



wwPDB EM Validation Summary Report ⓘ

Mar 17, 2026 – 05:11 PM UTC

PDB ID : 9C4K / pdb_00009c4k
EMDB ID : EMD-45190
Title : Yersinia entomophaga holotoxin complex in prepore conformation
Authors : Low, Y.S.; Landsberg, M.J.
Deposited on : 2024-06-04
Resolution : 4.60 Å (reported)
Based on initial model : 6OGD

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

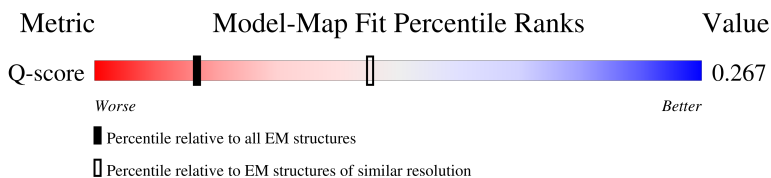
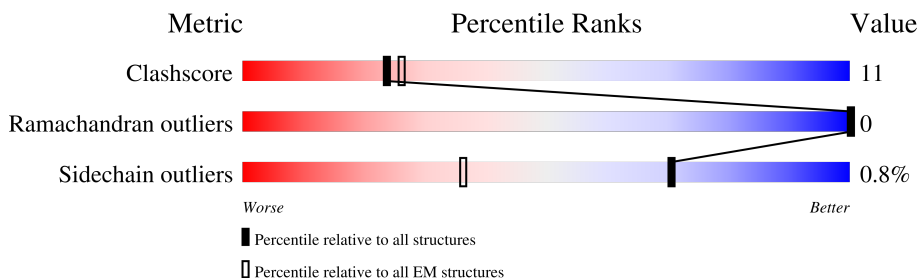
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 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.






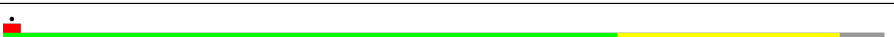
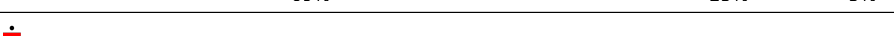
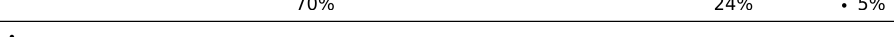





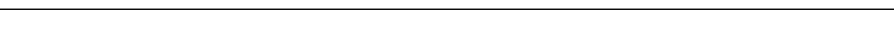
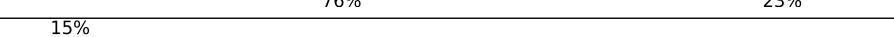
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2407 (4.10 - 5.10)

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

Mol	Chain	Length	Quality of chain
1	A	1164	 67% 21% 11%
1	D	1164	 68% 21% 11%
1	G	1164	 68% 21% 11%
1	J	1164	 68% 21% 11%

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Mol	Chain	Length	Quality of chain
1	M	1164	
2	B	1364	
2	E	1364	
2	H	1364	
2	K	1364	
2	N	1364	
3	C	633	
3	F	633	
3	I	633	
3	L	633	
3	O	633	
4	P	1487	
5	Q	970	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 133938 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	1033	Total	C	N	O	S	0	0
			8136	5186	1336	1591	23		
1	D	1033	Total	C	N	O	S	0	0
			8136	5186	1336	1591	23		
1	G	1033	Total	C	N	O	S	0	0
			8136	5186	1336	1591	23		
1	J	1033	Total	C	N	O	S	0	0
			8136	5186	1336	1591	23		
1	M	1033	Total	C	N	O	S	0	0
			8136	5186	1336	1591	23		

- Molecule 2 is a protein called Toxin subunit YenA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1289	Total	C	N	O	S	0	0
			10415	6606	1751	2022	36		
2	E	1289	Total	C	N	O	S	0	0
			10415	6606	1751	2022	36		
2	H	1289	Total	C	N	O	S	0	0
			10415	6606	1751	2022	36		
2	K	1289	Total	C	N	O	S	0	0
			10415	6606	1751	2022	36		
2	N	1289	Total	C	N	O	S	0	0
			10415	6606	1751	2022	36		

- Molecule 3 is a protein called Chitinase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	631	Total	C	N	O	S	0	0
			4896	3096	821	961	18		
3	F	631	Total	C	N	O	S	0	0
			4896	3096	821	961	18		
3	I	631	Total	C	N	O	S	0	0
			4896	3096	821	961	18		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	631	Total	C	N	O	S	0	0
			4896	3096	821	961	18		
3	O	631	Total	C	N	O	S	0	0
			4896	3096	821	961	18		

- Molecule 4 is a protein called Toxin subunit YenB.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	1476	Total	C	N	O	S	0	0
			11580	7325	1990	2228	37		

- Molecule 5 is a protein called Toxin subunit YenC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	668	Total	C	N	O	S	0	0
			5123	3197	895	1019	12		

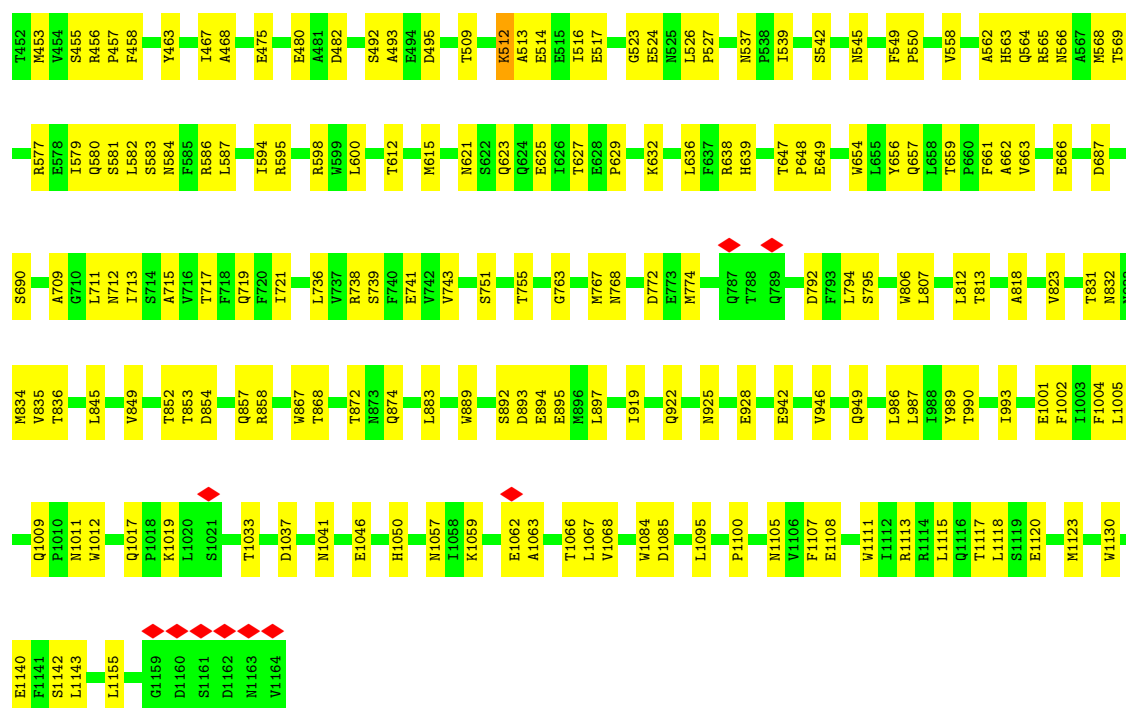
Chain D: 68% 21% 11%

[illegible]

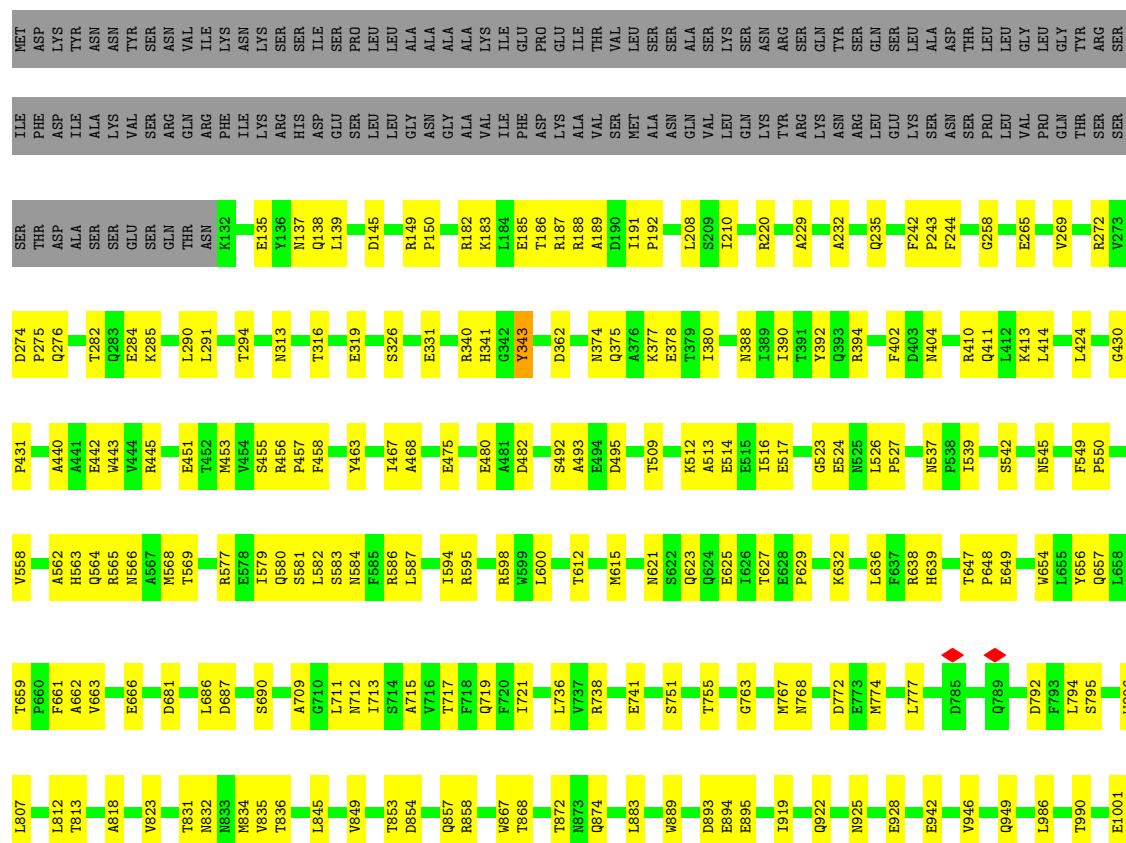
- Molecule 1: Toxin subunit YenA1

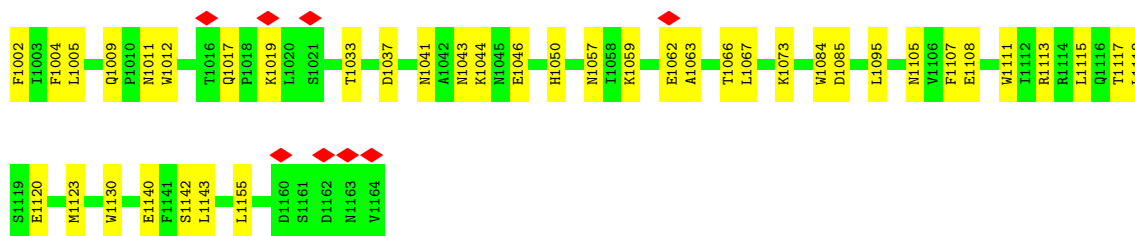
Chain G: 68% 21% 11%

	T282	T283	E284	K285	L290	N313	T316	E319	S326	E331	R340	H341	G342	Y343	D362	N375	K376	A376	K377	E378	I380	N388	I389	Y392	R393	R394	F402	D403	M404	R410	Q411	L424	G430	P431	A440	L441	E442	W443	V444	R445	C451									
SER	TSP	ASP	ALA	SER	SER	SER	GLN	THR	ASN	X132	E135	Y136	N137	Q138	D145	R149	P150	R182	K183	L184	T186	R187	R188	A189	D190	I191	P192	T210	R220	A229	A232	Q235	F242	P243	F244	G258	E265	V269	R272	D273	P275	C276								
ILE	PHE	ASP	ILE	ALA	LYS	VAL	GLN	ARG	PHE	ILE	LYS	ARG	SER	HIS	ASP	GLU	SER	LEU	GLY	ALA	GLY	ALA	VAL	ILE	PHE	ASP	LYS	ASN	ARG	GLN	TYR	SER	GLN	TYR	GLN	SER	LEU	ALA	ASP	THR	LEU	LEU	GLY	PRO	LEU	GLN	THR	GLY	SER	ASP



