



wwPDB EM Validation Summary Report ⓘ

Nov 15, 2022 – 01:06 PM JST

PDB ID : 6LAR
EMDB ID : EMD-0862
Title : Structure of ESX-3 complex
Authors : Wang, S.H.; Zhou, K.X.; Li, J.; Rao, Z.H.
Deposited on : 2019-11-13
Resolution : 3.70 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

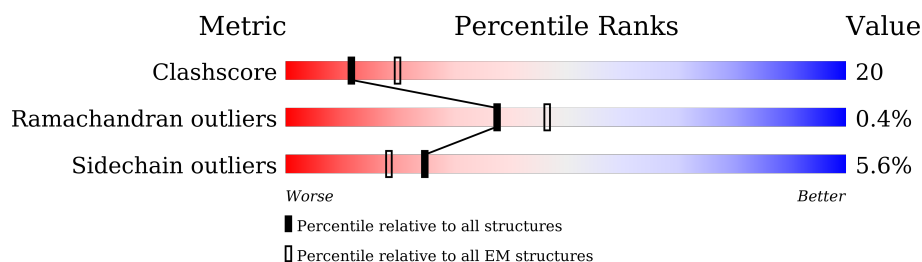
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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.



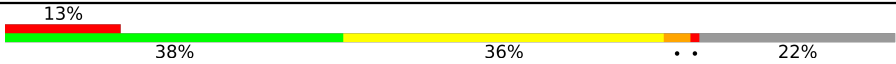

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$. 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	518	
1	I	518	
2	B	475	
2	C	475	
2	E	475	
2	H	475	
3	F	449	
3	J	449	

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Mol	Chain	Length	Quality of chain
4	D	309	
4	G	309	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22448 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 ESX-3 secretion system ATPase EccB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	81	Total	C	N	O	S	0	0
			642	402	127	110	3		
1	I	59	Total	C	N	O	S	0	0
			461	297	87	74	3		

- Molecule 2 is a protein called ESX-3 secretion system protein EccD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	427	Total	C	N	O	S	0	0
			3055	1986	527	534	8		
2	C	442	Total	C	N	O	S	0	0
			3168	2063	548	549	8		
2	E	427	Total	C	N	O	S	0	0
			3055	1986	527	534	8		
2	H	442	Total	C	N	O	S	0	0
			3168	2063	548	549	8		

- Molecule 3 is a protein called ESX-3 secretion system protein EccC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	336	Total	C	N	O	S	0	0
			2667	1671	501	491	4		
3	J	324	Total	C	N	O	S	0	0
			2574	1608	483	479	4		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	432	HIS	-	expression tag	UNP A0QQ40
F	433	LEU	-	expression tag	UNP A0QQ40
F	434	GLY	-	expression tag	UNP A0QQ40
F	435	GLY	-	expression tag	UNP A0QQ40
F	436	ILE	-	expression tag	UNP A0QQ40

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Chain	Residue	Modelled	Actual	Comment	Reference
F	437	LYS	-	expression tag	UNP A0QQ40
F	438	ALA	-	expression tag	UNP A0QQ40
F	439	PHE	-	expression tag	UNP A0QQ40
F	440	HIS	-	expression tag	UNP A0QQ40
F	441	HIS	-	expression tag	UNP A0QQ40
F	442	HIS	-	expression tag	UNP A0QQ40
F	443	HIS	-	expression tag	UNP A0QQ40
F	444	HIS	-	expression tag	UNP A0QQ40
F	445	HIS	-	expression tag	UNP A0QQ40
F	446	HIS	-	expression tag	UNP A0QQ40
F	447	HIS	-	expression tag	UNP A0QQ40
F	448	HIS	-	expression tag	UNP A0QQ40
F	449	HIS	-	expression tag	UNP A0QQ40
J	432	HIS	-	expression tag	UNP A0QQ40
J	433	LEU	-	expression tag	UNP A0QQ40
J	434	GLY	-	expression tag	UNP A0QQ40
J	435	GLY	-	expression tag	UNP A0QQ40
J	436	ILE	-	expression tag	UNP A0QQ40
J	437	LYS	-	expression tag	UNP A0QQ40
J	438	ALA	-	expression tag	UNP A0QQ40
J	439	PHE	-	expression tag	UNP A0QQ40
J	440	HIS	-	expression tag	UNP A0QQ40
J	441	HIS	-	expression tag	UNP A0QQ40
J	442	HIS	-	expression tag	UNP A0QQ40
J	443	HIS	-	expression tag	UNP A0QQ40
J	444	HIS	-	expression tag	UNP A0QQ40
J	445	HIS	-	expression tag	UNP A0QQ40
J	446	HIS	-	expression tag	UNP A0QQ40
J	447	HIS	-	expression tag	UNP A0QQ40
J	448	HIS	-	expression tag	UNP A0QQ40
J	449	HIS	-	expression tag	UNP A0QQ40

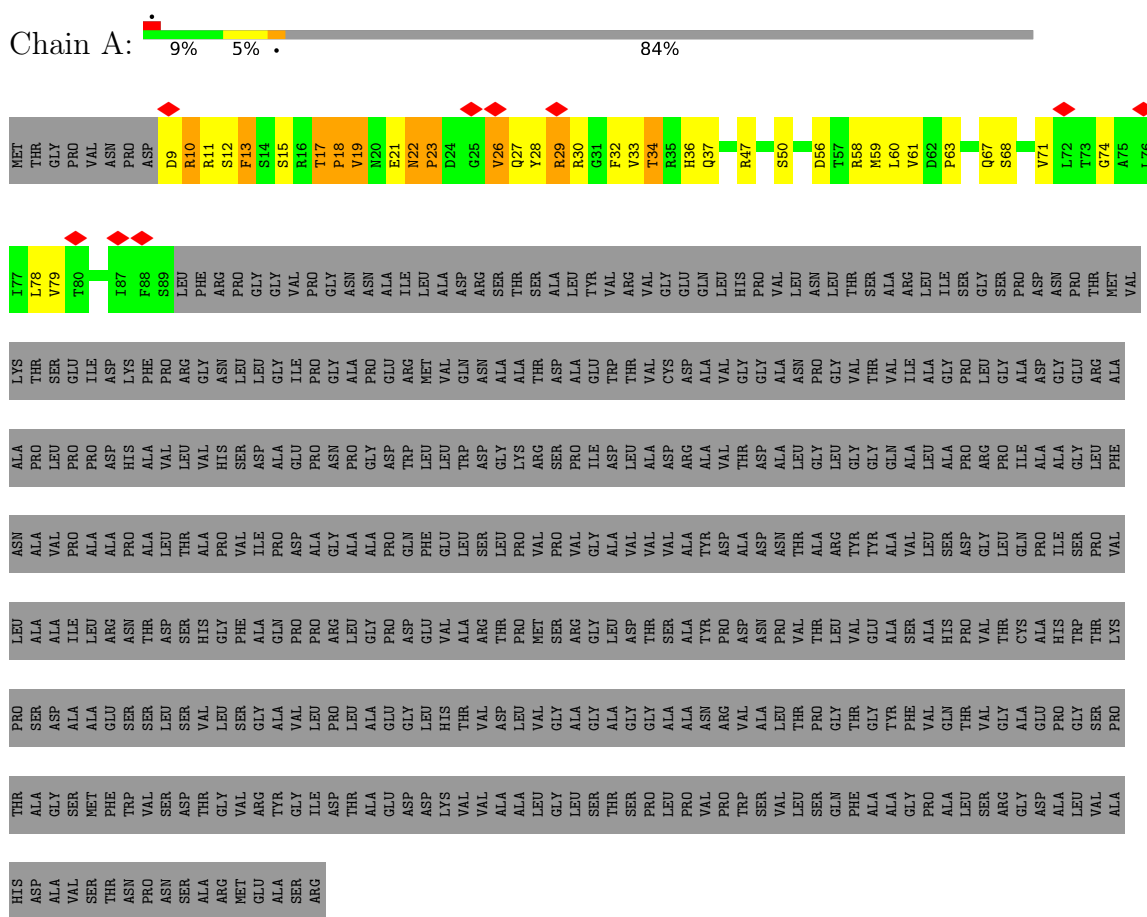
- Molecule 4 is a protein called ESX-3 secretion system protein EccE3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	241	Total	C	N	O	S	0	0
			1829	1160	336	328	5		
4	D	241	Total	C	N	O	S	0	0
			1829	1160	336	328	5		

