



Full wwPDB EM Validation Report ⓘ

May 27, 2024 – 05:59 AM EDT

PDB ID : 7SPU
EMDB ID : EMD-25372
Title : In situ cryo-EM structure of bacteriophage Sf6 gp3:gp7:gp5 complex in con-
formation 1 at 3.73Å resolution
Authors : Li, F.; Cingolani, G.; Hou, C.; Yang, R.
Deposited on : 2021-11-03
Resolution : 3.73 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 ⓘ symbol.

The types of validation reports are described at

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

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

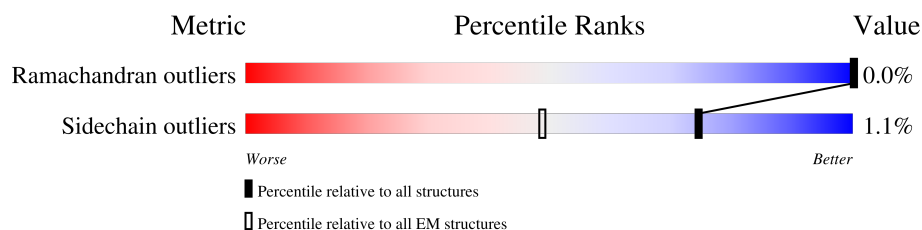
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

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 3.73 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 $\leq 5\%$. 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	0	160	<div> <div>30%</div> <div>90%</div> <div>8%</div> </div>
1	1	160	<div> <div>42%</div> <div>96%</div> <div>2%</div> </div>
1	Y	160	<div> <div>28%</div> <div>78%</div> <div>15%</div> <div>8%</div> </div>
1	f	160	<div> <div>34%</div> <div>96%</div> <div>2%</div> </div>
1	h	160	<div> <div>27%</div> <div>89%</div> <div>8%</div> </div>
1	n	160	<div> <div>30%</div> <div>90%</div> <div>8%</div> </div>
1	p	160	<div> <div>34%</div> <div>96%</div> <div>2%</div> </div>
1	r	160	<div> <div>32%</div> <div>92%</div> <div>8%</div> </div>
1	v	160	<div> <div>29%</div> <div>92%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	w	160	<div> <div>33%</div> <div>92%</div> <div>8%</div> </div>
1	x	160	<div> <div>34%</div> <div>98%</div> <div>..</div> </div>
1	z	160	<div> <div>39%</div> <div>99%</div> <div>.</div> </div>
2	A	708	<div> <div>46%</div> <div>87%</div> <div>11%</div> </div>
2	B	708	<div> <div>45%</div> <div>88%</div> <div>11%</div> </div>
2	C	708	<div> <div>45%</div> <div>87%</div> <div>11%</div> </div>
2	D	708	<div> <div>46%</div> <div>89%</div> <div>11%</div> </div>
2	E	708	<div> <div>45%</div> <div>87%</div> <div>11%</div> </div>
2	F	708	<div> <div>44%</div> <div>88%</div> <div>11%</div> </div>
2	G	708	<div> <div>46%</div> <div>88%</div> <div>11%</div> </div>
2	H	708	<div> <div>47%</div> <div>88%</div> <div>11%</div> </div>
2	I	708	<div> <div>47%</div> <div>87%</div> <div>11%</div> </div>
2	J	708	<div> <div>45%</div> <div>88%</div> <div>11%</div> </div>
2	K	708	<div> <div>44%</div> <div>88%</div> <div>11%</div> </div>
2	L	708	<div> <div>45%</div> <div>89%</div> <div>11%</div> </div>
3	M	423	<div> <div>18%</div> <div>98%</div> <div>.</div> </div>
3	N	423	<div> <div>19%</div> <div>100%</div> </div>
3	O	423	<div> <div>20%</div> <div>100%</div> </div>
3	P	423	<div> <div>17%</div> <div>100%</div> </div>
3	Q	423	<div> <div>22%</div> <div>100%</div> </div>
3	R	423	<div> <div>20%</div> <div>99%</div> <div>.</div> </div>
3	S	423	<div> <div>22%</div> <div>100%</div> </div>
3	T	423	<div> <div>23%</div> <div>100%</div> </div>
3	U	423	<div> <div>19%</div> <div>100%</div> </div>
3	V	423	<div> <div>21%</div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
3	W	423	21% 100%
3	X	423	20% 98%
3	Z	423	20% 99%
3	a	423	23% 99%
3	b	423	18% 99%
3	c	423	19% 99%
3	d	423	18% 99%
3	e	423	22% 96%
3	g	423	23% 98%
3	i	423	21% 97%
3	j	423	21% 98%
3	k	423	22% 97%
3	l	423	20% 96%
3	m	423	22% 100%
3	o	423	20% 100%
3	q	423	24% 99%
3	s	423	19% 100%
3	t	423	21% 98%
3	u	423	23% 99%
3	y	423	23% 99%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 169896 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 Gene 7 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	148	Total	C	N	O	S	0	0
			1161	732	191	232	6		
1	1	158	Total	C	N	O	S	0	0
			1232	777	202	247	6		
1	Y	148	Total	C	N	O	S	0	0
			1162	734	191	231	6		
1	f	158	Total	C	N	O	S	0	0
			1232	777	202	247	6		
1	h	148	Total	C	N	O	S	0	0
			1161	732	191	232	6		
1	n	148	Total	C	N	O	S	0	0
			1161	732	191	232	6		
1	p	158	Total	C	N	O	S	0	0
			1232	777	202	247	6		
1	r	148	Total	C	N	O	S	0	0
			1161	732	191	232	6		
1	v	148	Total	C	N	O	S	0	0
			1161	732	191	232	6		
1	w	148	Total	C	N	O	S	0	0
			1161	732	191	232	6		
1	x	158	Total	C	N	O	S	0	0
			1232	777	202	247	6		
1	z	158	Total	C	N	O	S	0	0
			1229	774	202	247	6		

- Molecule 2 is a protein called Gene 3 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		
2	B	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		
2	C	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		
2	E	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		
2	F	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		
2	G	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		
2	H	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		
2	I	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		
2	J	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		
2	K	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		
2	L	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		

- Molecule 3 is a protein called Gene 5 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	N	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	O	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	P	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	Q	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	R	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	S	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	T	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	U	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	V	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		

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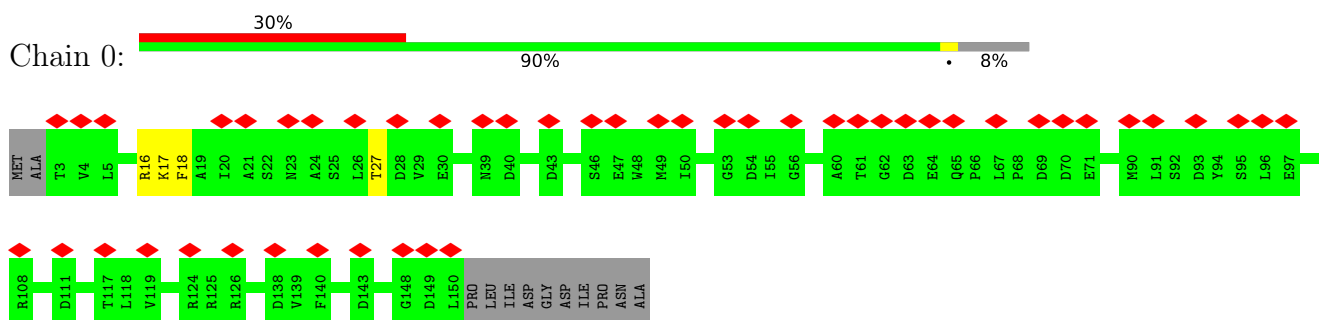
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	W	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	X	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	Z	421	Total	C	N	O	S	0	0
			3202	2013	549	630	10		
3	a	421	Total	C	N	O	S	0	0
			3202	2013	549	630	10		
3	b	421	Total	C	N	O	S	0	0
			3202	2013	549	630	10		
3	c	421	Total	C	N	O	S	0	0
			3202	2013	549	630	10		
3	d	421	Total	C	N	O	S	0	0
			3202	2013	549	630	10		
3	e	414	Total	C	N	O	S	0	0
			3149	1983	539	617	10		
3	g	414	Total	C	N	O	S	0	0
			3149	1983	539	617	10		
3	i	414	Total	C	N	O	S	0	0
			3149	1983	539	617	10		
3	j	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	k	414	Total	C	N	O	S	0	0
			3149	1983	539	617	10		
3	l	414	Total	C	N	O	S	0	0
			3149	1983	539	617	10		
3	m	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	o	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	q	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	s	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	t	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	u	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	y	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		

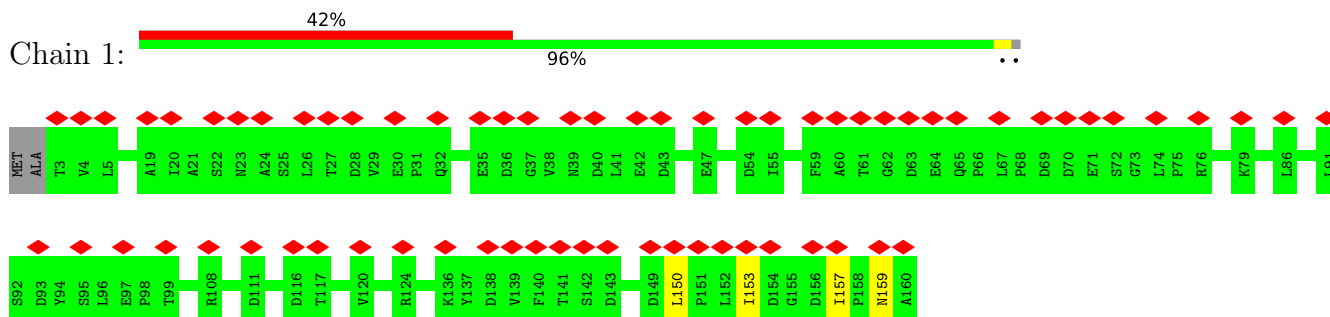
3 Residue-property plots [i](#)

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.

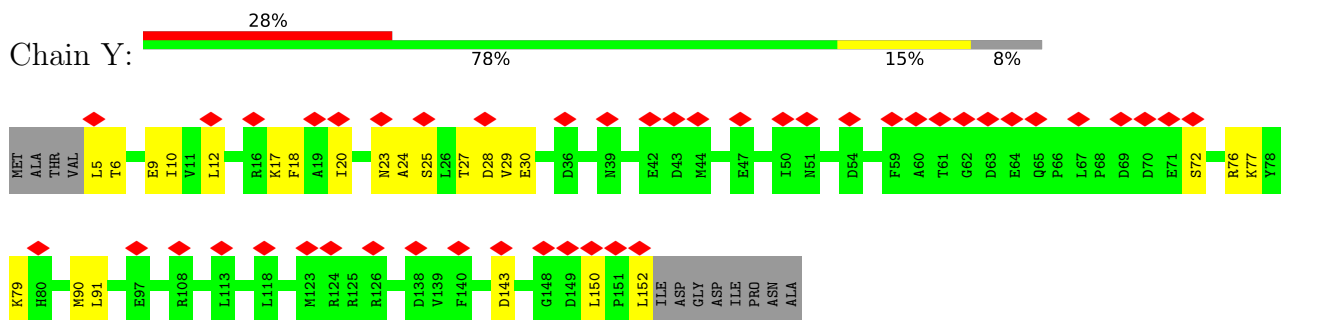
- Molecule 1: Gene 7 protein



- Molecule 1: Gene 7 protein

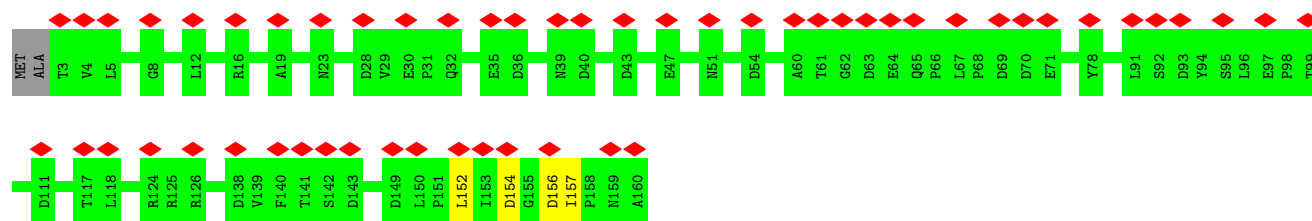


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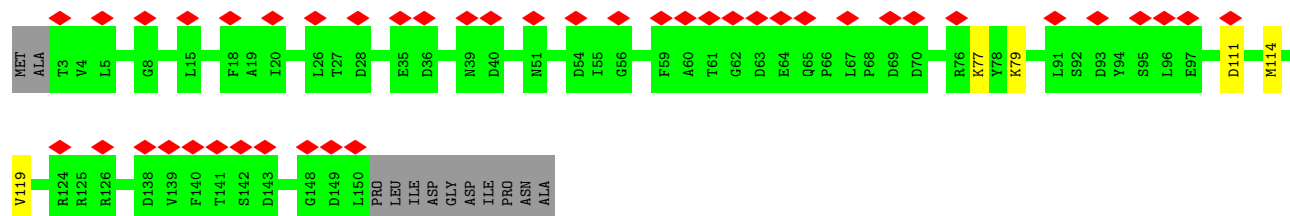
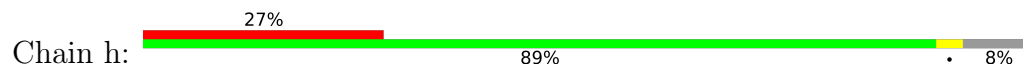


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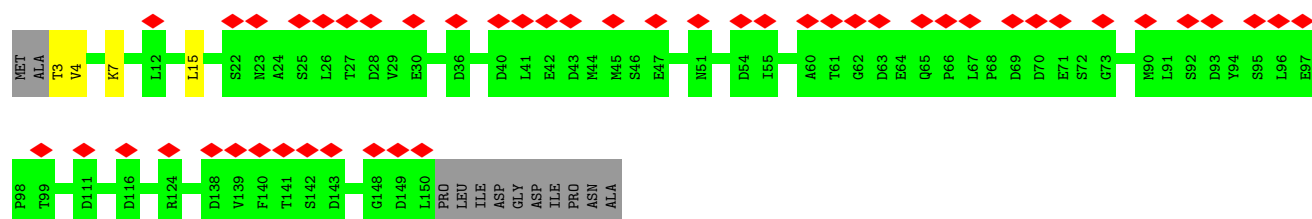
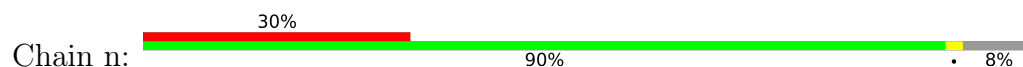




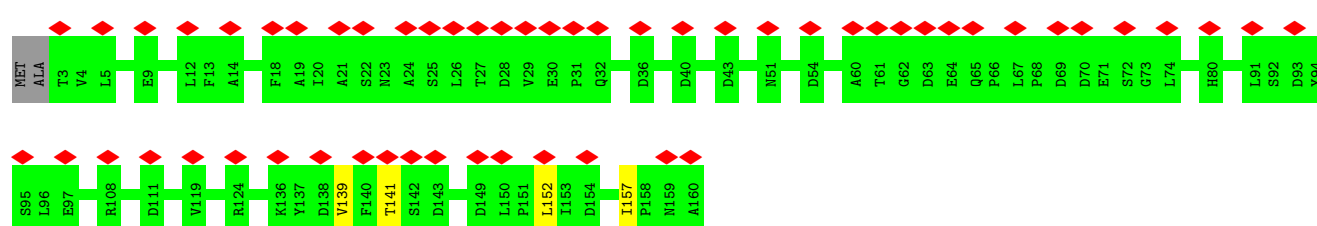
• Molecule 1: Gene 7 protein



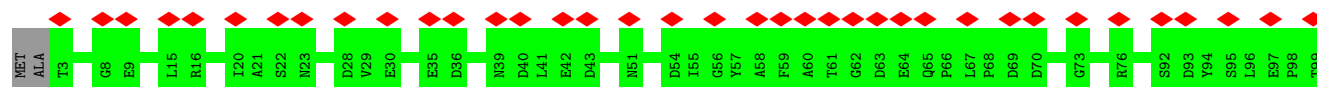
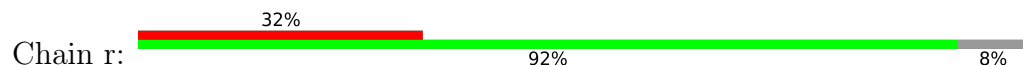
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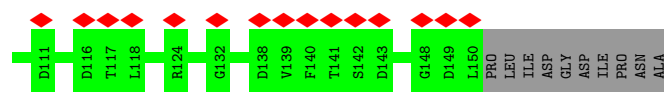


• Molecule 1: Gene 7 protein

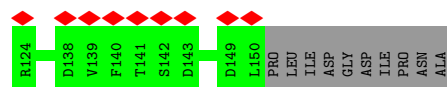
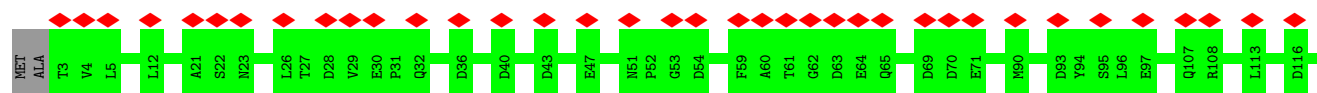


• Molecule 1: Gene 7 protein

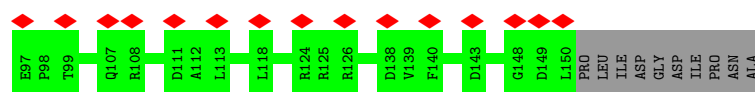
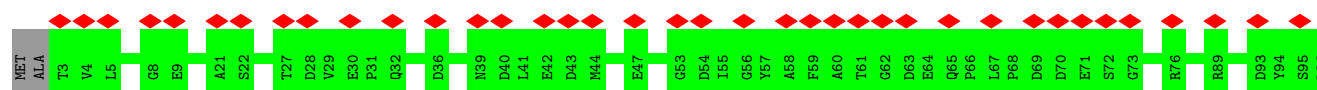
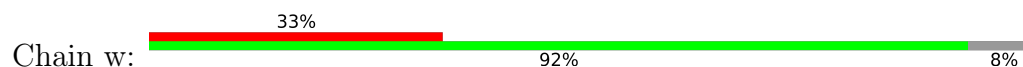




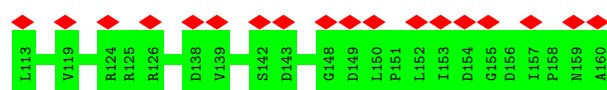
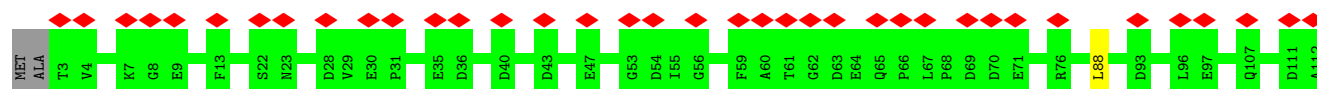
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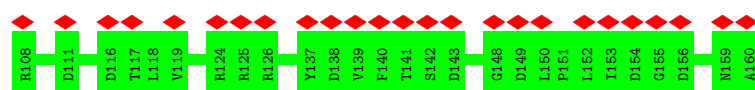
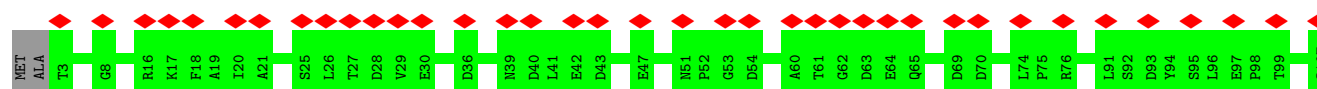
- Molecule 1: Gene 7 protein




