Full wwPDB EM Validation Report (i)

Dec 10, 2022 – 10:11 pm GMT

PDB ID	:	6QZ9
EMDB ID	:	EMD-4684
Title	:	The cryo-EM structure of the collar complex and tail axis in bacteriophage phi29
Authors	:	Xu, J.; Wang, D.; Gui, M.; Xiang, Y.
Deposited on	:	2019-03-11
Resolution	:	3.30 Å(reported)

This is a Full wwPDB EM Validation 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:

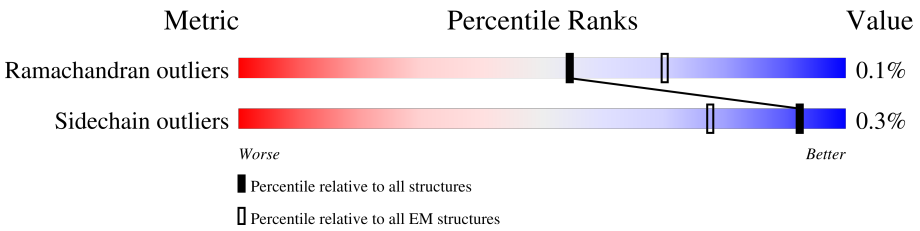
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.30 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0a	309	50% 85% 15%
1	0b	309	50% 85% 15%
1	0c	309	50% 85% 15%
1	0d	309	50% 85% 15%
1	0e	309	50% 85% 15%
1	0f	309	50% 85% 15%
1	0g	309	50% 85% 15%
1	0h	309	50% 85% 15%
1	0i	309	50% 85% 15%

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Mol	Chain	Length	Quality of chain
1	0j	309	50% 85% 15%
1	0k	309	50% 85% 15%
1	0l	309	50% 85% 15%
2	0A	293	99%
2	0B	293	99%
2	0C	293	5% 99%
2	0D	293	99%
2	0E	293	5% 99%
2	0F	293	99%
2	0G	293	99%
2	0H	293	99%
2	0I	293	5% 99%
2	0J	293	5% 99%
2	0K	293	5% 99%
2	0L	293	5% 99%
3	A	854	6% 94%
3	B	854	6% 93%
3	C	854	8% 92%
3	D	854	6% 94%
3	E	854	7% 93%
3	F	854	8% 92%
3	G	854	6% 94%
3	H	854	7% 93%
3	I	854	5% 8% 92%
3	J	854	6% 94%

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Mol	Chain	Length	Quality of chain
3	K	854	7% 93%
3	L	854	8% 92%
3	M	854	6% 94%
3	N	854	7% 93%
3	O	854	8% 92%
3	P	854	6% 94%
3	Q	854	7% 93%
3	R	854	5% 8% 92%
3	S	854	6% 94%
3	T	854	7% 93%
3	U	854	5% 8% 92%
3	V	854	6% 94%
3	W	854	7% 93%
3	X	854	8% 92%
3	Y	854	6% 94%
3	Z	854	7% 93%
3	a	854	8% 92%
3	b	854	6% 94%
3	c	854	7% 93%
3	d	854	8% 92%
3	e	854	6% 94%
3	f	854	6% 93%
3	g	854	8% 92%
3	h	854	6% 94%
3	i	854	7% 93%

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Mol	Chain	Length	Quality of chain
3	j	854	8% 92%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 71724 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0a	264	2163	1384	360	412	7	0	0
1	0b	264	2163	1384	360	412	7	0	0
1	0c	264	2163	1384	360	412	7	0	0
1	0d	264	2163	1384	360	412	7	0	0
1	0e	264	2163	1384	360	412	7	0	0
1	0f	264	2163	1384	360	412	7	0	0
1	0g	264	2163	1384	360	412	7	0	0
1	0h	264	2163	1384	360	412	7	0	0
1	0i	264	2163	1384	360	412	7	0	0
1	0j	264	2163	1384	360	412	7	0	0
1	0k	264	2163	1384	360	412	7	0	0
1	0l	264	2163	1384	360	412	7	0	0

- Molecule 2 is a protein called Proximal tail tube connector protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	0A	291	2296	1414	396	478	8	0	0
2	0B	291	2296	1414	396	478	8	0	0
2	0C	291	2296	1414	396	478	8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	0D	291	2296	1414	396	478	8	0	0
2	0E	291	2296	1414	396	478	8	0	0
2	0F	291	2296	1414	396	478	8	0	0
2	0G	291	2296	1414	396	478	8	0	0
2	0H	291	2296	1414	396	478	8	0	0
2	0I	291	2296	1414	396	478	8	0	0
2	0J	291	2296	1414	396	478	8	0	0
2	0K	291	2296	1414	396	478	8	0	0
2	0L	291	2296	1414	396	478	8	0	0

- Molecule 3 is a protein called Pre-neck appendage protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	51	433	281	67	83	2	0	0
3	B	57	482	312	74	92	4	0	0
3	C	71	603	391	94	114	4	0	0
3	D	51	433	281	67	83	2	0	0
3	E	57	482	312	74	92	4	0	0
3	F	71	603	391	94	114	4	0	0
3	G	51	433	281	67	83	2	0	0
3	H	57	482	312	74	92	4	0	0
3	I	71	603	391	94	114	4	0	0
3	J	51	433	281	67	83	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	K	57	482	312	74	92	4	0	0
			Total	C	N	O	S		
3	L	71	603	391	94	114	4	0	0
			Total	C	N	O	S		
3	M	51	433	281	67	83	2	0	0
			Total	C	N	O	S		
3	N	57	482	312	74	92	4	0	0
			Total	C	N	O	S		
3	O	71	603	391	94	114	4	0	0
			Total	C	N	O	S		
3	P	51	433	281	67	83	2	0	0
			Total	C	N	O	S		
3	Q	57	482	312	74	92	4	0	0
			Total	C	N	O	S		
3	R	71	603	391	94	114	4	0	0
			Total	C	N	O	S		
3	S	51	433	281	67	83	2	0	0
			Total	C	N	O	S		
3	T	57	482	312	74	92	4	0	0
			Total	C	N	O	S		
3	U	71	603	391	94	114	4	0	0
			Total	C	N	O	S		
3	V	51	433	281	67	83	2	0	0
			Total	C	N	O	S		
3	W	57	482	312	74	92	4	0	0
			Total	C	N	O	S		
3	X	71	603	391	94	114	4	0	0
			Total	C	N	O	S		
3	Y	51	433	281	67	83	2	0	0
			Total	C	N	O	S		
3	Z	57	482	312	74	92	4	0	0
			Total	C	N	O	S		
3	a	71	603	391	94	114	4	0	0
			Total	C	N	O	S		
3	b	51	433	281	67	83	2	0	0
			Total	C	N	O	S		
3	c	57	482	312	74	92	4	0	0
			Total	C	N	O	S		
3	d	71	603	391	94	114	4	0	0
			Total	C	N	O	S		
3	e	51	433	281	67	83	2	0	0

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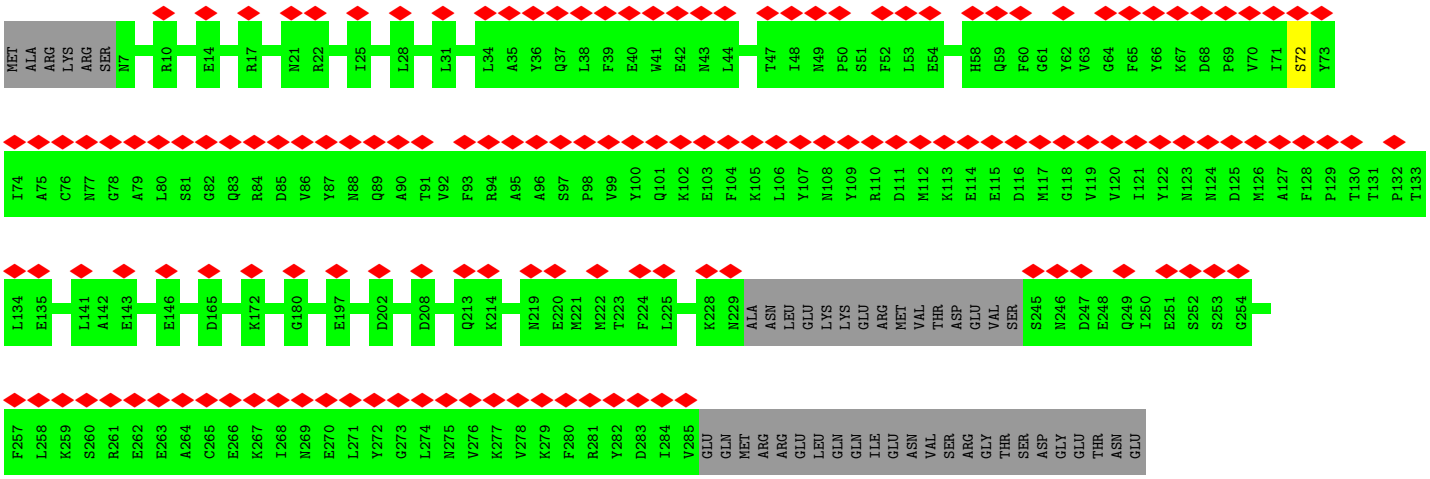
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	f	57	482	312	74	92	4	0	0
			Total	C	N	O	S		
3	g	71	603	391	94	114	4	0	0
			Total	C	N	O	S		
3	h	51	433	281	67	83	2	0	0
			Total	C	N	O	S		
3	i	57	482	312	74	92	4	0	0
			Total	C	N	O	S		
3	j	71	603	391	94	114	4	0	0

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.

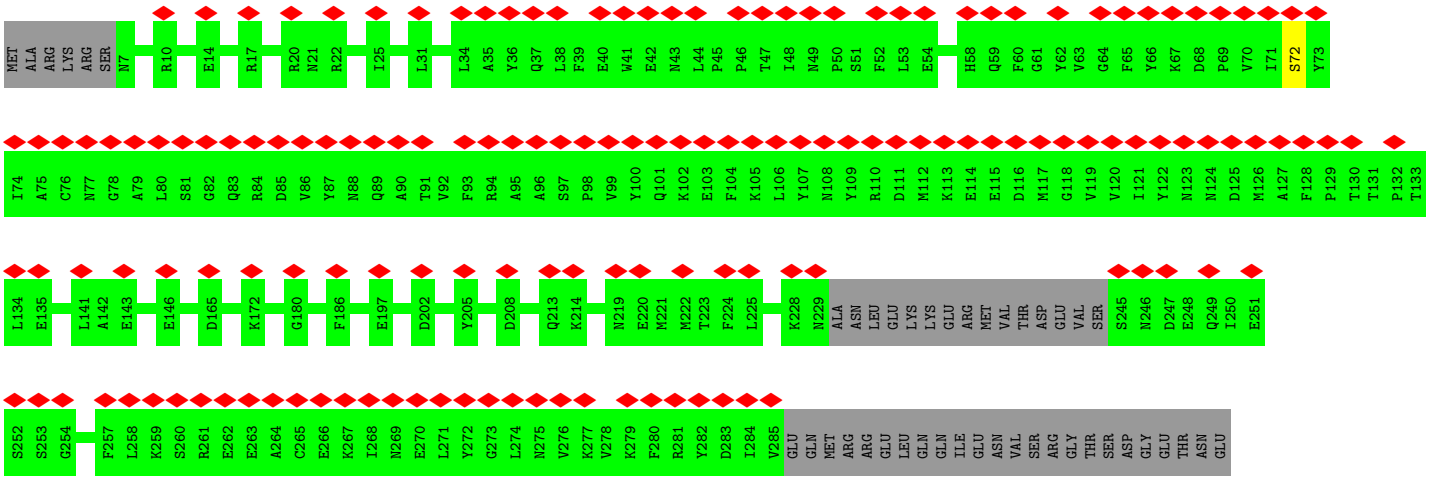
- Molecule 1: Portal protein

Chain 0a:



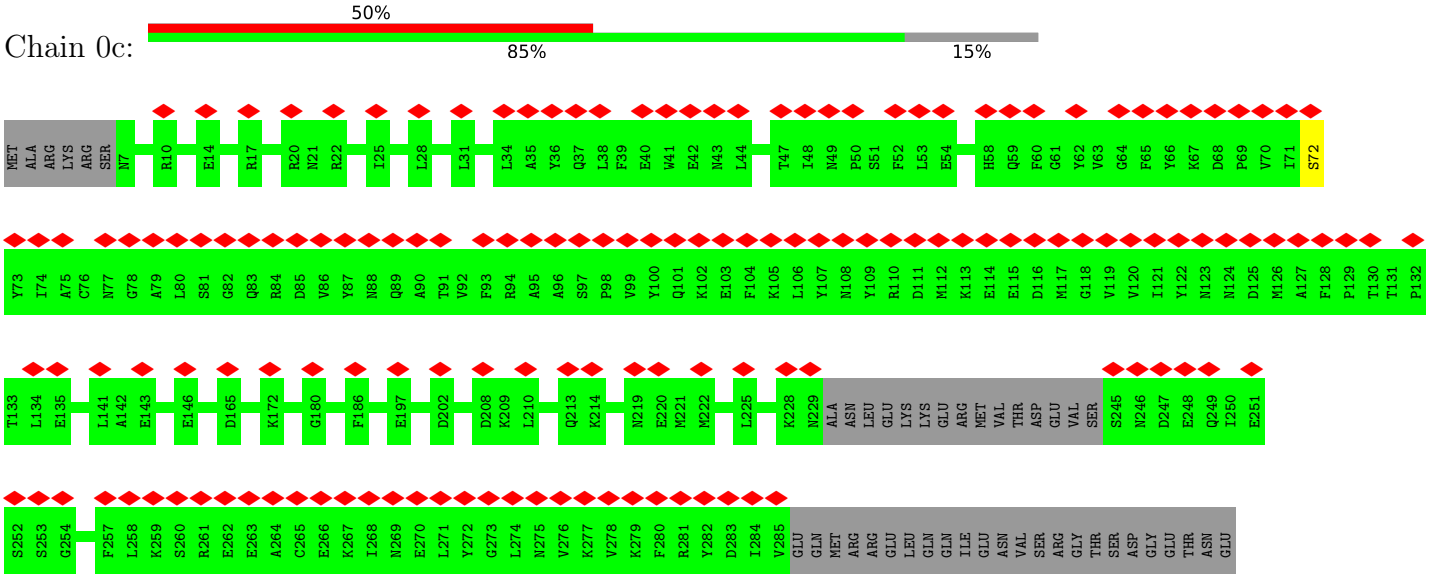
- Molecule 1: Portal protein

Chain 0b:



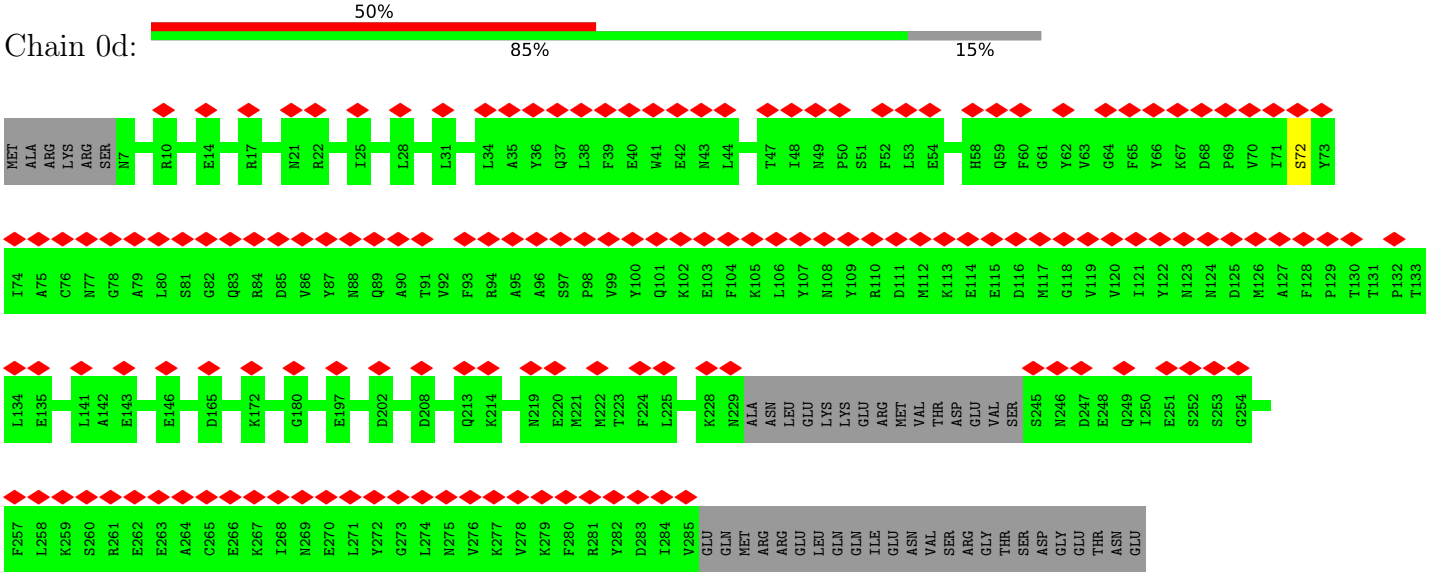
- Molecule 1: Portal protein

Chain 0c:



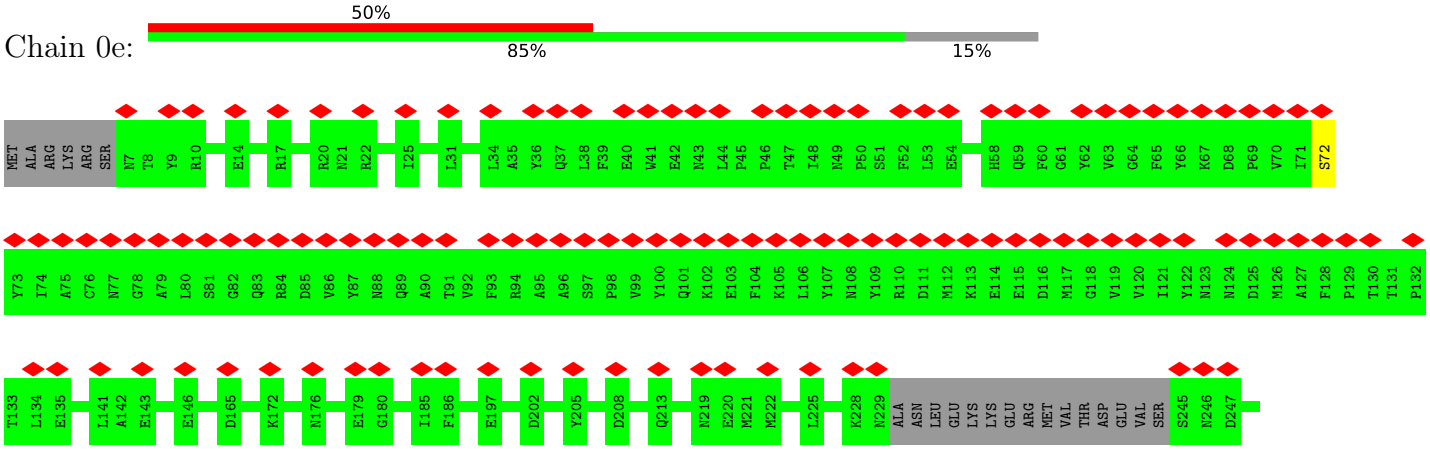
- Molecule 1: Portal protein

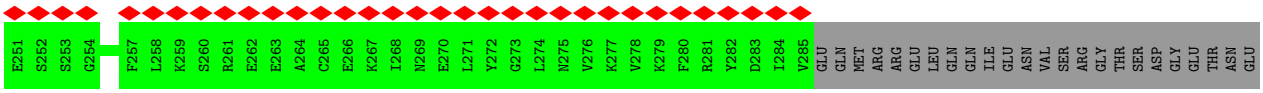
Chain 0d:



- Molecule 1: Portal protein

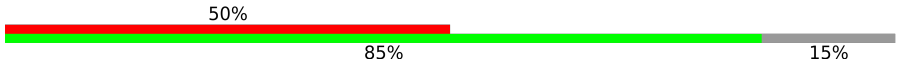
Chain 0e:

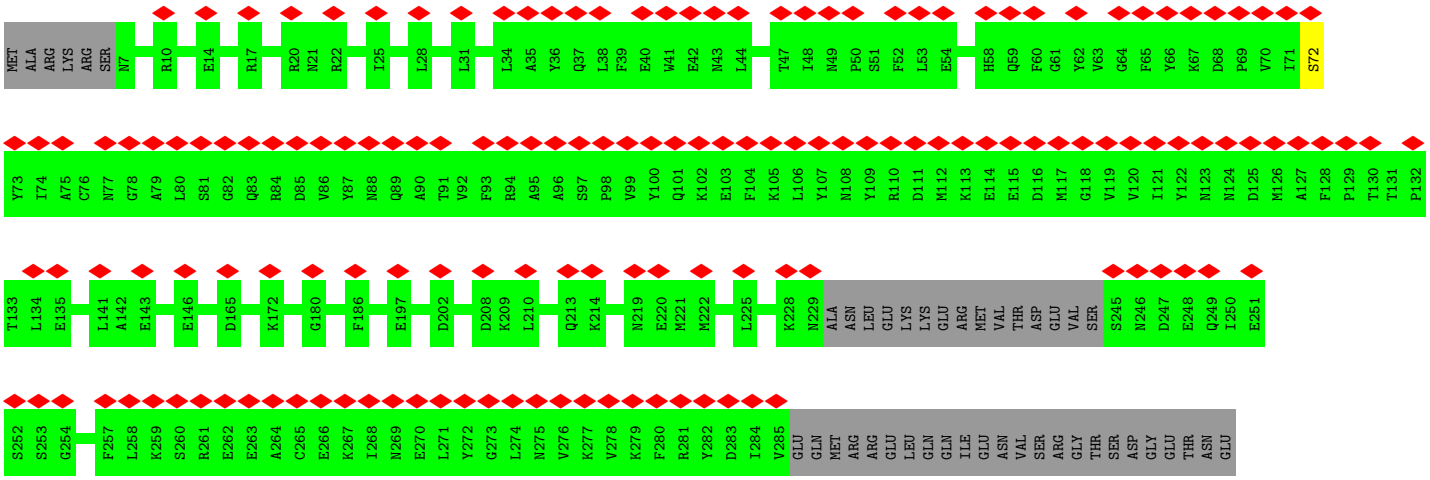




- Molecule 1: Portal protein

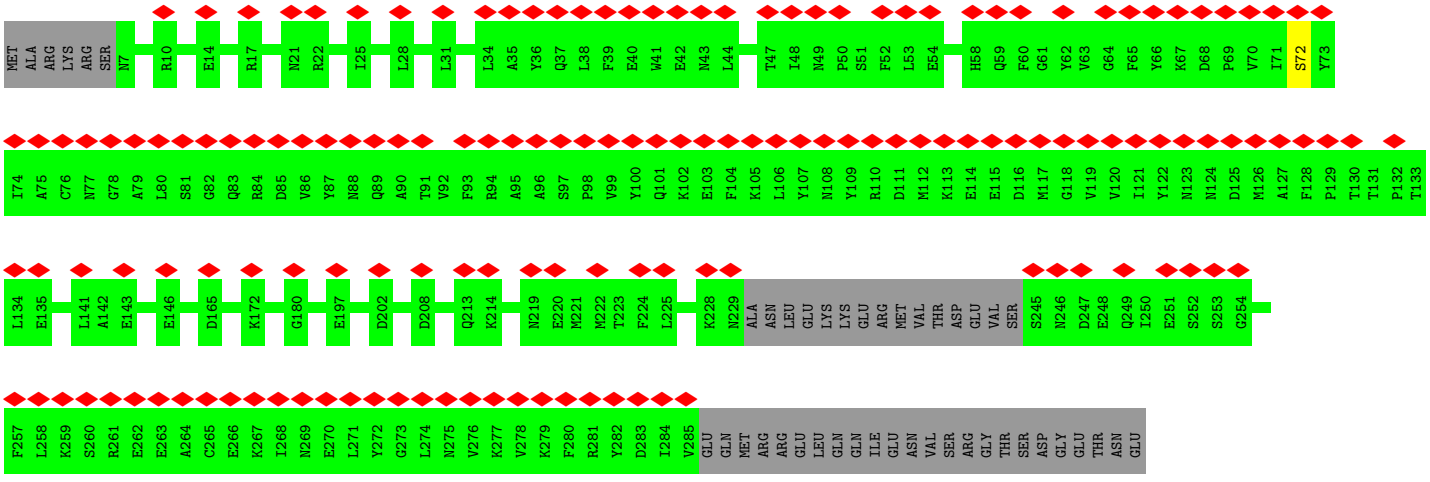
Chain 0f:





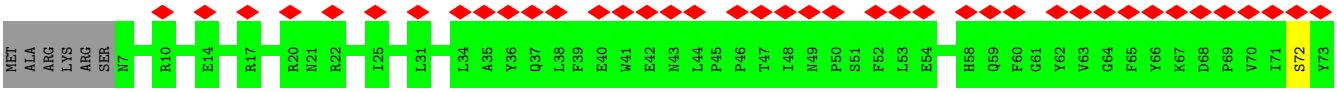
- Molecule 1: Portal protein

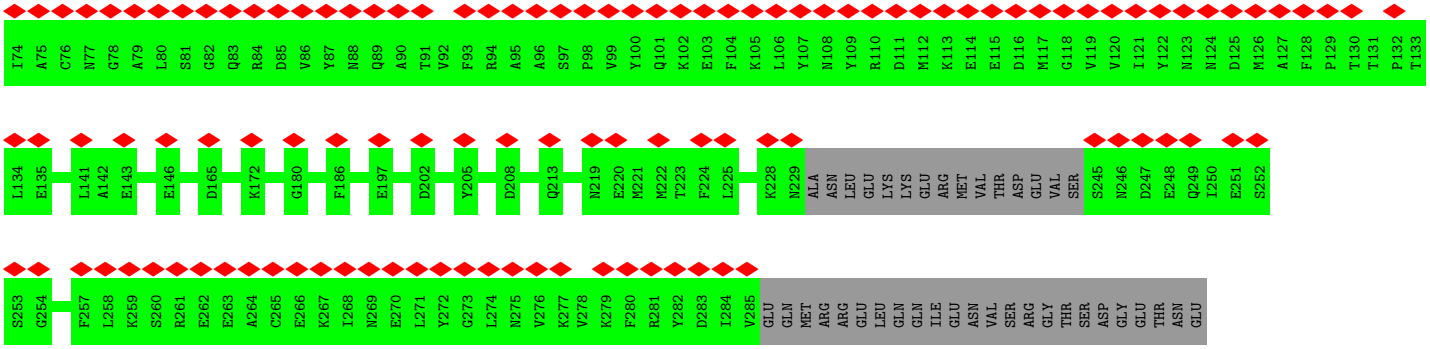
Chain 0g:



- Molecule 1: Portal protein

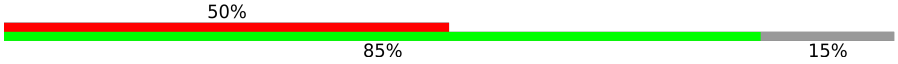
Chain 0h:

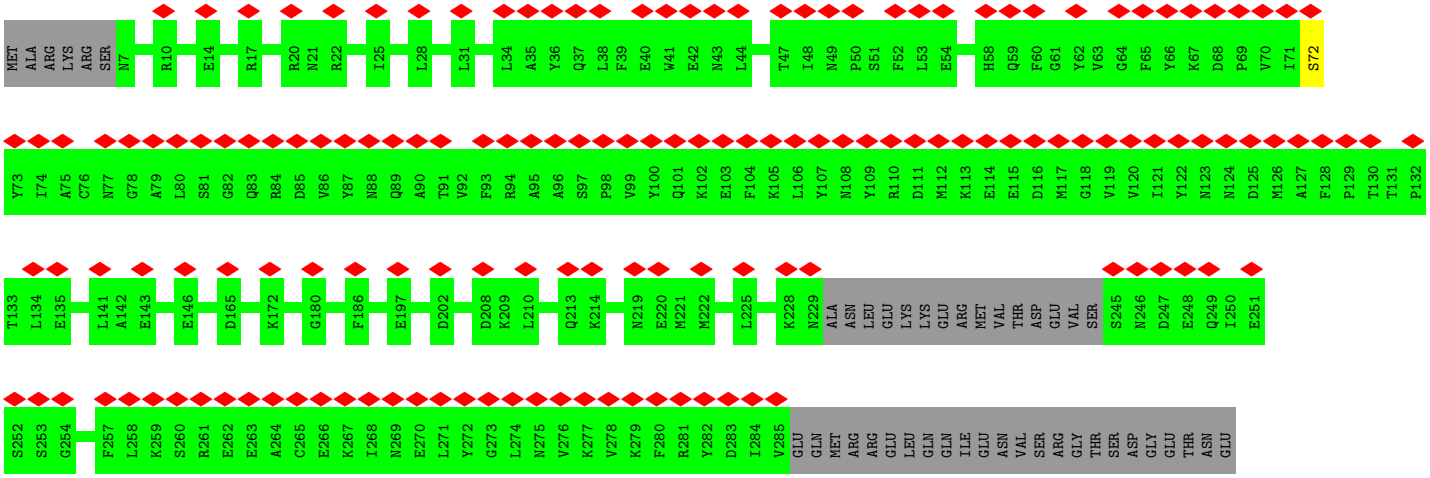




- Molecule 1: Portal protein

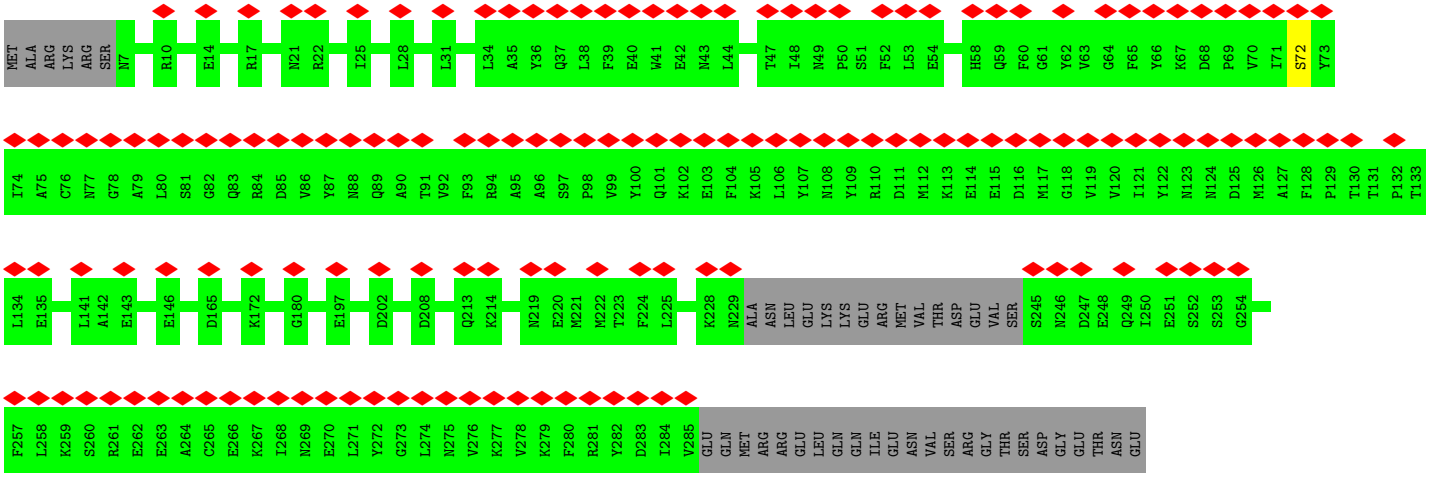
Chain 0i:





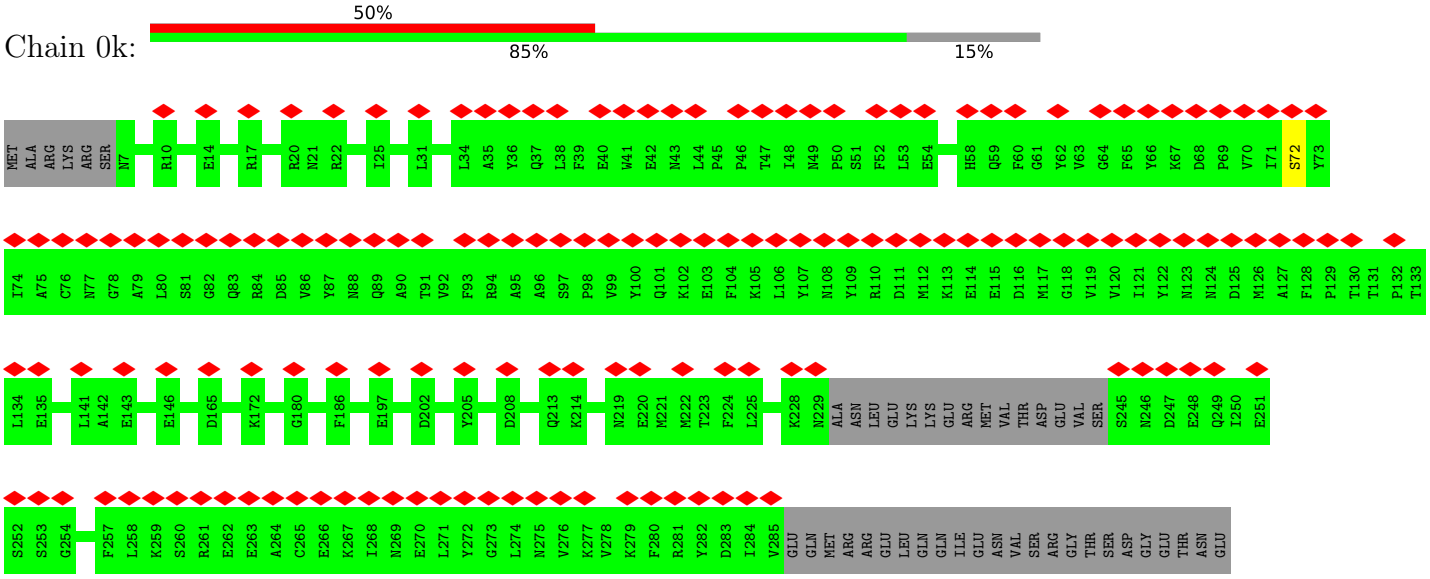
- Molecule 1: Portal protein

Chain 0j:



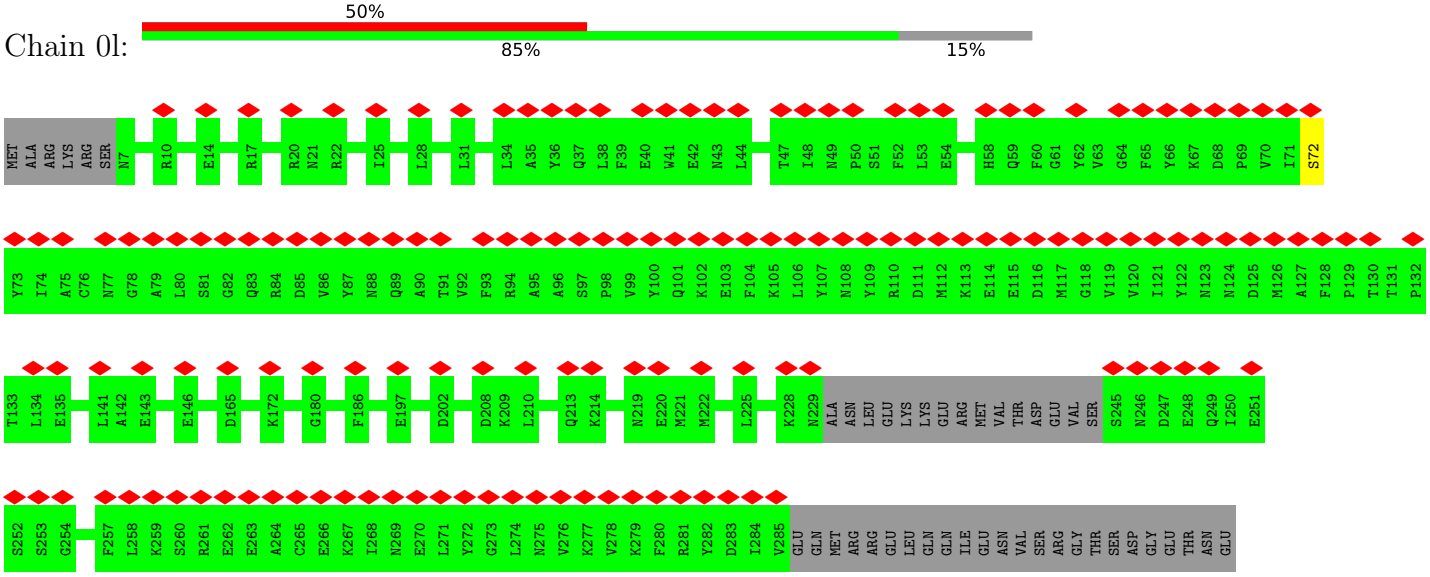
- Molecule 1: Portal protein

Chain 0k:



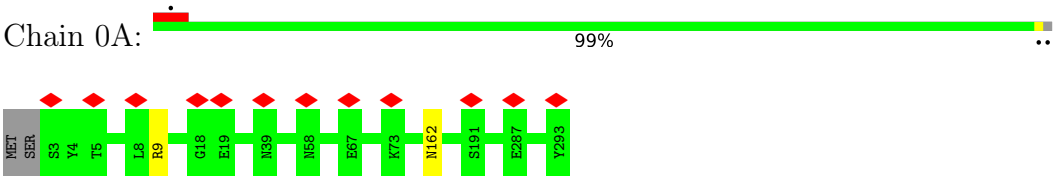
- Molecule 1: Portal protein

Chain 0l:



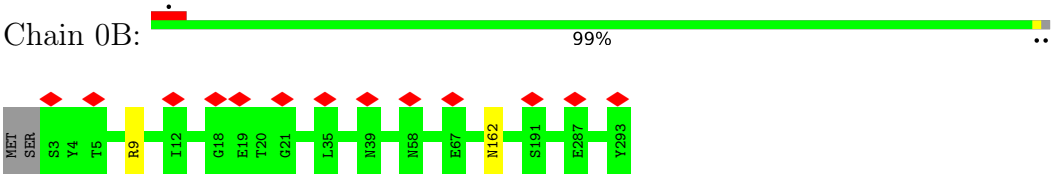
- Molecule 2: Proximal tail tube connector protein

Chain 0A:



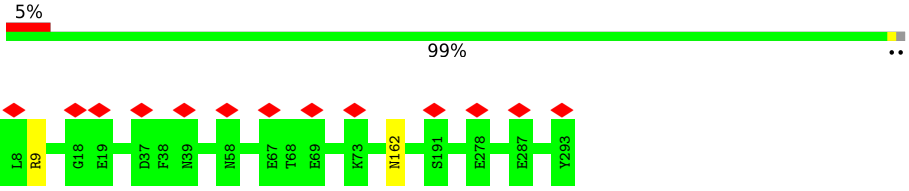
- Molecule 2: Proximal tail tube connector protein

Chain 0B:



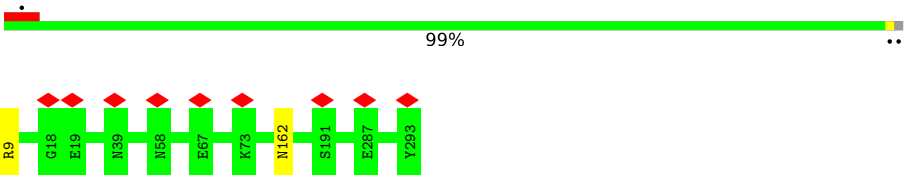
• Molecule 2: Proximal tail tube connector protein

Chain 0C:



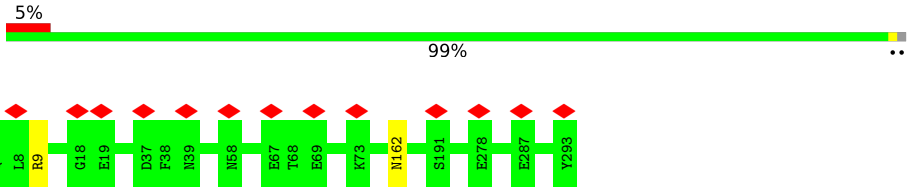
• Molecule 2: Proximal tail tube connector protein

Chain 0D:



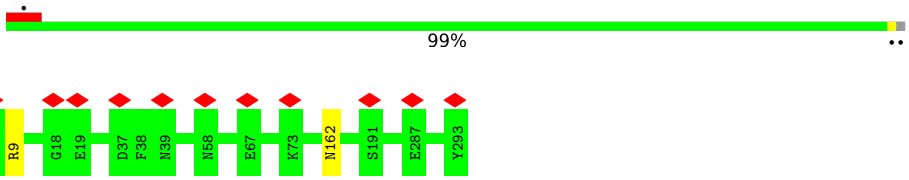
• Molecule 2: Proximal tail tube connector protein

Chain 0E:



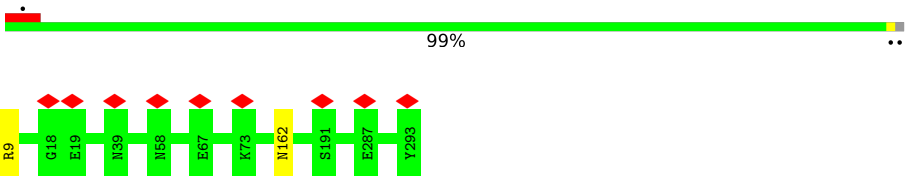
• Molecule 2: Proximal tail tube connector protein

Chain 0F:



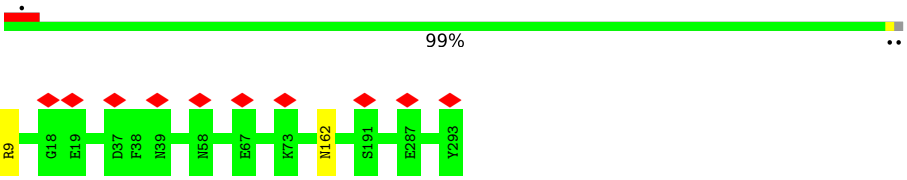
• Molecule 2: Proximal tail tube connector protein

Chain 0G:



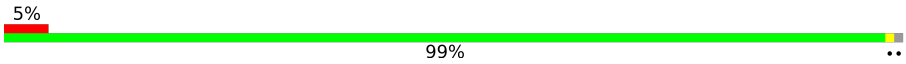
• Molecule 2: Proximal tail tube connector protein

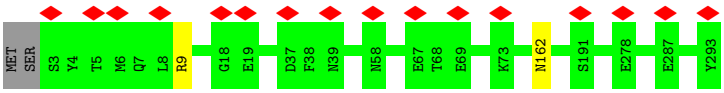
Chain 0H:



• Molecule 2: Proximal tail tube connector protein

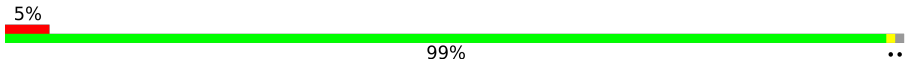
Chain 0I:

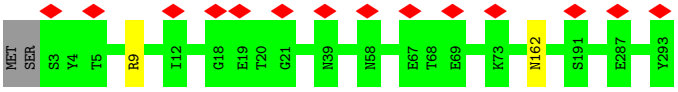




• Molecule 2: Proximal tail tube connector protein

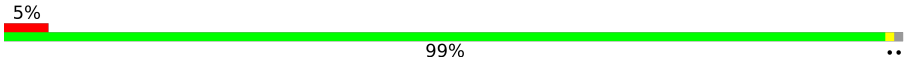
Chain 0J:

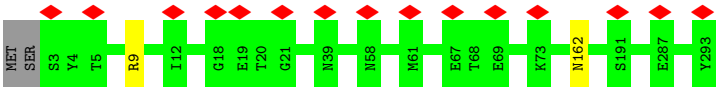




• Molecule 2: Proximal tail tube connector protein

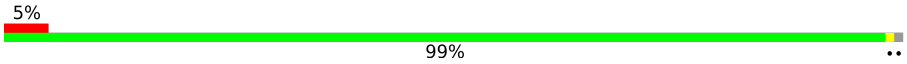
Chain 0K:

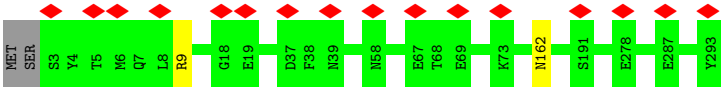




• Molecule 2: Proximal tail tube connector protein

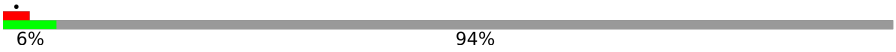
Chain 0L:

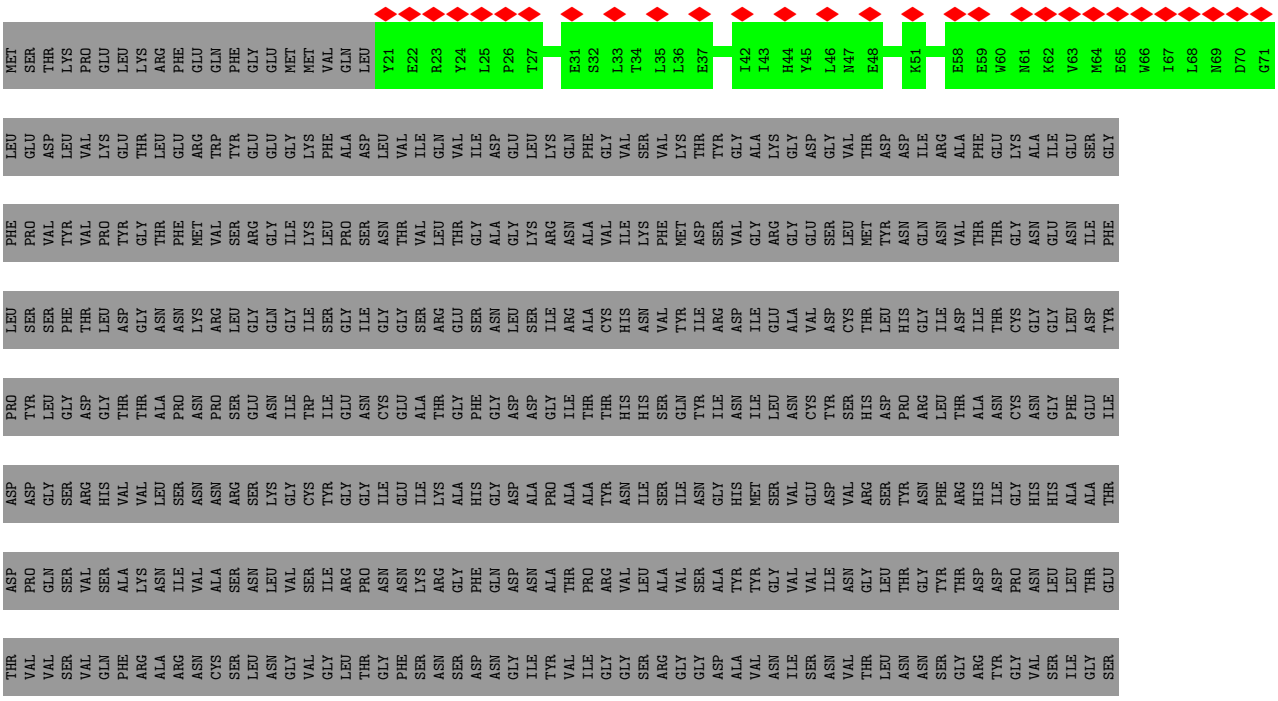




• Molecule 3: Pre-neck appendage protein

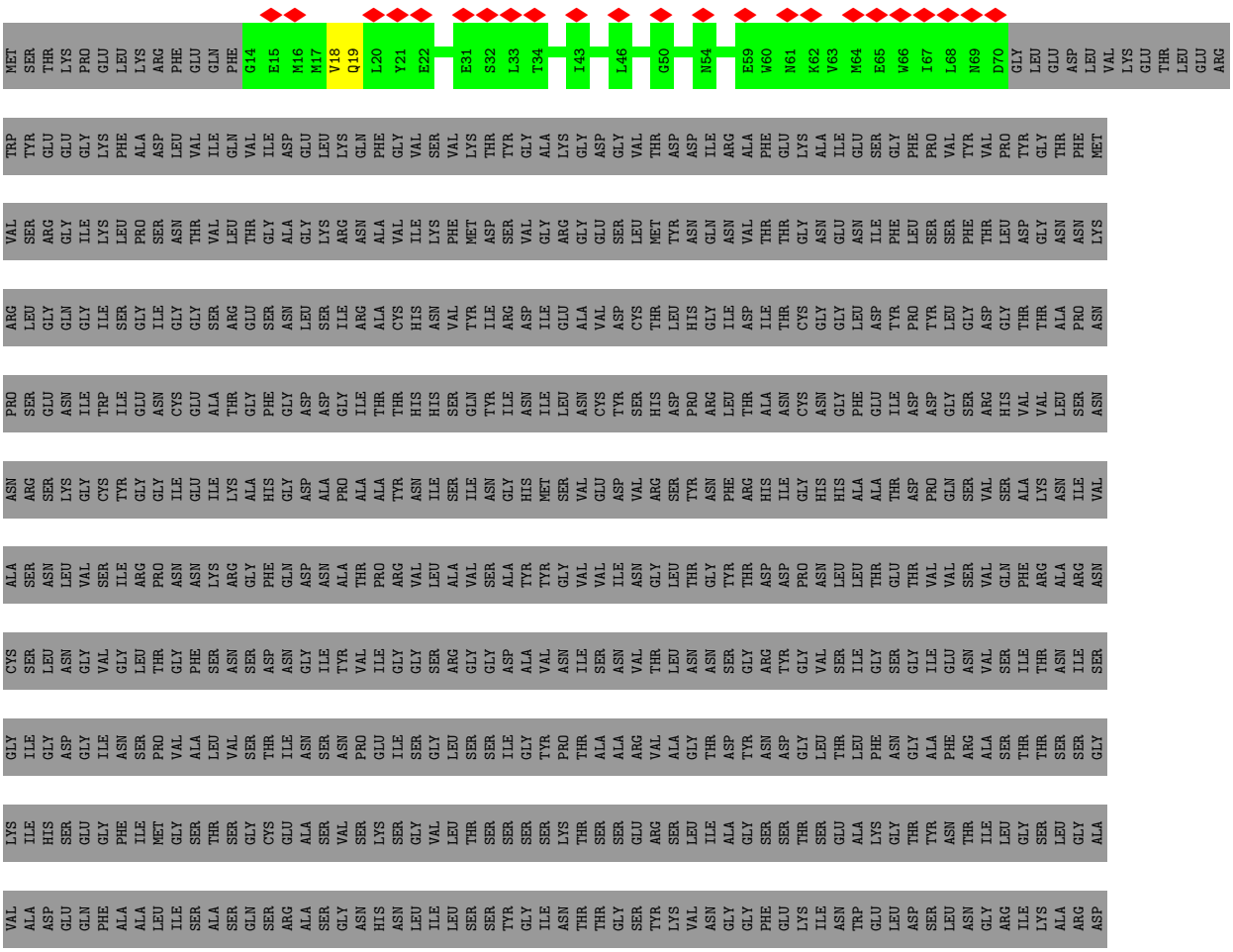
Chain A:

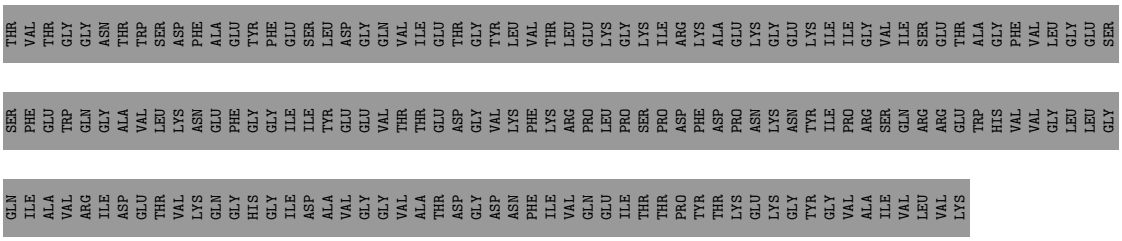




- Molecule 3: Pre-neck appendage protein

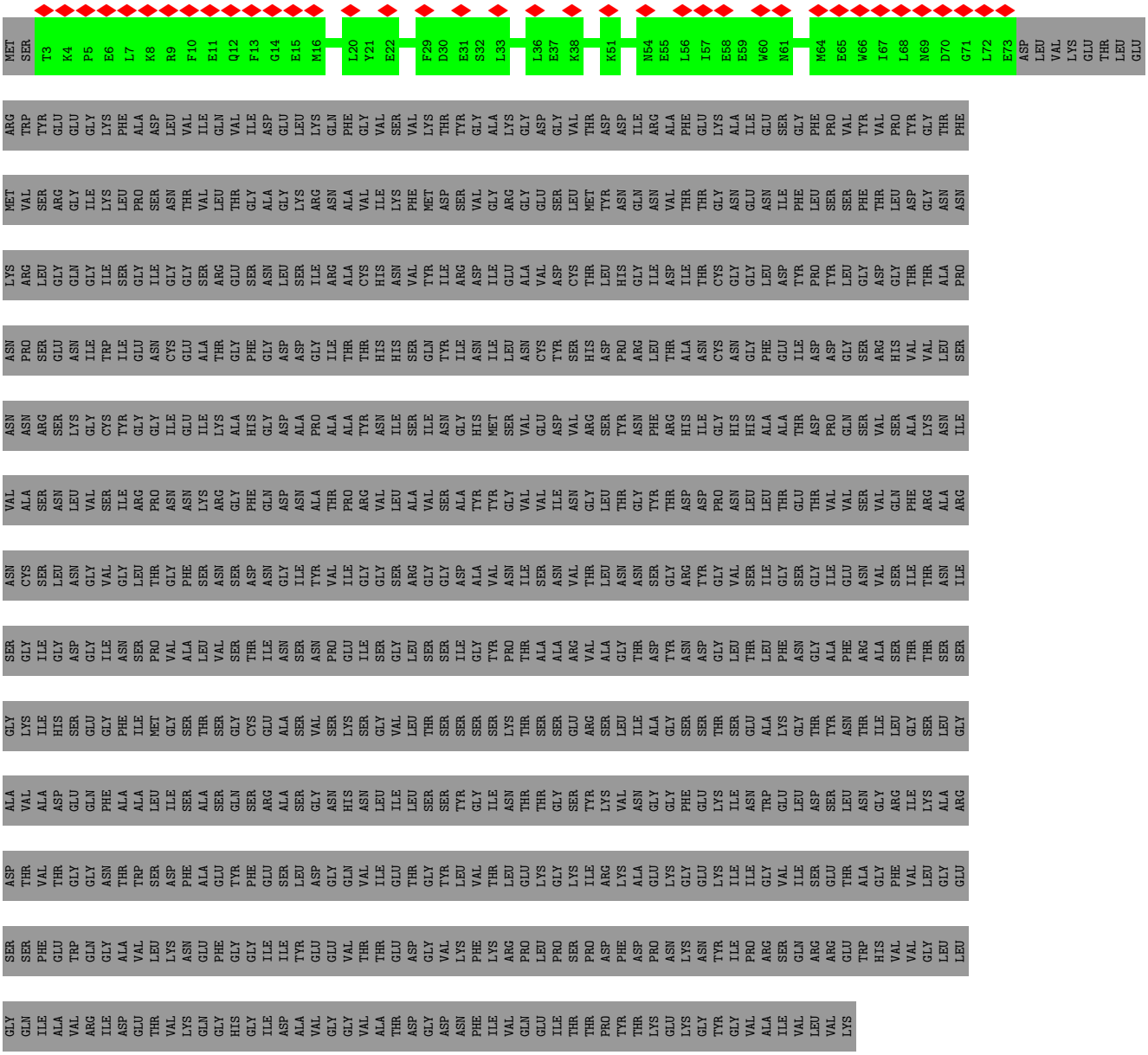
Chain B: 6% 93%





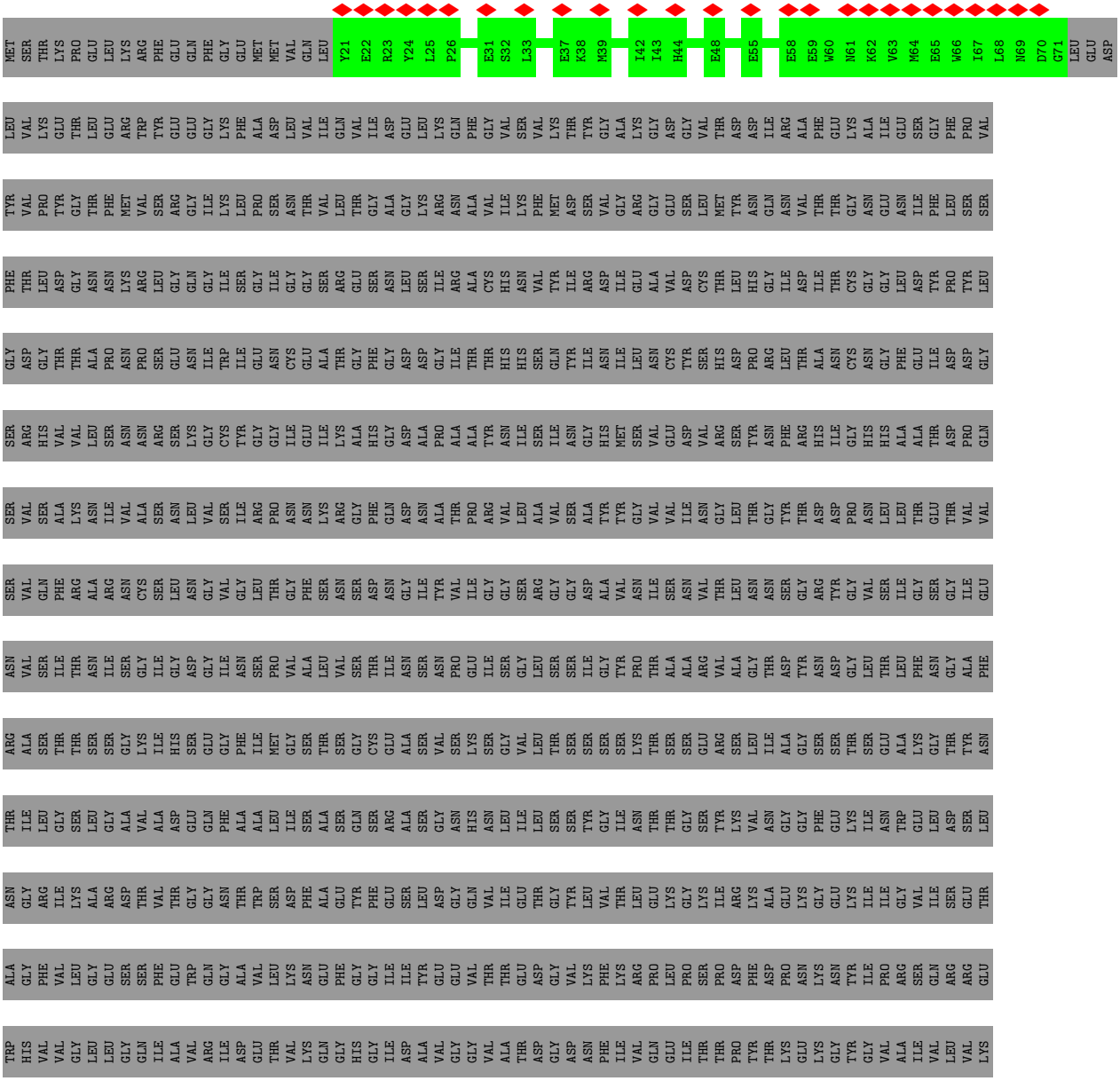
• Molecule 3: Pre-neck appendage protein

