wwPDB EM Validation Summary Report

Nov 3, 2026 – 03:32 pm GMT

PDB ID	:	31LY / pdb_000031ly
EMDB ID	:	EMD-58515
Title	:	Yersinia entomophaga holotoxin in its lollipop pore state
Authors	:	Ng'ang'a, P.N.; Raunser, S.; Bader, R.; Sitsel, O.
Deposited on	:	2026-06-12
Resolution	:	2.94 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:

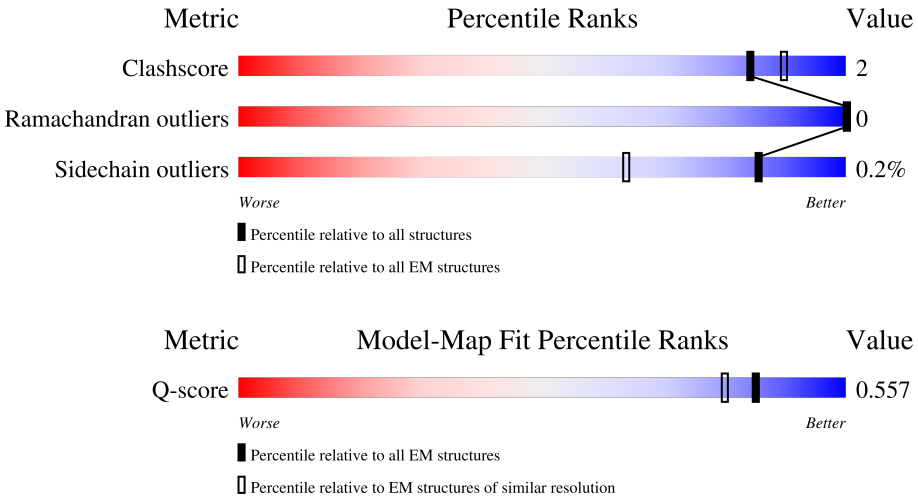
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & 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 2.94 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.



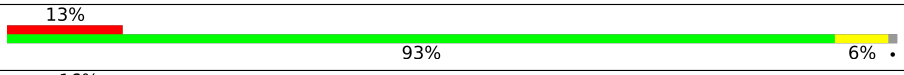
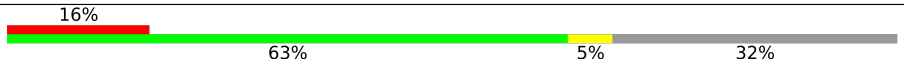
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13068 (2.44 - 3.44)

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	B	1364	32% 66%
1	G	1364	32% 66%
1	J	1364	32% 66%
1	M	1364	31% 66%

Continued on next page...

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Mol	Chain	Length	Quality of chain
1	P	1364	
2	D	1487	
3	E	970	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 35347 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 YenA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	464	Total	C	N	O	S	0	0
			3708	2336	626	732	14		
1	G	464	Total	C	N	O	S	0	0
			3708	2336	626	732	14		
1	J	464	Total	C	N	O	S	0	0
			3708	2336	626	732	14		
1	M	464	Total	C	N	O	S	0	0
			3708	2336	626	732	14		
1	P	464	Total	C	N	O	S	0	0
			3708	2336	626	732	14		

- Molecule 2 is a protein called Toxin subunit YenB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	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 3 is a protein called Toxin subunit YenC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	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

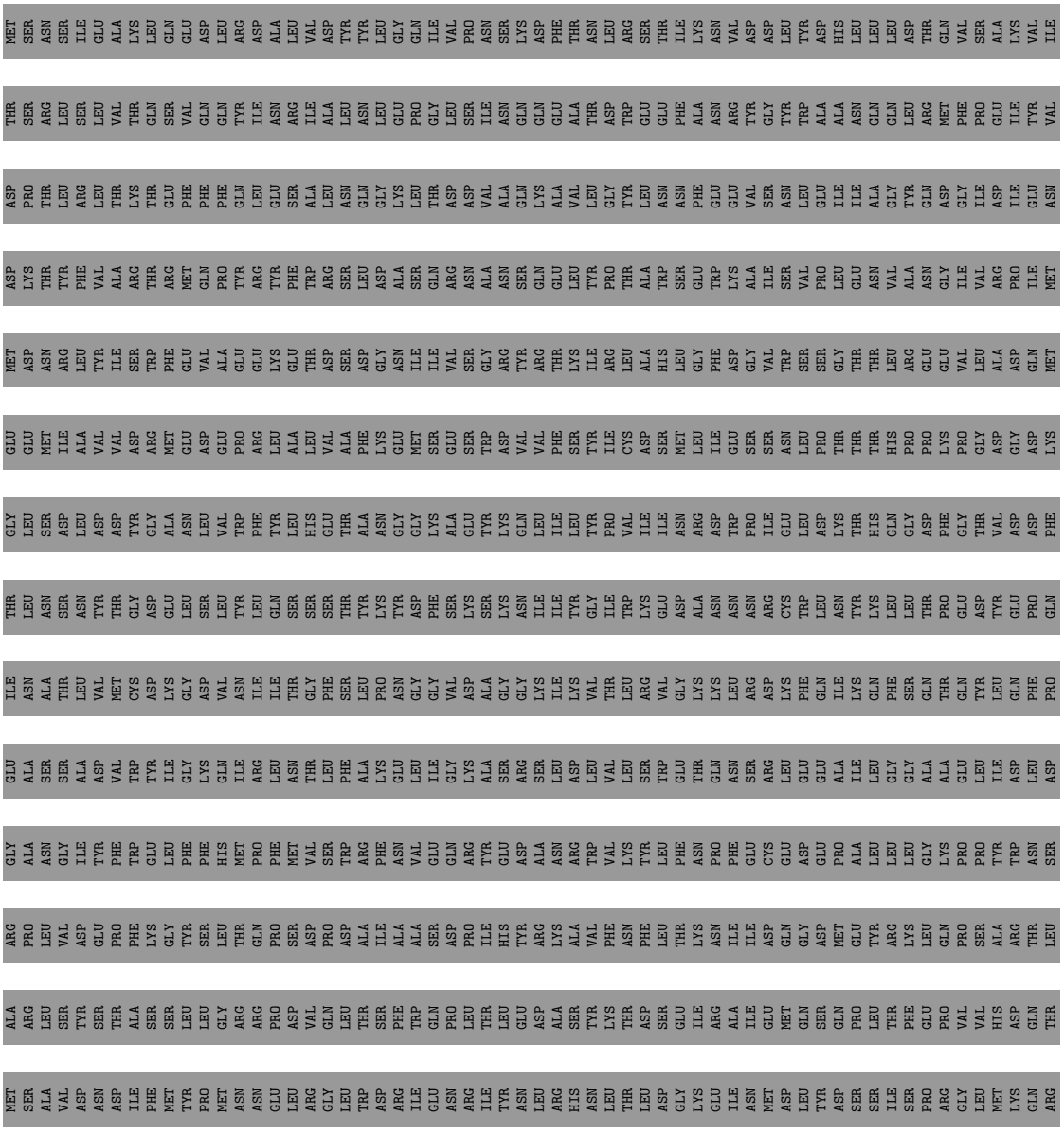
3 Residue-property plots (i)

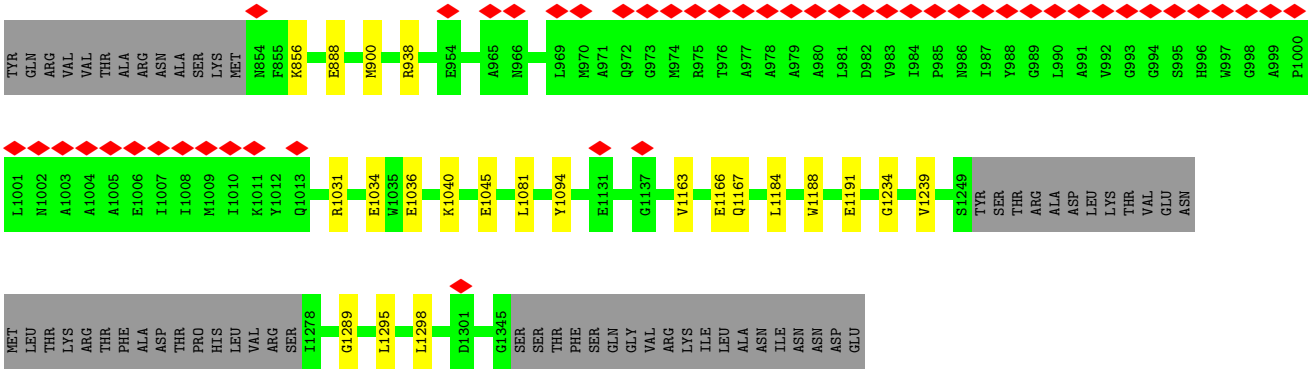
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 YenA2

Chain B:

