wwPDB EM Validation Summary Report

Nov 3, 2026 – 07:09 pm GMT

PDB ID	:	31OD / pdb_000031od
EMDB ID	:	EMD-58581
Title	:	Yersinia entomophaga holotoxin in its inverted pore state
Authors	:	Ng'ang'a, P.N.; Raunser, S.; Bader, R.; Sitsel, O.
Deposited on	:	2026-06-16
Resolution	:	4.09 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 ⓘ 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:

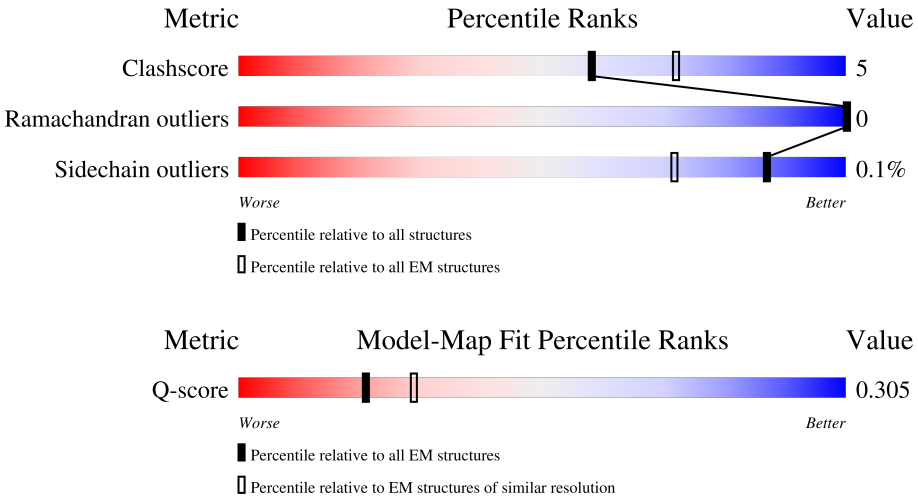
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 4.09 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.



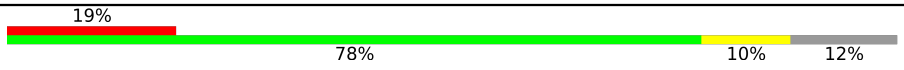
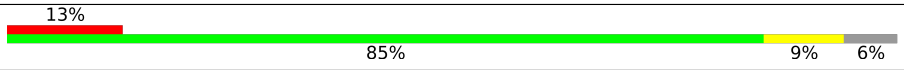
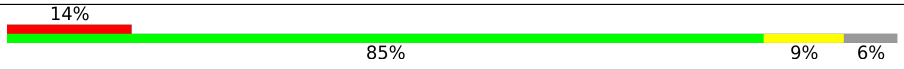
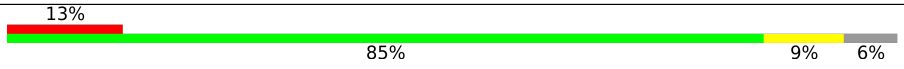
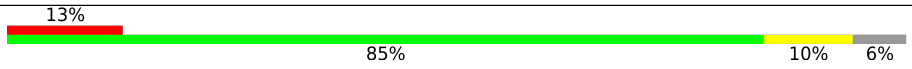
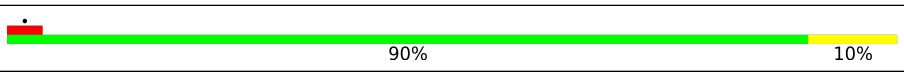
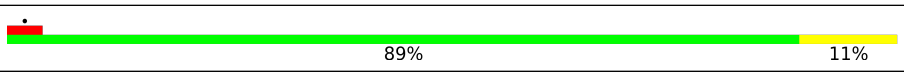
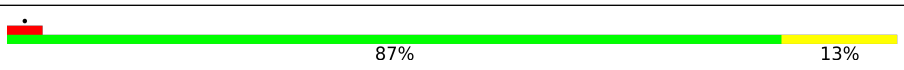
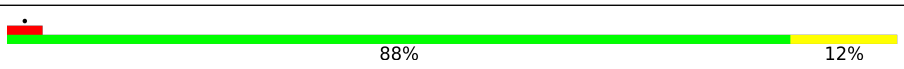
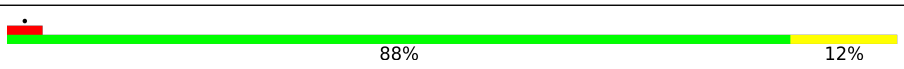
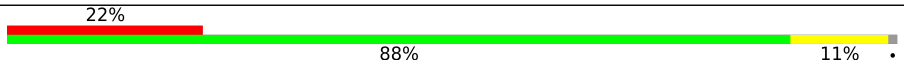
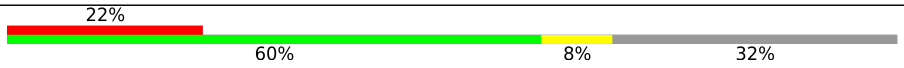
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6369 (3.59 - 4.59)

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	1164	18% 76% 12% 12%
1	F	1164	19% 77% 11% 12%
1	I	1164	18% 79% 10% 12%
1	L	1164	19% 79% 9% 12%

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Mol	Chain	Length	Quality of chain
1	O	1164	
2	B	1365	
2	G	1365	
2	J	1365	
2	M	1365	
2	P	1365	
3	C	633	
3	H	633	
3	K	633	
3	N	633	
3	Q	633	
4	D	1487	
5	E	970	
6	R	542	
6	S	542	
6	T	542	
6	U	542	
6	V	542	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 154987 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 Toxin subunit YenA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1026	Total	C	N	O	S	0	0
			8078	5154	1327	1574	23		
1	F	1026	Total	C	N	O	S	0	0
			8078	5154	1327	1574	23		
1	I	1026	Total	C	N	O	S	0	0
			8078	5154	1327	1574	23		
1	L	1026	Total	C	N	O	S	0	0
			8078	5154	1327	1574	23		
1	O	1026	Total	C	N	O	S	0	0
			8078	5154	1327	1574	23		

- Molecule 2 is a protein called Toxin subunit YenA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1286	Total	C	N	O	S	0	0
			10384	6587	1744	2017	36		
2	G	1286	Total	C	N	O	S	0	0
			10384	6587	1744	2017	36		
2	J	1286	Total	C	N	O	S	0	0
			10384	6587	1744	2017	36		
2	M	1286	Total	C	N	O	S	0	0
			10384	6587	1744	2017	36		
2	P	1286	Total	C	N	O	S	0	0
			10384	6587	1744	2017	36		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	351	THR	-	insertion	UNP B6A878
B	?	-	PRO	deletion	UNP B6A878
B	829	SER	-	insertion	UNP B6A878
G	351	THR	-	insertion	UNP B6A878
G	?	-	PRO	deletion	UNP B6A878
G	829	SER	-	insertion	UNP B6A878

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Chain	Residue	Modelled	Actual	Comment	Reference
J	351	THR	-	insertion	UNP B6A878
J	?	-	PRO	deletion	UNP B6A878
J	829	SER	-	insertion	UNP B6A878
M	351	THR	-	insertion	UNP B6A878
M	?	-	PRO	deletion	UNP B6A878
M	829	SER	-	insertion	UNP B6A878
P	351	THR	-	insertion	UNP B6A878
P	?	-	PRO	deletion	UNP B6A878
P	829	SER	-	insertion	UNP B6A878

- Molecule 3 is a protein called Chitinase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	633	Total	C	N	O	S	0	0
			4914	3107	824	964	19		
3	H	633	Total	C	N	O	S	0	0
			4914	3107	824	964	19		
3	K	633	Total	C	N	O	S	0	0
			4914	3107	824	964	19		
3	N	633	Total	C	N	O	S	0	0
			4914	3107	824	964	19		
3	Q	633	Total	C	N	O	S	0	0
			4914	3107	824	964	19		

- Molecule 4 is a protein called Toxin subunit YenB.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	1474	Total	C	N	O	S	0	0
			11696	7381	2021	2258	36		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1484	ASP	ASN	conflict	UNP B6A880

- Molecule 5 is a protein called Toxin subunit YenC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	658	Total	C	N	O	S	0	0
			5111	3187	895	1017	12		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	109	SER	LYS	conflict	UNP B6A882

- Molecule 6 is a protein called Chitinase 1.

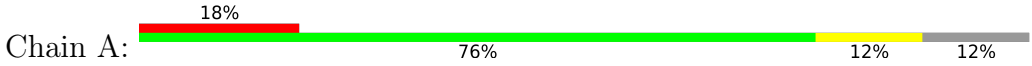
Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	542	Total	C	N	O	S	0	0
			4260	2691	706	850	13		
6	S	542	Total	C	N	O	S	0	0
			4260	2691	706	850	13		
6	T	542	Total	C	N	O	S	0	0
			4260	2691	706	850	13		
6	U	542	Total	C	N	O	S	0	0
			4260	2691	706	850	13		
6	V	542	Total	C	N	O	S	0	0
			4260	2691	706	850	13		

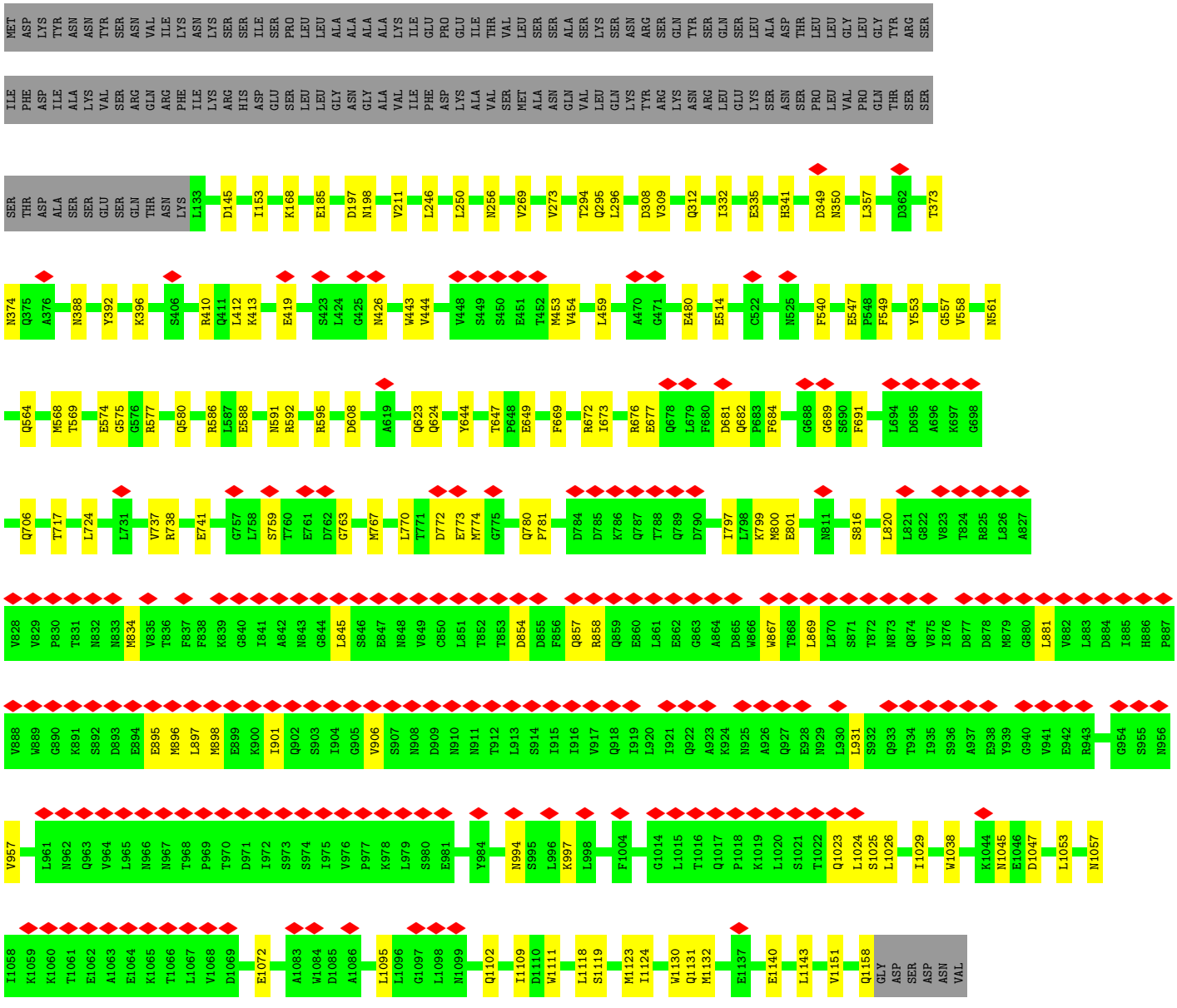
3 Residue-property plots (i)

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: Toxin subunit YenA1

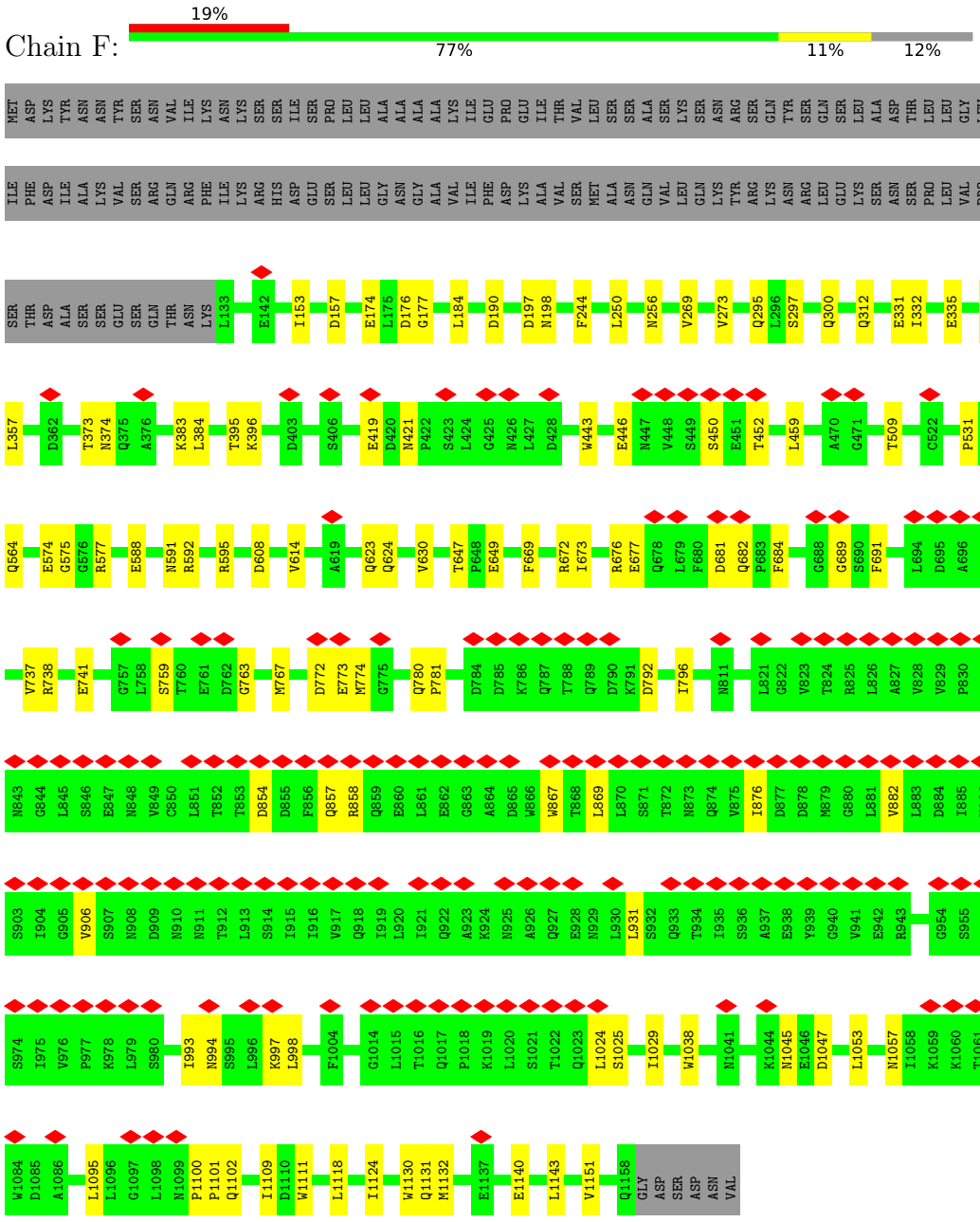
Chain A:





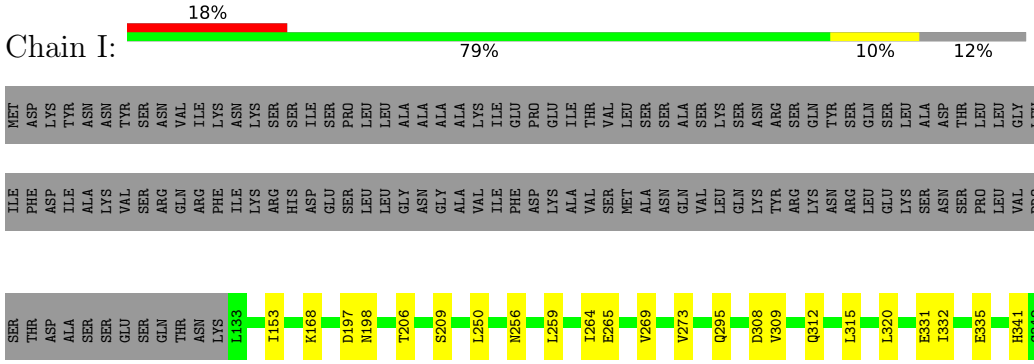
• Molecule 1: Toxin subunit YenA1

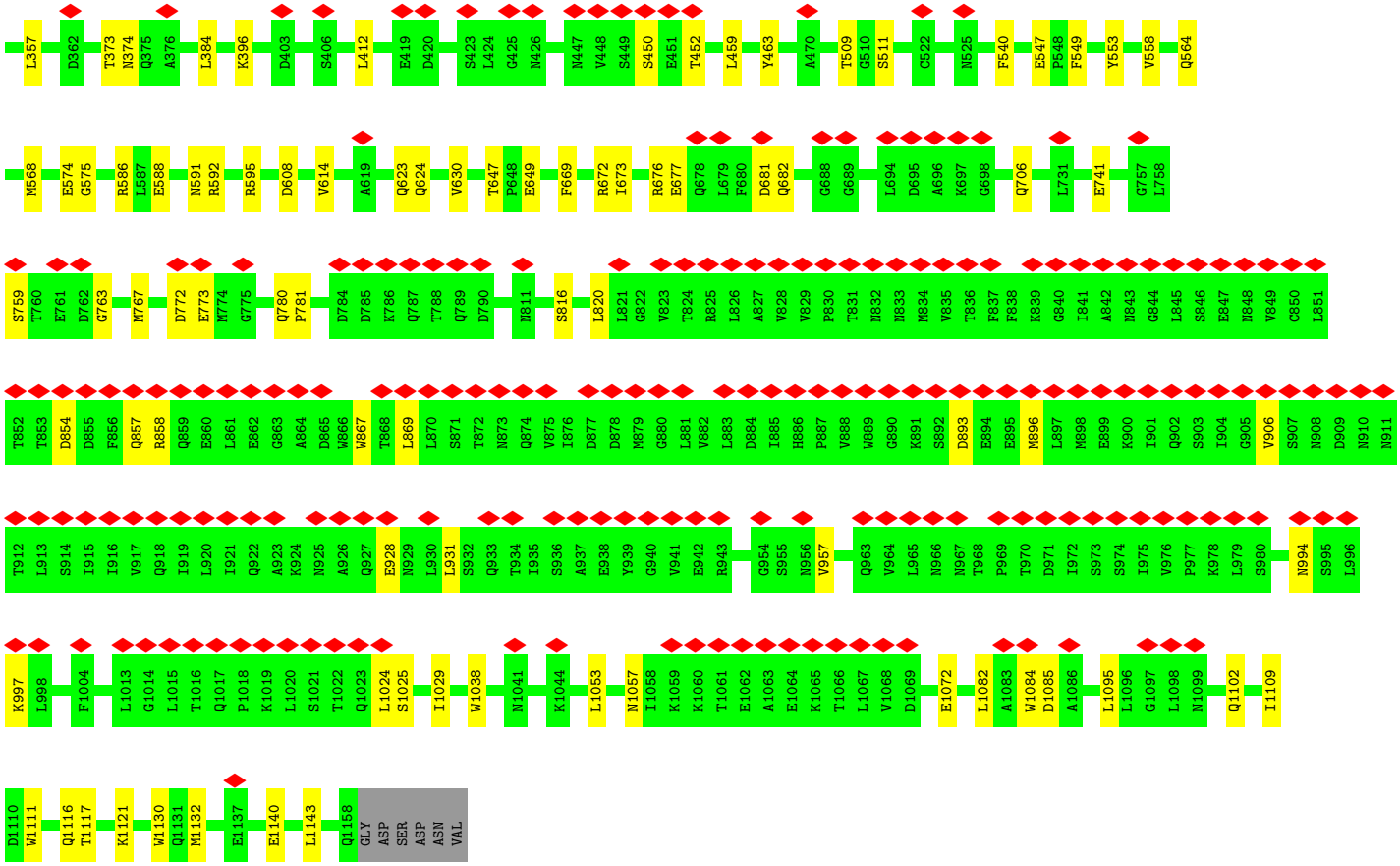
Chain F:



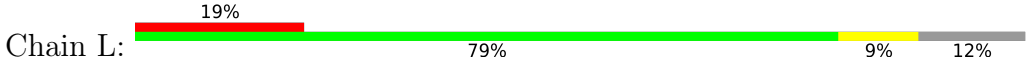
• Molecule 1: Toxin subunit YenA1

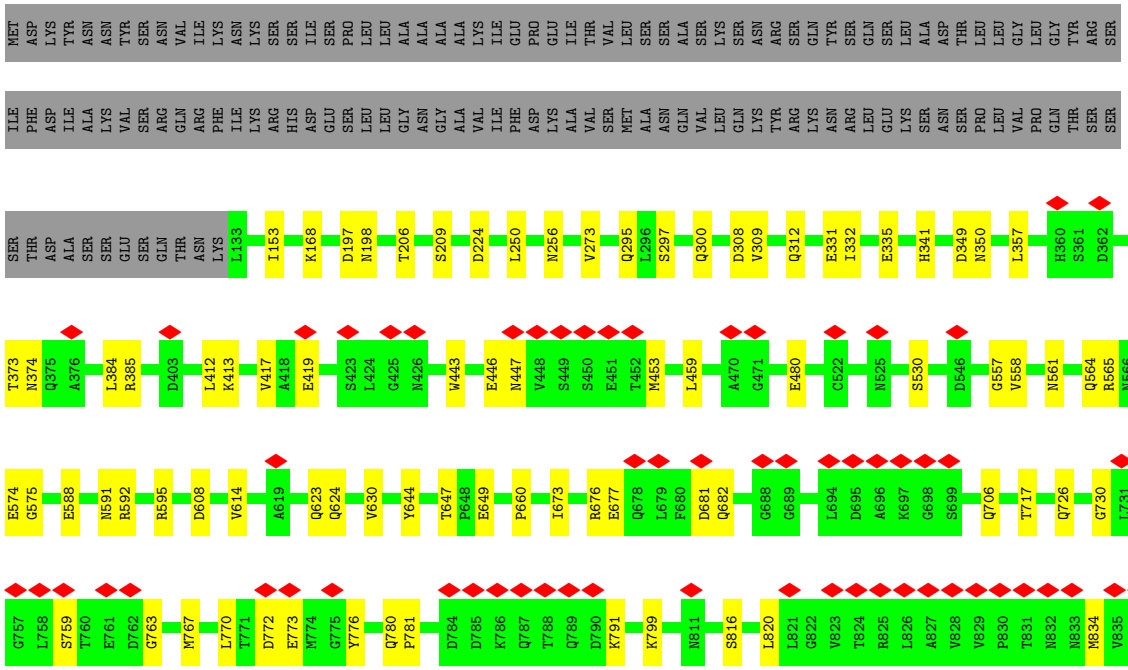
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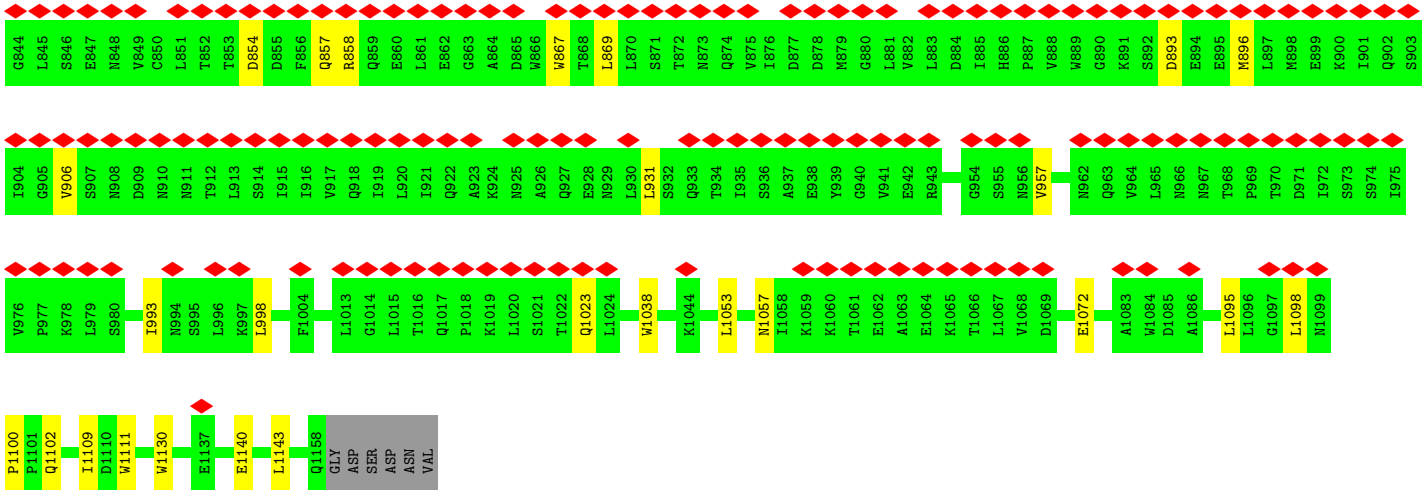




- Molecule 1: Toxin subunit YenA1



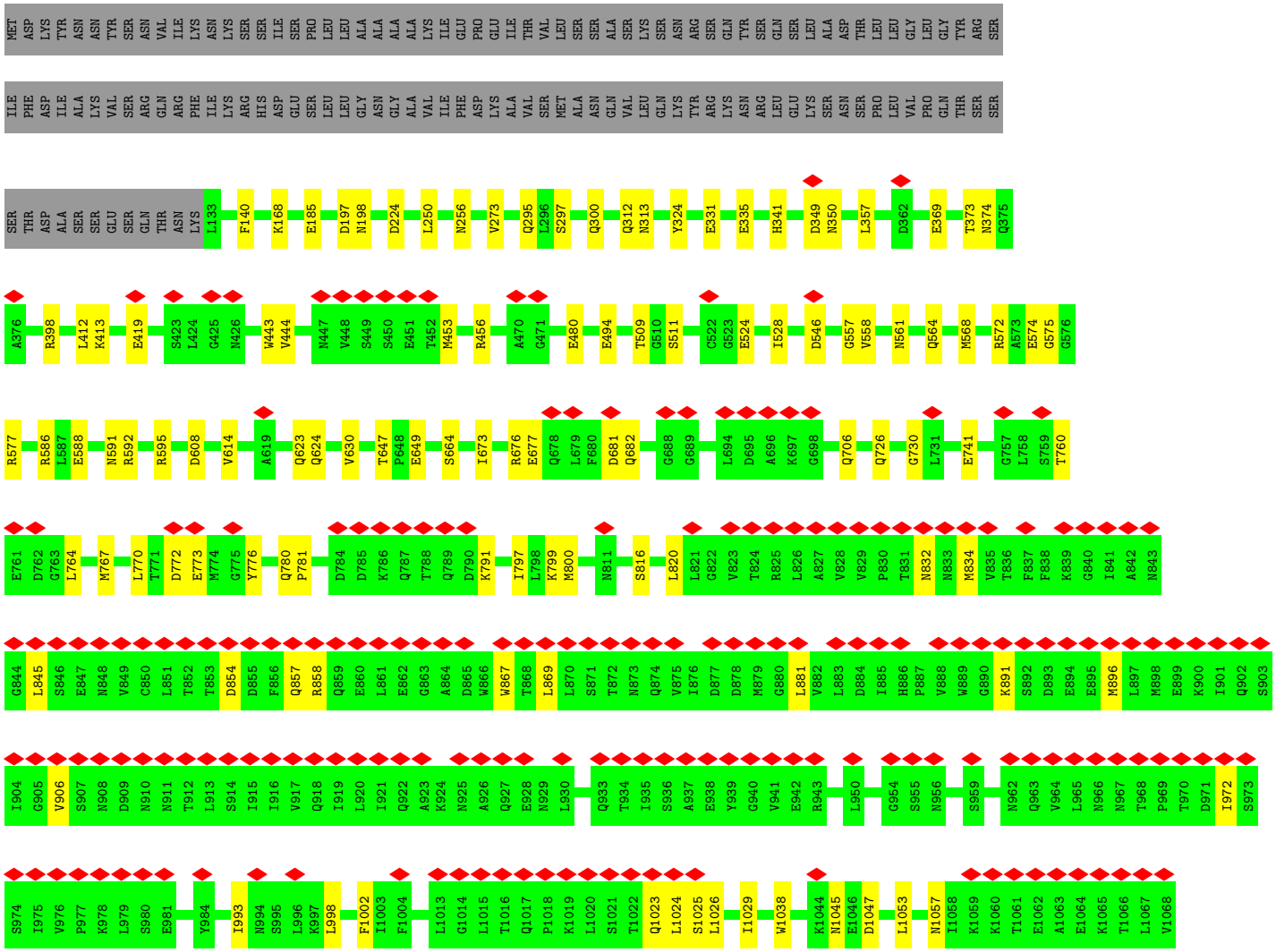


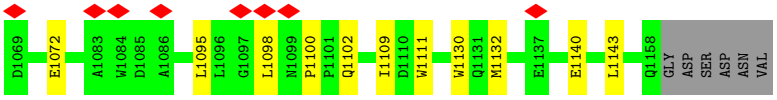


- Molecule 1: Toxin subunit YenA1

Chain O:



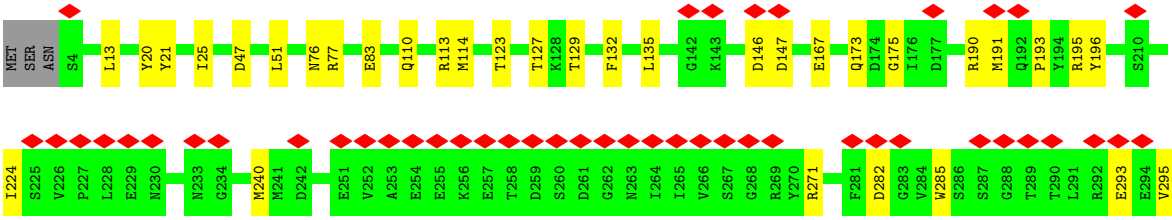


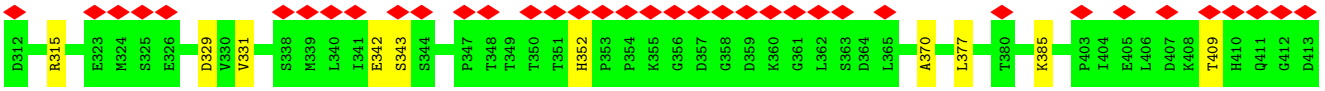


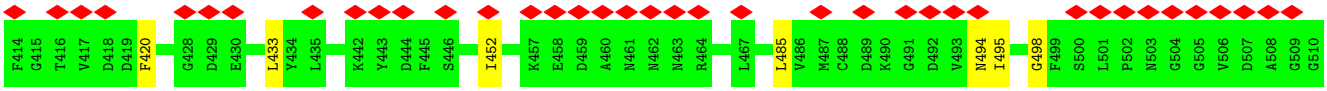
• Molecule 2: Toxin subunit YenA2

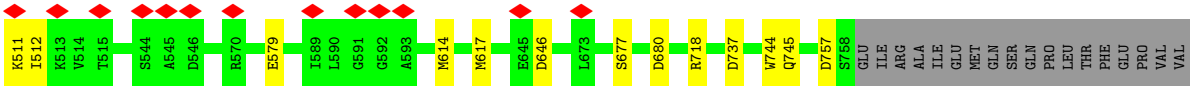
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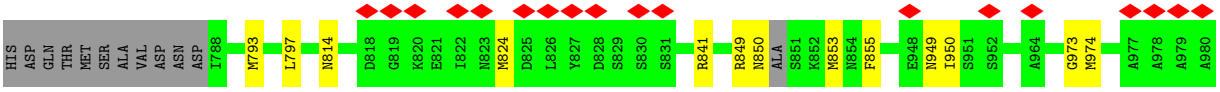


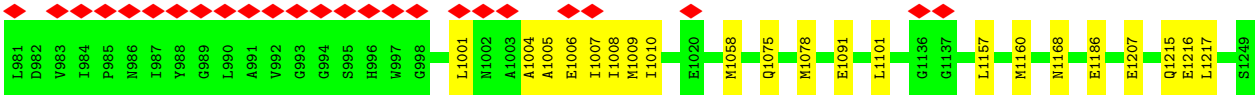


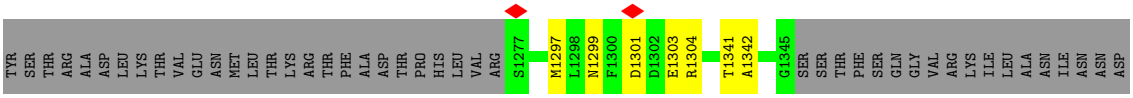












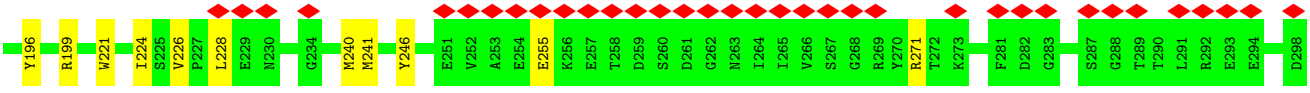


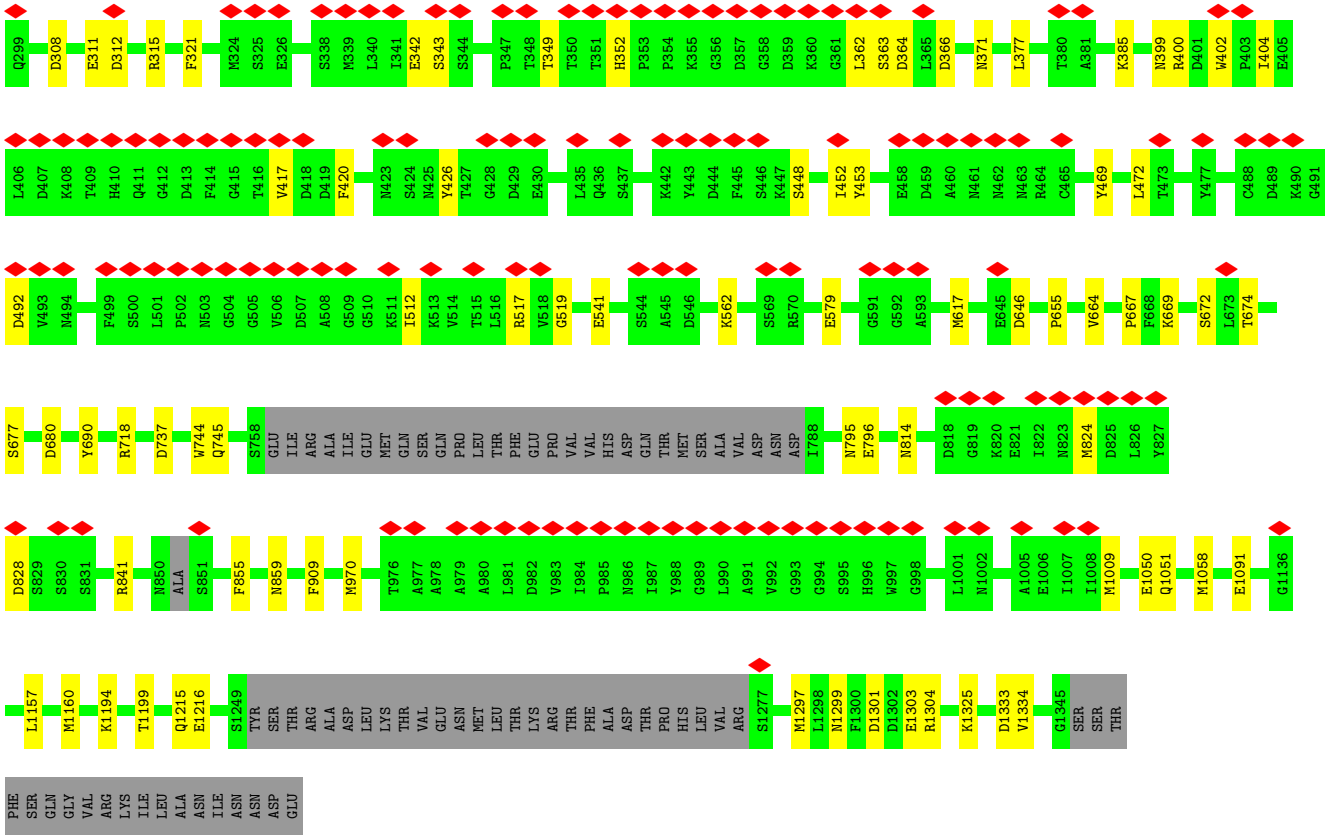
• Molecule 2: Toxin subunit YenA2

Chain G:





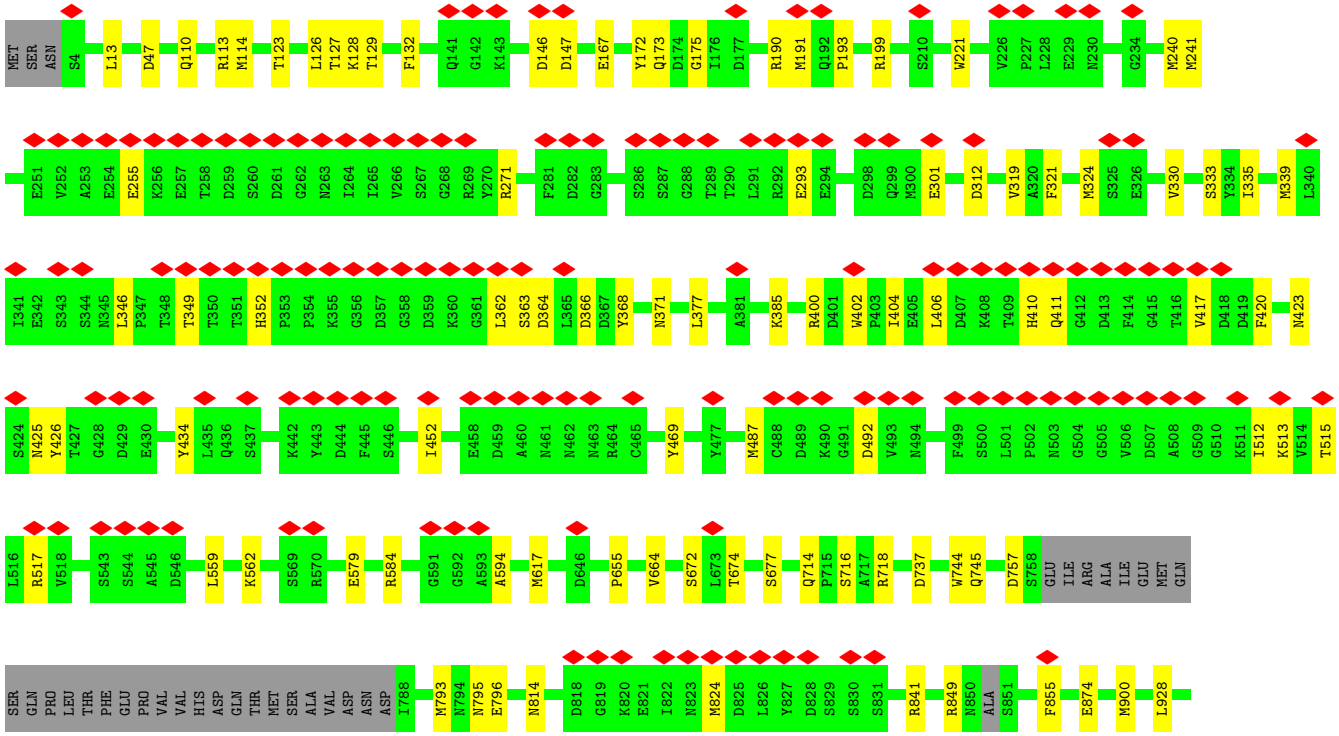


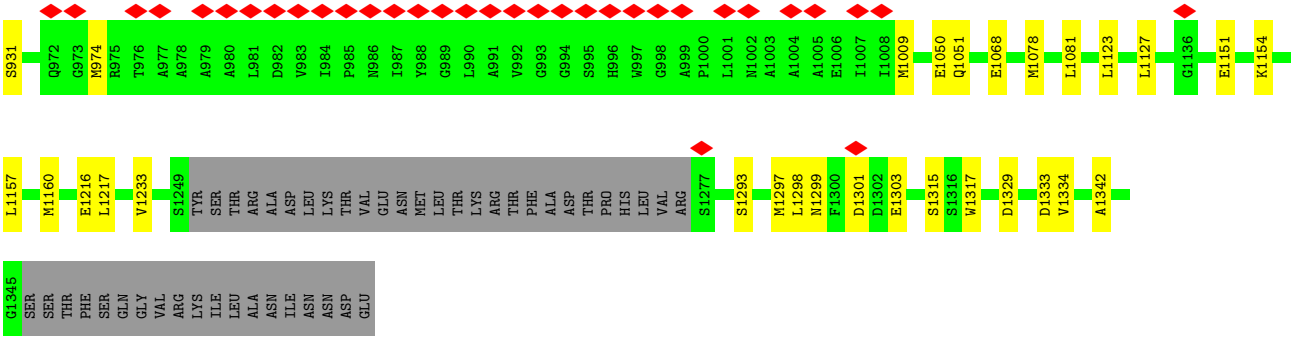


• Molecule 2: Toxin subunit YenA2

Chain J:



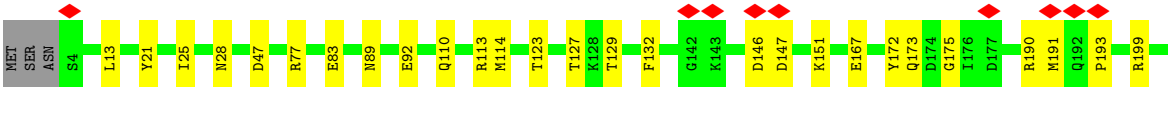


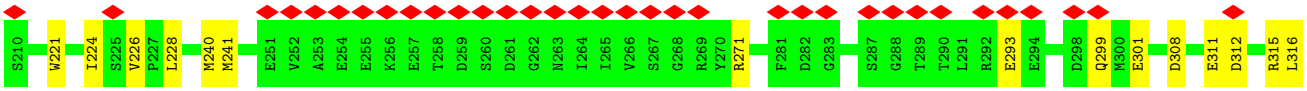


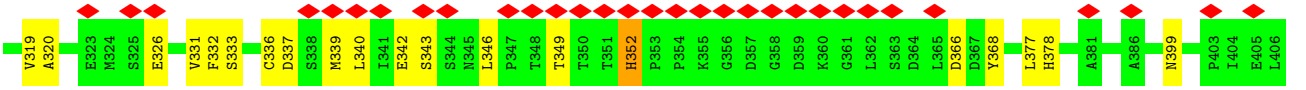
• Molecule 2: Toxin subunit YenA2

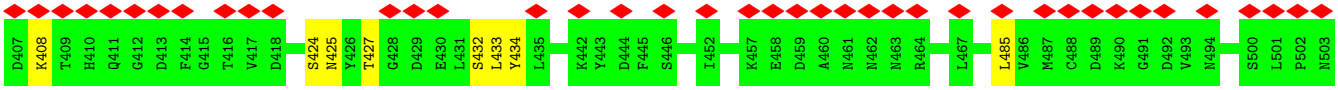
Chain M:

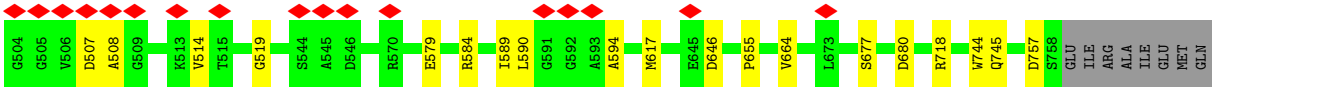


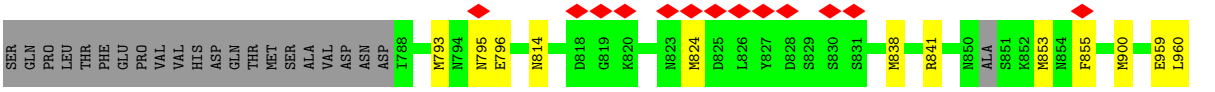


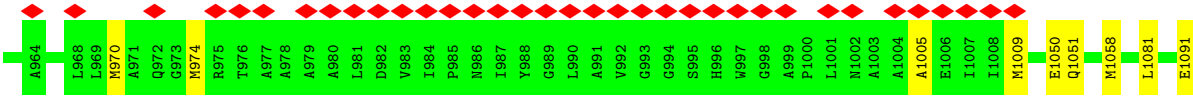


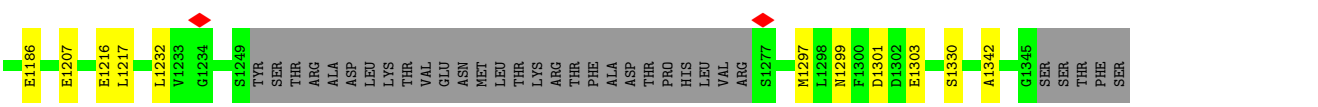




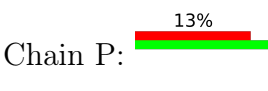








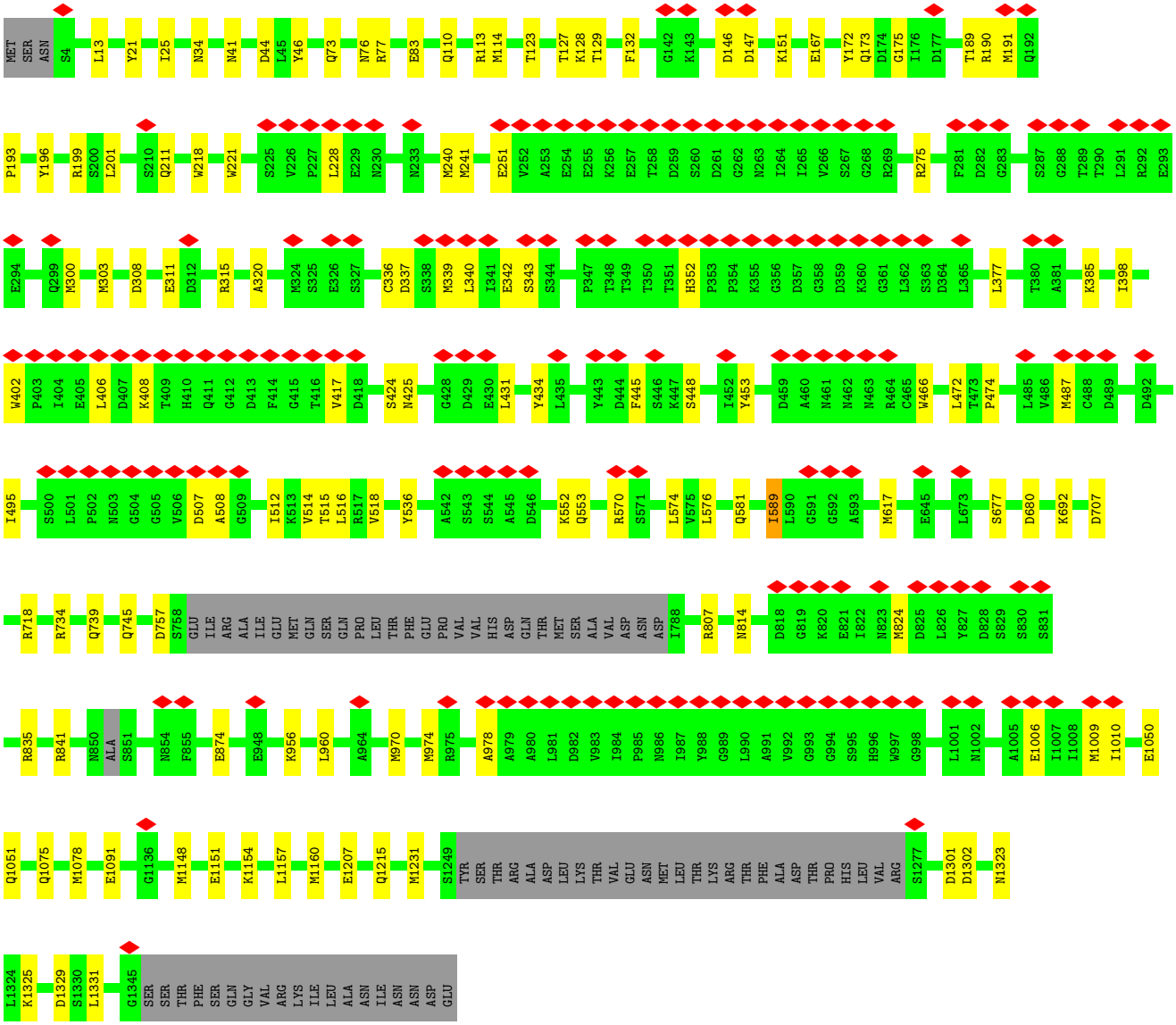




• Molecule 2: Toxin subunit YenA2

Chain P:

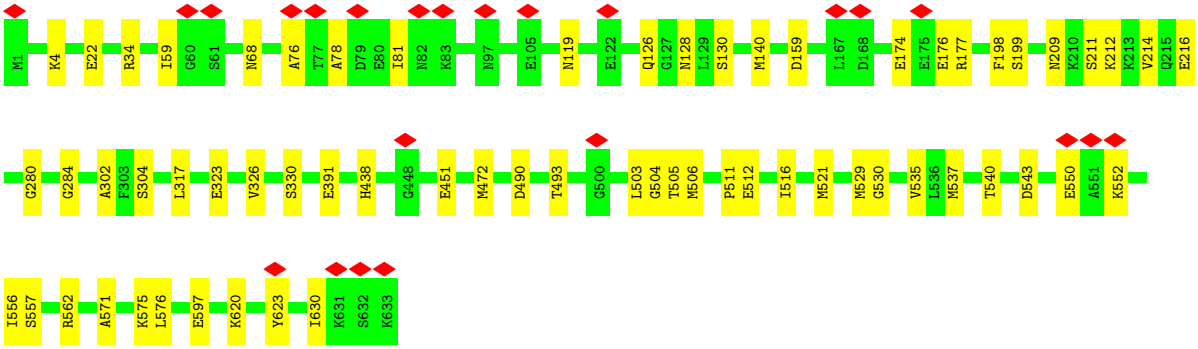




• Molecule 3: Chitinase 2

Chain C:

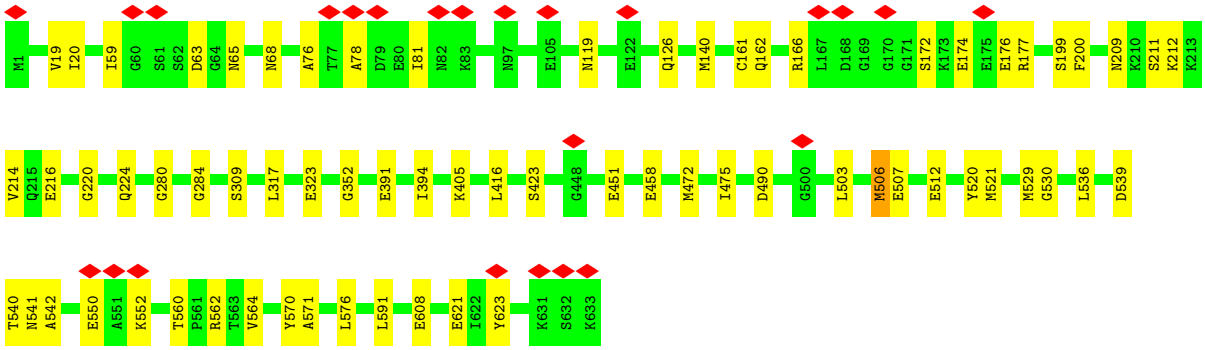




• Molecule 3: Chitinase 2

Chain H:

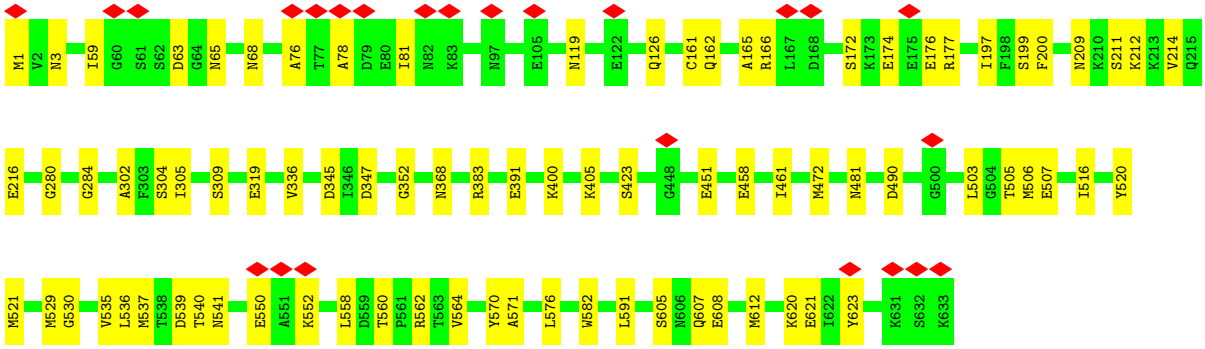




• Molecule 3: Chitinase 2

Chain K:

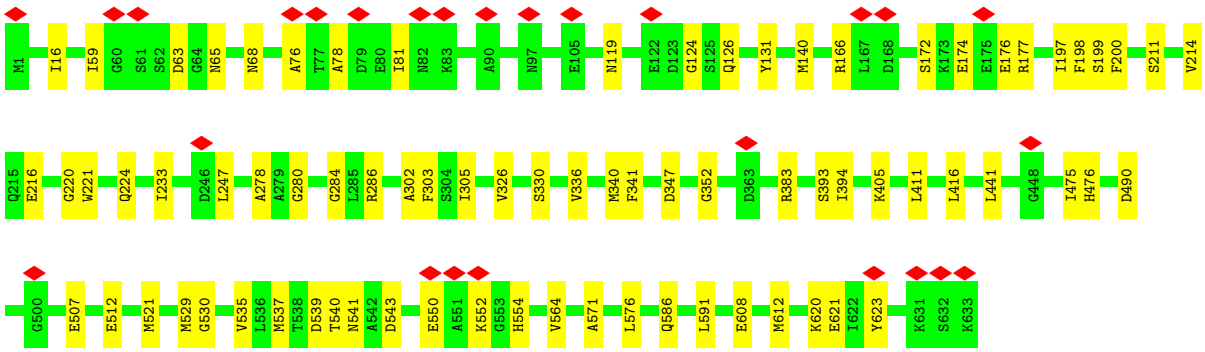




• Molecule 3: Chitinase 2

Chain N:

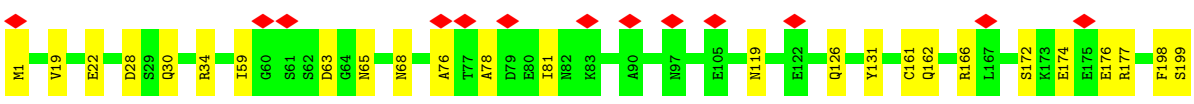


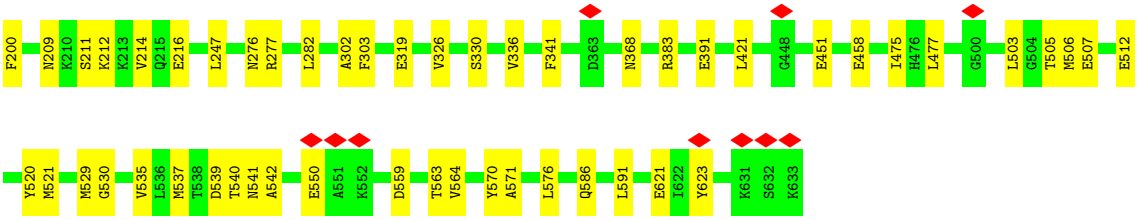


• Molecule 3: Chitinase 2

Chain Q:



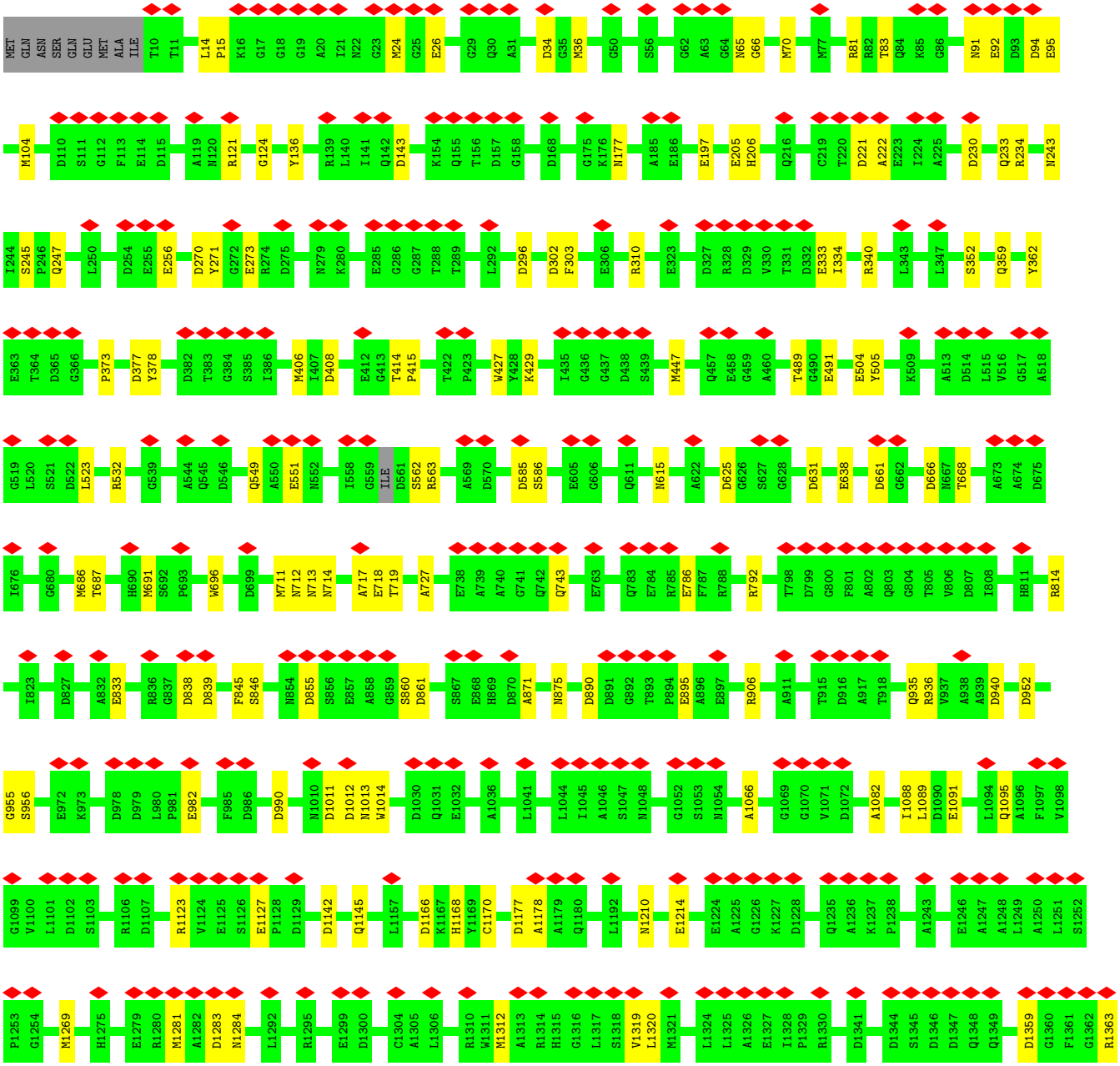


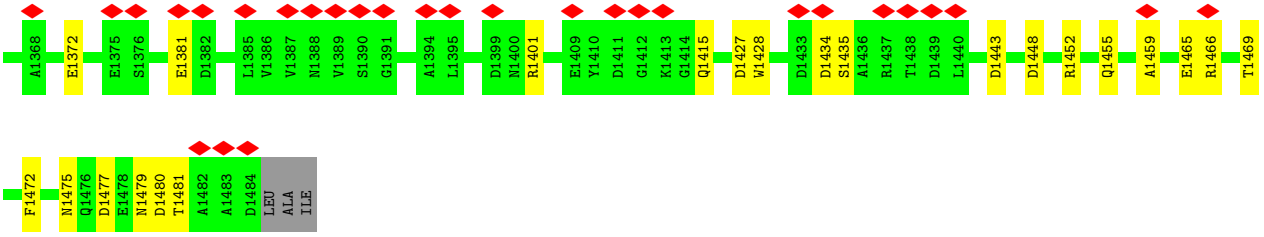


• Molecule 4: Toxin subunit YenB

Chain D:



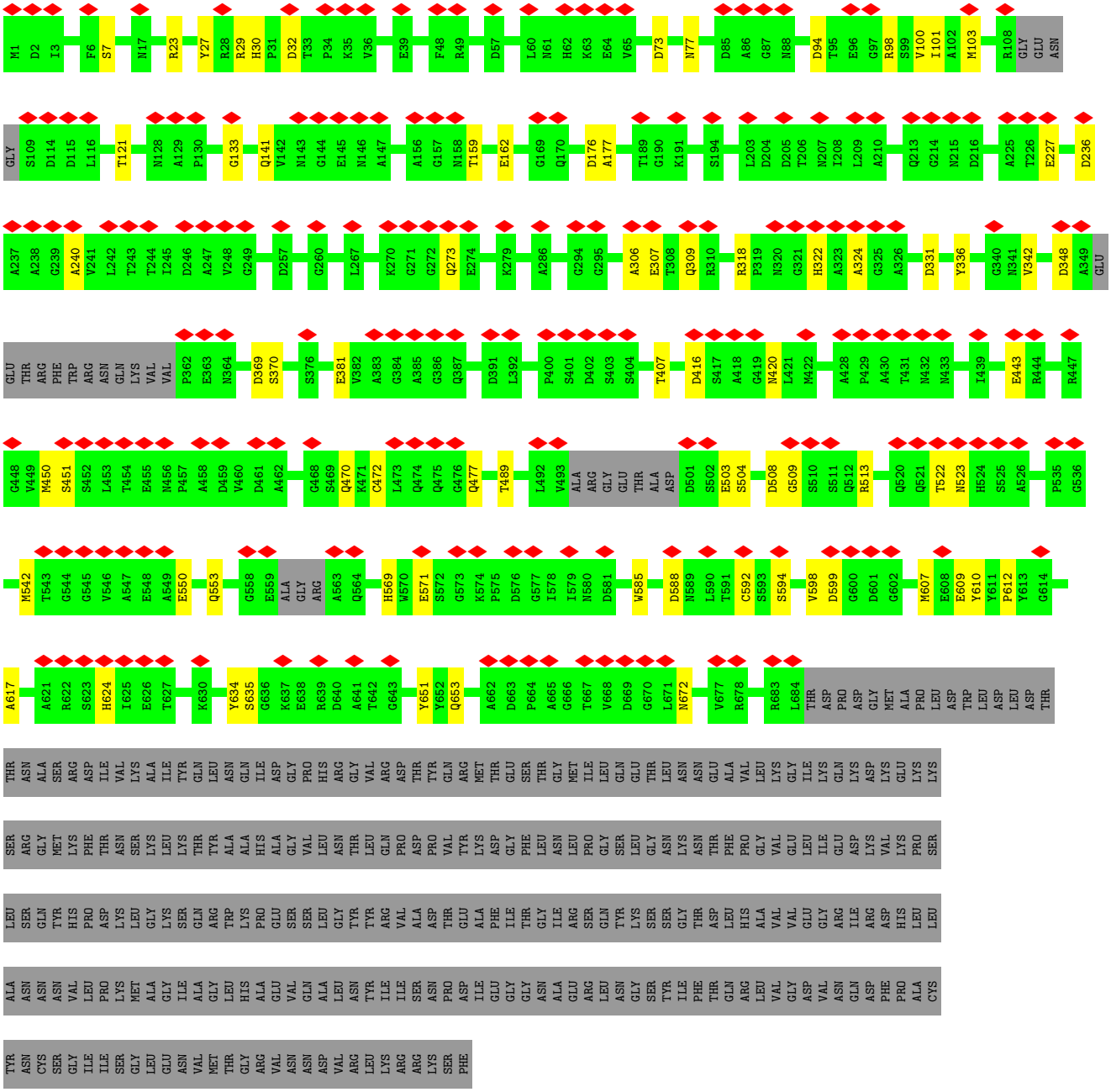




• Molecule 5: Toxin subunit YenC2

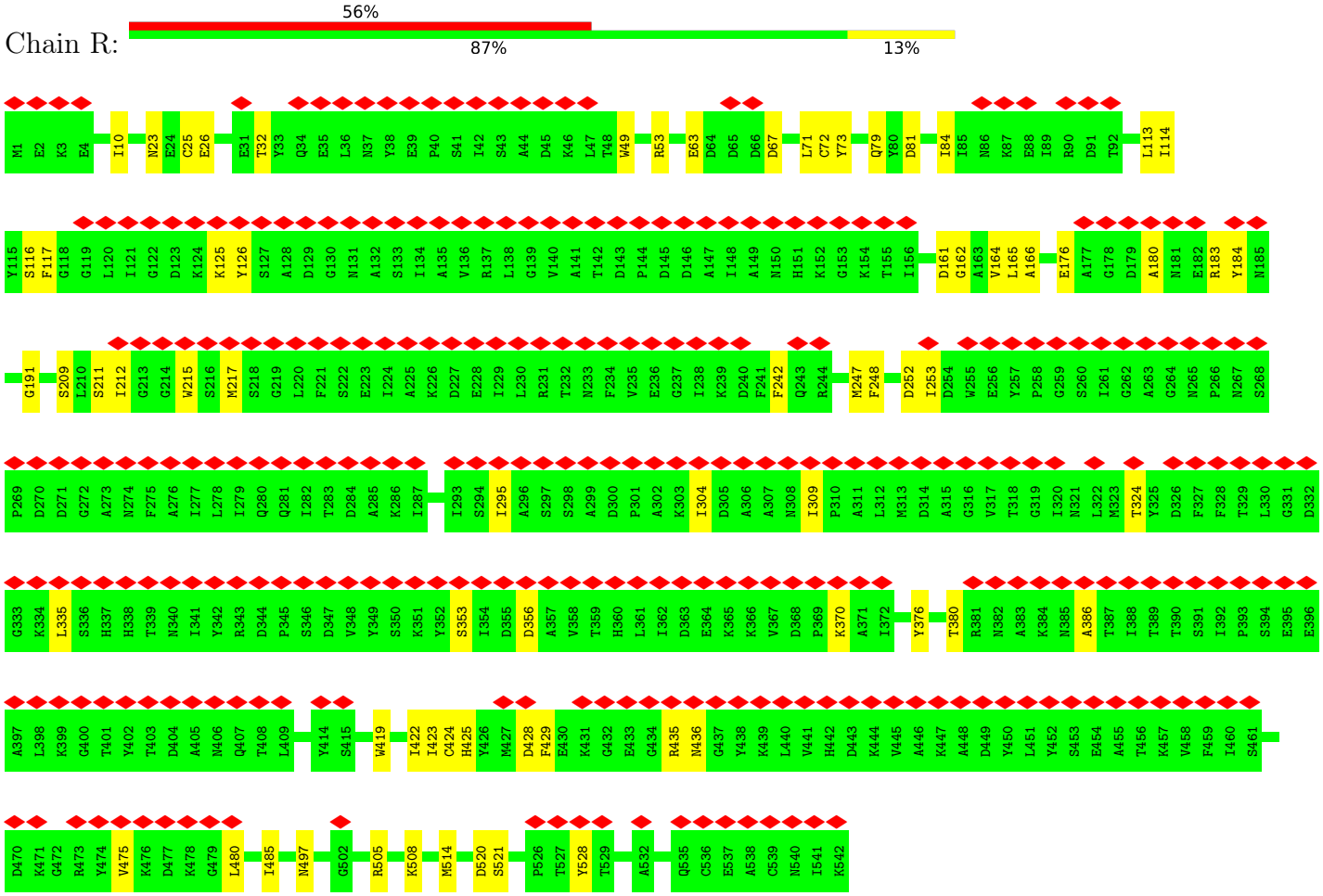
Chain E:





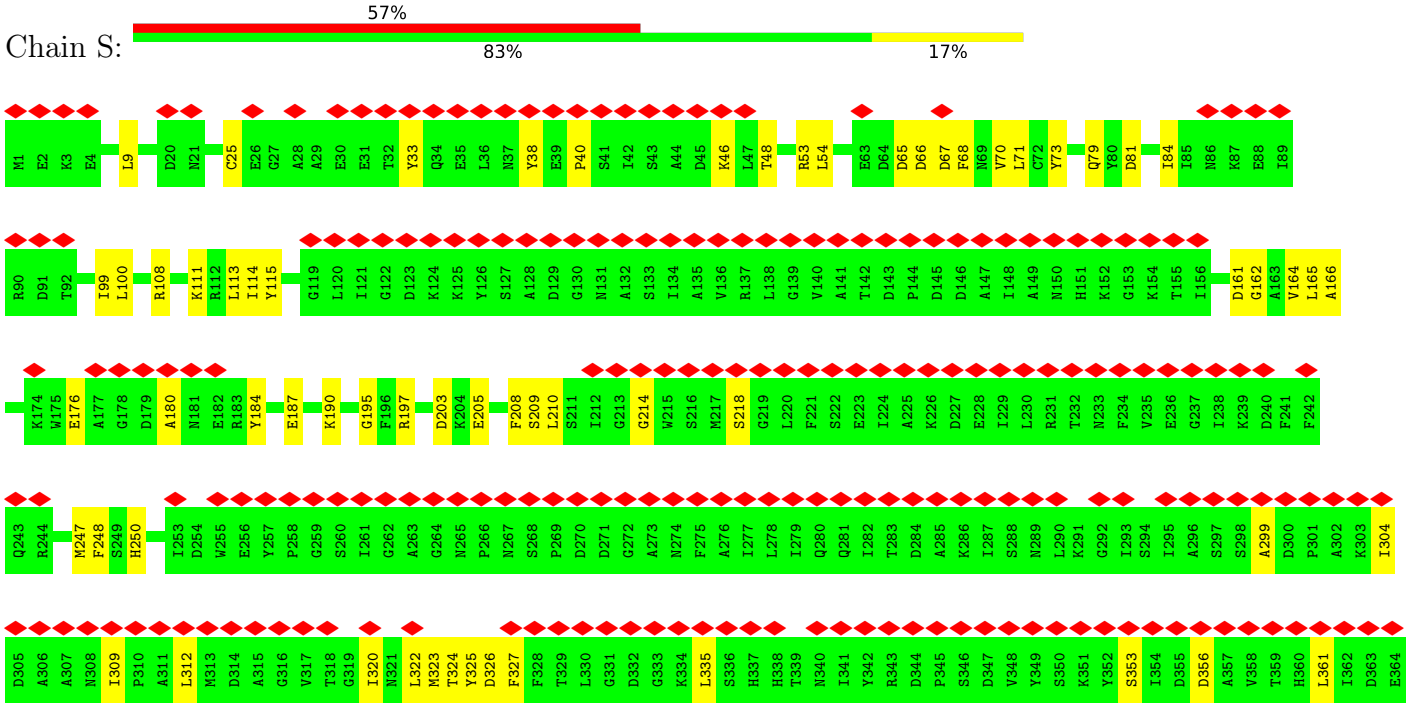
• Molecule 6: Chitinase 1

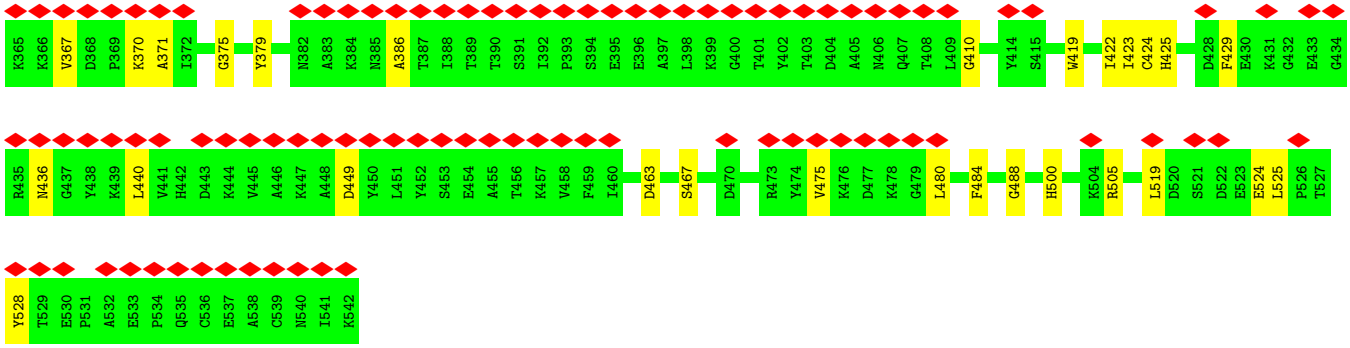
Chain R:



• Molecule 6: Chitinase 1

Chain S:

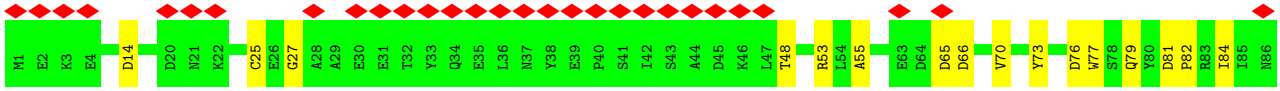


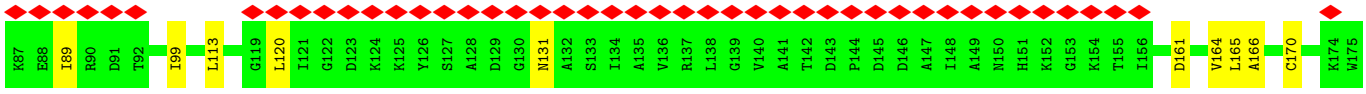


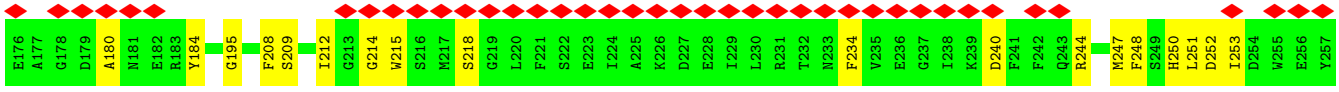
• Molecule 6: Chitinase 1

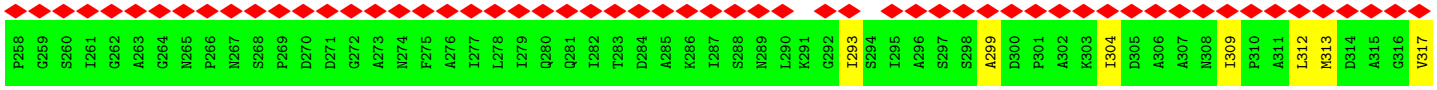
Chain T:



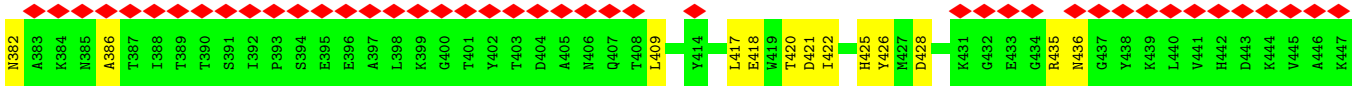


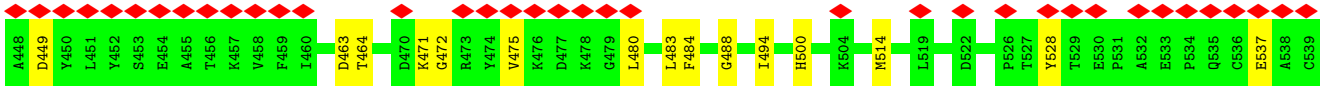








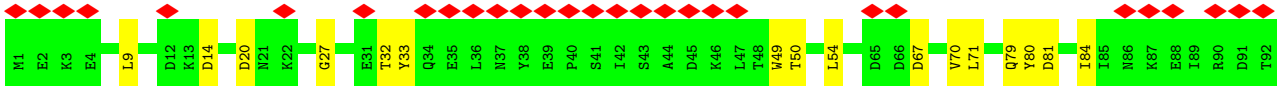


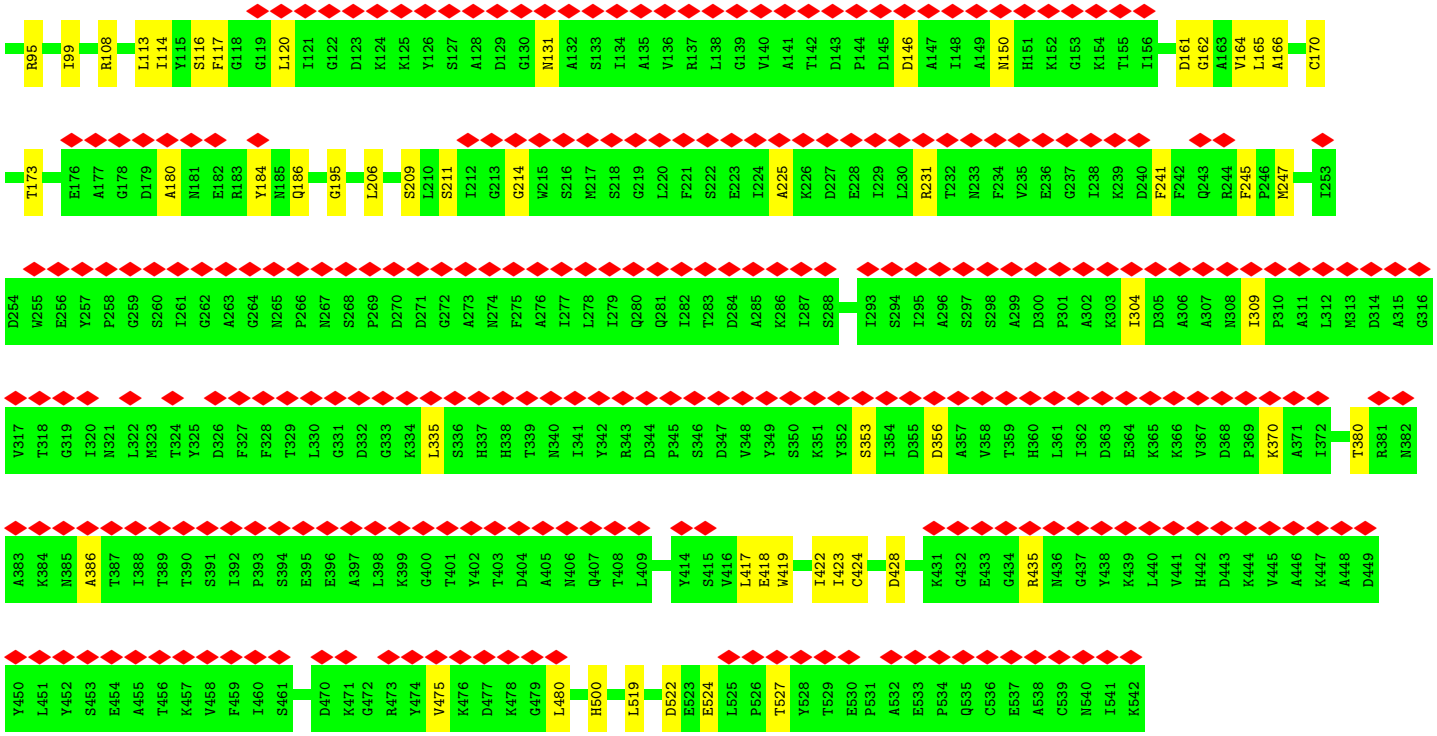


• Molecule 6: Chitinase 1

Chain U:



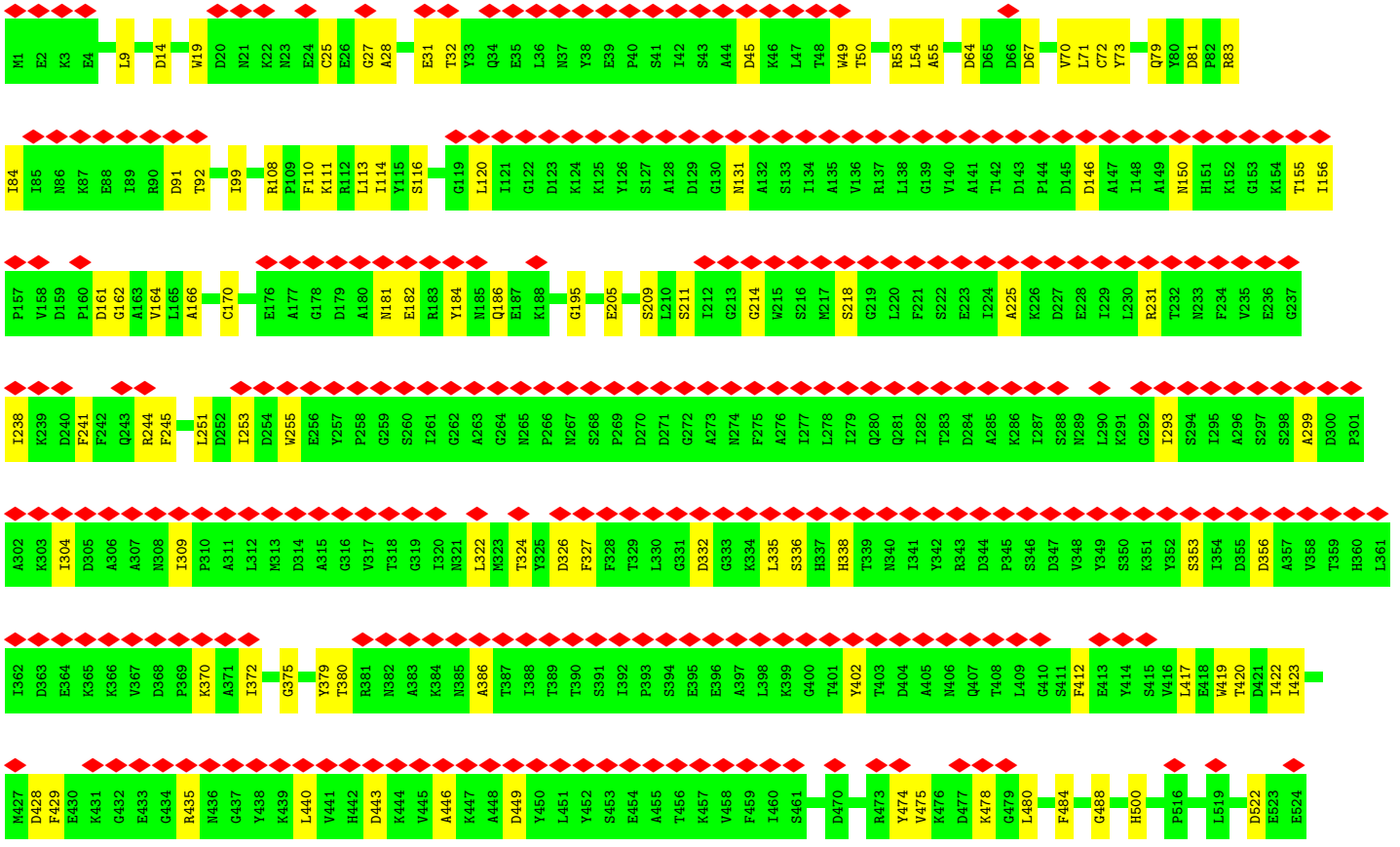


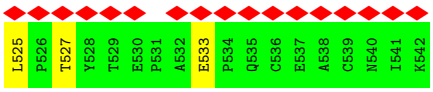


• Molecule 6: Chitinase 1

Chain V:






L525
P526
T527
Y528
T529
E530
P531
A532
E533
P534
Q535
C536
E537
A538
C539
N540
I541
K542

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	141722	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	63	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.599	Depositor
Minimum map value	0.000	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.0838	Depositor
Map size (Å)	528.0, 528.0, 528.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.13	0/8237	0.27	0/11204
1	F	0.12	0/8237	0.27	0/11204
1	I	0.13	0/8237	0.27	0/11204
1	L	0.12	0/8237	0.26	0/11204
1	O	0.12	0/8237	0.27	0/11204
2	B	0.15	0/10601	0.31	0/14366
2	G	0.16	0/10600	0.30	0/14363
2	J	0.16	0/10600	0.31	0/14363
2	M	0.16	0/10601	0.30	0/14366
2	P	0.15	0/10601	0.29	0/14366
3	C	0.13	0/5033	0.30	0/6818
3	H	0.13	0/5033	0.28	0/6818
3	K	0.13	0/5033	0.30	0/6818
3	N	0.13	0/5033	0.29	0/6818
3	Q	0.13	0/5033	0.28	0/6818
4	D	0.10	0/12010	0.25	0/16371
5	E	0.10	0/5207	0.27	0/7086
6	R	0.11	0/4356	0.29	0/5900
6	S	0.10	0/4356	0.28	0/5900
6	T	0.11	0/4356	0.29	0/5900
6	U	0.10	0/4356	0.26	0/5900
6	V	0.10	0/4356	0.27	0/5900
All	All	0.13	0/158350	0.28	0/214891

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)

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	8078	0	8029	89	0
1	F	8078	0	8029	77	0
1	I	8078	0	8029	75	0
1	L	8078	0	8029	67	0
1	O	8078	0	8029	83	0
2	B	10384	0	10134	83	0
2	G	10384	0	10133	86	0
2	J	10384	0	10133	96	0
2	M	10384	0	10134	84	0
2	P	10384	0	10134	91	0
3	C	4914	0	4716	42	0
3	H	4914	0	4716	49	0
3	K	4914	0	4716	59	0
3	N	4914	0	4716	52	0
3	Q	4914	0	4716	51	0
4	D	11696	0	11142	106	0
5	E	5111	0	4959	50	0
6	R	4260	0	4098	44	0
6	S	4260	0	4098	61	0
6	T	4260	0	4098	60	0
6	U	4260	0	4098	39	0
6	V	4260	0	4098	67	0
All	All	154987	0	150984	1451	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 5.

The worst 5 of 1451 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:A:1123:MET:HE1	1:A:1158:GLN:HB2	1.44	0.97
3:Q:529:MET:HE3	3:Q:530:GLY:H	1.36	0.91
2:M:339:MET:H	2:M:339:MET:HE3	1.37	0.89
1:A:1024:LEU:HD11	1:A:1029:ILE:HG13	1.55	0.87
3:H:529:MET:HE3	3:H:530:GLY:H	1.40	0.85

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	1024/1164 (88%)	1006 (98%)	18 (2%)	0	100	100
1	F	1024/1164 (88%)	1005 (98%)	19 (2%)	0	100	100
1	I	1024/1164 (88%)	1001 (98%)	23 (2%)	0	100	100
1	L	1024/1164 (88%)	1003 (98%)	21 (2%)	0	100	100
1	O	1024/1164 (88%)	1007 (98%)	17 (2%)	0	100	100
2	B	1280/1365 (94%)	1246 (97%)	34 (3%)	0	100	100
2	G	1278/1365 (94%)	1228 (96%)	50 (4%)	0	100	100
2	J	1278/1365 (94%)	1234 (97%)	44 (3%)	0	100	100
2	M	1280/1365 (94%)	1237 (97%)	43 (3%)	0	100	100
2	P	1280/1365 (94%)	1241 (97%)	39 (3%)	0	100	100
3	C	631/633 (100%)	606 (96%)	25 (4%)	0	100	100
3	H	631/633 (100%)	605 (96%)	26 (4%)	0	100	100
3	K	631/633 (100%)	604 (96%)	27 (4%)	0	100	100
3	N	631/633 (100%)	610 (97%)	21 (3%)	0	100	100
3	Q	631/633 (100%)	613 (97%)	18 (3%)	0	100	100
4	D	1472/1487 (99%)	1436 (98%)	36 (2%)	0	100	100
5	E	648/970 (67%)	630 (97%)	18 (3%)	0	100	100
6	R	540/542 (100%)	521 (96%)	19 (4%)	0	100	100
6	S	540/542 (100%)	519 (96%)	21 (4%)	0	100	100
6	T	540/542 (100%)	517 (96%)	23 (4%)	0	100	100
6	U	540/542 (100%)	516 (96%)	24 (4%)	0	100	100
6	V	540/542 (100%)	519 (96%)	21 (4%)	0	100	100
All	All	19491/20977 (93%)	18904 (97%)	587 (3%)	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	898/1022 (88%)	896 (100%)	2 (0%)	87	87
1	F	898/1022 (88%)	898 (100%)	0	100	100
1	I	898/1022 (88%)	898 (100%)	0	100	100
1	L	898/1022 (88%)	896 (100%)	2 (0%)	87	87
1	O	898/1022 (88%)	898 (100%)	0	100	100
2	B	1136/1210 (94%)	1133 (100%)	3 (0%)	86	85
2	G	1136/1210 (94%)	1135 (100%)	1 (0%)	88	89
2	J	1136/1210 (94%)	1136 (100%)	0	100	100
2	M	1136/1210 (94%)	1133 (100%)	3 (0%)	86	85
2	P	1136/1210 (94%)	1134 (100%)	2 (0%)	87	87
3	C	520/520 (100%)	520 (100%)	0	100	100
3	H	520/520 (100%)	519 (100%)	1 (0%)	87	87
3	K	520/520 (100%)	520 (100%)	0	100	100
3	N	520/520 (100%)	520 (100%)	0	100	100
3	Q	520/520 (100%)	520 (100%)	0	100	100
4	D	1255/1266 (99%)	1255 (100%)	0	100	100
5	E	551/818 (67%)	551 (100%)	0	100	100
6	R	455/455 (100%)	455 (100%)	0	100	100
6	S	455/455 (100%)	455 (100%)	0	100	100
6	T	455/455 (100%)	455 (100%)	0	100	100
6	U	455/455 (100%)	455 (100%)	0	100	100
6	V	455/455 (100%)	455 (100%)	0	100	100
All	All	16851/18119 (93%)	16837 (100%)	14 (0%)	87	89

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

Mol	Chain	Res	Type
1	L	644	TYR
1	L	717	THR
2	P	589	ILE
2	M	377	LEU
2	P	352	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 126 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	929	ASN
2	P	1326	GLN
3	K	481	ASN
2	P	1057	ASN
6	T	250	HIS

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	E	1
2	J	1
2	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	109:SER	C	114:ASP	N	5.53
1	J	299:GLN	C	300:MET	N	3.65
1	G	299:GLN	C	300:MET	N	3.64

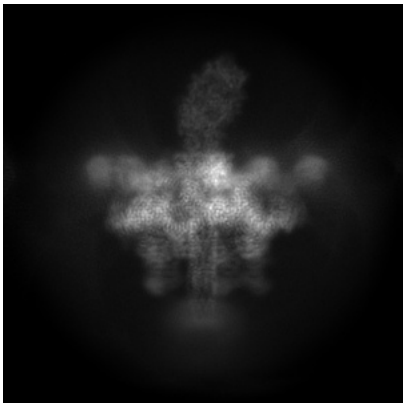
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-58581. These allow visual inspection of the internal detail of the map and identification of artifacts.

