wwPDB EM Validation Summary Report

Oct 7, 2024 – 09:28 pm BST

PDB ID	:	9GOA
EMDB ID	:	EMD-51495
Title	:	Pore state of alpha-Latrotoxin
Authors	:	Klink, B.U.; Gatsogiannis, C.; Kalyankumar, K.S.
Deposited on	:	2024-09-05
Resolution	:	3.20 Å(reported)
Based on initial model	:	.

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:

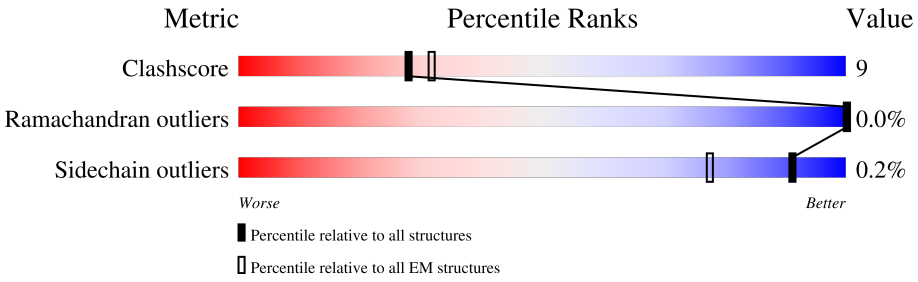
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.20 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1175	27% 73% 19% 8%
1	B	1175	22% 72% 20% 8%
1	C	1175	19% 74% 18% 8%
1	D	1175	15% 74% 18% 8%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 31628 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 Alpha-latrotoxin-Lt1a.

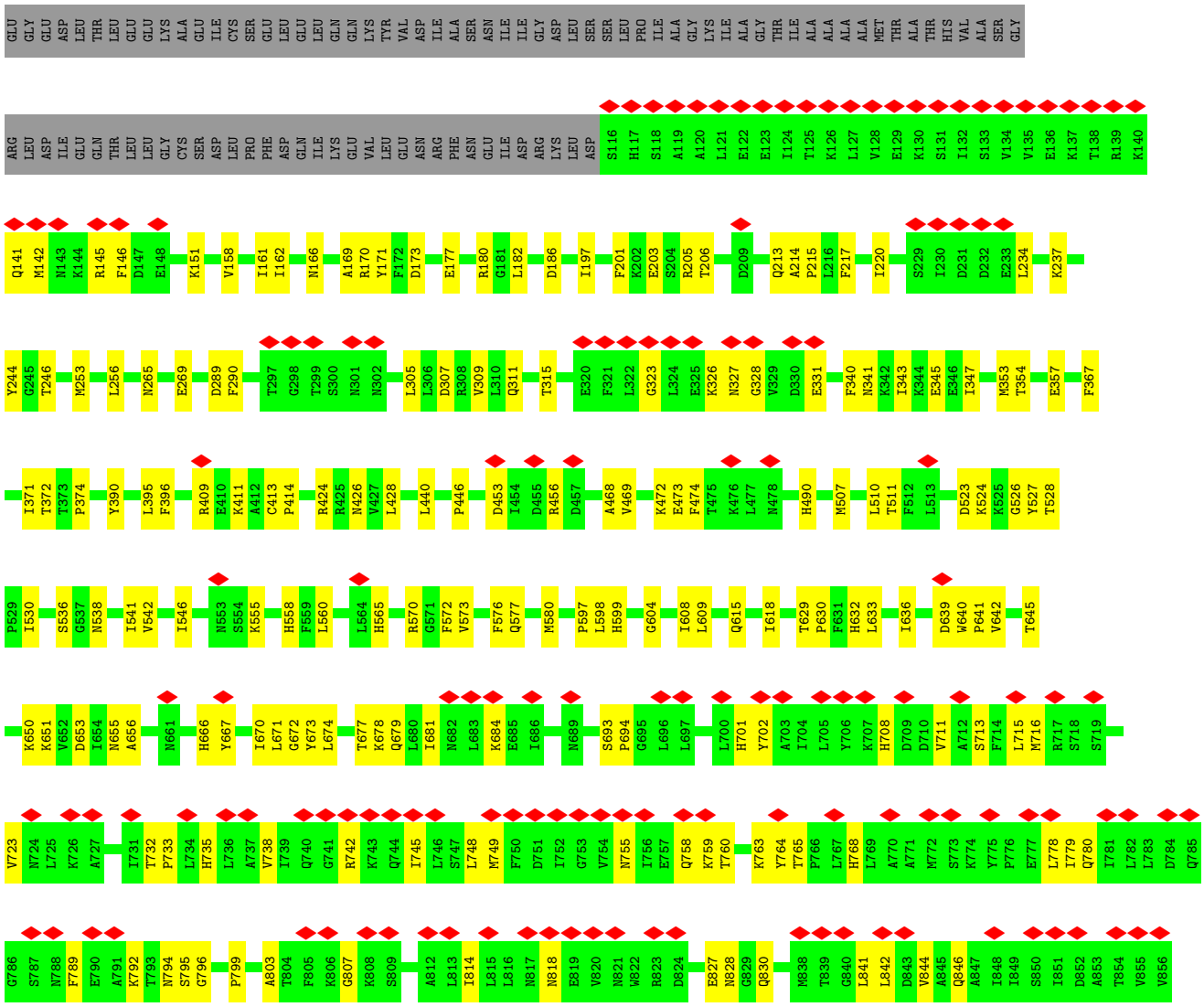
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1080	Total	C	N	O	S	0	0
			7907	4983	1374	1530	20		
1	B	1080	Total	C	N	O	S	0	0
			7907	4983	1374	1530	20		
1	C	1080	Total	C	N	O	S	0	0
			7907	4983	1374	1530	20		
1	D	1080	Total	C	N	O	S	0	0
			7907	4983	1374	1530	20		

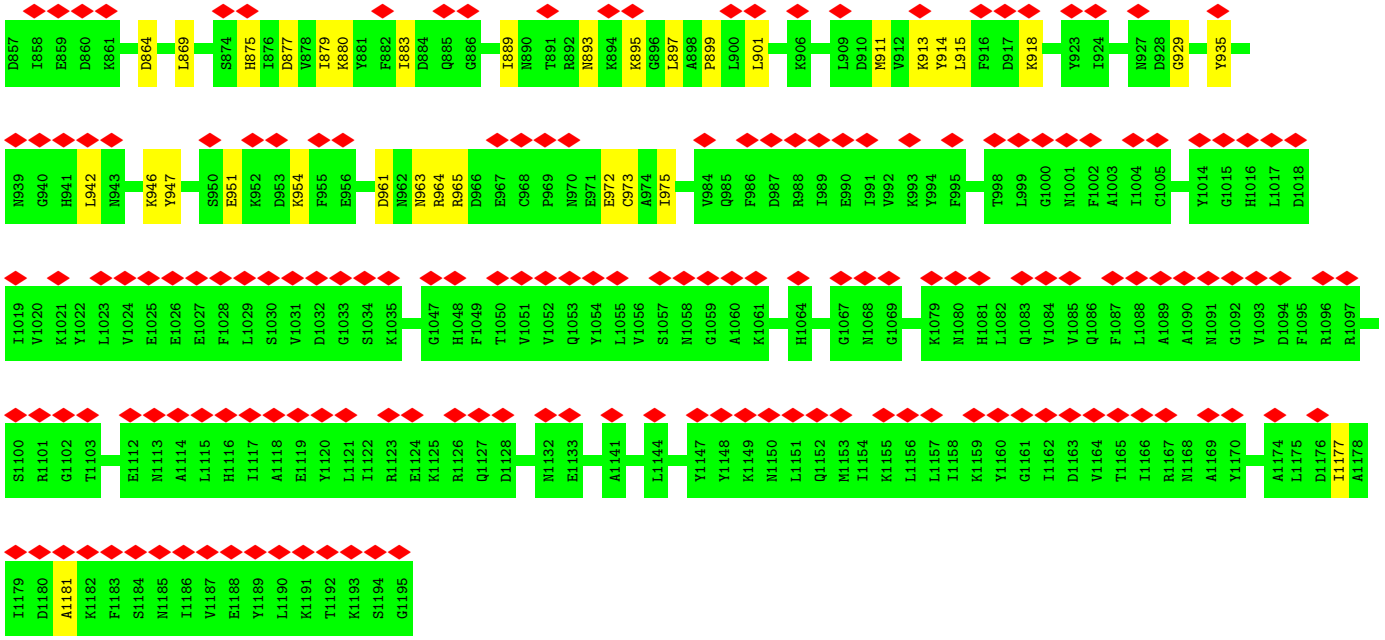
3 Residue-property plots (i)