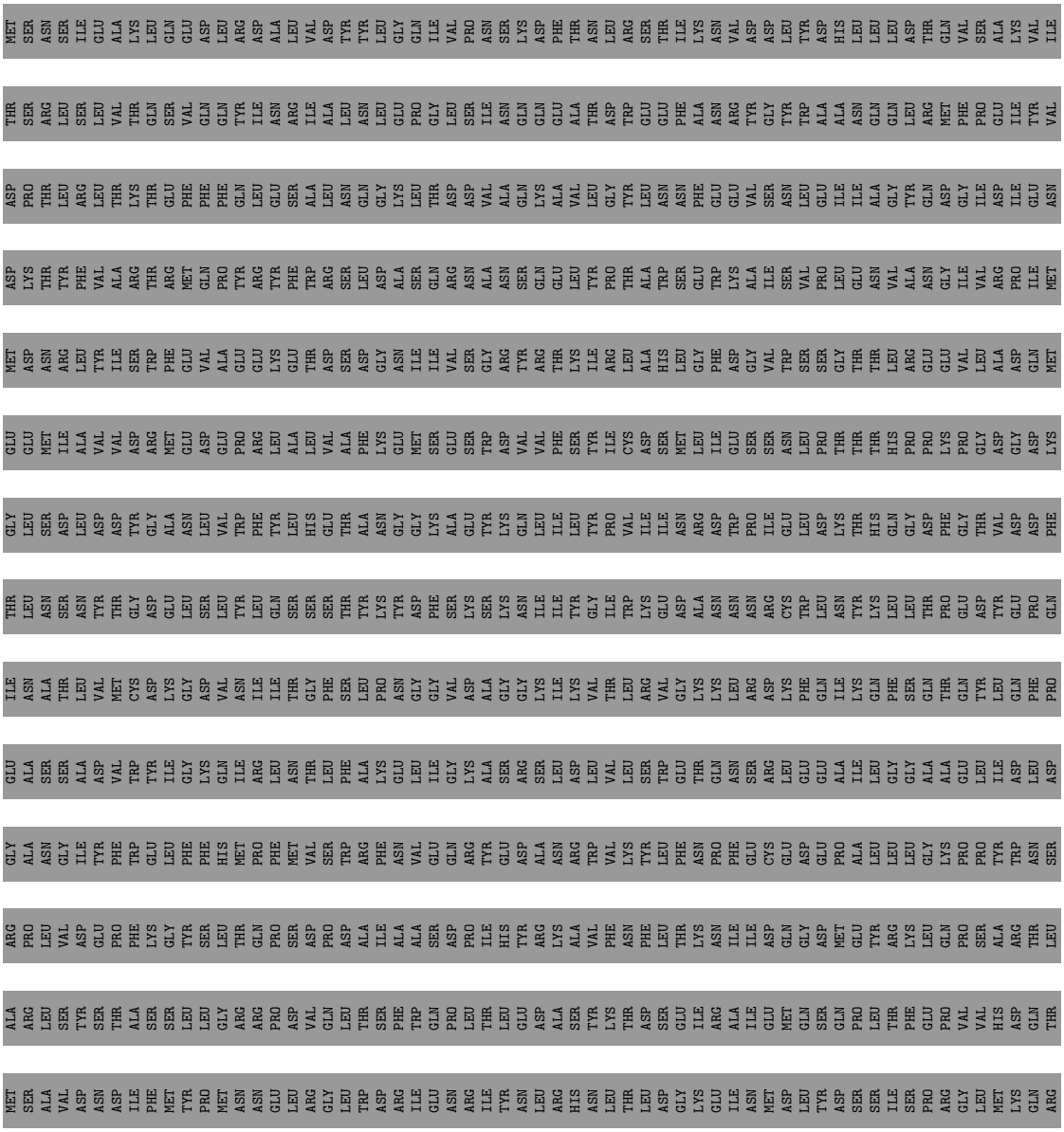


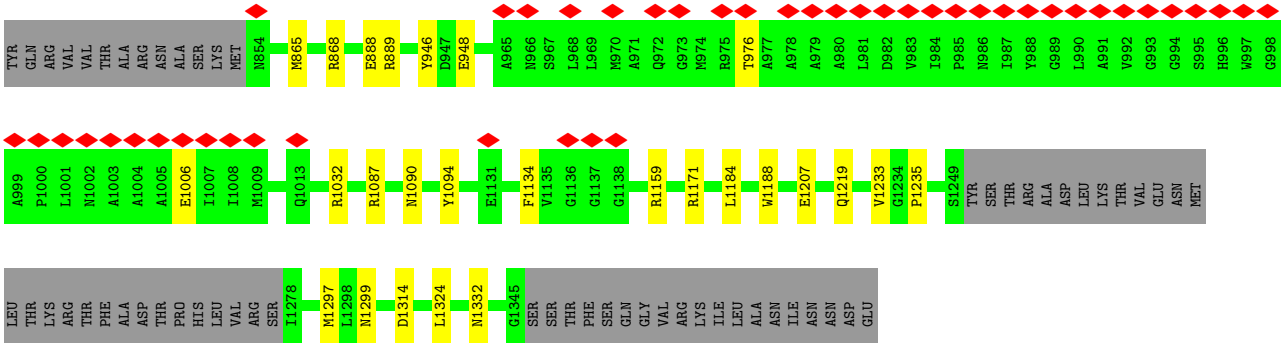




• Molecule 1: Toxin subunit YenA2

Chain G: 32% 66%

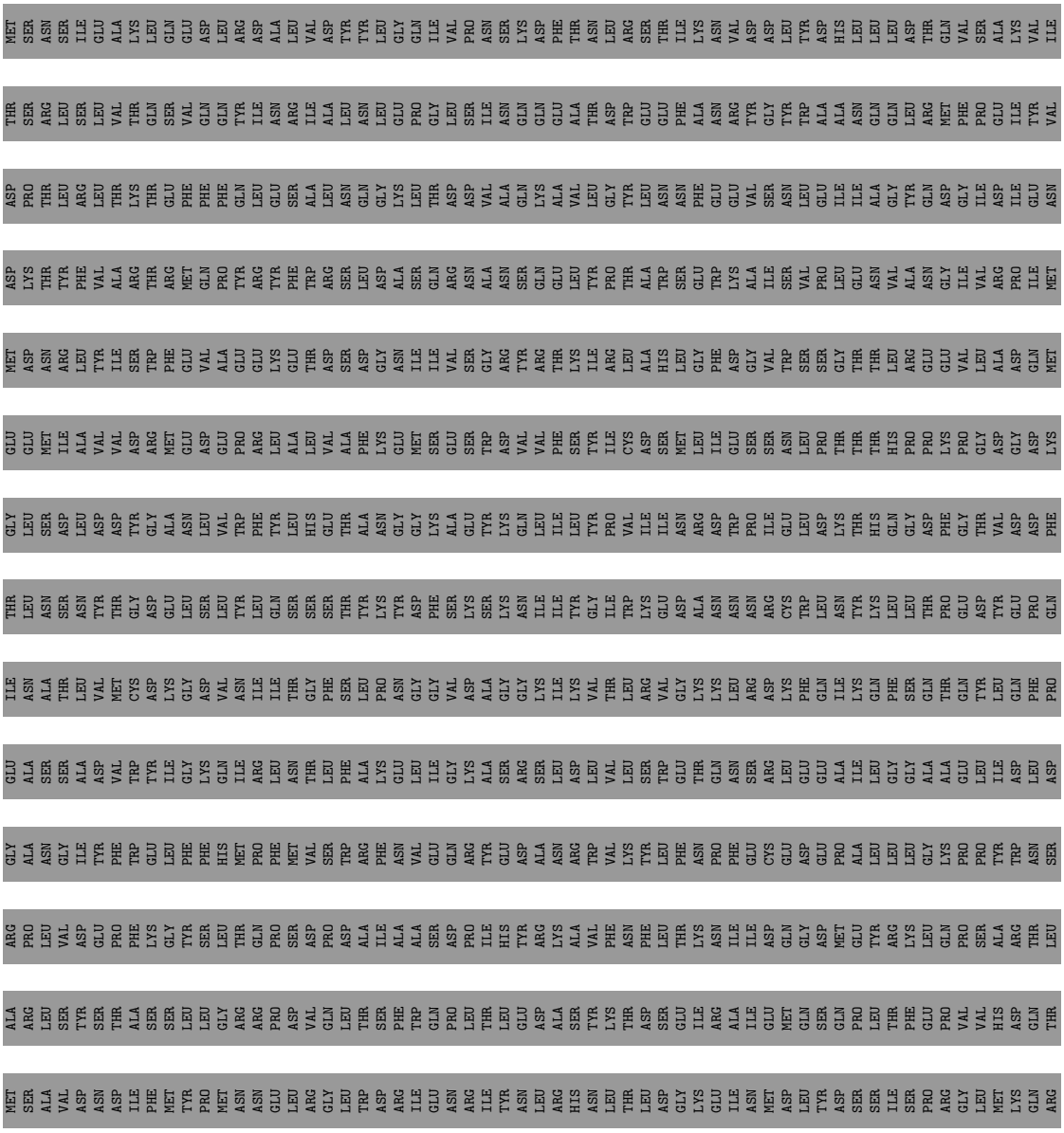


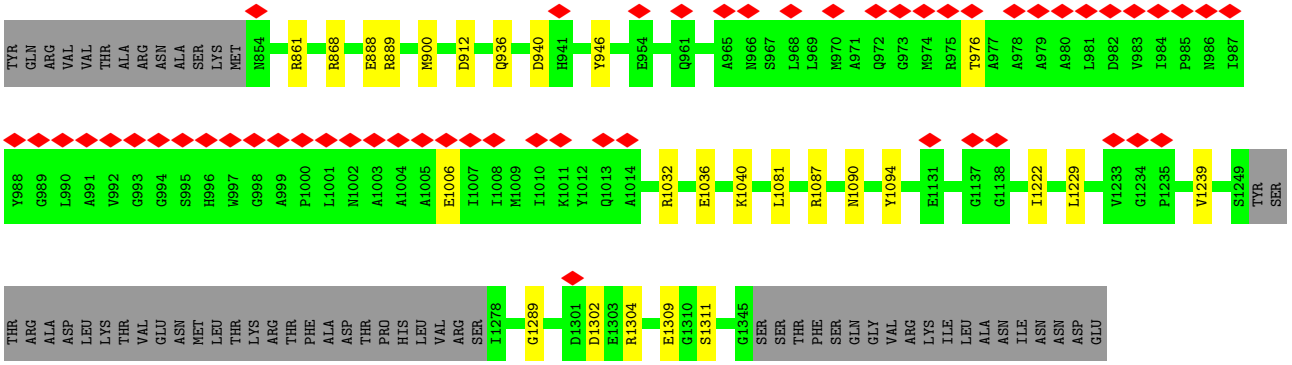


- Molecule 1: Toxin subunit YenA2

Chain J:



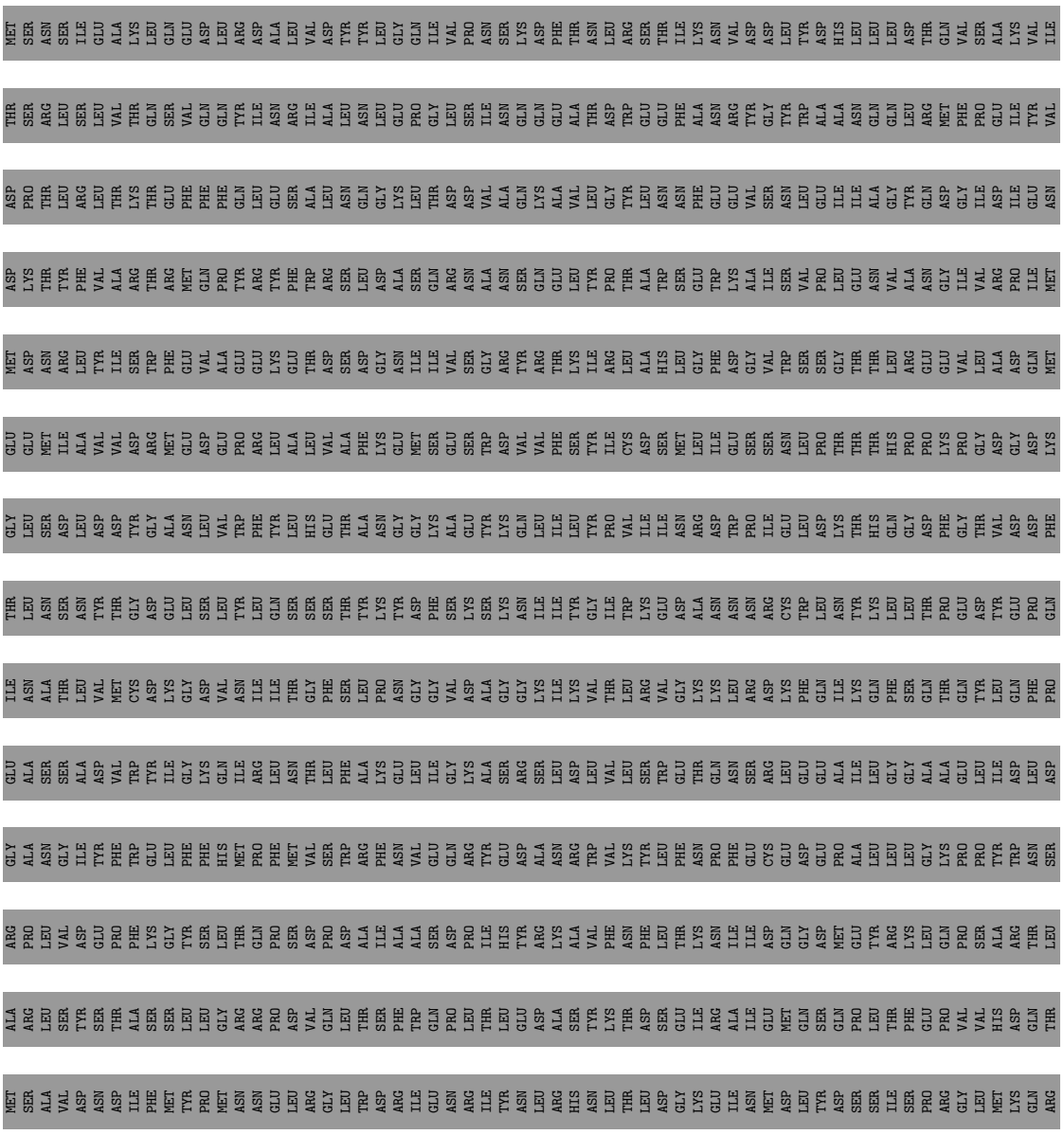


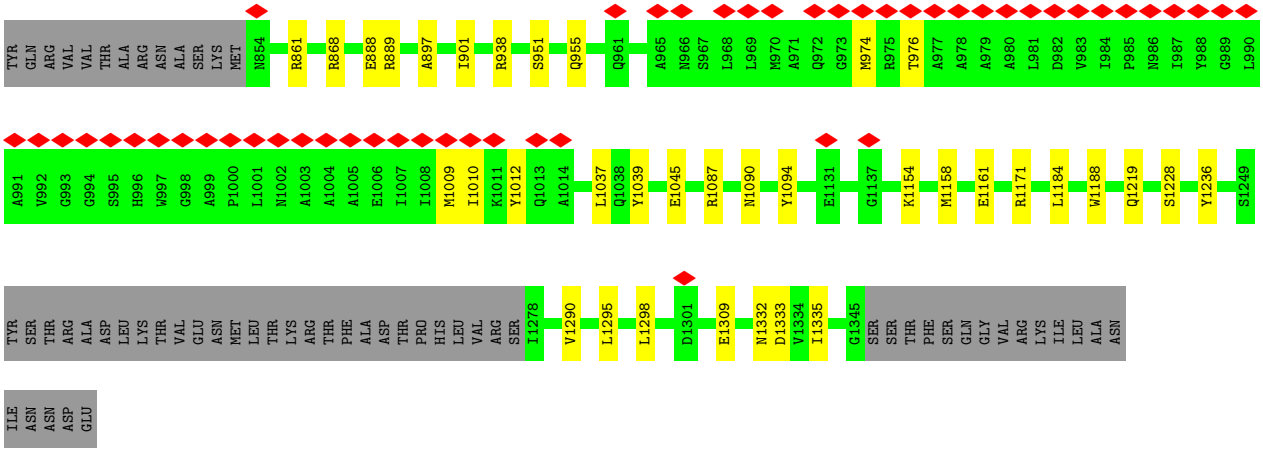


- Molecule 1: Toxin subunit YenA2

Chain M:



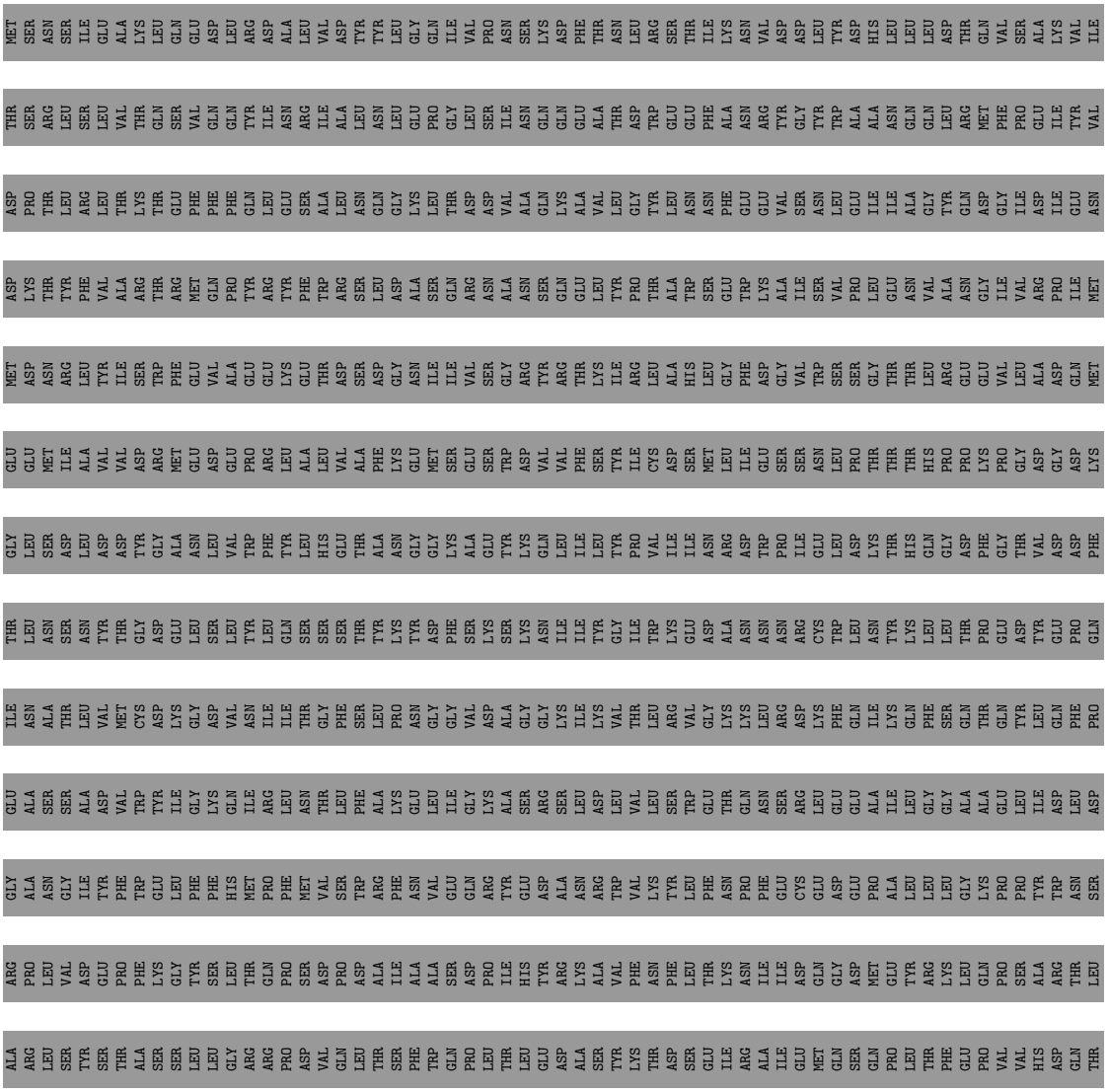


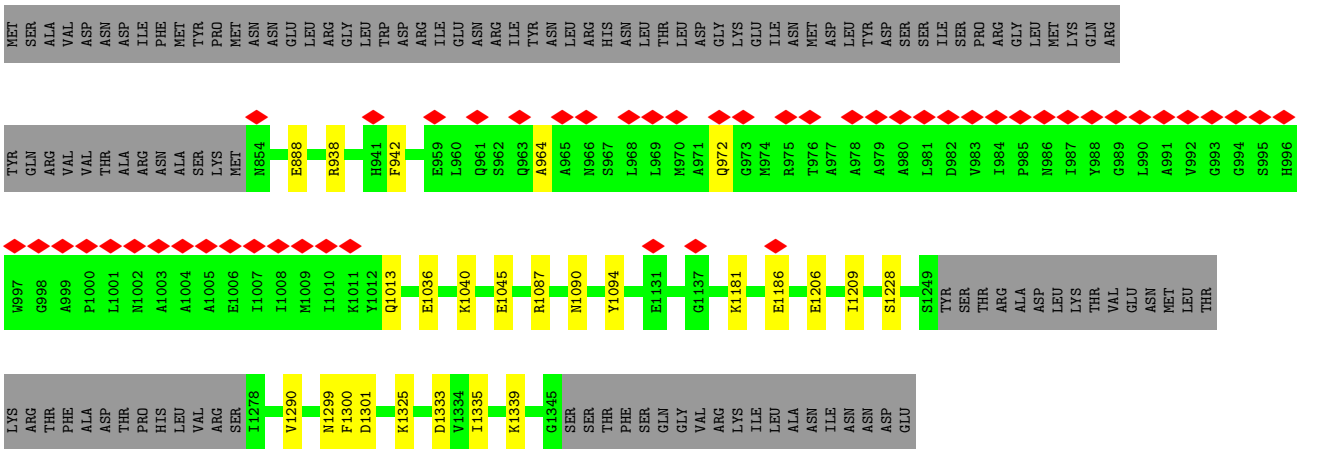


- Molecule 1: Toxin subunit YenA2

Chain P:

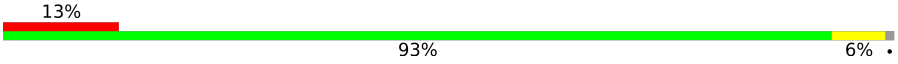


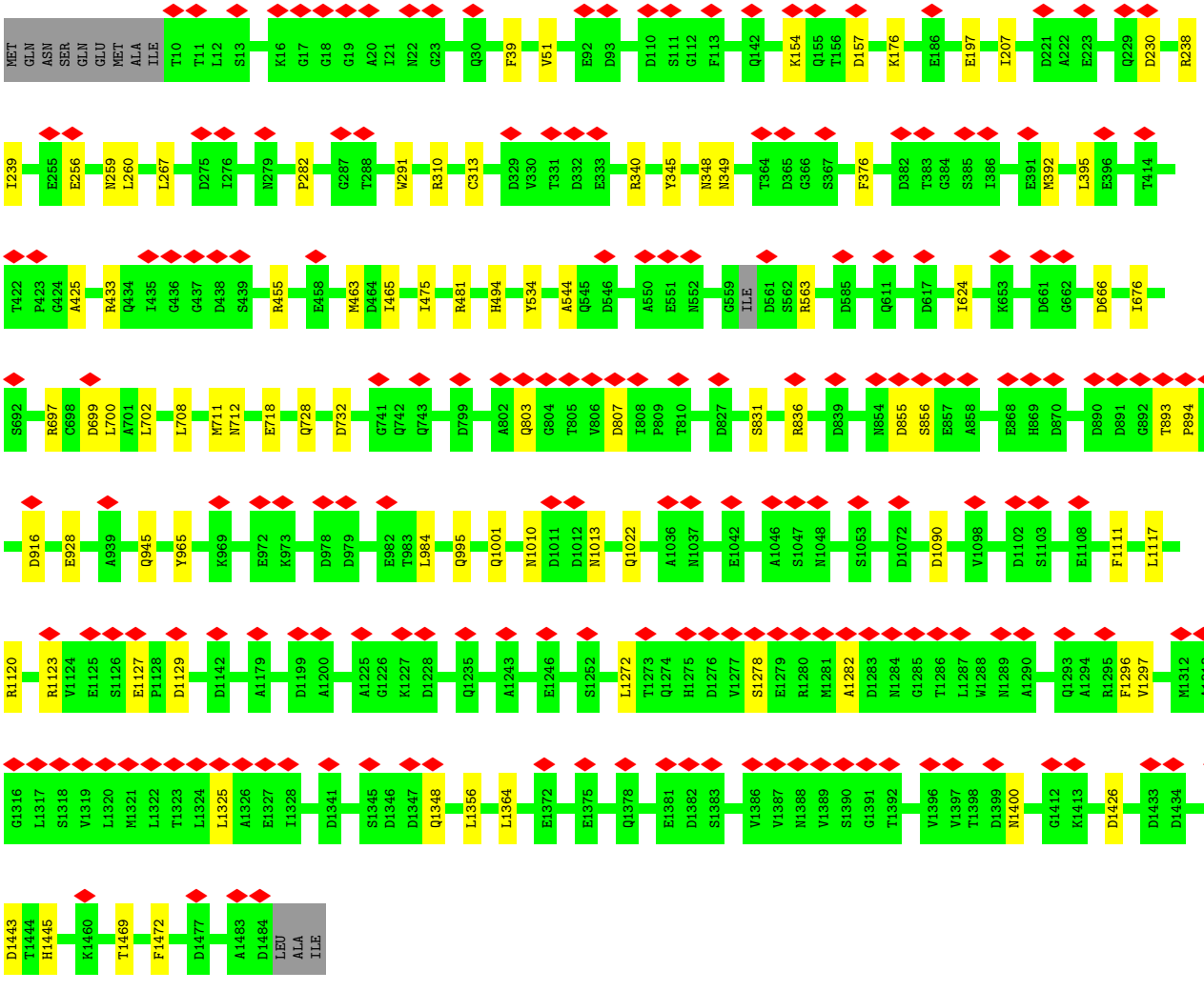




• Molecule 2: Toxin subunit YenB

Chain D:

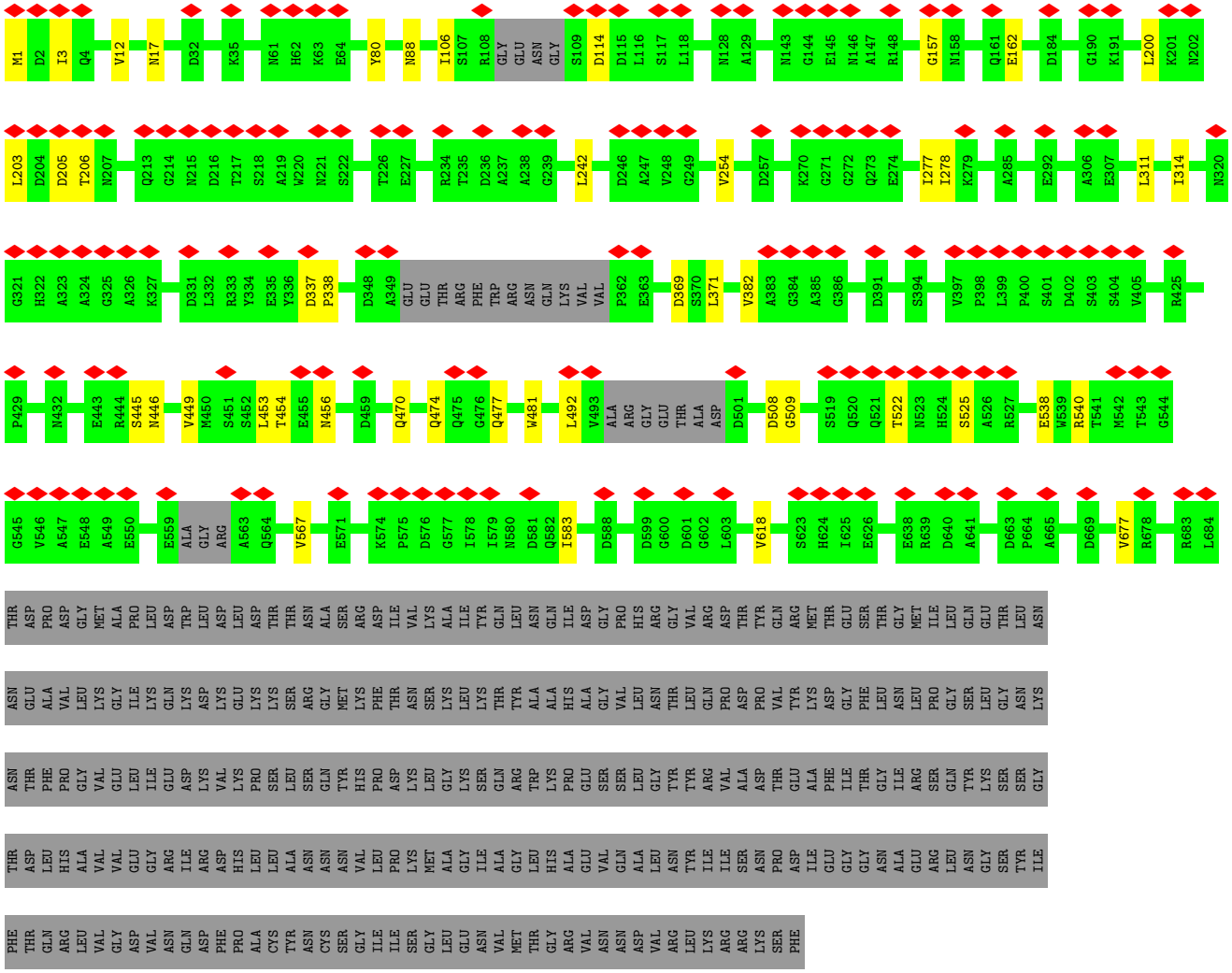




• Molecule 3: Toxin subunit YenC2

Chain E:




M1 D2 I3 Q4 V12 N17 D32 K35 N61 H62 K63 E64 Y80 N88 I106 S107 R108 GLY GLU ASN GLY S109 D114 D115 L116 S117 L118 N128 A129 N143 G144 E145 N146 A147 R148 G157 N158 Q161 E162 D184 G190 K191 L200 K201 N202
L203 D204 D205 T206 N207 Q213 G214 N215 D216 T217 S218 A219 W220 N221 S222 T226 E227 R234 T235 D236 A237 A238 G239 L242 D246 A247 V248 G249 V254 D257 K270 G271 G272 Q273 E274 I277 I278 K279 A285 E292 A306 E307 L311 I314 N320
G321 H322 A323 A324 G325 A326 K327 D331 L332 R333 Y334 E335 Y336 D337 P338 D348 A349 GLU GLU THR ARG PHE TRP ARG ASN GLN LYS VAL VAL P362 E363 D369 S370 L371 V382 A383 G384 A385 G386 D391 S394 V397 P398 L399 P400 S401 D402 S403 S404 V405 R425
P429 N432 E443 R444 S445 N446 V449 M450 S451 S452 L453 T454 E455 N456 D459 Q470 Q474 Q475 G476 Q477 W481 L492 V493 ALA ARG GLY GLU THR ALA ASP D501 D508 G509 S519 Q520 Q521 T522 N523 H524 S525 A526 R527 E538 W539 R540 T541 M542 T543 G544
G545 V546 A547 E548 A549 E550 E559 ALA GLY ARG A563 Q564 V567 E571 K574 P575 D576 G577 I578 I579 N580 D581 Q582 I583 D588 D599 G600 D601 G602 L603 V618 S623 H624 I625 E626 E638 R639 D640 A641 D663 P664 A665 D669 V677 R678 R683 L684
THR ASP PRO ASP GLY MET ALA PRO LEU ASP TRP LEU ASP LEU ASP THR THR ASN ALA SER ARG ASP ILE VAL LYS ALA ILE TYR GLN LEU ASN GLN ILE ASP GLY PRO HIS ARG GLY VAL ARG ASP THR TYR GLN ARG MET THR GLU SER THR GLY MET ILE LEU LEU GLN GLU THR LEU ASN
ASN GLU ALA VAL LEU LYS GLY ILE LYS GLN LYS ASP LYS GLU LYS LYS SER ARG GLY MET LYS PHE THR ASN SER LYS LEU LYS THR TYR ALA ALA HIS ALA GLY VAL LEU ASN THR LEU GLN PRO ASP PRO VAL TYR LYS ASP GLY PHE LEU ASN LEU PRO GLY SER LEU GLY ASN LYS
ASN THR PHE PRO GLY VAL GLU LEU ILE GLU ASP LYS VAL LYS PRO SER LEU SER GLN TYR HIS PRO ASP LYS LEU GLY LYS SER GLN ARG TRP LYS PRO GLU SER SER LEU GLY TYR TYR ARG VAL ALA ASP THR GLU ALA PHE ILE THR GLY ILE ARG SER GLN TYR LYS SER SER GLY
THR ASP LEU HIS ALA VAL VAL GLU GLY ARG ILE ARG ASP HIS LEU LEU ALA ASN ASN ASN VAL LEU PRO LYS MET ALA GLY ILE ALA GLY LEU HIS ALA GLU VAL GLN ALA LEU ASN TYR ILE ILE SER ASN PRO ASP ILE GLU GLY GLY ASN ALA GLU ARG LEU ASN GLY SER TYR ILE
PHE THR GLN ARG LEU VAL GLY ASP VAL ASN GLN ASP PHE PRO ALA CYS TYR ASN CYS SER GLY ILE ILE SER GLY LEU GLU ASN VAL MET THR GLY ARG VAL ASN ASN ASP VAL ARG LEU LYS ARG ARG LYS SER PHE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	147866	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 ($e^-/Å^2$)	44.7	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.223	Depositor
Minimum map value	0.000	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.232	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	B	0.14	0/3769	0.26	0/5092
1	G	0.14	0/3769	0.26	0/5092
1	J	0.15	0/3769	0.28	0/5092
1	M	0.15	0/3769	0.30	0/5092
1	P	0.14	0/3769	0.28	0/5092
2	D	0.11	0/12010	0.28	0/16371
3	E	0.10	0/5207	0.26	0/7086
All	All	0.13	0/36062	0.27	0/48917

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

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	B	3708	0	3649	14	0
1	G	3708	0	3649	18	0
1	J	3708	0	3649	18	0
1	M	3708	0	3649	24	0
1	P	3708	0	3649	16	0
2	D	11696	0	11142	61	0
3	E	5111	0	4959	27	0
All	All	35347	0	34346	157	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 2.

The worst 5 of 157 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)
3:E:508:ASP:OD1	3:E:509:GLY:N	2.18	0.77
1:G:1207:GLU:HG3	1:G:1314:ASP:HB2	1.69	0.75
1:B:1295:LEU:HD12	1:B:1298:LEU:HD12	1.73	0.70
1:J:861:ARG:NH2	1:J:1309:GLU:OE1	2.28	0.67
2:D:433:ARG:NH1	2:D:732:ASP:OD1	2.29	0.66

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	B	460/1364 (34%)	455 (99%)	5 (1%)	0	100	100
1	G	460/1364 (34%)	454 (99%)	6 (1%)	0	100	100
1	J	460/1364 (34%)	451 (98%)	9 (2%)	0	100	100
1	M	460/1364 (34%)	452 (98%)	8 (2%)	0	100	100
1	P	460/1364 (34%)	457 (99%)	3 (1%)	0	100	100
2	D	1472/1487 (99%)	1454 (99%)	18 (1%)	0	100	100
3	E	648/970 (67%)	633 (98%)	15 (2%)	0	100	100
All	All	4420/9277 (48%)	4356 (99%)	64 (1%)	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	B	408/1209 (34%)	408 (100%)	0	100 100
1	G	408/1209 (34%)	407 (100%)	1 (0%)	87 95
1	J	408/1209 (34%)	408 (100%)	0	100 100
1	M	408/1209 (34%)	405 (99%)	3 (1%)	76 86
1	P	408/1209 (34%)	407 (100%)	1 (0%)	87 95
2	D	1255/1266 (99%)	1253 (100%)	2 (0%)	87 95
3	E	551/818 (67%)	551 (100%)	0	100 100
All	All	3846/8129 (47%)	3839 (100%)	7 (0%)	85 95

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	1039	TYR
1	M	1184	LEU
1	P	1290	VAL
1	M	1290	VAL
1	G	1324	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	1283	GLN
1	M	921	ASN
1	G	1332	ASN
1	J	1141	ASN
1	M	1013	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	E	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	6.14

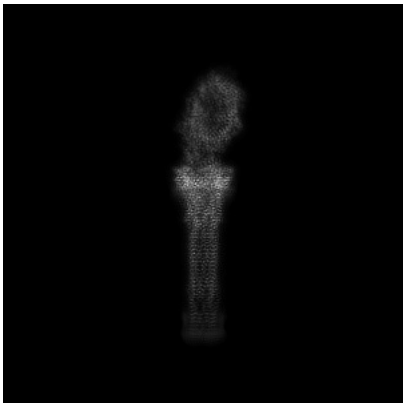
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-58515. These allow visual inspection of the internal detail of the map and identification of artifacts.

