wwPDB EM Validation Summary Report (i)

Mar 9, 2024 – 01:31 PM EST

PDB ID	:	6OGD
EMDB ID	:	EMD-20053
Title	:	Cryo-EM structure of YenTcA in its prepore state
Authors	:	Piper, S.J.; Brillault, L.; Box, J.K.; Landsberg, M.J.
Deposited on	:	2019-04-02
Resolution	:	4.40 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:

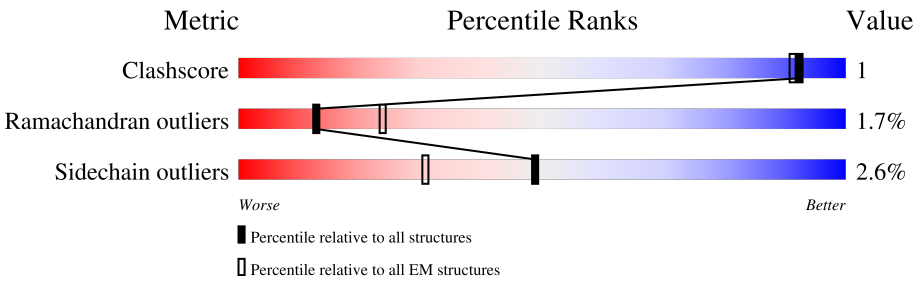
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 4.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	1164	6% 60% • 36%
1	D	1164	6% 60% • 36%
1	G	1164	6% 60% • 36%
1	J	1164	6% 60% • 36%
1	M	1164	6% 60% • 36%
2	B	1364	8% 70% 8% • 21%
2	E	1364	7% 70% 8% • 21%
2	H	1364	7% 71% 7% • 21%

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Mol	Chain	Length	Quality of chain
2	K	1364	8% 70% 8% • 21%
2	N	1364	7% 70% 8% • 21%
3	C	633	38% 80% • 15%
3	F	633	38% 80% 5% 15%
3	I	633	38% 80% 5% 15%
3	L	633	38% 80% 5% 15%
3	O	633	38% 80% • 15%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 94125 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
			Total	C	N	O	S		
1	A	748	5910	3766	983	1145	16	0	0
1	D	748	5910	3766	983	1145	16	0	0
1	G	748	5910	3766	983	1145	16	0	0
1	J	748	5910	3766	983	1145	16	0	0
1	M	748	5910	3766	983	1145	16	0	0

- Molecule 2 is a protein called Toxin subunit YenA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1078	8742	5535	1489	1688	30	0	0
2	E	1078	8742	5535	1489	1688	30	0	0
2	H	1078	8742	5535	1489	1688	30	0	0
2	K	1078	8742	5535	1489	1688	30	0	0
2	N	1078	8742	5535	1489	1688	30	0	0

- Molecule 3 is a protein called Chitinase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	538	4173	2641	697	818	17	0	0
3	F	538	4173	2641	697	818	17	0	0
3	I	538	4173	2641	697	818	17	0	0

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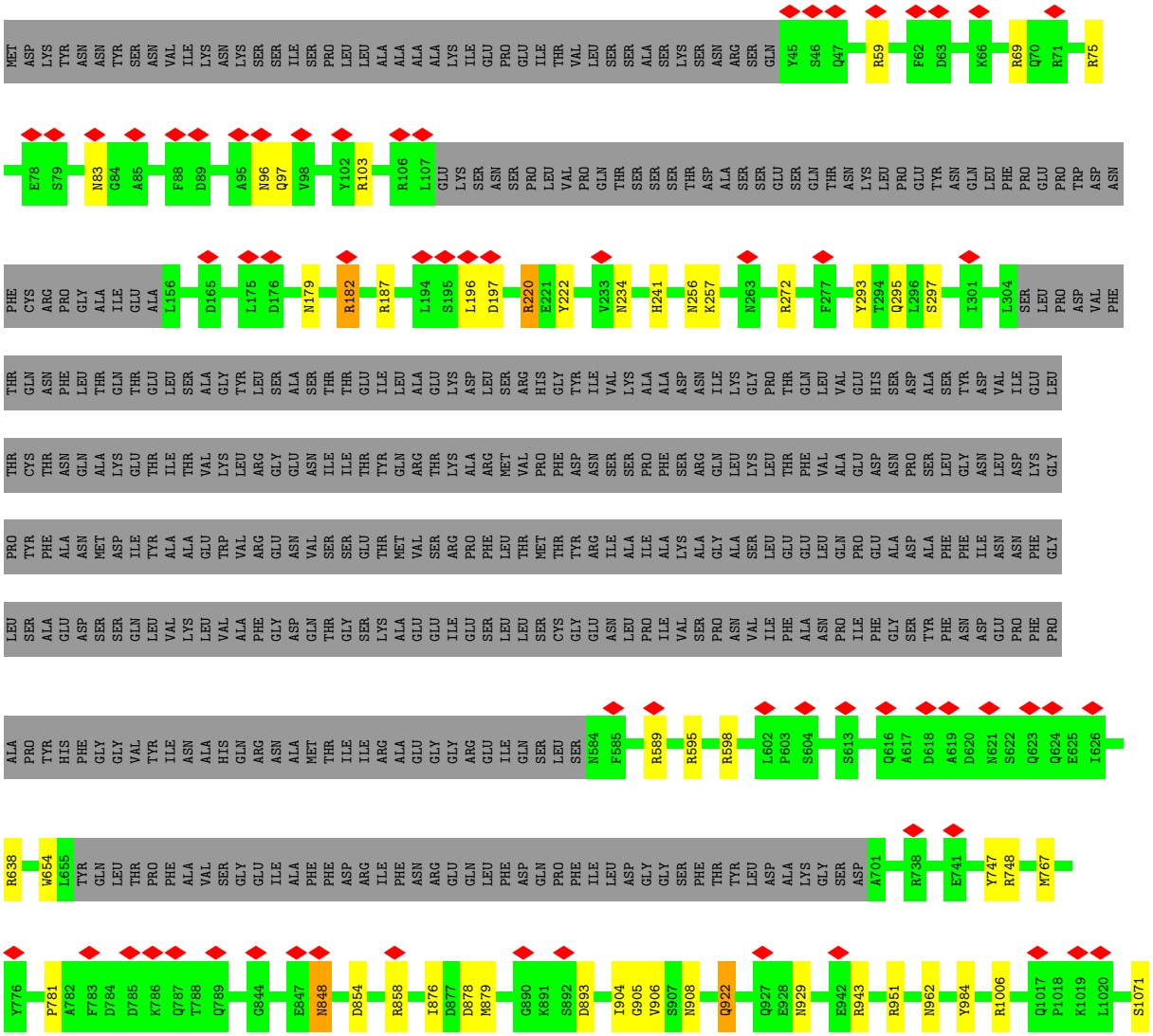
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	L	538	4173	2641	697	818	17	0	0
			Total	C	N	O	S		
3	O	538	4173	2641	697	818	17	0	0

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.

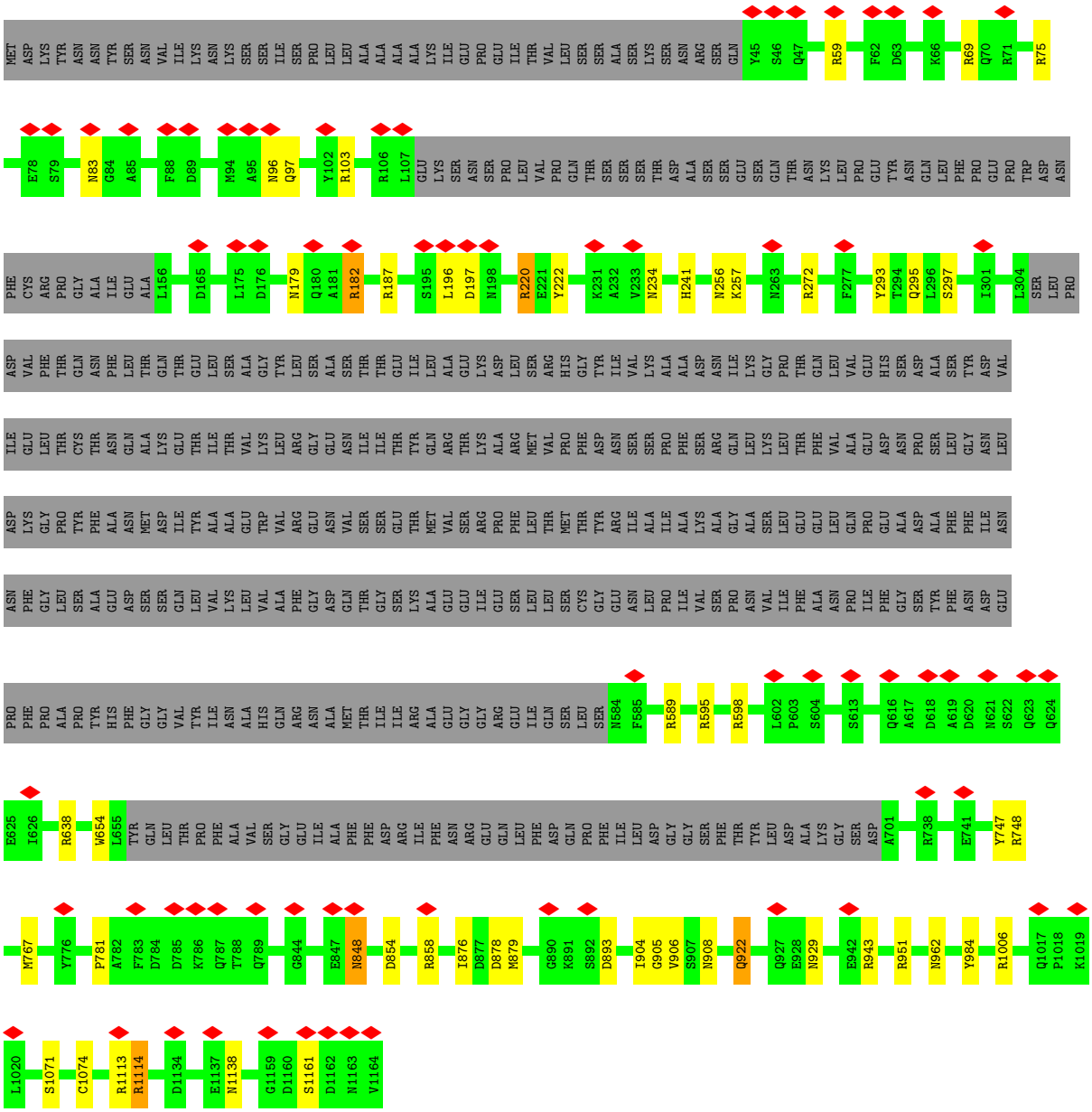
- Molecule 1: Toxin subunit YenA1

Chain A:



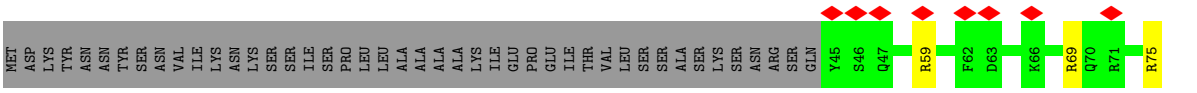
• Molecule 1: Toxin subunit YenA1

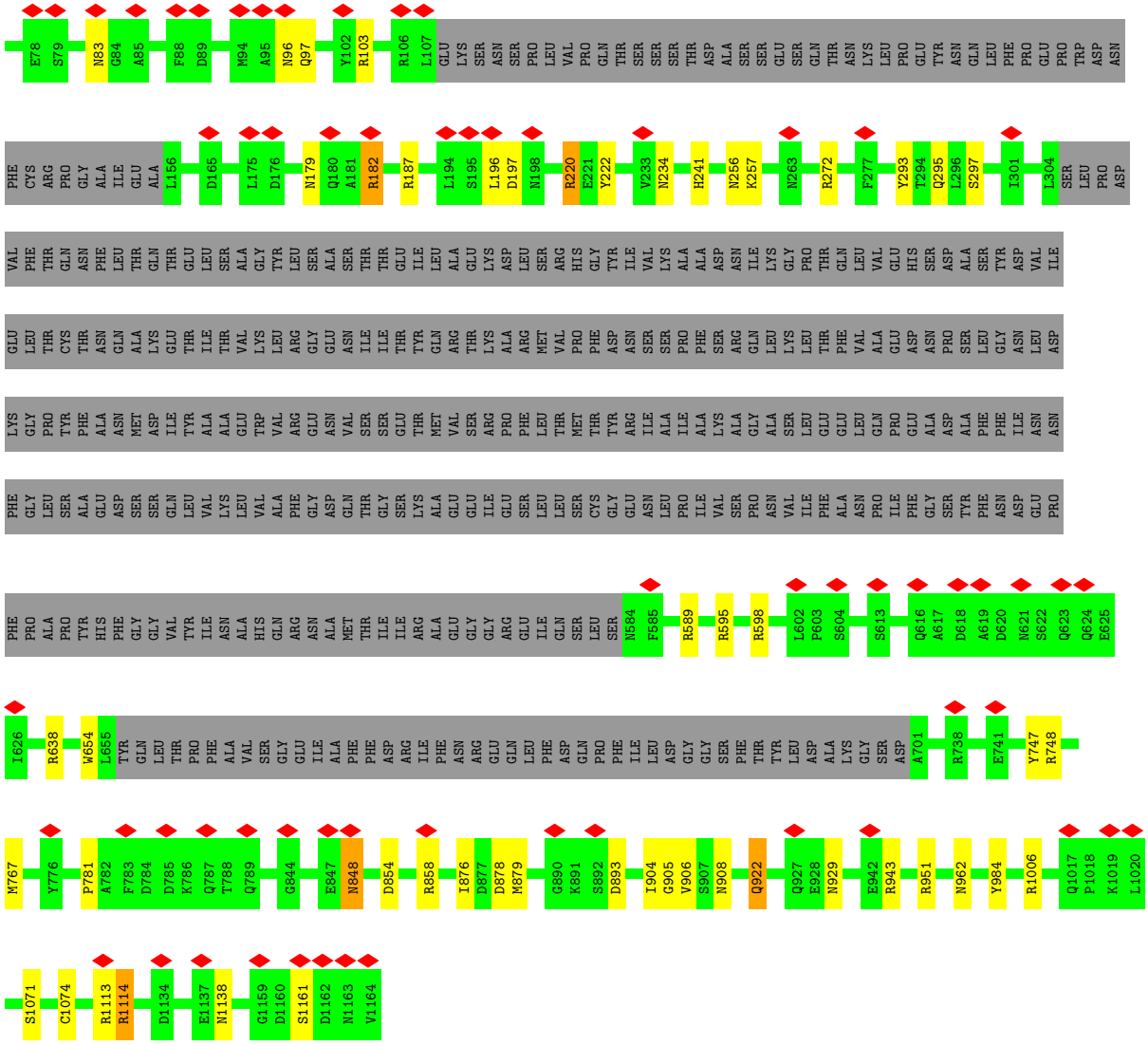
Chain D:



• Molecule 1: Toxin subunit YenA1

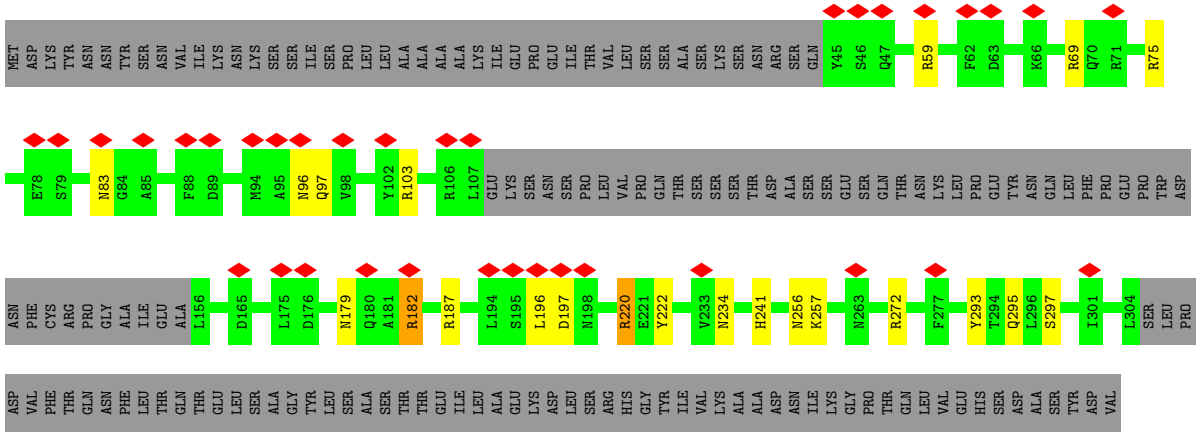
Chain G:

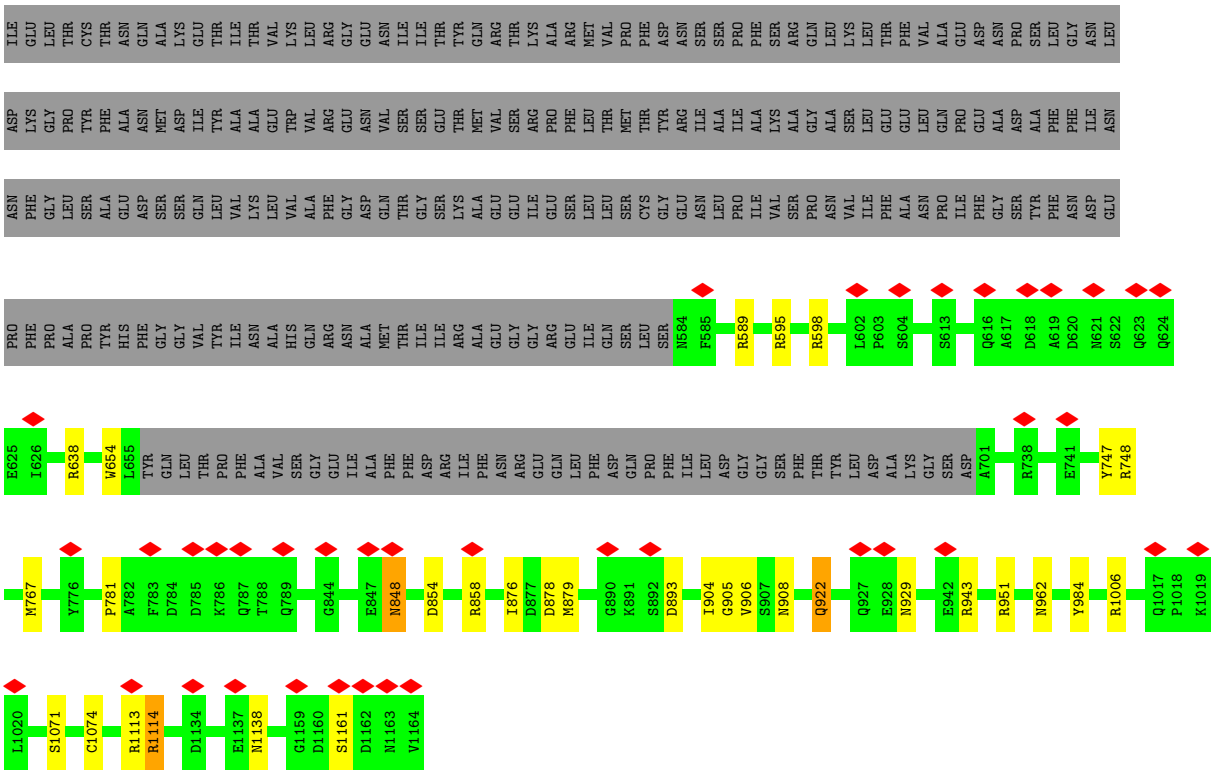




- Molecule 1: Toxin subunit YenA1

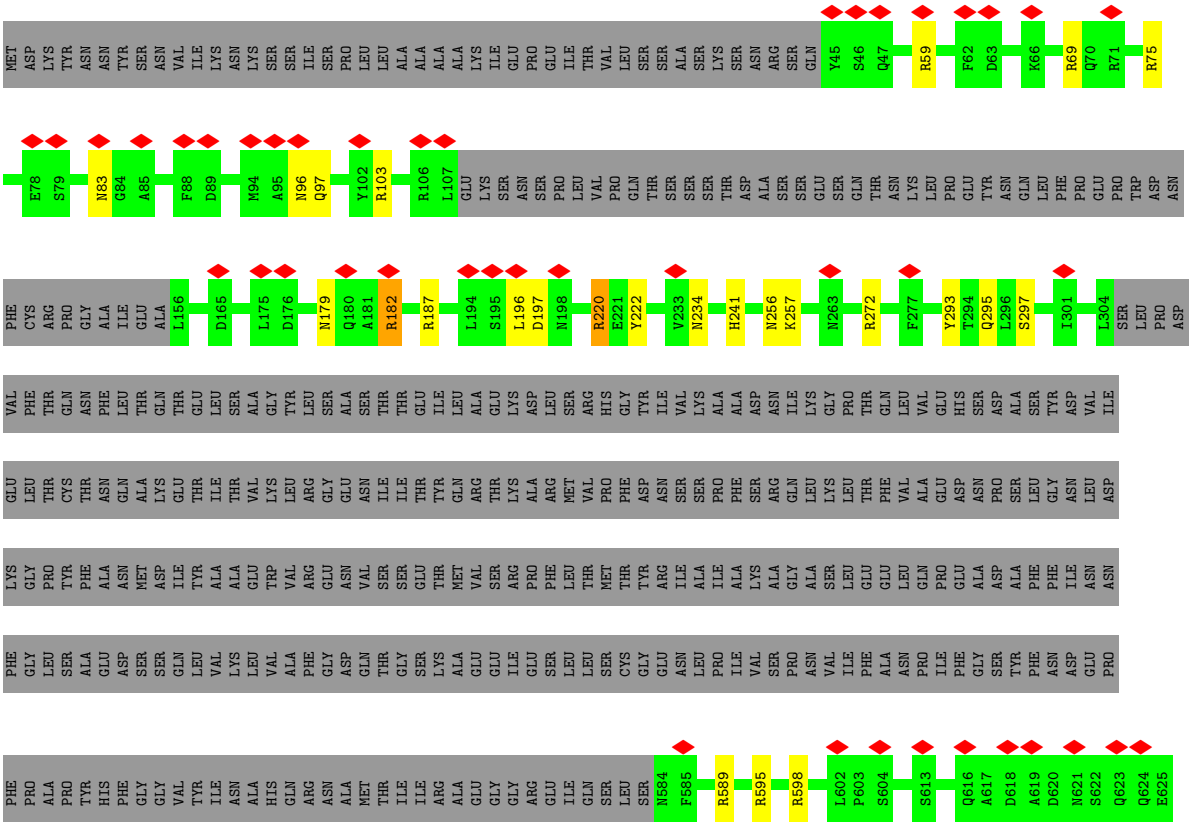
Chain J:

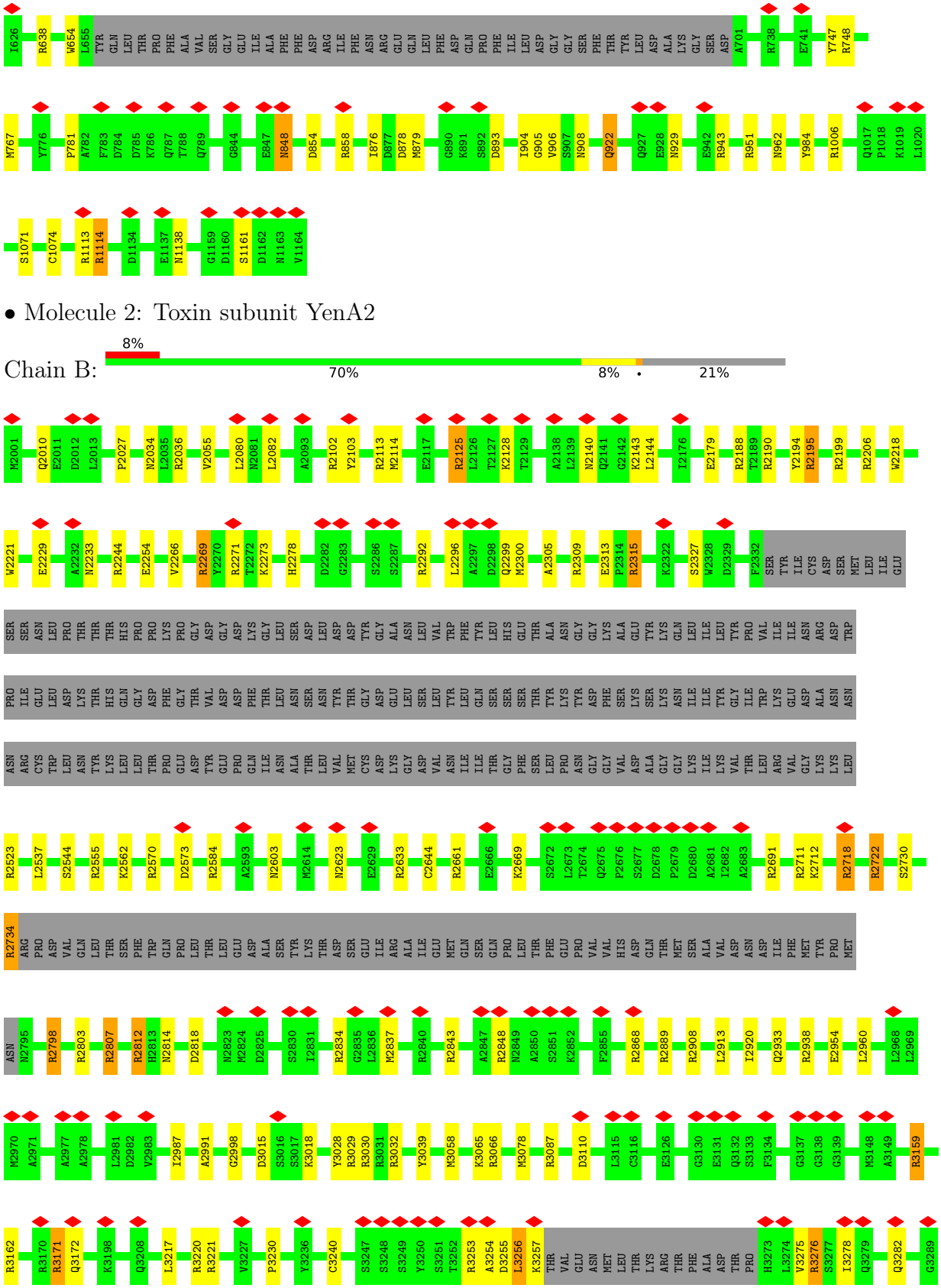




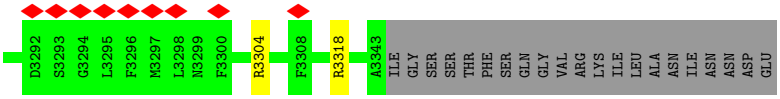
- Molecule 1: Toxin subunit YenA1

Chain M: 6% 60% 36%



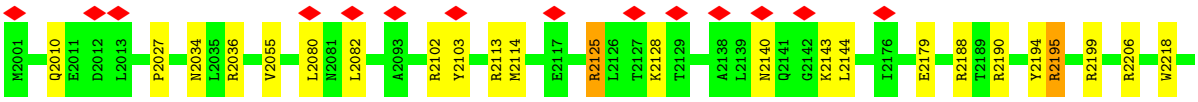


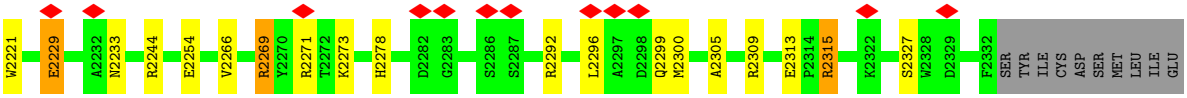
• Molecule 2: Toxin subunit YenA2

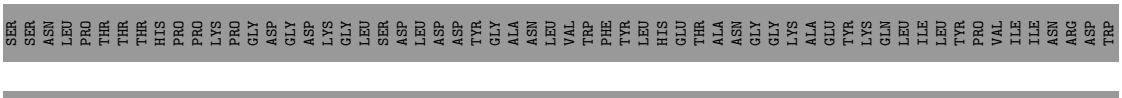


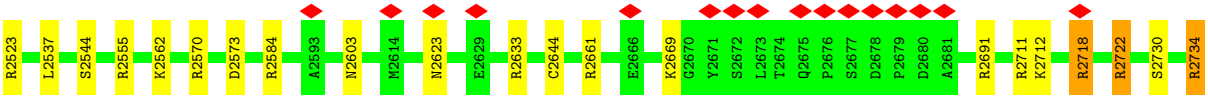
• Molecule 2: Toxin subunit YenA2

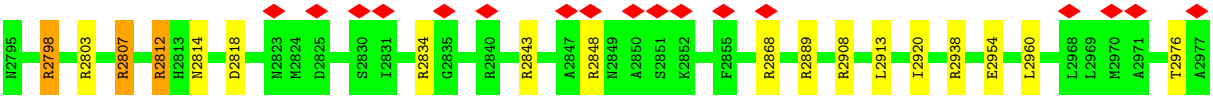
Chain E:

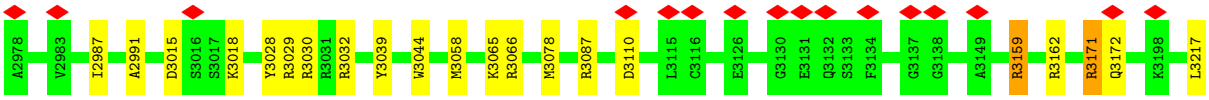


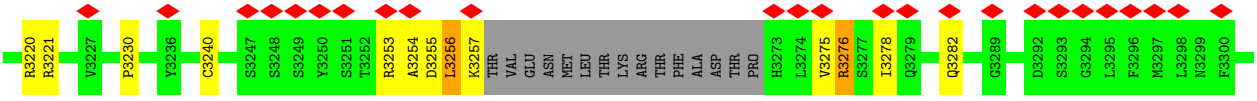


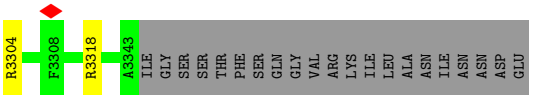






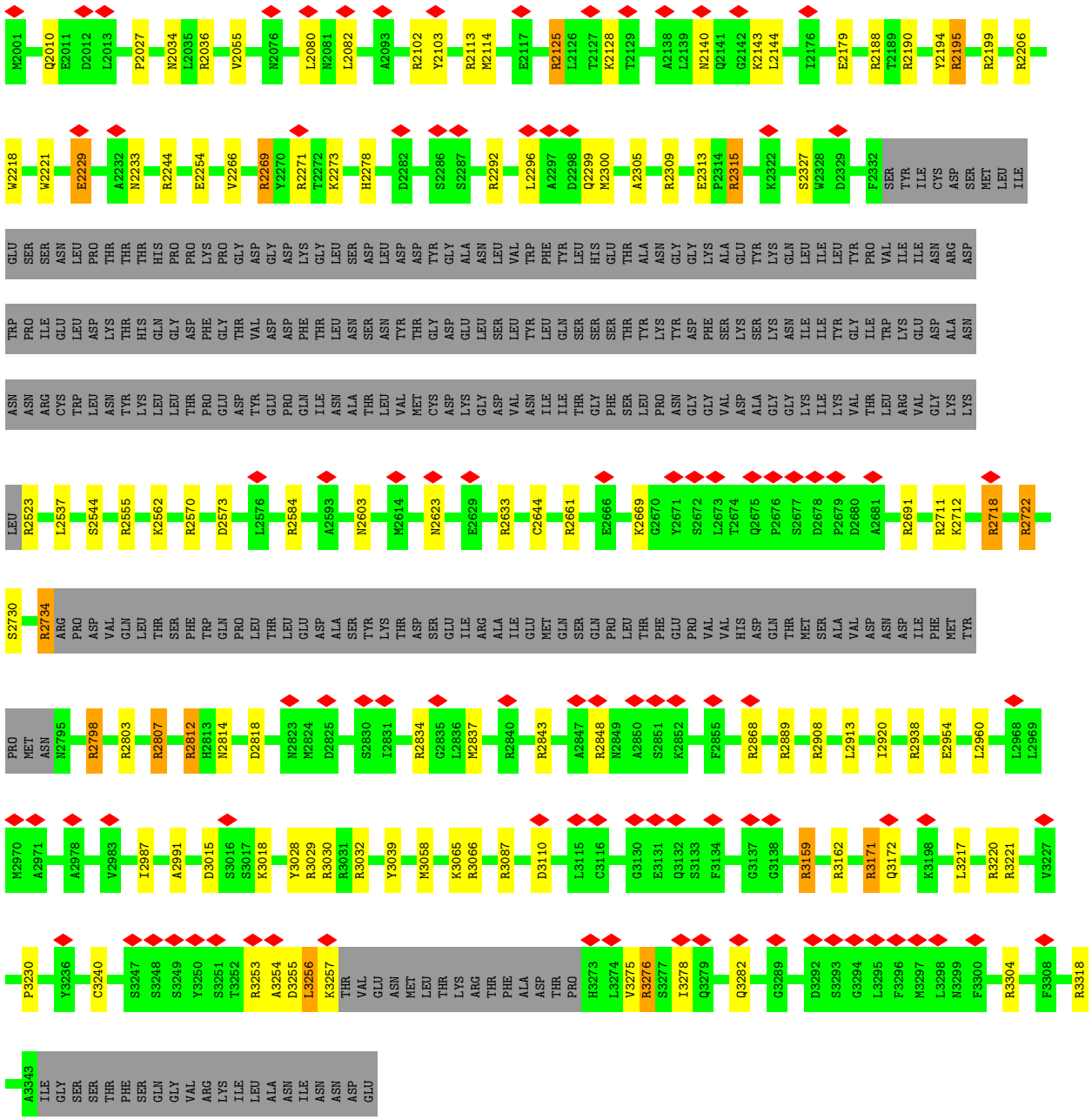






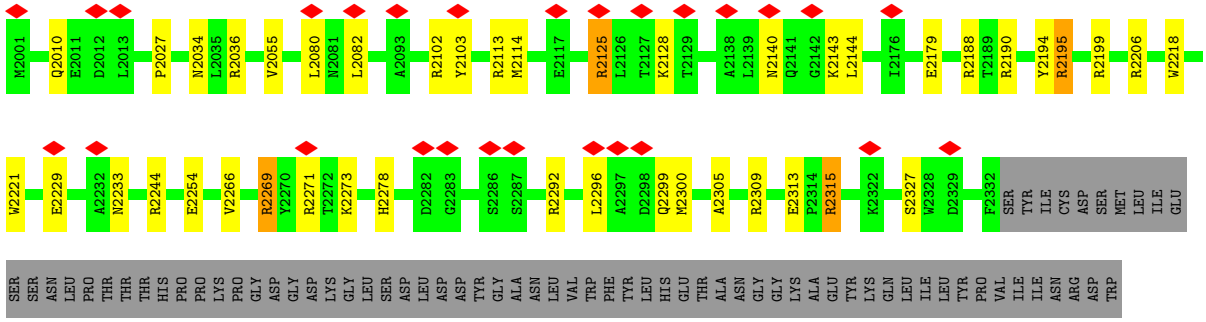
• Molecule 2: Toxin subunit YenA2

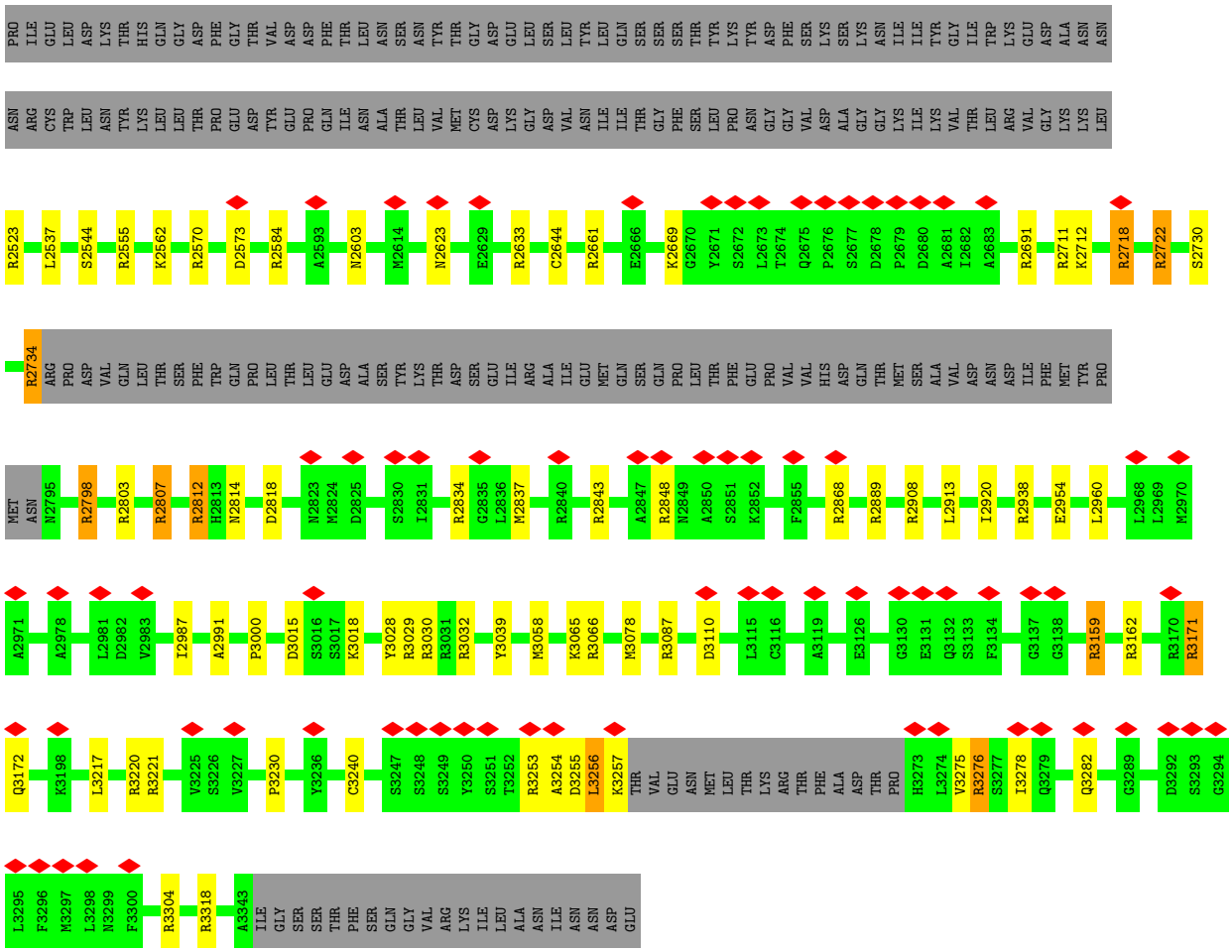
Chain H:



- Molecule 2: Toxin subunit YenA2

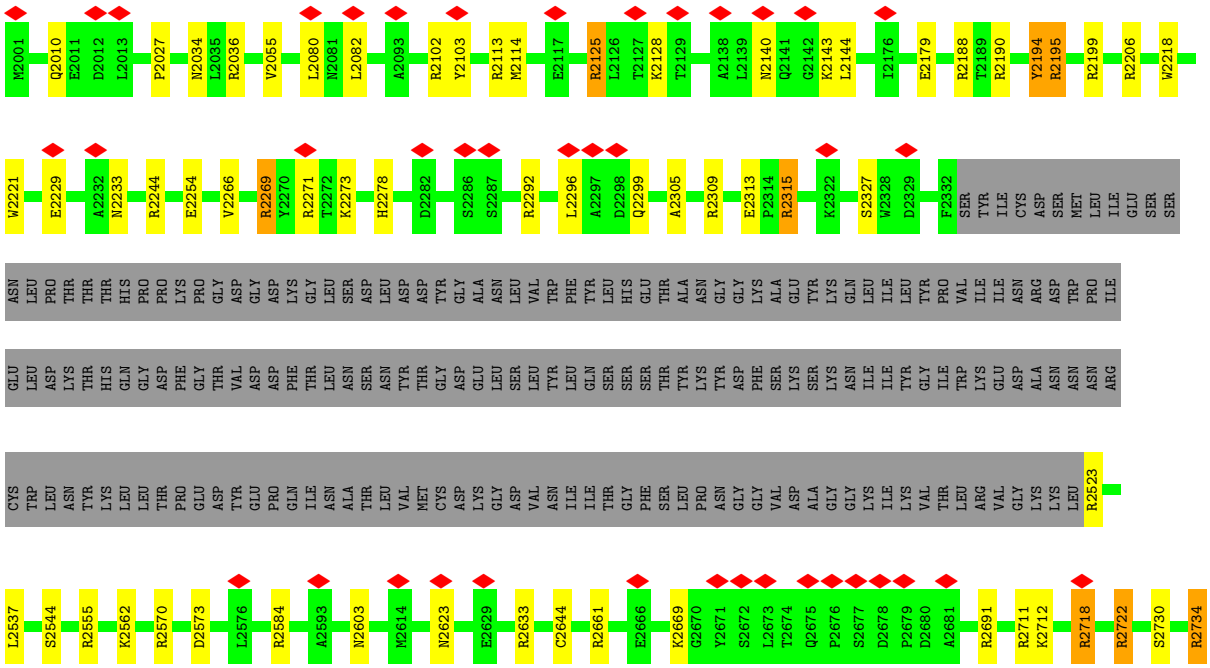
Chain K:

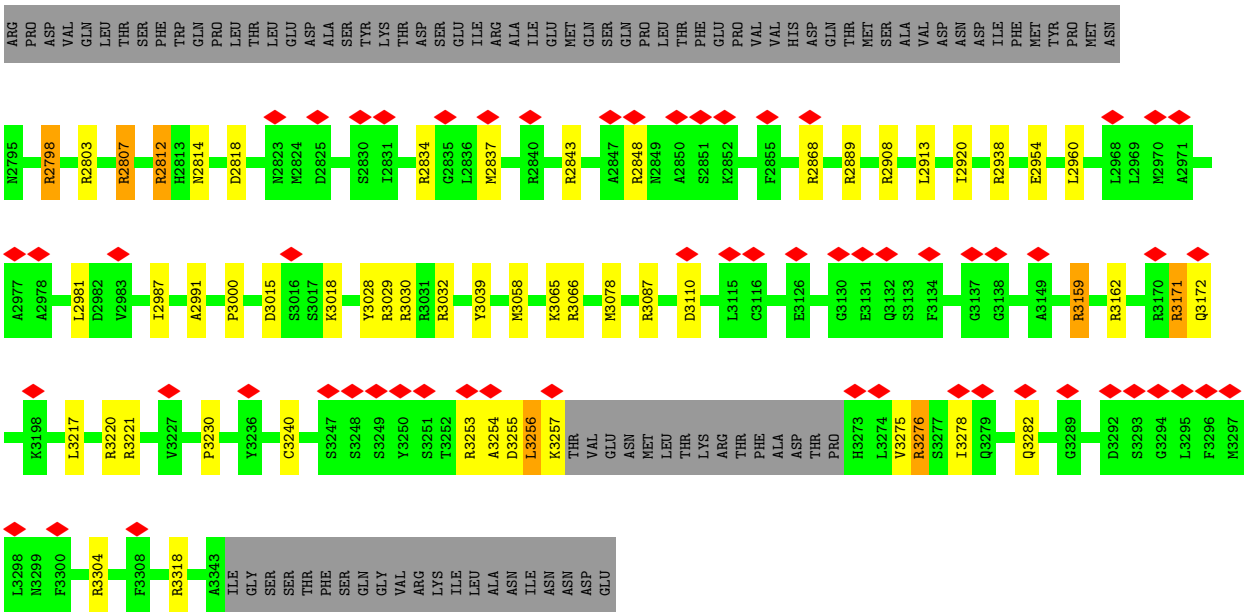




• Molecule 2: Toxin subunit YenA2

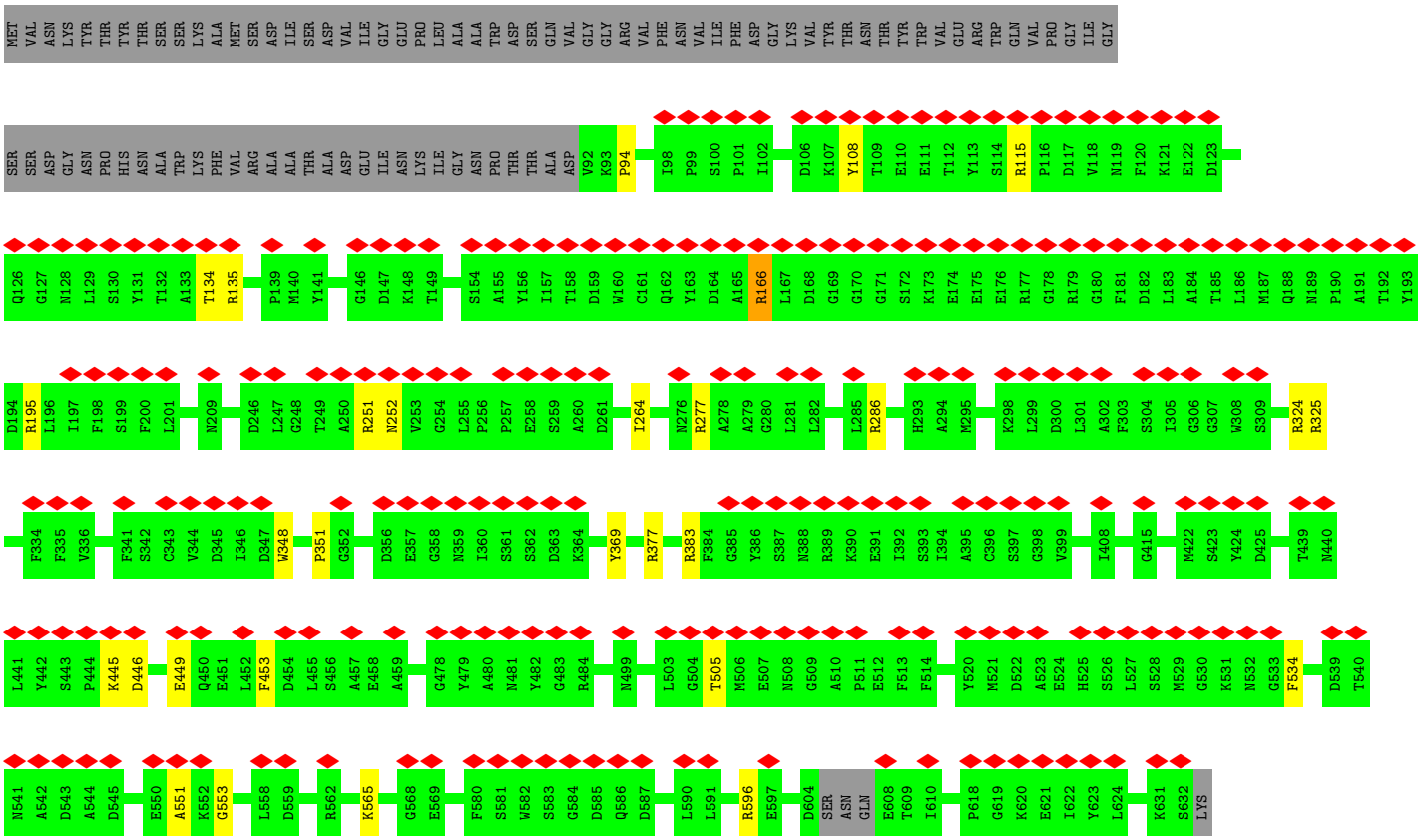
Chain N:





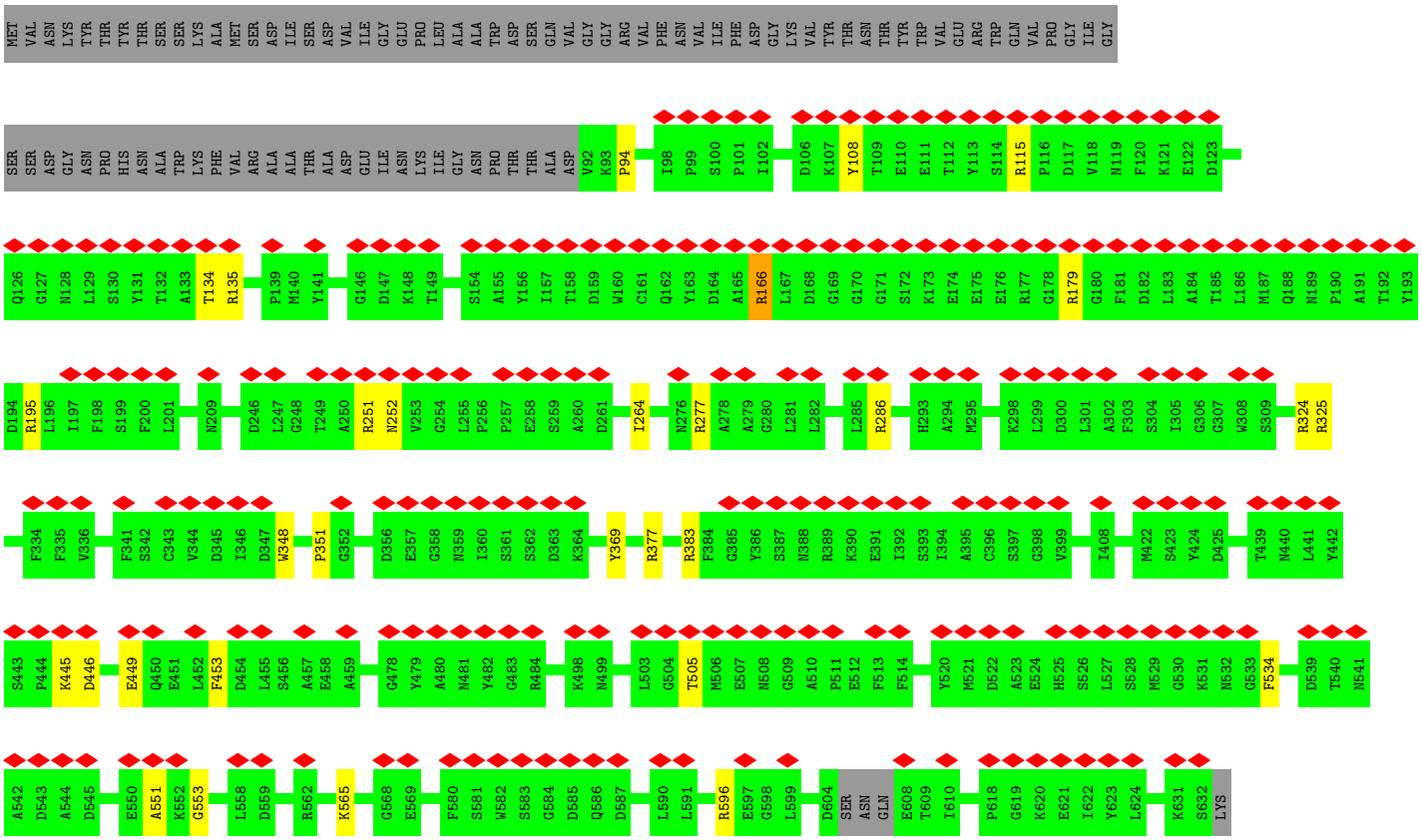
- Molecule 3: Chitinase 2

Chain C:



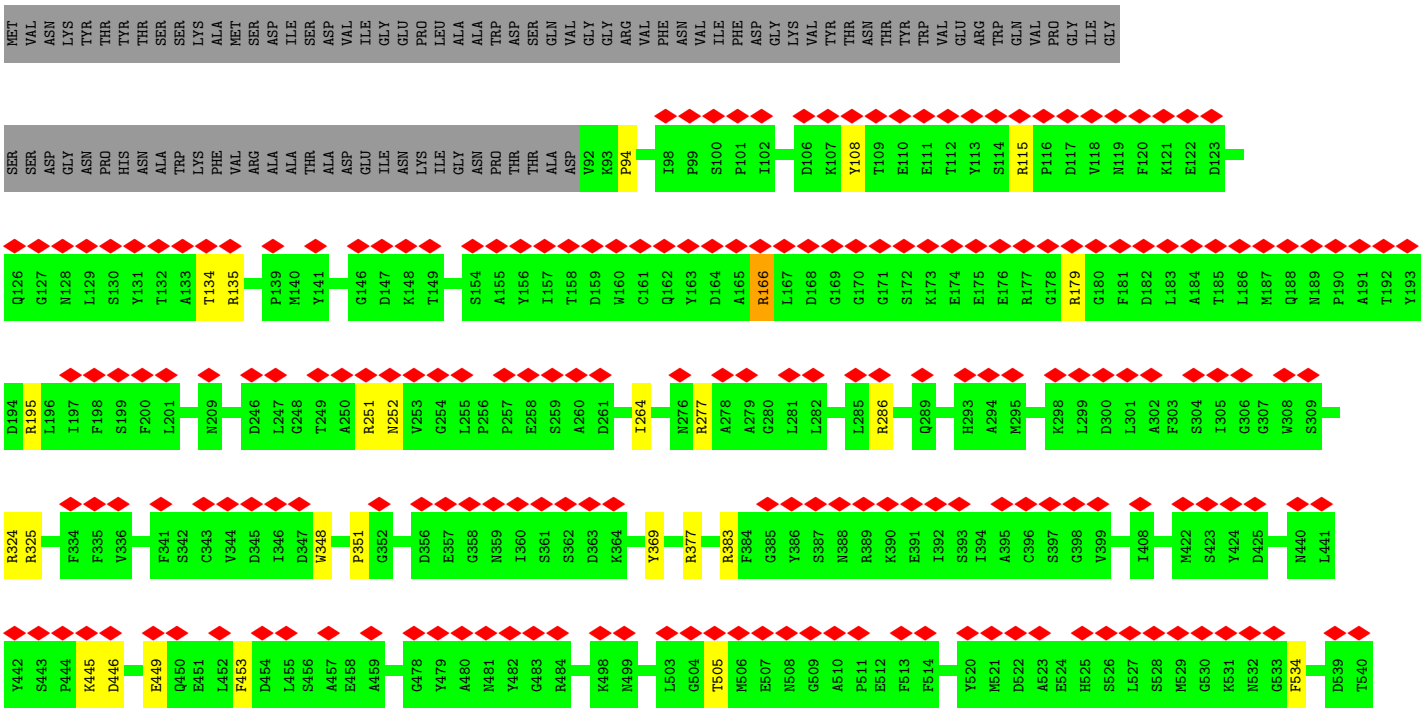
- Molecule 3: Chitinase 2

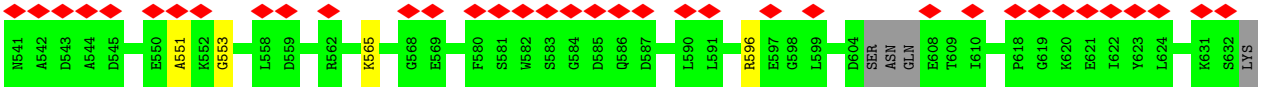
Chain F:



- Molecule 3: Chitinase 2

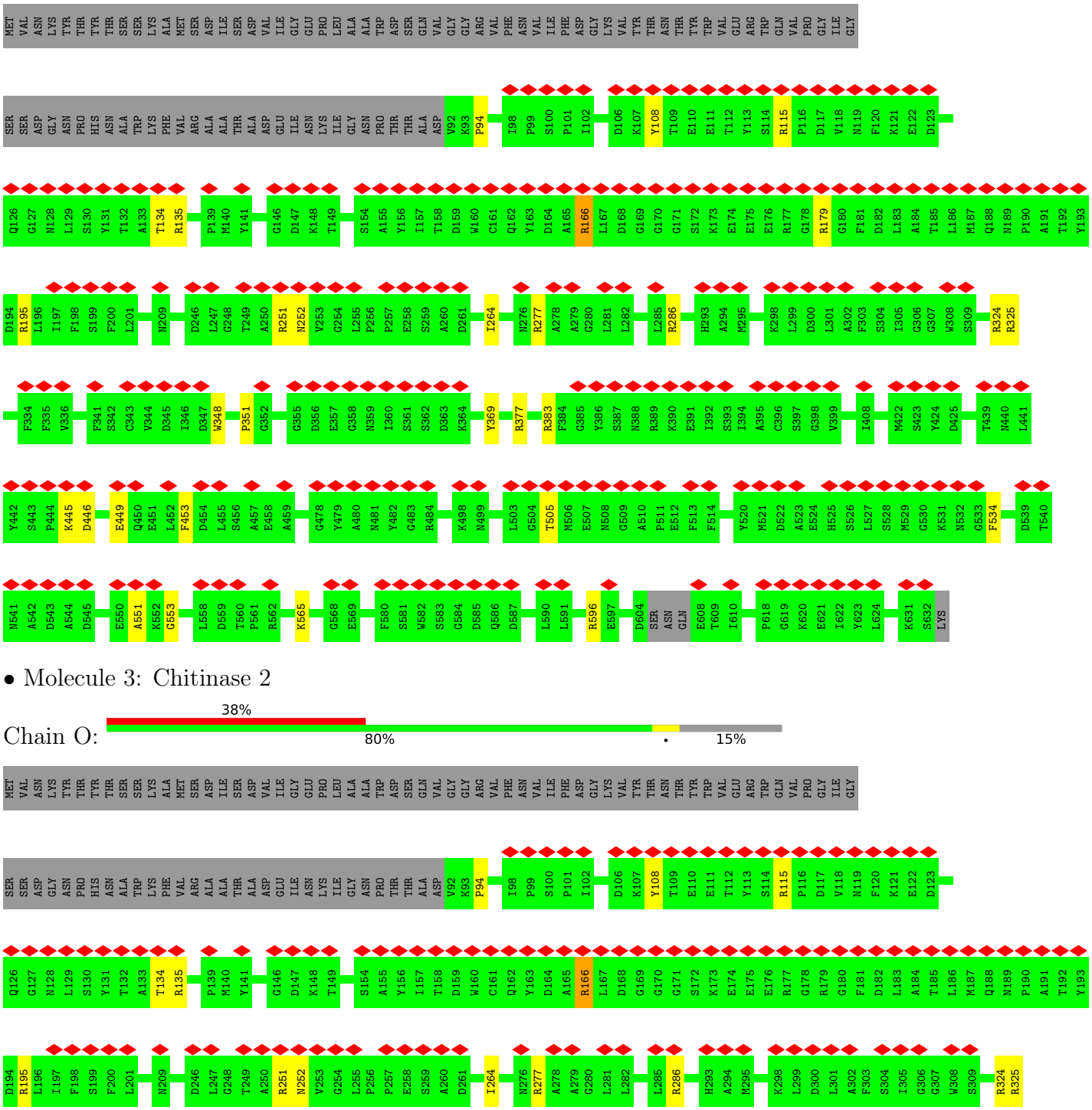
Chain I:





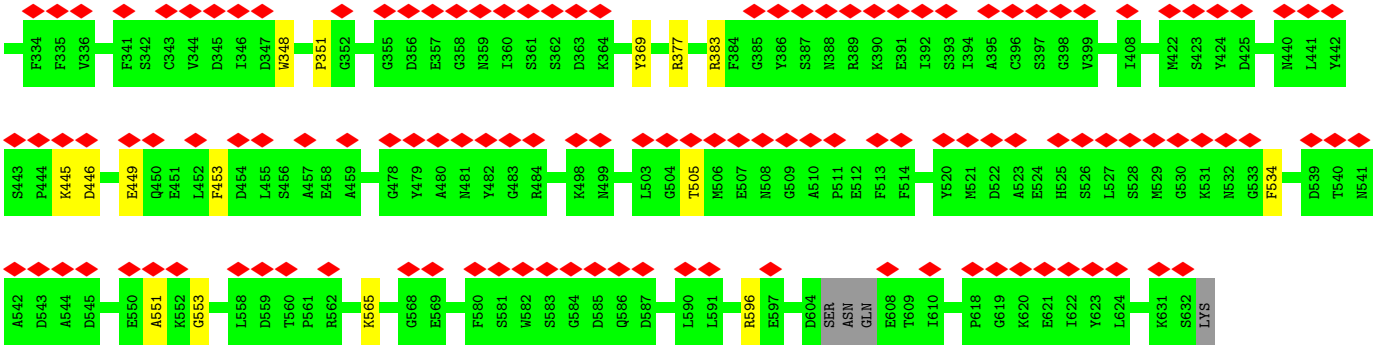
• Molecule 3: Chitinase 2

Chain L:



• Molecule 3: Chitinase 2

Chain O:


F334 F335 V336 F341 S342 C343 V344 D345 I346 D347 W348 P351 G352 G355 D356 E357 G358 N359 I360 S361 S362 D363 K364 Y369 R377 R383 F384 G385 Y386 S387 N388 R389 K390 E391 I392 S393 I394 A395 C396 S397 G398 V399 I408 M422 S423 Y424 D425 N440 L441 Y442
S443 P444 K445 D446 E449 Q450 E451 L452 F453 D454 L455 S456 A457 E458 A459 G478 Y479 A480 N481 Y482 G483 R484 K498 N499 L503 G504 T505 M506 E507 N508 G509 A510 P511 E512 F513 F514 Y520 M521 D522 A523 E524 H525 S526 L527 S528 M529 G530 K531 N532 G533 F534 D539 T540 N541
A542 D543 A544 D545 E550 A551 K552 G553 L558 D559 T560 P561 R562 K565 G568 E569 F580 S581 W582 S583 G584 D585 Q586 D587 L590 L591 R596 E597 D604 SER ASN GLN E608 T609 I610 P618 G619 K620 E621 I622 Y623 L624 K631 S632 LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	9856	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 ($e^-/Å^2$)	80	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	58.496	Depositor
Minimum map value	-45.992	Depositor
Average map value	0.004	Depositor
Map value standard deviation	1.654	Depositor
Recommended contour level	7.5	Depositor
Map size (Å)	557.44, 557.44, 557.44	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	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	0.68	0/6007	1.03	19/8156 (0.2%)
1	D	0.68	0/6007	1.03	19/8156 (0.2%)
1	G	0.69	0/6007	1.03	19/8156 (0.2%)
1	J	0.68	0/6007	1.03	19/8156 (0.2%)
1	M	0.68	0/6007	1.03	19/8156 (0.2%)
2	B	0.74	0/8915	1.08	52/12066 (0.4%)
2	E	0.74	0/8915	1.08	52/12066 (0.4%)
2	H	0.74	0/8915	1.08	51/12066 (0.4%)
2	K	0.74	0/8915	1.08	52/12066 (0.4%)
2	N	0.74	0/8915	1.08	52/12066 (0.4%)
3	C	0.76	0/4271	1.06	12/5778 (0.2%)
3	F	0.76	0/4271	1.06	13/5778 (0.2%)
3	I	0.76	0/4271	1.06	13/5778 (0.2%)
3	L	0.76	0/4271	1.06	13/5778 (0.2%)
3	O	0.76	0/4271	1.06	12/5778 (0.2%)
All	All	0.73	0/95965	1.06	417/130000 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	D	0	3
1	G	0	3
1	J	0	3
1	M	0	3
2	B	0	2
2	E	0	2
2	H	0	2
2	K	0	2
2	N	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
3	F	0	1
3	I	0	1
3	L	0	1
3	O	0	1
All	All	0	30

There are no bond length outliers.