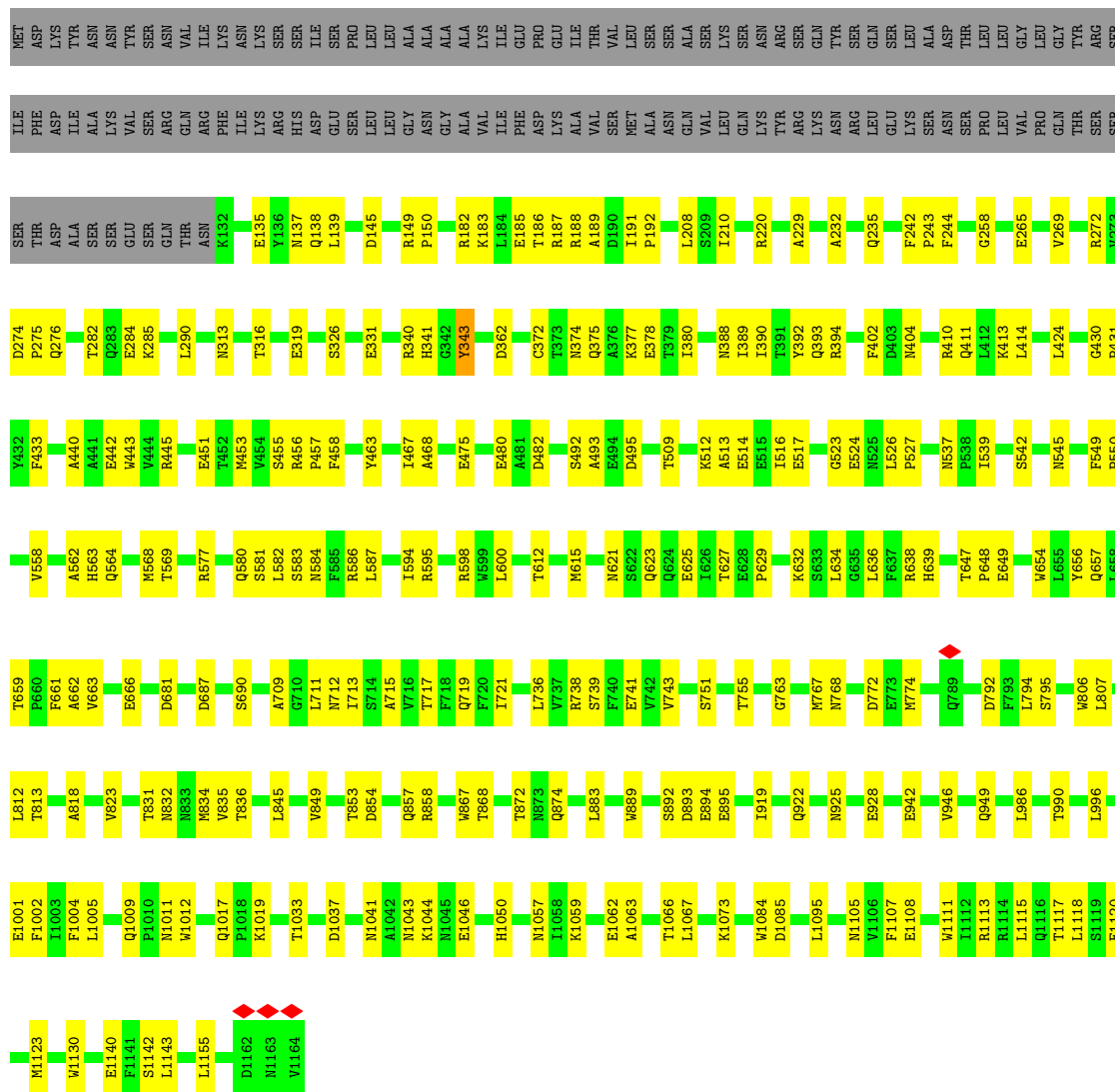
• Molecule 1: Toxin subunit YenA1





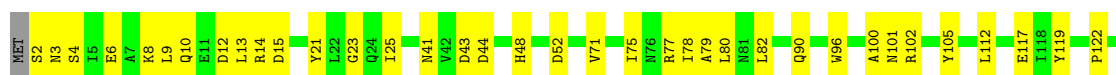
• Molecule 1: Toxin subunit YenA1

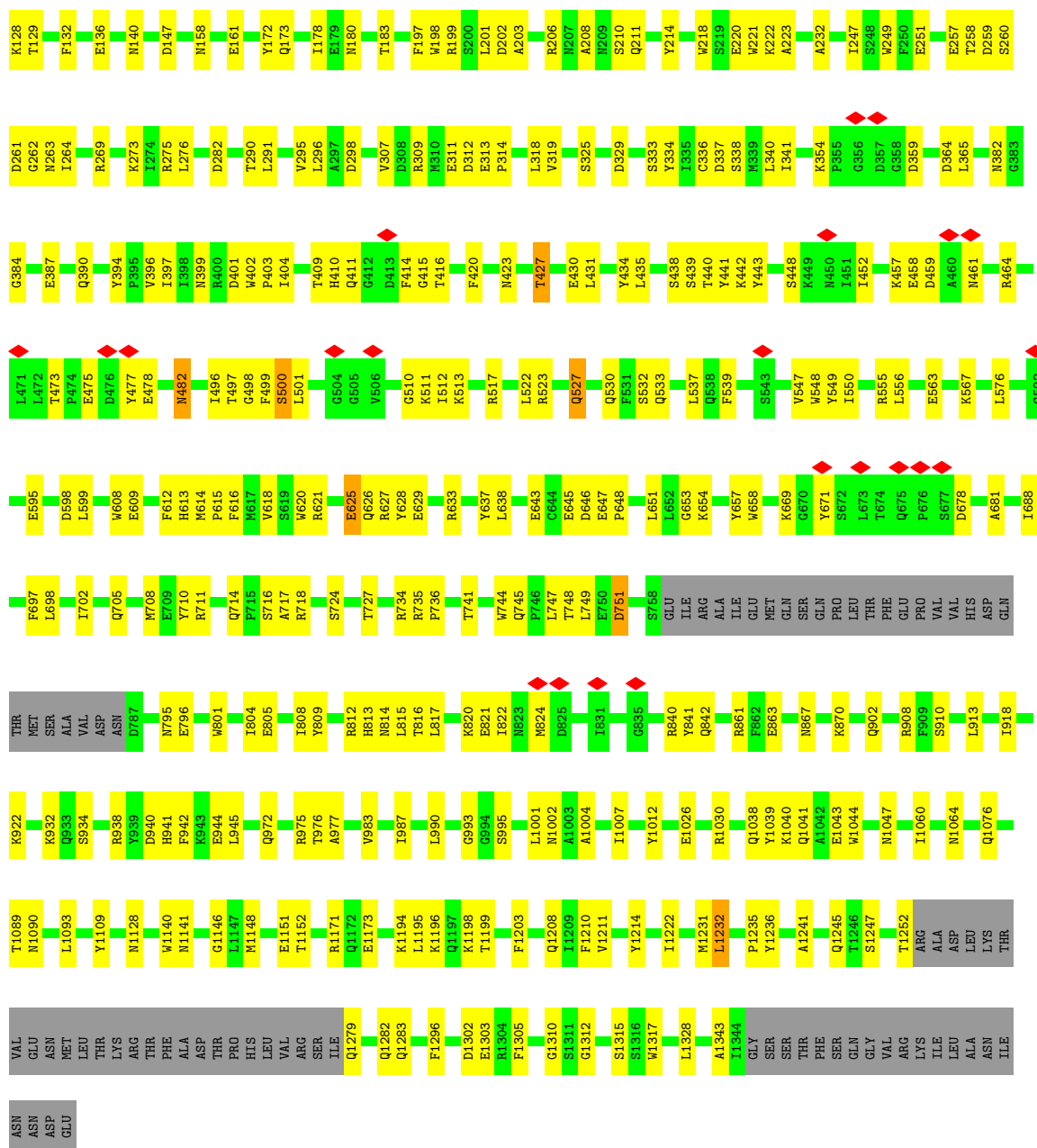
Chain M: 68% 21% 11%



• Molecule 2: Toxin subunit YenA2

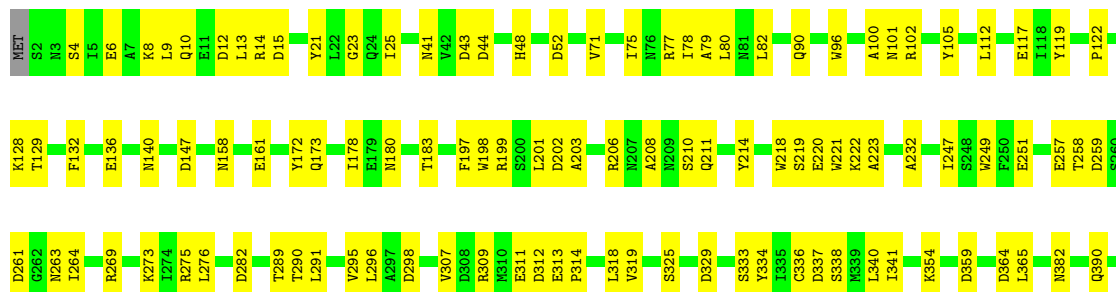
Chain B: 69% 25% 5%

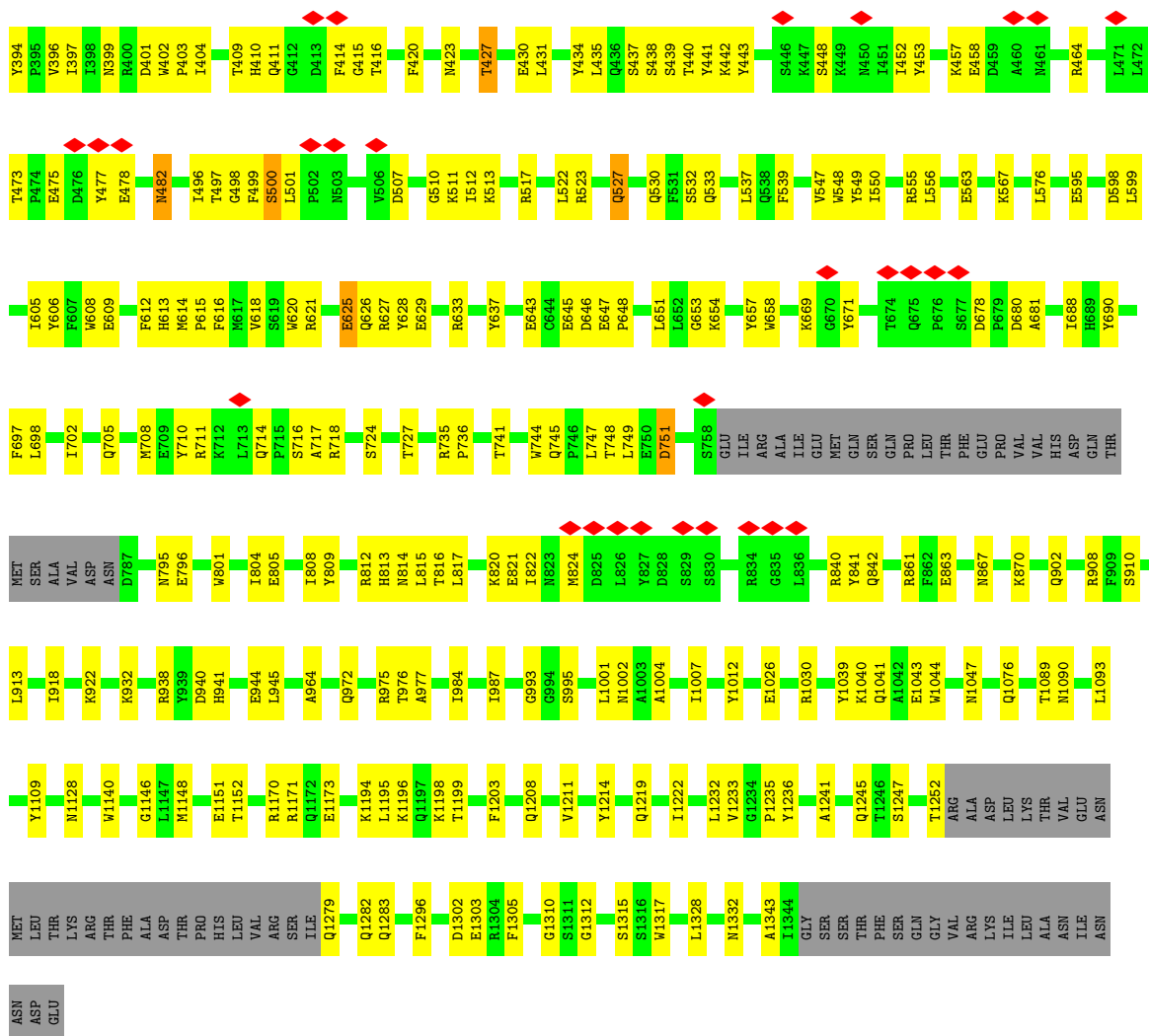




• Molecule 2: Toxin subunit YenA2

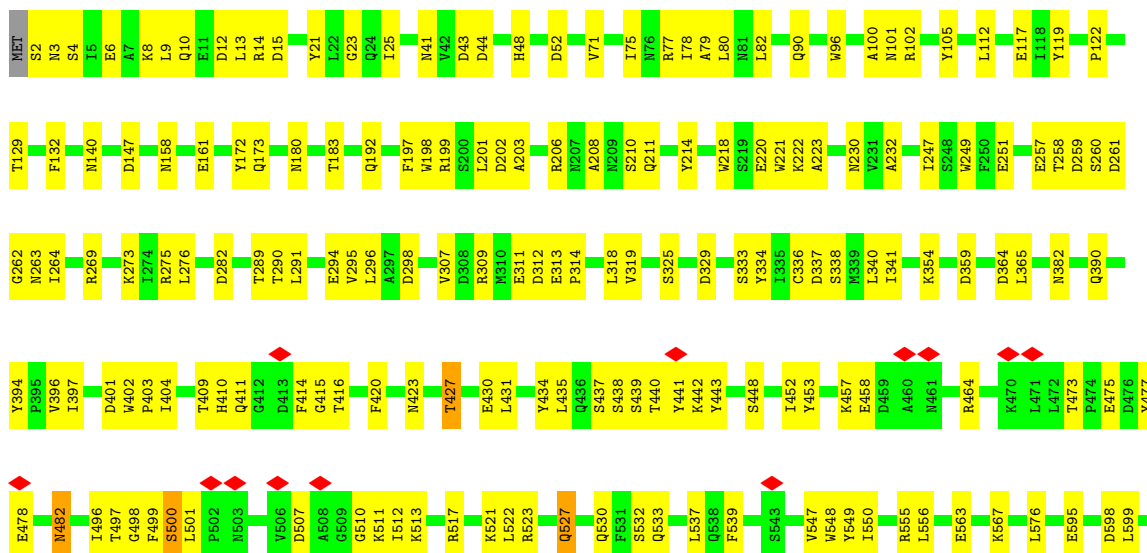
Chain E: 69% 25% 5%

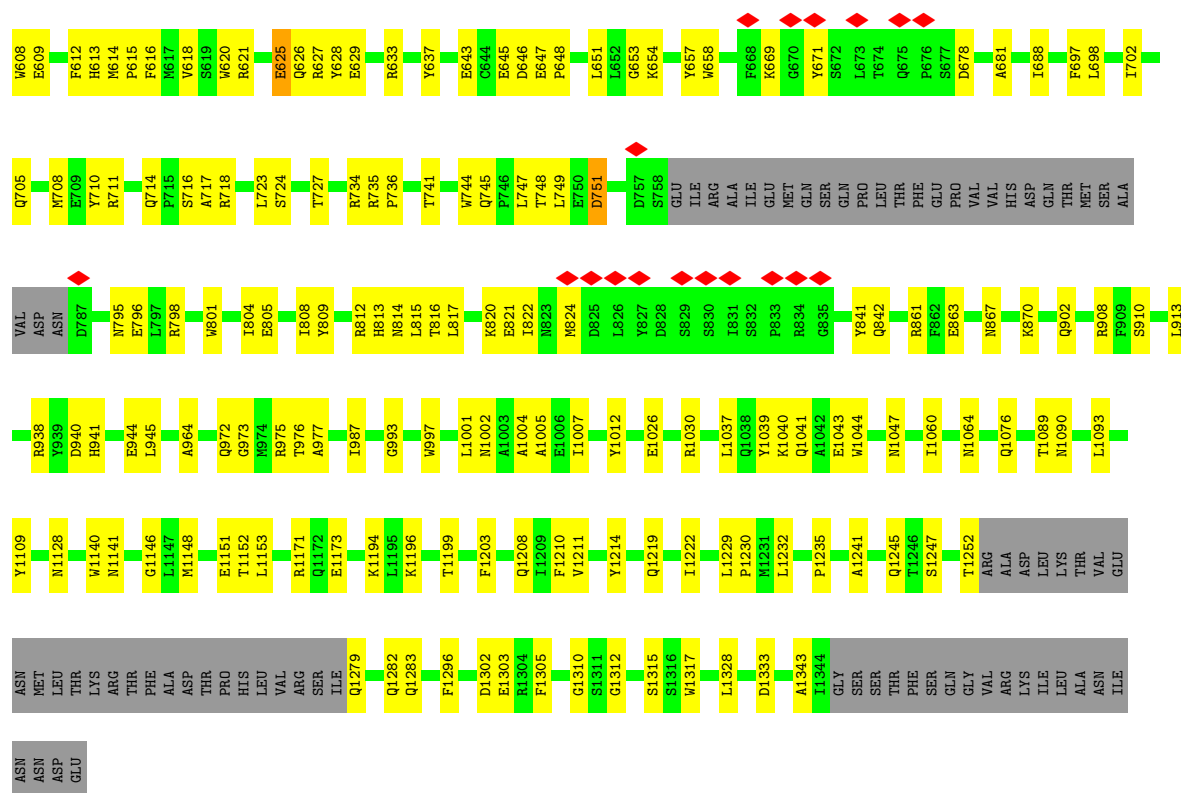


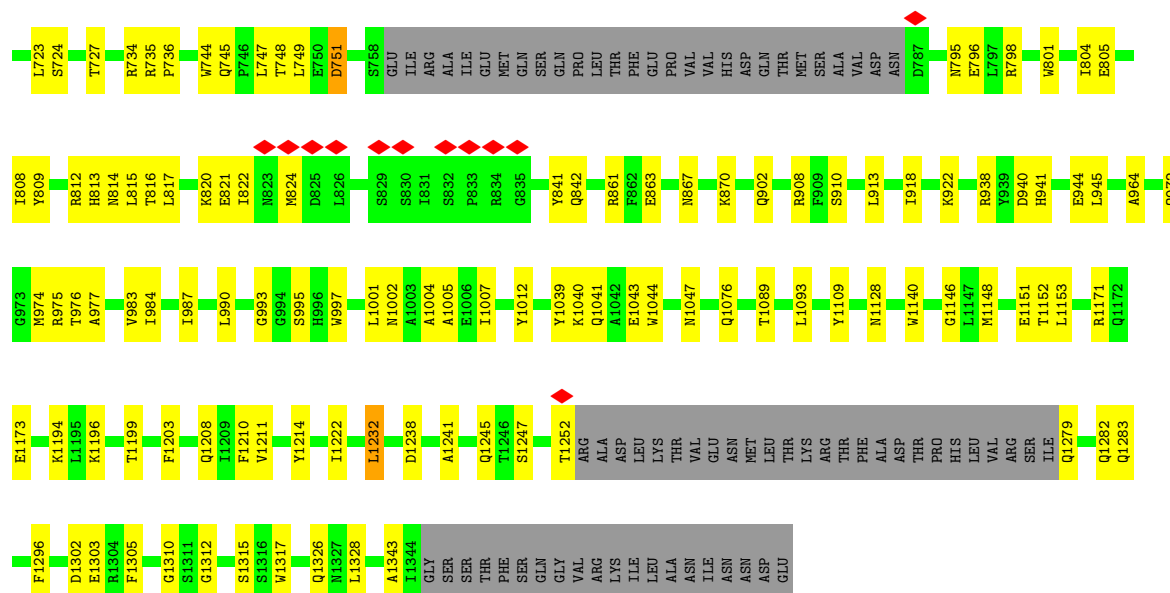


• Molecule 2: Toxin subunit YenA2

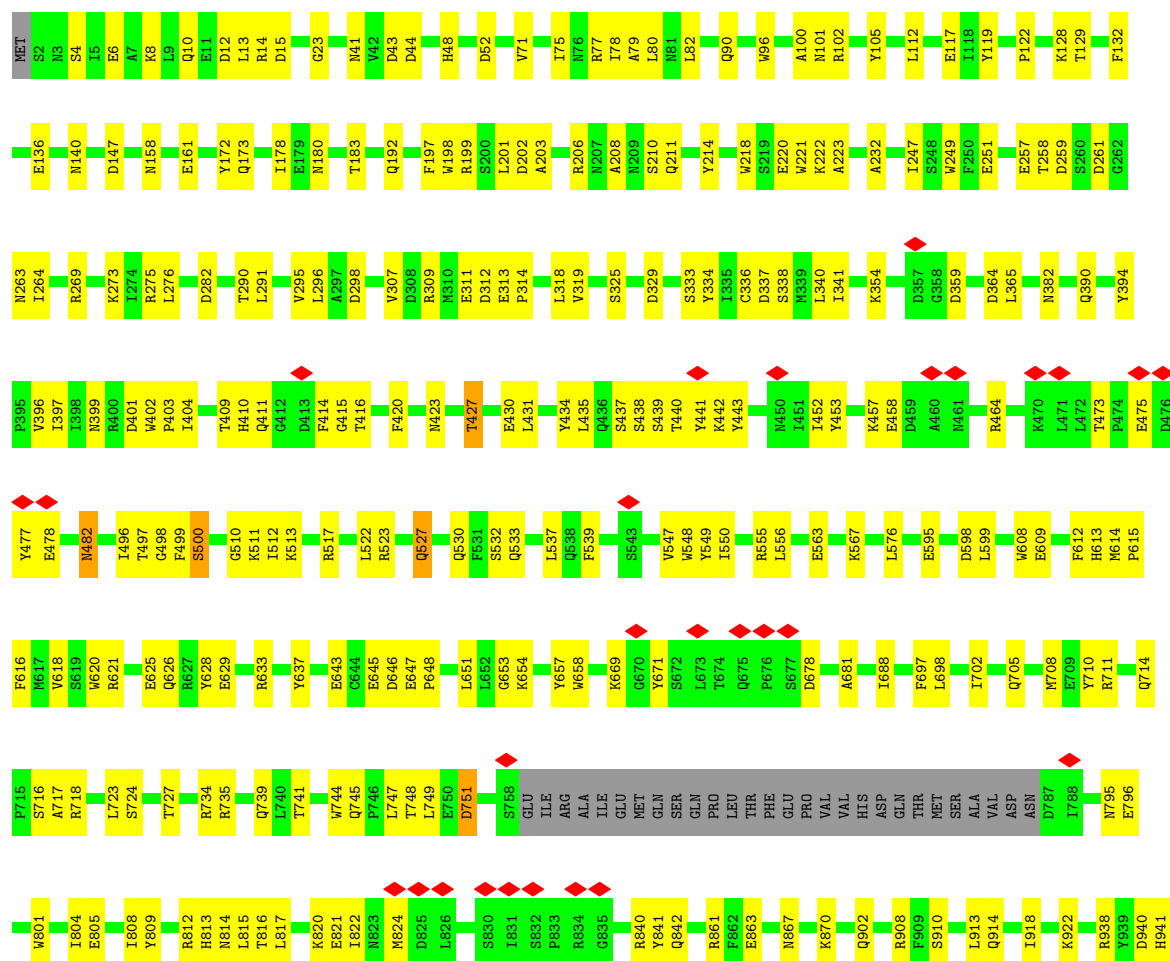
Chain H: 69% 25% 5%

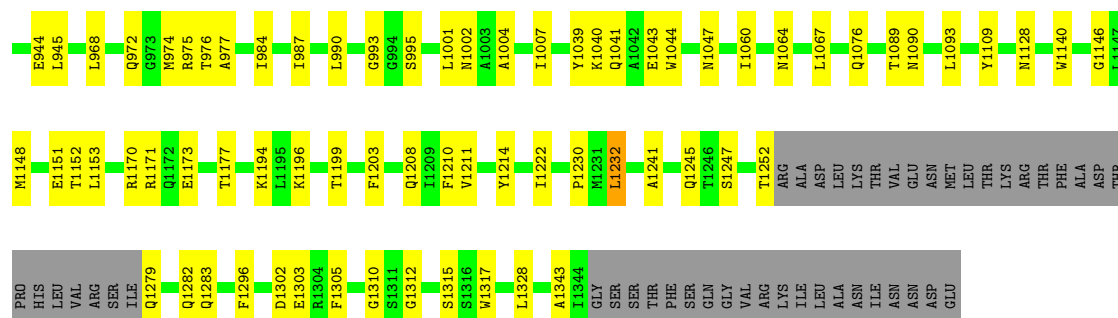






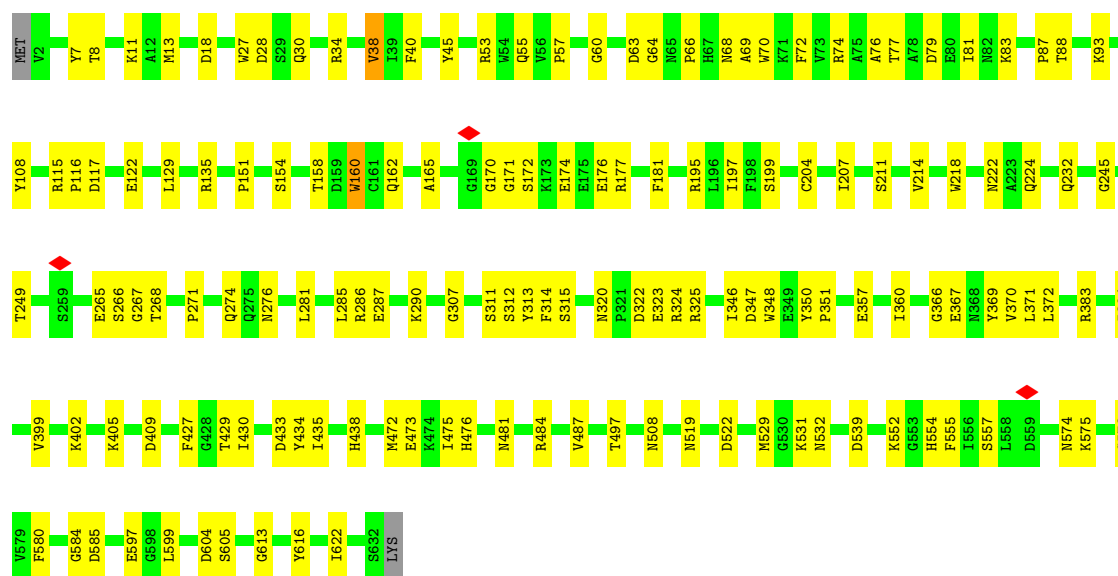
• Molecule 2: Toxin subunit YenA2





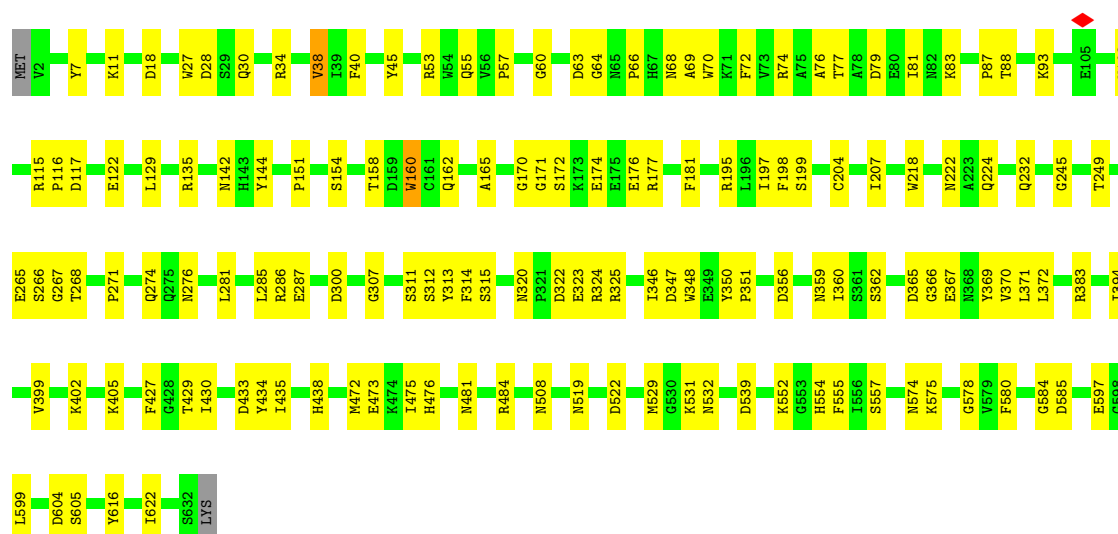
• Molecule 3: Chitinase 2

Chain C: 77% 23%

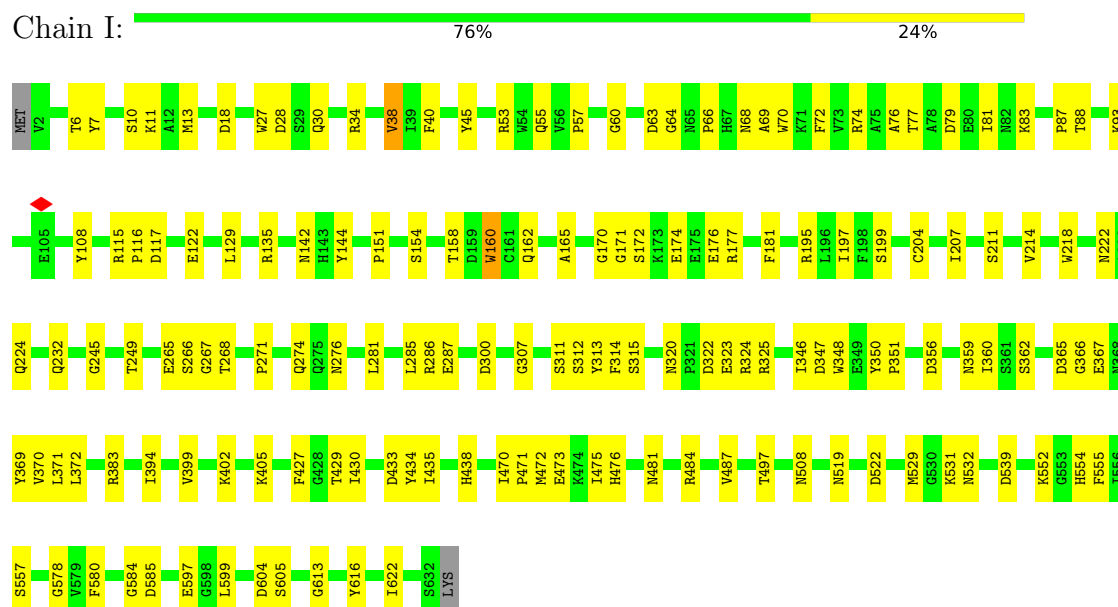


• Molecule 3: Chitinase 2

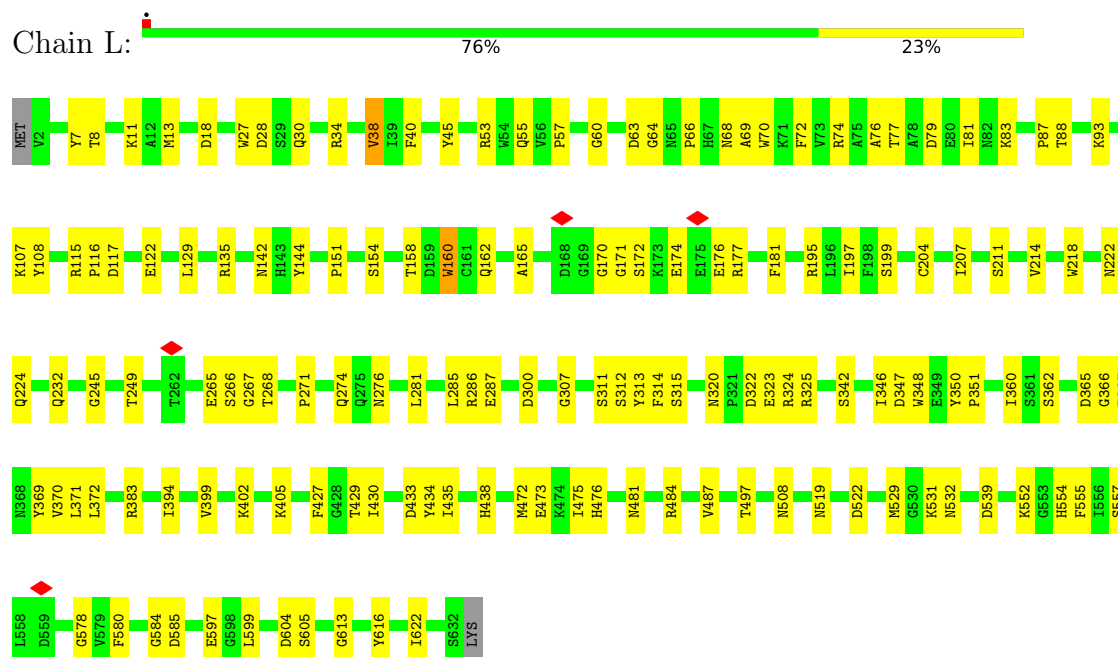
Chain F: 77% 22%



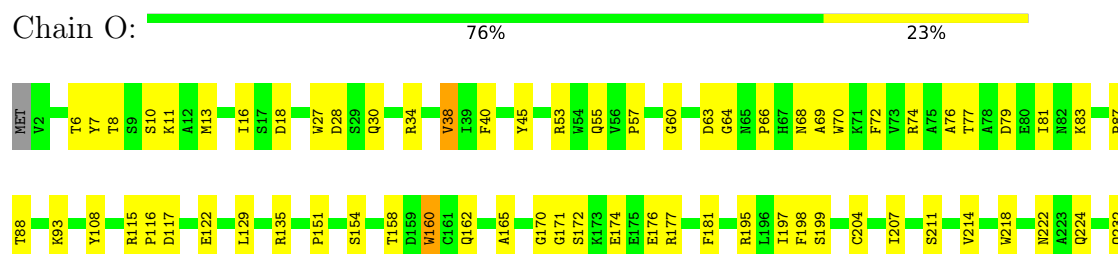
- Molecule 3: Chitinase 2

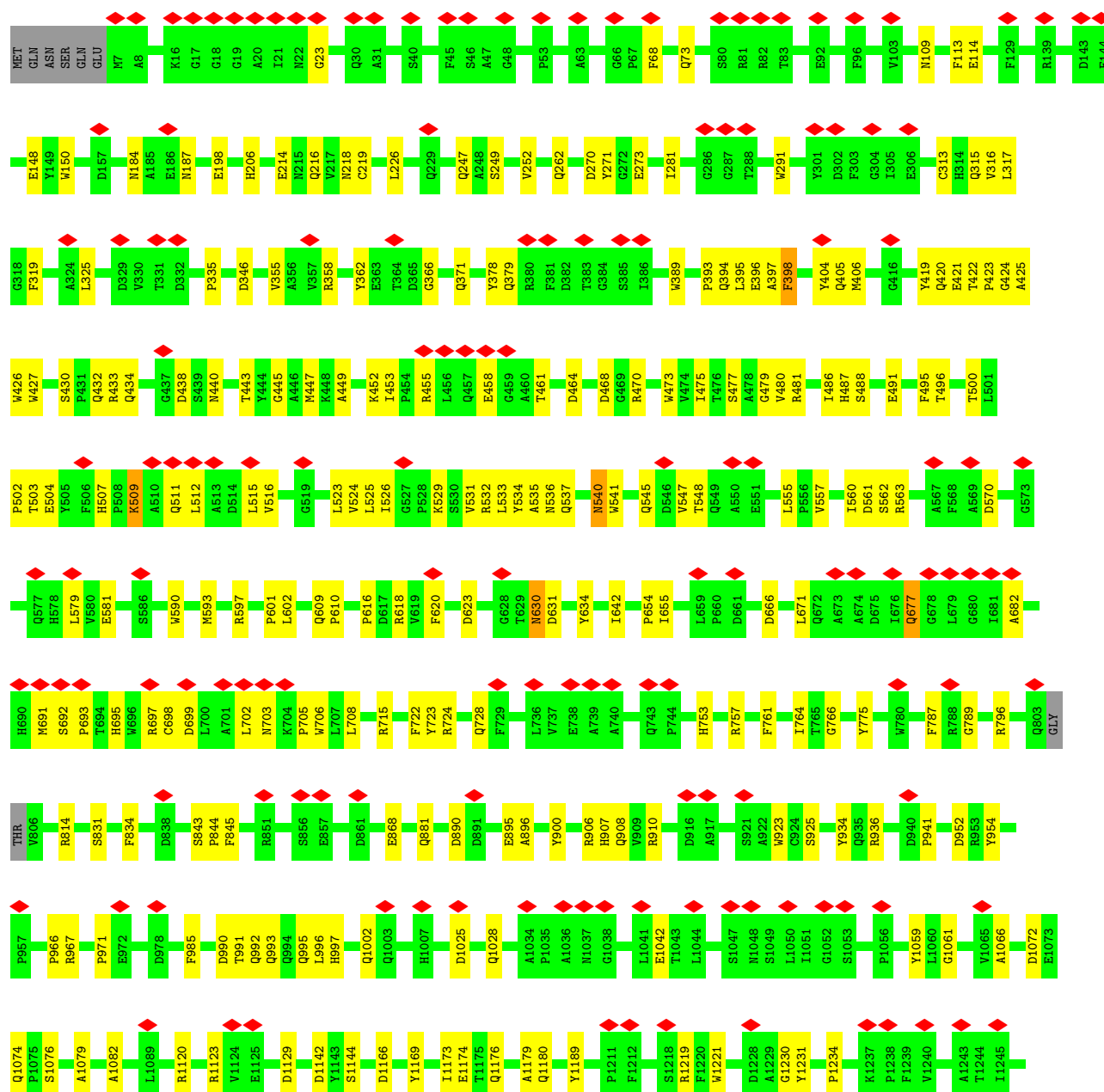


- Molecule 3: Chitinase 2

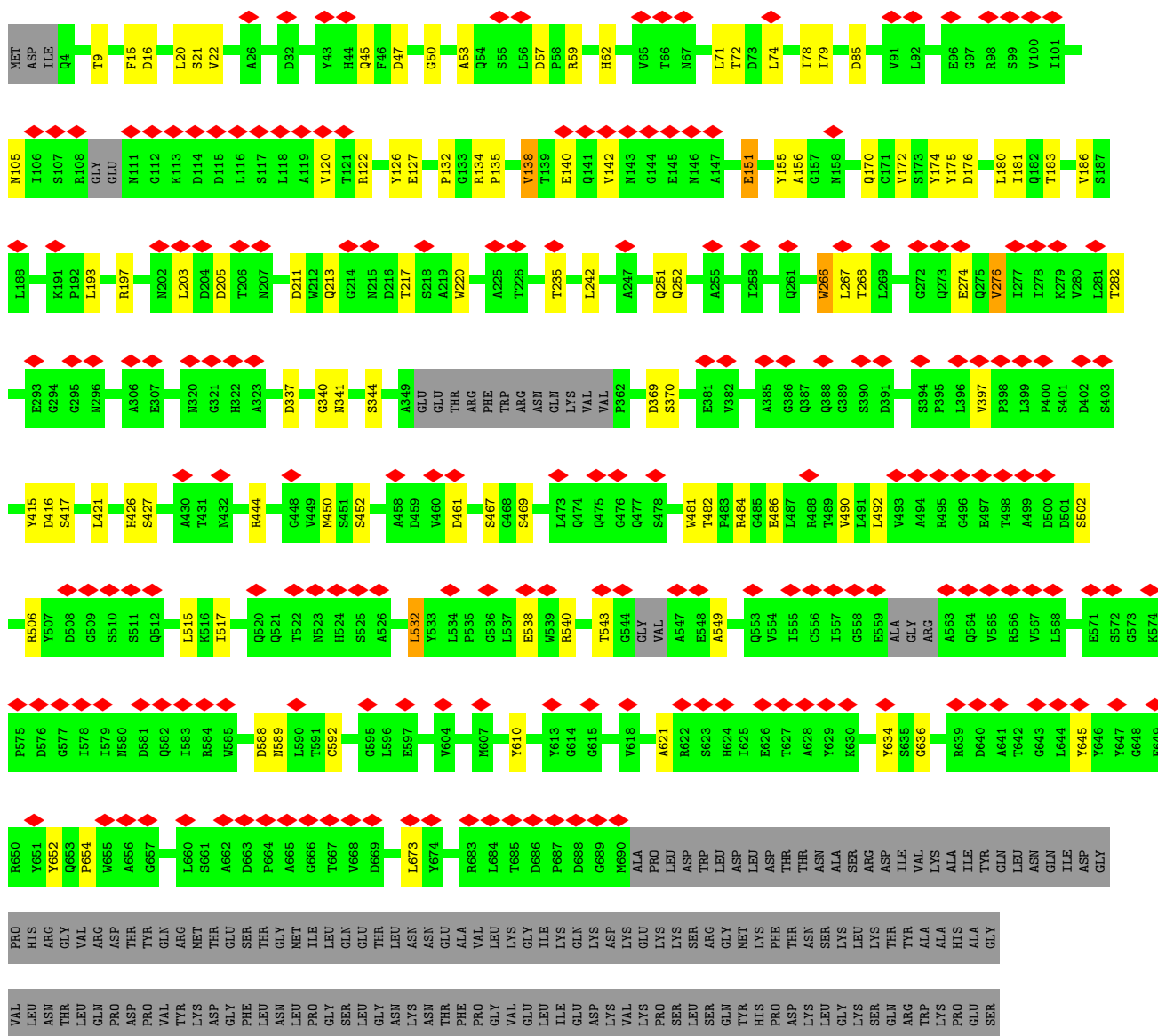


- Molecule 3: Chitinase 2





- Molecule 5: Toxin subunit YenC2



SER	GLN	ASN
LEU	ALA	ASP
GLY	LEU	VAL
TYR	ASN	ARG
TYR	LEU	LYS
ARG	ILE	ARG
VAL	ILE	ARG
ALA	SER	ARG
ASP	ASN	LYS
THR	PRO	SER
GLU	ASP	PHE
ALA	ILE	
PHE	GLU	
ILE	GLY	
THR	GLY	
GLY	ASN	
ILE	ALA	
ARG	GLU	
SER	ARG	
GLN	LEU	
TYR	ASN	
LYS	GLY	
SER	SER	
SER	TYR	
GLY	ILE	
THR	PHE	
ASP	THR	
LEU	GLN	
HIS	ARG	
ALA	LEU	
VAL	VAL	
VAL	GLY	
GLU	ASP	
GLY	VAL	
ARG	ASN	
ILE	GLN	
ARG	ASP	
ASP	PHE	
HIS	PRO	
LEU	ALA	
LEU	CYS	
ALA	TYR	
ASN	ASN	
ASN	CYS	
ASN	SER	
VAL	GLY	
LEU	ILE	
PRO	ILE	
LYS	SER	
MET	GLY	
ALA	LEU	
ILE	GLY	
ILE	ASN	
ALA	VAL	
GLY	MET	
LEU	THR	