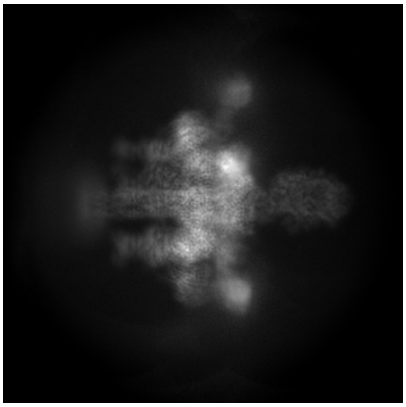
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

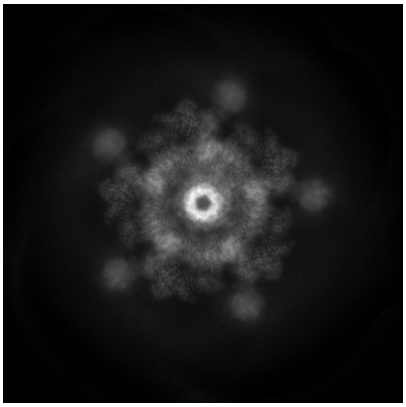
6.1.1 Primary map



X



Y

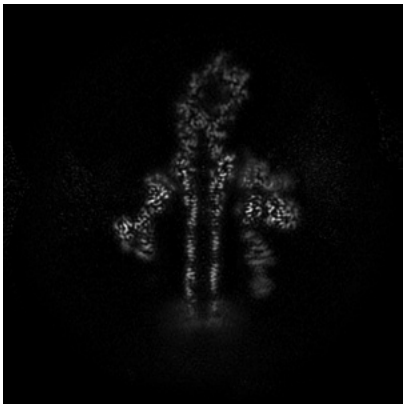


Z

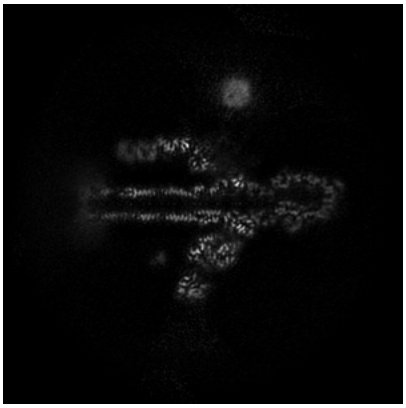
The images above show the map projected in three orthogonal directions.

6.2 Central slices

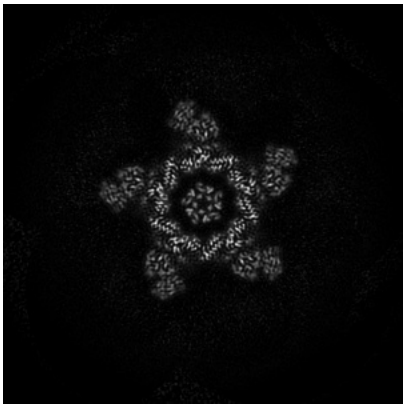
6.2.1 Primary map



X Index: 300



Y Index: 300



Z Index: 300

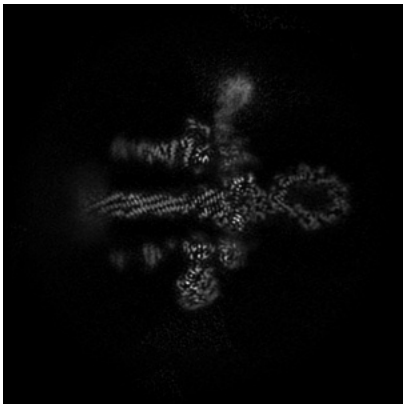
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

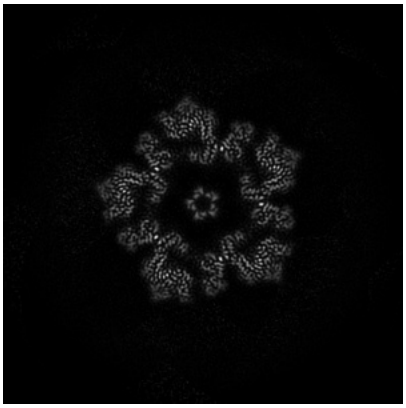
6.3.1 Primary map



X Index: 313



Y Index: 318

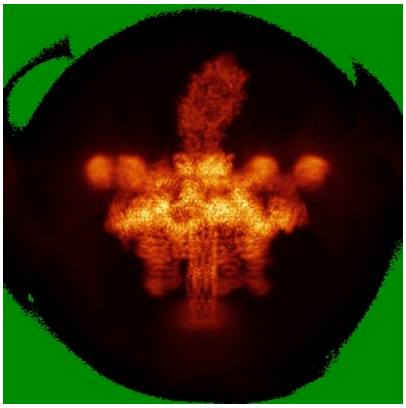


Z Index: 276

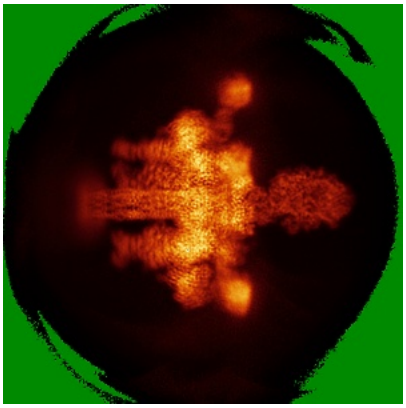
The images above show the largest variance slices of the map in three orthogonal directions.

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

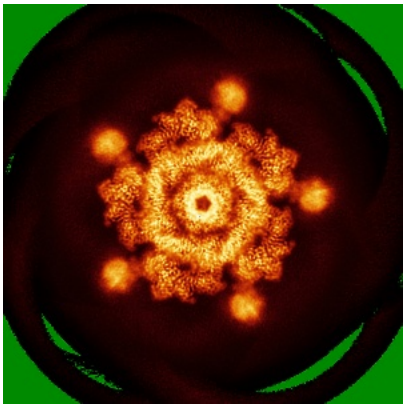
6.4.1 Primary map



X



Y

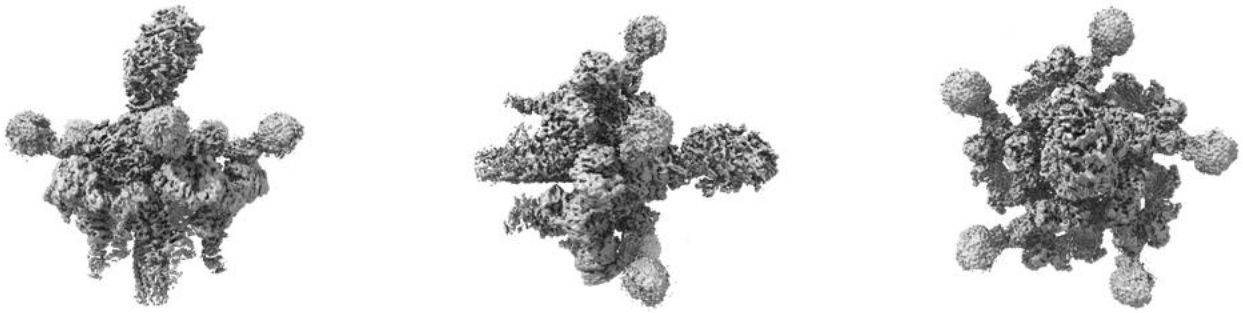


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0838. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

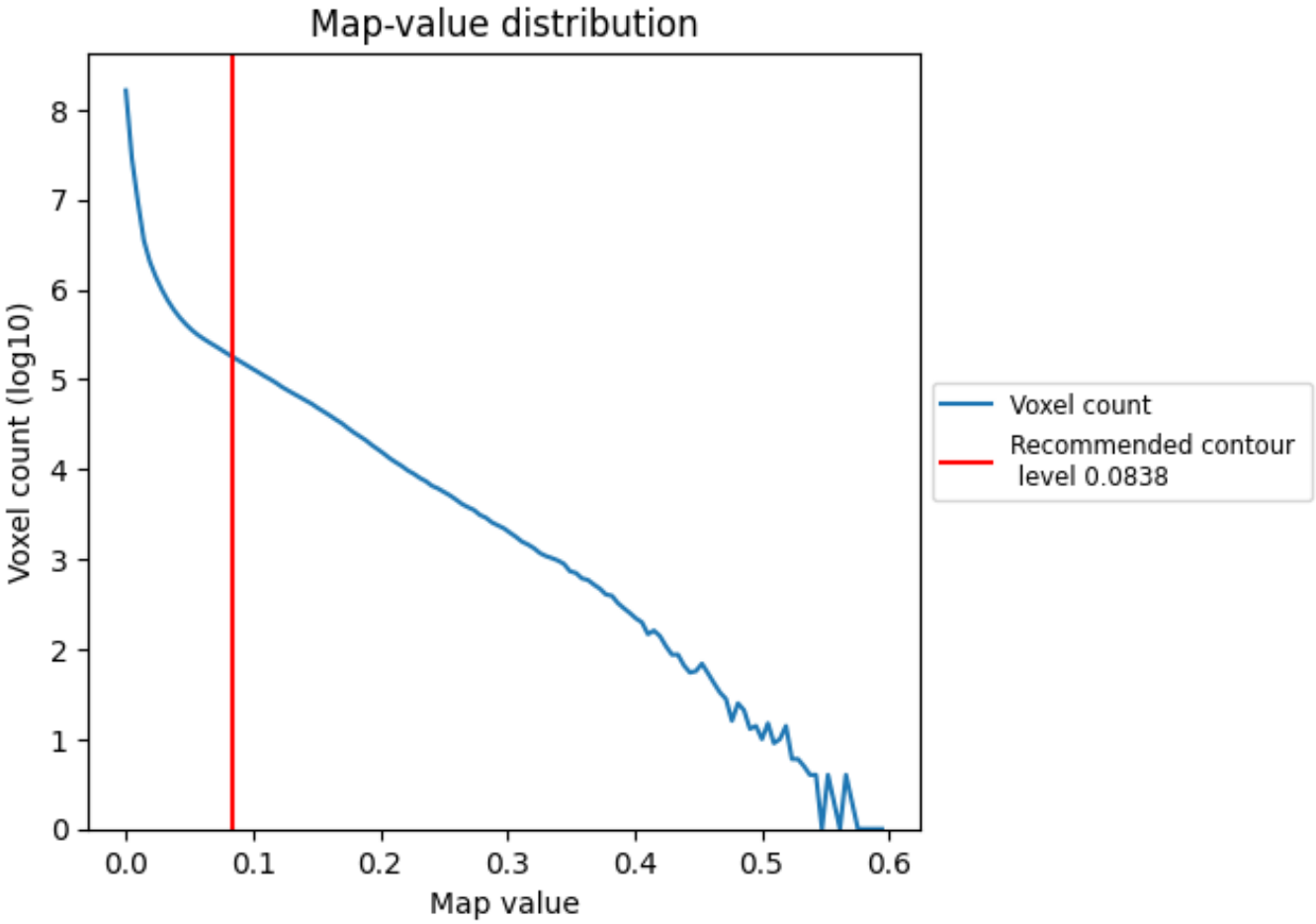
6.6 Mask visualisation (i)

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

7 Map analysis

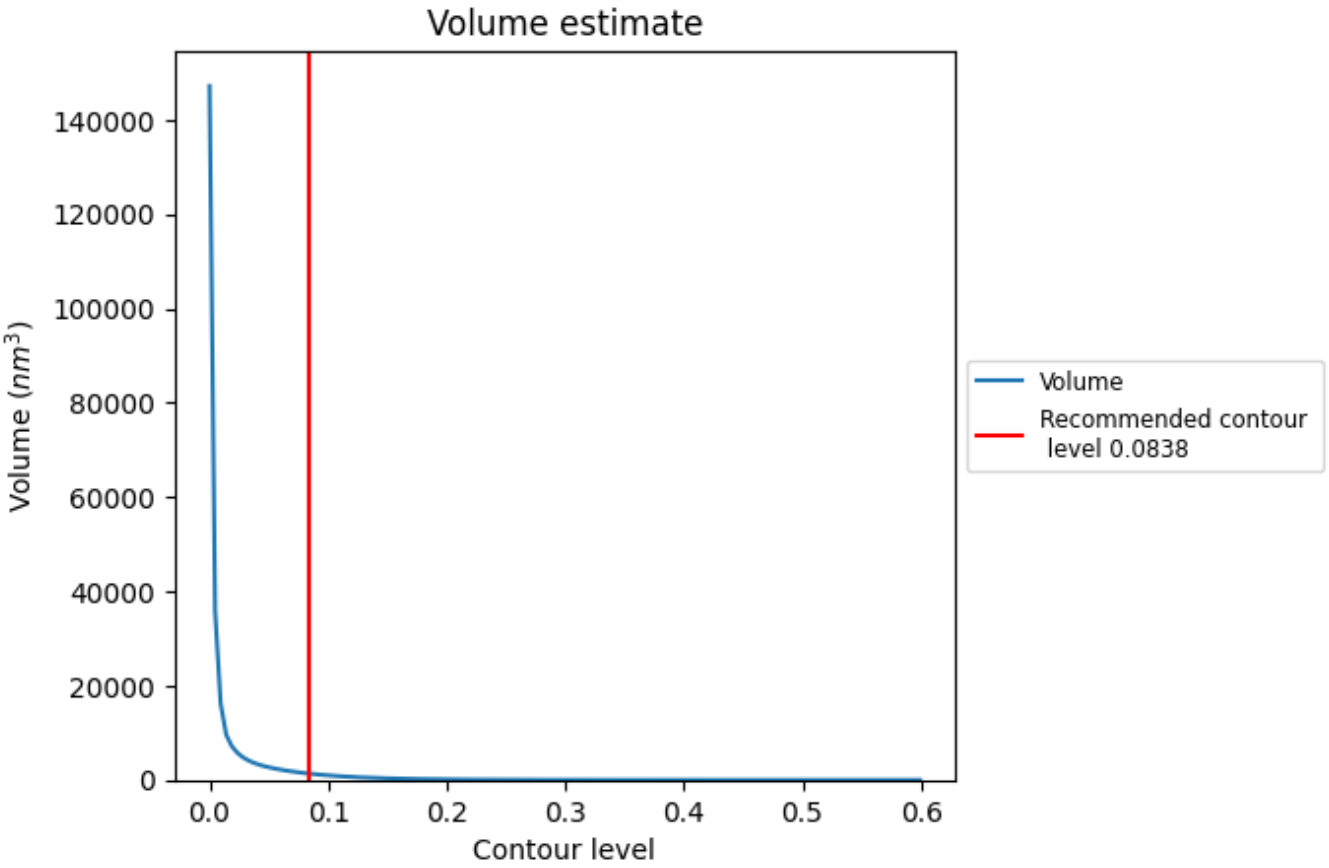
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

