



wwPDB EM Validation Summary Report ⓘ

Apr 21, 2025 – 02:30 PM JST

PDB ID : 8X9W / pdb_00008x9w
EMDB ID : EMD-38186
Title : portal vertex capsomer of the VZV C-Capsid
Authors : Nan, W.; Lei, C.; Jiangxi, W.
Deposited on : 2023-12-01
Resolution : 4.50 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.dev117
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) : 2.42

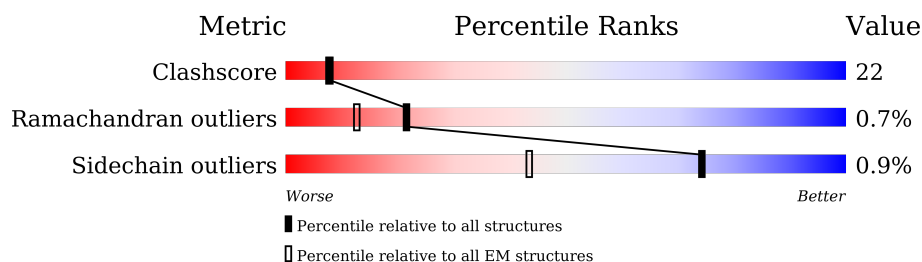
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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 $\leq 5\%$. 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	1387	<div> <div>5%</div> <div>57%</div> <div>40%</div> <div>.</div> </div>
1	C	1387	<div> <div>9%</div> <div>50%</div> <div>41%</div> <div>.</div> <div>7%</div> </div>
2	B	87	<div> <div>.</div> <div>98%</div> <div>.</div> </div>
2	H	87	<div> <div>6%</div> <div>98%</div> <div>.</div> </div>
2	I	87	<div> <div>5%</div> <div>98%</div> <div>.</div> </div>
2	J	87	<div> <div>.</div> <div>98%</div> <div>.</div> </div>
2	K	87	<div> <div>17%</div> <div>74%</div> <div>14%</div> <div>13%</div> </div>
2	L	87	<div> <div>17%</div> <div>76%</div> <div>11%</div> <div>13%</div> </div>

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Mol	Chain	Length	Quality of chain
2	Q	87	
2	R	87	
2	S	87	
2	T	87	
3	F	297	
4	O	307	
5	X	289	
6	k	550	
7	l	94	
7	m	94	
8	n	47	
8	o	47	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 37344 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 Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1347	Total	C	N	O	S	0	0
			10392	6579	1822	1927	64		
1	C	1287	Total	C	N	O	S	0	0
			9888	6258	1737	1829	64		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	ALA	-	expression tag	UNP P09245
A	9	ALA	-	expression tag	UNP P09245
A	10	ALA	-	expression tag	UNP P09245
A	11	ALA	-	expression tag	UNP P09245
A	12	ALA	-	expression tag	UNP P09245
A	13	ALA	-	expression tag	UNP P09245
A	22	ILE	LEU	conflict	UNP P09245
A	327	ASN	GLN	conflict	UNP P09245
A	329	ALA	THR	conflict	UNP P09245
A	343	SER	GLY	conflict	UNP P09245
A	344	LEU	MET	conflict	UNP P09245
A	348	GLY	ALA	conflict	UNP P09245
A	814	ALA	GLY	conflict	UNP P09245
C	8	ALA	-	expression tag	UNP P09245
C	9	ALA	-	expression tag	UNP P09245
C	10	ALA	-	expression tag	UNP P09245
C	11	ALA	-	expression tag	UNP P09245
C	12	ALA	-	expression tag	UNP P09245
C	13	ALA	-	expression tag	UNP P09245
C	22	ILE	LEU	conflict	UNP P09245
C	323	ASN	GLN	conflict	UNP P09245
C	325	ALA	THR	conflict	UNP P09245
C	339	SER	GLY	conflict	UNP P09245
C	340	LEU	MET	conflict	UNP P09245
C	344	GLY	ALA	conflict	UNP P09245
C	814	ALA	GLY	conflict	UNP P09245

- Molecule 2 is a protein called coiled-coil domain of portal.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	87	Total	C	N	O	0	0
			435	261	87	87		
2	H	87	Total	C	N	O	0	0
			435	261	87	87		
2	I	87	Total	C	N	O	0	0
			435	261	87	87		
2	J	87	Total	C	N	O	0	0
			435	261	87	87		
2	K	76	Total	C	N	O	0	0
			380	228	76	76		
2	L	76	Total	C	N	O	0	0
			380	228	76	76		
2	Q	76	Total	C	N	O	0	0
			380	228	76	76		
2	R	76	Total	C	N	O	0	0
			380	228	76	76		
2	S	76	Total	C	N	O	0	0
			380	228	76	76		
2	T	87	Total	C	N	O	0	0
			435	261	87	87		

- Molecule 3 is a protein called Tri2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	297	Total	C	N	O	S	0	0
			2124	1367	365	383	9		

- Molecule 4 is a protein called Tri2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	307	Total	C	N	O	S	0	0
			2279	1456	399	413	11		

- Molecule 5 is a protein called Tri1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	X	289	Total	C	N	O	S	0	0
			2198	1392	397	395	14		

- Molecule 6 is a protein called CVC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	k	550	Total	C	N	O	S	0	0
			4206	2674	764	747	21		

- Molecule 7 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	l	94	Total	C	N	O	S	0	0
			766	486	138	138	4		
7	m	80	Total	C	N	O	S	0	0
			648	410	121	115	2		

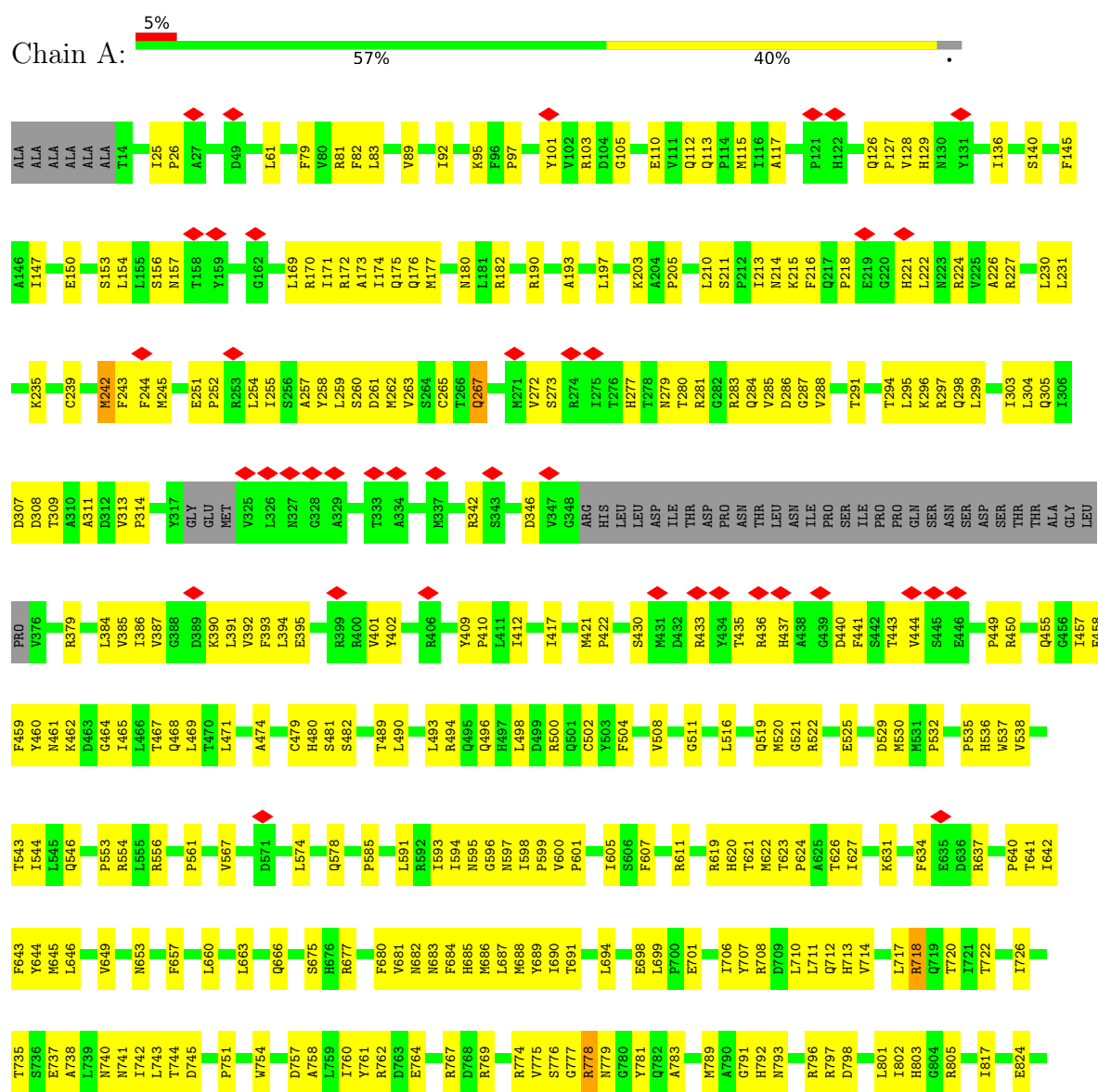
- Molecule 8 is a protein called Large tegument protein deneddylase.

