wwPDB EM Validation Summary Report (i)

Mar 25, 2026 – 12:48 AM UTC

PDB ID	:	6HCG / pdb_00006hcg
EMDB ID	:	EMD-0193
Title	:	Klebsiella pneumoniae type II secretion system outer membrane complex. PulD, PulS and PulC HR domain.
Authors	:	Chernyatina, A.A.; Low, H.H.
Deposited on	:	2018-08-15
Resolution	:	4.30 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

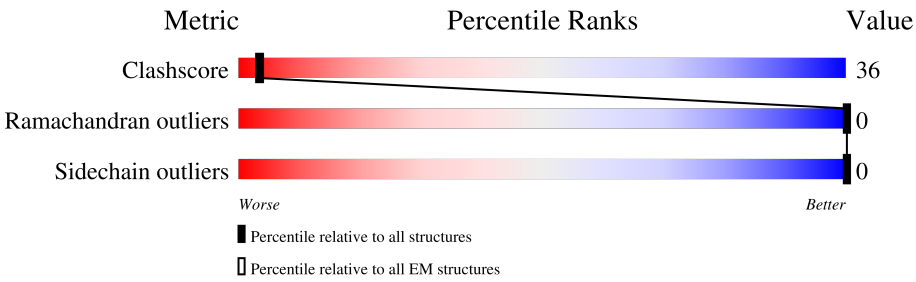
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

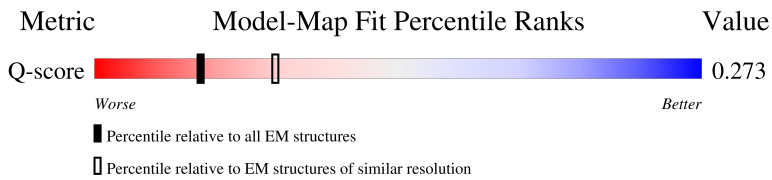
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.30 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

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

Mol	Chain	Length	Quality of chain
1	A	657	6% 41% 49% 10%
1	B	657	7% 42% 48% 10%
1	C	657	7% 41% 49% 10%
1	D	657	7% 42% 48% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	657	8% 42% 48% 10%
1	F	657	8% 42% 48% 10%
1	G	657	9% 41% 49% 10%
1	H	657	9% 41% 49% 10%
1	I	657	8% 41% 49% 10%
1	J	657	9% 40% 50% 10%
1	K	657	8% 41% 49% 10%
1	L	657	9% 41% 49% 10%
1	M	657	8% 41% 49% 10%
1	N	657	8% 41% 49% 10%
1	O	657	8% 41% 49% 10%
2	P	143	37% 46% 17% • 35%
2	Q	143	35% 46% 17% • 35%
2	R	143	36% 46% 17% • 35%
2	S	143	38% 46% 18% • 35%
2	T	143	38% 46% 17% • 35%
2	U	143	34% 46% 17% • 35%
2	V	143	35% 46% 17% • 35%
2	W	143	31% 46% 17% • 35%
2	X	143	32% 46% 17% • 35%
2	Y	143	35% 46% 17% • 35%
2	Z	143	39% 46% 17% • 35%
2	a	143	36% 45% 18% • 35%
2	b	143	37% 45% 18% • 35%
2	c	143	38% 46% 17% • 35%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	d	143	36% 45% 18% • 35%
3	e	280	19% 19% 6% 76%
3	f	280	19% 19% 6% 76%
3	g	280	19% 19% 5% 76%
3	h	280	19% 19% 6% 76%
3	i	280	17% 19% 5% 76%
3	j	280	18% 19% 6% 76%
3	k	280	17% 19% 6% 76%
3	l	280	17% 19% 5% 76%
3	m	280	17% 19% 6% 76%
3	n	280	18% 19% 5% 76%
3	o	280	20% 19% 6% 76%
3	p	280	20% 19% 5% 76%
3	q	280	19% 19% 5% 76%
3	r	280	20% 19% 5% 76%
3	s	280	19% 19% 5% 76%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 85185 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 Type II secretion system protein D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	592	4447	2780	779	878	10	0	0
1	B	592	4447	2780	779	878	10	0	0
1	C	592	4447	2780	779	878	10	0	0
1	D	592	4447	2780	779	878	10	0	0
1	E	592	4447	2780	779	878	10	0	0
1	F	592	4447	2780	779	878	10	0	0
1	G	592	4447	2780	779	878	10	0	0
1	H	592	4447	2780	779	878	10	0	0
1	I	592	4447	2780	779	878	10	0	0
1	J	592	4447	2780	779	878	10	0	0
1	K	592	4447	2780	779	878	10	0	0
1	L	592	4447	2780	779	878	10	0	0
1	M	592	4447	2780	779	878	10	0	0
1	N	592	4447	2780	779	878	10	0	0
1	O	592	4447	2780	779	878	10	0	0

- Molecule 2 is a protein called Pullulanase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	P	93	720	441	134	143	2	0	0
2	Q	93	720	441	134	143	2	0	0
2	R	93	720	441	134	143	2	0	0
2	S	93	720	441	134	143	2	0	0
2	T	93	720	441	134	143	2	0	0
2	U	93	720	441	134	143	2	0	0
2	V	93	720	441	134	143	2	0	0
2	W	93	720	441	134	143	2	0	0
2	X	93	720	441	134	143	2	0	0
2	Y	93	720	441	134	143	2	0	0
2	Z	93	720	441	134	143	2	0	0
2	a	93	720	441	134	143	2	0	0
2	b	93	720	441	134	143	2	0	0
2	c	93	720	441	134	143	2	0	0
2	d	93	720	441	134	143	2	0	0

- Molecule 3 is a protein called Pectic enzymes secretion protein OutC.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	e	68	512	326	92	94	0	0
3	f	68	512	326	92	94	0	0
3	g	68	512	326	92	94	0	0
3	h	68	512	326	92	94	0	0
3	i	68	512	326	92	94	0	0

Continued on next page...

Continued from previous page...

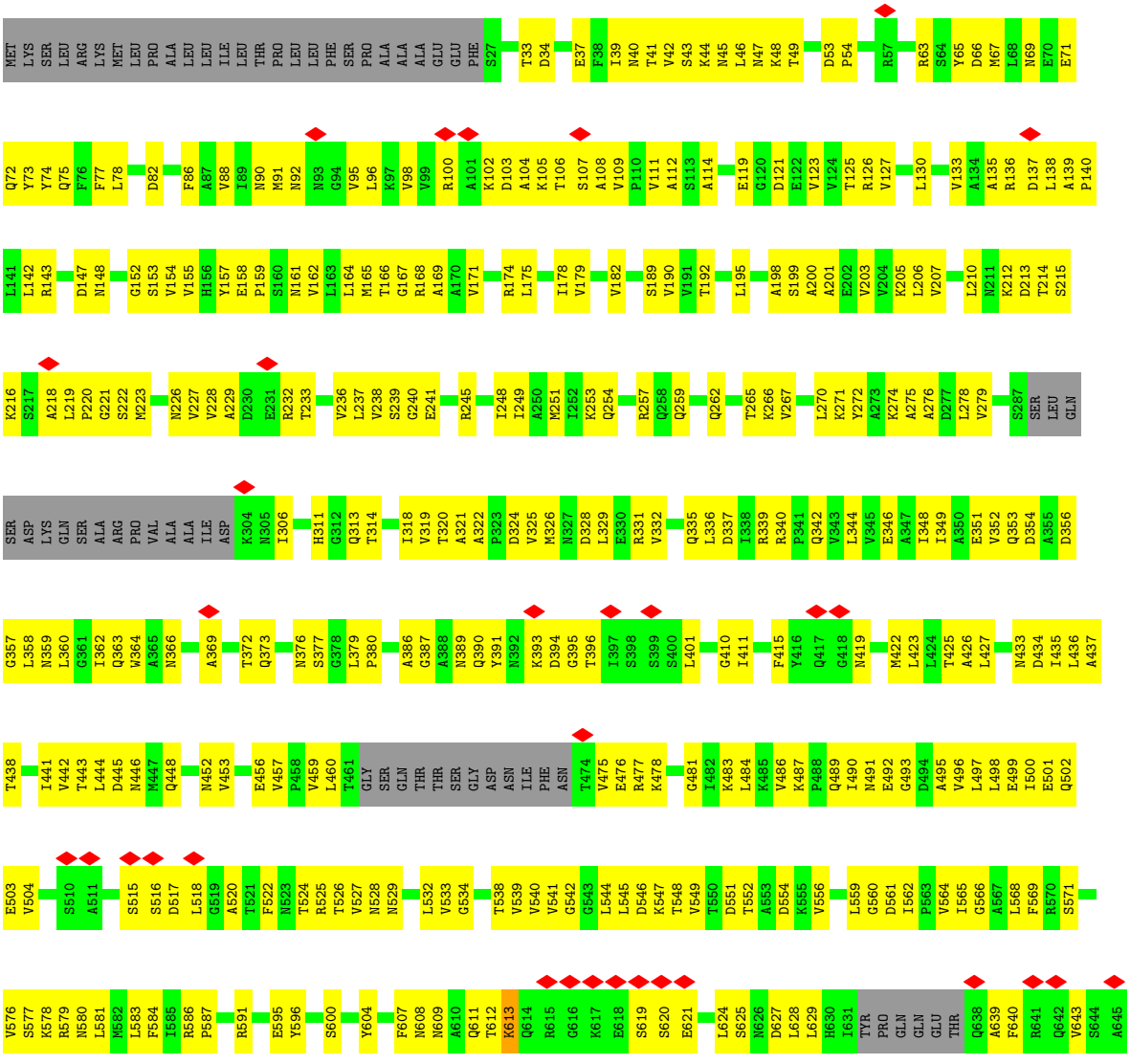
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	j	68	512	326	92	94	0	0
3	k	68	512	326	92	94	0	0
3	l	68	512	326	92	94	0	0
3	m	68	512	326	92	94	0	0
3	n	68	512	326	92	94	0	0
3	o	68	512	326	92	94	0	0
3	p	68	512	326	92	94	0	0
3	q	68	512	326	92	94	0	0
3	r	68	512	326	92	94	0	0
3	s	68	512	326	92	94	0	0

3 Residue-property plots (i)

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

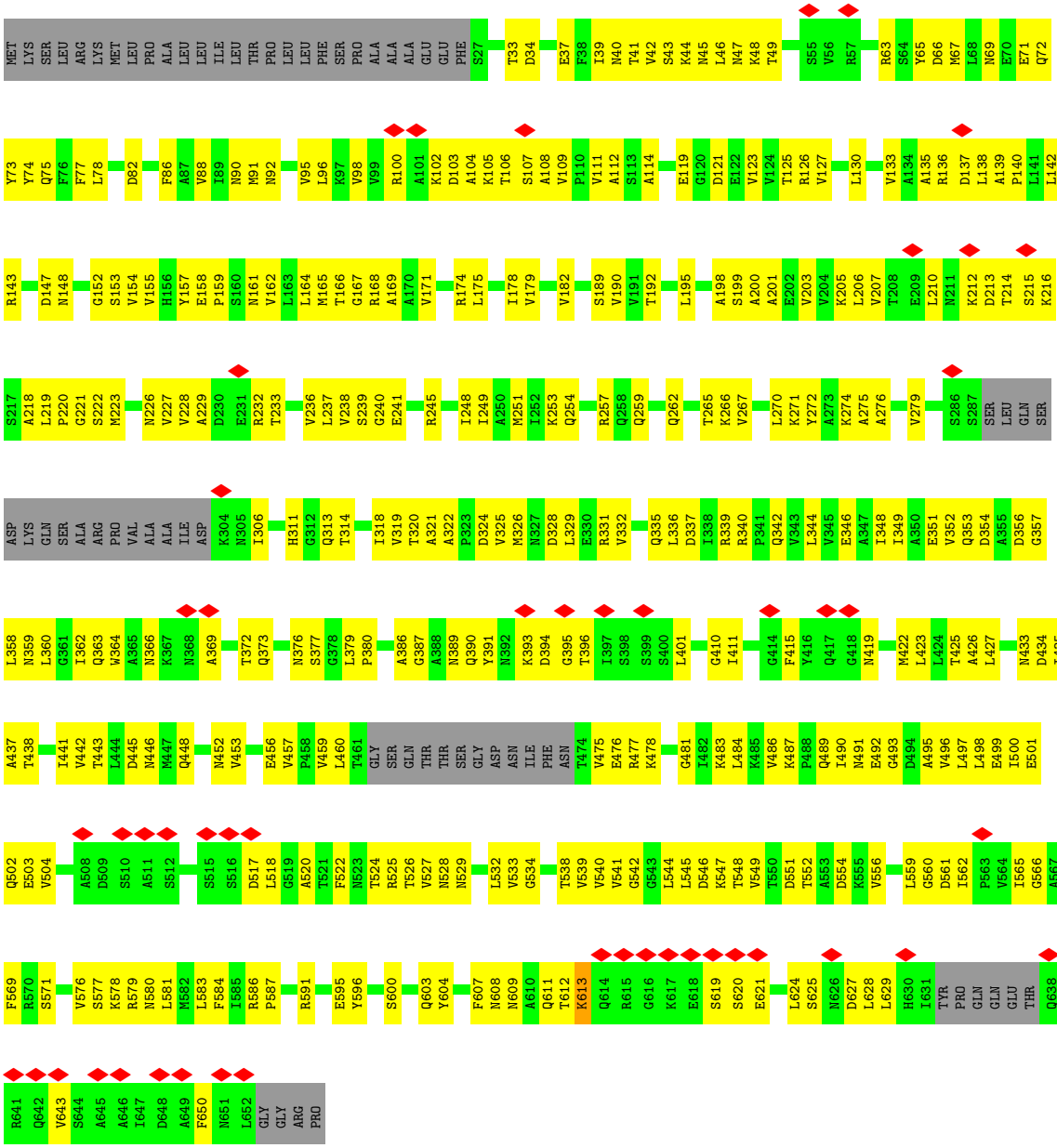
- Molecule 1: Type II secretion system protein D

Chain A: 6% 41% 49% 10%



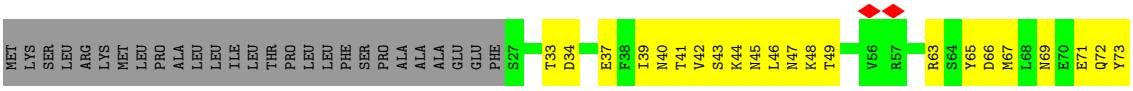
• Molecule 1: Type II secretion system protein D

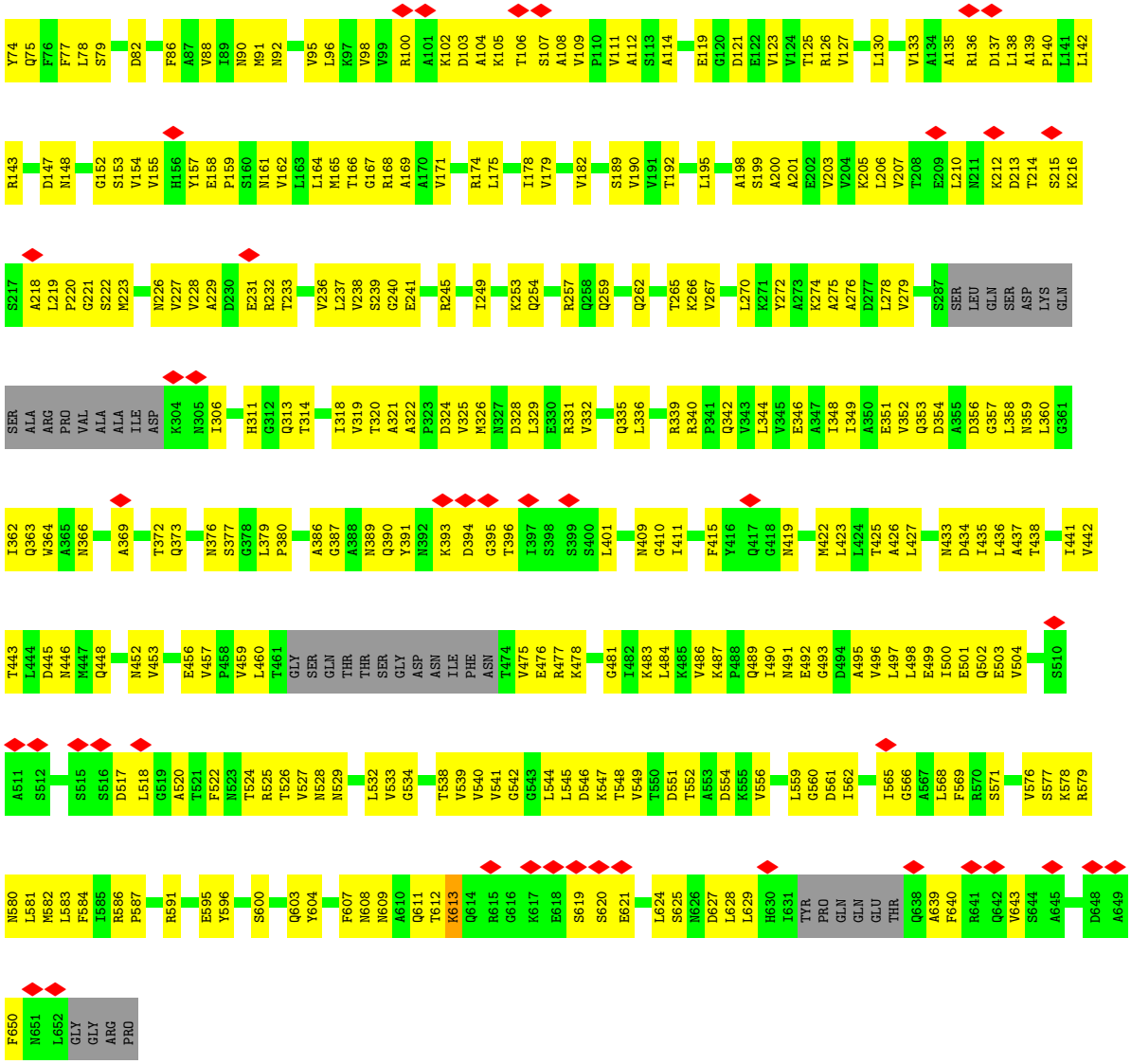
Chain B:



• Molecule 1: Type II secretion system protein D

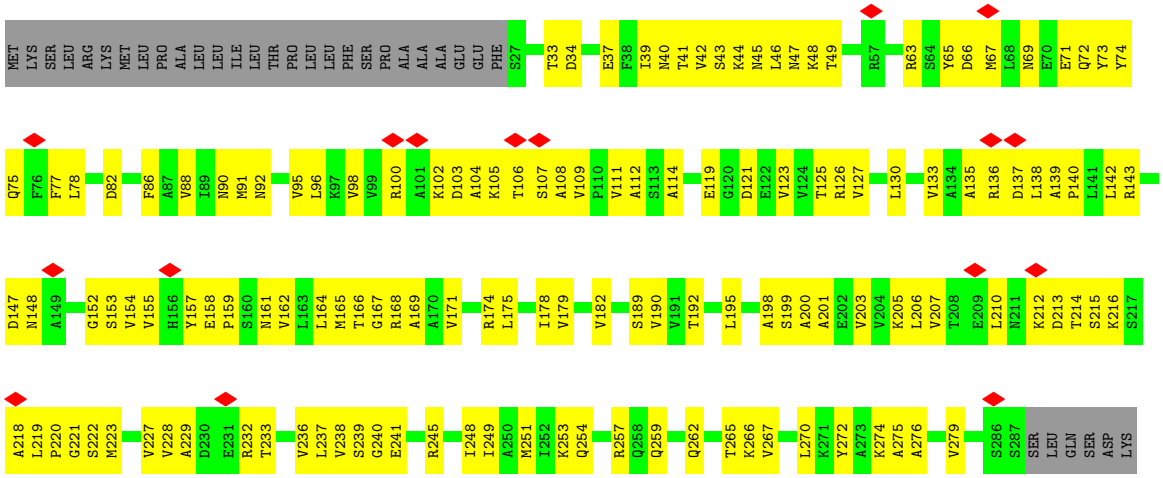
Chain C:

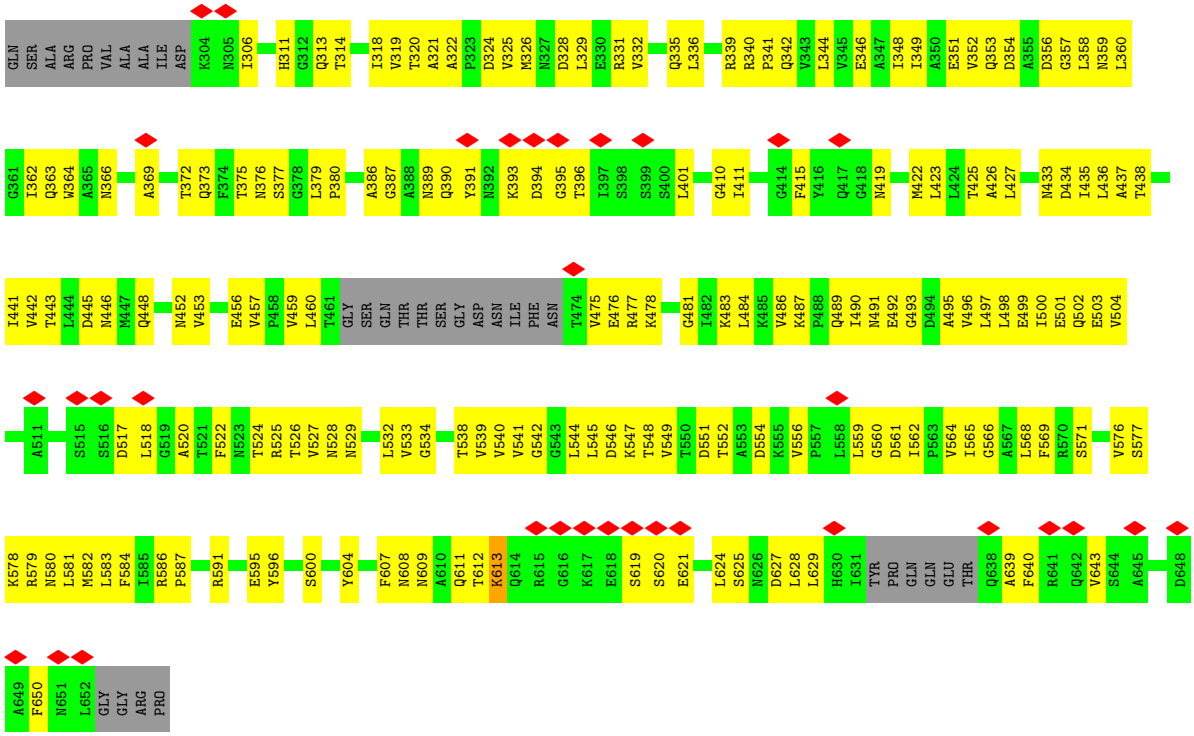




- Molecule 1: Type II secretion system protein D

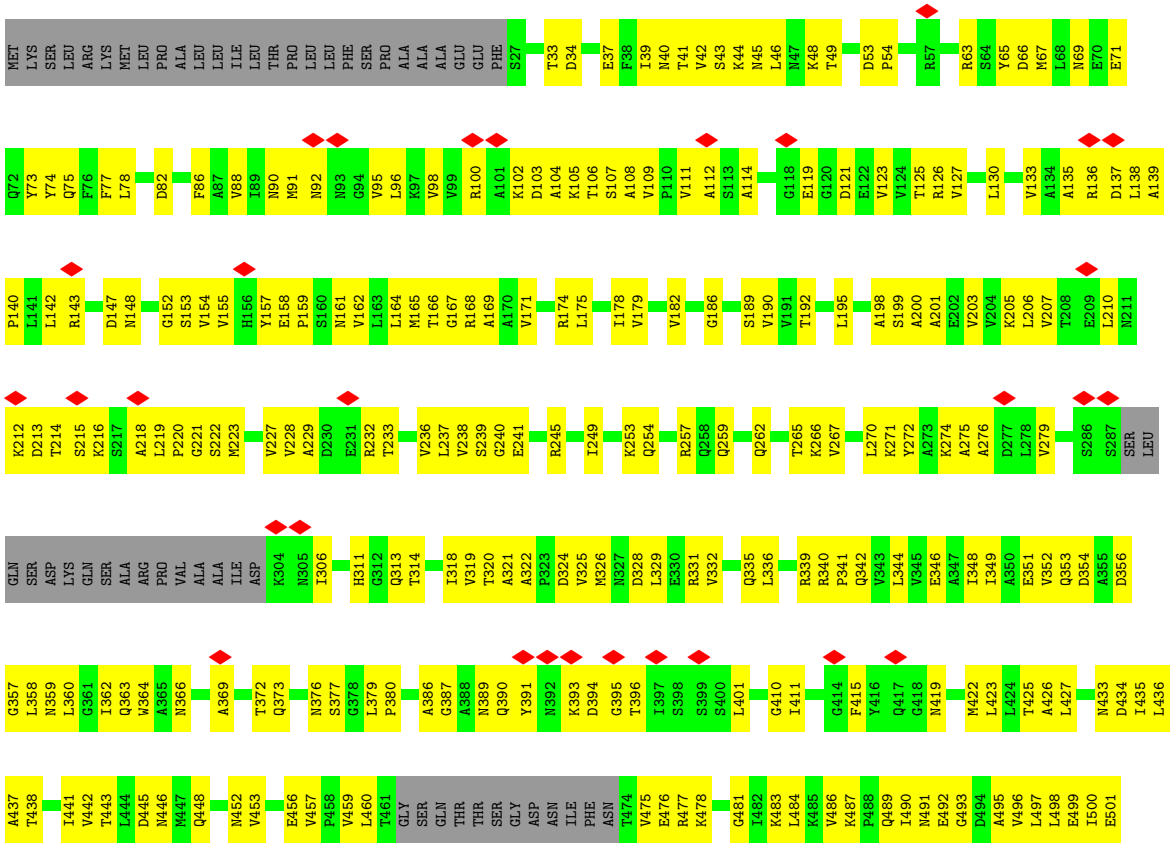
Chain D:

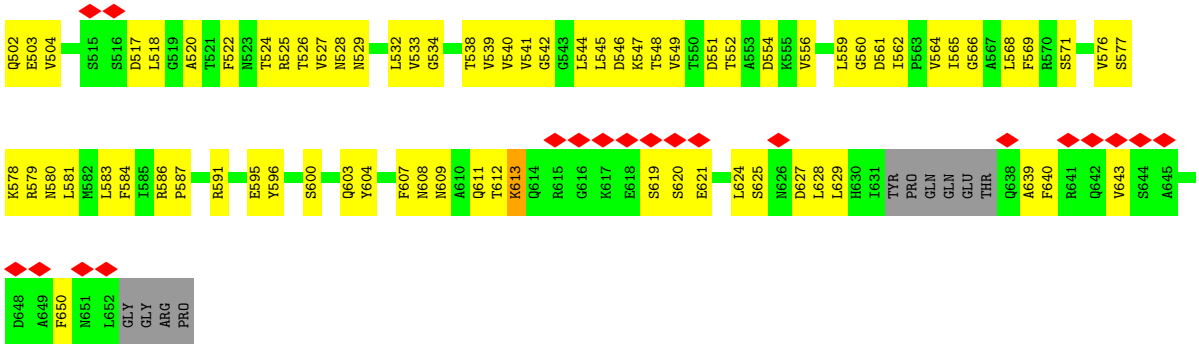




- Molecule 1: Type II secretion system protein D

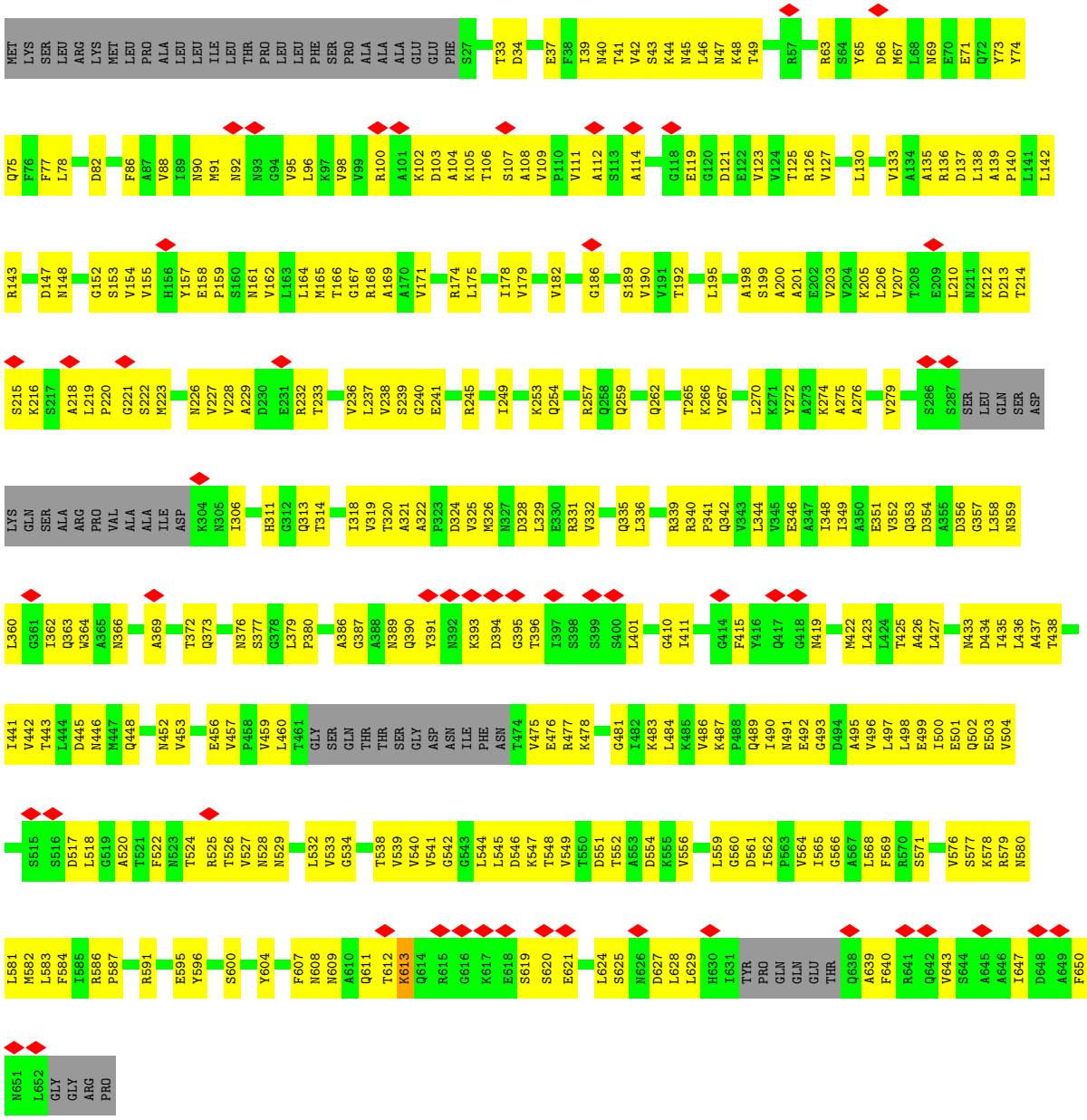
Chain E:





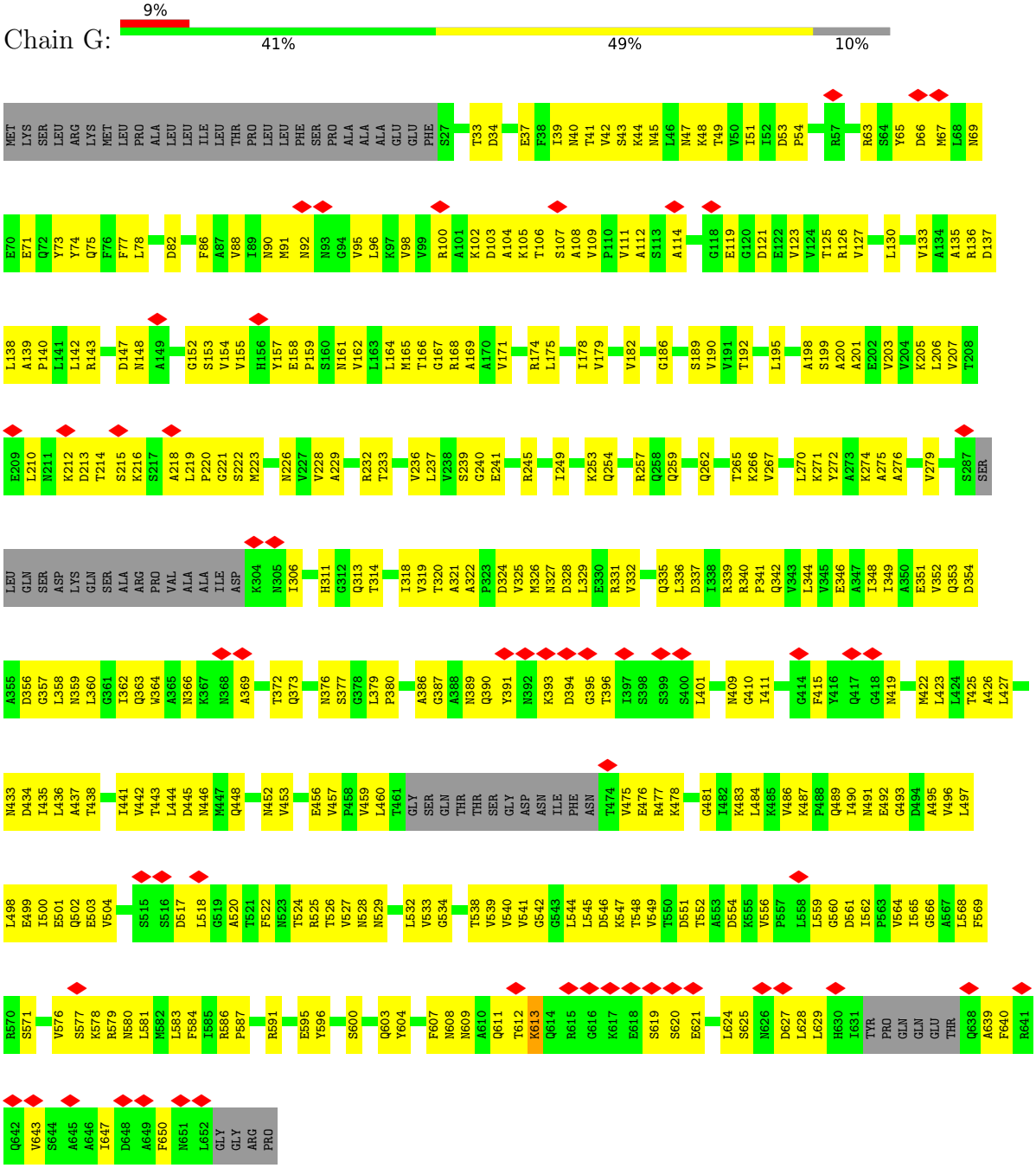
• Molecule 1: Type II secretion system protein D

Chain F:



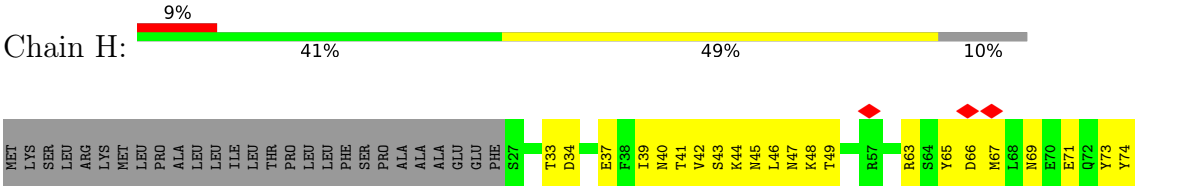
- Molecule 1: Type II secretion system protein D

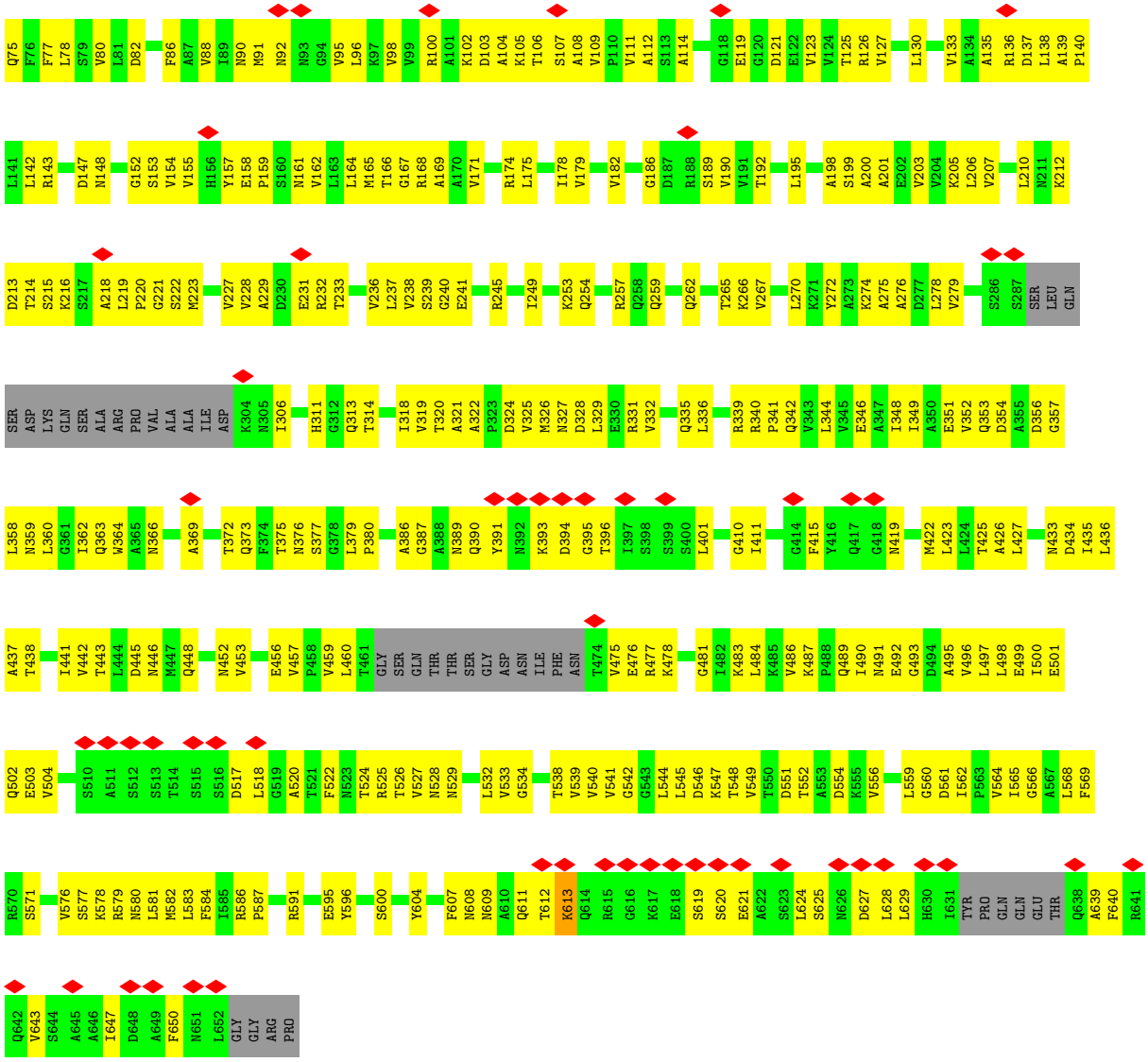
Chain G:



- Molecule 1: Type II secretion system protein D

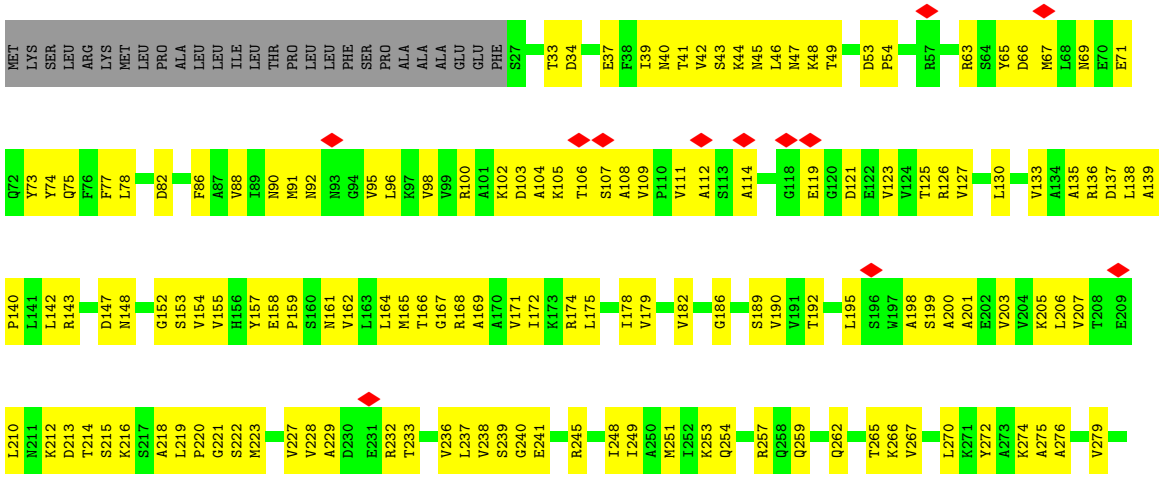
Chain H:

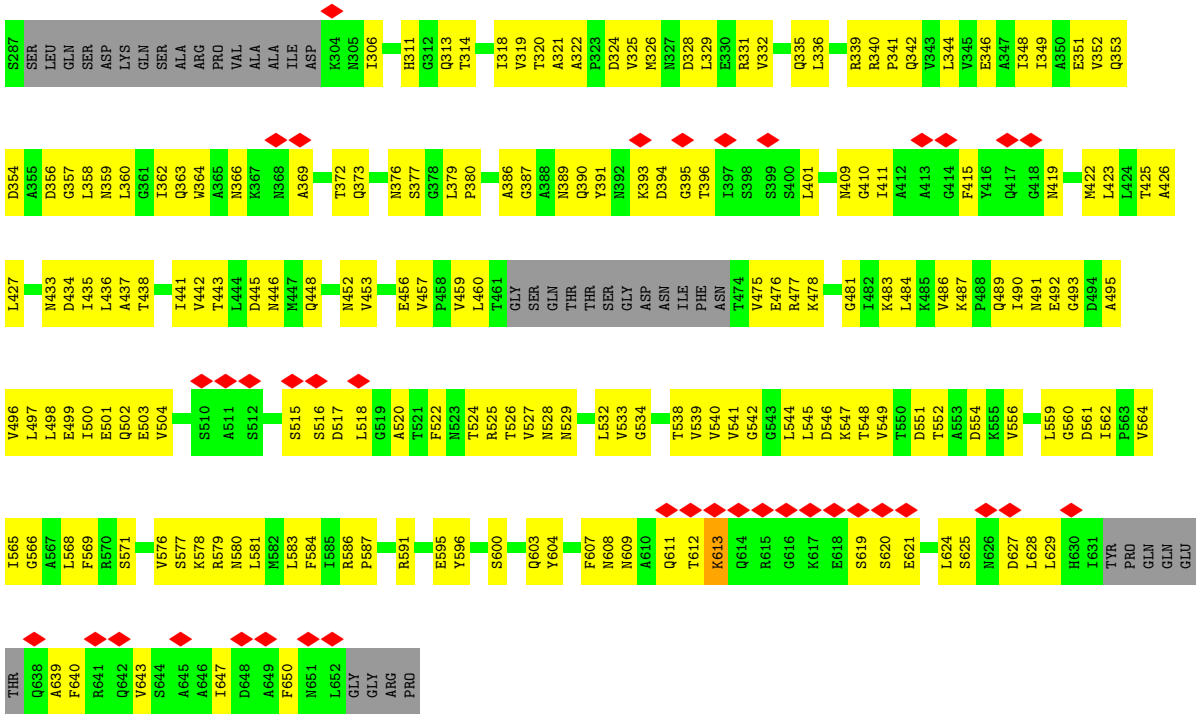




- Molecule 1: Type II secretion system protein D

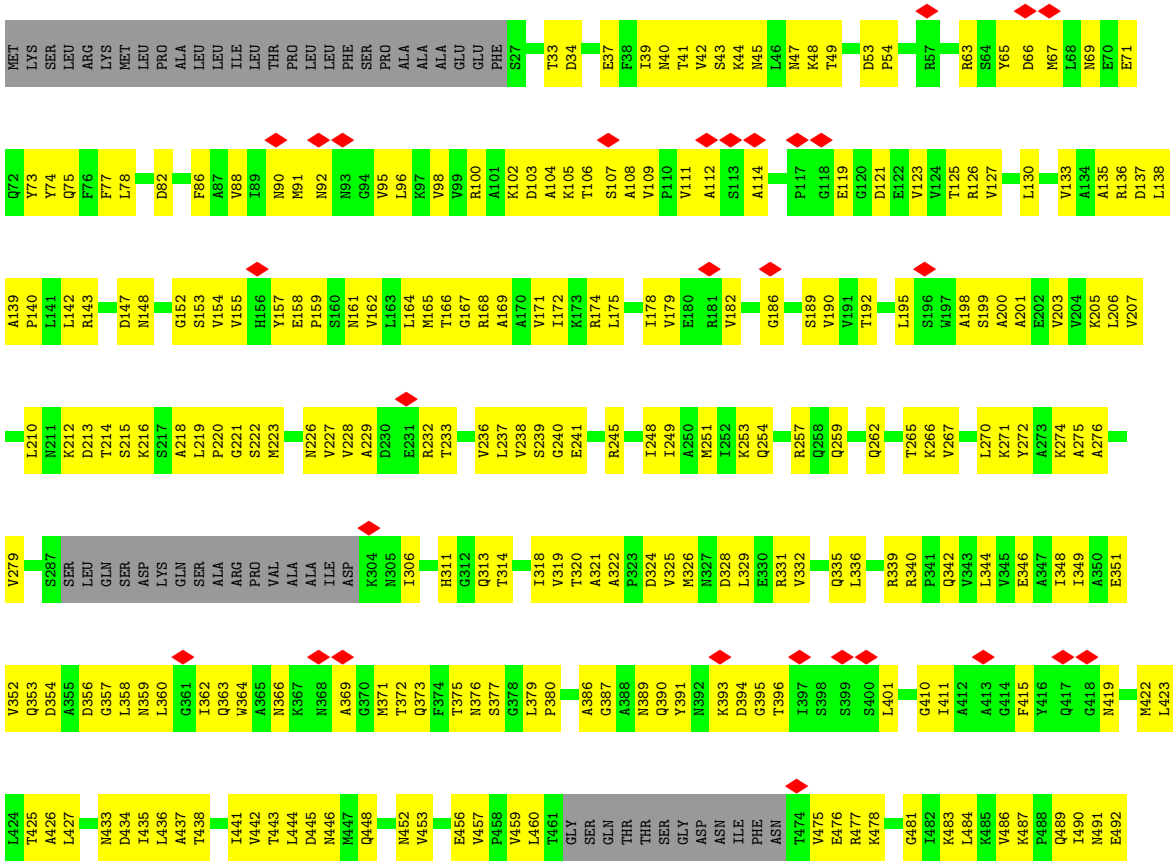
Chain I:

