



wwPDB EM Validation Summary Report ⓘ

Feb 25, 2024 – 11:43 AM EST

PDB ID : 6X64
EMDB ID : EMD-22069
Title : Legionella pneumophila Dot T4SS PR
Authors : Durie, C.L.; Sheedlo, M.J.; Chung, J.M.; Byrne, B.G.; Su, M.; Knight, T.; Swanson, M.S.; Lacy, D.B.; Ohi, M.D.
Deposited on : 2020-05-27
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.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

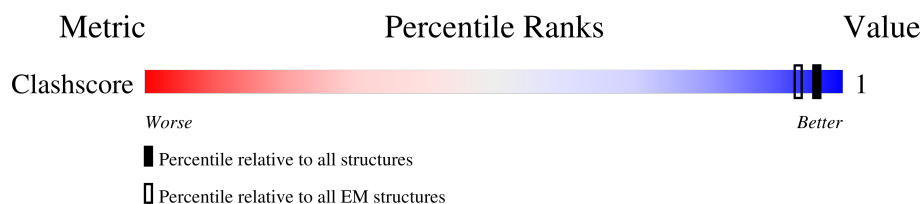
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY


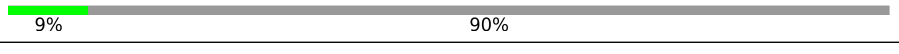
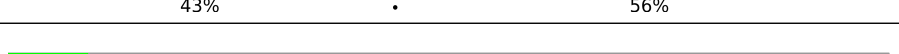

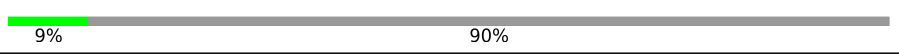





The reported resolution of this entry is 3.70 Å.

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

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	AV	330	
1	AW	330	
1	BV	330	
1	BW	330	
1	CV	330	
1	CW	330	
1	DV	330	
1	DW	330	
1	EV	330	
1	EW	330	

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Mol	Chain	Length	Quality of chain
1	FV	330	
1	FW	330	
1	GV	330	
1	GW	330	
1	HV	330	
1	HW	330	
1	IV	330	
1	IW	330	
1	JV	330	
1	JW	330	
1	KV	330	
1	KW	330	
1	LV	330	
1	LW	330	
1	MV	330	
1	MW	330	
1	NV	330	
1	NW	330	
1	OV	330	
1	OW	330	
1	PV	330	
1	PW	330	
1	QV	330	
1	QW	330	
1	RV	330	

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Mol	Chain	Length	Quality of chain
1	RW	330	<div><div></div><div>10%</div><div>90%</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15840 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 Type IV secretion system unknown protein fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	AV	144	Total	C	N	O	0	0
			720	432	144	144		
1	AW	32	Total	C	N	O	0	0
			160	96	32	32		
1	BV	144	Total	C	N	O	0	0
			720	432	144	144		
1	BW	32	Total	C	N	O	0	0
			160	96	32	32		
1	CV	144	Total	C	N	O	0	0
			720	432	144	144		
1	CW	32	Total	C	N	O	0	0
			160	96	32	32		
1	DV	144	Total	C	N	O	0	0
			720	432	144	144		
1	DW	32	Total	C	N	O	0	0
			160	96	32	32		
1	EV	144	Total	C	N	O	0	0
			720	432	144	144		
1	EW	32	Total	C	N	O	0	0
			160	96	32	32		
1	FV	144	Total	C	N	O	0	0
			720	432	144	144		
1	FW	32	Total	C	N	O	0	0
			160	96	32	32		
1	GV	144	Total	C	N	O	0	0
			720	432	144	144		
1	GW	32	Total	C	N	O	0	0
			160	96	32	32		
1	HV	144	Total	C	N	O	0	0
			720	432	144	144		
1	HW	32	Total	C	N	O	0	0
			160	96	32	32		
1	IV	144	Total	C	N	O	0	0
			720	432	144	144		

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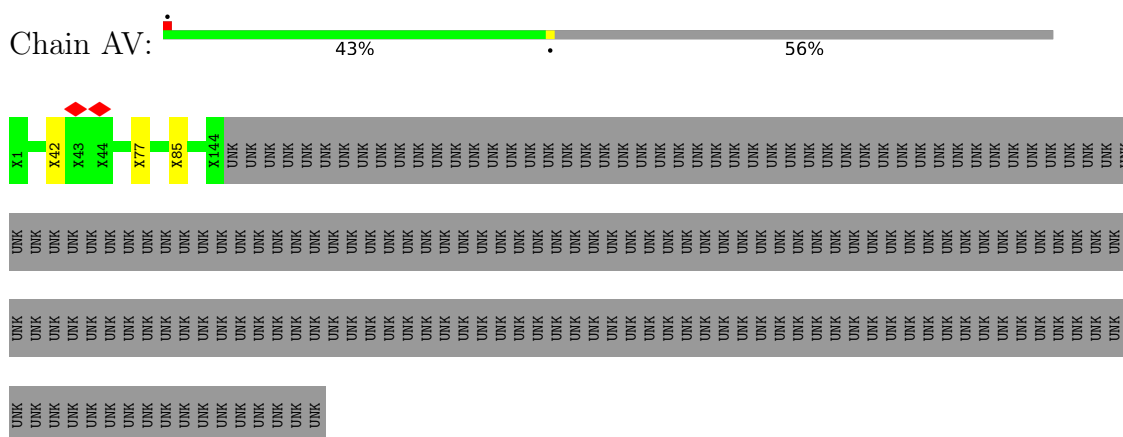
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Mol	Chain	Residues	Atoms				AltConf	Trace
1	IW	32	Total	C	N	O	0	0
			160	96	32	32		
1	JV	144	Total	C	N	O	0	0
			720	432	144	144		
1	JW	32	Total	C	N	O	0	0
			160	96	32	32		
1	KV	144	Total	C	N	O	0	0
			720	432	144	144		
1	KW	32	Total	C	N	O	0	0
			160	96	32	32		
1	LV	144	Total	C	N	O	0	0
			720	432	144	144		
1	LW	32	Total	C	N	O	0	0
			160	96	32	32		
1	MV	144	Total	C	N	O	0	0
			720	432	144	144		
1	MW	32	Total	C	N	O	0	0
			160	96	32	32		
1	NV	144	Total	C	N	O	0	0
			720	432	144	144		
1	NW	32	Total	C	N	O	0	0
			160	96	32	32		
1	OV	144	Total	C	N	O	0	0
			720	432	144	144		
1	OW	32	Total	C	N	O	0	0
			160	96	32	32		
1	PV	144	Total	C	N	O	0	0
			720	432	144	144		
1	PW	32	Total	C	N	O	0	0
			160	96	32	32		
1	QV	144	Total	C	N	O	0	0
			720	432	144	144		
1	QW	32	Total	C	N	O	0	0
			160	96	32	32		
1	RV	144	Total	C	N	O	0	0
			720	432	144	144		
1	RW	32	Total	C	N	O	0	0
			160	96	32	32		

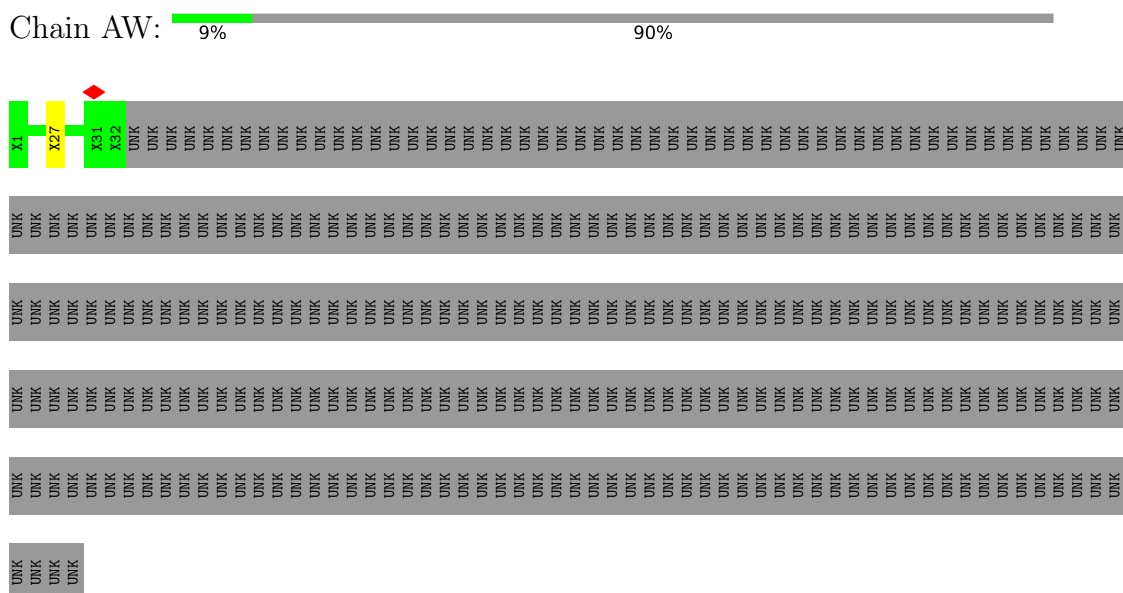
3 Residue-property plots [i](#)

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.