HIS	GLY	
ALA	ARG	
GLU	VAL	
VAL	ASN	

ASN
ASP
VAL
ARG
LEU
LYS
ARG
ARG
LYS
SER
PHE

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	60315	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.400	Depositor
Minimum map value	-0.590	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.345	Depositor
Map size (Å)	804.96, 804.96, 804.96	wwPDB
Map dimensions	468, 468, 468	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.72, 1.72, 1.72	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	0.44	0/8295	0.67	1/11281 (0.0%)
1	D	0.44	0/8295	0.67	1/11281 (0.0%)
1	G	0.44	0/8295	0.67	1/11281 (0.0%)
1	J	0.44	0/8295	0.67	1/11281 (0.0%)
1	M	0.44	0/8295	0.67	1/11281 (0.0%)
2	B	0.42	0/10634	0.66	0/14412
2	E	0.42	0/10634	0.66	0/14412
2	H	0.42	0/10634	0.66	0/14412
2	K	0.42	0/10634	0.66	0/14412
2	N	0.42	0/10634	0.67	0/14412
3	C	0.28	0/5015	0.61	0/6797
3	F	0.29	0/5015	0.60	0/6797
3	I	0.29	0/5015	0.61	0/6797
3	L	0.29	0/5015	0.60	0/6797
3	O	0.29	0/5015	0.60	0/6797
4	P	0.26	0/11893	0.60	0/16229
5	Q	0.24	0/5220	0.61	0/7111
All	All	0.39	0/136833	0.65	5/185790 (0.0%)

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
2	B	0	1
2	E	0	1
2	H	0	1
2	K	0	1
2	N	0	1
All	All	0	5

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	1063	ALA	N-CA-C	-5.32	100.50	109.07
1	J	1063	ALA	N-CA-C	-5.32	100.51	109.07
1	D	1063	ALA	N-CA-C	-5.30	100.53	109.07
1	A	1063	ALA	N-CA-C	-5.30	100.54	109.07
1	G	1063	ALA	N-CA-C	-5.28	100.57	109.07

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	908	ARG	Sidechain
2	E	908	ARG	Sidechain
2	H	908	ARG	Sidechain
2	K	908	ARG	Sidechain
2	N	908	ARG	Sidechain

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	A	8136	0	8081	192	0
1	D	8136	0	8081	187	0
1	G	8136	0	8081	190	0
1	J	8136	0	8081	193	0
1	M	8136	0	8081	194	0
2	B	10415	0	10160	266	0
