



## wwPDB EM Validation Summary Report ⓘ

Sep 3, 2025 – 05:38 PM EDT

PDB ID : 9AY5 / pdb\_00009ay5  
EMDB ID : EMD-43960  
Title : Tail-Baseplate of P1 bacteriophage  
Authors : Nakamura, T.; Sen, A.; Terashi, G.; Kihara, D.  
Deposited on : 2024-03-07  
Resolution : 6.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev126  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

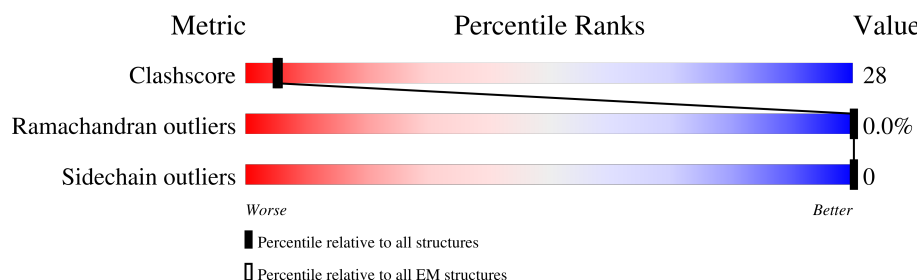
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	203	<div> <div>51%</div> <div>40%</div> <div>48%</div> <div>11%</div> </div>
1	B	203	<div> <div>52%</div> <div>37%</div> <div>51%</div> <div>11%</div> </div>
1	C	203	<div> <div>53%</div> <div>36%</div> <div>52%</div> <div>11%</div> </div>
1	D	203	<div> <div>51%</div> <div>39%</div> <div>50%</div> <div>11%</div> </div>
1	E	203	<div> <div>52%</div> <div>39%</div> <div>50%</div> <div>11%</div> </div>
1	F	203	<div> <div>53%</div> <div>38%</div> <div>51%</div> <div>11%</div> </div>
2	G	193	<div> <div>54%</div> <div>39%</div> <div>42%</div> <div>18%</div> </div>
2	H	193	<div> <div>52%</div> <div>40%</div> <div>41%</div> <div>18%</div> </div>

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Mol	Chain	Length	Quality of chain
2	I	193	
2	J	193	
2	K	193	
2	L	193	
3	M	118	
3	N	118	
3	O	118	
3	P	118	
3	Q	118	
3	R	118	
4	S	125	
4	T	125	
4	U	125	
4	V	125	
4	W	125	
4	X	125	
5	0	477	
5	1	477	
5	2	477	
5	3	477	
5	4	477	
5	5	477	
5	6	477	
5	7	477	
5	8	477	

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Mol	Chain	Length	Quality of chain
5	9	477	
5	Y	477	
5	Z	477	
6	a	278	
6	b	278	
6	c	278	
6	d	278	
6	e	278	
6	f	278	
7	AA	529	
7	BA	529	
7	CA	529	
7	DA	529	
7	EA	529	
7	FA	529	
7	GA	529	
7	HA	529	
7	IA	529	
7	JA	529	
7	KA	529	
7	LA	529	
7	MA	529	
7	NA	529	
7	OA	529	
7	PA	529	

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Mol	Chain	Length	Quality of chain
7	QA	529	
7	RA	529	
7	g	529	
7	h	529	
7	i	529	
7	j	529	
7	k	529	
7	l	529	
7	m	529	
7	n	529	
7	o	529	
7	p	529	
7	q	529	
7	r	529	
8	AB	169	
8	BB	169	
8	CB	169	
8	DB	169	
8	EB	169	
8	FB	169	
8	GB	169	
8	HB	169	
8	IB	169	
8	JB	169	
8	KB	169	

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Mol	Chain	Length	Quality of chain
8	LB	169	
8	MB	169	
8	NB	169	
8	OB	169	
8	PB	169	
8	QB	169	
8	RB	169	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 225414 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 Tub.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	180	Total	C	N	O	S	0	0
			1409	900	229	274	6		
1	B	180	Total	C	N	O	S	0	0
			1409	900	229	274	6		
1	C	180	Total	C	N	O	S	0	0
			1409	900	229	274	6		
1	D	180	Total	C	N	O	S	0	0
			1409	900	229	274	6		
1	E	180	Total	C	N	O	S	0	0
			1409	900	229	274	6		
1	F	180	Total	C	N	O	S	0	0
			1409	900	229	274	6		

- Molecule 2 is a protein called PmgG.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	158	Total	C	N	O	S	0	0
			1202	764	199	235	4		
2	H	158	Total	C	N	O	S	0	0
			1202	764	199	235	4		
2	I	158	Total	C	N	O	S	0	0
			1202	764	199	235	4		
2	J	158	Total	C	N	O	S	0	0
			1202	764	199	235	4		
2	K	158	Total	C	N	O	S	0	0
			1202	764	199	235	4		
2	L	158	Total	C	N	O	S	0	0
			1202	764	199	235	4		

- Molecule 3 is a protein called PmgA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	112	Total	C	N	O	S	0	0
			888	571	142	174	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	112	Total	C	N	O	S	0	0
			888	571	142	174	1		
3	O	112	Total	C	N	O	S	0	0
			888	571	142	174	1		
3	P	112	Total	C	N	O	S	0	0
			888	571	142	174	1		
3	Q	112	Total	C	N	O	S	0	0
			888	571	142	174	1		
3	R	112	Total	C	N	O	S	0	0
			888	571	142	174	1		

- Molecule 4 is a protein called Gp26.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	115	Total	C	N	O	S	0	0
			944	602	163	173	6		
4	T	115	Total	C	N	O	S	0	0
			944	602	163	173	6		
4	U	115	Total	C	N	O	S	0	0
			944	602	163	173	6		
4	V	115	Total	C	N	O	S	0	0
			944	602	163	173	6		
4	W	115	Total	C	N	O	S	0	0
			944	602	163	173	6		
4	X	115	Total	C	N	O	S	0	0
			944	602	163	173	6		

- Molecule 5 is a protein called BplA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	477	Total	C	N	O	S	0	0
			3780	2426	601	741	12		
5	Z	477	Total	C	N	O	S	0	0
			3780	2426	601	741	12		
5	0	477	Total	C	N	O	S	0	0
			3780	2426	601	741	12		
5	1	477	Total	C	N	O	S	0	0
			3780	2426	601	741	12		
5	2	477	Total	C	N	O	S	0	0
			3780	2426	601	741	12		
5	3	477	Total	C	N	O	S	0	0
			3780	2426	601	741	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	477	Total	C	N	O	S	0	0
			3780	2426	601	741	12		
5	5	477	Total	C	N	O	S	0	0
			3780	2426	601	741	12		
5	6	477	Total	C	N	O	S	0	0
			3780	2426	601	741	12		
5	7	477	Total	C	N	O	S	0	0
			3780	2426	601	741	12		
5	8	477	Total	C	N	O	S	0	0
			3780	2426	601	741	12		
5	9	477	Total	C	N	O	S	0	0
			3780	2426	601	741	12		

- Molecule 6 is a protein called Gp16.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	a	204	Total	C	N	O	S	0	0
			1652	1056	279	309	8		
6	b	204	Total	C	N	O	S	0	0
			1652	1056	279	309	8		
6	c	204	Total	C	N	O	S	0	0
			1652	1056	279	309	8		
6	d	204	Total	C	N	O	S	0	0
			1652	1056	279	309	8		
6	e	204	Total	C	N	O	S	0	0
			1652	1056	279	309	8		
6	f	204	Total	C	N	O	S	0	0
			1652	1056	279	309	8		

- Molecule 7 is a protein called Gp22.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	528	Total	C	N	O	S	0	0
			3995	2525	668	784	18		
7	h	528	Total	C	N	O	S	0	0
			3995	2525	668	784	18		
7	i	528	Total	C	N	O	S	0	0
			3995	2525	668	784	18		
7	j	528	Total	C	N	O	S	0	0
			3995	2525	668	784	18		
7	k	528	Total	C	N	O	S	0	0
			3995	2525	668	784	18		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	l	528	Total 3995	C 2525	N 668	O 784	S 18	0	0
7	m	528	Total 3995	C 2525	N 668	O 784	S 18	0	0
7	n	528	Total 3995	C 2525	N 668	O 784	S 18	0	0
7	o	528	Total 3995	C 2525	N 668	O 784	S 18	0	0
7	p	528	Total 3995	C 2525	N 668	O 784	S 18	0	0
7	q	528	Total 3995	C 2525	N 668	O 784	S 18	0	0
7	r	528	Total 3995	C 2525	N 668	O 784	S 18	0	0
7	AA	528	Total 3995	C 2525	N 668	O 784	S 18	0	0
7	BA	528	Total 3995	C 2525	N 668	O 784	S 18	0	0
7	CA	528	Total 3995	C 2525	N 668	O 784	S 18	0	0
7	DA	528	Total 3995	C 2525	N 668	O 784	S 18	0	0
7	EA	528	Total 3995	C 2525	N 668	O 784	S 18	0	0
7	FA	528	Total 3995	C 2525	N 668	O 784	S 18	0	0
7	GA	528	Total 3995	C 2525	N 668	O 784	S 18	0	0
7	HA	528	Total 3995	C 2525	N 668	O 784	S 18	0	0
7	IA	528	Total 3995	C 2525	N 668	O 784	S 18	0	0
7	JA	528	Total 3995	C 2525	N 668	O 784	S 18	0	0
7	KA	528	Total 3995	C 2525	N 668	O 784	S 18	0	0
7	LA	528	Total 3995	C 2525	N 668	O 784	S 18	0	0
7	MA	528	Total 3995	C 2525	N 668	O 784	S 18	0	0
7	NA	528	Total 3995	C 2525	N 668	O 784	S 18	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	OA	528	Total	C	N	O	S	0	0
			3995	2525	668	784	18		
7	PA	528	Total	C	N	O	S	0	0
			3995	2525	668	784	18		
7	QA	528	Total	C	N	O	S	0	0
			3995	2525	668	784	18		
7	RA	528	Total	C	N	O	S	0	0
			3995	2525	668	784	18		

- Molecule 8 is a protein called BplB.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AB	168	Total	C	N	O	S	0	0
			1313	819	227	262	5		
8	BB	168	Total	C	N	O	S	0	0
			1313	819	227	262	5		
8	CB	168	Total	C	N	O	S	0	0
			1313	819	227	262	5		
8	DB	168	Total	C	N	O	S	0	0
			1313	819	227	262	5		
8	EB	168	Total	C	N	O	S	0	0
			1313	819	227	262	5		
8	FB	168	Total	C	N	O	S	0	0
			1313	819	227	262	5		
8	GB	168	Total	C	N	O	S	0	0
			1313	819	227	262	5		
8	HB	168	Total	C	N	O	S	0	0
			1313	819	227	262	5		
8	IB	168	Total	C	N	O	S	0	0
			1313	819	227	262	5		
8	JB	168	Total	C	N	O	S	0	0
			1313	819	227	262	5		
8	KB	168	Total	C	N	O	S	0	0
			1313	819	227	262	5		
8	LB	168	Total	C	N	O	S	0	0
			1313	819	227	262	5		
8	MB	168	Total	C	N	O	S	0	0
			1313	819	227	262	5		
8	NB	168	Total	C	N	O	S	0	0
			1313	819	227	262	5		
8	OB	168	Total	C	N	O	S	0	0
			1313	819	227	262	5		

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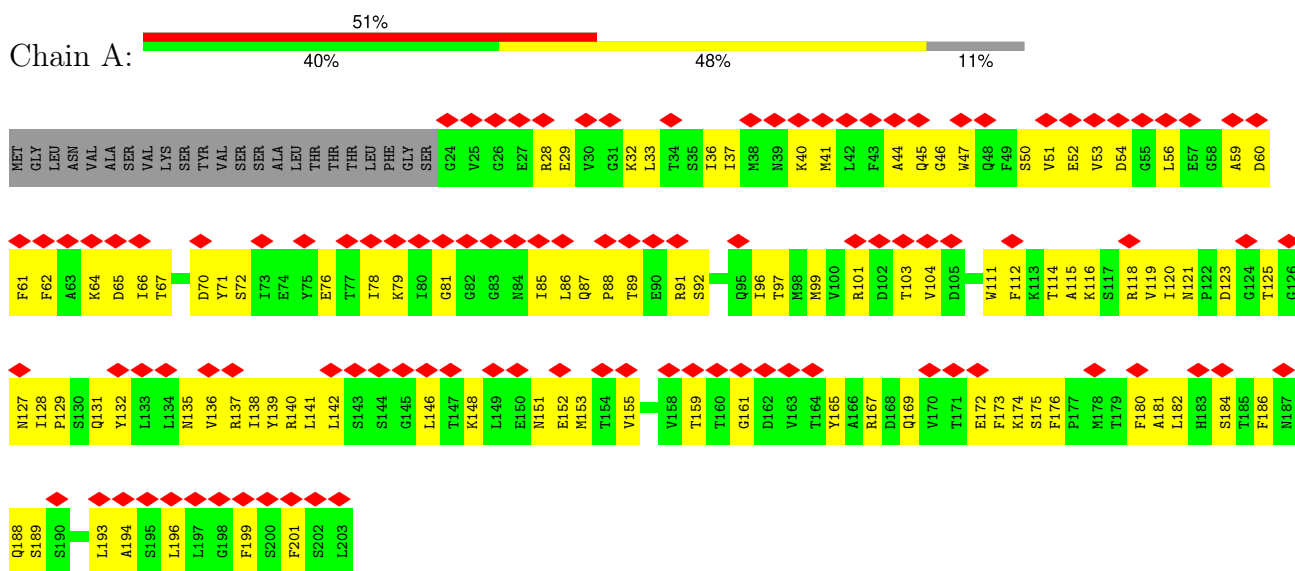
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Mol	Chain	Residues	Atoms					AltConf	Trace
8	PB	168	Total	C	N	O	S	0	0
			1313	819	227	262	5		
8	QB	168	Total	C	N	O	S	0	0
			1313	819	227	262	5		
8	RB	168	Total	C	N	O	S	0	0
			1313	819	227	262	5		

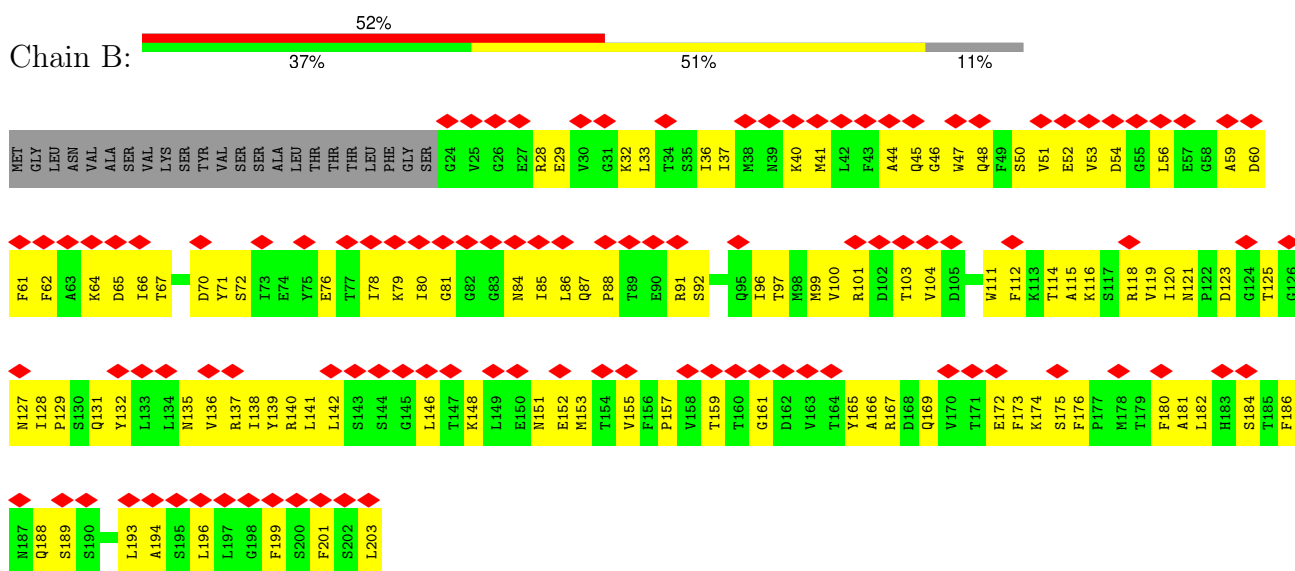
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

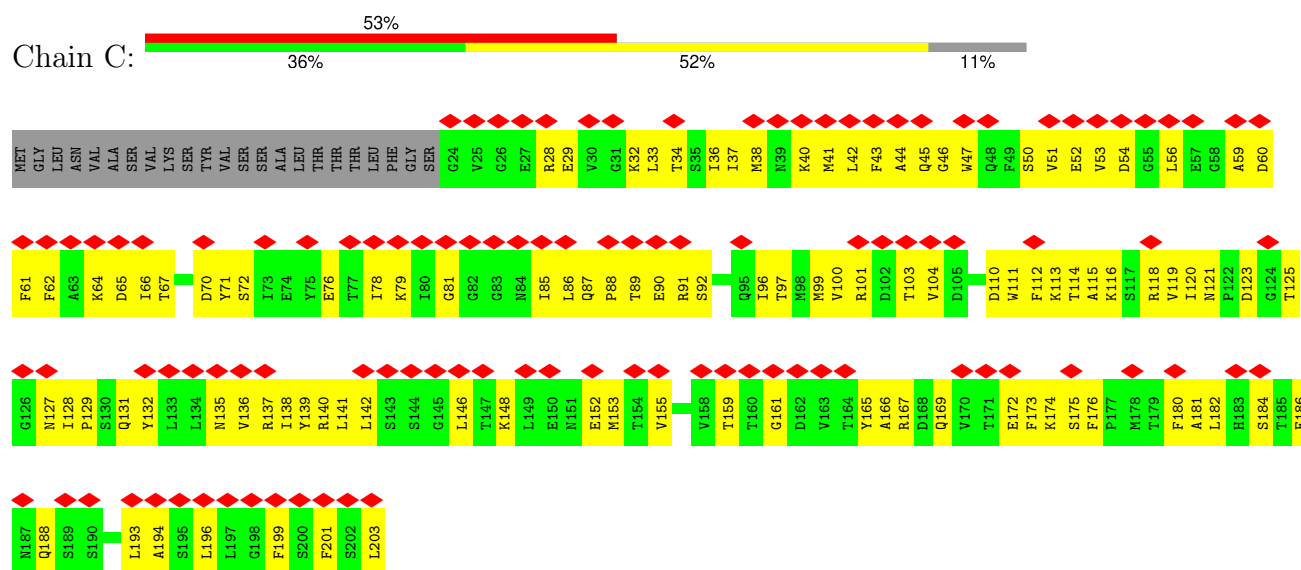
#### • Molecule 1: Tub



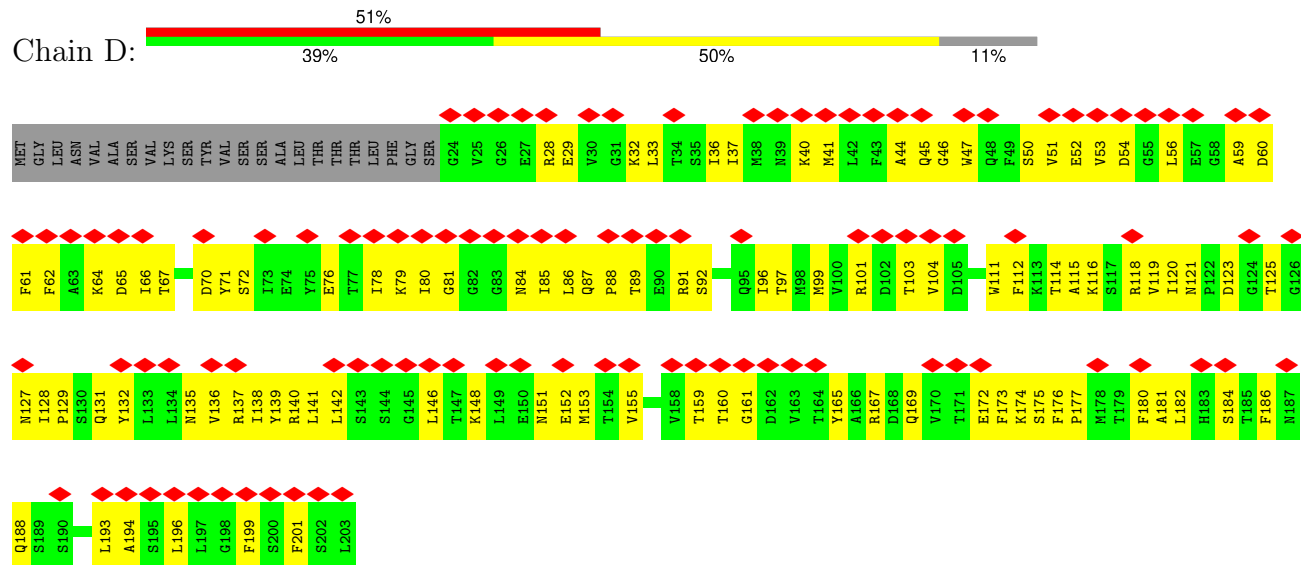
#### • Molecule 1: Tub



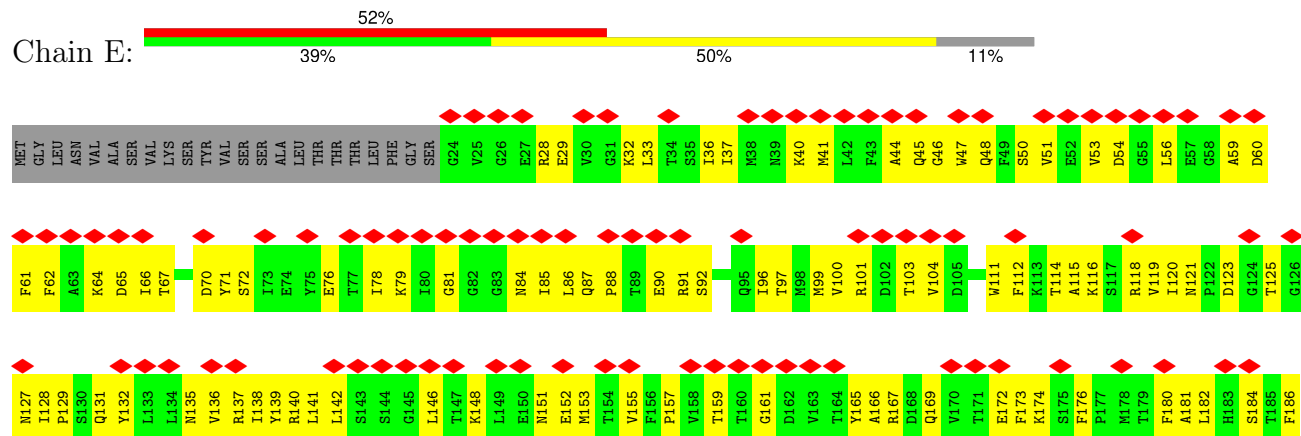
#### • Molecule 1: Tub



• Molecule 1: Tub

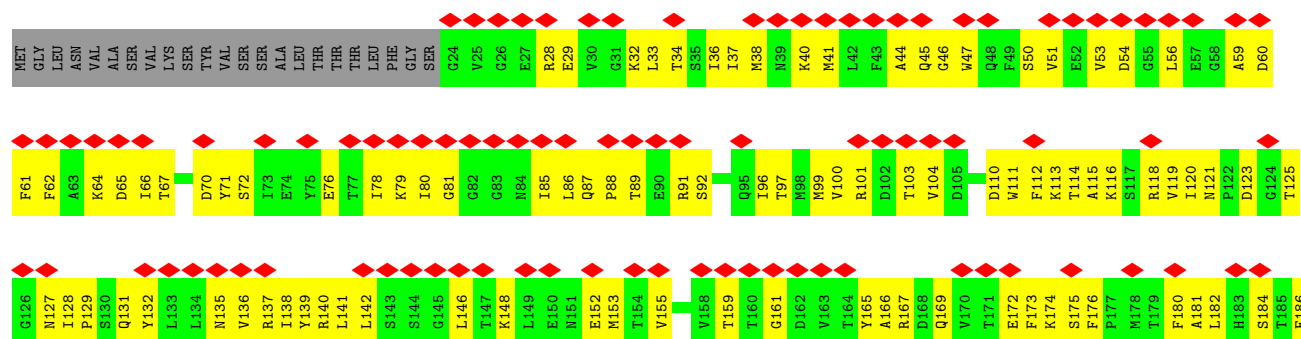
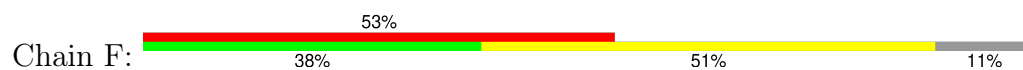


• Molecule 1: Tub

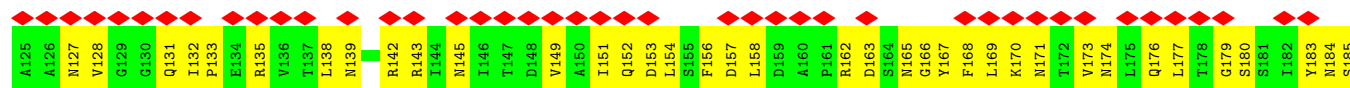
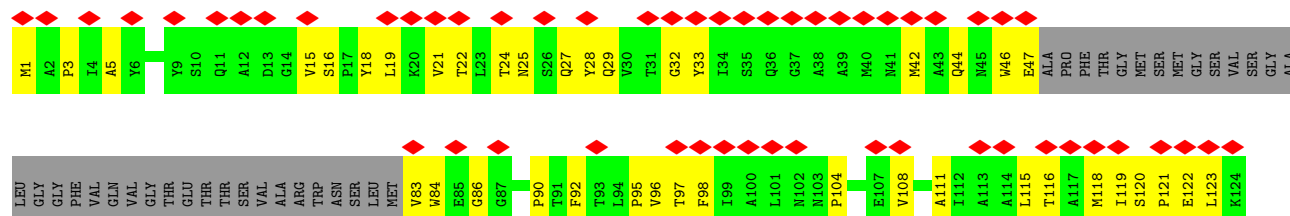




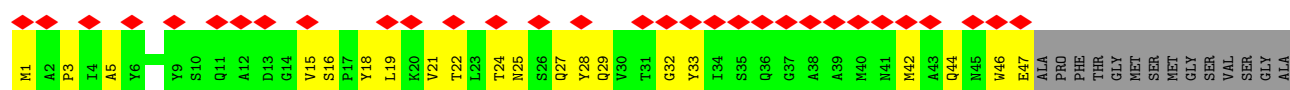
• Molecule 1: Tub

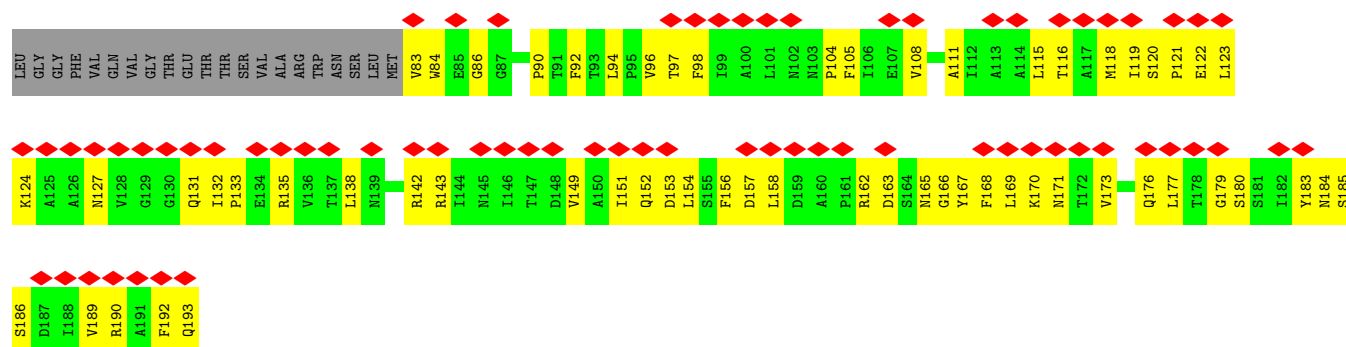


• Molecule 2: PmgG

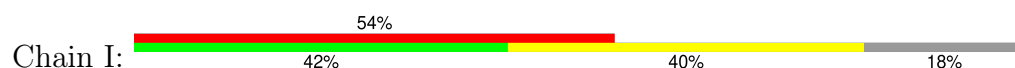


• Molecule 2: PmgG

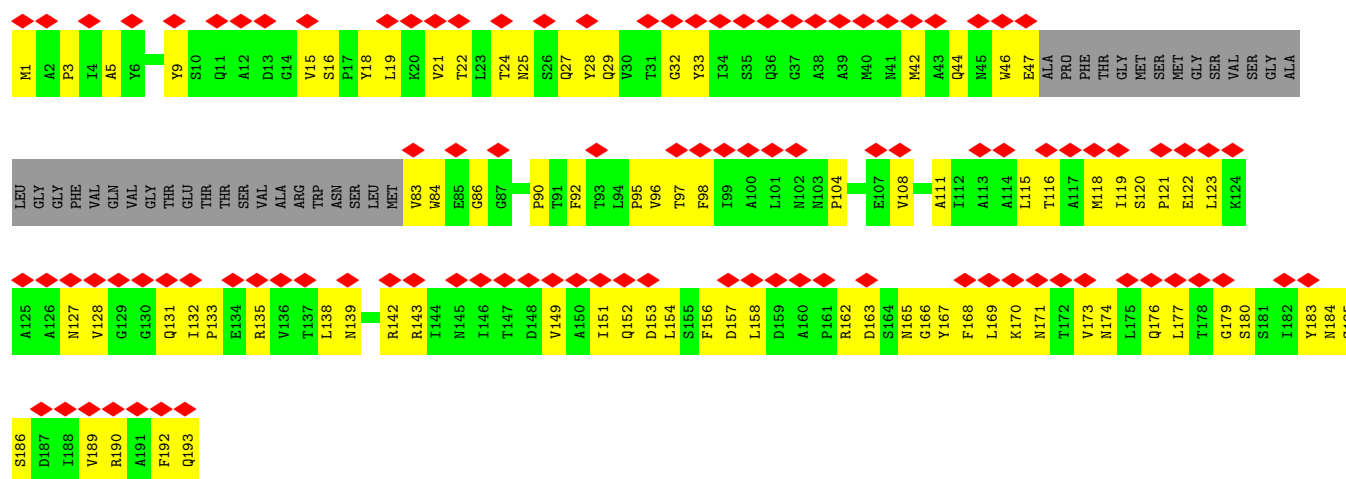




• Molecule 2: PmgG

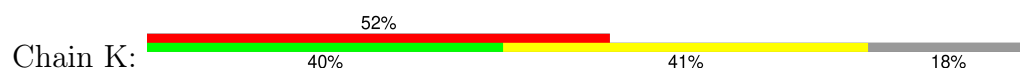


• Molecule 2: PmgG

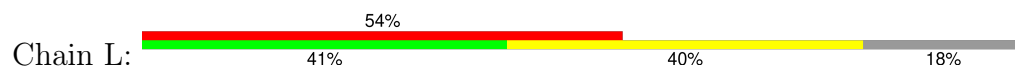


• Molecule 2: PmgG

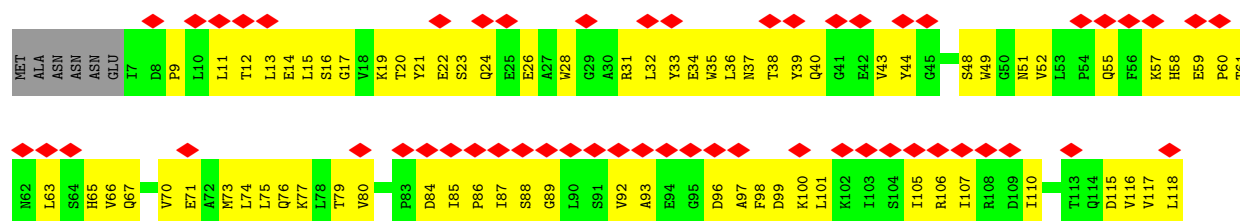




• Molecule 2: PmgG

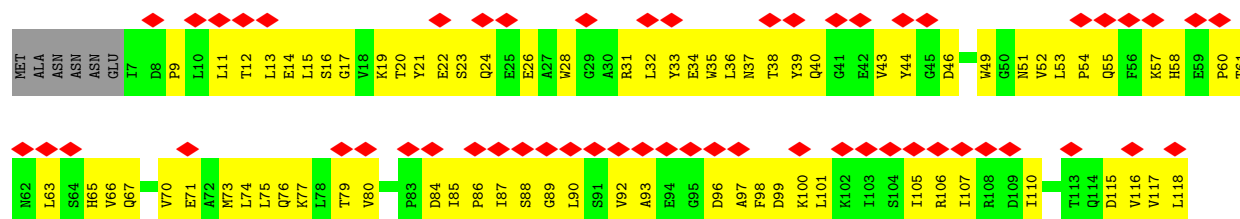


• Molecule 3: PmgA

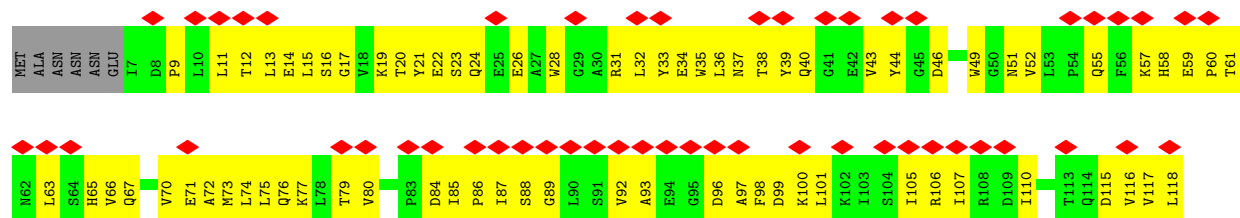
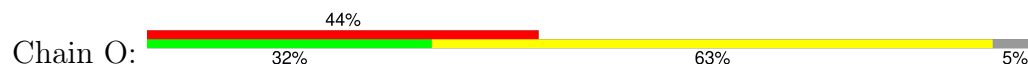