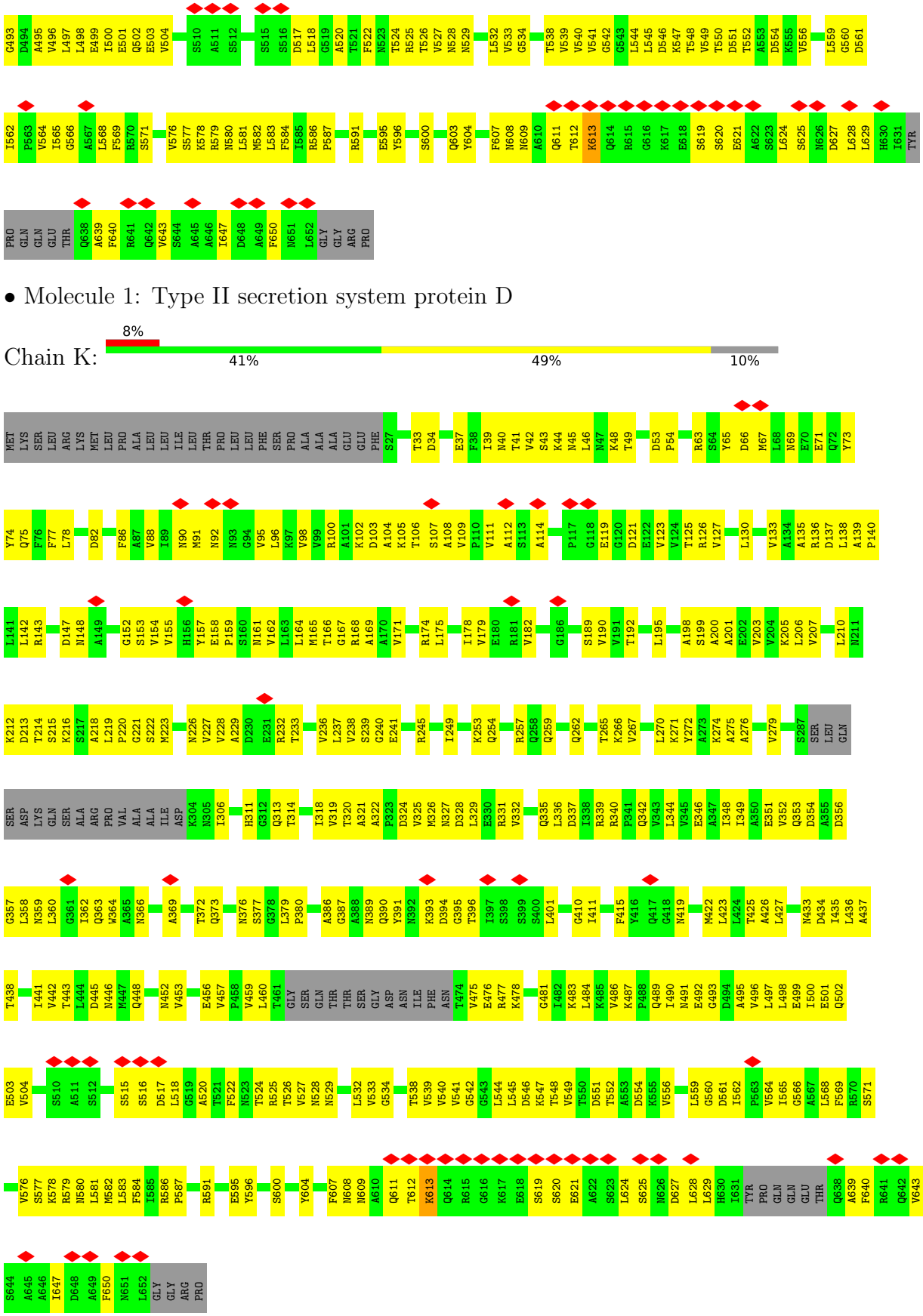




- Molecule 1: Type II secretion system protein D

Chain J:



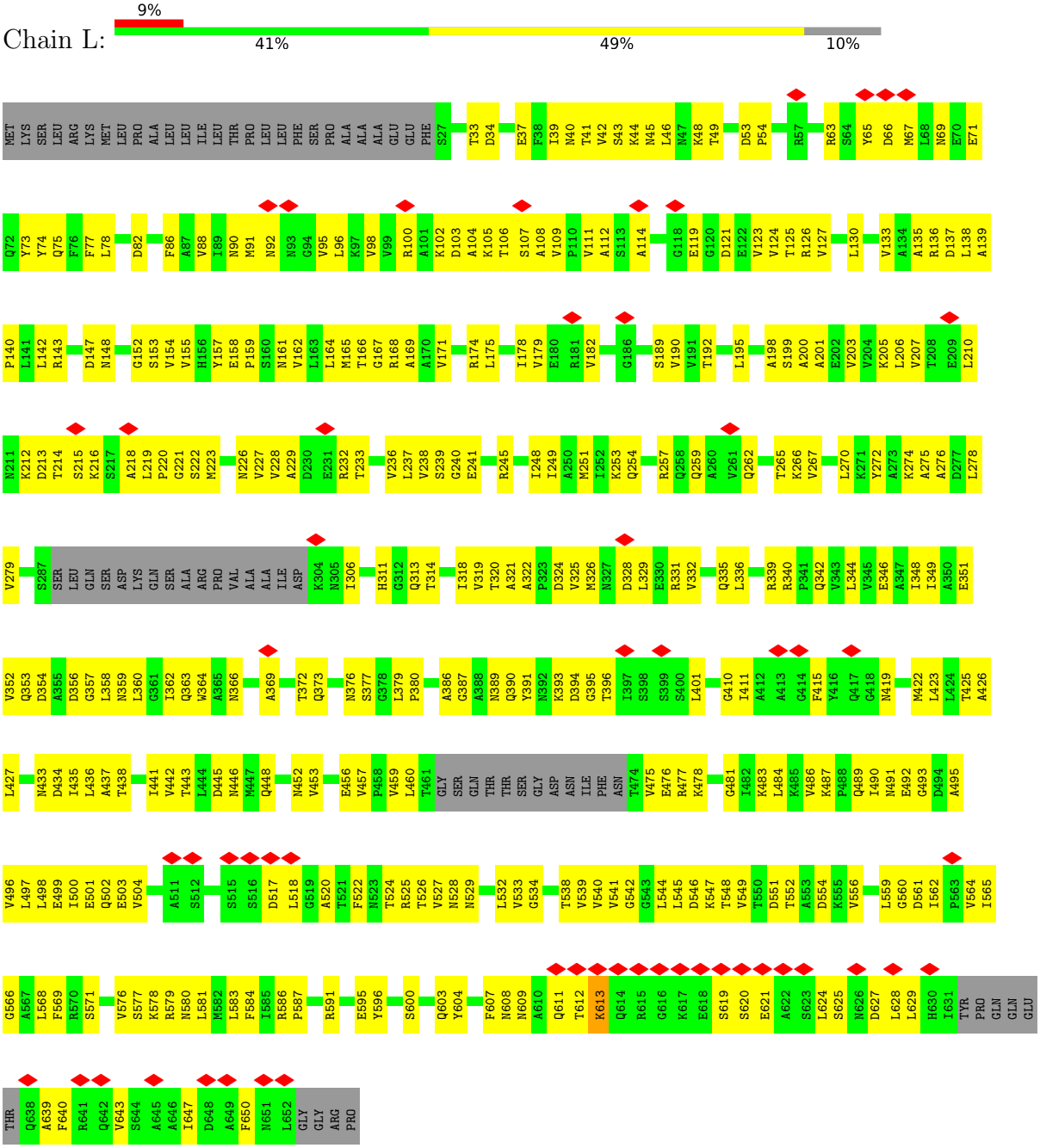


• Molecule 1: Type II secretion system protein D

Chain K: 8% 41% 49% 10%

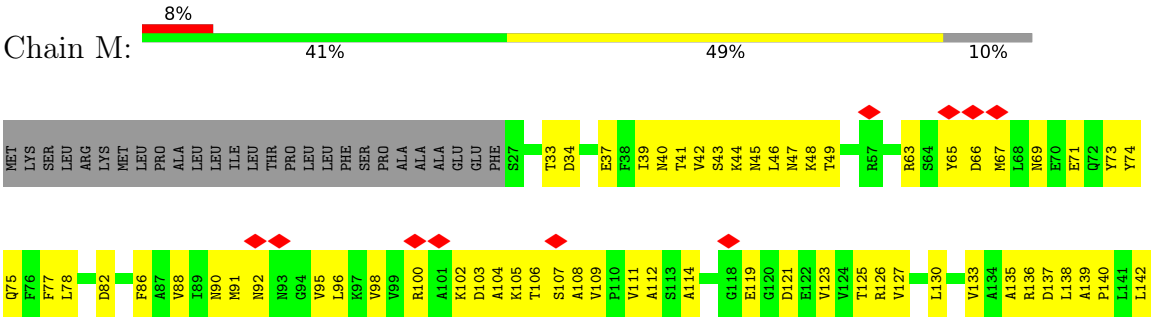
- Molecule 1: Type II secretion system protein D

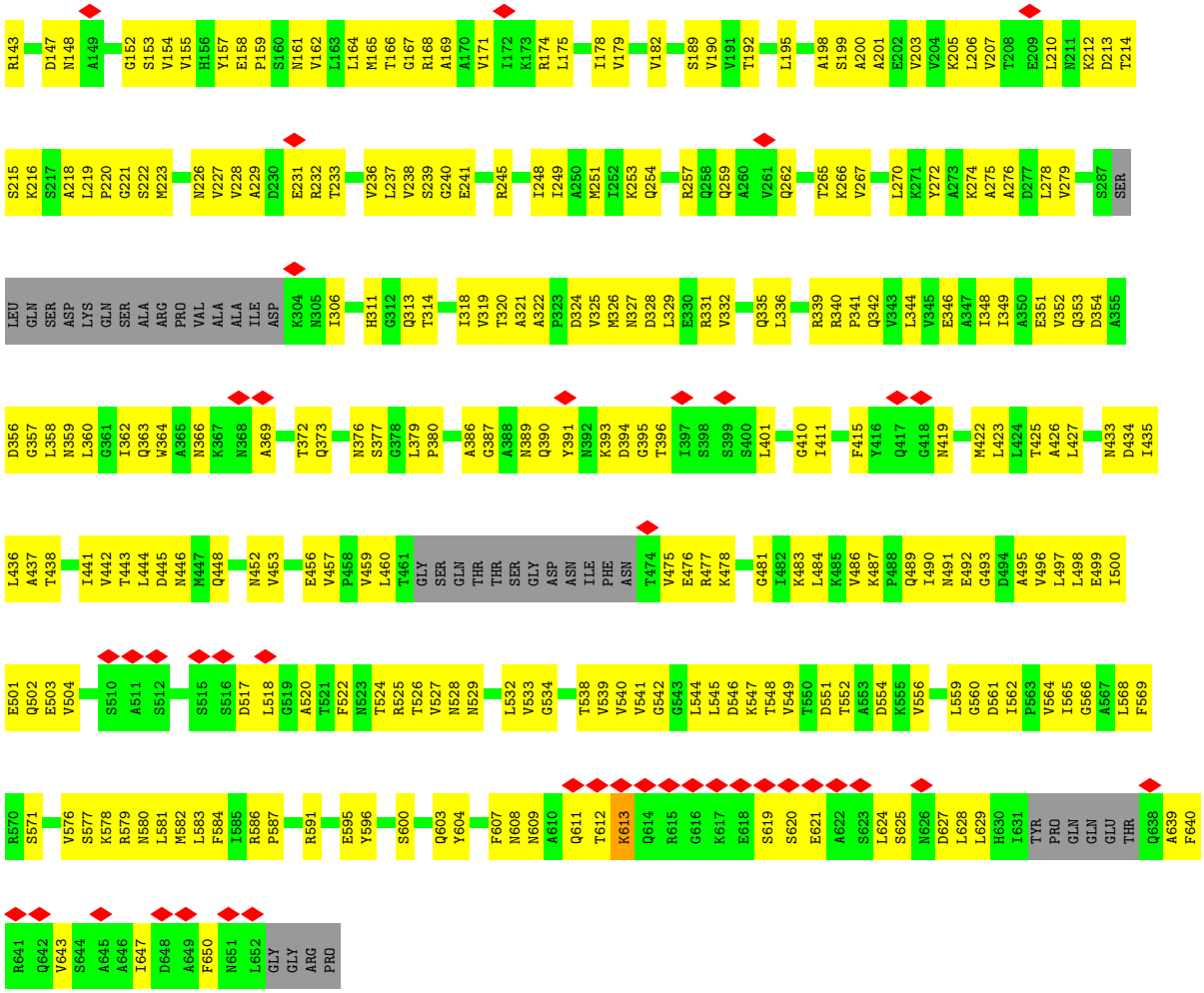
Chain L:



- Molecule 1: Type II secretion system protein D

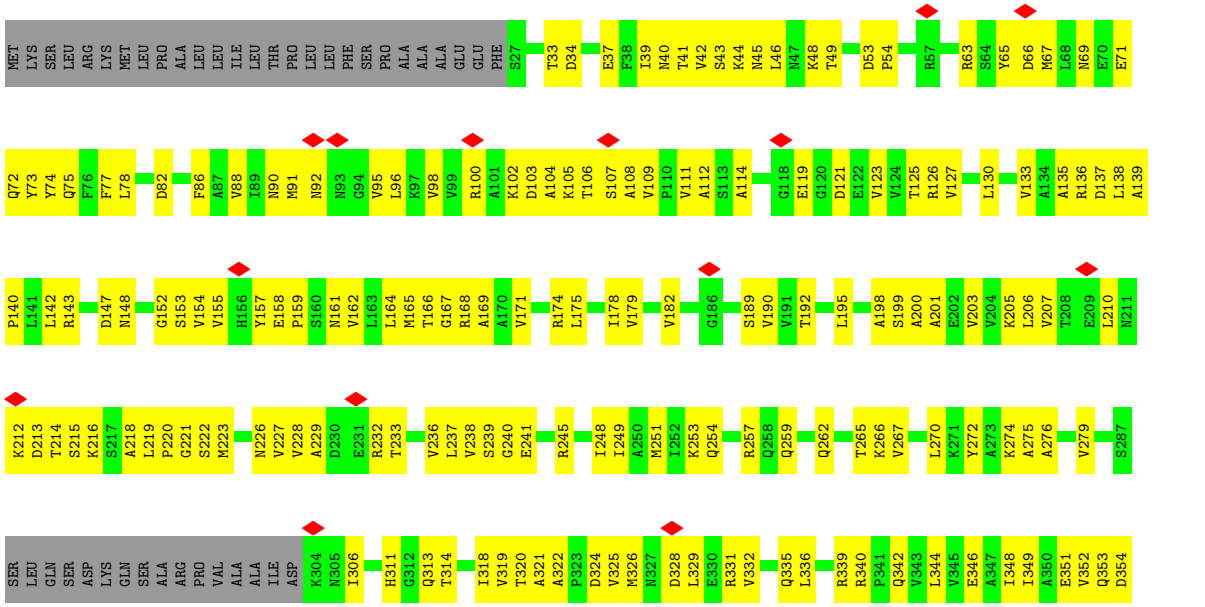
Chain M:

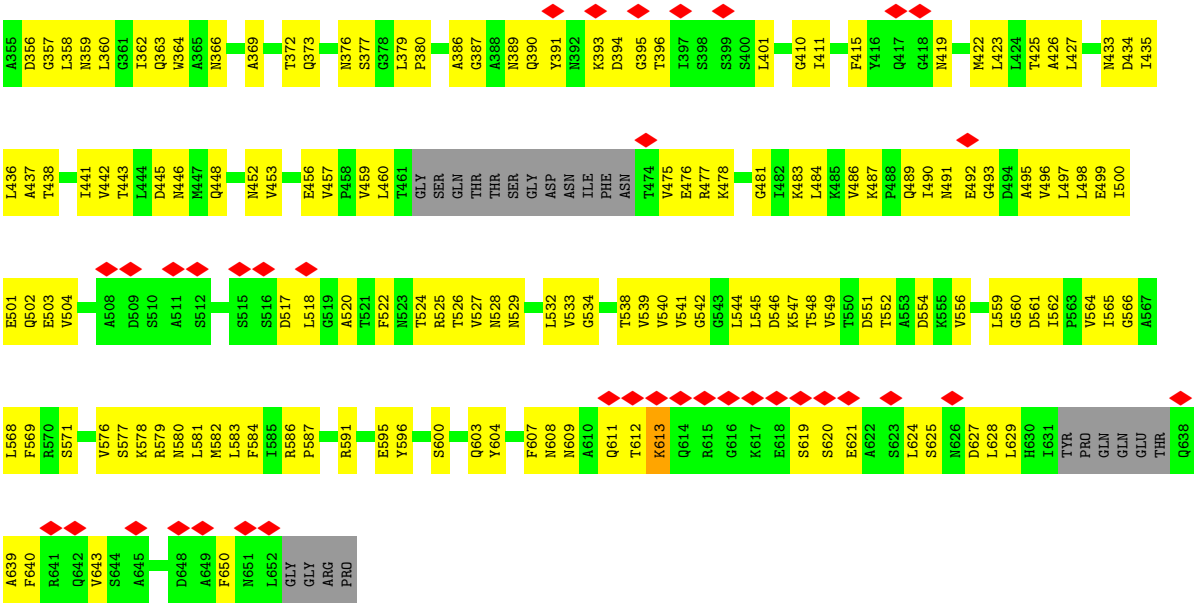




- Molecule 1: Type II secretion system protein D

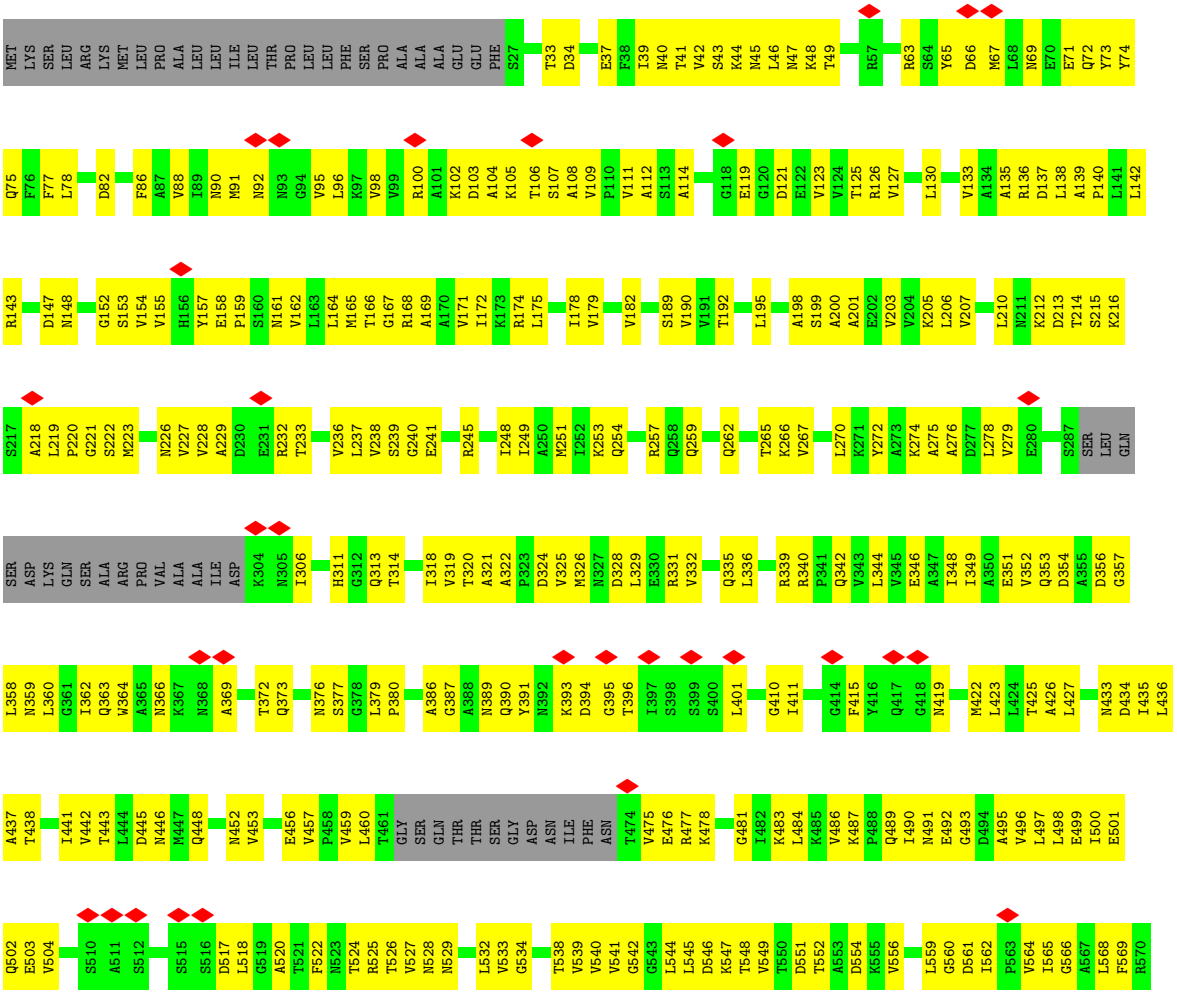
Chain N:

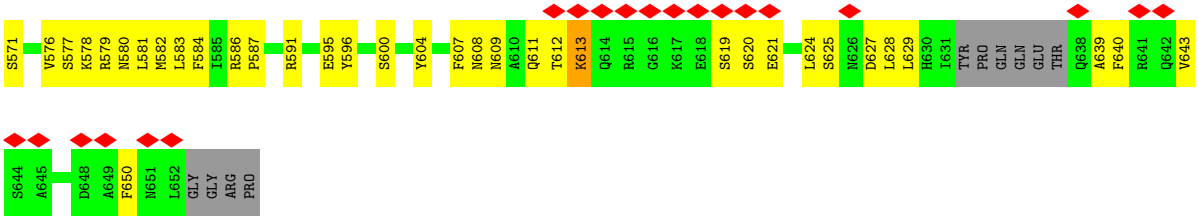




- Molecule 1: Type II secretion system protein D

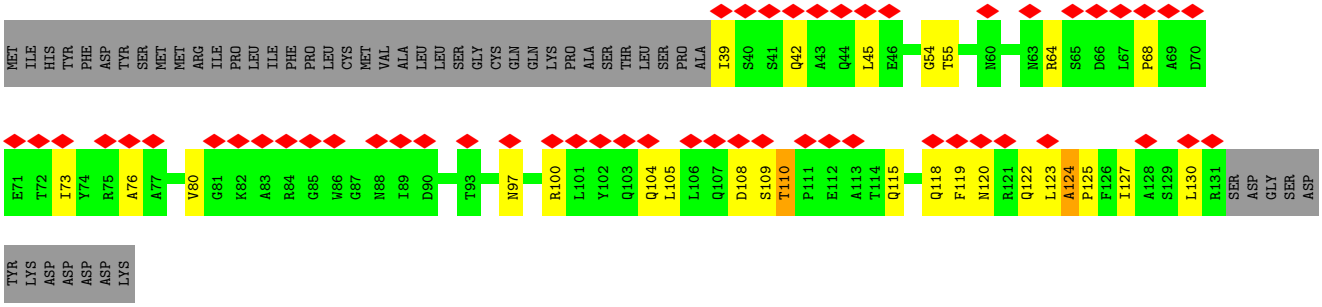
Chain O:





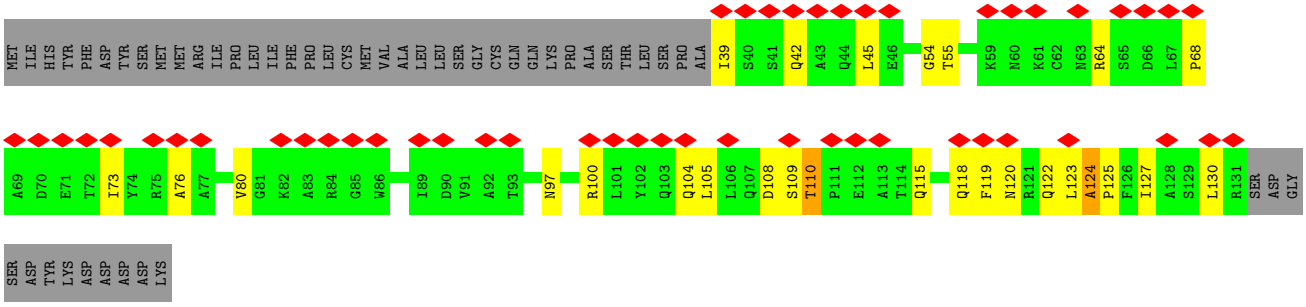
- Molecule 2: Pullulanase

Chain P:



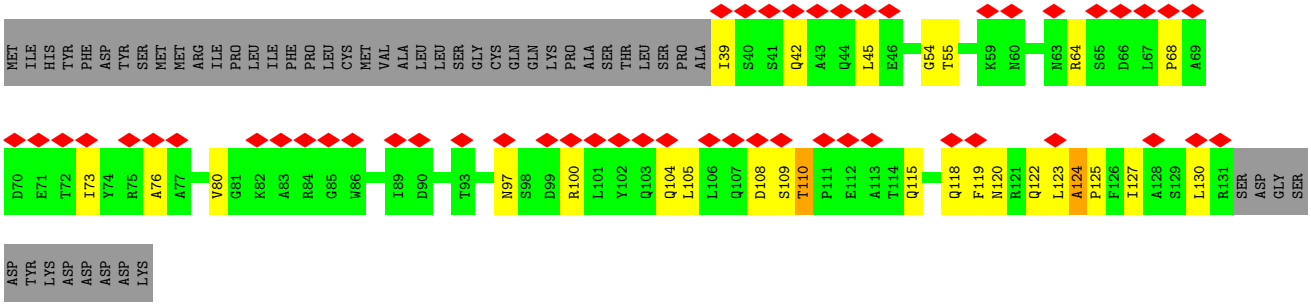
- Molecule 2: Pullulanase

Chain Q:



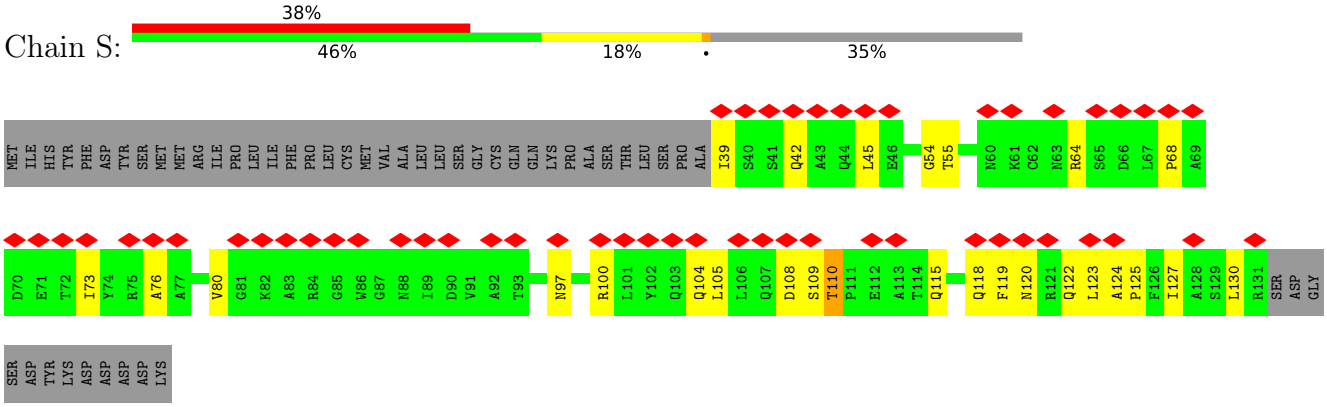
- Molecule 2: Pullulanase

Chain R:



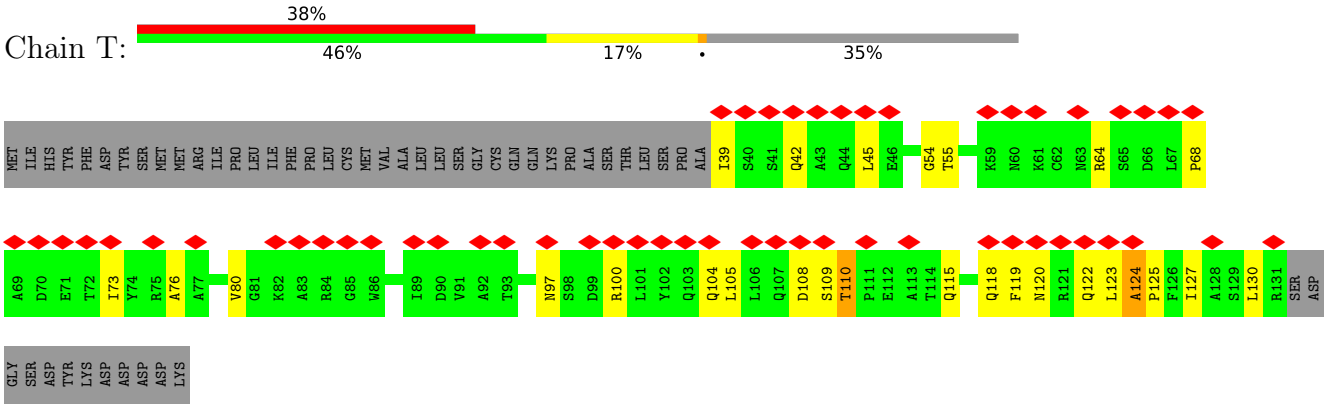
- Molecule 2: Pullulanase

Chain S:



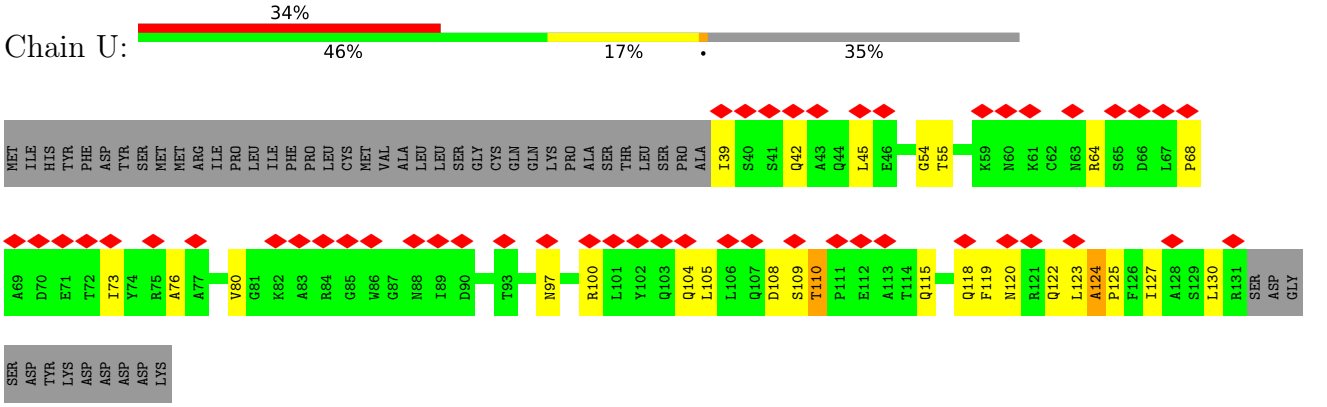
- Molecule 2: Pullulanase

Chain T:



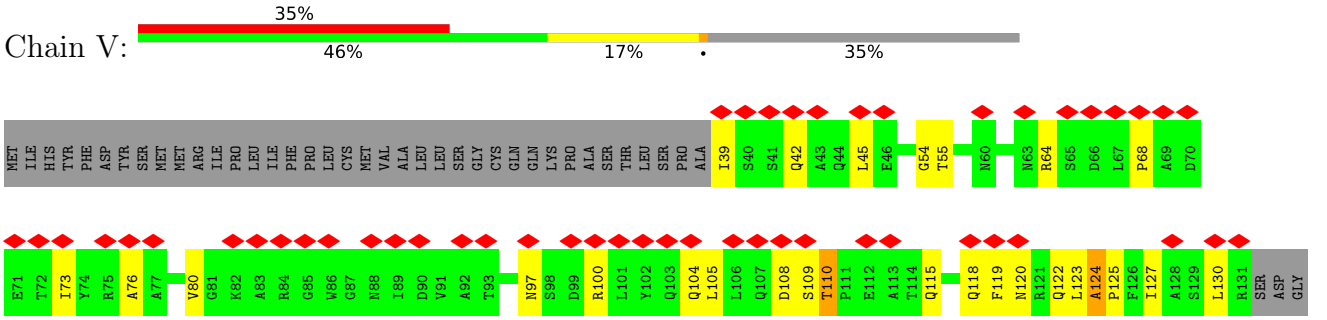
- Molecule 2: Pullulanase

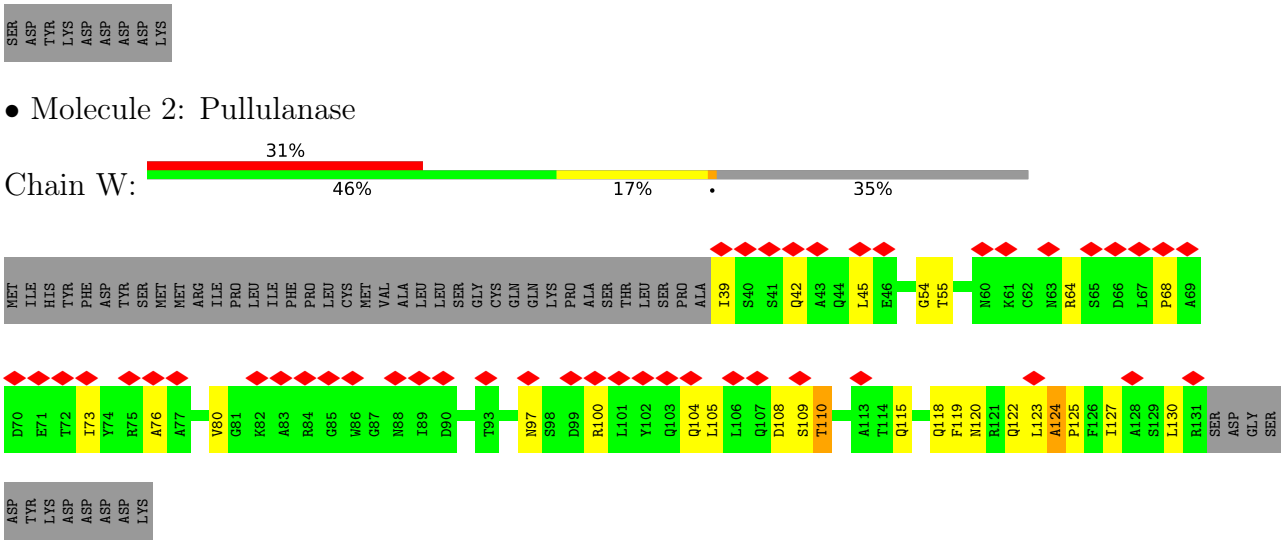
Chain U:

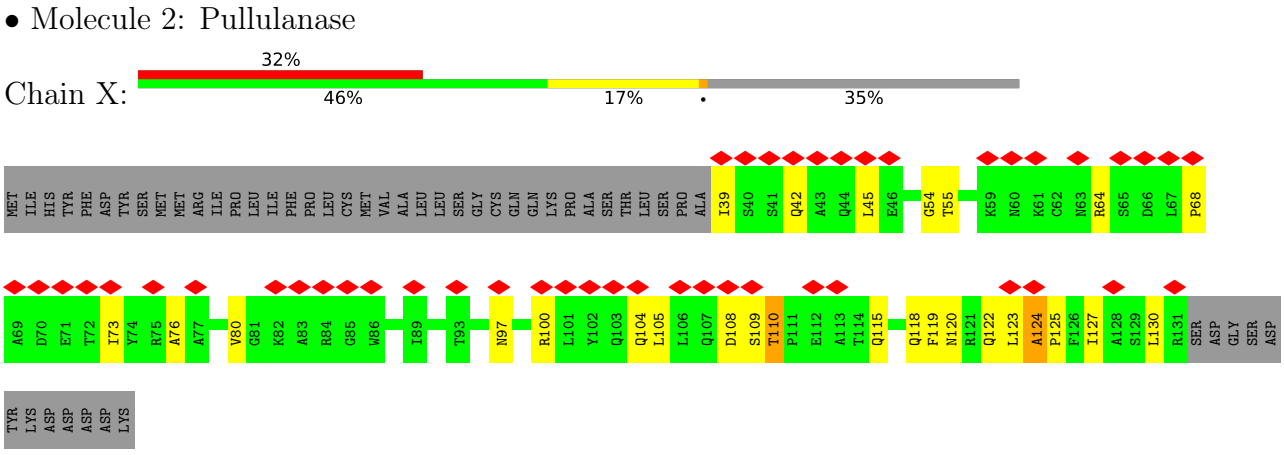


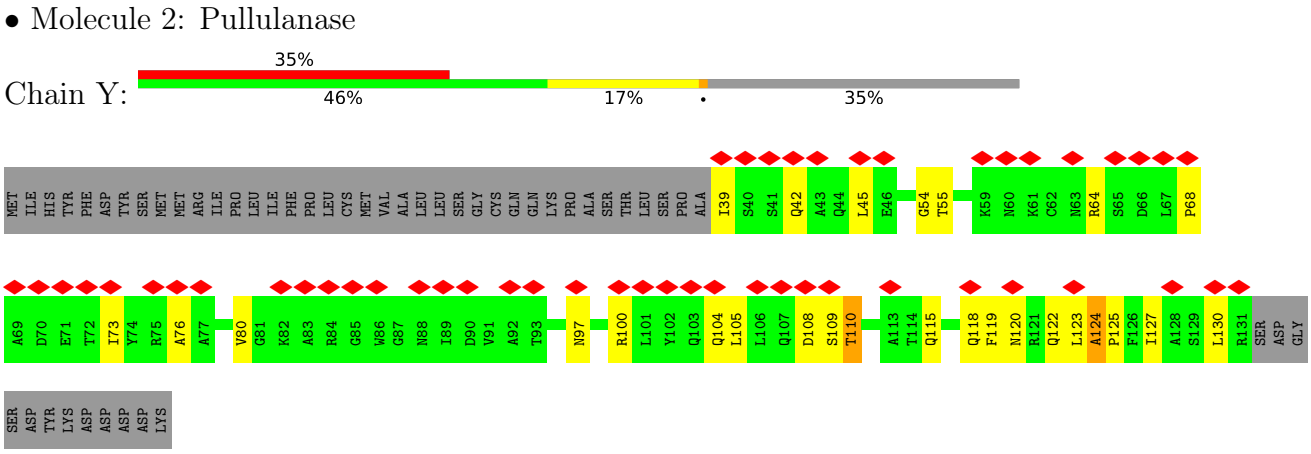
- Molecule 2: Pullulanase

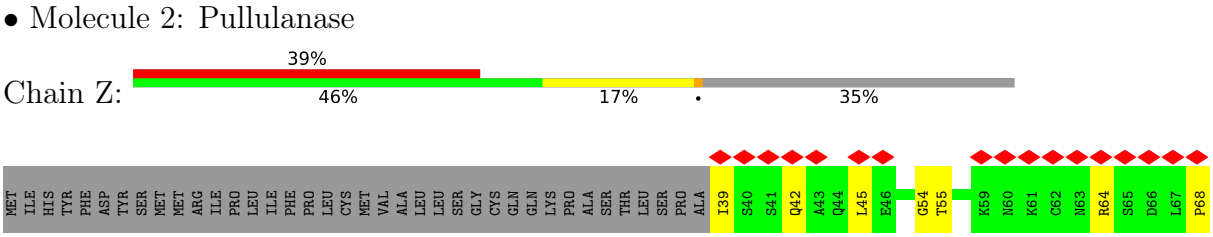
Chain V:

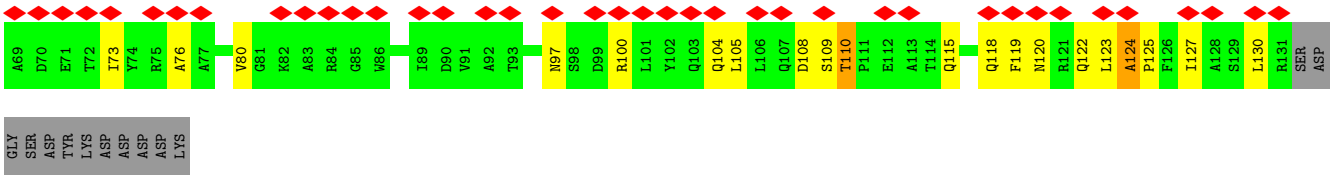



SER ASP TYR LYS ASP ASP ASP ASP LYS
• Molecule 2: Pullulanase
Chain W:
31%
46%
17%
35%
MET ILE HIS TYR PHE ASP TYR SER MET MET ARG ILE PRO LEU ILE PHE PRO LEU CYS MET VAL ALA LEU LEU SER GLY CYS GLN GLN LYS PRO ALA SER THR LEU SER PRO ALA I39 S40 S41 Q42 A43 Q44 L45 E46 G54 T55 N60 K61 C62 N63 R64 S65 D66 L67 P68 A69
D70 E71 T72 I73 Y74 R75 A76 A77 V80 G81 K82 A83 R84 G85 W86 G87 N88 I89 D90 T93 N97 S98 D99 R100 L101 Y102 Q103 Q104 L105 L106 Q107 D108 S109 T110 A113 T114 Q115 Q118 F119 N120 R121 Q122 L123 A124 P125 F126 I127 A128 S129 L130 R131 SER ASP GLY SER
ASP TYR LYS ASP ASP ASP ASP LYS


• Molecule 2: Pullulanase
Chain X:
32%
46%
17%
35%
MET ILE HIS TYR PHE ASP TYR SER MET MET ARG ILE PRO LEU ILE PHE PRO LEU CYS MET VAL ALA LEU LEU SER GLY CYS GLN GLN LYS PRO ALA SER THR LEU SER PRO ALA I39 S40 S41 Q42 A43 Q44 L45 E46 G54 T55 K59 N60 K61 C62 N63 R64 S65 D66 L67 P68
A69 D70 E71 T72 I73 Y74 R75 A76 A77 V80 G81 K82 A83 R84 G85 W86 I89 T93 N97 R100 L101 Y102 Q103 Q104 L105 L106 Q107 D108 S109 T110 P111 E112 A113 T114 Q115 Q118 F119 N120 R121 Q122 L123 A124 P125 F126 I127 A128 S129 L130 R131 SER ASP GLY SER ASP
TYR LYS ASP ASP ASP ASP LYS

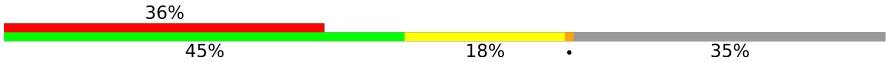

• Molecule 2: Pullulanase
Chain Y:
35%
46%
17%
35%
MET ILE HIS TYR PHE ASP TYR SER MET MET ARG ILE PRO LEU ILE PHE PRO LEU CYS MET VAL ALA LEU LEU SER GLY CYS GLN GLN LYS PRO ALA SER THR LEU SER PRO ALA I39 S40 S41 Q42 A43 Q44 L45 E46 G54 T55 K59 N60 K61 C62 N63 R64 S65 D66 L67 P68
A69 D70 E71 T72 I73 Y74 R75 A76 A77 V80 G81 K82 A83 R84 G85 W86 G87 N88 I89 D90 V91 A92 T93 N97 R100 L101 Y102 Q103 Q104 L105 L106 Q107 D108 S109 T110 A113 T114 Q115 Q118 F119 N120 R121 Q122 L123 A124 P125 F126 I127 A128 S129 L130 R131 SER ASP GLY
SER ASP TYR LYS ASP ASP ASP ASP LYS

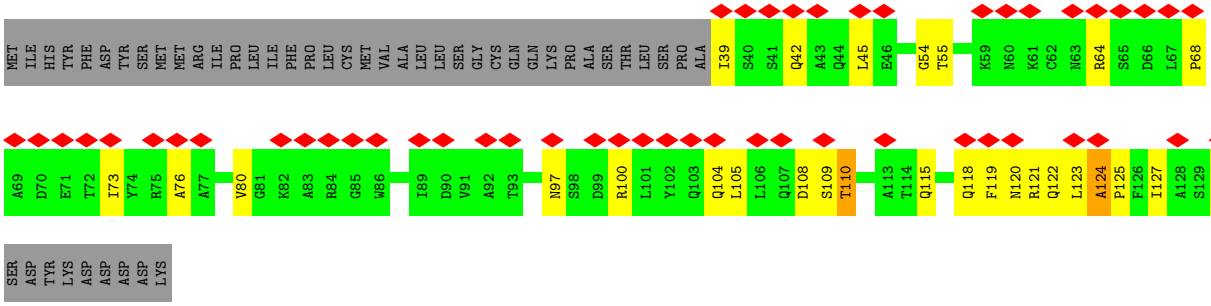

• Molecule 2: Pullulanase
Chain Z:
39%
46%
17%
35%
MET ILE HIS TYR PHE ASP TYR SER MET MET ARG ILE PRO LEU ILE PHE PRO LEU CYS MET VAL ALA LEU LEU SER GLY CYS GLN GLN LYS PRO ALA SER THR LEU SER PRO ALA I39 S40 S41 Q42 A43 Q44 L45 E46 G54 T55 K59 N60 K61 C62 N63 R64 S65 D66 L67 P68



