAL PHE GLY PRO GLU LEU VAL SER LEU GLY PRO GLU GLU GLN PHE THR VAL LEU SER LEU SER ALA GLY ARG PRO LYS ARG PRO HIS ALA ARG ARG ARG ALA LEU CYS LEU LEU LEU GLY PRO ASP PHE PHE THR ASP VAL ILE THR ILE GLU THR ALA ASP HIS ALA ARG LEU GLN LEU GLN

LEU ALA TYR ASN TRP HIS PHE GLU VAL ASN ASP ARG LYS ASP PRO GLN GLU THR ALA LYS LEU PHE SER VAL PRO ASP PHE VAL GLY ASP ALA CYS LYS ALA ILE ALA SER ARG VAL ARG GLY ALA VAL ALA SER VAL THR PHE ASP ASP PHE HIS LYS ASN SER ALA ARG ILE ILE ARG

THR ALA VAL PHE GLY PHE GLU THR SER GLU ALA LYS GLY PRO ASP GLY MET ALA LEU PRO ARG PRO ARG ASP GLN ALA VAL PHE PRO GLN ASN GLY LEU VAL VAL SER SER VAL ASP VAL GLN SER VAL GLU PRO VAL ASP GLN ARG THR ARG ASP ALA LEU GLN ARG SER VAL GLN LEU

ALA ILE GLU ILE THR THR ASN SER GLN GLU ALA ALA ALA LYS HIS GLU ALA GLN ARG LEU GLU GLN GLU ALA ARG GLY ARG LEU GLU ARG GLN LYS ILE LEU ASP GLN SER GLU ALA GLU LYS ALA ARG LYS GLU LEU LEU GLU LEU GLU GLU ALA LEU SER MET ALA VAL GLU SER THR GLY

THR ALA LYS ALA GLU ALA GLU SER ARG ALA GLU GLU ALA ALA GLY SER VAL LEU GLN ALA LYS LEU LYS ALA GLN ALA LEU ALA ILE GLU THR GLU ALA GLU LEU GLN ARG VAL GLN LYS VAL ARG GLU LEU E769 L770 V771 R774 E789 V790 E791 E800

R808 D809 L810 D834 GLY SER THR PRO ILE ASN LEU PHE ASN THR ALA PHE GLY LEU LEU GLY MET GLY PRO GLU GLY GLN PRO LEU GLY ARG ARG VAL ALA SER GLY PRO SER PRO GLY GLU GLY ILE SER PRO GLN SER ALA GLN ALA PRO GLN ALA PRO GLY ASP ASN HIS VAL VAL

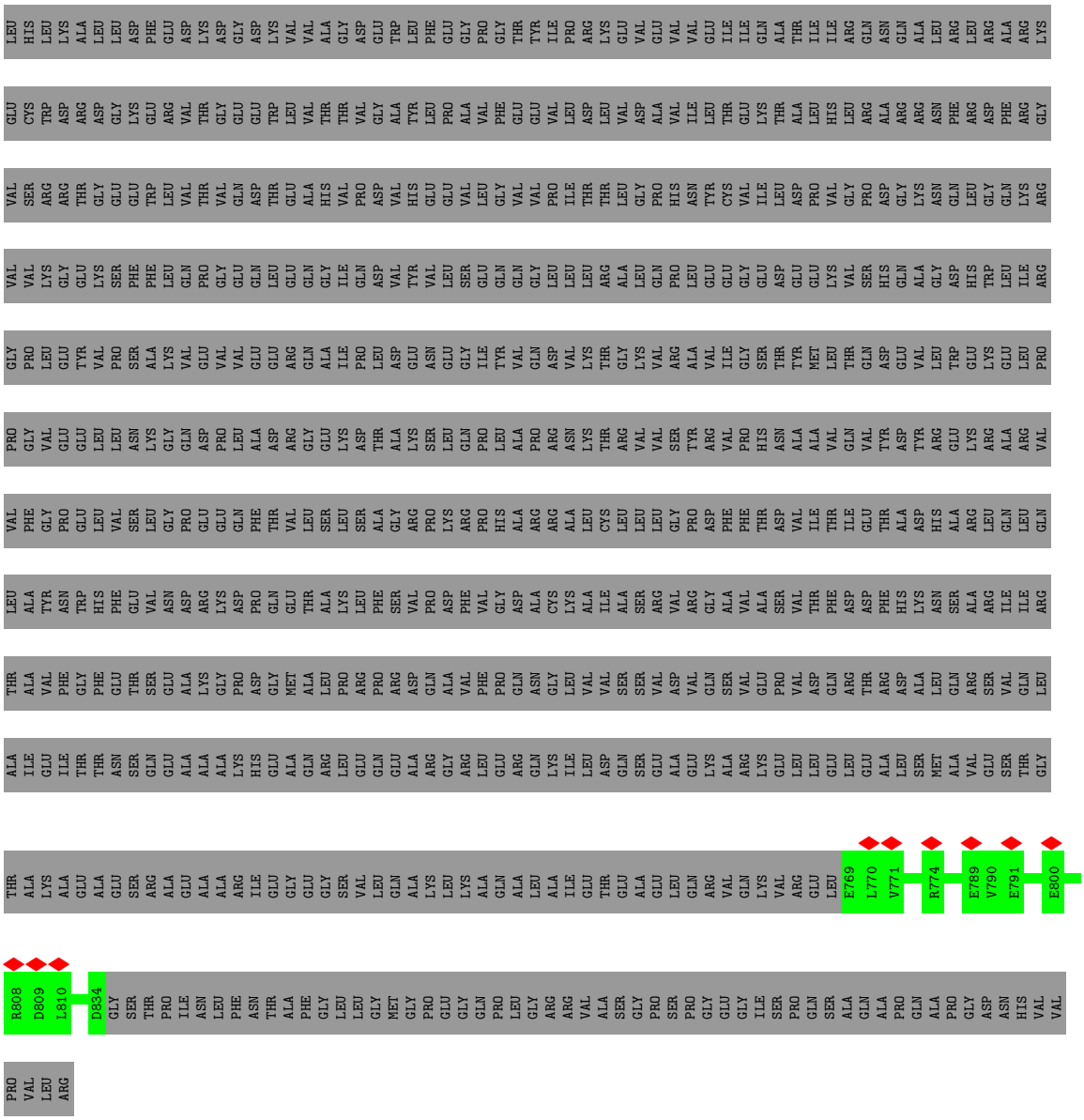
PRO VAL LEU ARG

• Molecule 1: Major vault protein

Chain Av: 7% 93%

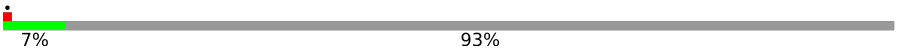
MET ALA THR GLU GLU PHE ILE ILE ARG ILE PRO PRO TYR HIS TYR ILE HIS VAL LEU ASP GLN ASN SER ASN VAL SER ARG VAL GLU VAL GLY PRO LYS THR TYR ILE ARG GLN ASP ASN GLU ARG VAL LEU PHE ALA PRO MET ARG MET VAL THR VAL PRO PRO ARG HIS TYR CYS THR

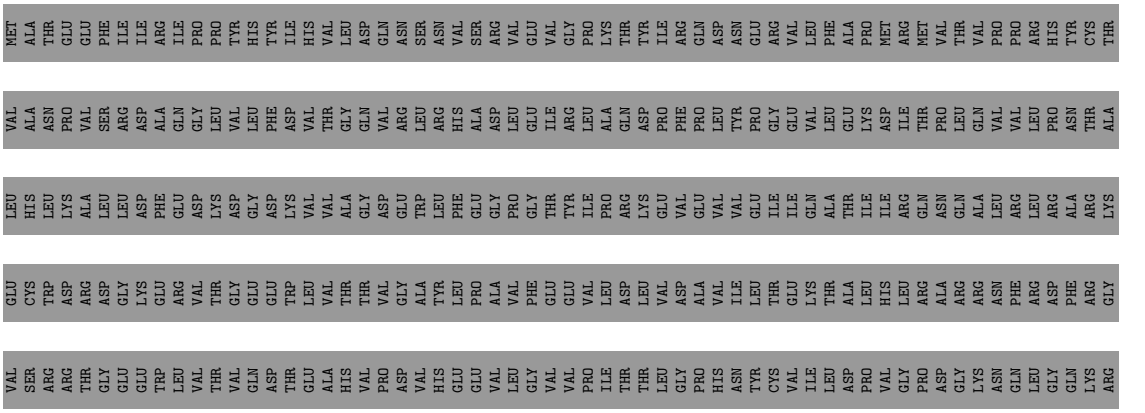
VAL ALA ASN PRO VAL SER ARG ASP ALA GLN GLY LEU VAL LEU PHE ASP VAL THR GLY GLN VAL ARG LEU ARG HIS ALA ASP LEU GLU ILE ARG LEU ALA GLN ASP PRO PHE PRO LEU TYR PRO GLY GLU VAL LEU GLU LYS ASP ILE THR PRO LEU GLN VAL VAL LEU PRO ASN THR ALA

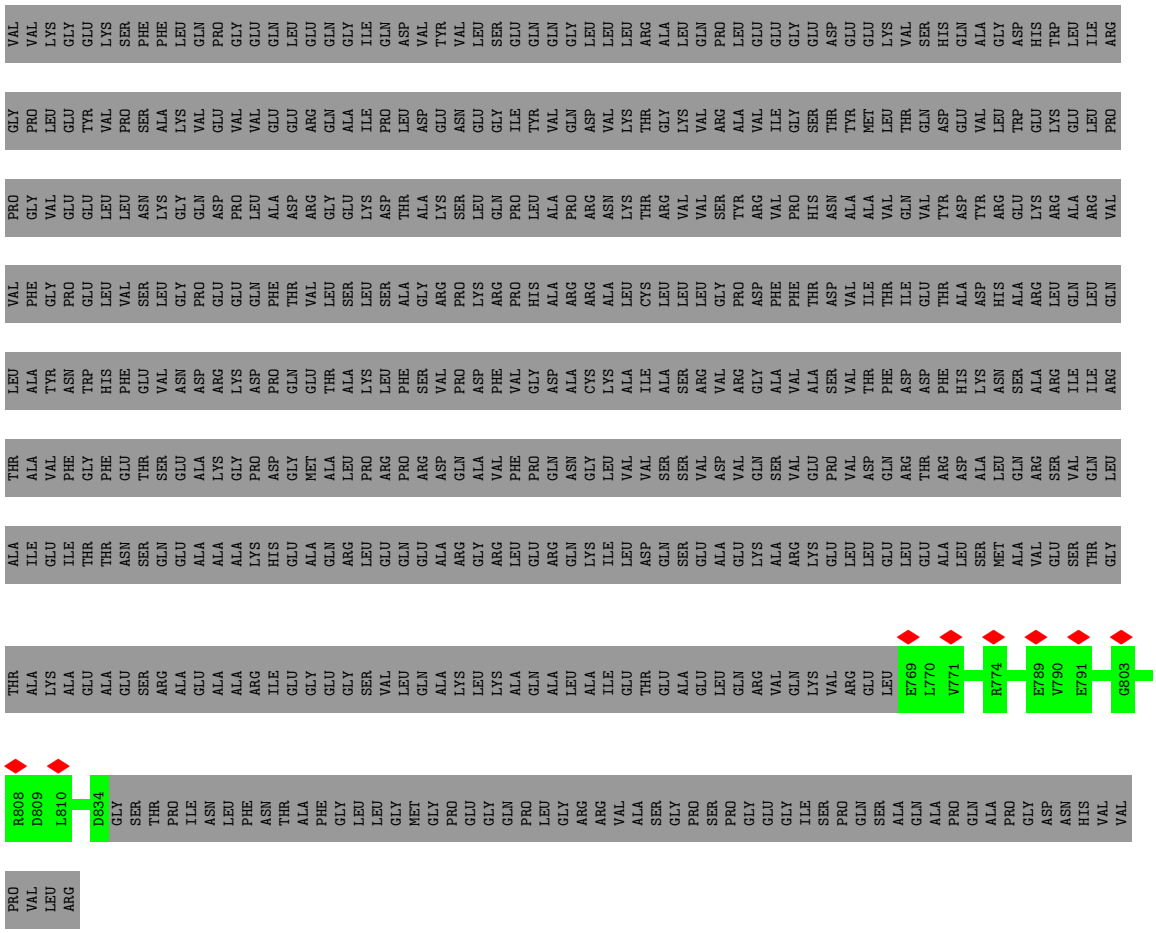


- Molecule 1: Major vault protein

Chain Aw:

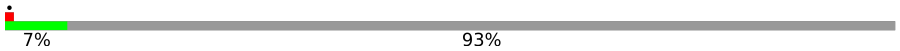


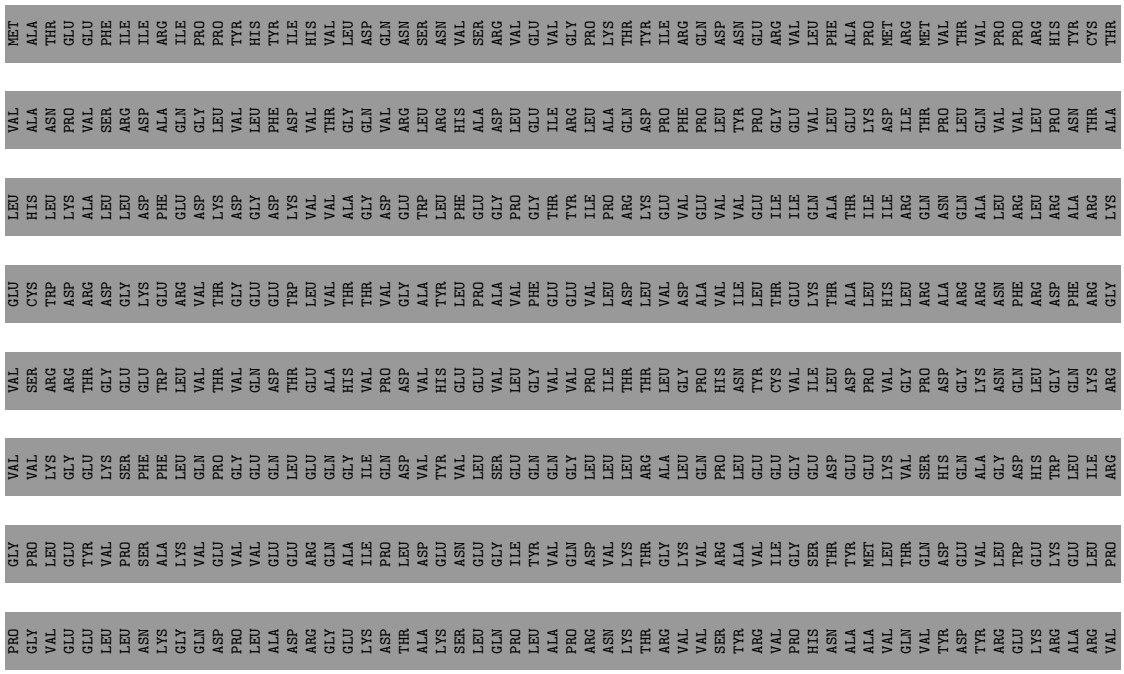


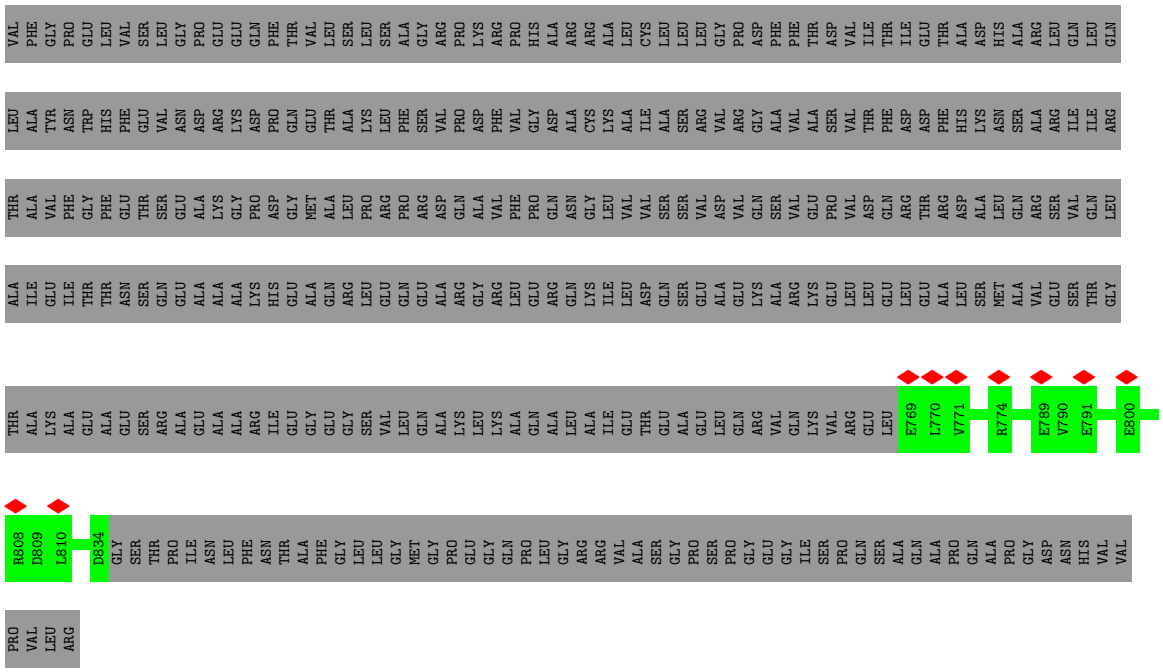


• Molecule 1: Major vault protein

Chain Ax:

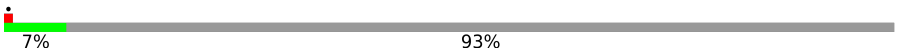


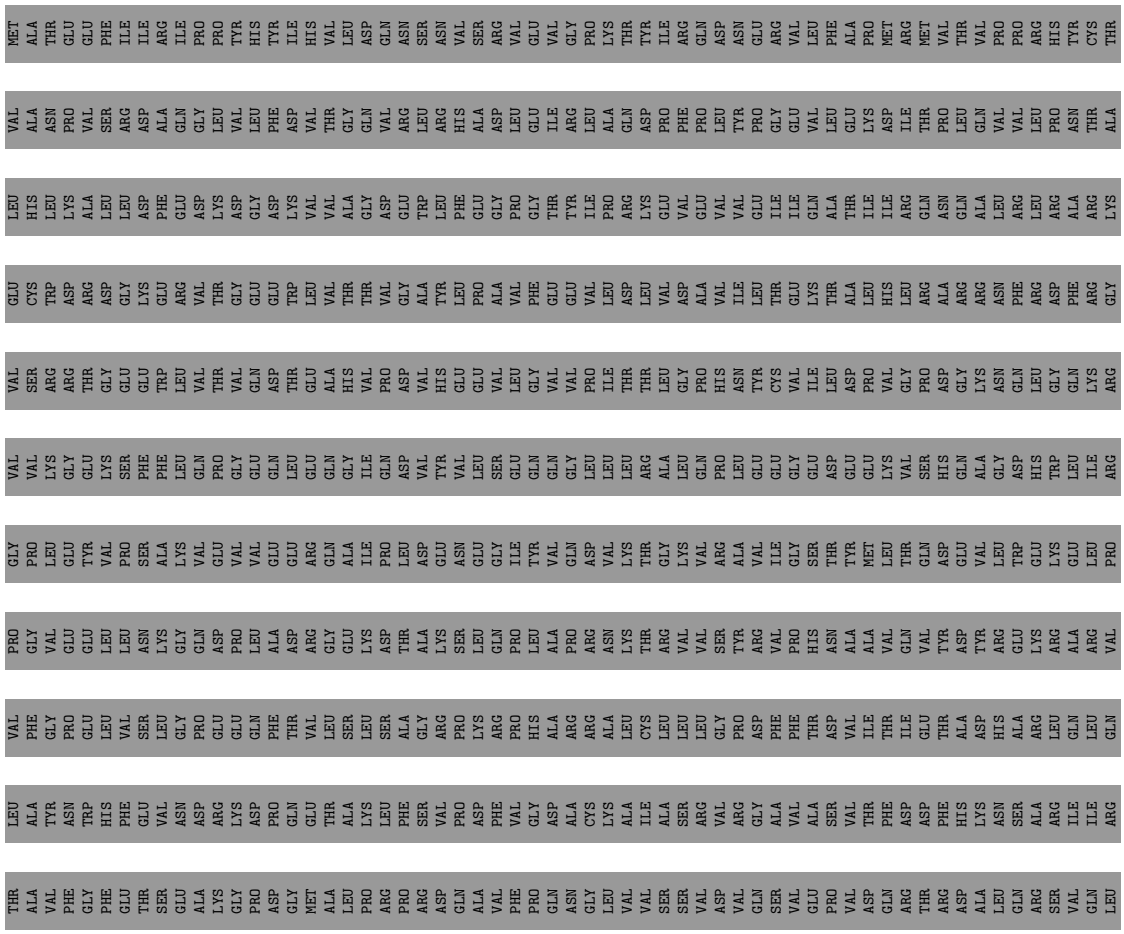


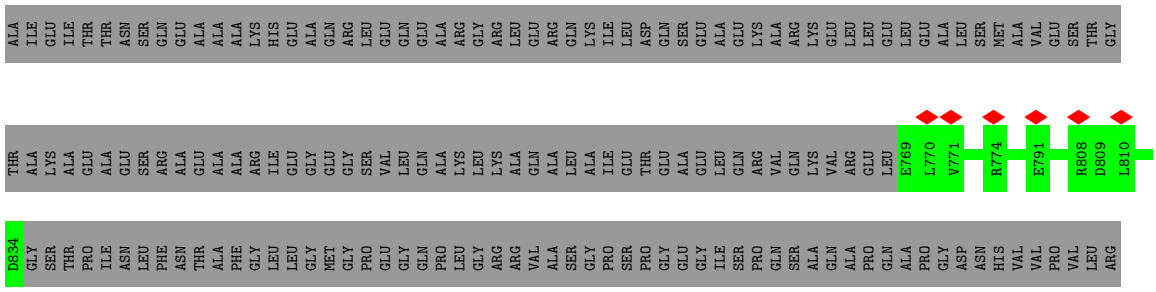


• Molecule 1: Major vault protein

Chain Ay:

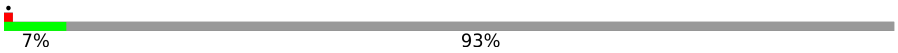


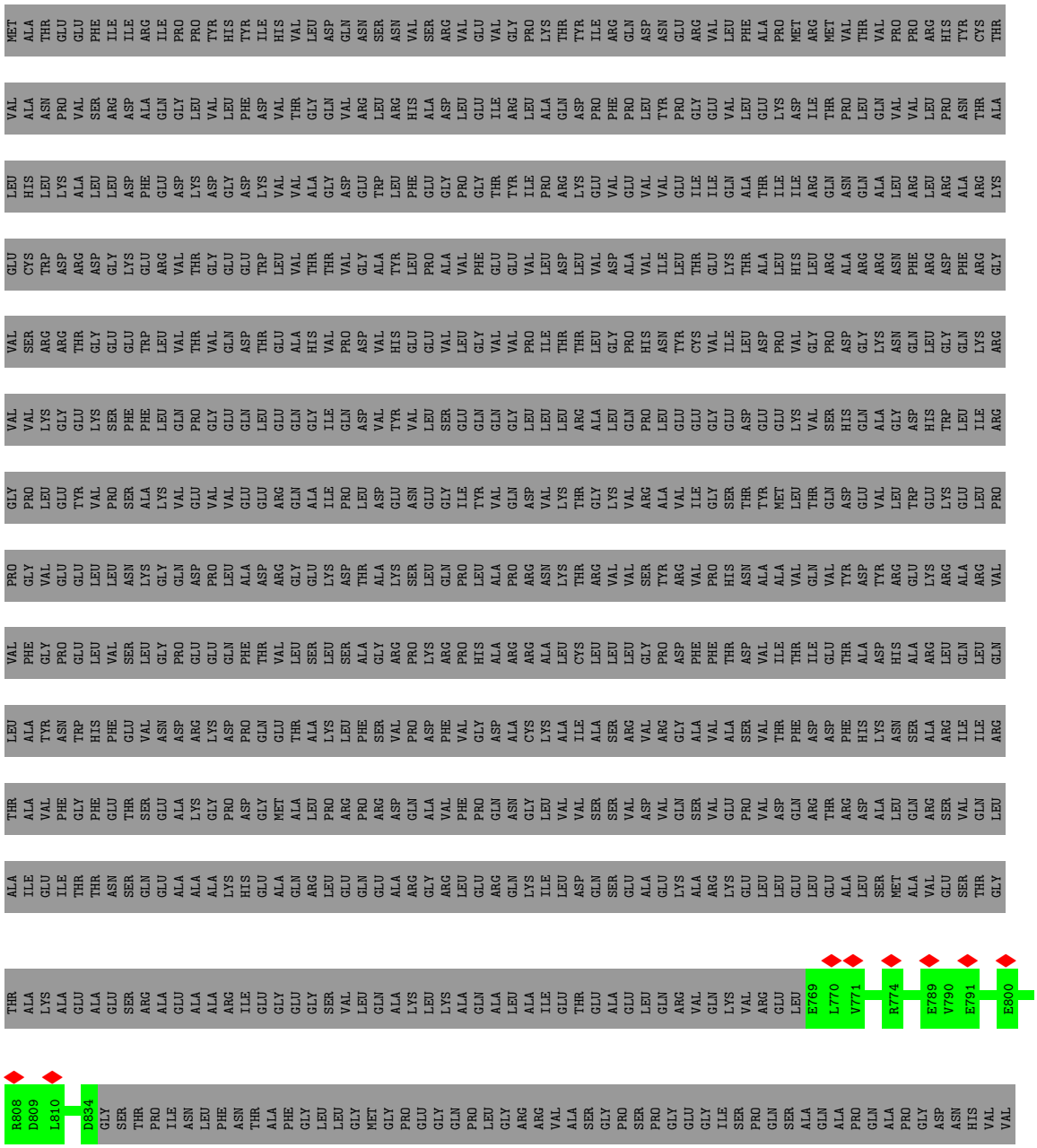


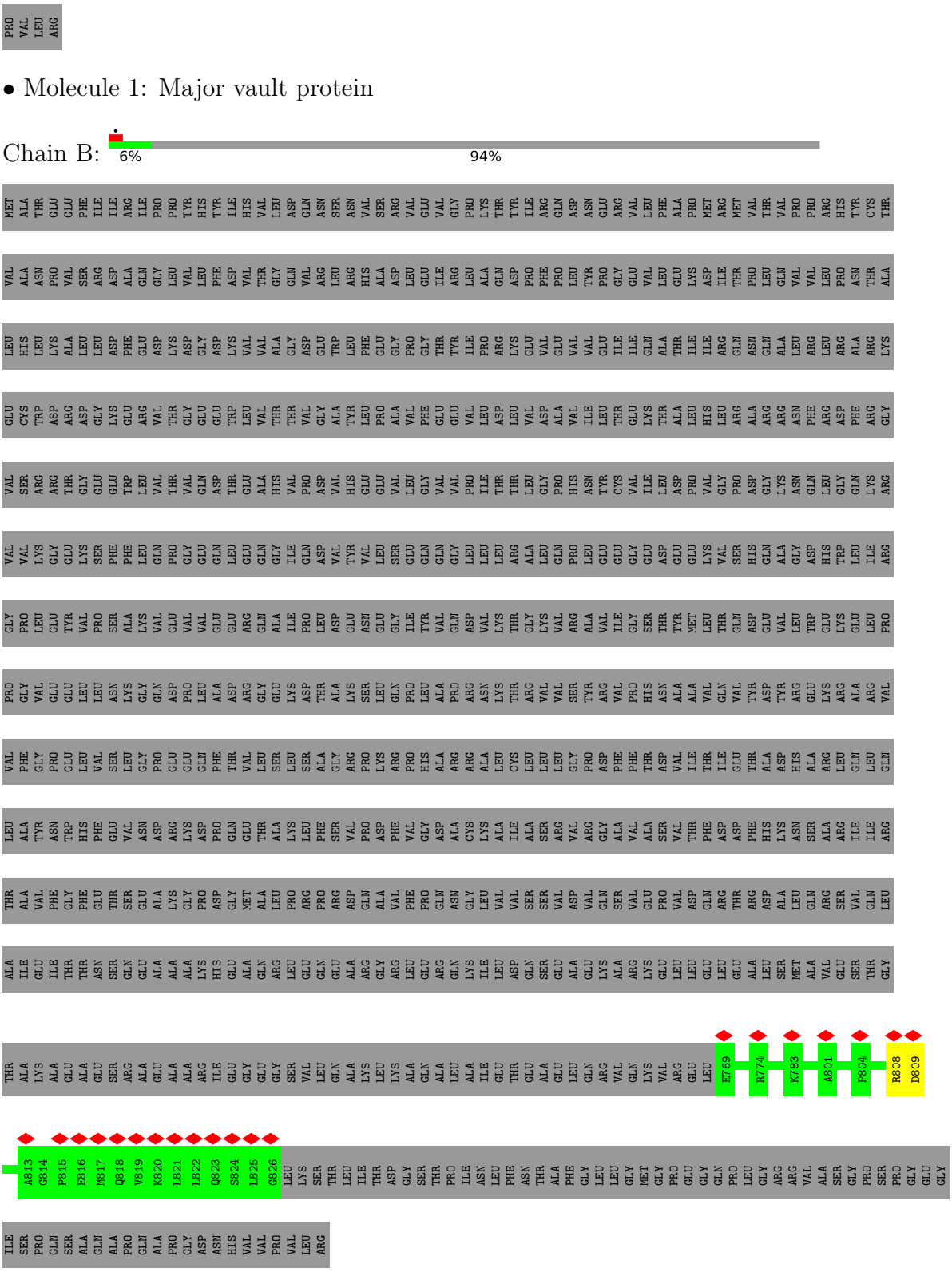


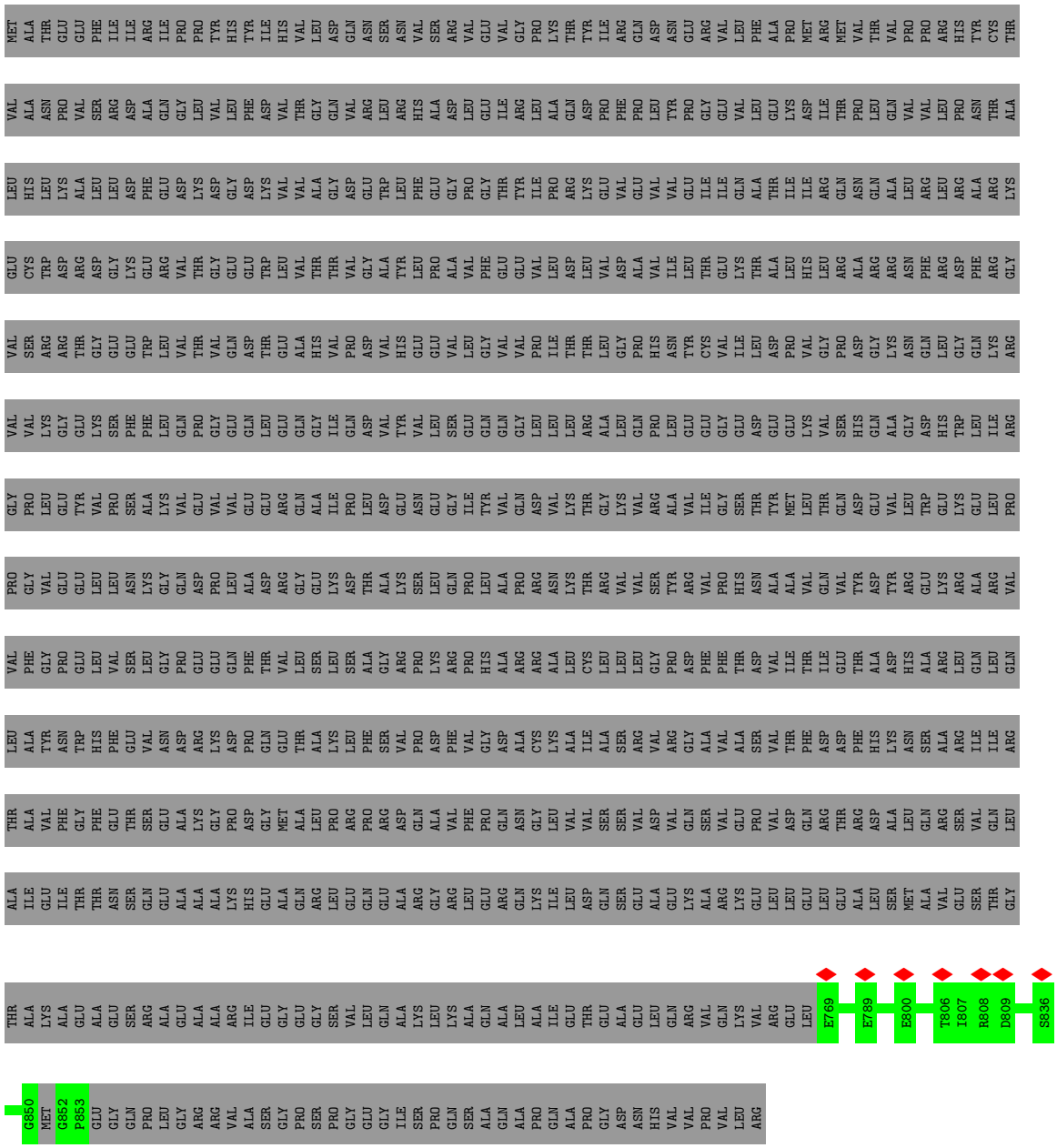
- Molecule 1: Major vault protein

Chain Az:



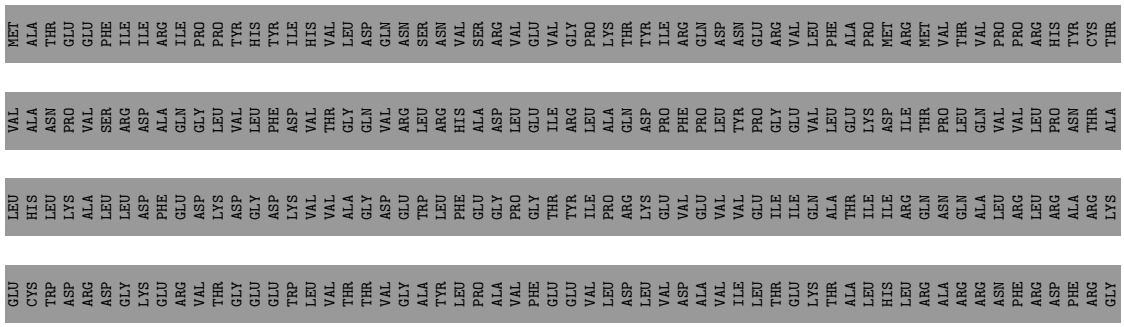


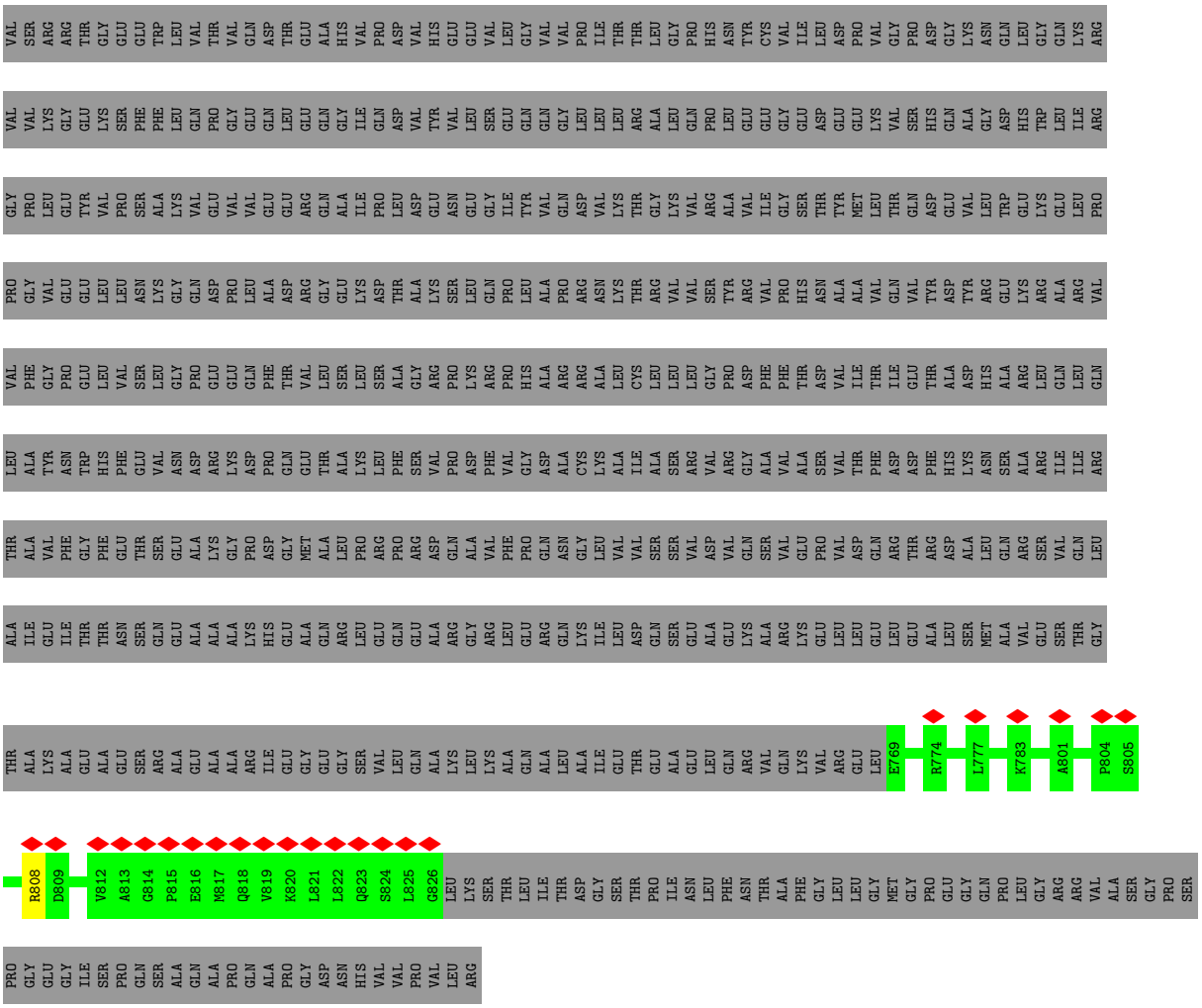

PRO VAL LEU ARG
• Molecule 1: Major vault protein
Chain B:
6%
94%
E769
R774
K783
A801
P804
R808
D809
A813
G814
P815
E816
M817
Q818
V819
K820
L821
L822
Q823
S824
L825
G826
• Molecule 1: Major vault protein
Chain C:
9%
91%



- Molecule 1: Major vault protein

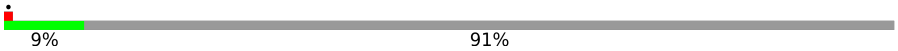
Chain D: 6% 94%

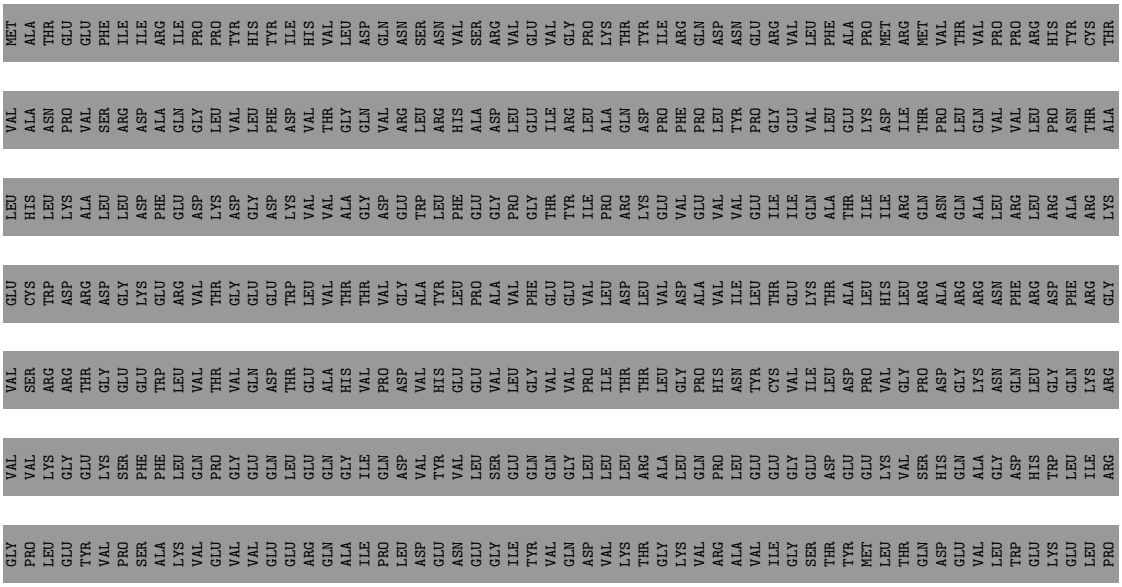


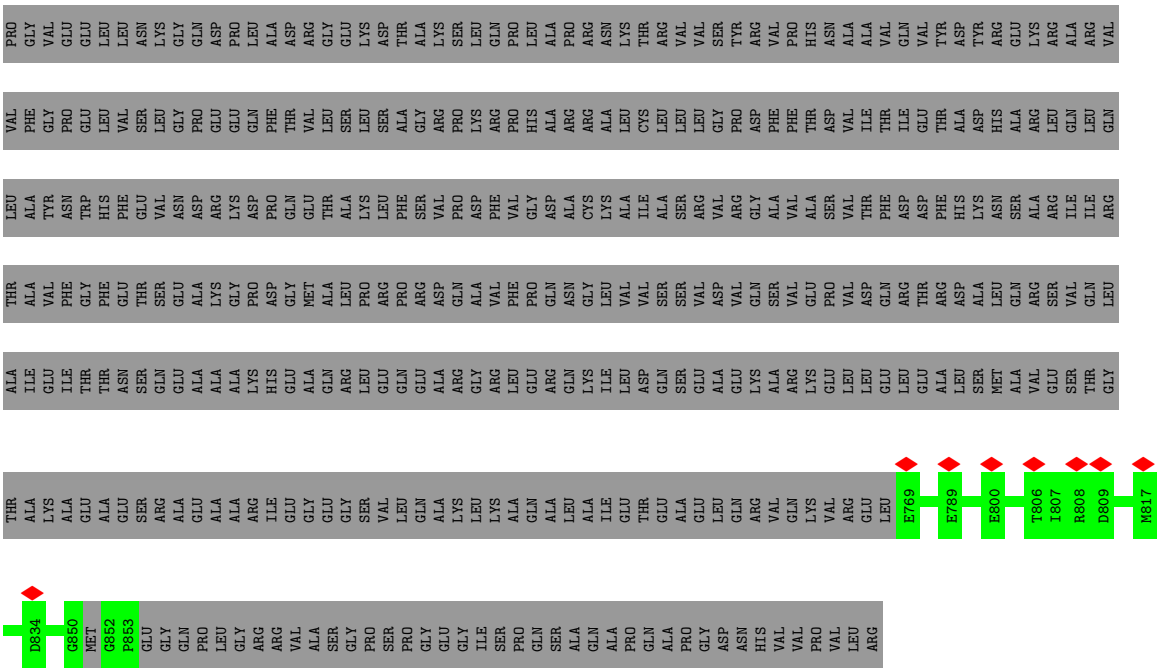


• Molecule 1: Major vault protein

Chain E:

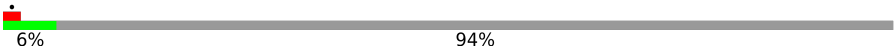


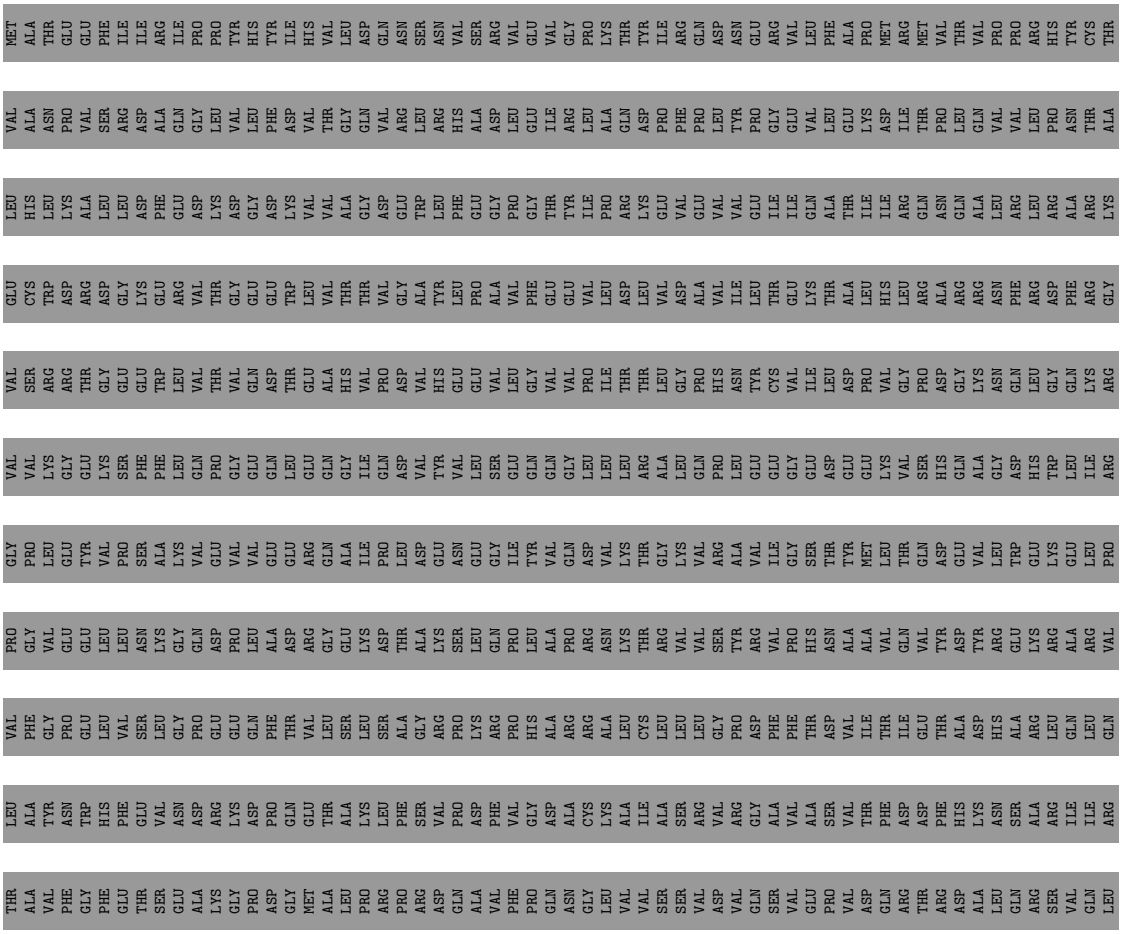


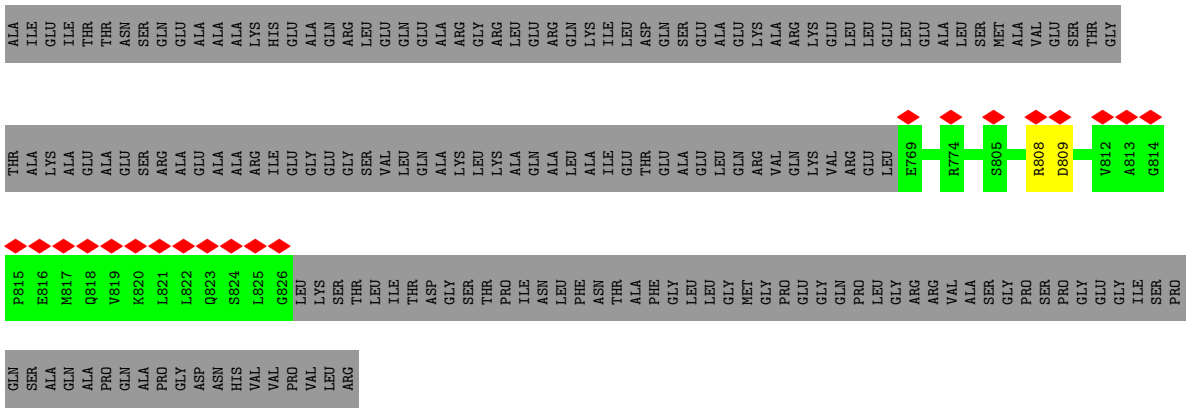


• Molecule 1: Major vault protein

Chain F:

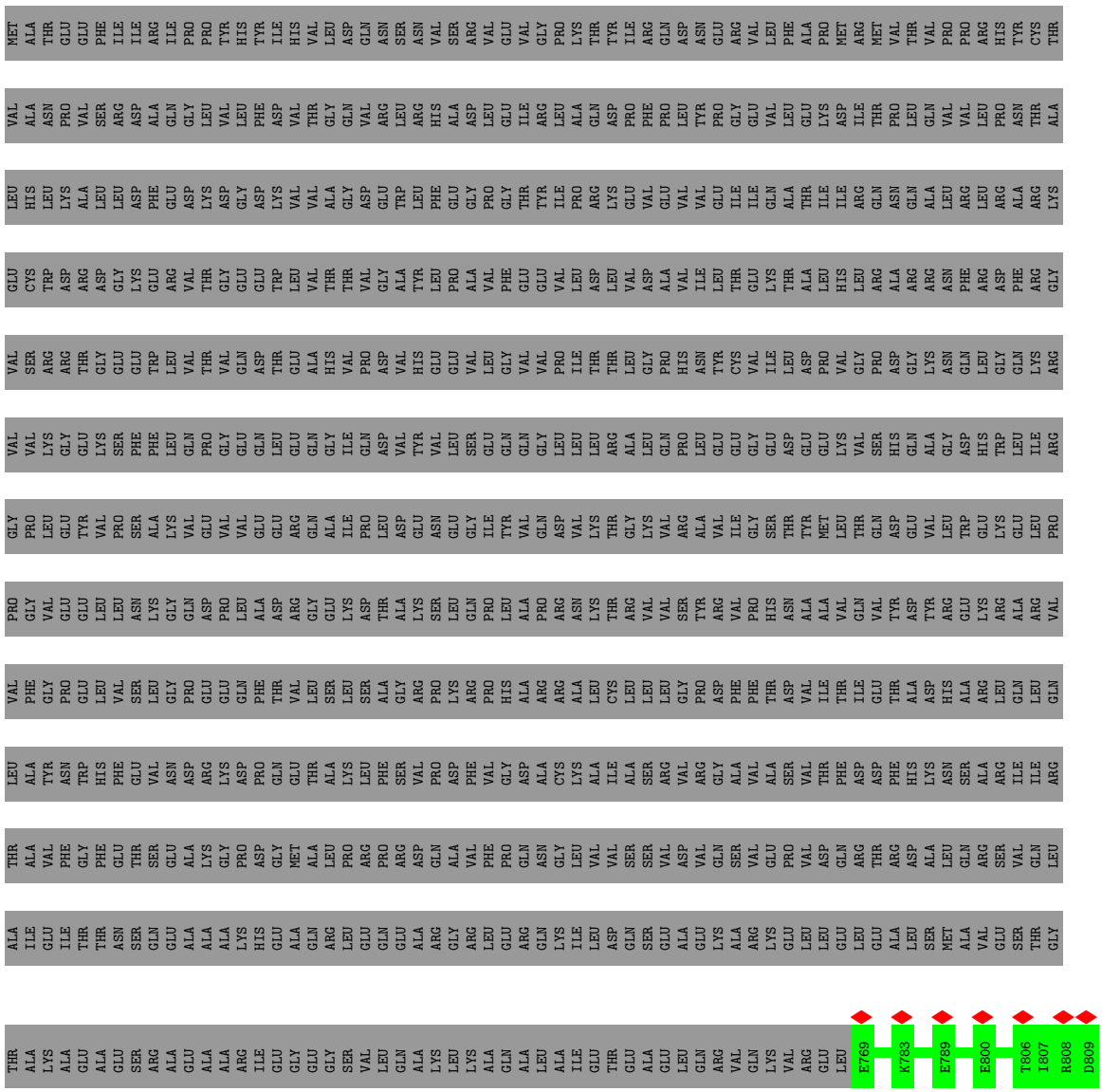


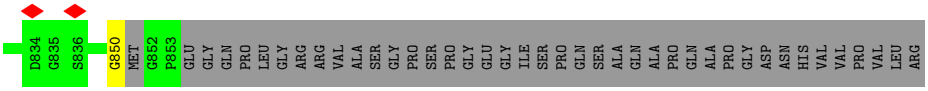




- Molecule 1: Major vault protein

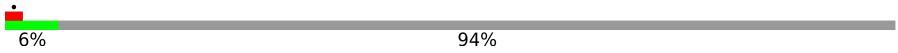
Chain G: 9% 91%

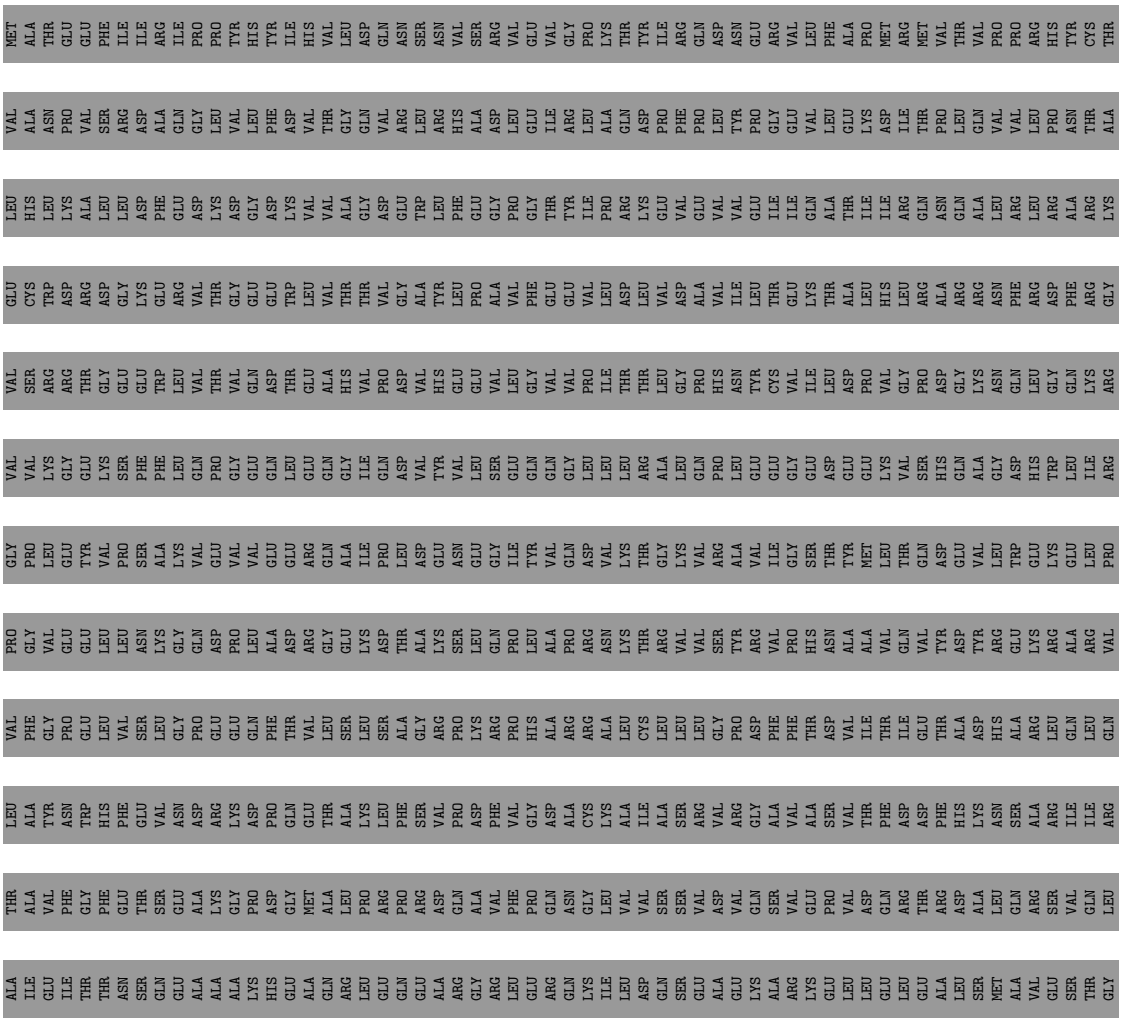




- Molecule 1: Major vault protein

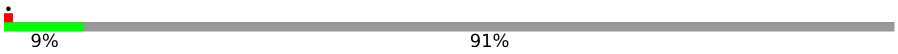
Chain H:

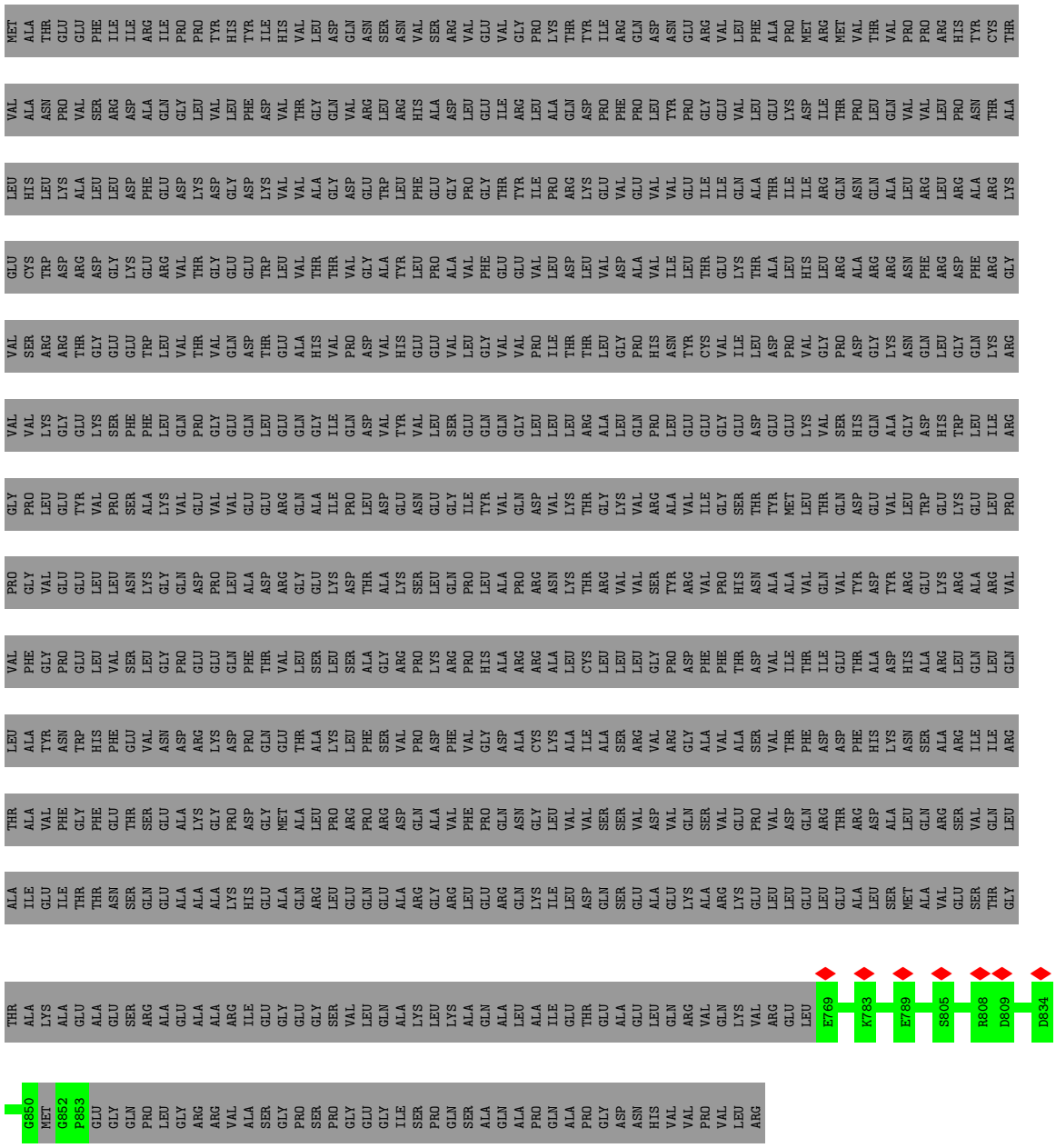




- Molecule 1: Major vault protein

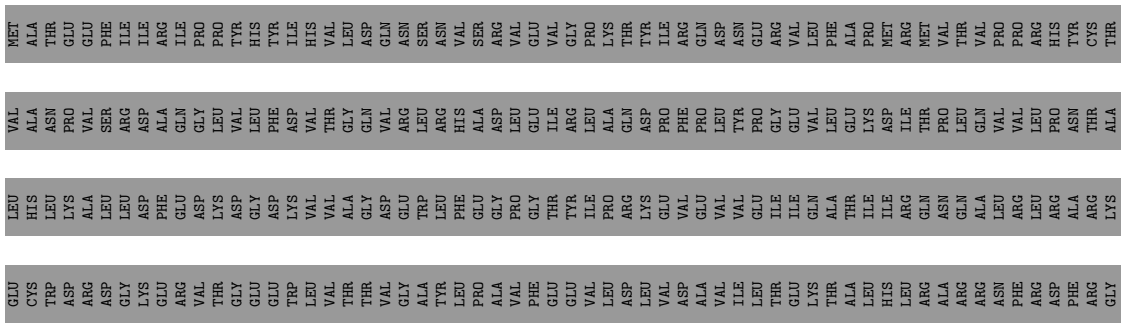
Chain I:





- Molecule 1: Major vault protein

Chain J: 6% 94%



VAL SER ARG ARG THR GLY GLU GLU TRP LEU VAL THR VAL GLN ASP THR GLU ALA HIS VAL PRO ASP VAL HIS GLU GLU VAL LEU GLY VAL VAL PRO ILE THR THR LEU GLY PRO HIS ASN TYR CYS VAL ILE LEU ASP PRO VAL GLY PRO ASP GLY LYS ASN GLN LEU GLY GLN LYS ARG

VAL VAL LYS GLY GLU LYS SER PHE PHE LEU GLN PRO GLY GLU GLN LEU GLU GLN GLN GLY ILE GLN ASP VAL TYR VAL LEU SER GLU GLN GLN GLY LEU LEU LEU ARG ALA LEU GLN PRO LEU GLU GLU GLY GLU ASP GLU GLU LYS VAL SER HIS GLN ALA GLY ASP HIS TRP LEU ILE ARG

GLY PRO LEU GLU TYR VAL PRO SER ALA LYS VAL GLU VAL VAL GLU GLU ARG GLN ALA ILE PRO LEU ASP GLU ASN GLU GLY ILE TYR VAL GLN ASP VAL LYS THR GLY LYS VAL ARG ALA VAL ILE GLY SER THR TYR MET LEU THR GLN ASP GLU VAL LEU TRP GLU LYS ARG GLU LEU PRO

PRO GLY VAL GLU GLU LEU LEU ASN LYS GLY GLN ASP PRO LEU ALA ASP ARG GLY GLU LYS ASP THR ALA LYS SER LEU GLN PRO LEU ALA PRO ARG ASN LYS THR ARG VAL VAL SER TYR ARG VAL PRO HIS ASN ALA ALA VAL GLN VAL TYR ASP TYR ARG GLU LYS ARG ALA ARG VAL

VAL PHE GLY PRO GLU LEU VAL SER LEU GLY PRO GLU GLU GLN PHE THR VAL LEU SER LEU SER ALA GLY ARG PRO LYS ARG PRO HIS ALA ARG ARG ALA LEU CYS LEU LEU LEU GLY PRO ASP PHE PHE THR ASP VAL ALA ILE THR ILE GLU THR ALA ASP HIS ALA ARG LEU GLN LEU GLN

LEU ALA TYR ASN TRP HIS PHE GLU VAL ASN ASP ARG LYS ASP PRO GLN GLU THR ALA LYS LEU PHE SER VAL PRO ASP PHE VAL GLY ASP ALA ASP ARG ARG ALA LEU LYS SER ARG ARG VAL ASP ASP PHE HIS ALA ILE ILE ALA SER ARG VAL ALA ALA SER VAL THR PHE ASP ASP PHE HIS LYS ASN SER ALA ARG ILE ILE ARG

THR ALA VAL PHE GLY PHE GLU THR SER GLU ALA LYS GLY PRO ASP GLY MET ALA LEU PRO ARG PRO ARG ASP GLN ALA VAL PHE PRO GLN ASN GLY LEU VAL VAL SER SER VAL ASP VAL GLN SER VAL GLU PRO VAL ASP GLN ARG THR ARG ASP ALA LEU GLN ARG SER VAL GLN LEU

ALA ILE GLU ILE THR THR ASN SER GLN GLU ALA ALA ALA ALA LYS HIS GLU ALA GLN ARG LEU GLU GLN GLU ALA ARG GLY ARG LEU GLU ARG GLN LYS ILE LEU ASP GLN SER GLU ALA GLU LYS ALA ARG LYS GLU LEU LEU LEU GLU ALA LEU SER MET ALA VAL GLU SER THR GLY

THR ALA LYS ALA GLU ALA GLU SER ARG ALA GLU ALA ALA ARG ILE GLU GLY GLU GLY SER VAL LEU GLN ALA LYS LEU LYS ALA GLN ALA LEU ALA ILE GLU THR GLU ALA GLU LEU GLN ARG VAL GLN LYS VAL ARG GLU LEU E769 R774 L777 E780 P804 R808 D809

V812 A813 G814 P815 E816 M817 Q818 V819 K820 L821 L822 Q823 S824 L825 G826 LEU LYS SER THR LEU ILE THR ASP GLY SER THR PRO ILE ASN LEU PHE ASN THR ALA PHE GLY LEU LEU GLY MET GLY PRO GLU GLY GLN PRO LEU GLY ARG ARG VAL ALA SER GLY PRO SER PRO GLY GLU

GLY ILE SER PRO GLN SER ALA GLN ALA PRO GLN ALA PRO GLY ASP ASN HIS VAL VAL PRO VAL LEU ARG

- Molecule 1: Major vault protein

Chain K: 9% 91%

MET ALA THR GLU GLU PHE ILE ILE ARG ILE PRO PRO TYR HIS TYR ILE HIS VAL LEU ASP GLN ASN SER ASN VAL SER ARG VAL GLU VAL GLY PRO LYS THR TYR ILE ARG GLN ASP ASN GLU ARG VAL LEU PHE ALA PRO MET ARG MET VAL THR VAL PRO PRO ARG HIS TYR CYS THR

VAL ALA ASN PRO VAL SER ARG ASP ALA GLN GLY LEU VAL LEU PHE ASP VAL THR GLY GLN VAL ARG LEU GLU ILE ARG LEU ALA GLN ASP PRO PHE PRO LEU TYR PRO GLY GLU VAL LEU GLU LYS ASP ILE THR PRO LEU GLN VAL VAL LEU PRO ASN THR ALA

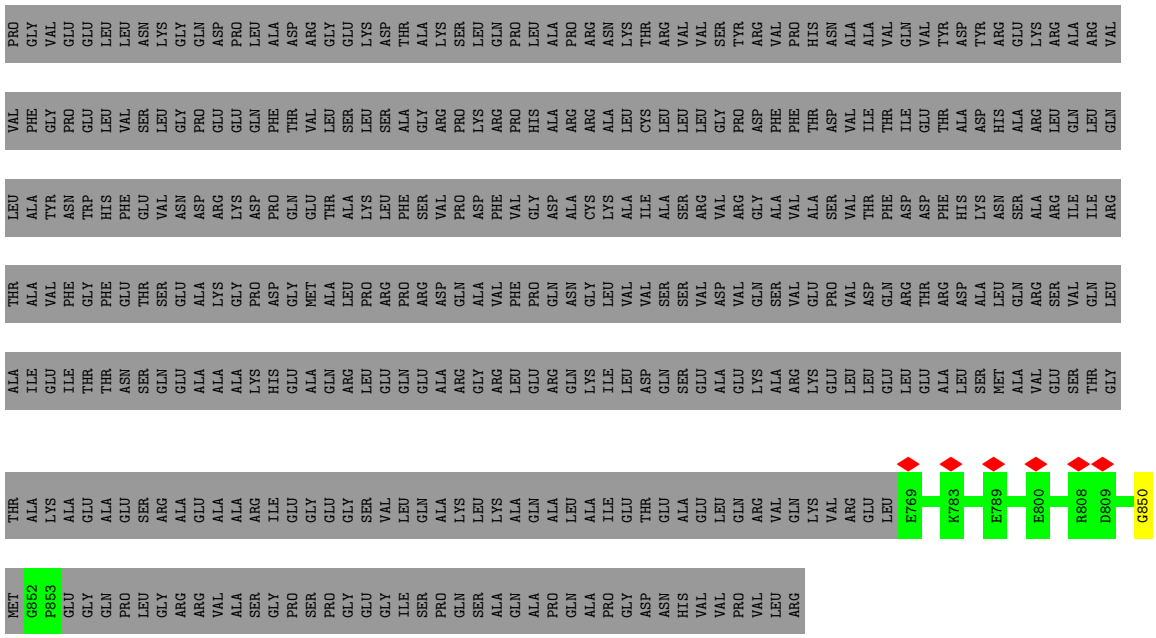
LEU HIS LEU LYS ALA LEU LEU ASP PHE GLU ASP LYS ASP GLY ASP LYS VAL VAL ALA GLY ASP GLU GLY GLY THR TYR ILE PRO ARG LYS GLU VAL GLU VAL VAL GLU ILE ILE GLN ALA THR ILE ILE ARG GLN ASN GLN ALA LEU ARG LYS ALA

GLU CYS TRP ASP ARG ASP GLY LYS GLU ARG VAL THR GLY GLU GLU TRP LEU VAL THR THR VAL GLY VAL PHE GLU GLU VAL LEU ASP LEU VAL ASP ALA VAL ILE LEU THR GLU LYS THR ALA HIS LEU ARG ALA ARG ARG ASN PHE ARG ASP PHE ARG GLY

VAL SER ARG ARG THR GLY GLU GLU TRP LEU VAL THR VAL GLN ASP THR GLU ALA HIS VAL PRO ASP VAL HIS GLU GLU VAL LEU GLY VAL VAL PRO ILE THR THR LEU GLY PRO HIS ASN TYR CYS VAL ILE LEU ASP PRO VAL GLY PRO ASP GLY LYS ASN GLN LEU GLY GLN LYS ARG

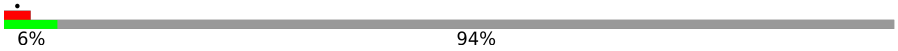
VAL VAL LYS GLY GLU LYS SER PHE PHE LEU GLN PRO GLY GLU GLN LEU GLU GLN GLN GLY LEU LEU LEU ARG ALA LEU GLN PRO LEU GLU GLU GLY GLU ASP GLU GLU LYS VAL SER HIS GLN ALA GLY ASP HIS TRP LEU ILE ARG