The worst 5 of 417 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2661	ARG	NE-CZ-NH1	9.12	124.86	120.30
2	H	2661	ARG	NE-CZ-NH1	9.09	124.84	120.30
2	B	2661	ARG	NE-CZ-NH1	9.07	124.83	120.30
2	K	2661	ARG	NE-CZ-NH1	9.05	124.83	120.30
2	N	2661	ARG	NE-CZ-NH1	9.00	124.80	120.30

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1114	ARG	Sidechain
1	A	241	HIS	Peptide
1	A	984	TYR	Sidechain
2	B	2718	ARG	Sidechain
2	B	2807	ARG	Sidechain

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	5910	0	5971	10	0
1	D	5910	0	5971	12	0
1	G	5910	0	5971	11	0
1	J	5910	0	5971	10	0
1	M	5910	0	5971	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8742	0	8563	89	0
2	E	8742	0	8563	91	0
2	H	8742	0	8563	85	0
2	K	8742	0	8563	87	0
2	N	8742	0	8563	89	0
3	C	4173	0	4010	1	0
3	F	4173	0	4010	1	0
3	I	4173	0	4010	1	0
3	L	4173	0	4010	1	0
3	O	4173	0	4010	1	0
All	All	94125	0	92720	257	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 1.

The worst 5 of 257 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)
2:B:2812:ARG:HD2	2:E:2055:VAL:CB	1.62	1.28
2:K:2812:ARG:HD2	2:N:2055:VAL:CB	1.66	1.25
2:B:2812:ARG:HD2	2:E:2055:VAL:CG1	1.67	1.23
2:E:2812:ARG:HD2	2:H:2055:VAL:CB	1.67	1.22
2:K:2812:ARG:HD2	2:N:2055:VAL:CG1	1.69	1.21

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	740/1164 (64%)	665 (90%)	66 (9%)	9 (1%)	13 50
1	D	740/1164 (64%)	665 (90%)	66 (9%)	9 (1%)	13 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	740/1164 (64%)	665 (90%)	66 (9%)	9 (1%)	13	50
1	J	740/1164 (64%)	665 (90%)	66 (9%)	9 (1%)	13	50
1	M	740/1164 (64%)	665 (90%)	66 (9%)	9 (1%)	13	50
2	B	1070/1364 (78%)	934 (87%)	115 (11%)	21 (2%)	7	40
2	E	1070/1364 (78%)	934 (87%)	115 (11%)	21 (2%)	7	40
2	H	1070/1364 (78%)	934 (87%)	115 (11%)	21 (2%)	7	40
2	K	1070/1364 (78%)	934 (87%)	115 (11%)	21 (2%)	7	40
2	N	1070/1364 (78%)	934 (87%)	116 (11%)	20 (2%)	8	41
3	C	534/633 (84%)	475 (89%)	50 (9%)	9 (2%)	9	43
3	F	534/633 (84%)	475 (89%)	50 (9%)	9 (2%)	9	43
3	I	534/633 (84%)	475 (89%)	50 (9%)	9 (2%)	9	43
3	L	534/633 (84%)	475 (89%)	50 (9%)	9 (2%)	9	43
3	O	534/633 (84%)	475 (89%)	50 (9%)	9 (2%)	9	43
All	All	11720/15805 (74%)	10370 (88%)	1156 (10%)	194 (2%)	13	43

5 of 194 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	2669	LYS
2	E	2669	LYS
2	H	2669	LYS
2	K	2669	LYS
2	N	2669	LYS

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	664/1022 (65%)	644 (97%)	20 (3%)	41	63
1	D	664/1022 (65%)	644 (97%)	20 (3%)	41	63
1	G	664/1022 (65%)	644 (97%)	20 (3%)	41	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	664/1022 (65%)	644 (97%)	20 (3%)	41	63
1	M	664/1022 (65%)	644 (97%)	20 (3%)	41	63
2	B	953/1209 (79%)	925 (97%)	28 (3%)	42	64
2	E	953/1209 (79%)	925 (97%)	28 (3%)	42	64
2	H	953/1209 (79%)	925 (97%)	28 (3%)	42	64
2	K	953/1209 (79%)	925 (97%)	28 (3%)	42	64
2	N	953/1209 (79%)	925 (97%)	28 (3%)	42	64
3	C	441/520 (85%)	435 (99%)	6 (1%)	67	81
3	F	441/520 (85%)	435 (99%)	6 (1%)	67	81
3	I	441/520 (85%)	435 (99%)	6 (1%)	67	81
3	L	441/520 (85%)	435 (99%)	6 (1%)	67	81
3	O	441/520 (85%)	435 (99%)	6 (1%)	67	81
All	All	10290/13755 (75%)	10020 (97%)	270 (3%)	49	67

5 of 270 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	893	ASP
2	N	2103	TYR
2	N	3217	LEU
2	E	3039	TYR
2	E	2722	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
2	K	2024	GLN
3	L	97	ASN
2	K	3323	ASN
2	N	2024	GLN
2	E	2134	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

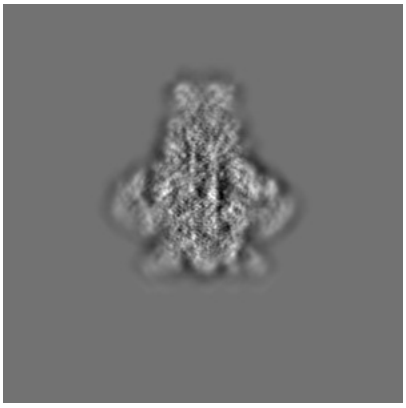
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-20053. These allow visual inspection of the internal detail of the map and identification of artifacts.

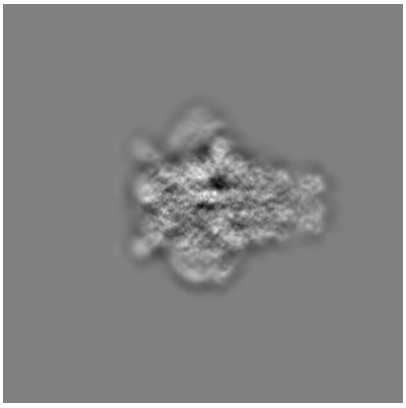
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

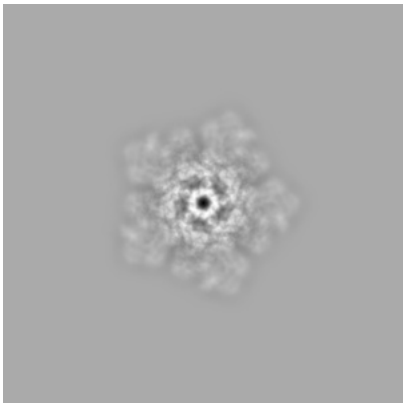
6.1.1 Primary map



X



Y

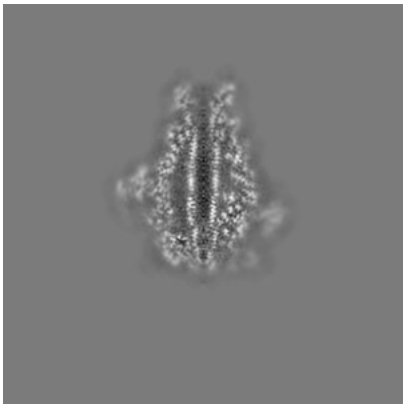


Z

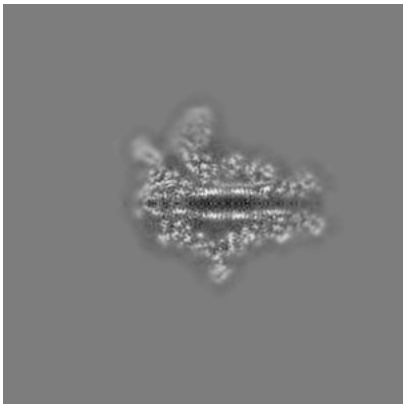
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

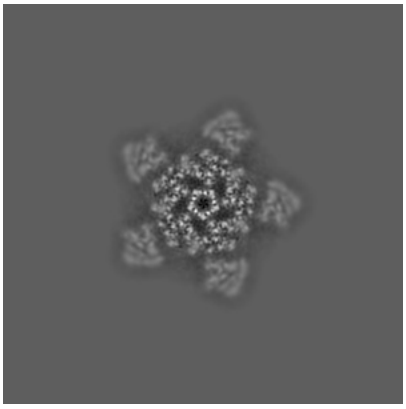
6.2.1 Primary map



X Index: 208



Y Index: 208

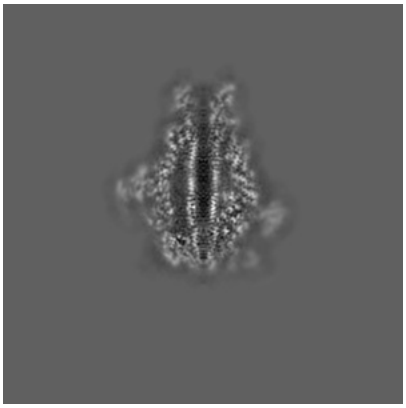


Z Index: 208

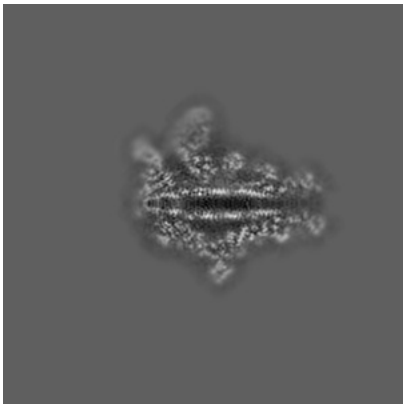
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

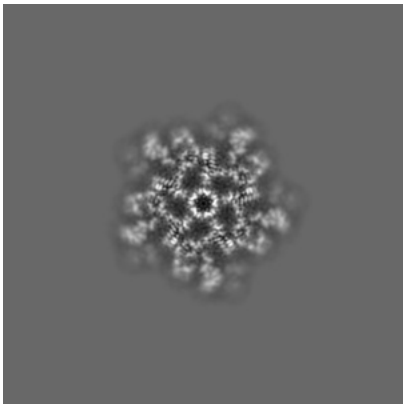
6.3.1 Primary map



X Index: 209



Y Index: 206

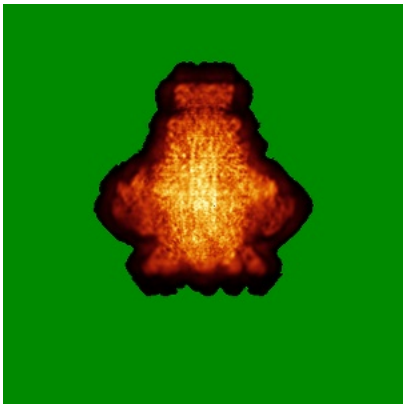


Z Index: 218

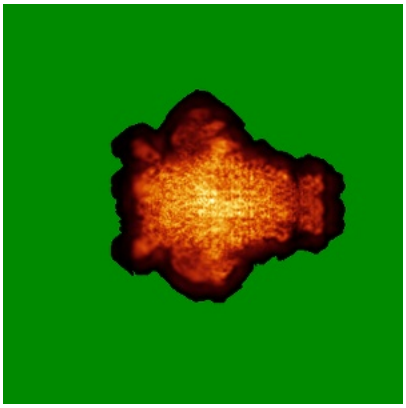
The images above show the largest variance slices of the map in three orthogonal directions.