• Molecule 3: PmgA

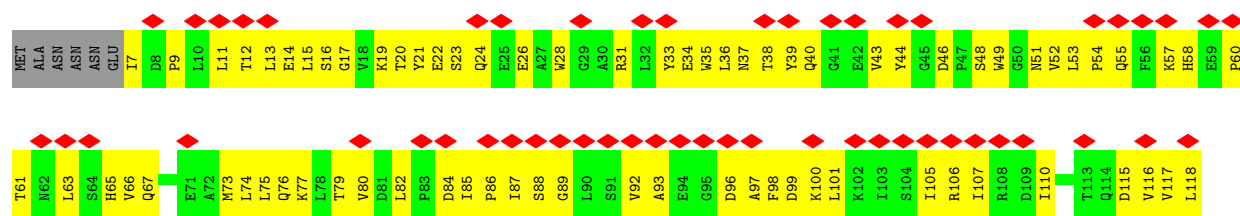




• Molecule 3: PmgA



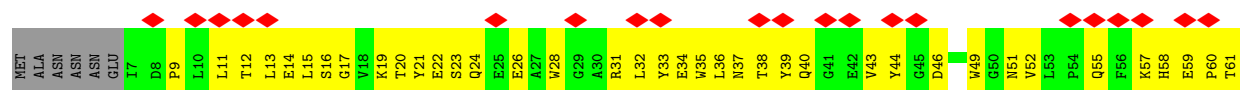
• Molecule 3: PmgA

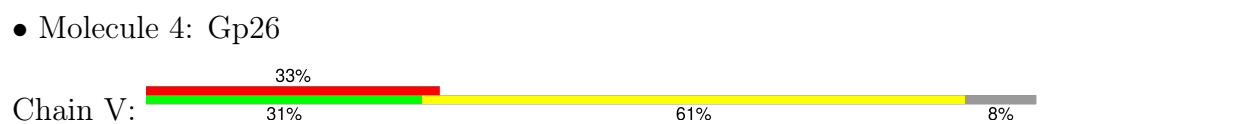
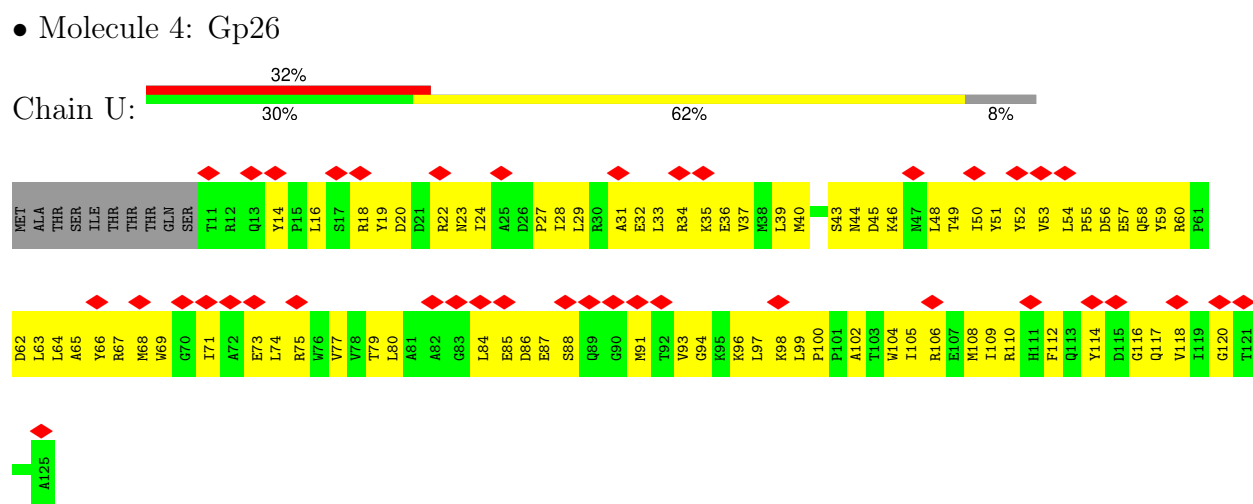
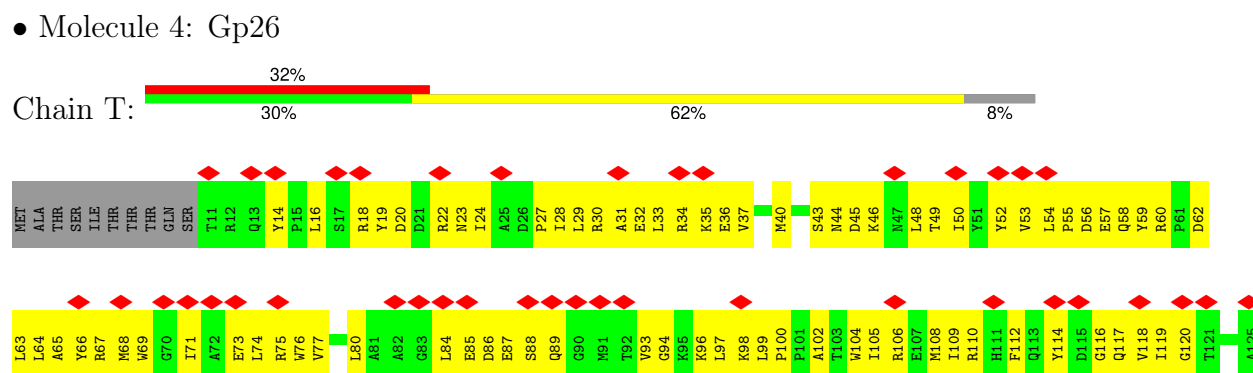
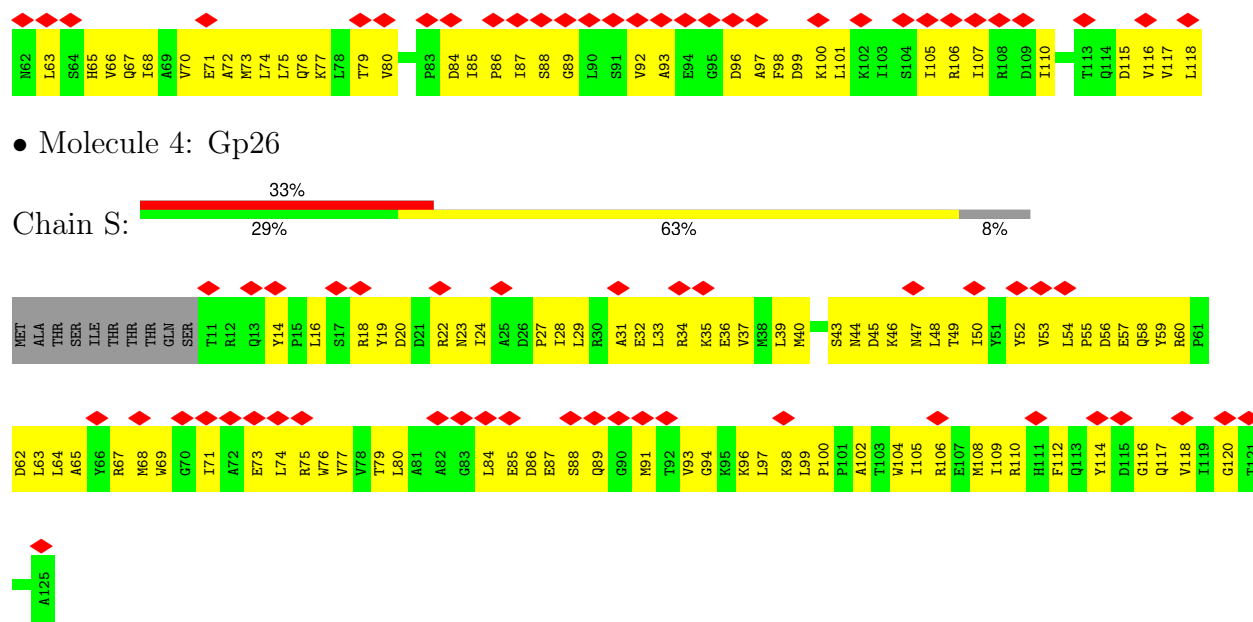


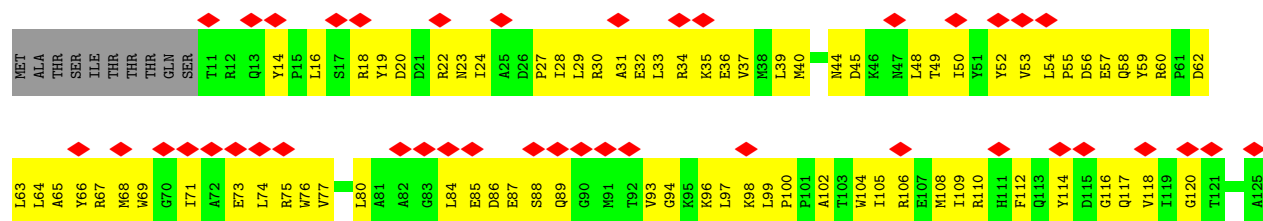
• Molecule 3: PmgA



• Molecule 3: PmgA



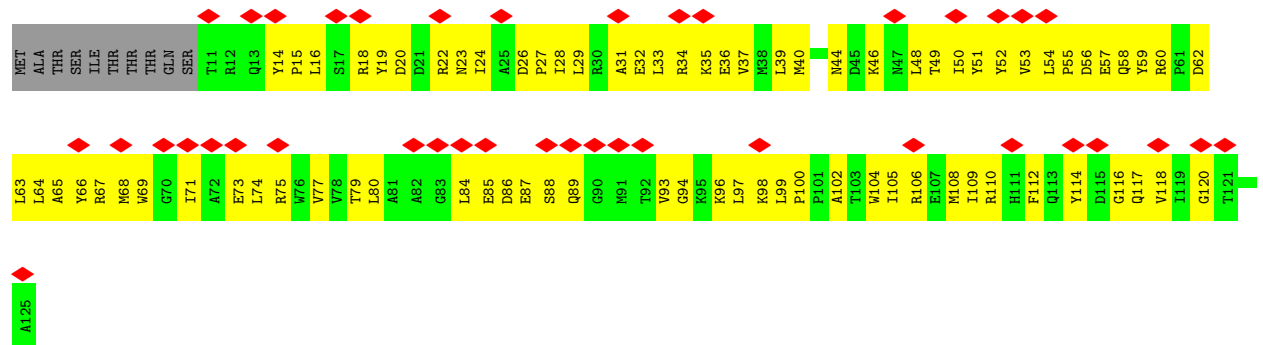




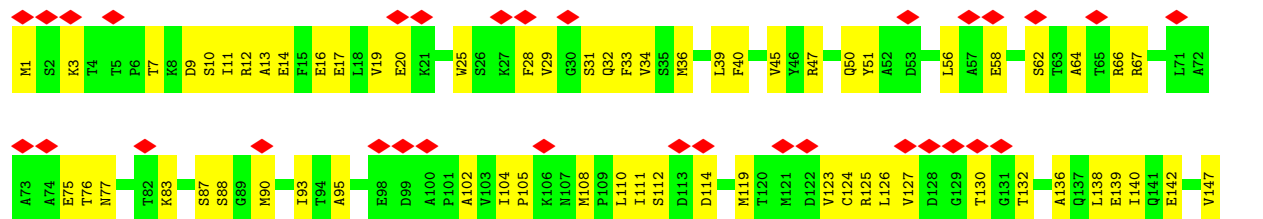
## • Molecule 4: Gp26

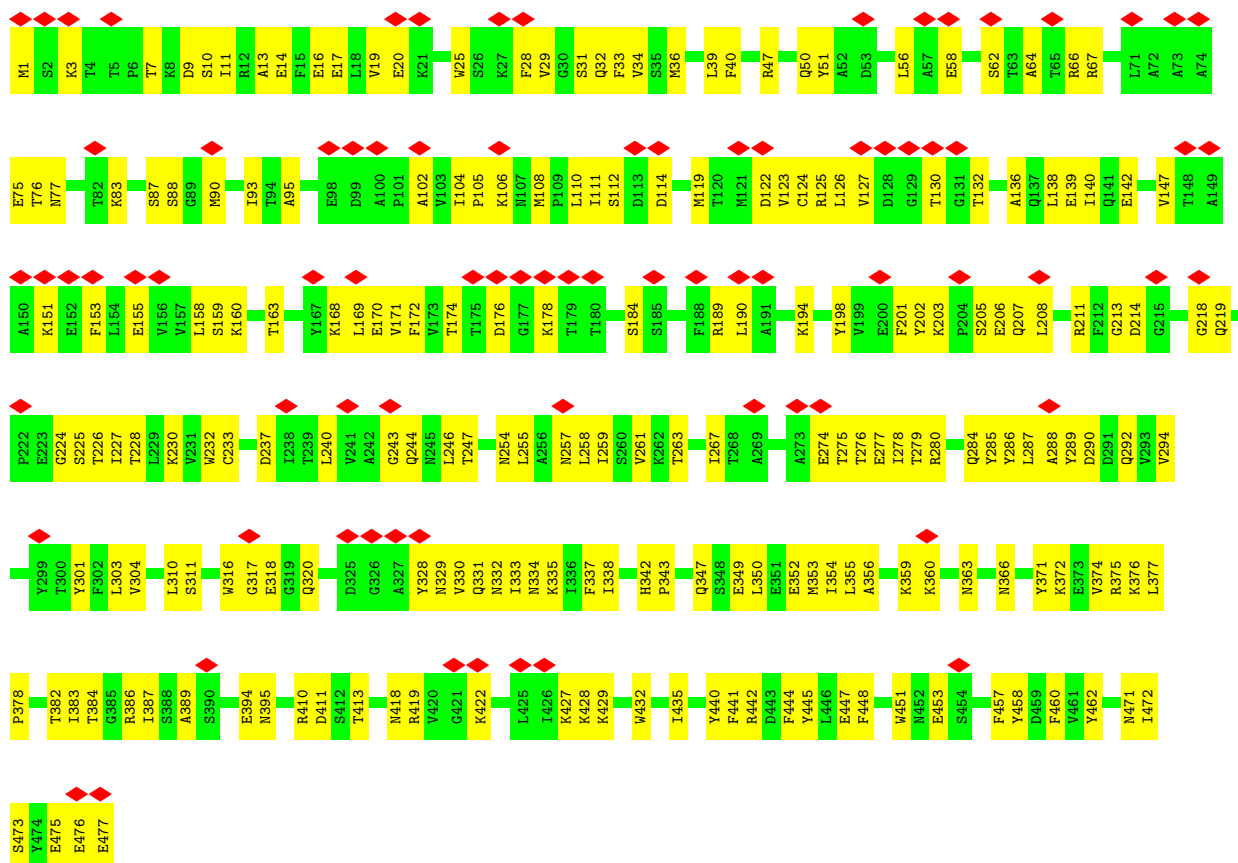
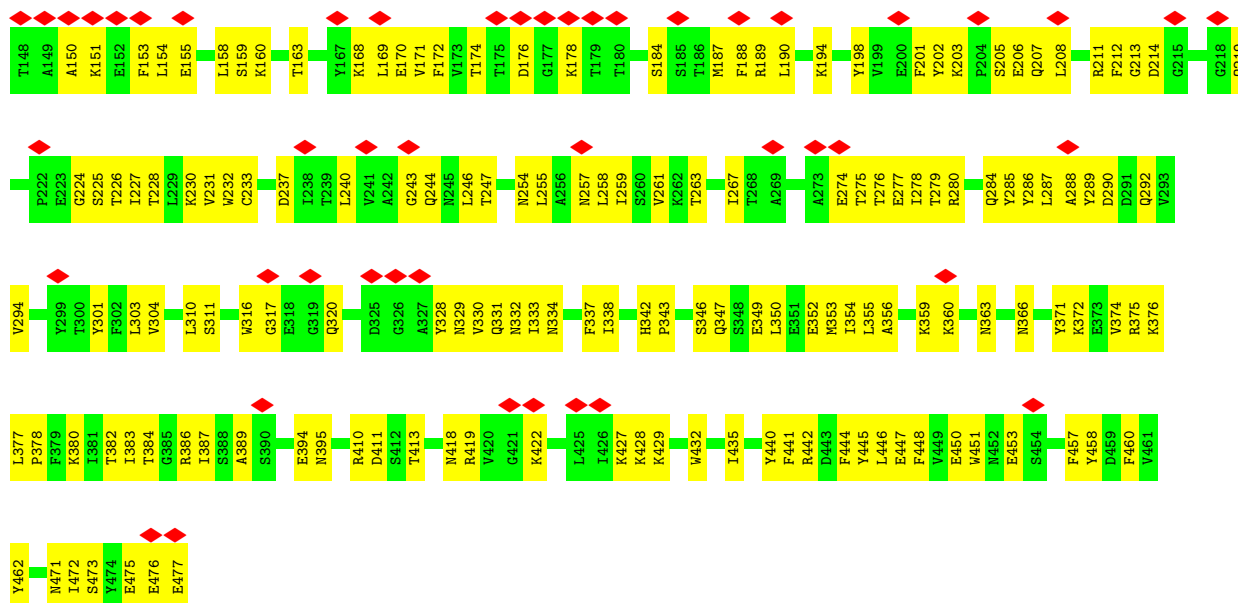