2	E	10415	0	10160	256	0
2	H	10415	0	10160	258	0
2	K	10415	0	10160	256	0
2	N	10415	0	10160	253	0
3	C	4896	0	4691	106	0
3	F	4896	0	4691	105	0
3	I	4896	0	4691	112	0
3	L	4896	0	4691	107	0
3	O	4896	0	4691	107	0
4	P	11580	0	10922	194	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Q	5123	0	4909	64	0
All	All	133938	0	130491	2868	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 11.

The worst 5 of 2868 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:E:1235:PRO:HA	4:P:424:GLY:HA3	1.24	1.17
2:B:1235:PRO:HD3	4:P:500:THR:HB	1.38	1.05
2:B:1236:TYR:CE1	4:P:480:VAL:HA	1.99	0.96
2:B:1236:TYR:HE1	4:P:480:VAL:HA	1.32	0.92
2:N:1232:LEU:HD12	4:P:557:VAL:HB	1.51	0.90

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	1031/1164 (89%)	966 (94%)	65 (6%)	0	100	100
1	D	1031/1164 (89%)	967 (94%)	64 (6%)	0	100	100
1	G	1031/1164 (89%)	966 (94%)	65 (6%)	0	100	100
1	J	1031/1164 (89%)	967 (94%)	64 (6%)	0	100	100
1	M	1031/1164 (89%)	967 (94%)	64 (6%)	0	100	100
2	B	1283/1364 (94%)	1201 (94%)	82 (6%)	0	100	100
2	E	1283/1364 (94%)	1202 (94%)	81 (6%)	0	100	100
2	H	1283/1364 (94%)	1200 (94%)	83 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	1283/1364 (94%)	1200 (94%)	83 (6%)	0	100	100
2	N	1283/1364 (94%)	1201 (94%)	82 (6%)	0	100	100
3	C	629/633 (99%)	581 (92%)	48 (8%)	0	100	100
3	F	629/633 (99%)	581 (92%)	48 (8%)	0	100	100
3	I	629/633 (99%)	581 (92%)	48 (8%)	0	100	100
3	L	629/633 (99%)	582 (92%)	47 (8%)	0	100	100
3	O	629/633 (99%)	582 (92%)	47 (8%)	0	100	100
4	P	1472/1487 (99%)	1361 (92%)	111 (8%)	0	100	100
5	Q	658/970 (68%)	608 (92%)	50 (8%)	0	100	100
All	All	16845/18262 (92%)	15713 (93%)	1132 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	906/1022 (89%)	902 (100%)	4 (0%)	84	82
1	D	906/1022 (89%)	902 (100%)	4 (0%)	84	82
1	G	906/1022 (89%)	902 (100%)	4 (0%)	84	82