- Molecule 2: Pullulanase

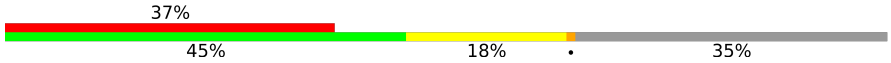
Chain a:

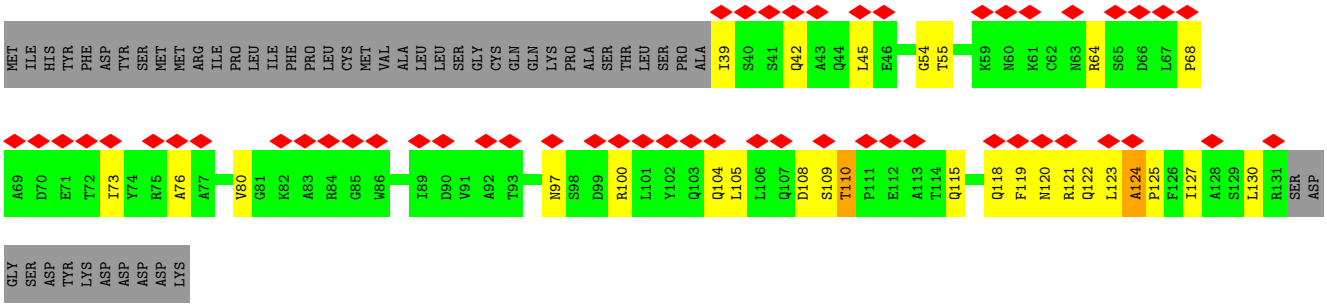




- Molecule 2: Pullulanase

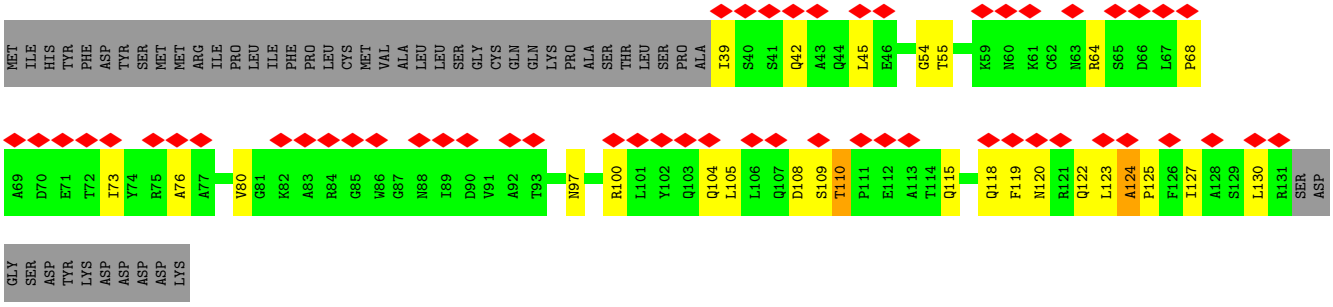
Chain b:





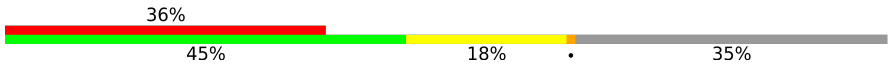
- Molecule 2: Pullulanase

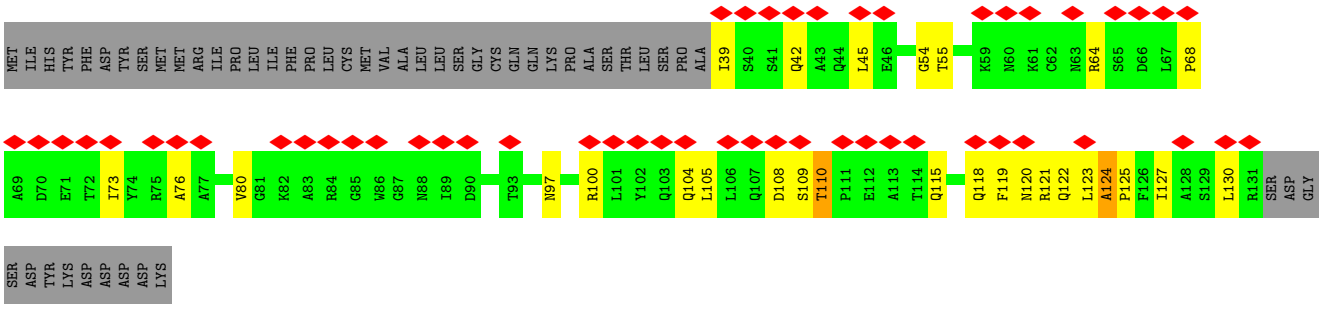
Chain c:



- Molecule 2: Pullulanase

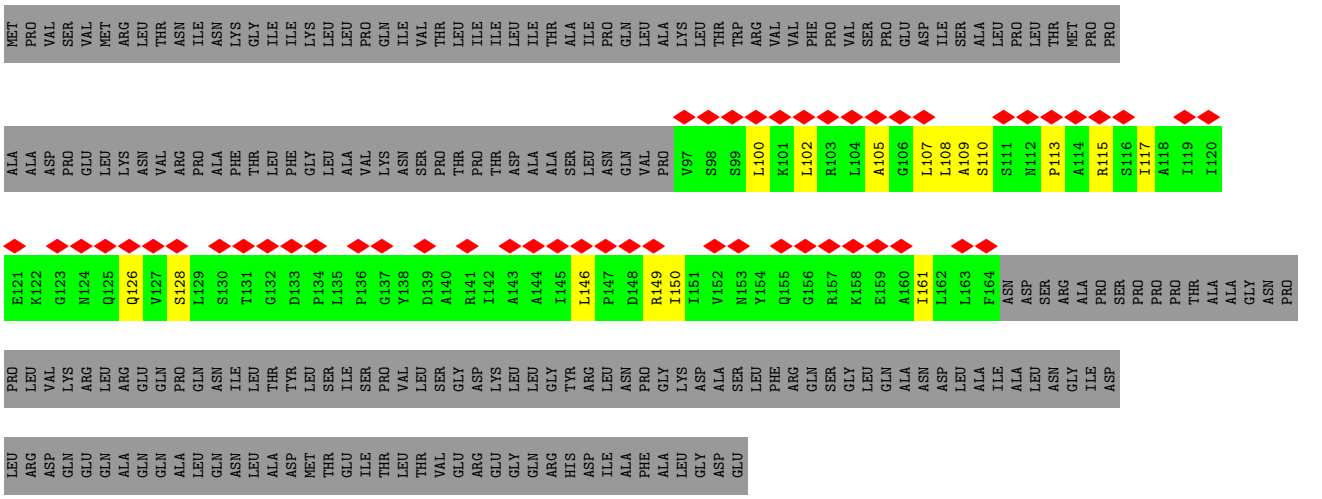
Chain d:





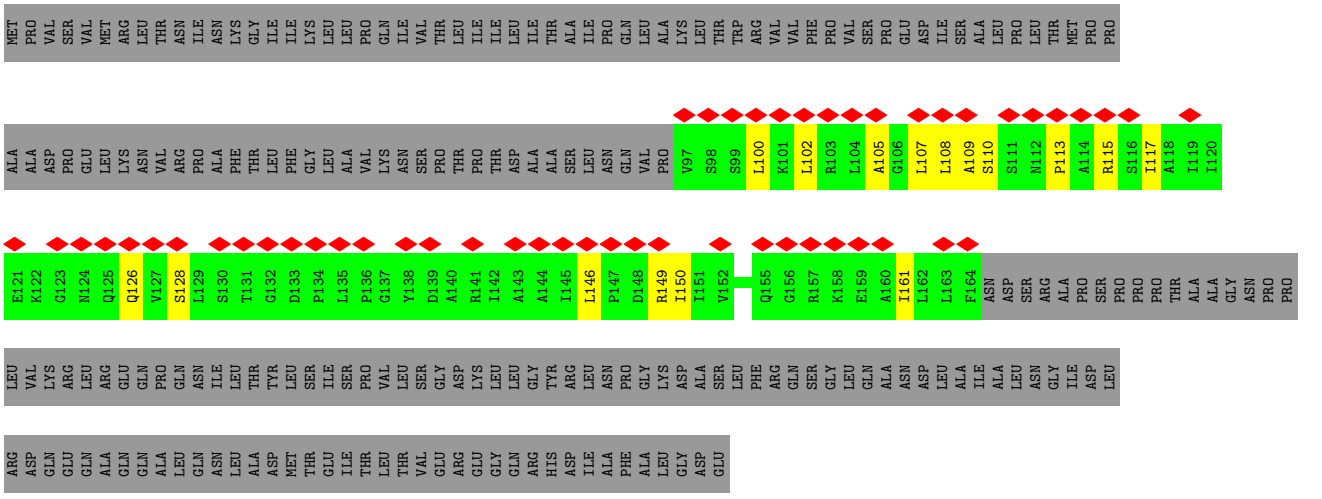
• Molecule 3: Pectic enzymes secretion protein OutC

Chain e:



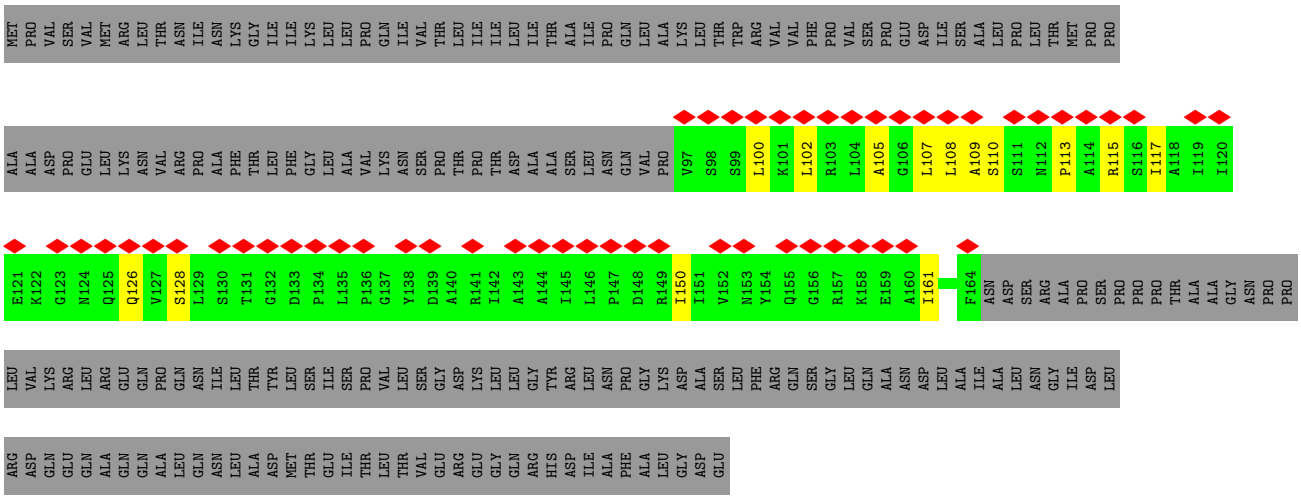
• Molecule 3: Pectic enzymes secretion protein OutC

Chain f:



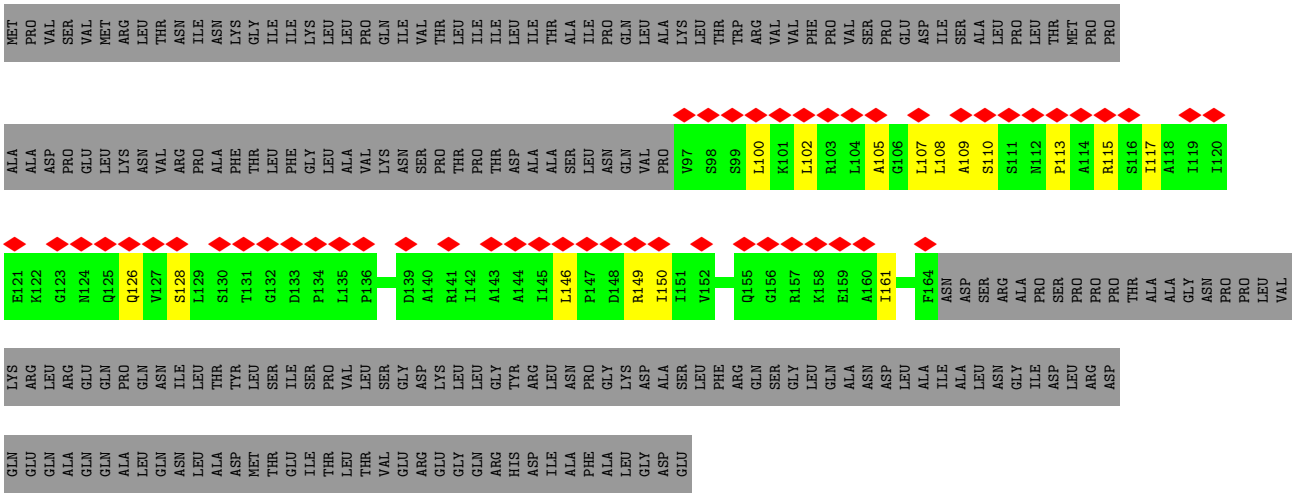
• Molecule 3: Pectic enzymes secretion protein OutC

Chain g:



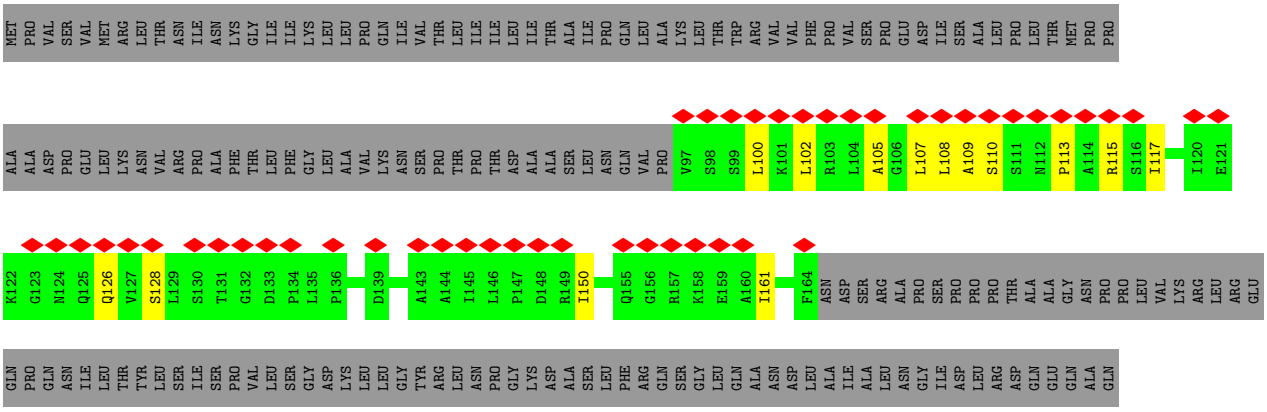
- Molecule 3: Pectic enzymes secretion protein OutC

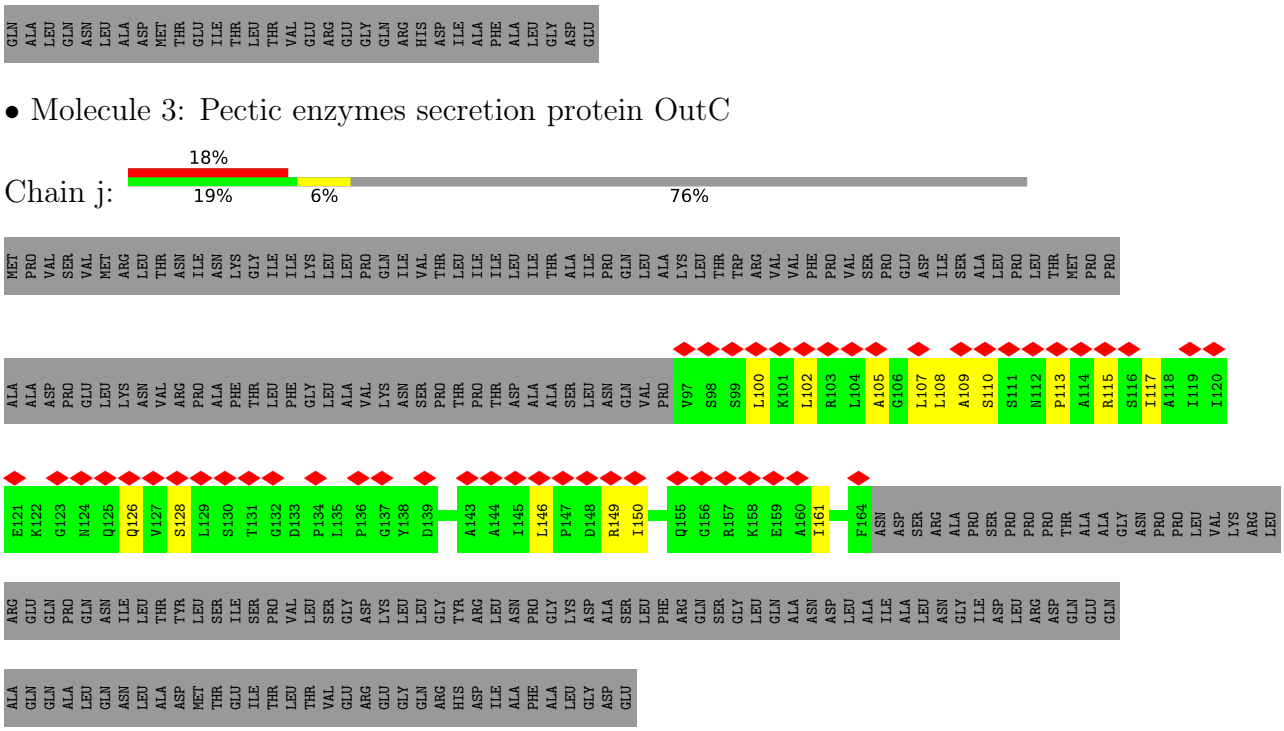
Chain h:



- Molecule 3: Pectic enzymes secretion protein OutC

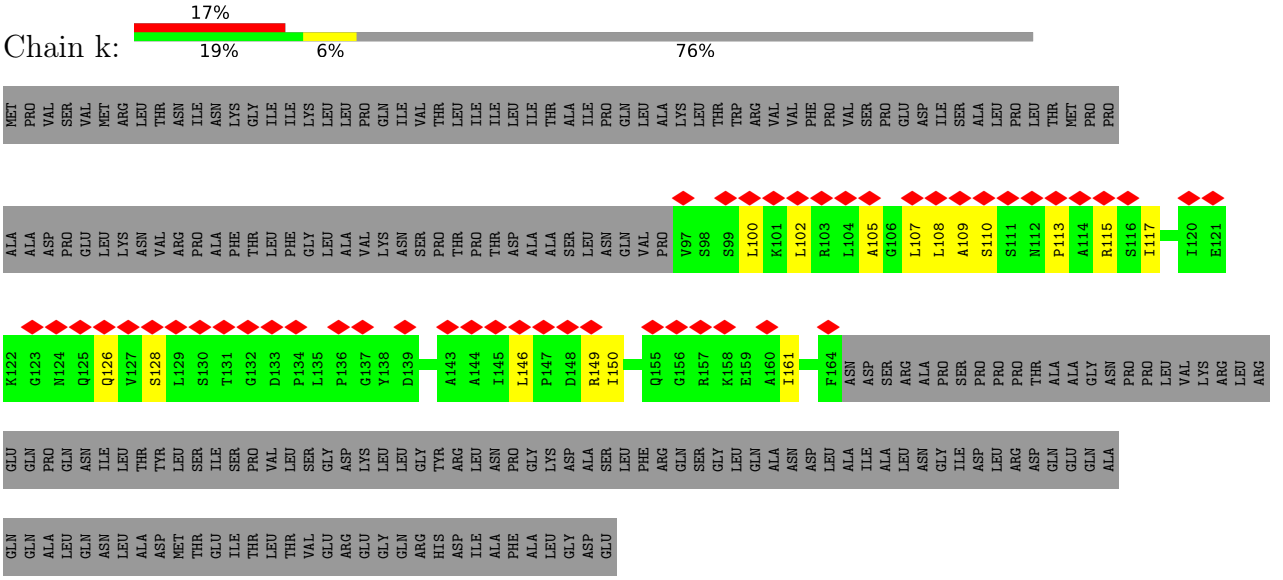
Chain i:



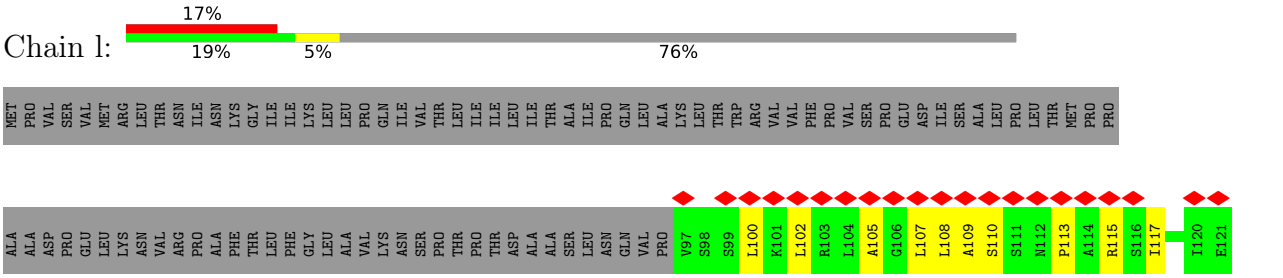


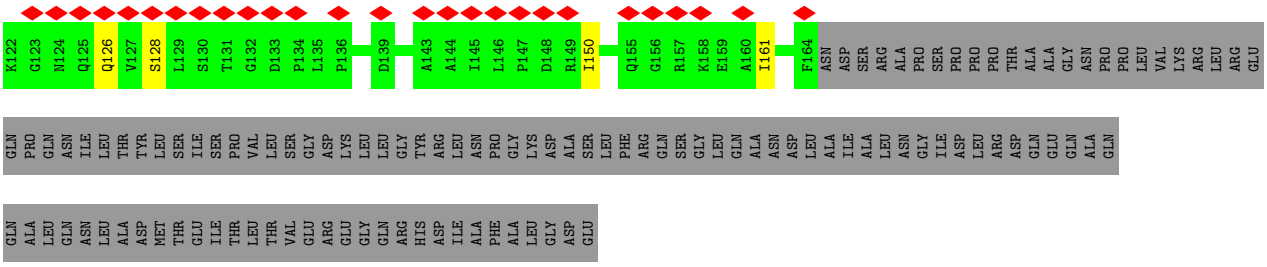
• Molecule 3: Pectic enzymes secretion protein OutC