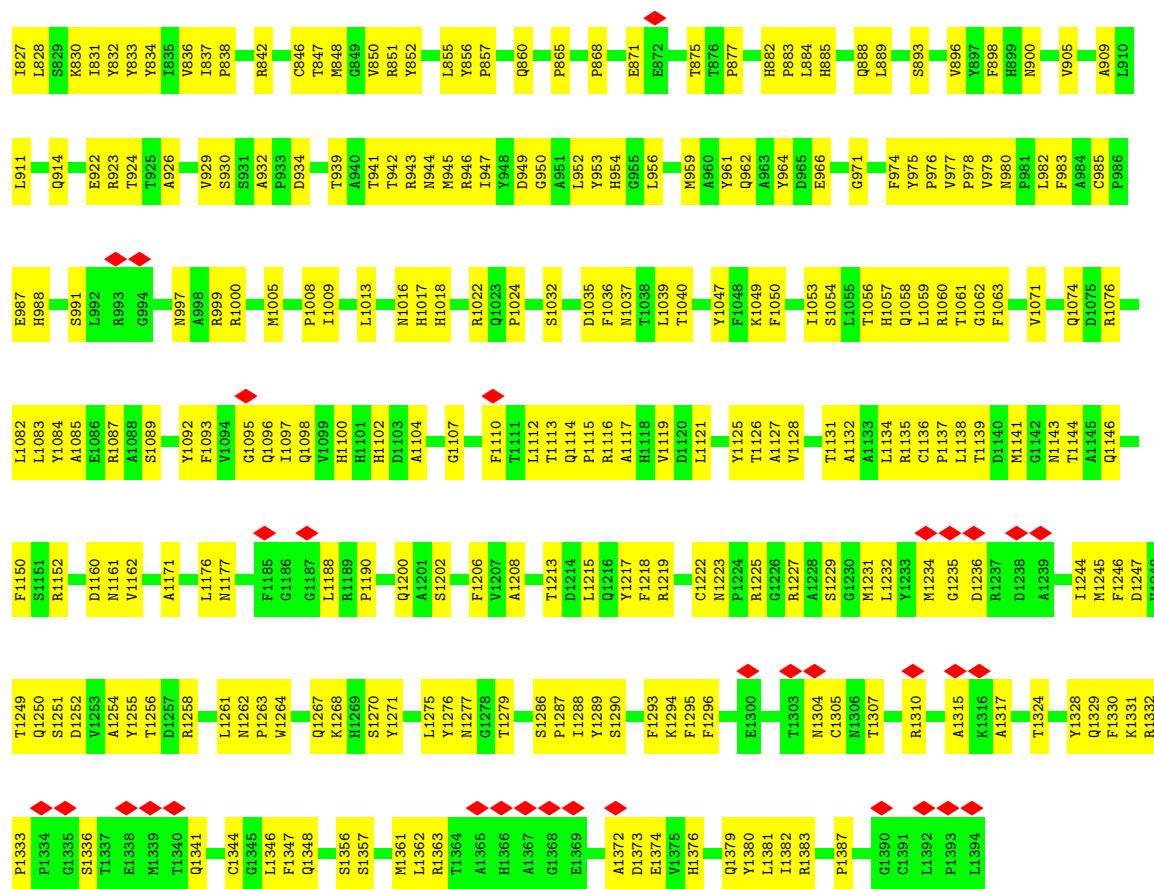
Mol	Chain	Residues	Atoms					AltConf	Trace
8	n	47	Total	C	N	O	S	0	0
			384	237	84	61	2		
8	o	47	Total	C	N	O	S	0	0
			384	237	84	61	2		

3 Residue-property plots

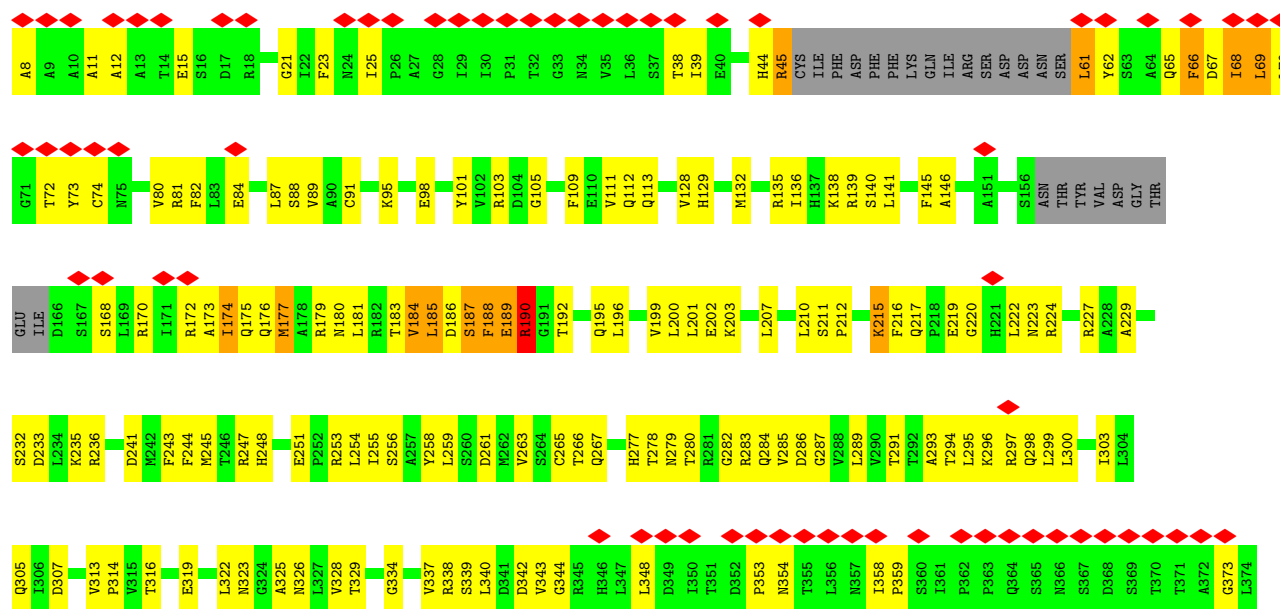
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

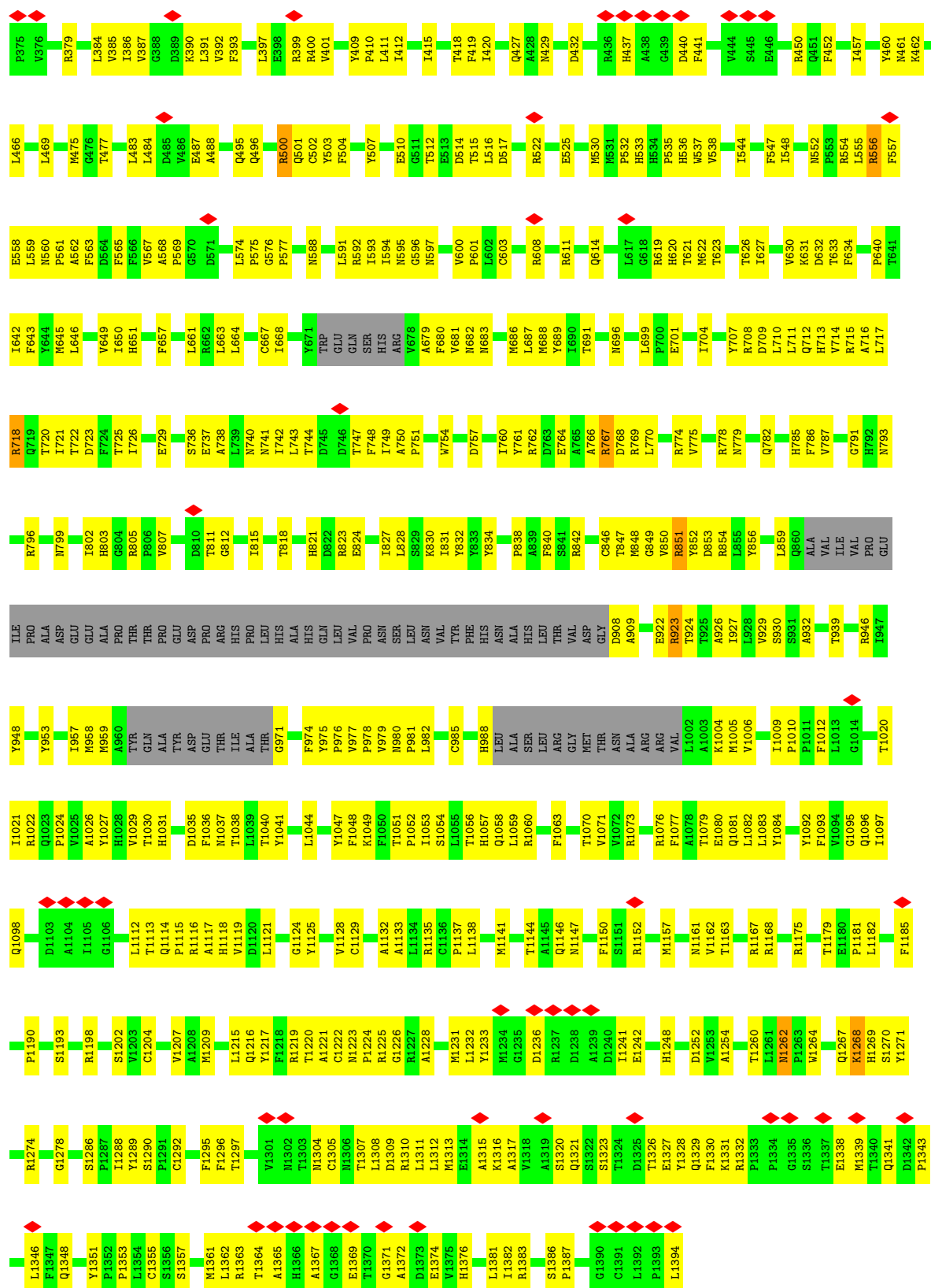
• Molecule 1: Major capsid protein





• Molecule 1: Major capsid protein

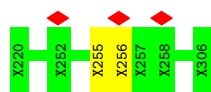




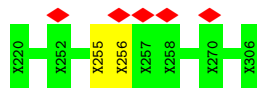
• Molecule 2: coiled-coil domain of portal