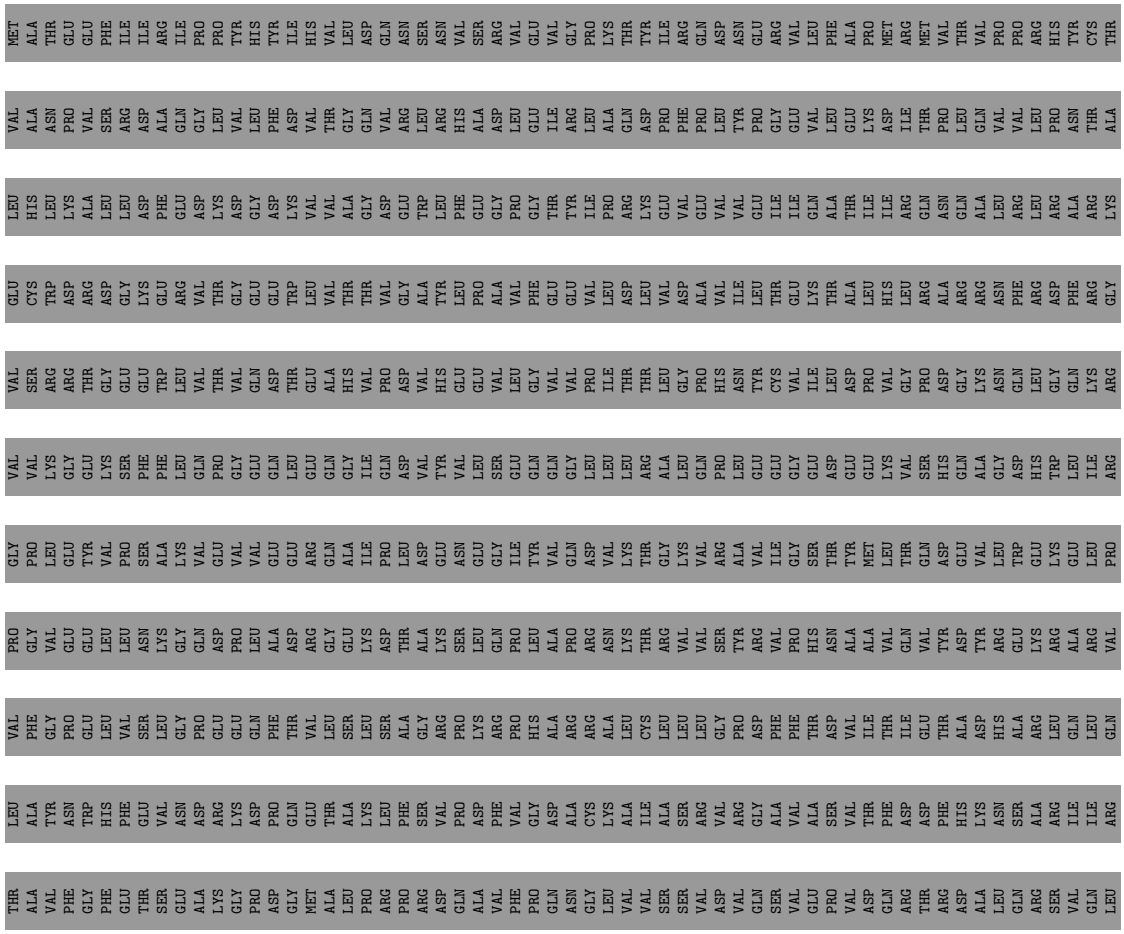
GLY PRO LEU GLU TYR VAL PRO SER ALA LYS VAL GLU VAL VAL GLU GLU ARG GLN ALA ILE PRO LEU ASP GLU ASN GLU GLY ILE TYR VAL GLN ASP VAL LYS THR GLY LYS VAL ARG ALA VAL ILE GLY SER THR TYR MET LEU THR GLN ASP GLU VAL LEU TRP GLU LYS GLU LEU PRO

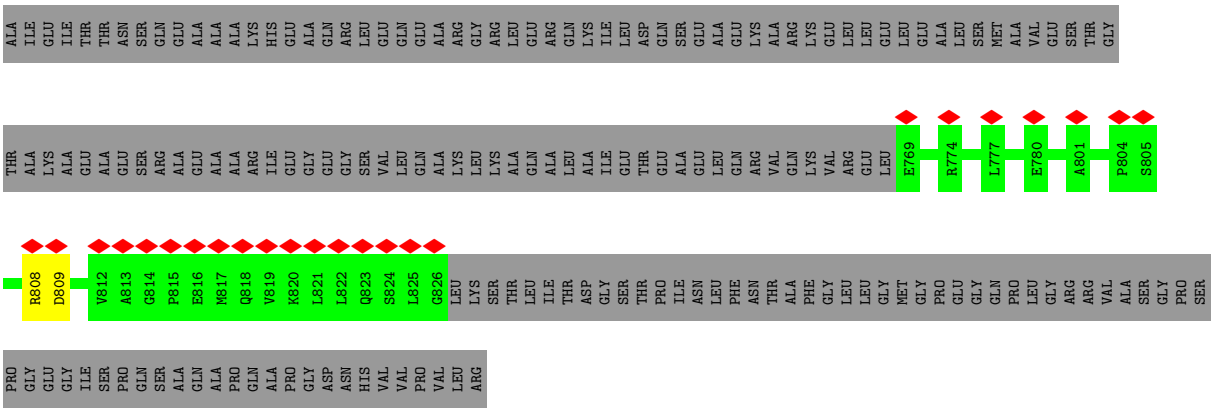


- Molecule 1: Major vault protein

Chain L:

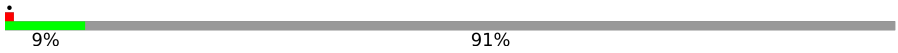


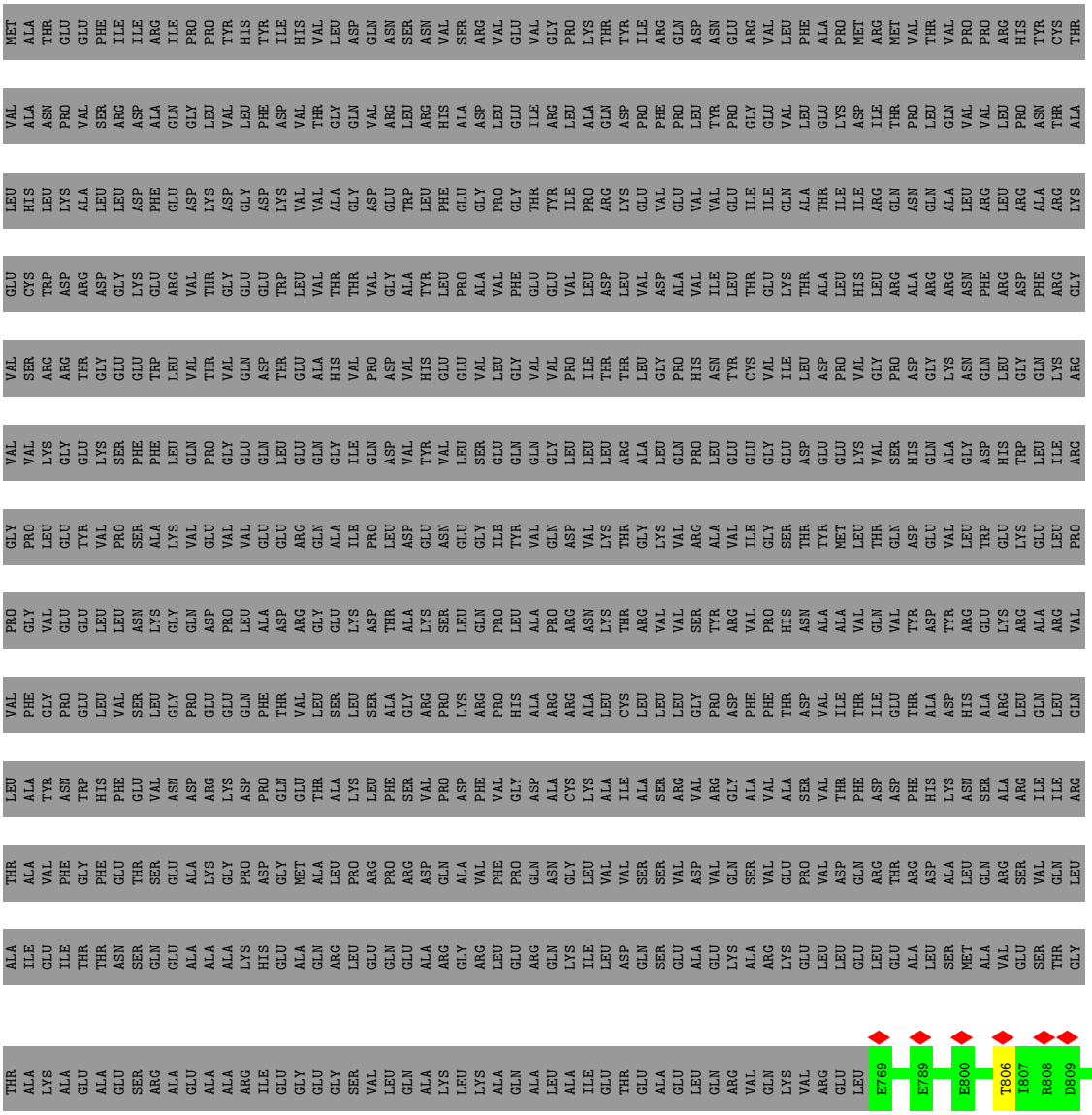


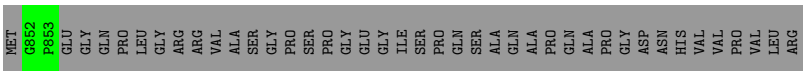


• Molecule 1: Major vault protein

Chain M:

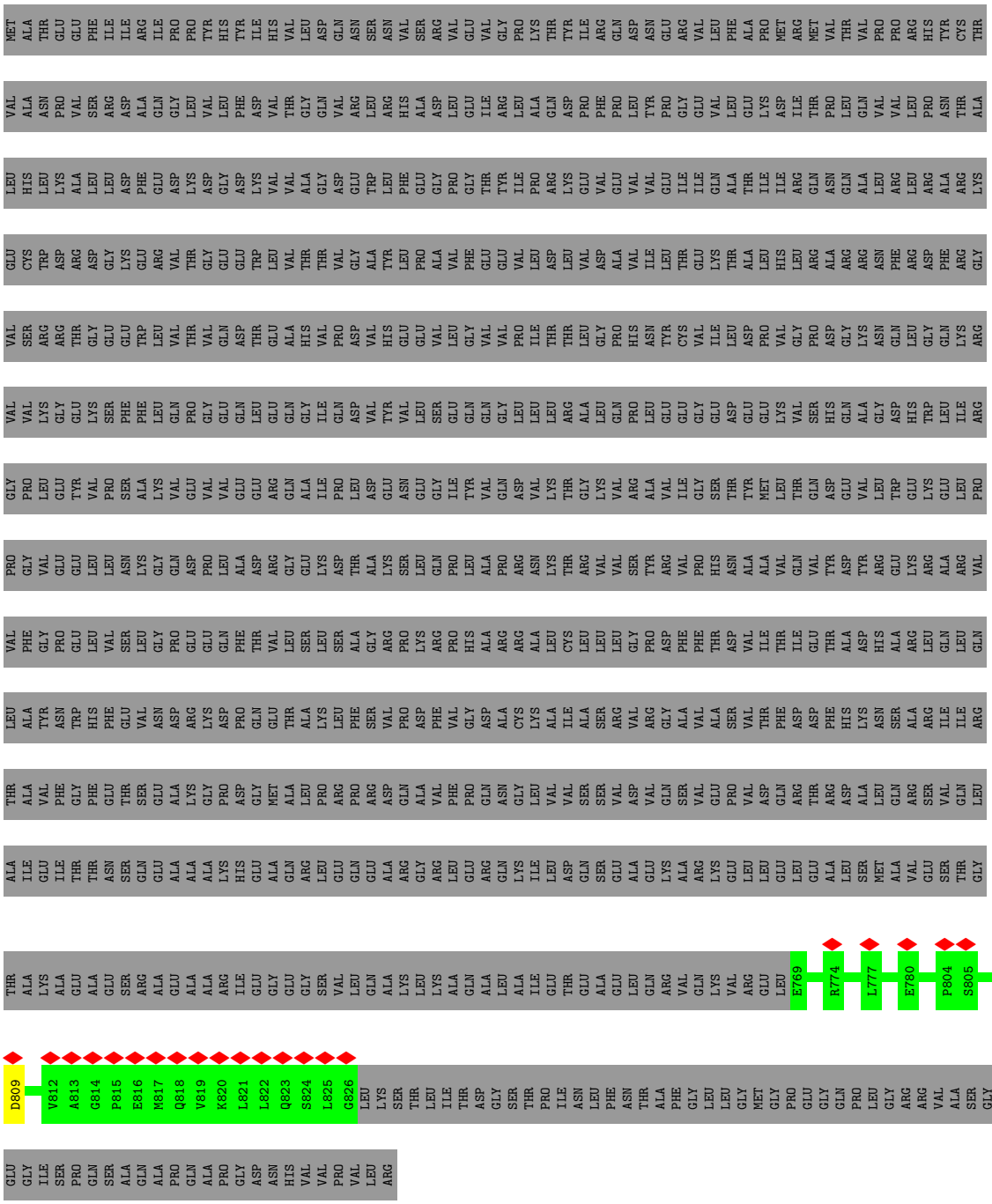






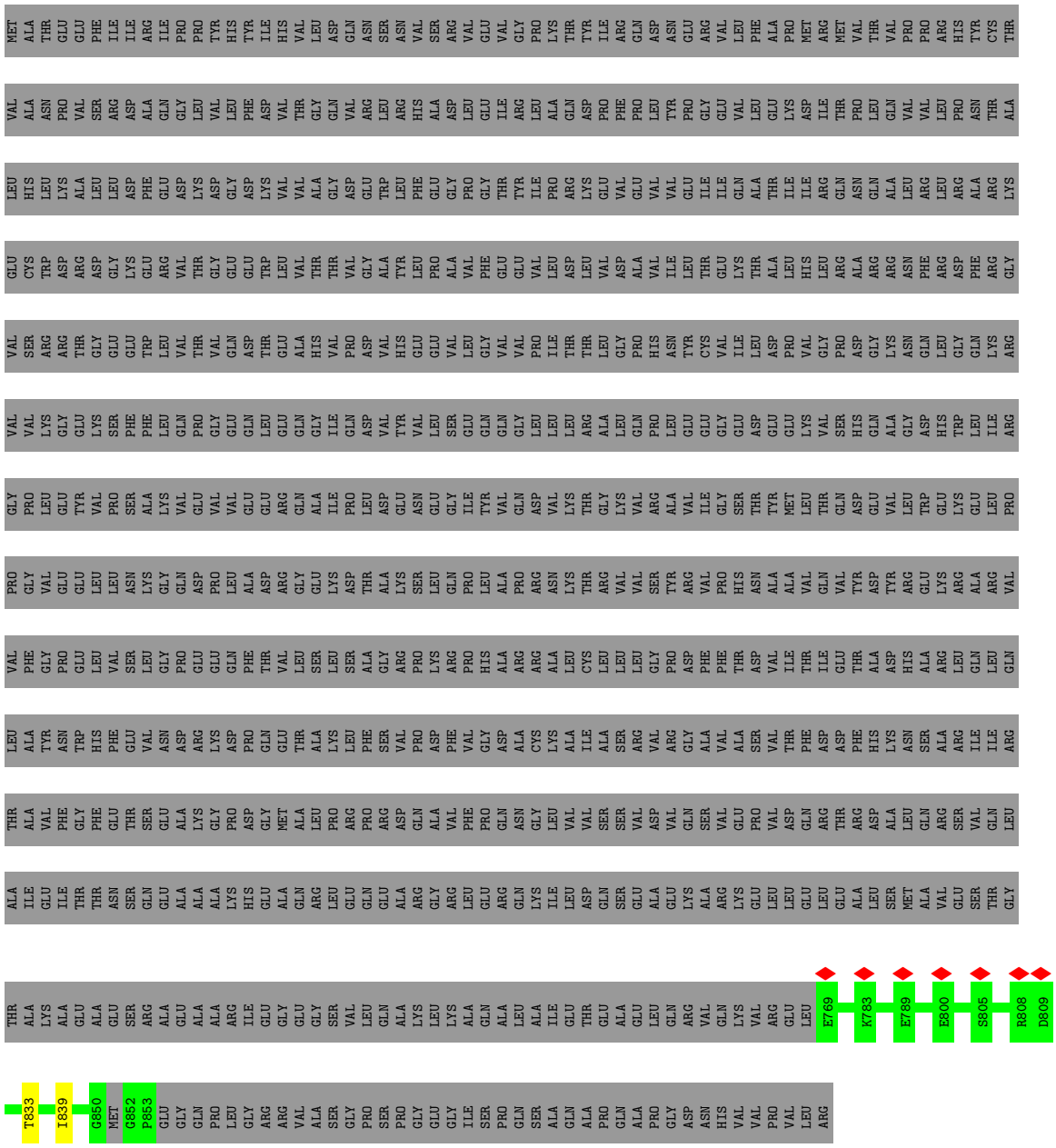
• Molecule 1: Major vault protein

Chain N: 6% 94%



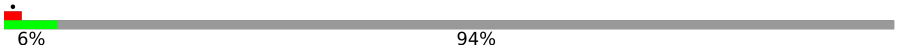
• Molecule 1: Major vault protein

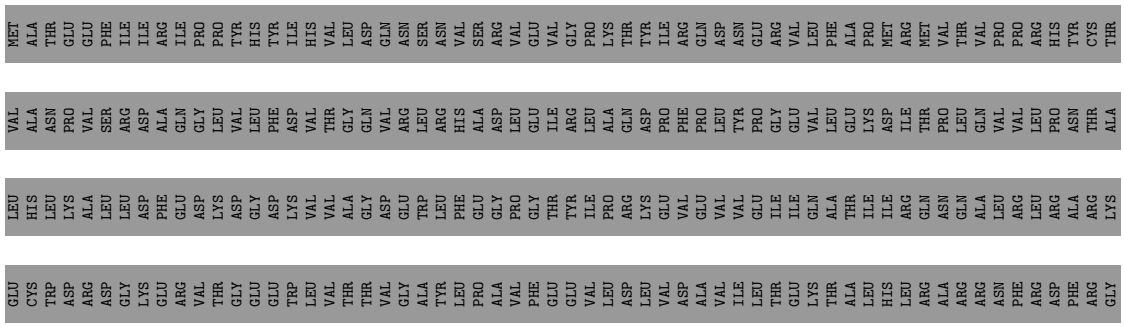
Chain O: 9% 91%

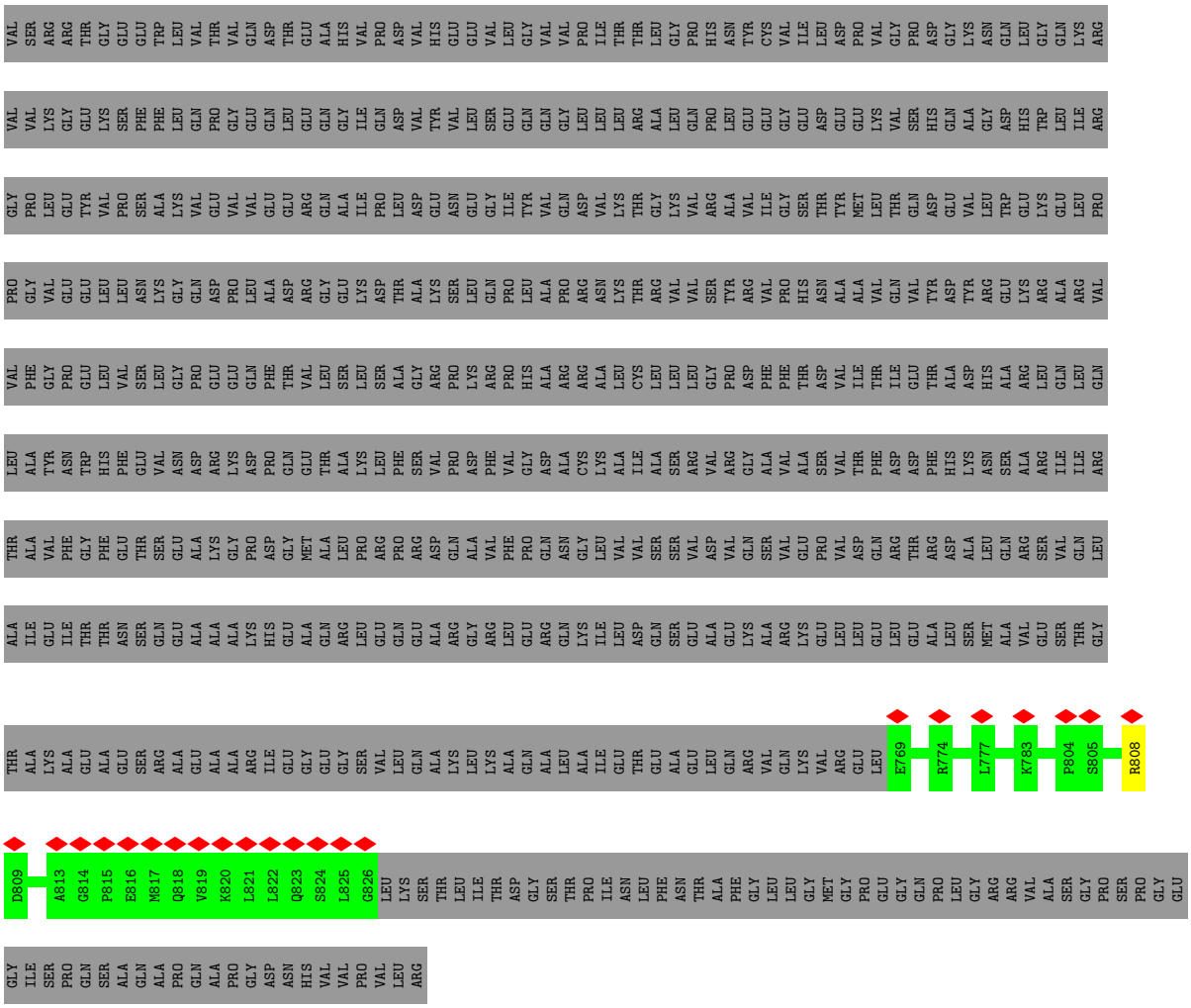


• Molecule 1: Major vault protein

Chain P:

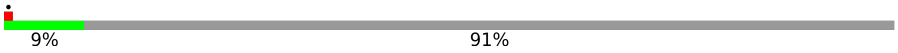


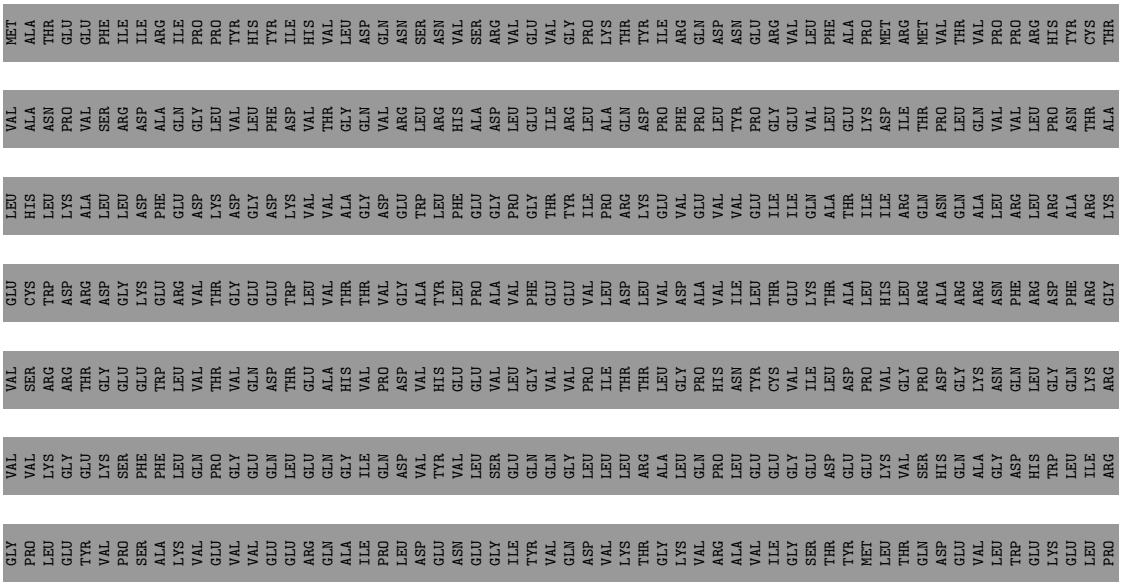


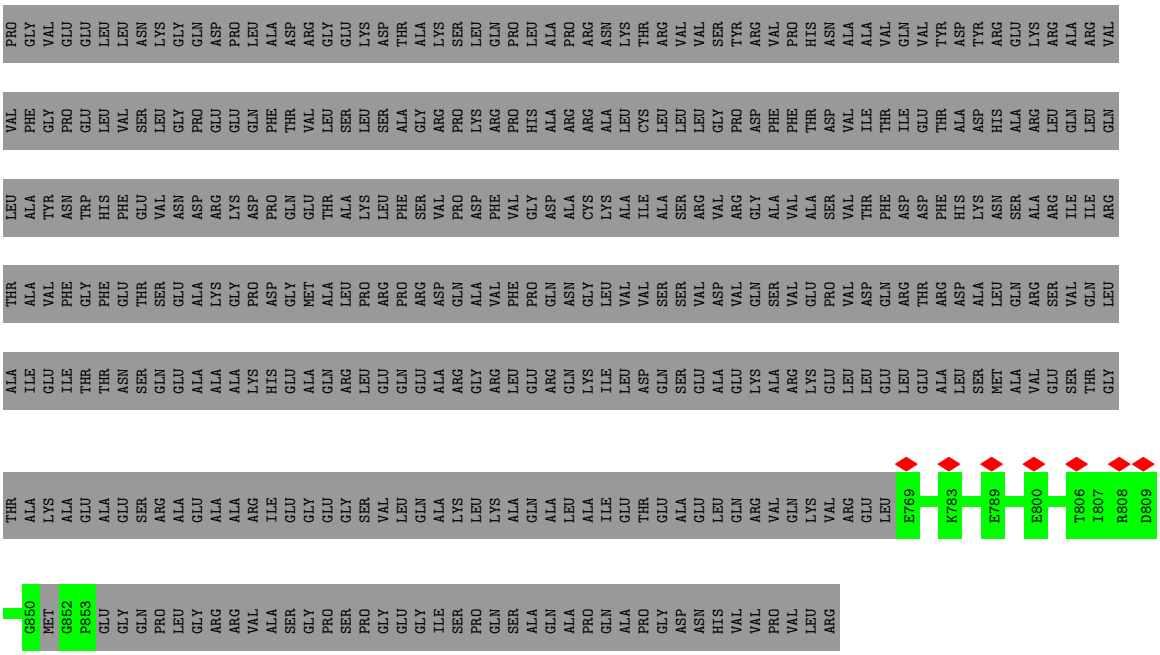


- Molecule 1: Major vault protein

Chain Q:

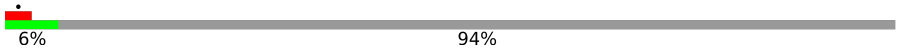


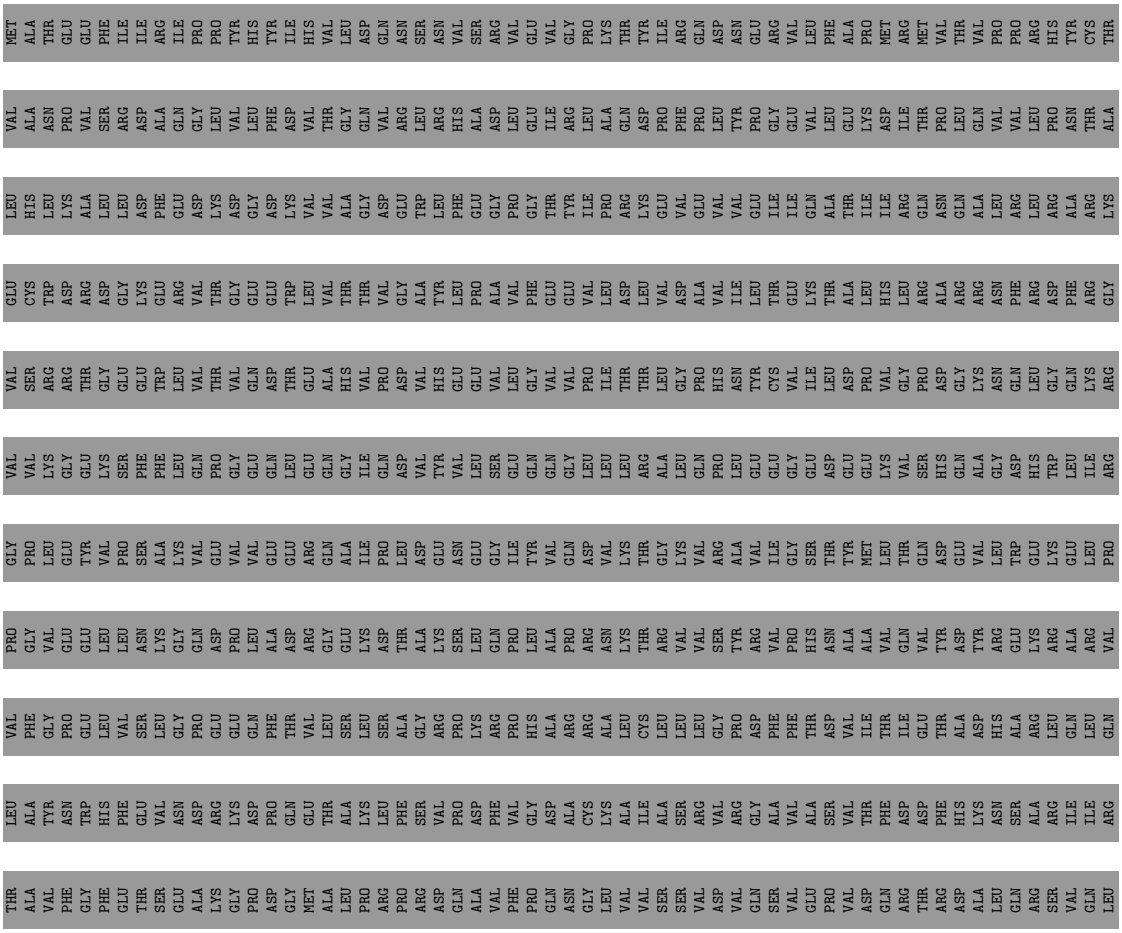


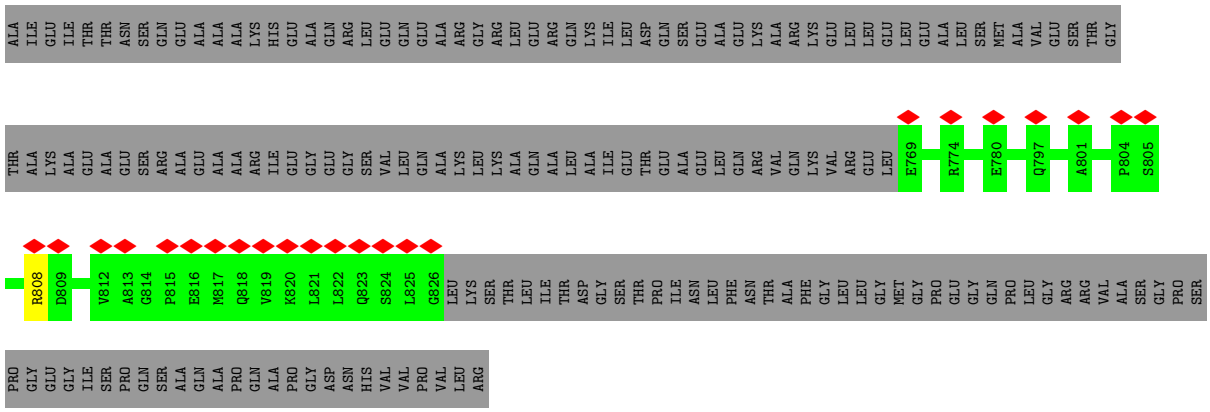


- Molecule 1: Major vault protein

Chain R:

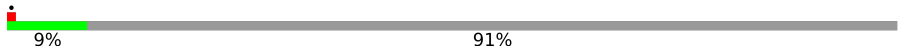


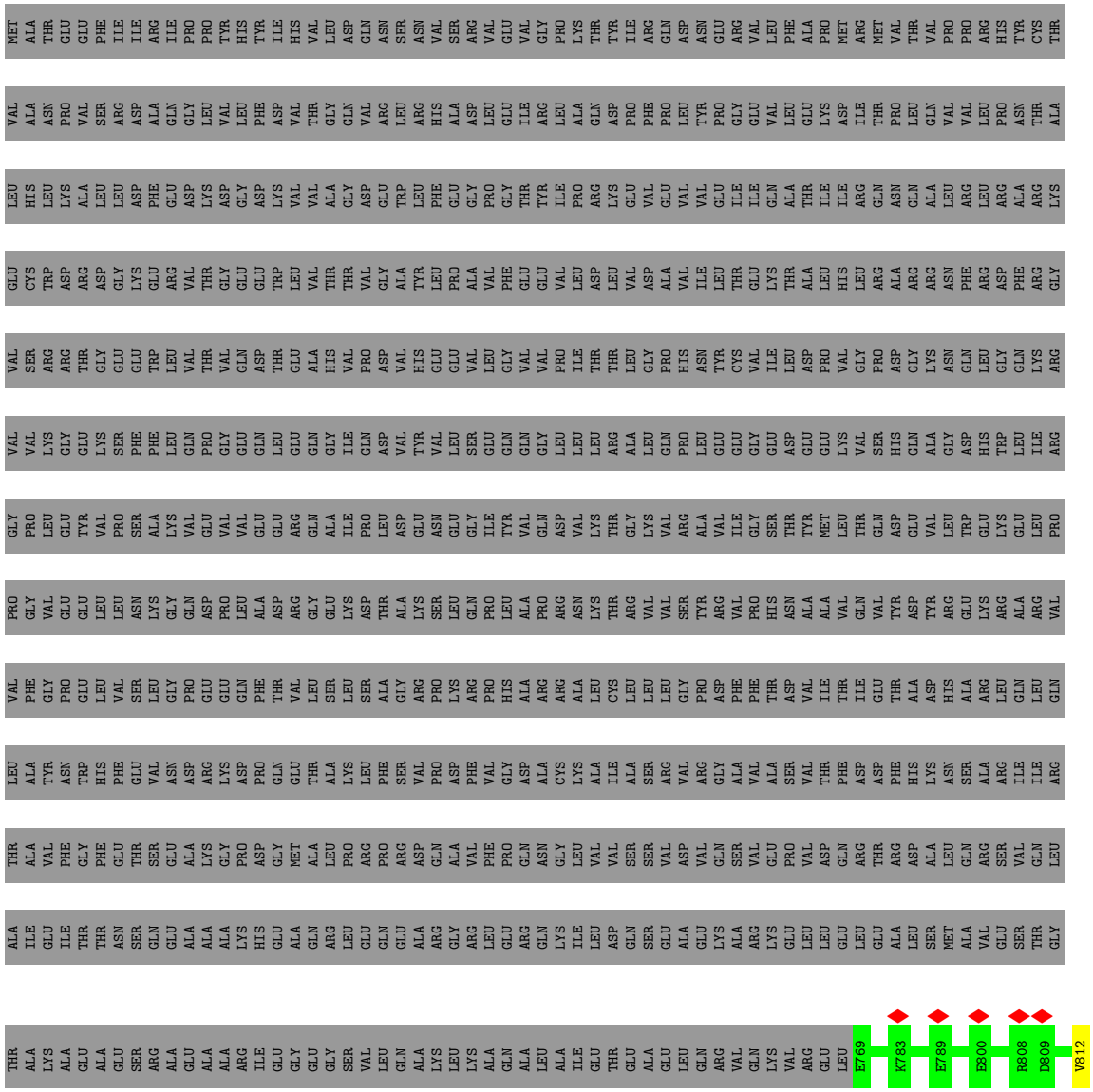


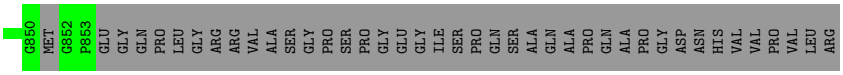


- Molecule 1: Major vault protein

Chain S:

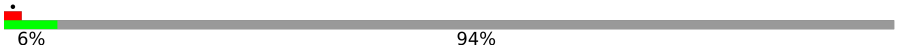


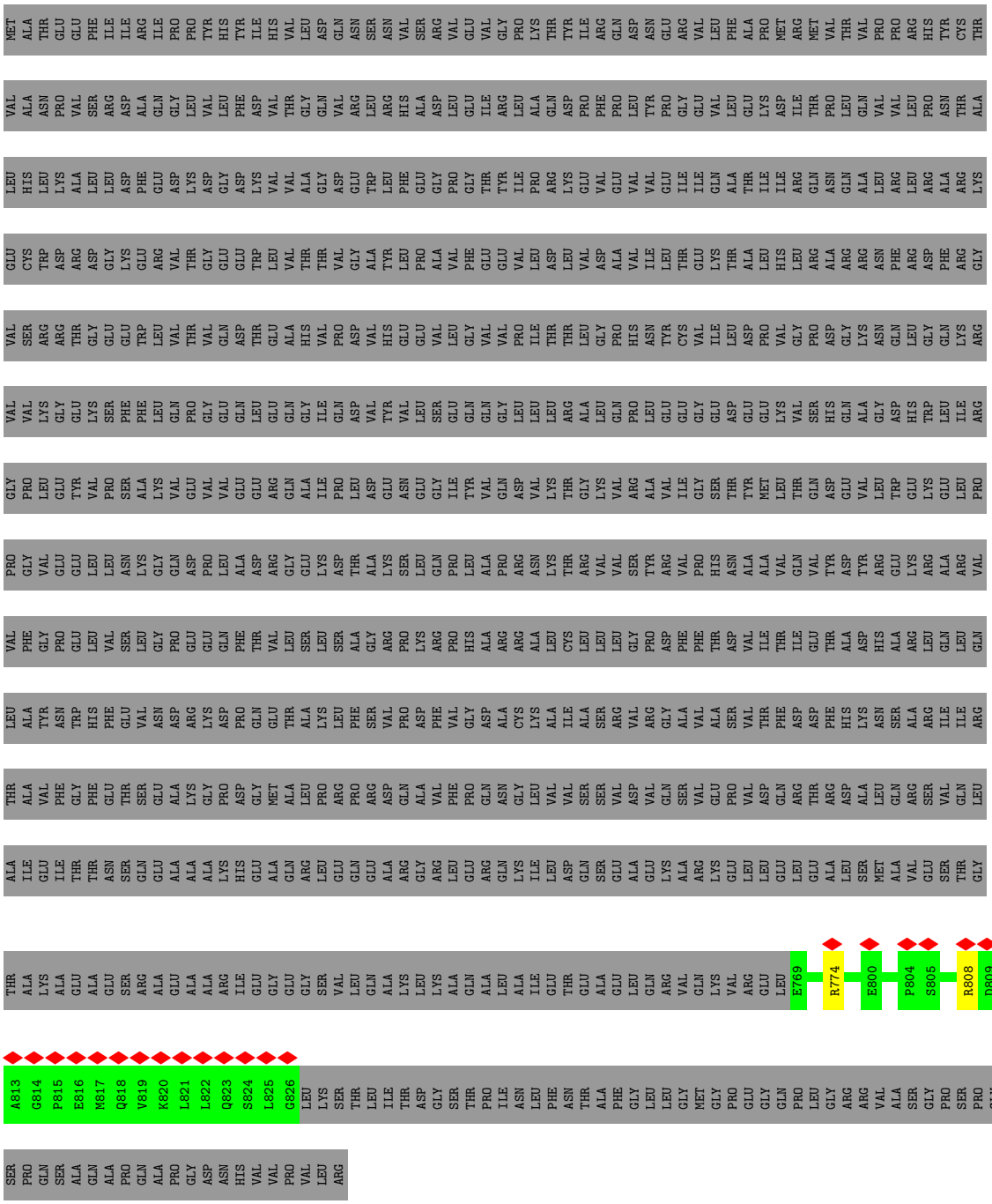




• Molecule 1: Major vault protein

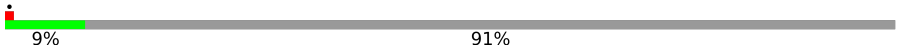
Chain T:

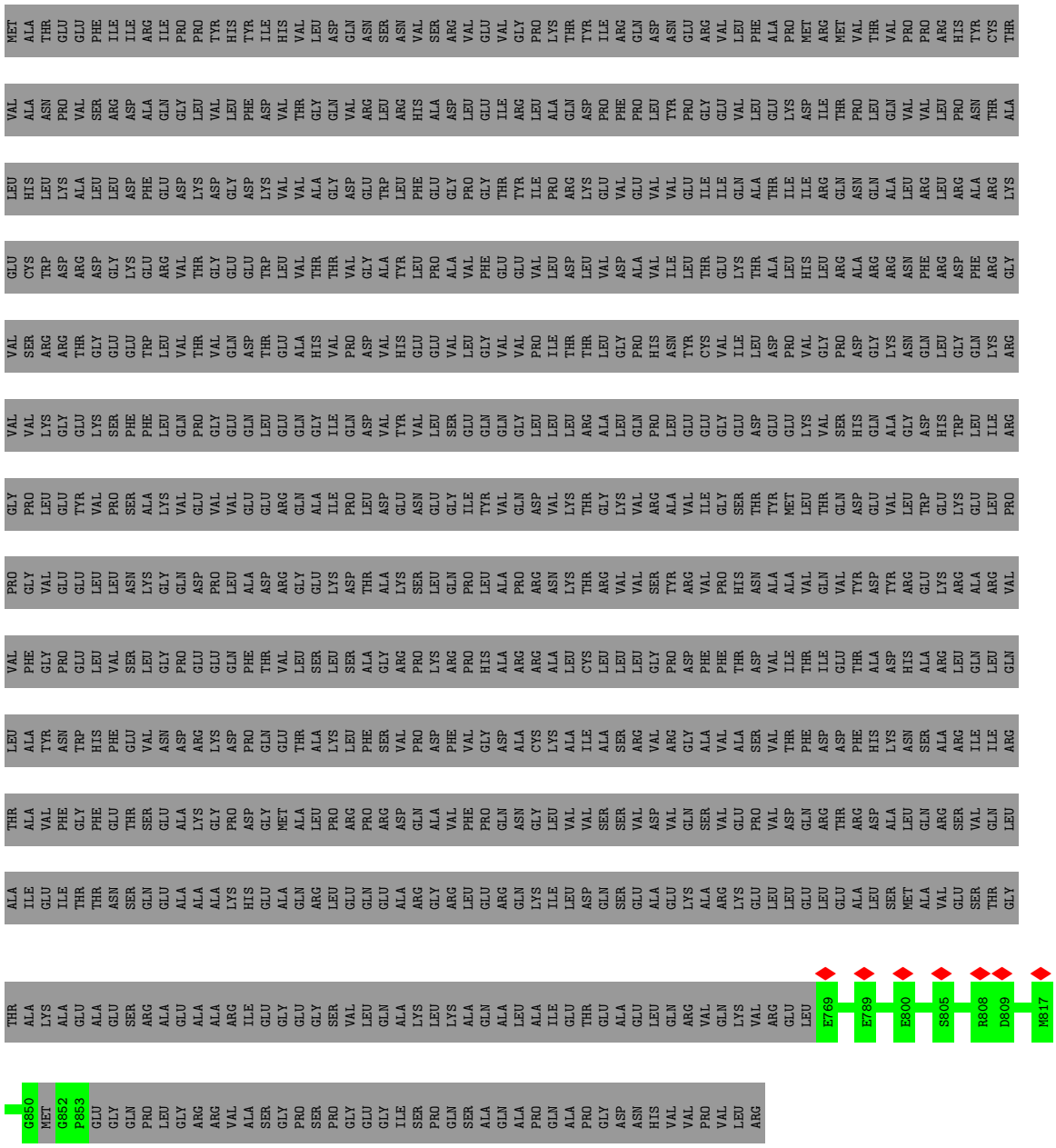




• Molecule 1: Major vault protein

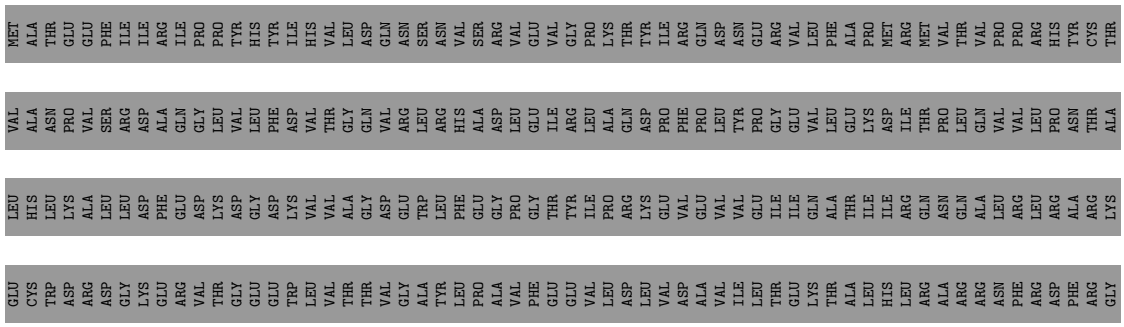
Chain U:

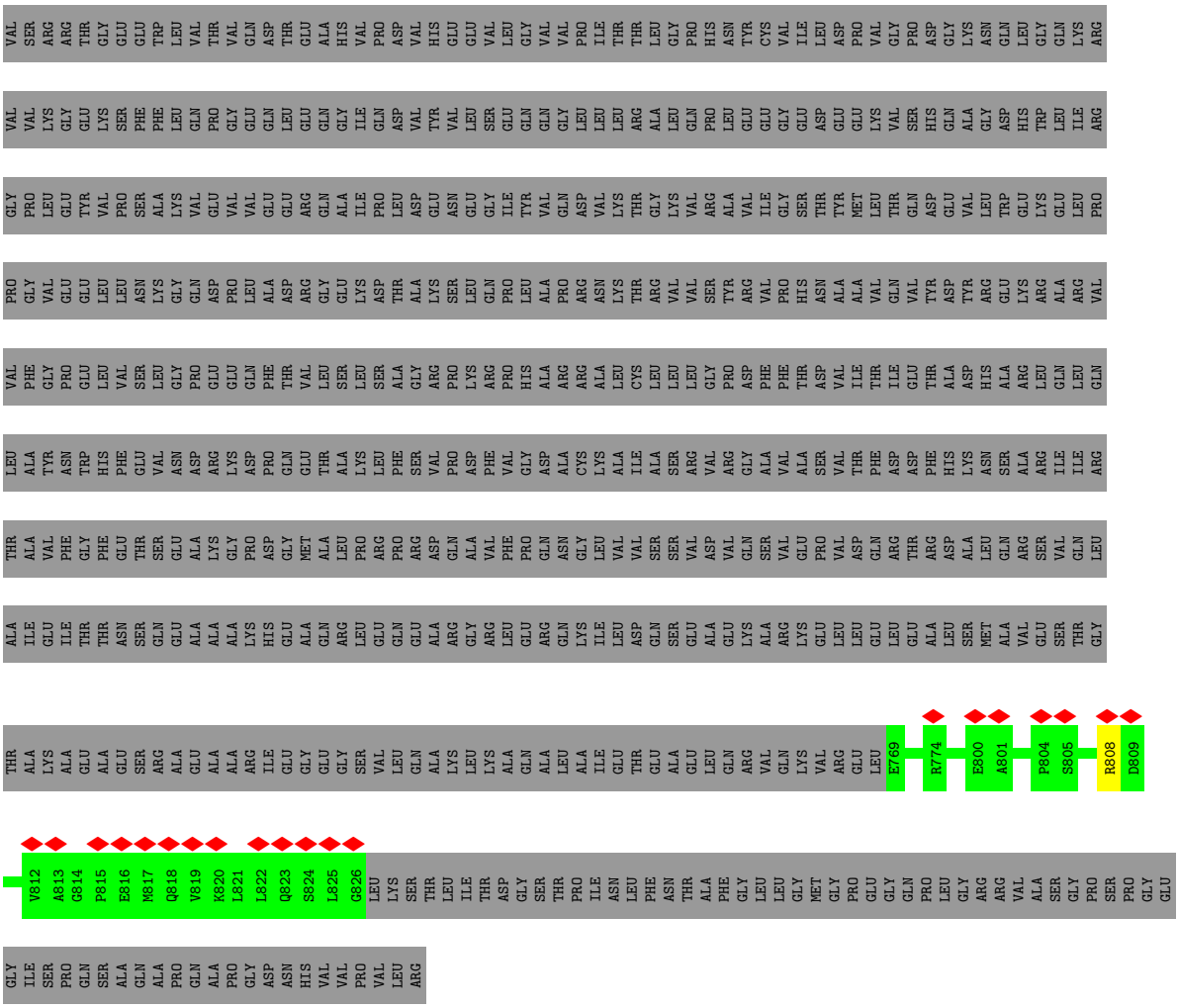




- Molecule 1: Major vault protein

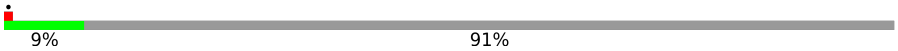
Chain V: 6% 94%

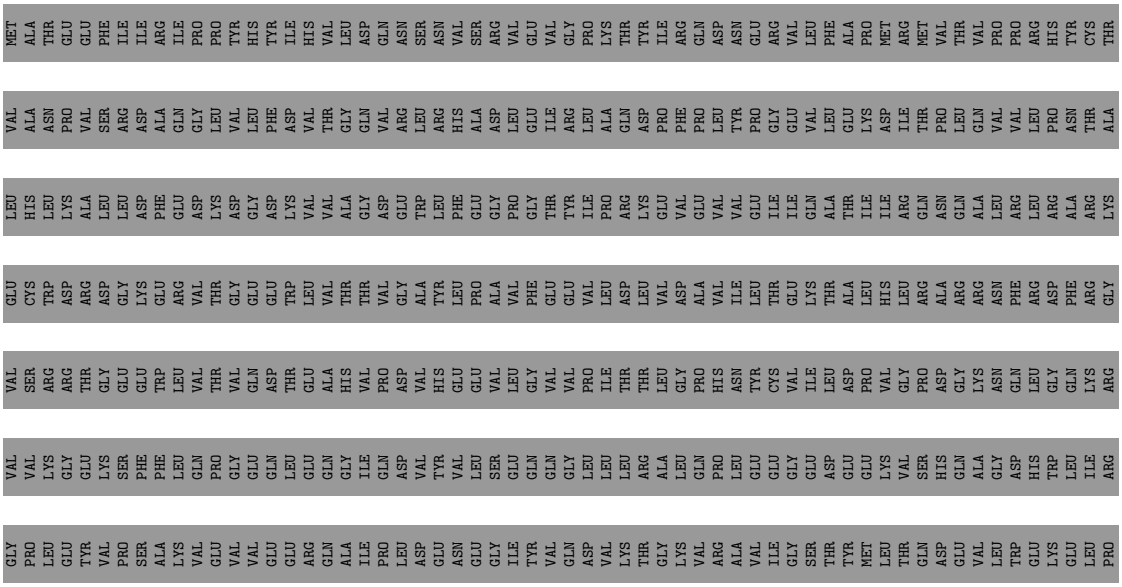




- Molecule 1: Major vault protein

Chain W:





PRO GLY VAL GLU GLU LEU LEU ASN LYS GLY GLN ASP PRO LEU ALA ASP ARG GLY GLU LYS ASP THR ALA LYS SER LEU GLN PRO LEU ALA PRO ARG ASN LYS THR ARG VAL VAL SER TYR ARG VAL PRO HIS ASN ALA ALA VAL GLN VAL TYR ASP TYR ARG GLU LYS ARG ALA ARG VAL

VAL PHE GLY PRO GLU LEU VAL SER LEU GLY PRO GLU GLU GLN PHE THR VAL LEU SER LEU SER ALA GLY ARG PRO LYS ARG PRO HIS ALA ARG ARG ALA LEU CYS LEU LEU LEU GLY PRO ASP PHE PHE THR ASP VAL ILE THR ILE GLU THR ALA ASP HIS ALA ARG LEU GLN GLN

LEU ALA TYR ASN TRP HIS PHE GLU VAL ASN ASP ARG LYS ASP PRO GLN GLU THR ALA LYS LEU PHE SER VAL PRO ASP PHE VAL GLY ASP ALA CYS LYS ALA ILE ALA SER ARG VAL ARG GLY ALA VAL ALA SER VAL THR PHE ASP ASP PHE HIS LYS ASN SER ALA ARG ILE ILE ARG

THR ALA VAL PHE GLY PHE GLU THR SER GLU ALA LYS GLY PRO ASP GLY MET ALA LEU PRO ARG PRO ARG ASP GLN ASN GLY LEU VAL VAL SER SER VAL ASP VAL GLN SER VAL GLU PRO VAL ASP GLN ARG THR ARG ASP ALA LEU GLN ARG SER VAL GLU LEU

ALA ILE GLU ILE THR THR ASN SER GLN GLU ALA ALA ALA LYS HIS GLU ALA GLN ARG LEU GLU GLN GLU ALA ARG GLY ARG LEU GLU ARG GLN LYS ILE LEU ASP GLN SER GLU ALA GLU LYS ALA ARG LYS GLU LEU GLU LEU GLU LEU GLU LEU GLU ALA LEU SER MET ALA VAL GLU SER THR GLY

THR ALA LYS ALA GLU ALA GLU SER ARG ALA GLU ALA ALA ARG ILE GLU GLY GLU GLY SER VAL LEU GLN ALA LYS LEU LYS ALA GLN ALA LEU ALA ILE GLU THR GLU ALA GLU LEU GLN ARG VAL GLN LYS VAL ARG GLU LEU E769 E789 E800 T806 I807 R808 D809 G850

MET G852 P853 GLU GLY GLN PRO LEU GLY ARG ARG VAL ALA SER GLY PRO SER PRO GLY GLU GLY ILE SER PRO GLN SER ALA GLN ALA PRO GLN ALA PRO GLY ASP ASN HIS VAL VAL PRO VAL LEU ARG

- Molecule 1: Major vault protein

Chain X: 6% 94%

MET ALA THR GLU GLU PHE ILE ILE ARG ILE PRO PRO TYR HIS TYR ILE HIS VAL LEU ASP GLN ASN SER ASN VAL SER ARG VAL GLU VAL GLY PRO LYS THR TYR ILE ARG GLN ASP ASN GLU ARG VAL LEU PHE ALA PRO MET ARG MET VAL THR VAL PRO PRO ARG HIS TYR CYS THR

VAL ALA ASN PRO VAL SER ARG ASP ALA GLN GLY LEU VAL LEU PHE ASP VAL THR GLY GLN VAL ARG LEU ARG HIS ALA ASP LEU GLU ILE ARG LEU ALA GLN ASP PRO PHE PRO LEU TYR PRO GLY GLU VAL LEU GLU LYS ASP ILE THR PRO LEU GLN VAL VAL LEU PRO ASN THR ALA

LEU HIS LEU LYS ALA LEU LEU ASP PHE GLU ASP LYS ASP GLY ASP LYS VAL VAL ALA GLY ASP GLU TRP LEU PHE GLU GLY PRO GLY THR TYR ILE PRO ARG LYS GLU VAL GLU VAL VAL GLU ILE ILE GLN ALA THR ILE ILE ARG GLN ASN GLN ALA LEU ARG LEU ARG ALA ARG LYS

GLU CYS TRP ASP ARG ASP GLY LYS GLU ARG VAL THR GLY GLU GLU TRP LEU VAL THR THR VAL GLY ALA TYR LEU PRO ALA VAL PHE GLU GLU VAL THR LEU ASP ALA VAL ILE LEU THR GLU LYS THR ALA HIS LEU ARG ALA ARG ARG ASN PHE ARG ASP PHE ARG GLY

VAL SER ARG ARG THR GLY GLU GLU TRP LEU VAL THR VAL GLN ASP THR GLU ALA HIS VAL PRO ASP VAL HIS GLU GLU VAL LEU GLY VAL VAL PRO ILE THR THR LEU GLY PRO HIS ASN TYR CYS VAL ILE LEU ASP PRO VAL GLY PRO ASP GLY LYS ASN GLN LEU GLY GLN LYS ARG

VAL VAL LYS GLY GLU LYS SER PHE PHE LEU GLN PRO GLY GLU GLN LEU GLU GLN GLY ILE GLN ASP VAL TYR VAL LEU SER GLU GLU GLN GLN GLY LEU LEU LEU ARG ALA LEU GLN PRO LEU GLU GLU GLY GLU GLU ASP GLU GLU LYS VAL SER HIS GLN ALA GLY ASP HIS TRP LEU ILE ARG

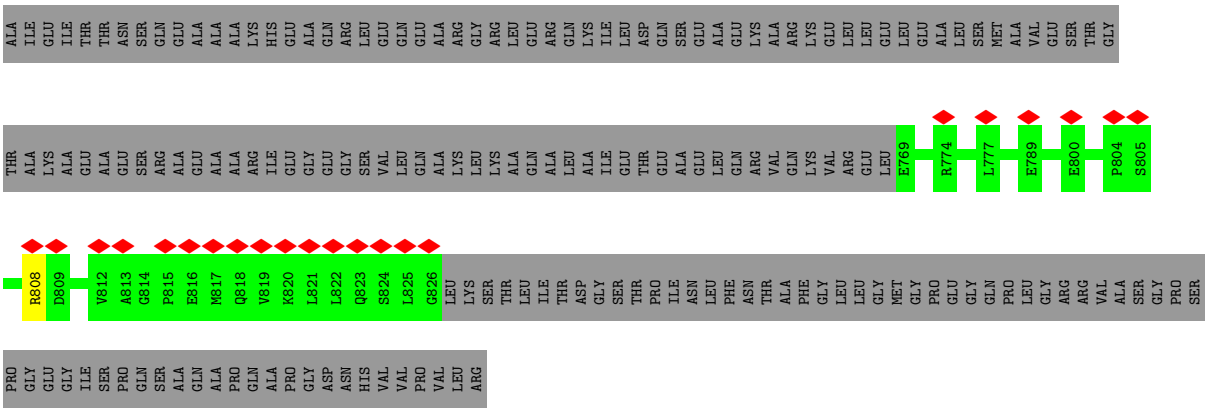
GLY PRO LEU GLU TYR VAL PRO SER ALA LYS VAL GLU VAL VAL GLU GLU ARG GLN ALA ILE PRO LEU ASP ASP GLU VAL ASN GLU GLU GLY ILE TYR VAL GLN ASP VAL LYS THR GLY LYS VAL ARG ALA VAL ILE GLY SER THR TYR GLU GLU LEU TRP GLU LYS ARG LEU GLU LEU PRO

PRO GLY VAL GLU GLU LEU LEU ASN LYS GLY GLN ASP PRO LEU ALA ASP ARG GLY GLU LYS ASP THR ALA LYS SER LEU GLN PRO LEU ALA PRO ARG ASN LYS THR ARG VAL VAL SER TYR ARG VAL PRO HIS ASN ALA ALA VAL GLN VAL TYR ASP TYR ARG GLU LYS ARG ALA ARG VAL

VAL PHE GLY PRO GLU LEU VAL SER LEU GLY PRO GLU GLU GLN PHE THR VAL LEU SER LEU SER ALA GLY ARG PRO LYS ARG PRO HIS ALA ARG ARG ALA LEU CYS LEU LEU LEU GLY PRO ASP PHE PHE THR ASP VAL ILE THR ILE GLU THR ALA ASP HIS ALA ARG LEU GLN GLN

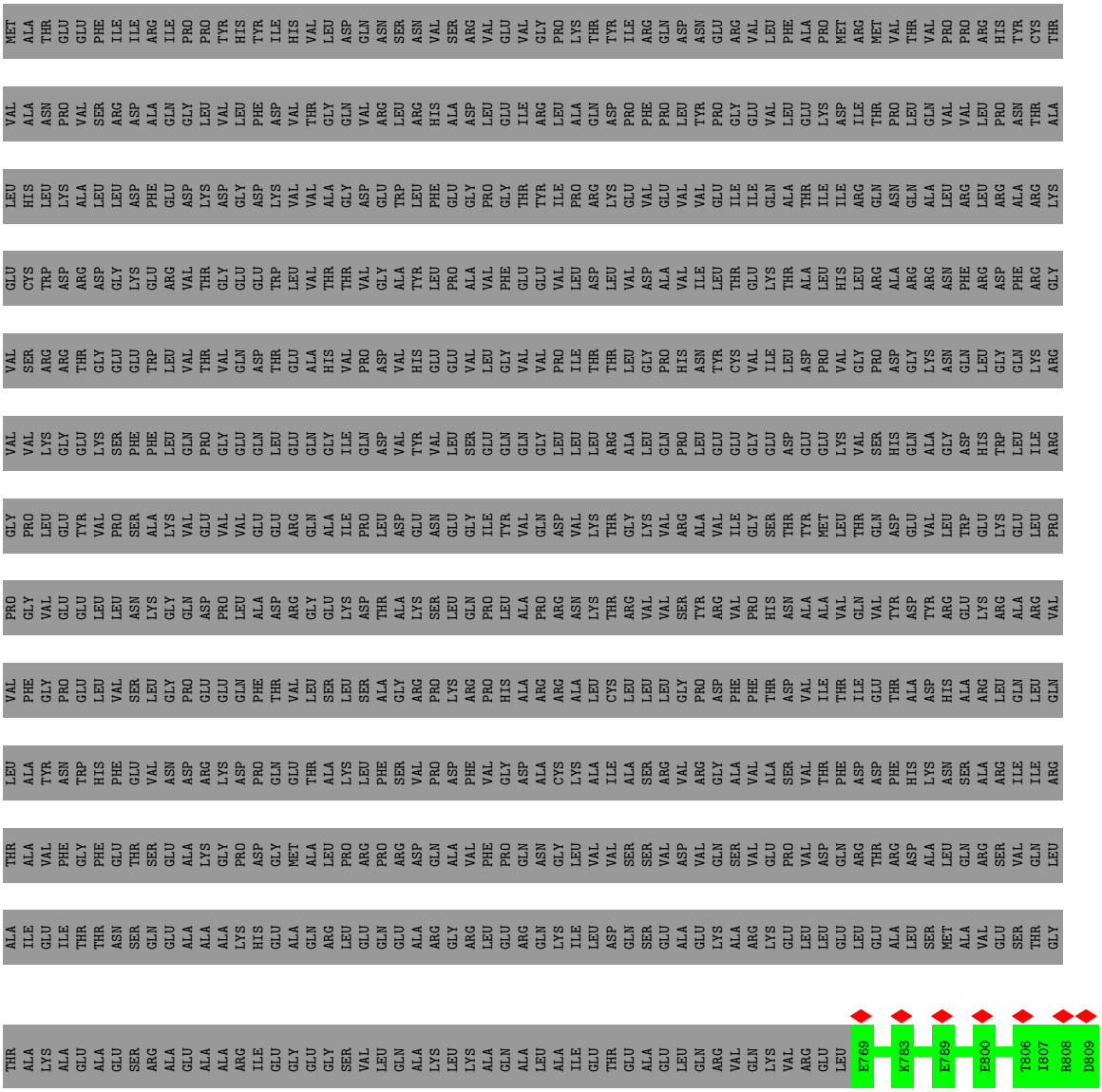
LEU ALA TYR ASN TRP HIS PHE GLU VAL ASN ASP ARG LYS ASP PRO GLN GLU THR ALA LYS LEU PHE SER VAL PRO ASP PHE VAL GLY ASP ALA CYS LYS ALA ILE ALA SER ARG VAL ARG GLY ALA VAL ALA SER VAL THR PHE ASP ASP PHE HIS LYS ASN SER ALA ARG ILE ILE ARG

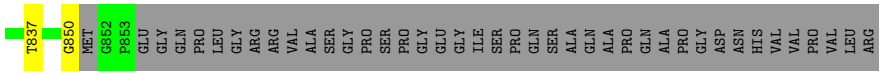
THR ALA VAL PHE GLY PHE GLU THR SER GLU ALA LYS GLY PRO ASP GLY MET ALA LEU PRO ARG PRO ARG ASP GLN ASN GLY LEU VAL VAL SER SER VAL ASP VAL GLN SER VAL GLU PRO VAL ASP GLN ARG THR ARG ASP ALA LEU GLN ARG SER VAL GLU LEU



- Molecule 1: Major vault protein

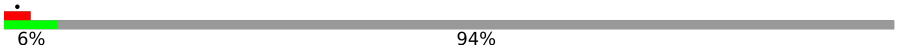
Chain Y: 9% 91%

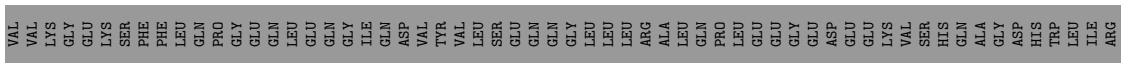


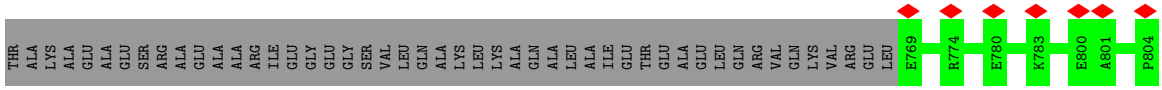


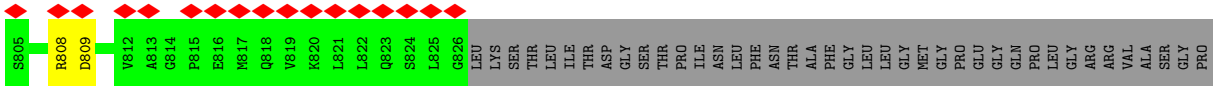
- Molecule 1: Major vault protein

Chain Z:









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65387	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.259	Depositor
Minimum map value	-0.208	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	0.65	0/639	1.22	0/863
1	A1	0.63	0/510	1.26	0/686
1	A2	0.64	0/510	1.26	0/686
1	A3	0.63	0/510	1.26	0/686
1	A4	0.62	0/510	1.22	0/686
1	Ar	0.63	0/510	1.23	0/686
1	As	0.63	0/510	1.25	0/686
1	At	0.63	0/510	1.25	0/686
1	Au	0.63	0/510	1.25	0/686
1	Av	0.63	0/510	1.27	0/686
1	Aw	0.64	0/510	1.26	0/686
1	Ax	0.64	0/510	1.25	0/686
1	Ay	0.63	0/510	1.26	0/686
1	Az	0.63	0/510	1.26	0/686
1	B	0.65	0/449	1.31	1/603 (0.2%)
1	C	0.65	0/639	1.23	0/863
1	D	0.68	0/449	1.36	1/603 (0.2%)
1	E	0.64	0/639	1.21	0/863
1	F	0.65	0/449	1.34	1/603 (0.2%)
1	G	0.65	0/639	1.22	0/863
1	H	0.65	0/449	1.33	2/603 (0.3%)
1	I	0.65	0/639	1.19	0/863
1	J	0.64	0/449	1.28	1/603 (0.2%)
1	K	0.66	0/639	1.20	0/863
1	L	0.65	0/449	1.34	1/603 (0.2%)
1	M	0.64	0/639	1.21	0/863
1	N	0.65	0/449	1.32	1/603 (0.2%)
1	O	0.64	0/639	1.24	0/863
1	P	0.65	0/449	1.34	0/603
1	Q	0.64	0/639	1.22	0/863
1	R	0.65	0/449	1.34	0/603
1	S	0.65	0/639	1.26	0/863
1	T	0.65	0/449	1.35	1/603 (0.2%)
1	U	0.65	0/639	1.22	0/863

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	V	0.65	0/449	1.33	0/603
1	W	0.64	0/639	1.22	0/863
1	X	0.65	0/449	1.34	0/603
1	Y	0.65	0/639	1.22	0/863
1	Z	0.65	0/449	1.35	1/603 (0.2%)
All	All	0.64	0/20774	1.26	10/27976 (0.0%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Z	809	ASP	CA-CB-CG	5.50	118.10	112.60
1	F	809	ASP	CA-CB-CG	5.25	117.85	112.60
1	J	808	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	D	808	ARG	NE-CZ-NH2	5.15	123.84	119.20
1	B	809	ASP	CA-CB-CG	5.12	117.72	112.60

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	632	665	664	1	0
1	A1	507	541	540	0	0
1	A2	507	541	540	1	0
1	A3	507	541	540	0	0
1	A4	507	541	540	0	0
1	Ar	507	541	540	0	0
1	As	507	541	540	1	0
1	At	507	541	540	0	0
1	Au	507	541	540	0	0
1	Av	507	541	540	0	0
1	Aw	507	541	540	0	0
1	Ax	507	541	540	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ay	507	541	540	0	0
1	Az	507	541	540	0	0
1	B	446	472	471	0	0
1	C	632	665	664	0	0
1	D	446	472	471	0	0
1	E	632	665	664	0	0
1	F	446	472	471	0	0
1	G	632	665	664	0	0
1	H	446	472	471	0	0
1	I	632	665	664	0	0
1	J	446	472	471	0	0
1	K	632	665	664	0	0
1	L	446	472	471	0	0
1	M	632	665	664	0	0
1	N	446	472	471	0	0
1	O	632	665	664	1	0
1	P	446	472	471	0	0
1	Q	632	665	664	0	0
1	R	446	472	471	0	0
1	S	632	665	664	1	0
1	T	446	472	471	0	0
1	U	632	665	664	0	0
1	V	446	472	471	0	0
1	W	632	665	664	0	0
1	X	446	472	471	0	0
1	Y	632	665	664	0	0
1	Z	446	472	471	0	0
All	All	20605	21814	21775	3	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 0.