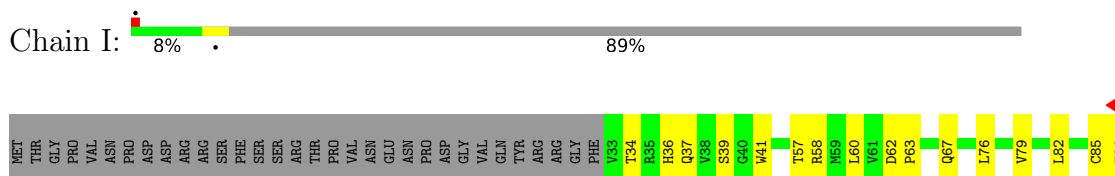
3 Residue-property plots

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.

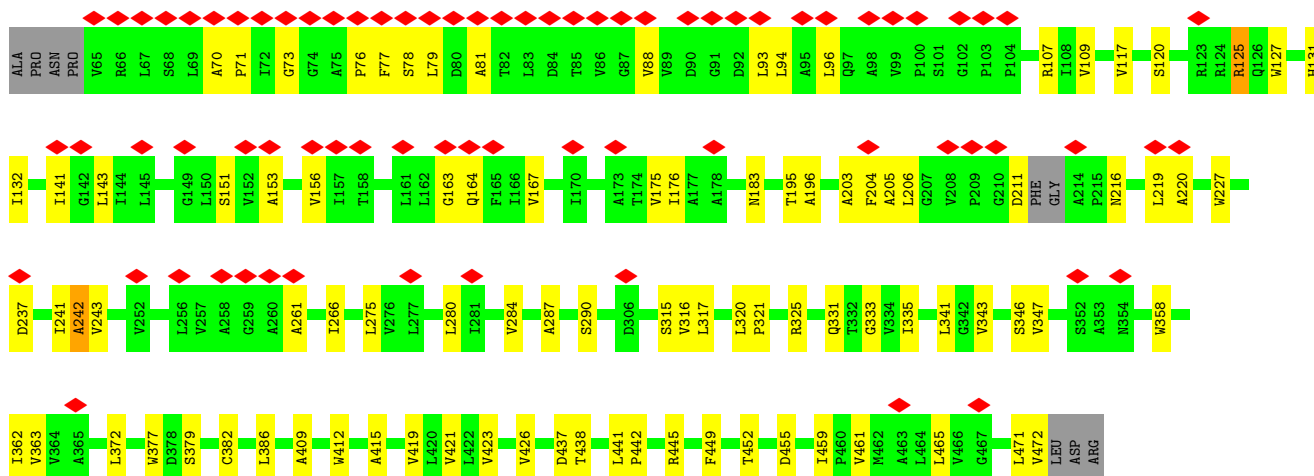
• Molecule 1: ESX-3 secretion system ATPase EccB3



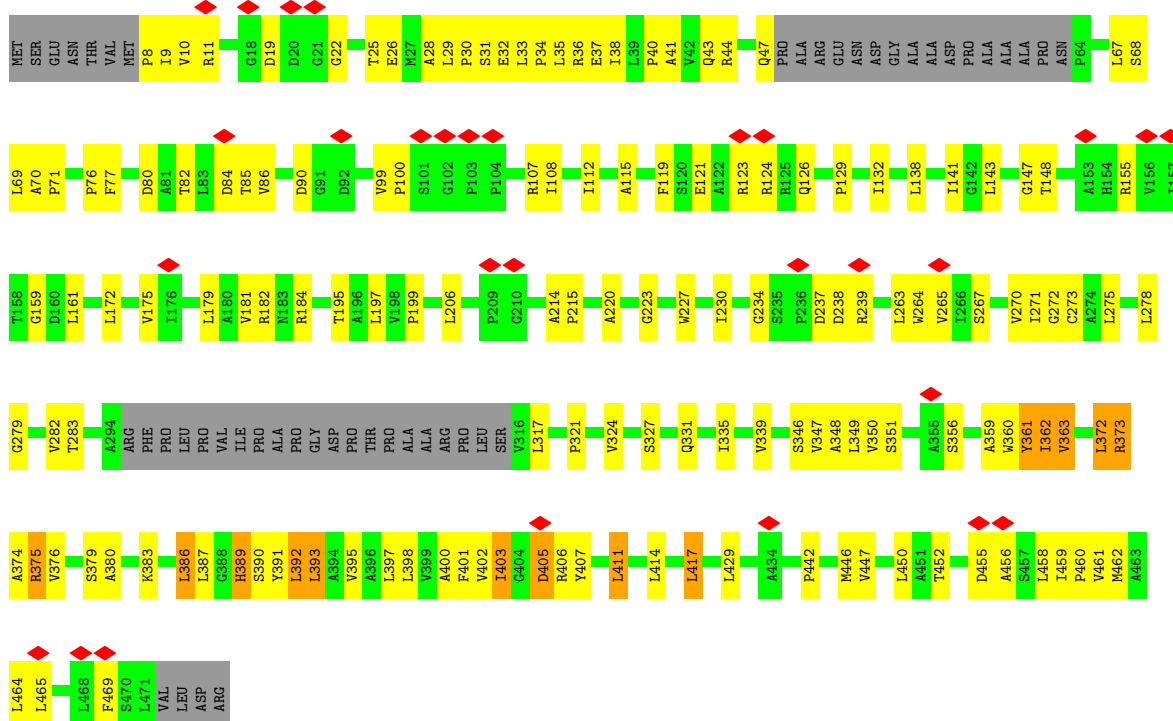
• Molecule 1: ESX-3 secretion system ATPase EccB3