Chain B:

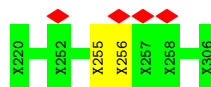
98%



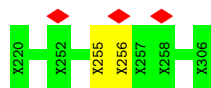
- Molecule 2: coiled-coil domain of portal



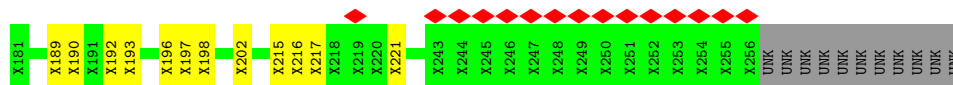
- Molecule 2: coiled-coil domain of portal



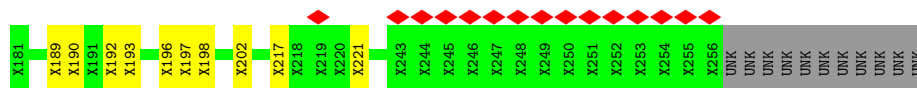
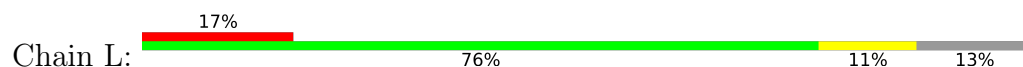
- Molecule 2: coiled-coil domain of portal



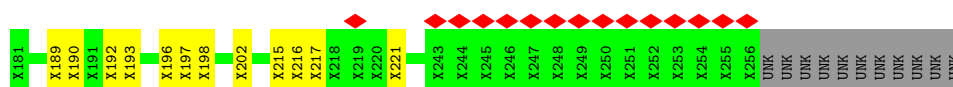
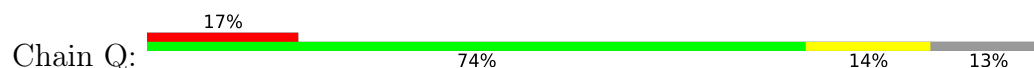
- Molecule 2: coiled-coil domain of portal



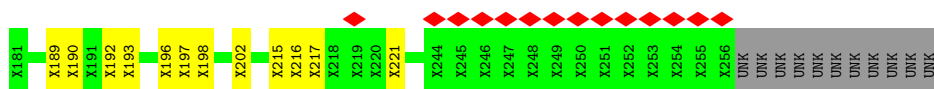
- Molecule 2: coiled-coil domain of portal



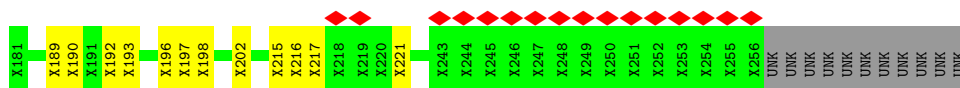
- Molecule 2: coiled-coil domain of portal



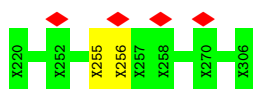
- Molecule 2: coiled-coil domain of portal



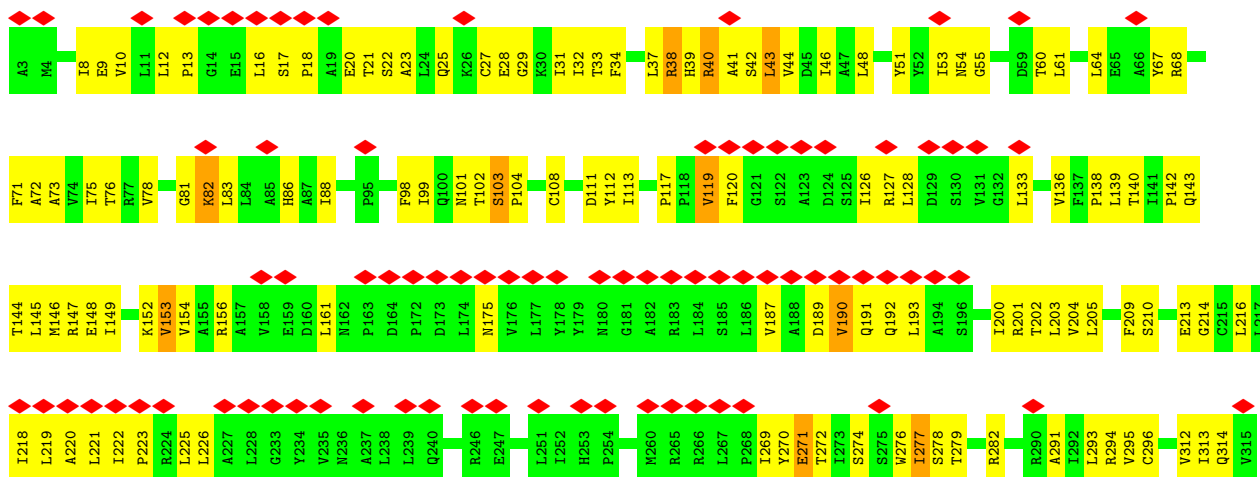
- Chain S:



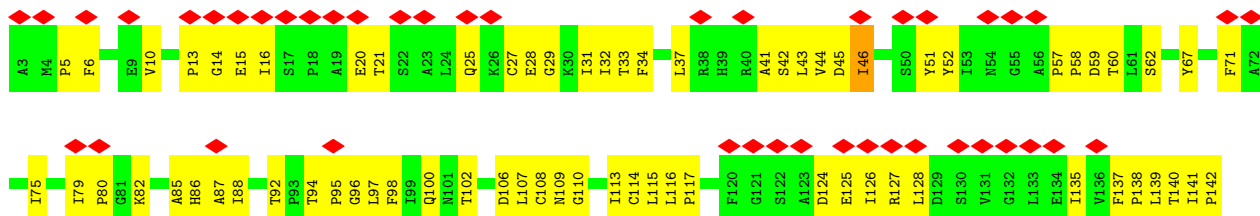
- Chain T:  5% 98%

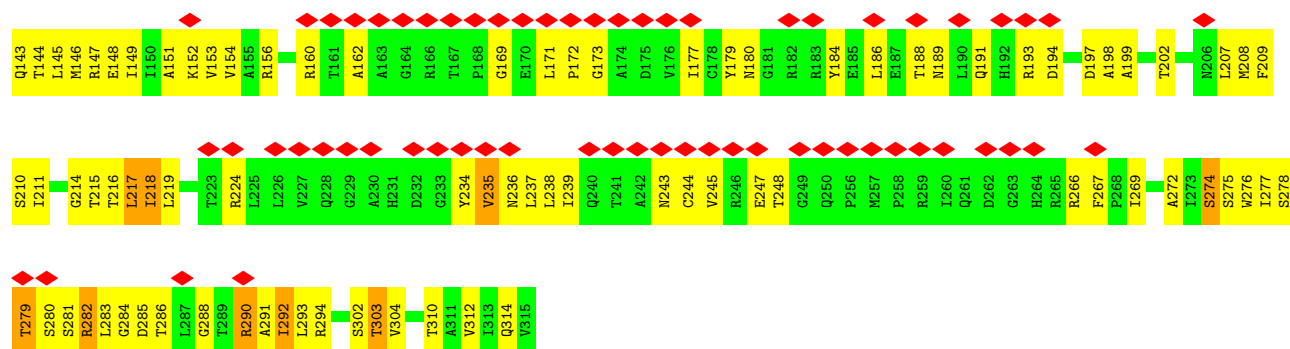


- Chain F:  28% 57% 15%

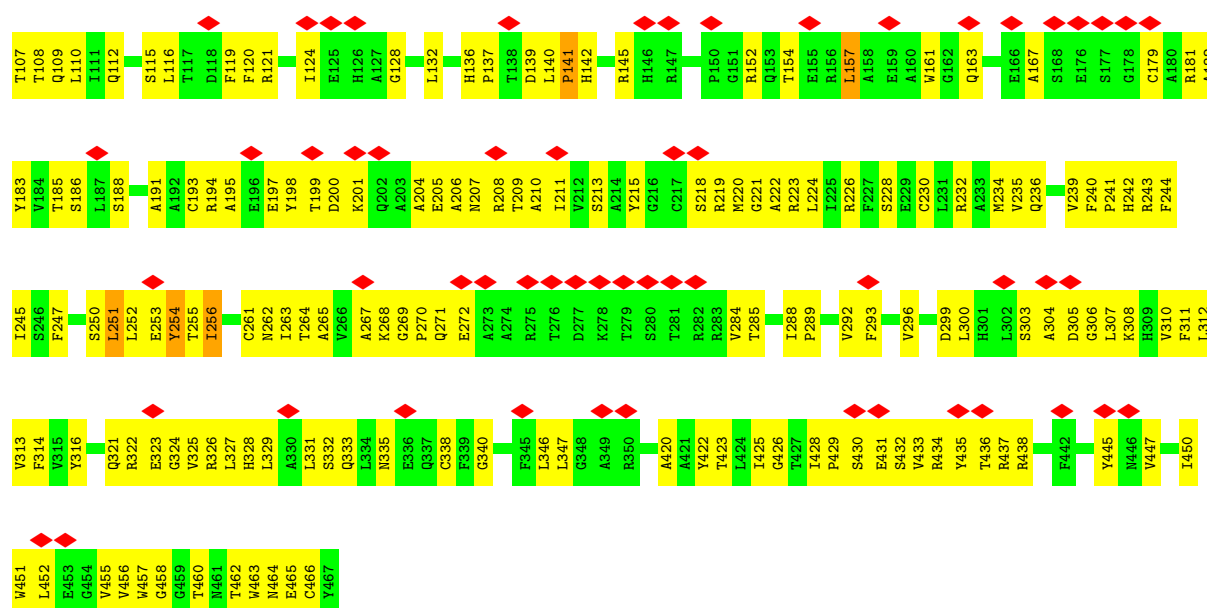


- Chain O:  35% 50% 47%

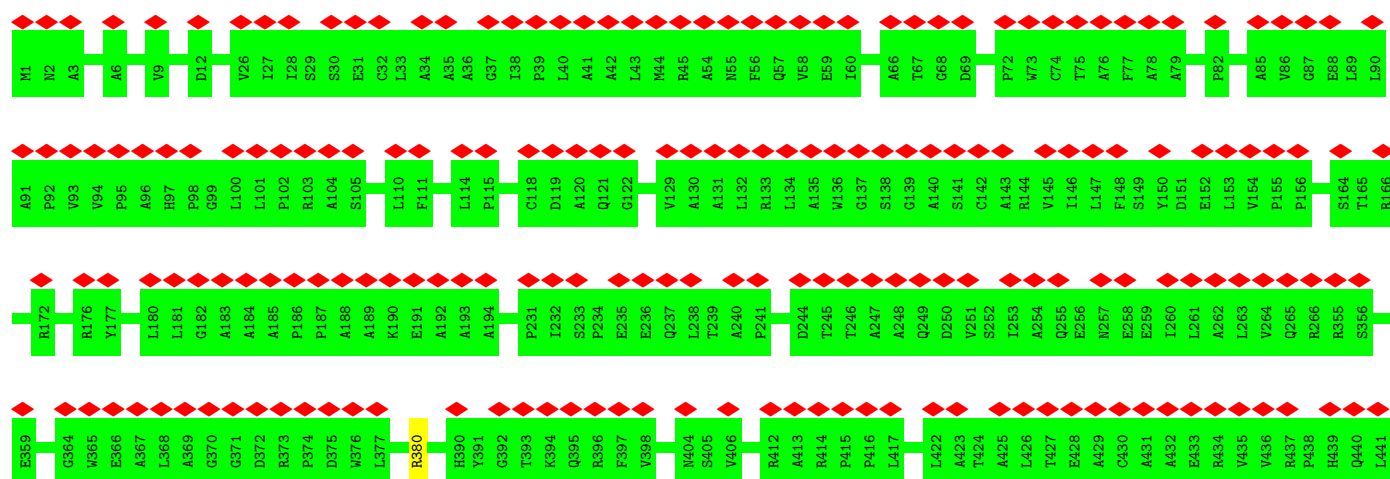


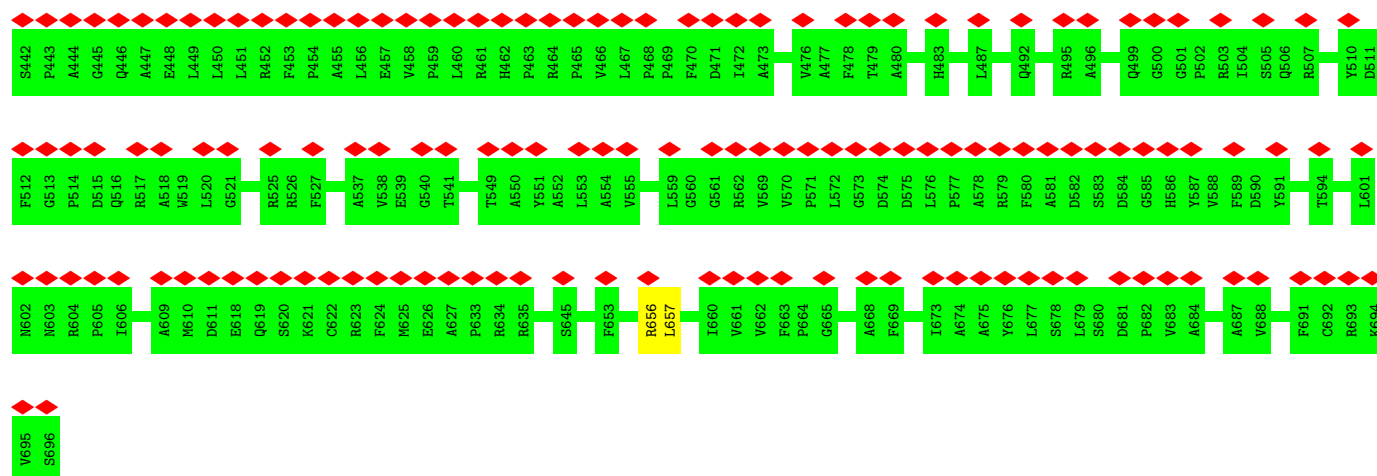


• Molecule 5: Tri1

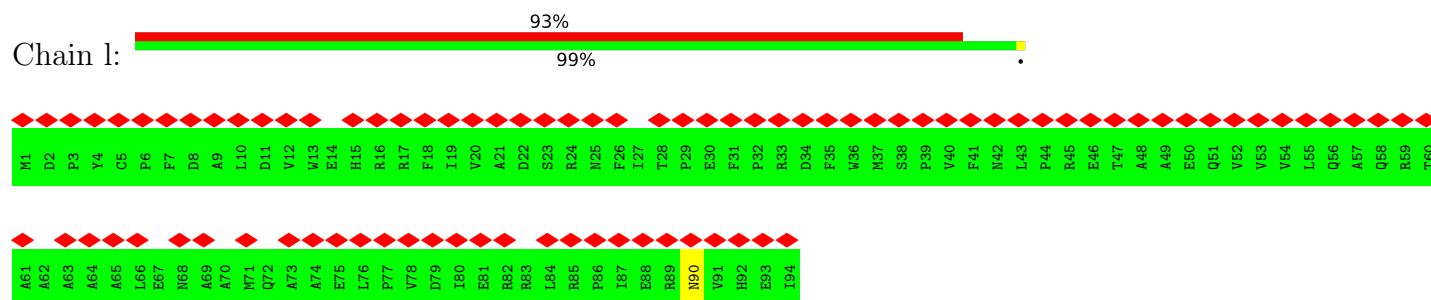


• Molecule 6: CVC1

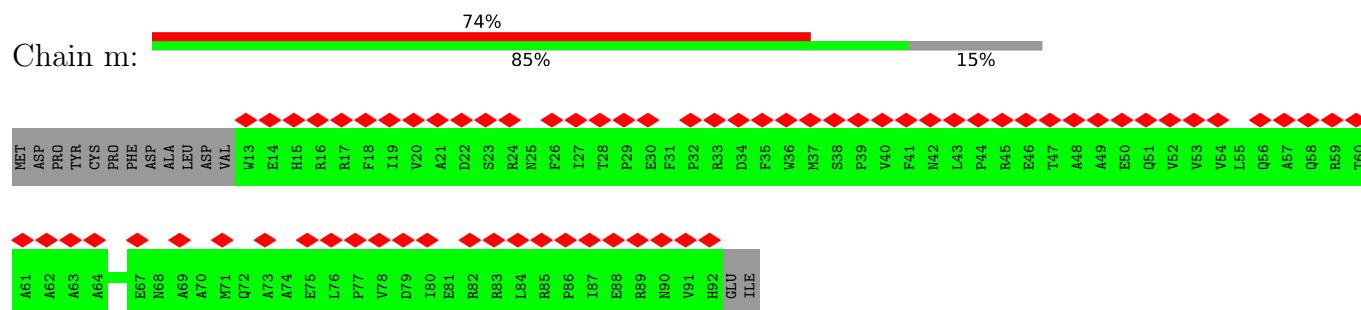




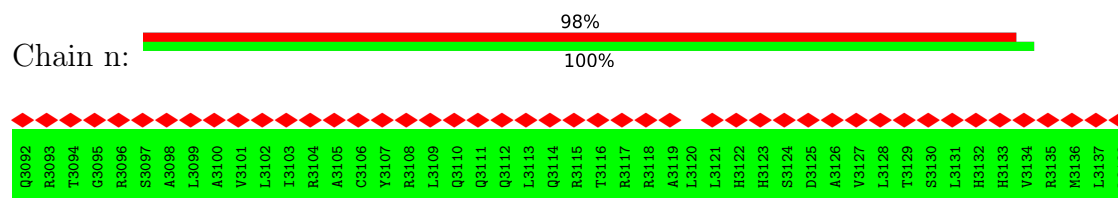
- Molecule 7: Capsid vertex component 2



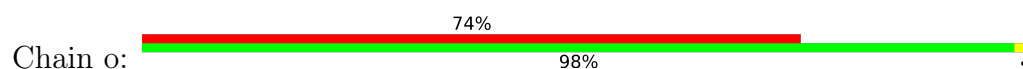
- Molecule 7: Capsid vertex component 2



- Molecule 8: Large tegument protein deneddylase



- Molecule 8: Large tegument protein deneddylase



Q3092	R3093	T3094	G3095	R3096	S3097	A3098	L3099	A3100	V3101	L3102	T3103	R3104	V3107	R3108	L3109	Q3110	G3111	Q3112	L3113	Q3114	R3115	T3116	R3117	R3118	A3119	L3120	L3121	H3122	H3123	S3124	D3125	A3126	V3127	L3128	T3129	S3130	H3133	V3134	L3138
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28556	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	0.031	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	345.6, 345.6, 345.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	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	0.32	0/10642	0.57	1/14510 (0.0%)
1	C	0.33	0/10114	0.58	0/13779
3	F	0.29	0/2158	0.64	2/2951 (0.1%)
4	O	0.28	0/2320	0.68	1/3165 (0.0%)
5	X	0.30	0/2244	0.65	1/3050 (0.0%)
6	k	0.27	0/4307	0.54	1/5866 (0.0%)
7	l	0.27	0/786	0.56	0/1072
7	m	0.27	0/664	0.58	0/905
8	n	0.21	0/388	0.56	0/521
8	o	0.23	0/388	0.57	0/521
All	All	0.31	0/34011	0.59	6/46340 (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
1	C	0	1
3	F	0	1
4	O	0	2
All	All	0	4

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	217	LEU	C-N-CA	6.98	139.16	121.70
3	F	277	ILE	C-N-CA	5.91	136.47	121.70
3	F	43	LEU	CA-CB-CG	5.71	128.44	115.30
1	A	242	MET	CA-CB-CG	5.47	122.60	113.30
6	k	657	LEU	CA-CB-CG	5.40	127.72	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	45	ARG	Sidechain
3	F	271	GLU	Peptide
4	O	218	ILE	Peptide
4	O	86	HIS	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	10392	0	10096	458	0
1	C	9888	0	9673	502	0
2	B	435	0	90	1	0
2	H	435	0	90	1	0
2	I	435	0	90	1	0
2	J	435	0	90	1	0
2	K	380	0	80	6	0
2	L	380	0	80	5	0
2	Q	380	0	80	6	0
2	R	380	0	80	6	0
2	S	380	0	80	6	0
2	T	435	0	90	1	0
3	F	2124	0	2111	112	0
4	O	2279	0	2316	138	0
5	X	2198	0	2124	163	0
6	k	4206	0	4190	0	0
7	l	766	0	745	0	0
7	m	648	0	631	0	0
8	n	384	0	410	0	0
8	o	384	0	410	0	0
All	All	37344	0	33556	1374	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 22.