- Molecule 1: Gene 7 protein

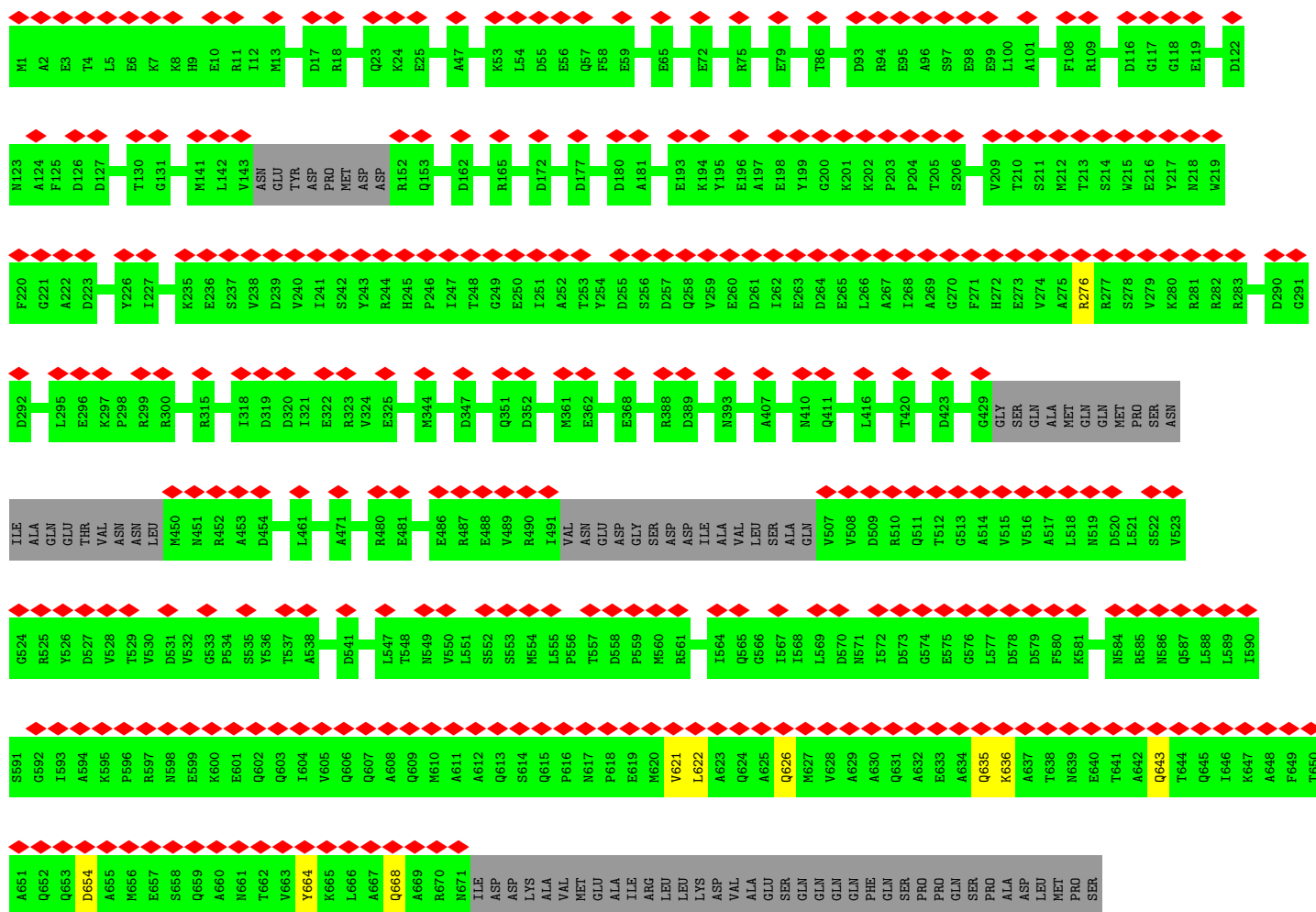


- Molecule 1: Gene 7 protein




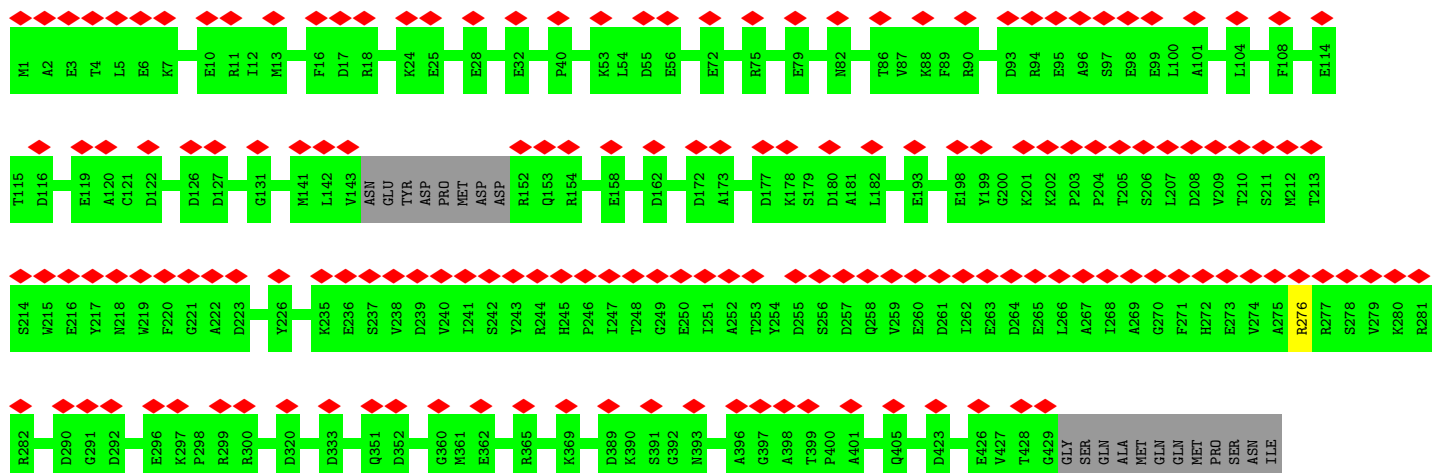
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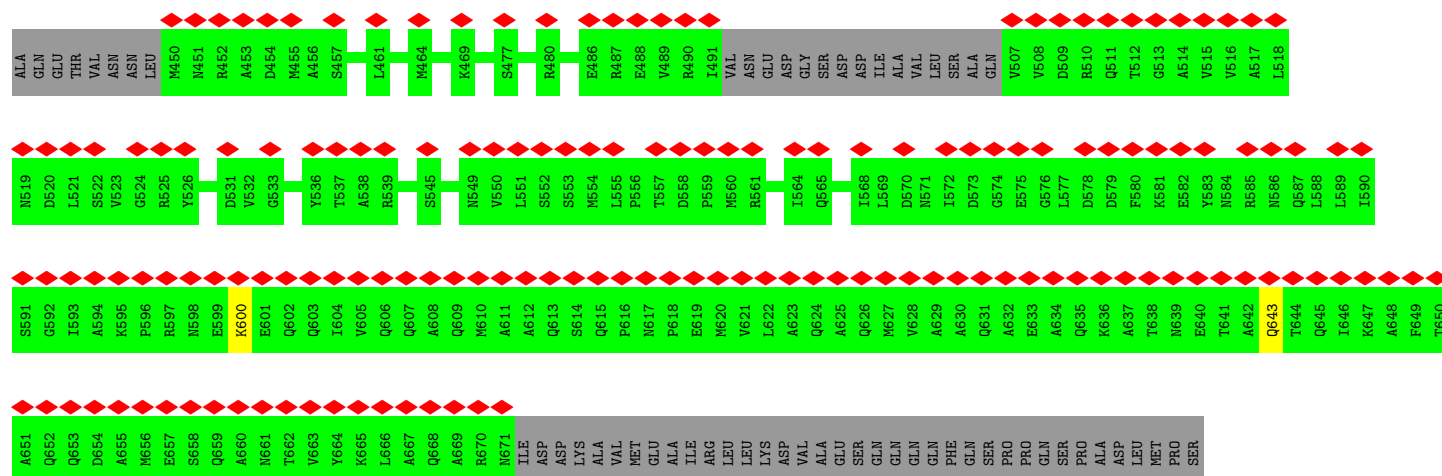
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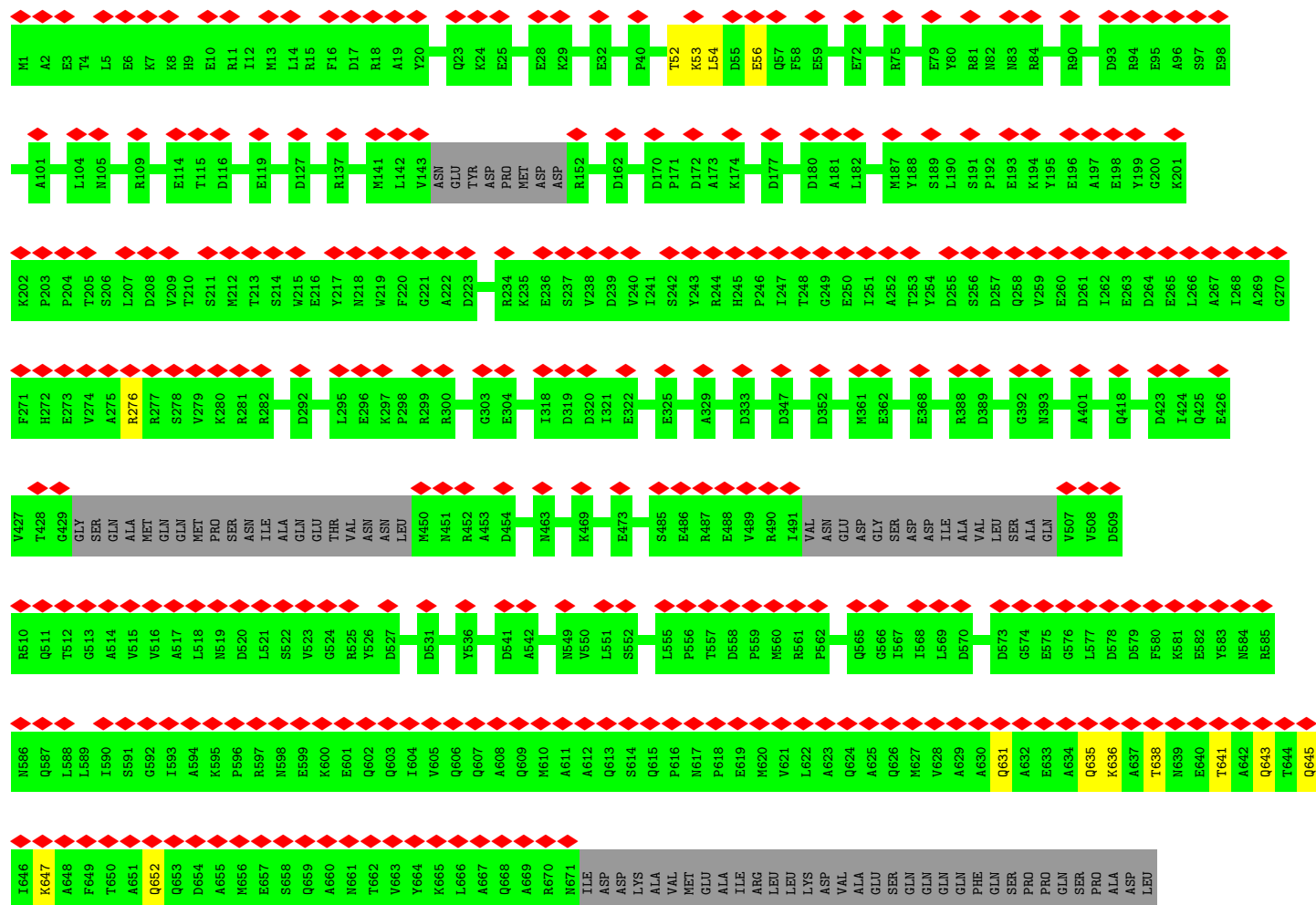
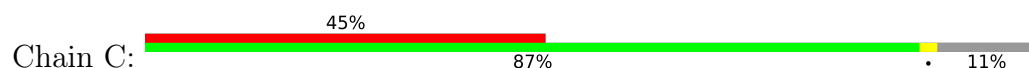
• Molecule 2: Gene 3 protein

Chain B: 



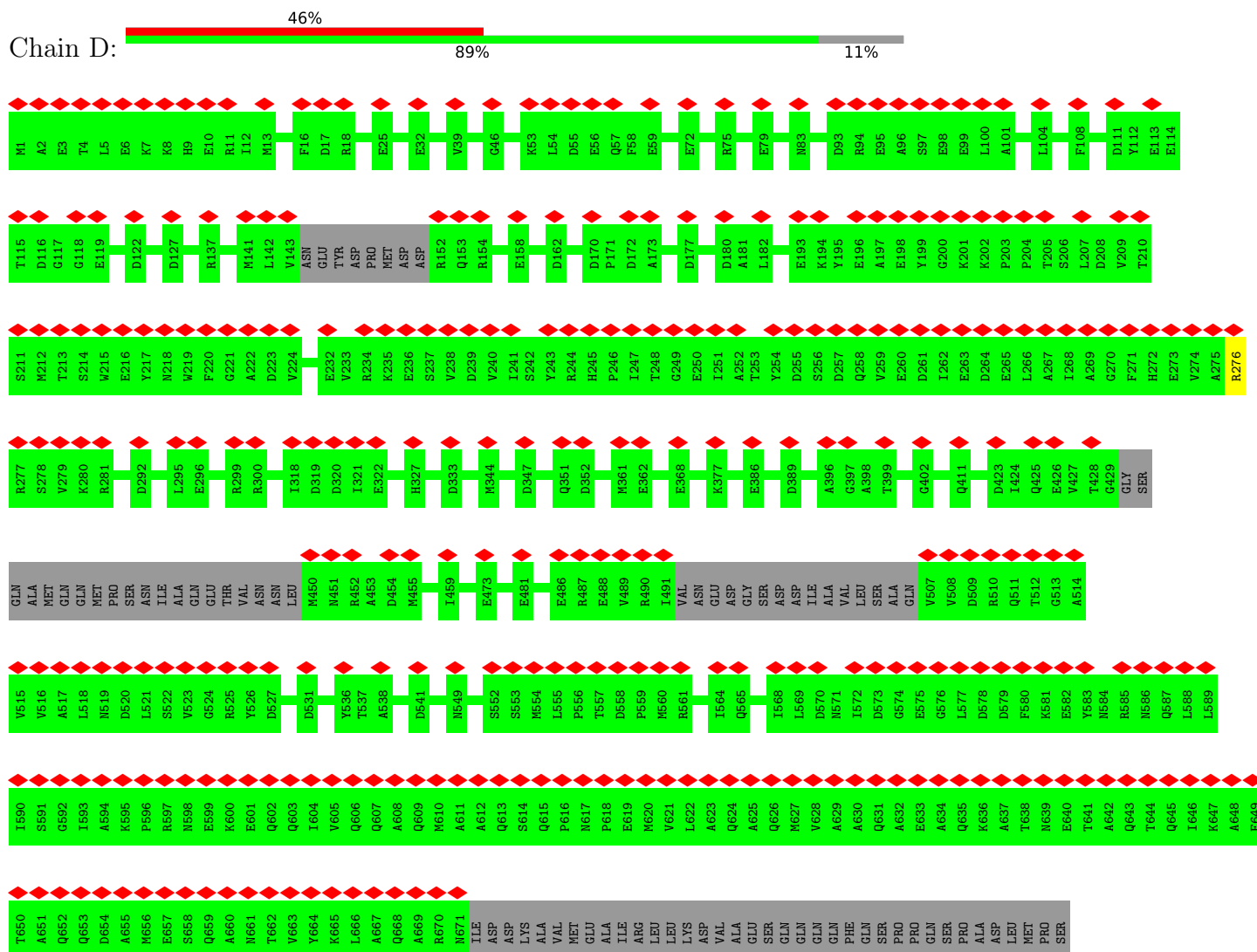


• Molecule 2: Gene 3 protein



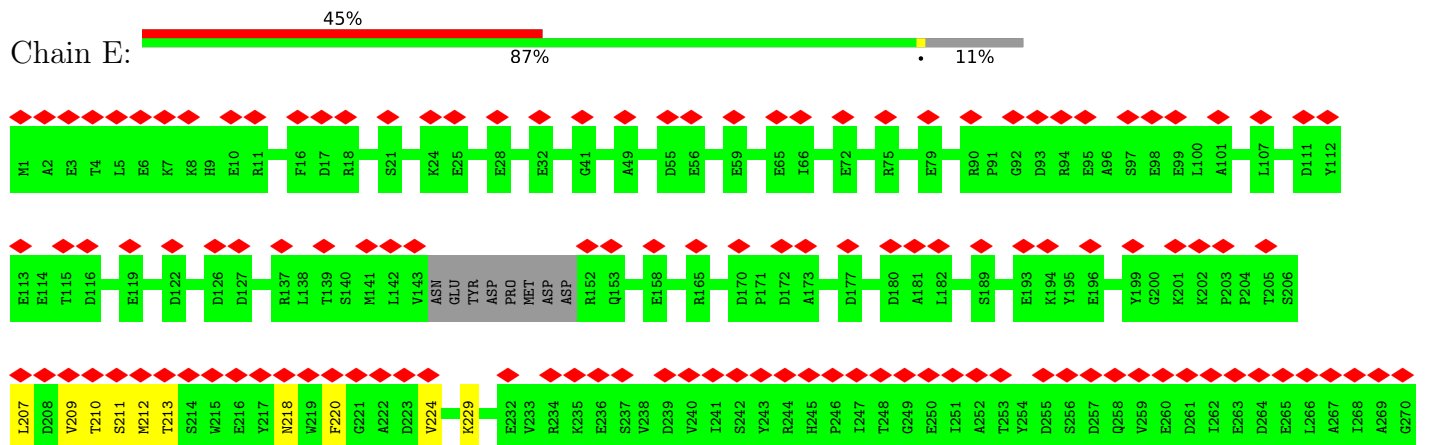
- Molecule 2: Gene 3 protein

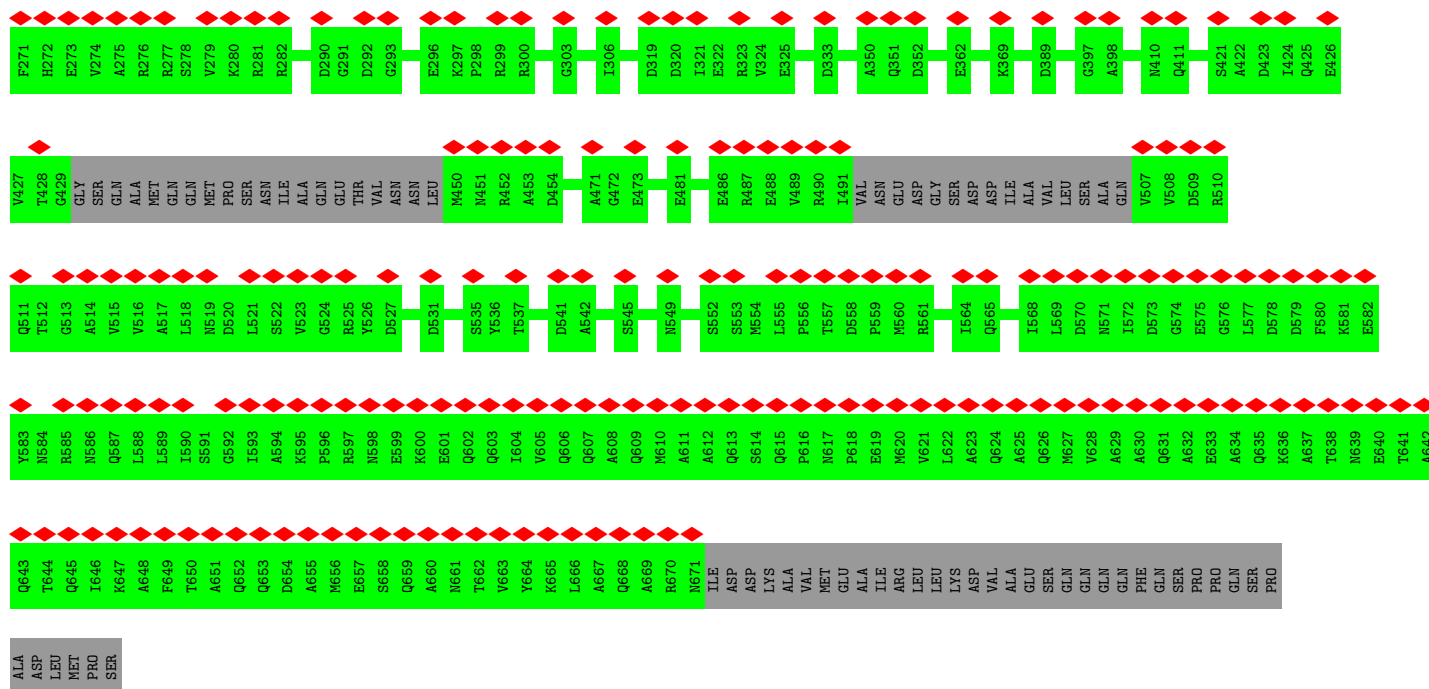
Chain D:



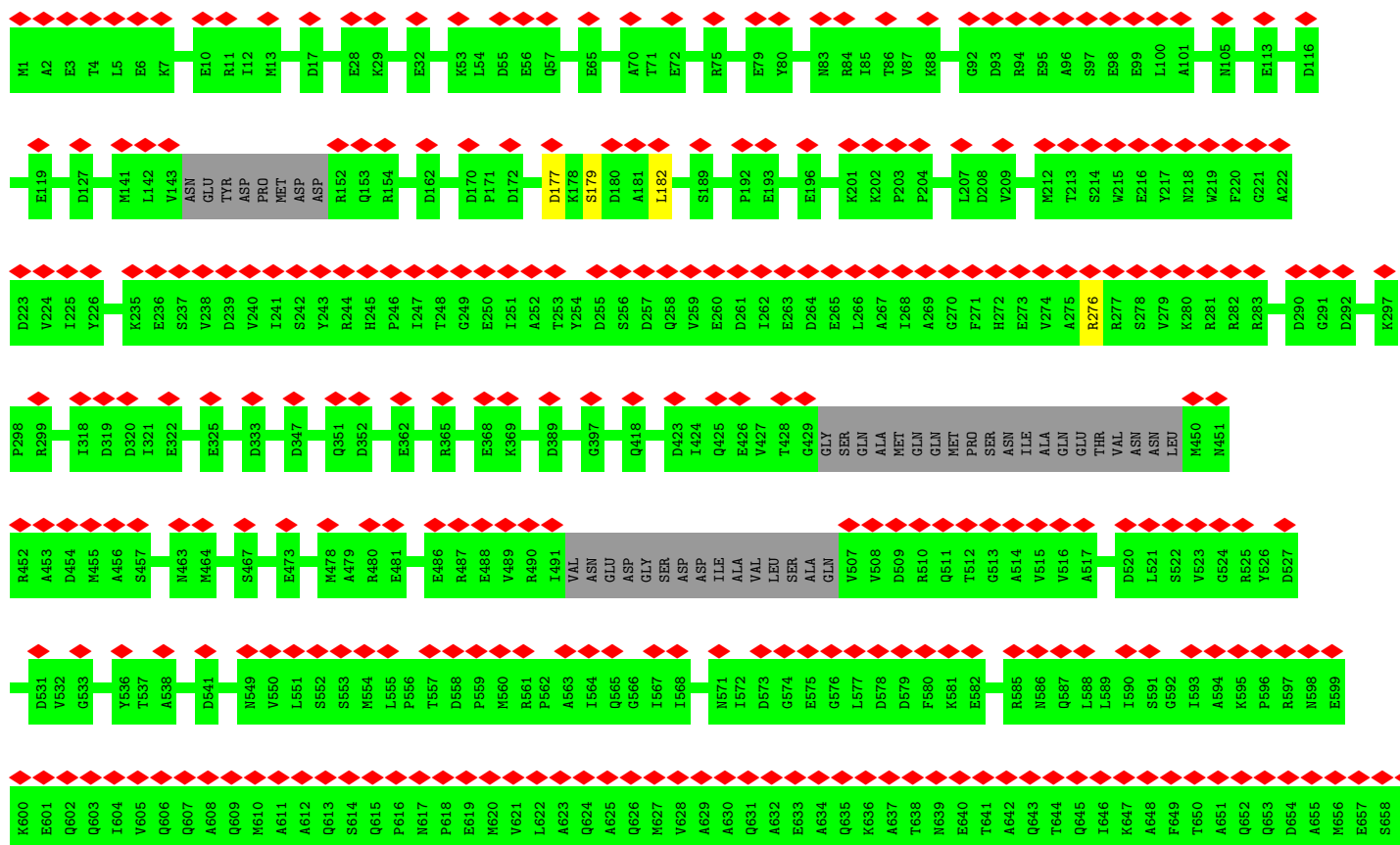
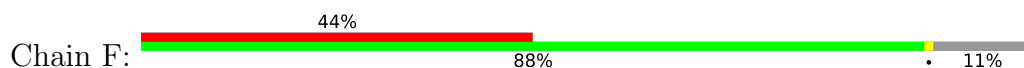
- Molecule 2: Gene 3 protein

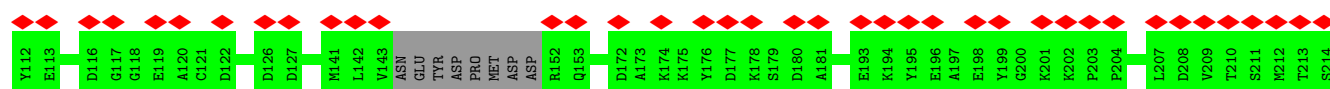
Chain E:

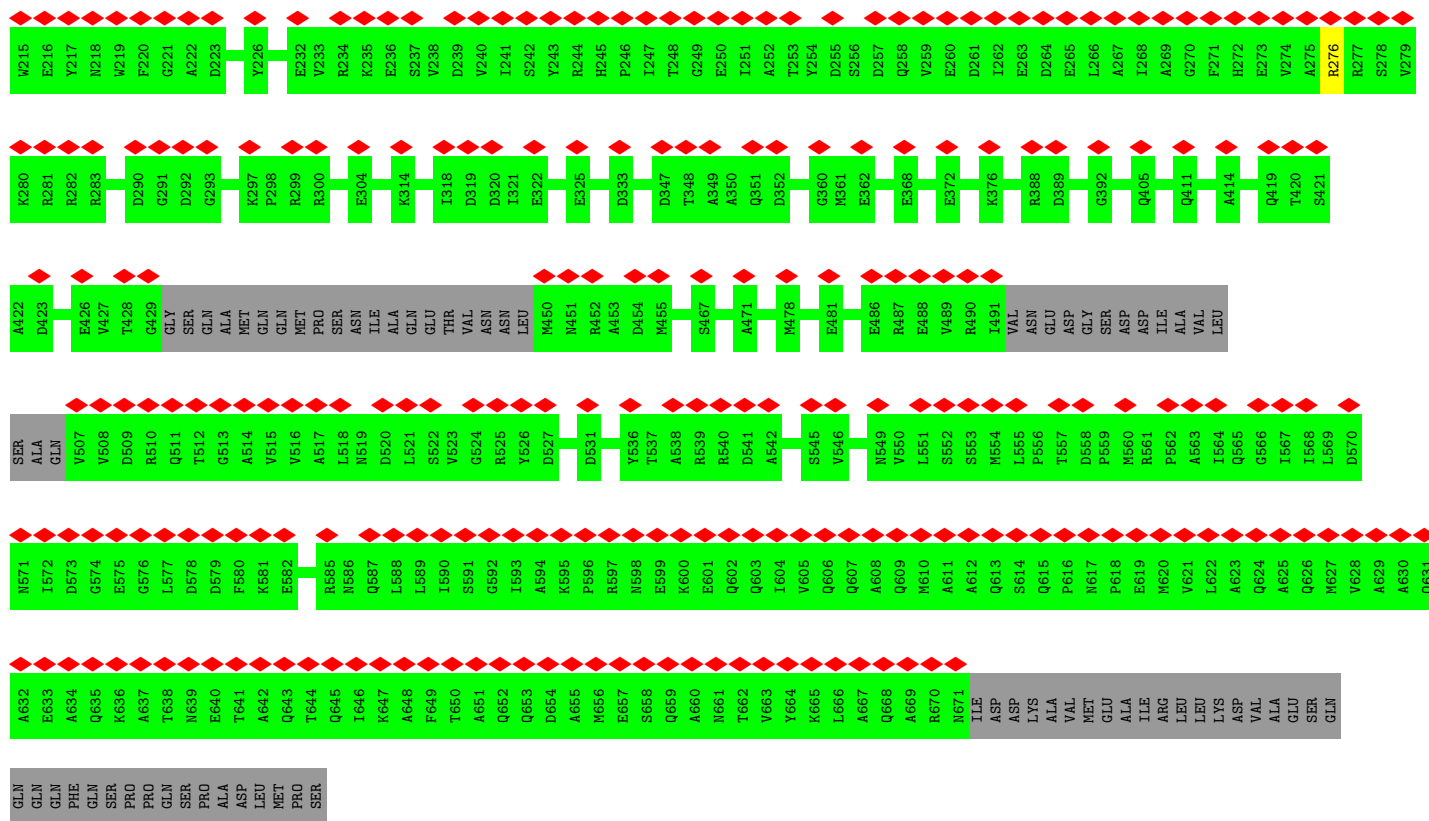




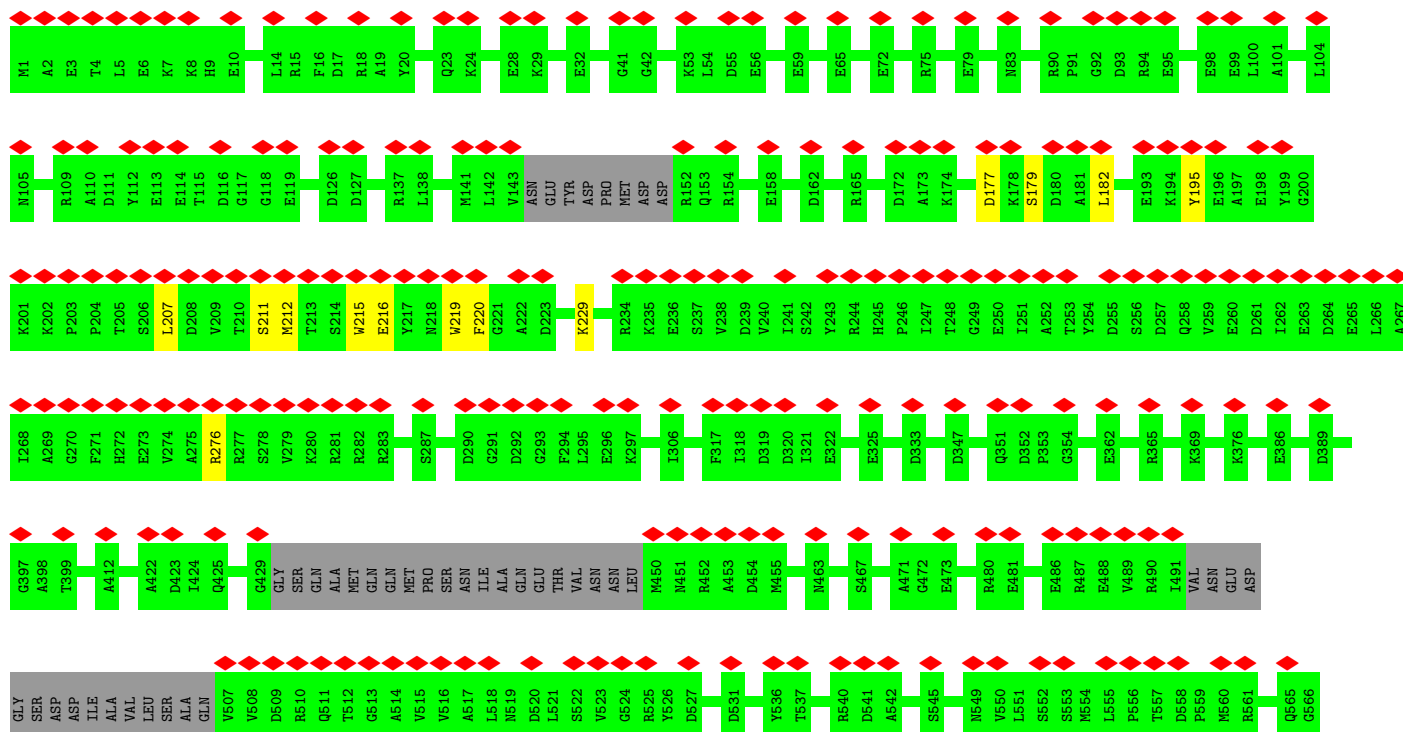
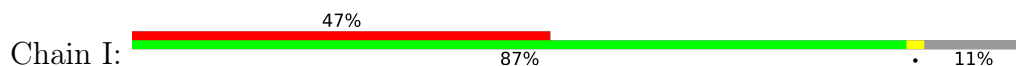
• Molecule 2: Gene 3 protein



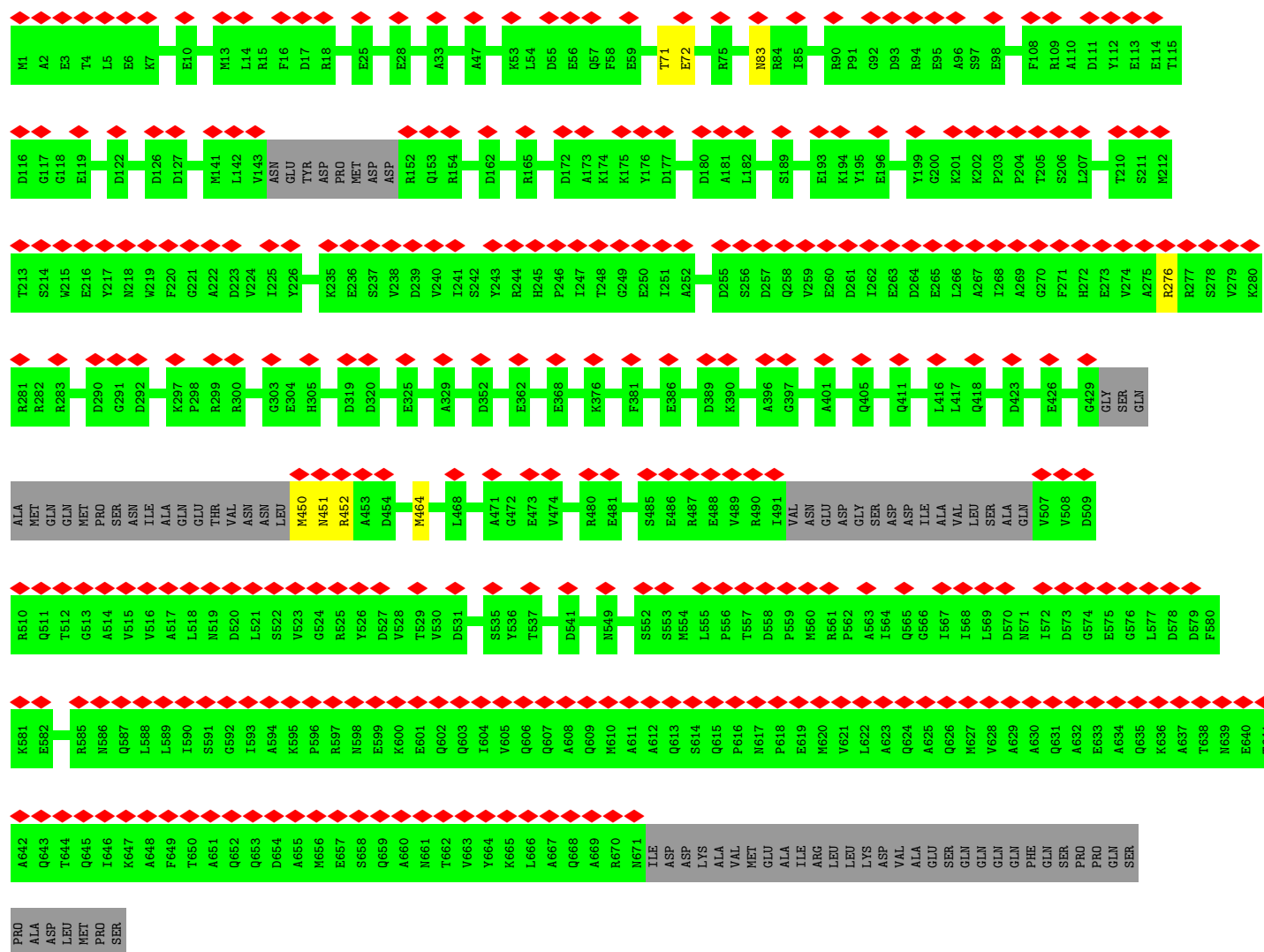
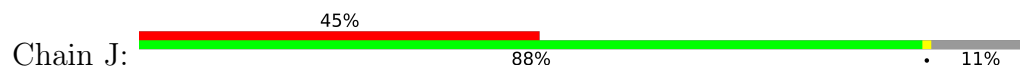