• Molecule 3: Pectic enzymes secretion protein OutC



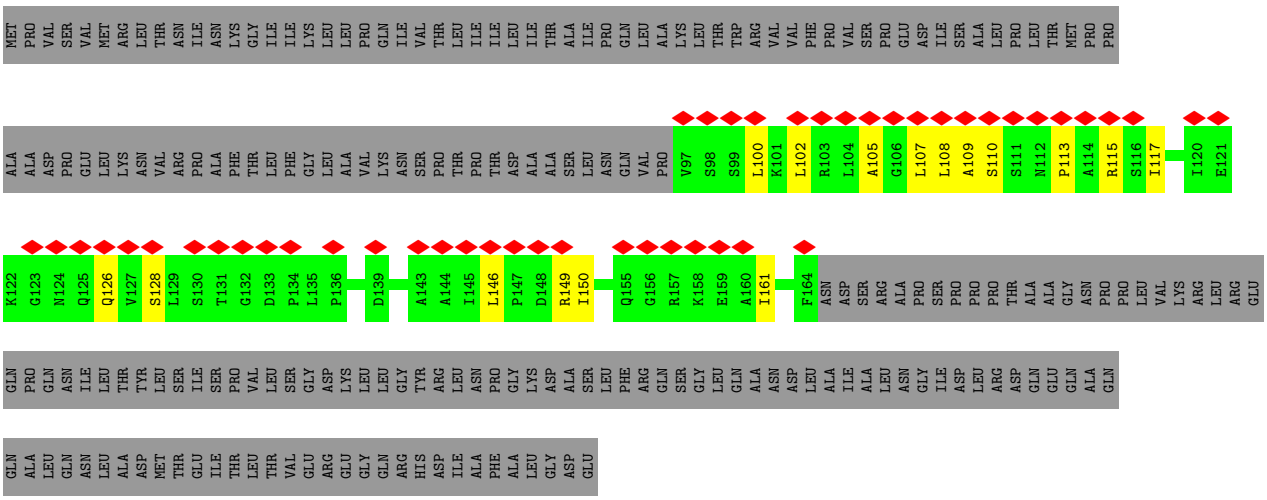
• Molecule 3: Pectic enzymes secretion protein OutC





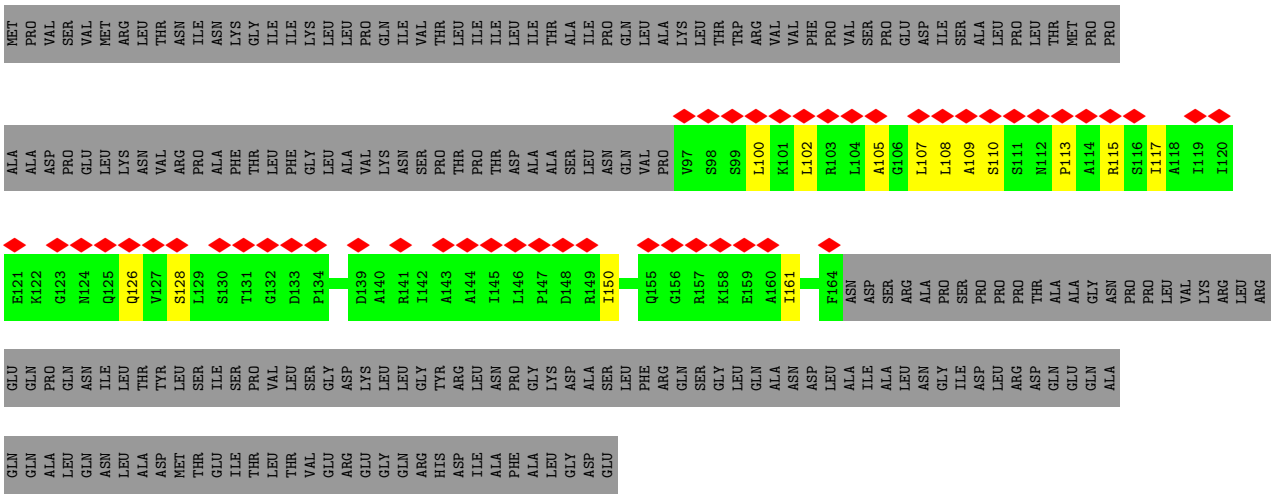
• Molecule 3: Pectic enzymes secretion protein OutC

Chain m:



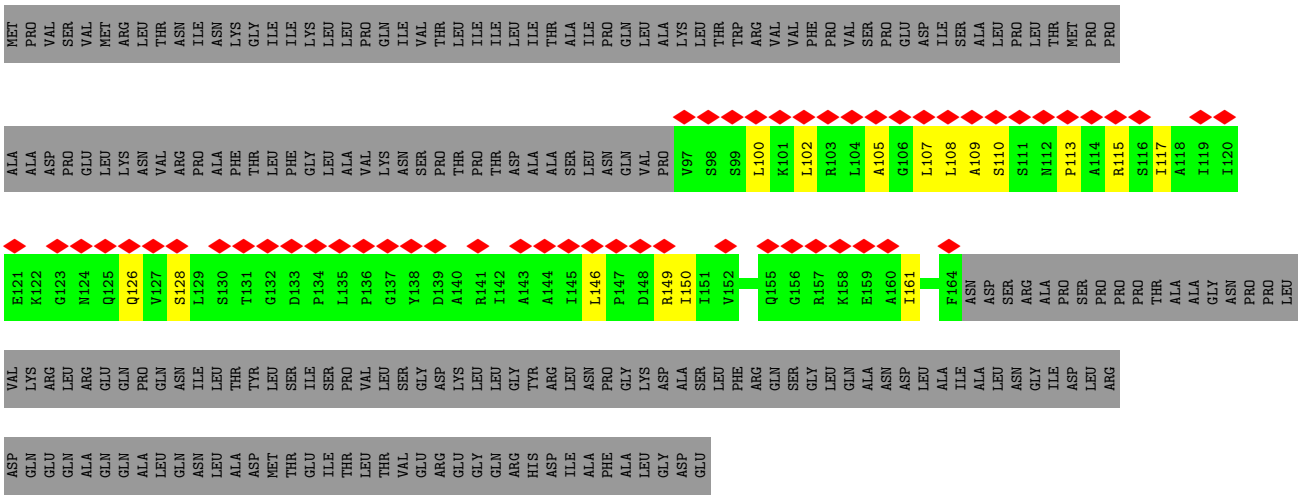
• Molecule 3: Pectic enzymes secretion protein OutC

Chain n:



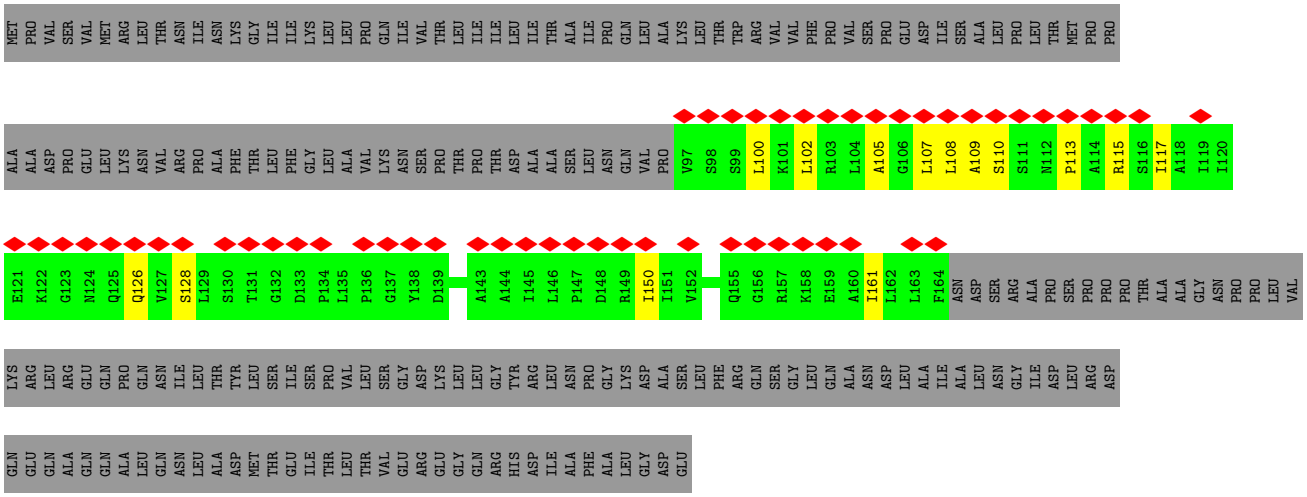
• Molecule 3: Pectic enzymes secretion protein OutC

Chain o:



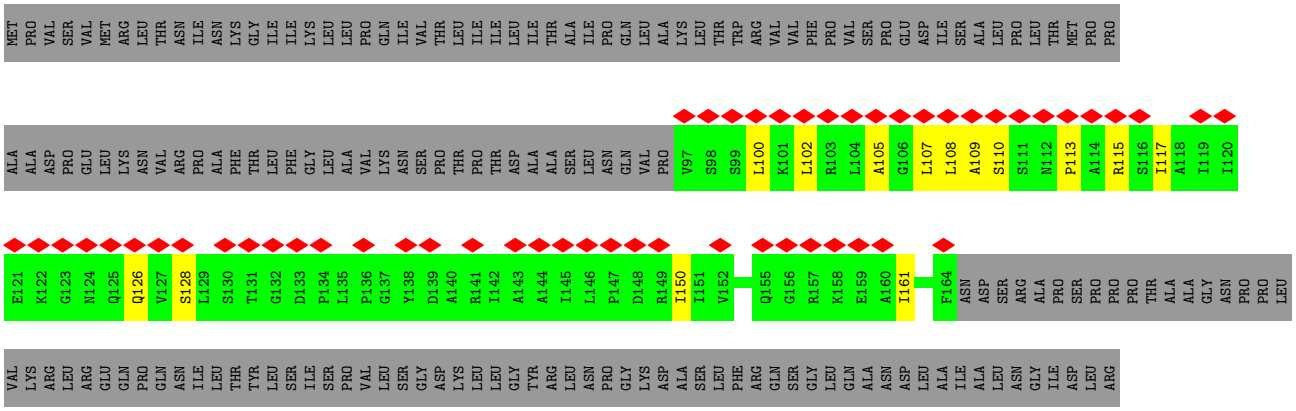
• Molecule 3: Pectic enzymes secretion protein OutC

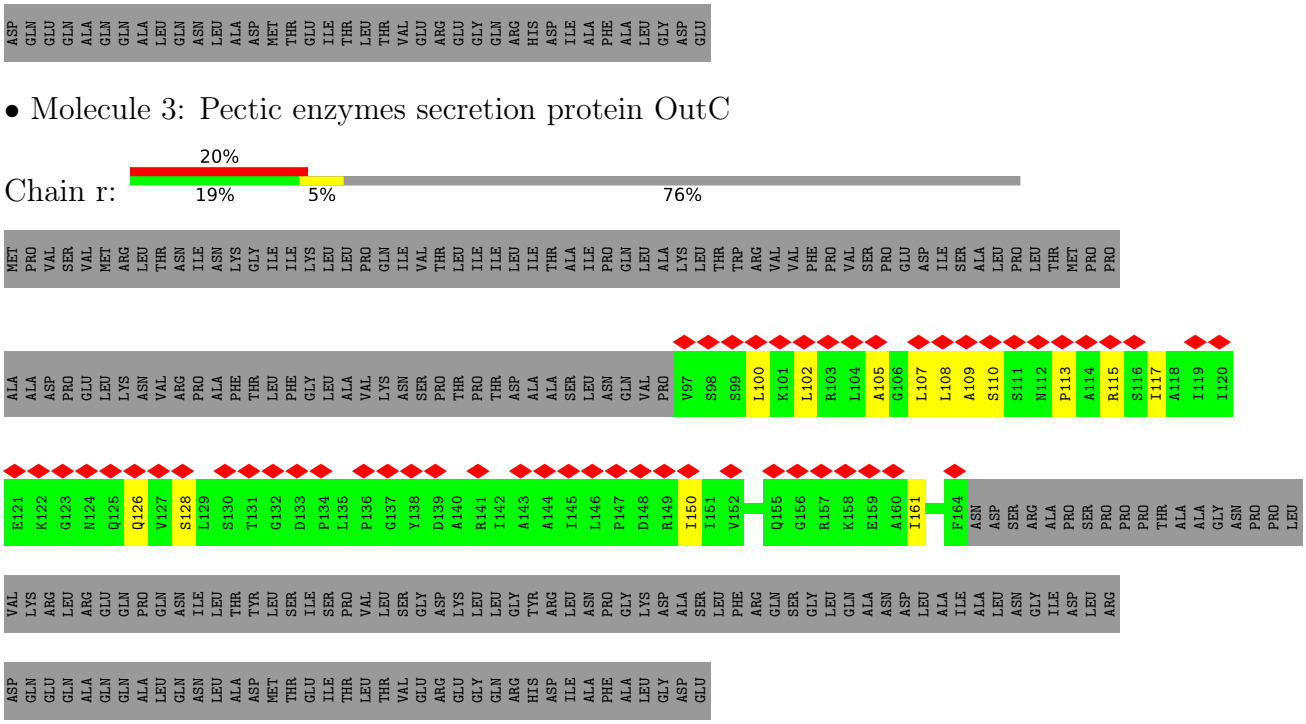
Chain p:

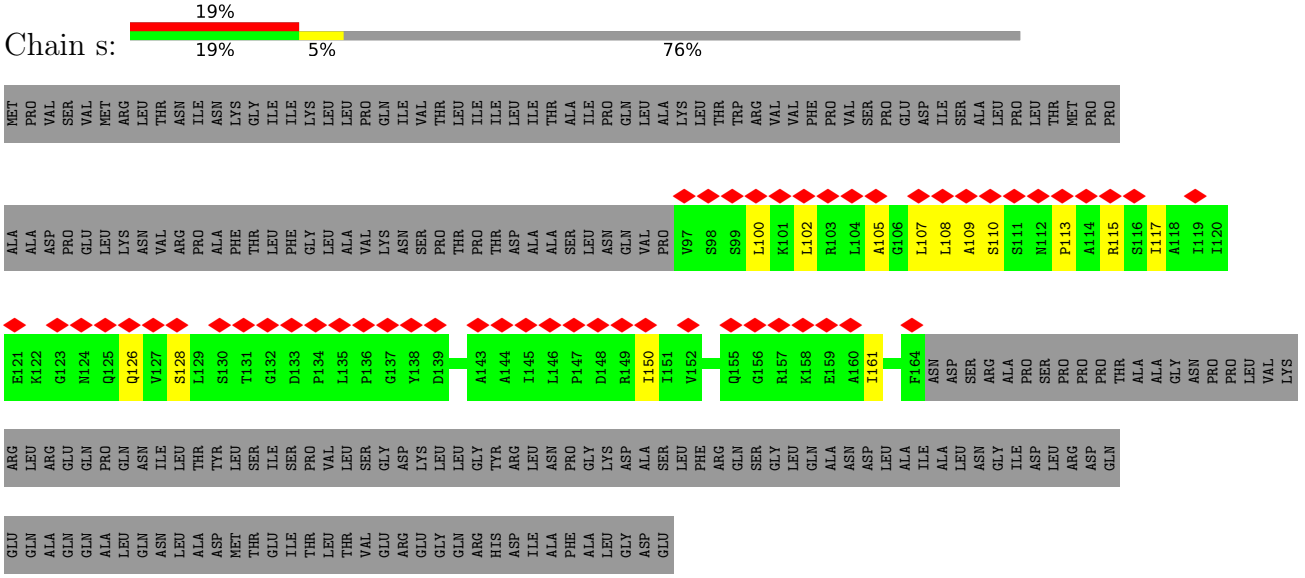


• Molecule 3: Pectic enzymes secretion protein OutC

Chain q:




ASP GLN GLU GLN ALA GLN GLN ALA LEU GLN LEU ALA ASP MET THR GLU ILE THR LEU THR VAL GLU ARG GLU GLY GLN ARG HIS ASP ILE ALA PHE ALA LEU GLY ASP GLU
• Molecule 3: Pectic enzymes secretion protein OutC
Chain r:
20%
19%
5%
76


• Molecule 3: Pectic enzymes secretion protein OutC
Chain s:
19%
19%
5%
76

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C15	Depositor
Number of particles used	7284	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	23.619	Depositor
Minimum map value	-13.503	Depositor
Average map value	0.124	Depositor
Map value standard deviation	0.884	Depositor
Recommended contour level	4.3	Depositor
Map size (Å)	409.4, 409.4, 409.4	wwPDB
Map dimensions	230, 230, 230	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.78, 1.78, 1.78	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	0.54	0/4496	0.75	4/6106 (0.1%)
1	B	0.54	0/4496	0.75	4/6106 (0.1%)
1	C	0.54	0/4496	0.75	4/6106 (0.1%)
1	D	0.54	0/4496	0.75	4/6106 (0.1%)
1	E	0.54	0/4496	0.75	4/6106 (0.1%)
1	F	0.54	0/4496	0.75	4/6106 (0.1%)
1	G	0.54	0/4496	0.75	4/6106 (0.1%)
1	H	0.54	0/4496	0.75	4/6106 (0.1%)
1	I	0.54	0/4496	0.75	4/6106 (0.1%)
1	J	0.54	0/4496	0.75	4/6106 (0.1%)
1	K	0.54	0/4496	0.75	4/6106 (0.1%)
1	L	0.54	0/4496	0.75	4/6106 (0.1%)
1	M	0.54	0/4496	0.75	4/6106 (0.1%)
1	N	0.54	0/4496	0.75	4/6106 (0.1%)
1	O	0.54	0/4496	0.75	4/6106 (0.1%)
2	P	0.86	1/729 (0.1%)	1.42	4/987 (0.4%)
2	Q	0.86	1/729 (0.1%)	1.42	4/987 (0.4%)
2	R	0.86	1/729 (0.1%)	1.42	6/987 (0.6%)
2	S	0.87	1/729 (0.1%)	1.42	3/987 (0.3%)
2	T	0.87	1/729 (0.1%)	1.42	4/987 (0.4%)
2	U	0.87	1/729 (0.1%)	1.42	4/987 (0.4%)
2	V	0.87	1/729 (0.1%)	1.42	4/987 (0.4%)
2	W	0.86	1/729 (0.1%)	1.42	4/987 (0.4%)
2	X	0.87	1/729 (0.1%)	1.42	4/987 (0.4%)
2	Y	0.87	1/729 (0.1%)	1.42	4/987 (0.4%)
2	Z	0.87	1/729 (0.1%)	1.42	4/987 (0.4%)
2	a	0.87	1/729 (0.1%)	1.42	4/987 (0.4%)
2	b	0.86	1/729 (0.1%)	1.42	6/987 (0.6%)
2	c	0.87	1/729 (0.1%)	1.42	4/987 (0.4%)
2	d	0.87	1/729 (0.1%)	1.42	4/987 (0.4%)
3	e	0.14	0/518	0.37	0/701
3	f	0.13	0/518	0.37	0/701
3	g	0.14	0/518	0.37	0/701
3	h	0.14	0/518	0.37	0/701

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	i	0.13	0/518	0.37	0/701
3	j	0.14	0/518	0.37	0/701
3	k	0.14	0/518	0.37	0/701
3	l	0.14	0/518	0.37	0/701
3	m	0.14	0/518	0.37	0/701
3	n	0.13	0/518	0.37	0/701
3	o	0.14	0/518	0.37	0/701
3	p	0.13	0/518	0.37	0/701
3	q	0.13	0/518	0.37	0/701
3	r	0.14	0/518	0.37	0/701
3	s	0.14	0/518	0.37	0/701
All	All	0.57	15/86145 (0.0%)	0.84	123/116910 (0.1%)

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	100	ARG	CD-NE	5.16	1.53	1.46
2	X	100	ARG	CD-NE	5.15	1.53	1.46
2	a	100	ARG	CD-NE	5.15	1.53	1.46
2	U	100	ARG	CD-NE	5.14	1.53	1.46
2	P	100	ARG	CD-NE	5.13	1.53	1.46

The worst 5 of 123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	619	SER	N-CA-C	6.53	119.65	108.02
1	O	619	SER	N-CA-C	6.53	119.64	108.02
1	K	619	SER	N-CA-C	6.52	119.63	108.02
1	H	619	SER	N-CA-C	6.52	119.62	108.02
1	J	619	SER	N-CA-C	6.52	119.62	108.02

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4447	0	4545	438	0
1	B	4447	0	4545	430	0
1	C	4447	0	4545	441	0
1	D	4447	0	4545	437	0
1	E	4447	0	4545	429	0
1	F	4447	0	4545	430	0
1	G	4447	0	4545	440	0
1	H	4447	0	4545	442	0
1	I	4447	0	4545	441	0
1	J	4447	0	4545	448	0
1	K	4447	0	4545	438	0
1	L	4447	0	4545	430	0
1	M	4447	0	4545	431	0
1	N	4447	0	4545	438	0
1	O	4447	0	4545	438	0
2	P	720	0	709	43	0
2	Q	720	0	709	42	0
2	R	720	0	709	43	0
2	S	720	0	709	44	0
2	T	720	0	709	43	0
2	U	720	0	709	44	0
2	V	720	0	709	45	0
2	W	720	0	709	45	0
2	X	720	0	709	44	0
2	Y	720	0	709	44	0
2	Z	720	0	709	45	0
2	a	720	0	709	44	0
2	b	720	0	709	45	0
2	c	720	0	709	43	0
2	d	720	0	709	44	0
3	e	512	0	546	32	0
3	f	512	0	546	31	0
3	g	512	0	546	31	0
3	h	512	0	546	33	0
3	i	512	0	546	31	0
3	j	512	0	546	32	0
3	k	512	0	546	33	0
3	l	512	0	546	31	0
3	m	512	0	546	33	0
3	n	512	0	546	31	0
3	o	512	0	546	30	0
3	p	512	0	546	30	0
3	q	512	0	546	33	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	r	512	0	546	31	0
3	s	512	0	546	31	0
All	All	85185	0	87000	6151	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 36.