The worst 5 of 1374 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:C:337:VAL:CG2	1:C:340:LEU:HD21	1.31	1.58
1:C:337:VAL:CG2	1:C:340:LEU:CD2	1.82	1.55
1:C:337:VAL:HG22	1:C:340:LEU:CD2	1.58	1.17
1:C:337:VAL:HG21	1:C:340:LEU:CD2	1.80	1.07
1:C:337:VAL:CG2	1:C:340:LEU:HD23	1.66	1.06

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	1341/1387 (97%)	1196 (89%)	144 (11%)	1 (0%)	48	83
1	C	1273/1387 (92%)	1142 (90%)	126 (10%)	5 (0%)	30	68
3	F	287/297 (97%)	222 (77%)	56 (20%)	9 (3%)	3	22
4	O	299/307 (97%)	247 (83%)	44 (15%)	8 (3%)	4	26
5	X	283/289 (98%)	237 (84%)	41 (14%)	5 (2%)	7	34
6	k	534/550 (97%)	508 (95%)	26 (5%)	0	100	100
7	l	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
7	m	78/94 (83%)	75 (96%)	3 (4%)	0	100	100
8	n	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
8	o	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
All	All	4277/4499 (95%)	3799 (89%)	450 (10%)	28 (1%)	21	56

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	66	PHE
3	F	38	ARG
3	F	103	SER

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Mol	Chain	Res	Type
3	F	119	VAL
3	F	190	VAL

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	1101/1168 (94%)	1097 (100%)	4 (0%)	89	90
1	C	1050/1168 (90%)	1028 (98%)	22 (2%)	48	67
3	F	212/252 (84%)	211 (100%)	1 (0%)	86	89
4	O	242/258 (94%)	240 (99%)	2 (1%)	79	84
5	X	220/240 (92%)	220 (100%)	0	100	100
6	k	429/429 (100%)	427 (100%)	2 (0%)	86	89
7	l	80/80 (100%)	79 (99%)	1 (1%)	65	77
7	m	66/80 (82%)	66 (100%)	0	100	100
8	n	41/41 (100%)	41 (100%)	0	100	100
8	o	41/41 (100%)	40 (98%)	1 (2%)	44	63
All	All	3482/3757 (93%)	3449 (99%)	33 (1%)	74	83

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	O	290	ARG
6	k	380	ARG
8	o	3115	ARG
1	C	185	LEU
1	C	184	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	44	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1146	GLN
6	k	61	GLN
1	C	112	GLN
1	C	1321	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	k	7
3	F	4
4	O	3
5	X	2

The worst 5 of 16 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	k	266:ARG	C	355:ARG	N	36.83
1	O	250:GLN	C	256:PRO	N	16.00
1	k	200:LEU	C	230:PRO	N	14.76
1	X	351:ILE	C	417:CYS	N	12.96
1	F	260:MET	C	265:ARG	N	11.08

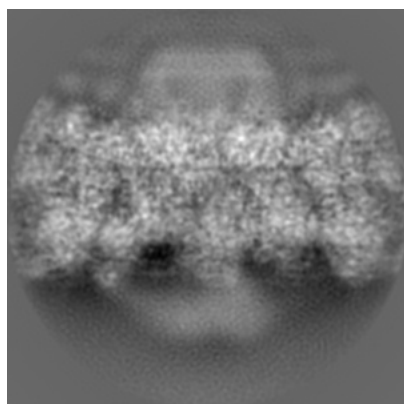
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38186. These allow visual inspection of the internal detail of the map and identification of artifacts.

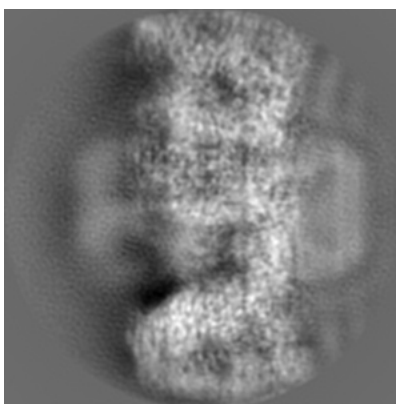
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

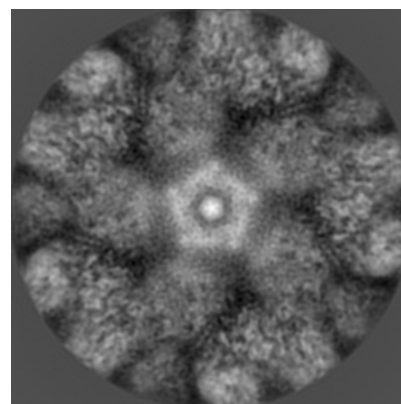
6.1.1 Primary map



X

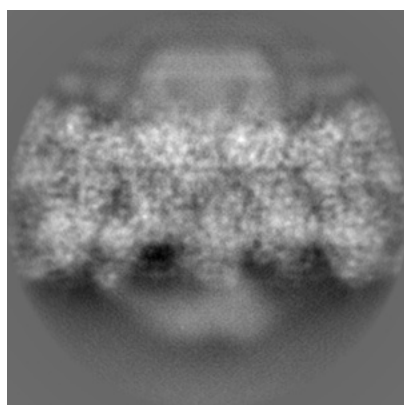


Y

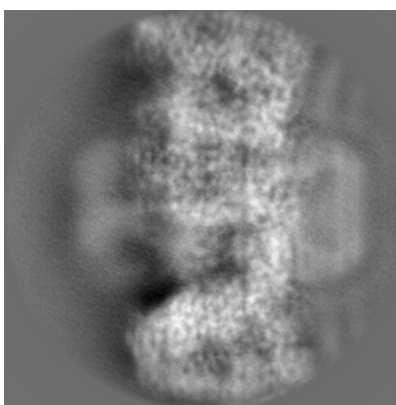


Z

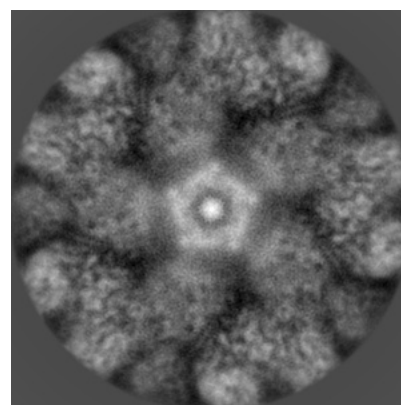
6.1.2 Raw map



X



Y

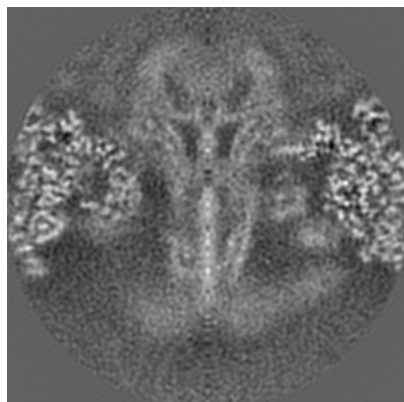


Z

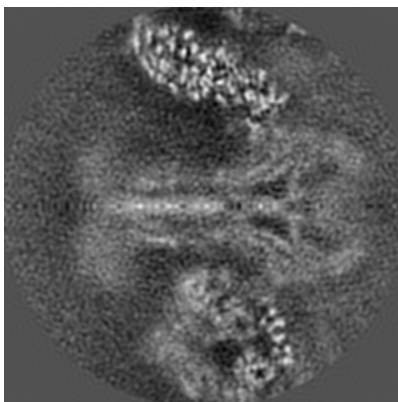
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