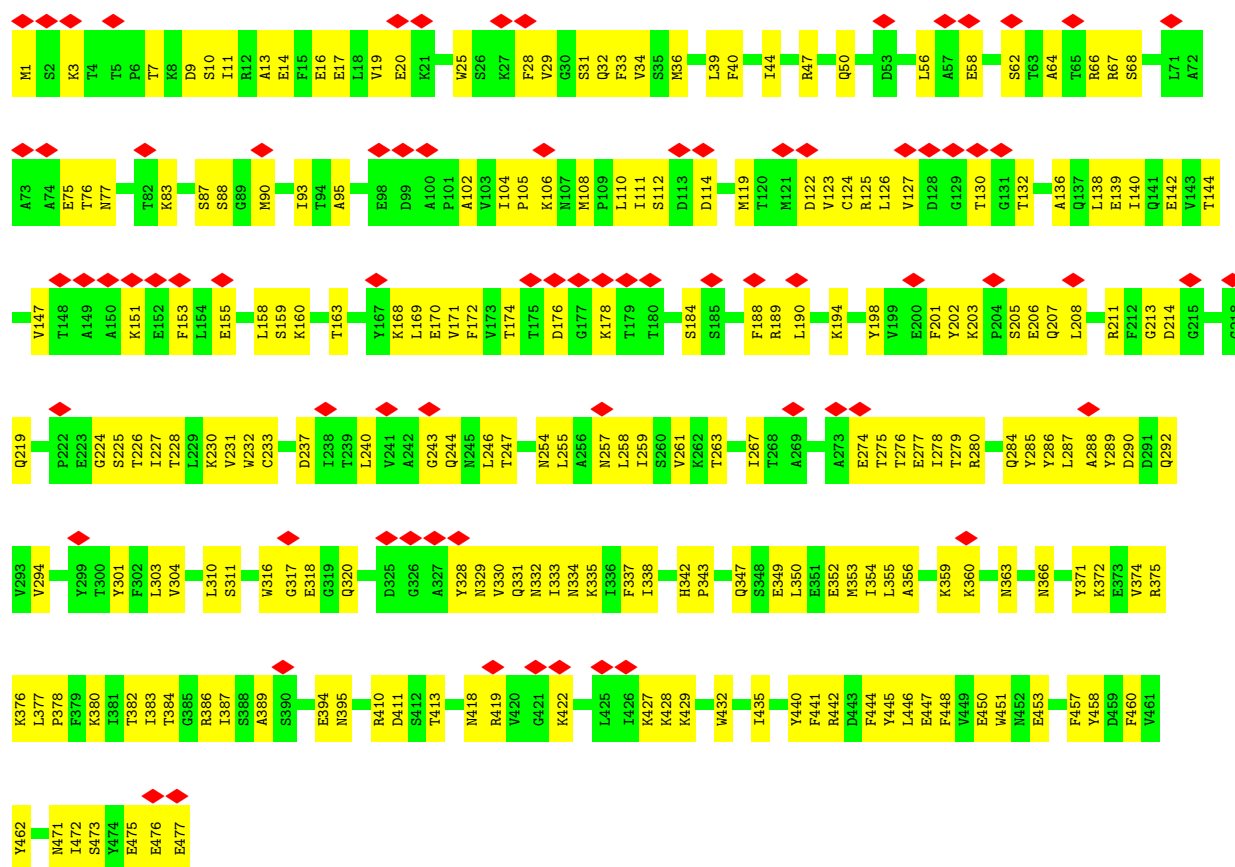
## • Molecule 4: Gp26



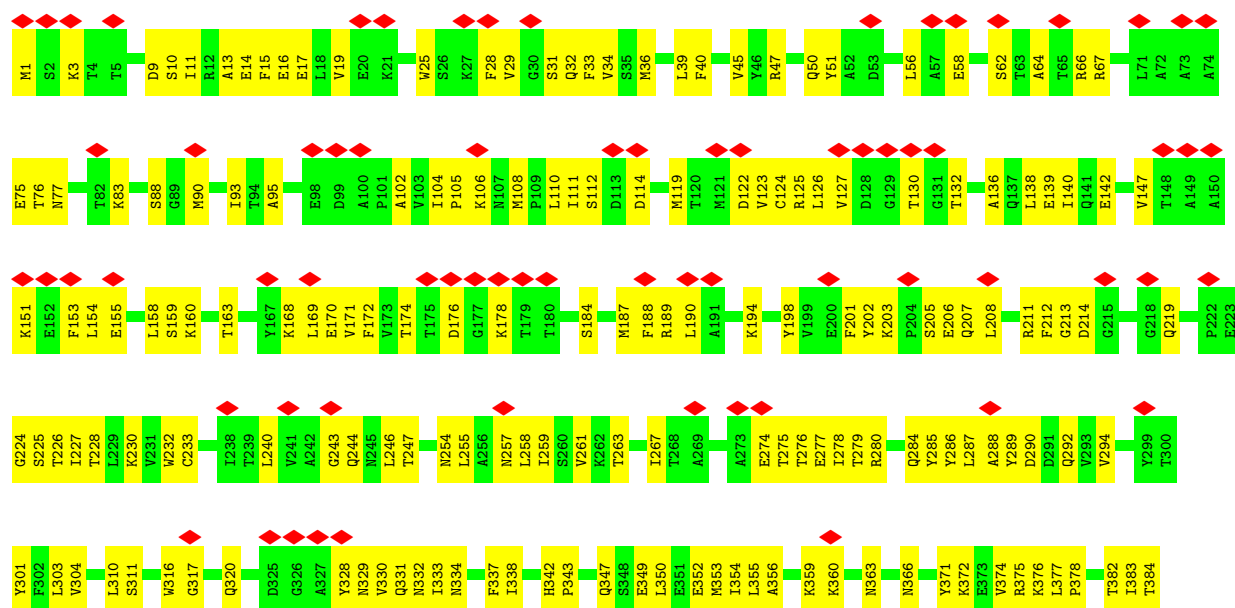
## • Molecule 5: Bp1A





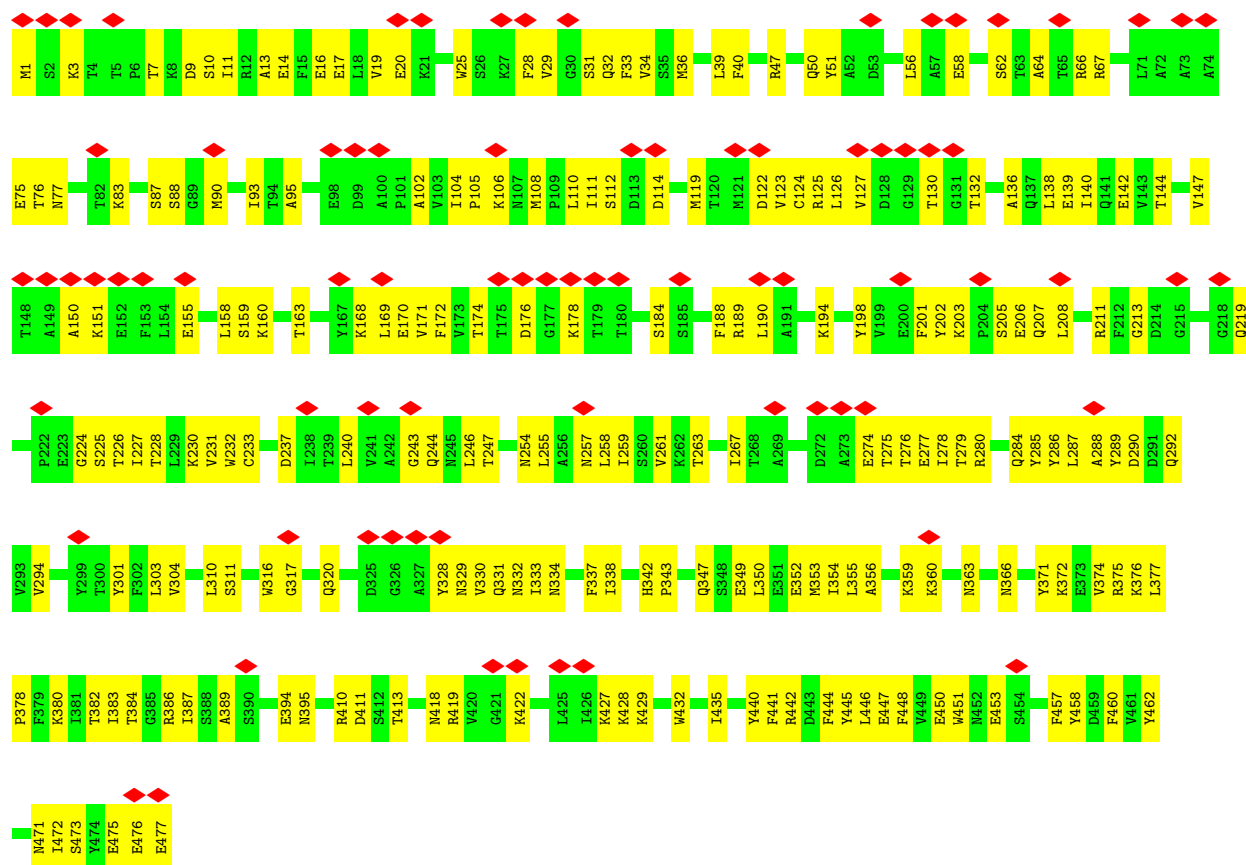


• Molecule 5: BplA

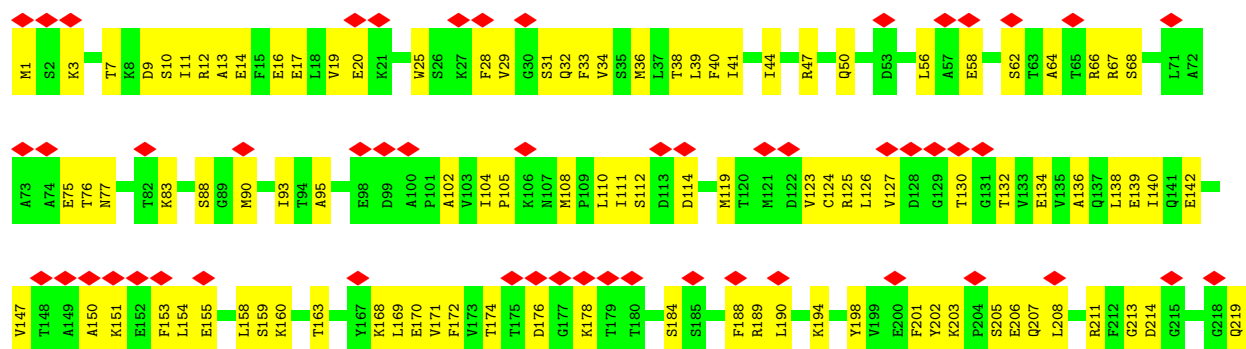


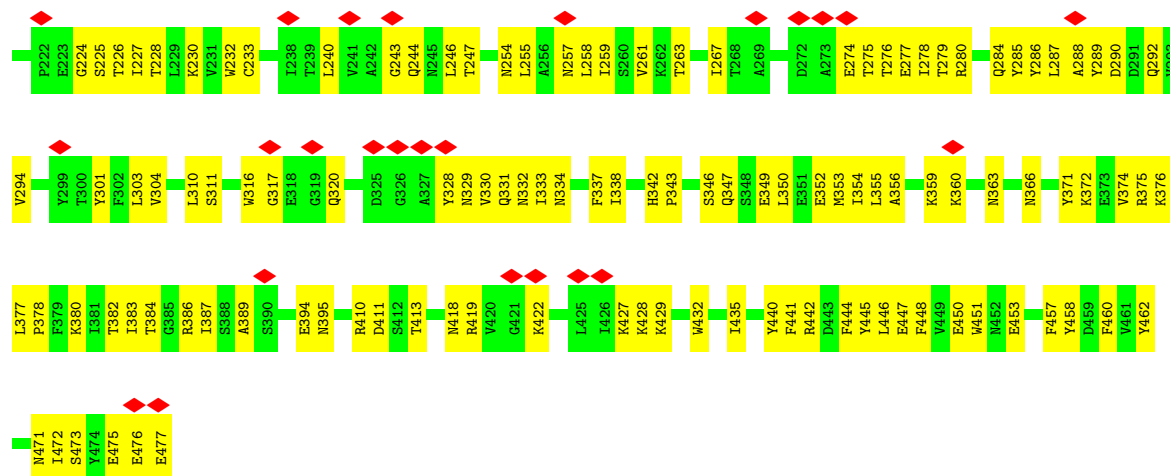


• Molecule 5: BplA

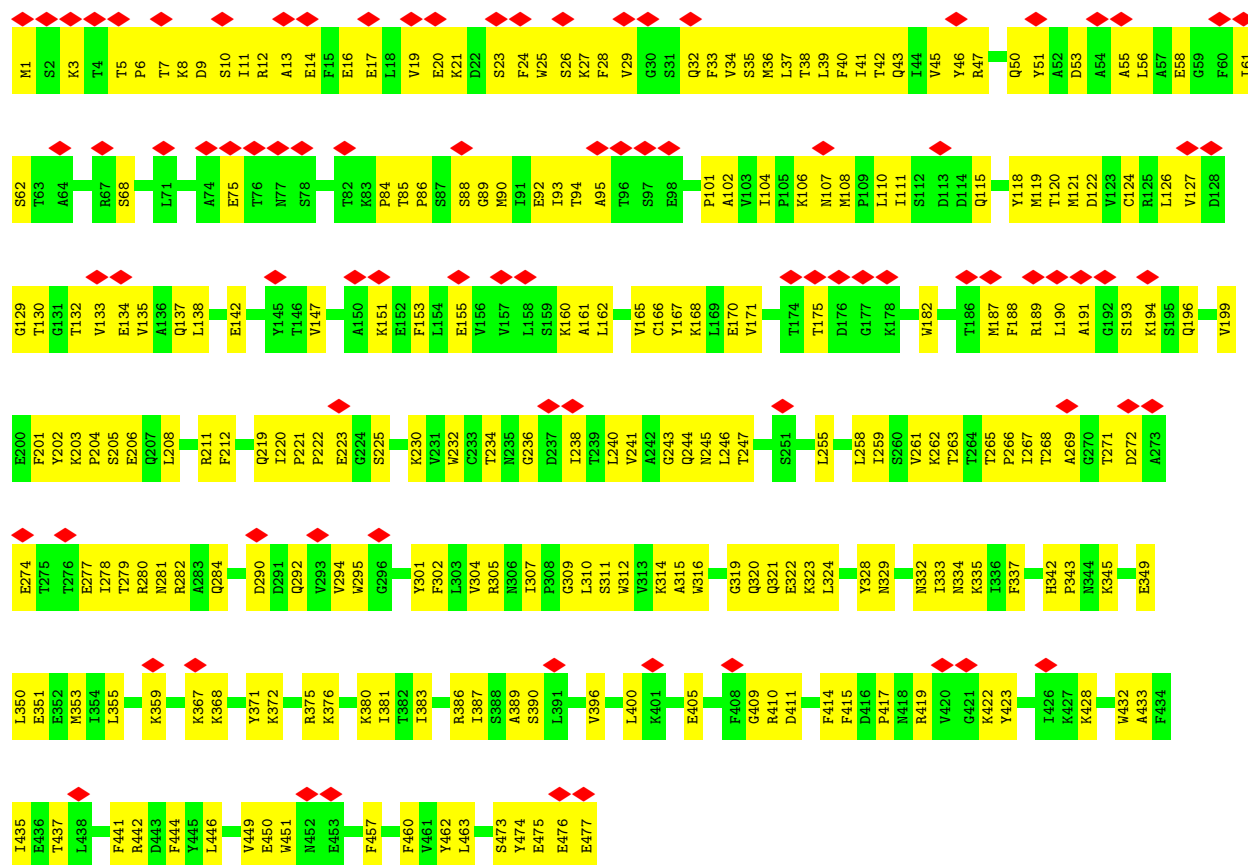


• Molecule 5: BplA





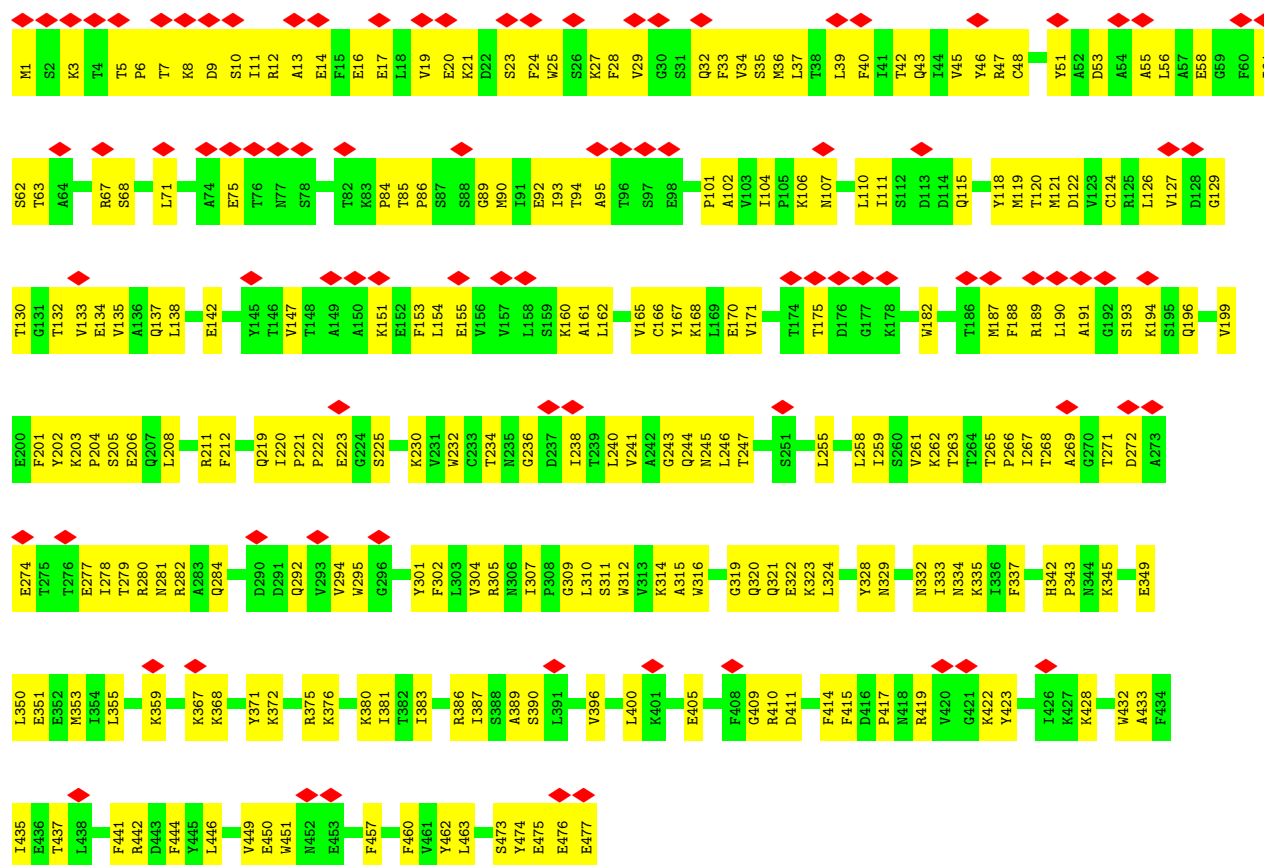
### • Molecule 5: BplA



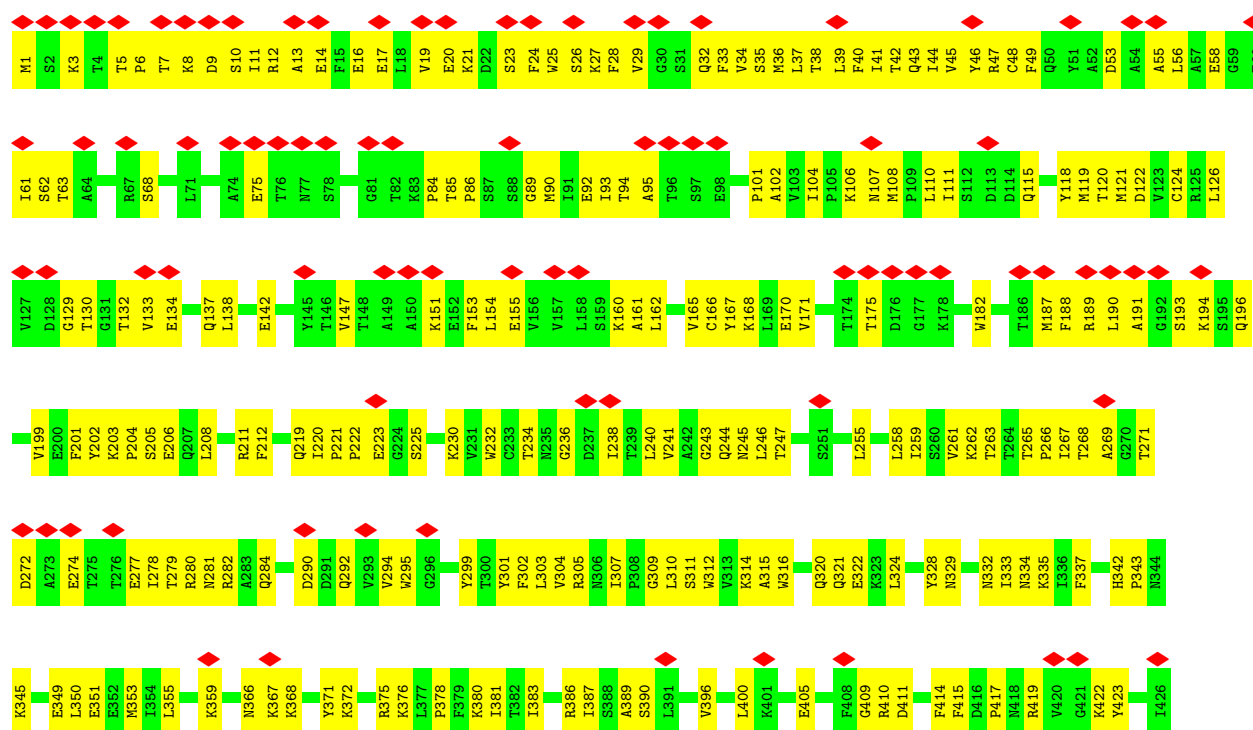
### • Molecule 5: BplA

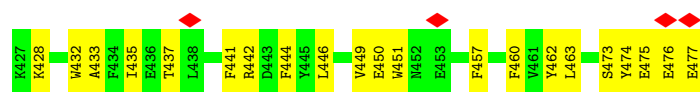




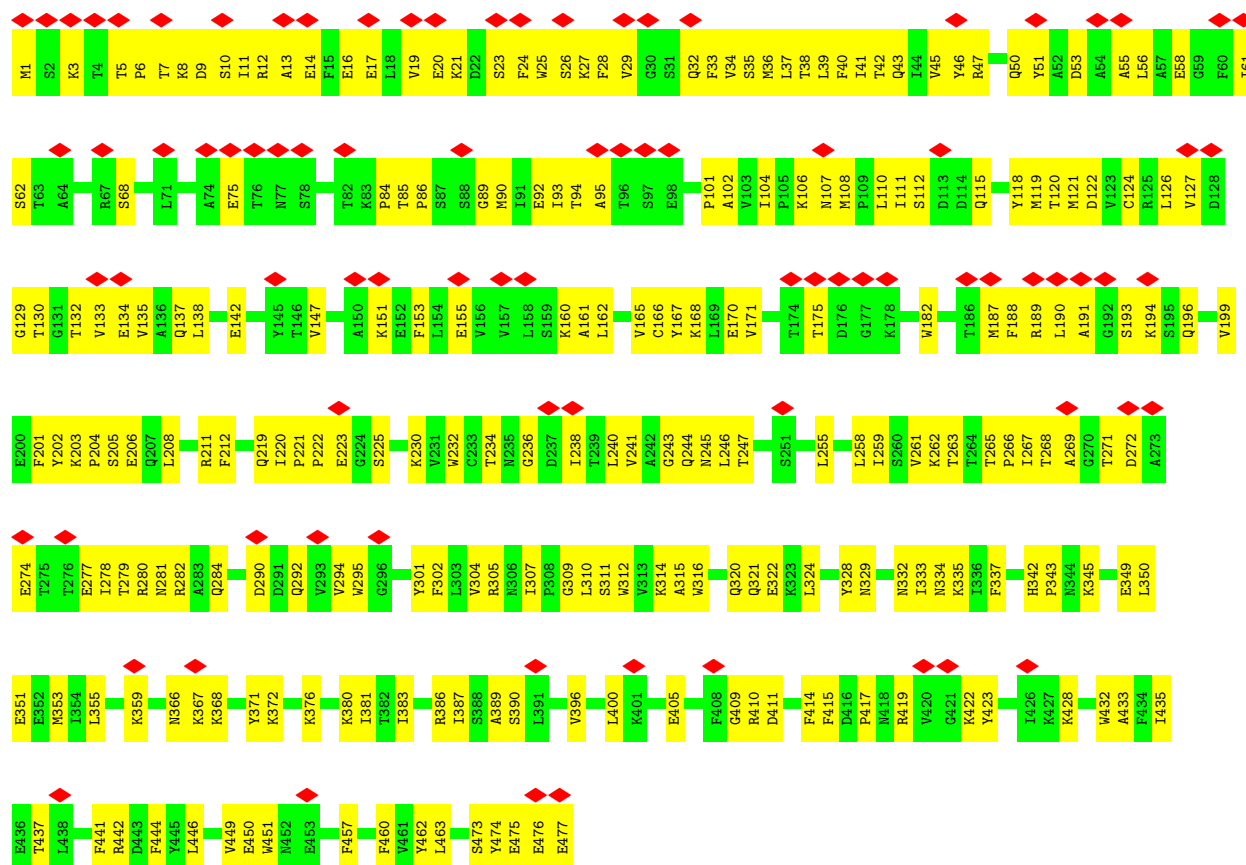


• Molecule 5: BplA

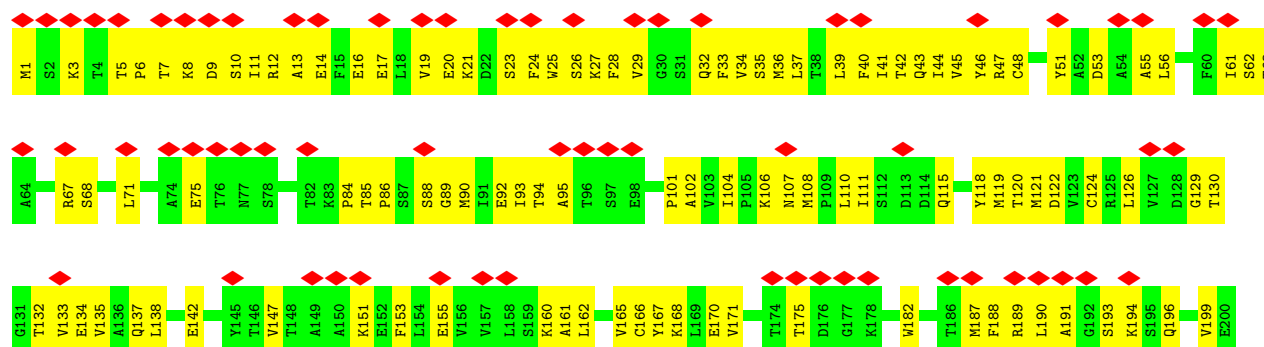


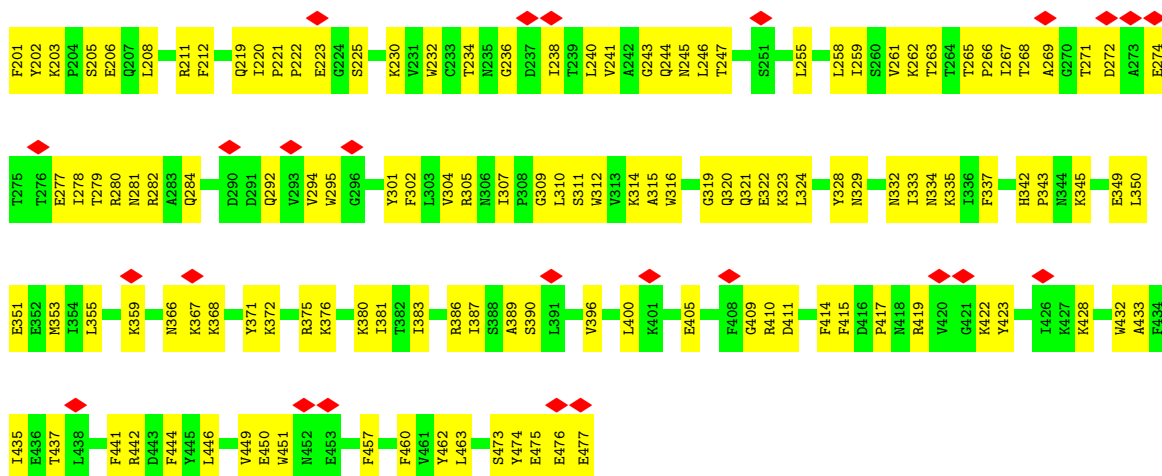


• Molecule 5: BplA

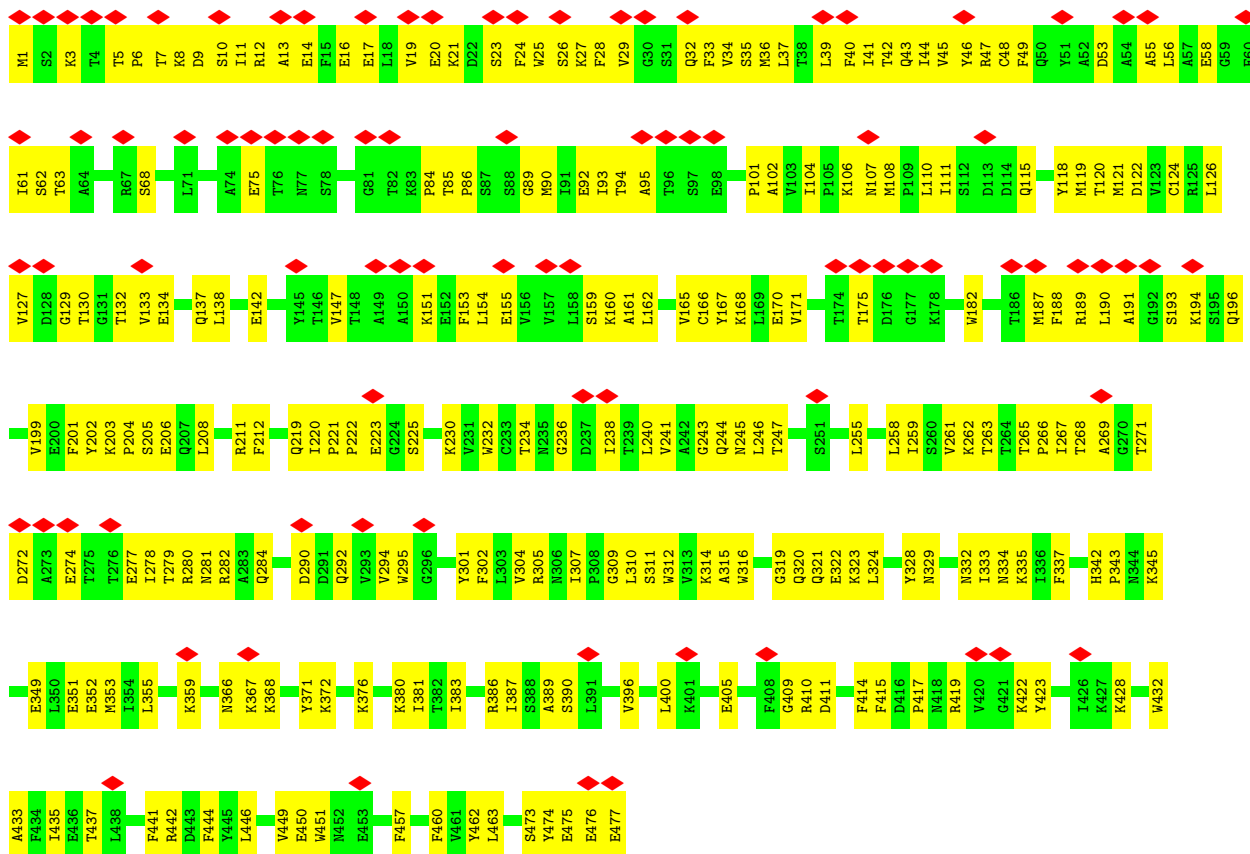


• Molecule 5: BplA

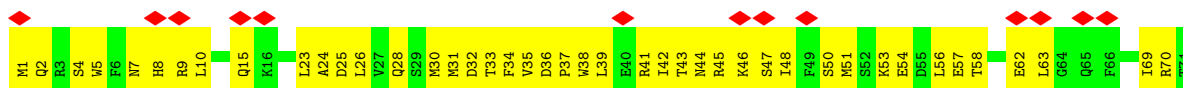




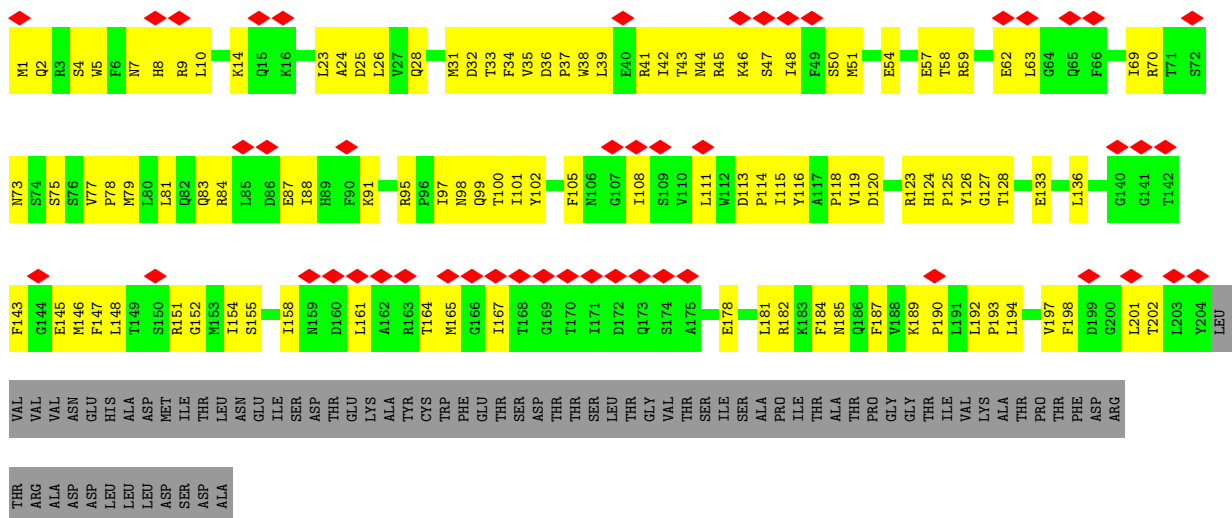
### • Molecule 5: Bp1A



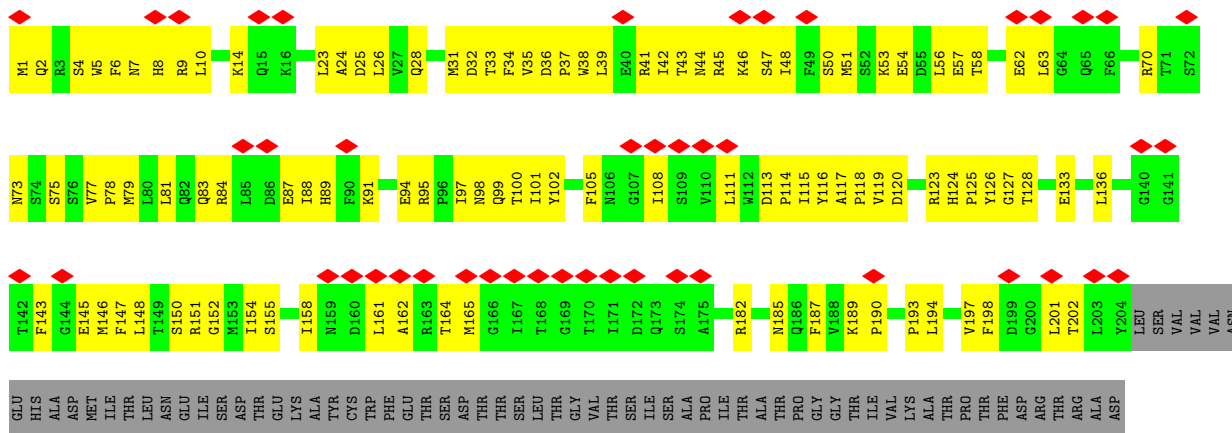
### • Molecule 6: Gp16



- Molecule 6: Gp16



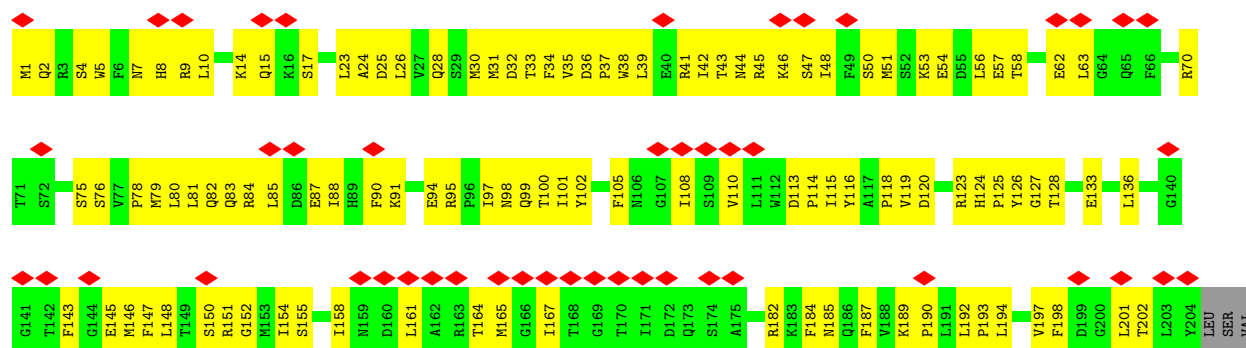
- Molecule 6: Gp16



ASP  
LEU  
LEU  
LEU  
ASP  
SER  
ASP  
ALA

• Molecule 6: Gp16

Chain d: 17% 33% 40% 27%



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

• Molecule 6: Gp16

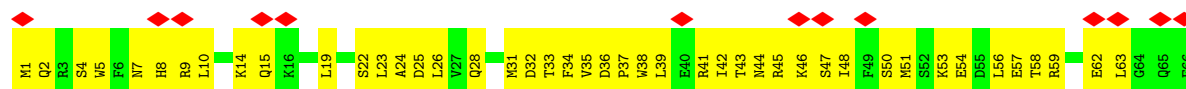
Chain e: 17% 35% 38% 27%



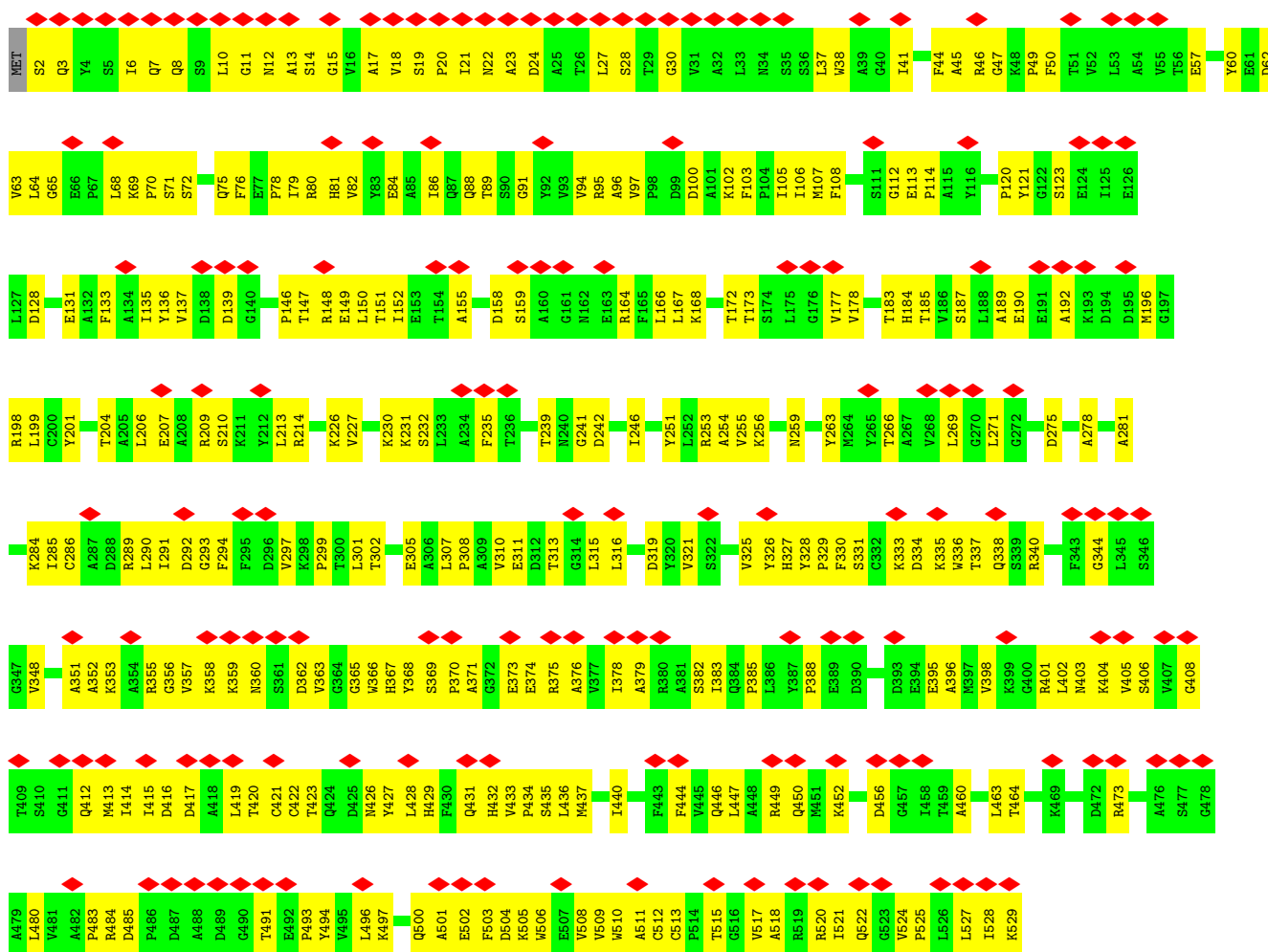
HIS  
ALA  
ASP  
MET  
ILE  
THR  
LEU  
ASN  
GLU  
ILE  
SER  
THR  
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THR  
GLU  
LYS  
ALA  
TYR  
CYS  
TRP  
PHE  
GLU  
THR  
SER  
ASP  
THR  
THR  
SER  
LEU  
THR  
GLY  
VAL  
THR  
SER  
SER  
ILE  
SER  
ALA  
PRO  
THR  
ILE  
THR  
THR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