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

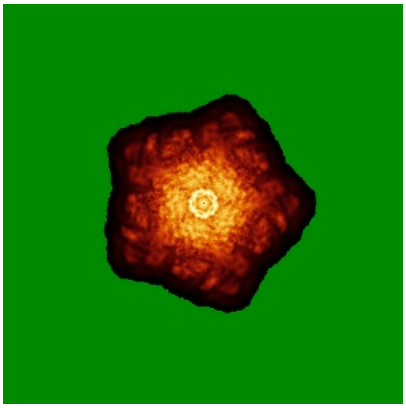
6.4.1 Primary map



X



Y

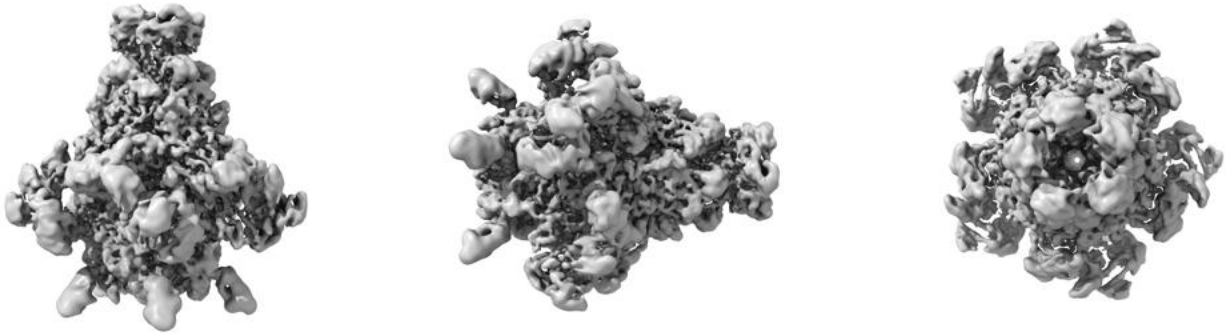


Z

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 7.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

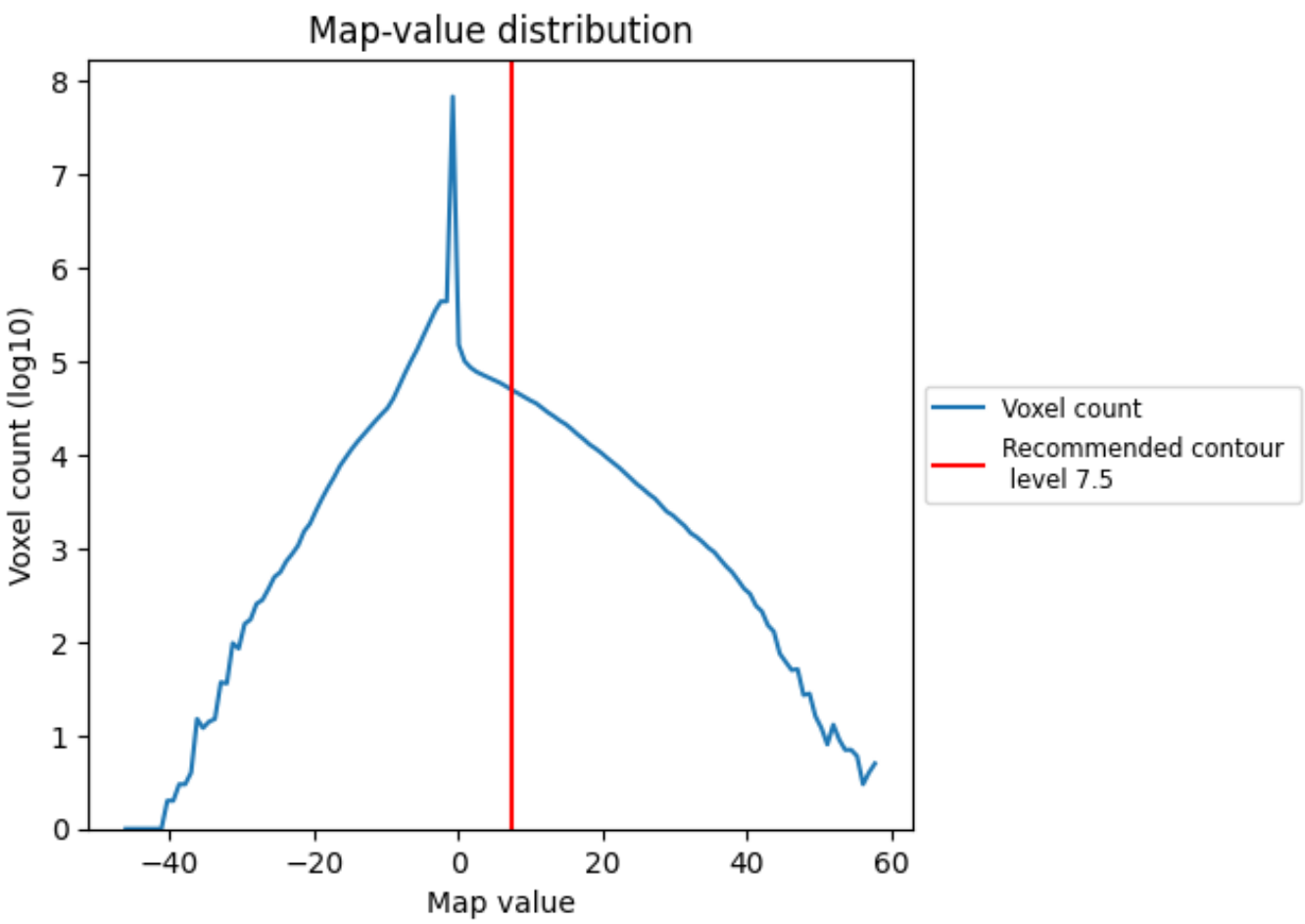
6.6 Mask visualisation (i)

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

7 Map analysis (i)

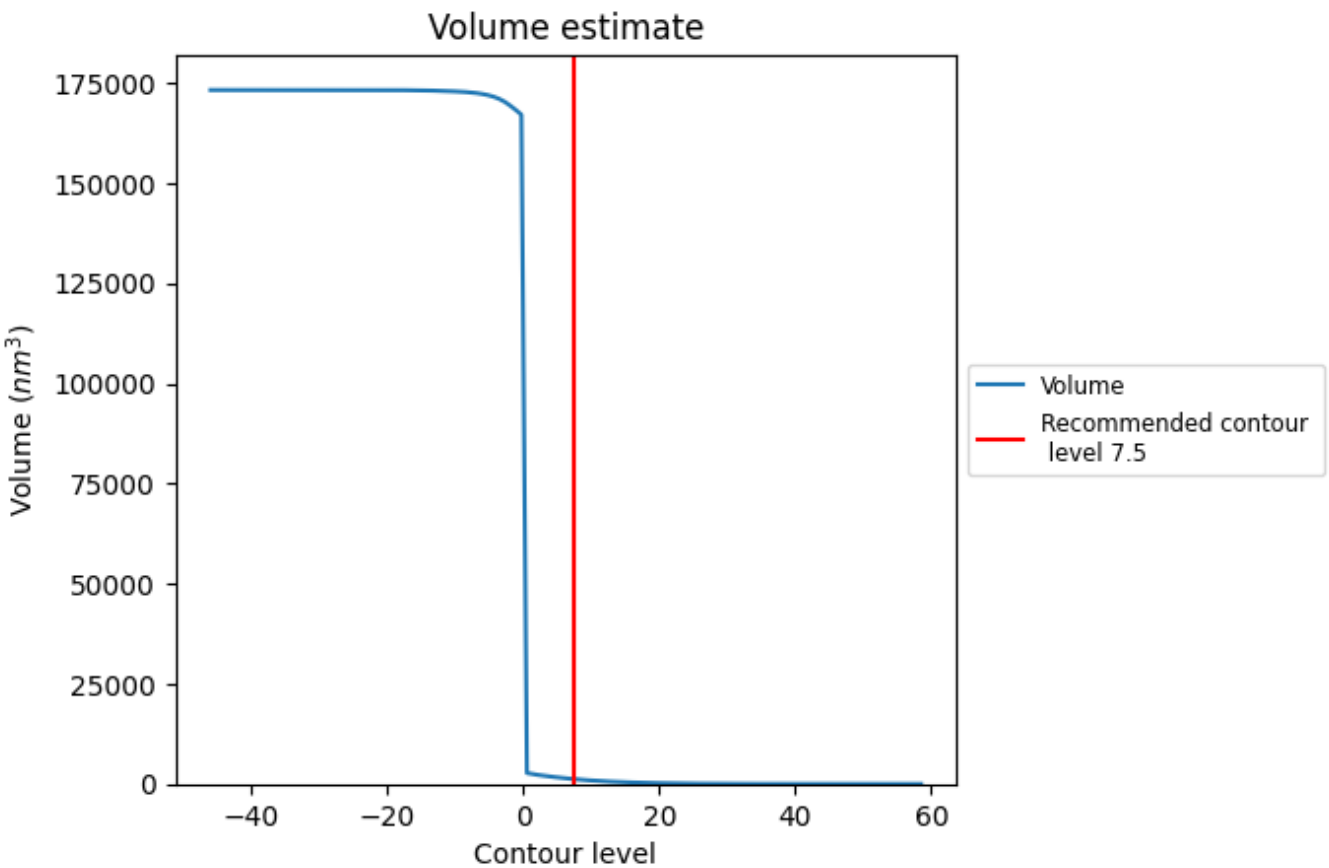
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

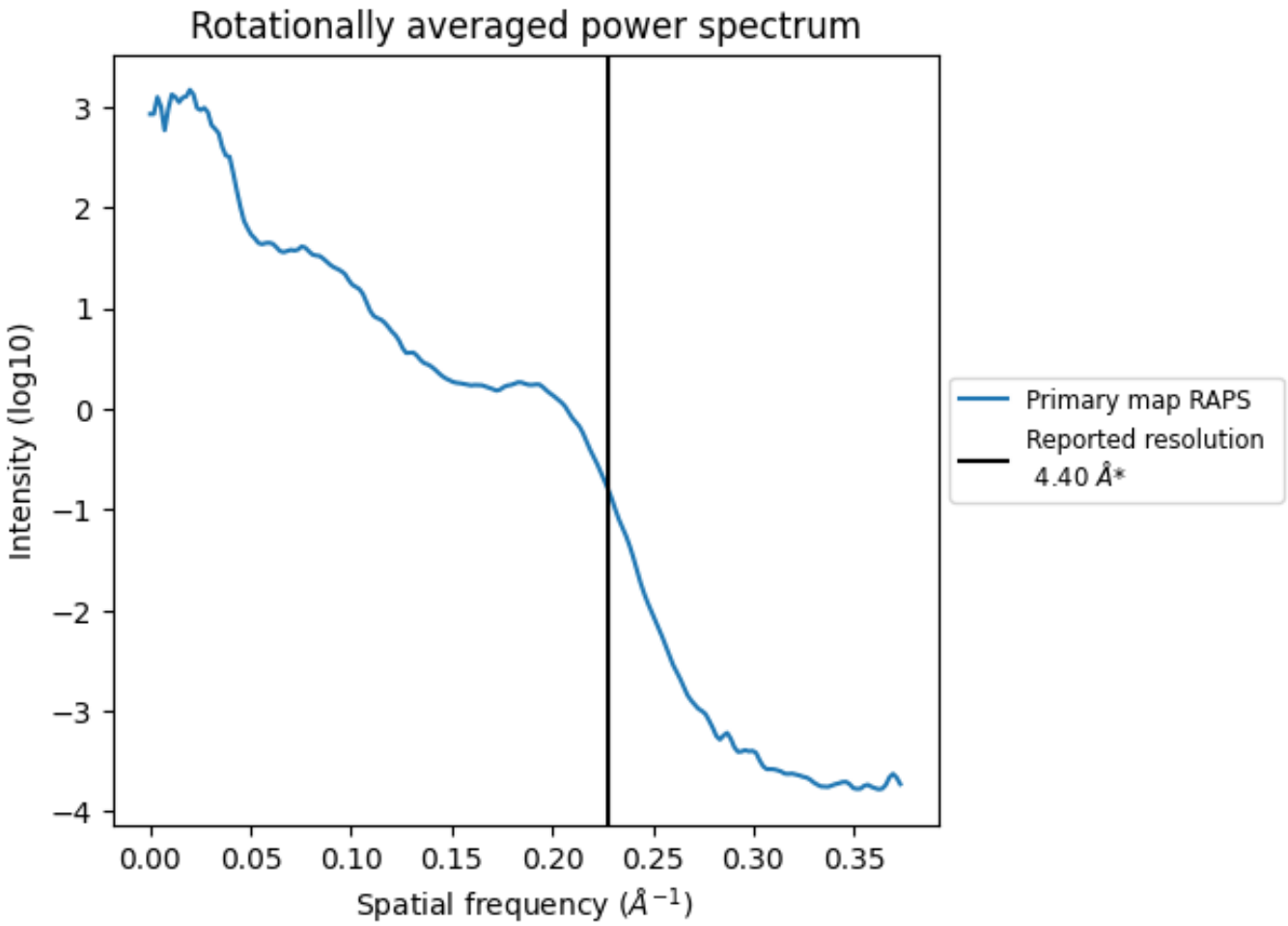
7.2 Volume estimate (i)



The volume at the recommended contour level is 1210 nm^3; this corresponds to an approximate mass of 1093 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)