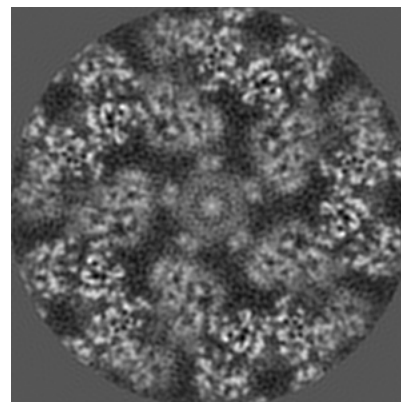
6.2.1 Primary map



X Index: 128

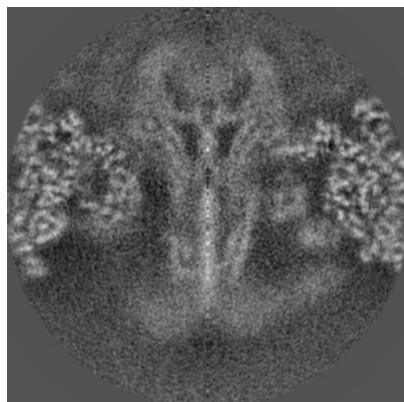


Y Index: 128

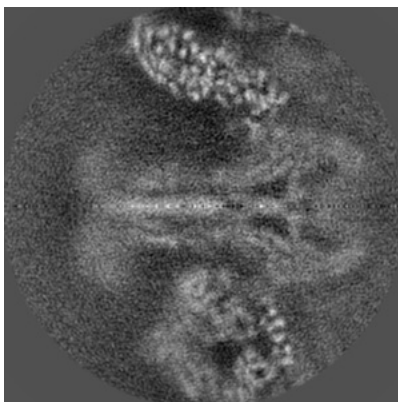


Z Index: 128

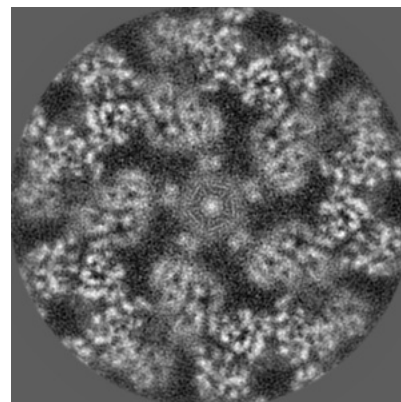
6.2.2 Raw map



X Index: 128



Y Index: 128

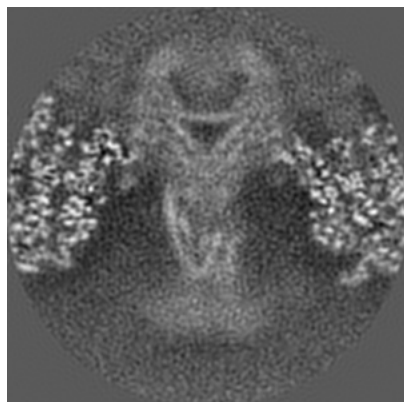


Z Index: 128

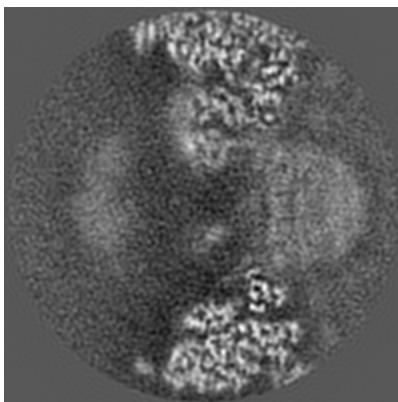
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

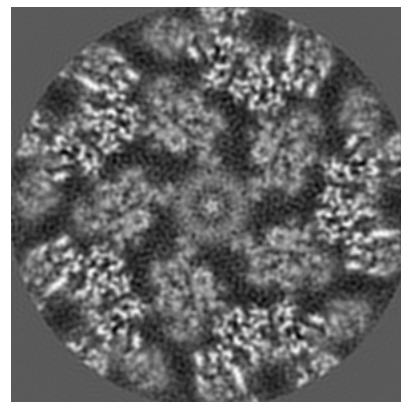
6.3.1 Primary map



X Index: 143

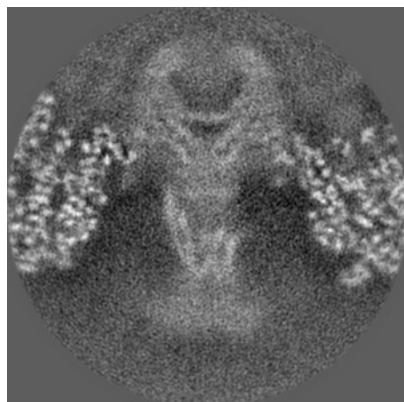


Y Index: 96

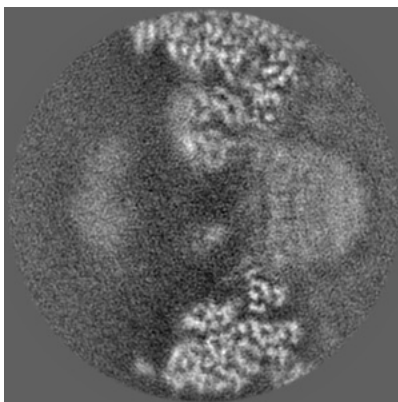


Z Index: 133

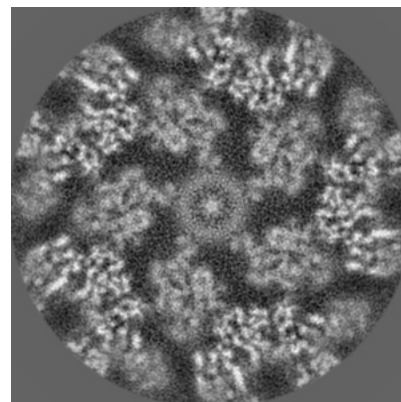
6.3.2 Raw map



X Index: 144



Y Index: 96

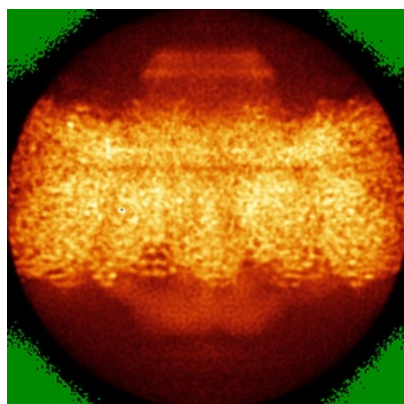


Z Index: 133

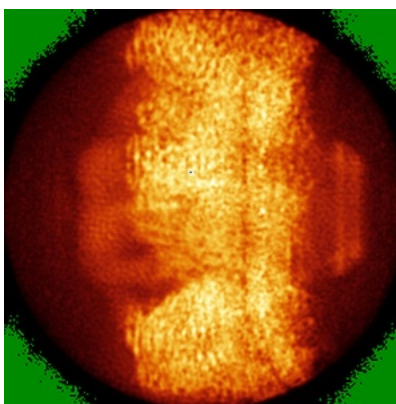
The images above show the largest variance slices of the map in three orthogonal directions.

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

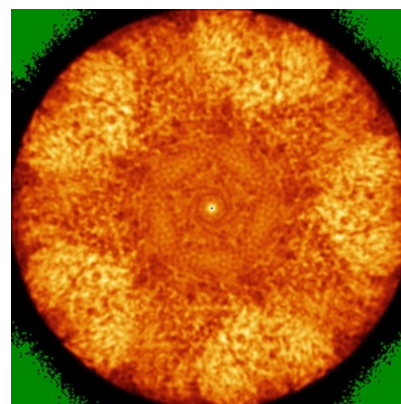
6.4.1 Primary map



X

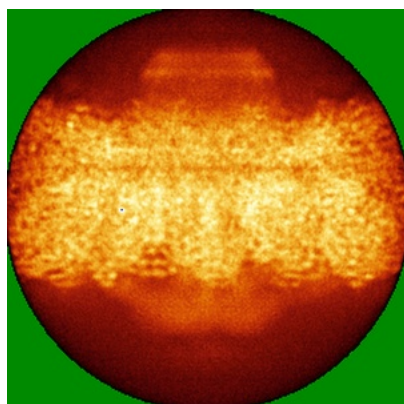


Y

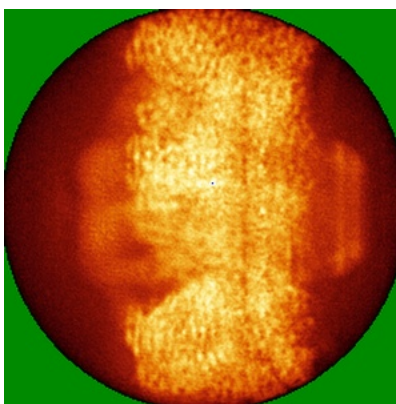


Z

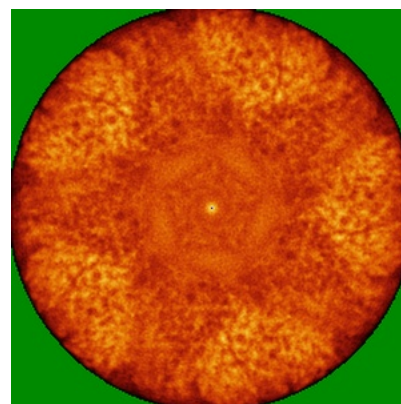
6.4.2 Raw map



X



Y

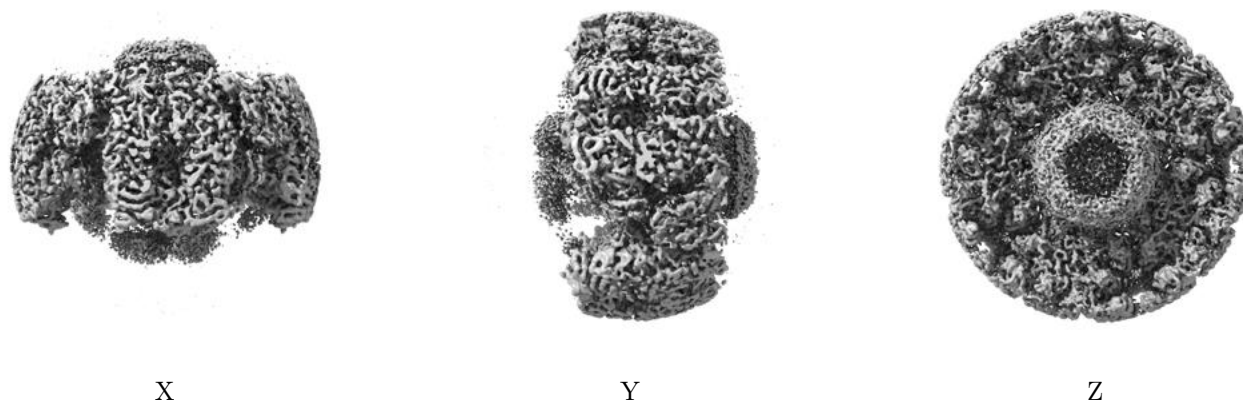


Z

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.