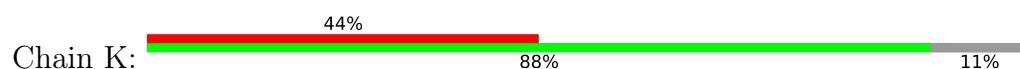
• Molecule 2: Gene 3 protein

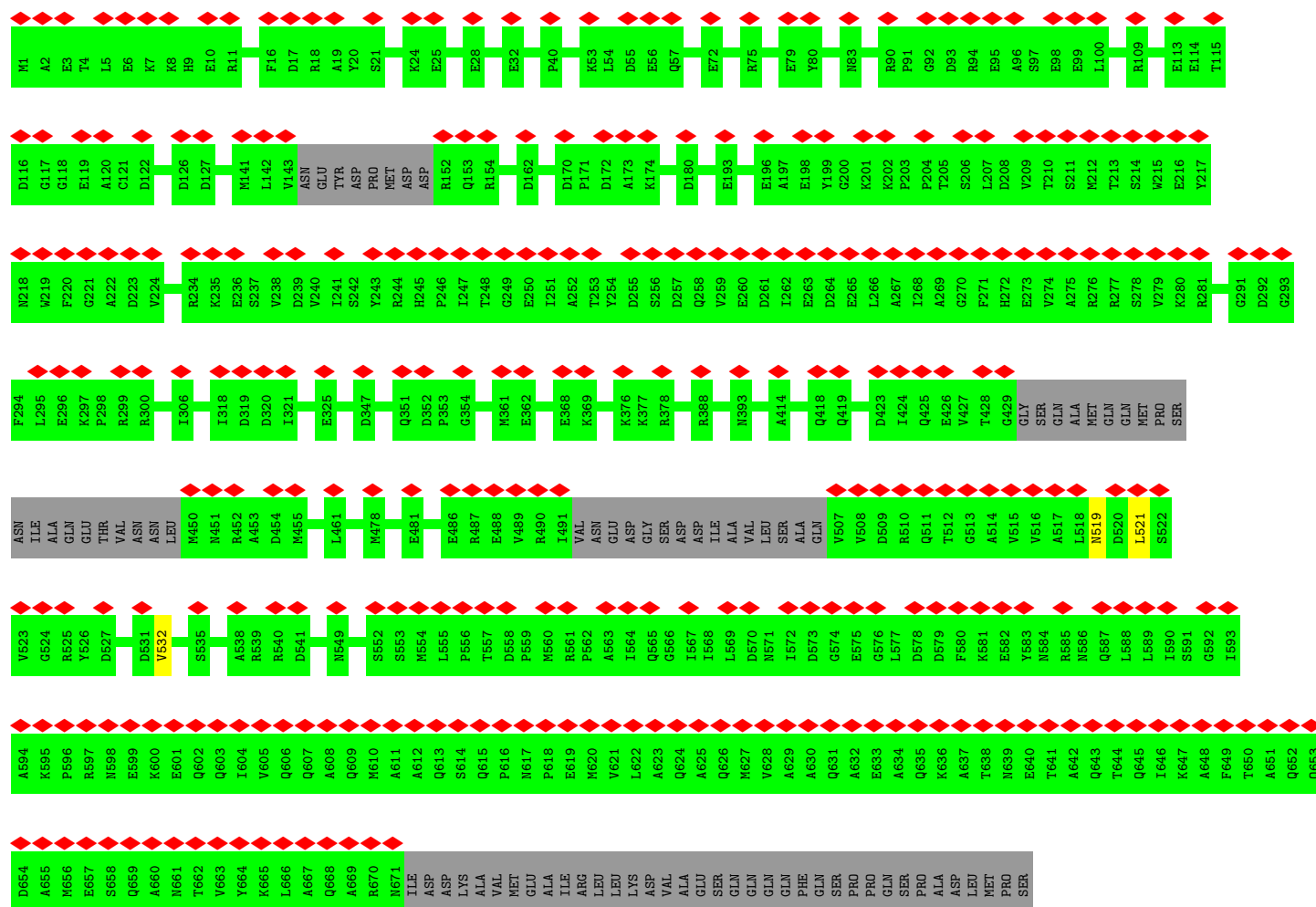


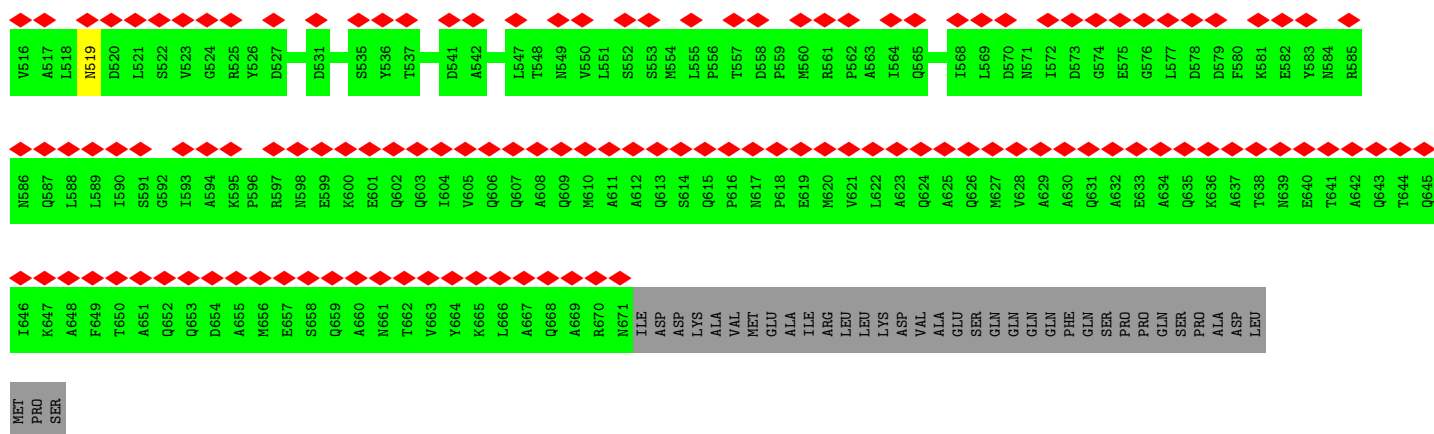
- Molecule 2: Gene 3 protein



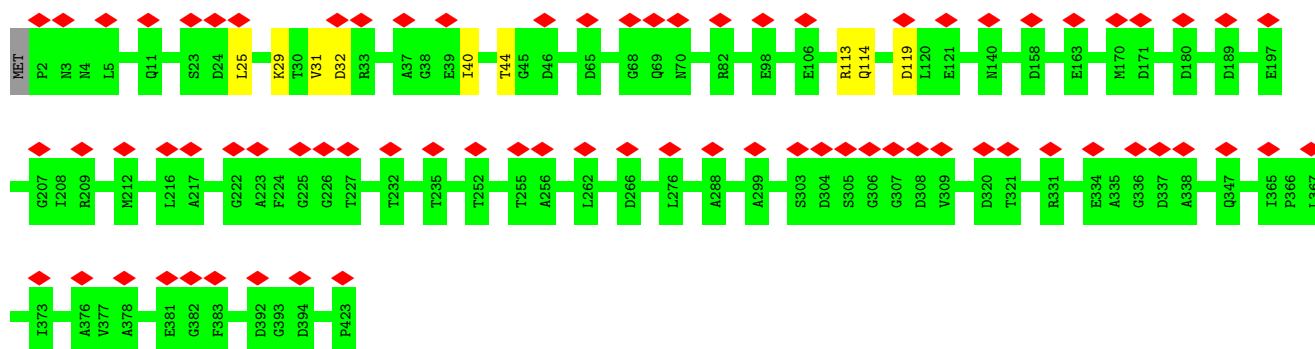
- Molecule 2: Gene 3 protein



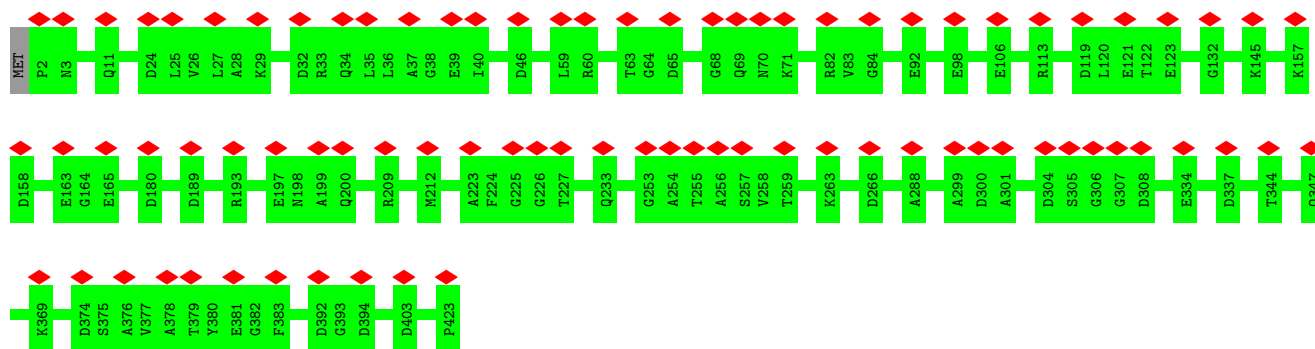




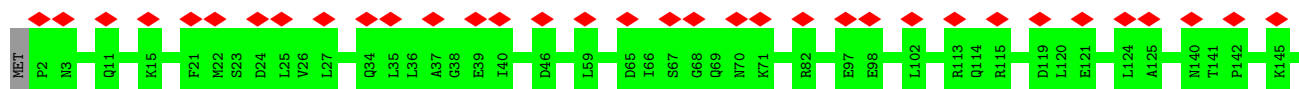
• Molecule 3: Gene 5 protein

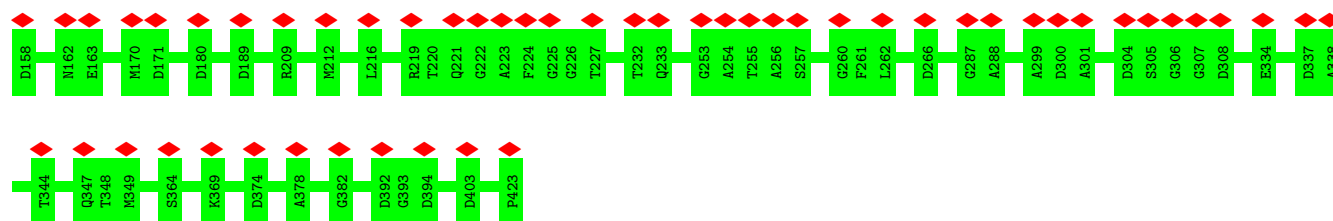


• Molecule 3: Gene 5 protein

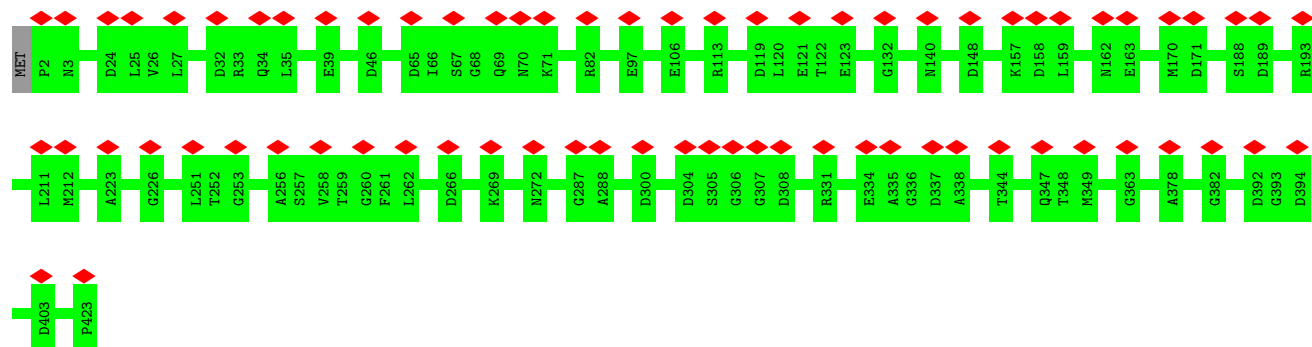


• Molecule 3: Gene 5 protein

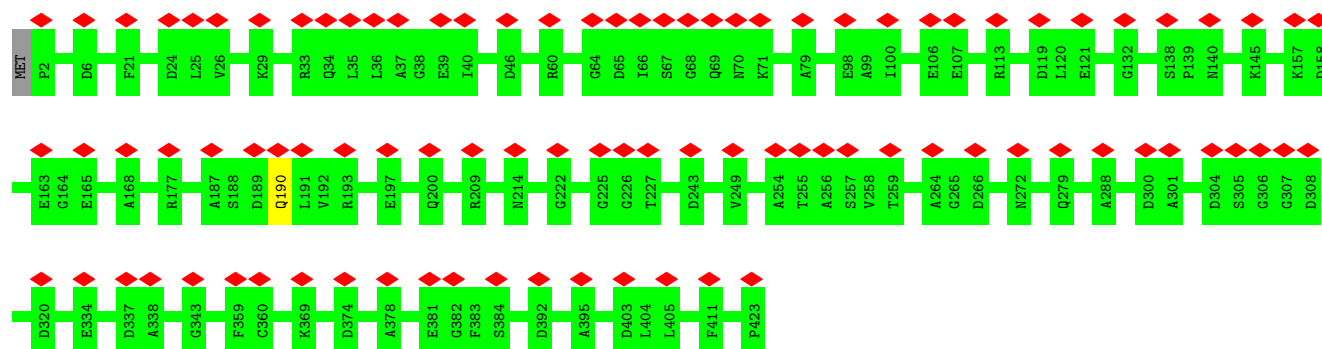




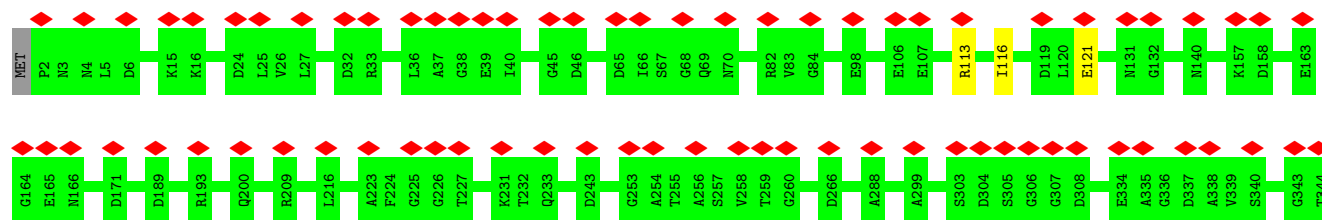
• Molecule 3: Gene 5 protein

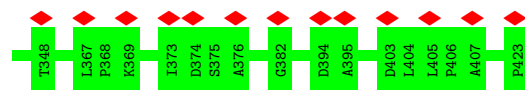


• Molecule 3: Gene 5 protein

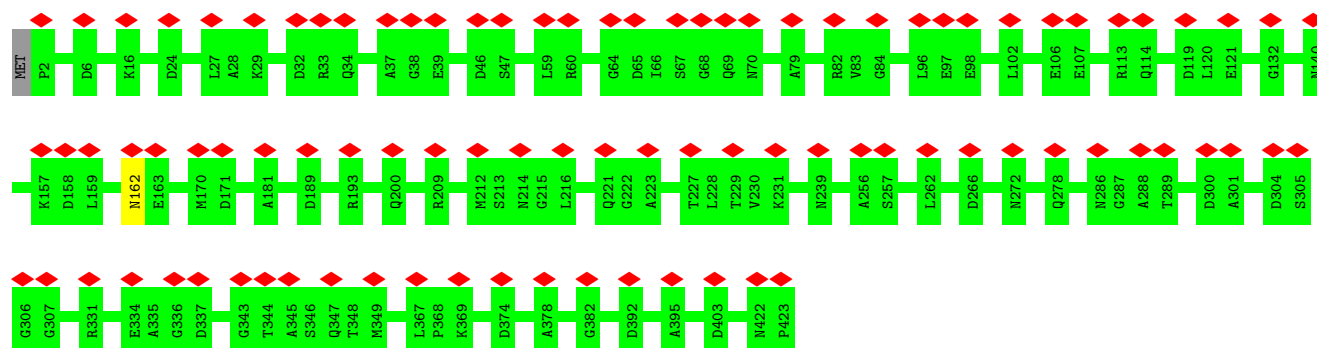


• Molecule 3: Gene 5 protein

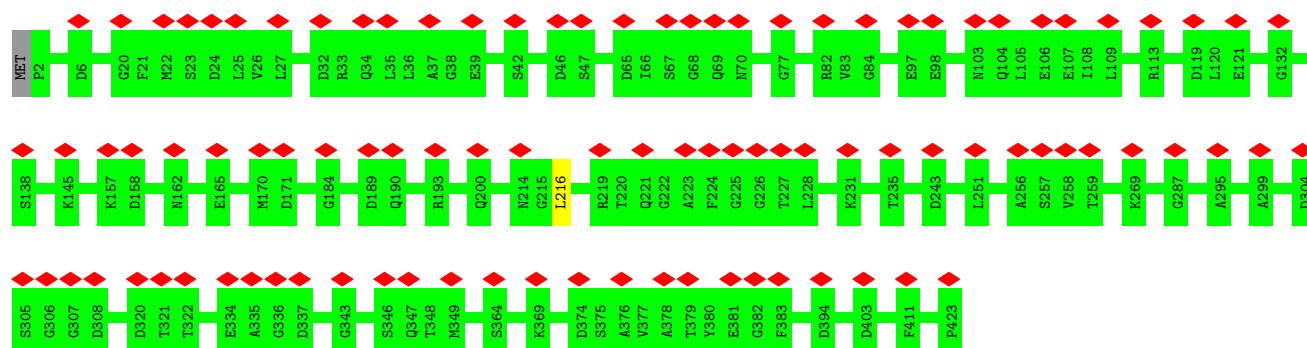




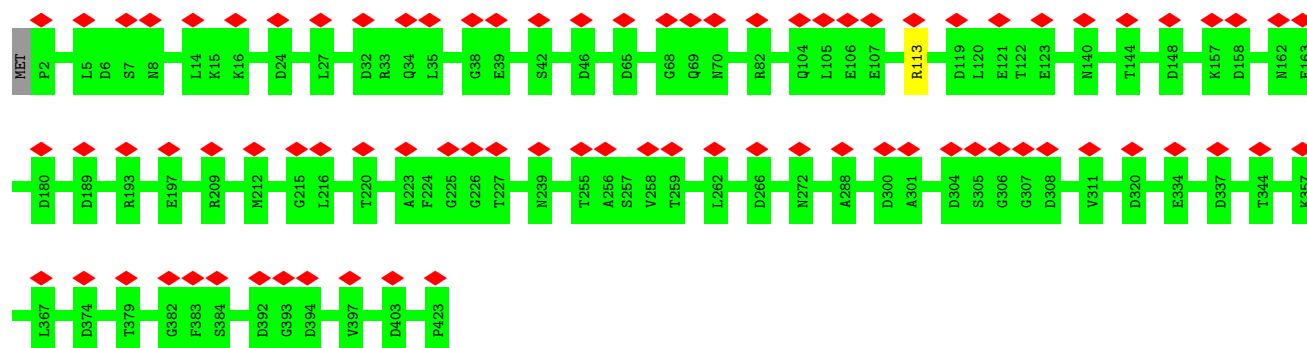
- Molecule 3: Gene 5 protein



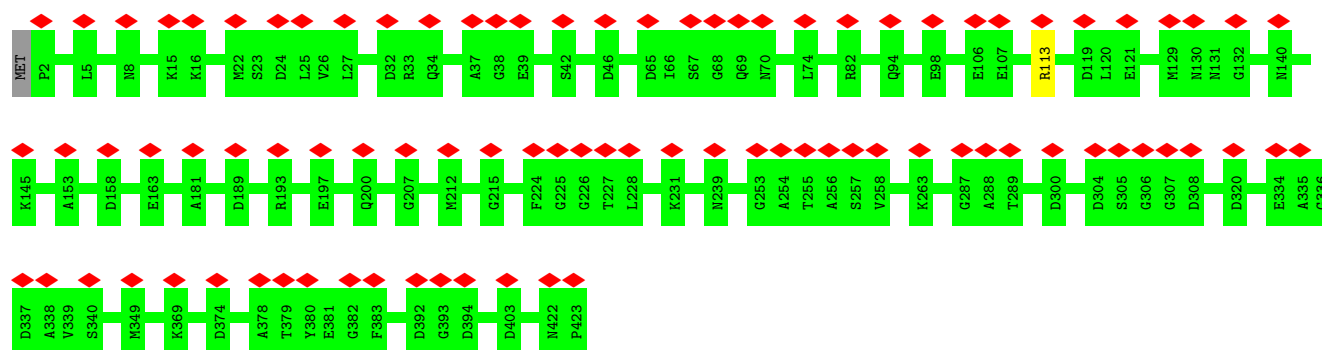
- Molecule 3: Gene 5 protein



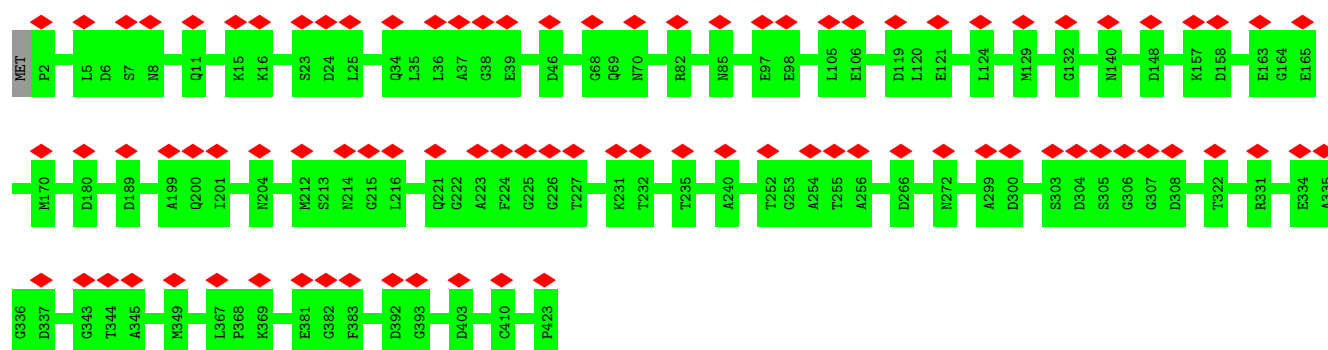
- Molecule 3: Gene 5 protein



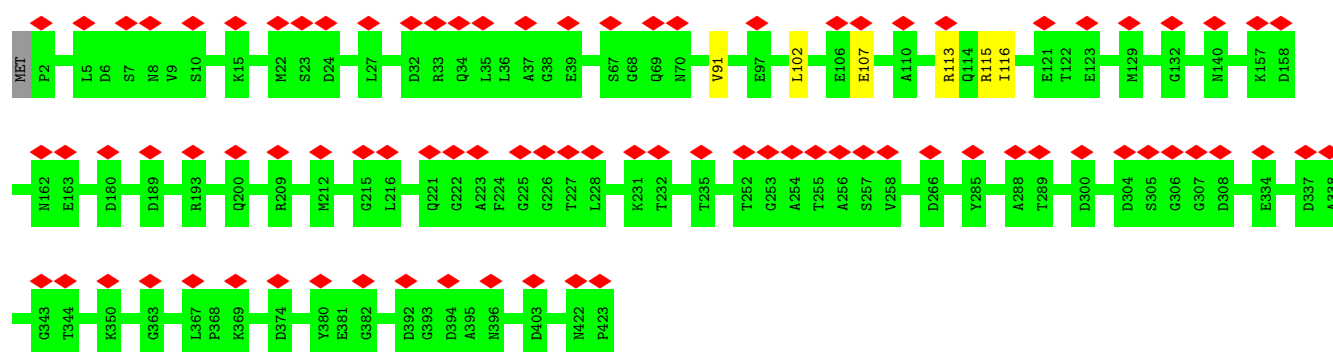
- Molecule 3: Gene 5 protein



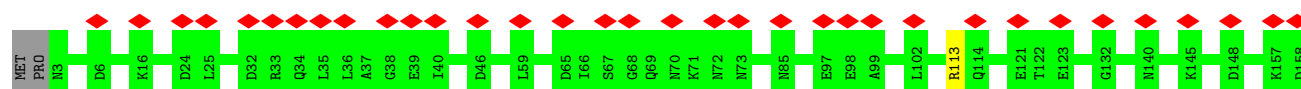
• Molecule 3: Gene 5 protein