1	J	906/1022 (89%)	902 (100%)	4 (0%)	84	82
1	M	906/1022 (89%)	902 (100%)	4 (0%)	84	82
2	B	1139/1209 (94%)	1128 (99%)	11 (1%)	68	76
2	E	1139/1209 (94%)	1128 (99%)	11 (1%)	68	76
2	H	1139/1209 (94%)	1128 (99%)	11 (1%)	68	76
2	K	1139/1209 (94%)	1128 (99%)	11 (1%)	68	76
2	N	1139/1209 (94%)	1128 (99%)	11 (1%)	68	76
3	C	518/520 (100%)	515 (99%)	3 (1%)	78	80
3	F	518/520 (100%)	515 (99%)	3 (1%)	78	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	518/520 (100%)	515 (99%)	3 (1%)	78	80
3	L	518/520 (100%)	515 (99%)	3 (1%)	78	80
3	O	518/520 (100%)	515 (99%)	3 (1%)	78	80
4	P	1218/1266 (96%)	1204 (99%)	14 (1%)	65	74
5	Q	539/818 (66%)	527 (98%)	12 (2%)	45	64
All	All	14572/15839 (92%)	14456 (99%)	116 (1%)	70	77

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	1123	MET
5	Q	344	SER
3	L	372	LEU
5	Q	282	THR
4	P	677	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 144 such sidechains are listed below:

Mol	Chain	Res	Type
2	N	527	GLN
5	Q	446	ASN
2	N	1038	GLN
4	P	402	GLN
1	G	375	GLN

5.3.3 RNA ⓘ

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 [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.

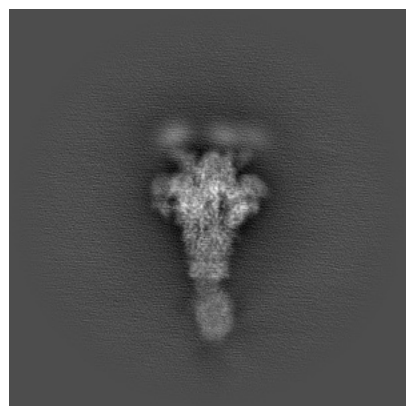
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45190. These allow visual inspection of the internal detail of the map and identification of artifacts.

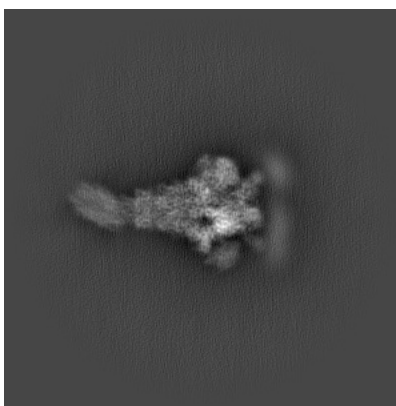
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

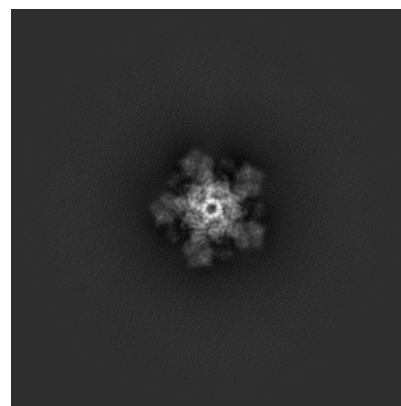
6.1.1 Primary map



X

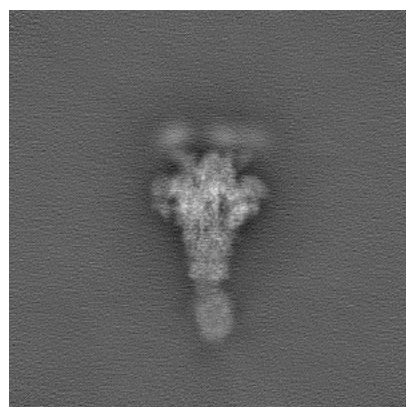


Y

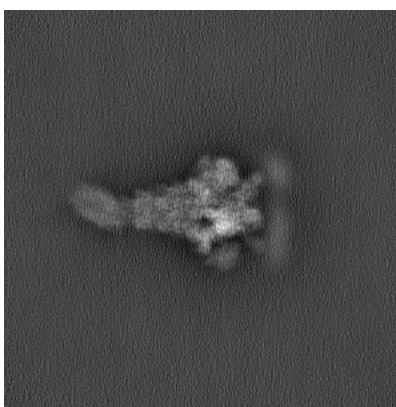


Z

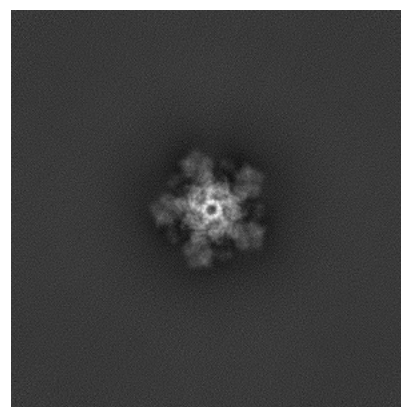
6.1.2 Raw map



X



Y

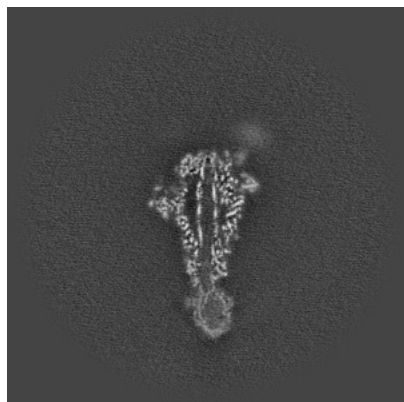


Z

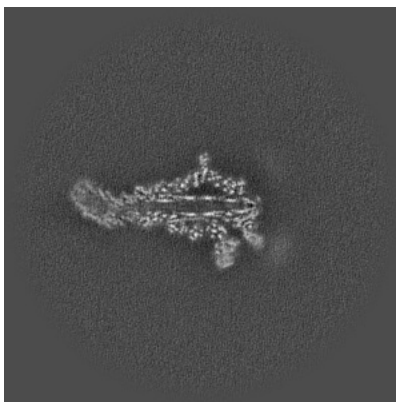
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