Chain C: 8% 92%



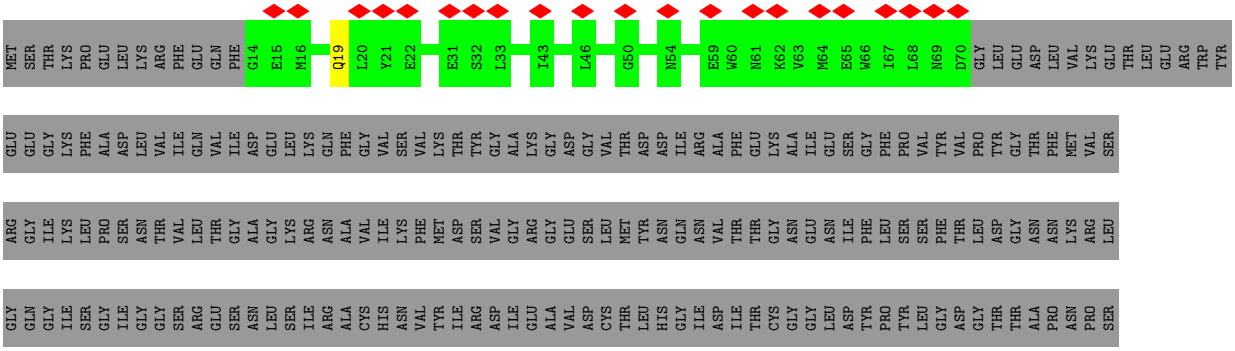
• Molecule 3: Pre-neck appendage protein

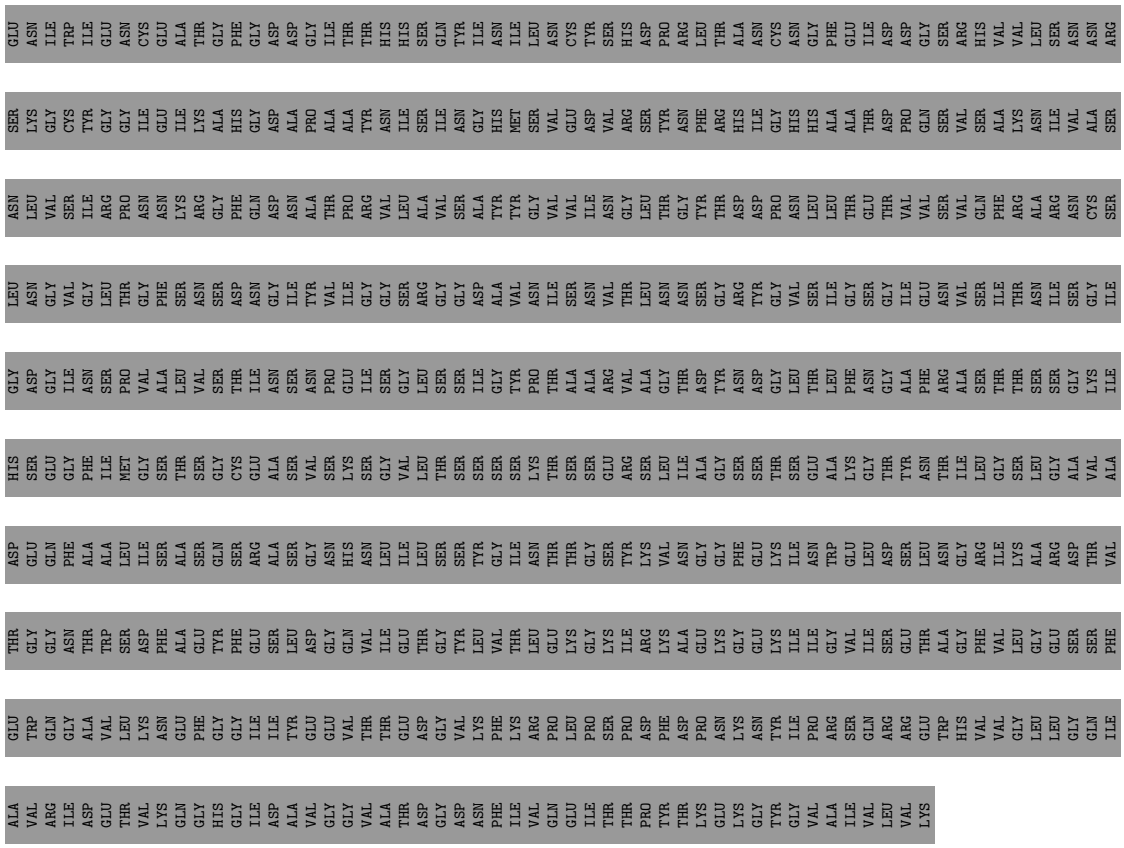
Chain D: 6% 94%



- Molecule 3: Pre-neck appendage protein

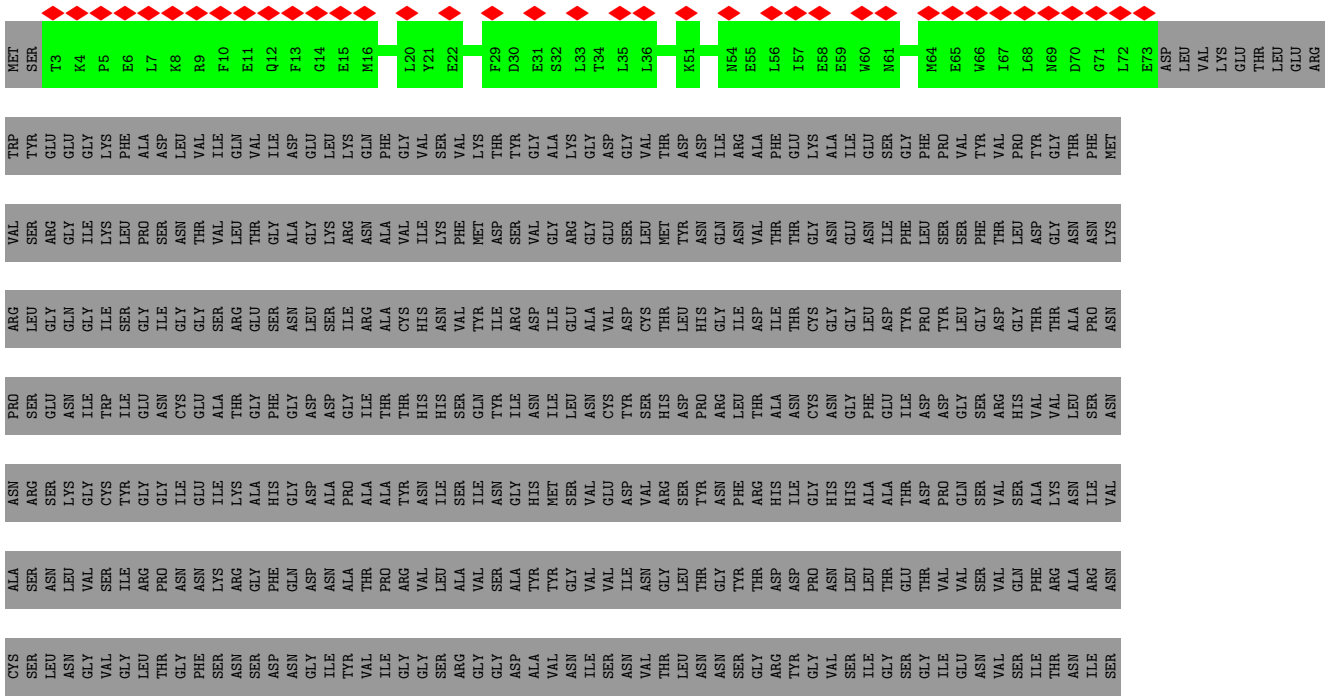
Chain E: 7% 93%

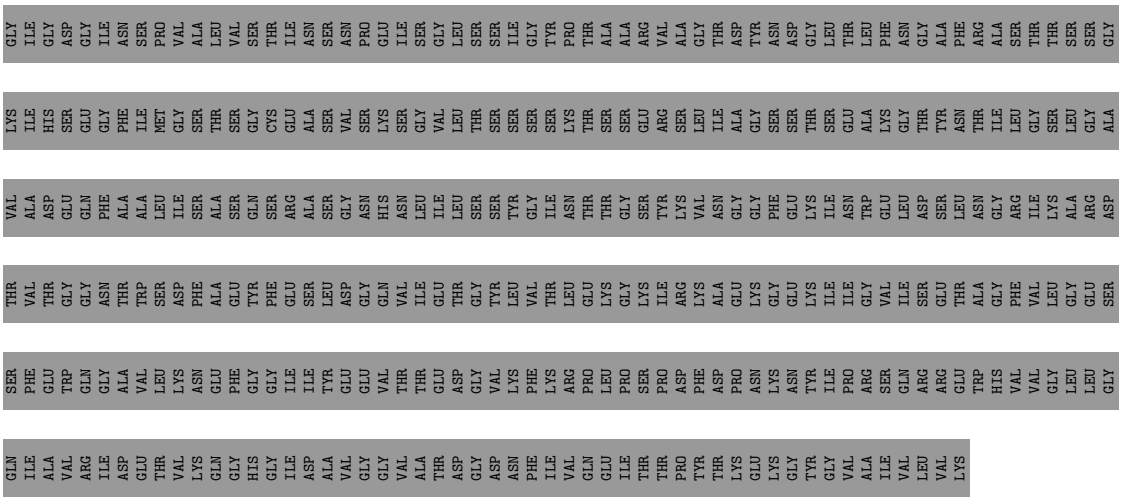




- Molecule 3: Pre-neck appendage protein

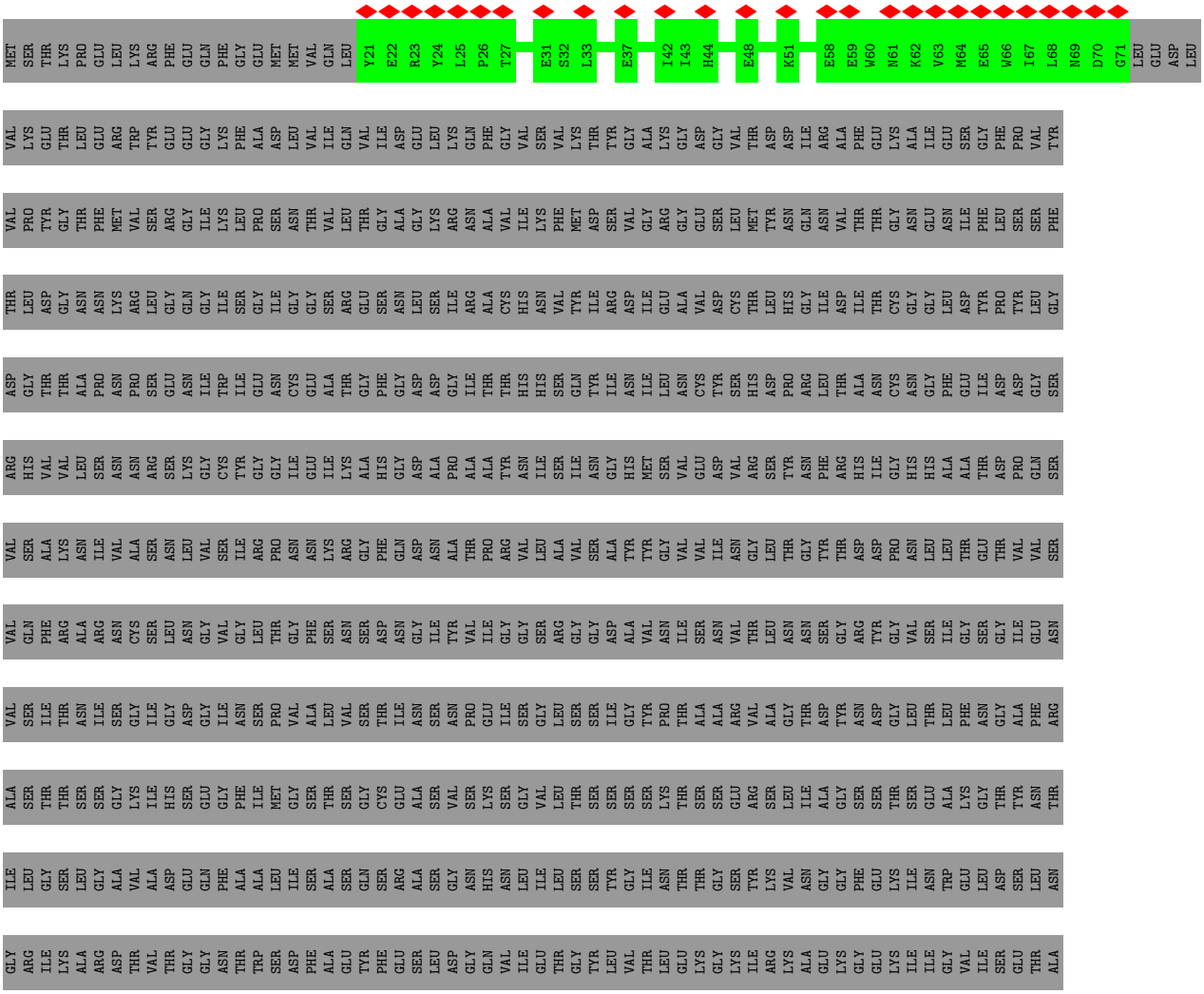
Chain F: 8% 92%

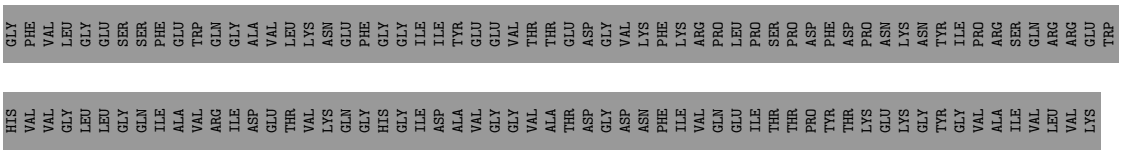




- Molecule 3: Pre-neck appendage protein

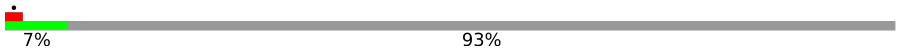
Chain G: 6% 94%

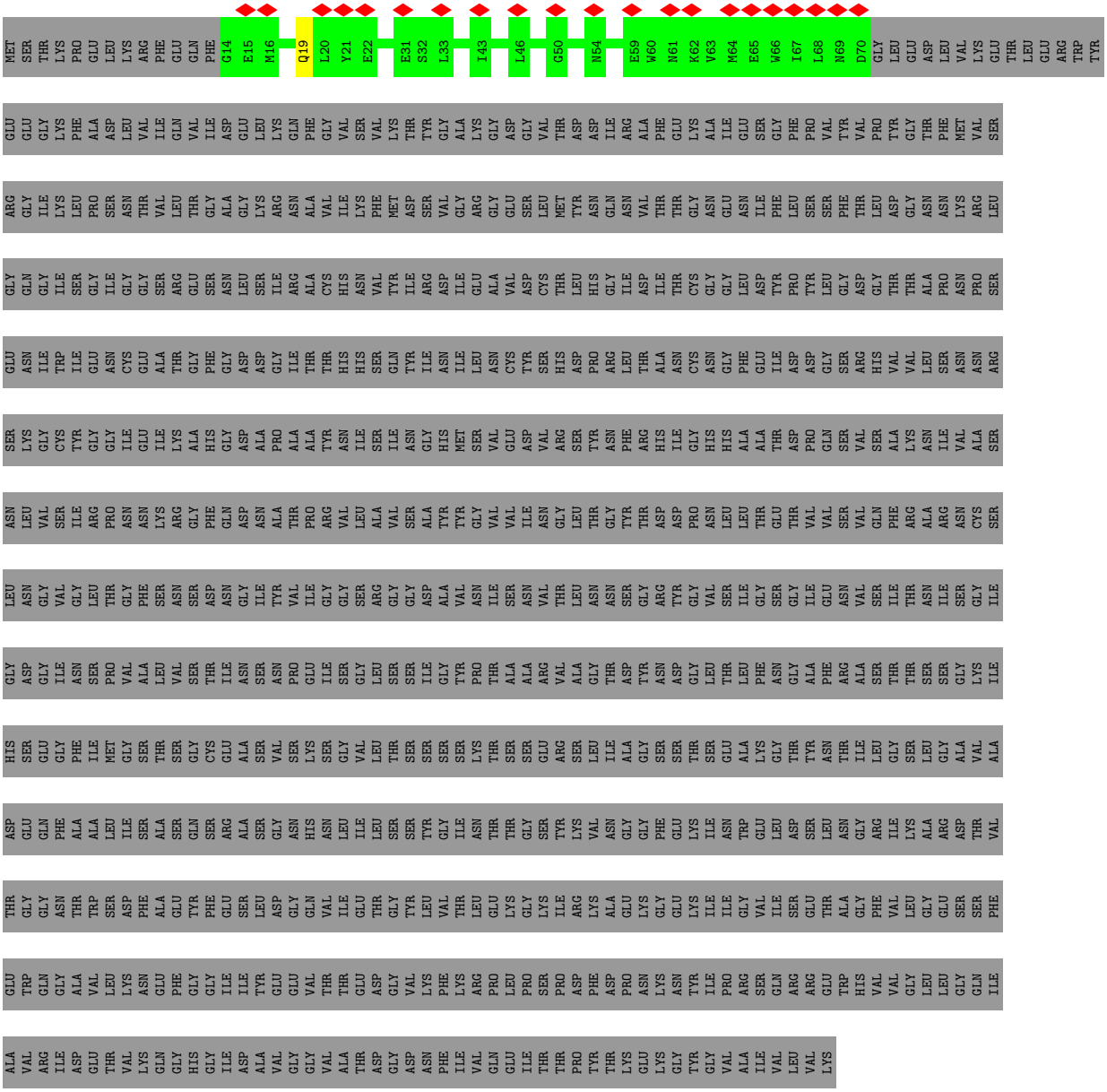




• Molecule 3: Pre-neck appendage protein

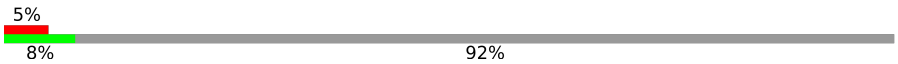
Chain H:

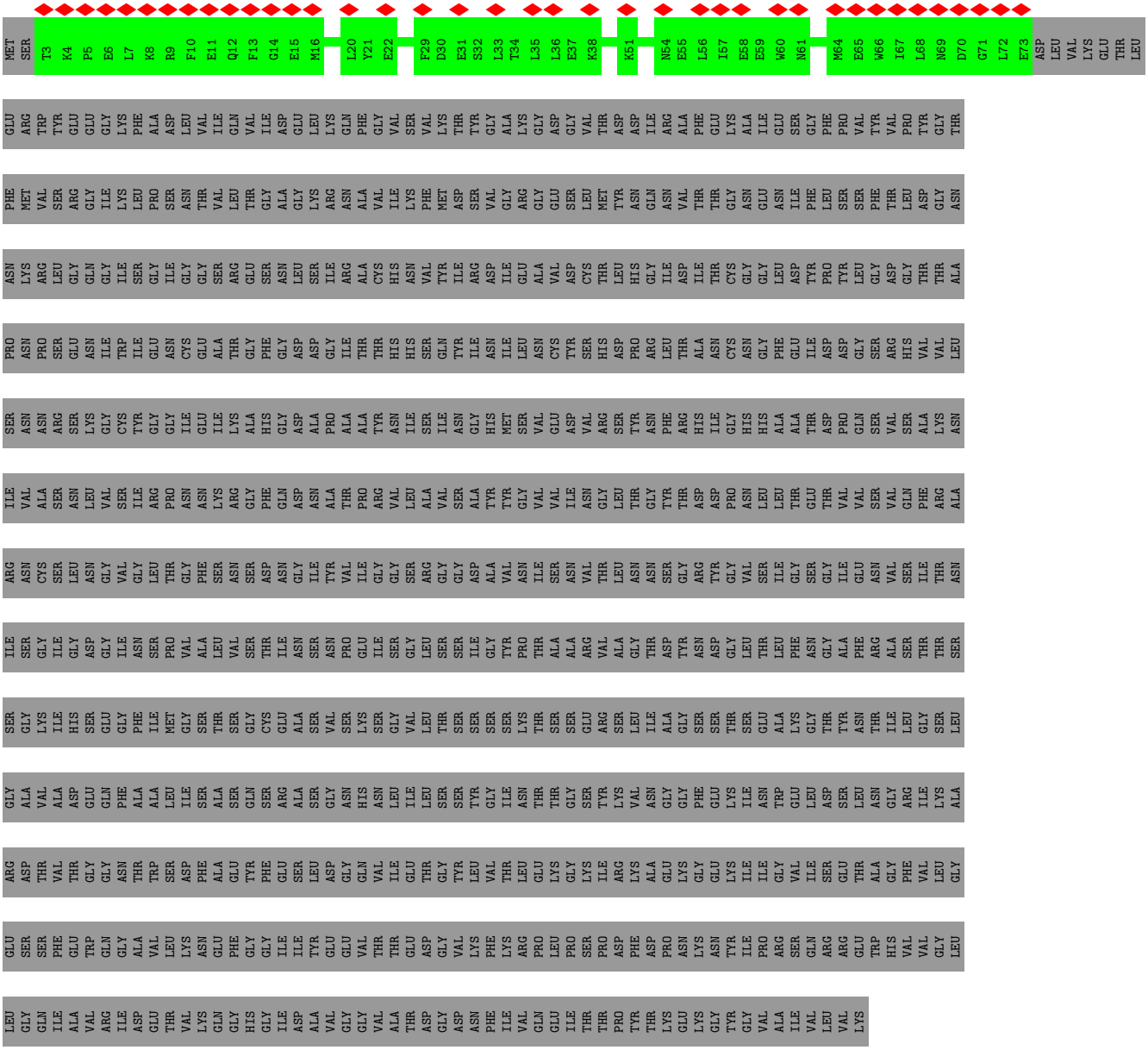




• Molecule 3: Pre-neck appendage protein

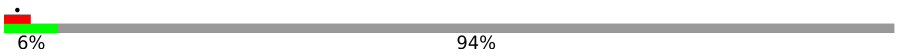
Chain I:

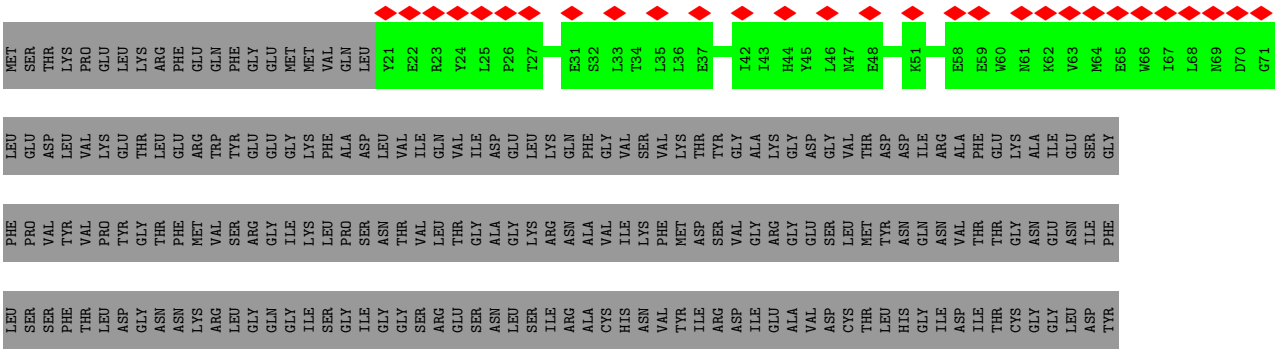




- Molecule 3: Pre-neck appendage protein

Chain J:





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

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

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

THR VAL VAL SER VAL GLN PHE ARG ALA ARG ASN CYS SER LEU ASN GLY VAL GLY LEU THR GLY PHE SER ASN SER ASP ASN GLY ILE TYR VAL ILE GLY GLY SER ARG GLY GLY ASP ALA VAL ASN ILE SER SER ASN VAL THR LEU ASN ASN SER GLY ARG TYR GLY VAL SER ILE GLY

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

GLY ALA PHE ARG ALA SER THR THR SER SER GLY LYS ILE HIS SER GLU GLY PHE ILE MET GLY SER THR SER GLY CYS GLU ALA SER VAL SER LYS THR SER SER SER GLU ARG VAL ALA GLY THR SER THR SER SER GLU ALA LYS GLY

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

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

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

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

LEU VAL LYS

- Molecule 3: Pre-neck appendage protein

Chain K: 7% 93%

MET SER THR LYS PRO GLU LEU LYS ARG PHE GLU GLN PHE G14 E15 M16 Q19 L20 Y21 E22 E31 S32 L33 T34 I43 L46 G50 N54 E59 W60 N61 K62 V63 M64 E65 W66 I67 L68 N69 D70 GLY LEU GLU ASP LEU VAL LYS GLU THR LEU GLU ARG TRP

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

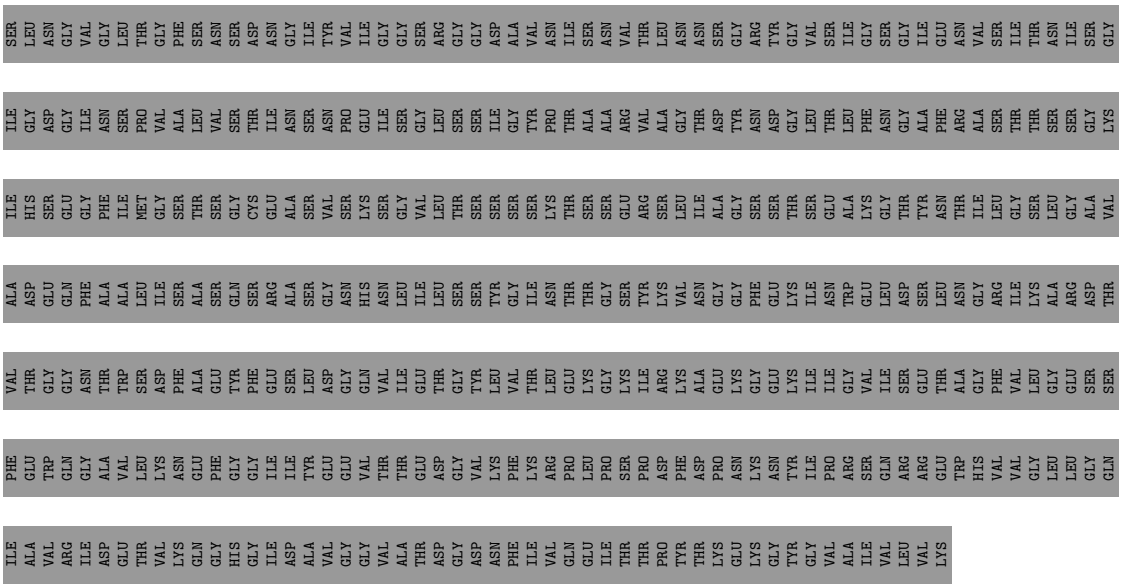
SER ARG GLY ILE LYS LEU PRO SER ASN THR VAL LEU THR GLY ALA GLY LYS ARG ASN ALA VAL ILE LYS PHE MET ASP SER VAL GLY ARG GLY GLU SER LEU MET TYR ASN GLN ASN VAL THR THR GLY ASN GLU ASN ILE PHE LEU SER SER PHE THR LEU ASP GLY ASN ASN LYS ARG