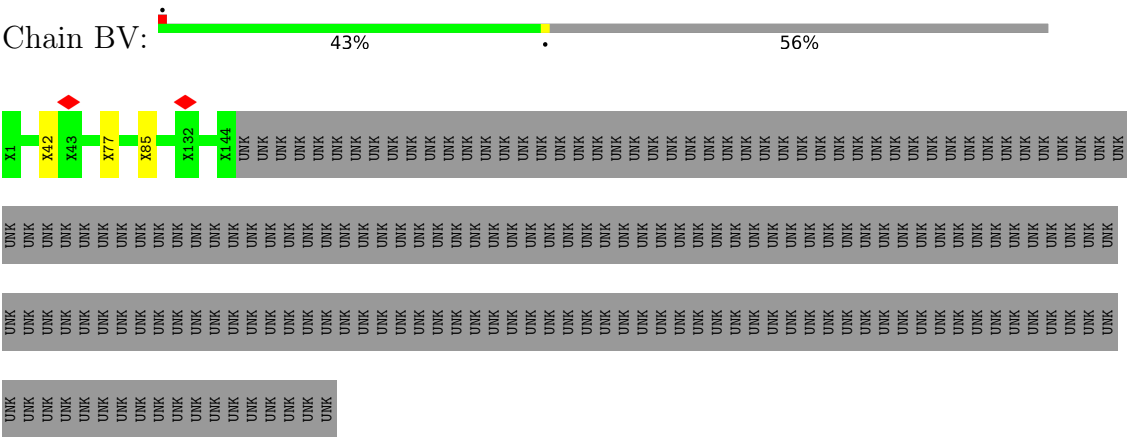
- Molecule 1: Type IV secretion system unknown protein fragment



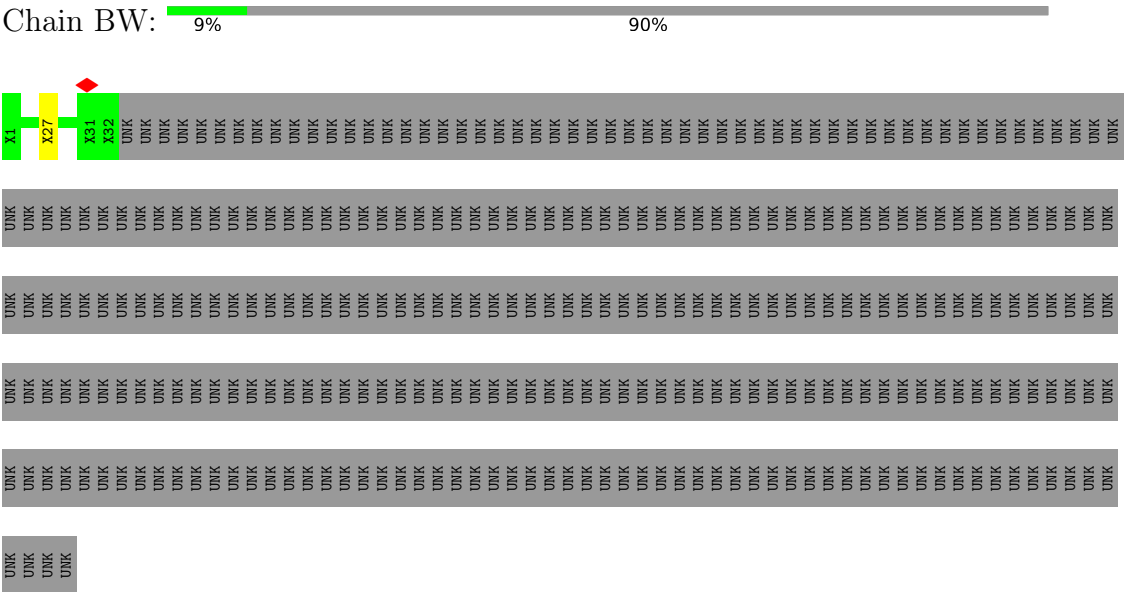
- Molecule 1: Type IV secretion system unknown protein fragment



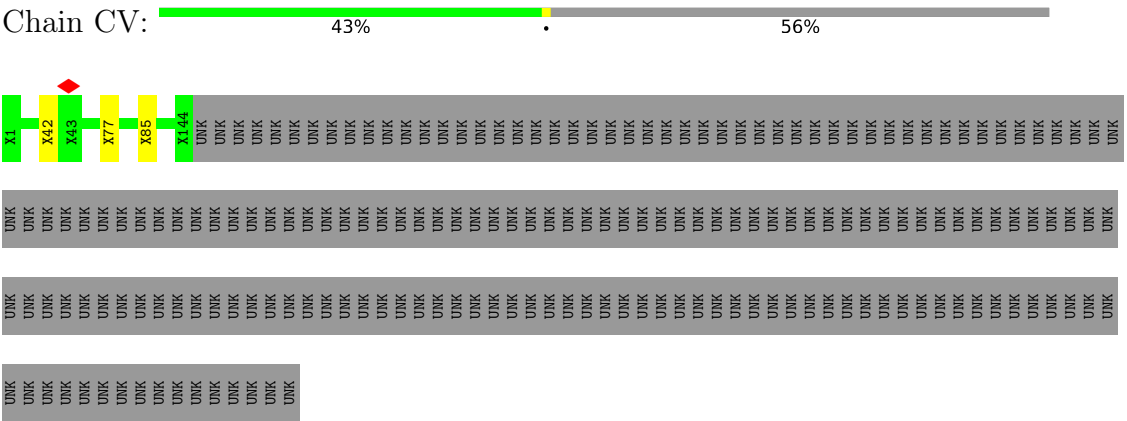
- Molecule 1: Type IV secretion system unknown protein fragment



• Molecule 1: Type IV secretion system unknown protein fragment

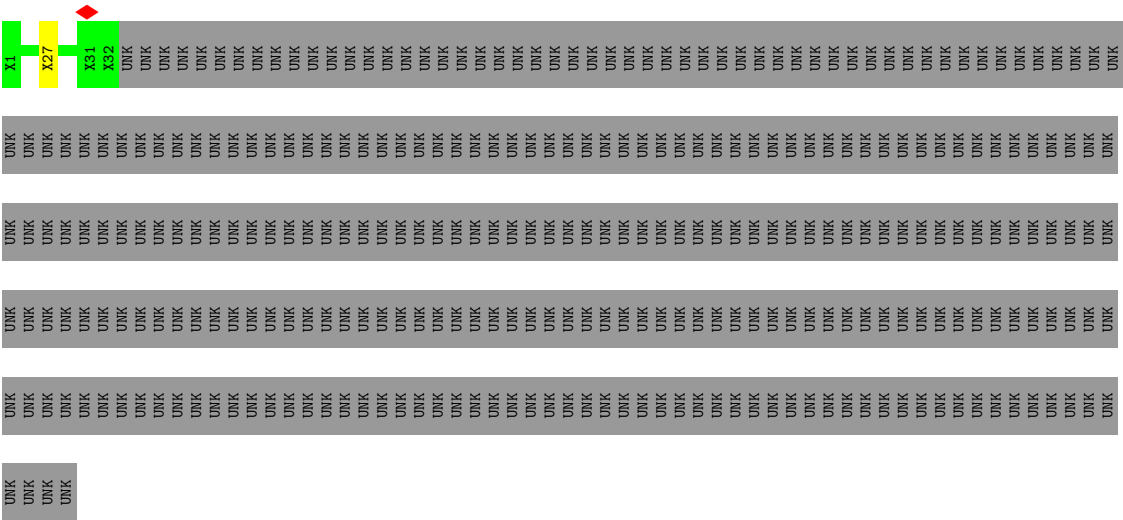


• Molecule 1: Type IV secretion system unknown protein fragment



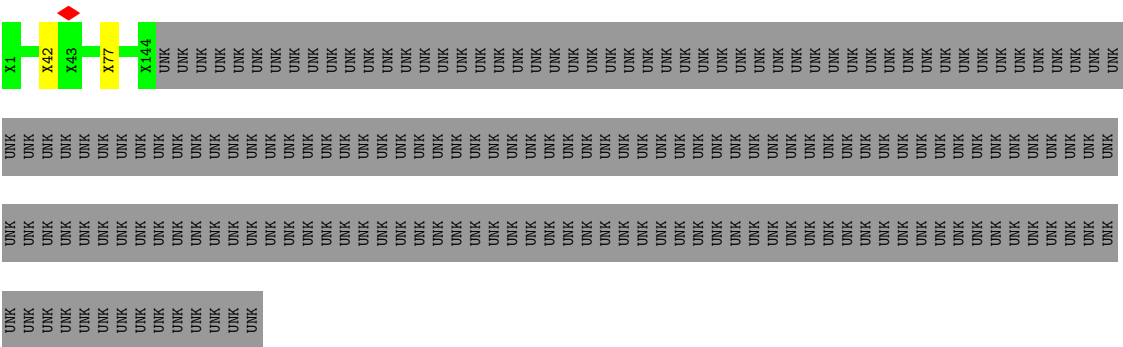
• Molecule 1: Type IV secretion system unknown protein fragment

Chain CW: 9% 90%



- Molecule 1: Type IV secretion system unknown protein fragment

Chain DV: 43% 56%



- Molecule 1: Type IV secretion system unknown protein fragment

Chain DW: 10% 90%

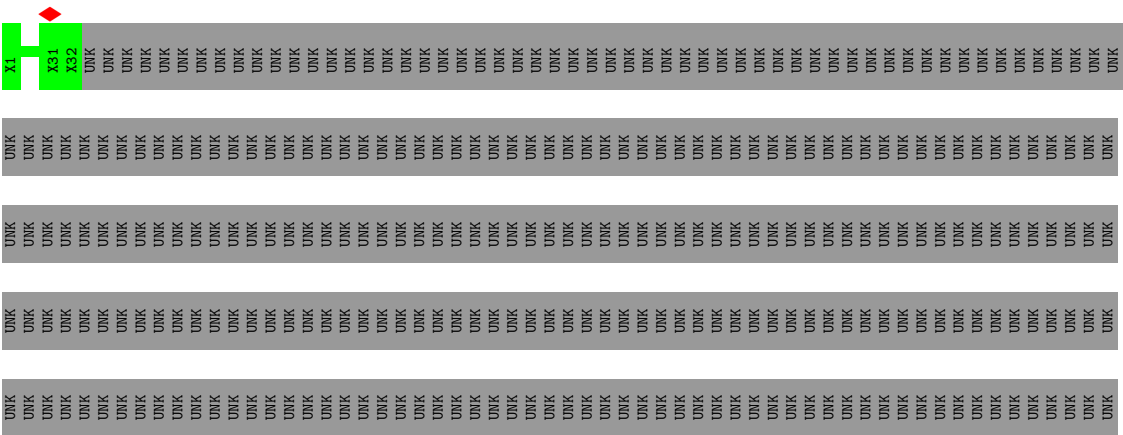
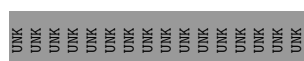


Diagram illustrating a 1D CNN layer with kernel size 3 and stride 2. The input is a 1x16 grid of gray cells. The output is a 1x8 grid of colored cells, where the first five cells are labeled x_1 , x_{42} , x_{43} , x_{77} , and x_{144} , and the remaining three cells are labeled UNK. A red diamond is positioned above the third cell (x_{43}), and a yellow diamond is positioned above the fourth cell (x_{77}). Arrows indicate the sliding window for each output cell: x_1 uses cells 1-3; x_{42} uses cells 4-6; x_{43} uses cells 5-7; x_{77} uses cells 8-10; x_{144} uses cells 11-13; and the remaining UNK cells use cells 14-16 in groups of three.