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: Alpha-latrotoxin-Lt1a

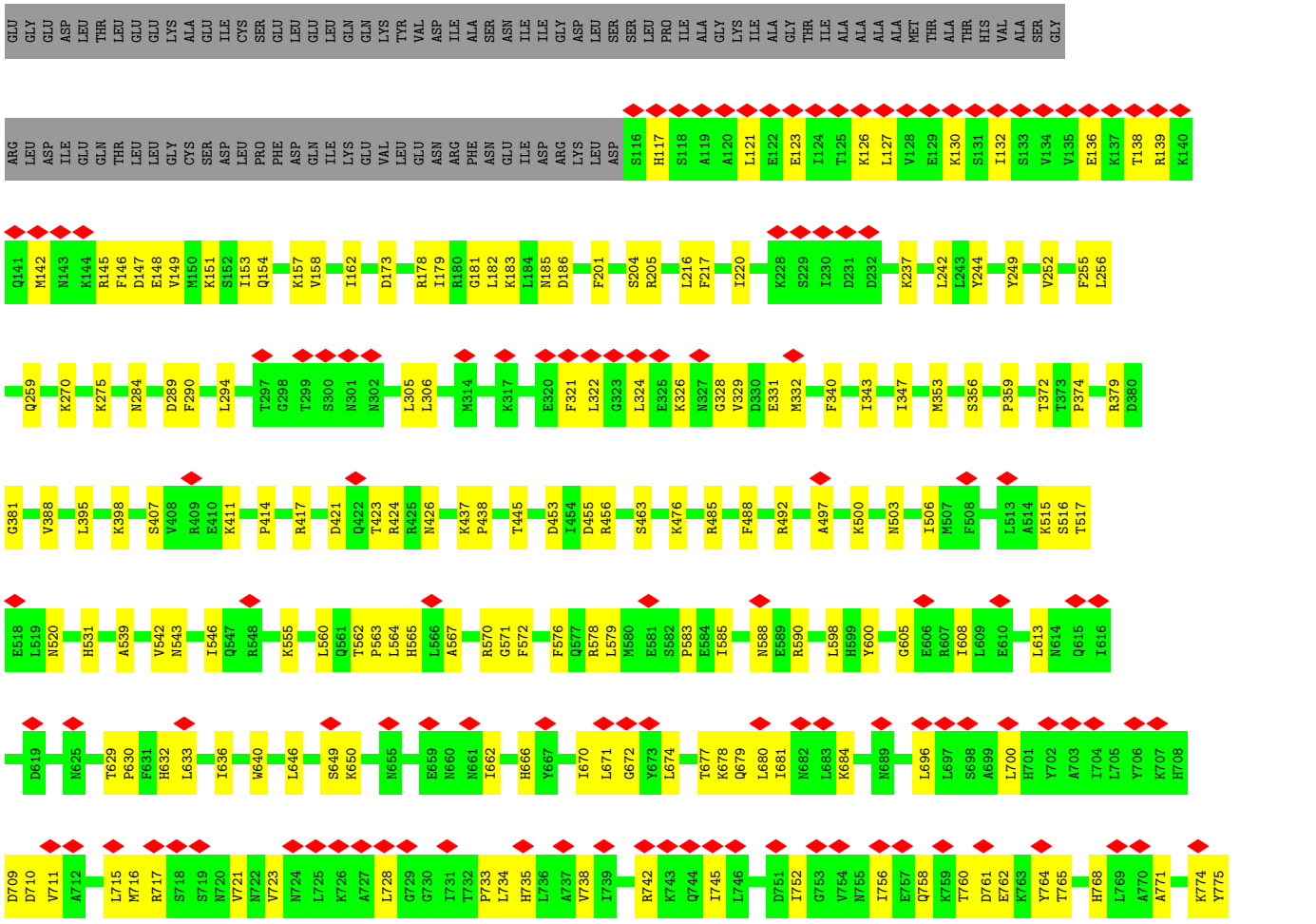
Chain A:

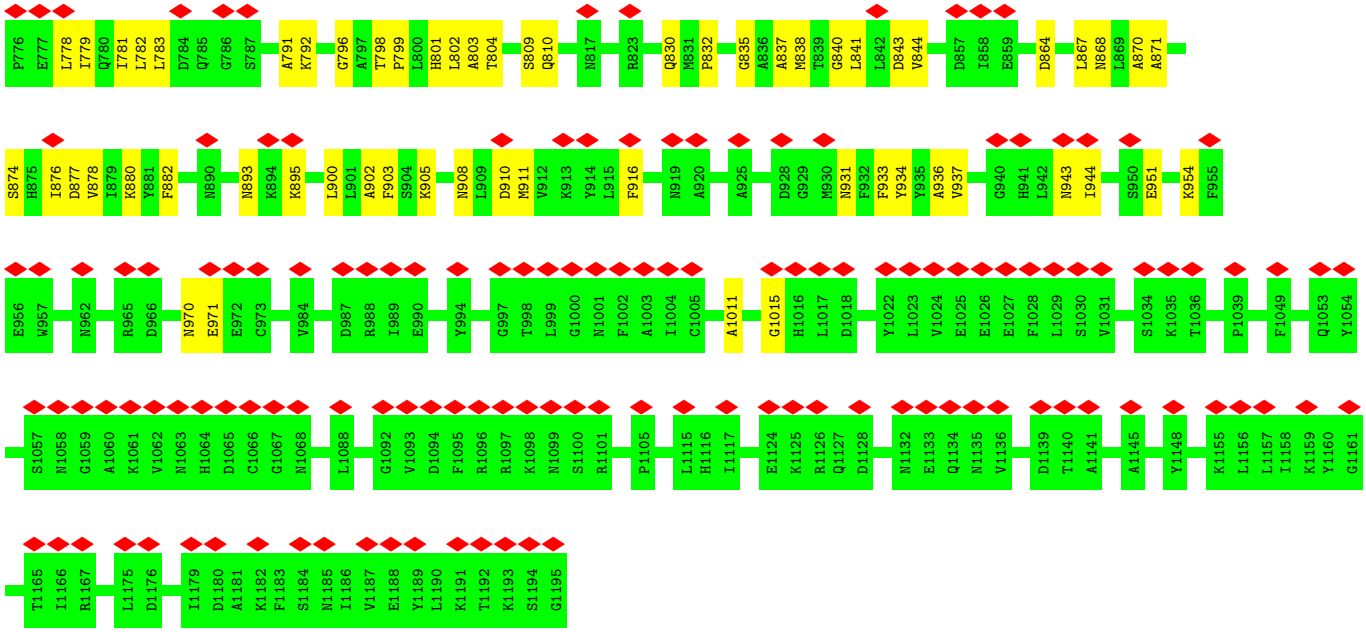




- Molecule 1: Alpha-latrotoxin-Lt1a

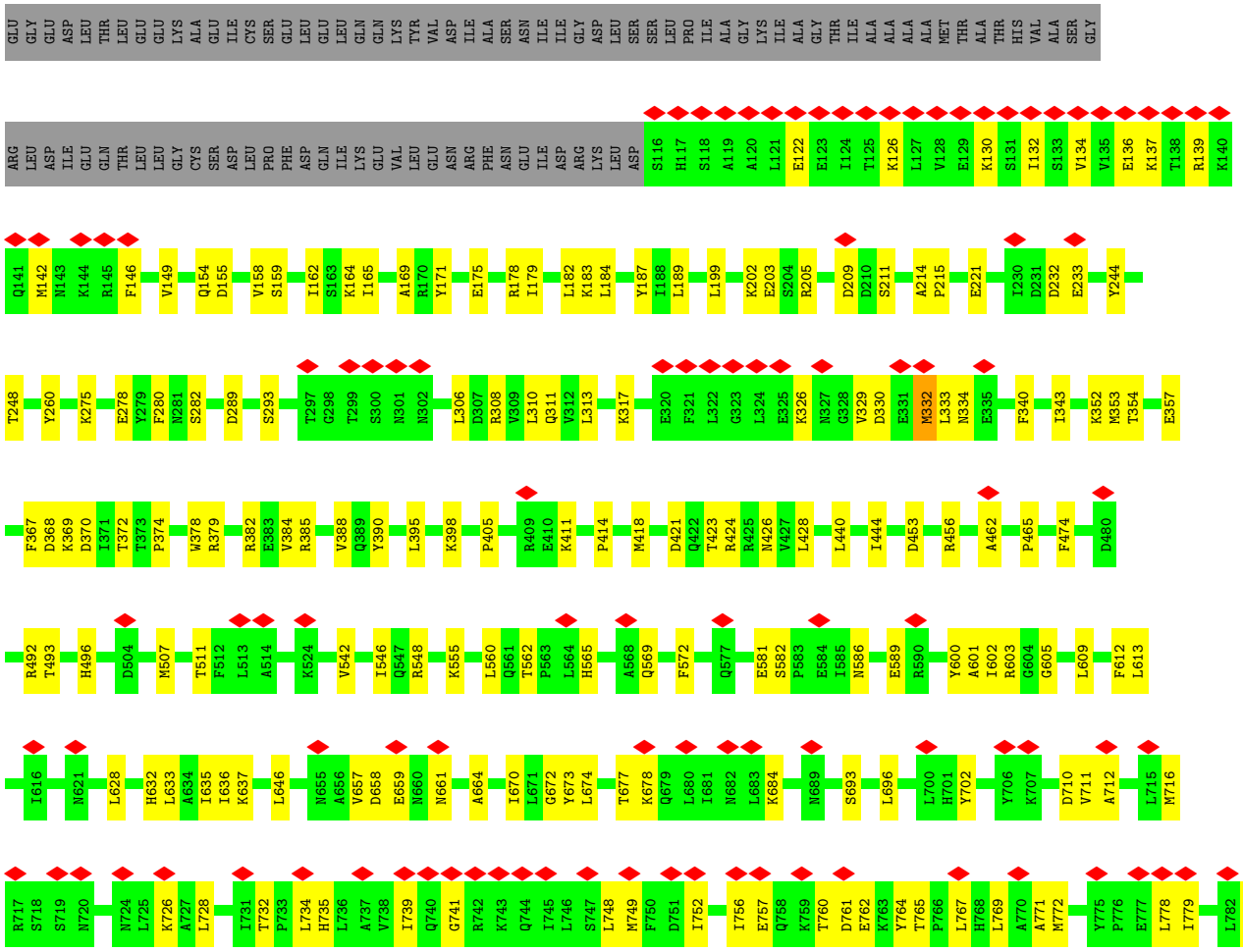
Chain B:

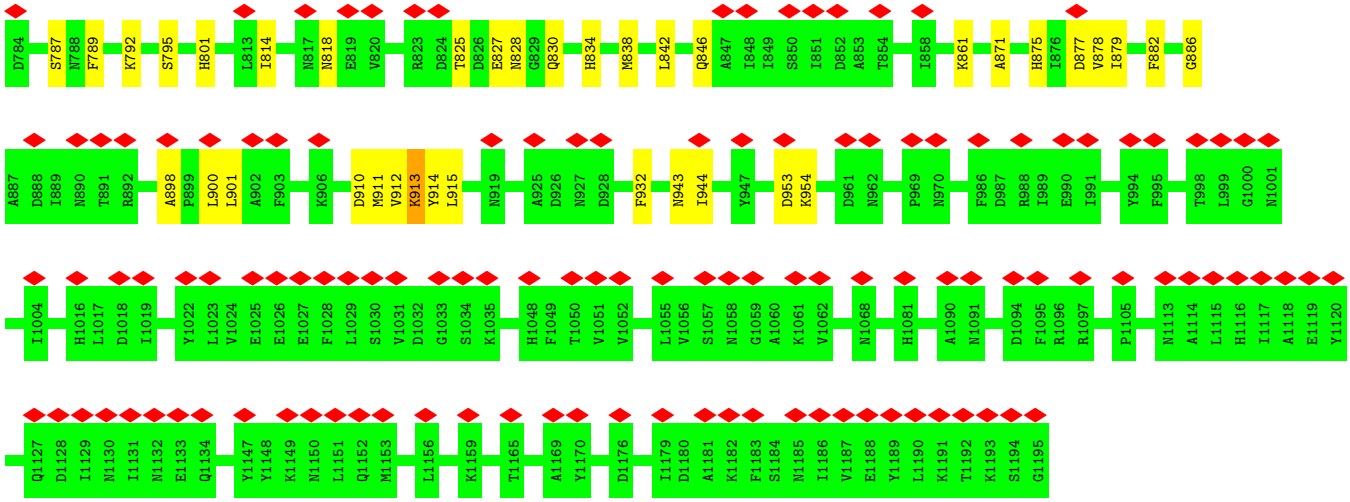




- Molecule 1: Alpha-latrotoxin-Lt1a

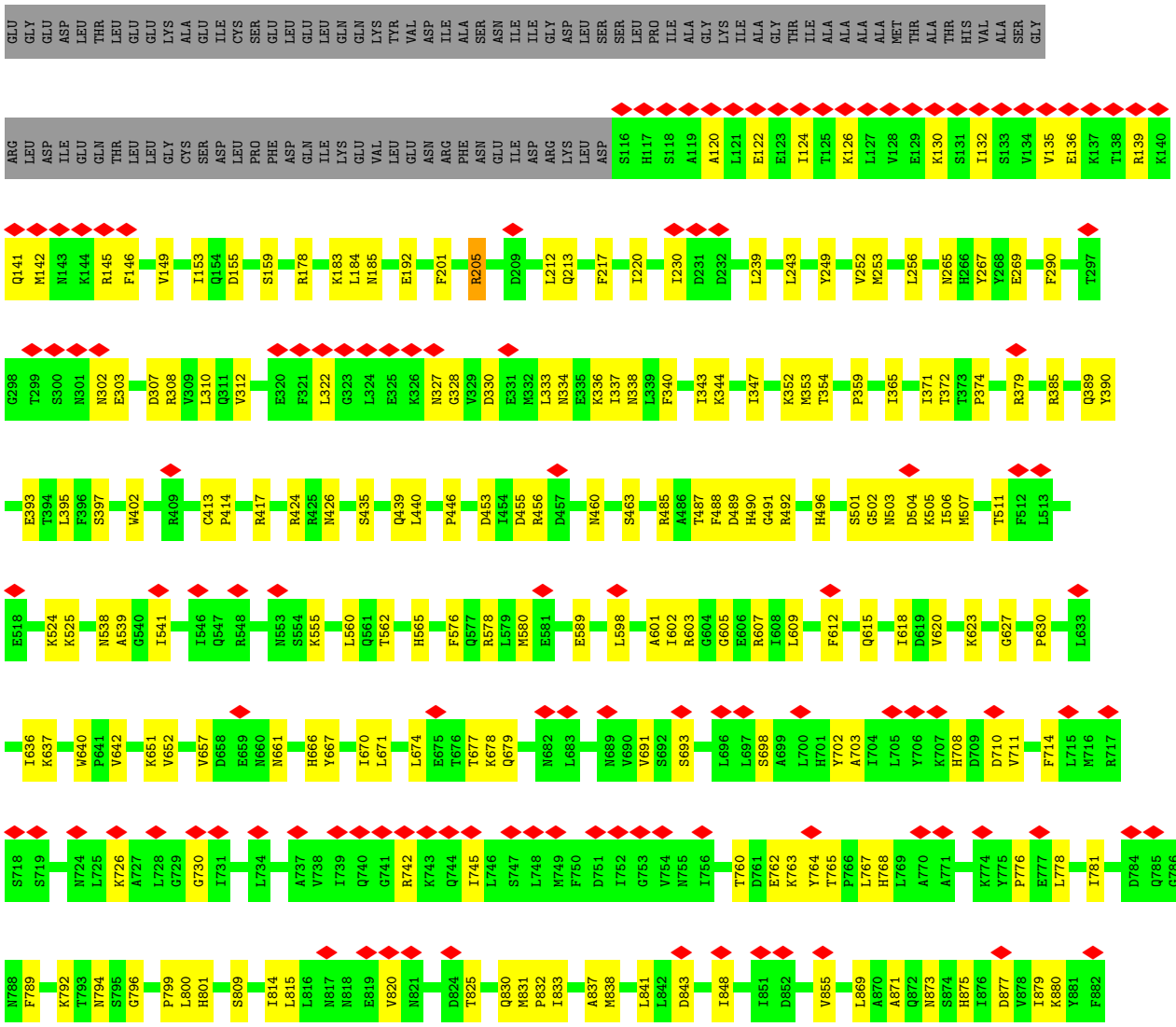
Chain C:

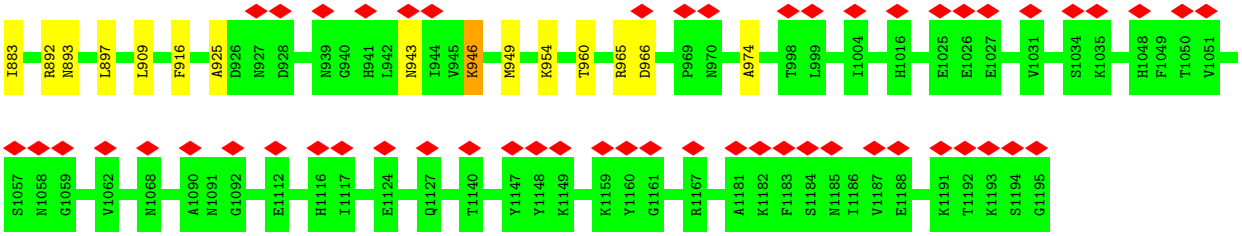




• Molecule 1: Alpha-latrotoxin-Lt1a

Chain D:




I883
R892
N893
L897
L909
F916
A925
D926
N927
D928
N939
G940
H941
L942
N943
I944
V945
K946
M949
K954
T960
R965
D966
P969
N970
A974
T998
L999
I1004
H1016
E1025
E1026
E1027
V1031
S1034
K1035
H1048
F1049
T1050
V1051
S1057
N1058
G1059
V1062
N1068
A1090
N1091
G1092
E1112
H1116
I1117
E1124
Q1127
T1140
Y1147
Y1148
K1149
K1159
Y1160
G1161
R1167
A1181
K1182
F1183
S1184
N1185
I1186
V1187
E1188
K1191
T1192
K1193
S1194
G1195

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	70971	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	215000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	48.701	Depositor
Minimum map value	-34.334	Depositor
Average map value	-0.007	Depositor
Map value standard deviation	1.201	Depositor
Recommended contour level	6.9	Depositor
Map size (Å)	324.8, 324.8, 324.8	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.58, 0.58, 0.58	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	0.25	0/8039	0.47	1/10921 (0.0%)
1	B	0.25	0/8039	0.49	0/10921
1	C	0.29	2/8039 (0.0%)	0.55	5/10921 (0.0%)
1	D	0.25	0/8039	0.48	0/10921
All	All	0.26	2/32156 (0.0%)	0.50	6/43684 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	465	PRO	CB-CG	-11.73	0.91	1.50
1	C	465	PRO	CG-CD	-8.21	1.23	1.50

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	465	PRO	CB-CG-CD	18.69	179.38	106.50
1	C	465	PRO	N-CD-CG	-16.32	78.72	103.20
1	C	465	PRO	CA-CB-CG	-14.88	75.74	104.00
1	C	465	PRO	CA-N-CD	-6.41	102.52	111.50
1	C	332	MET	CA-CB-CG	5.89	123.31	113.30

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	A	7907	0	7305	149	0
1	B	7907	0	7305	165	0
1	C	7907	0	7305	141	0
1	D	7907	0	7305	135	0
All	All	31628	0	29220	572	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 9.

The worst 5 of 572 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:760:THR:HG22	1:D:764:TYR:H	1.51	0.75
1:A:650:LYS:HG2	1:A:651:LYS:H	1.52	0.74
1:B:182:LEU:HD23	1:B:186:ASP:HB3	1.68	0.74
1:B:778:LEU:HA	1:B:781:ILE:HG22	1.69	0.74
1:A:173:ASP:OD1	1:A:244:TYR:OH	2.07	0.73

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	1078/1175 (92%)	1034 (96%)	43 (4%)	1 (0%)	48 80
1	B	1078/1175 (92%)	1033 (96%)	45 (4%)	0	100 100
1	C	1078/1175 (92%)	1050 (97%)	28 (3%)	0	100 100
1	D	1078/1175 (92%)	1035 (96%)	43 (4%)	0	100 100
All	All	4312/4700 (92%)	4152 (96%)	159 (4%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	558	HIS

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	750/1015 (74%)	750 (100%)	0	100	100
1	B	750/1015 (74%)	749 (100%)	1 (0%)	92	98
1	C	750/1015 (74%)	749 (100%)	1 (0%)	92	98
1	D	750/1015 (74%)	746 (100%)	4 (0%)	86	93
All	All	3000/4060 (74%)	2994 (100%)	6 (0%)	91	97

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	485	ARG
1	D	607	ARG
1	D	946	LYS
1	C	913	LYS
1	B	456	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	908	ASN
1	D	460	ASN
1	C	908	ASN
1	B	735	HIS
1	D	439	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 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.