• Molecule 6: Gp16

Chain f: 17% 34% 39% 27%

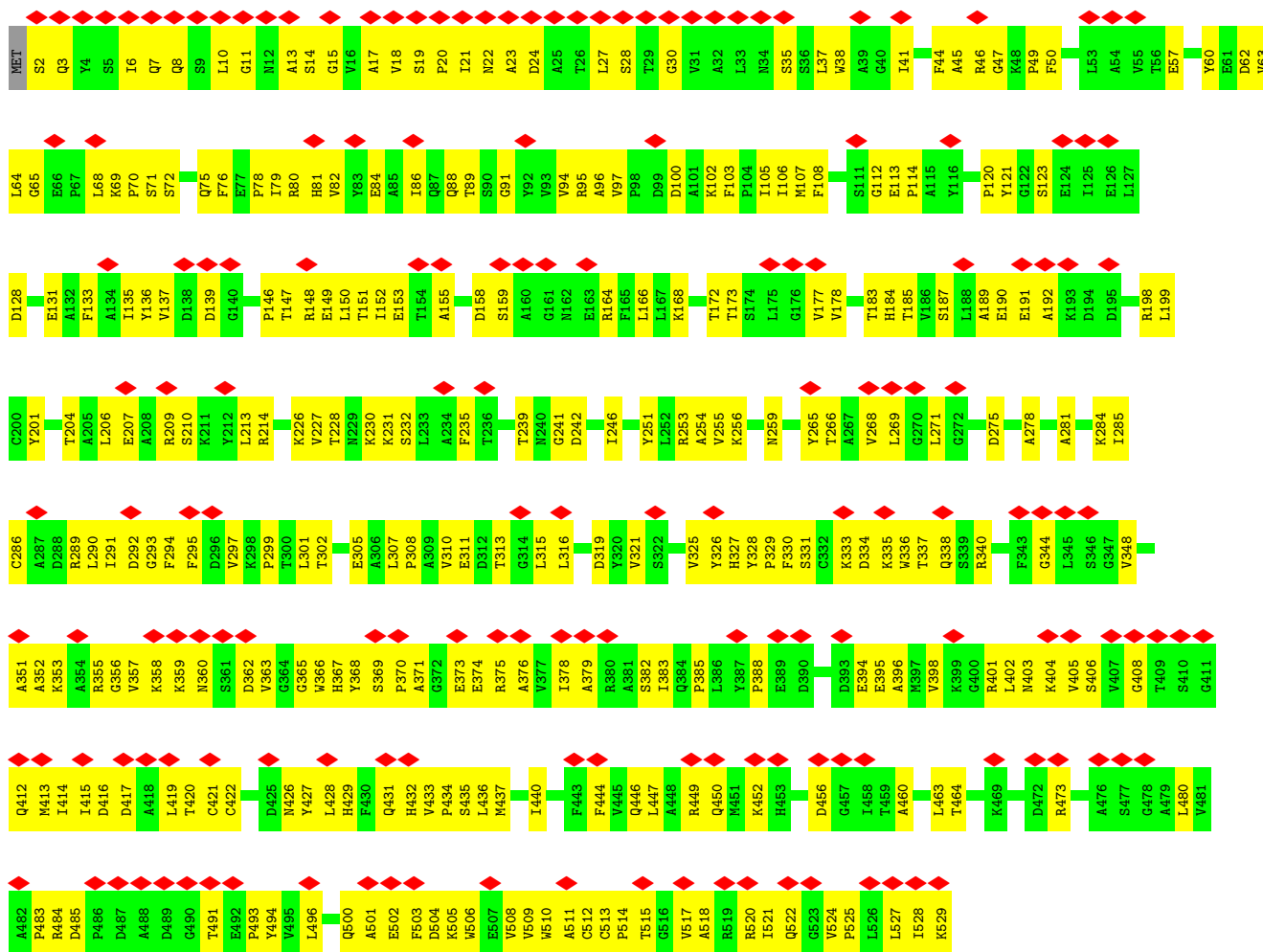


- Molecule 7: Gp22

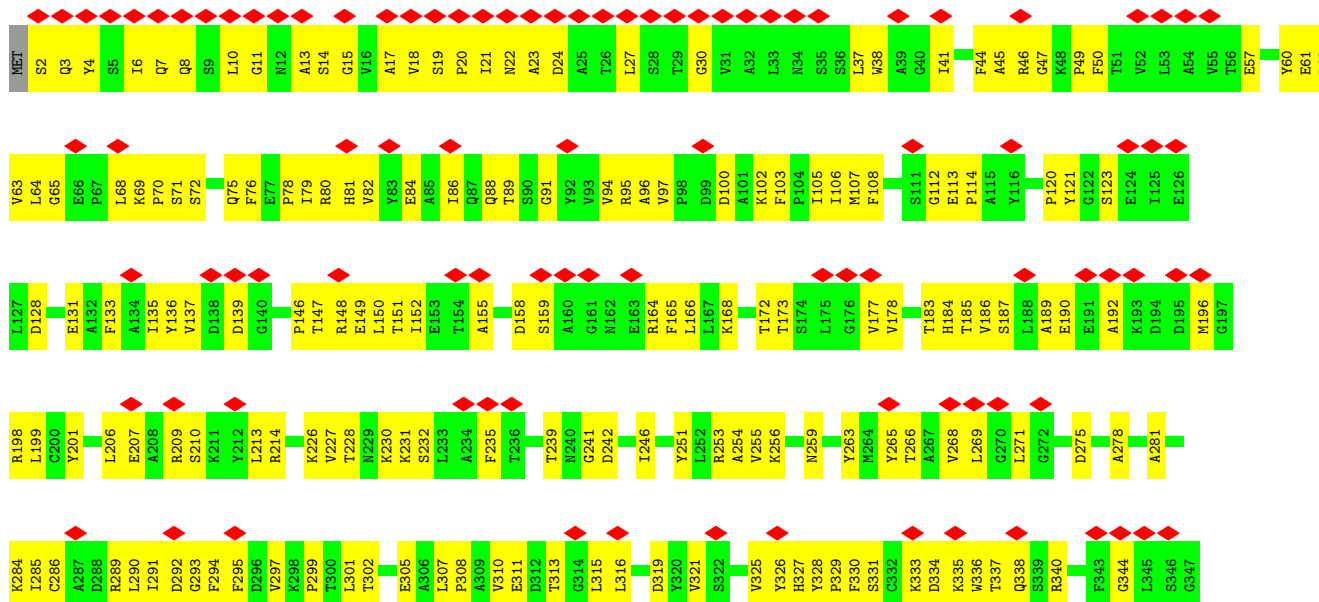


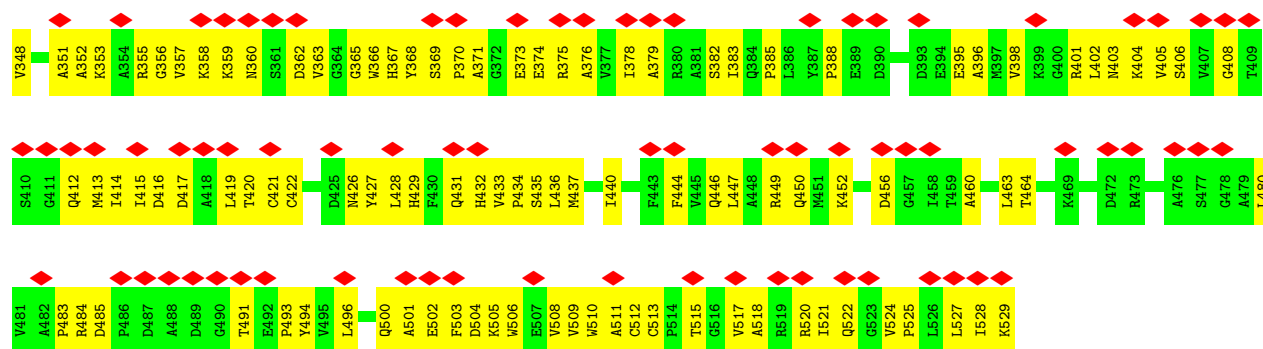
- Molecule 7: Gp22



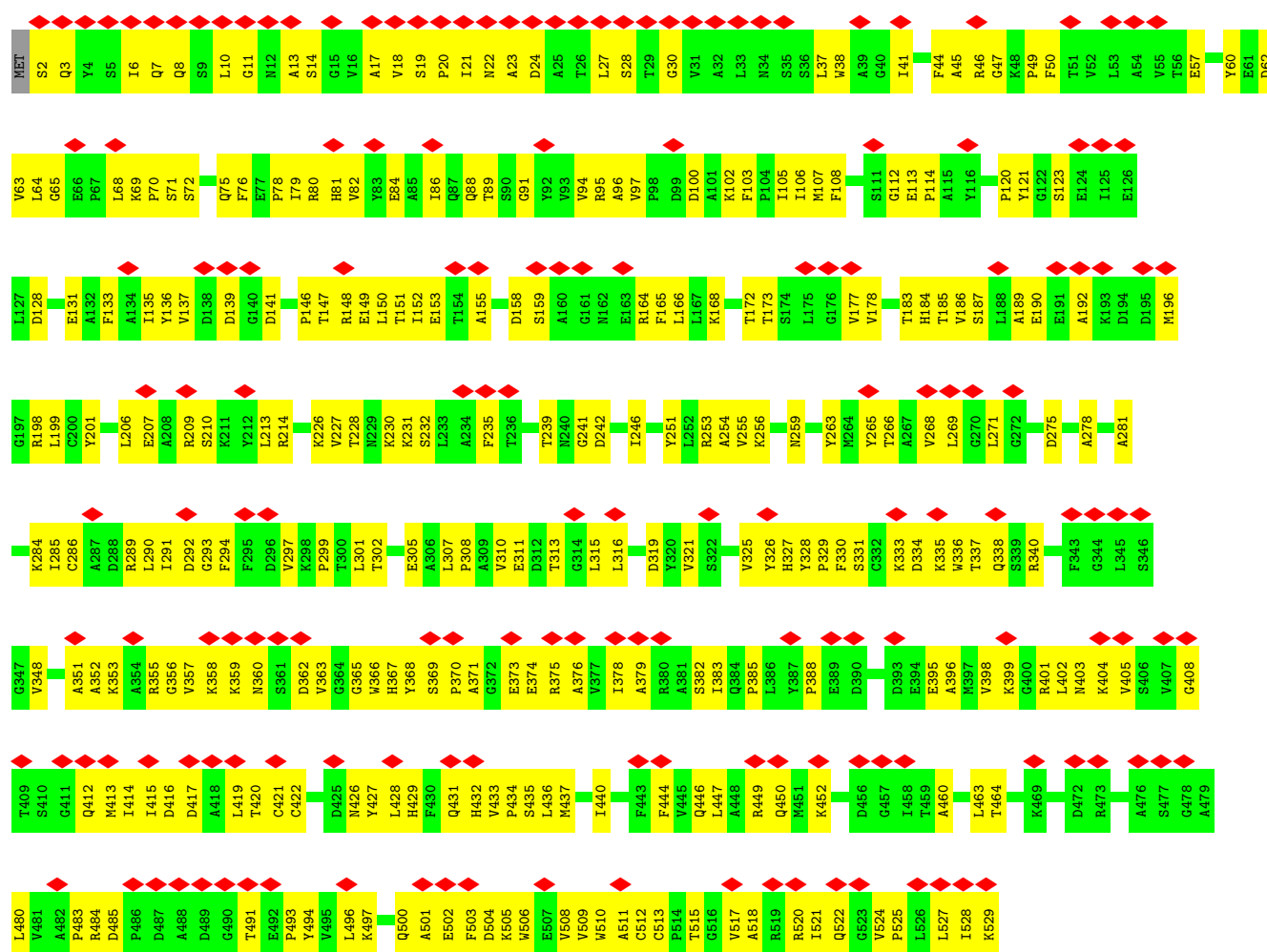


# Molecule 7: Gp22





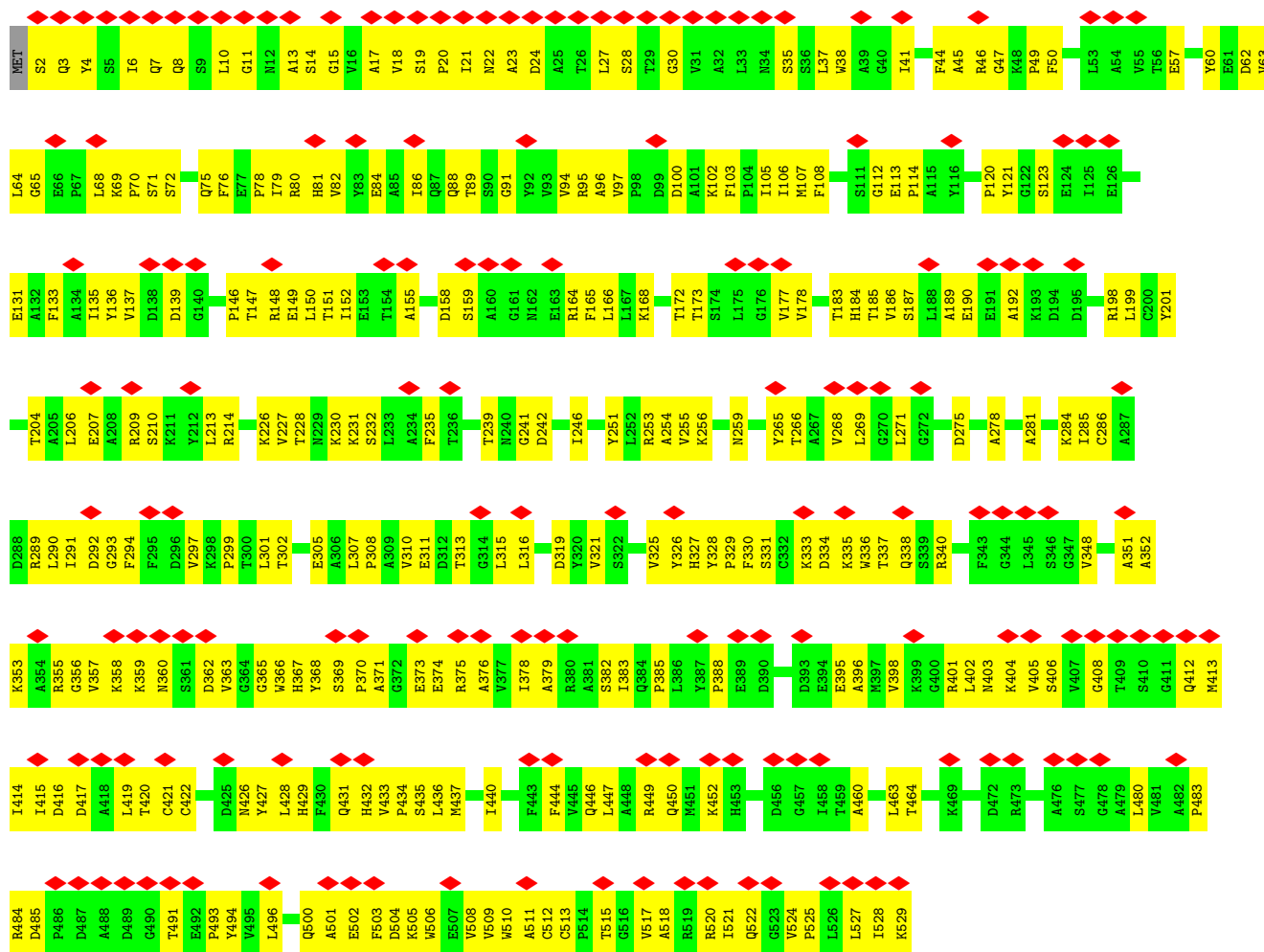
• Molecule 7: Gp22



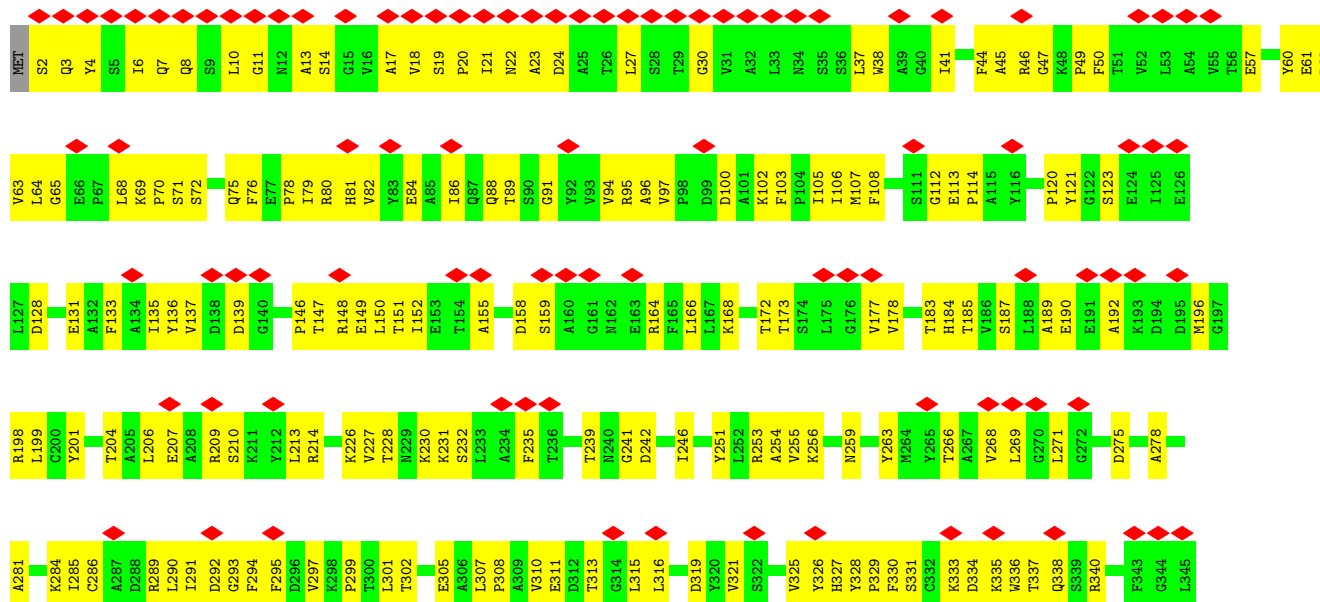
• Molecule 7: Gp22



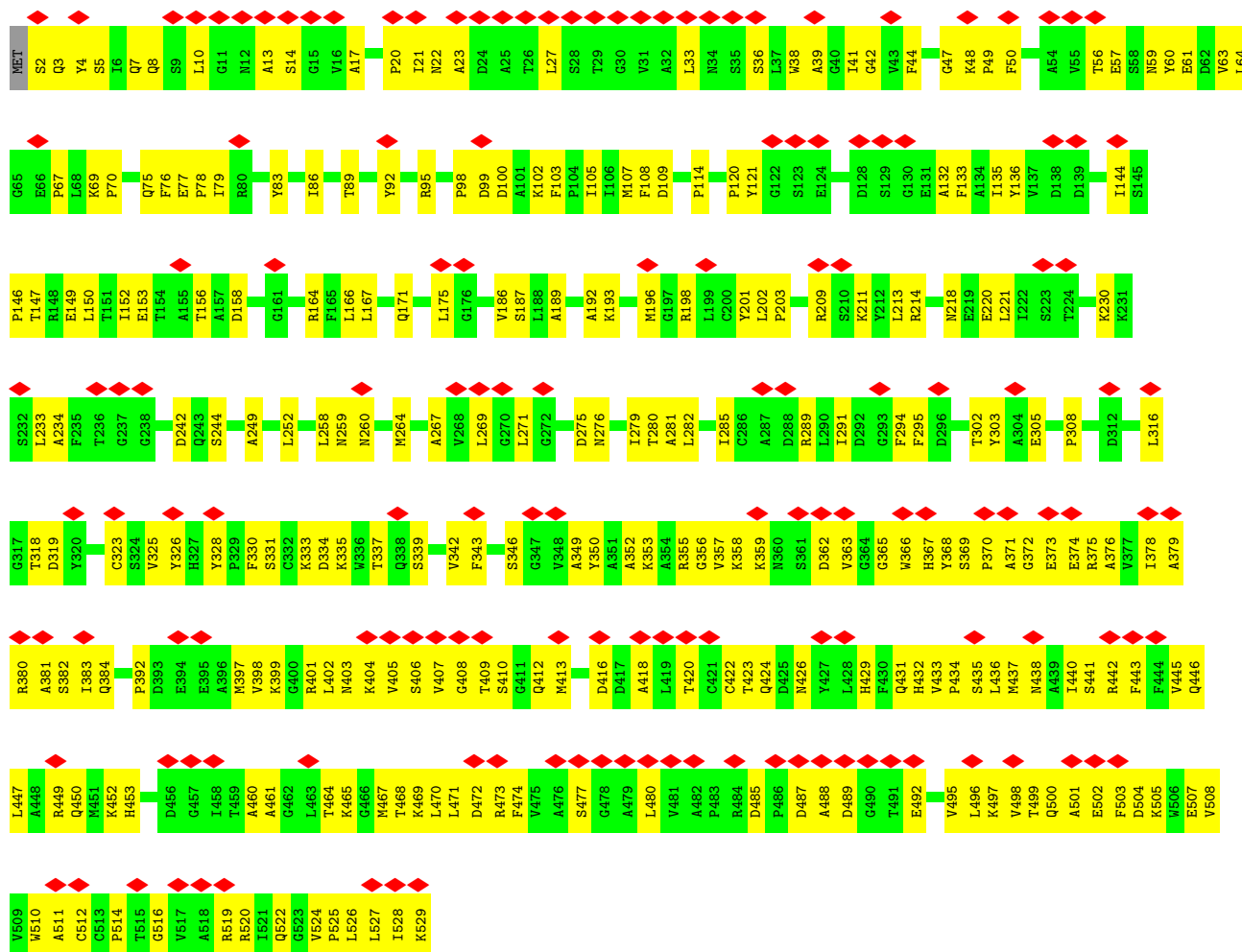




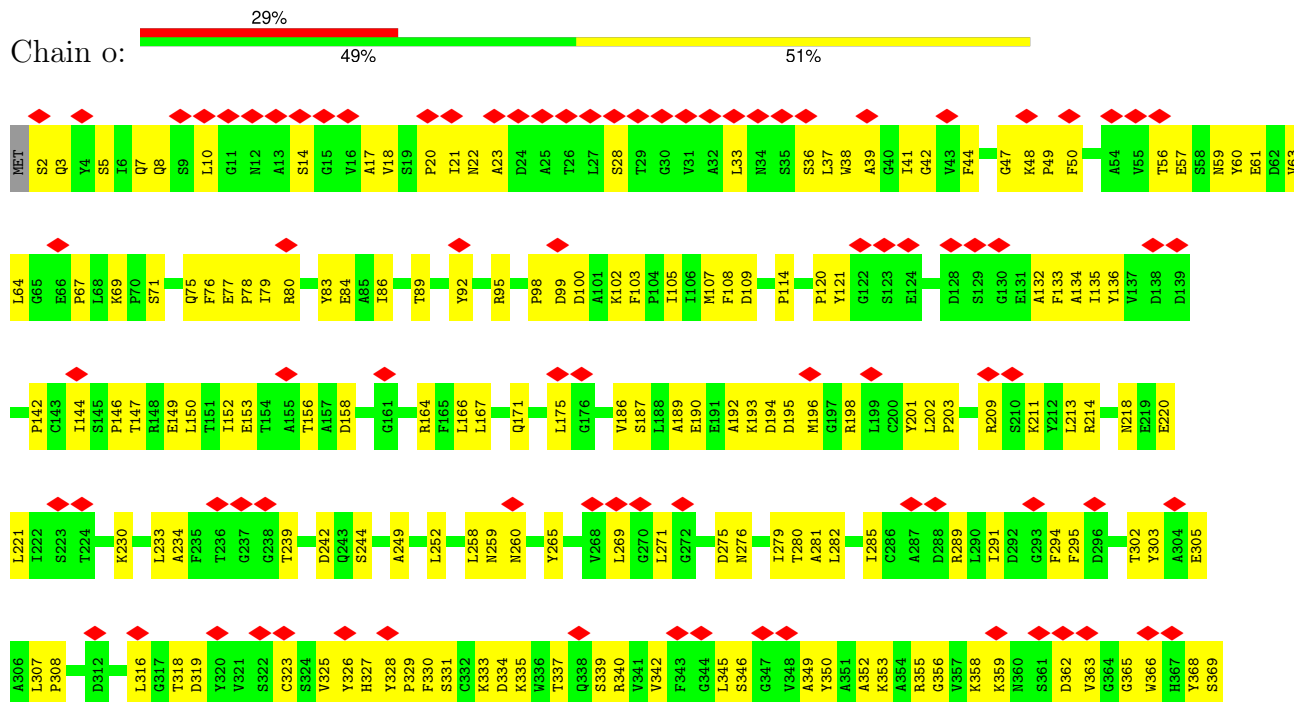
### • Molecule 7: Gp22

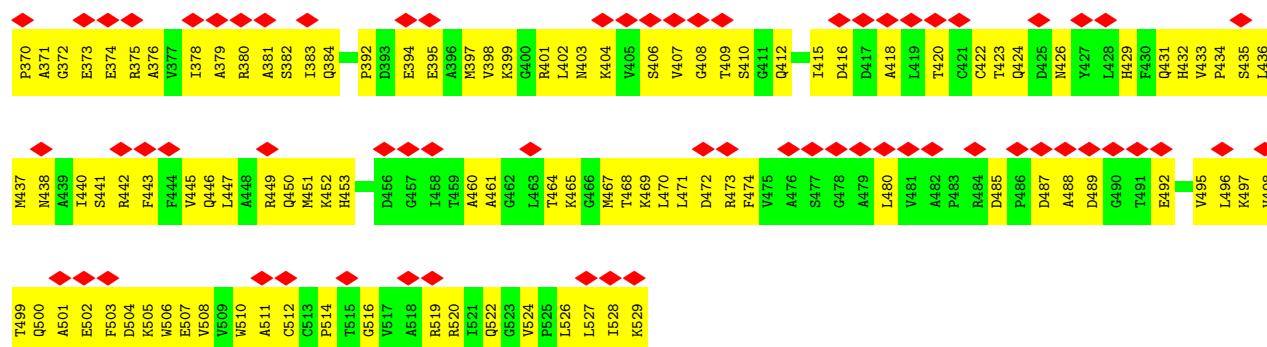




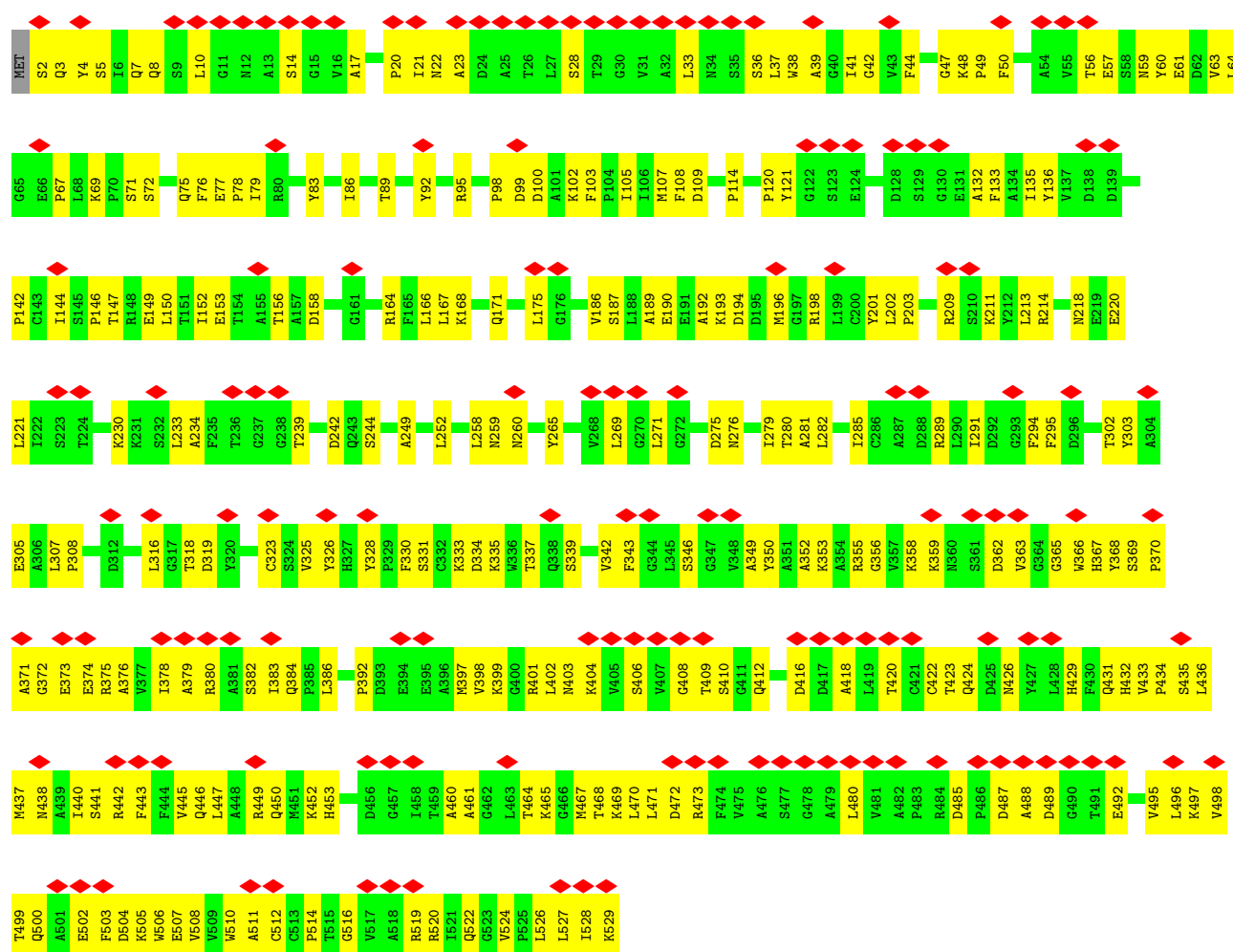


• Molecule 7: Gp22



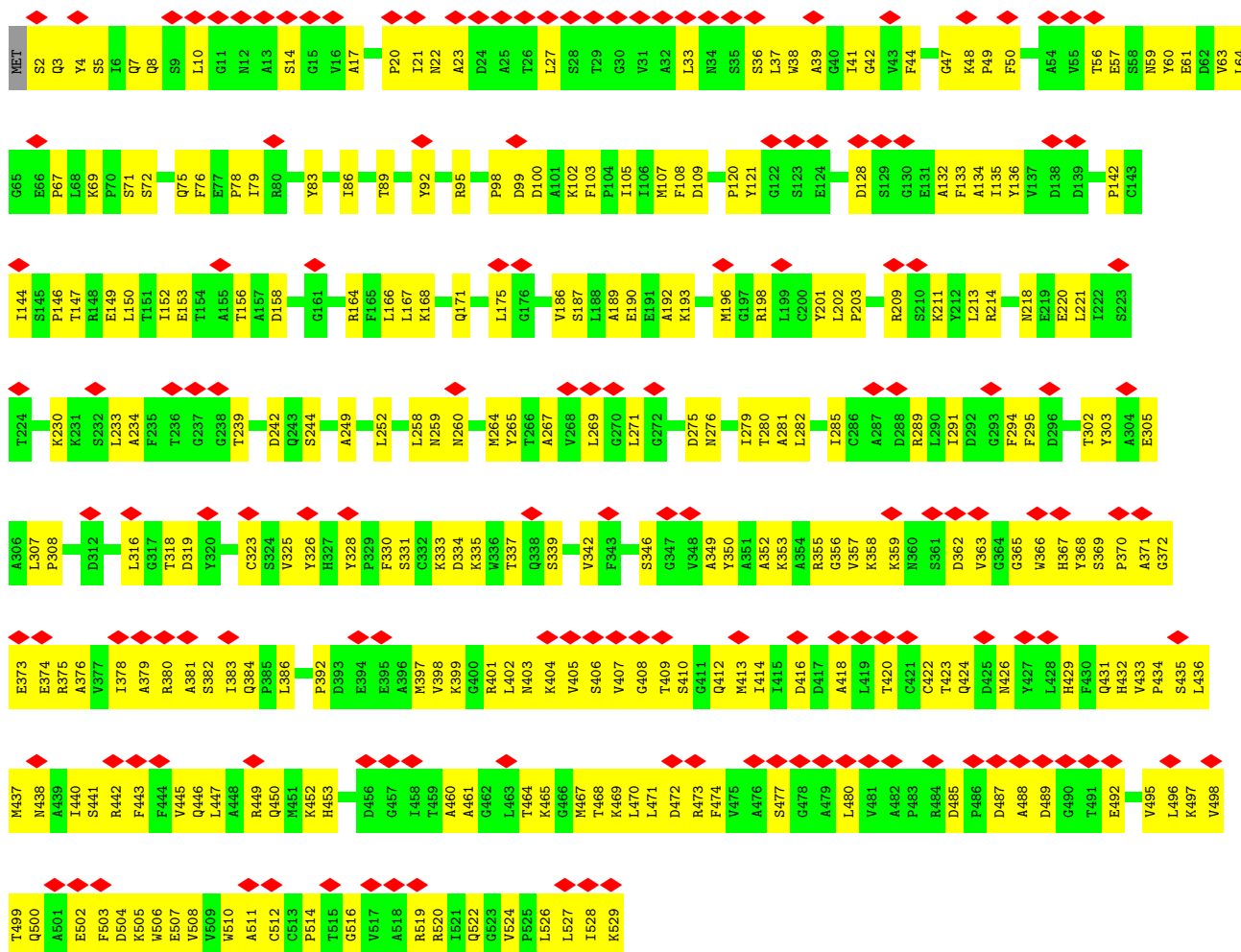


• Molecule 7: Gp22

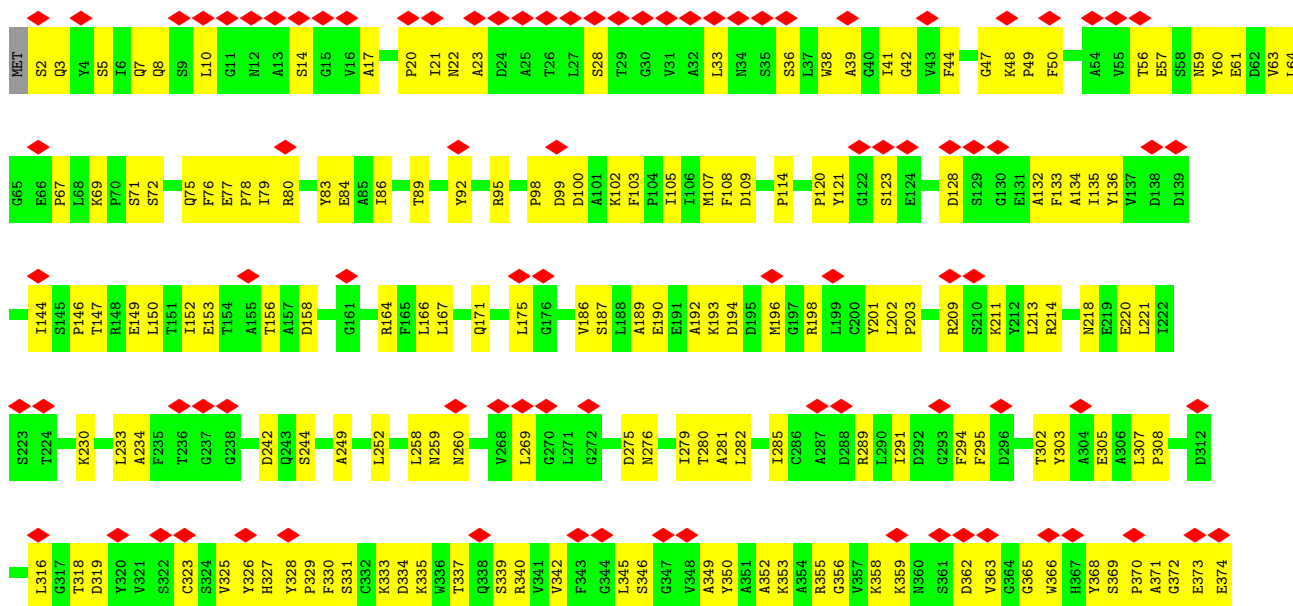


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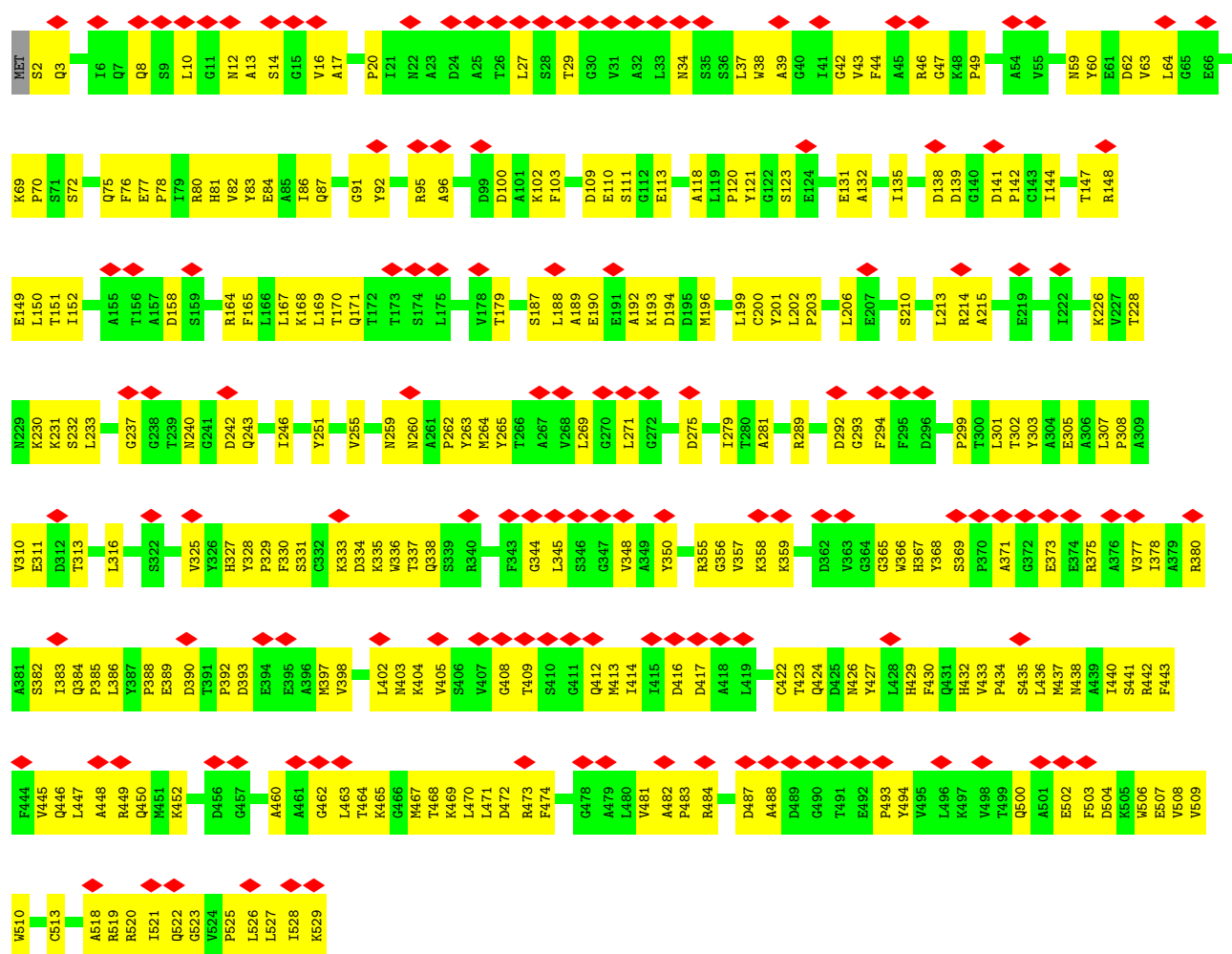