[illegible]

UNK	UNK	UNK	UNK
-----	-----	-----	-----

- Chain HV:  43% . 56%



- Chain HW:  9% 90%



- Chain IV: 42% 56%



[illegible]

- Chain IW:

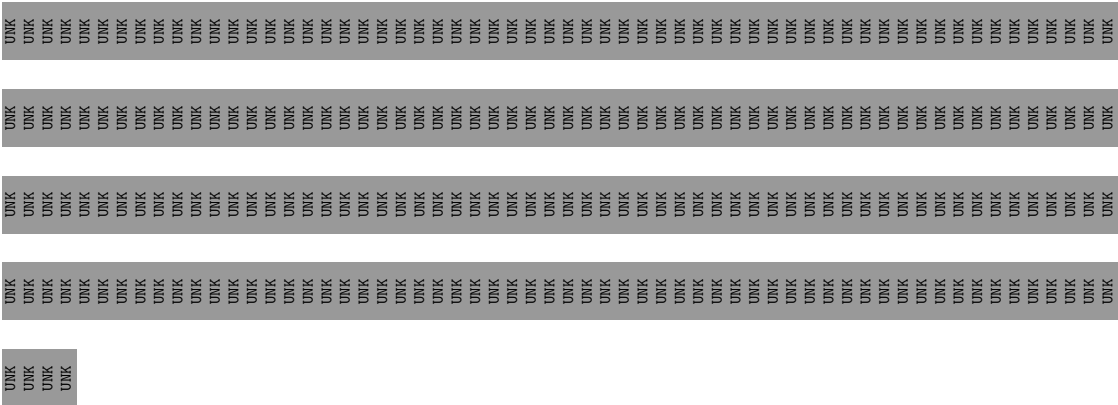
UNK
UNK
UNK
UNK

- Chain JV:  43% 56%

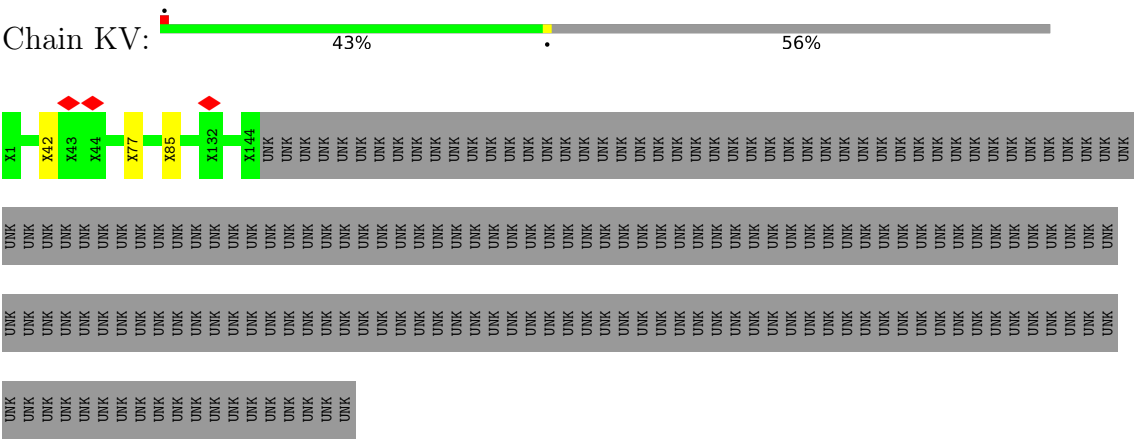
UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK

- Chain JW:

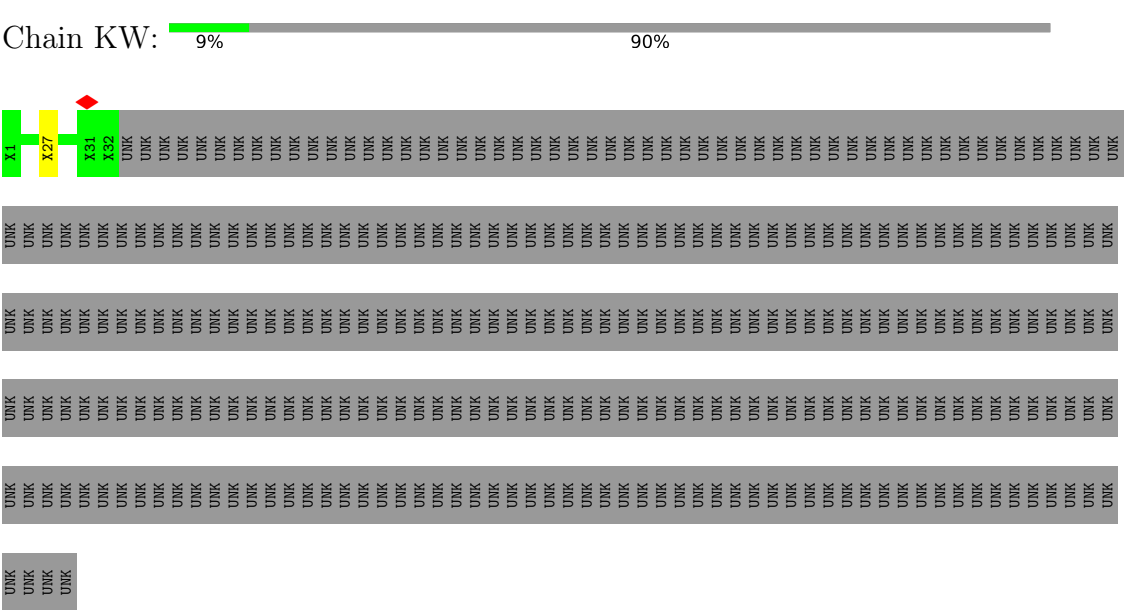
[illegible]



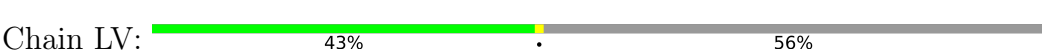
● Molecule 1: Type IV secretion system unknown protein fragment