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

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

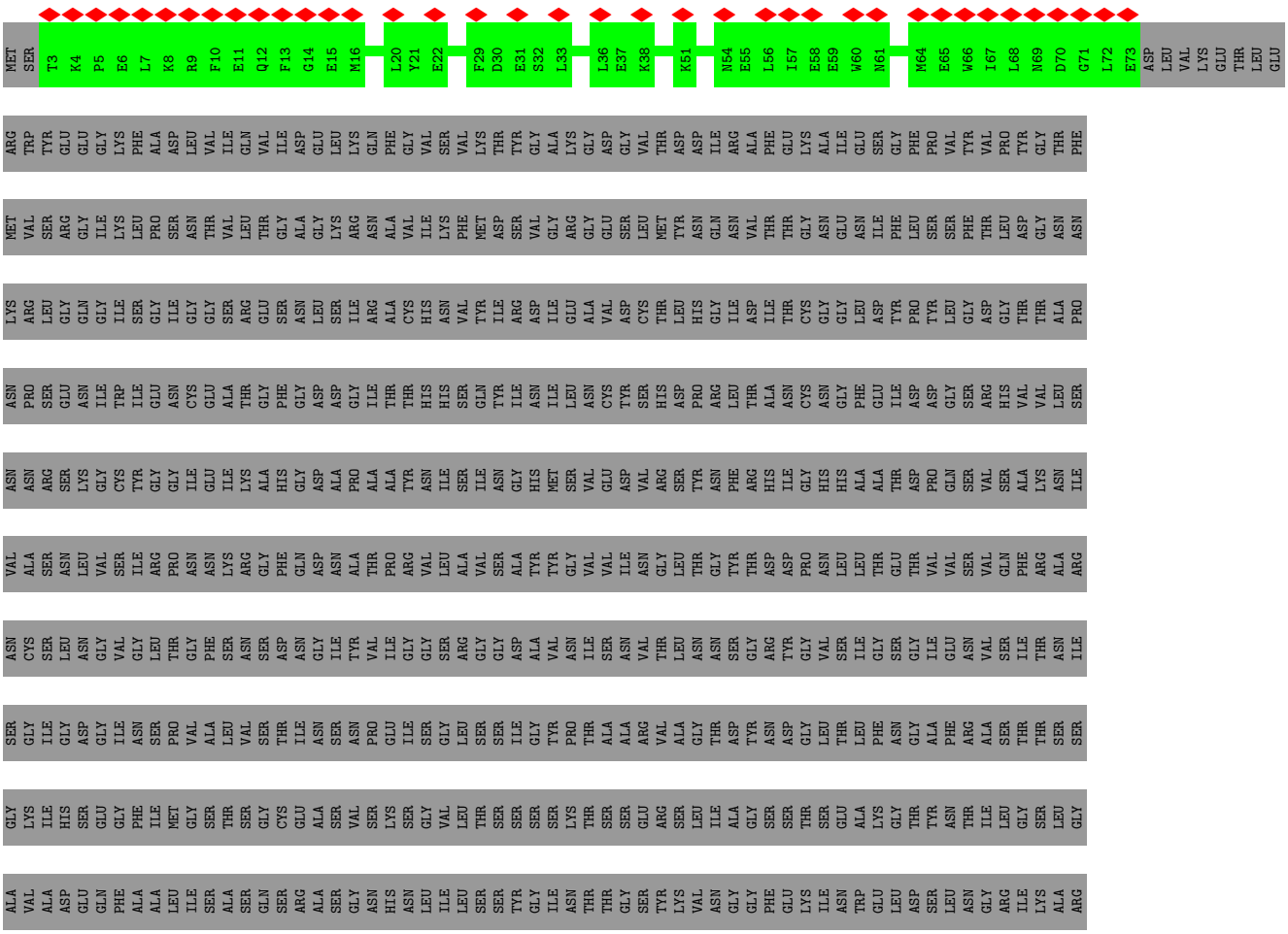
ARG SER LYS GLY CYS TYR GLY GLY ILE GLU ILE LYS ALA HIS GLY ASP ALA PRO ALA TYR ASN ILE SER ILE ASN GLY HIS MET SER VAL GLU ASP VAL ARG SER TYR ASN PHE ARG HIS ILE GLY HIS HIS ALA ALA THR ASP PRO GLN SER VAL SER ALA LYS ASN ILE LEU VAL ALA

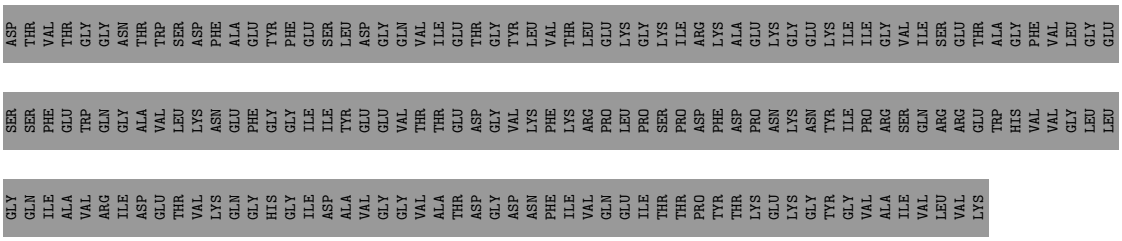
SER ASN LEU VAL SER ILE ARG PRO ASN ASN LYS ARG GLY PHE GLN ASP ASN ALA THR PRO ARG VAL LEU ALA VAL SER ALA TYR TYR GLY VAL VAL ILE ASN GLY LEU THR GLY TYR THR ASP ASP PRO ASN LEU LEU THR GLU THR VAL VAL SER VAL GLN PHE ARG ALA ARG ASN CYS



- Molecule 3: Pre-neck appendage protein

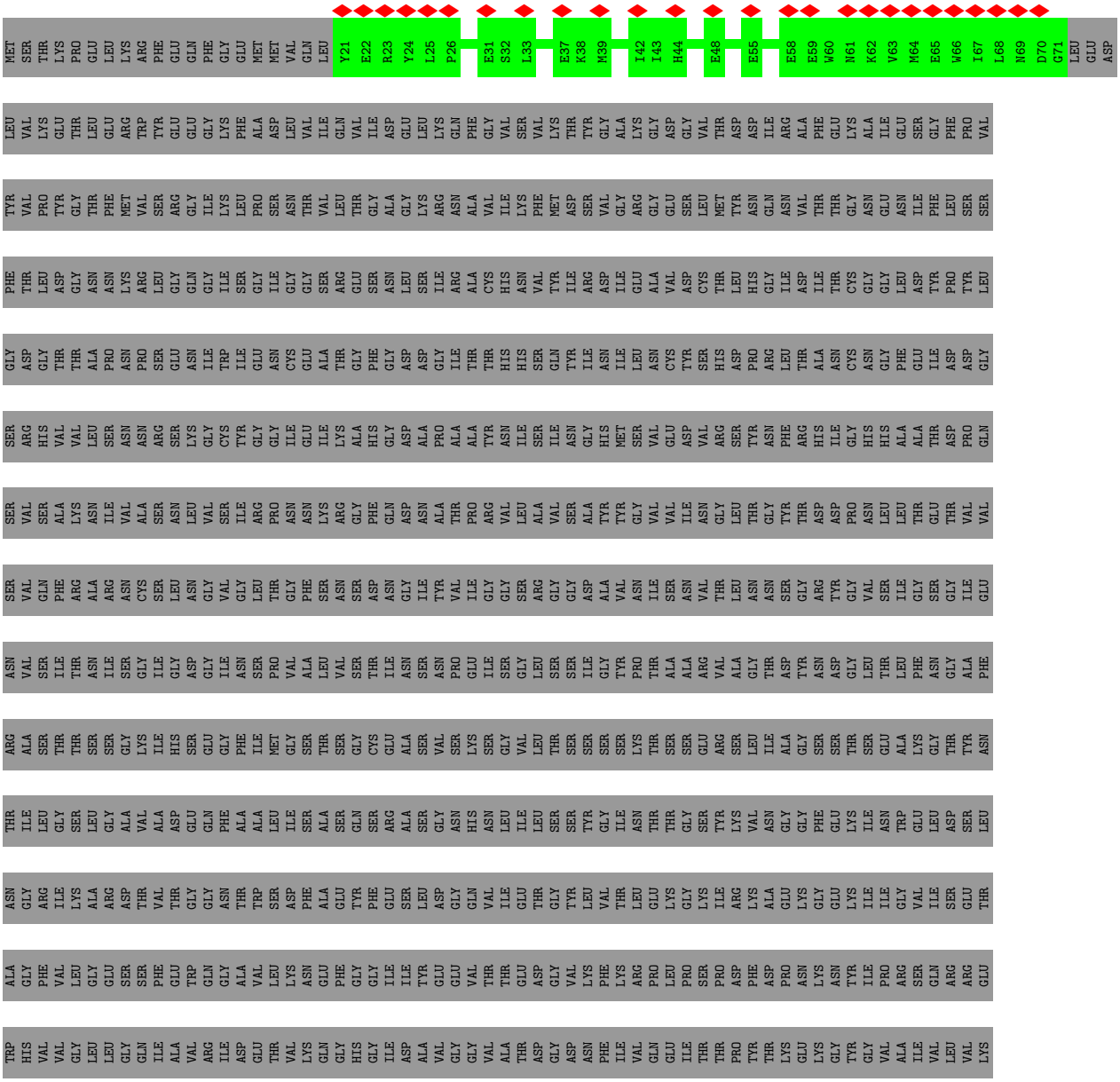
Chain L: 8% 92%





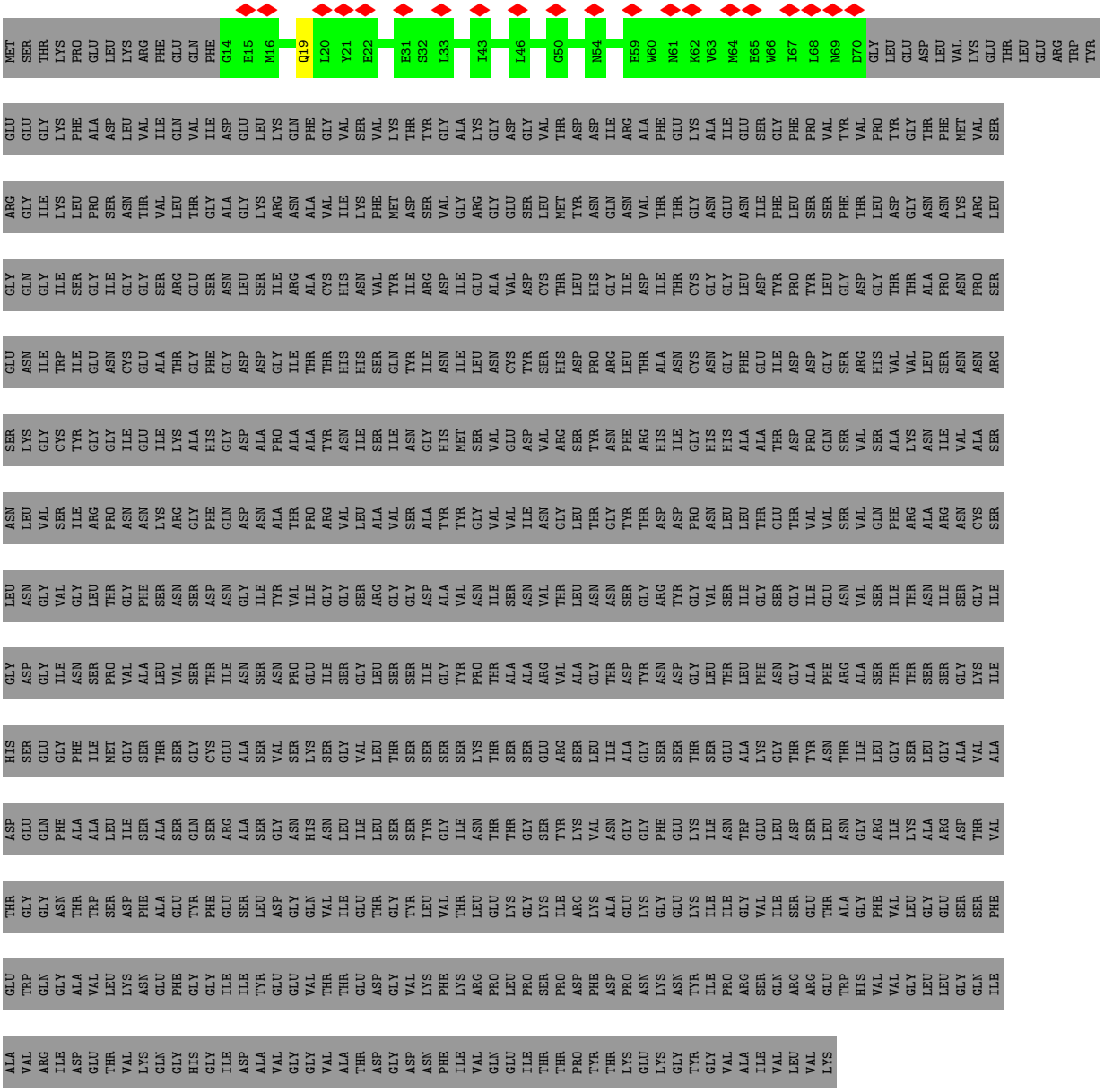
• Molecule 3: Pre-neck appendage protein

Chain M: 6% 94%



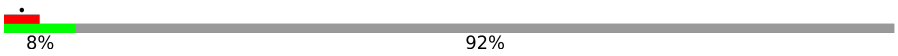
• Molecule 3: Pre-neck appendage protein

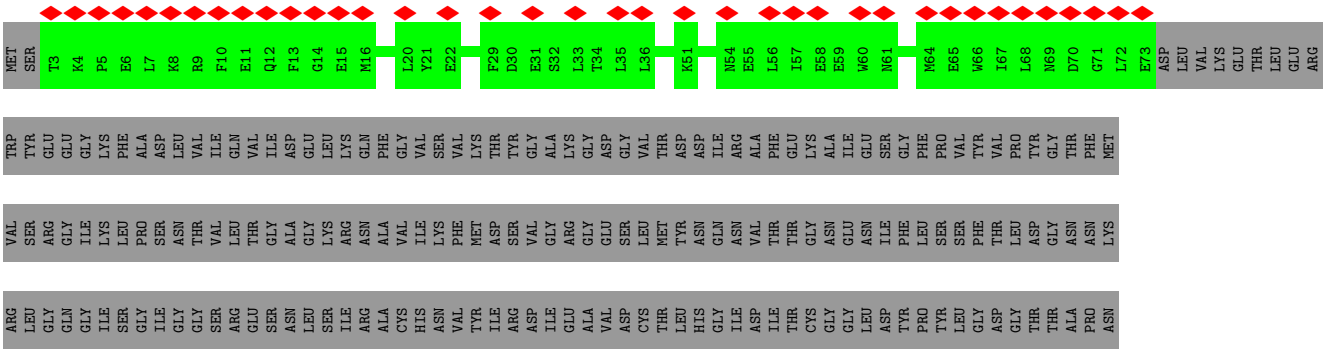
Chain N: 7% 93%



- Molecule 3: Pre-neck appendage protein

Chain O:





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

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

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

CYS SER LEU ASN GLY VAL GLY LEU THR GLY PHE SER ASN SER ASP ASN GLY ILE TYR VAL ILE GLY GLY SER ARG GLY GLY ASP ALA VAL ASN VAL THR LEU ASN ASN SER GLY ARG TYR GLY VAL SER ILE GLY SER GLY ILE GLU ASN VAL SER ILE THR ASN SER

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

LYS ILE HIS SER GLU GLY PHE ILE MET GLY SER THR SER GLY CYS GLU ALA SER VAL SER LYS SER GLY VAL LEU THR SER SER SER LYS THR SER SER GLU GLU ARG SER LEU ILE ALA GLY SER SER THR SER GLU ALA LYS GLY THR ASN THR ILE LEU GLY SER LEU GLY ALA

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

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

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

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

• Molecule 3: Pre-neck appendage protein

Chain P: 6% 94%

MET SER THR LYS PRO GLU LEU LYS ARG PHE GLU GLN PHE GLY GLU MET MET VAL GLN LEU Y21 E22 R23 Y24 L25 P26 T27 E31 S32 L33 E37 I42 I43 H44 E48 K51 E58 E59 W60 N61 K62 V63 M64 E65 W66 I67 L68 N69 D70 G71 LEU GLU ASP LEU

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

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

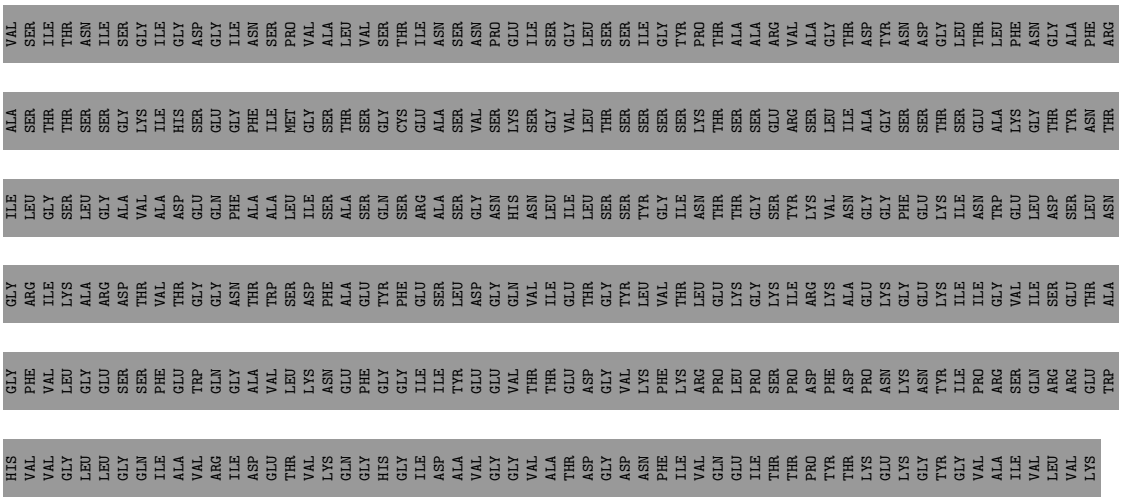
THR LEU ASP GLY ASN ASN LYS ARG LEU GLY GLN GLY ILE SER GLY ILE GLY GLY SER ARG GLU SER ASN LEU SER ILE ARG ALA CYS HIS ASN VAL TYR ILE ARG ASP ILE GLU ALA VAL ASP CYS THR LEU HIS GLY ILE ASP ILE THR CYS GLY GLY LEU ASP TYR PRO TYR LEU GLY

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

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

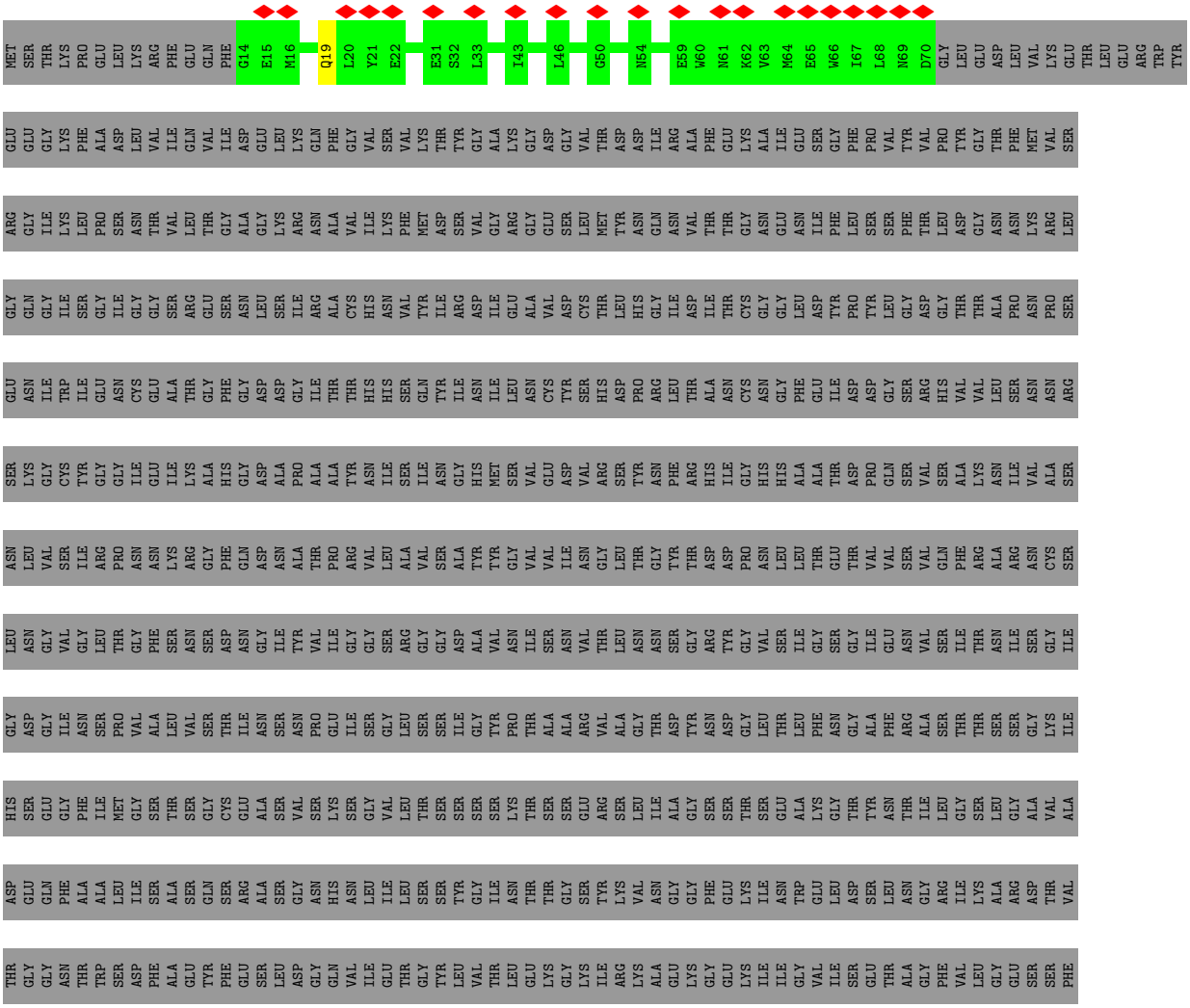
VAL SER ALA LYS ASN ILE VAL SER ASN LEU VAL SER ILE ARG PRO ASN ASN LYS ARG GLY PHE GLN ASP ASN ALA THR PRO ARG VAL LEU ALA VAL SER ALA TYR TYR GLY VAL VAL ILE ASN GLY LEU THR GLY TYR THR ASP ASP PRO ASN LEU LEU THR GLU THR VAL SER

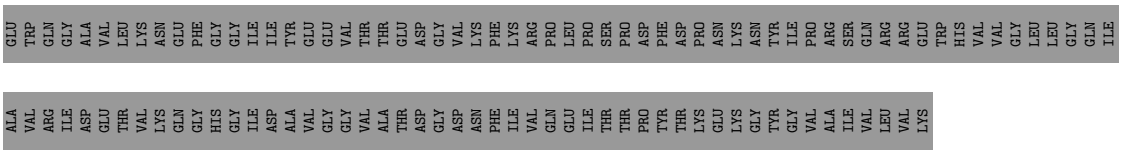
VAL GLN PHE ARG ALA ARG ASN CYS SER LEU ASN GLY VAL GLY ILE TYR VAL ILE GLY GLY SER ARG GLY GLY ASP ALA VAL ALA ASN VAL THR LEU ASN ASN SER GLY ARG TYR GLY VAL SER ILE GLY SER GLY ILE GLU ASN



- Molecule 3: Pre-neck appendage protein

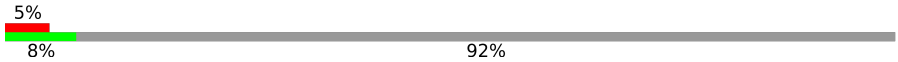
Chain Q: 7% 93%

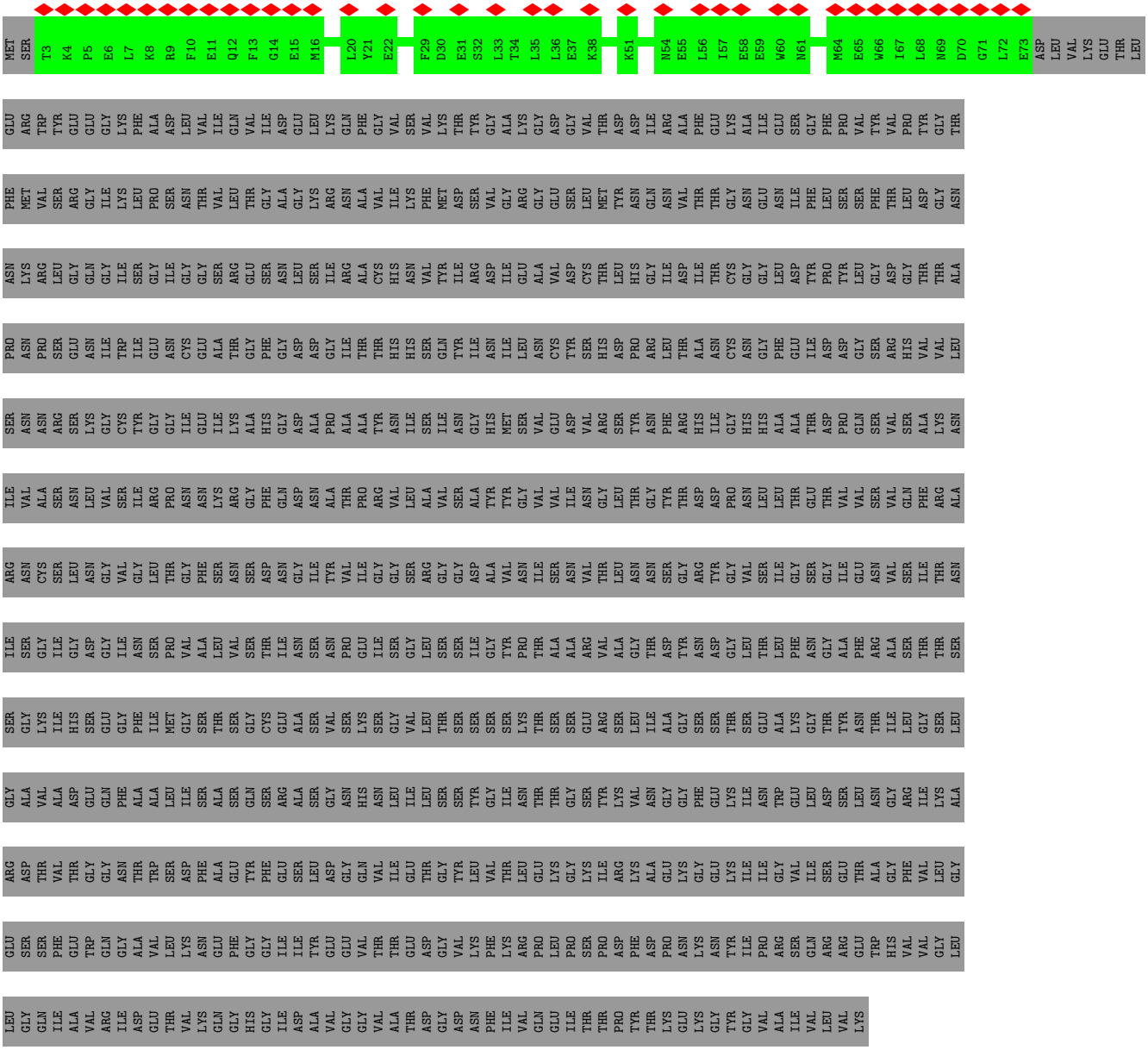




• Molecule 3: Pre-neck appendage protein

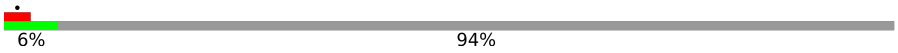
Chain R:

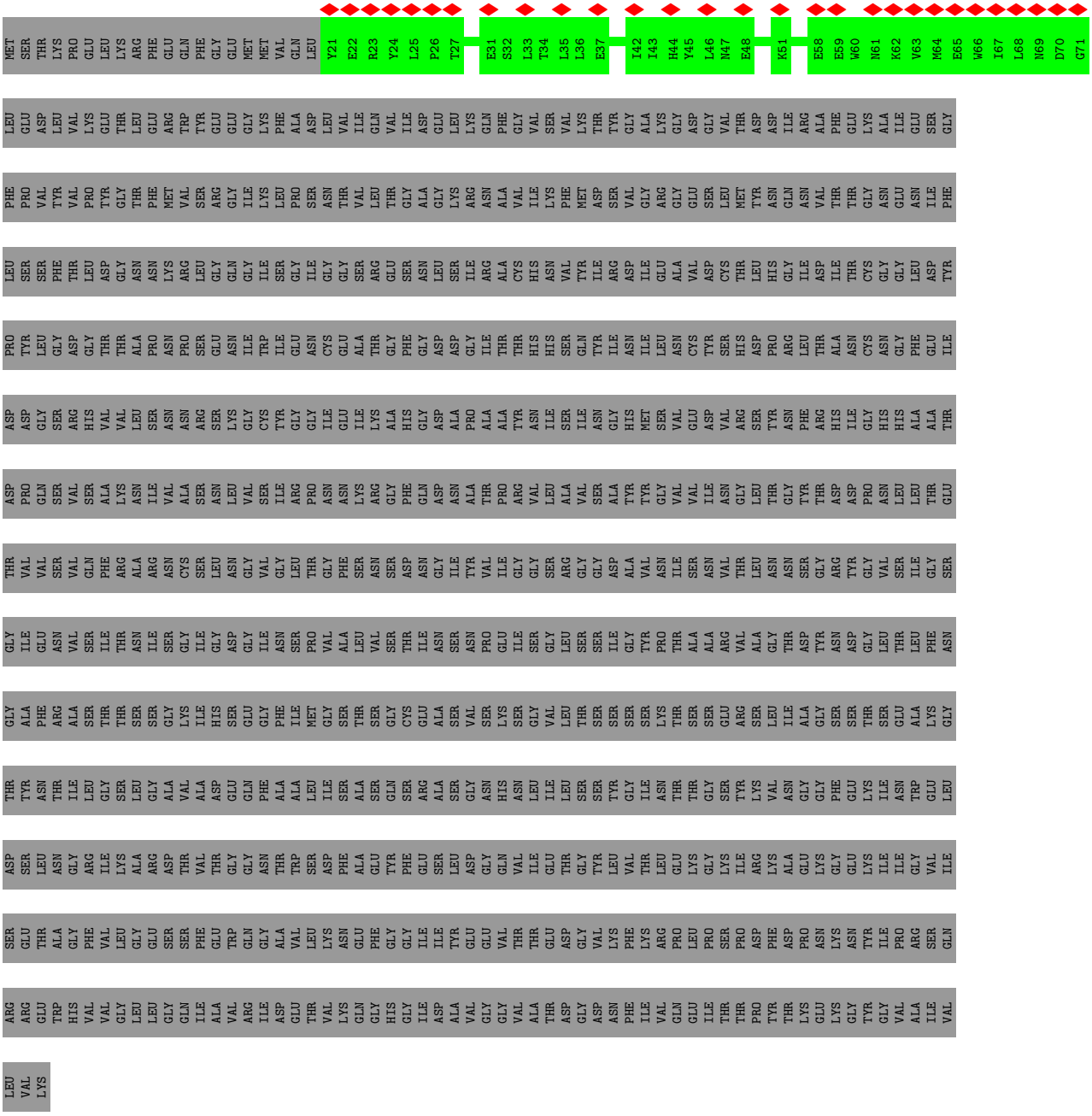




• Molecule 3: Pre-neck appendage protein

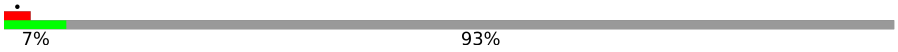
Chain S:

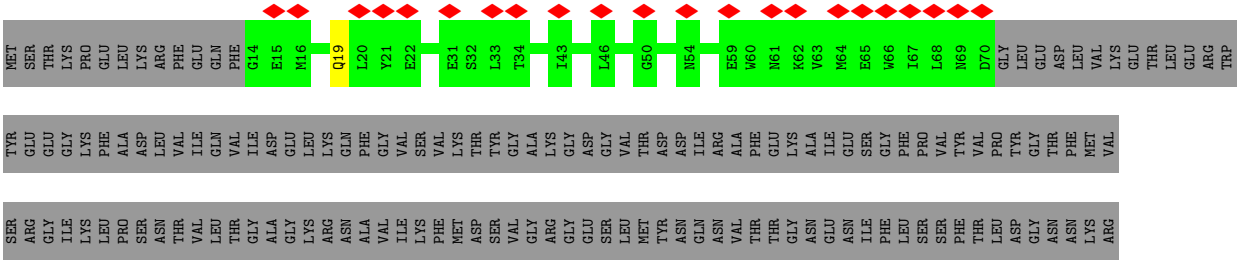


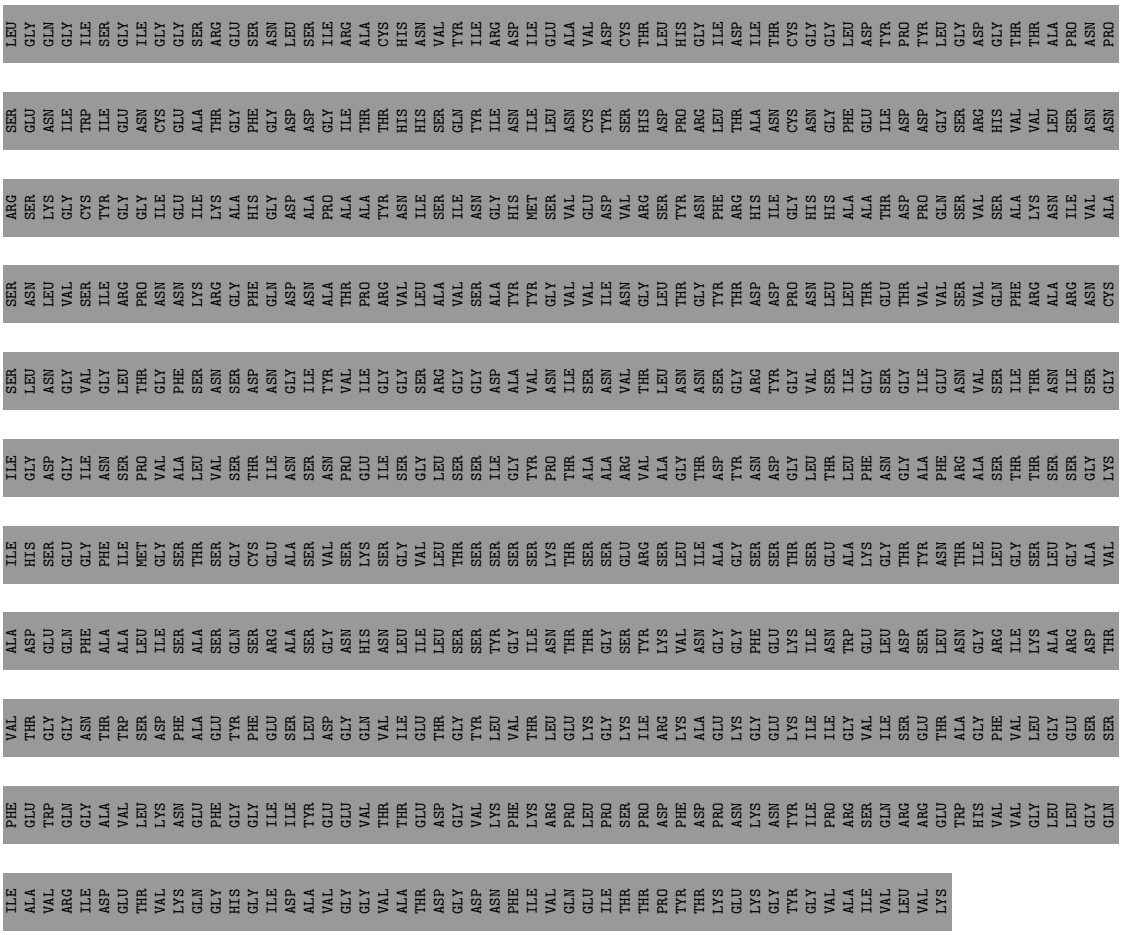


• Molecule 3: Pre-neck appendage protein

Chain T:

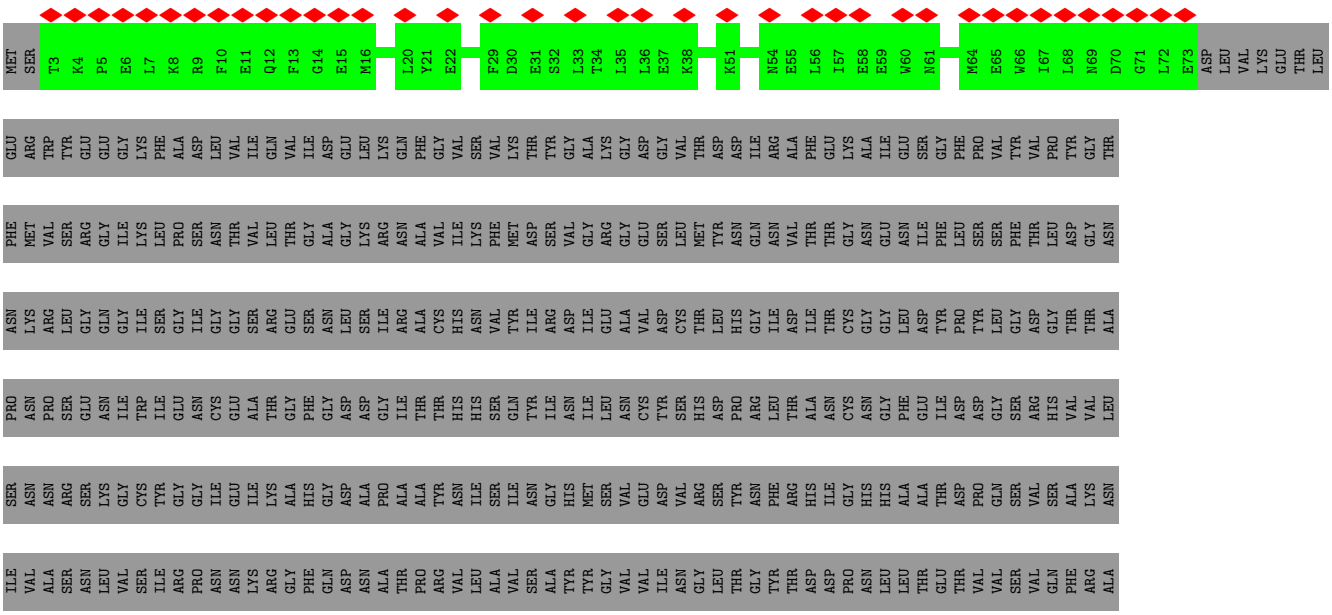


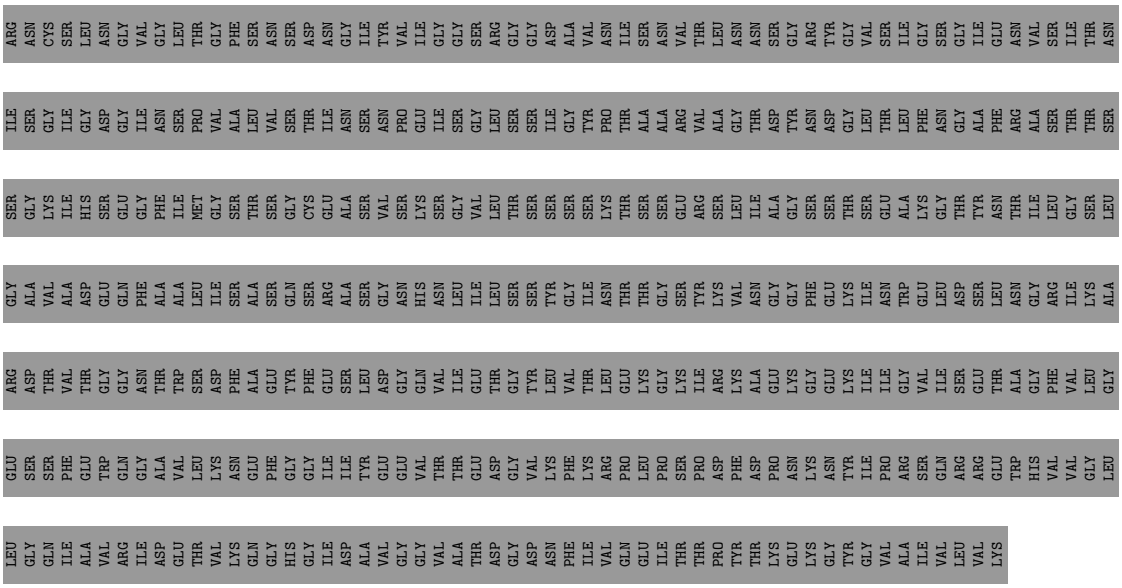




• Molecule 3: Pre-neck appendage protein

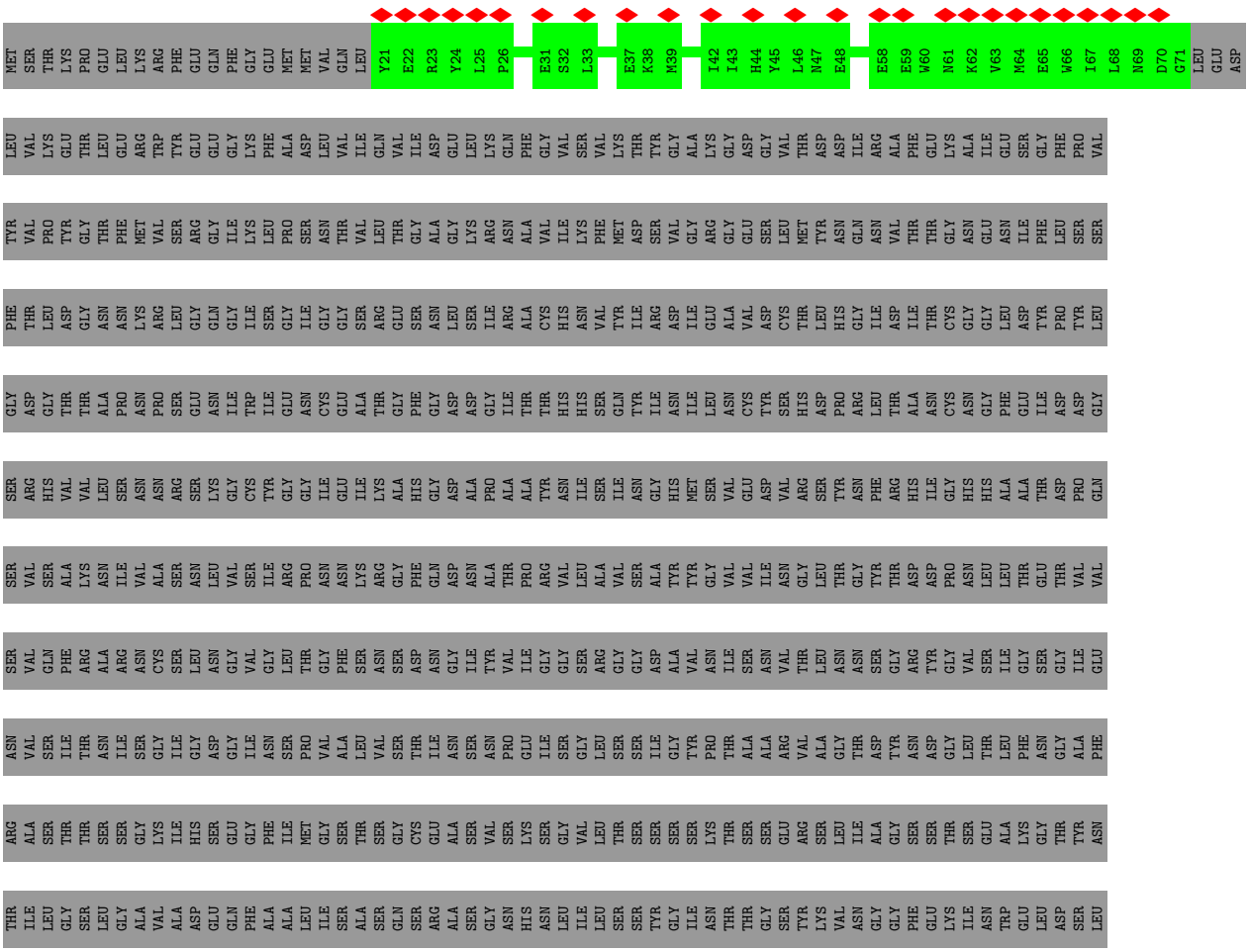
Chain U: 5% 8% 92%

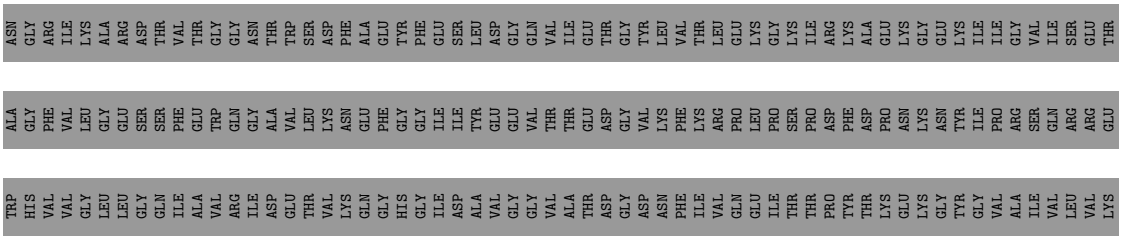




• Molecule 3: Pre-neck appendage protein

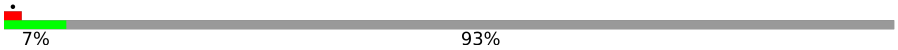
Chain V: 6% 94%

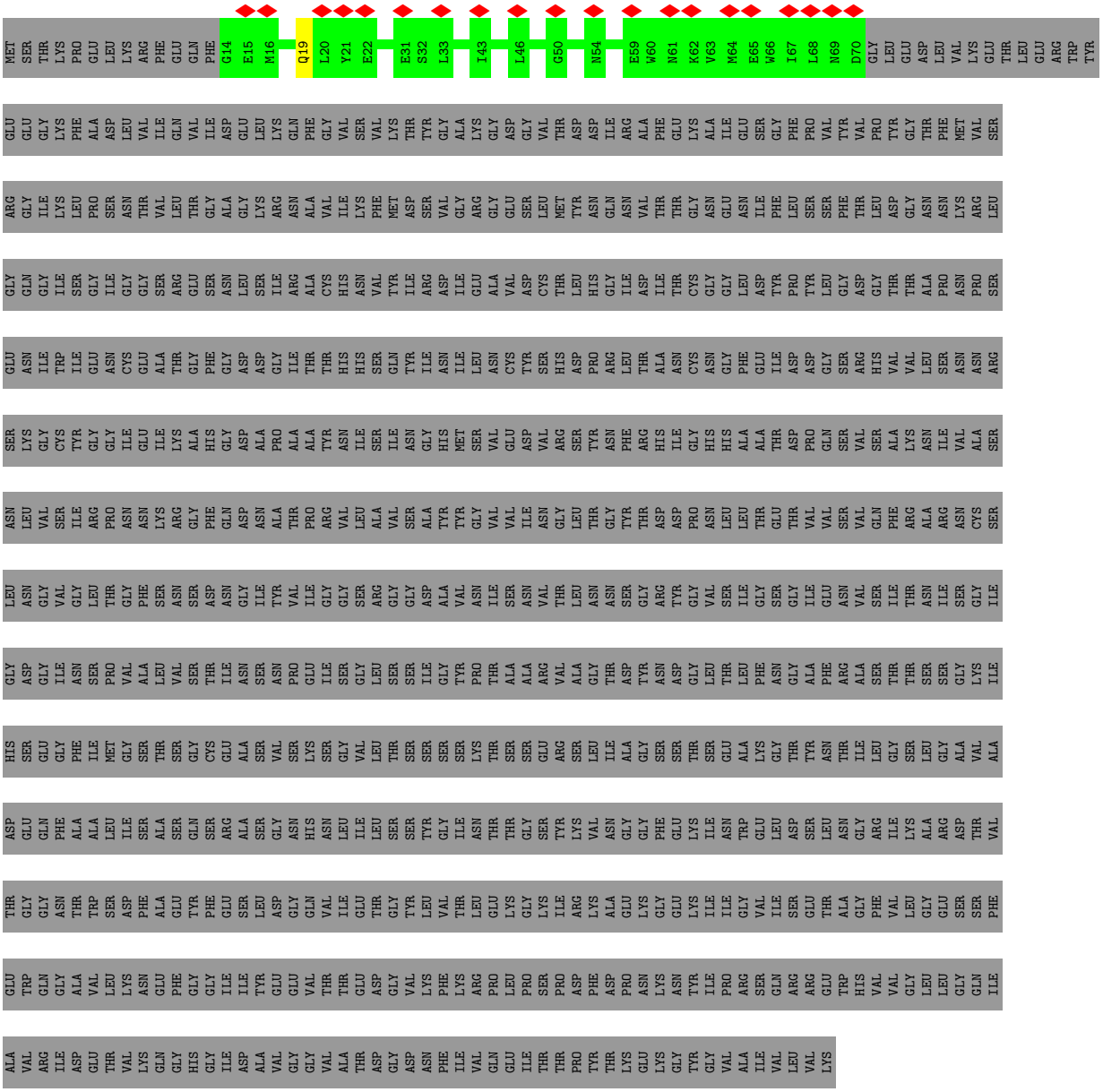




• Molecule 3: Pre-neck appendage protein

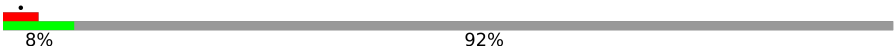
Chain W:

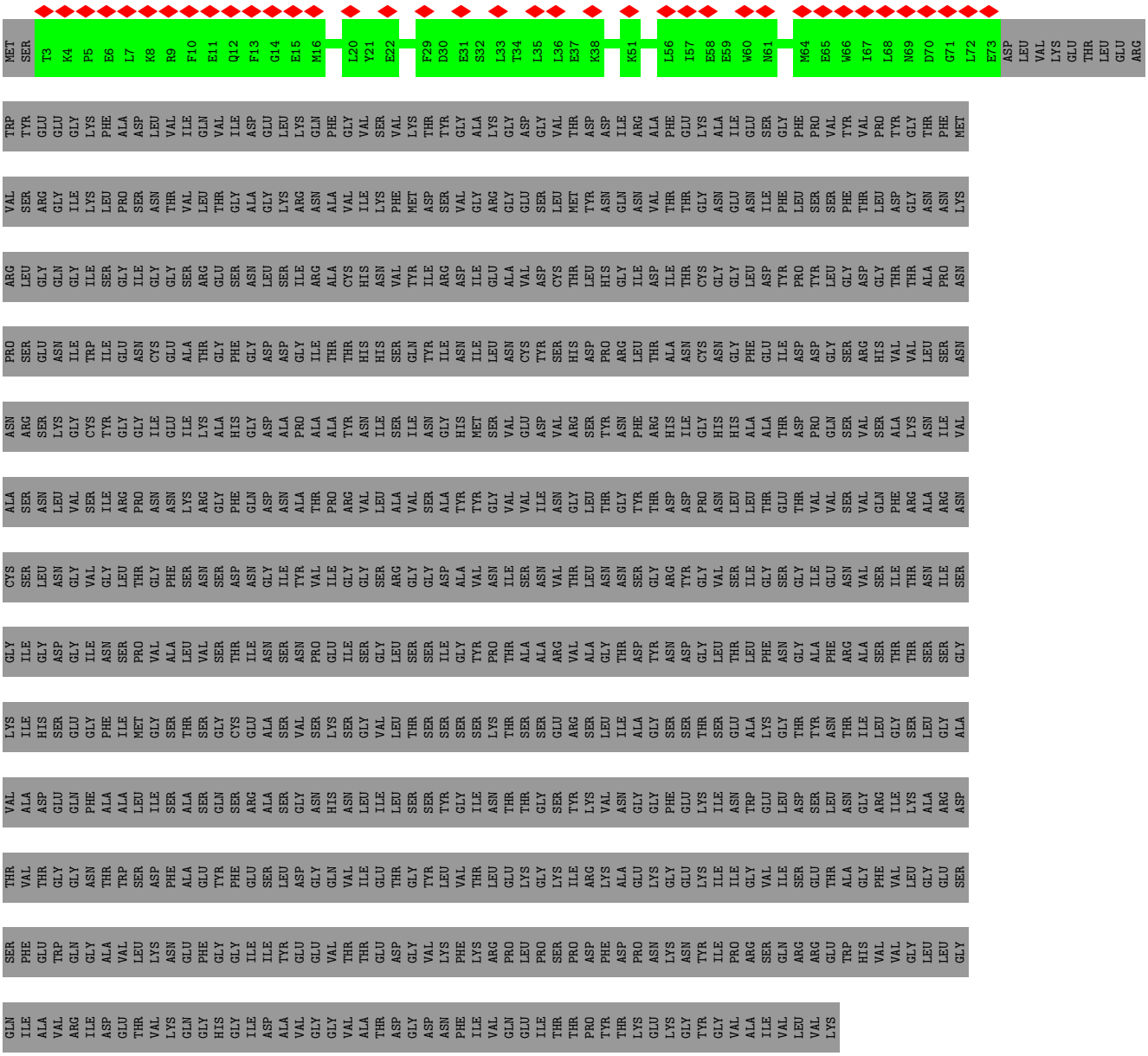




• Molecule 3: Pre-neck appendage protein

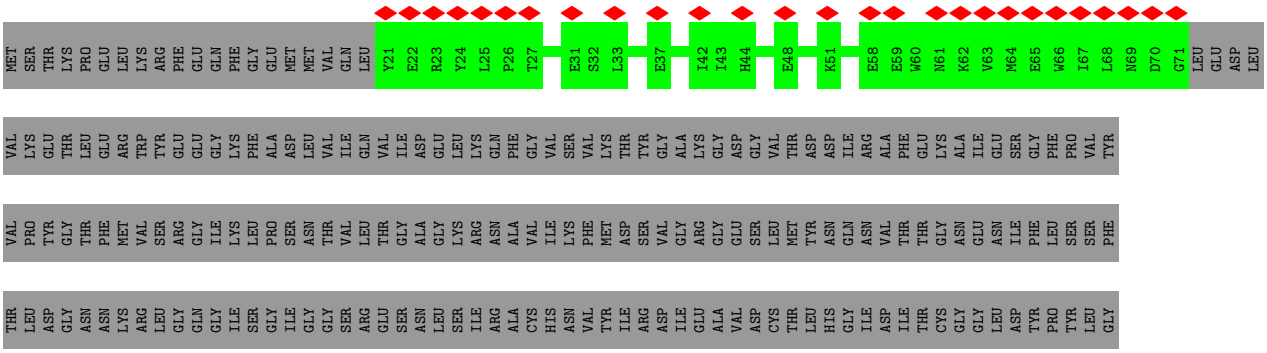
Chain X:

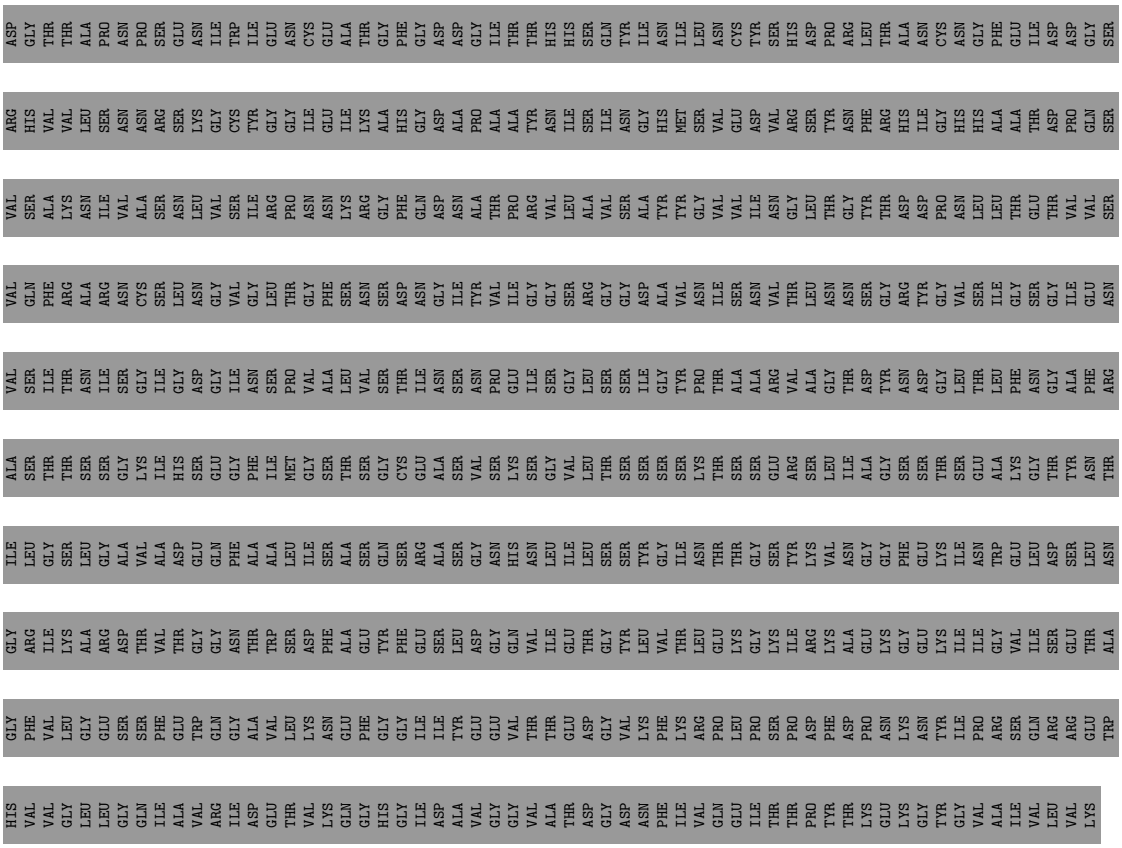




- Molecule 3: Pre-neck appendage protein

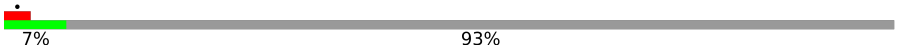
Chain Y: 6% 94%

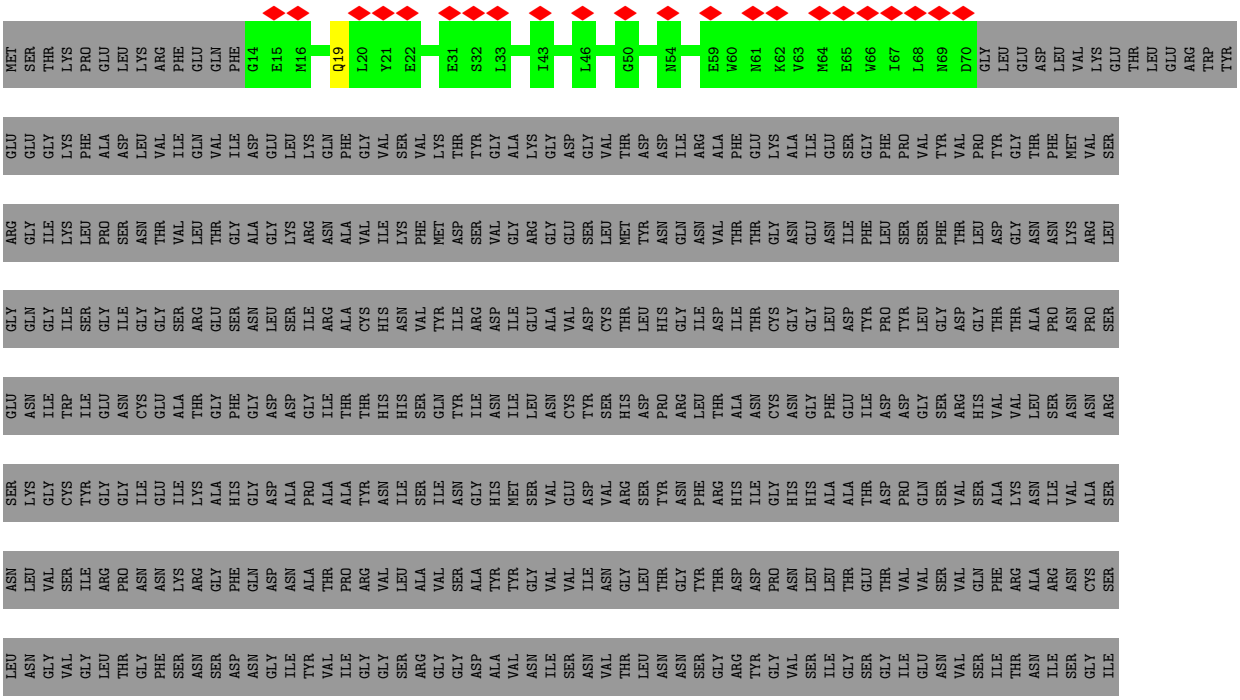


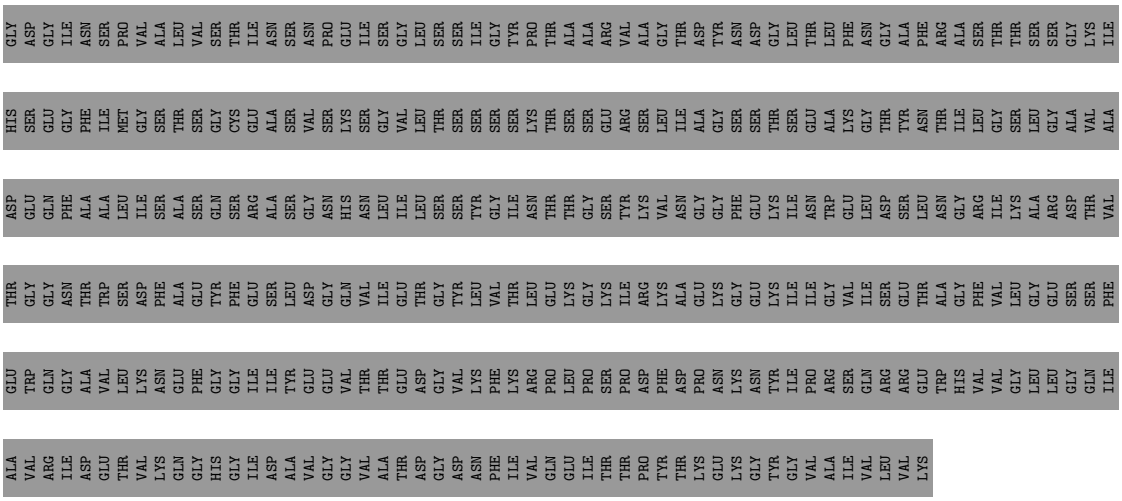


- Molecule 3: Pre-neck appendage protein

Chain Z:

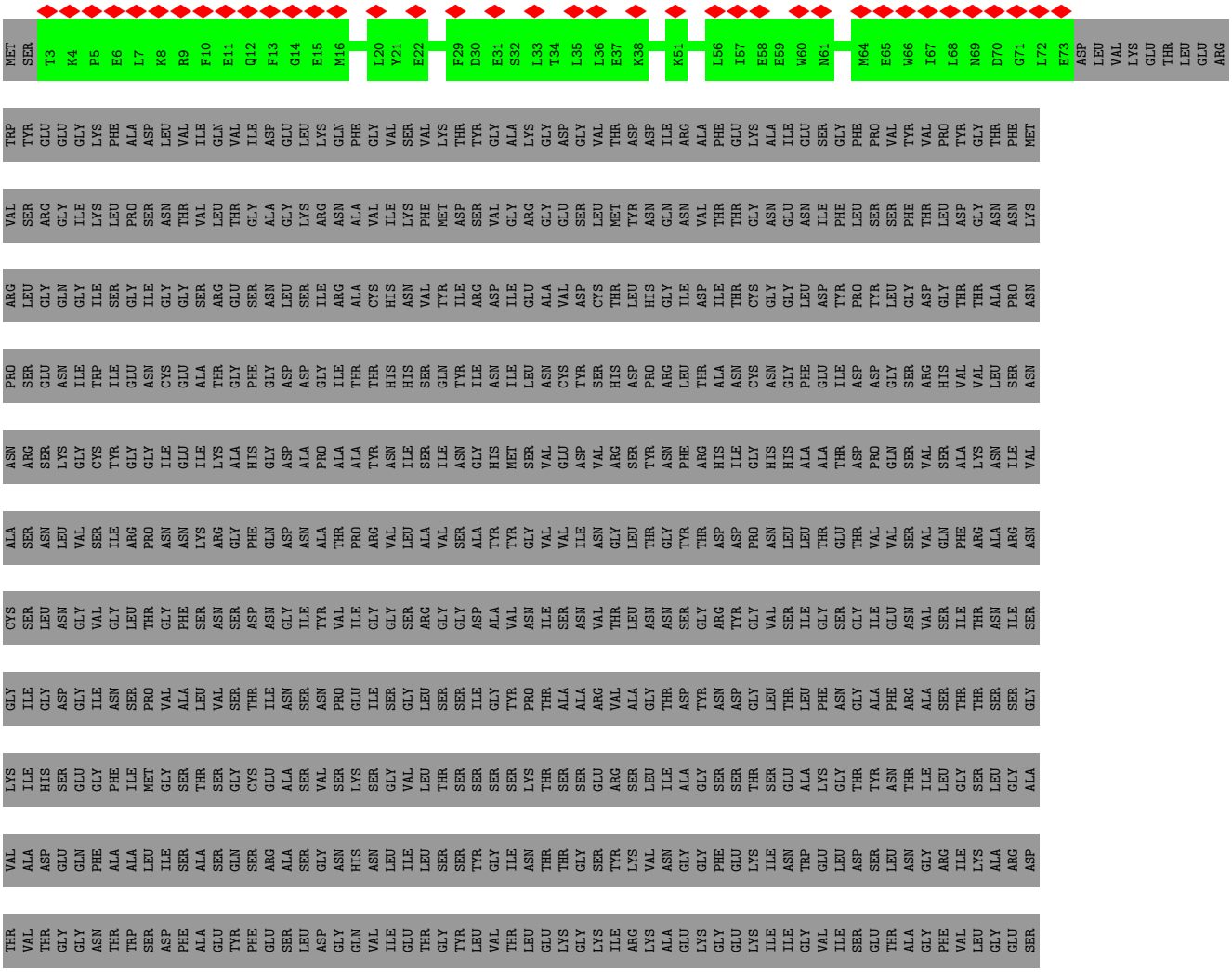


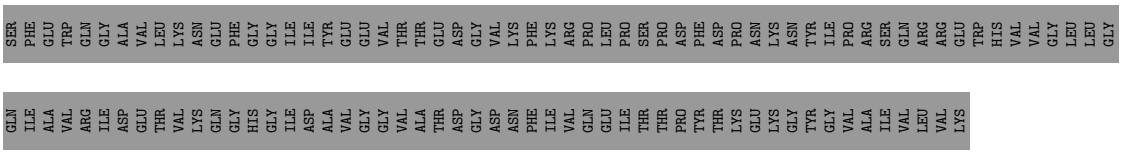




- Molecule 3: Pre-neck appendage protein

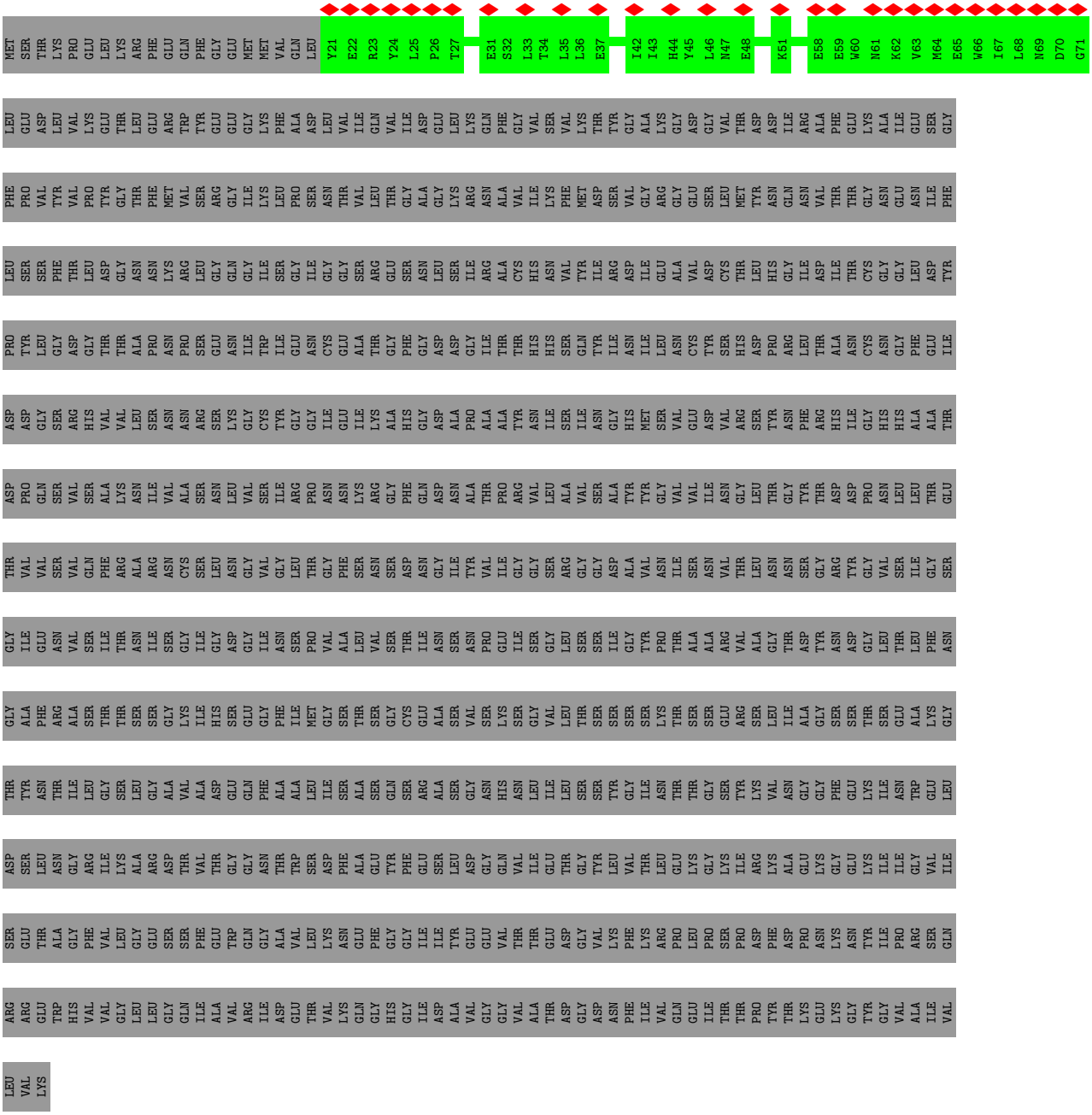
Chain a: 8% 92%





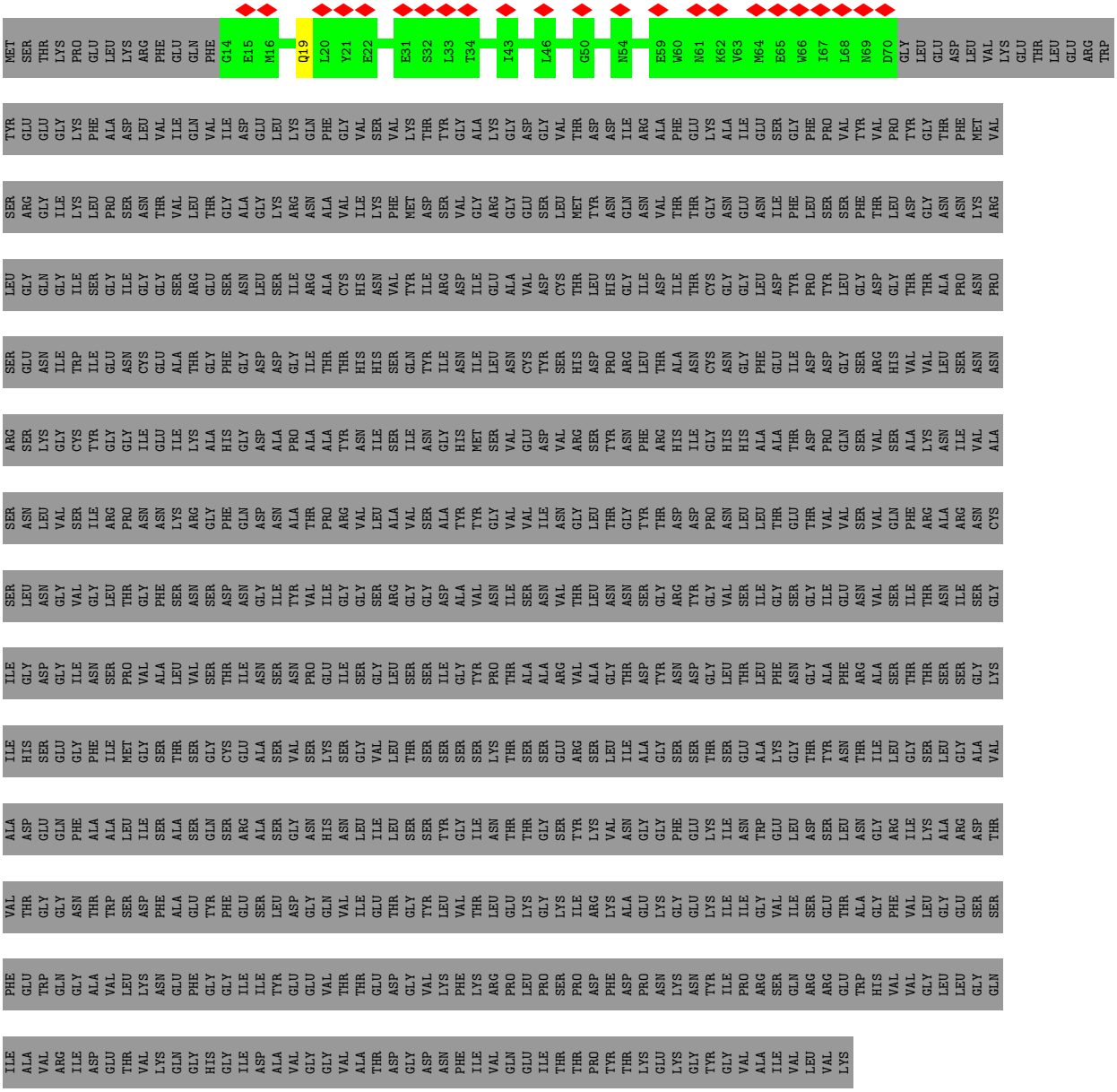
• Molecule 3: Pre-neck appendage protein

Chain b: 6% 94%



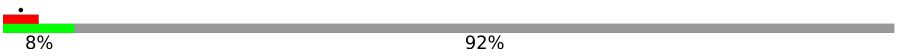
• Molecule 3: Pre-neck appendage protein

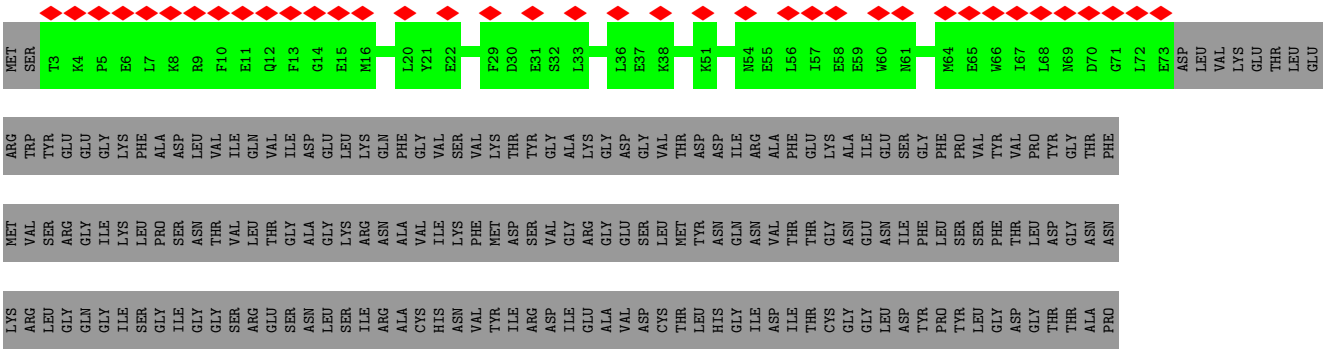
Chain c: 7% 93%

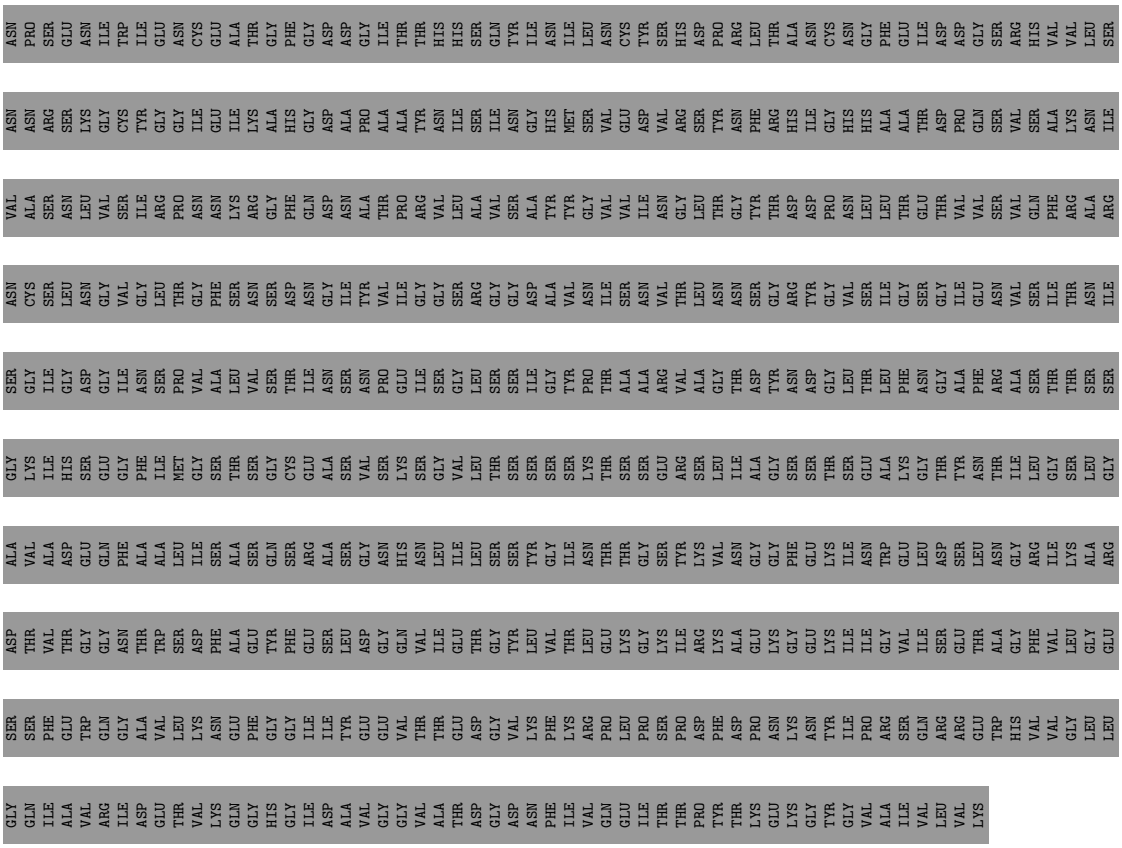


• Molecule 3: Pre-neck appendage protein

Chain d:

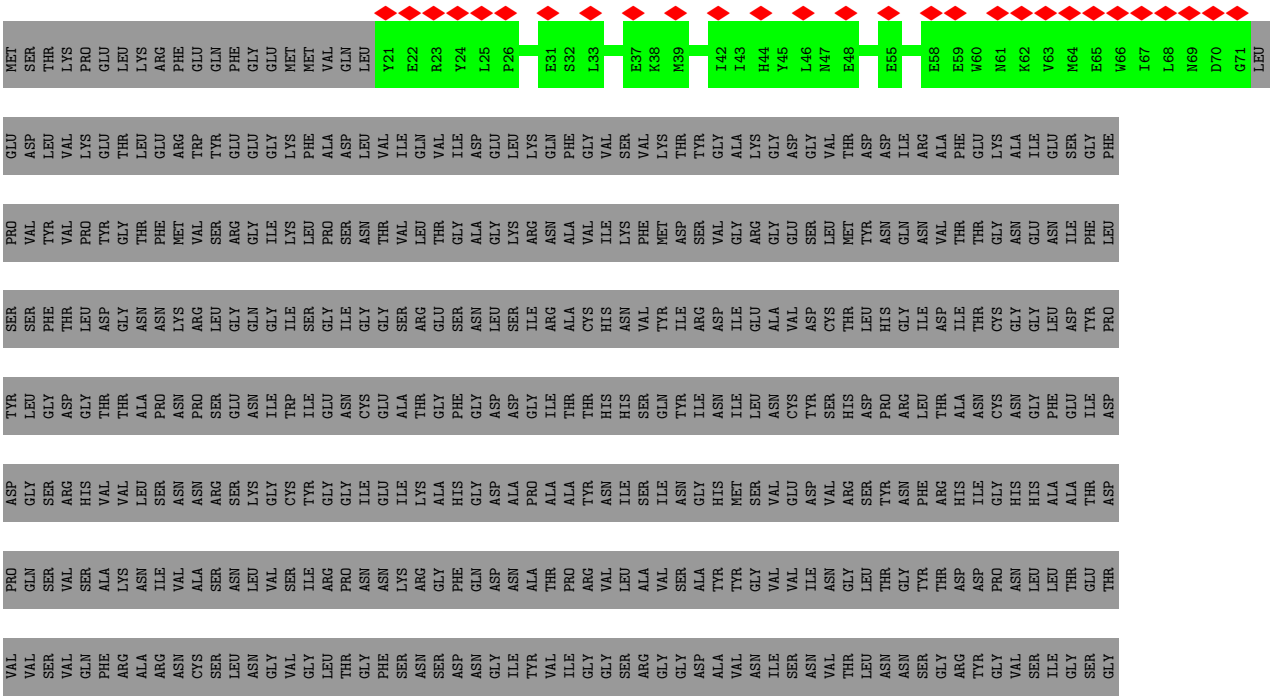






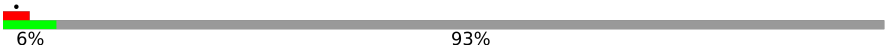
- Molecule 3: Pre-neck appendage protein

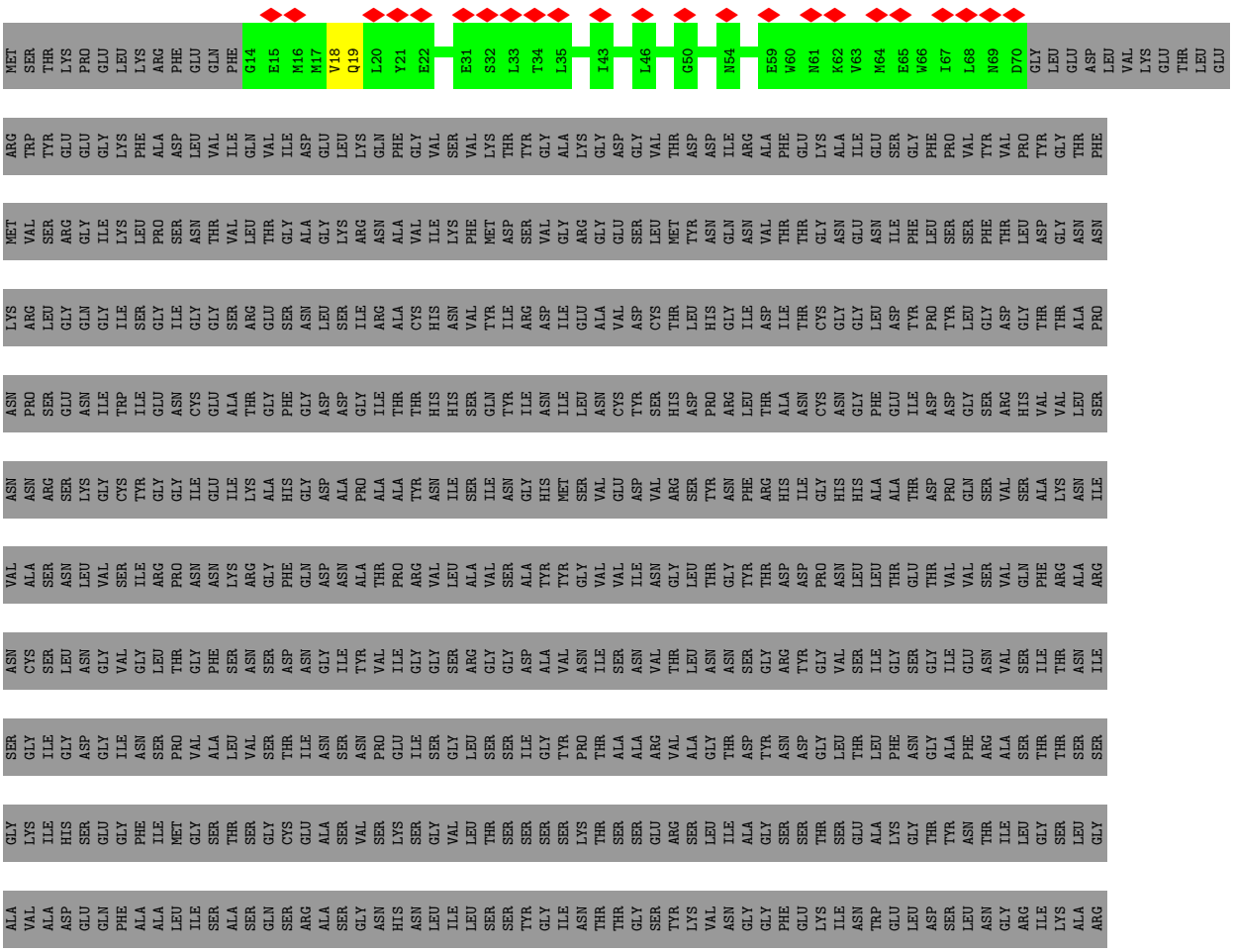
Chain e: 6% 94%

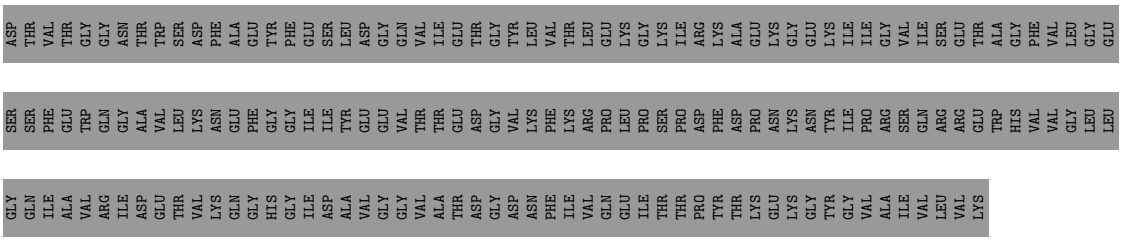


- Molecule 3: Pre-neck appendage protein

Chain f:

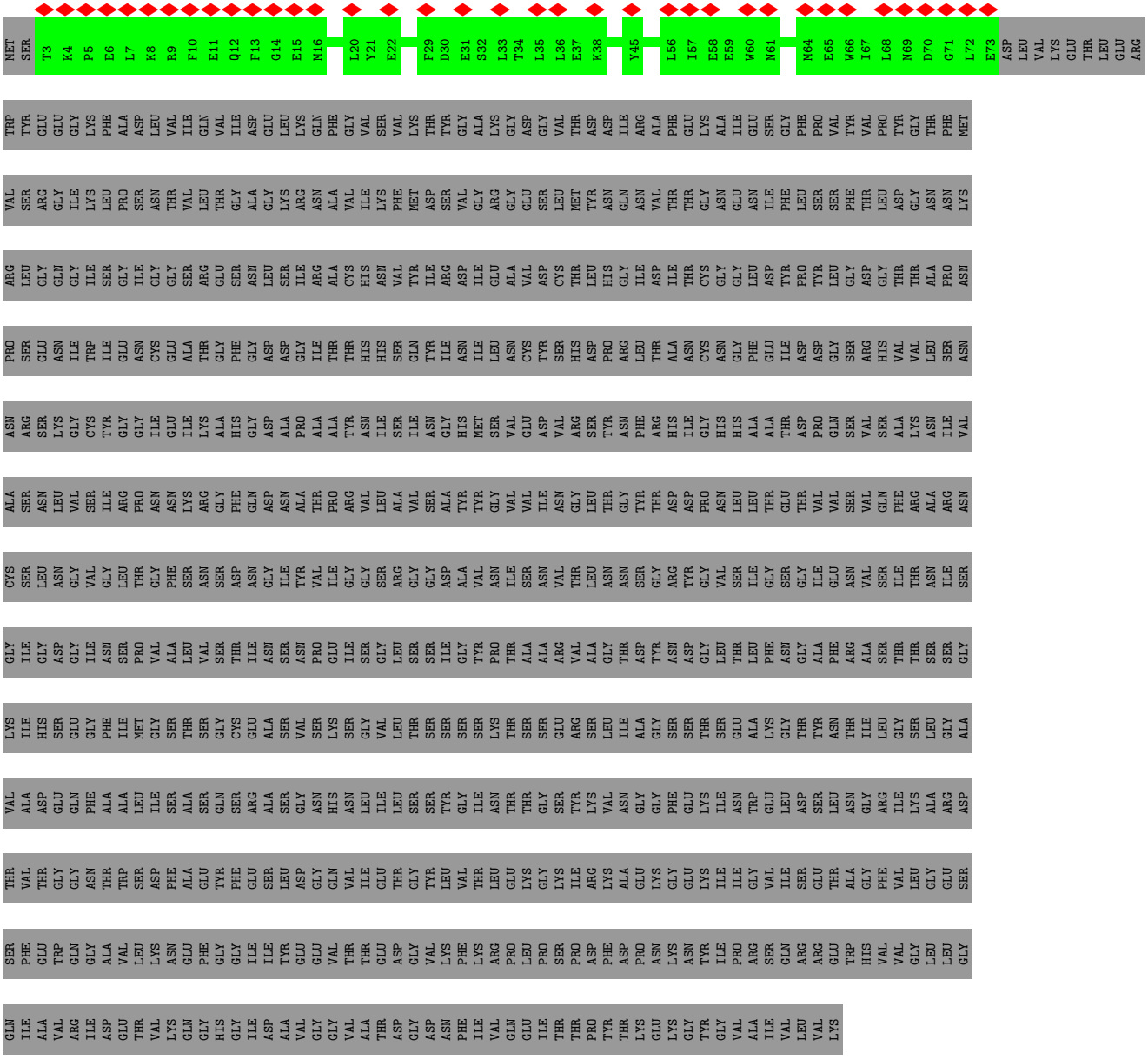






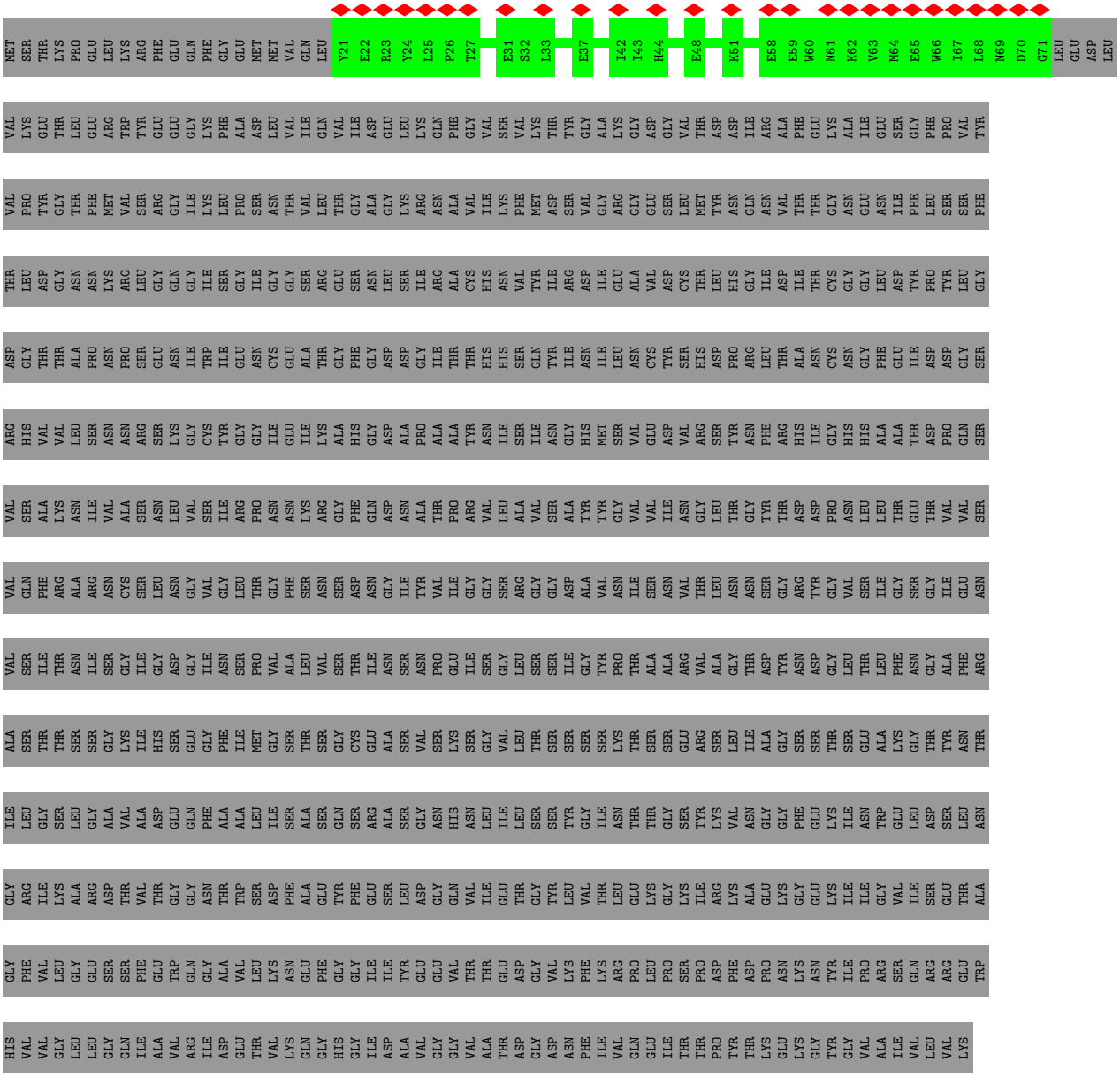
• Molecule 3: Pre-neck appendage protein

Chain g: 8% 92%



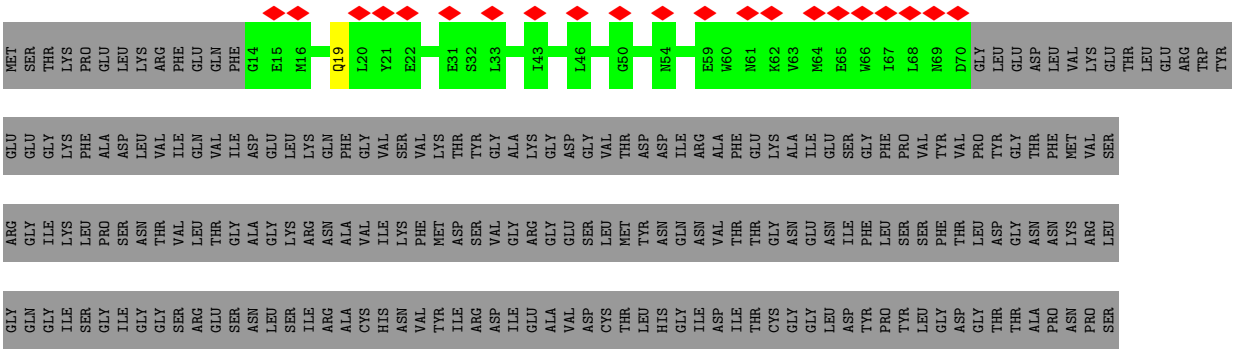
• Molecule 3: Pre-neck appendage protein

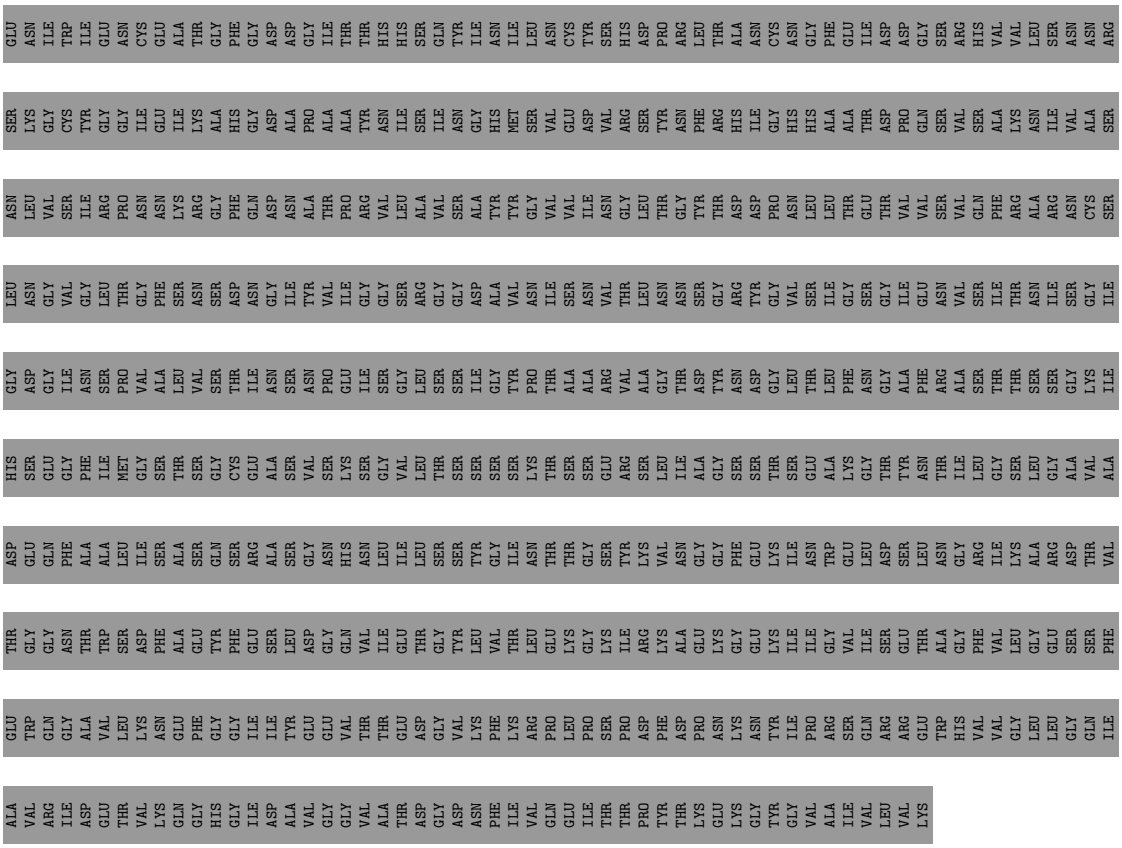
Chain h: 6% 94%



- Molecule 3: Pre-neck appendage protein

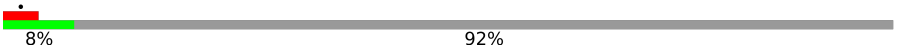
Chain i: 7% 93%

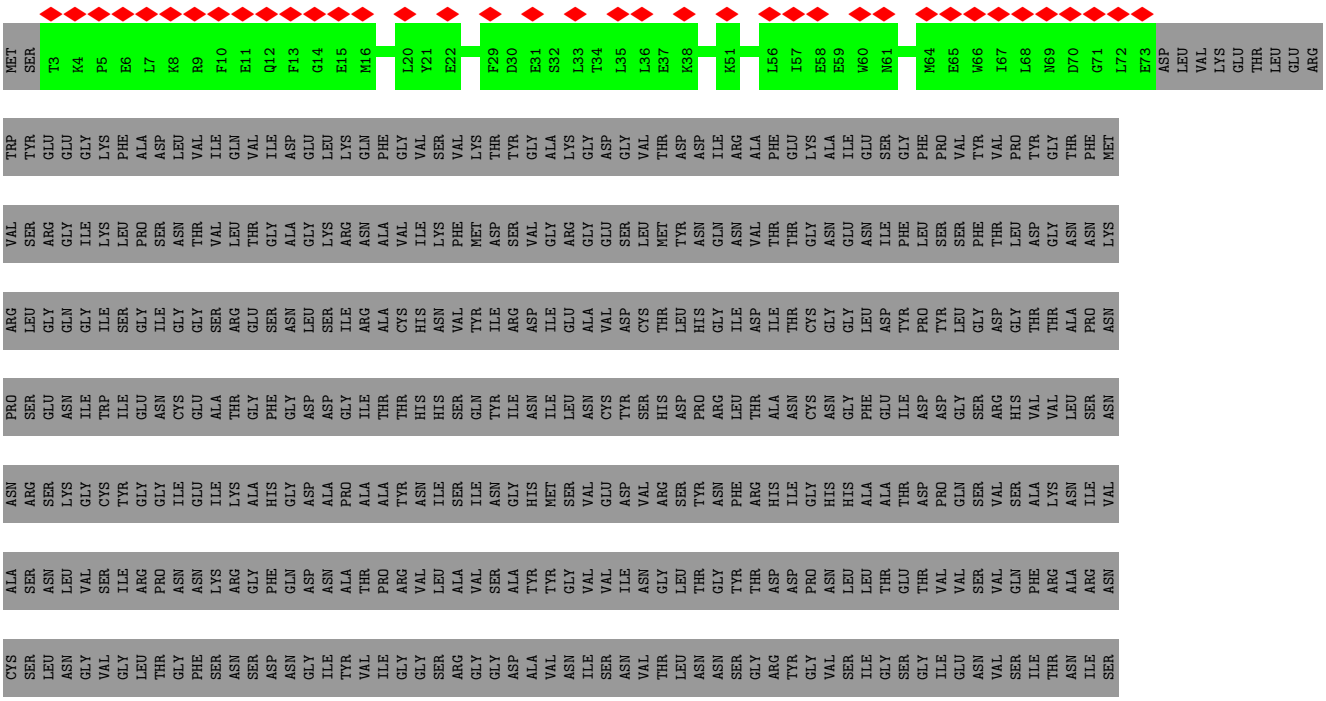




- Molecule 3: Pre-neck appendage protein

Chain j:





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

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

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

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

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

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

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36370	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	120.855	Depositor
Minimum map value	-0.428	Depositor
Average map value	0.025	Depositor
Map value standard deviation	0.514	Depositor
Recommended contour level	6.0	Depositor
Map size (Å)	740.8544, 740.8544, 740.8544	wwPDB
Map dimensions	572, 572, 572	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2952, 1.2952, 1.2952	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	0a	0.30	0/2211	0.48	0/2996
1	0b	0.30	0/2211	0.48	0/2996
1	0c	0.30	0/2211	0.48	0/2996
1	0d	0.30	0/2211	0.48	0/2996
1	0e	0.30	0/2211	0.48	0/2996
1	0f	0.30	0/2211	0.49	0/2996
1	0g	0.30	0/2211	0.49	0/2996
1	0h	0.30	0/2211	0.49	0/2996
1	0i	0.30	0/2211	0.49	0/2996
1	0j	0.30	0/2211	0.49	0/2996
1	0k	0.30	0/2211	0.49	0/2996
1	0l	0.30	0/2211	0.48	0/2996
2	0A	0.36	0/2331	0.56	0/3144
2	0B	0.36	0/2331	0.56	0/3144
2	0C	0.36	0/2331	0.56	0/3144
2	0D	0.36	0/2331	0.56	0/3144
2	0E	0.36	0/2331	0.56	0/3144
2	0F	0.36	0/2331	0.56	0/3144
2	0G	0.36	0/2331	0.56	0/3144
2	0H	0.36	0/2331	0.56	0/3144
2	0I	0.36	0/2331	0.56	0/3144
2	0J	0.36	0/2331	0.56	0/3144
2	0K	0.36	0/2331	0.56	0/3144
2	0L	0.36	0/2331	0.56	0/3144
3	A	0.32	0/442	0.59	0/598
3	B	0.38	0/491	0.60	0/663
3	C	0.29	0/615	0.48	0/828
3	D	0.32	0/442	0.58	0/598
3	E	0.35	0/491	0.60	0/663
3	F	0.29	0/615	0.48	0/828
3	G	0.32	0/442	0.58	0/598
3	H	0.37	0/491	0.60	0/663
3	I	0.29	0/615	0.48	0/828
3	J	0.32	0/442	0.59	0/598

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	K	0.37	0/491	0.60	0/663
3	L	0.29	0/615	0.48	0/828
3	M	0.32	0/442	0.58	0/598
3	N	0.37	0/491	0.60	0/663
3	O	0.29	0/615	0.48	0/828
3	P	0.32	0/442	0.58	0/598
3	Q	0.37	0/491	0.60	0/663
3	R	0.29	0/615	0.48	0/828
3	S	0.32	0/442	0.59	0/598
3	T	0.36	0/491	0.60	0/663
3	U	0.29	0/615	0.48	0/828
3	V	0.32	0/442	0.59	0/598
3	W	0.35	0/491	0.60	0/663
3	X	0.29	0/615	0.48	0/828
3	Y	0.32	0/442	0.59	0/598
3	Z	0.37	0/491	0.60	0/663
3	a	0.29	0/615	0.48	0/828
3	b	0.32	0/442	0.58	0/598
3	c	0.38	0/491	0.60	0/663
3	d	0.29	0/615	0.48	0/828
3	e	0.33	0/442	0.60	0/598
3	f	0.34	0/491	0.59	0/663
3	g	0.29	0/615	0.48	0/828
3	h	0.32	0/442	0.59	0/598
3	i	0.35	0/491	0.60	0/663
3	j	0.29	0/615	0.48	0/828
All	All	0.33	0/73080	0.53	0/98748

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	0a	0	1
1	0b	0	1
1	0c	0	1
1	0d	0	1
1	0e	0	1
1	0f	0	1
1	0g	0	1
1	0h	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0i	0	1
1	0j	0	1
1	0k	0	1
1	0l	0	1
3	B	0	1
3	f	0	1
All	All	0	14

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0a	72	SER	Peptide
1	0b	72	SER	Peptide
1	0c	72	SER	Peptide
1	0d	72	SER	Peptide
1	0e	72	SER	Peptide
1	0f	72	SER	Peptide
1	0g	72	SER	Peptide
1	0h	72	SER	Peptide
1	0i	72	SER	Peptide
1	0j	72	SER	Peptide
1	0k	72	SER	Peptide
1	0l	72	SER	Peptide
3	B	18	VAL	Peptide
3	f	18	VAL	Peptide

5.2 Too-close contacts (i)

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

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	0a	260/309 (84%)	243 (94%)	17 (6%)	0	100	100
1	0b	260/309 (84%)	243 (94%)	17 (6%)	0	100	100
1	0c	260/309 (84%)	243 (94%)	17 (6%)	0	100	100
1	0d	260/309 (84%)	243 (94%)	17 (6%)	0	100	100
1	0e	260/309 (84%)	243 (94%)	17 (6%)	0	100	100
1	0f	260/309 (84%)	243 (94%)	17 (6%)	0	100	100
1	0g	260/309 (84%)	243 (94%)	17 (6%)	0	100	100
1	0h	260/309 (84%)	243 (94%)	17 (6%)	0	100	100
1	0i	260/309 (84%)	243 (94%)	17 (6%)	0	100	100
1	0j	260/309 (84%)	243 (94%)	17 (6%)	0	100	100
1	0k	260/309 (84%)	243 (94%)	17 (6%)	0	100	100
1	0l	260/309 (84%)	243 (94%)	17 (6%)	0	100	100
2	0A	289/293 (99%)	272 (94%)	17 (6%)	0	100	100
2	0B	289/293 (99%)	272 (94%)	17 (6%)	0	100	100
2	0C	289/293 (99%)	272 (94%)	17 (6%)	0	100	100
2	0D	289/293 (99%)	272 (94%)	17 (6%)	0	100	100
2	0E	289/293 (99%)	272 (94%)	17 (6%)	0	100	100
2	0F	289/293 (99%)	272 (94%)	17 (6%)	0	100	100
2	0G	289/293 (99%)	272 (94%)	17 (6%)	0	100	100
2	0H	289/293 (99%)	272 (94%)	17 (6%)	0	100	100
2	0I	289/293 (99%)	272 (94%)	17 (6%)	0	100	100
2	0J	289/293 (99%)	272 (94%)	17 (6%)	0	100	100
2	0K	289/293 (99%)	272 (94%)	17 (6%)	0	100	100
2	0L	289/293 (99%)	272 (94%)	17 (6%)	0	100	100
3	A	49/854 (6%)	42 (86%)	7 (14%)	0	100	100
3	B	55/854 (6%)	52 (94%)	2 (4%)	1 (2%)	8	35
3	C	69/854 (8%)	63 (91%)	6 (9%)	0	100	100
3	D	49/854 (6%)	42 (86%)	7 (14%)	0	100	100
3	E	55/854 (6%)	51 (93%)	3 (6%)	1 (2%)	8	35
3	F	69/854 (8%)	63 (91%)	6 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	49/854 (6%)	42 (86%)	7 (14%)	0	100	100
3	H	55/854 (6%)	52 (94%)	2 (4%)	1 (2%)	8	35
3	I	69/854 (8%)	63 (91%)	6 (9%)	0	100	100
3	J	49/854 (6%)	42 (86%)	7 (14%)	0	100	100
3	K	55/854 (6%)	52 (94%)	2 (4%)	1 (2%)	8	35
3	L	69/854 (8%)	63 (91%)	6 (9%)	0	100	100
3	M	49/854 (6%)	42 (86%)	7 (14%)	0	100	100
3	N	55/854 (6%)	52 (94%)	2 (4%)	1 (2%)	8	35
3	O	69/854 (8%)	63 (91%)	6 (9%)	0	100	100
3	P	49/854 (6%)	42 (86%)	7 (14%)	0	100	100
3	Q	55/854 (6%)	52 (94%)	2 (4%)	1 (2%)	8	35
3	R	69/854 (8%)	63 (91%)	6 (9%)	0	100	100
3	S	49/854 (6%)	42 (86%)	7 (14%)	0	100	100
3	T	55/854 (6%)	52 (94%)	2 (4%)	1 (2%)	8	35
3	U	69/854 (8%)	63 (91%)	6 (9%)	0	100	100
3	V	49/854 (6%)	42 (86%)	7 (14%)	0	100	100
3	W	55/854 (6%)	52 (94%)	2 (4%)	1 (2%)	8	35
3	X	69/854 (8%)	63 (91%)	6 (9%)	0	100	100
3	Y	49/854 (6%)	42 (86%)	7 (14%)	0	100	100
3	Z	55/854 (6%)	52 (94%)	2 (4%)	1 (2%)	8	35
3	a	69/854 (8%)	63 (91%)	6 (9%)	0	100	100
3	b	49/854 (6%)	42 (86%)	7 (14%)	0	100	100
3	c	55/854 (6%)	52 (94%)	2 (4%)	1 (2%)	8	35
3	d	69/854 (8%)	63 (91%)	6 (9%)	0	100	100
3	e	49/854 (6%)	42 (86%)	7 (14%)	0	100	100
3	f	55/854 (6%)	52 (94%)	2 (4%)	1 (2%)	8	35
3	g	69/854 (8%)	63 (91%)	6 (9%)	0	100	100
3	h	49/854 (6%)	42 (86%)	7 (14%)	0	100	100
3	i	55/854 (6%)	52 (94%)	2 (4%)	1 (2%)	8	35
3	j	69/854 (8%)	63 (91%)	6 (9%)	0	100	100
All	All	8664/37968 (23%)	8063 (93%)	589 (7%)	12 (0%)	54	81

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	19	GLN
3	E	19	GLN
3	H	19	GLN
3	K	19	GLN
3	N	19	GLN
3	Q	19	GLN
3	T	19	GLN
3	W	19	GLN
3	Z	19	GLN
3	c	19	GLN
3	f	19	GLN
3	i	19	GLN

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	0a	236/277 (85%)	236 (100%)	0	100	100
1	0b	236/277 (85%)	236 (100%)	0	100	100
1	0c	236/277 (85%)	236 (100%)	0	100	100
1	0d	236/277 (85%)	236 (100%)	0	100	100
1	0e	236/277 (85%)	236 (100%)	0	100	100
1	0f	236/277 (85%)	236 (100%)	0	100	100
1	0g	236/277 (85%)	236 (100%)	0	100	100
1	0h	236/277 (85%)	236 (100%)	0	100	100
1	0i	236/277 (85%)	236 (100%)	0	100	100
1	0j	236/277 (85%)	236 (100%)	0	100	100
1	0k	236/277 (85%)	236 (100%)	0	100	100
1	0l	236/277 (85%)	236 (100%)	0	100	100
2	0A	249/270 (92%)	247 (99%)	2 (1%)	81	89
2	0B	249/270 (92%)	247 (99%)	2 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	0C	249/270 (92%)	247 (99%)	2 (1%)	81	89
2	0D	249/270 (92%)	247 (99%)	2 (1%)	81	89
2	0E	249/270 (92%)	247 (99%)	2 (1%)	81	89
2	0F	249/270 (92%)	247 (99%)	2 (1%)	81	89
2	0G	249/270 (92%)	247 (99%)	2 (1%)	81	89
2	0H	249/270 (92%)	247 (99%)	2 (1%)	81	89
2	0I	249/270 (92%)	247 (99%)	2 (1%)	81	89
2	0J	249/270 (92%)	247 (99%)	2 (1%)	81	89
2	0K	249/270 (92%)	247 (99%)	2 (1%)	81	89
2	0L	249/270 (92%)	247 (99%)	2 (1%)	81	89
3	A	48/706 (7%)	48 (100%)	0	100	100
3	B	54/706 (8%)	54 (100%)	0	100	100
3	C	67/706 (10%)	67 (100%)	0	100	100
3	D	48/706 (7%)	48 (100%)	0	100	100
3	E	54/706 (8%)	54 (100%)	0	100	100
3	F	67/706 (10%)	67 (100%)	0	100	100
3	G	48/706 (7%)	48 (100%)	0	100	100
3	H	54/706 (8%)	54 (100%)	0	100	100
3	I	67/706 (10%)	67 (100%)	0	100	100
3	J	48/706 (7%)	48 (100%)	0	100	100
3	K	54/706 (8%)	54 (100%)	0	100	100
3	L	67/706 (10%)	67 (100%)	0	100	100
3	M	48/706 (7%)	48 (100%)	0	100	100
3	N	54/706 (8%)	54 (100%)	0	100	100
3	O	67/706 (10%)	67 (100%)	0	100	100
3	P	48/706 (7%)	48 (100%)	0	100	100
3	Q	54/706 (8%)	54 (100%)	0	100	100
3	R	67/706 (10%)	67 (100%)	0	100	100
3	S	48/706 (7%)	48 (100%)	0	100	100
3	T	54/706 (8%)	54 (100%)	0	100	100
3	U	67/706 (10%)	67 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	V	48/706 (7%)	48 (100%)	0	100	100
3	W	54/706 (8%)	54 (100%)	0	100	100
3	X	67/706 (10%)	67 (100%)	0	100	100
3	Y	48/706 (7%)	48 (100%)	0	100	100
3	Z	54/706 (8%)	54 (100%)	0	100	100
3	a	67/706 (10%)	67 (100%)	0	100	100
3	b	48/706 (7%)	48 (100%)	0	100	100
3	c	54/706 (8%)	54 (100%)	0	100	100
3	d	67/706 (10%)	67 (100%)	0	100	100
3	e	48/706 (7%)	48 (100%)	0	100	100
3	f	54/706 (8%)	54 (100%)	0	100	100
3	g	67/706 (10%)	67 (100%)	0	100	100
3	h	48/706 (7%)	48 (100%)	0	100	100
3	i	54/706 (8%)	54 (100%)	0	100	100
3	j	67/706 (10%)	67 (100%)	0	100	100
All	All	7848/31980 (24%)	7824 (100%)	24 (0%)	92	96