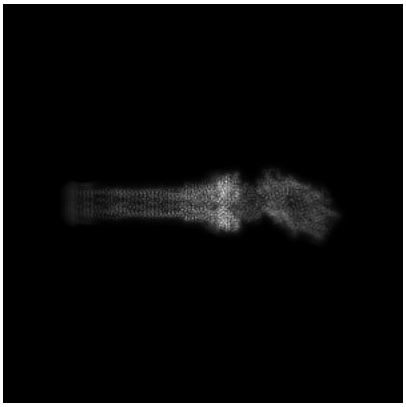
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

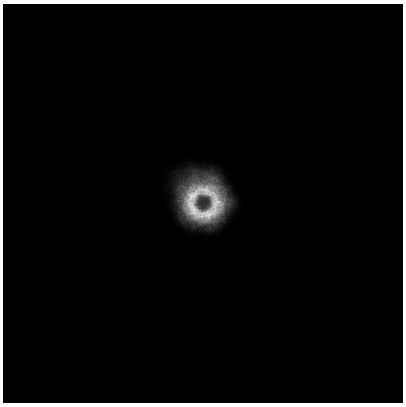
6.1.1 Primary map



X



Y



Z

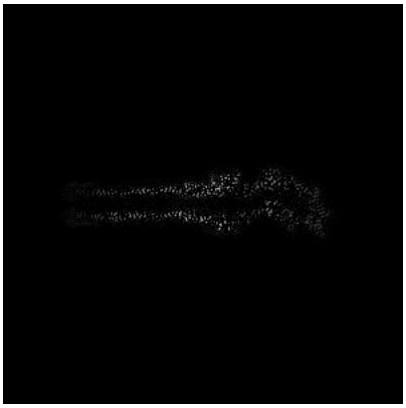
The images above show the map projected in three orthogonal directions.

6.2 Central slices

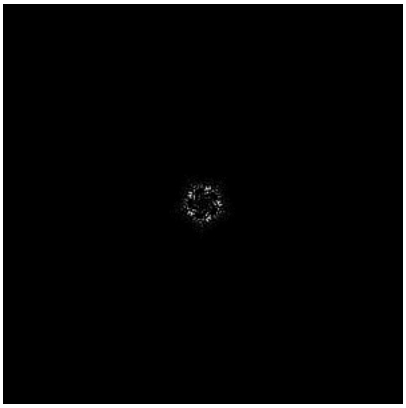
6.2.1 Primary map



X Index: 300



Y Index: 300



Z Index: 300

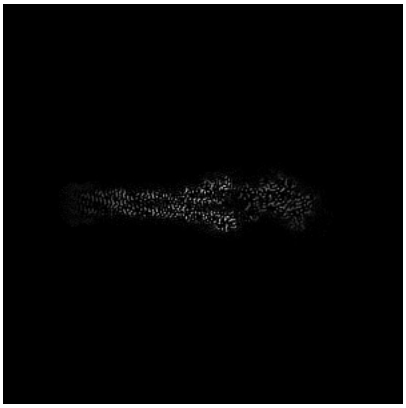
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

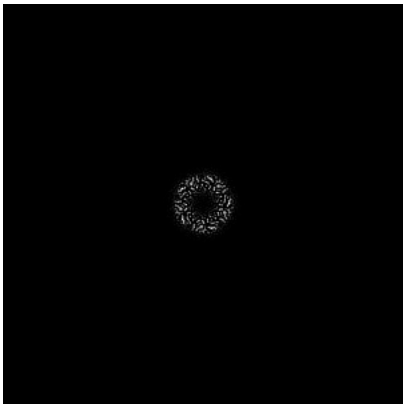
6.3.1 Primary map



X Index: 286



Y Index: 286

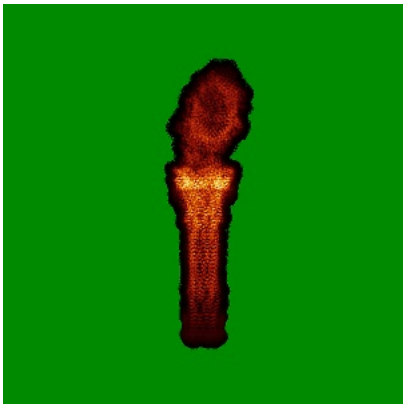


Z Index: 334

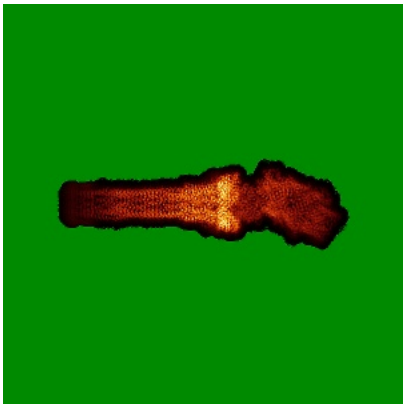
The images above show the largest variance slices of the map in three orthogonal directions.