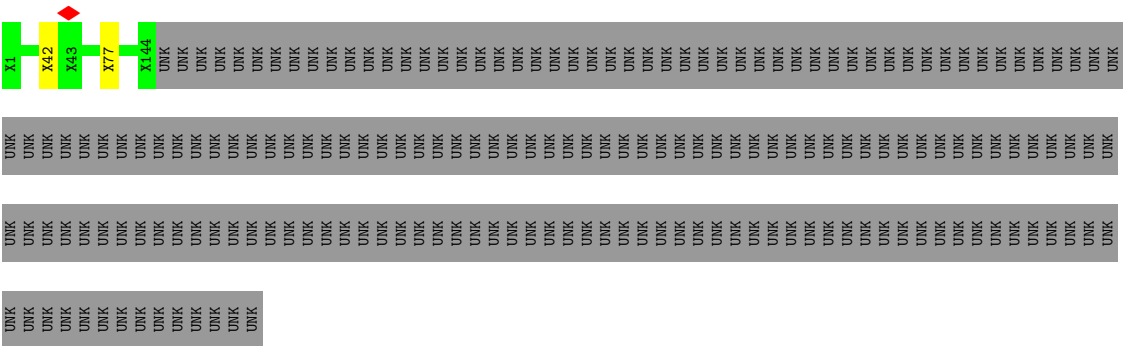


● Molecule 1: Type IV secretion system unknown protein fragment

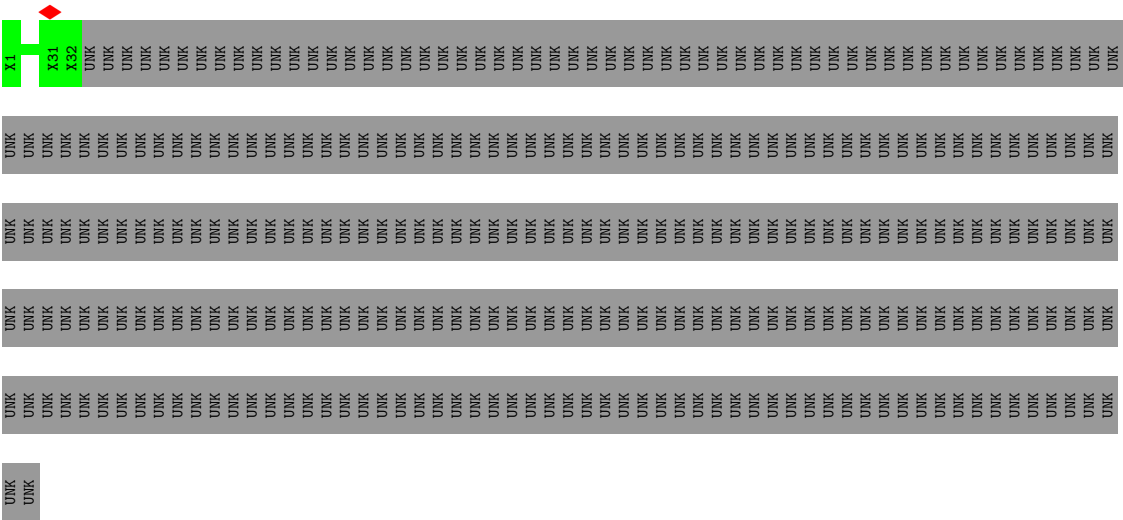


● Molecule 1: Type IV secretion system unknown protein fragment

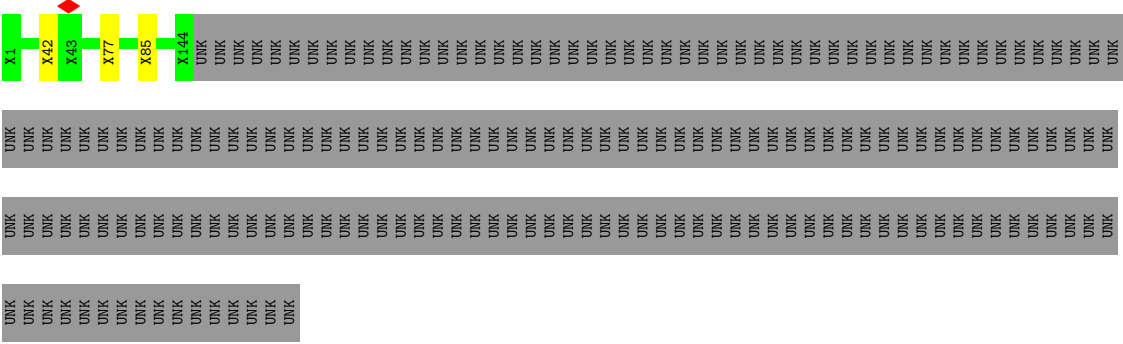




● Molecule 1: Type IV secretion system unknown protein fragment

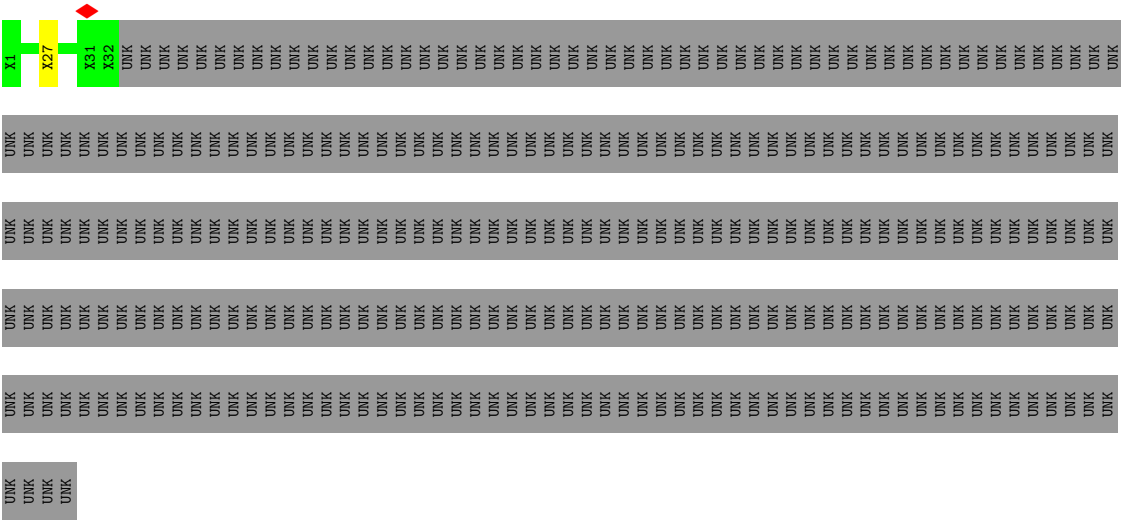


● Molecule 1: Type IV secretion system unknown protein fragment



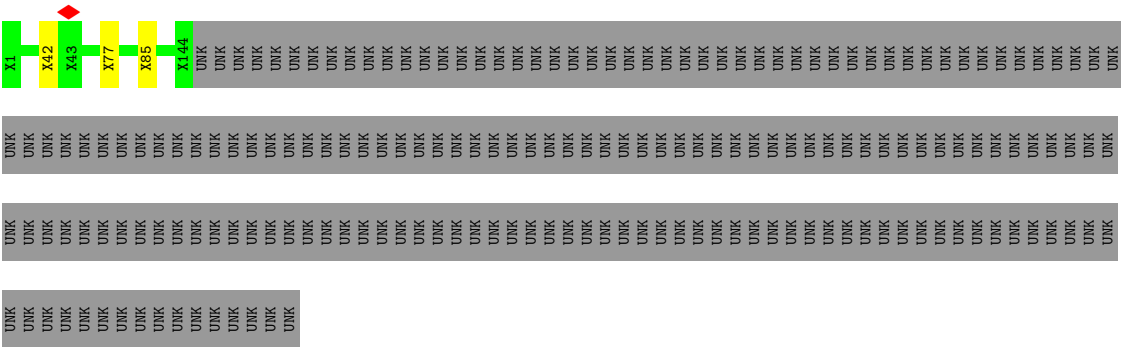
● Molecule 1: Type IV secretion system unknown protein fragment





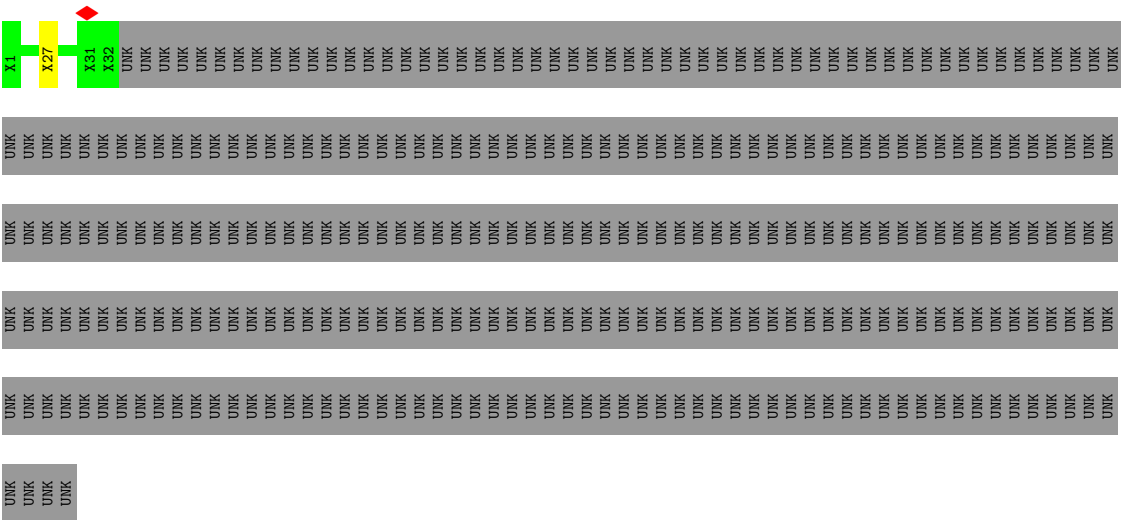
● Molecule 1: Type IV secretion system unknown protein fragment

Chain NV: 43% 56%

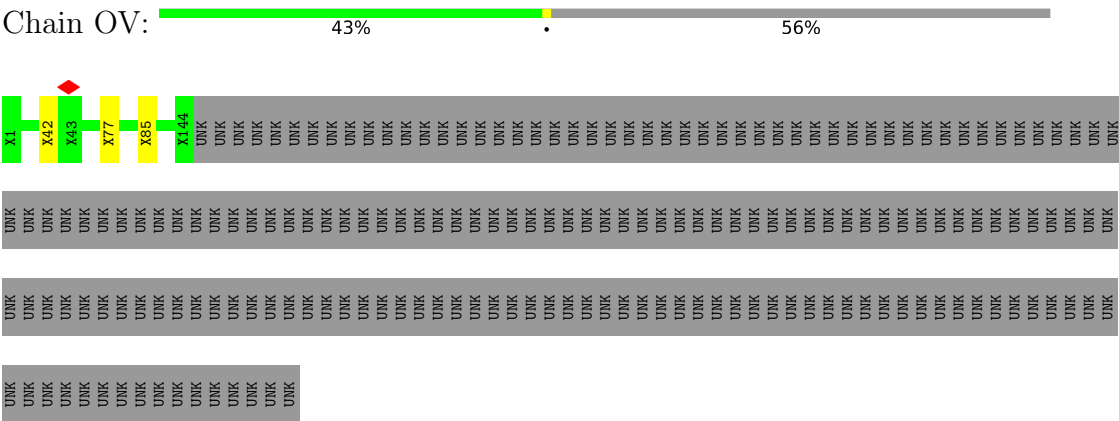


● Molecule 1: Type IV secretion system unknown protein fragment

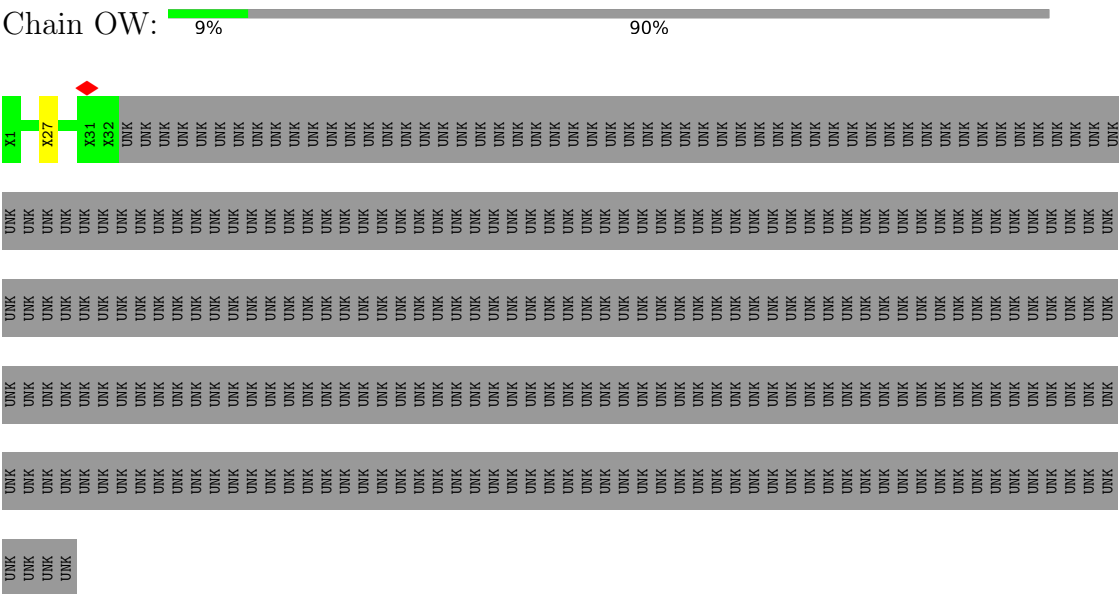
Chain NW: 9% 90%



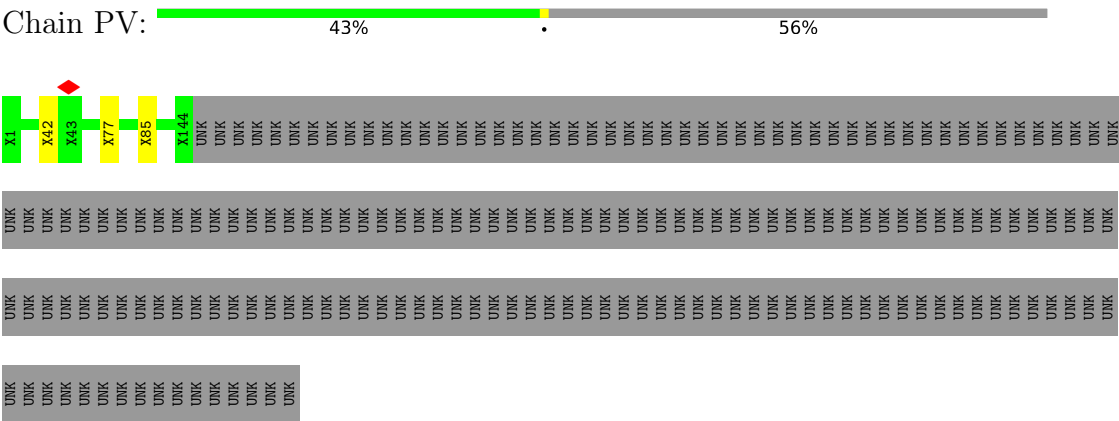
• Molecule 1: Type IV secretion system unknown protein fragment