The worst 5 of 6151 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:45:ASN:CB	3:l:108:LEU:HD21	1.69	1.23
1:B:45:ASN:CB	3:g:108:LEU:HD21	1.69	1.22
1:C:45:ASN:CB	3:e:108:LEU:HD21	1.69	1.22
1:G:45:ASN:CB	3:k:108:LEU:HD21	1.69	1.22
1:I:45:ASN:CB	3:m:108:LEU:HD21	1.69	1.22

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	584/657 (89%)	516 (88%)	68 (12%)	0	100	100
1	B	584/657 (89%)	515 (88%)	69 (12%)	0	100	100
1	C	584/657 (89%)	516 (88%)	68 (12%)	0	100	100
1	D	584/657 (89%)	516 (88%)	68 (12%)	0	100	100
1	E	584/657 (89%)	516 (88%)	68 (12%)	0	100	100
1	F	584/657 (89%)	515 (88%)	69 (12%)	0	100	100
1	G	584/657 (89%)	516 (88%)	68 (12%)	0	100	100
1	H	584/657 (89%)	516 (88%)	68 (12%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	584/657 (89%)	516 (88%)	68 (12%)	0	100	100
1	J	584/657 (89%)	516 (88%)	68 (12%)	0	100	100
1	K	584/657 (89%)	516 (88%)	68 (12%)	0	100	100
1	L	584/657 (89%)	516 (88%)	68 (12%)	0	100	100
1	M	584/657 (89%)	516 (88%)	68 (12%)	0	100	100
1	N	584/657 (89%)	516 (88%)	68 (12%)	0	100	100
1	O	584/657 (89%)	516 (88%)	68 (12%)	0	100	100
2	P	91/143 (64%)	89 (98%)	2 (2%)	0	100	100
2	Q	91/143 (64%)	89 (98%)	2 (2%)	0	100	100
2	R	91/143 (64%)	89 (98%)	2 (2%)	0	100	100
2	S	91/143 (64%)	89 (98%)	2 (2%)	0	100	100
2	T	91/143 (64%)	89 (98%)	2 (2%)	0	100	100
2	U	91/143 (64%)	89 (98%)	2 (2%)	0	100	100
2	V	91/143 (64%)	89 (98%)	2 (2%)	0	100	100
2	W	91/143 (64%)	89 (98%)	2 (2%)	0	100	100
2	X	91/143 (64%)	89 (98%)	2 (2%)	0	100	100
2	Y	91/143 (64%)	89 (98%)	2 (2%)	0	100	100
2	Z	91/143 (64%)	89 (98%)	2 (2%)	0	100	100
2	a	91/143 (64%)	89 (98%)	2 (2%)	0	100	100
2	b	91/143 (64%)	89 (98%)	2 (2%)	0	100	100
2	c	91/143 (64%)	89 (98%)	2 (2%)	0	100	100
2	d	91/143 (64%)	89 (98%)	2 (2%)	0	100	100
3	e	66/280 (24%)	63 (96%)	3 (4%)	0	100	100
3	f	66/280 (24%)	63 (96%)	3 (4%)	0	100	100
3	g	66/280 (24%)	63 (96%)	3 (4%)	0	100	100
3	h	66/280 (24%)	63 (96%)	3 (4%)	0	100	100
3	i	66/280 (24%)	63 (96%)	3 (4%)	0	100	100
3	j	66/280 (24%)	63 (96%)	3 (4%)	0	100	100
3	k	66/280 (24%)	63 (96%)	3 (4%)	0	100	100
3	l	66/280 (24%)	63 (96%)	3 (4%)	0	100	100
3	m	66/280 (24%)	63 (96%)	3 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	n	66/280 (24%)	63 (96%)	3 (4%)	0	100	100
3	o	66/280 (24%)	63 (96%)	3 (4%)	0	100	100
3	p	66/280 (24%)	63 (96%)	3 (4%)	0	100	100
3	q	66/280 (24%)	63 (96%)	3 (4%)	0	100	100
3	r	66/280 (24%)	63 (96%)	3 (4%)	0	100	100
3	s	66/280 (24%)	63 (96%)	3 (4%)	0	100	100
All	All	11115/16200 (69%)	10018 (90%)	1097 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	490/544 (90%)	490 (100%)	0	100	100
1	B	490/544 (90%)	490 (100%)	0	100	100
1	C	490/544 (90%)	490 (100%)	0	100	100
1	D	490/544 (90%)	490 (100%)	0	100	100
1	E	490/544 (90%)	490 (100%)	0	100	100
1	F	490/544 (90%)	490 (100%)	0	100	100
1	G	490/544 (90%)	490 (100%)	0	100	100
1	H	490/544 (90%)	490 (100%)	0	100	100
1	I	490/544 (90%)	490 (100%)	0	100	100
1	J	490/544 (90%)	490 (100%)	0	100	100
1	K	490/544 (90%)	490 (100%)	0	100	100
1	L	490/544 (90%)	490 (100%)	0	100	100
1	M	490/544 (90%)	490 (100%)	0	100	100
1	N	490/544 (90%)	490 (100%)	0	100	100
1	O	490/544 (90%)	490 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	78/123 (63%)	78 (100%)	0	100	100
2	Q	78/123 (63%)	78 (100%)	0	100	100
2	R	78/123 (63%)	78 (100%)	0	100	100
2	S	78/123 (63%)	78 (100%)	0	100	100
2	T	78/123 (63%)	78 (100%)	0	100	100
2	U	78/123 (63%)	78 (100%)	0	100	100
2	V	78/123 (63%)	78 (100%)	0	100	100
2	W	78/123 (63%)	78 (100%)	0	100	100
2	X	78/123 (63%)	78 (100%)	0	100	100
2	Y	78/123 (63%)	78 (100%)	0	100	100
2	Z	78/123 (63%)	78 (100%)	0	100	100
2	a	78/123 (63%)	78 (100%)	0	100	100
2	b	78/123 (63%)	78 (100%)	0	100	100
2	c	78/123 (63%)	78 (100%)	0	100	100
2	d	78/123 (63%)	78 (100%)	0	100	100
3	e	55/236 (23%)	55 (100%)	0	100	100
3	f	55/236 (23%)	55 (100%)	0	100	100
3	g	55/236 (23%)	55 (100%)	0	100	100
3	h	55/236 (23%)	55 (100%)	0	100	100
3	i	55/236 (23%)	55 (100%)	0	100	100
3	j	55/236 (23%)	55 (100%)	0	100	100
3	k	55/236 (23%)	55 (100%)	0	100	100
3	l	55/236 (23%)	55 (100%)	0	100	100
3	m	55/236 (23%)	55 (100%)	0	100	100
3	n	55/236 (23%)	55 (100%)	0	100	100
3	o	55/236 (23%)	55 (100%)	0	100	100
3	p	55/236 (23%)	55 (100%)	0	100	100
3	q	55/236 (23%)	55 (100%)	0	100	100
3	r	55/236 (23%)	55 (100%)	0	100	100
3	s	55/236 (23%)	55 (100%)	0	100	100
All	All	9345/13545 (69%)	9345 (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 260 such sidechains are listed below:

Mol	Chain	Res	Type
2	W	104	GLN
2	Y	97	ASN
1	H	144	GLN
1	H	47	ASN
2	Z	97	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

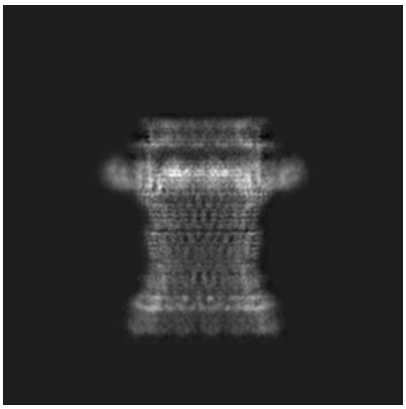
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0193. These allow visual inspection of the internal detail of the map and identification of artifacts.

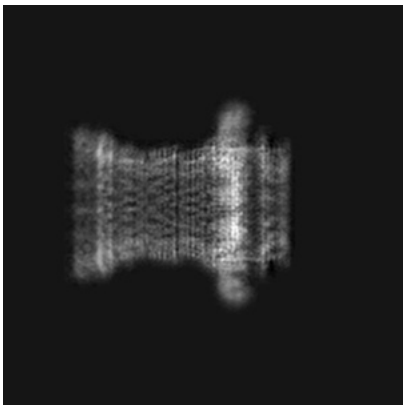
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

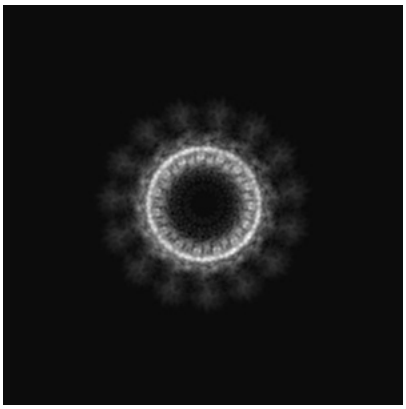
6.1.1 Primary map



X

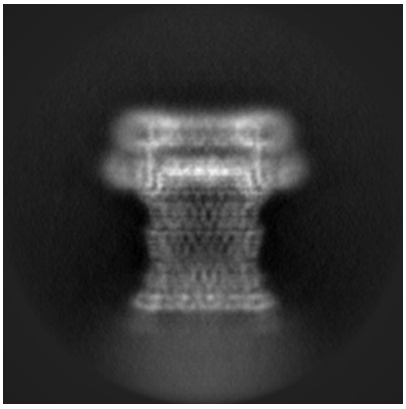


Y

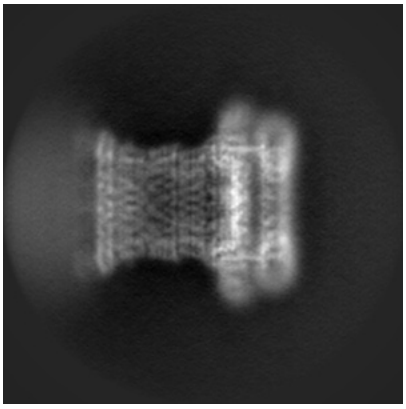


Z

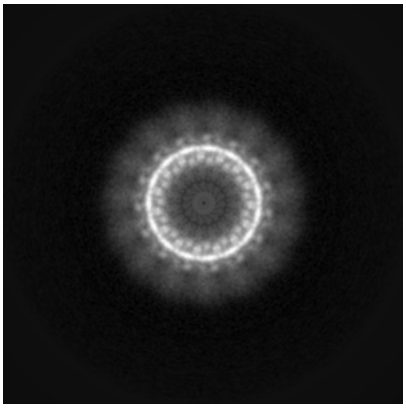
6.1.2 Raw map



X



Y



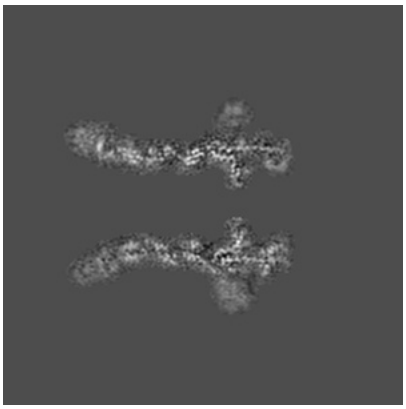
Z

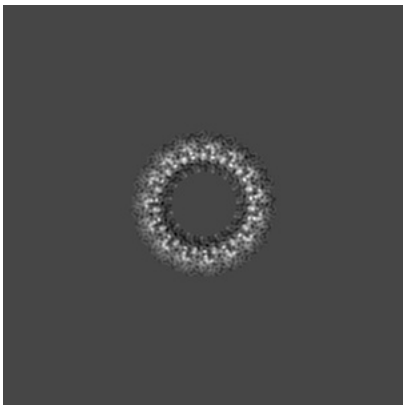
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

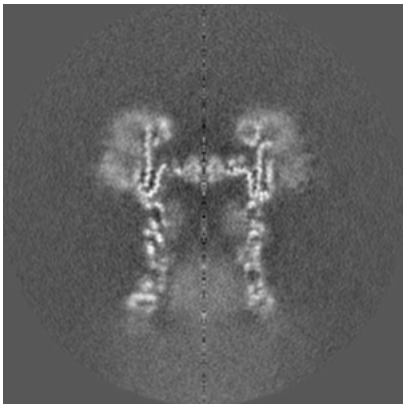
6.2.1 Primary map

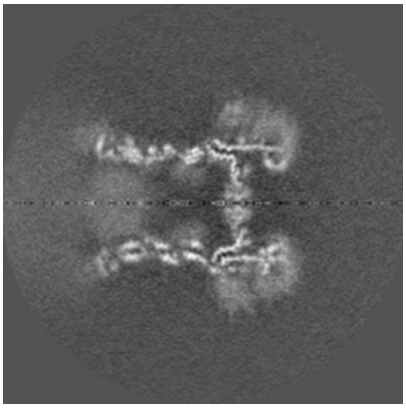
X Index: 115

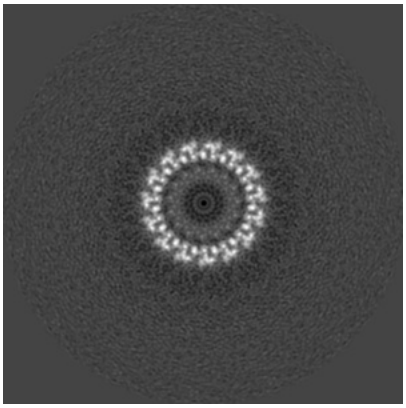

Y Index: 115


Z Index: 115

6.2.2 Raw map


X Index: 115

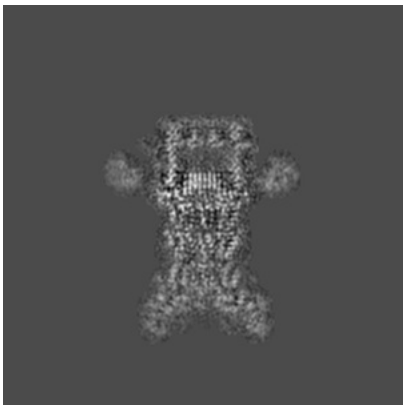

Y Index: 115


Z Index: 115

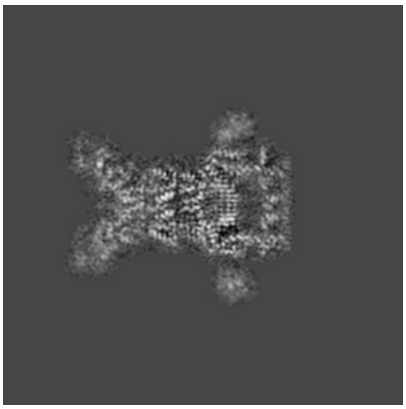
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

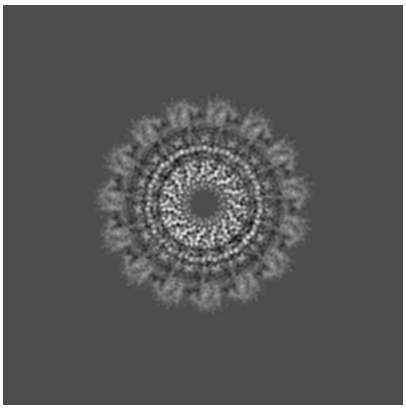
6.3.1 Primary map



X Index: 141

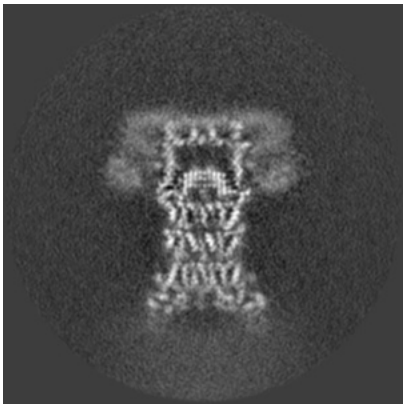


Y Index: 140

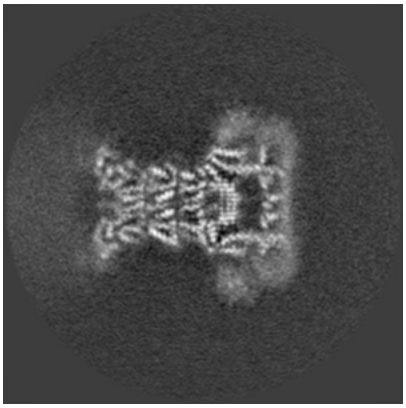


Z Index: 134

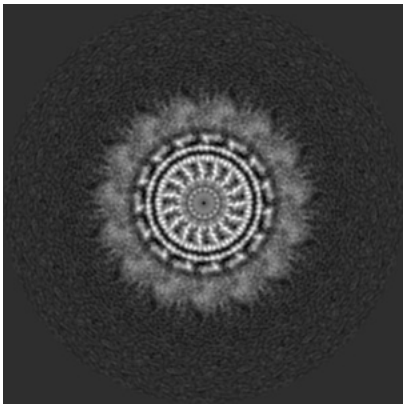
6.3.2 Raw map



X Index: 140



Y Index: 140

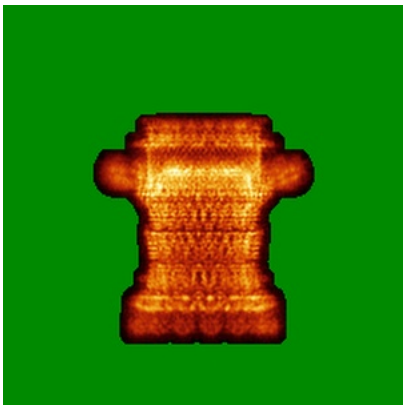


Z Index: 132

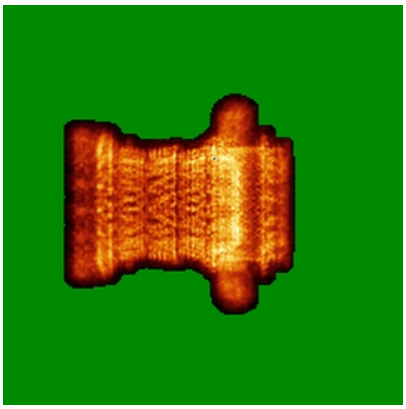
The images above show the largest variance slices of the map in three orthogonal directions.

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

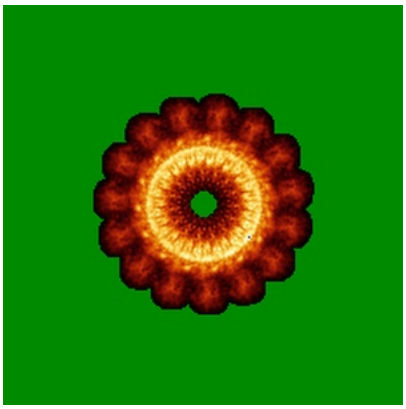
6.4.1 Primary map



X

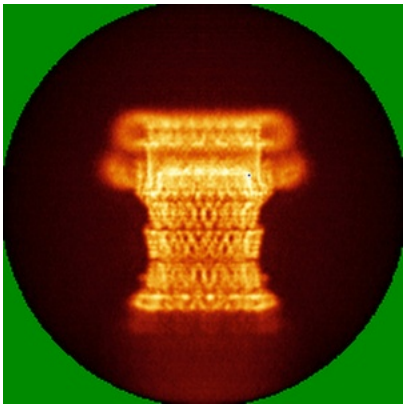


Y

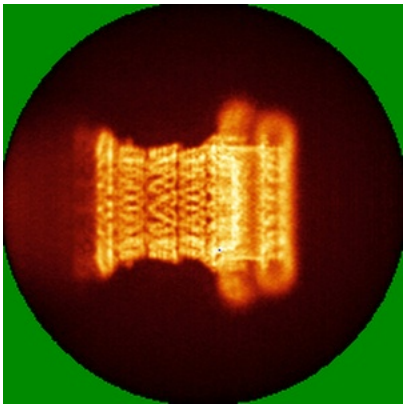


Z

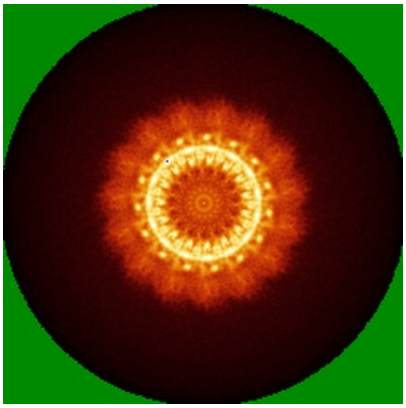
6.4.2 Raw map



X



Y

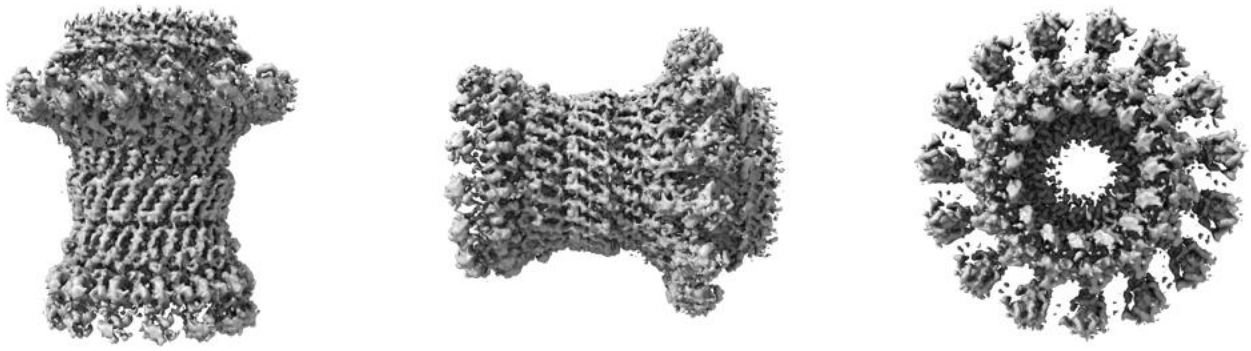


Z

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)

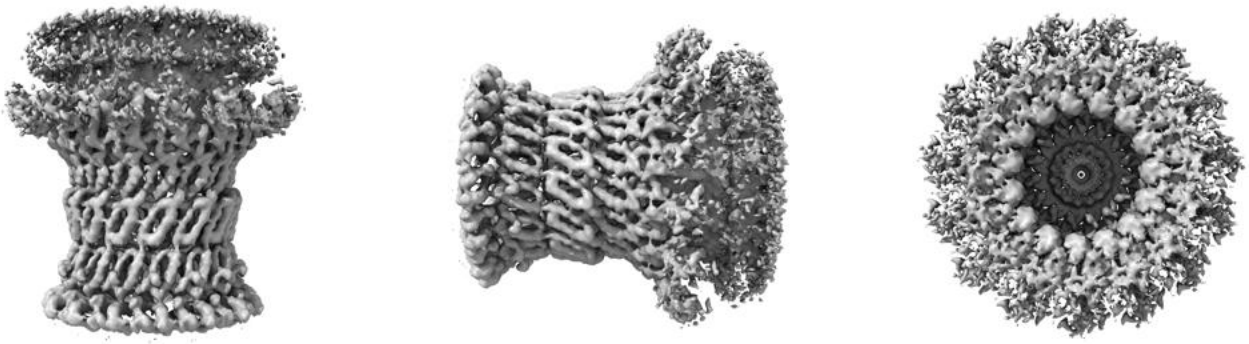
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 4.3. 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.