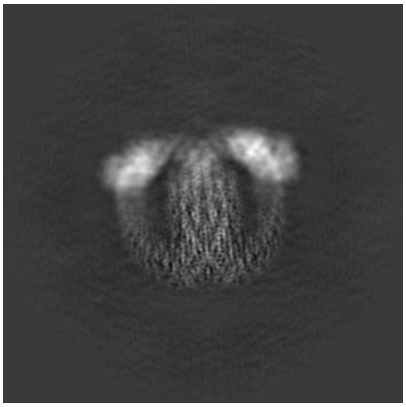
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51495. These allow visual inspection of the internal detail of the map and identification of artifacts.

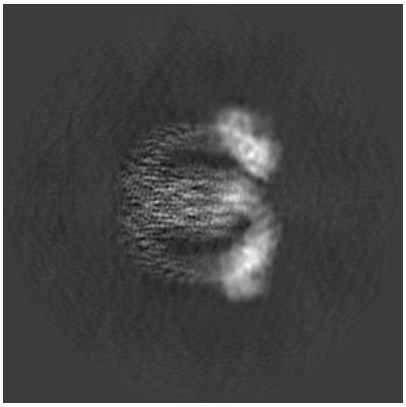
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

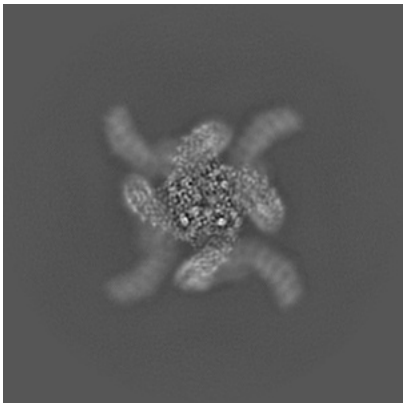
6.1.1 Primary map



X



Y

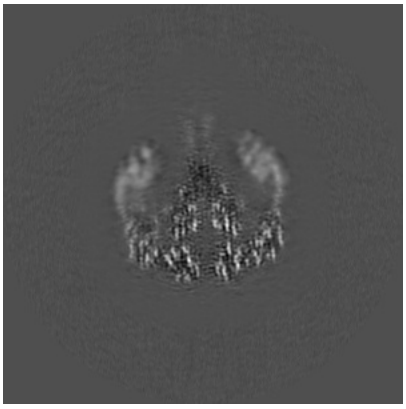


Z

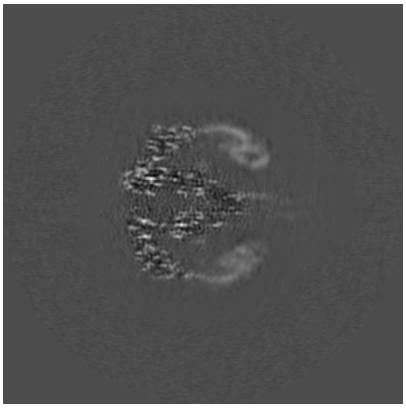
The images above show the map projected in three orthogonal directions.

6.2 Central slices

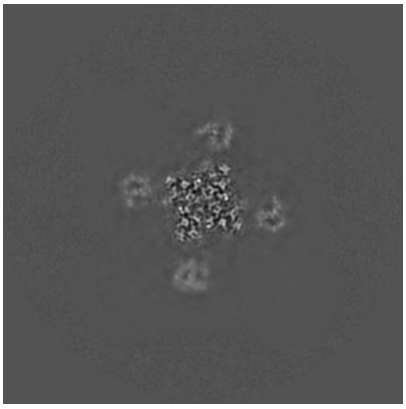
6.2.1 Primary map



X Index: 280



Y Index: 280

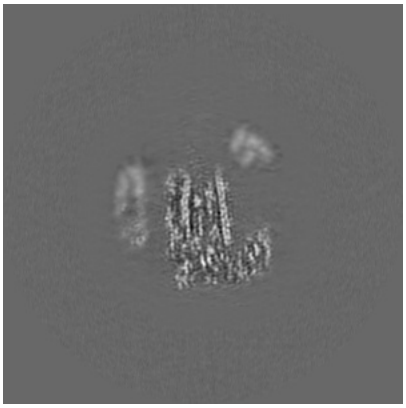


Z Index: 280

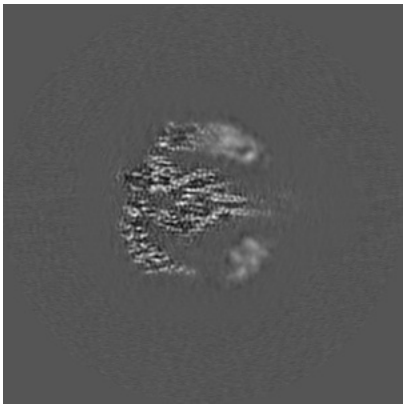
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

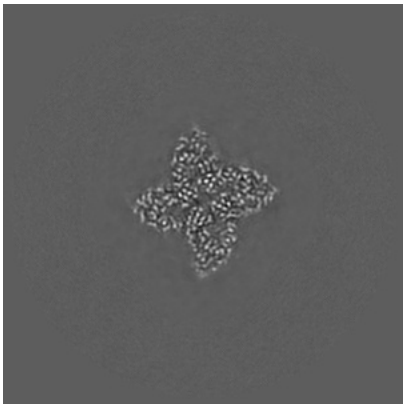
6.3.1 Primary map



X Index: 256



Y Index: 268

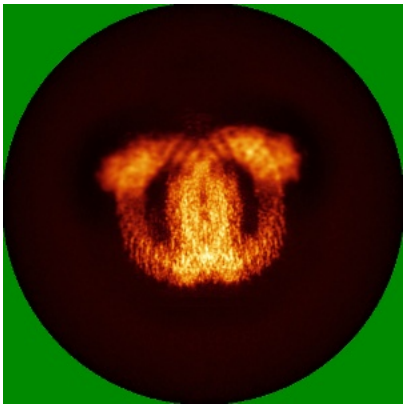


Z Index: 204

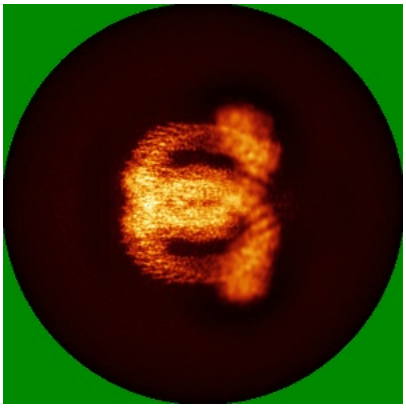
The images above show the largest variance slices of the map in three orthogonal directions.