• Molecule 7: Gp22



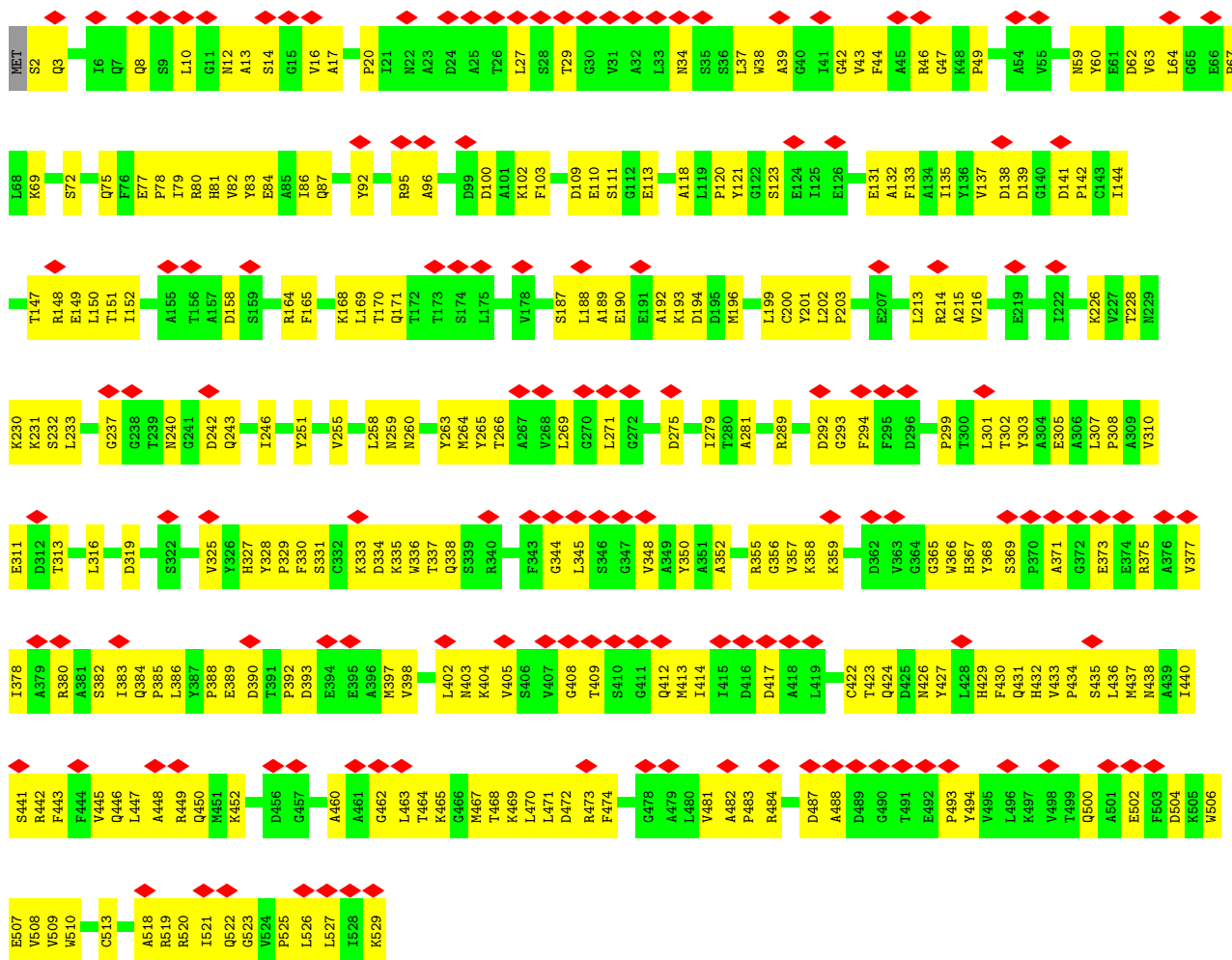


• Molecule 7: Gp22

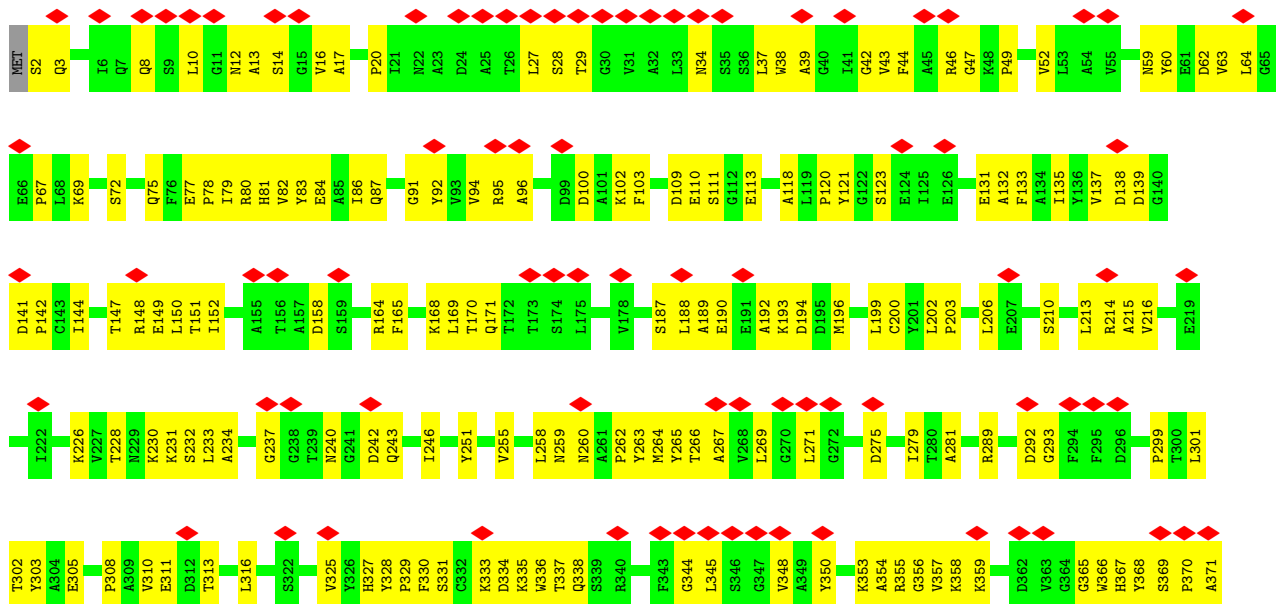


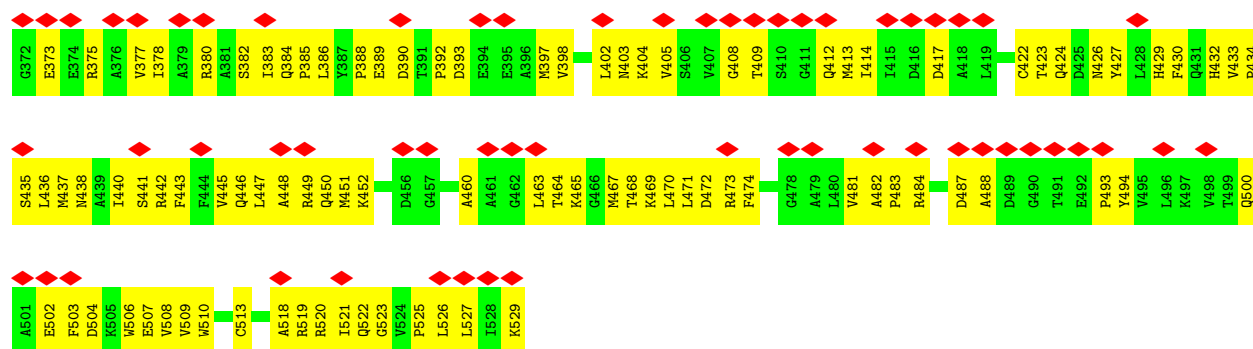
• Molecule 7: Gp22



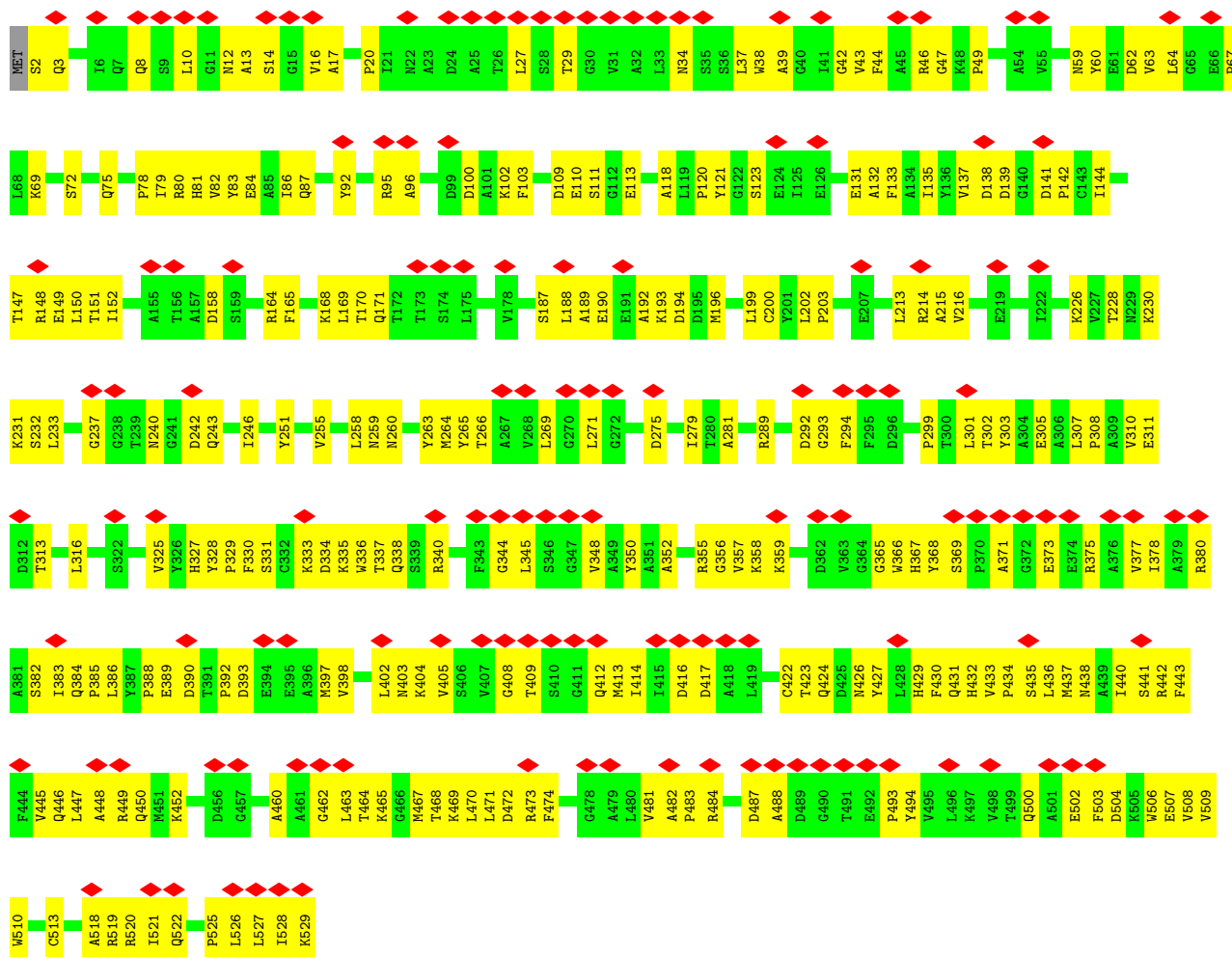


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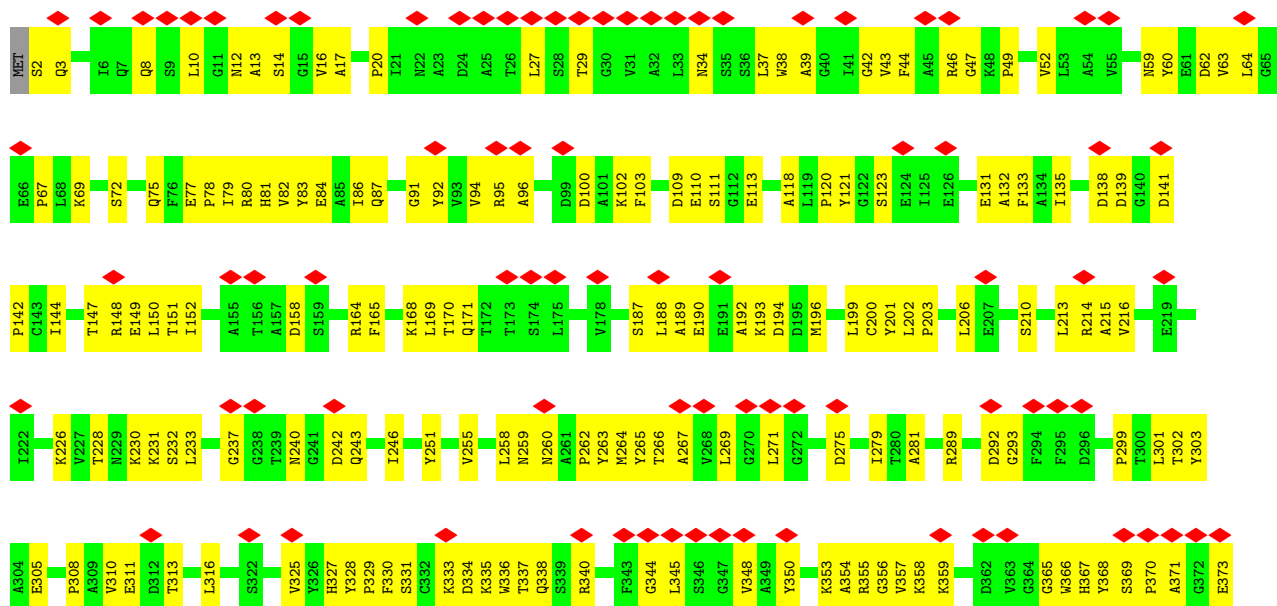


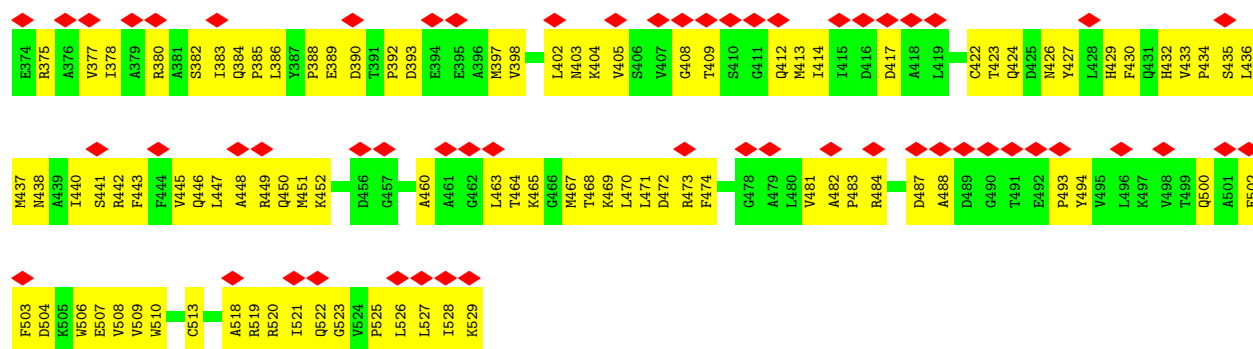




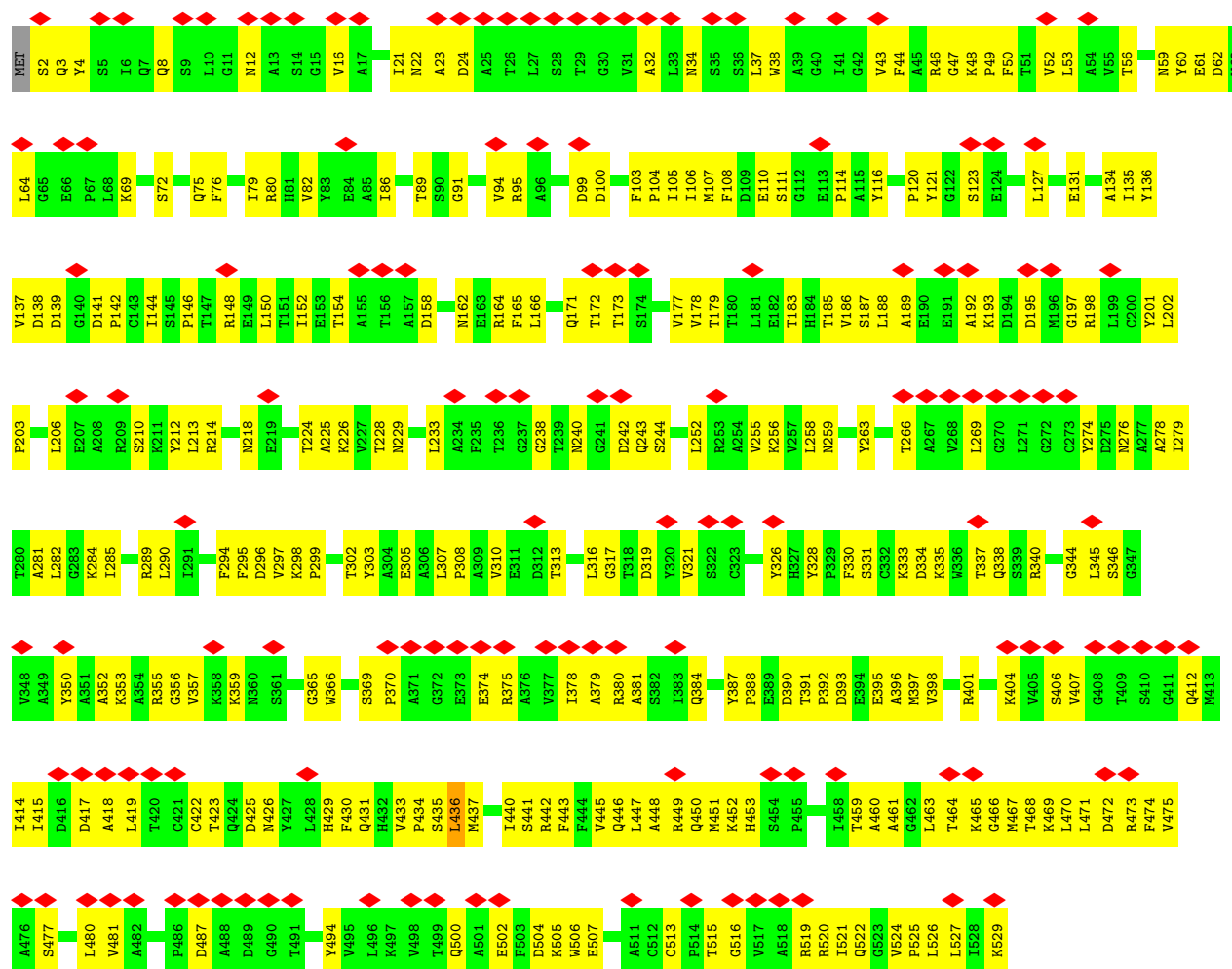


### • Molecule 7: Gp22



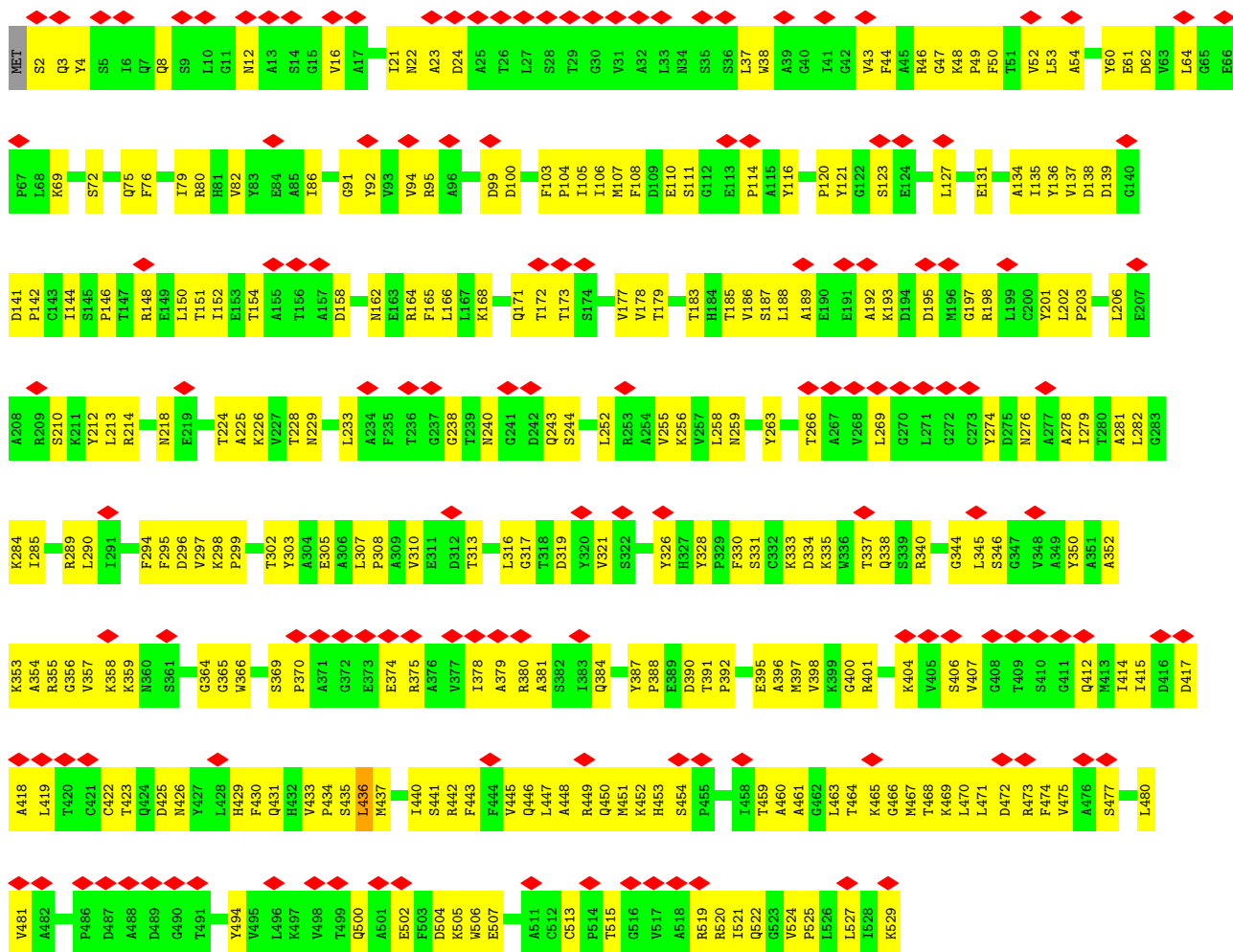


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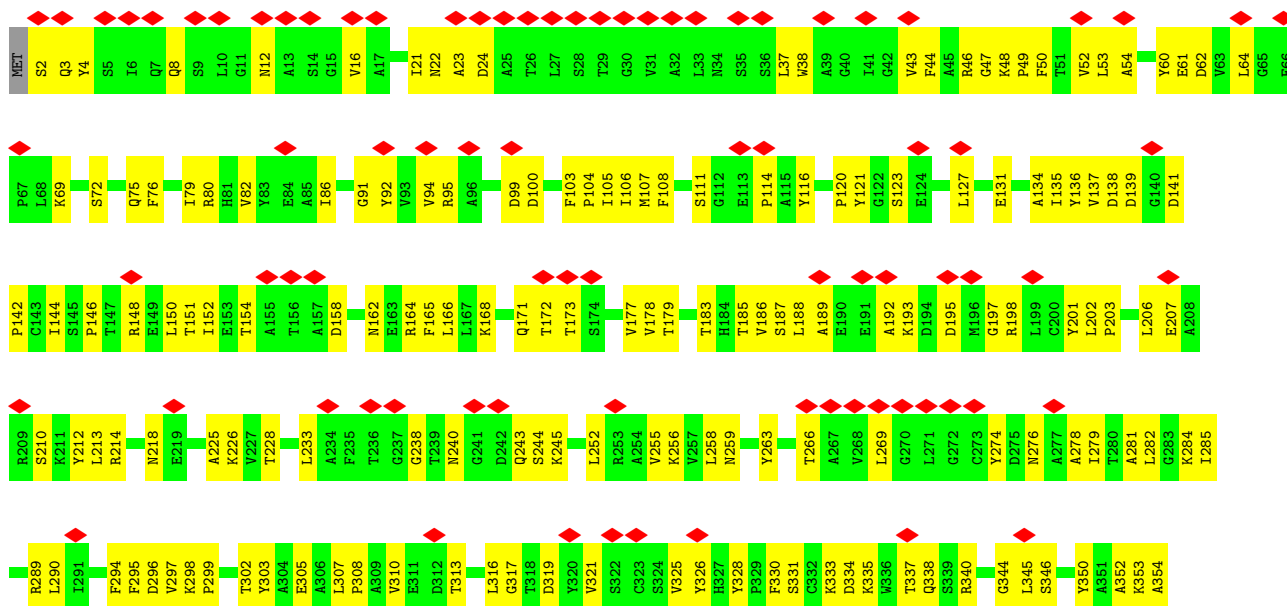


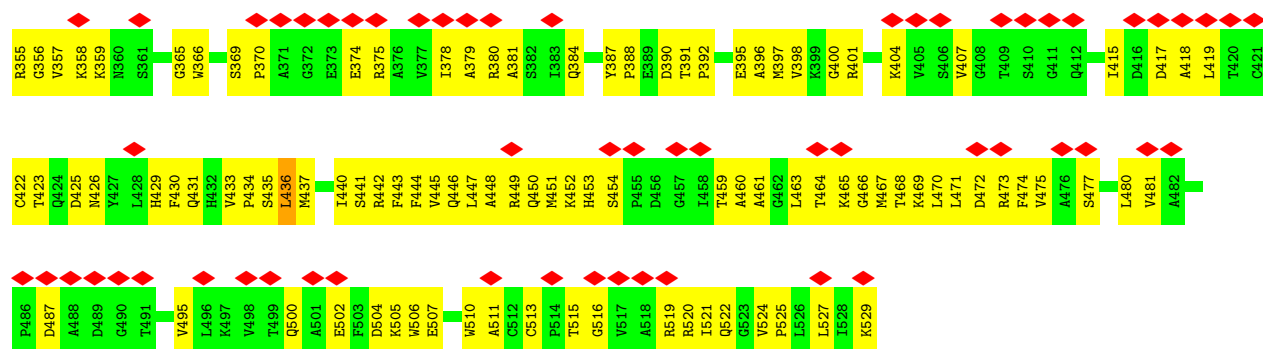
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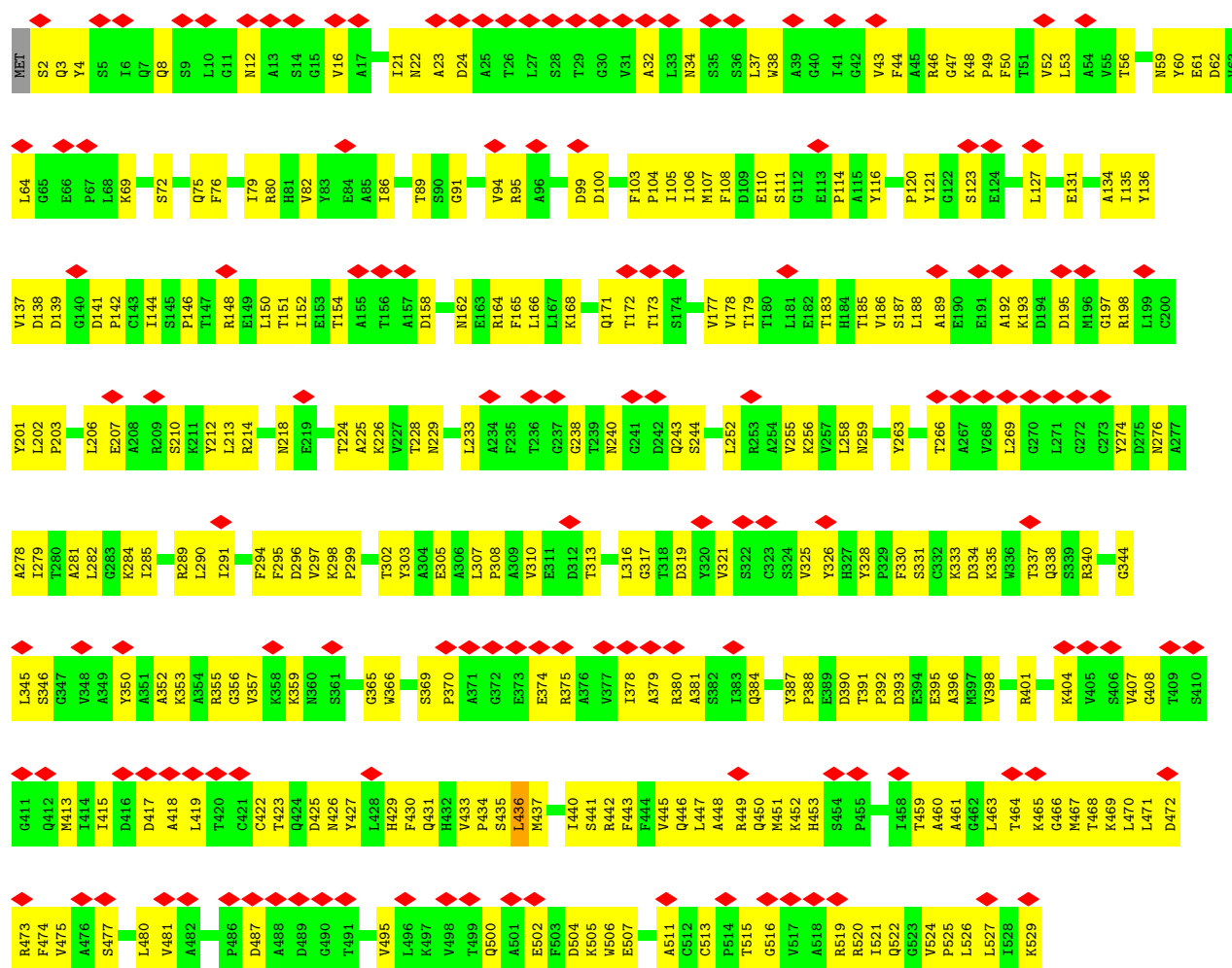


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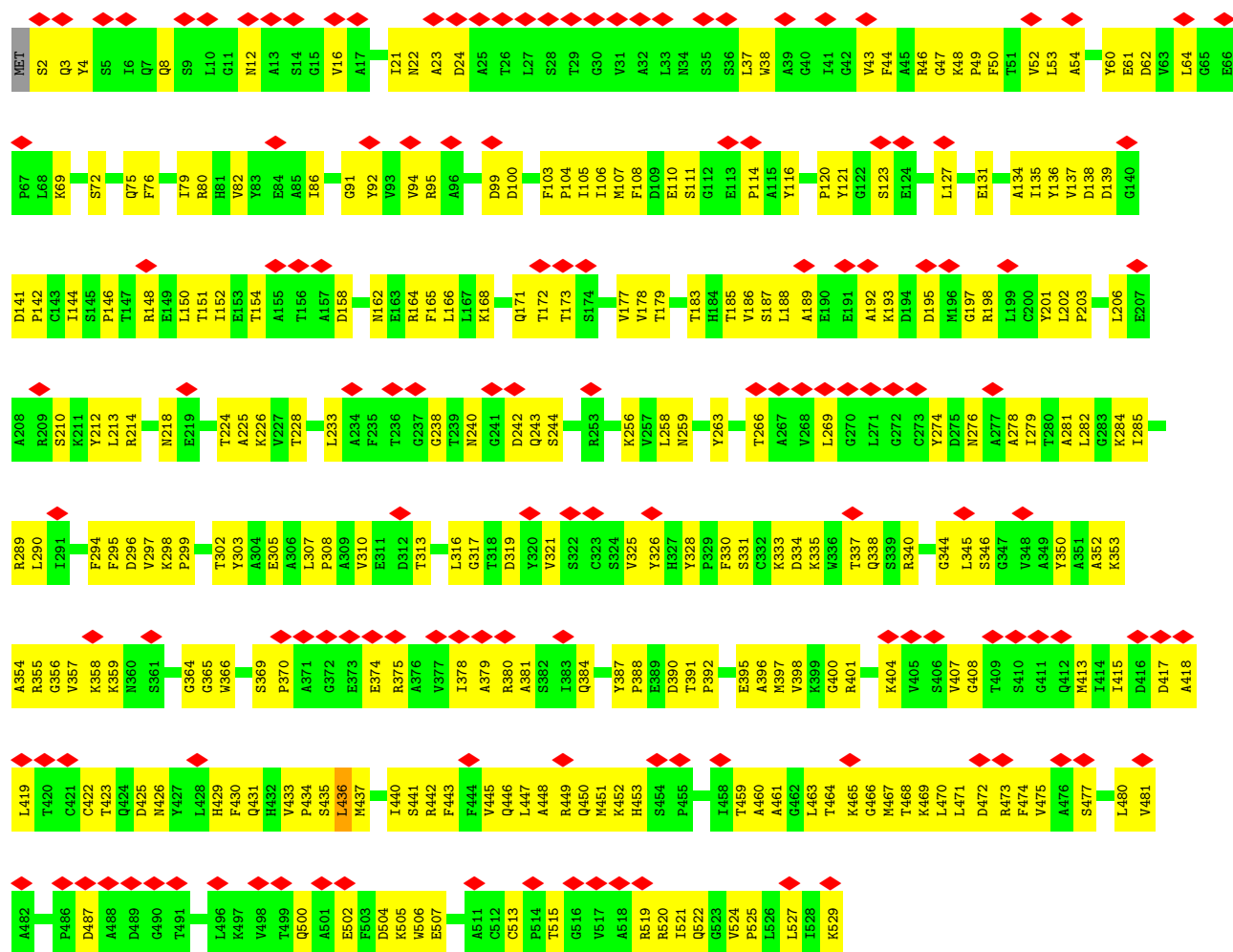


• Molecule 7: Gp22

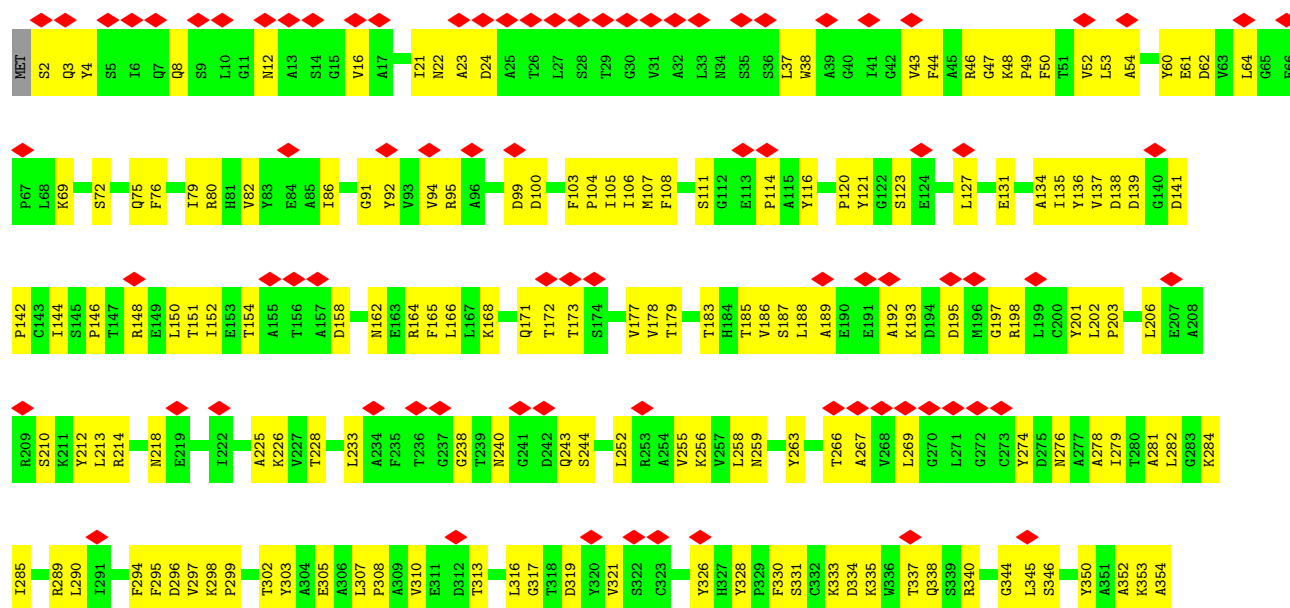


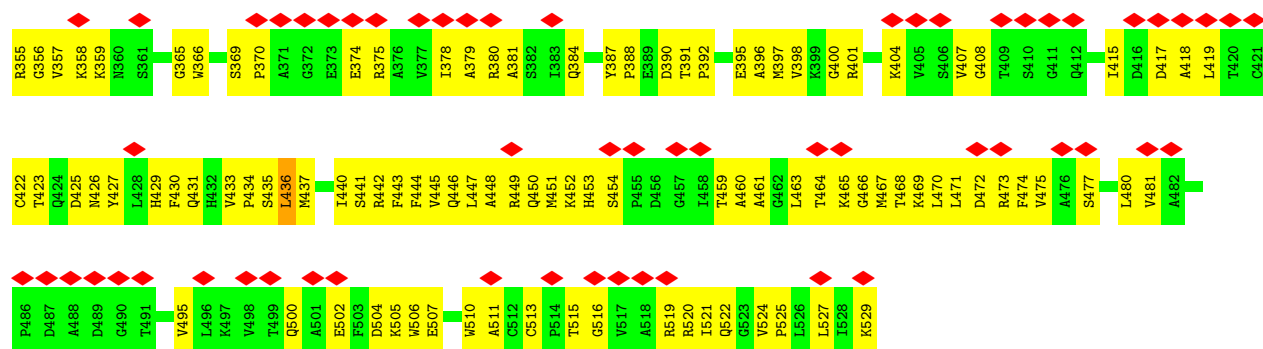
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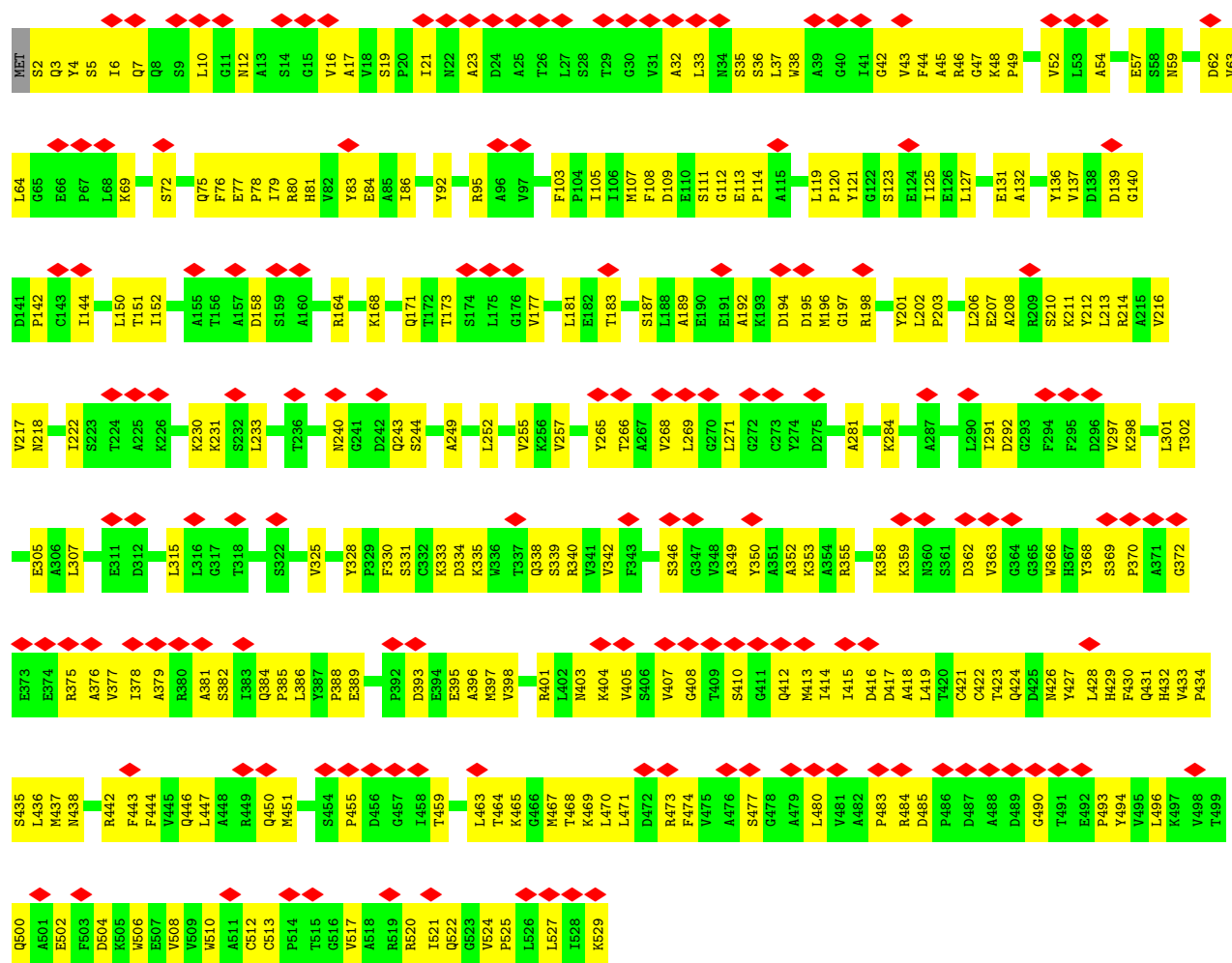