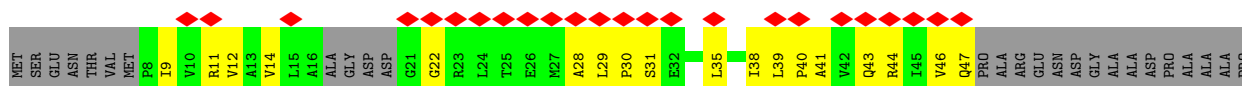


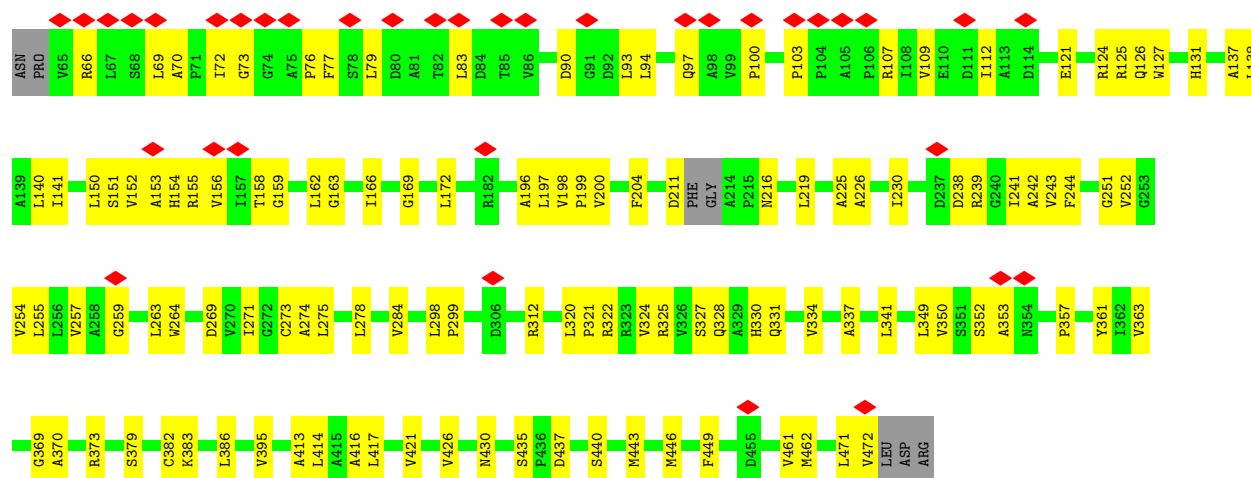


• Molecule 2: ESX-3 secretion system protein EccD3

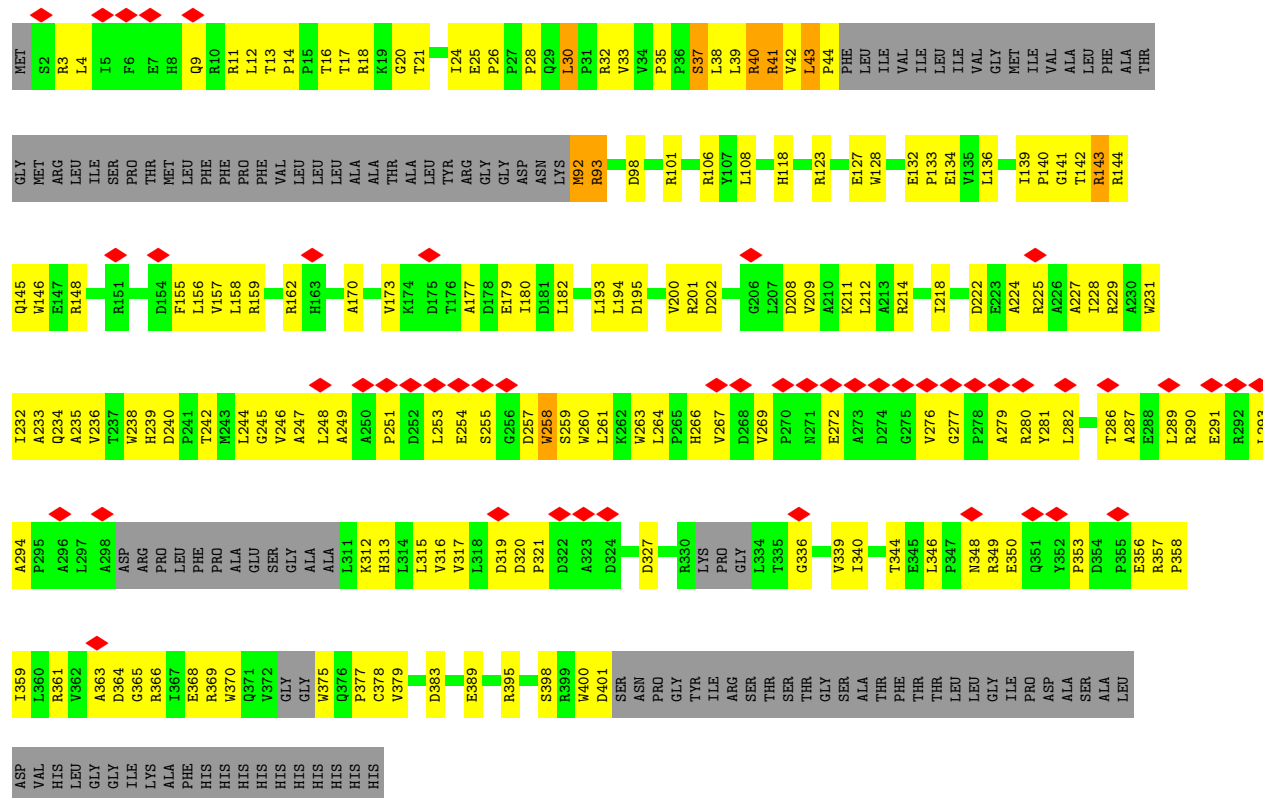


• Molecule 2: ESX-3 secretion system protein EccD3

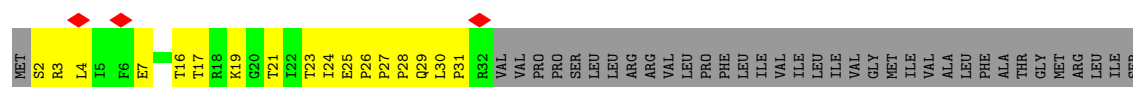


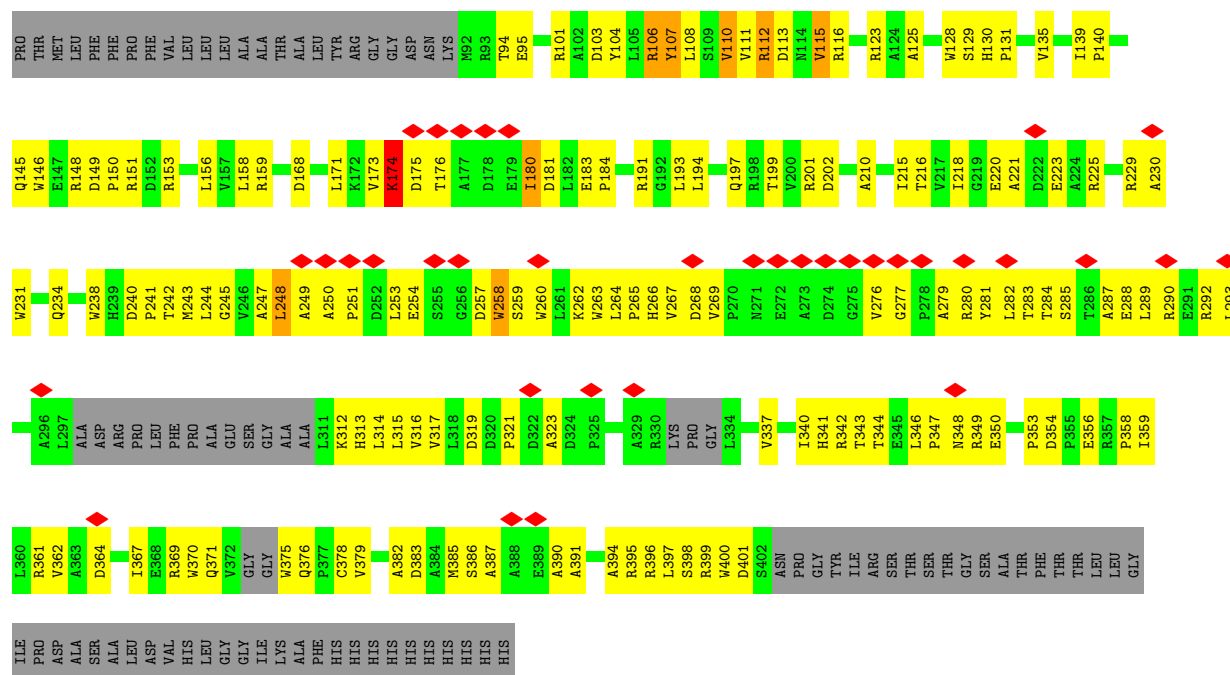


• Molecule 3: ESX-3 secretion system protein EccC3

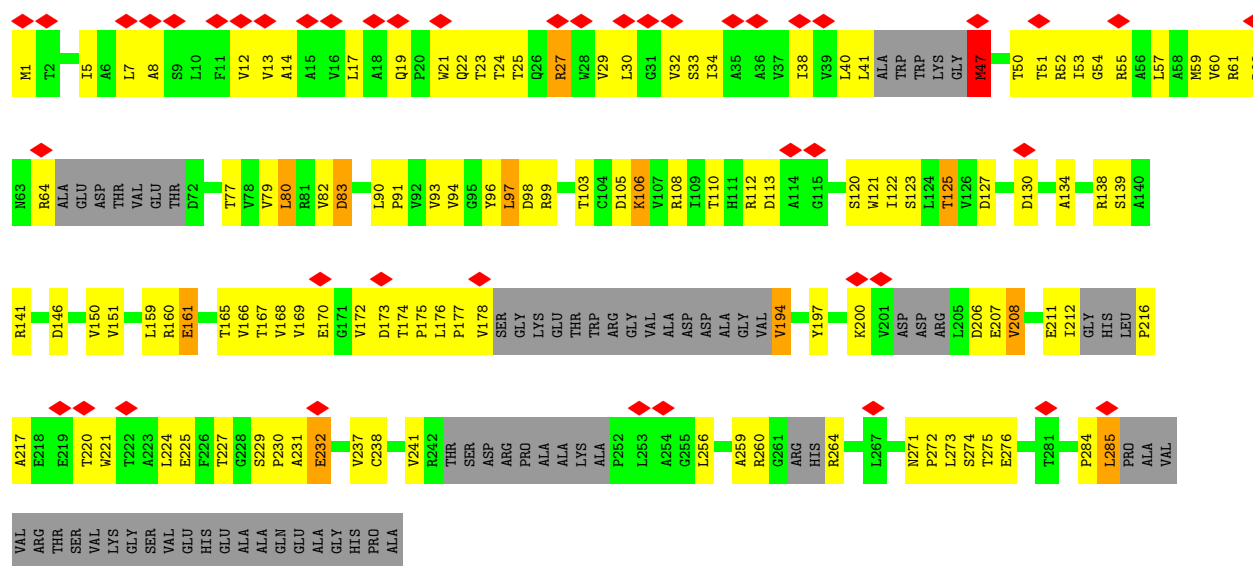


• Molecule 3: ESX-3 secretion system protein EccC3

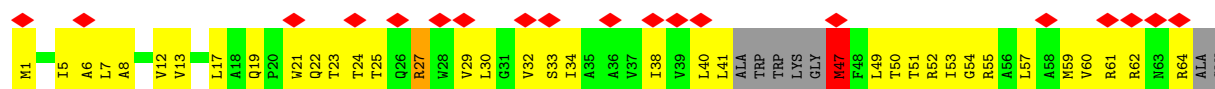




• Molecule 4: ESX-3 secretion system protein EccE3



• Molecule 4: ESX-3 secretion system protein EccE3





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	215839	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	29000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.173	Depositor
Minimum map value	-0.113	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size (\AA)	360.8, 360.8, 360.8	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.82, 0.82, 0.82	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	0.52	0/654	0.56	0/883
1	I	0.42	0/469	0.50	0/634
2	B	0.34	0/3111	0.52	0/4271
2	C	0.36	0/3229	0.51	0/4438
2	E	0.40	0/3111	0.52	0/4271
2	H	0.41	0/3229	0.52	0/4438
3	F	0.38	0/2727	0.54	0/3727
3	J	0.40	0/2631	0.57	1/3593 (0.0%)
4	D	0.35	0/1855	0.56	2/2531 (0.1%)
4	G	0.35	0/1855	0.56	2/2531 (0.1%)
All	All	0.38	0/22871	0.53	5/31317 (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
3	J	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	232	GLU	CA-CB-CG	7.09	129.01	113.40