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

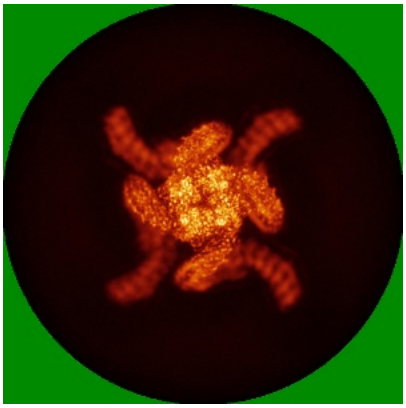
6.4.1 Primary map



X



Y

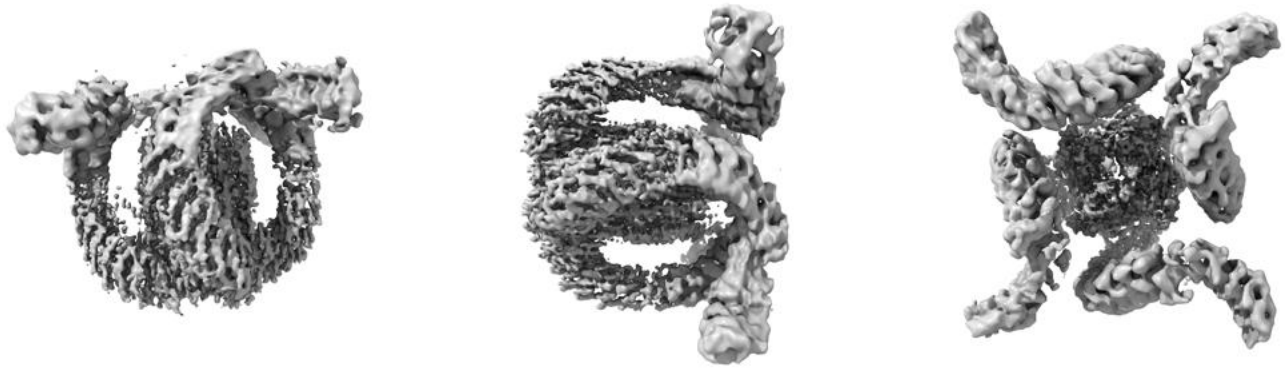


Z

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

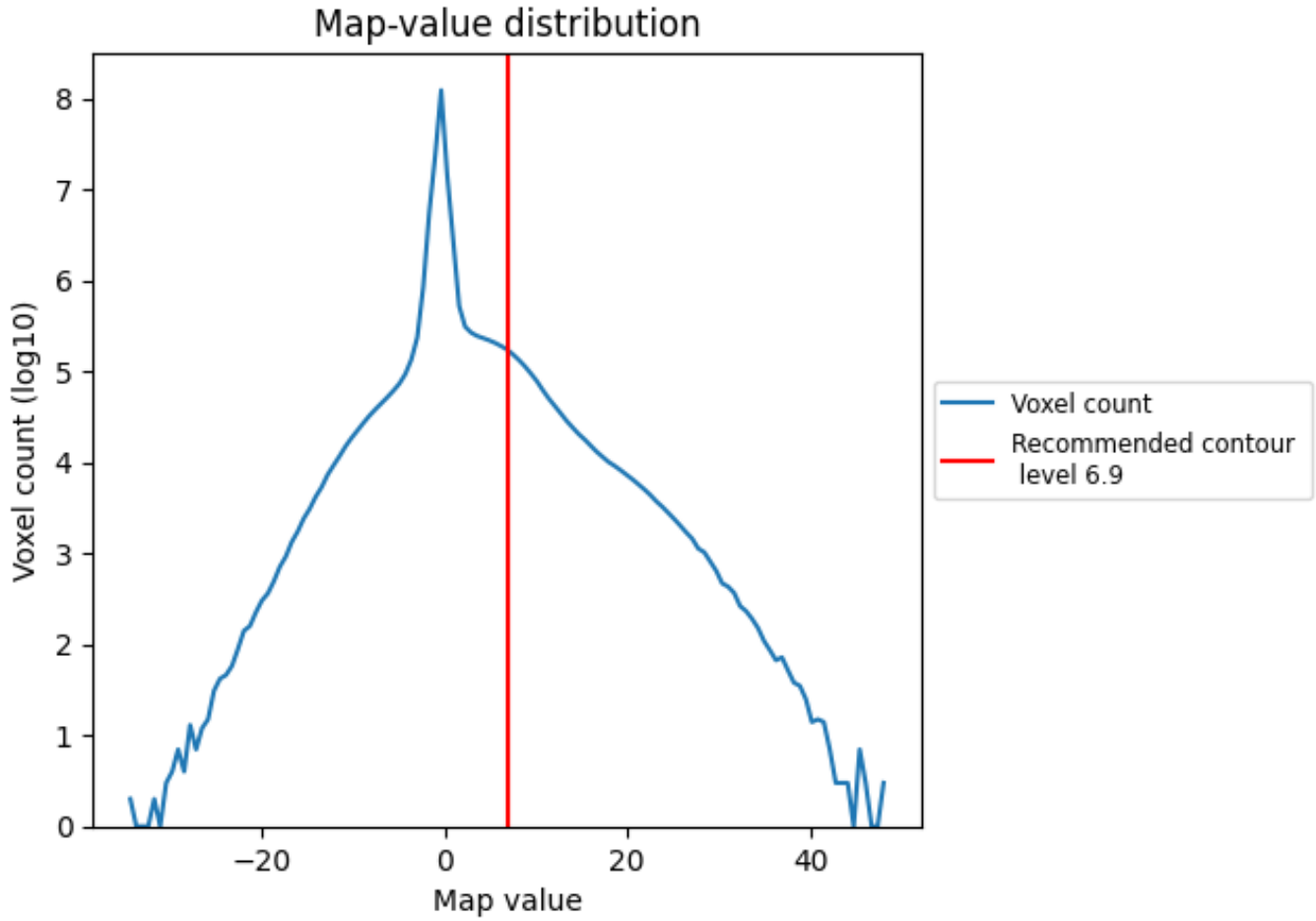
6.6 Mask visualisation (i)

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

7 Map analysis

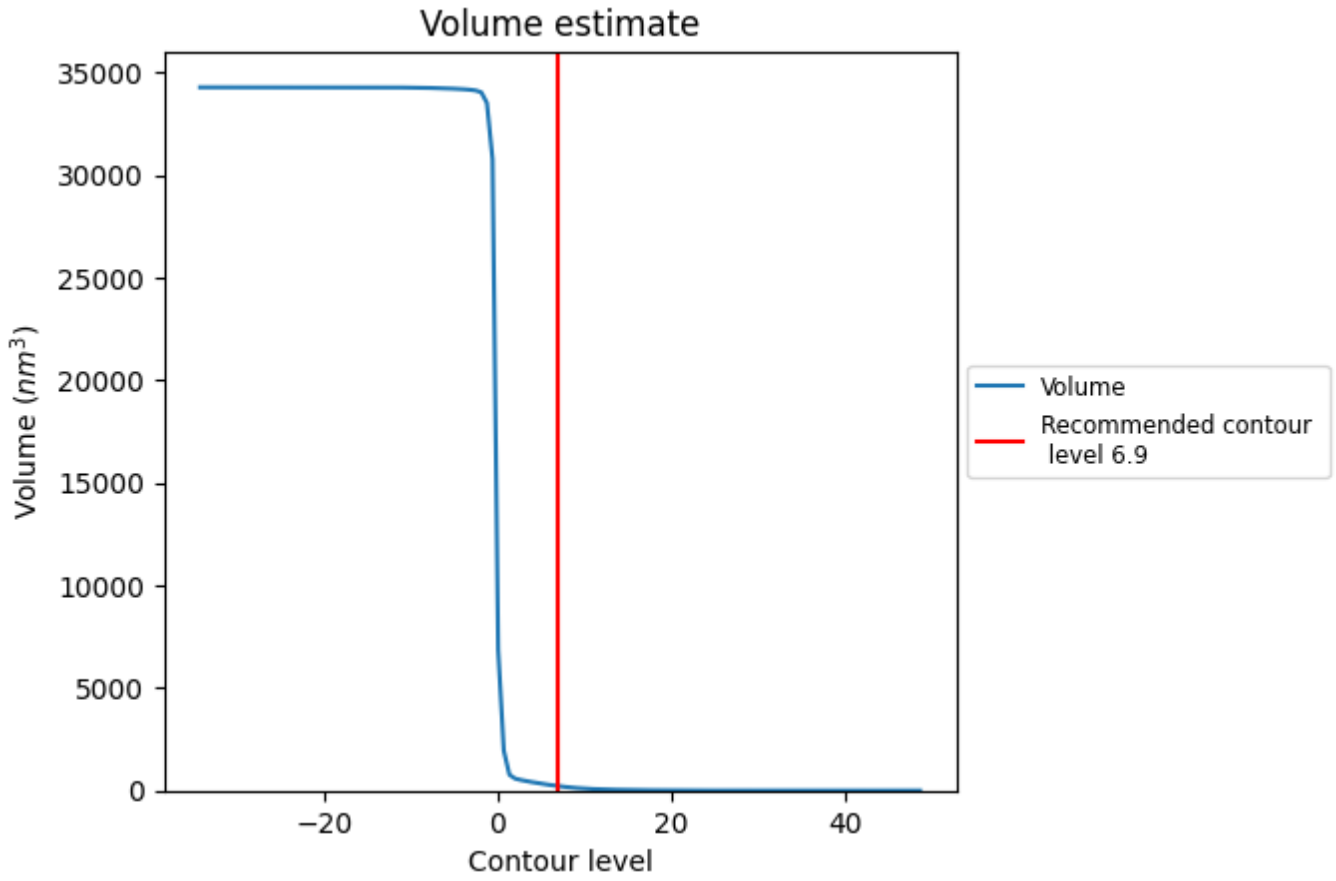
This section contains the results of statistical analysis of the map.