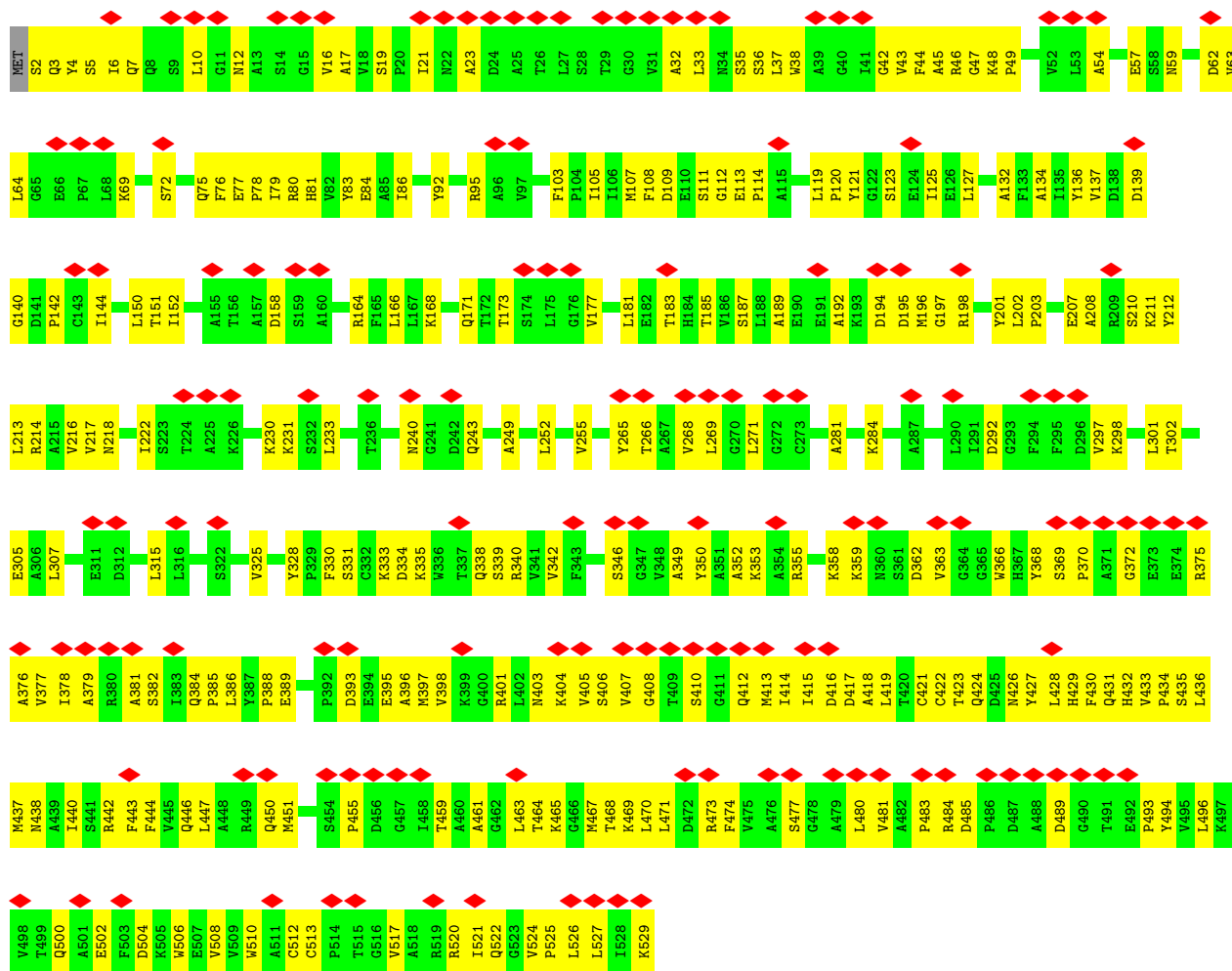
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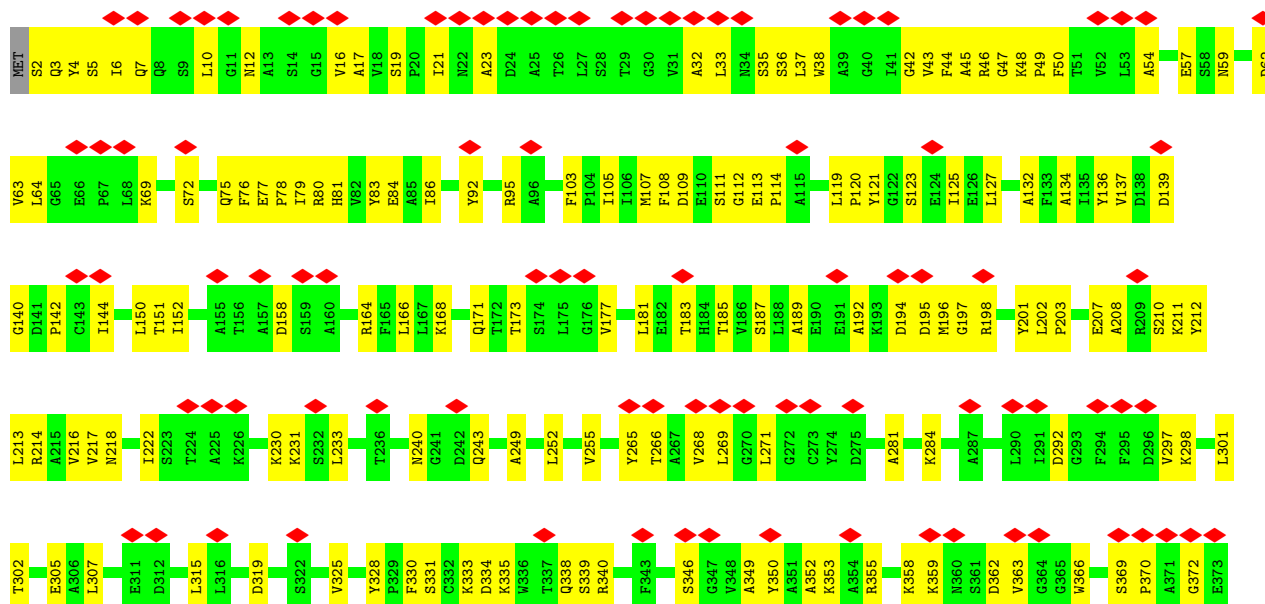


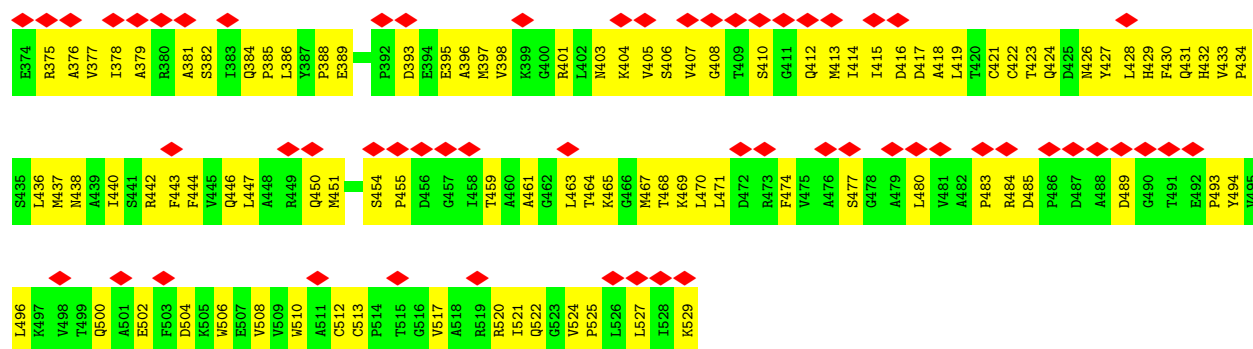
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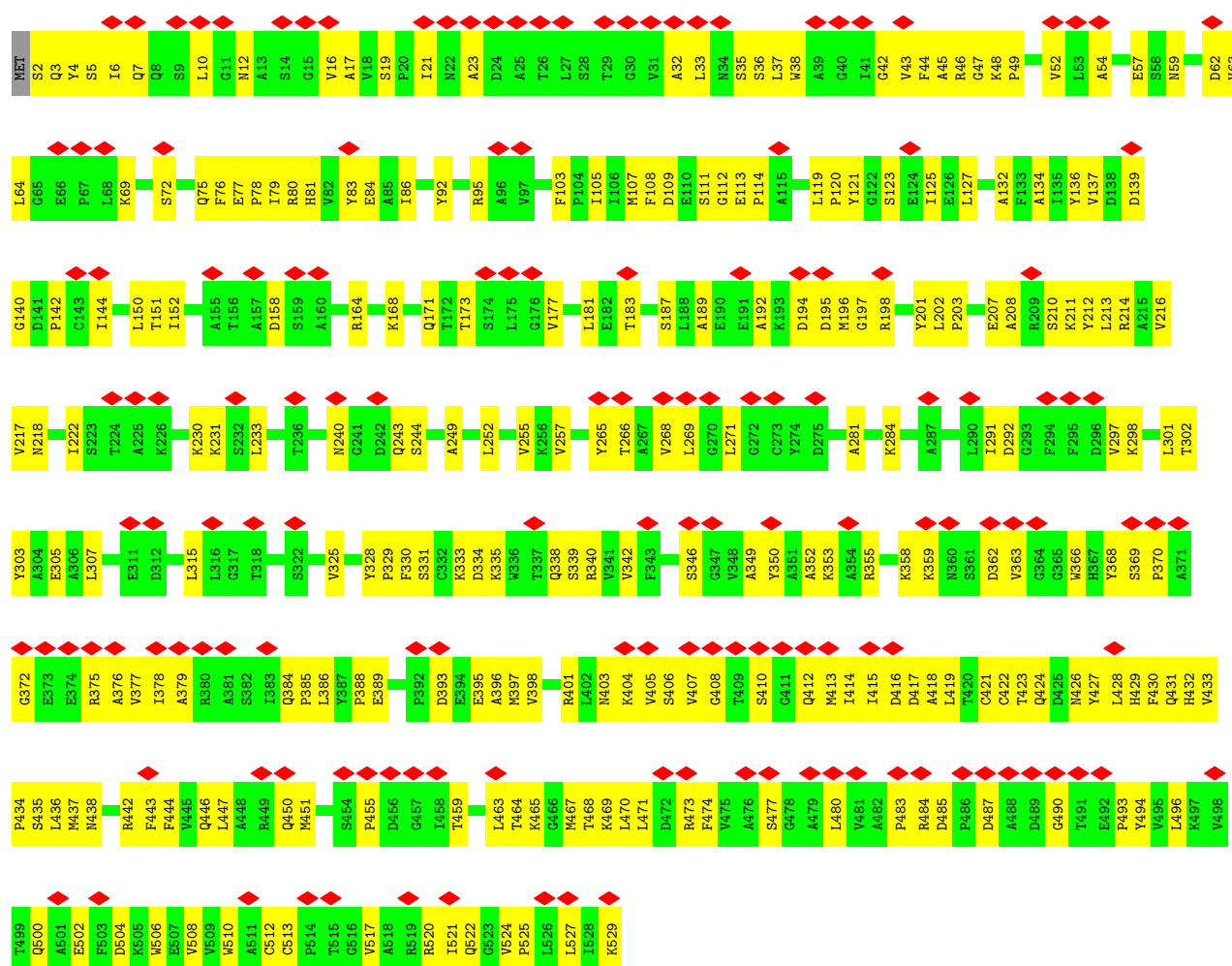


• Molecule 7: Gp22





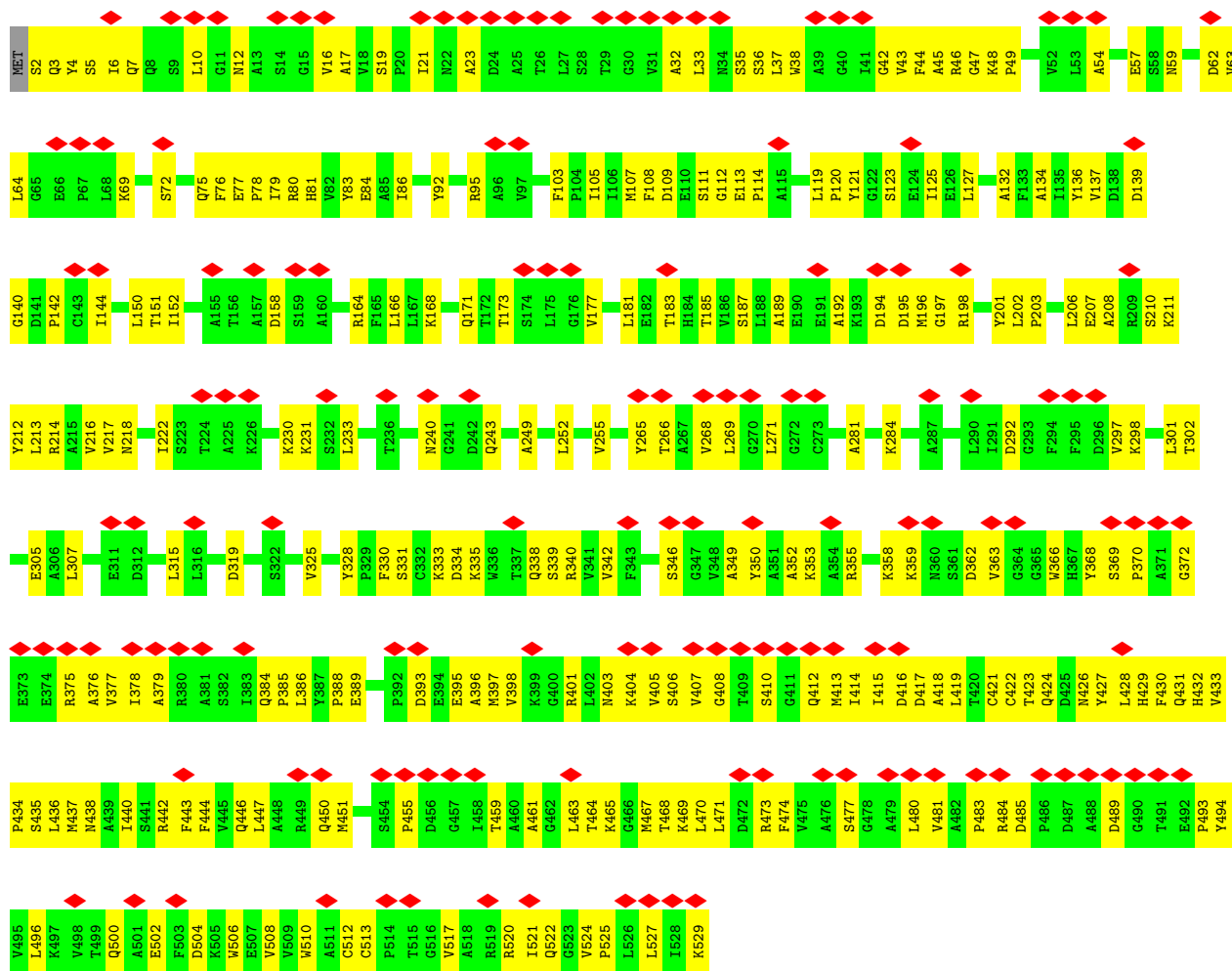
• Molecule 7: Gp22



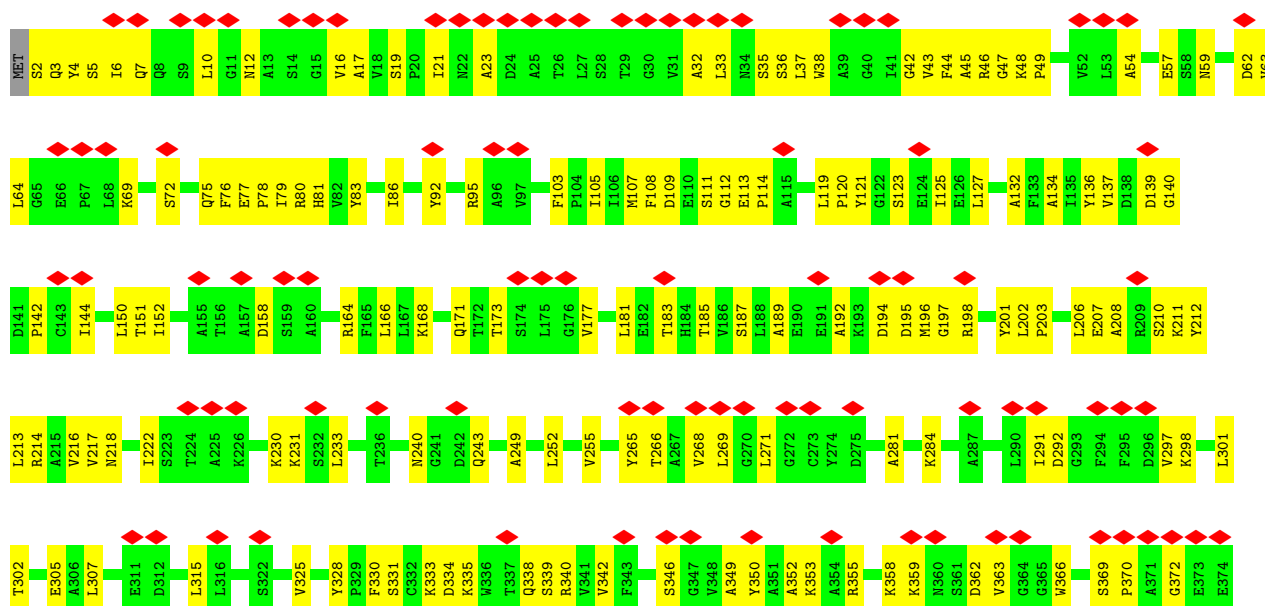
• Molecule 7: Gp22

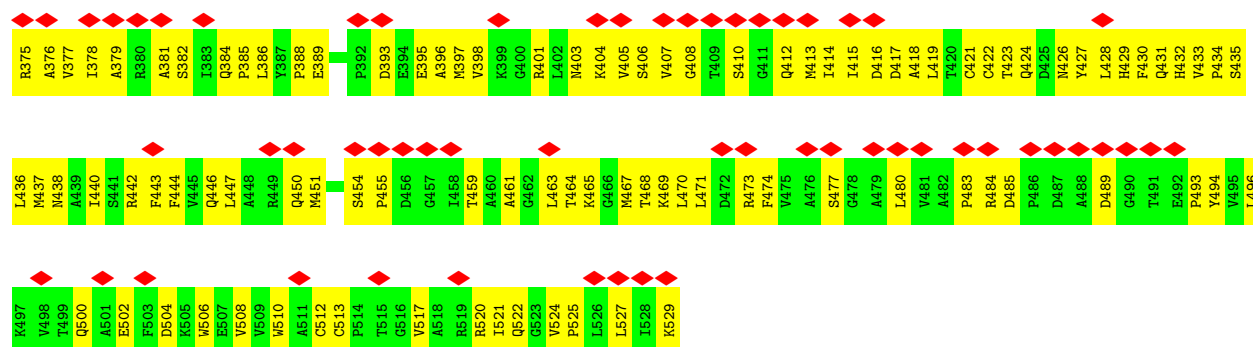




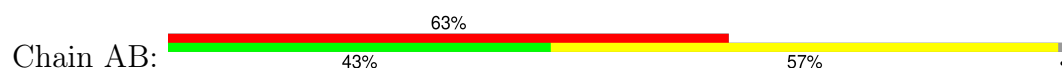


### • Molecule 7: Gp22

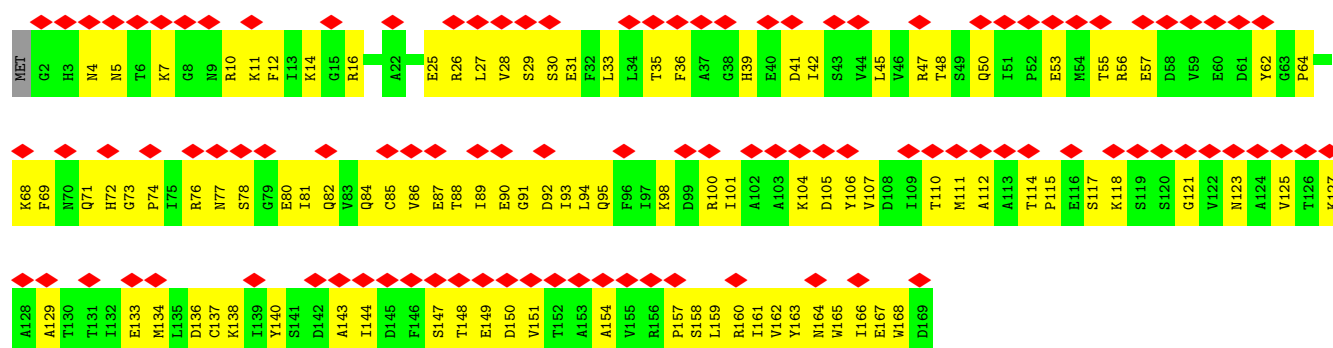




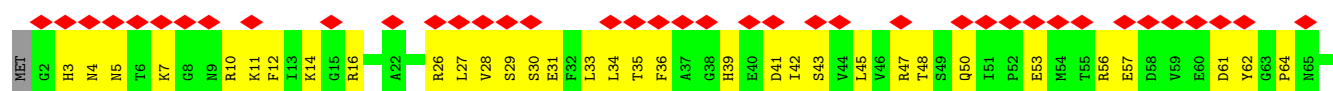
• Molecule 8: BplB

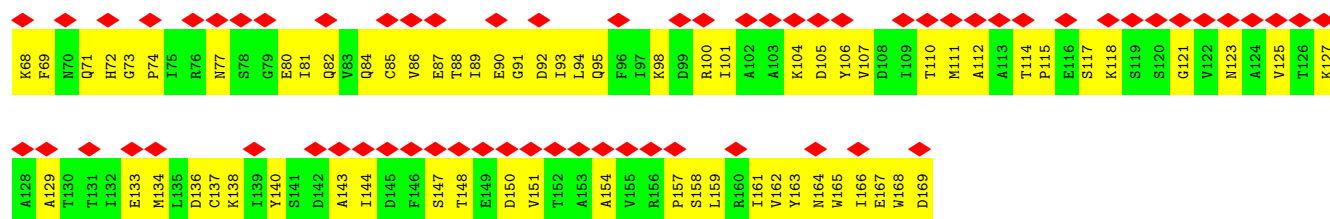


• Molecule 8: BplB

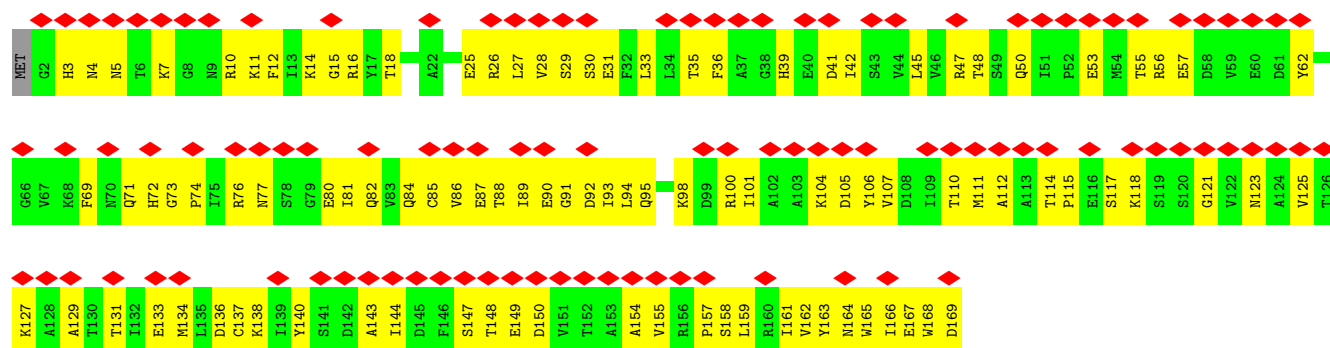


• Molecule 8: BplB

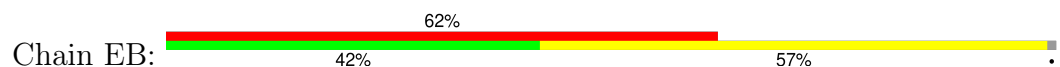




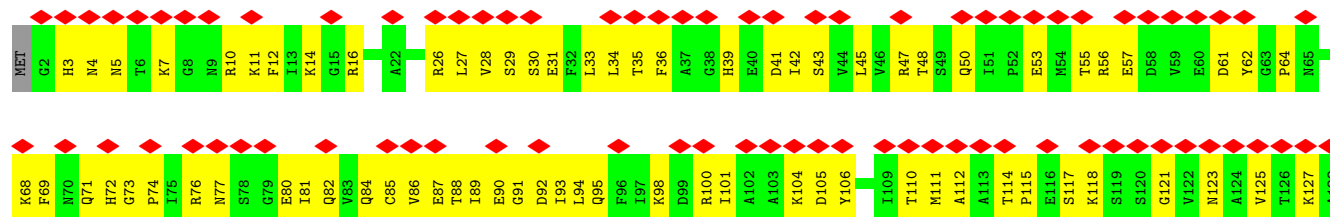
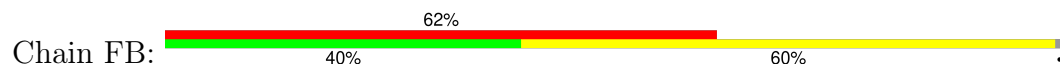
• Molecule 8: BplB



• Molecule 8: BplB

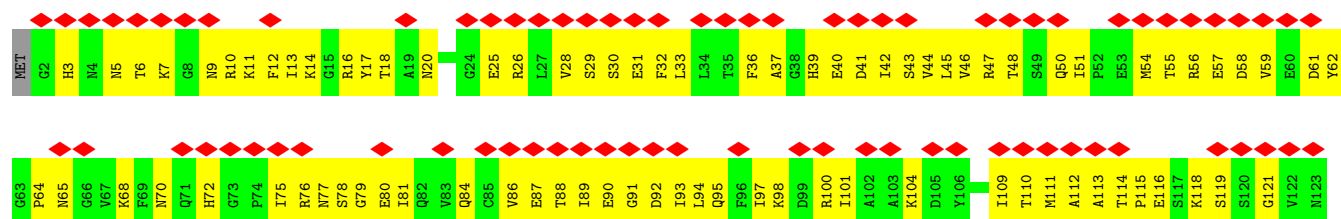


• Molecule 8: BplB

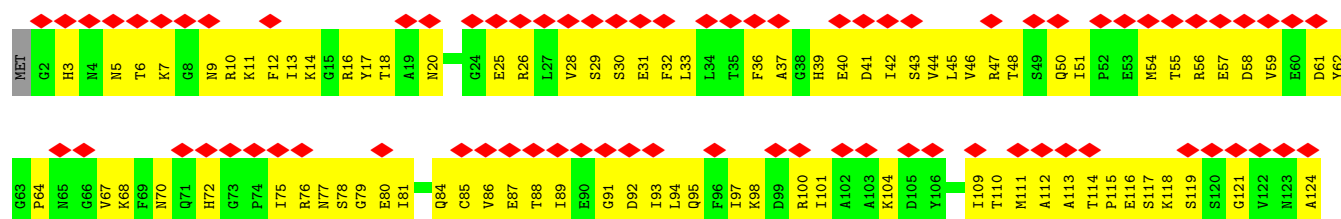




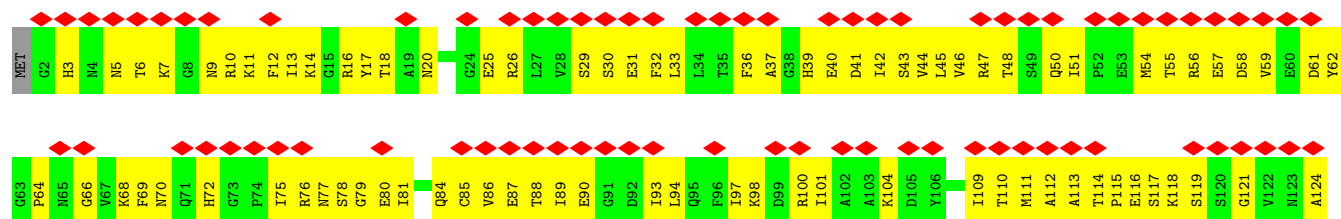
## • Molecule 8: BplB



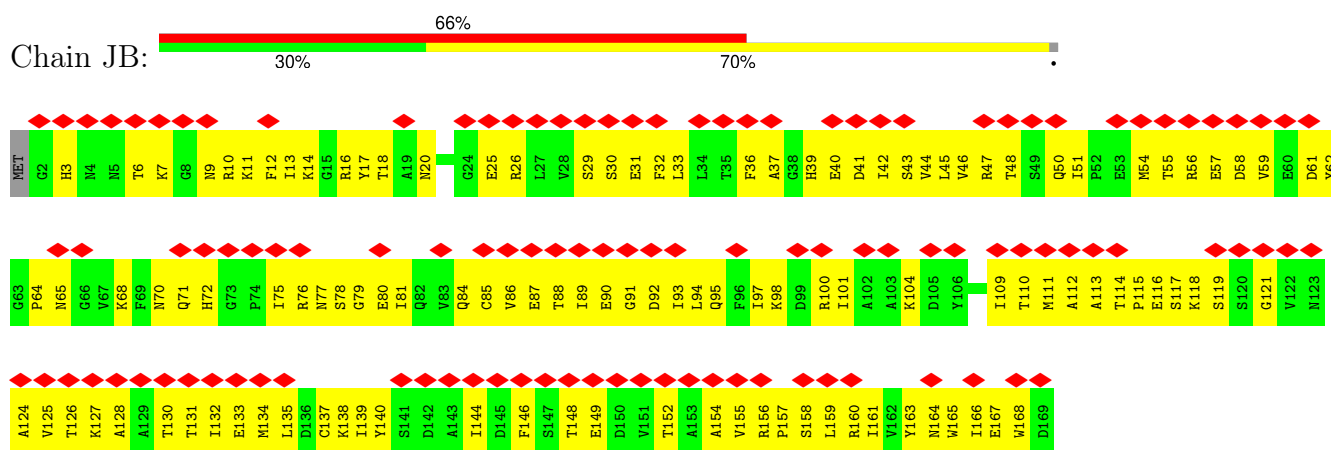
## • Molecule 8: BplB



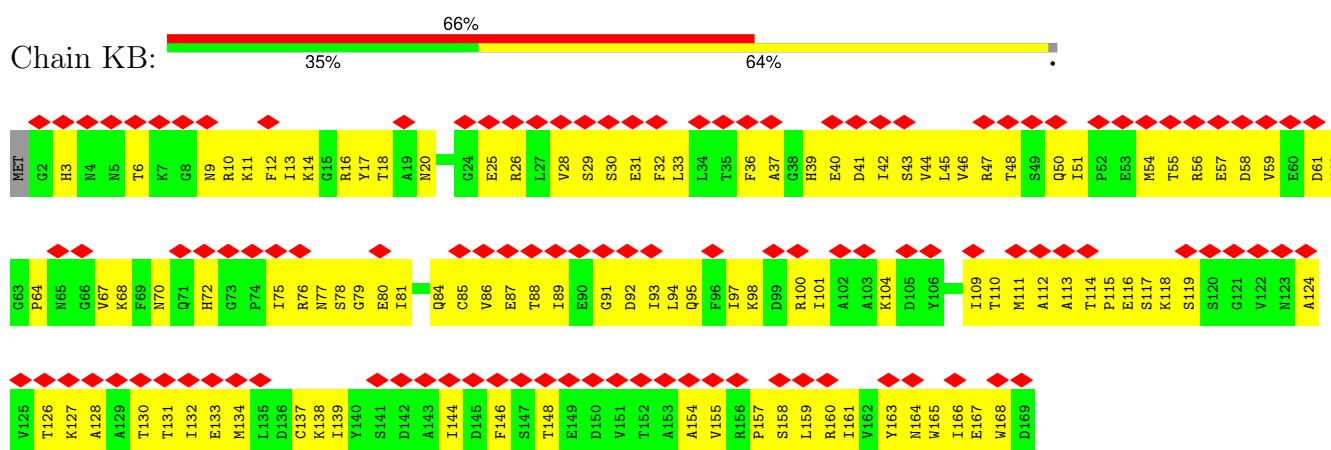
## • Molecule 8: BplB



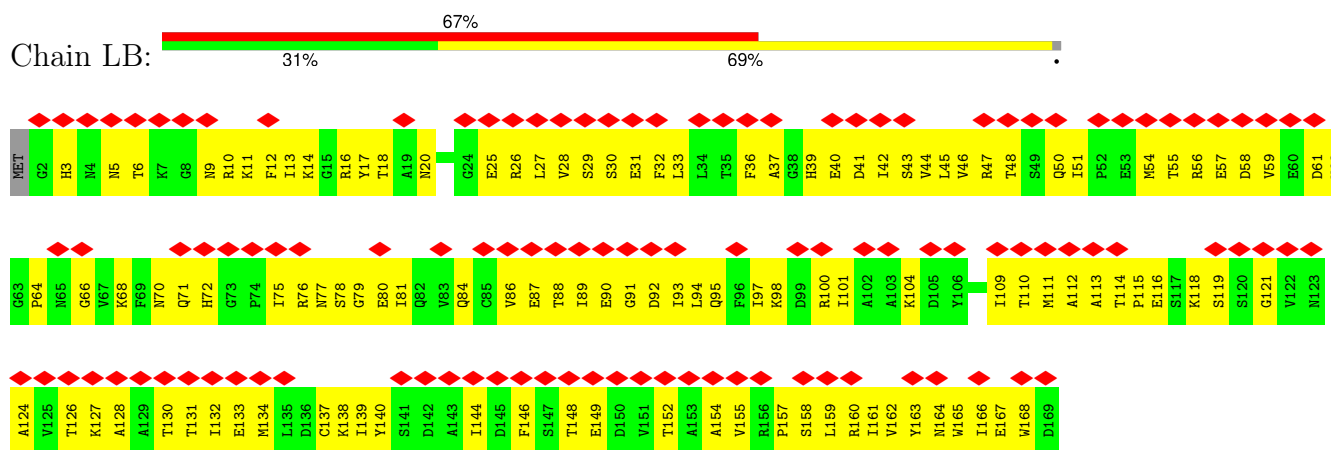
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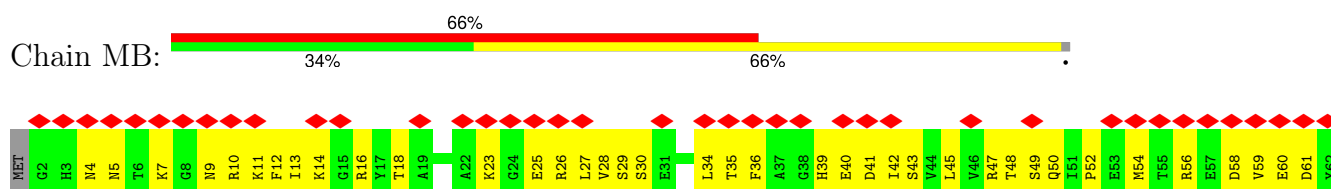
• Molecule 8: BplB