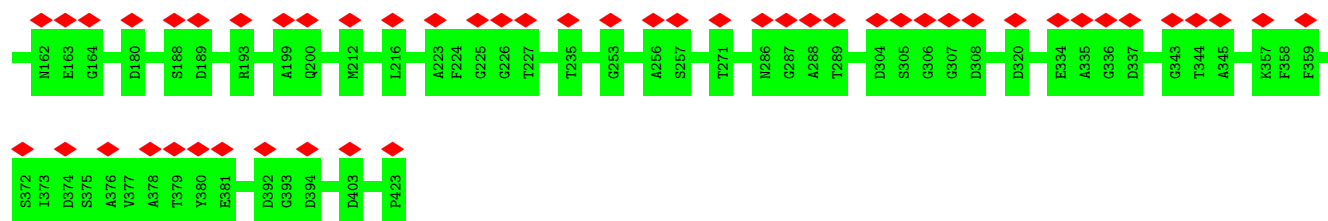


• Molecule 3: Gene 5 protein



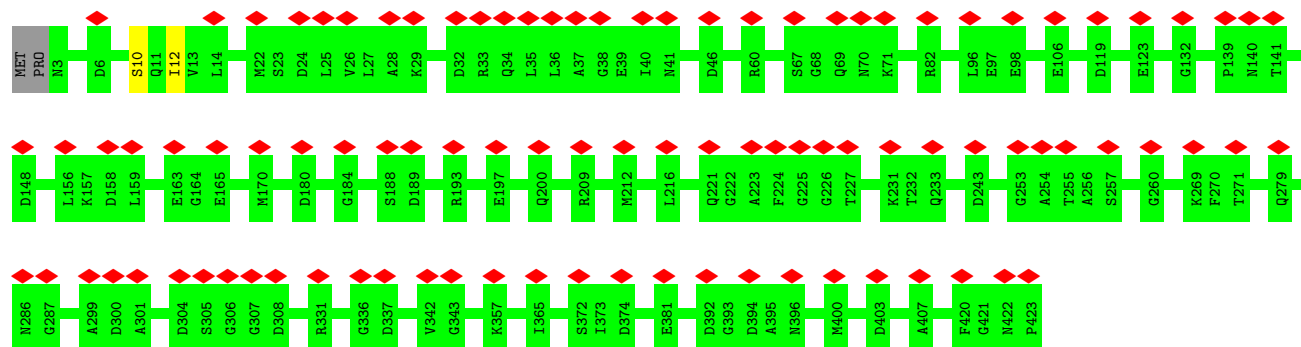
• Molecule 3: Gene 5 protein





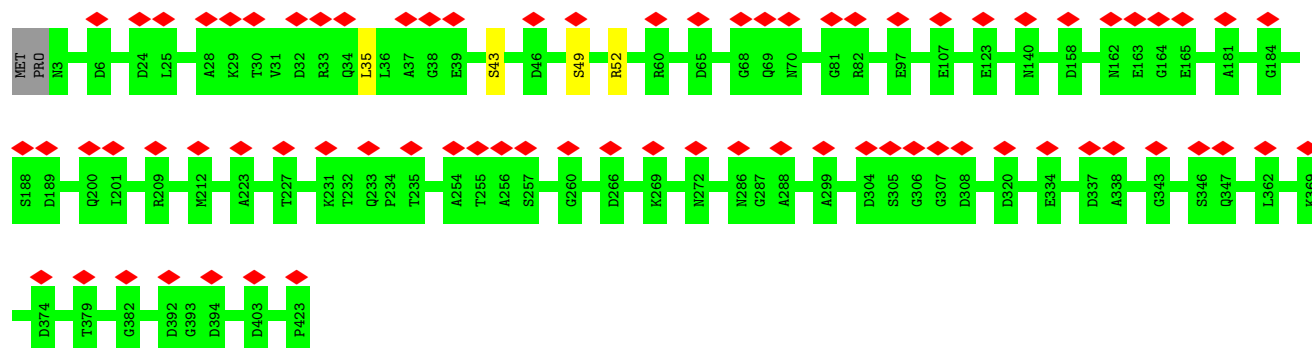
• Molecule 3: Gene 5 protein

Chain a: 23% 99%



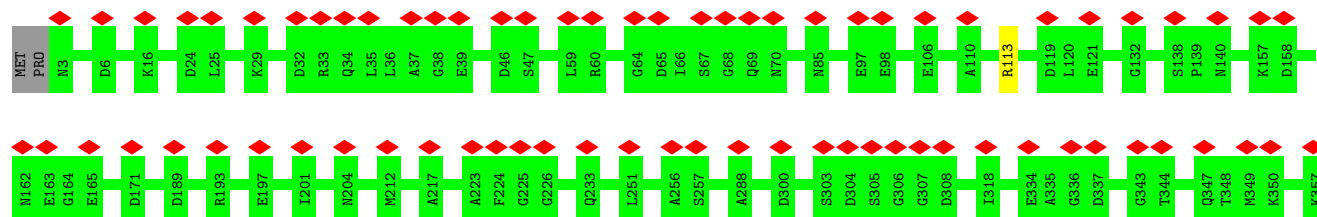
• Molecule 3: Gene 5 protein

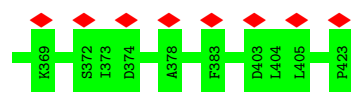
Chain b: 18% 99%



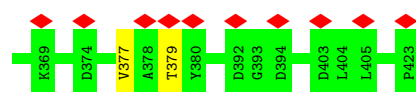
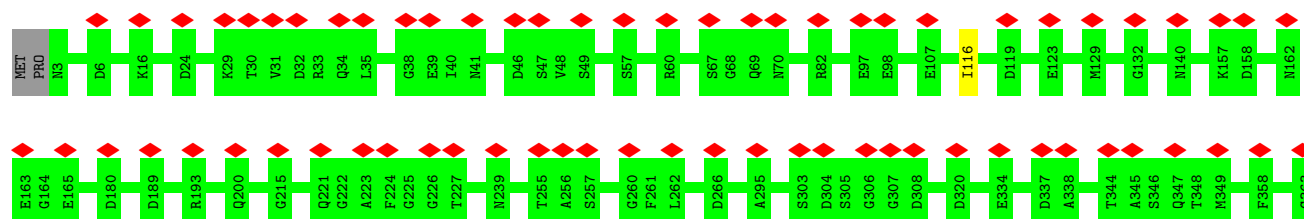
• Molecule 3: Gene 5 protein

Chain c: 19% 99%

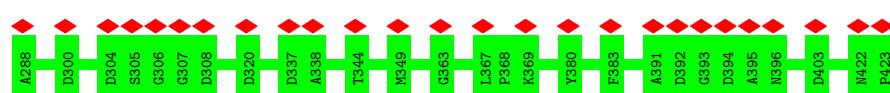
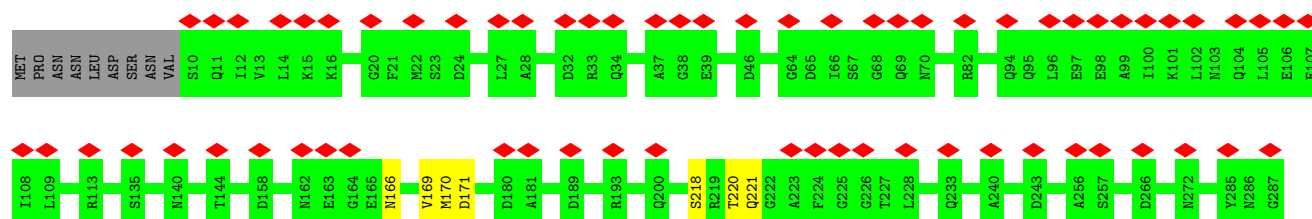




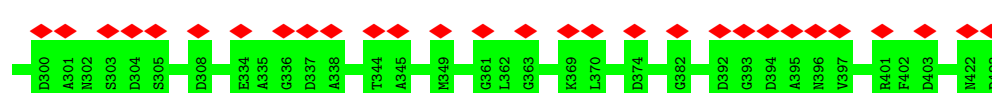
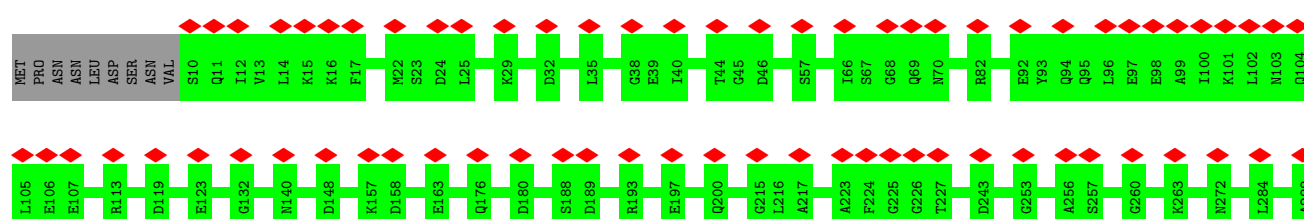
• Molecule 3: Gene 5 protein



• Molecule 3: Gene 5 protein

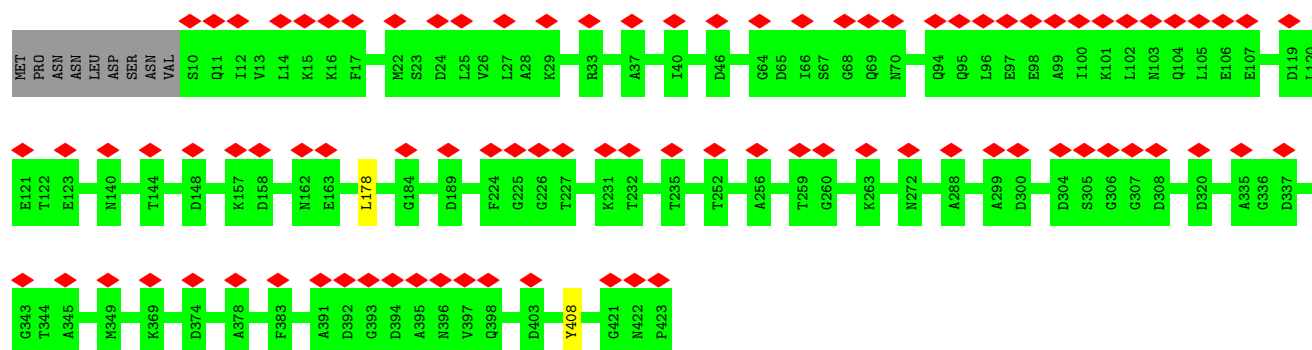


• Molecule 3: Gene 5 protein



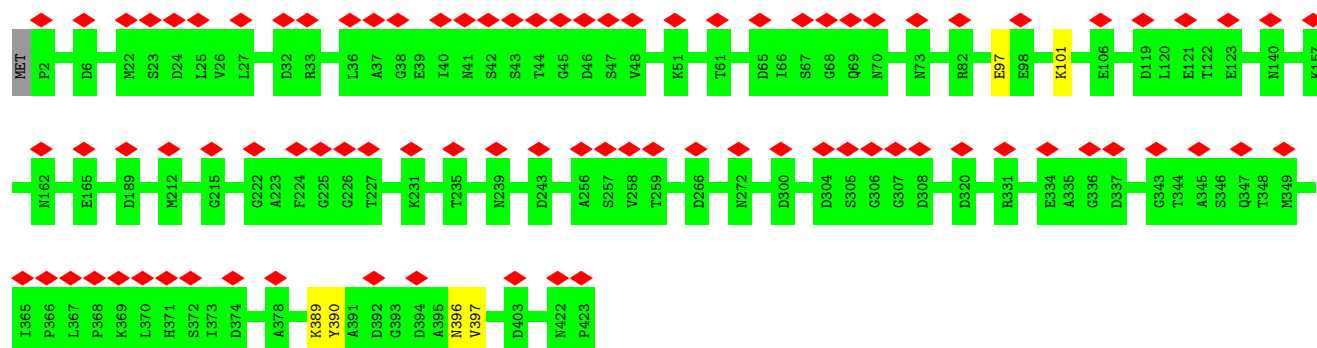
• Molecule 3: Gene 5 protein

Chain i: 



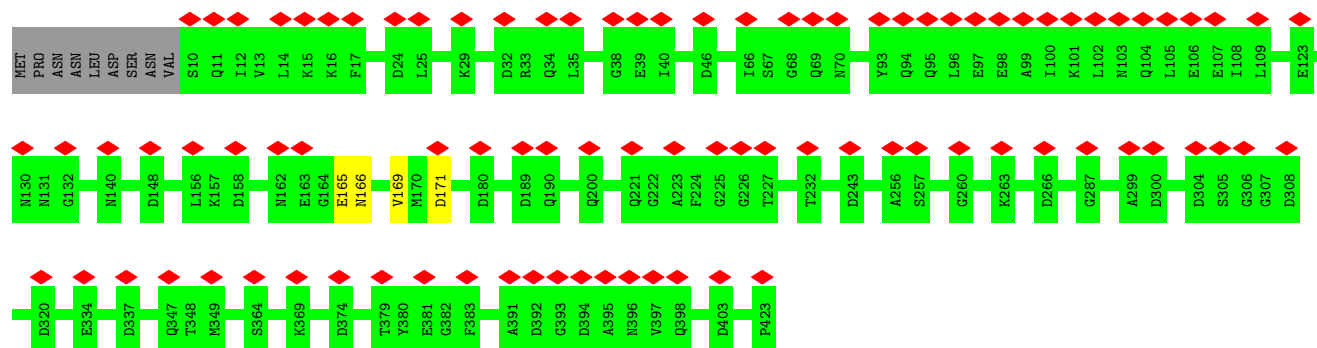
• Molecule 3: Gene 5 protein

Chain j: 



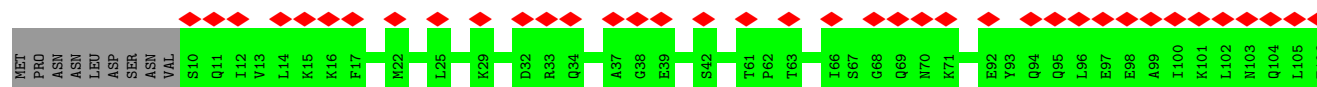
• Molecule 3: Gene 5 protein

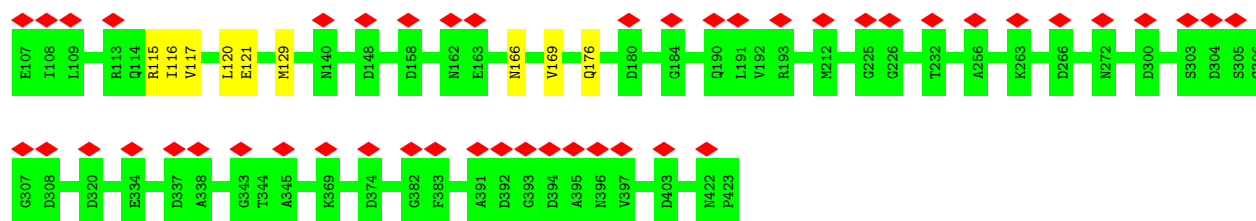
Chain k: 



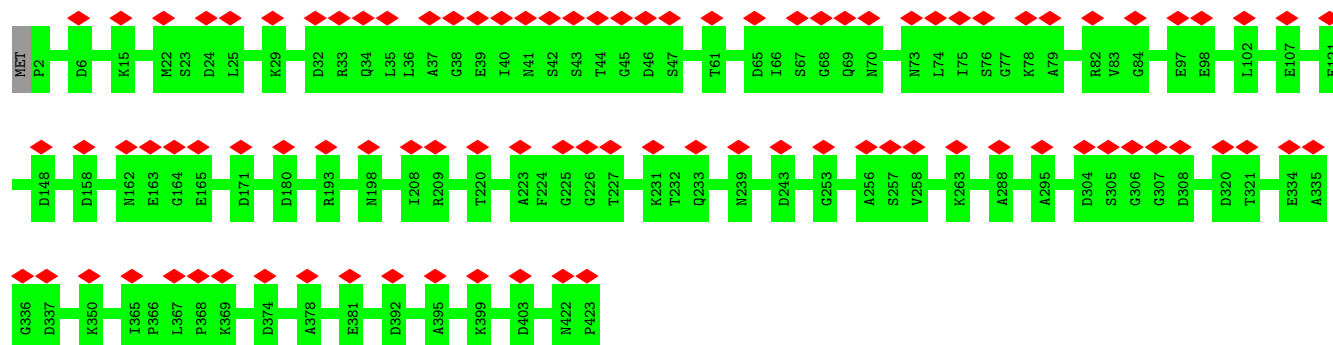
• Molecule 3: Gene 5 protein

Chain l: 