4	D	232	GLU	CA-CB-CG	7.07	128.94	113.40
3	J	248	LEU	CA-CB-CG	5.40	127.73	115.30
4	D	47	MET	CA-CB-CG	5.40	122.47	113.30
4	G	47	MET	CA-CB-CG	5.38	122.45	113.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	J	323	ALA	Peptide

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	642	0	653	56	0
1	I	461	0	487	16	0
2	B	3055	0	3235	95	0
2	C	3168	0	3367	75	0
2	E	3055	0	3235	151	0
2	H	3168	0	3367	100	0
3	F	2667	0	2661	143	0
3	J	2574	0	2549	197	0
4	D	1829	0	1907	83	0
4	G	1829	0	1907	74	0
All	All	22448	0	23368	903	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 20.

The worst 5 of 903 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:PHE:CE2	3:J:104:TYR:HD1	1.39	1.39
2:E:346:SER:OG	2:E:363:VAL:HG12	1.20	1.33
2:E:346:SER:OG	2:E:363:VAL:CG1	1.86	1.24
1:A:13:PHE:CE2	3:J:104:TYR:CD1	2.30	1.18
2:E:107:ARG:NE	3:J:116:ARG:HH21	1.39	1.17

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	79/518 (15%)	68 (86%)	6 (8%)	5 (6%)	1	17
1	I	57/518 (11%)	55 (96%)	2 (4%)	0	100	100
2	B	421/475 (89%)	384 (91%)	37 (9%)	0	100	100
2	C	434/475 (91%)	386 (89%)	47 (11%)	1 (0%)	47	78
2	E	421/475 (89%)	362 (86%)	58 (14%)	1 (0%)	47	78
2	H	434/475 (91%)	371 (86%)	63 (14%)	0	100	100
3	F	326/449 (73%)	263 (81%)	62 (19%)	1 (0%)	41	74
3	J	314/449 (70%)	256 (82%)	55 (18%)	3 (1%)	15	51
4	D	225/309 (73%)	196 (87%)	29 (13%)	0	100	100
4	G	225/309 (73%)	196 (87%)	29 (13%)	0	100	100
All	All	2936/4452 (66%)	2537 (86%)	388 (13%)	11 (0%)	38	69