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.

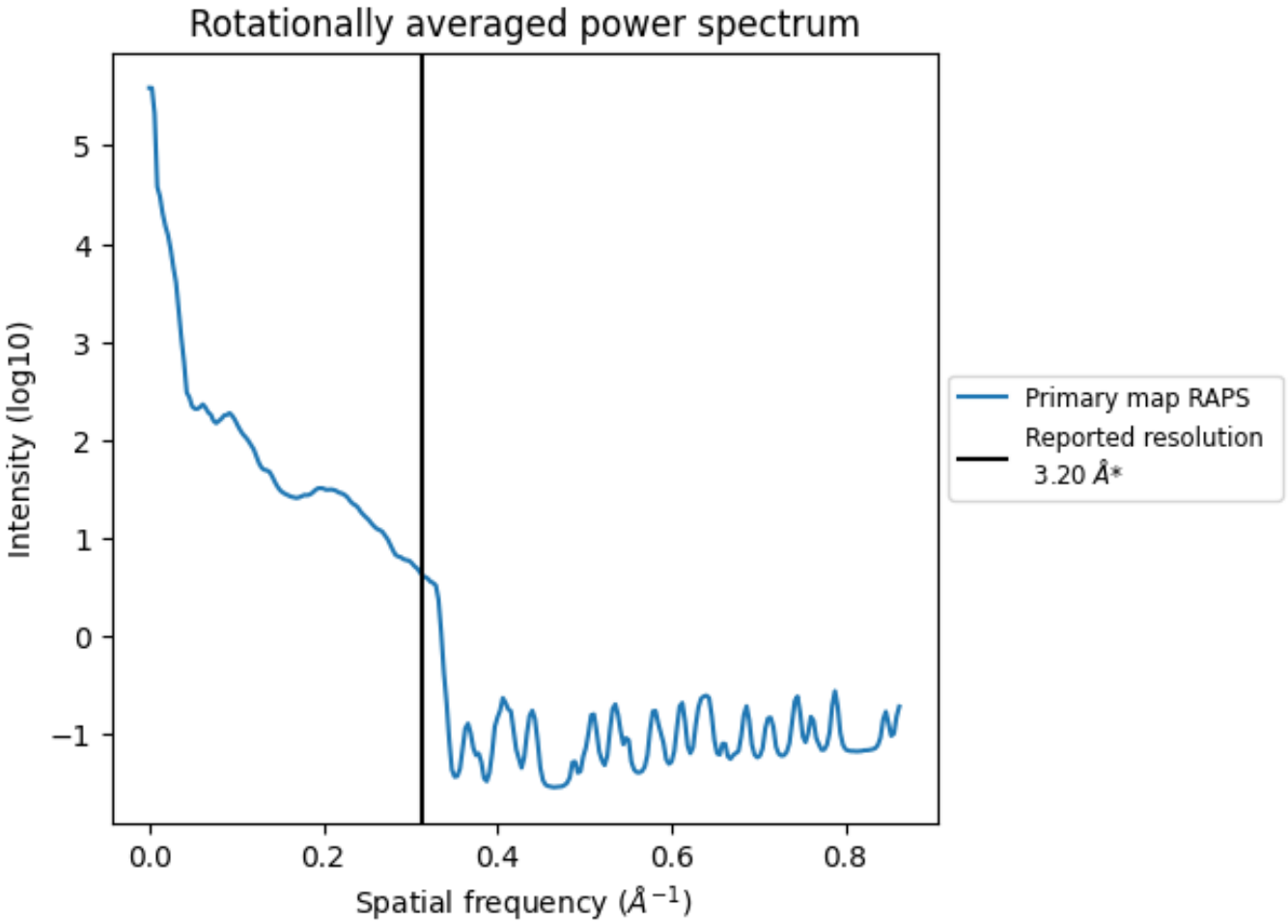
7.2 Volume estimate (i)



The volume at the recommended contour level is 222 nm^3; this corresponds to an approximate mass of 201 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 0.312 $Å^{-1}$

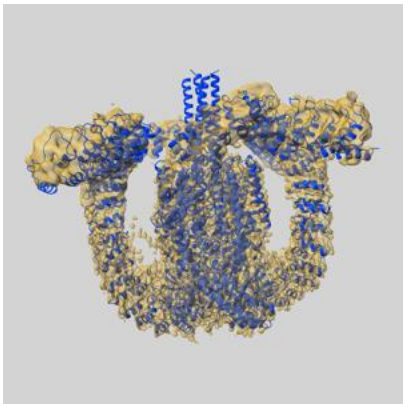
8 Fourier-Shell correlation (i)

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

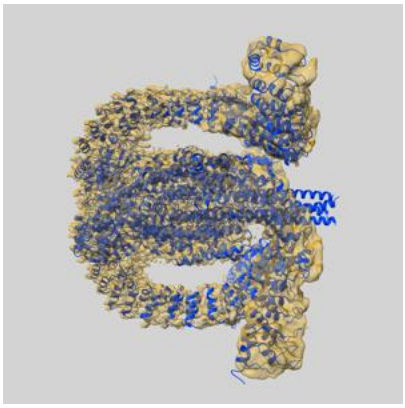
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51495 and PDB model 9GOA. Per-residue inclusion information can be found in section 3 on page 4.