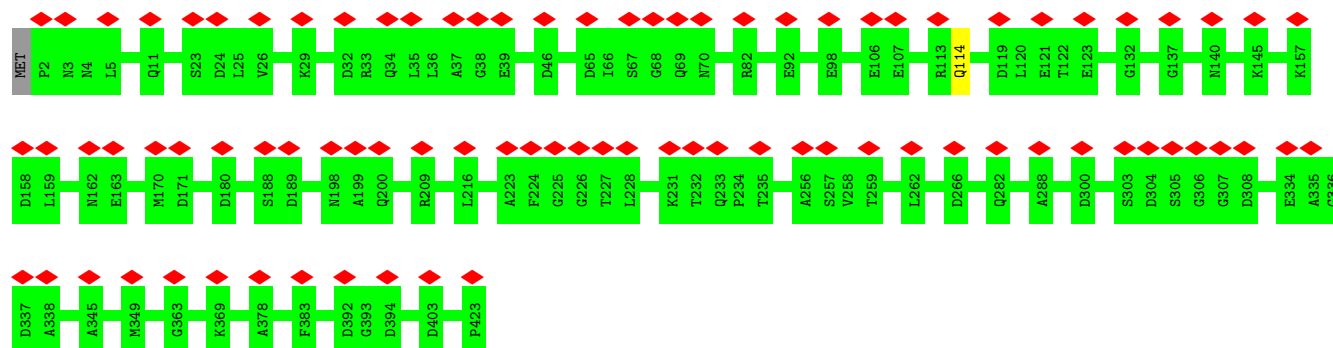




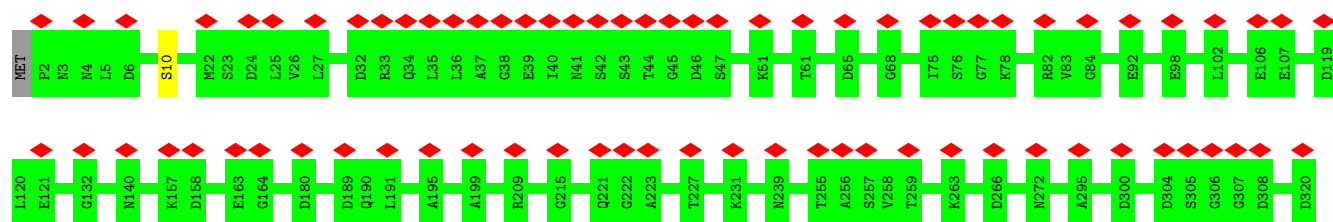
• Molecule 3: Gene 5 protein

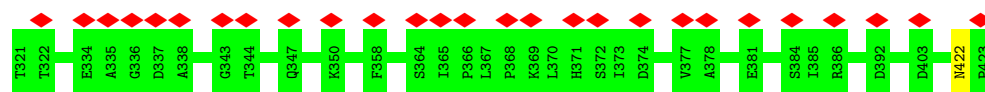


• Molecule 3: Gene 5 protein

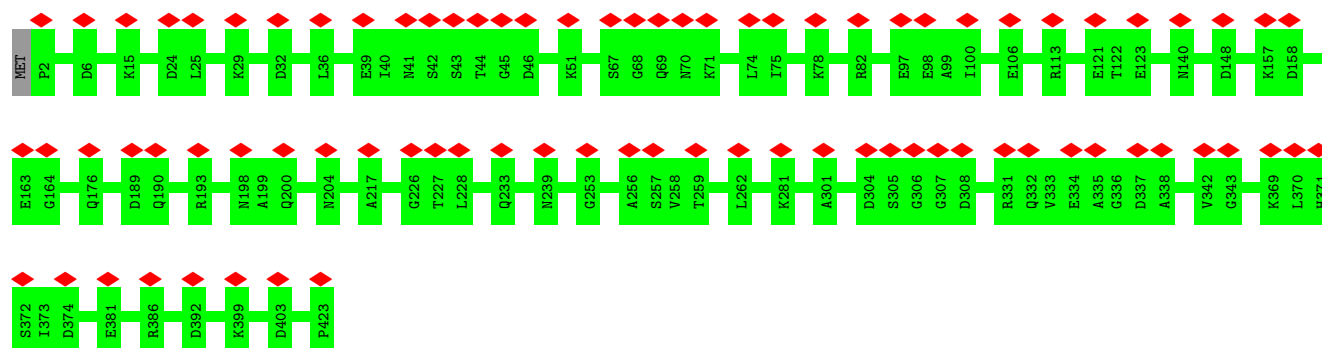


• Molecule 3: Gene 5 protein

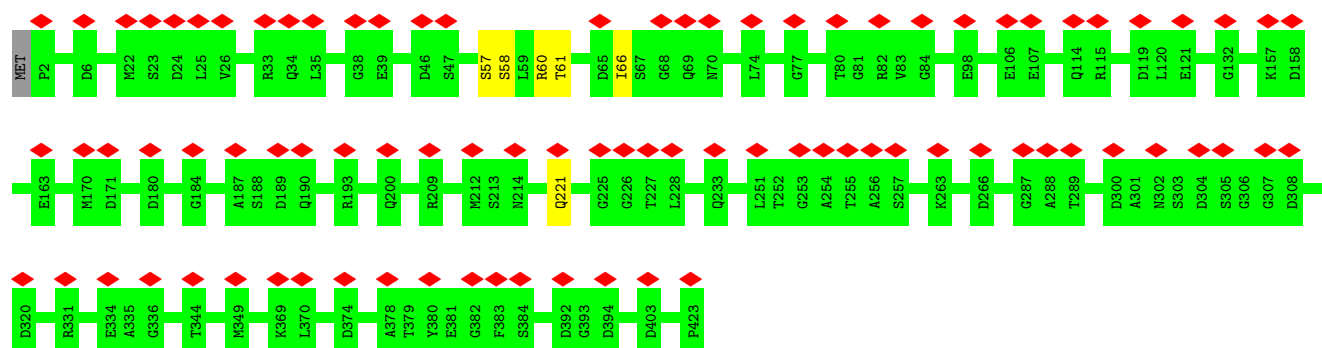




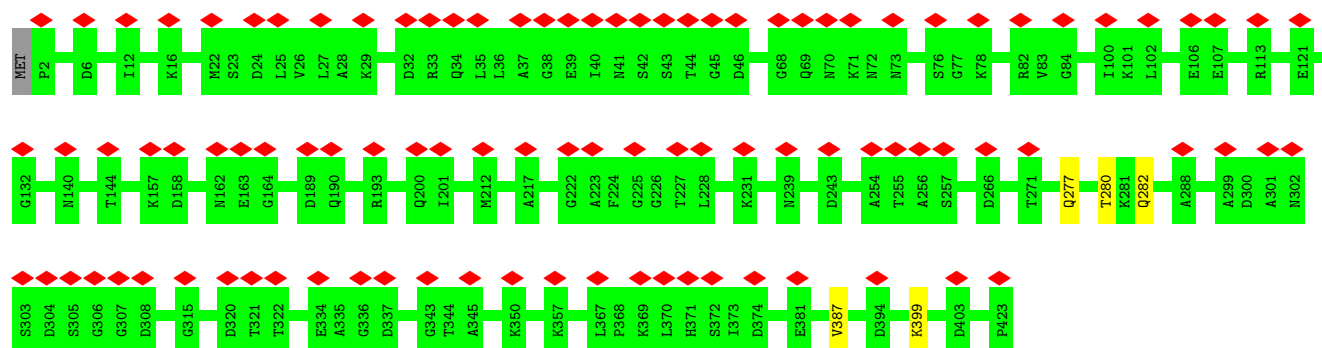
• Molecule 3: Gene 5 protein



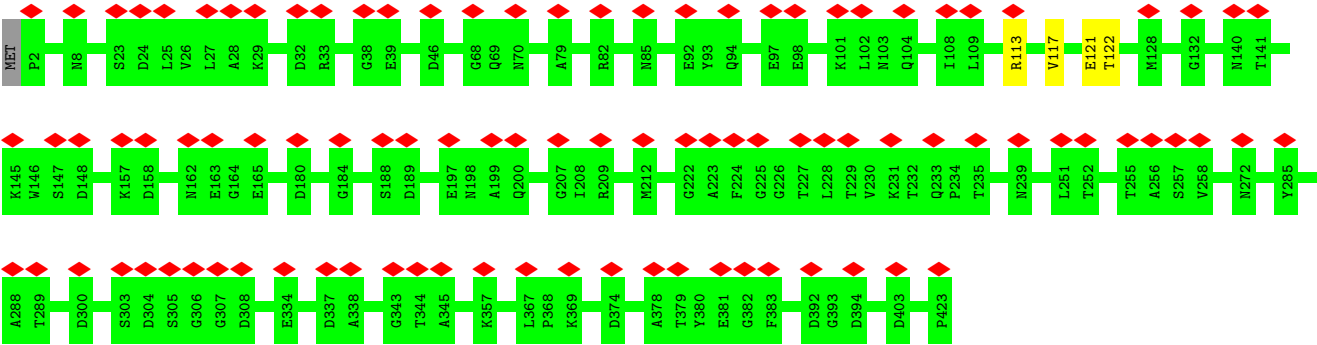
• Molecule 3: Gene 5 protein



• Molecule 3: Gene 5 protein



• Molecule 3: Gene 5 protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	14.559	Depositor
Minimum map value	-8.202	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.62	Depositor
Map size (\AA)	574.464, 574.464, 574.464	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.122, 1.122, 1.122	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	0	0.36	0/1186	0.56	0/1611
1	1	0.35	0/1259	0.56	0/1713
1	Y	0.45	0/1188	0.62	0/1614
1	f	0.29	0/1259	0.50	0/1713
1	h	0.32	0/1186	0.52	0/1611
1	n	0.29	0/1186	0.52	0/1611
1	p	0.32	0/1259	0.55	0/1713
1	r	0.25	0/1186	0.48	0/1611
1	v	0.26	0/1186	0.48	0/1611
1	w	0.26	0/1186	0.50	0/1611
1	x	0.31	0/1259	0.53	0/1713
1	z	0.27	0/1256	0.50	0/1709
2	A	0.30	0/5064	0.54	0/6846
2	B	0.26	0/5064	0.51	0/6846
2	C	0.29	0/5064	0.53	0/6846
2	D	0.25	0/5064	0.51	0/6846
2	E	0.28	0/5064	0.53	0/6846
2	F	0.26	0/5064	0.51	0/6846
2	G	0.25	0/5064	0.51	0/6846
2	H	0.26	0/5064	0.52	0/6846
2	I	0.31	0/5064	0.54	0/6846
2	J	0.27	0/5064	0.52	0/6846
2	K	0.27	0/5064	0.51	0/6846
2	L	0.26	0/5064	0.51	0/6846
3	M	0.31	0/3274	0.51	0/4455
3	N	0.26	0/3274	0.49	0/4455
3	O	0.25	0/3274	0.48	0/4455
3	P	0.26	0/3274	0.49	0/4455
3	Q	0.25	0/3274	0.49	0/4455
3	R	0.27	0/3274	0.50	0/4455
3	S	0.25	0/3274	0.48	0/4455
3	T	0.27	0/3274	0.49	0/4455
3	U	0.25	0/3274	0.48	0/4455
3	V	0.26	0/3274	0.48	0/4455

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	W	0.25	0/3274	0.48	0/4455
3	X	0.29	0/3274	0.51	0/4455
3	Z	0.25	0/3266	0.49	0/4444
3	a	0.27	0/3266	0.49	0/4444
3	b	0.29	0/3266	0.49	0/4444
3	c	0.25	0/3266	0.49	0/4444
3	d	0.32	0/3266	0.52	0/4444
3	e	0.29	0/3213	0.51	0/4371
3	g	0.27	0/3213	0.49	0/4371
3	i	0.29	0/3213	0.51	0/4371
3	j	0.29	0/3274	0.50	0/4455
3	k	0.28	0/3213	0.50	0/4371
3	l	0.29	0/3213	0.51	0/4371
3	m	0.26	0/3274	0.48	0/4455
3	o	0.25	0/3274	0.48	0/4455
3	q	0.27	0/3274	0.49	0/4455
3	s	0.26	0/3274	0.49	0/4455
3	t	0.28	0/3274	0.50	0/4455
3	u	0.29	0/3274	0.52	0/4455
3	y	0.26	0/3274	0.49	0/4455
All	All	0.28	0/173239	0.51	0/235168

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	0	146/160 (91%)	138 (94%)	8 (6%)	0	100	100
1	1	156/160 (98%)	146 (94%)	10 (6%)	0	100	100
1	Y	146/160 (91%)	135 (92%)	10 (7%)	1 (1%)	22	59
1	f	156/160 (98%)	150 (96%)	6 (4%)	0	100	100
1	h	146/160 (91%)	142 (97%)	4 (3%)	0	100	100
1	n	146/160 (91%)	135 (92%)	11 (8%)	0	100	100
1	p	156/160 (98%)	146 (94%)	10 (6%)	0	100	100
1	r	146/160 (91%)	143 (98%)	3 (2%)	0	100	100
1	v	146/160 (91%)	141 (97%)	5 (3%)	0	100	100
1	w	146/160 (91%)	137 (94%)	9 (6%)	0	100	100
1	x	156/160 (98%)	143 (92%)	13 (8%)	0	100	100
1	z	156/160 (98%)	142 (91%)	14 (9%)	0	100	100
2	A	620/708 (88%)	590 (95%)	30 (5%)	0	100	100
2	B	620/708 (88%)	586 (94%)	34 (6%)	0	100	100
2	C	620/708 (88%)	587 (95%)	33 (5%)	0	100	100
2	D	620/708 (88%)	589 (95%)	31 (5%)	0	100	100
2	E	620/708 (88%)	594 (96%)	26 (4%)	0	100	100
2	F	620/708 (88%)	590 (95%)	30 (5%)	0	100	100
2	G	620/708 (88%)	589 (95%)	31 (5%)	0	100	100
2	H	620/708 (88%)	599 (97%)	20 (3%)	1 (0%)	47	78
2	I	620/708 (88%)	591 (95%)	28 (4%)	1 (0%)	47	78
2	J	620/708 (88%)	587 (95%)	33 (5%)	0	100	100
2	K	620/708 (88%)	582 (94%)	38 (6%)	0	100	100
2	L	620/708 (88%)	594 (96%)	26 (4%)	0	100	100
3	M	420/423 (99%)	402 (96%)	18 (4%)	0	100	100
3	N	420/423 (99%)	405 (96%)	15 (4%)	0	100	100
3	O	420/423 (99%)	404 (96%)	16 (4%)	0	100	100
3	P	420/423 (99%)	405 (96%)	15 (4%)	0	100	100
3	Q	420/423 (99%)	407 (97%)	13 (3%)	0	100	100
3	R	420/423 (99%)	410 (98%)	10 (2%)	0	100	100
3	S	420/423 (99%)	412 (98%)	8 (2%)	0	100	100
3	T	420/423 (99%)	406 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	U	420/423 (99%)	401 (96%)	19 (4%)	0	100	100
3	V	420/423 (99%)	401 (96%)	19 (4%)	0	100	100
3	W	420/423 (99%)	401 (96%)	19 (4%)	0	100	100
3	X	420/423 (99%)	398 (95%)	22 (5%)	0	100	100
3	Z	419/423 (99%)	401 (96%)	18 (4%)	0	100	100
3	a	419/423 (99%)	405 (97%)	14 (3%)	0	100	100
3	b	419/423 (99%)	402 (96%)	17 (4%)	0	100	100
3	c	419/423 (99%)	403 (96%)	16 (4%)	0	100	100
3	d	419/423 (99%)	400 (96%)	19 (4%)	0	100	100
3	e	412/423 (97%)	390 (95%)	22 (5%)	0	100	100
3	g	412/423 (97%)	394 (96%)	18 (4%)	0	100	100
3	i	412/423 (97%)	393 (95%)	19 (5%)	0	100	100
3	j	420/423 (99%)	407 (97%)	13 (3%)	0	100	100
3	k	412/423 (97%)	386 (94%)	26 (6%)	0	100	100
3	l	412/423 (97%)	388 (94%)	24 (6%)	0	100	100
3	m	420/423 (99%)	409 (97%)	11 (3%)	0	100	100
3	o	420/423 (99%)	403 (96%)	17 (4%)	0	100	100
3	q	420/423 (99%)	411 (98%)	9 (2%)	0	100	100
3	s	420/423 (99%)	404 (96%)	16 (4%)	0	100	100
3	t	420/423 (99%)	410 (98%)	10 (2%)	0	100	100
3	u	420/423 (99%)	402 (96%)	18 (4%)	0	100	100
3	y	420/423 (99%)	402 (96%)	18 (4%)	0	100	100
All	All	21797/23106 (94%)	20838 (96%)	956 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	211	SER
1	Y	24	ALA
2	H	55	ASP

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	0	128/137 (93%)	124 (97%)	4 (3%)	40	65
1	1	136/137 (99%)	132 (97%)	4 (3%)	42	66
1	Y	128/137 (93%)	105 (82%)	23 (18%)	1	11
1	f	136/137 (99%)	132 (97%)	4 (3%)	42	66
1	h	128/137 (93%)	123 (96%)	5 (4%)	32	60
1	n	128/137 (93%)	124 (97%)	4 (3%)	40	65
1	p	136/137 (99%)	132 (97%)	4 (3%)	42	66
1	r	128/137 (93%)	128 (100%)	0	100	100
1	v	128/137 (93%)	128 (100%)	0	100	100
1	w	128/137 (93%)	128 (100%)	0	100	100
1	x	136/137 (99%)	135 (99%)	1 (1%)	84	91
1	z	135/137 (98%)	135 (100%)	0	100	100
2	A	522/592 (88%)	512 (98%)	10 (2%)	57	76
2	B	522/592 (88%)	519 (99%)	3 (1%)	86	92
2	C	522/592 (88%)	508 (97%)	14 (3%)	44	68
2	D	522/592 (88%)	521 (100%)	1 (0%)	93	97
2	E	522/592 (88%)	512 (98%)	10 (2%)	57	76
2	F	522/592 (88%)	518 (99%)	4 (1%)	81	89
2	G	522/592 (88%)	520 (100%)	2 (0%)	91	95
2	H	522/592 (88%)	517 (99%)	5 (1%)	76	86
2	I	522/592 (88%)	510 (98%)	12 (2%)	50	71
2	J	522/592 (88%)	514 (98%)	8 (2%)	65	81
2	K	522/592 (88%)	519 (99%)	3 (1%)	86	92
2	L	522/592 (88%)	521 (100%)	1 (0%)	93	97
3	M	350/351 (100%)	341 (97%)	9 (3%)	46	69
3	N	350/351 (100%)	350 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	O	350/351 (100%)	350 (100%)	0	100	100
3	P	350/351 (100%)	350 (100%)	0	100	100
3	Q	350/351 (100%)	349 (100%)	1 (0%)	92	96
3	R	350/351 (100%)	347 (99%)	3 (1%)	78	88
3	S	350/351 (100%)	349 (100%)	1 (0%)	92	96
3	T	350/351 (100%)	349 (100%)	1 (0%)	92	96
3	U	350/351 (100%)	349 (100%)	1 (0%)	92	96
3	V	350/351 (100%)	349 (100%)	1 (0%)	92	96
3	W	350/351 (100%)	350 (100%)	0	100	100
3	X	350/351 (100%)	344 (98%)	6 (2%)	60	79
3	Z	349/351 (99%)	348 (100%)	1 (0%)	92	96
3	a	349/351 (99%)	347 (99%)	2 (1%)	86	92
3	b	349/351 (99%)	345 (99%)	4 (1%)	73	85
3	c	349/351 (99%)	348 (100%)	1 (0%)	92	96
3	d	349/351 (99%)	346 (99%)	3 (1%)	78	88
3	e	342/351 (97%)	335 (98%)	7 (2%)	55	75
3	g	342/351 (97%)	342 (100%)	0	100	100
3	i	342/351 (97%)	340 (99%)	2 (1%)	86	92
3	j	350/351 (100%)	344 (98%)	6 (2%)	60	79
3	k	342/351 (97%)	338 (99%)	4 (1%)	71	84
3	l	342/351 (97%)	333 (97%)	9 (3%)	46	69
3	m	350/351 (100%)	350 (100%)	0	100	100
3	o	350/351 (100%)	349 (100%)	1 (0%)	92	96
3	q	350/351 (100%)	348 (99%)	2 (1%)	86	92
3	s	350/351 (100%)	350 (100%)	0	100	100
3	t	350/351 (100%)	344 (98%)	6 (2%)	60	79
3	u	350/351 (100%)	345 (99%)	5 (1%)	67	82
3	y	350/351 (100%)	346 (99%)	4 (1%)	73	85
All	All	18294/19278 (95%)	18092 (99%)	202 (1%)	74	85

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	16	ARG
1	0	17	LYS
1	0	18	PHE
1	0	27	THR
1	1	150	LEU
1	1	153	ILE
1	1	157	ILE
1	1	159	ASN
2	A	276	ARG
2	A	621	VAL
2	A	622	LEU
2	A	626	GLN
2	A	635	GLN
2	A	636	LYS
2	A	643	GLN
2	A	654	ASP
2	A	664	TYR
2	A	668	GLN
2	B	276	ARG
2	B	600	LYS
2	B	643	GLN
2	C	52	THR
2	C	53	LYS
2	C	54	LEU
2	C	56	GLU
2	C	276	ARG
2	C	631	GLN
2	C	635	GLN
2	C	636	LYS
2	C	638	THR
2	C	641	THR
2	C	643	GLN
2	C	645	GLN
2	C	647	LYS
2	C	652	GLN
2	D	276	ARG
2	E	207	LEU
2	E	209	VAL
2	E	210	THR
2	E	211	SER
2	E	212	MET
2	E	213	THR
2	E	218	ASN