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	18	PRO
1	A	26	VAL
3	F	258	TRP
2	C	242	ALA

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	70/398 (18%)	60 (86%)	10 (14%)	3	19
1	I	50/398 (13%)	49 (98%)	1 (2%)	55	74
2	B	305/342 (89%)	304 (100%)	1 (0%)	92	96
2	C	319/342 (93%)	318 (100%)	1 (0%)	92	96
2	E	305/342 (89%)	286 (94%)	19 (6%)	18	49
2	H	319/342 (93%)	318 (100%)	1 (0%)	92	96
3	F	281/369 (76%)	271 (96%)	10 (4%)	35	63
3	J	270/369 (73%)	257 (95%)	13 (5%)	25	56
4	D	192/241 (80%)	155 (81%)	37 (19%)	1	9
4	G	192/241 (80%)	155 (81%)	37 (19%)	1	9
All	All	2303/3384 (68%)	2173 (94%)	130 (6%)	25	53

5 of 130 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	161	GLU
4	D	178	VAL
4	G	178	VAL
4	G	168	VAL
4	D	200	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	131	HIS
3	J	271	ASN
4	D	19	GLN
3	J	371	GLN
3	J	187	HIS

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 [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.

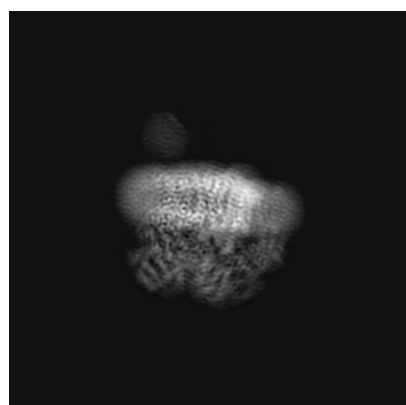
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0862. These allow visual inspection of the internal detail of the map and identification of artifacts.

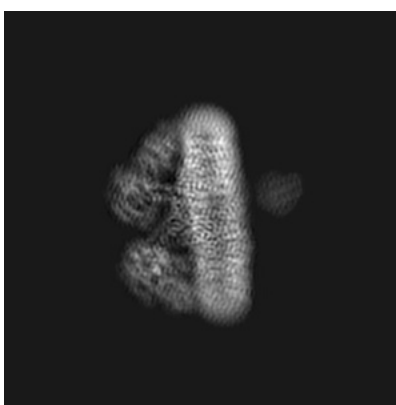
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

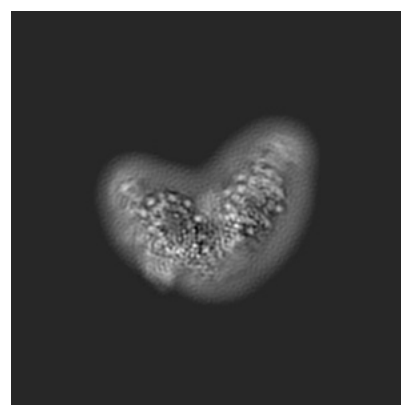
6.1.1 Primary map



X



Y

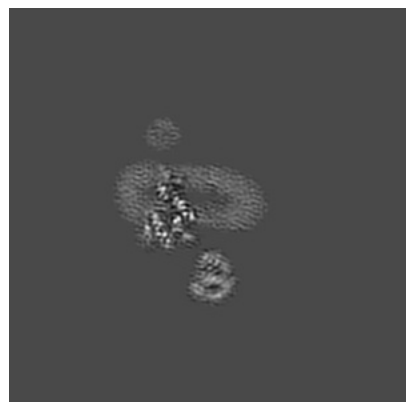


Z

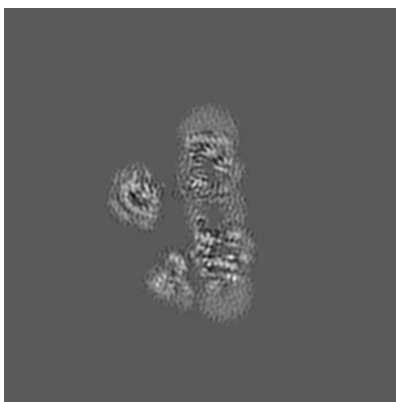
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

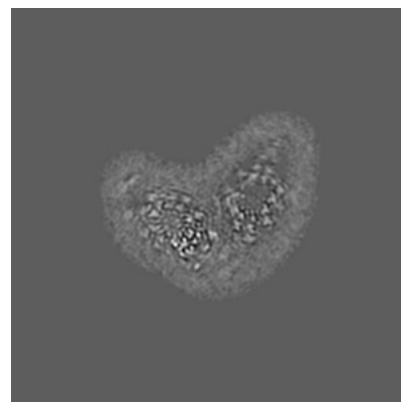
6.2.1 Primary map



X Index: 220



Y Index: 220

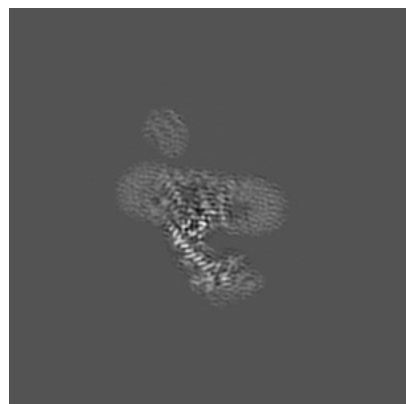


Z Index: 220

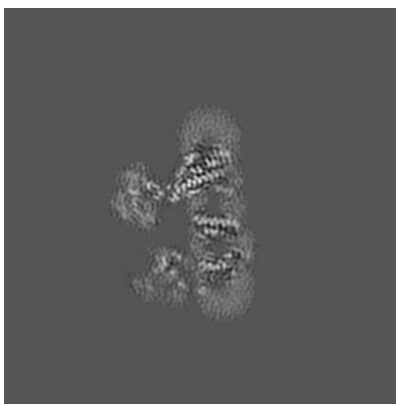
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

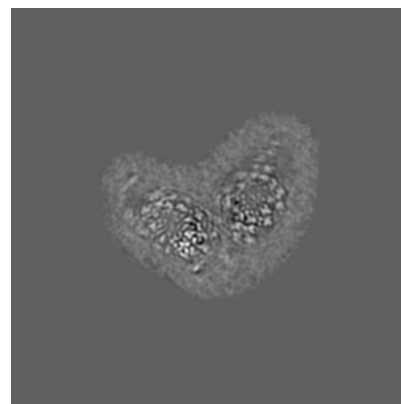
6.3.1 Primary map



X Index: 244



Y Index: 211



Z Index: 218

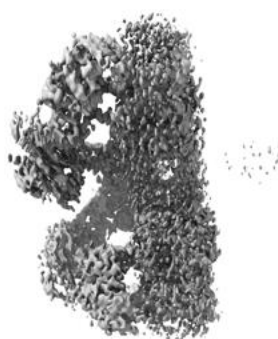
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