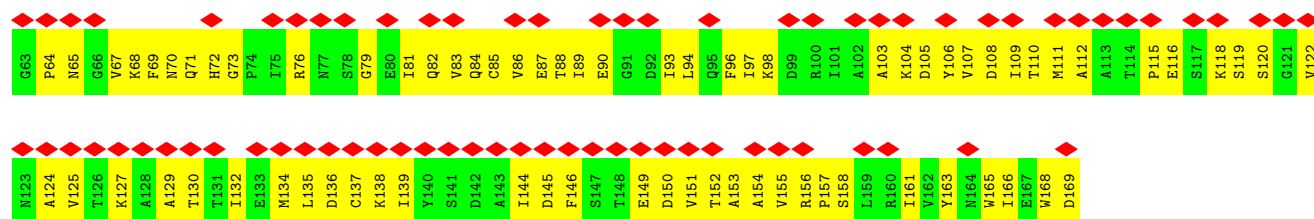


• Molecule 8: BplB

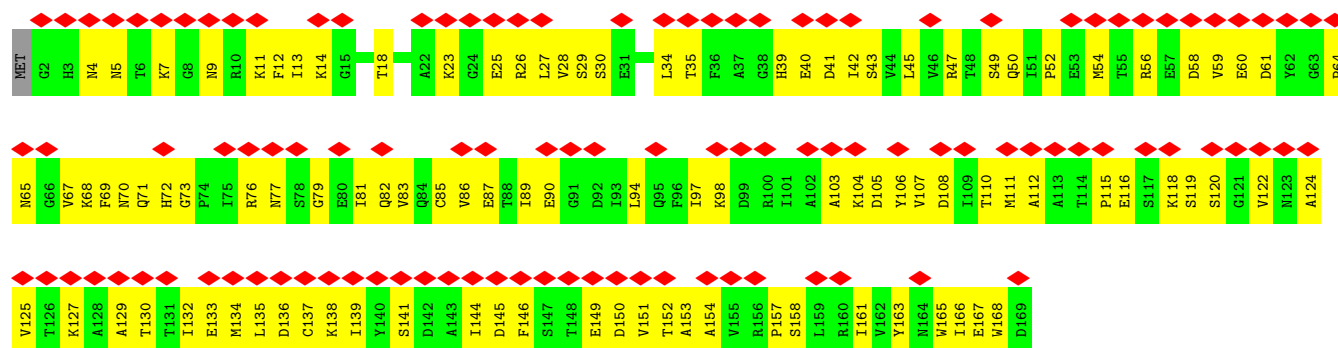


• Molecule 8: BplB

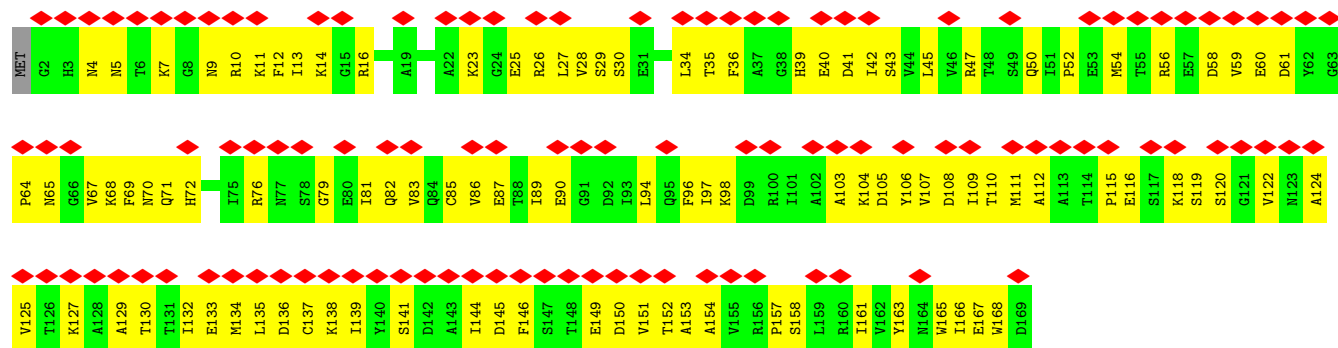




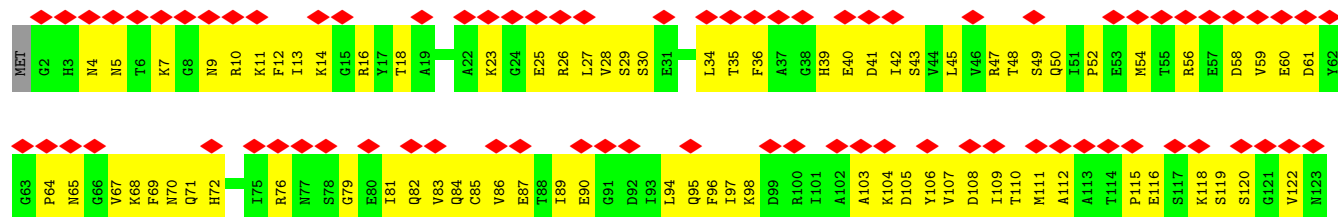
• Molecule 8: BplB



• Molecule 8: BplB

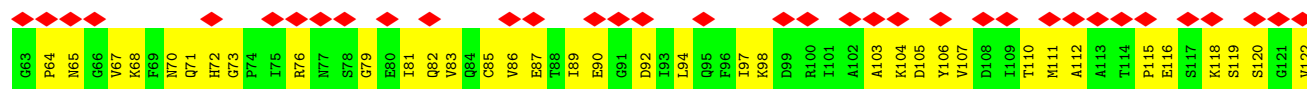
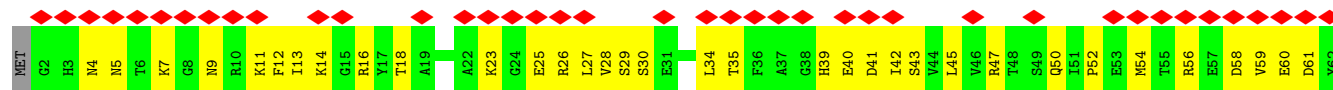
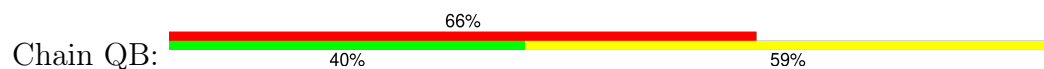


• Molecule 8: BplB

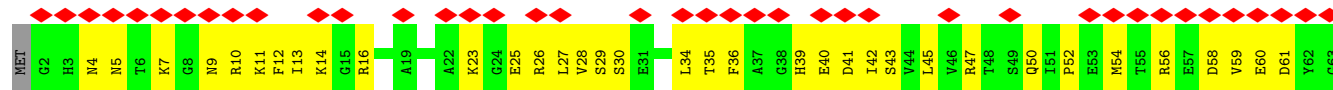




## ● Molecule 8: BplB



## ● Molecule 8: BplB



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12800	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.659	Depositor
Minimum map value	-0.362	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.22	Depositor
Map size (Å)	711.1168, 711.1168, 711.1168	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3889, 1.3889, 1.3889	Depositor



## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.20	0/1438	0.39	0/1945
1	B	0.19	0/1438	0.39	0/1945
1	C	0.20	0/1438	0.40	0/1945
1	D	0.20	0/1438	0.39	0/1945
1	E	0.19	0/1438	0.39	0/1945
1	F	0.20	0/1438	0.41	0/1945
2	G	0.20	0/1226	0.42	0/1673
2	H	0.20	0/1226	0.43	0/1673
2	I	0.20	0/1226	0.44	0/1673
2	J	0.20	0/1226	0.43	0/1673
2	K	0.20	0/1226	0.43	0/1673
2	L	0.20	0/1226	0.44	0/1673
3	M	0.22	0/907	0.59	0/1237
3	N	0.24	0/907	0.59	0/1237
3	O	0.22	0/907	0.60	0/1237
3	P	0.25	0/907	0.59	0/1237
3	Q	0.24	0/907	0.59	0/1237
3	R	0.22	0/907	0.60	0/1237
4	S	0.22	0/964	0.55	0/1305
4	T	0.22	0/964	0.53	0/1305
4	U	0.21	0/964	0.50	0/1305
4	V	0.23	0/964	0.56	0/1305
4	W	0.22	0/964	0.55	0/1305
4	X	0.21	0/964	0.51	0/1305
5	0	0.16	0/3864	0.35	0/5250
5	1	0.17	0/3864	0.38	2/5250 (0.0%)
5	2	0.16	0/3864	0.35	0/5250
5	3	0.16	0/3864	0.35	0/5250
5	4	0.17	0/3864	0.35	0/5250
5	5	0.17	0/3864	0.35	0/5250
5	6	0.18	0/3864	0.36	0/5250
5	7	0.17	0/3864	0.35	0/5250
5	8	0.17	0/3864	0.35	0/5250
5	9	0.17	0/3864	0.36	0/5250

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
5	Y	0.17	0/3864	0.35	0/5250
5	Z	0.16	0/3864	0.34	0/5250
6	a	0.17	0/1688	0.41	0/2286
6	b	0.16	0/1688	0.39	0/2286
6	c	0.16	0/1688	0.41	0/2286
6	d	0.17	0/1688	0.41	0/2286
6	e	0.17	0/1688	0.40	0/2286
6	f	0.16	0/1688	0.39	0/2286
7	AA	0.19	0/4077	0.41	0/5549
7	BA	0.19	0/4077	0.42	0/5549
7	CA	0.19	0/4077	0.42	0/5549
7	DA	0.19	0/4077	0.41	0/5549
7	EA	0.19	0/4077	0.42	0/5549
7	FA	0.19	0/4077	0.42	0/5549
7	GA	0.18	0/4077	0.40	2/5549 (0.0%)
7	HA	0.18	0/4077	0.40	2/5549 (0.0%)
7	IA	0.18	0/4077	0.41	2/5549 (0.0%)
7	JA	0.17	0/4077	0.39	2/5549 (0.0%)
7	KA	0.17	0/4077	0.39	2/5549 (0.0%)
7	LA	0.18	0/4077	0.41	2/5549 (0.0%)
7	MA	0.18	0/4077	0.39	1/5549 (0.0%)
7	NA	0.18	0/4077	0.39	1/5549 (0.0%)
7	OA	0.18	0/4077	0.38	1/5549 (0.0%)
7	PA	0.18	0/4077	0.39	1/5549 (0.0%)
7	QA	0.18	0/4077	0.38	1/5549 (0.0%)
7	RA	0.18	0/4077	0.38	1/5549 (0.0%)
7	g	0.17	0/4077	0.35	0/5549
7	h	0.17	0/4077	0.35	0/5549
7	i	0.17	0/4077	0.34	0/5549
7	j	0.17	0/4077	0.35	0/5549
7	k	0.17	0/4077	0.35	0/5549
7	l	0.17	0/4077	0.35	0/5549
7	m	0.19	0/4077	0.40	0/5549
7	n	0.20	0/4077	0.42	0/5549
7	o	0.19	0/4077	0.38	0/5549
7	p	0.19	0/4077	0.40	0/5549
7	q	0.19	0/4077	0.40	0/5549
7	r	0.18	0/4077	0.38	0/5549
8	AB	0.20	0/1335	0.41	0/1806
8	BB	0.20	0/1335	0.41	0/1806
8	CB	0.20	0/1335	0.40	0/1806
8	DB	0.21	0/1335	0.41	0/1806
8	EB	0.20	0/1335	0.43	0/1806

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
8	FB	0.21	0/1335	0.42	0/1806
8	GB	0.22	0/1335	0.51	0/1806
8	HB	0.20	0/1335	0.47	0/1806
8	IB	0.20	0/1335	0.47	0/1806
8	JB	0.20	0/1335	0.49	0/1806
8	KB	0.20	0/1335	0.49	0/1806
8	LB	0.23	0/1335	0.51	0/1806
8	MB	0.19	0/1335	0.46	0/1806
8	NB	0.20	0/1335	0.46	0/1806
8	OB	0.21	0/1335	0.46	0/1806
8	PB	0.20	0/1335	0.48	0/1806
8	QB	0.21	0/1335	0.49	0/1806
8	RB	0.19	0/1335	0.45	0/1806
All	All	0.18	0/230046	0.40	20/312654 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	1
1	F	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	PA	455	PRO	CA-N-CD	-5.63	104.12	112.00
7	MA	455	PRO	CA-N-CD	-5.62	104.13	112.00
7	NA	455	PRO	CA-N-CD	-5.59	104.17	112.00
7	QA	455	PRO	CA-N-CD	-5.58	104.18	112.00
7	OA	455	PRO	CA-N-CD	-5.55	104.23	112.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	89	THR	Peptide
1	C	89	THR	Peptide
1	D	89	THR	Peptide
1	F	89	THR	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1409	0	1389	97	0
1	B	1409	0	1389	106	0
1	C	1409	0	1389	107	0
1	D	1409	0	1389	103	0
1	E	1409	0	1389	99	0
1	F	1409	0	1389	105	0
2	G	1202	0	1186	84	0
2	H	1202	0	1186	79	0
2	I	1202	0	1186	77	0
2	J	1202	0	1186	80	0
2	K	1202	0	1186	83	0
2	L	1202	0	1186	76	0
3	M	888	0	884	97	0
3	N	888	0	884	99	0
3	O	888	0	884	98	0
3	P	888	0	884	97	0
3	Q	888	0	884	99	0
3	R	888	0	884	98	0
4	S	944	0	949	87	0
4	T	944	0	949	93	0
4	U	944	0	949	94	0
4	V	944	0	949	95	0
4	W	944	0	949	88	0
4	X	944	0	949	93	0
5	0	3780	0	3720	180	0
5	1	3780	0	3720	178	0
5	2	3780	0	3720	180	0
5	3	3780	0	3720	181	0
5	4	3780	0	3720	210	0
5	5	3780	0	3720	210	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	6	3780	0	3720	218	0
5	7	3780	0	3720	213	0
5	8	3780	0	3720	214	0
5	9	3780	0	3720	218	0
5	Y	3780	0	3720	187	0
5	Z	3780	0	3720	176	0
6	a	1652	0	1661	103	0
6	b	1652	0	1661	93	0
6	c	1652	0	1661	97	0
6	d	1652	0	1661	99	0
6	e	1652	0	1661	100	0
6	f	1652	0	1661	96	0
7	AA	3995	0	3951	252	0
7	BA	3995	0	3951	249	0
7	CA	3995	0	3951	262	0
7	DA	3995	0	3951	255	0
7	EA	3995	0	3951	247	0
7	FA	3995	0	3951	262	0
7	GA	3995	0	3951	228	0
7	HA	3995	0	3951	224	0
7	IA	3995	0	3951	229	0
7	JA	3995	0	3951	226	0
7	KA	3995	0	3951	224	0
7	LA	3995	0	3951	230	0
7	MA	3995	0	3951	218	0
7	NA	3995	0	3951	224	0
7	OA	3995	0	3951	219	0
7	PA	3995	0	3951	218	0
7	QA	3995	0	3951	222	0
7	RA	3995	0	3951	219	0
7	g	3995	0	3951	275	0
7	h	3995	0	3951	273	0
7	i	3995	0	3951	274	0
7	j	3995	0	3951	266	0
7	k	3995	0	3951	267	0
7	l	3995	0	3951	270	0
7	m	3995	0	3951	238	0
7	n	3995	0	3951	247	0
7	o	3995	0	3951	249	0
7	p	3995	0	3951	241	0
7	q	3995	0	3951	239	0
7	r	3995	0	3951	246	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	AB	1313	0	1286	110	0
8	BB	1313	0	1286	114	0
8	CB	1313	0	1286	111	0
8	DB	1313	0	1286	122	0
8	EB	1313	0	1286	118	0
8	FB	1313	0	1286	115	0
8	GB	1313	0	1286	151	0
8	HB	1313	0	1286	145	0
8	IB	1313	0	1286	149	0
8	JB	1313	0	1286	153	0
8	KB	1313	0	1286	150	0
8	LB	1313	0	1286	154	0
8	MB	1313	0	1286	143	0
8	NB	1313	0	1286	137	0
8	OB	1313	0	1286	139	0
8	PB	1313	0	1286	142	0
8	QB	1313	0	1286	129	0
8	RB	1313	0	1286	134	0
All	All	225414	0	222732	12747	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 28.

The worst 5 of 12747 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)
8:FB:48:THR:HB	8:FB:84:GLN:HB3	1.48	0.96
8:EB:48:THR:HB	8:EB:84:GLN:HB3	1.48	0.95
8:BB:48:THR:HB	8:BB:84:GLN:HB3	1.48	0.95
8:CB:48:THR:HB	8:CB:84:GLN:HB3	1.48	0.94
8:DB:48:THR:HB	8:DB:84:GLN:HB3	1.48	0.94

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	178/203 (88%)	165 (93%)	13 (7%)	0	100	100
1	B	178/203 (88%)	164 (92%)	14 (8%)	0	100	100
1	C	178/203 (88%)	164 (92%)	14 (8%)	0	100	100
1	D	178/203 (88%)	165 (93%)	13 (7%)	0	100	100
1	E	178/203 (88%)	164 (92%)	14 (8%)	0	100	100
1	F	178/203 (88%)	164 (92%)	14 (8%)	0	100	100
2	G	154/193 (80%)	140 (91%)	14 (9%)	0	100	100
2	H	154/193 (80%)	141 (92%)	13 (8%)	0	100	100
2	I	154/193 (80%)	142 (92%)	12 (8%)	0	100	100
2	J	154/193 (80%)	140 (91%)	14 (9%)	0	100	100
2	K	154/193 (80%)	141 (92%)	13 (8%)	0	100	100
2	L	154/193 (80%)	141 (92%)	13 (8%)	0	100	100
3	M	110/118 (93%)	97 (88%)	13 (12%)	0	100	100
3	N	110/118 (93%)	95 (86%)	15 (14%)	0	100	100
3	O	110/118 (93%)	96 (87%)	14 (13%)	0	100	100
3	P	110/118 (93%)	95 (86%)	15 (14%)	0	100	100
3	Q	110/118 (93%)	95 (86%)	15 (14%)	0	100	100
3	R	110/118 (93%)	96 (87%)	14 (13%)	0	100	100
4	S	113/125 (90%)	102 (90%)	11 (10%)	0	100	100
4	T	113/125 (90%)	102 (90%)	10 (9%)	1 (1%)	14	51
4	U	113/125 (90%)	103 (91%)	10 (9%)	0	100	100
4	V	113/125 (90%)	104 (92%)	9 (8%)	0	100	100
4	W	113/125 (90%)	102 (90%)	11 (10%)	0	100	100
4	X	113/125 (90%)	103 (91%)	10 (9%)	0	100	100
5	0	475/477 (100%)	462 (97%)	13 (3%)	0	100	100
5	1	475/477 (100%)	462 (97%)	13 (3%)	0	100	100
5	2	475/477 (100%)	461 (97%)	14 (3%)	0	100	100
5	3	475/477 (100%)	462 (97%)	13 (3%)	0	100	100
5	4	475/477 (100%)	450 (95%)	25 (5%)	0	100	100
5	5	475/477 (100%)	451 (95%)	24 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	6	475/477 (100%)	451 (95%)	24 (5%)	0	100	100
5	7	475/477 (100%)	450 (95%)	25 (5%)	0	100	100
5	8	475/477 (100%)	451 (95%)	24 (5%)	0	100	100
5	9	475/477 (100%)	452 (95%)	23 (5%)	0	100	100
5	Y	475/477 (100%)	462 (97%)	13 (3%)	0	100	100
5	Z	475/477 (100%)	461 (97%)	14 (3%)	0	100	100
6	a	202/278 (73%)	191 (95%)	11 (5%)	0	100	100
6	b	202/278 (73%)	193 (96%)	9 (4%)	0	100	100
6	c	202/278 (73%)	191 (95%)	11 (5%)	0	100	100
6	d	202/278 (73%)	190 (94%)	12 (6%)	0	100	100
6	e	202/278 (73%)	191 (95%)	11 (5%)	0	100	100
6	f	202/278 (73%)	191 (95%)	11 (5%)	0	100	100
7	AA	526/529 (99%)	497 (94%)	29 (6%)	0	100	100
7	BA	526/529 (99%)	497 (94%)	29 (6%)	0	100	100
7	CA	526/529 (99%)	497 (94%)	29 (6%)	0	100	100
7	DA	526/529 (99%)	497 (94%)	29 (6%)	0	100	100
7	EA	526/529 (99%)	498 (95%)	28 (5%)	0	100	100
7	FA	526/529 (99%)	498 (95%)	28 (5%)	0	100	100
7	GA	526/529 (99%)	498 (95%)	28 (5%)	0	100	100
7	HA	526/529 (99%)	500 (95%)	26 (5%)	0	100	100
7	IA	526/529 (99%)	500 (95%)	26 (5%)	0	100	100
7	JA	526/529 (99%)	498 (95%)	28 (5%)	0	100	100
7	KA	526/529 (99%)	500 (95%)	26 (5%)	0	100	100
7	LA	526/529 (99%)	500 (95%)	26 (5%)	0	100	100
7	MA	526/529 (99%)	493 (94%)	33 (6%)	0	100	100
7	NA	526/529 (99%)	494 (94%)	32 (6%)	0	100	100
7	OA	526/529 (99%)	493 (94%)	33 (6%)	0	100	100
7	PA	526/529 (99%)	492 (94%)	34 (6%)	0	100	100
7	QA	526/529 (99%)	494 (94%)	32 (6%)	0	100	100
7	RA	526/529 (99%)	493 (94%)	33 (6%)	0	100	100
7	g	526/529 (99%)	488 (93%)	38 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	h	526/529 (99%)	488 (93%)	38 (7%)	0	100	100
7	i	526/529 (99%)	489 (93%)	37 (7%)	0	100	100
7	j	526/529 (99%)	488 (93%)	38 (7%)	0	100	100
7	k	526/529 (99%)	488 (93%)	38 (7%)	0	100	100
7	l	526/529 (99%)	490 (93%)	36 (7%)	0	100	100
7	m	526/529 (99%)	492 (94%)	34 (6%)	0	100	100
7	n	526/529 (99%)	490 (93%)	36 (7%)	0	100	100
7	o	526/529 (99%)	490 (93%)	36 (7%)	0	100	100
7	p	526/529 (99%)	491 (93%)	35 (7%)	0	100	100
7	q	526/529 (99%)	490 (93%)	36 (7%)	0	100	100
7	r	526/529 (99%)	491 (93%)	35 (7%)	0	100	100
8	AB	166/169 (98%)	159 (96%)	7 (4%)	0	100	100
8	BB	166/169 (98%)	159 (96%)	7 (4%)	0	100	100
8	CB	166/169 (98%)	159 (96%)	7 (4%)	0	100	100
8	DB	166/169 (98%)	159 (96%)	7 (4%)	0	100	100
8	EB	166/169 (98%)	159 (96%)	7 (4%)	0	100	100
8	FB	166/169 (98%)	159 (96%)	7 (4%)	0	100	100
8	GB	166/169 (98%)	158 (95%)	8 (5%)	0	100	100
8	HB	166/169 (98%)	158 (95%)	8 (5%)	0	100	100
8	IB	166/169 (98%)	156 (94%)	10 (6%)	0	100	100
8	JB	166/169 (98%)	158 (95%)	8 (5%)	0	100	100
8	KB	166/169 (98%)	156 (94%)	10 (6%)	0	100	100
8	LB	166/169 (98%)	156 (94%)	10 (6%)	0	100	100
8	MB	166/169 (98%)	155 (93%)	11 (7%)	0	100	100
8	NB	166/169 (98%)	153 (92%)	13 (8%)	0	100	100
8	OB	166/169 (98%)	155 (93%)	11 (7%)	0	100	100
8	PB	166/169 (98%)	155 (93%)	11 (7%)	0	100	100
8	QB	166/169 (98%)	154 (93%)	12 (7%)	0	100	100
8	RB	166/169 (98%)	156 (94%)	10 (6%)	0	100	100
All	All	29010/30138 (96%)	27281 (94%)	1728 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	T	119	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	157/176 (89%)	157 (100%)	0	100	100
1	B	157/176 (89%)	157 (100%)	0	100	100
1	C	157/176 (89%)	157 (100%)	0	100	100
1	D	157/176 (89%)	157 (100%)	0	100	100
1	E	157/176 (89%)	157 (100%)	0	100	100
1	F	157/176 (89%)	157 (100%)	0	100	100
2	G	130/156 (83%)	130 (100%)	0	100	100
2	H	130/156 (83%)	130 (100%)	0	100	100
2	I	130/156 (83%)	130 (100%)	0	100	100
2	J	130/156 (83%)	130 (100%)	0	100	100
2	K	130/156 (83%)	130 (100%)	0	100	100
2	L	130/156 (83%)	130 (100%)	0	100	100
3	M	99/104 (95%)	99 (100%)	0	100	100
3	N	99/104 (95%)	99 (100%)	0	100	100
3	O	99/104 (95%)	99 (100%)	0	100	100
3	P	99/104 (95%)	99 (100%)	0	100	100
3	Q	99/104 (95%)	99 (100%)	0	100	100
3	R	99/104 (95%)	99 (100%)	0	100	100
4	S	101/110 (92%)	101 (100%)	0	100	100
4	T	101/110 (92%)	101 (100%)	0	100	100
4	U	101/110 (92%)	101 (100%)	0	100	100
4	V	101/110 (92%)	101 (100%)	0	100	100
4	W	101/110 (92%)	101 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	X	101/110 (92%)	101 (100%)	0	100	100
5	0	416/416 (100%)	416 (100%)	0	100	100
5	1	416/416 (100%)	416 (100%)	0	100	100
5	2	416/416 (100%)	416 (100%)	0	100	100
5	3	416/416 (100%)	416 (100%)	0	100	100
5	4	416/416 (100%)	416 (100%)	0	100	100
5	5	416/416 (100%)	416 (100%)	0	100	100
5	6	416/416 (100%)	416 (100%)	0	100	100
5	7	416/416 (100%)	416 (100%)	0	100	100
5	8	416/416 (100%)	416 (100%)	0	100	100
5	9	416/416 (100%)	416 (100%)	0	100	100
5	Y	416/416 (100%)	416 (100%)	0	100	100
5	Z	416/416 (100%)	416 (100%)	0	100	100
6	a	188/252 (75%)	188 (100%)	0	100	100
6	b	188/252 (75%)	188 (100%)	0	100	100
6	c	188/252 (75%)	188 (100%)	0	100	100
6	d	188/252 (75%)	188 (100%)	0	100	100
6	e	188/252 (75%)	188 (100%)	0	100	100
6	f	188/252 (75%)	188 (100%)	0	100	100
7	AA	429/430 (100%)	429 (100%)	0	100	100
7	BA	429/430 (100%)	429 (100%)	0	100	100
7	CA	429/430 (100%)	429 (100%)	0	100	100
7	DA	429/430 (100%)	429 (100%)	0	100	100
7	EA	429/430 (100%)	429 (100%)	0	100	100
7	FA	429/430 (100%)	429 (100%)	0	100	100
7	GA	429/430 (100%)	429 (100%)	0	100	100
7	HA	429/430 (100%)	429 (100%)	0	100	100
7	IA	429/430 (100%)	429 (100%)	0	100	100
7	JA	429/430 (100%)	429 (100%)	0	100	100
7	KA	429/430 (100%)	429 (100%)	0	100	100
7	LA	429/430 (100%)	429 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	MA	429/430 (100%)	429 (100%)	0	100	100
7	NA	429/430 (100%)	429 (100%)	0	100	100
7	OA	429/430 (100%)	429 (100%)	0	100	100
7	PA	429/430 (100%)	429 (100%)	0	100	100
7	QA	429/430 (100%)	429 (100%)	0	100	100
7	RA	429/430 (100%)	429 (100%)	0	100	100
7	g	429/430 (100%)	429 (100%)	0	100	100
7	h	429/430 (100%)	429 (100%)	0	100	100
7	i	429/430 (100%)	429 (100%)	0	100	100
7	j	429/430 (100%)	429 (100%)	0	100	100
7	k	429/430 (100%)	429 (100%)	0	100	100
7	l	429/430 (100%)	429 (100%)	0	100	100
7	m	429/430 (100%)	429 (100%)	0	100	100
7	n	429/430 (100%)	429 (100%)	0	100	100
7	o	429/430 (100%)	429 (100%)	0	100	100
7	p	429/430 (100%)	429 (100%)	0	100	100
7	q	429/430 (100%)	429 (100%)	0	100	100
7	r	429/430 (100%)	429 (100%)	0	100	100
8	AB	143/144 (99%)	143 (100%)	0	100	100
8	BB	143/144 (99%)	143 (100%)	0	100	100
8	CB	143/144 (99%)	143 (100%)	0	100	100
8	DB	143/144 (99%)	143 (100%)	0	100	100
8	EB	143/144 (99%)	143 (100%)	0	100	100
8	FB	143/144 (99%)	143 (100%)	0	100	100
8	GB	143/144 (99%)	143 (100%)	0	100	100
8	HB	143/144 (99%)	143 (100%)	0	100	100
8	IB	143/144 (99%)	143 (100%)	0	100	100
8	JB	143/144 (99%)	143 (100%)	0	100	100
8	KB	143/144 (99%)	143 (100%)	0	100	100
8	LB	143/144 (99%)	143 (100%)	0	100	100
8	MB	143/144 (99%)	143 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	NB	143/144 (99%)	143 (100%)	0	100	100
8	OB	143/144 (99%)	143 (100%)	0	100	100
8	PB	143/144 (99%)	143 (100%)	0	100	100
8	QB	143/144 (99%)	143 (100%)	0	100	100
8	RB	143/144 (99%)	143 (100%)	0	100	100
All	All	24486/25272 (97%)	24486 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 225 such sidechains are listed below:

Mol	Chain	Res	Type
7	m	88	GLN
8	PB	82	GLN
7	r	403	ASN
8	OB	65	ASN
7	RA	3	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 ⓘ

There are no chain breaks in this entry.

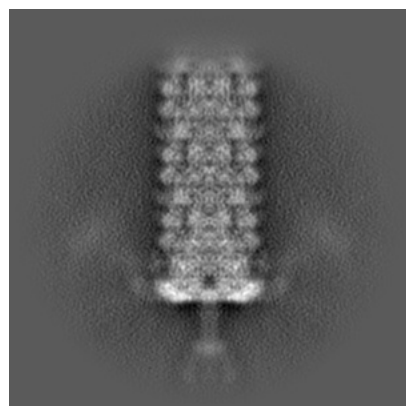
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43960. These allow visual inspection of the internal detail of the map and identification of artifacts.

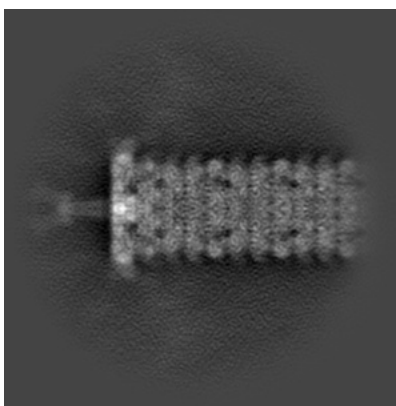
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

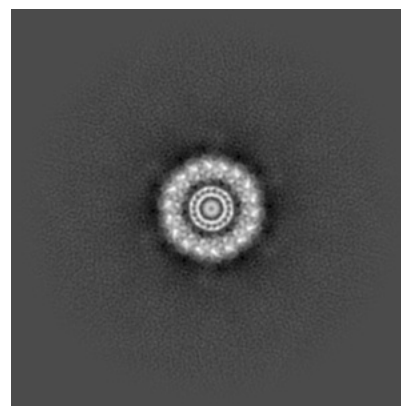
#### 6.1.1 Primary map



X

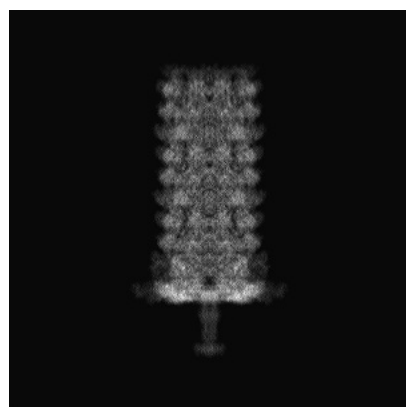


Y

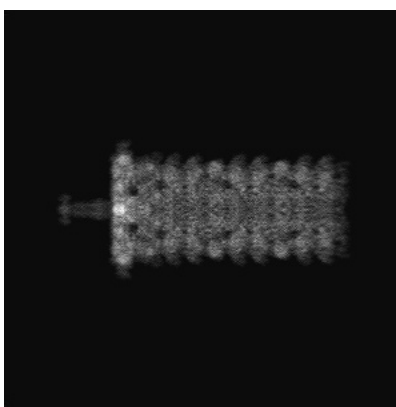


Z

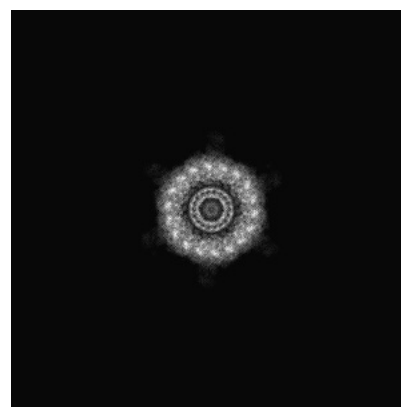
#### 6.1.2 Raw map



X



Y

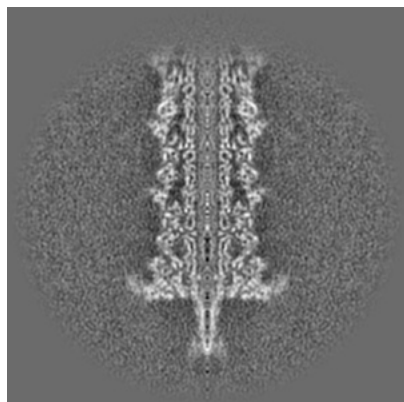


Z

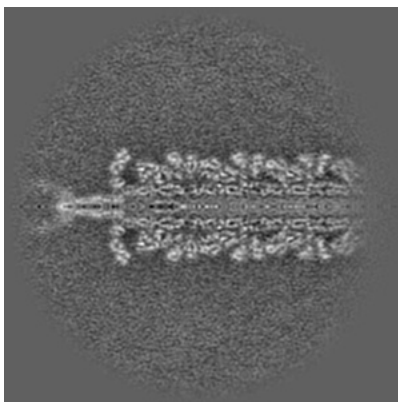
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