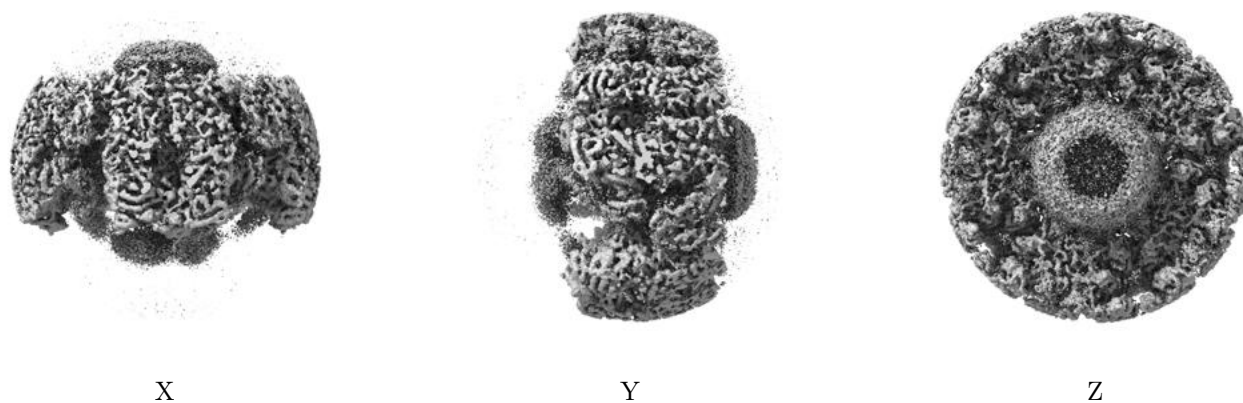
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. 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.

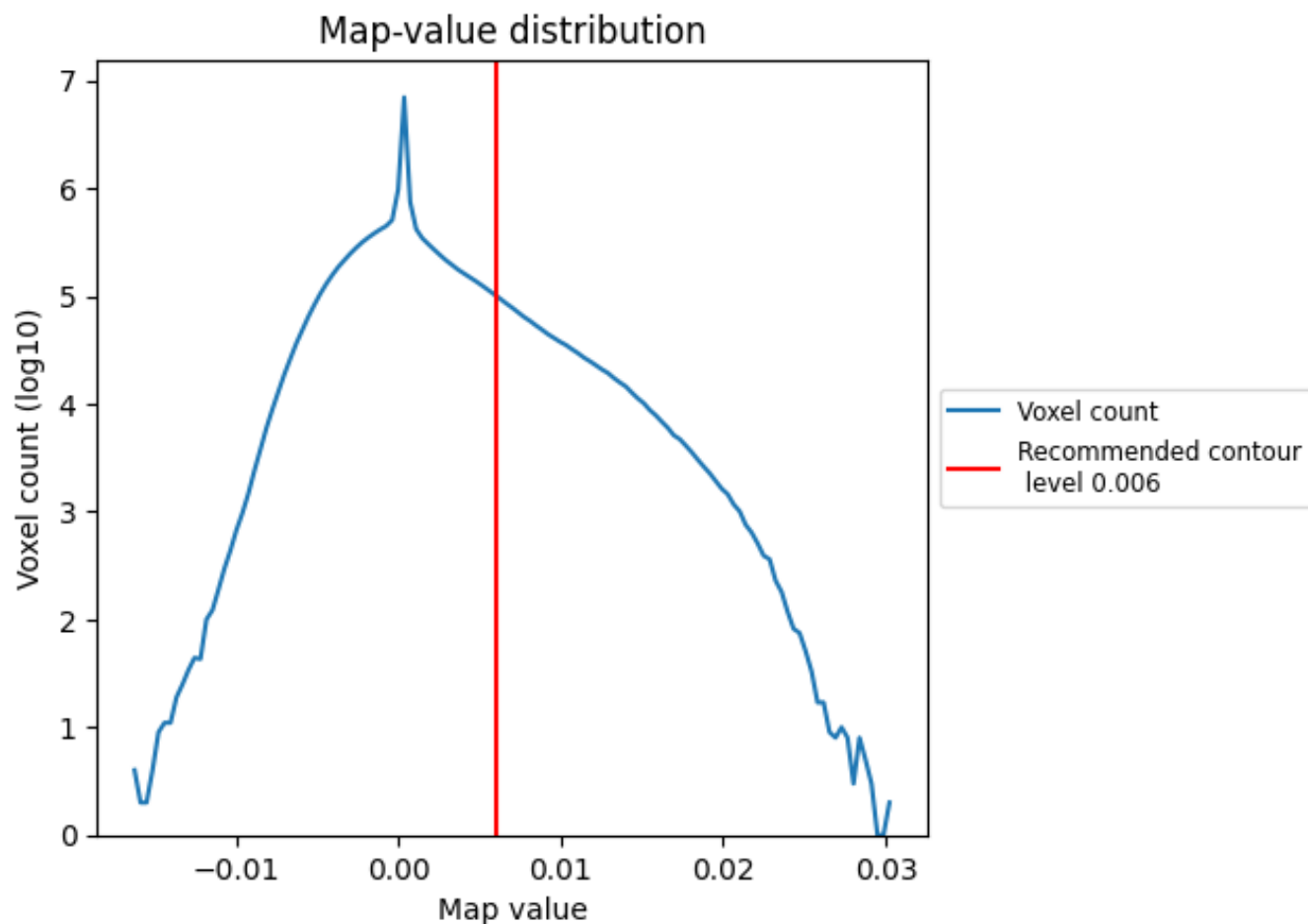
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

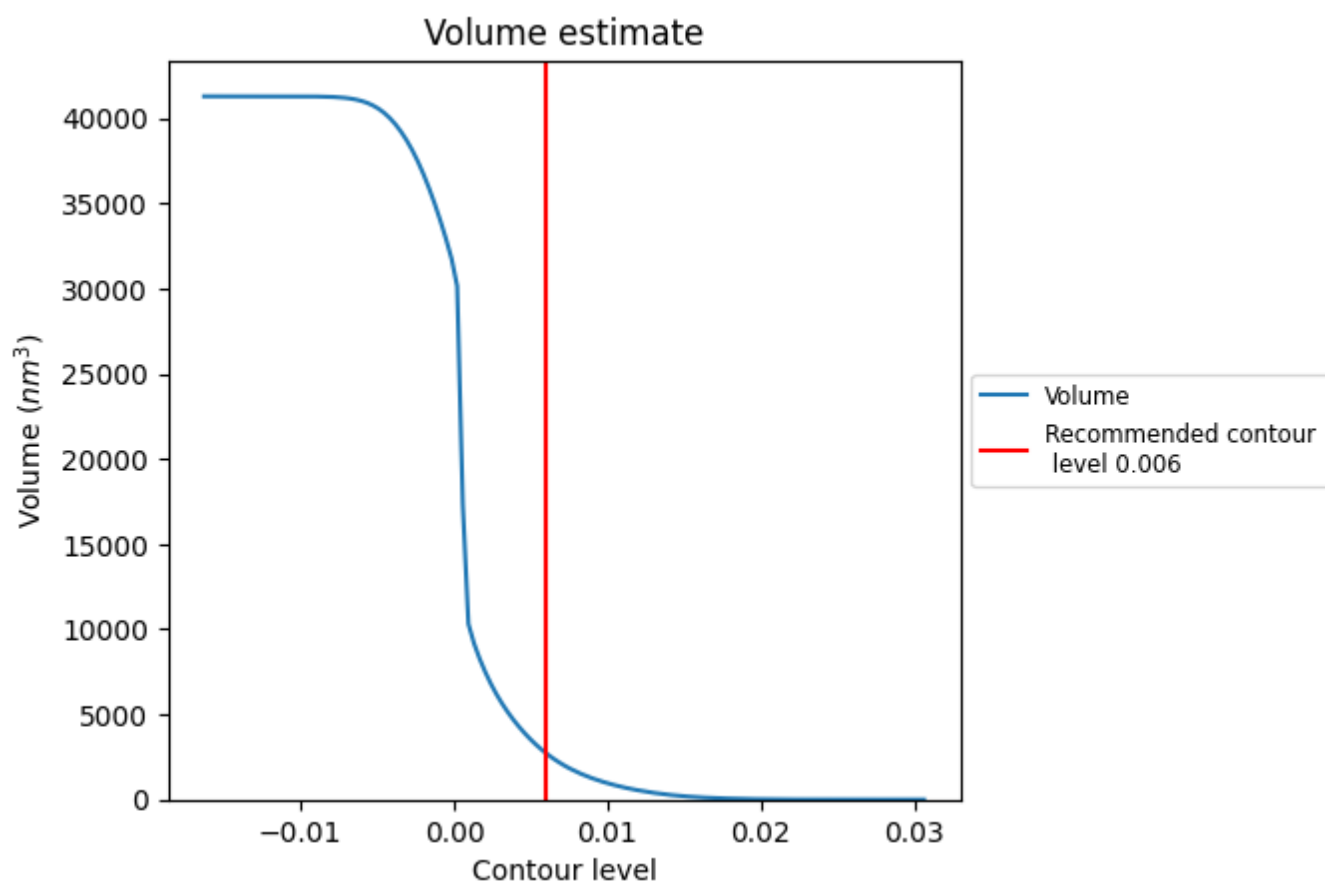
This section contains the results of statistical analysis of the map.

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.