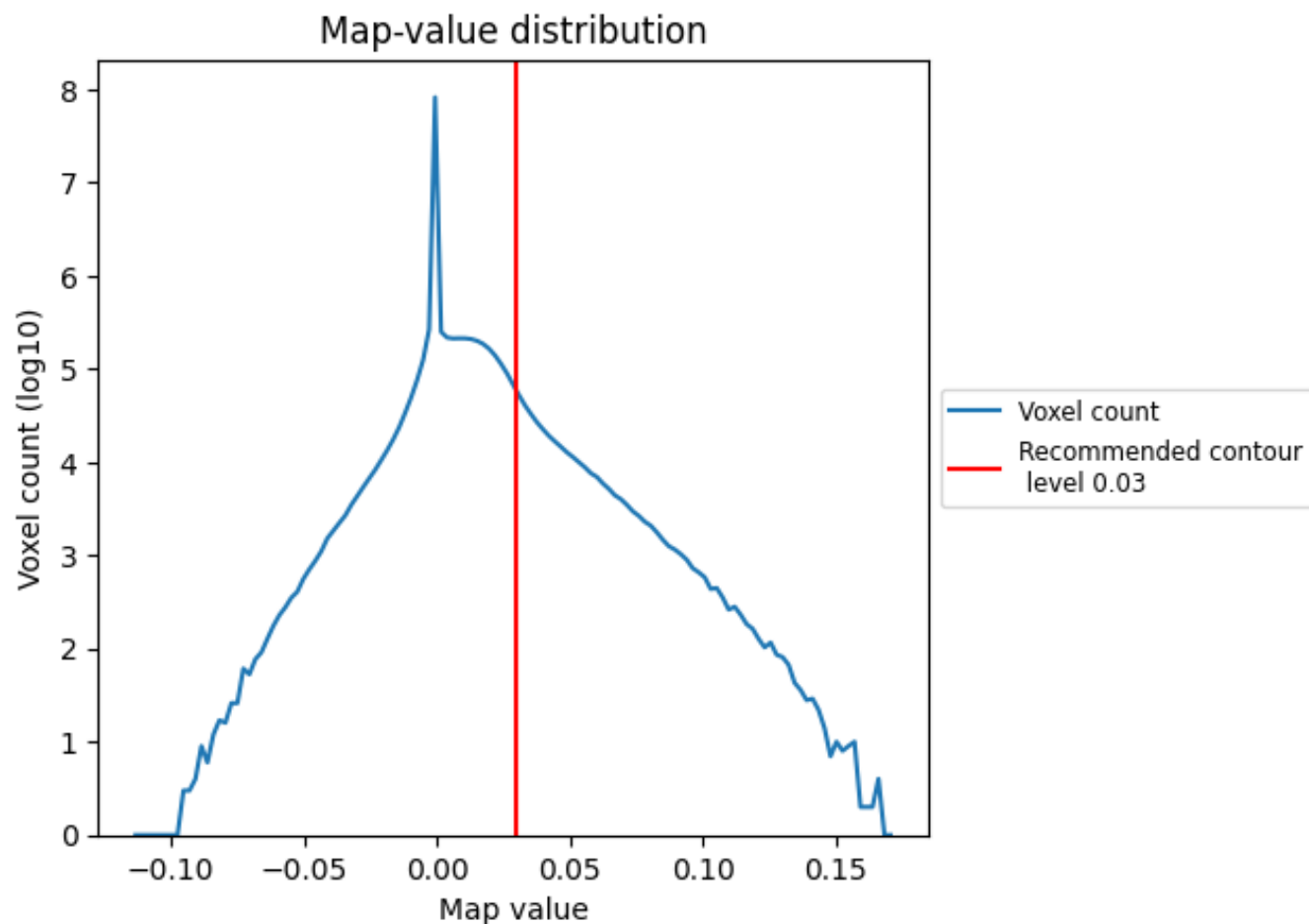
6.5 Mask visualisation

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

7 Map analysis [i](#)

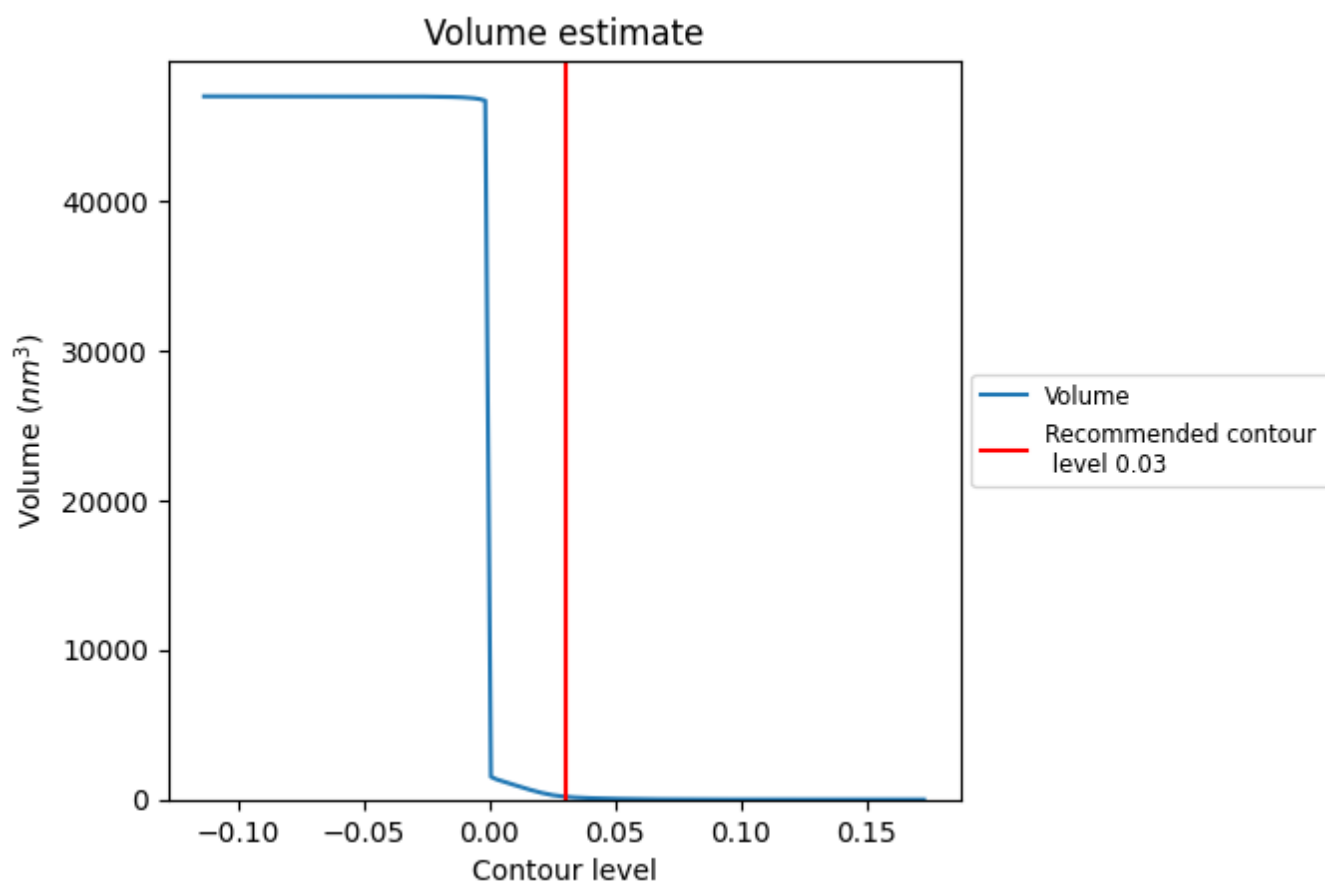
This section contains the results of statistical analysis of the map.