• Molecule 1: Type IV secretion system unknown protein fragment

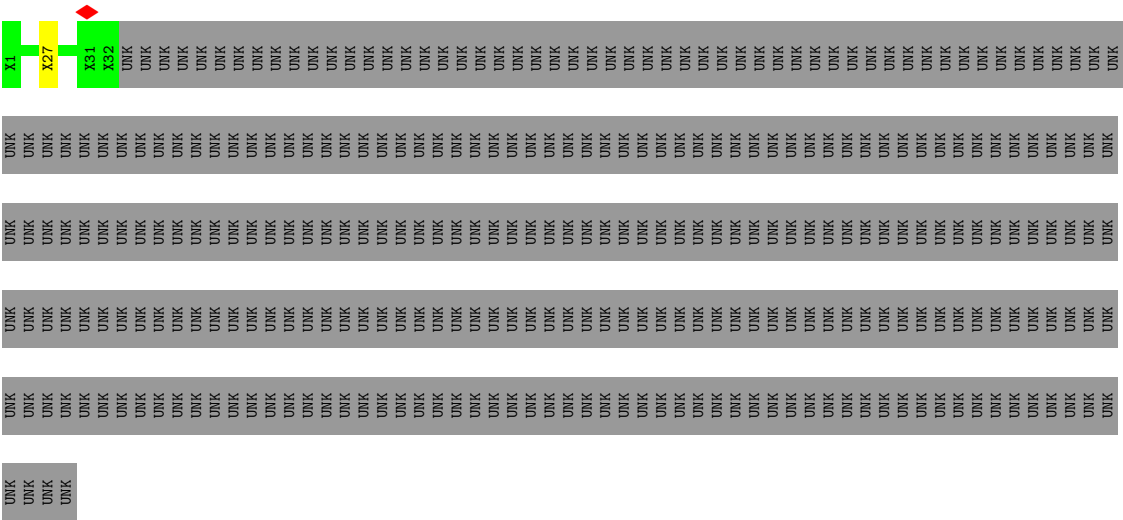


• Molecule 1: Type IV secretion system unknown protein fragment



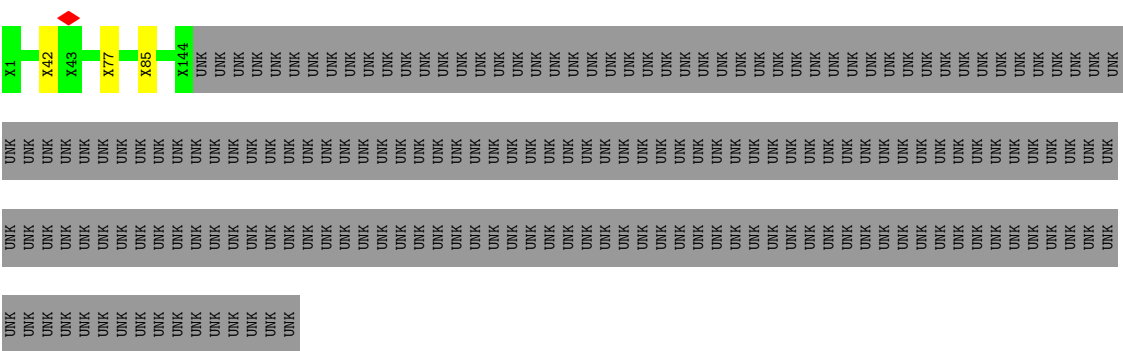
• Molecule 1: Type IV secretion system unknown protein fragment

Chain PW: 9% 90%



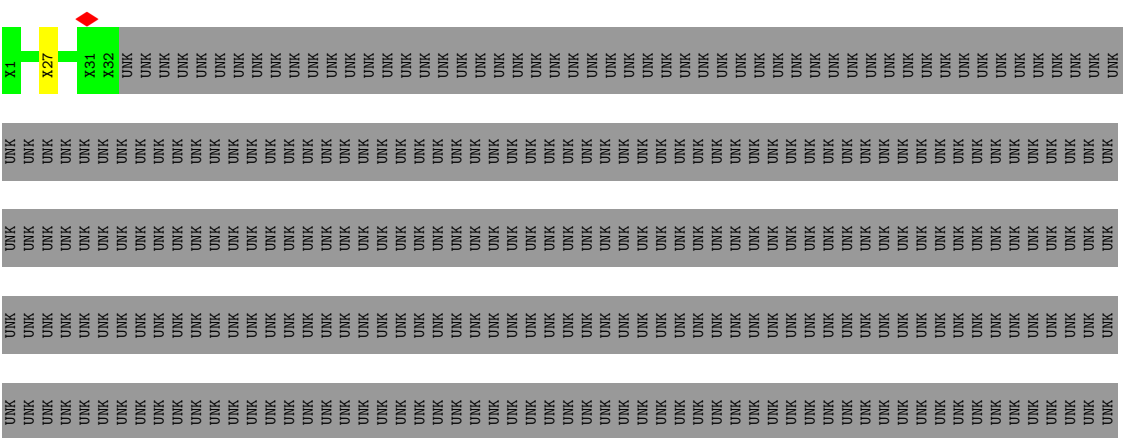
● Molecule 1: Type IV secretion system unknown protein fragment

Chain QV: 43% 56%



● Molecule 1: Type IV secretion system unknown protein fragment

Chain QW: 9% 90%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C18	Depositor
Number of particles used	6850	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 ($e^-/\text{\AA}^2$)	58.1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.084	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	836.39996, 836.39996, 836.39996	wwPDB
Map dimensions	510, 510, 510	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.64, 1.64, 1.64	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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AV	0	2
1	BV	0	2
1	CV	0	2
1	DV	0	2
1	EV	0	2
1	FV	0	2
1	GV	0	2
1	HV	0	2
1	IV	0	2
1	JV	0	2
1	KV	0	2
1	LV	0	2
1	MV	0	2
1	NV	0	2
1	OV	0	2
1	PV	0	2
1	QV	0	2
1	RV	0	2
All	All	0	36

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AV	42	UNK	Peptide
1	AV	77	UNK	Peptide
1	BV	42	UNK	Peptide
1	BV	77	UNK	Peptide
1	CV	42	UNK	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	AV	720	0	160	1	0
1	AW	160	0	35	1	0
1	BV	720	0	160	1	0
1	BW	160	0	35	1	0
1	CV	720	0	160	1	0
1	CW	160	0	35	1	0
1	DV	720	0	160	0	0
1	DW	160	0	35	0	0
1	EV	720	0	160	1	0
1	EW	160	0	35	1	0
1	FV	720	0	160	0	0
1	FW	160	0	35	0	0
1	GV	720	0	160	2	0
1	GW	160	0	35	1	0
1	HV	720	0	160	1	0
1	HW	160	0	35	1	0
1	IV	720	0	160	2	0
1	IW	160	0	35	1	0
1	JV	720	0	160	1	0
1	JW	160	0	35	1	0
1	KV	720	0	160	1	0
1	KW	160	0	35	1	0
1	LV	720	0	160	0	0
1	LW	160	0	35	0	0
1	MV	720	0	160	1	0
1	MW	160	0	35	1	0
1	NV	720	0	160	1	0
1	NW	160	0	35	1	0
1	OV	720	0	160	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	OW	160	0	35	1	0
1	PV	720	0	160	1	0
1	PW	160	0	35	1	0
1	QV	720	0	160	1	0
1	QW	160	0	35	1	0
1	RV	720	0	160	0	0
1	RW	160	0	35	0	0
All	All	15840	0	3510	16	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 16 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:PV:85:UNK:HA	1:PW:27:UNK:O	2.06	0.55
1:IV:85:UNK:HA	1:IW:27:UNK:O	2.07	0.54
1:JV:85:UNK:HA	1:JW:27:UNK:O	2.14	0.48
1:MV:85:UNK:HA	1:MW:27:UNK:O	2.14	0.47
1:AV:85:UNK:HA	1:AW:27:UNK:O	2.15	0.46

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

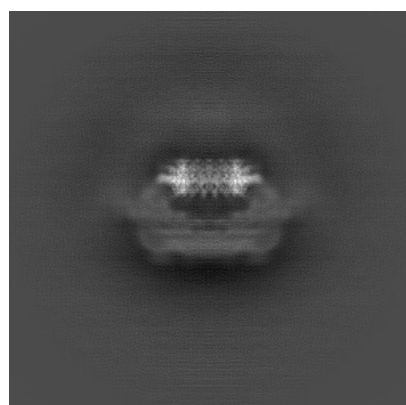
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22069. These allow visual inspection of the internal detail of the map and identification of artifacts.

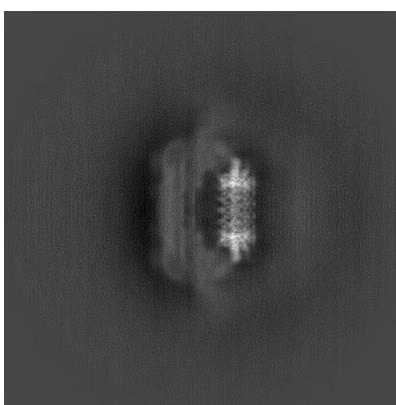
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

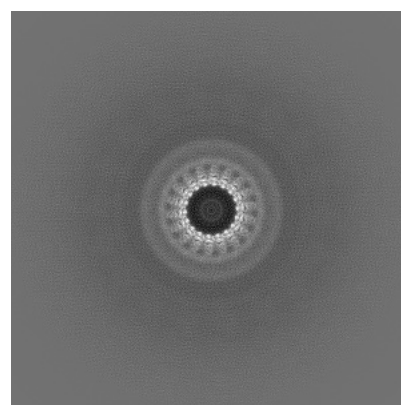
6.1.1 Primary map



X



Y



Z

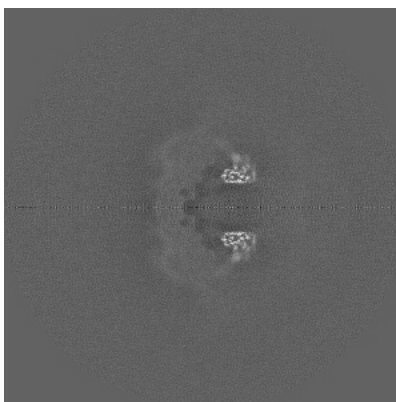
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