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

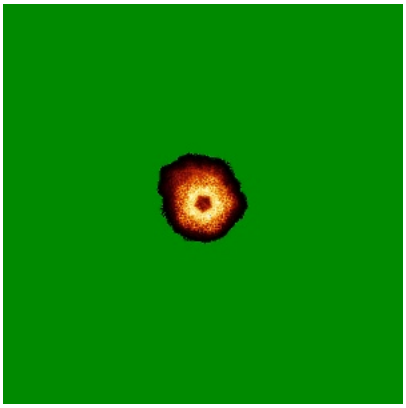
6.4.1 Primary map



X



Y

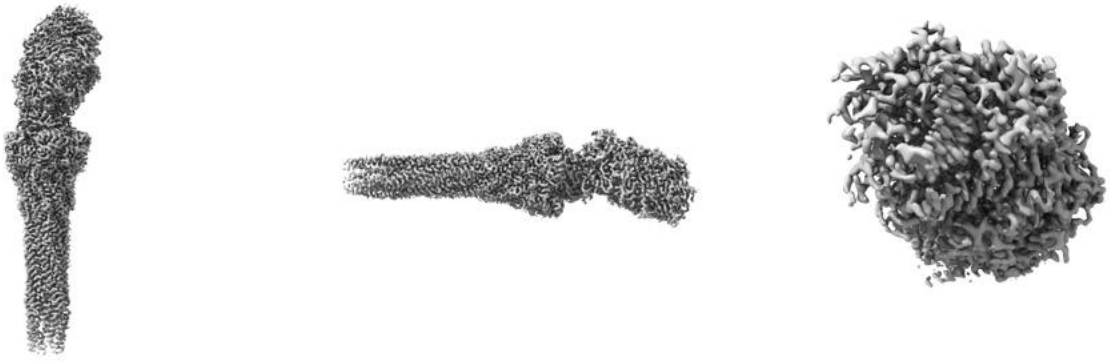


Z

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

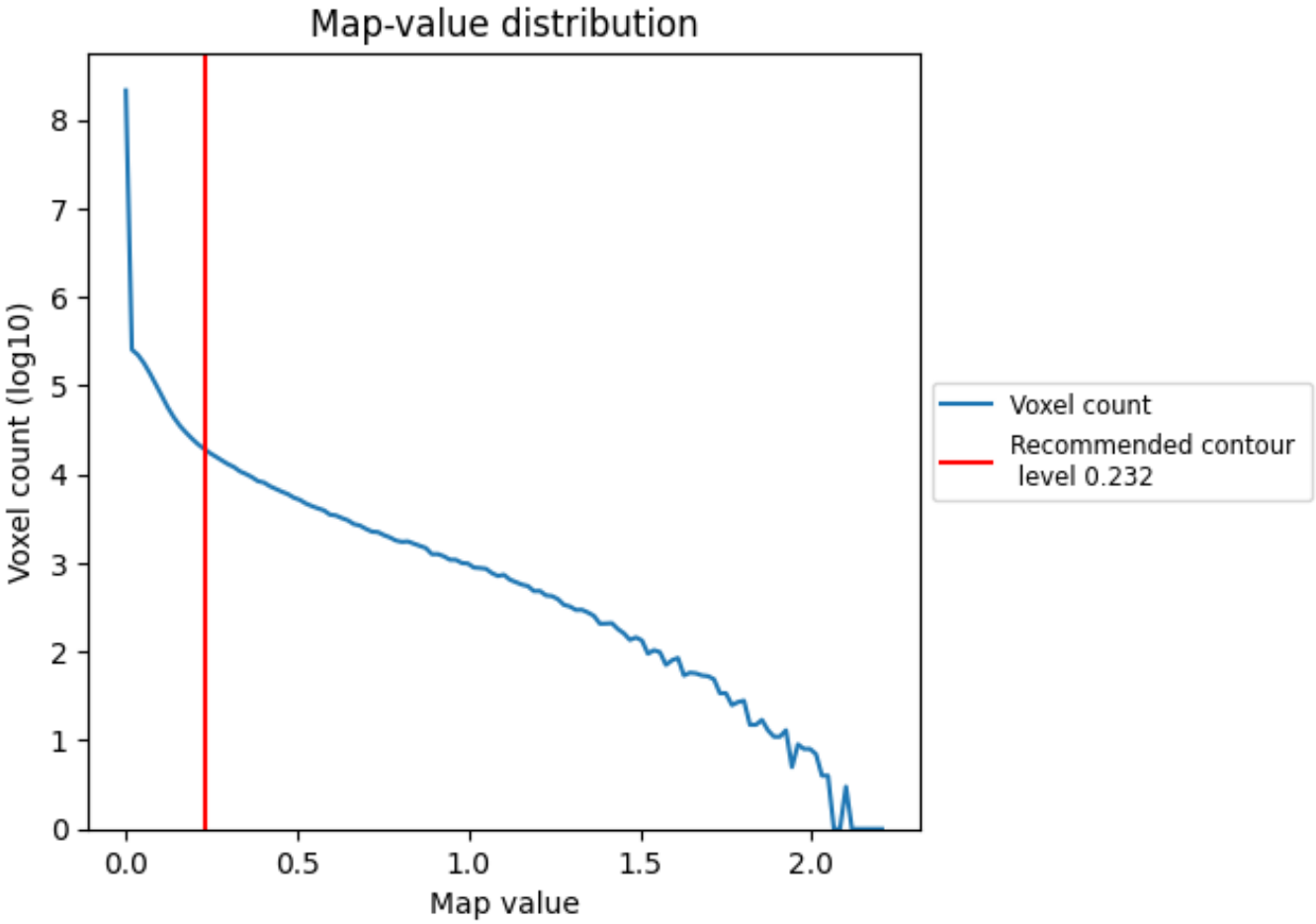
6.6 Mask visualisation (i)

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

7 Map analysis

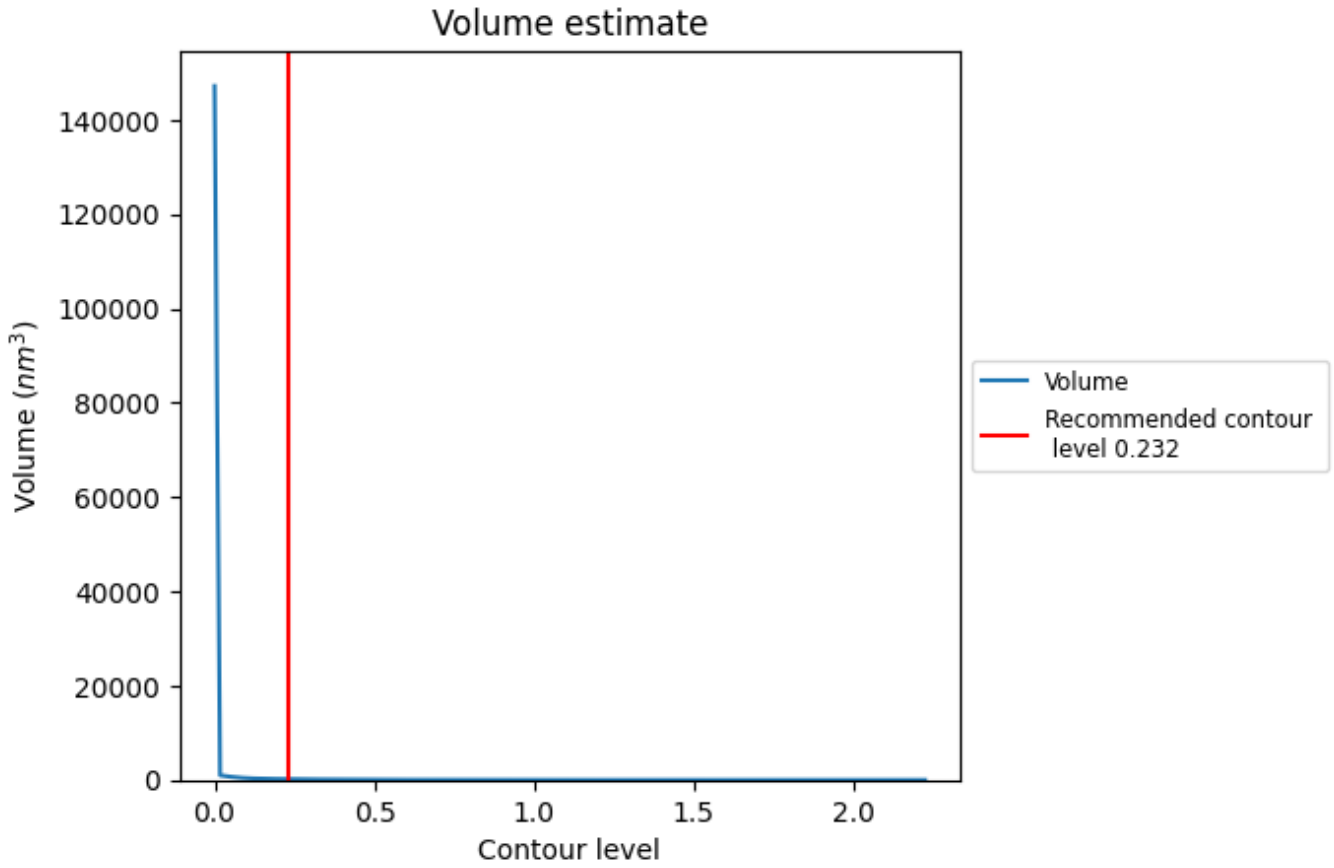
This section contains the results of statistical analysis of the map.

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.

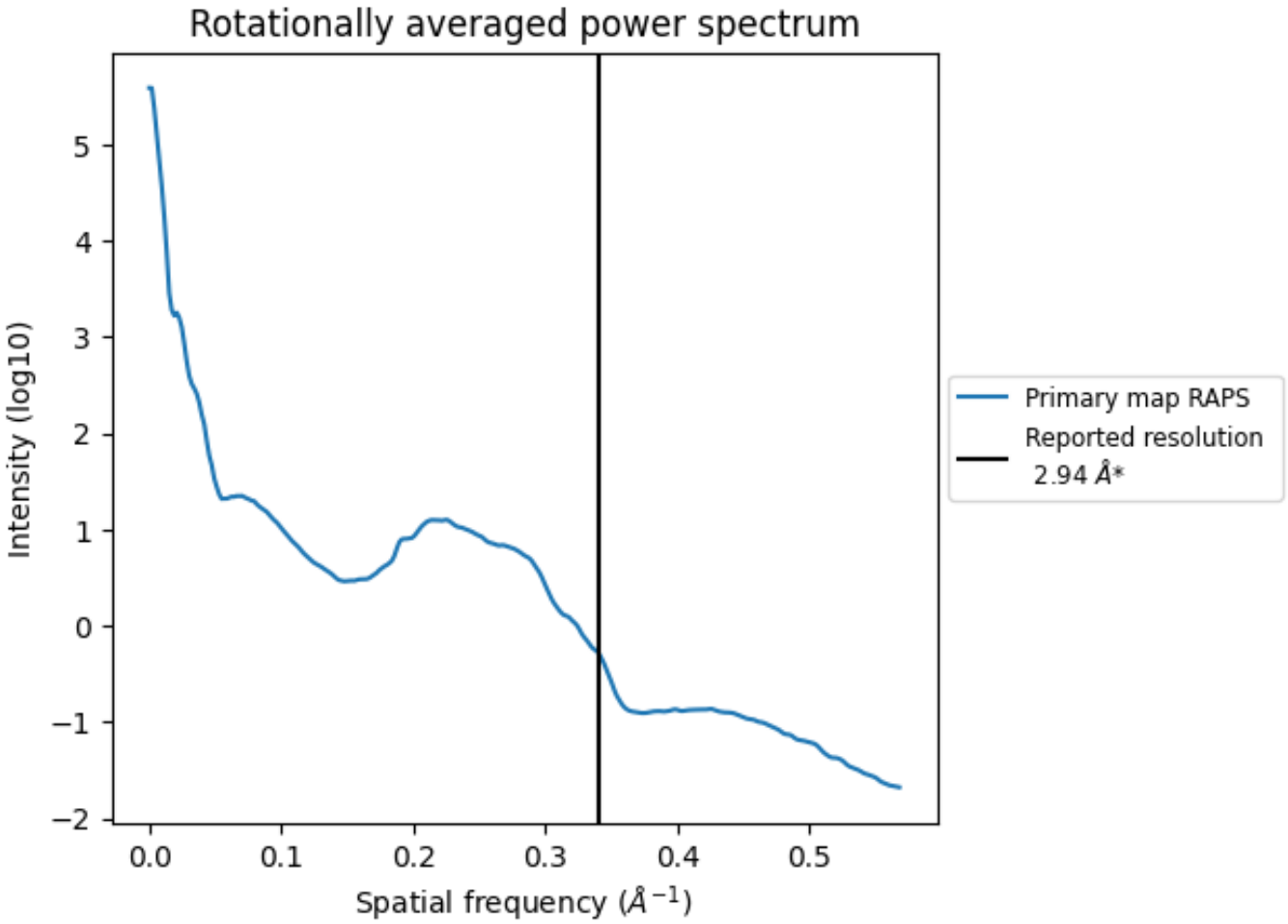
7.2 Volume estimate



The volume at the recommended contour level is 170 nm^3; this corresponds to an approximate mass of 154 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 0.340 Å^{-1}