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.

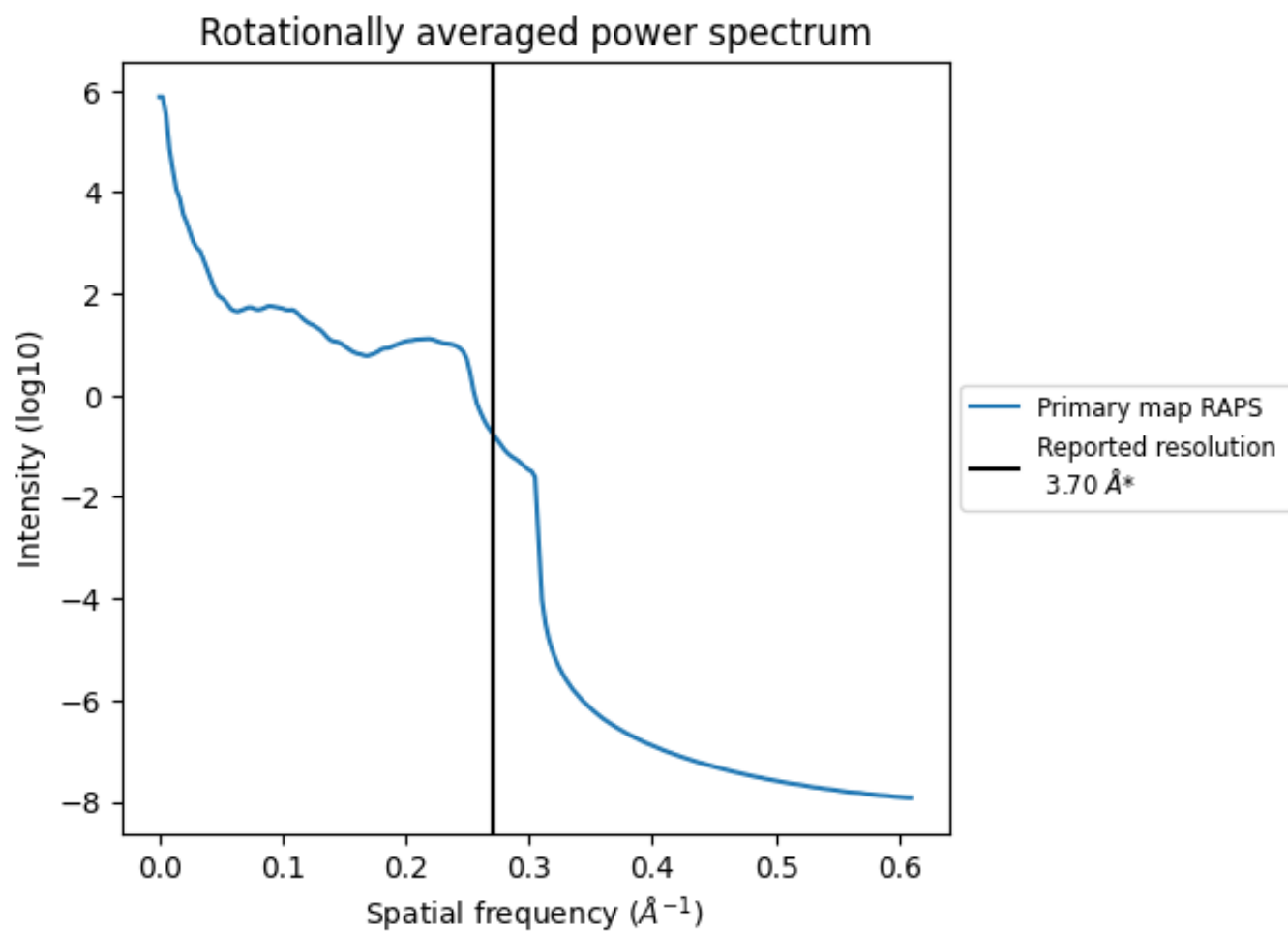
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 194 nm³; this corresponds to an approximate mass of 175 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 0.270 Å⁻¹

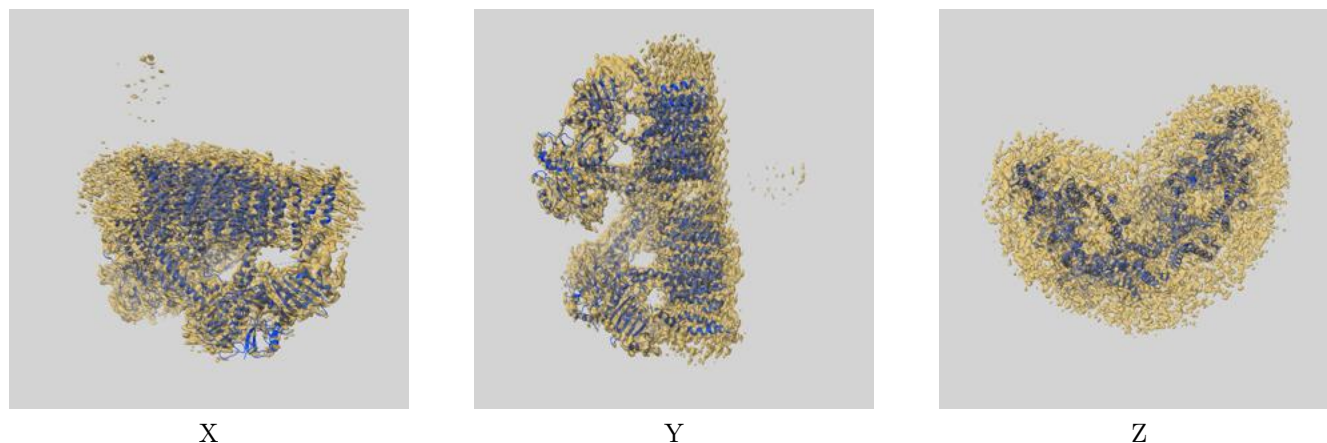
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