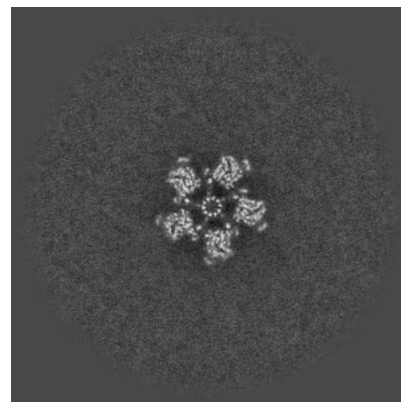
6.2.1 Primary map



X Index: 234

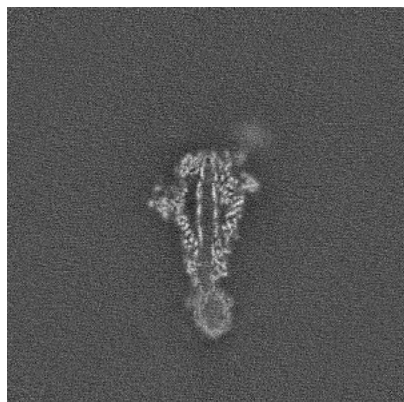


Y Index: 234

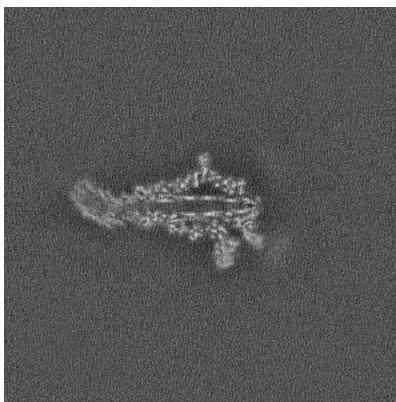


Z Index: 234

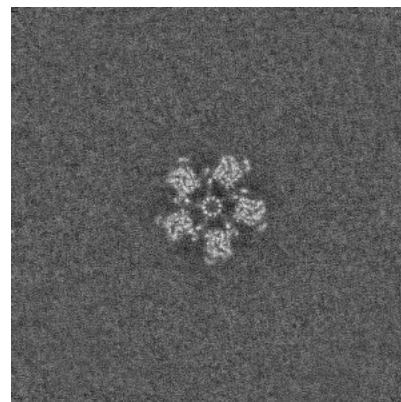
6.2.2 Raw map



X Index: 234



Y Index: 234

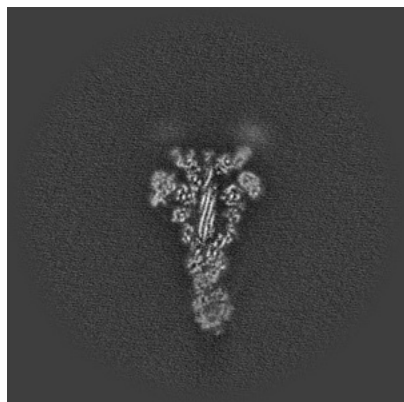


Z Index: 234

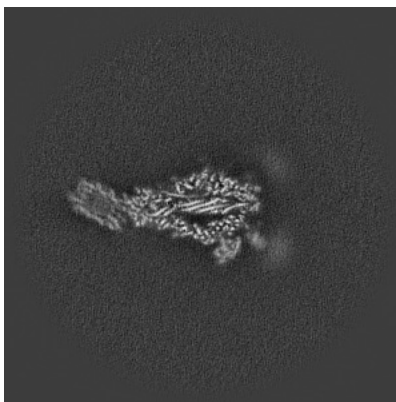
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

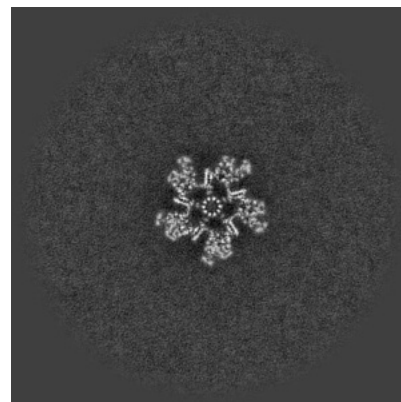
6.3.1 Primary map



X Index: 226

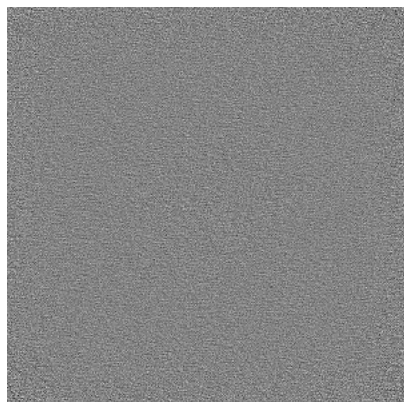


Y Index: 243

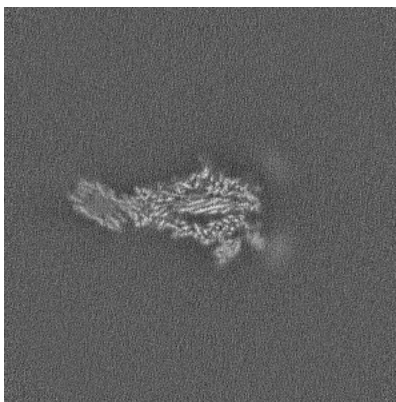


Z Index: 237

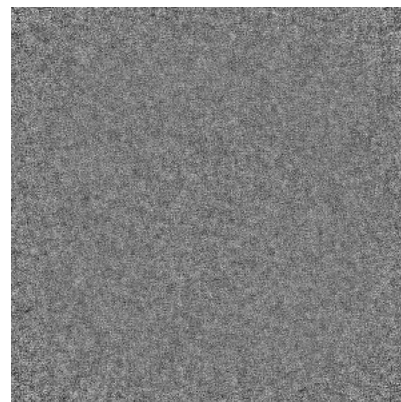
6.3.2 Raw map



X Index: 0



Y Index: 242

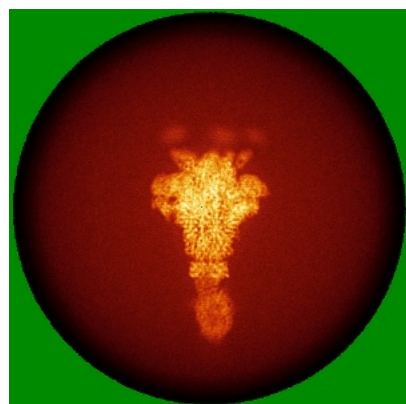


Z Index: 0

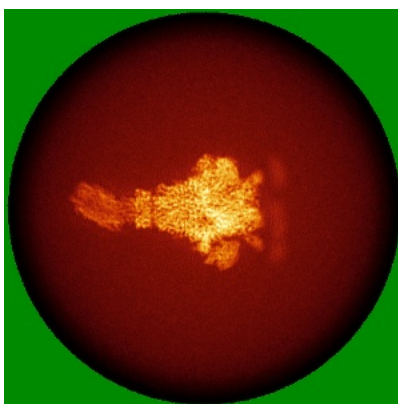
The images above show the largest variance slices of the map in three orthogonal directions.

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

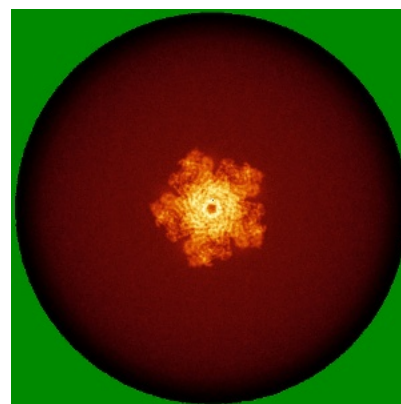
6.4.1 Primary map



X

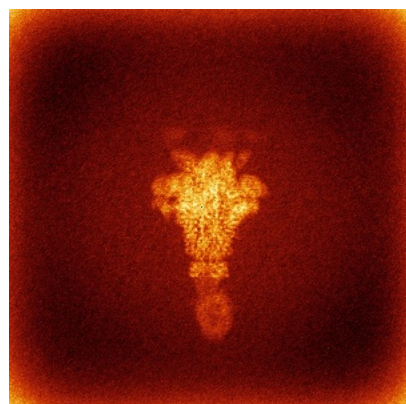


Y

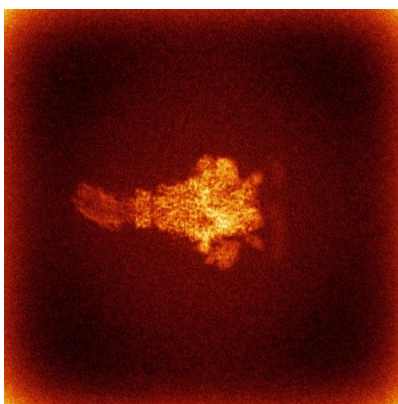


Z

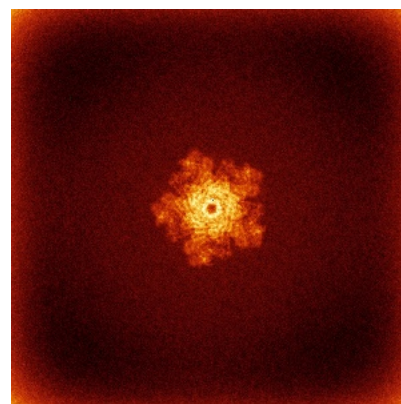
6.4.2 Raw map



X



Y

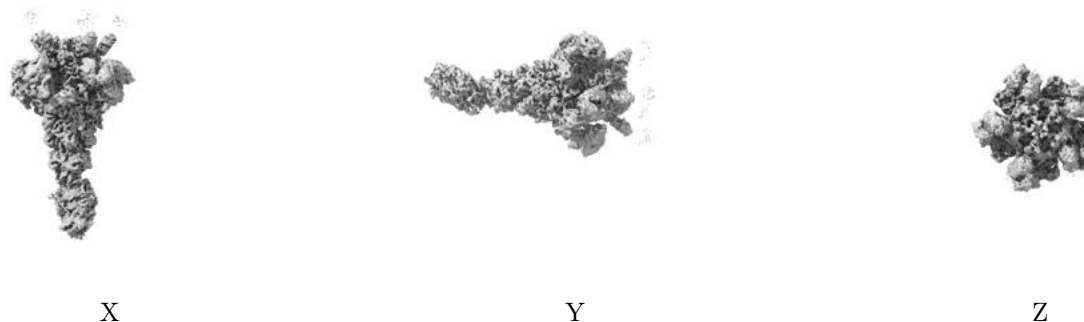


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

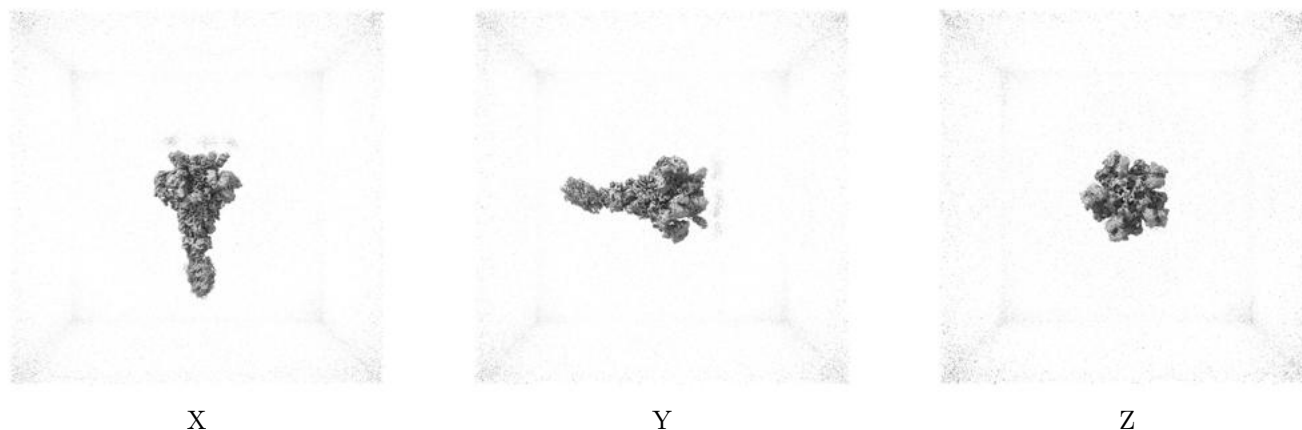
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.345. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