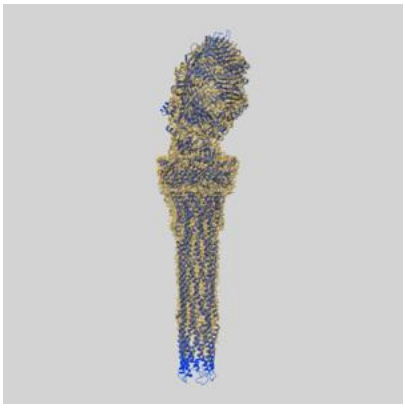
8 Fourier-Shell correlation

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

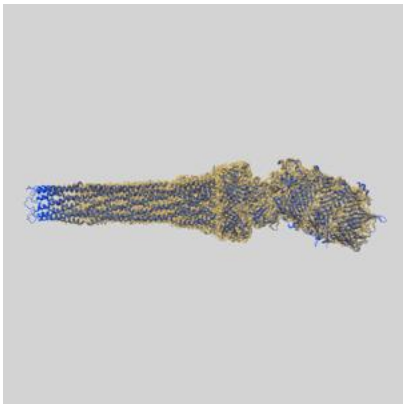
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-58515 and PDB model 31LY. Per-residue inclusion information can be found in section 3 on page 5.

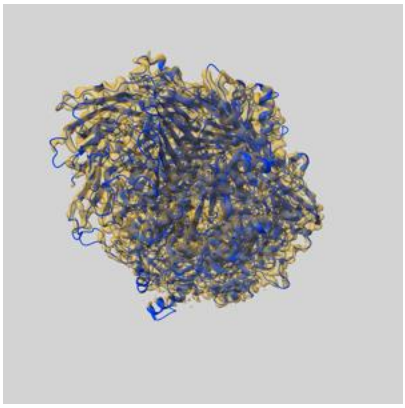
9.1 Map-model overlay



X



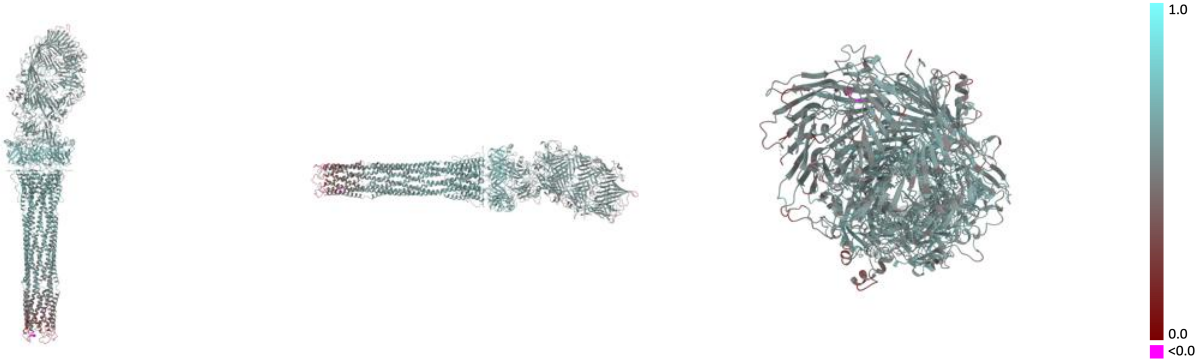
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.232 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.

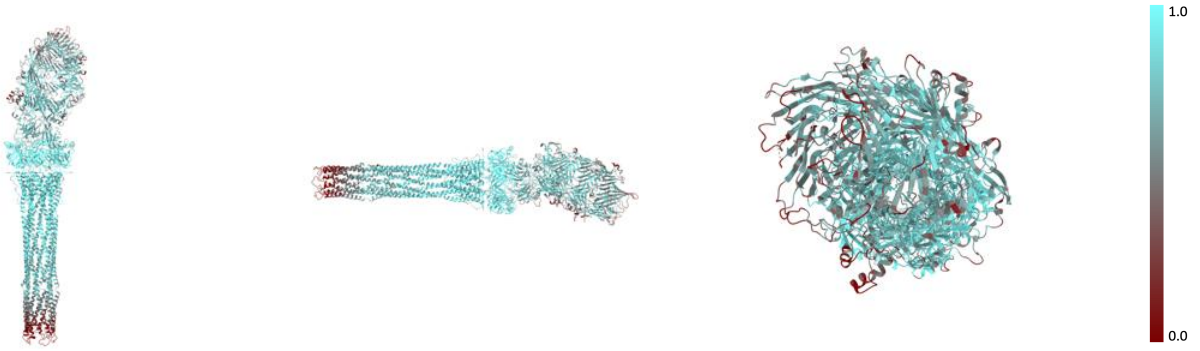
9.2 Q-score mapped to coordinate model



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.

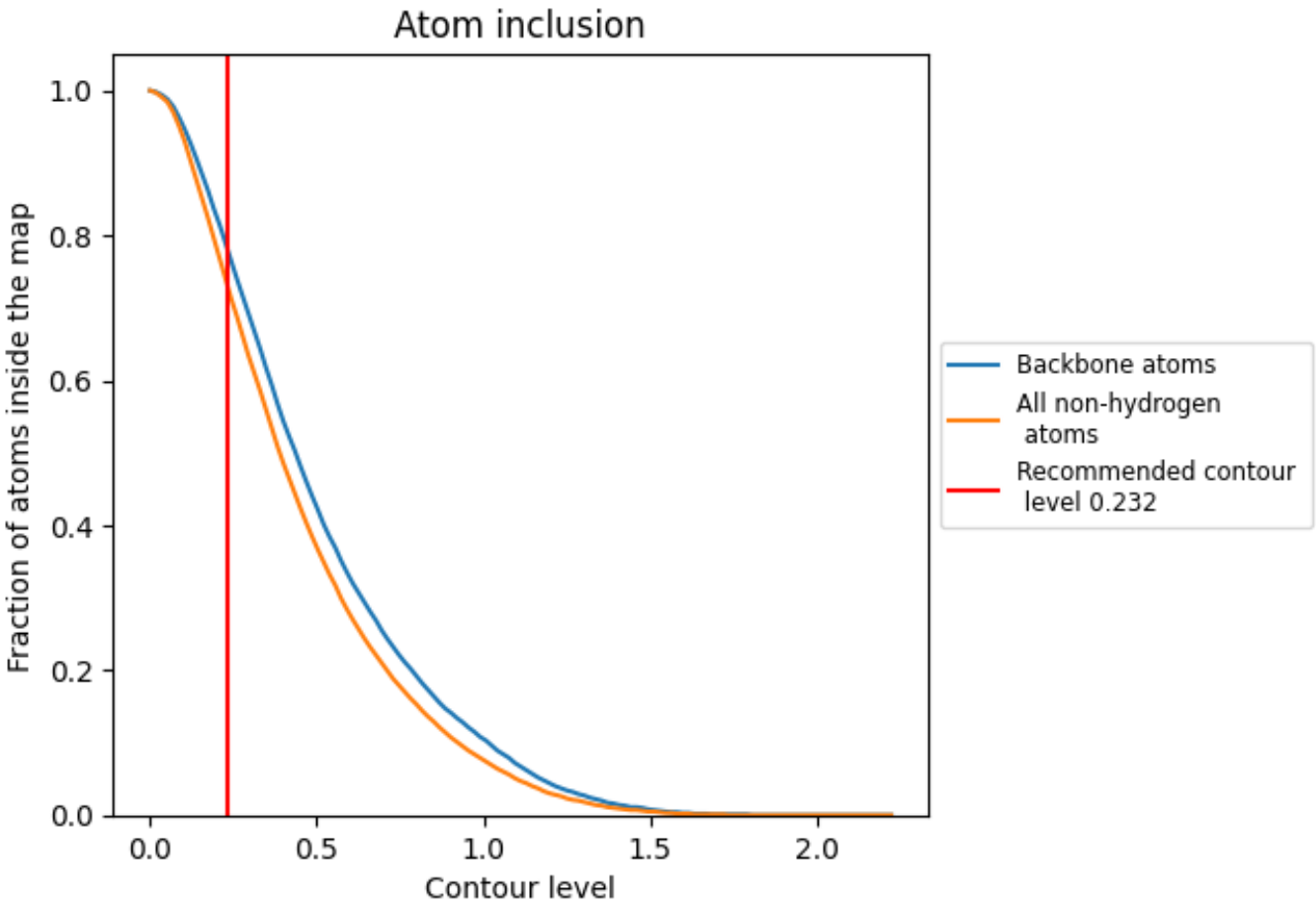
9.3 Atom inclusion mapped to coordinate model



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 (0.232).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 73% 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 (0.232) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7310	0.5570
B	0.8070	0.5760
D	0.6820	0.5450
E	0.5840	0.5250
G	0.8050	0.5780
J	0.7980	0.5690
M	0.8010	0.5740
P	0.8040	0.5710