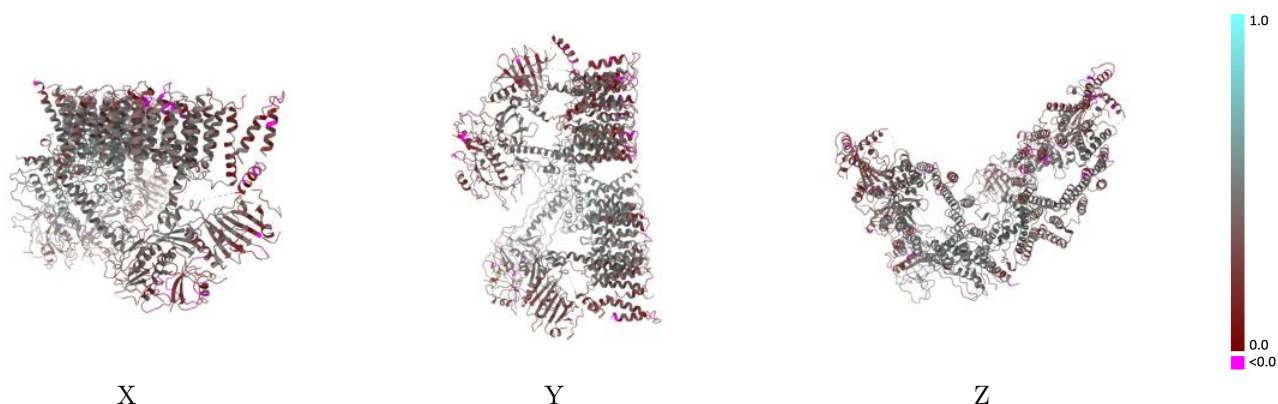
This section contains information regarding the fit between EMDB map EMD-0862 and PDB model 6LAR. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



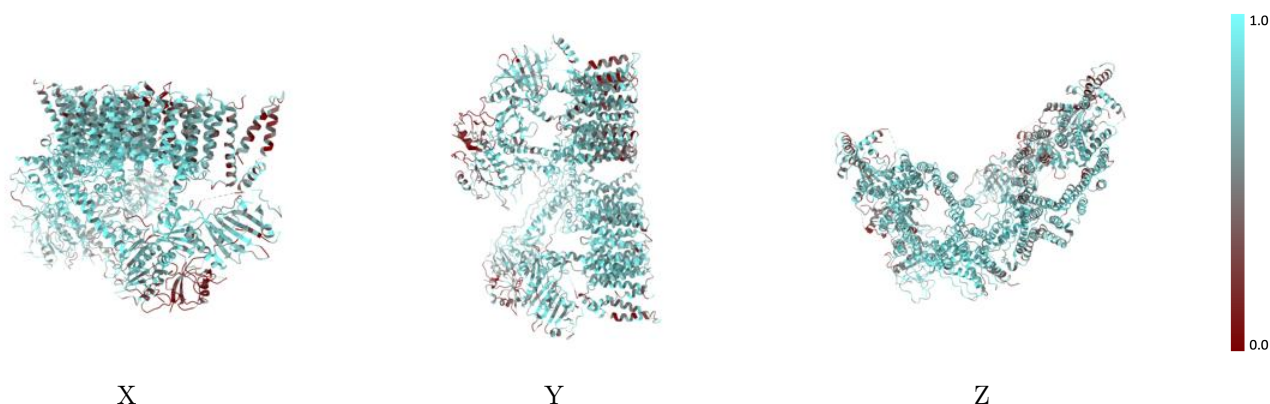
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



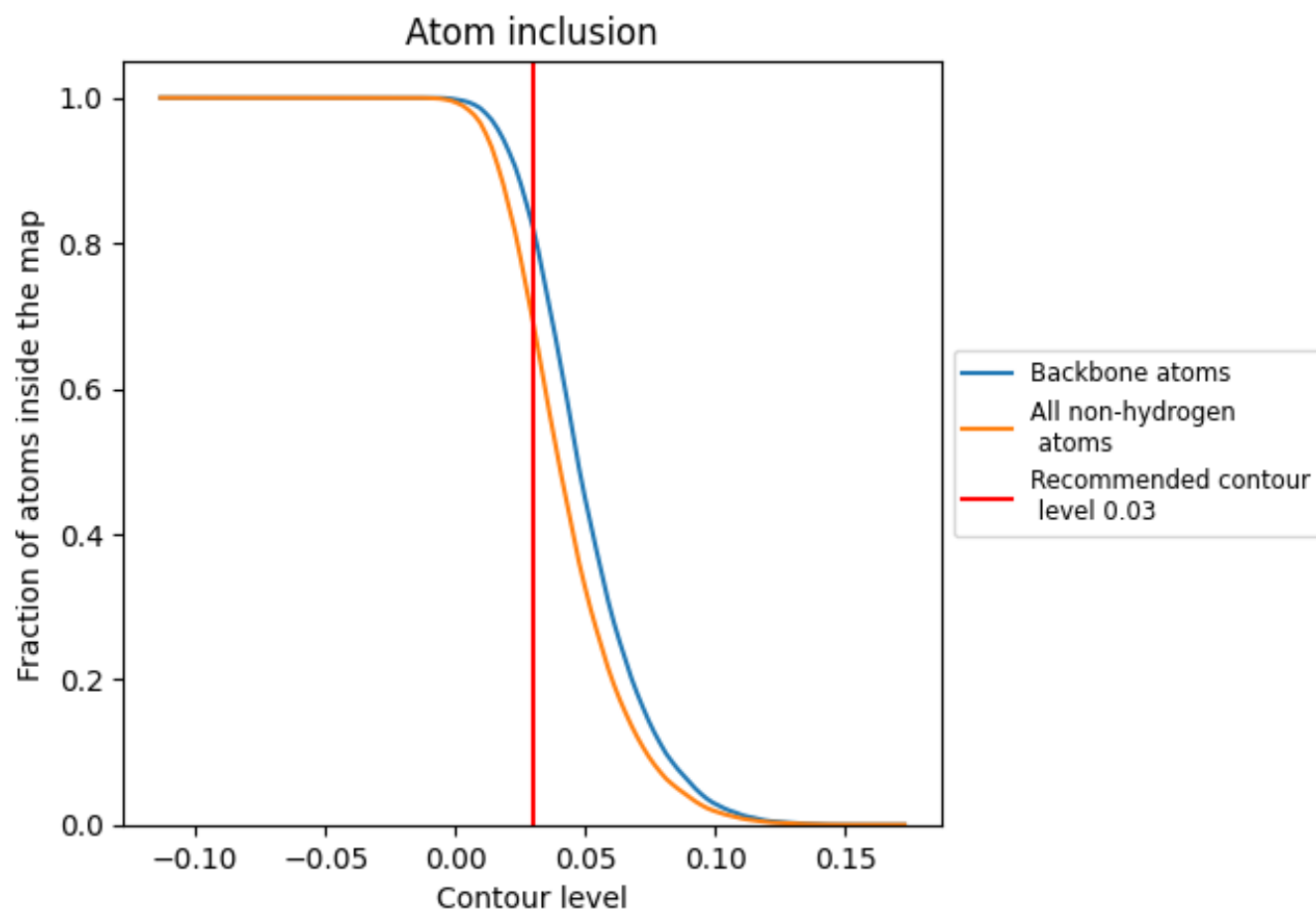
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 69% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6896	<div></div> 0.3780
A	<div></div> 0.7760	<div></div> 0.4450
B	<div></div> 0.6817	<div></div> 0.3860
C	<div></div> 0.6037	<div></div> 0.3620
D	<div></div> 0.6537	<div></div> 0.3160
E	<div></div> 0.7407	<div></div> 0.4070
F	<div></div> 0.6866	<div></div> 0.3640
G	<div></div> 0.6306	<div></div> 0.3110
H	<div></div> 0.7215	<div></div> 0.4260
I	<div></div> 0.7892	<div></div> 0.4410
J	<div></div> 0.7361	<div></div> 0.3740

1.0
0.0
<0.0