All (3) 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:O:833:THR:HG22	1:O:839:ILE:HD12	1.96	0.48
1:A2:817:MET:HE1	1:S:812:VAL:HG13	1.99	0.45
1:A:770:LEU:HD21	1:As:775:ALA:HB1	2.01	0.42

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	82/893 (9%)	78 (95%)	4 (5%)	0	100	100
1	A1	64/893 (7%)	61 (95%)	3 (5%)	0	100	100
1	A2	64/893 (7%)	62 (97%)	2 (3%)	0	100	100
1	A3	64/893 (7%)	61 (95%)	3 (5%)	0	100	100
1	A4	64/893 (7%)	61 (95%)	3 (5%)	0	100	100
1	Ar	64/893 (7%)	62 (97%)	2 (3%)	0	100	100
1	As	64/893 (7%)	62 (97%)	2 (3%)	0	100	100
1	At	64/893 (7%)	62 (97%)	2 (3%)	0	100	100
1	Au	64/893 (7%)	60 (94%)	4 (6%)	0	100	100
1	Av	64/893 (7%)	62 (97%)	2 (3%)	0	100	100
1	Aw	64/893 (7%)	62 (97%)	2 (3%)	0	100	100
1	Ax	64/893 (7%)	63 (98%)	1 (2%)	0	100	100
1	Ay	64/893 (7%)	61 (95%)	3 (5%)	0	100	100
1	Az	64/893 (7%)	62 (97%)	2 (3%)	0	100	100
1	B	56/893 (6%)	56 (100%)	0	0	100	100
1	C	82/893 (9%)	79 (96%)	3 (4%)	0	100	100
1	D	56/893 (6%)	53 (95%)	3 (5%)	0	100	100
1	E	82/893 (9%)	78 (95%)	4 (5%)	0	100	100
1	F	56/893 (6%)	53 (95%)	3 (5%)	0	100	100
1	G	82/893 (9%)	78 (95%)	3 (4%)	1 (1%)	10	41
1	H	56/893 (6%)	52 (93%)	4 (7%)	0	100	100
1	I	82/893 (9%)	79 (96%)	3 (4%)	0	100	100
1	J	35/893 (4%)	35 (100%)	0	0	100	100
1	K	82/893 (9%)	80 (98%)	1 (1%)	1 (1%)	10	41
1	L	56/893 (6%)	53 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	82/893 (9%)	78 (95%)	4 (5%)	0	100	100
1	N	56/893 (6%)	53 (95%)	3 (5%)	0	100	100
1	O	82/893 (9%)	78 (95%)	4 (5%)	0	100	100
1	P	56/893 (6%)	53 (95%)	3 (5%)	0	100	100
1	Q	82/893 (9%)	79 (96%)	3 (4%)	0	100	100
1	R	56/893 (6%)	53 (95%)	3 (5%)	0	100	100
1	S	82/893 (9%)	78 (95%)	4 (5%)	0	100	100
1	T	56/893 (6%)	53 (95%)	3 (5%)	0	100	100
1	U	82/893 (9%)	78 (95%)	4 (5%)	0	100	100
1	V	56/893 (6%)	52 (93%)	4 (7%)	0	100	100
1	W	82/893 (9%)	76 (93%)	6 (7%)	0	100	100
1	X	56/893 (6%)	52 (93%)	4 (7%)	0	100	100
1	Y	82/893 (9%)	78 (95%)	3 (4%)	1 (1%)	10	41
1	Z	56/893 (6%)	54 (96%)	2 (4%)	0	100	100
All	All	2605/34827 (8%)	2490 (96%)	112 (4%)	3 (0%)	49	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Y	850	GLY
1	G	850	GLY
1	K	850	GLY

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	69/755 (9%)	69 (100%)	0	100	100
1	A1	56/755 (7%)	56 (100%)	0	100	100
1	A2	56/755 (7%)	55 (98%)	1 (2%)	51	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A3	56/755 (7%)	56 (100%)	0	100	100
1	A4	56/755 (7%)	56 (100%)	0	100	100
1	Ar	56/755 (7%)	56 (100%)	0	100	100
1	As	56/755 (7%)	56 (100%)	0	100	100
1	At	56/755 (7%)	56 (100%)	0	100	100
1	Au	56/755 (7%)	56 (100%)	0	100	100
1	Av	56/755 (7%)	56 (100%)	0	100	100
1	Aw	56/755 (7%)	56 (100%)	0	100	100
1	Ax	56/755 (7%)	56 (100%)	0	100	100
1	Ay	56/755 (7%)	56 (100%)	0	100	100
1	Az	56/755 (7%)	56 (100%)	0	100	100
1	B	48/755 (6%)	47 (98%)	1 (2%)	47	65
1	C	69/755 (9%)	69 (100%)	0	100	100
1	D	48/755 (6%)	48 (100%)	0	100	100
1	E	69/755 (9%)	69 (100%)	0	100	100
1	F	48/755 (6%)	47 (98%)	1 (2%)	47	65
1	G	69/755 (9%)	69 (100%)	0	100	100
1	H	48/755 (6%)	47 (98%)	1 (2%)	47	65
1	I	69/755 (9%)	69 (100%)	0	100	100
1	J	48/755 (6%)	48 (100%)	0	100	100
1	K	69/755 (9%)	69 (100%)	0	100	100
1	L	48/755 (6%)	47 (98%)	1 (2%)	47	65
1	M	69/755 (9%)	68 (99%)	1 (1%)	59	71
1	N	48/755 (6%)	47 (98%)	1 (2%)	47	65
1	O	69/755 (9%)	69 (100%)	0	100	100
1	P	48/755 (6%)	47 (98%)	1 (2%)	47	65
1	Q	69/755 (9%)	69 (100%)	0	100	100
1	R	48/755 (6%)	47 (98%)	1 (2%)	47	65
1	S	69/755 (9%)	69 (100%)	0	100	100
1	T	48/755 (6%)	47 (98%)	1 (2%)	47	65
1	U	69/755 (9%)	69 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	V	48/755 (6%)	47 (98%)	1 (2%)	47	65
1	W	69/755 (9%)	69 (100%)	0	100	100
1	X	48/755 (6%)	47 (98%)	1 (2%)	47	65
1	Y	69/755 (9%)	68 (99%)	1 (1%)	59	71
1	Z	48/755 (6%)	47 (98%)	1 (2%)	47	65
All	All	2249/29445 (8%)	2235 (99%)	14 (1%)	76	79

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	808	ARG
1	R	808	ARG
1	Z	808	ARG
1	X	808	ARG
1	Y	837	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	823	GLN
1	Y	786	GLN
1	L	797	GLN
1	X	797	GLN
1	T	823	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

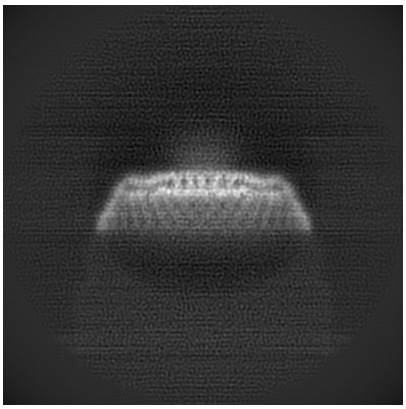
6 Map visualisation (i)

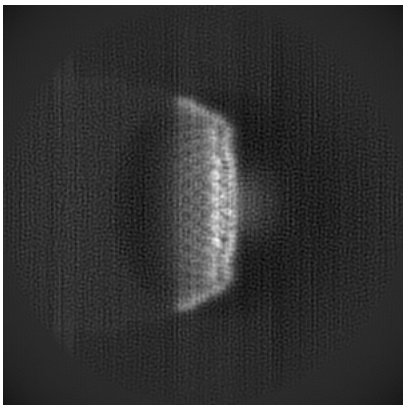
This section contains visualisations of the EMDB entry EMD-53806. These allow visual inspection of the internal detail of the map and identification of artifacts.

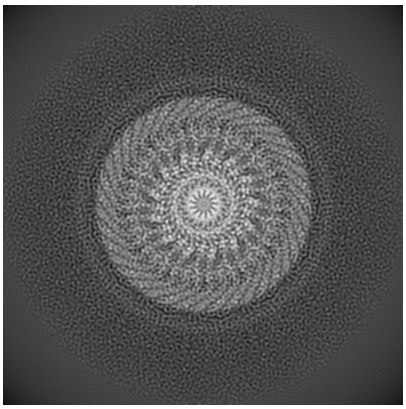
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

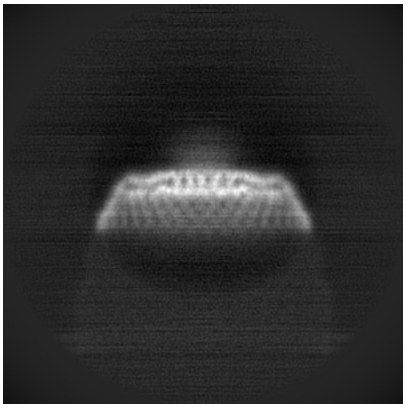
6.1.1 Primary map

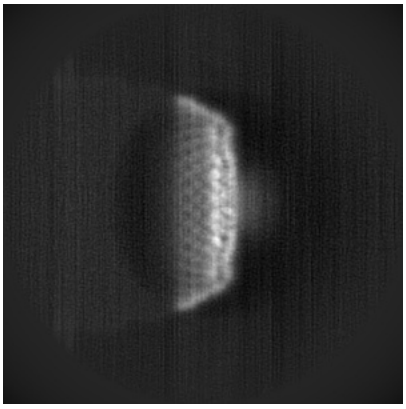

X

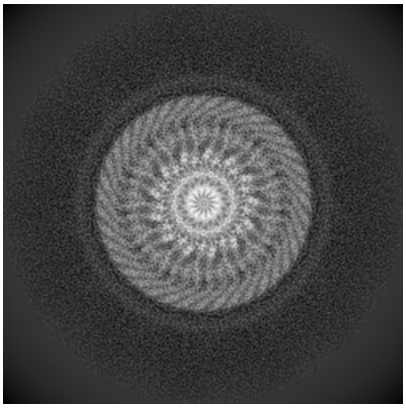

Y


Z

6.1.2 Raw map


X

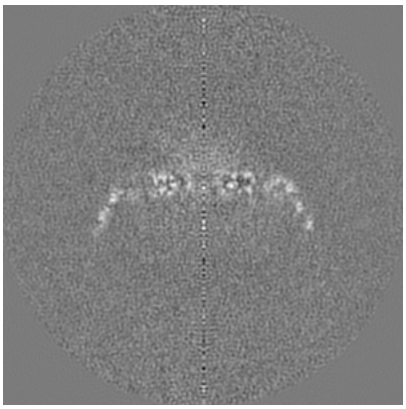

Y

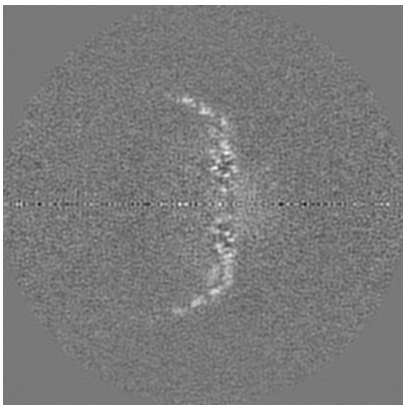

Z

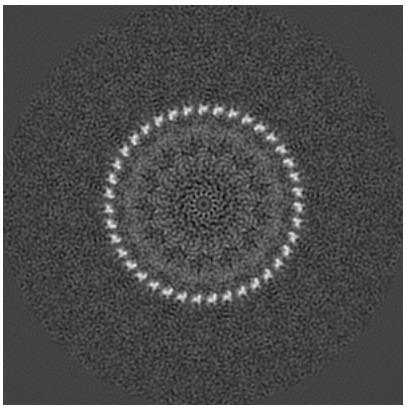
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

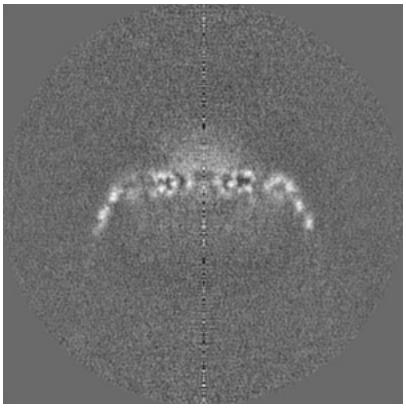
6.2.1 Primary map

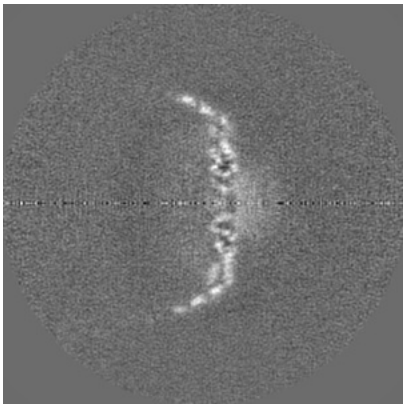

X Index: 128

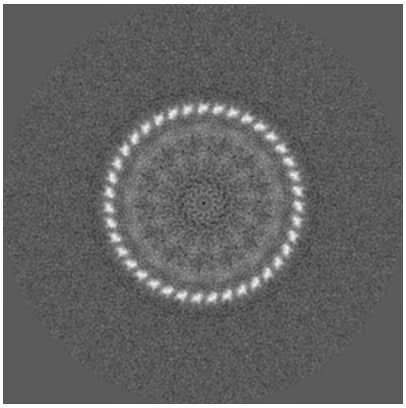

Y Index: 128


Z Index: 128

6.2.2 Raw map


X Index: 128

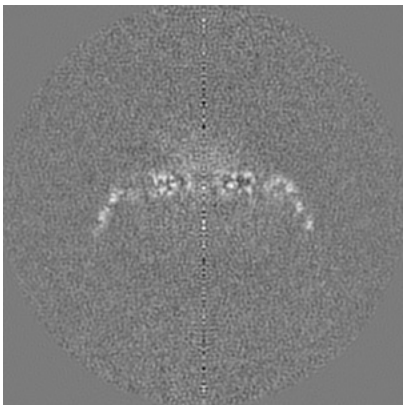

Y Index: 128

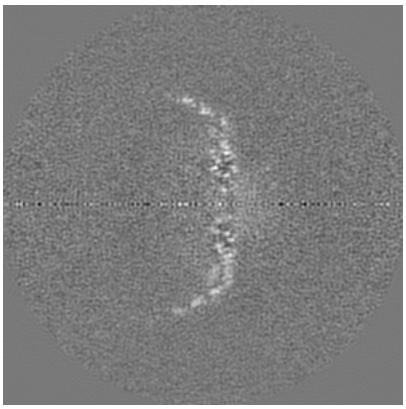

Z Index: 128

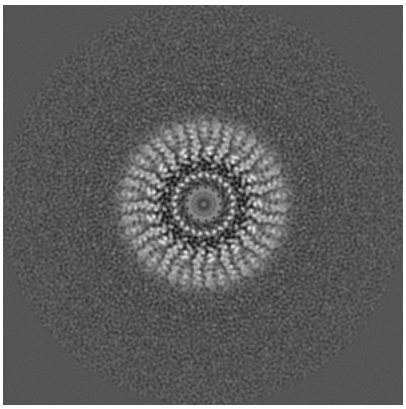
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

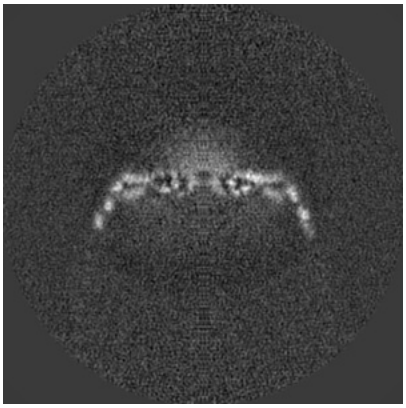
6.3.1 Primary map

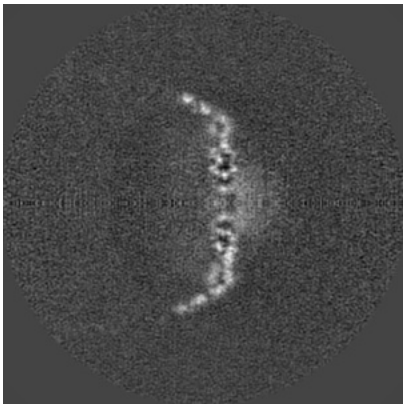

X Index: 128

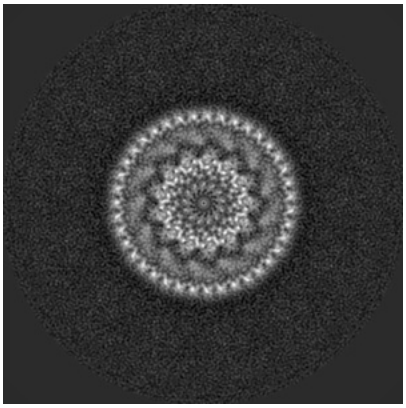

Y Index: 128


Z Index: 143

6.3.2 Raw map


X Index: 123

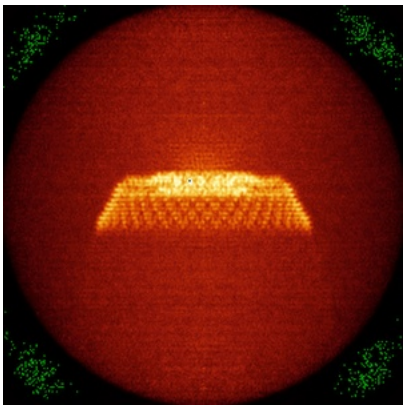

Y Index: 127

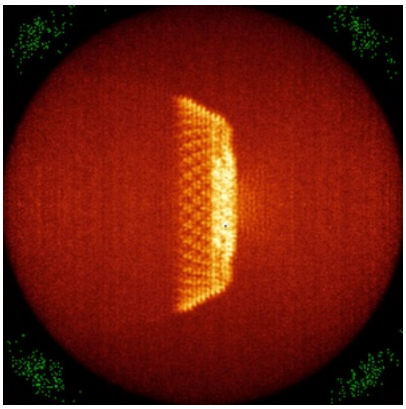

Z Index: 136

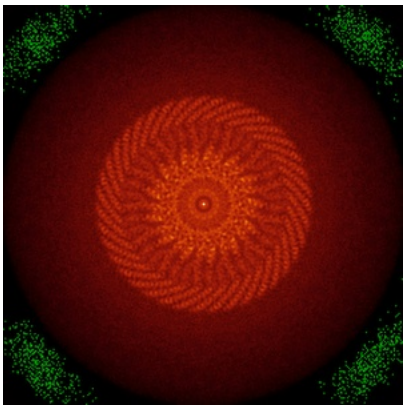
The images above show the largest variance slices of the map in three orthogonal directions.

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

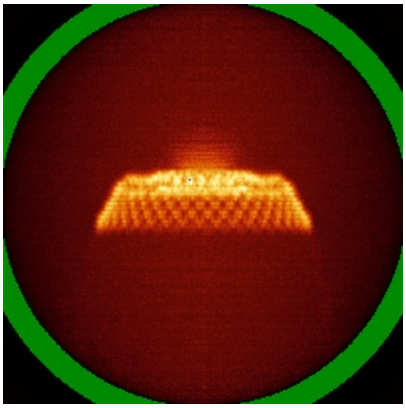
6.4.1 Primary map

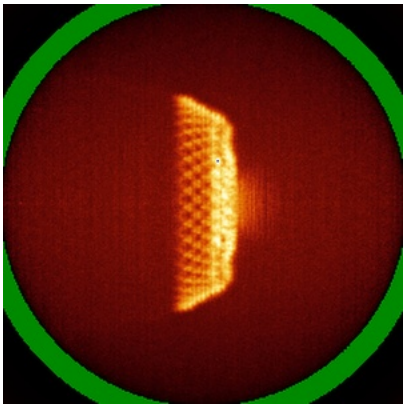

X

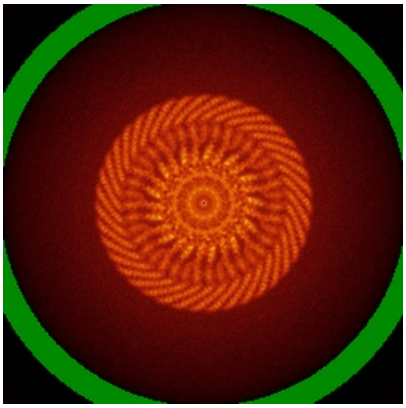

Y


Z

6.4.2 Raw map


X

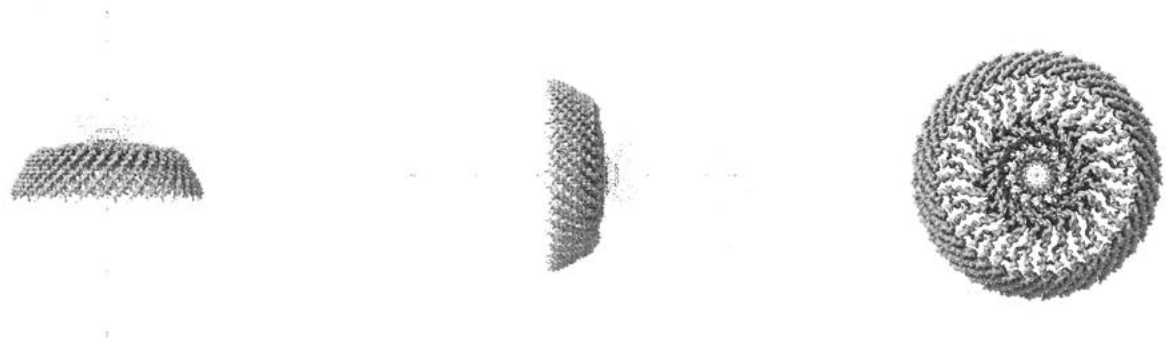

Y


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)

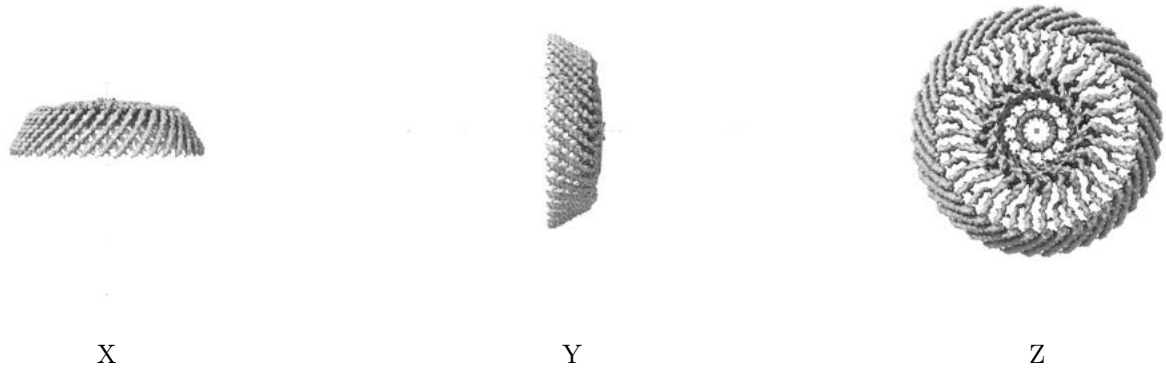
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. 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.