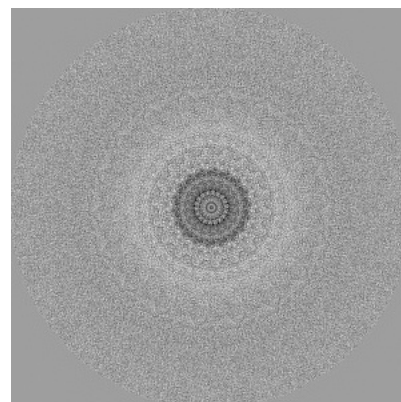
6.2.1 Primary map



X Index: 255



Y Index: 255

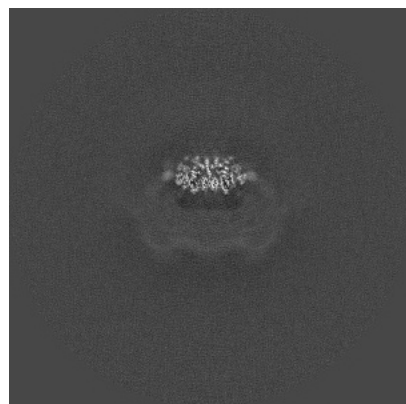


Z Index: 255

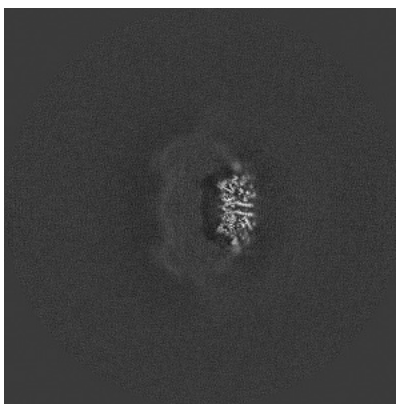
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

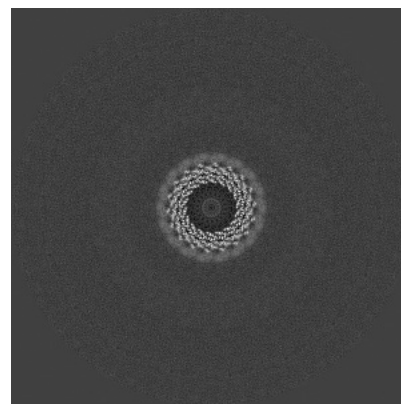
6.3.1 Primary map



X Index: 221



Y Index: 288

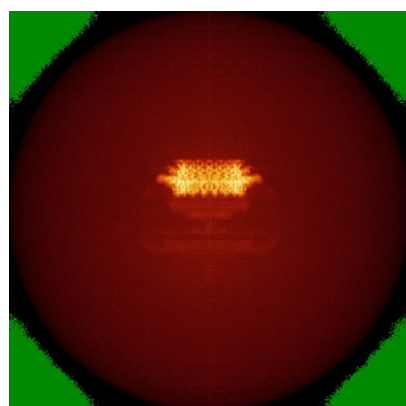


Z Index: 292

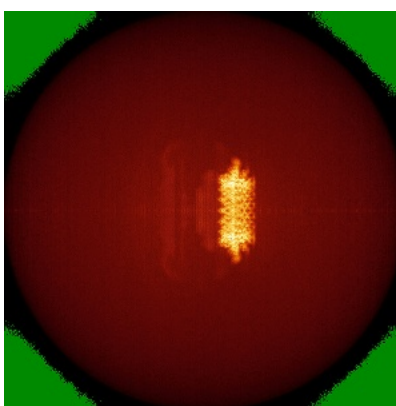
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

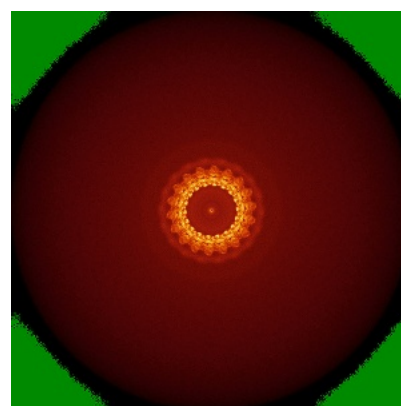
6.4.1 Primary map



X



Y

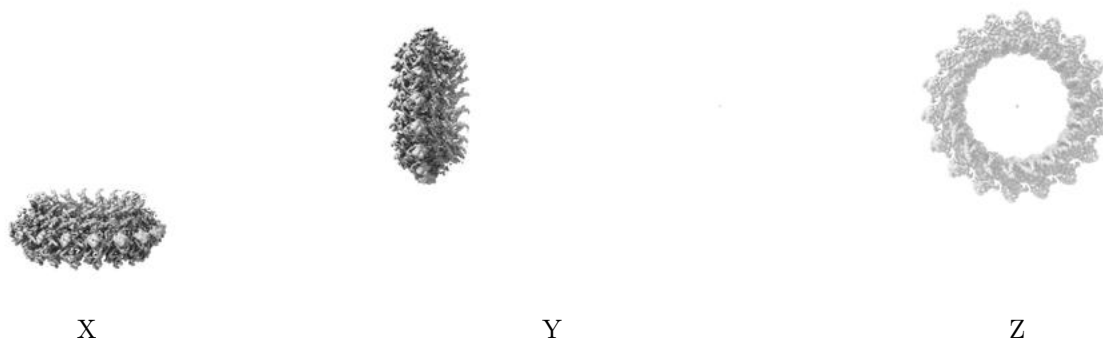


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

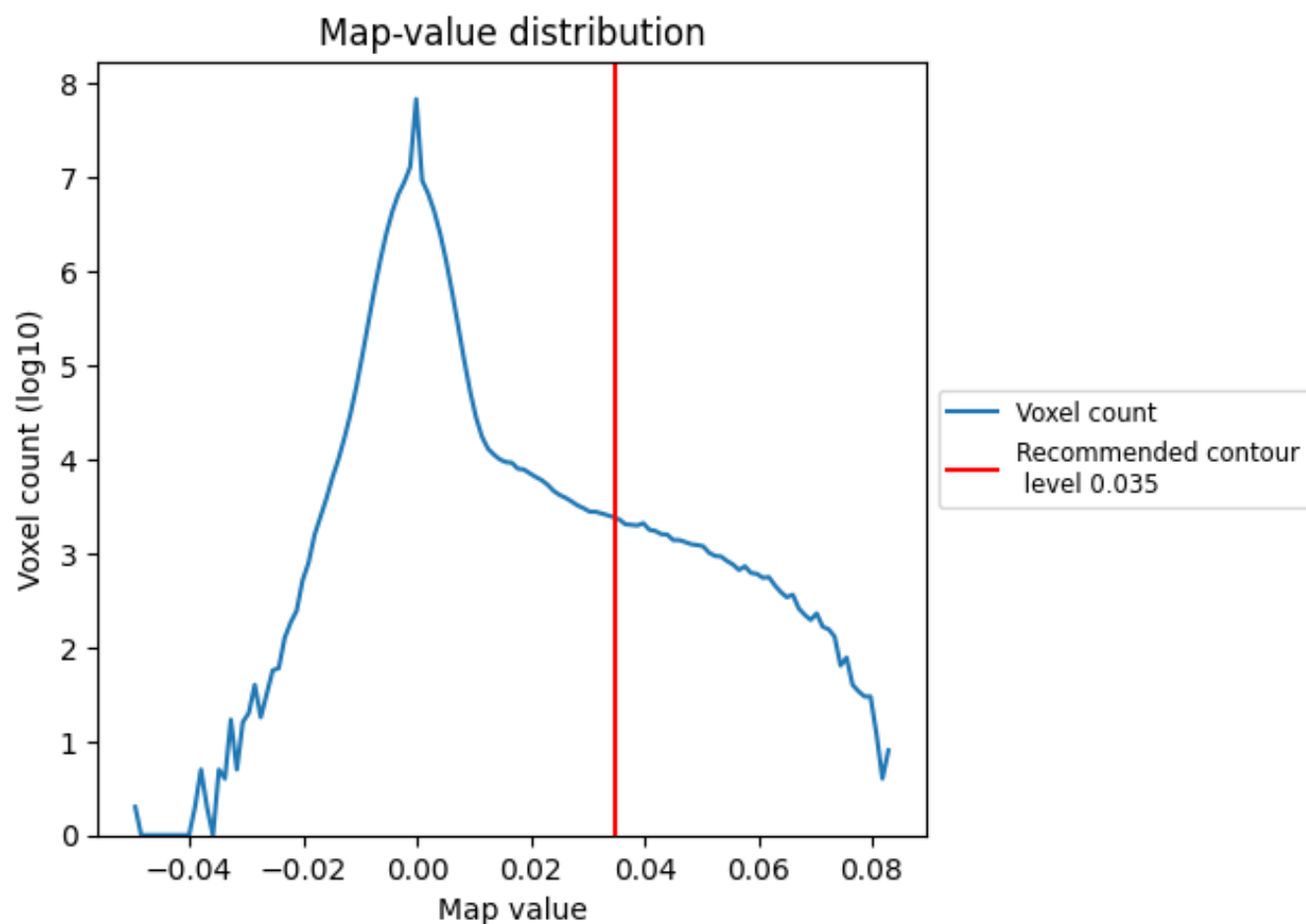
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