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Mol	Chain	Res	Type
2	E	220	PHE
2	E	224	VAL
2	E	229	LYS
2	F	177	ASP
2	F	179	SER
2	F	182	LEU
2	F	276	ARG
2	G	201	LYS
2	G	510	ARG
2	H	53	LYS
2	H	54	LEU
2	H	55	ASP
2	H	65	GLU
2	H	276	ARG
2	I	177	ASP
2	I	179	SER
2	I	182	LEU
2	I	195	TYR
2	I	207	LEU
2	I	212	MET
2	I	215	TRP
2	I	216	GLU
2	I	219	TRP
2	I	220	PHE
2	I	229	LYS
2	I	276	ARG
2	J	71	THR
2	J	72	GLU
2	J	83	ASN
2	J	276	ARG
2	J	450	MET
2	J	451	ASN
2	J	452	ARG
2	J	464	MET
2	K	519	ASN
2	K	521	LEU
2	K	532	VAL
2	L	519	ASN
3	M	25	LEU
3	M	29	LYS
3	M	31	VAL
3	M	32	ASP

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Mol	Chain	Res	Type
3	M	40	ILE
3	M	44	THR
3	M	113	ARG
3	M	114	GLN
3	M	119	ASP
3	Q	190	GLN
3	R	113	ARG
3	R	116	ILE
3	R	121	GLU
3	S	162	ASN
3	T	216	LEU
3	U	113	ARG
3	V	113	ARG
3	X	91	VAL
3	X	102	LEU
3	X	107	GLU
3	X	113	ARG
3	X	115	ARG
3	X	116	ILE
1	Y	5	LEU
1	Y	6	THR
1	Y	9	GLU
1	Y	10	ILE
1	Y	12	LEU
1	Y	17	LYS
1	Y	18	PHE
1	Y	20	ILE
1	Y	23	ASN
1	Y	25	SER
1	Y	27	THR
1	Y	28	ASP
1	Y	29	VAL
1	Y	30	GLU
1	Y	72	SER
1	Y	76	ARG
1	Y	77	LYS
1	Y	79	LYS
1	Y	90	MET
1	Y	91	LEU
1	Y	143	ASP
1	Y	150	LEU
1	Y	152	LEU

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Mol	Chain	Res	Type
3	Z	113	ARG
3	a	10	SER
3	a	12	ILE
3	b	35	LEU
3	b	43	SER
3	b	49	SER
3	b	52	ARG
3	c	113	ARG
3	d	116	ILE
3	d	377	VAL
3	d	379	THR
3	e	166	ASN
3	e	169	VAL
3	e	170	MET
3	e	171	ASP
3	e	218	SER
3	e	220	THR
3	e	221	GLN
1	f	152	LEU
1	f	154	ASP
1	f	156	ASP
1	f	157	ILE
1	h	77	LYS
1	h	79	LYS
1	h	111	ASP
1	h	114	MET
1	h	119	VAL
3	i	178	LEU
3	i	408	TYR
3	j	97	GLU
3	j	101	LYS
3	j	389	LYS
3	j	390	TYR
3	j	396	ASN
3	j	397	VAL
3	k	165	GLU
3	k	166	ASN
3	k	169	VAL
3	k	171	ASP
3	l	115	ARG
3	l	116	ILE
3	l	117	VAL

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Mol	Chain	Res	Type
3	l	120	LEU
3	l	121	GLU
3	l	129	MET
3	l	166	ASN
3	l	169	VAL
3	l	176	GLN
1	n	3	THR
1	n	4	VAL
1	n	7	LYS
1	n	15	LEU
3	o	114	GLN
1	p	139	VAL
1	p	141	THR
1	p	152	LEU
1	p	157	ILE
3	q	10	SER
3	q	422	ASN
3	t	57	SER
3	t	58	SER
3	t	60	ARG
3	t	61	THR
3	t	66	ILE
3	t	221	GLN
3	u	277	GLN
3	u	280	THR
3	u	282	GLN
3	u	387	VAL
3	u	399	LYS
1	x	88	LEU
3	y	113	ARG
3	y	117	VAL
3	y	121	GLU
3	y	122	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	101	GLN
1	0	105	ASN
2	A	602	GLN
2	C	643	GLN
2	C	661	ASN

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Mol	Chain	Res	Type
2	D	609	GLN
2	E	661	ASN
2	G	606	GLN
2	I	218	ASN
3	M	114	GLN
3	M	221	GLN
3	M	267	GLN
3	M	418	GLN
3	O	114	GLN
3	S	162	ASN
3	T	347	GLN
3	W	186	HIS
3	W	279	GLN
3	X	186	HIS
1	Y	101	GLN
1	Y	107	GLN
3	d	388	HIS
3	e	221	GLN
3	g	332	GLN
3	g	396	ASN
1	h	39	ASN
3	i	332	GLN
3	j	114	GLN
3	j	388	HIS
3	k	166	ASN
3	k	356	ASN
3	l	114	GLN
3	l	166	ASN
3	l	356	ASN
3	m	233	GLN
3	o	279	GLN
1	p	23	ASN
3	q	398	GLN
3	s	186	HIS
3	t	55	GLN
3	t	69	GLN
3	t	140	ASN
3	u	182	GLN
3	u	186	HIS
3	u	282	GLN
3	u	398	GLN
3	y	356	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.

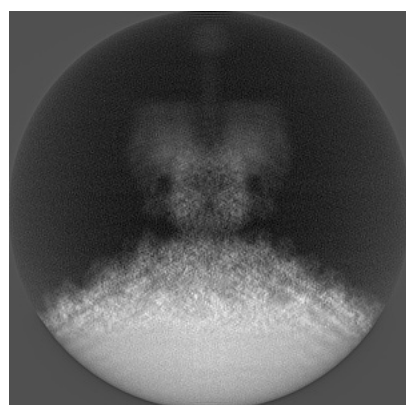
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25372. These allow visual inspection of the internal detail of the map and identification of artifacts.

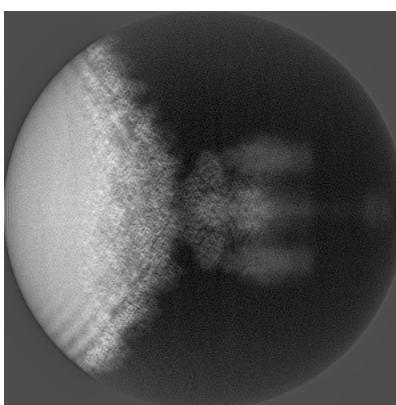
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

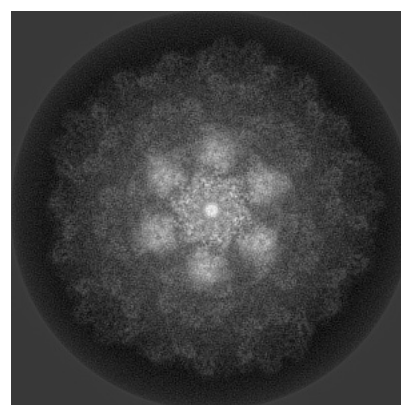
6.1.1 Primary map



X



Y

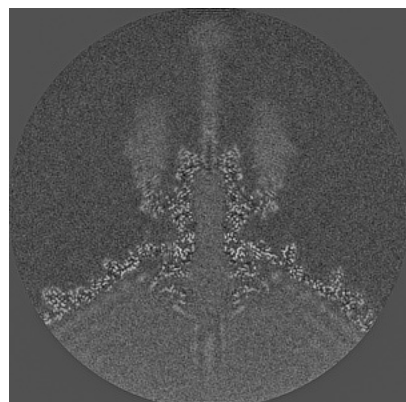


Z

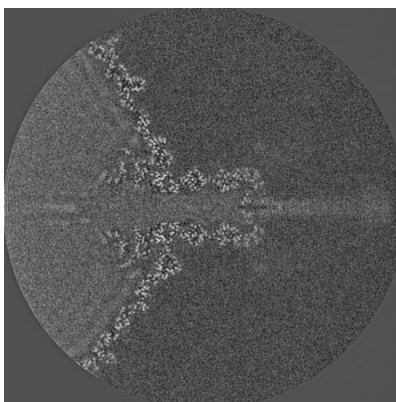
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

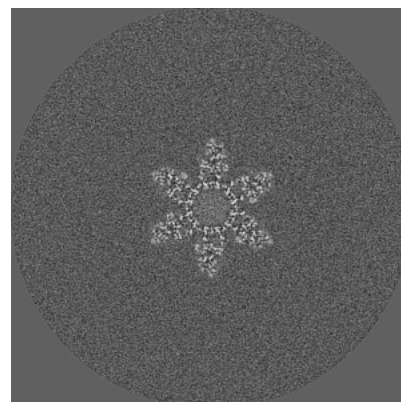
6.2.1 Primary map



X Index: 256



Y Index: 256

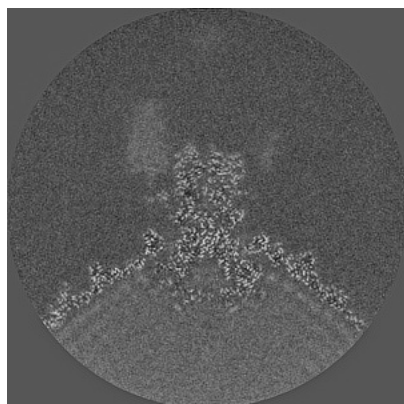


Z Index: 256

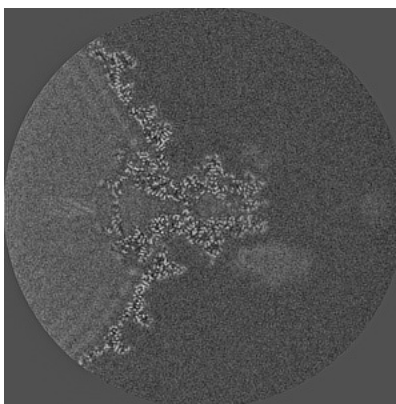
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

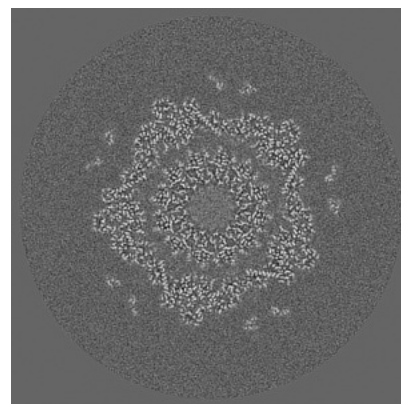
6.3.1 Primary map



X Index: 235



Y Index: 239

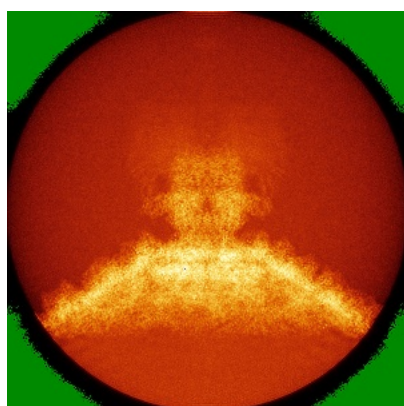


Z Index: 178

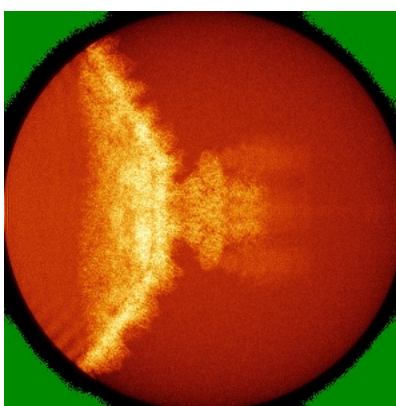
The images above show the largest variance slices of the map in three orthogonal directions.

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

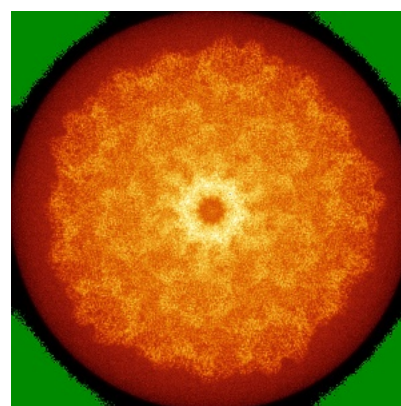
6.4.1 Primary map



X



Y

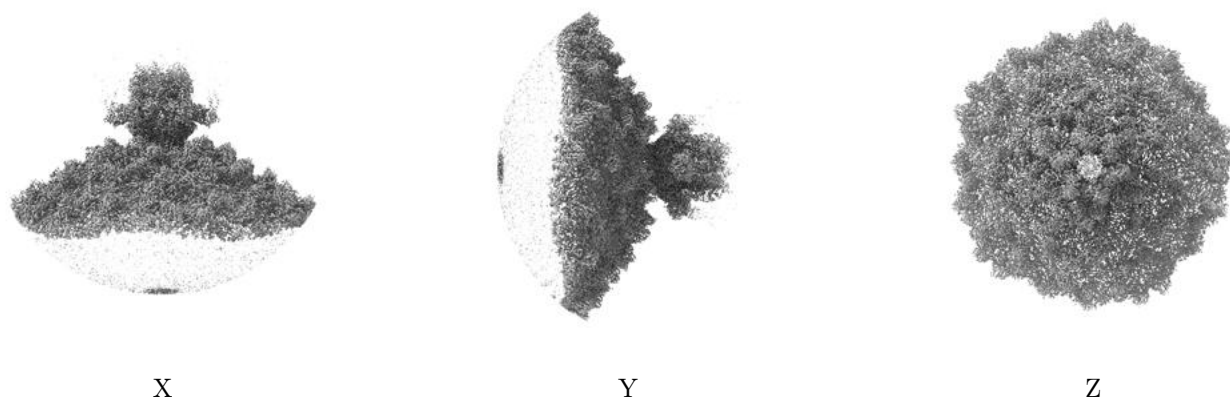


Z

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



The images above show the 3D surface view of the map at the recommended contour level 4.62. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

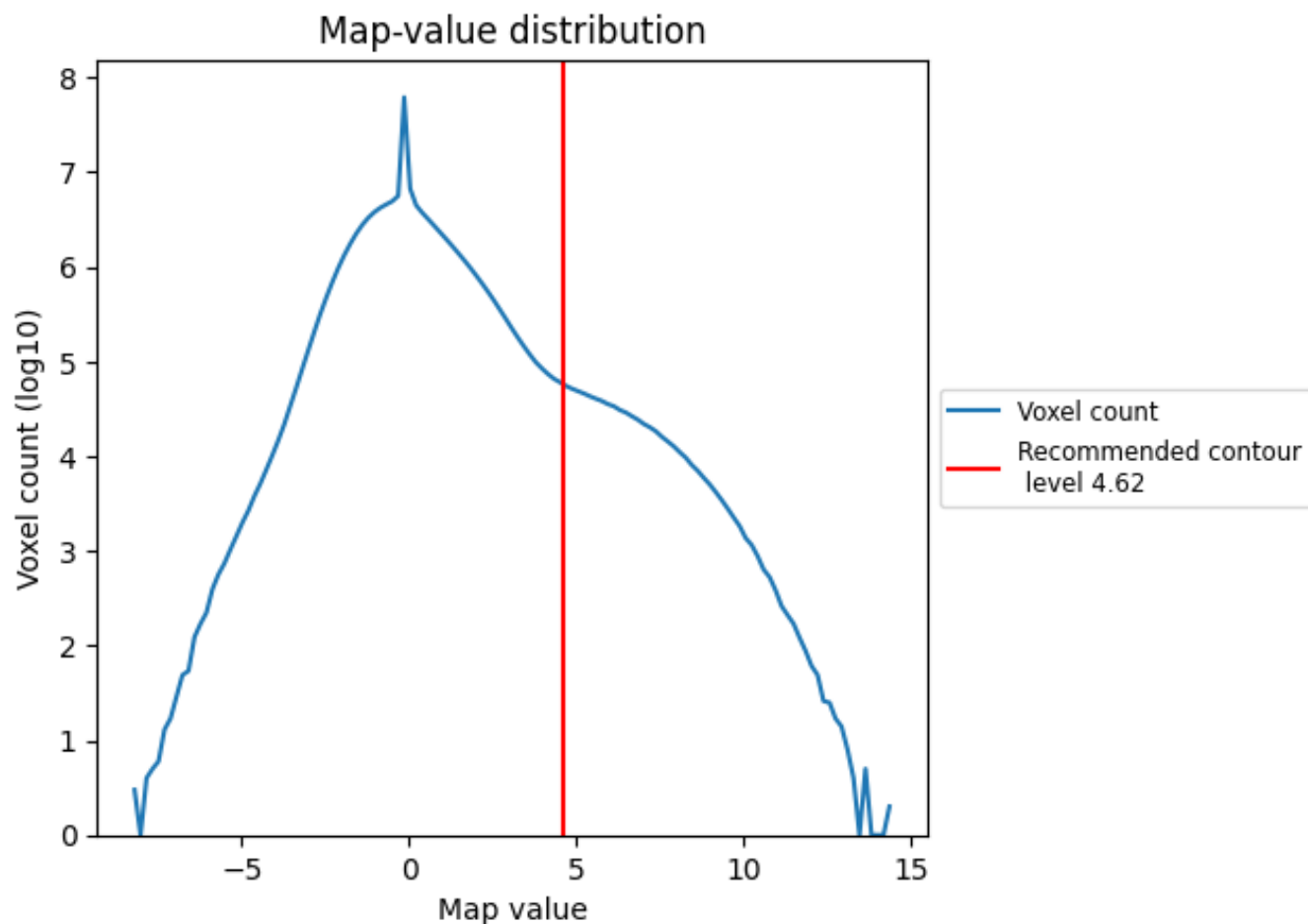
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

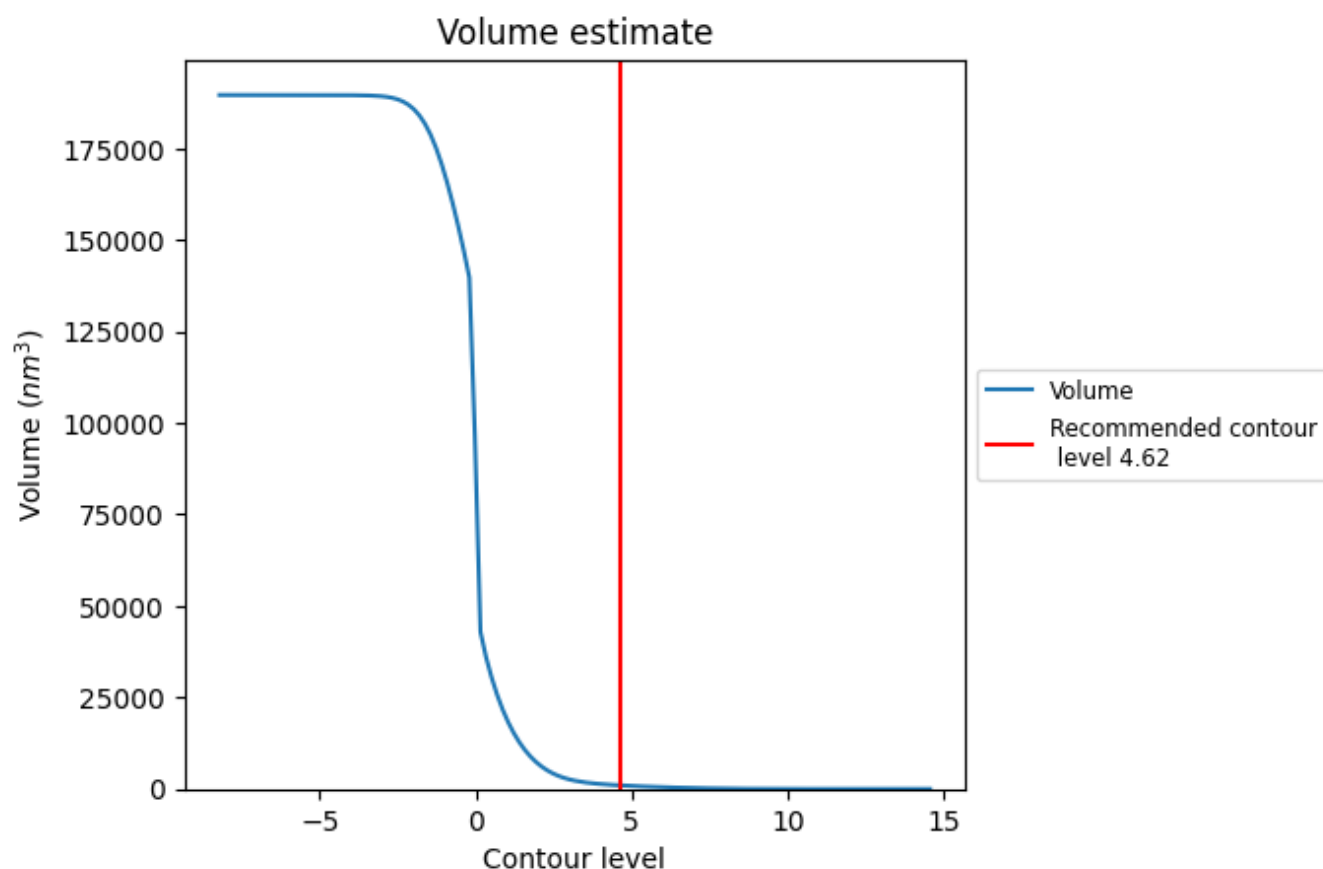
This section contains the results of statistical analysis of the map.