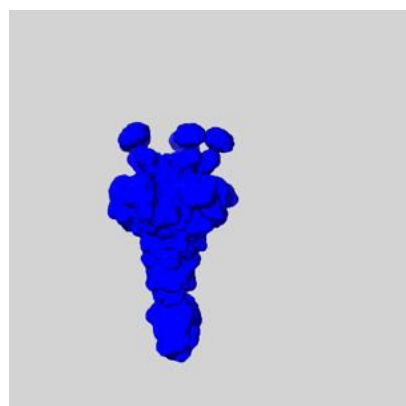
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

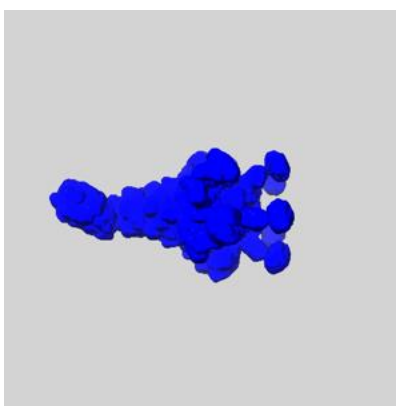
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

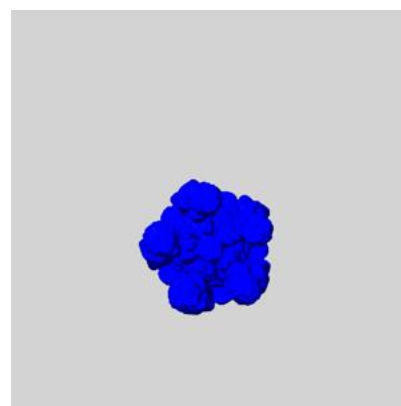
6.6.1 emd_45190_msk_1.map [i](#)



X



Y

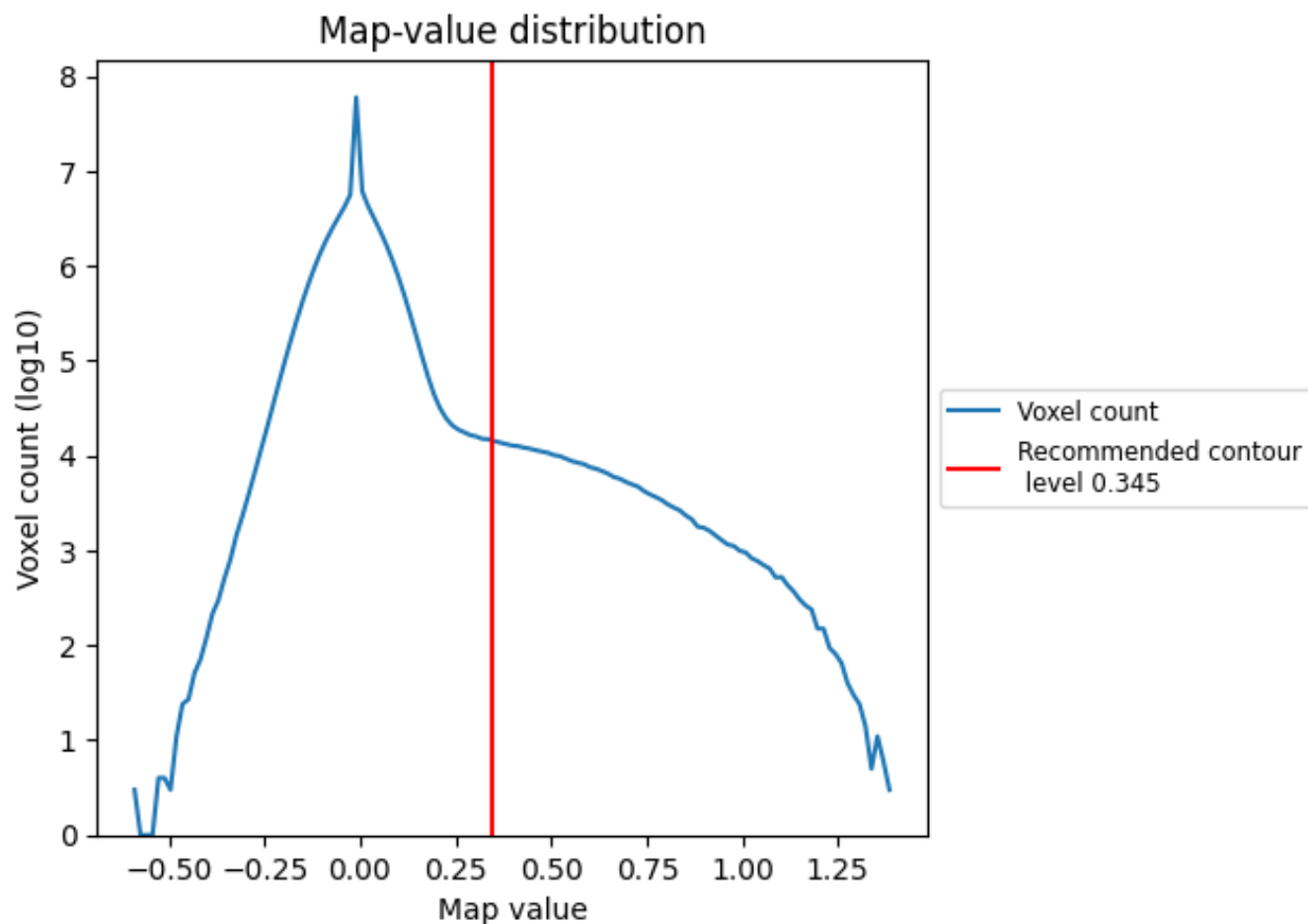


Z

7 Map analysis [i](#)

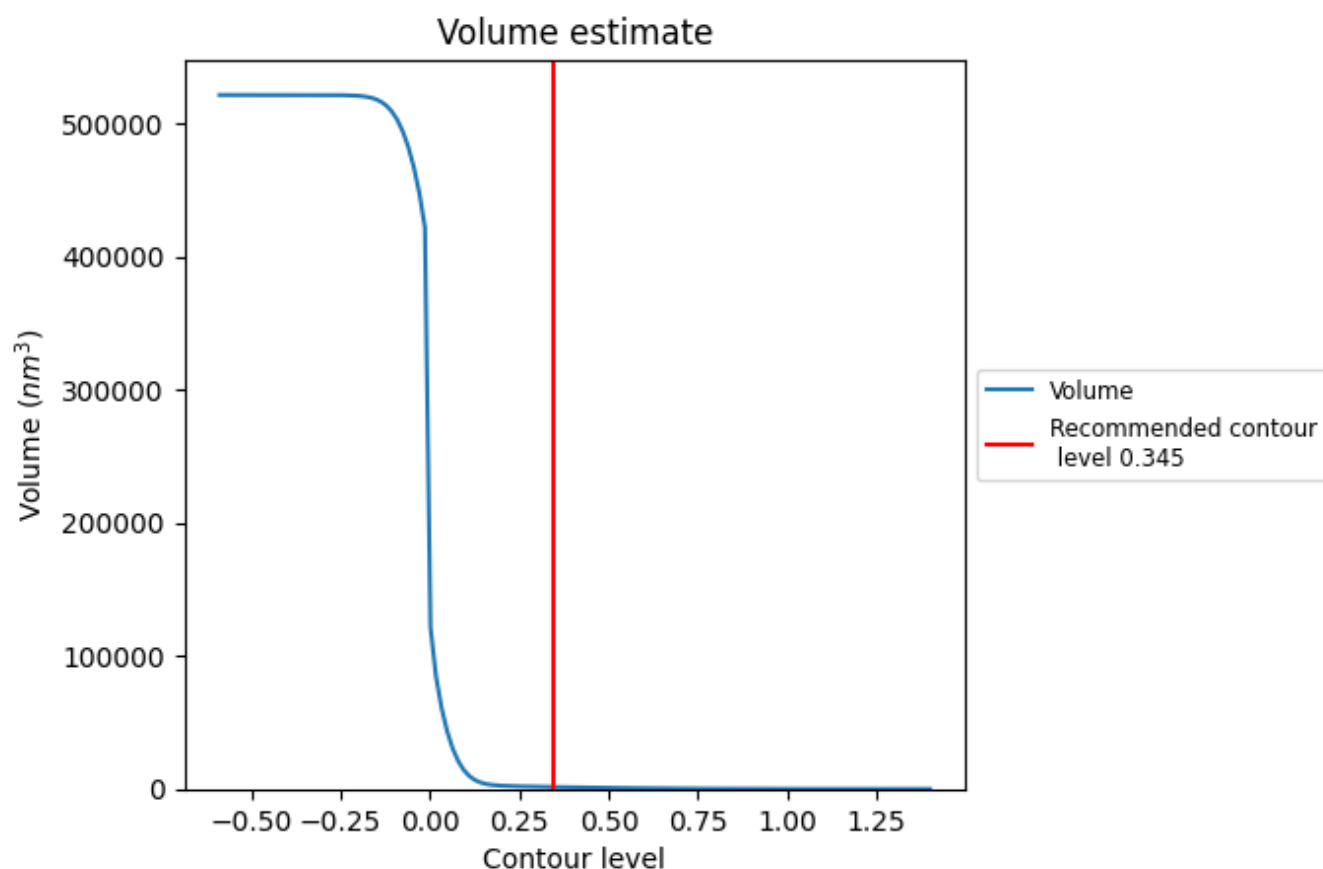
This section contains the results of statistical analysis of the map.

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.

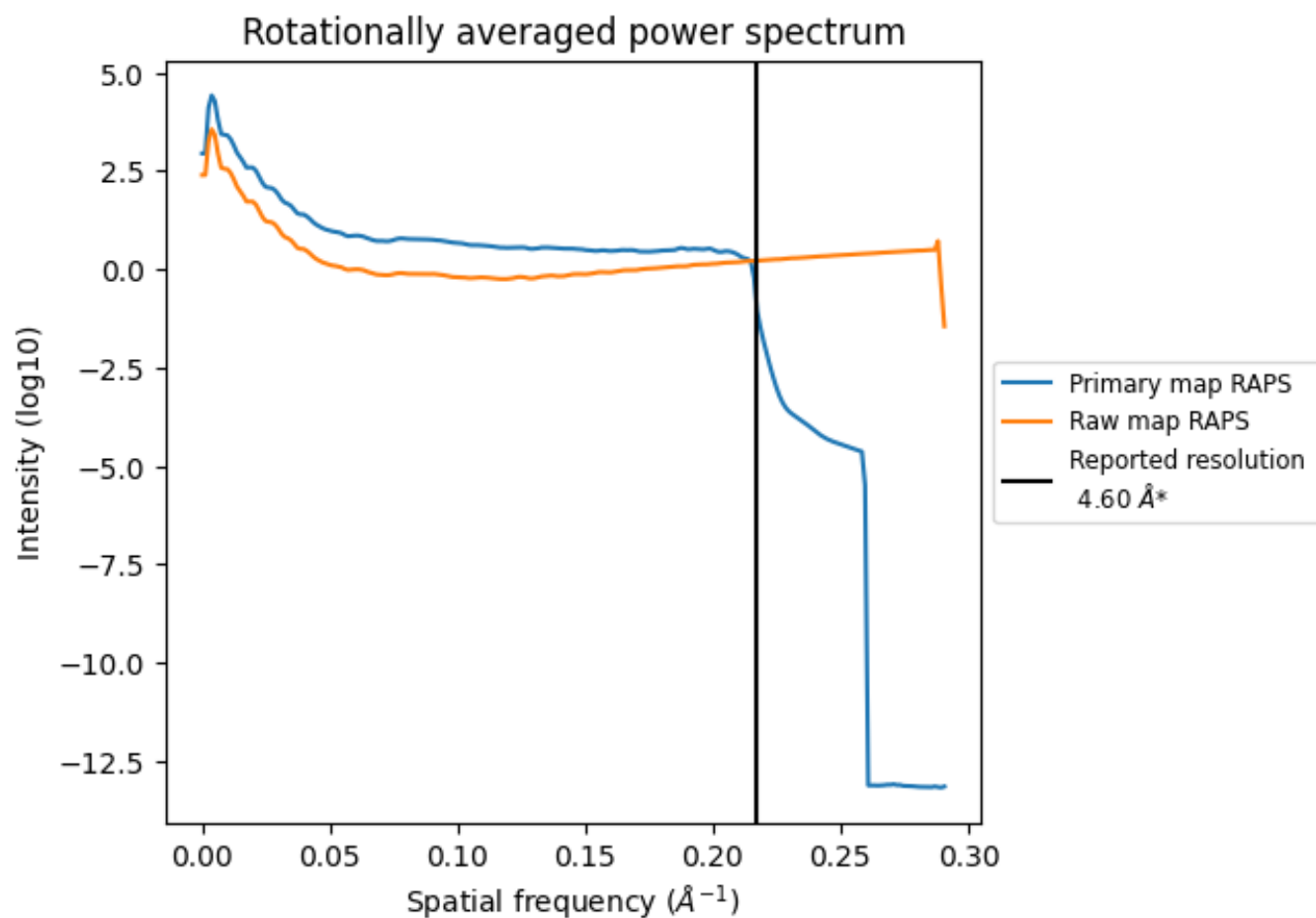
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1450 nm^3 ; this corresponds to an approximate mass of 1310 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