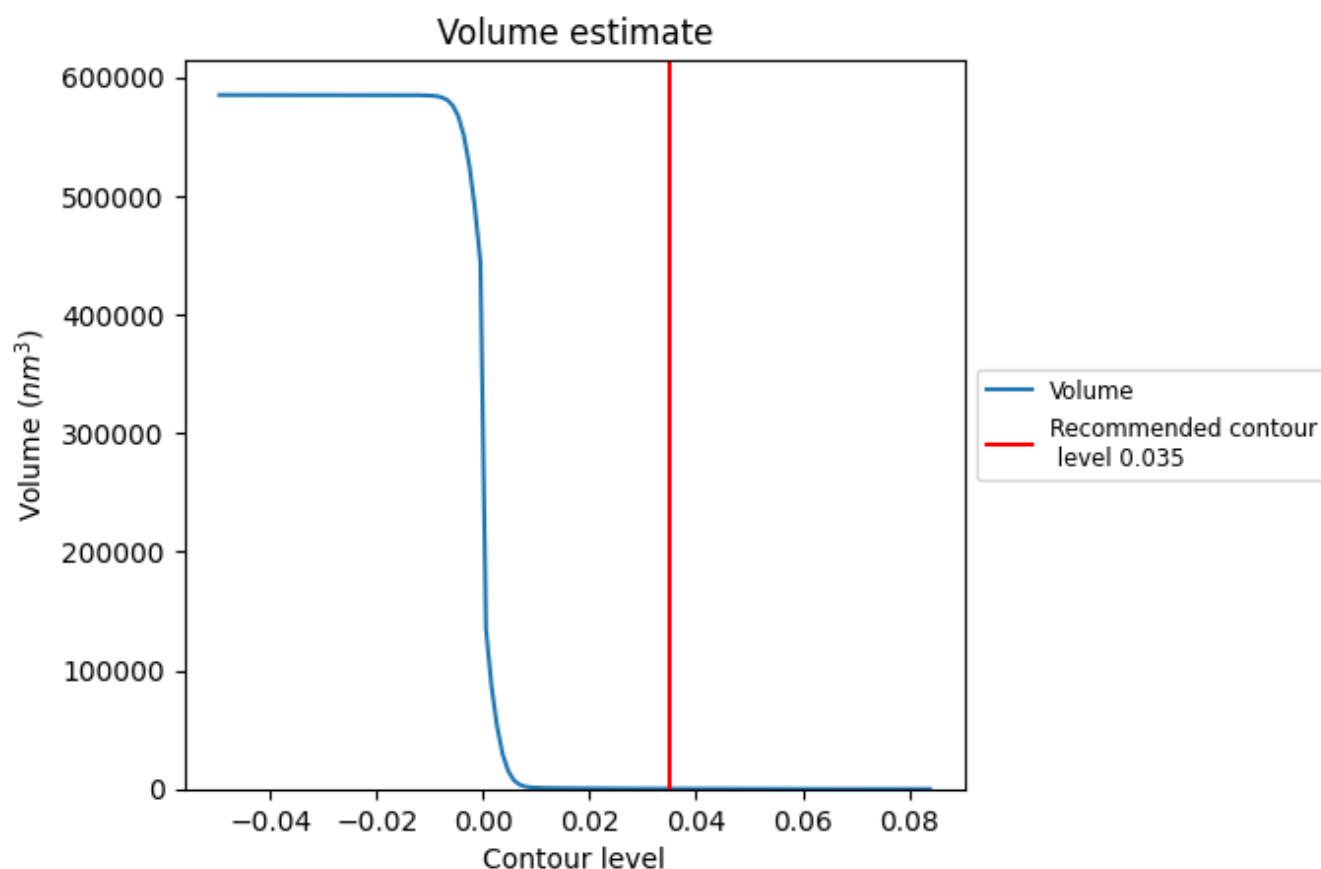
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

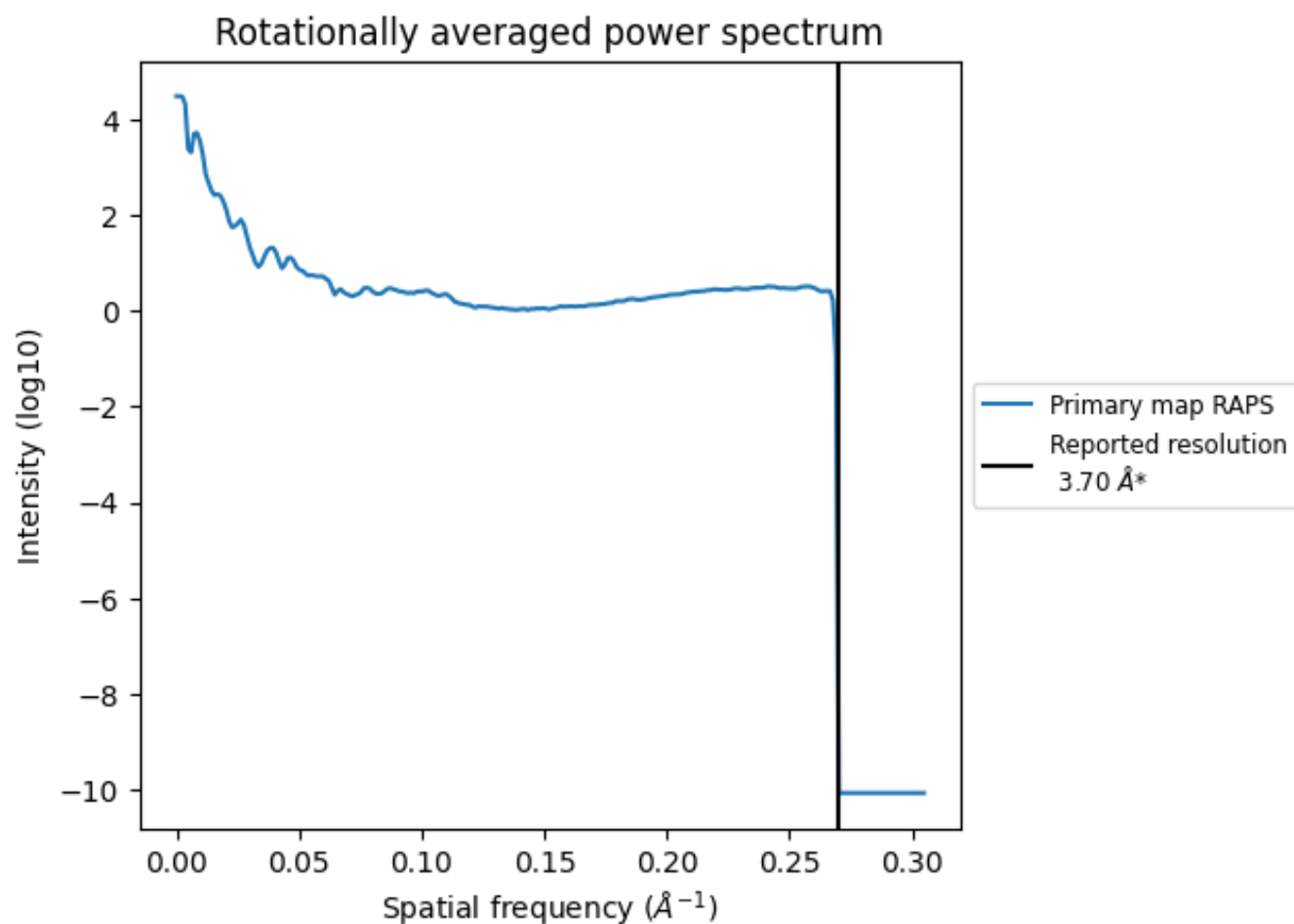
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 167 nm³; this corresponds to an approximate mass of 151 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 ⓘ

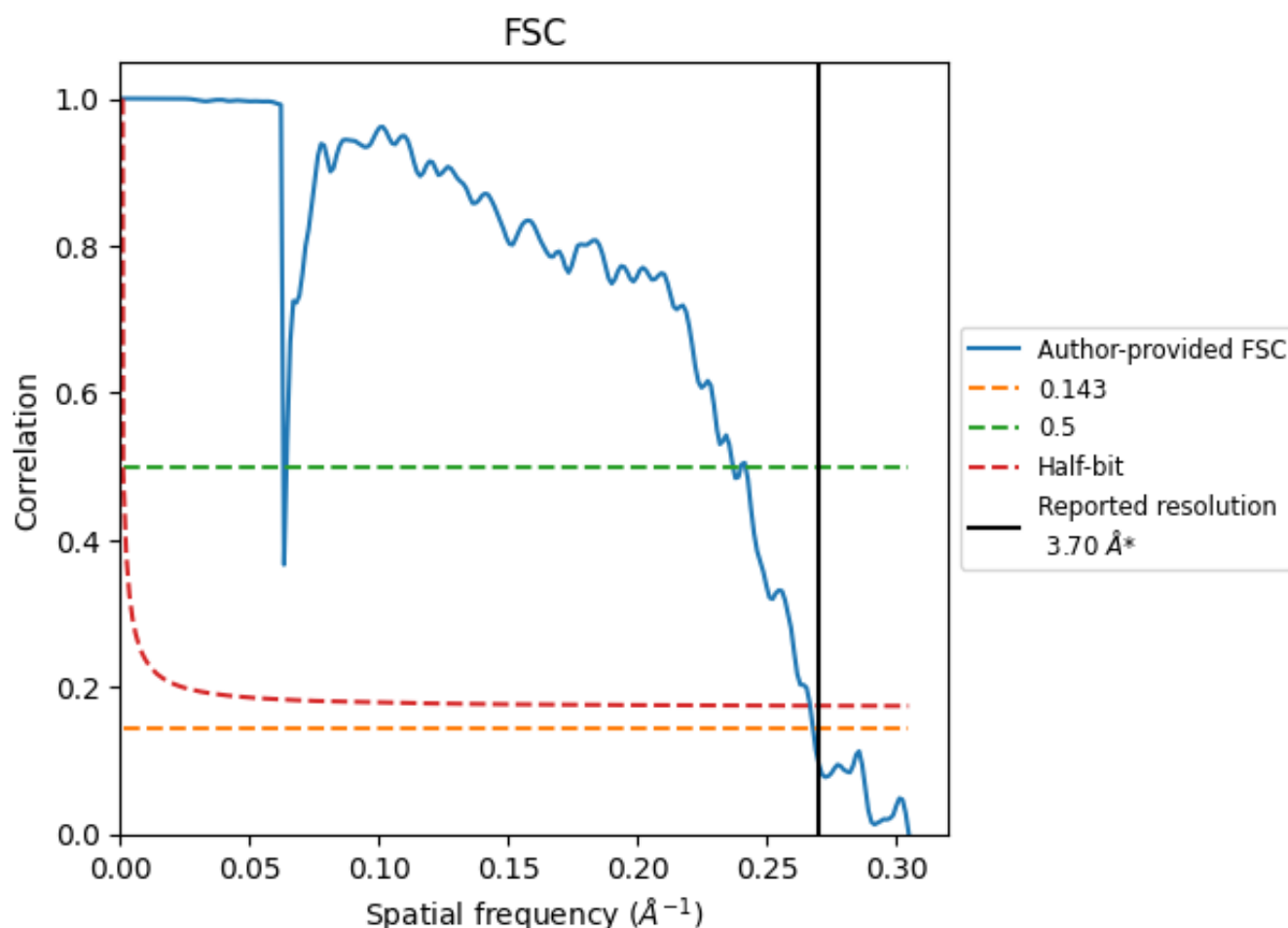


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation [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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