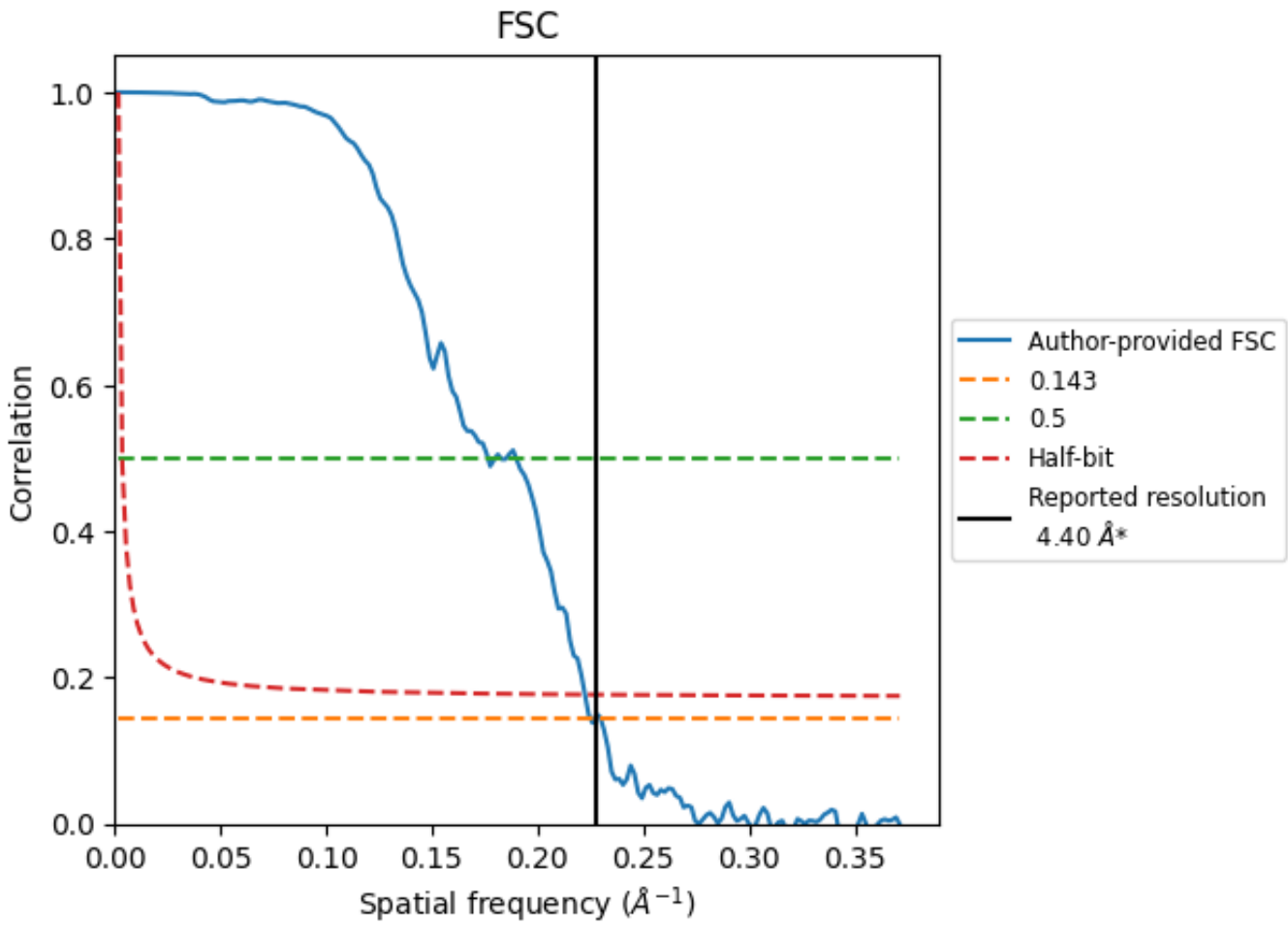


*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

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 0.227 Å^{-1}

8.2 Resolution estimates (i)

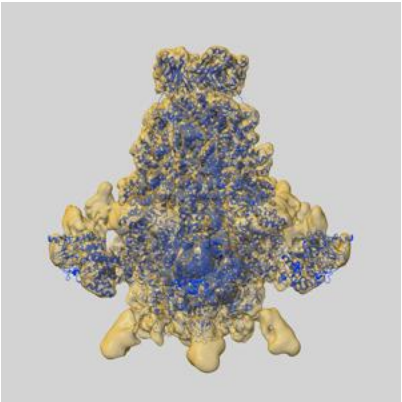
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.44	5.67	4.49
Unmasked-calculated*	-	-	-

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

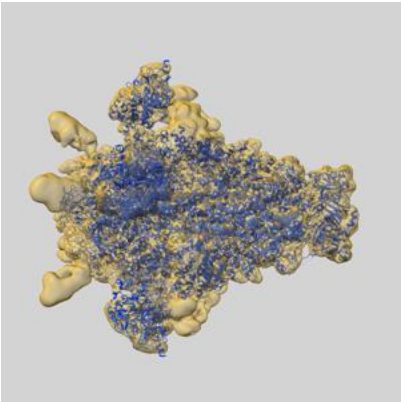
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20053 and PDB model 6OGD. Per-residue inclusion information can be found in section 3 on page 6.

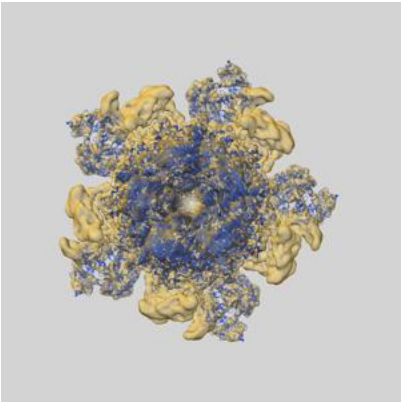
9.1 Map-model overlay (i)



X



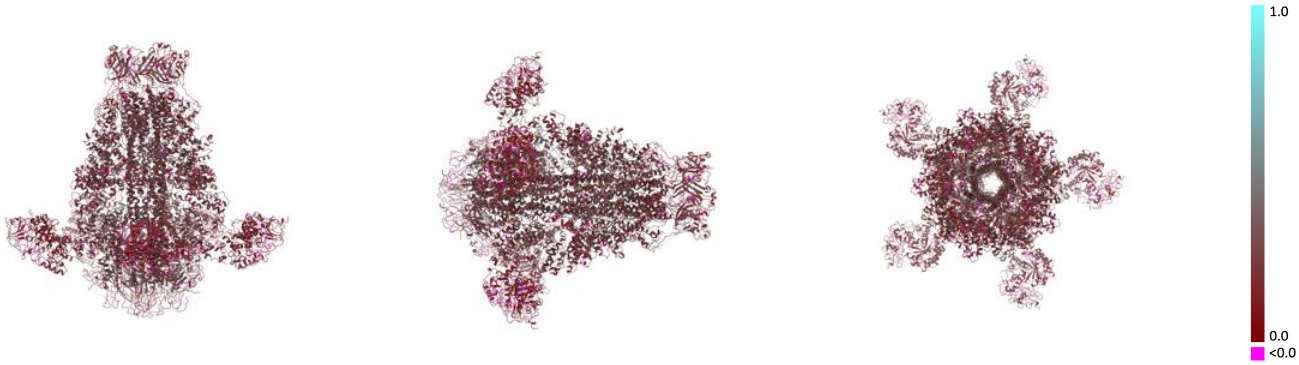
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 7.5 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.

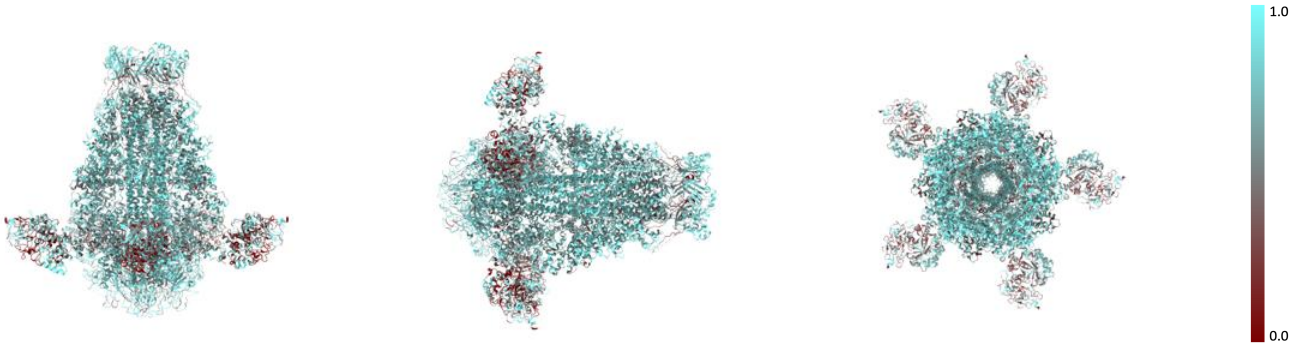
9.2 Q-score mapped to coordinate model (i)



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.

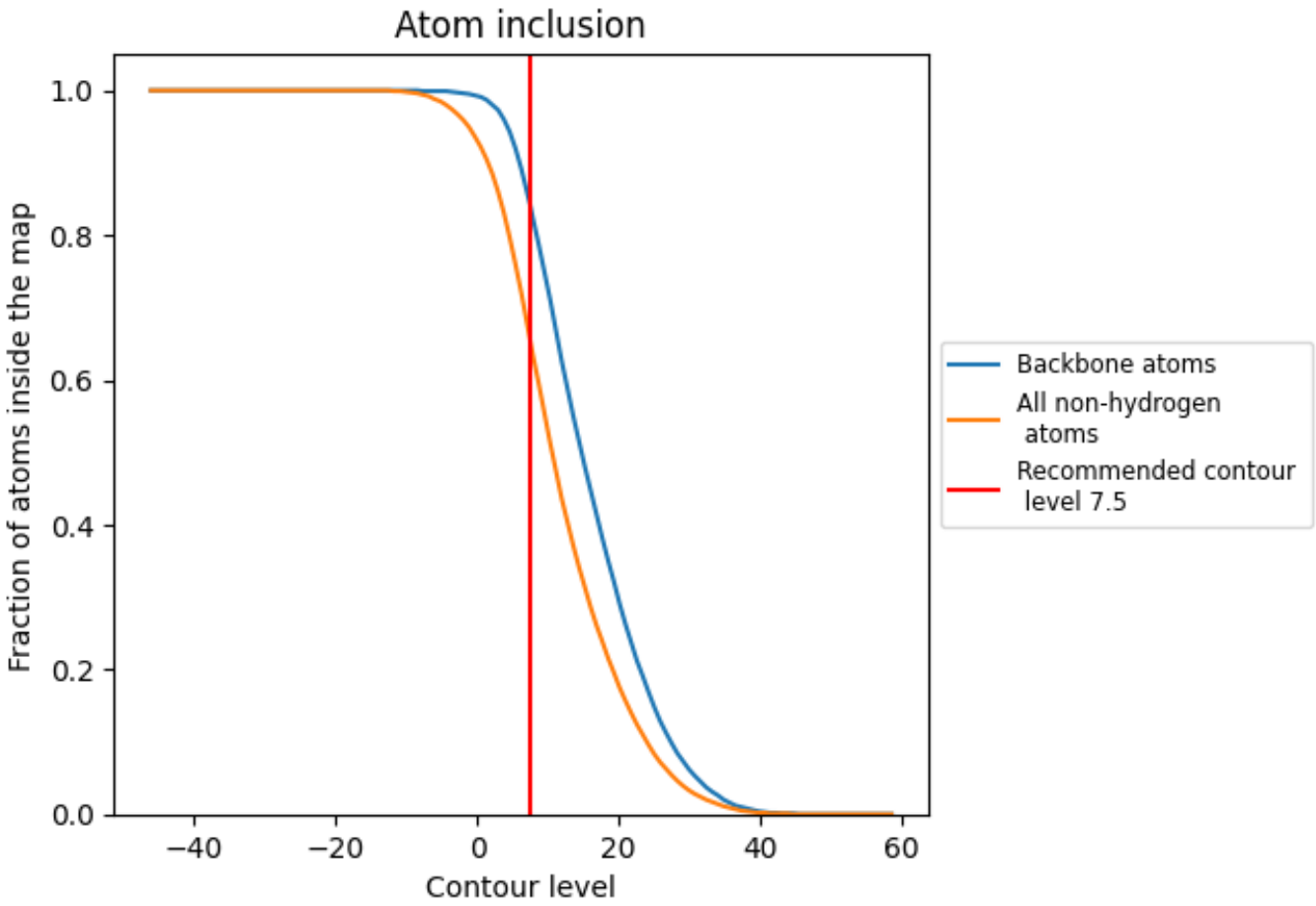
9.3 Atom inclusion mapped to coordinate model (i)



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 (7.5).

9.4 Atom inclusion (i)



At the recommended contour level, 84% 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 (7.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6560	0.2300
A	0.7130	0.2370
B	0.7110	0.2640
C	0.4590	0.1490
D	0.7130	0.2380
E	0.7120	0.2630
F	0.4580	0.1470
G	0.7130	0.2390
H	0.7130	0.2630
I	0.4550	0.1480
J	0.7120	0.2380
K	0.7110	0.2640
L	0.4580	0.1480
M	0.7120	0.2380
N	0.7120	0.2640
O	0.4590	0.1490