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.

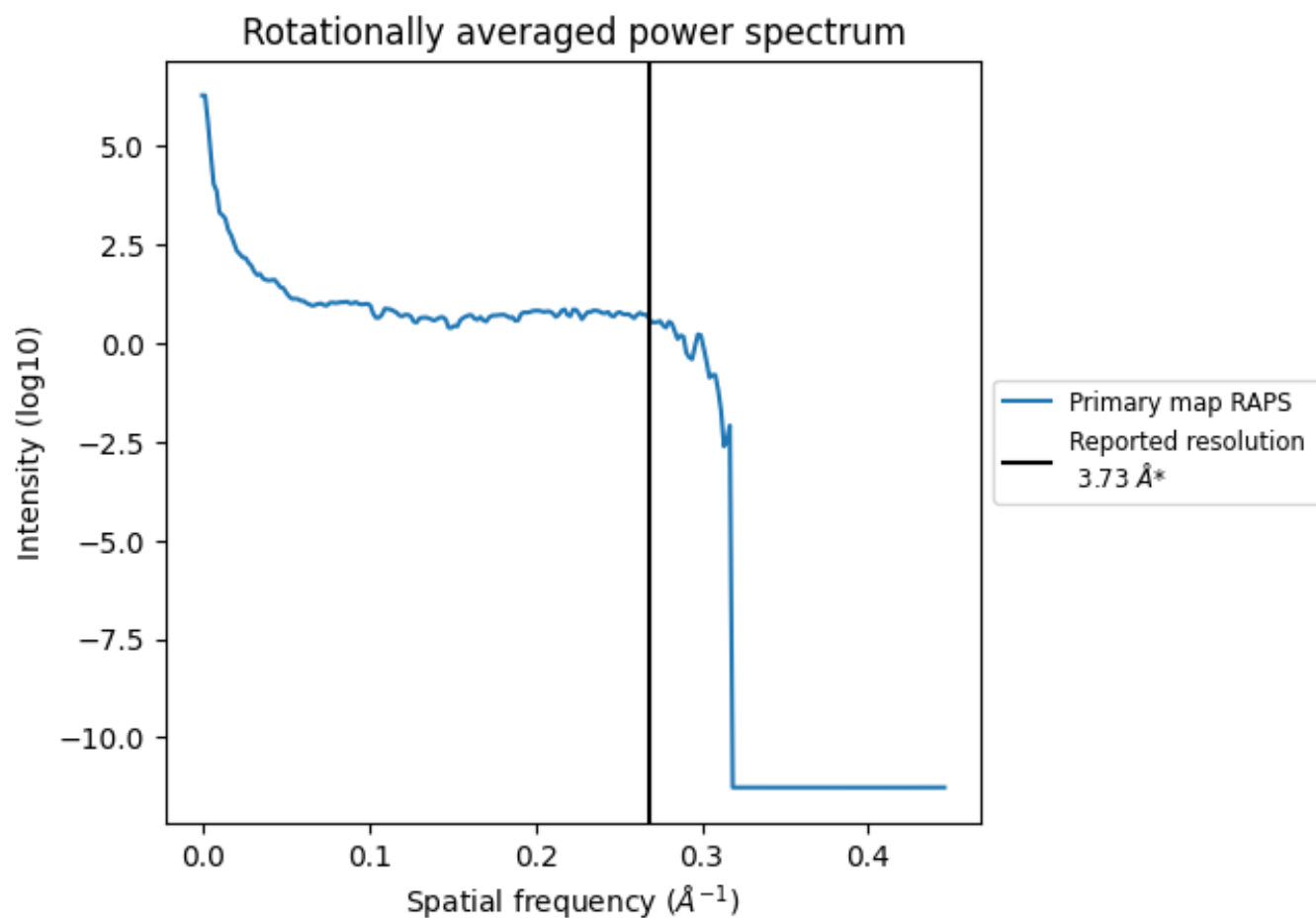
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 990 nm^3 ; this corresponds to an approximate mass of 895 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 ⓘ

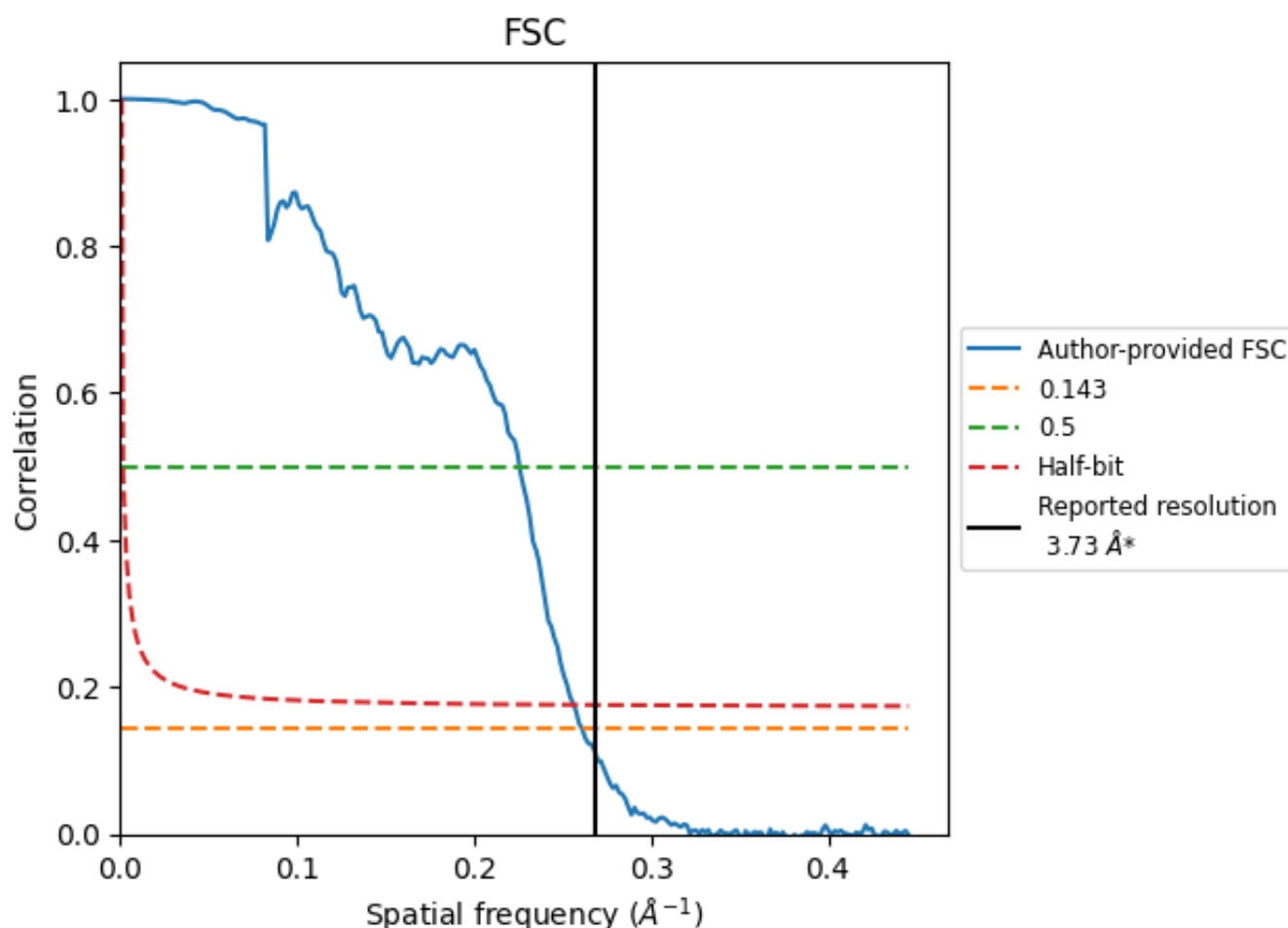


*Reported resolution corresponds to spatial frequency of 0.268 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.268 Å⁻¹

8.2 Resolution estimates [i](#)

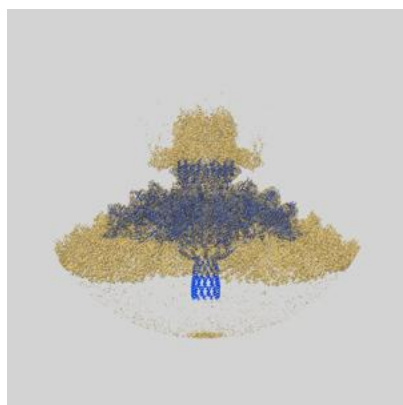
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.73	-	-
Author-provided FSC curve	3.83	4.43	3.90
Unmasked-calculated*	-	-	-

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

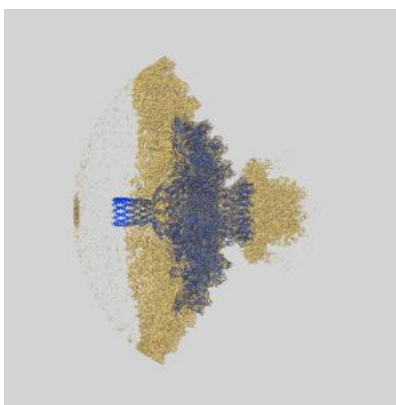
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25372 and PDB model 7SPU. Per-residue inclusion information can be found in section [3](#) on page [8](#).

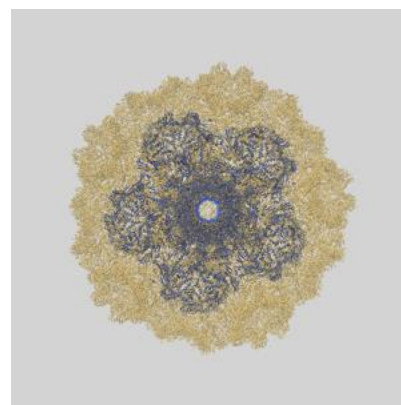
9.1 Map-model overlay [i](#)



X



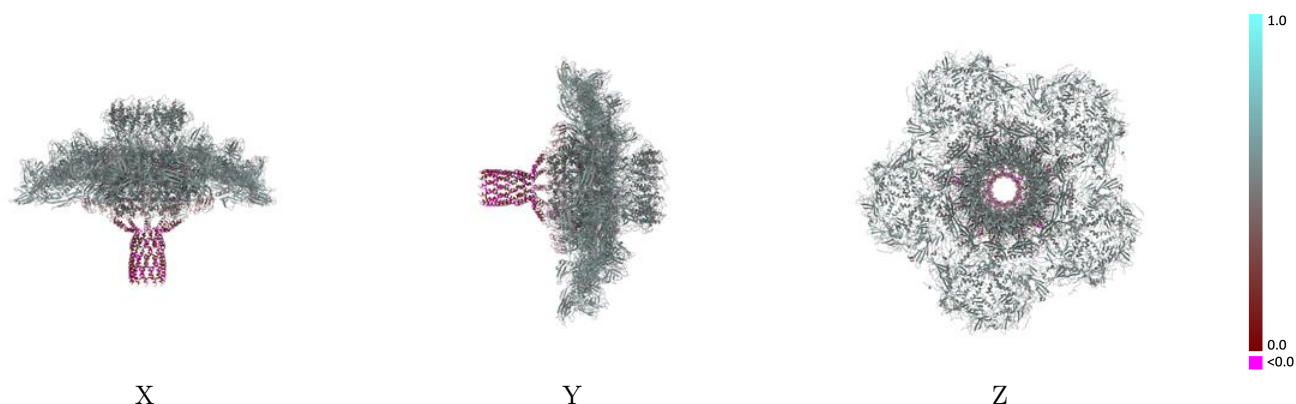
Y



Z

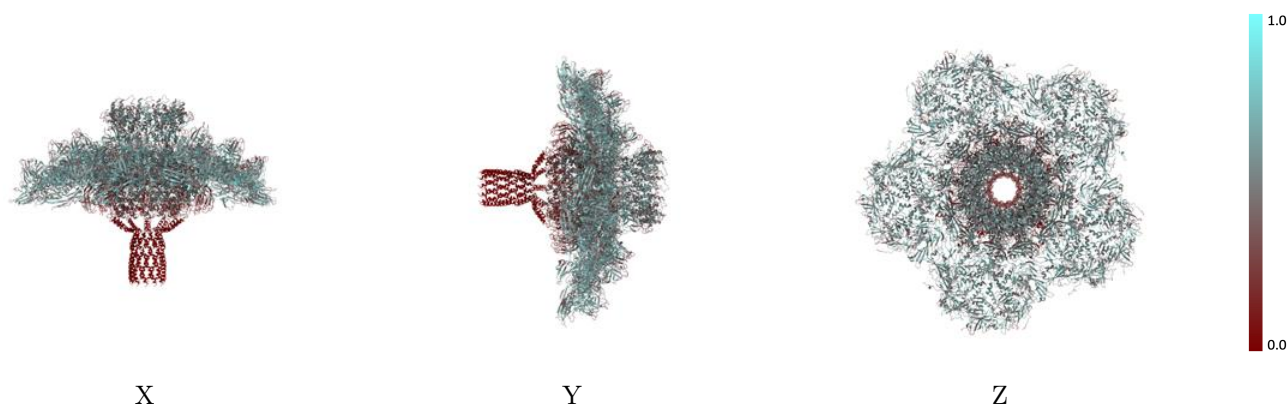
The images above show the 3D surface view of the map at the recommended contour level 4.62 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



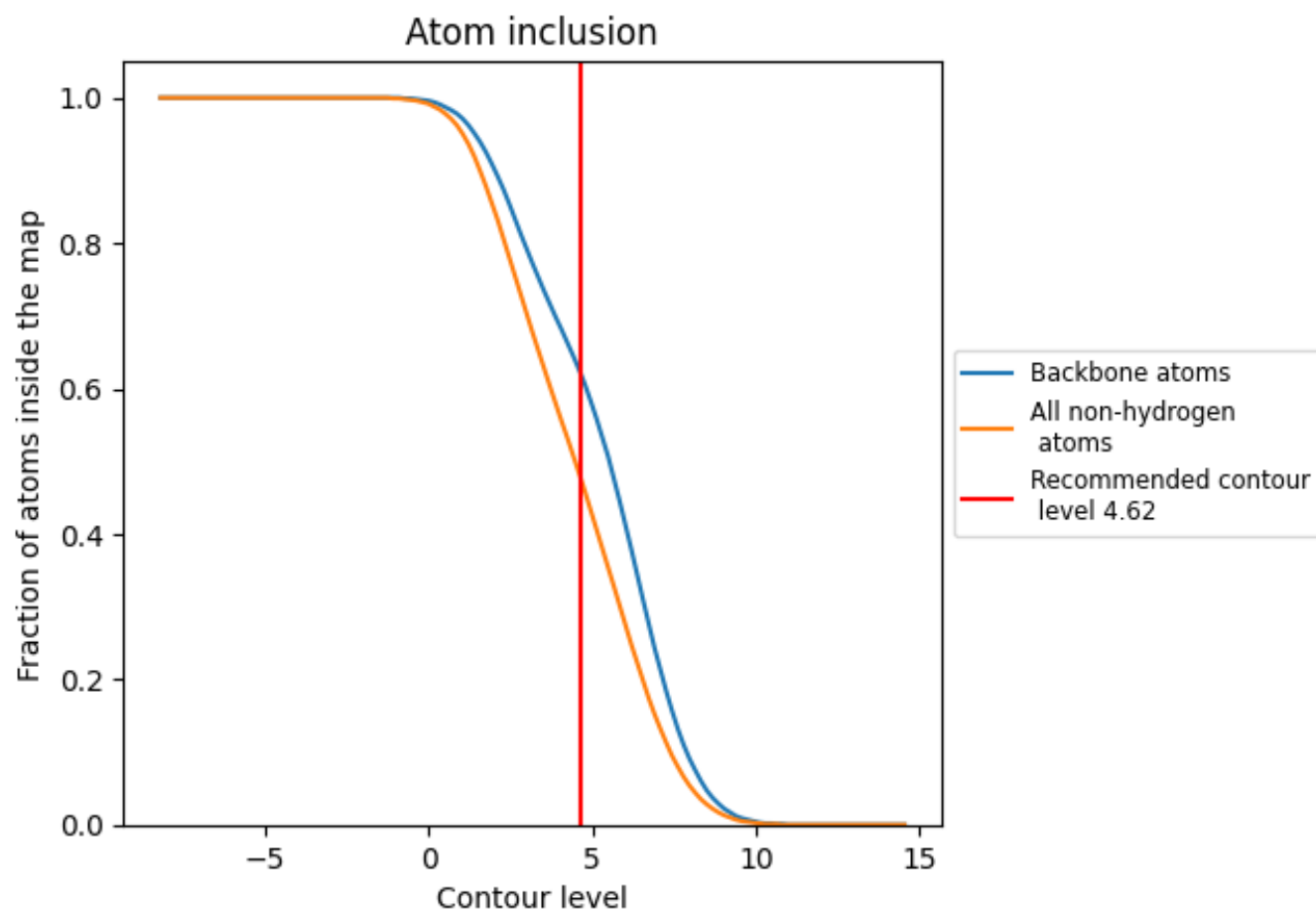
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.62).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 48% 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 (4.62) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4810	 0.4950
0	 0.5000	 0.5130
1	 0.4640	 0.5000
A	 0.3730	 0.4510
B	 0.3720	 0.4420
C	 0.3670	 0.4480
D	 0.3680	 0.4420
E	 0.3750	 0.4510
F	 0.3860	 0.4460
G	 0.3760	 0.4450
H	 0.3680	 0.4450
I	 0.3680	 0.4490
J	 0.3660	 0.4500
K	 0.3730	 0.4430
L	 0.3810	 0.4450
M	 0.5620	 0.5280
N	 0.5600	 0.5270
O	 0.5570	 0.5270
P	 0.5640	 0.5290
Q	 0.5360	 0.5250
R	 0.5460	 0.5300
S	 0.5400	 0.5270
T	 0.5400	 0.5270
U	 0.5470	 0.5220
V	 0.5450	 0.5240
W	 0.5360	 0.5220
X	 0.5350	 0.5220
Y	 0.5000	 0.5160
Z	 0.5580	 0.5300
a	 0.5420	 0.5270
b	 0.5460	 0.5280
c	 0.5600	 0.5320
d	 0.5570	 0.5310
e	 0.5400	 0.4960
f	 0.4820	 0.5160



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Chain	Atom inclusion	Q-score
g	 0.5320	 0.5130
h	 0.4940	 0.5150
i	 0.5390	 0.5090
j	 0.5530	 0.5270
k	 0.5320	 0.5080
l	 0.5360	 0.5070
m	 0.5550	 0.5300
n	 0.4860	 0.5050
o	 0.5640	 0.5290
p	 0.4850	 0.5070
q	 0.5420	 0.5280
r	 0.4820	 0.5110
s	 0.5560	 0.5290
t	 0.5420	 0.5280
u	 0.5420	 0.5270
v	 0.4910	 0.5030
w	 0.4840	 0.5140
x	 0.4870	 0.5110
y	 0.5350	 0.5230
z	 0.4790	 0.5030