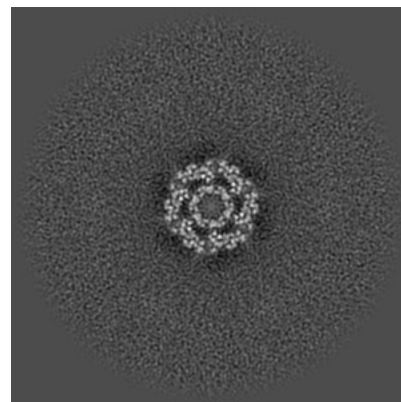
### 6.2.1 Primary map



X Index: 256

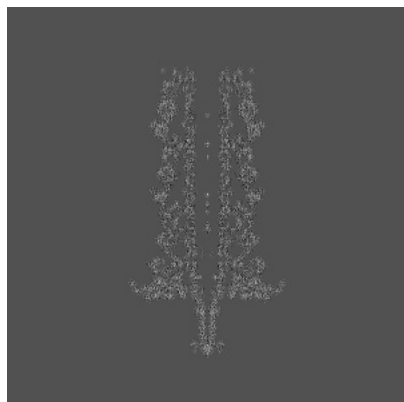


Y Index: 256

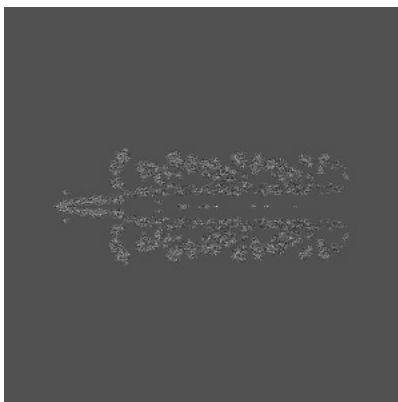


Z Index: 256

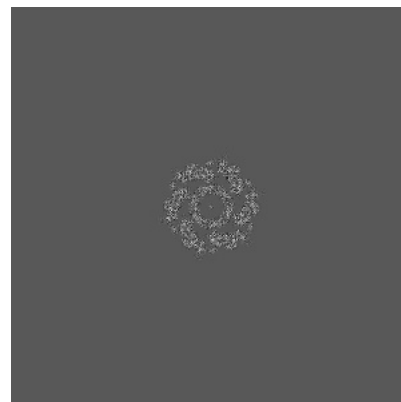
### 6.2.2 Raw map



X Index: 256



Y Index: 256



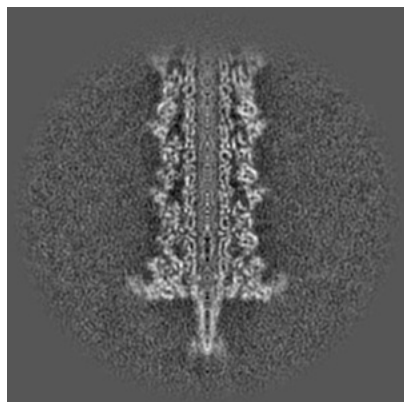
Z Index: 256

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

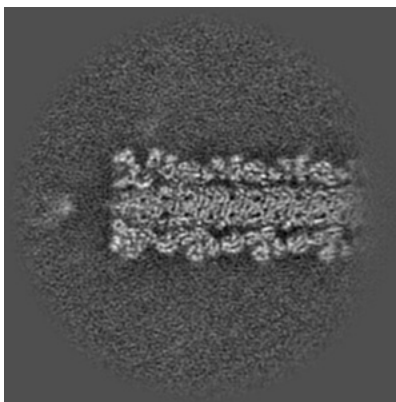


## 6.3 Largest variance slices [i](#)

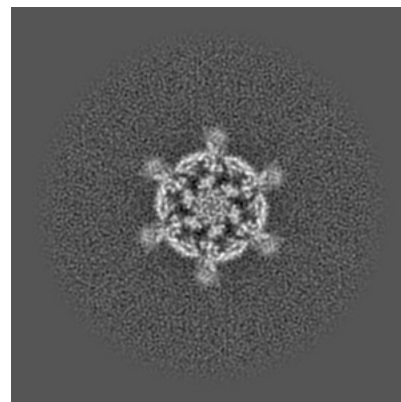
### 6.3.1 Primary map



X Index: 255



Y Index: 238

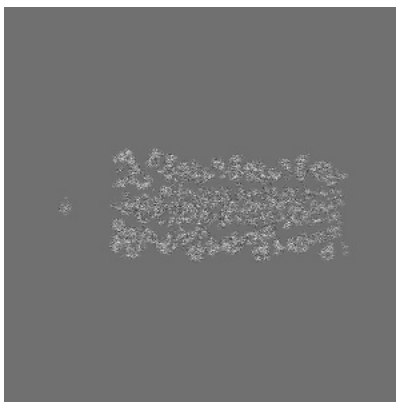


Z Index: 151

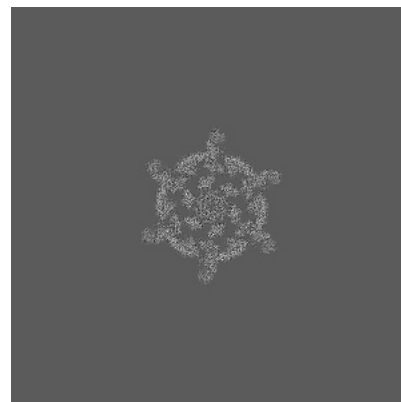
### 6.3.2 Raw map



X Index: 272



Y Index: 238

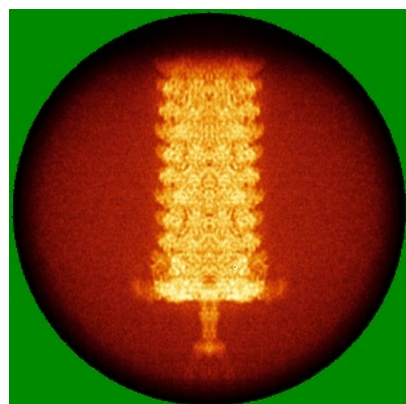


Z Index: 150

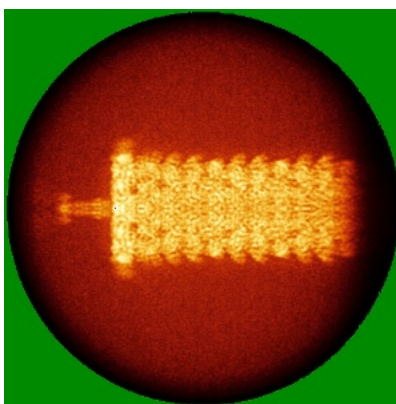
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

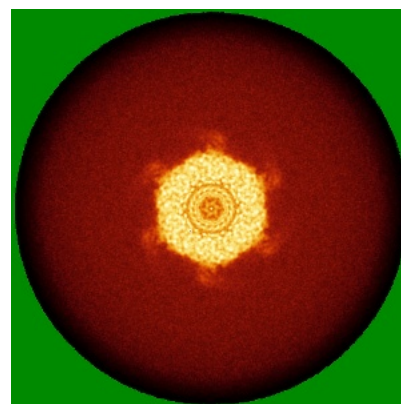
### 6.4.1 Primary map



X

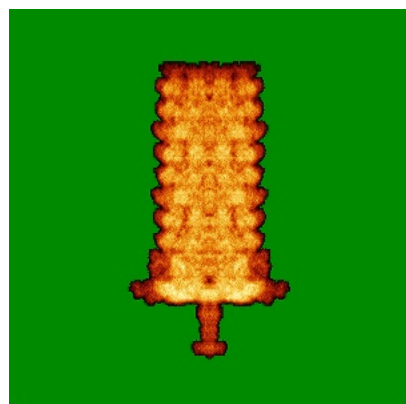


Y

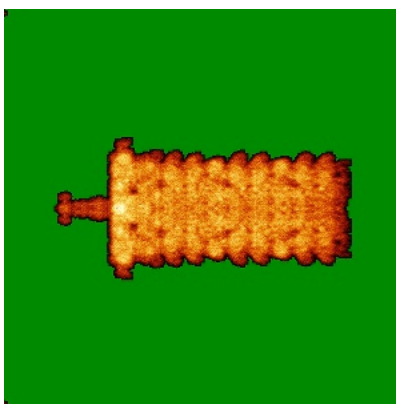


Z

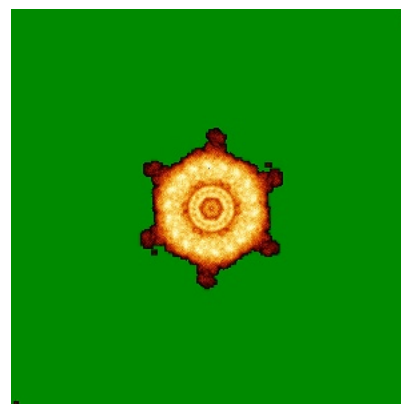
### 6.4.2 Raw map



X



Y

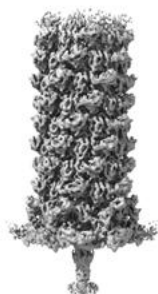


Z

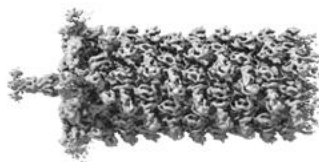
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



Y



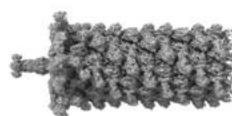
Z

The images above show the 3D surface view of the map at the recommended contour level 0.22. 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.

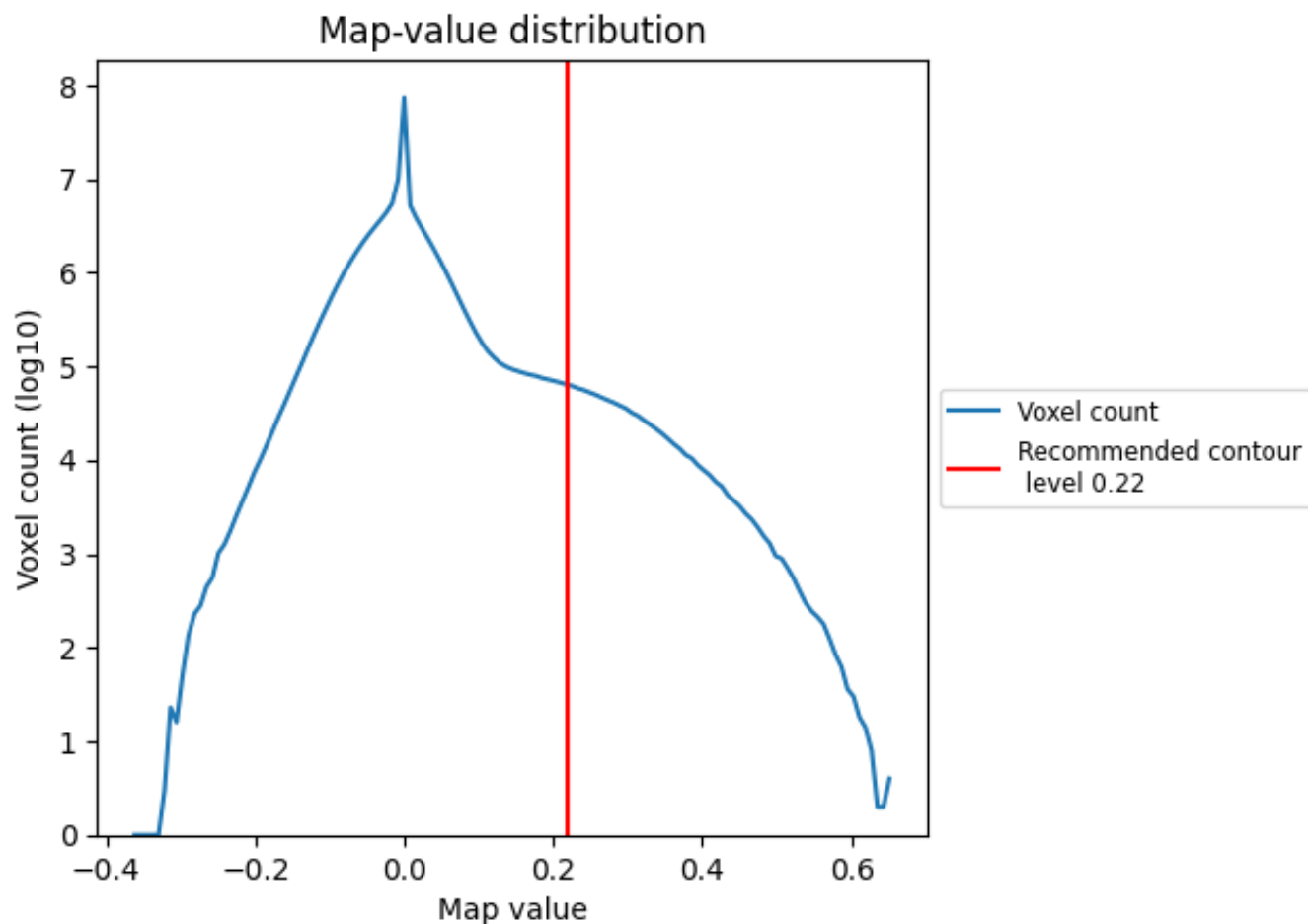
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

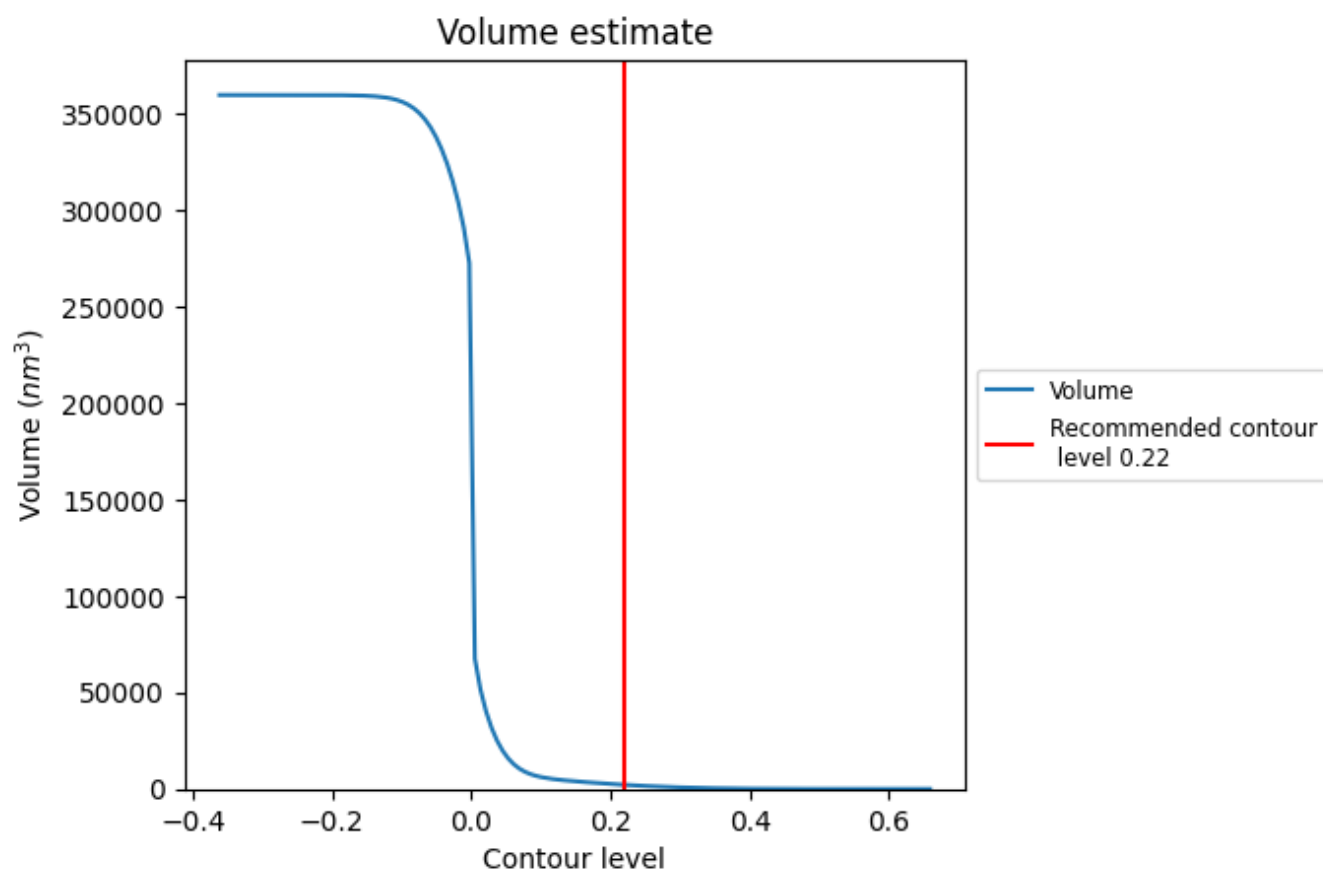
This section contains the results of statistical analysis of the map.

### 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.

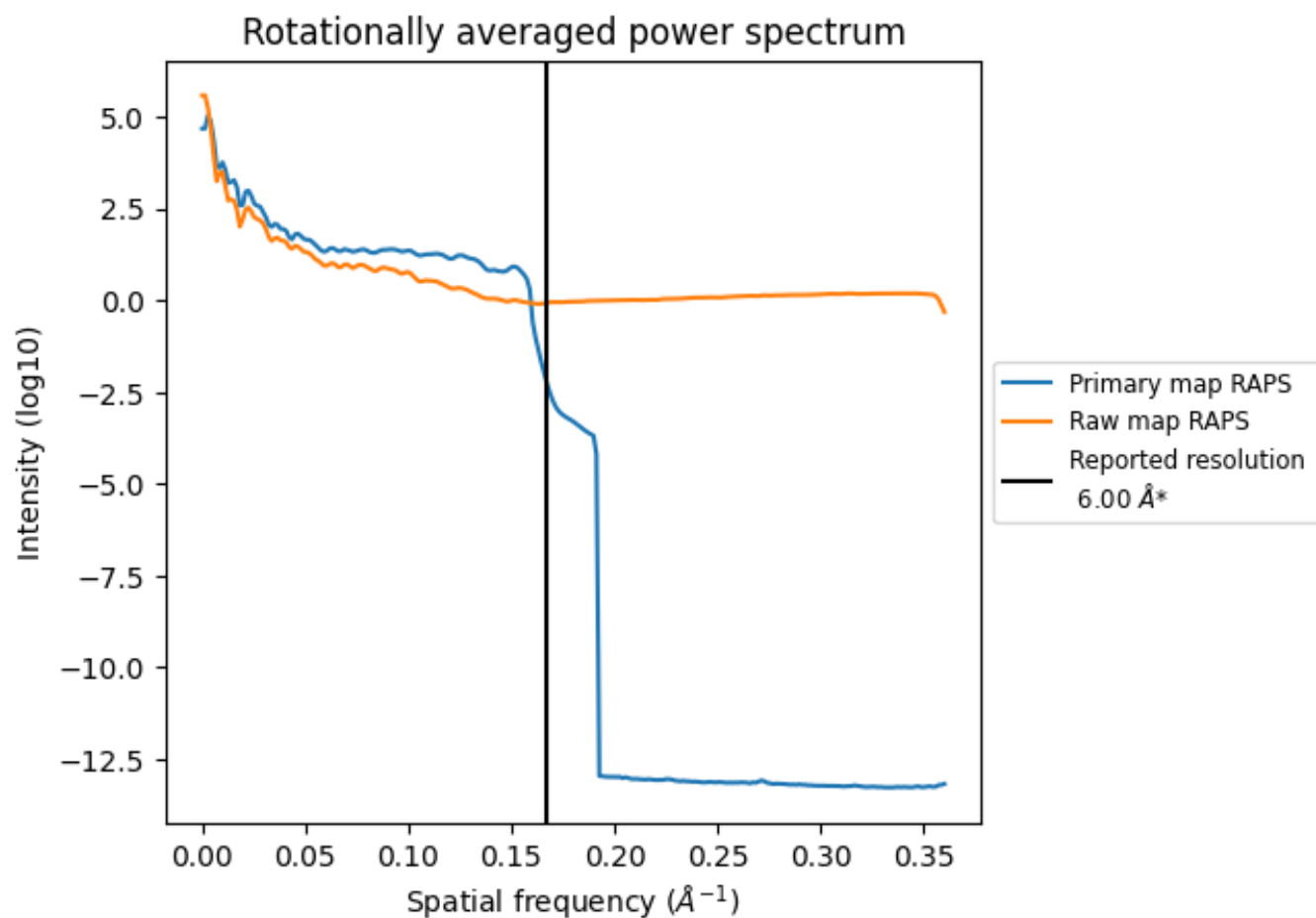
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2145  $\text{nm}^3$ ; this corresponds to an approximate mass of 1938 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

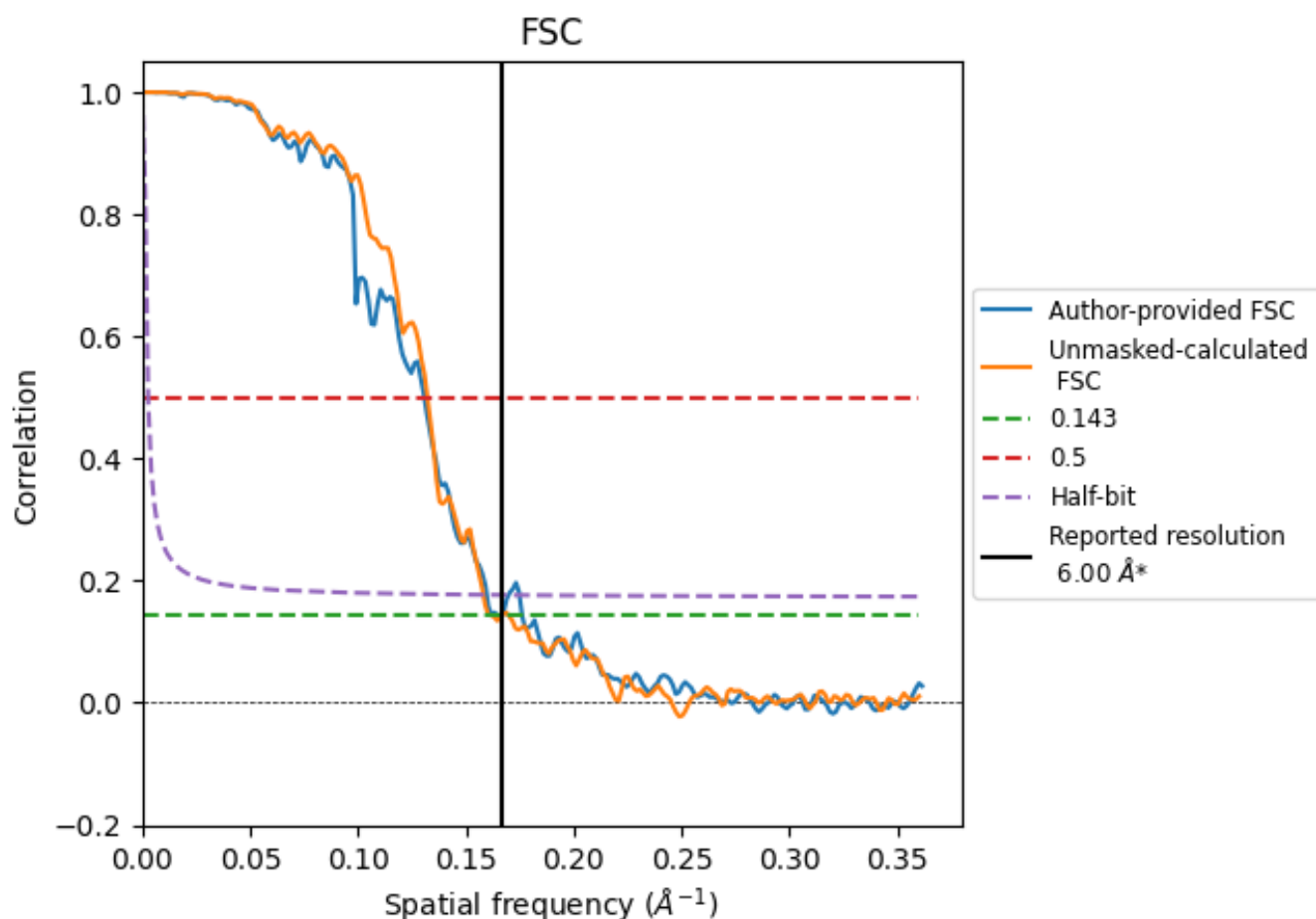


\*Reported resolution corresponds to spatial frequency of 0.167 Å<sup>-1</sup>

## 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  $0.167 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.00	-	-
Author-provided FSC curve	6.07	7.65	6.27
Unmasked-calculated*	6.18	7.56	6.33

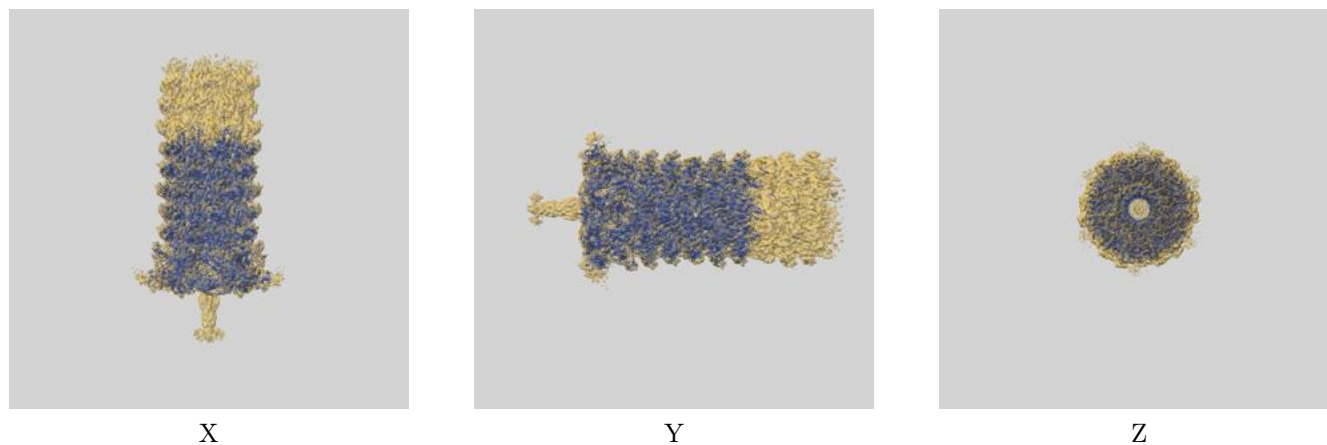
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



## 9 Map-model fit [i](#)

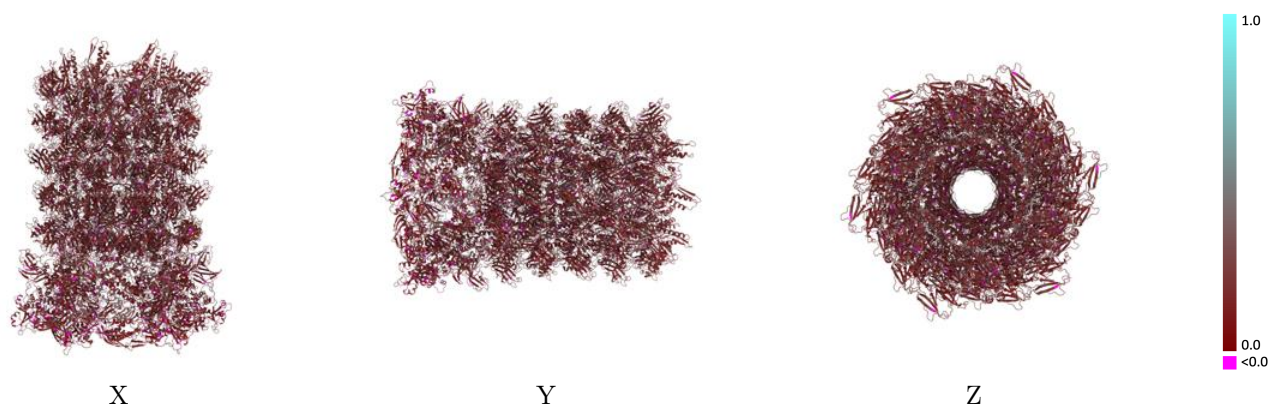
This section contains information regarding the fit between EMDB map EMD-43960 and PDB model 9AY5. Per-residue inclusion information can be found in section [3](#) on page [13](#).

### 9.1 Map-model overlay [i](#)



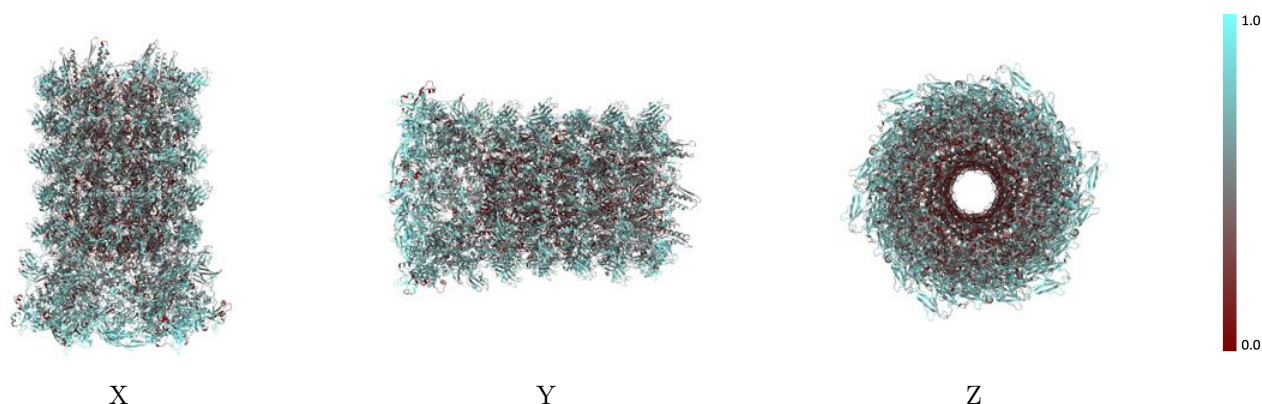
The images above show the 3D surface view of the map at the recommended contour level 0.22 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



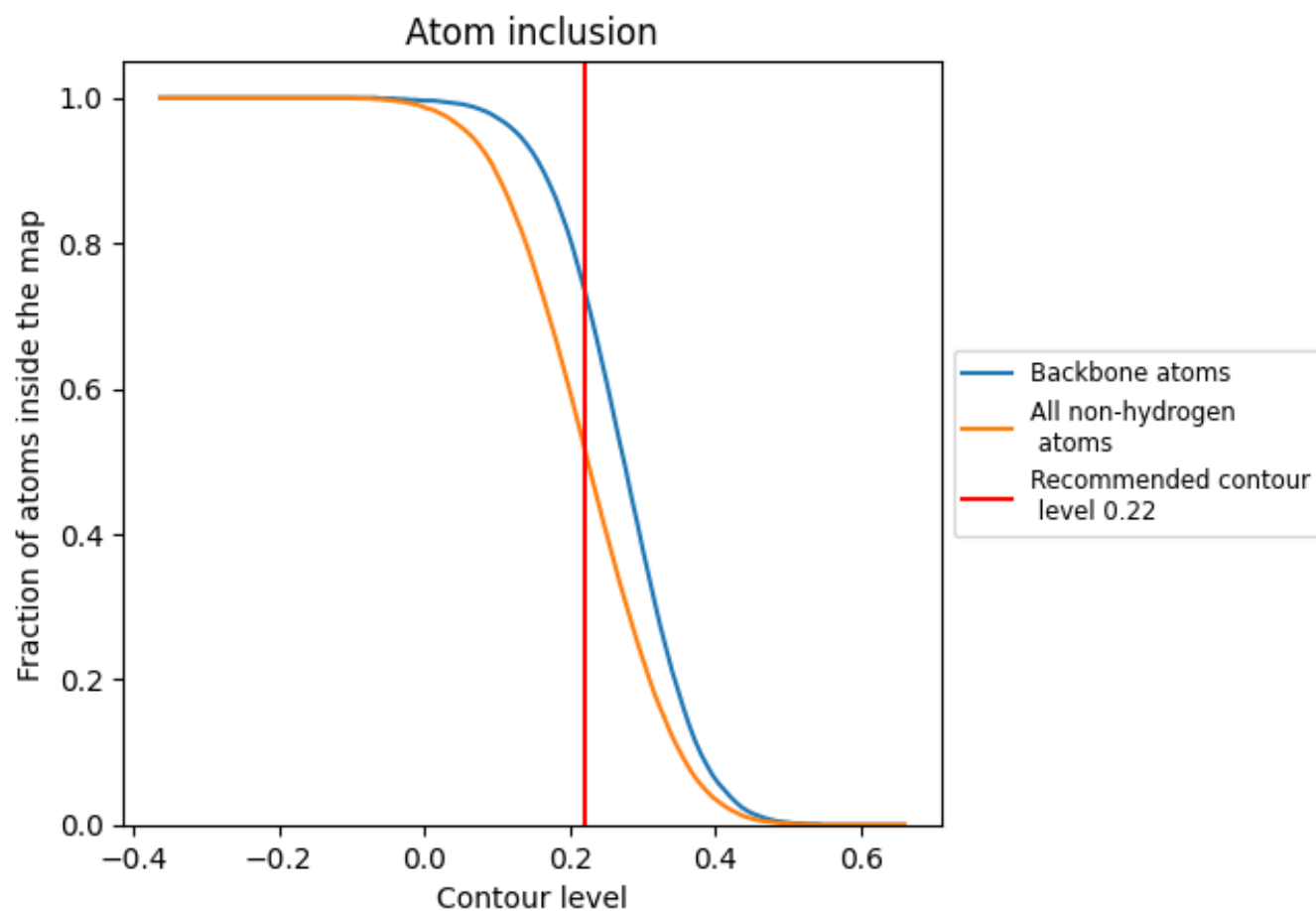
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.22).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 52% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5170	 0.2000
0	 0.6340	 0.1920
1	 0.6330	 0.1920
2	 0.6320	 0.1920
3	 0.6310	 0.1920
4	 0.6420	 0.1830
5	 0.6400	 0.1830
6	 0.6410	 0.1830
7	 0.6440	 0.1830
8	 0.6410	 0.1830
9	 0.6420	 0.1840
A	 0.3290	 0.1980
AA	 0.5470	 0.2090
AB	 0.3180	 0.2000
B	 0.3300	 0.1970
BA	 0.5440	 0.2080
BB	 0.3210	 0.1970
C	 0.3300	 0.1990
CA	 0.5470	 0.2090
CB	 0.3240	 0.2000
D	 0.3290	 0.1980
DA	 0.5460	 0.2090
DB	 0.3190	 0.2010
E	 0.3300	 0.1990
EA	 0.5450	 0.2090
EB	 0.3220	 0.2000
F	 0.3300	 0.1960
FA	 0.5460	 0.2100
FB	 0.3240	 0.2020
G	 0.3240	 0.1960
GA	 0.5400	 0.2100
GB	 0.3060	 0.2010
H	 0.3230	 0.1950
HA	 0.5400	 0.2100
HB	 0.3030	 0.2000































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Chain	Atom inclusion	Q-score
I	 0.3220	 0.1930
IA	 0.5390	 0.2100
IB	 0.3010	 0.2010
J	 0.3240	 0.1940
JA	 0.5410	 0.2090
JB	 0.3060	 0.2030
K	 0.3240	 0.1940
KA	 0.5400	 0.2090
KB	 0.3040	 0.2010
L	 0.3210	 0.1940
LA	 0.5400	 0.2090
LB	 0.3040	 0.2000
M	 0.4050	 0.1920
MA	 0.5510	 0.2130
MB	 0.3000	 0.2010
N	 0.4110	 0.1920
NA	 0.5550	 0.2140
NB	 0.3030	 0.2010
O	 0.4090	 0.1930
OA	 0.5520	 0.2140
OB	 0.3030	 0.2010
P	 0.4050	 0.1920
PA	 0.5520	 0.2140
PB	 0.3000	 0.2020
Q	 0.4110	 0.1890
QA	 0.5550	 0.2150
QB	 0.3020	 0.2040
R	 0.4090	 0.1920
RA	 0.5510	 0.2130
RB	 0.3020	 0.2010
S	 0.4800	 0.2150
T	 0.4880	 0.2110
U	 0.4840	 0.2120
V	 0.4790	 0.2100
W	 0.4880	 0.2110
X	 0.4850	 0.2130
Y	 0.6300	 0.1920
Z	 0.6310	 0.1930
a	 0.5890	 0.1760
b	 0.5940	 0.1750
c	 0.5960	 0.1780
d	 0.5890	 0.1780

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Chain	Atom inclusion	Q-score
e	 0.5950	 0.1760
f	 0.5960	 0.1770
g	 0.5160	 0.1950
h	 0.5170	 0.1940
i	 0.5170	 0.1940
j	 0.5160	 0.1940
k	 0.5170	 0.1930
l	 0.5170	 0.1940
m	 0.5330	 0.2110
n	 0.5340	 0.2100
o	 0.5330	 0.2110
p	 0.5330	 0.2110
q	 0.5340	 0.2110
r	 0.5330	 0.2110