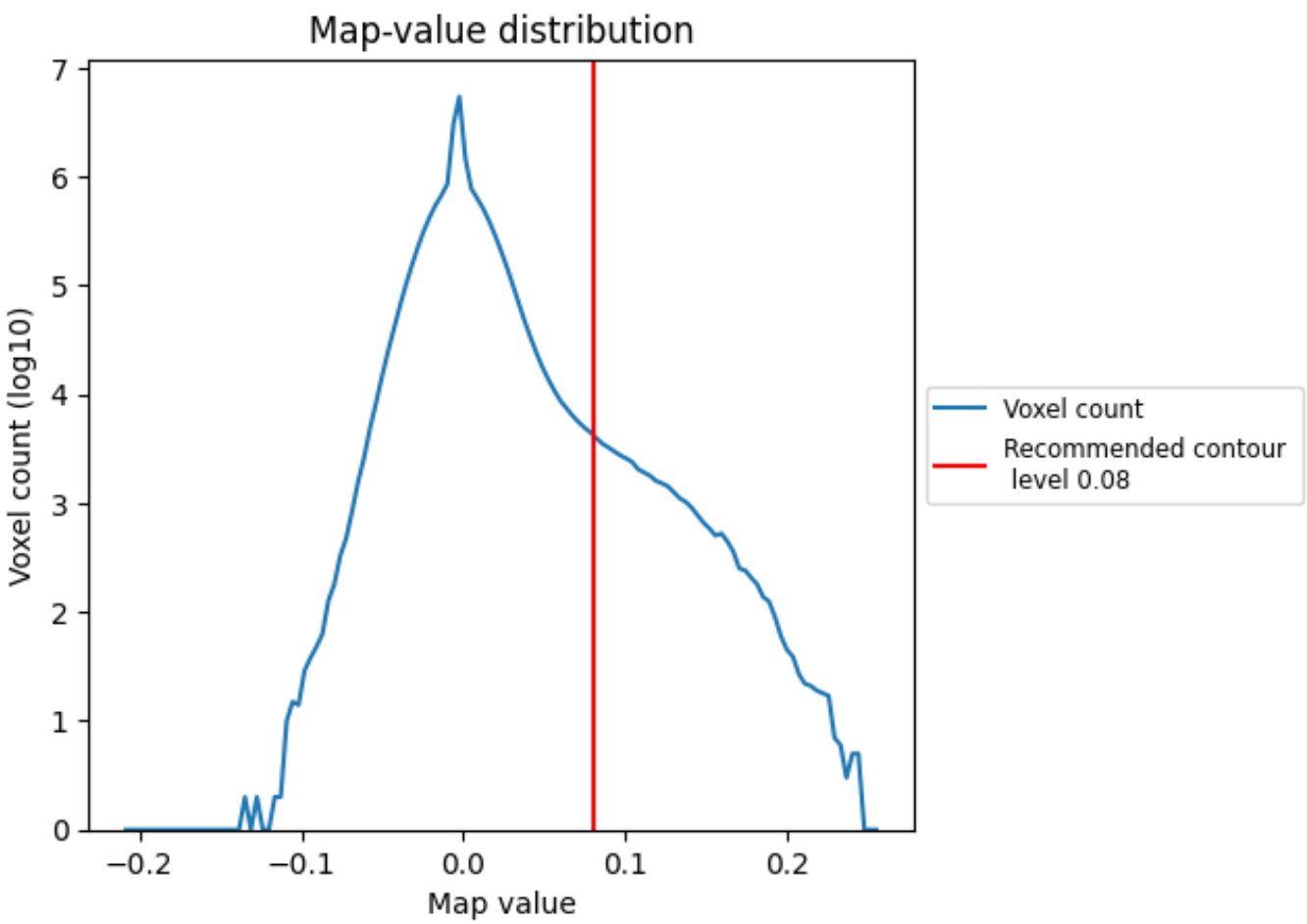
6.6 Mask visualisation (i)

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

7 Map analysis (i)

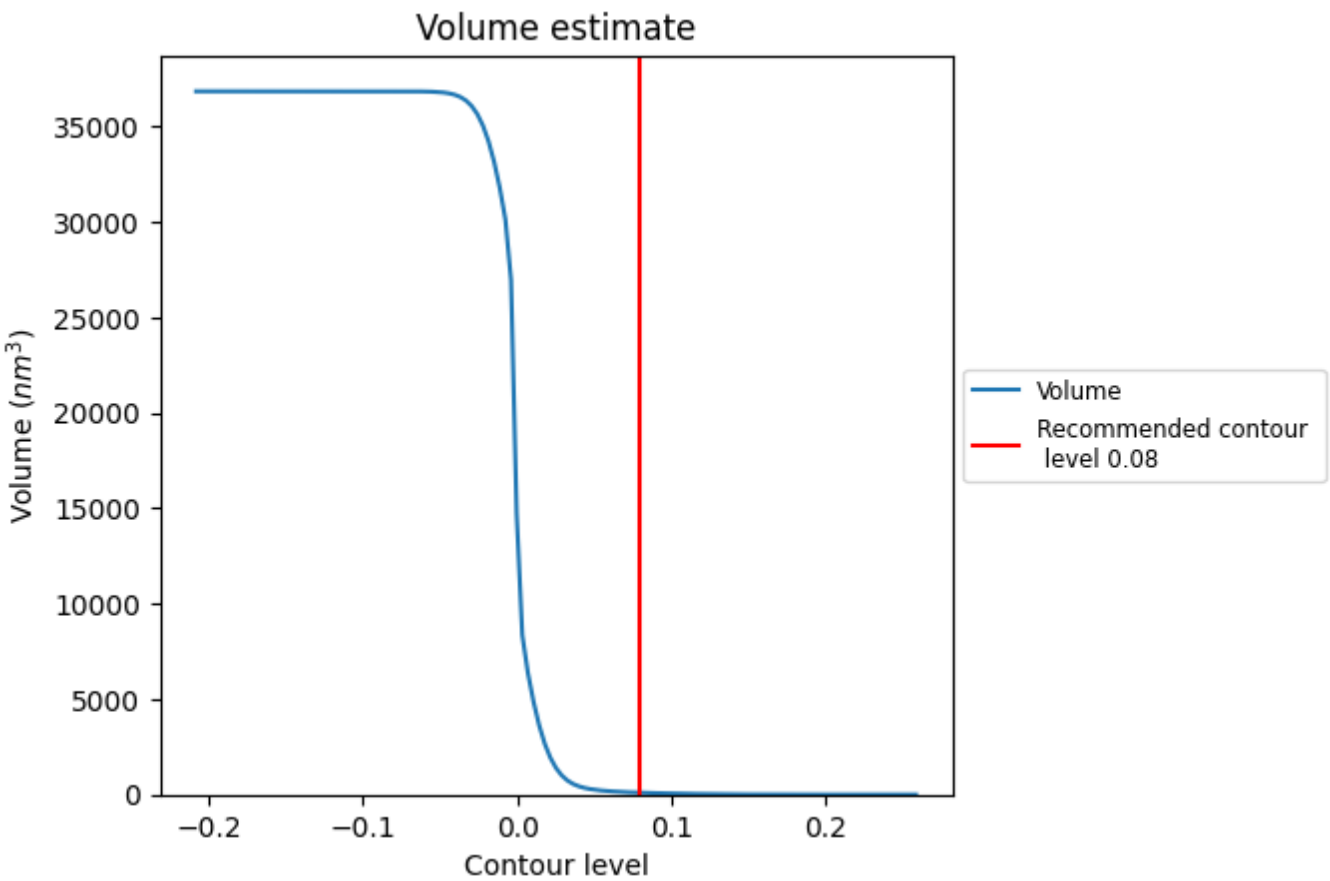
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

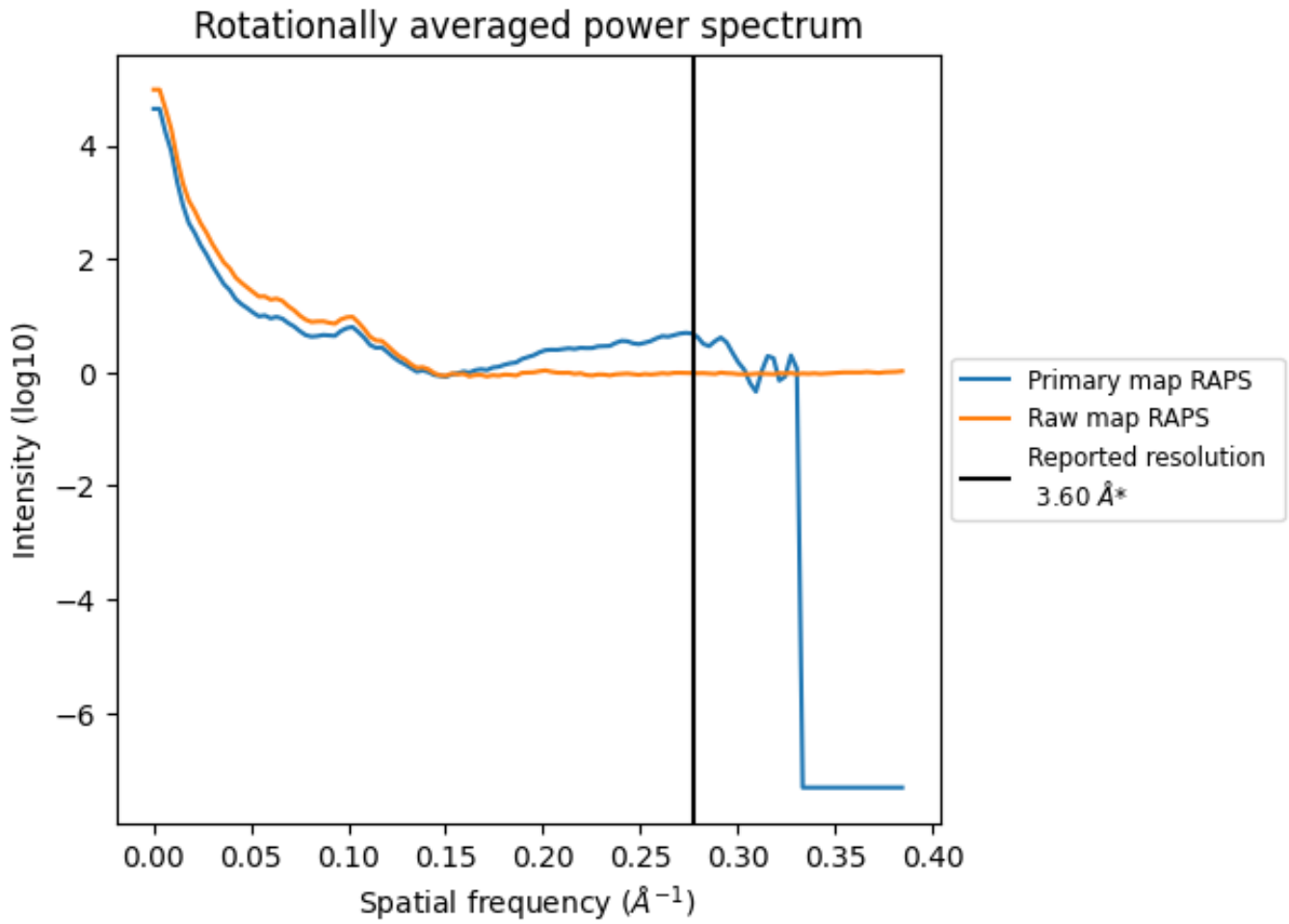
7.2 Volume estimate (i)



The volume at the recommended contour level is 97 nm^3; this corresponds to an approximate mass of 88 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)

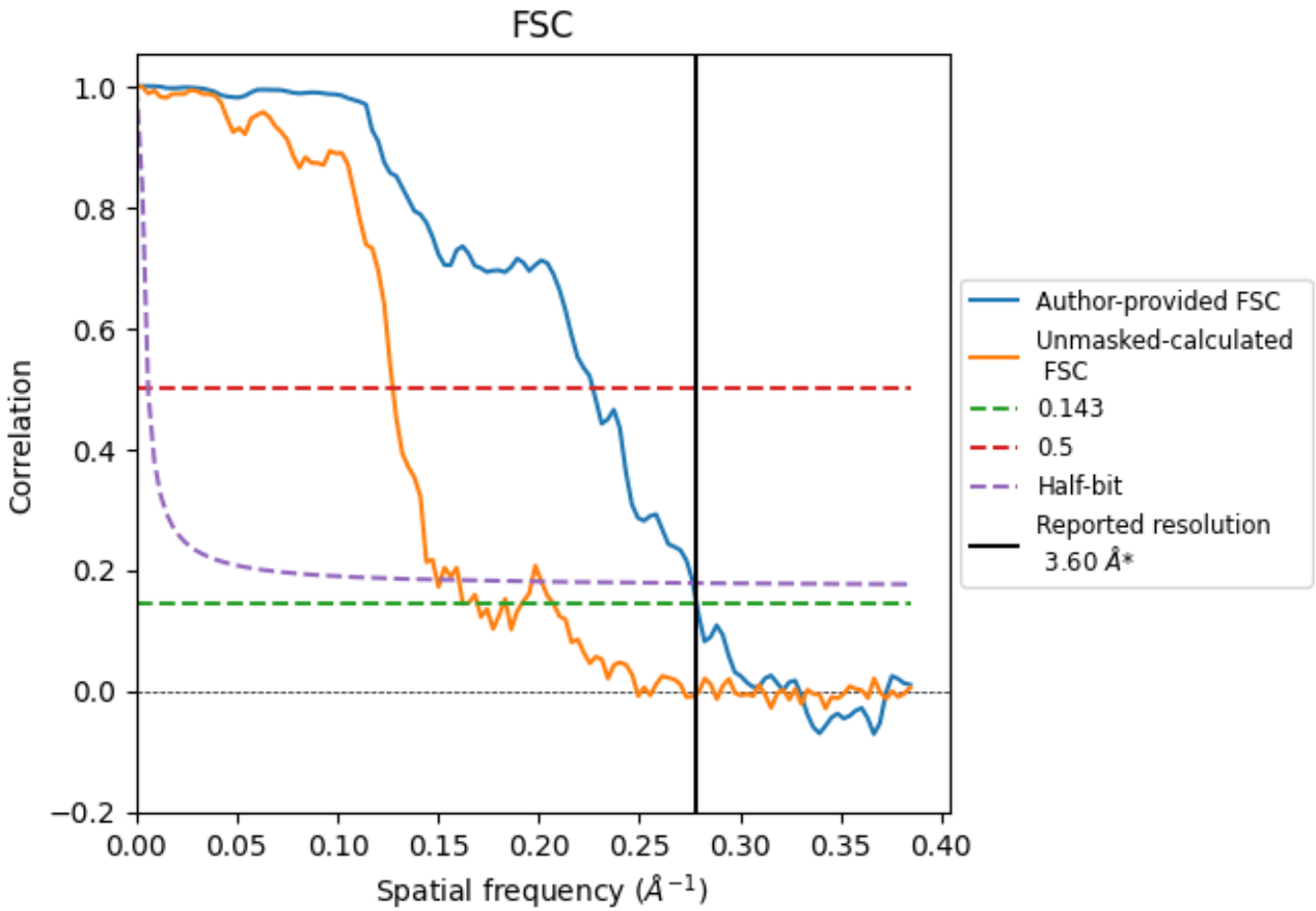


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

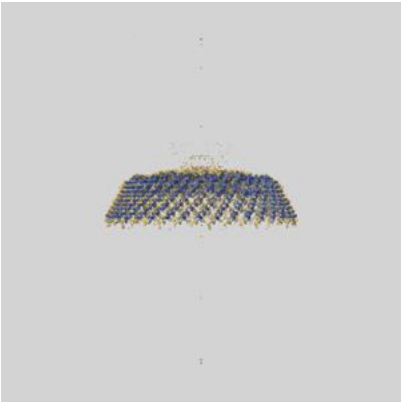
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.59	4.41	3.62
Unmasked-calculated*	5.90	7.84	6.69

*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 5.90 differs from the reported value 3.6 by more than 10 %

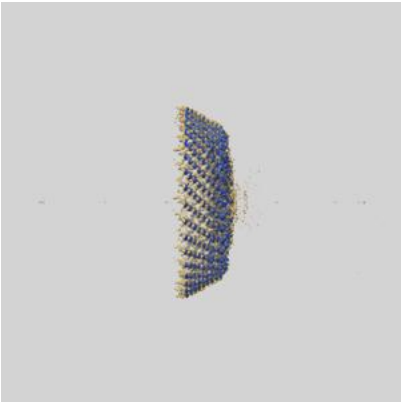
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-53806 and PDB model 9R87. Per-residue inclusion information can be found in section 3 on page 8.

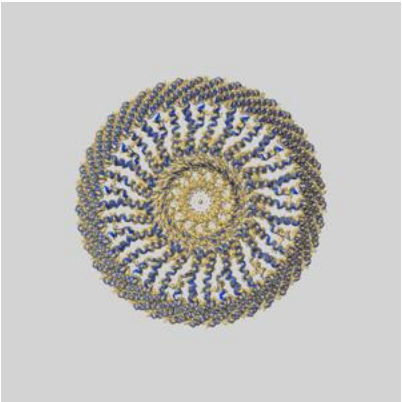
9.1 Map-model overlay (i)



X



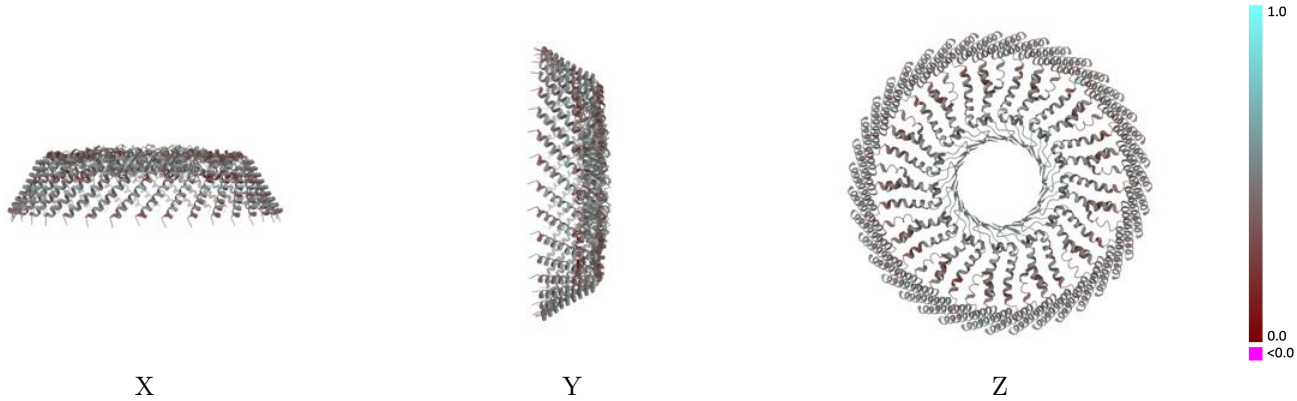
Y



Z

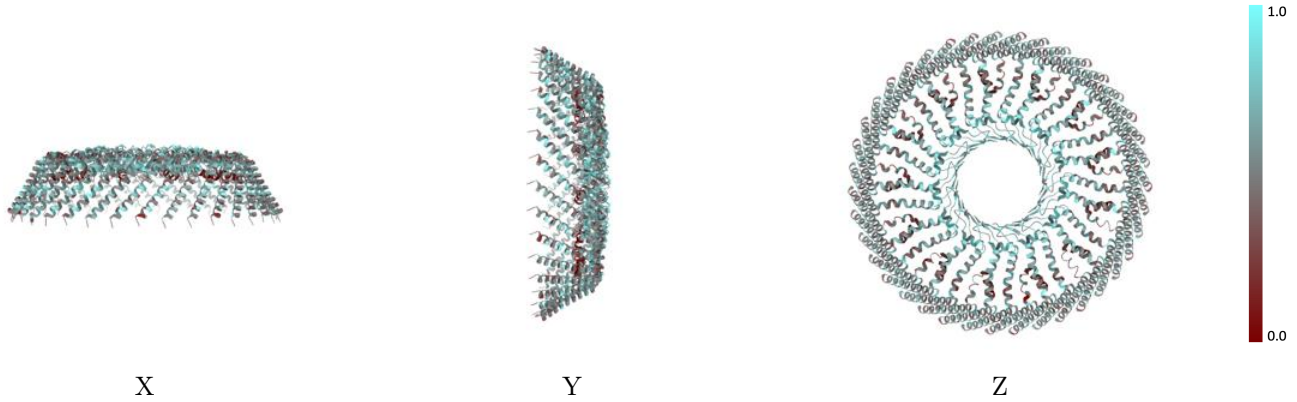
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



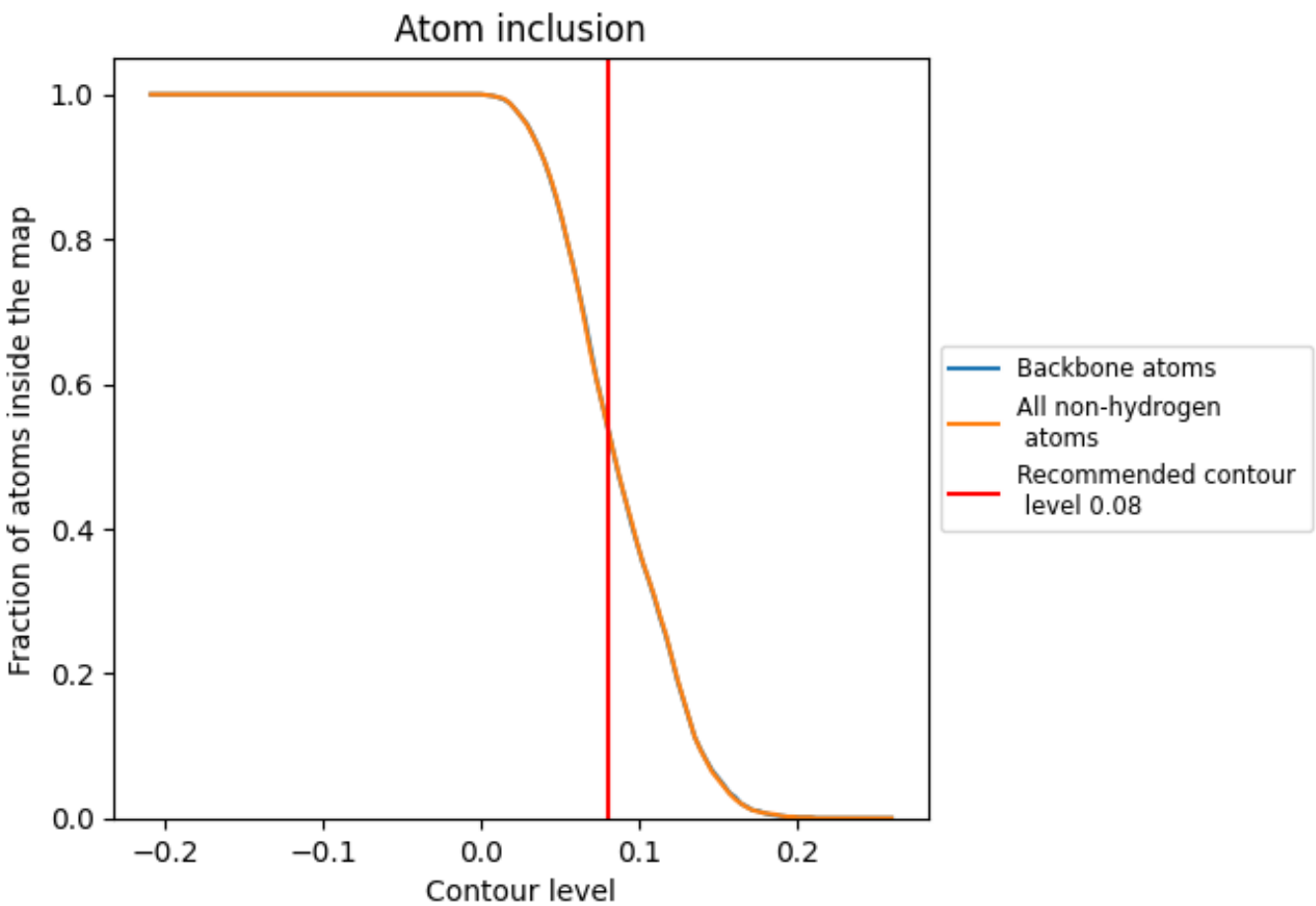
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (i)



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 (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 54% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5380	0.4540
A	0.6030	0.4740
A1	0.5620	0.4550
A2	0.5900	0.4590
A3	0.5800	0.4530
A4	0.5700	0.4550
Ar	0.5720	0.4620
As	0.5680	0.4560
At	0.5680	0.4620
Au	0.5620	0.4590
Av	0.5740	0.4630
Aw	0.5740	0.4590
Ax	0.5720	0.4590
Ay	0.5820	0.4570
Az	0.5840	0.4540
B	0.4420	0.4300
C	0.6000	0.4670
D	0.4240	0.4250
E	0.6010	0.4720
F	0.4220	0.4280
G	0.5920	0.4710
H	0.4420	0.4380
I	0.5930	0.4690
J	0.4330	0.4340
K	0.5980	0.4720
L	0.4150	0.4220
M	0.6080	0.4760
N	0.4310	0.4240
O	0.6050	0.4720
P	0.4380	0.4240
Q	0.5970	0.4730
R	0.4240	0.4230
S	0.6140	0.4720
T	0.4420	0.4240
U	0.5970	0.4680

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Chain	Atom inclusion	Q-score
V	0.4400	0.4220
W	0.6010	0.4680
X	0.4290	0.4150
Y	0.6010	0.4690
Z	0.4330	0.4260