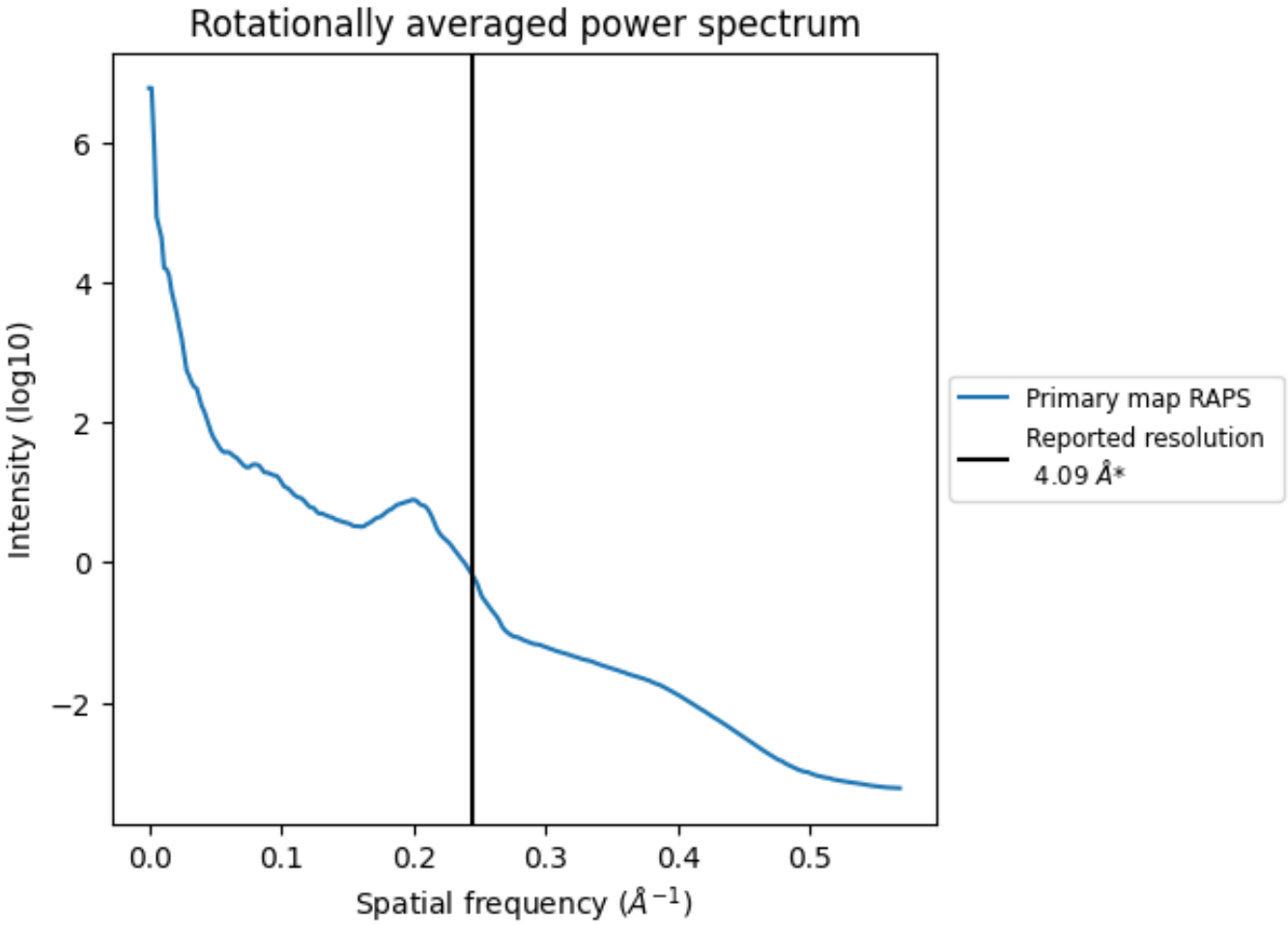
7.2 Volume estimate



The volume at the recommended contour level is 1347 nm^3; this corresponds to an approximate mass of 1217 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 0.244 Å^{-1}

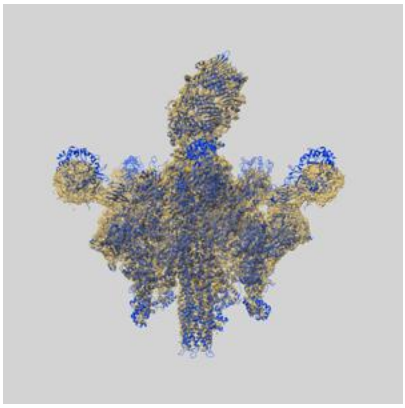
8 Fourier-Shell correlation (i)

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

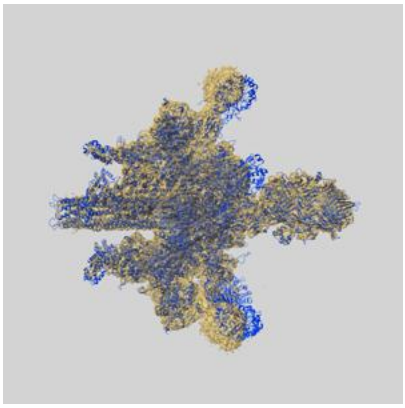
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-58581 and PDB model 31OD. Per-residue inclusion information can be found in section 3 on page 7.

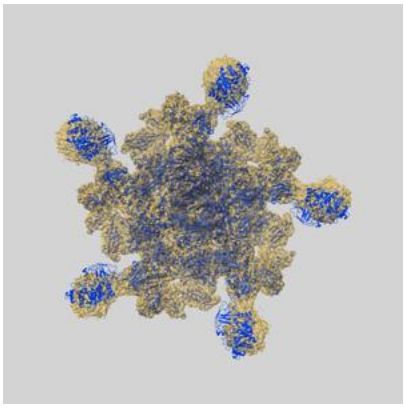
9.1 Map-model overlay



X



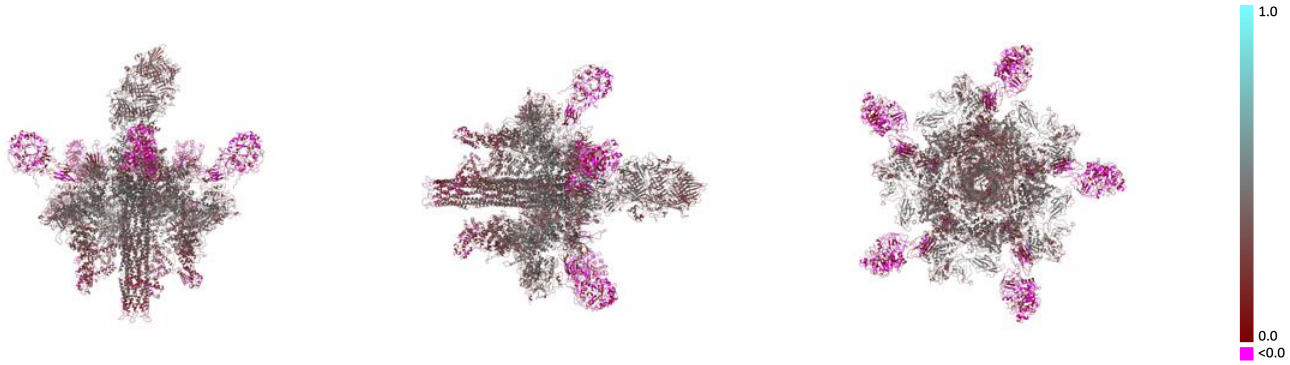
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0838 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.

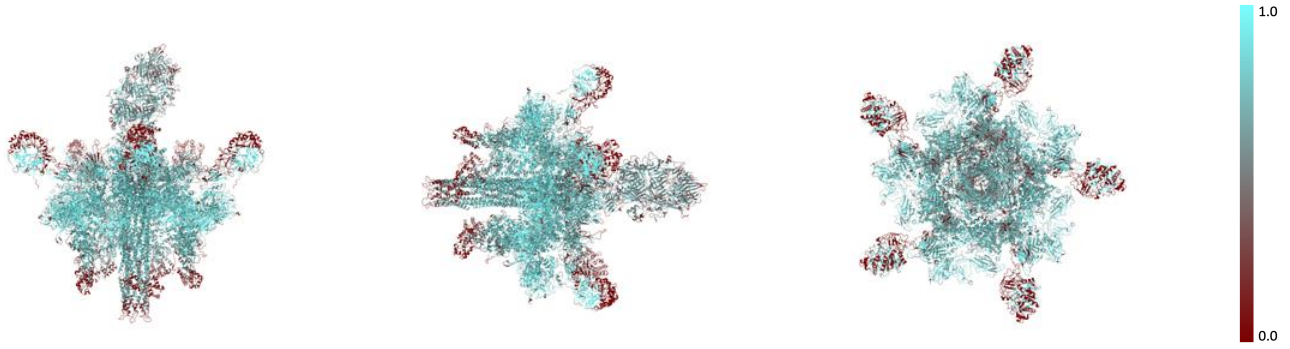
9.2 Q-score mapped to coordinate model (i)



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.

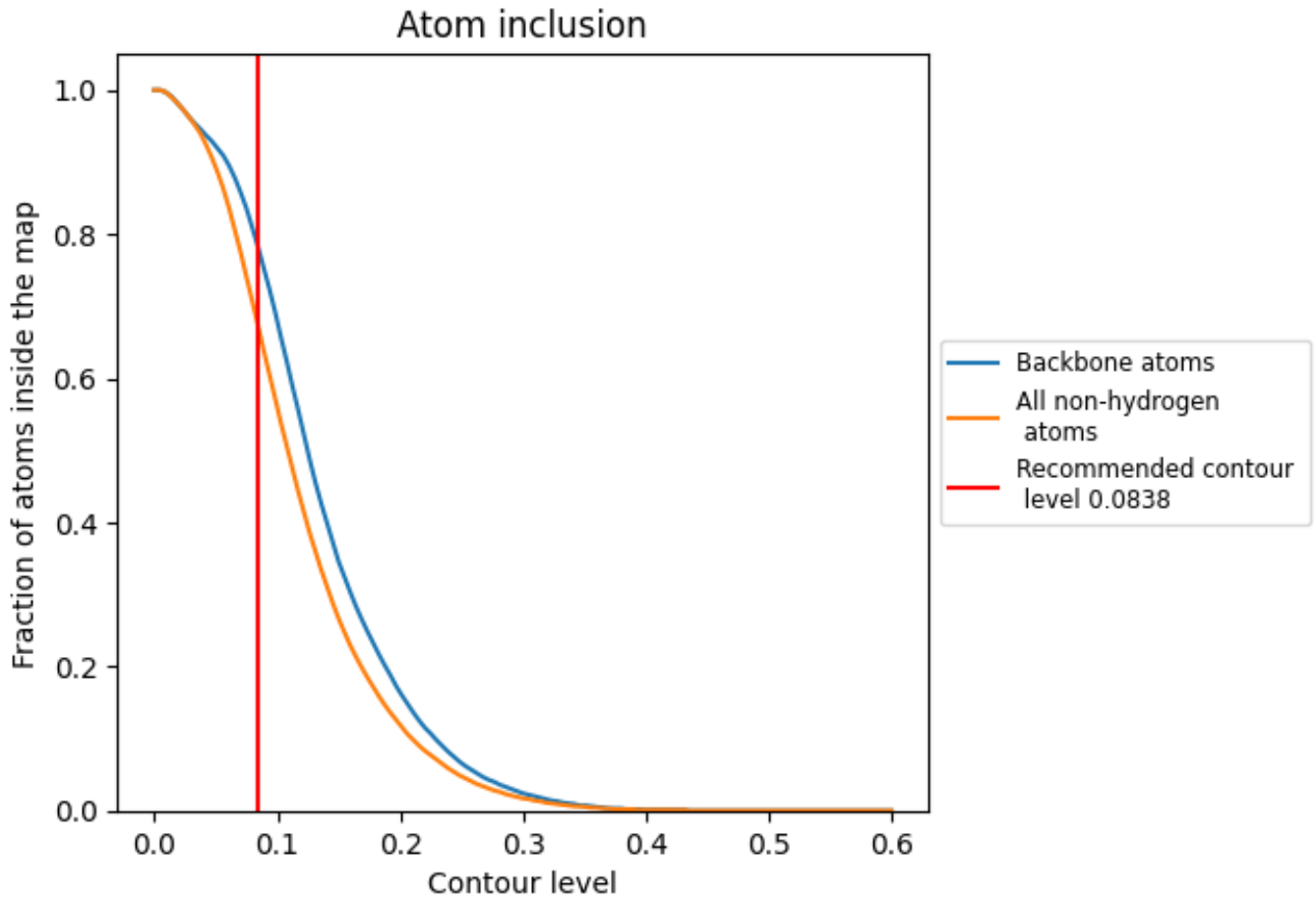
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0838).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0838) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6780	0.3050
A	0.6840	0.3300
B	0.7430	0.3520
C	0.8460	0.3750
D	0.5810	0.3620
E	0.5040	0.3230
F	0.6810	0.3300
G	0.7380	0.3460
H	0.8410	0.3740
I	0.6810	0.3290
J	0.7410	0.3470
K	0.8440	0.3730
L	0.6810	0.3300
M	0.7430	0.3440
N	0.8430	0.3740
O	0.6810	0.3300
P	0.7400	0.3470
Q	0.8450	0.3740
R	0.4300	0.0480
S	0.4200	0.0320
T	0.4300	0.0410
U	0.4190	0.0370
V	0.3870	0.0390