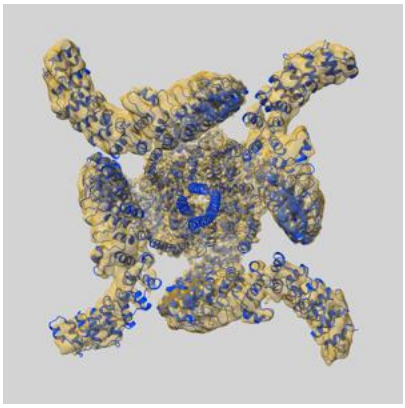
9.1 Map-model overlay



X



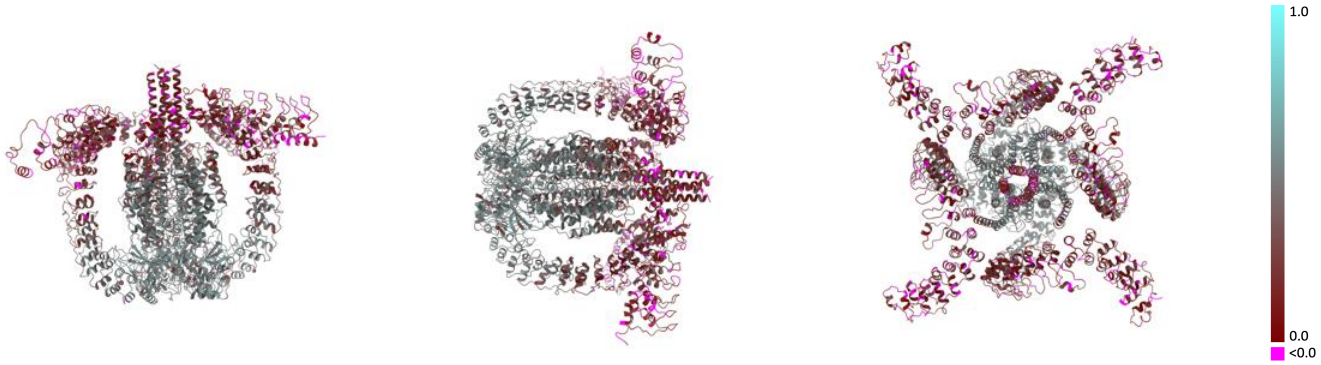
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.9 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.

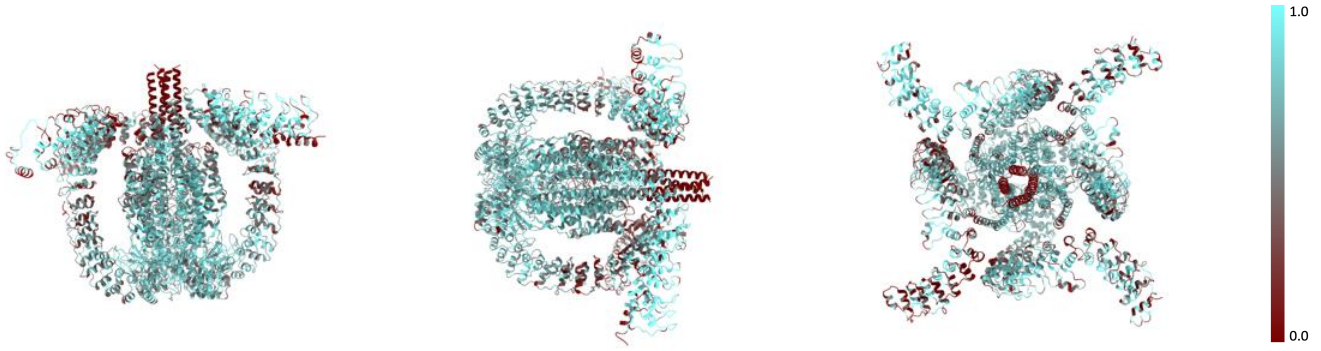
9.2 Q-score mapped to coordinate model (i)



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.

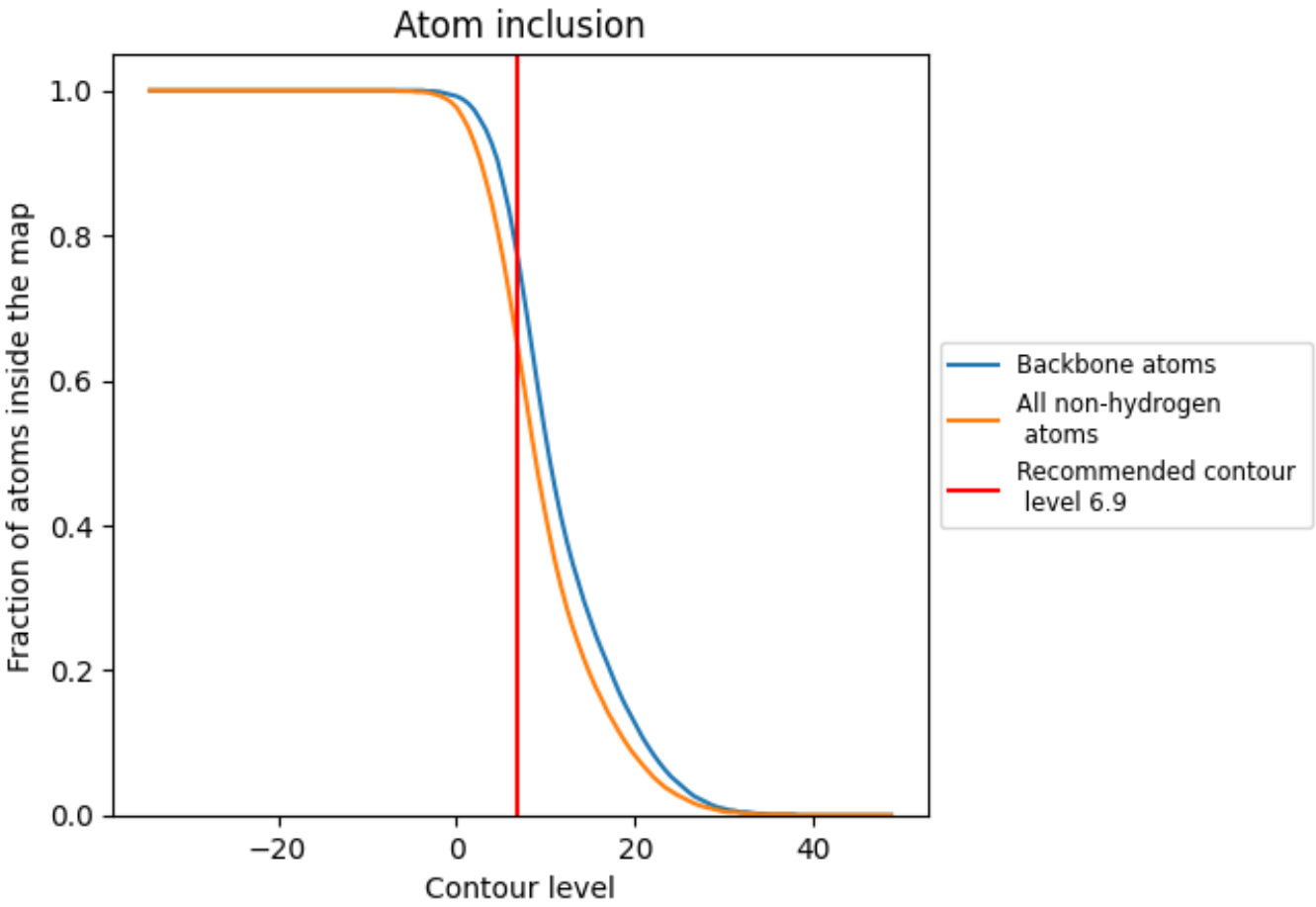
9.3 Atom inclusion mapped to coordinate model (i)



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 (6.9).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 64% 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 (6.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6440	0.3510
A	0.5950	0.3570
B	0.6350	0.3370
C	0.6610	0.3540
D	0.6850	0.3560