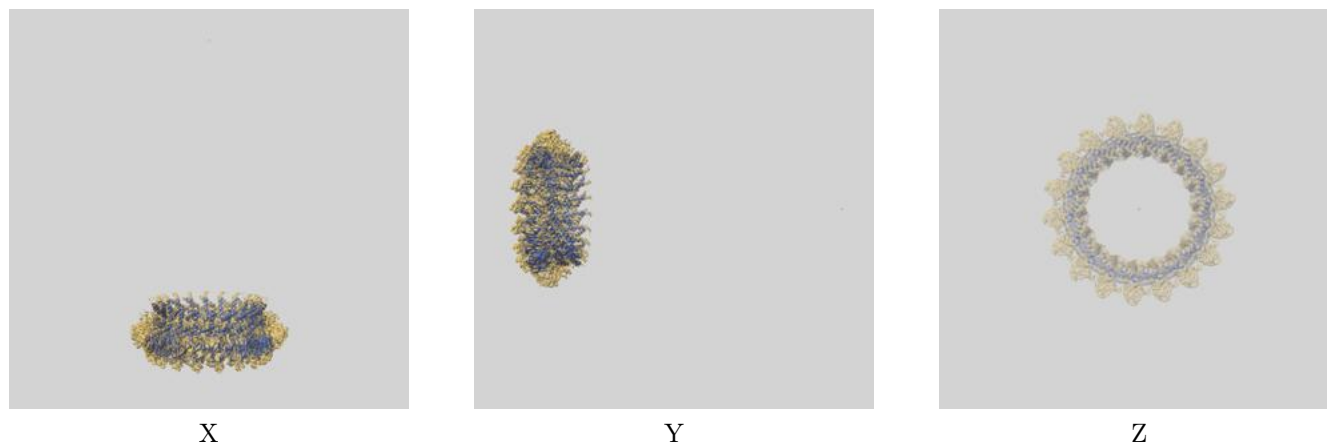
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.73	15.85	3.75
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

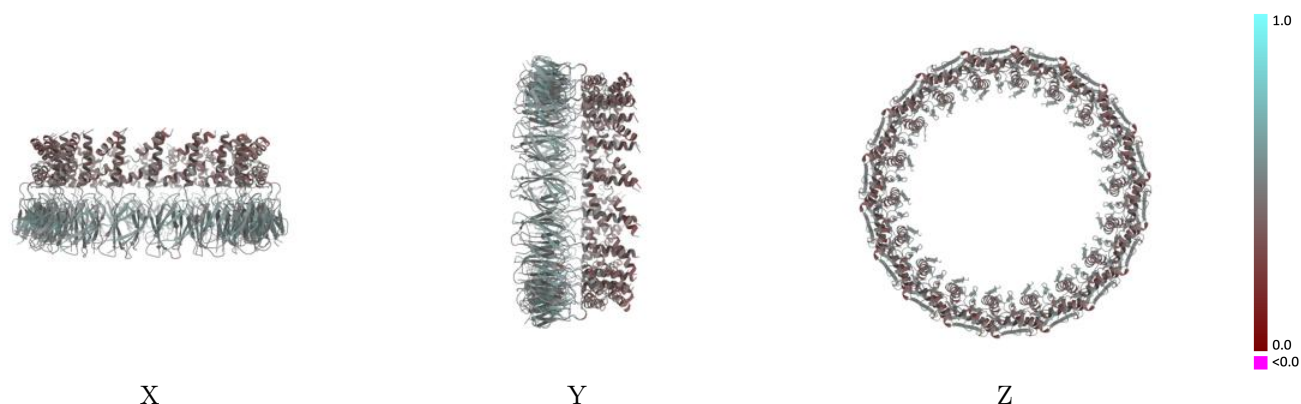
This section contains information regarding the fit between EMDB map EMD-22069 and PDB model 6X64. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



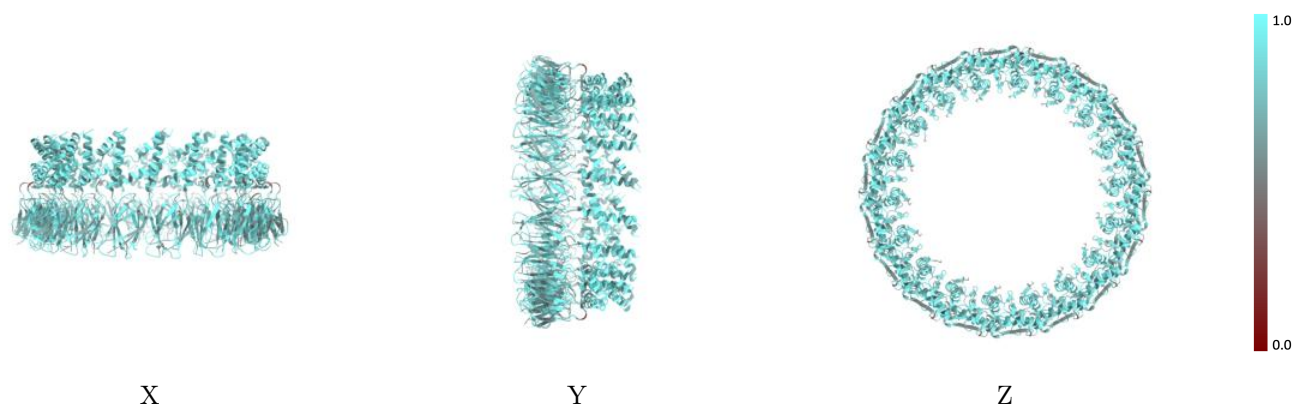
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



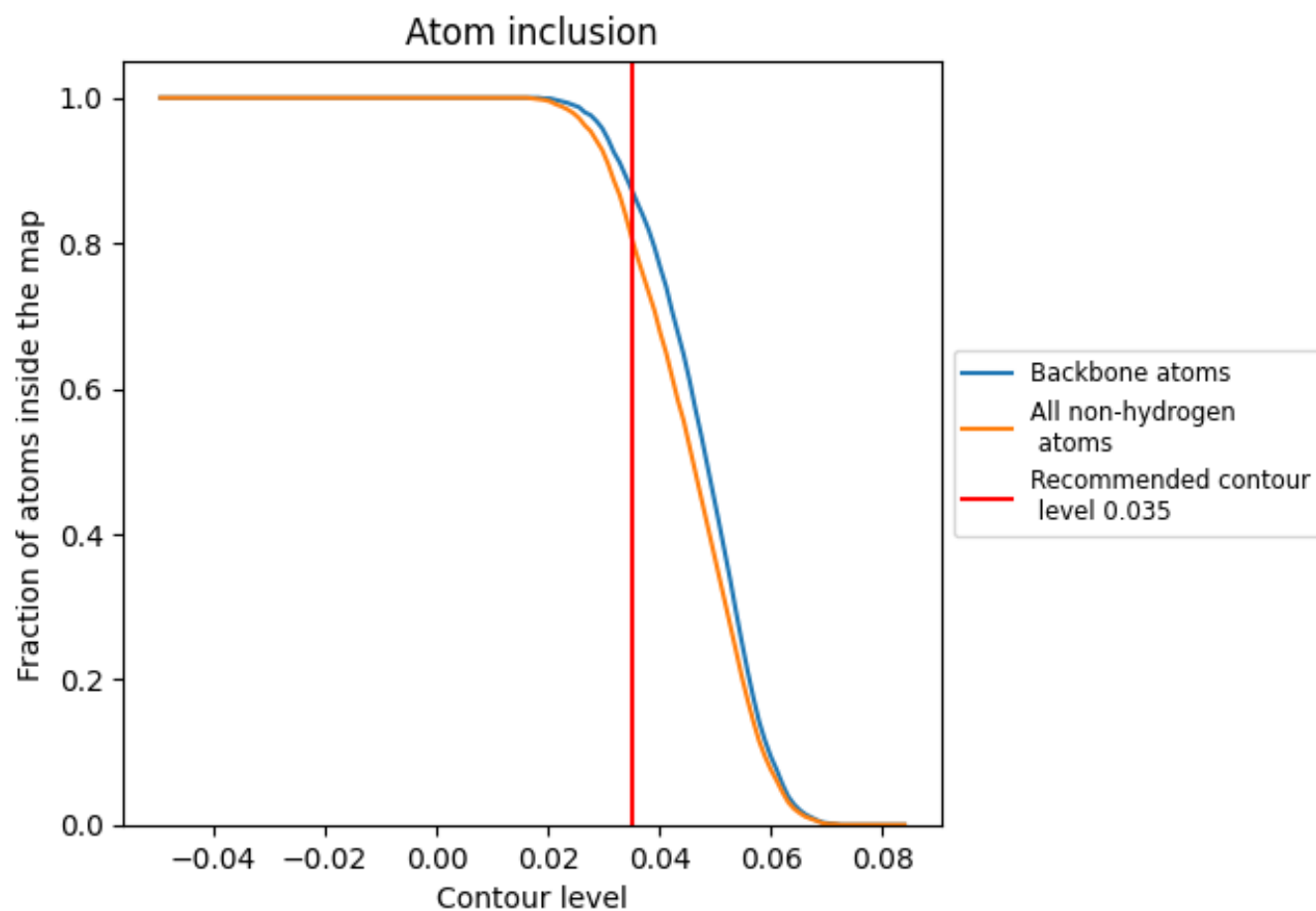
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 81% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8080	 0.4760
AV	 0.8060	 0.4880
AW	 0.8440	 0.4430
BV	 0.8010	 0.4850
BW	 0.8190	 0.4460
CV	 0.8060	 0.4860
CW	 0.8310	 0.4500
DV	 0.8070	 0.4820
DW	 0.8190	 0.4460
EV	 0.8070	 0.4860
EW	 0.8310	 0.4450
FV	 0.8080	 0.4830
FW	 0.8440	 0.4450
GV	 0.8040	 0.4830
GW	 0.8310	 0.4360
HV	 0.8000	 0.4840
HW	 0.8250	 0.4420
IV	 0.8010	 0.4810
IW	 0.8250	 0.4420
JV	 0.8060	 0.4880
JW	 0.8500	 0.4380
KV	 0.8030	 0.4830
KW	 0.8060	 0.4390
LV	 0.8060	 0.4860
LW	 0.8250	 0.4390
MV	 0.8070	 0.4860
MW	 0.8310	 0.4430
NV	 0.8070	 0.4810
NW	 0.8120	 0.4410
OV	 0.8040	 0.4810
OW	 0.8190	 0.4460
PV	 0.8040	 0.4830
PW	 0.8310	 0.4400
QV	 0.7990	 0.4830
QW	 0.8310	 0.4460



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Chain	Atom inclusion	Q-score
RV	 0.7970	 0.4820
RW	 0.8380	 0.4540