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	0A	9	ARG
2	0A	162	ASN
2	0B	9	ARG
2	0B	162	ASN
2	0C	9	ARG
2	0C	162	ASN
2	0D	9	ARG
2	0D	162	ASN
2	0E	9	ARG
2	0E	162	ASN
2	0F	9	ARG
2	0F	162	ASN
2	0G	9	ARG
2	0G	162	ASN
2	0H	9	ARG
2	0H	162	ASN
2	0I	9	ARG

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Mol	Chain	Res	Type
2	0I	162	ASN
2	0J	9	ARG
2	0J	162	ASN
2	0K	9	ARG
2	0K	162	ASN
2	0L	9	ARG
2	0L	162	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
2	0A	162	ASN
2	0A	196	HIS
2	0A	279	GLN
2	0B	17	GLN
2	0B	162	ASN
2	0B	196	HIS
2	0C	162	ASN
2	0C	196	HIS
2	0C	199	ASN
2	0C	279	GLN
2	0D	162	ASN
2	0D	196	HIS
2	0E	162	ASN
2	0E	196	HIS
2	0F	162	ASN
2	0F	196	HIS
2	0G	162	ASN
2	0G	196	HIS
2	0H	162	ASN
2	0H	196	HIS
2	0H	279	GLN
2	0I	162	ASN
2	0I	196	HIS
2	0I	199	ASN
2	0I	279	GLN
2	0J	17	GLN
2	0J	162	ASN
2	0J	196	HIS
2	0K	162	ASN
2	0K	196	HIS
2	0L	162	ASN

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Mol	Chain	Res	Type
2	0L	196	HIS
3	B	54	ASN
3	B	61	ASN
3	E	54	ASN
3	E	61	ASN
3	H	54	ASN
3	H	61	ASN
3	K	54	ASN
3	K	61	ASN
3	N	54	ASN
3	N	61	ASN
3	Q	54	ASN
3	Q	61	ASN
3	T	54	ASN
3	T	61	ASN
3	W	54	ASN
3	W	61	ASN
3	Z	54	ASN
3	Z	61	ASN
3	c	54	ASN
3	c	61	ASN
3	f	54	ASN
3	f	61	ASN
3	i	54	ASN
3	i	61	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation (i)

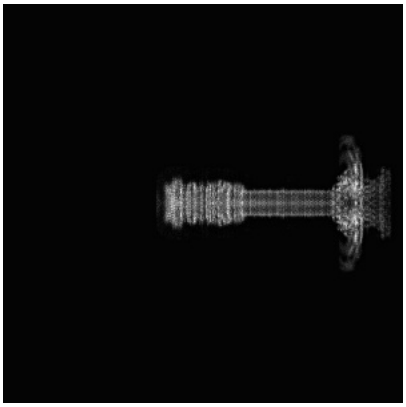
This section contains visualisations of the EMDB entry EMD-4684. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

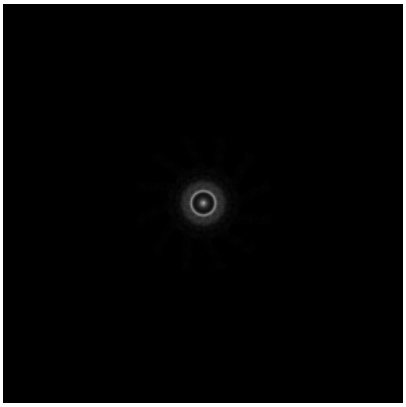
6.1 Orthogonal projections (i)

6.1.1 Primary map

X



Y

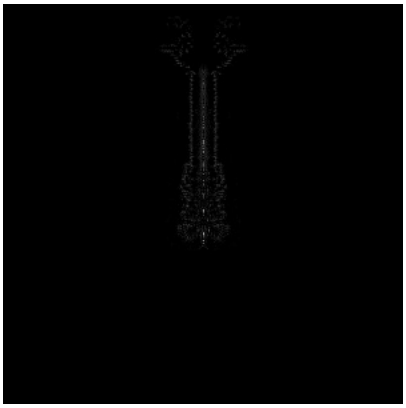


Z

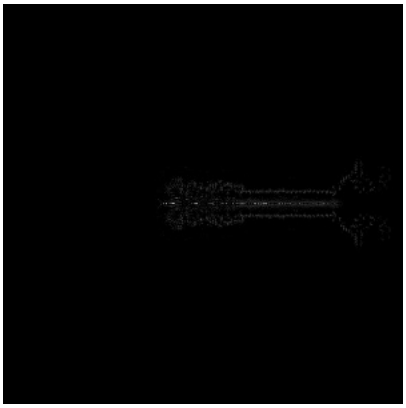
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

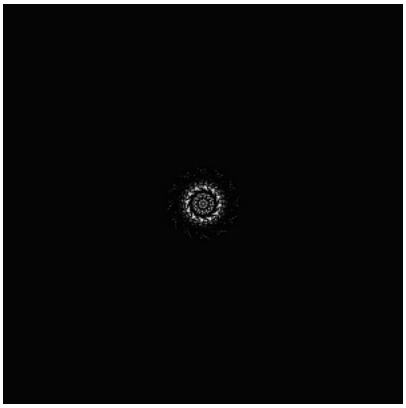
6.2.1 Primary map



X Index: 286



Y Index: 286

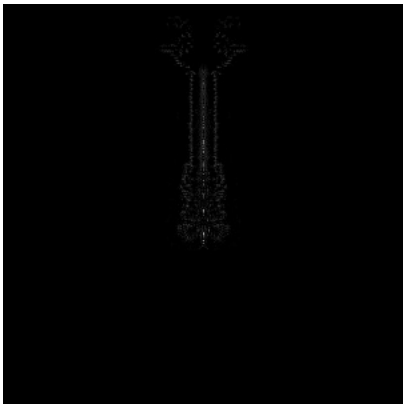


Z Index: 286

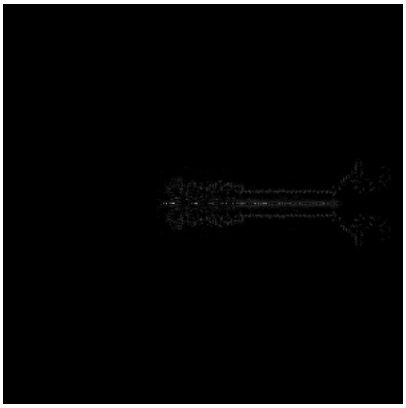
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

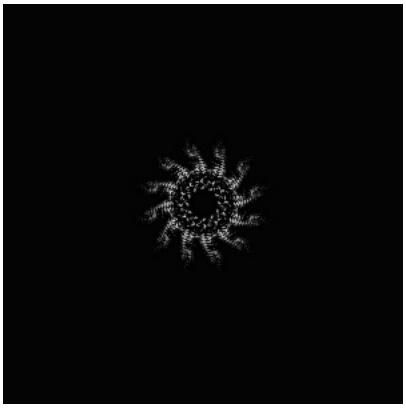
6.3.1 Primary map



X Index: 286



Y Index: 286

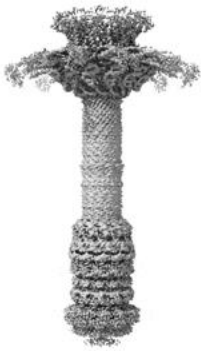


Z Index: 504

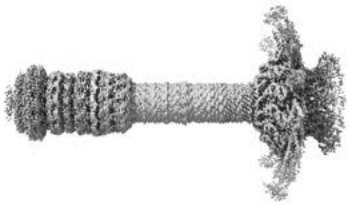
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

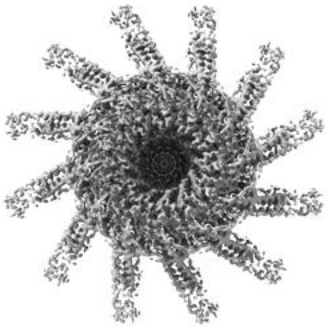
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

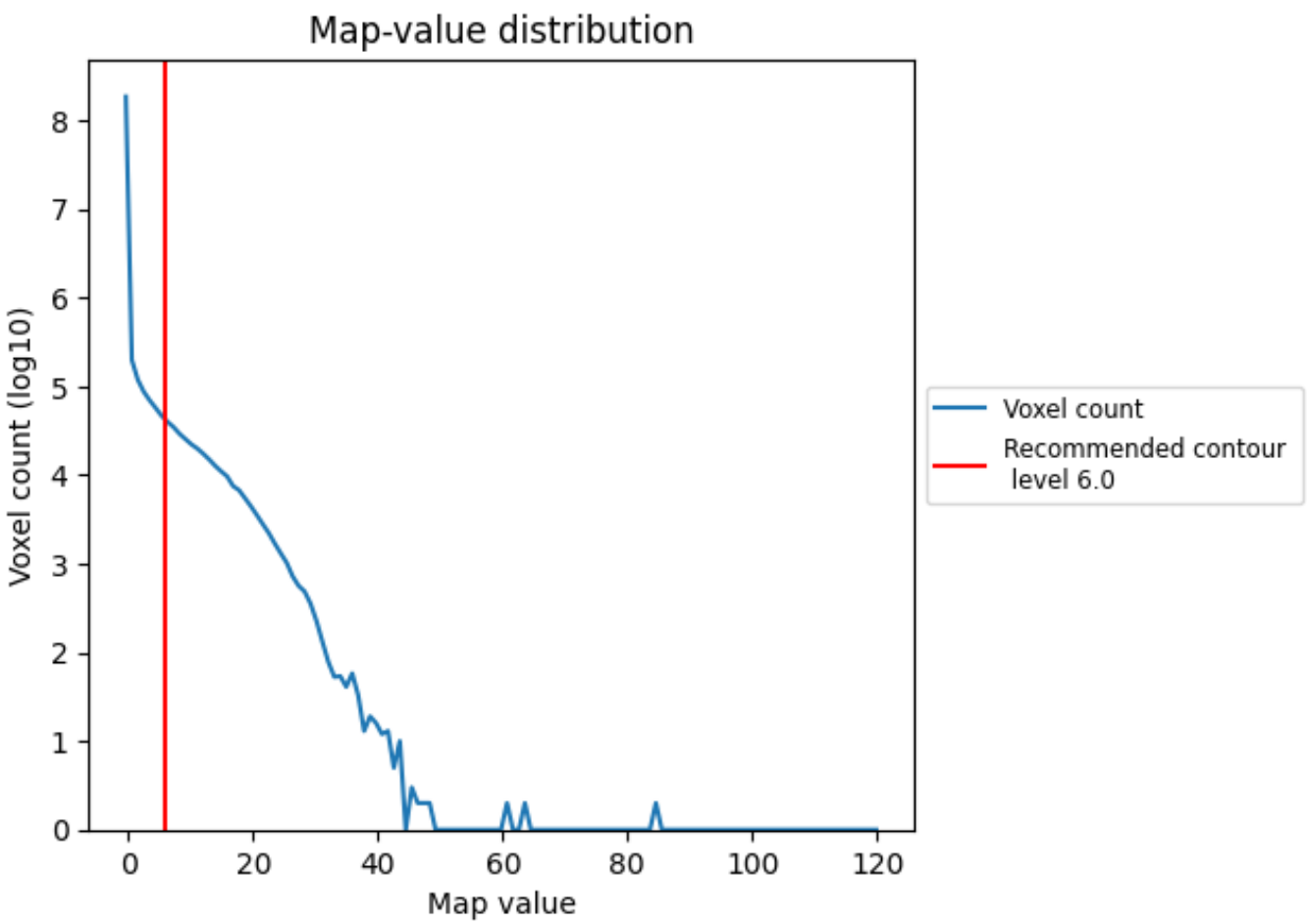
6.5 Mask visualisation (i)

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

7 Map analysis (i)

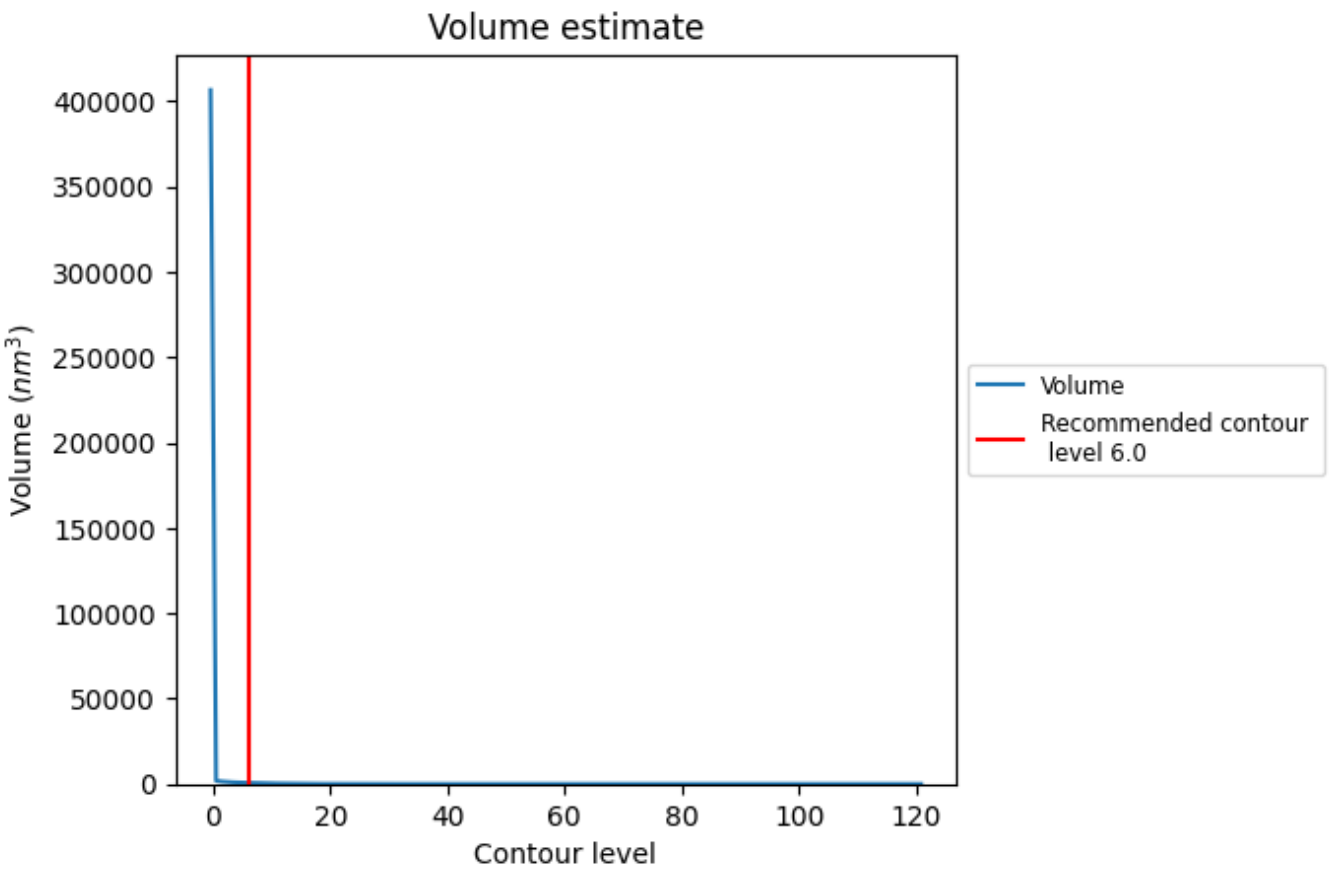
This section contains the results of statistical analysis of the map.

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.

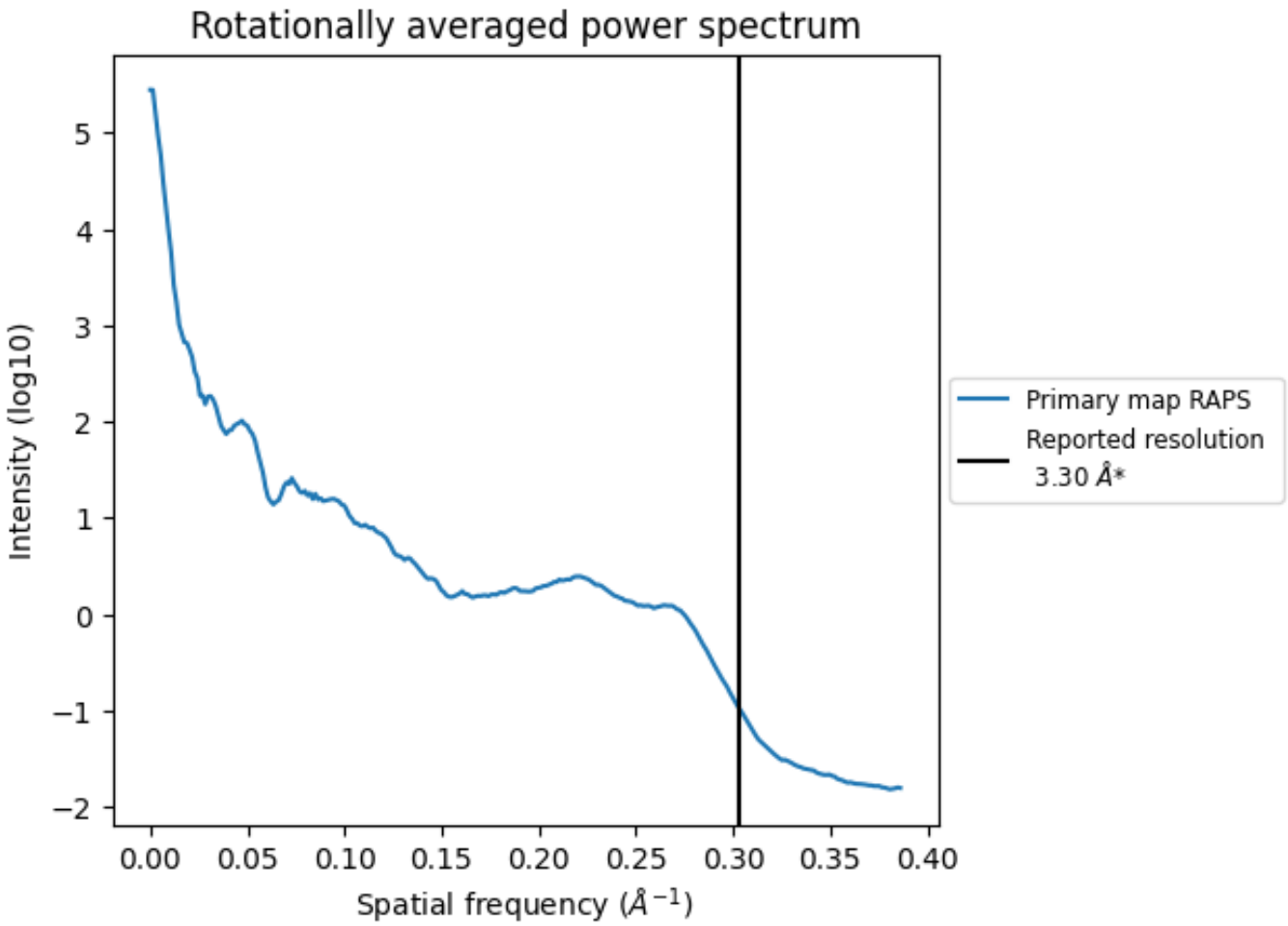
7.2 Volume estimate (i)



The volume at the recommended contour level is 630 nm^3; this corresponds to an approximate mass of 569 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 0.303 Å^{-1}

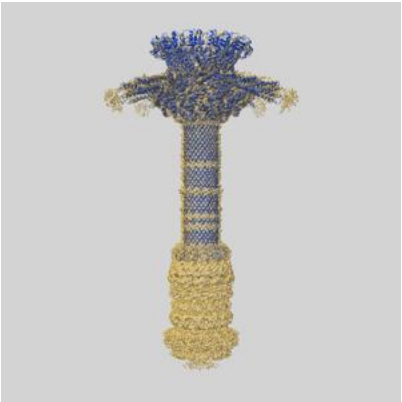
8 Fourier-Shell correlation (i)

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

9 Map-model fit (i)

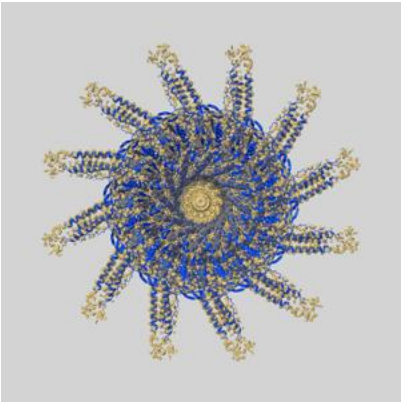
This section contains information regarding the fit between EMDB map EMD-4684 and PDB model 6QZ9. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay (i)



X

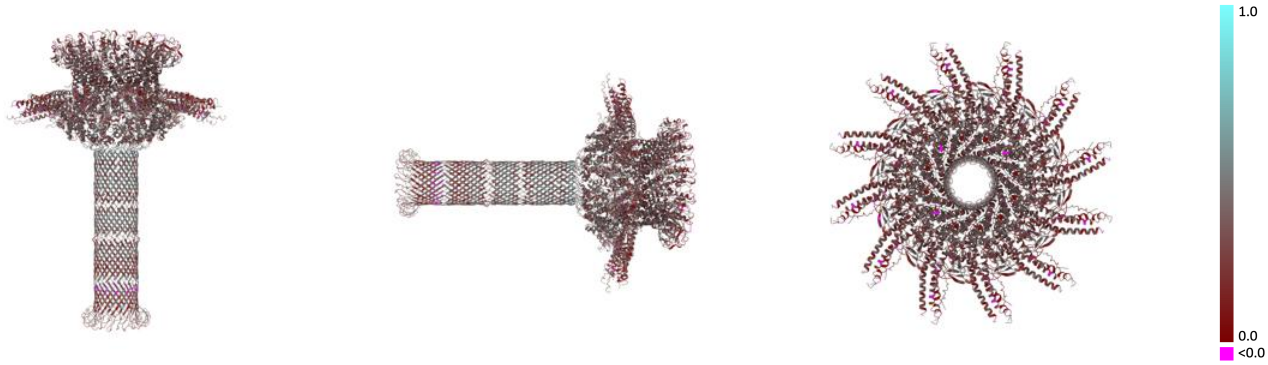
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0 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.

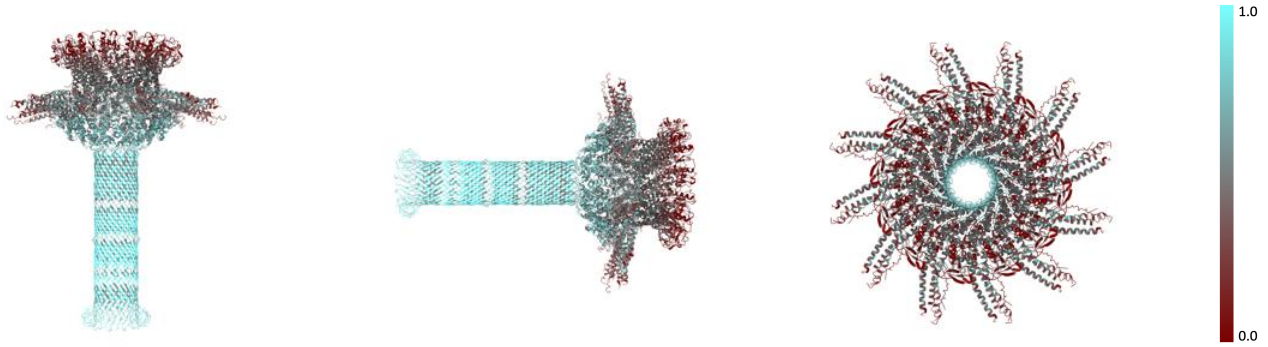
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

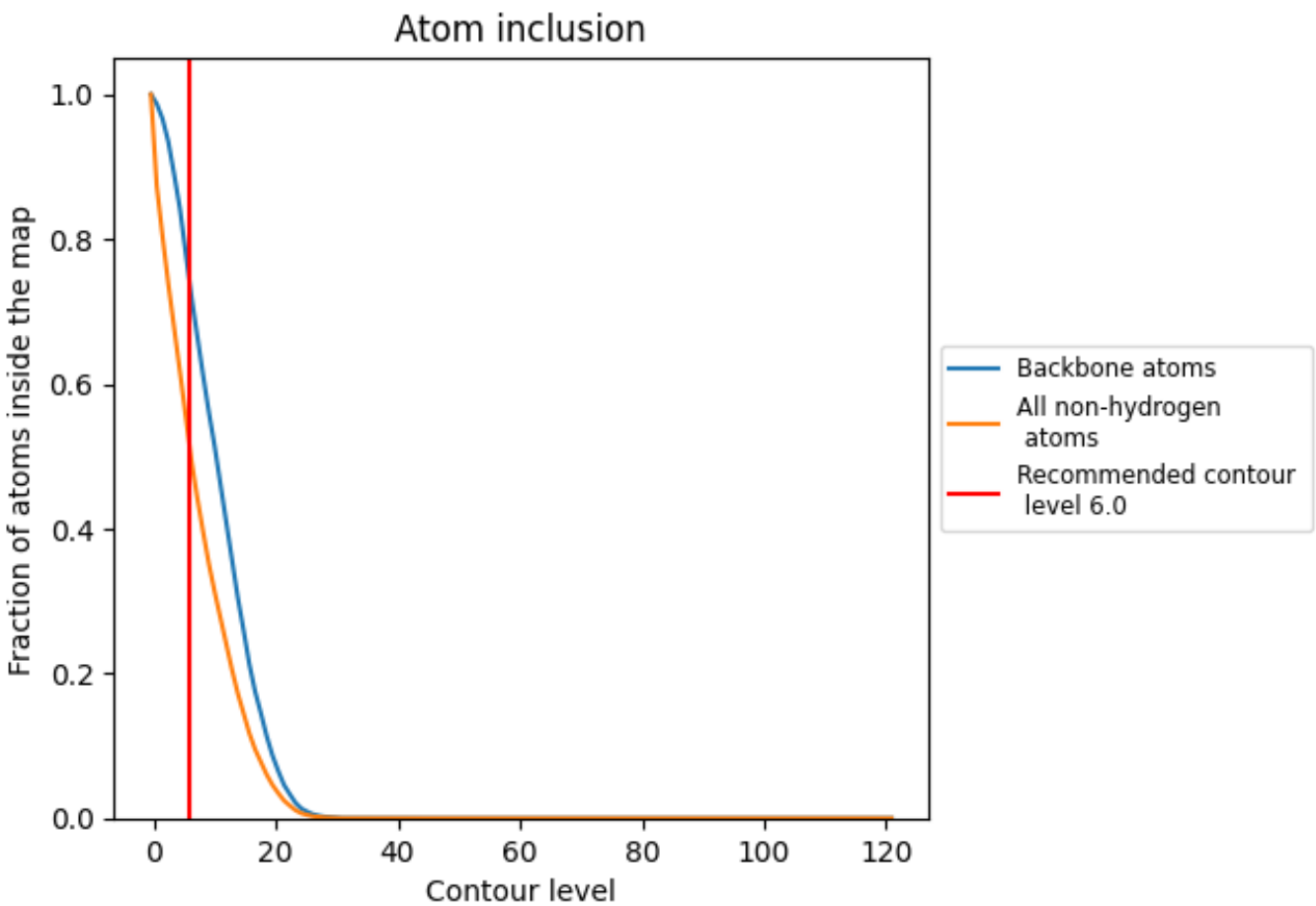
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6.0).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 51% 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 (6.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5070	0.3310
0A	0.7324	0.3750
0B	0.7266	0.3720
0C	0.7332	0.3750
0D	0.7319	0.3750
0E	0.7328	0.3750
0F	0.7341	0.3740
0G	0.7319	0.3730
0H	0.7332	0.3730
0I	0.7324	0.3730
0J	0.7297	0.3730
0K	0.7253	0.3710
0L	0.7328	0.3740
0a	0.3373	0.3190
0b	0.3363	0.3170
0c	0.3377	0.3160
0d	0.3368	0.3180
0e	0.3373	0.3170
0f	0.3377	0.3160
0g	0.3368	0.3180
0h	0.3358	0.3180
0i	0.3373	0.3170
0j	0.3373	0.3190
0k	0.3358	0.3180
0l	0.3373	0.3180
A	0.4249	0.2620
B	0.4589	0.2920
C	0.3620	0.3070
D	0.4202	0.2620
E	0.4589	0.2880
F	0.3653	0.3080
G	0.4272	0.2610
H	0.4547	0.2910
I	0.3586	0.3070
J	0.4249	0.2660

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Chain	Atom inclusion	Q-score
K	0.4611	0.2900
L	0.3620	0.3050
M	0.4225	0.2610
N	0.4611	0.2880
O	0.3653	0.3060
P	0.4296	0.2600
Q	0.4526	0.2880
R	0.3586	0.3040
S	0.4249	0.2640
T	0.4611	0.2910
U	0.3636	0.3030
V	0.4202	0.2600
W	0.4611	0.2870
X	0.3670	0.3060
Y	0.4272	0.2600
Z	0.4484	0.2880
a	0.3636	0.3020
b	0.4202	0.2580
c	0.4611	0.2880
d	0.3620	0.3060
e	0.4155	0.2610
f	0.4547	0.2880
g	0.3721	0.3020
h	0.4272	0.2570
i	0.4526	0.2910
j	0.3620	0.3050