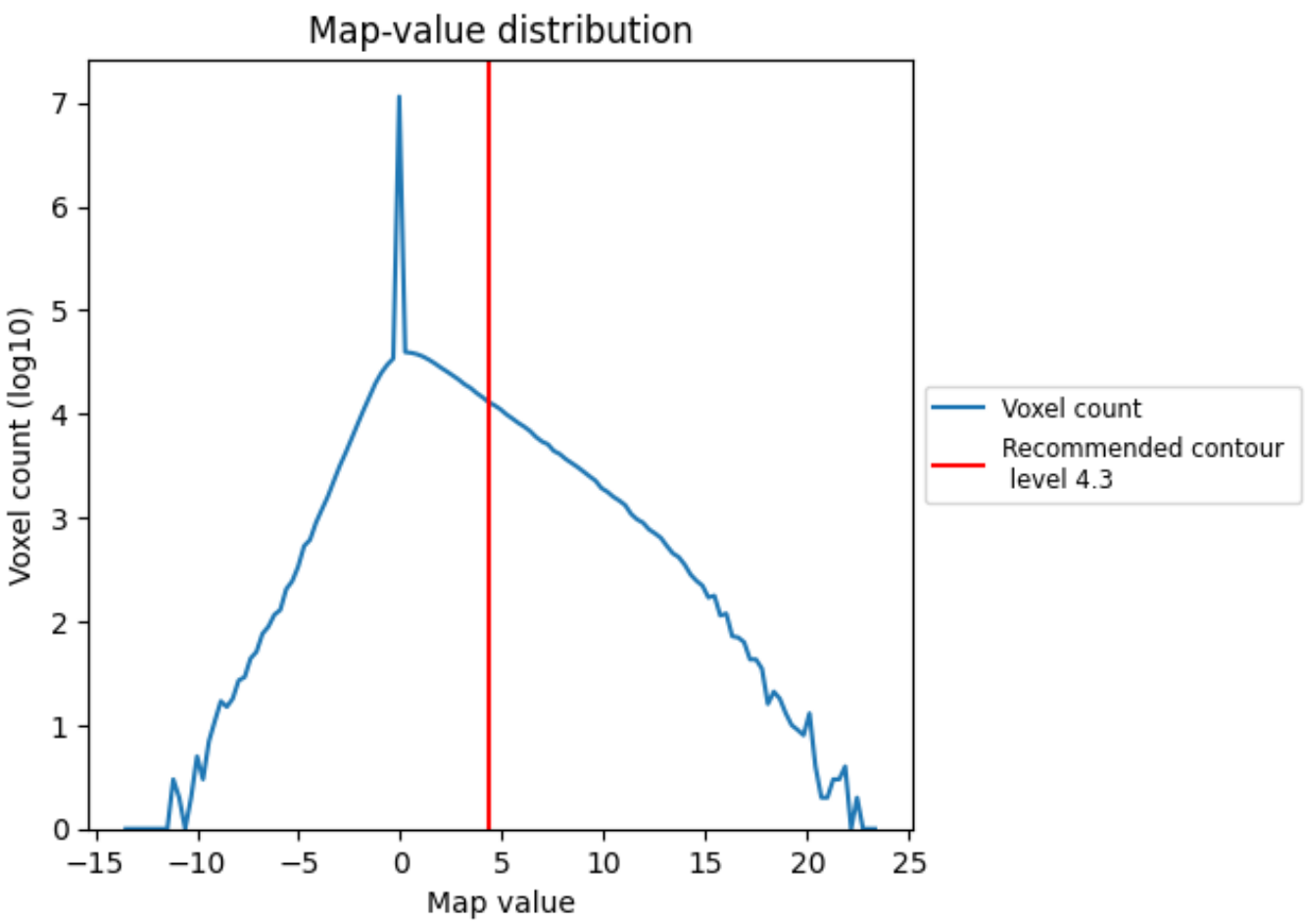
6.6 Mask visualisation (i)

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

7 Map analysis (i)

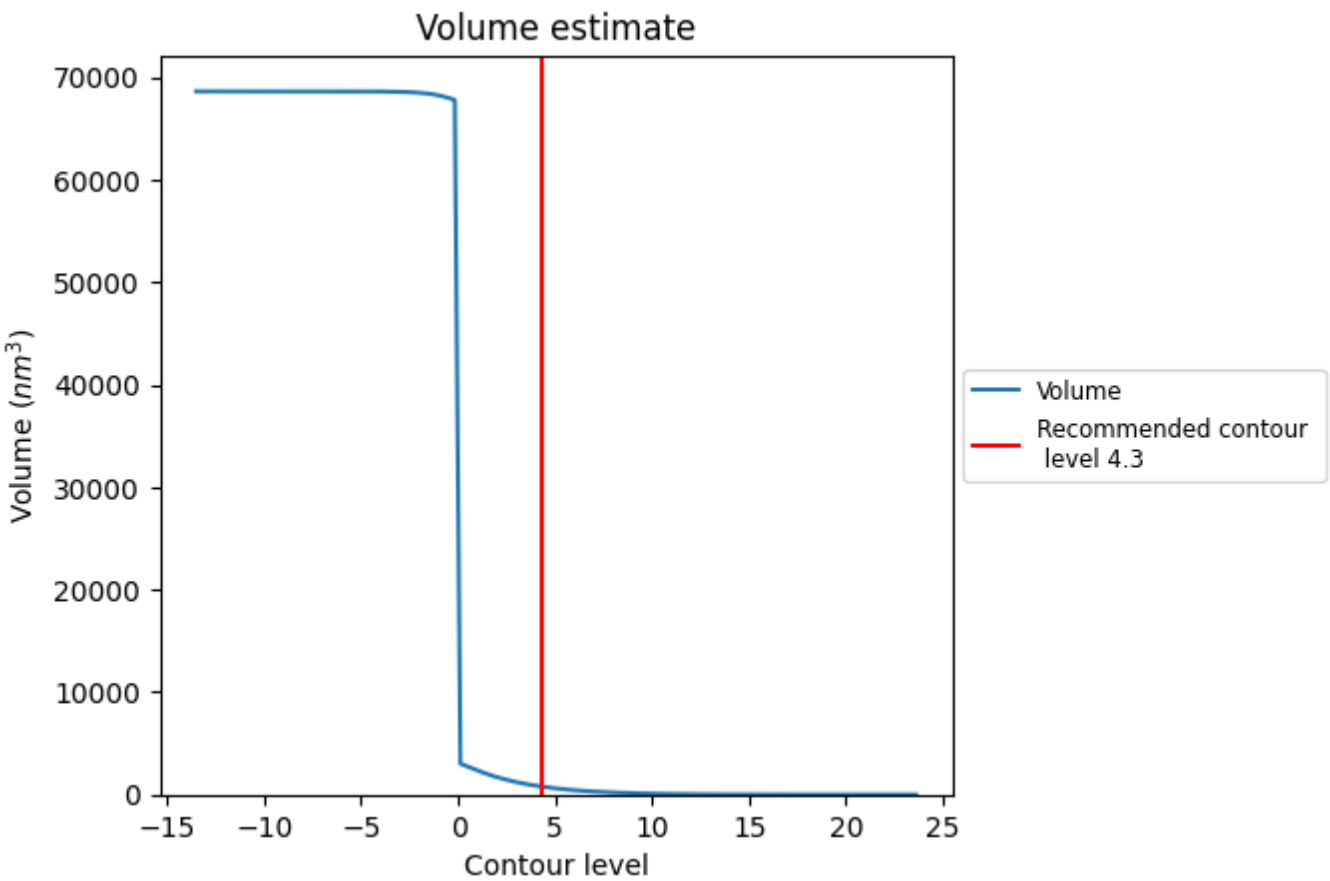
This section contains the results of statistical analysis of the map.

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.

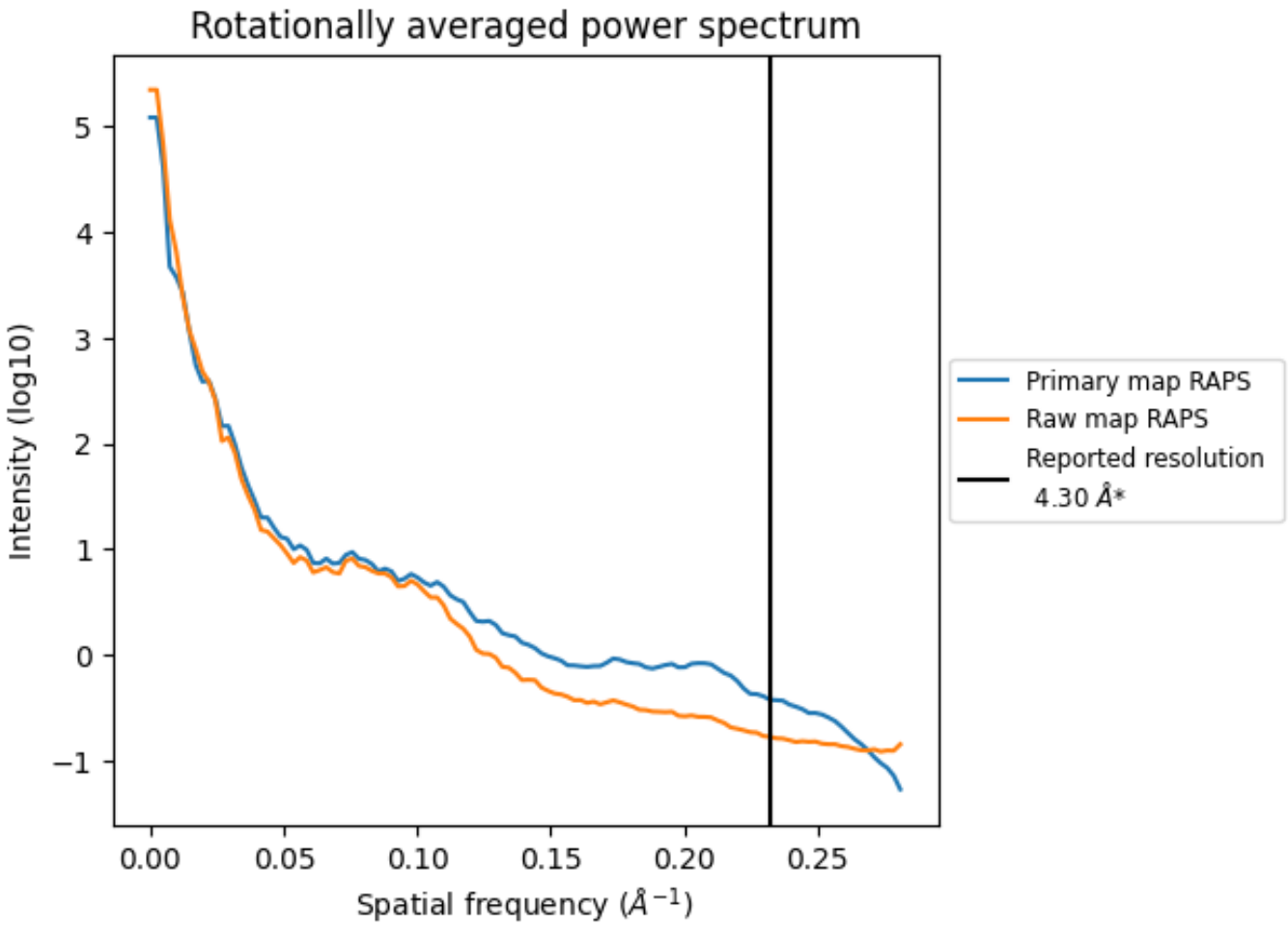
7.2 Volume estimate (i)



The volume at the recommended contour level is 783 nm^3; this corresponds to an approximate mass of 707 kDa.

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

7.3 Rotationally averaged power spectrum (i)

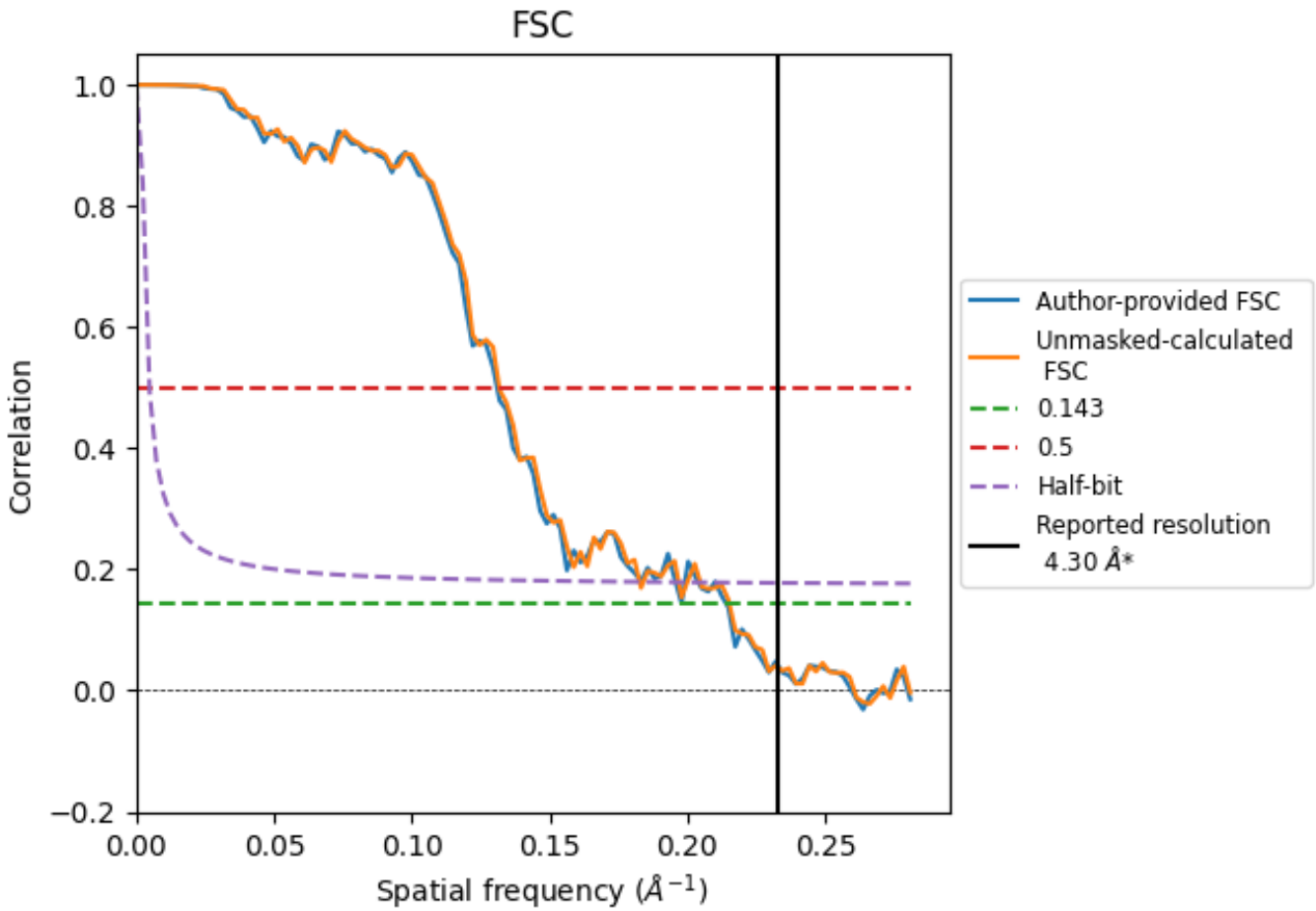


*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

8.2 Resolution estimates (i)

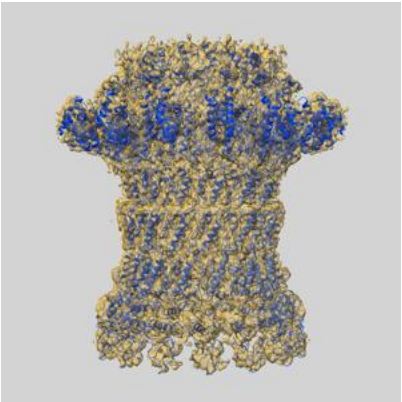
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.67	7.64	5.11
Unmasked-calculated*	4.64	7.59	5.47

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

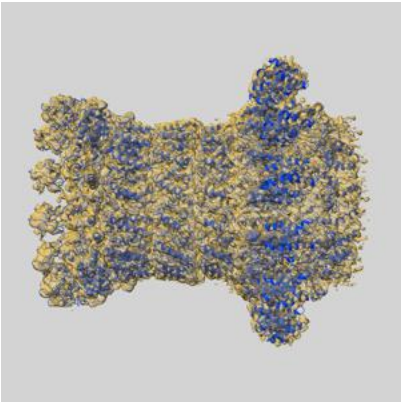
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0193 and PDB model 6HCG. Per-residue inclusion information can be found in section 3 on page 8.

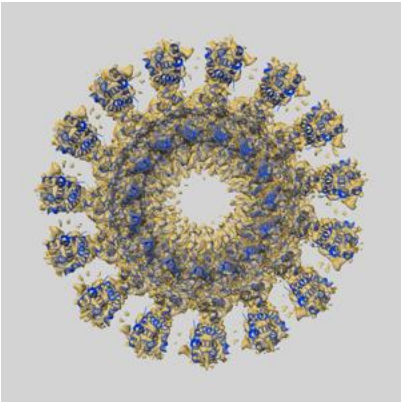
9.1 Map-model overlay (i)



X



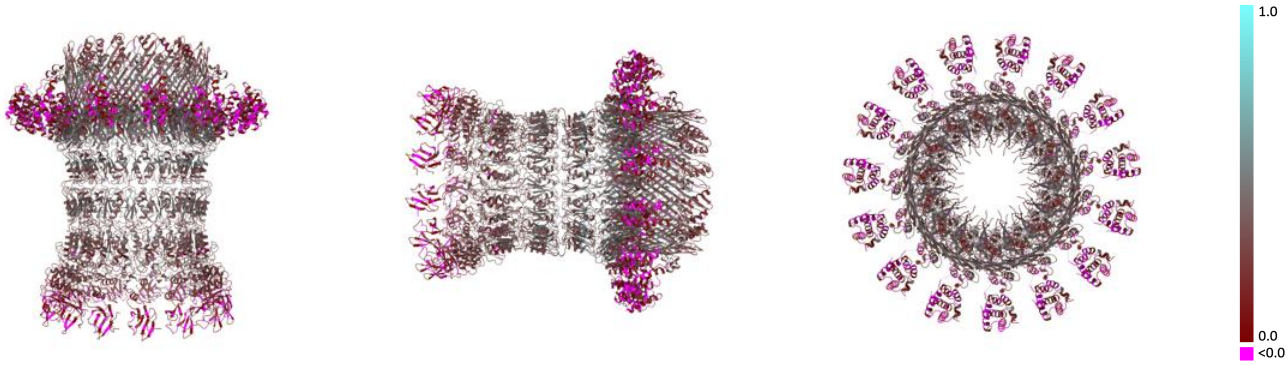
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

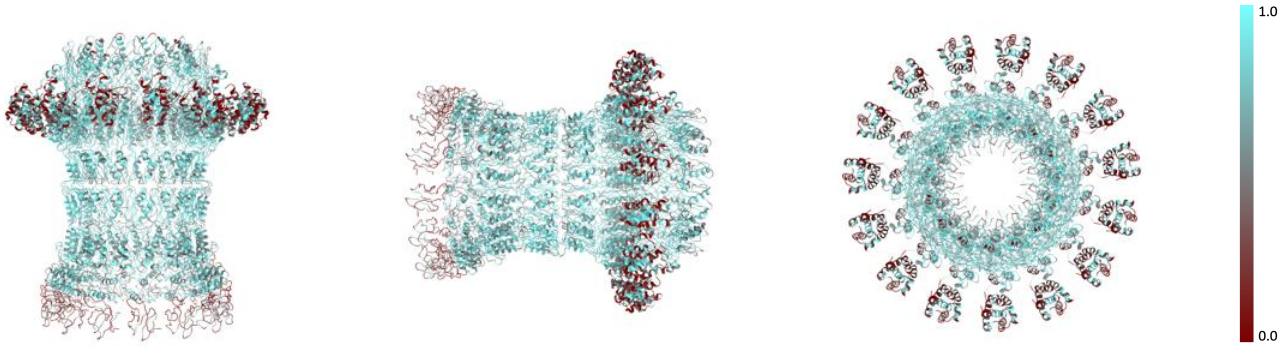
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

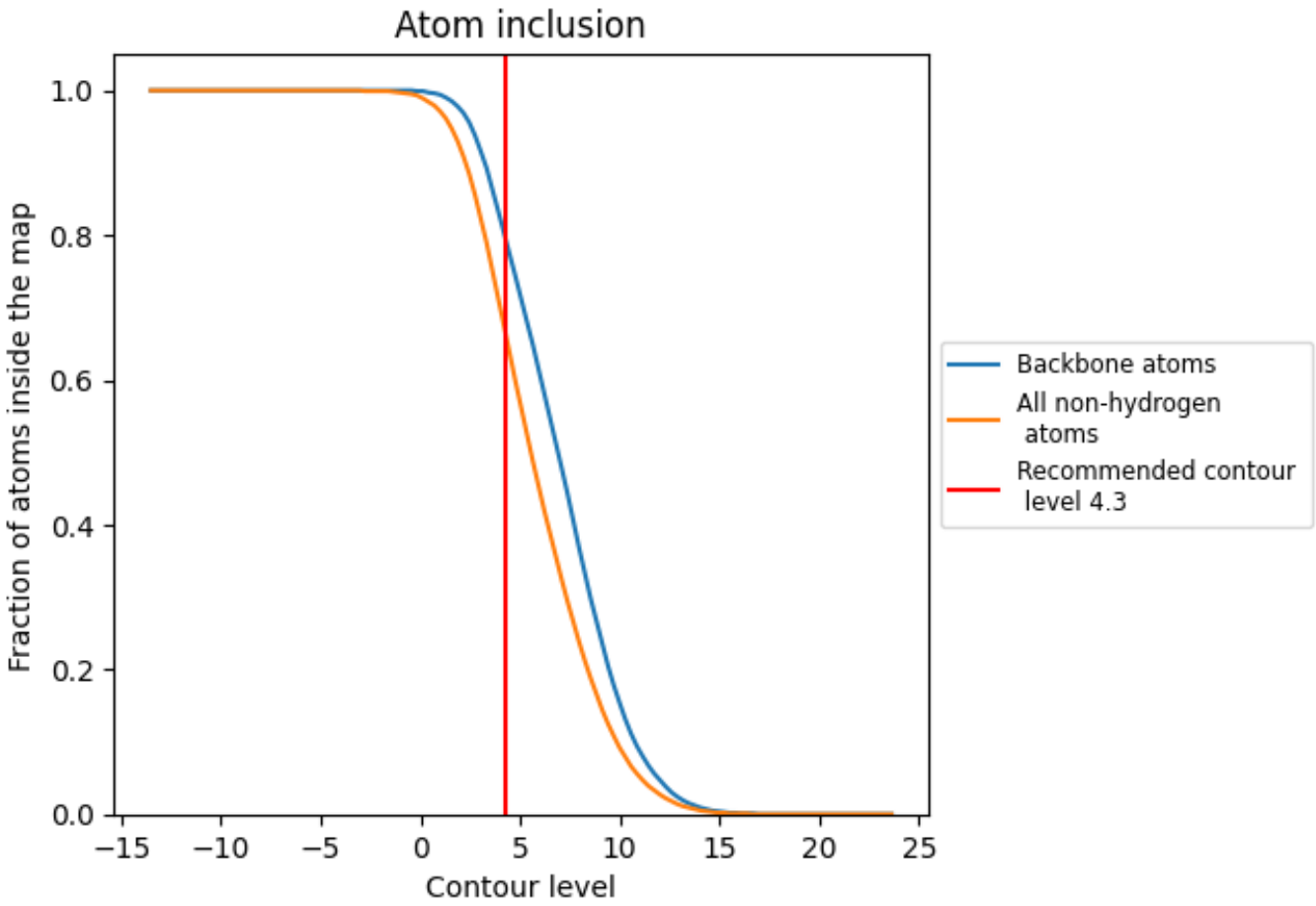
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.3).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (4.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6600	0.2730
A	0.7570	0.3210
B	0.7560	0.3230
C	0.7600	0.3280
D	0.7520	0.3310
E	0.7490	0.3250
F	0.7500	0.3240
G	0.7440	0.3250
H	0.7450	0.3230
I	0.7480	0.3240
J	0.7410	0.3220
K	0.7480	0.3230
L	0.7440	0.3240
M	0.7450	0.3250
N	0.7450	0.3230
O	0.7430	0.3260
P	0.3850	0.0770
Q	0.4100	0.0790
R	0.3960	0.0830
S	0.3800	0.0760
T	0.3900	0.0790
U	0.3880	0.0810
V	0.4090	0.0730
W	0.4260	0.0850
X	0.4300	0.0780
Y	0.4060	0.0810
Z	0.3690	0.0660
a	0.3790	0.0730
b	0.3730	0.0710
c	0.3620	0.0770
d	0.3800	0.0740
e	0.2640	0.1000
f	0.2440	0.0950
g	0.2480	0.1100
h	0.2580	0.1020

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	0.2600	0.0910
j	0.2800	0.1030
k	0.3100	0.0970
l	0.2920	0.1010
m	0.2820	0.0970
n	0.2840	0.1100
o	0.2200	0.0980
p	0.2540	0.0910
q	0.2460	0.1040
r	0.2300	0.0920
s	0.2360	0.1040