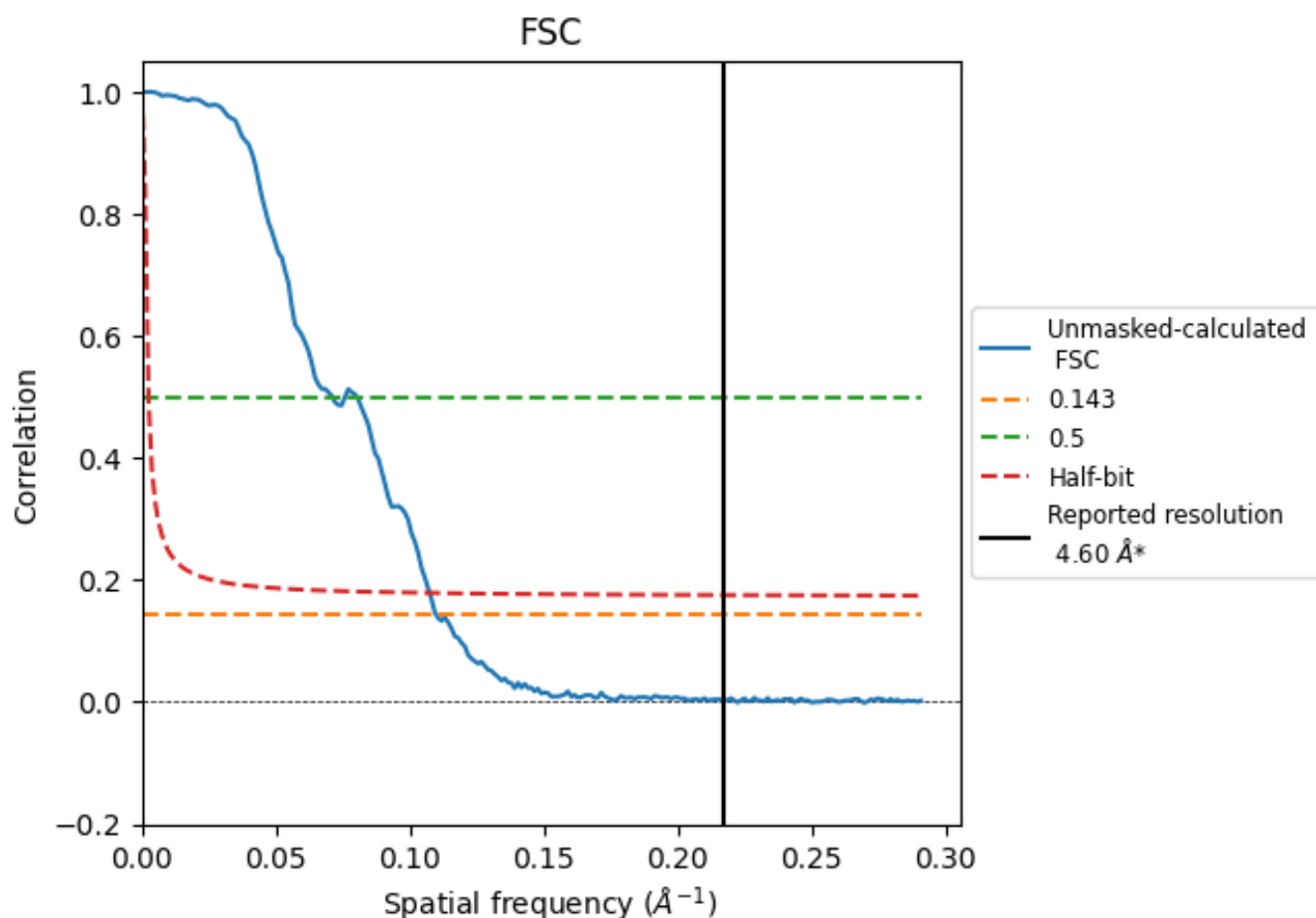


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

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 0.217 Å⁻¹

8.2 Resolution estimates [i](#)

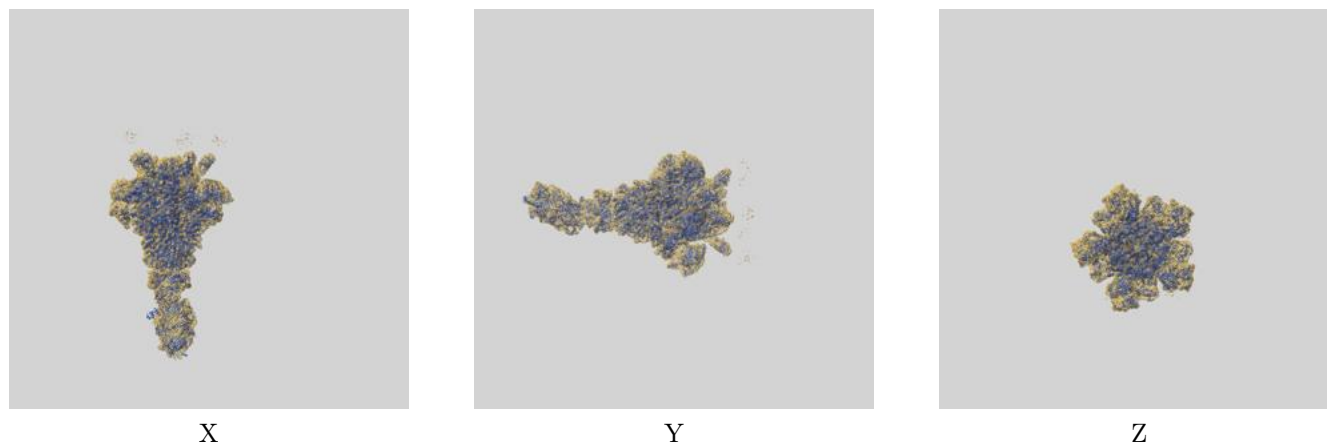
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.11	14.08	9.31

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.11 differs from the reported value 4.6 by more than 10 %

9 Map-model fit [i](#)

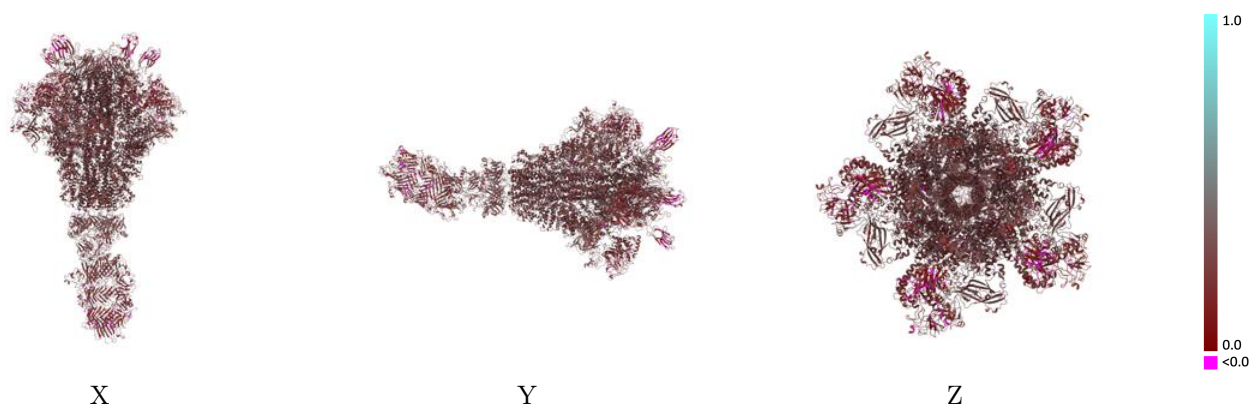
This section contains information regarding the fit between EMDB map EMD-45190 and PDB model 9C4K. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



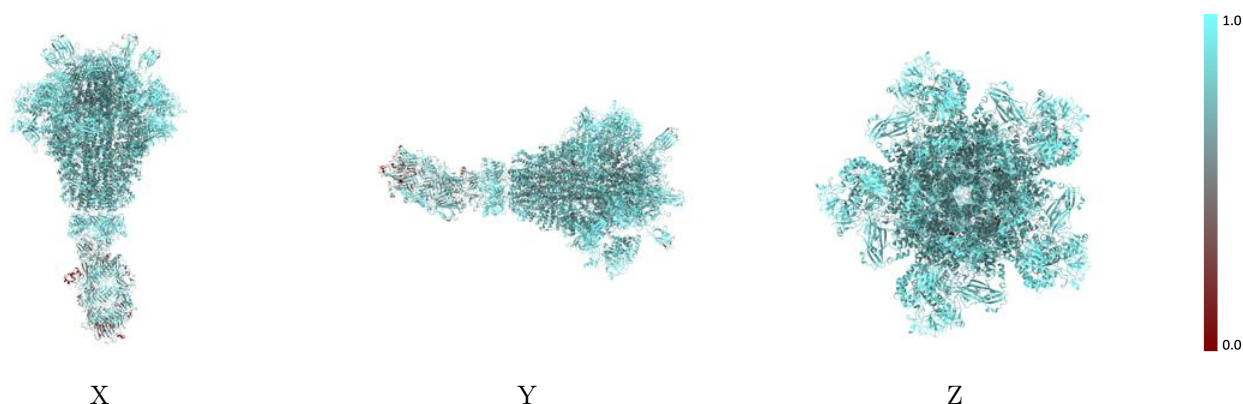
The images above show the 3D surface view of the map at the recommended contour level 0.345 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



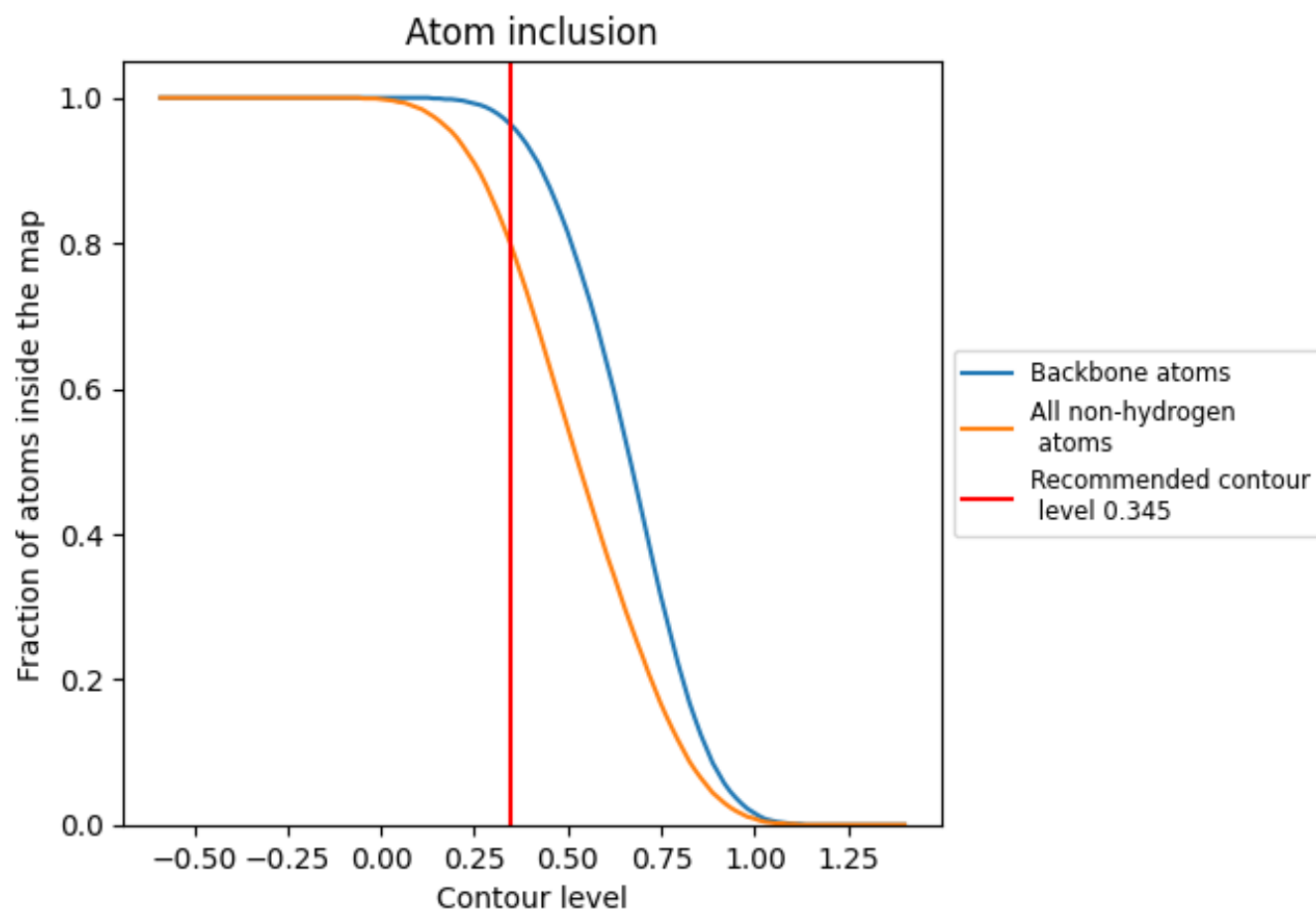
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.345).





































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 80% 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 (0.345) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8010	 0.2670
A	 0.8230	 0.2930
B	 0.8040	 0.2820
C	 0.8860	 0.2410
D	 0.8250	 0.2840
E	 0.7850	 0.2710
F	 0.8890	 0.2260
G	 0.8200	 0.2840
H	 0.7810	 0.2680
I	 0.8900	 0.2280
J	 0.8230	 0.2880
K	 0.7870	 0.2730
L	 0.8810	 0.2250
M	 0.8310	 0.2850
N	 0.7920	 0.2740
O	 0.8850	 0.2250
P	 0.6800	 0.2640
Q	 0.5800	 0.2210