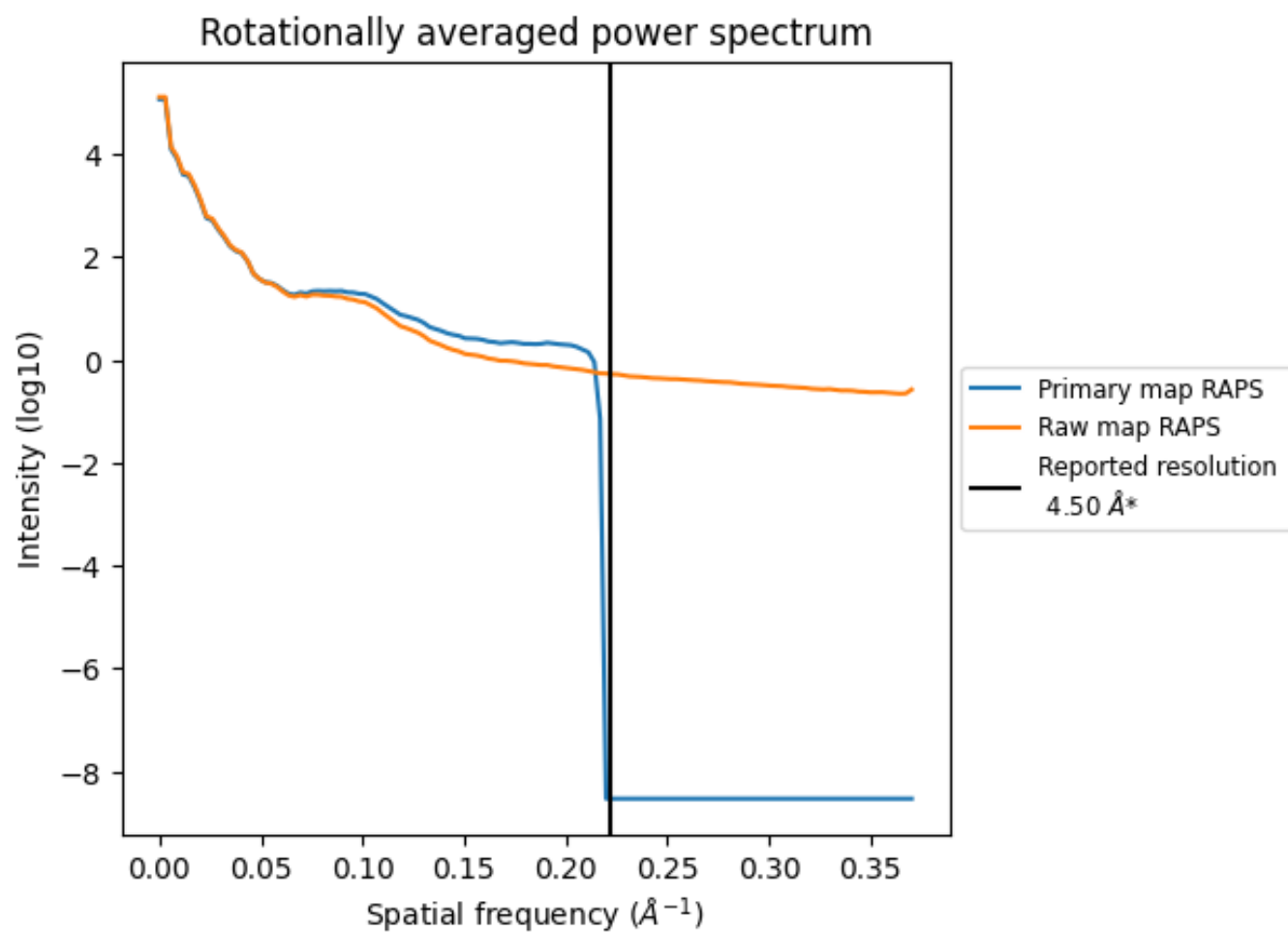
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2723 nm³; this corresponds to an approximate mass of 2460 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 ⓘ

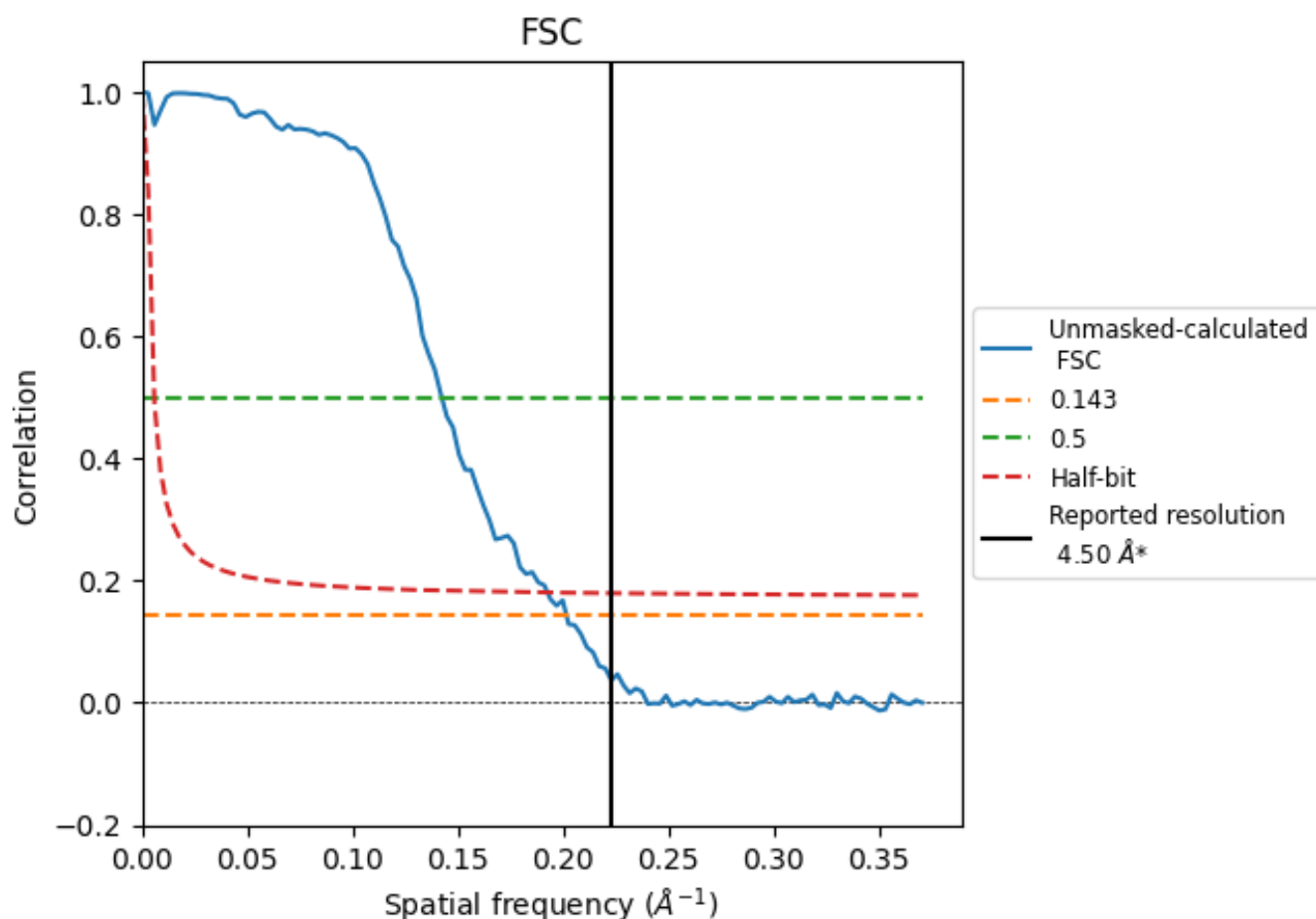


*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

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 0.222 Å⁻¹

8.2 Resolution estimates [i](#)

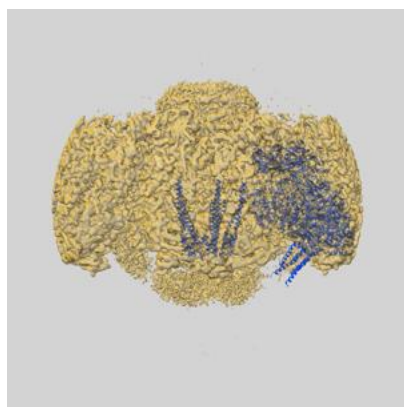
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.96	7.03	5.19

*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 4.96 differs from the reported value 4.5 by more than 10 %

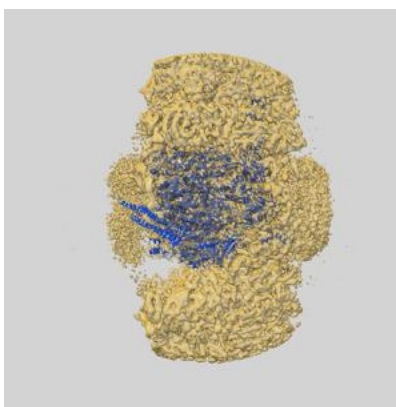
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38186 and PDB model 8X9W. Per-residue inclusion information can be found in section [3](#) on page [7](#).

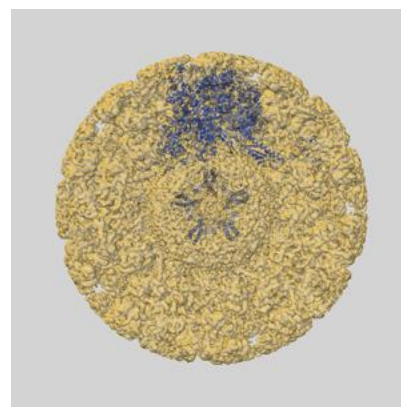
9.1 Map-model overlay [i](#)



X



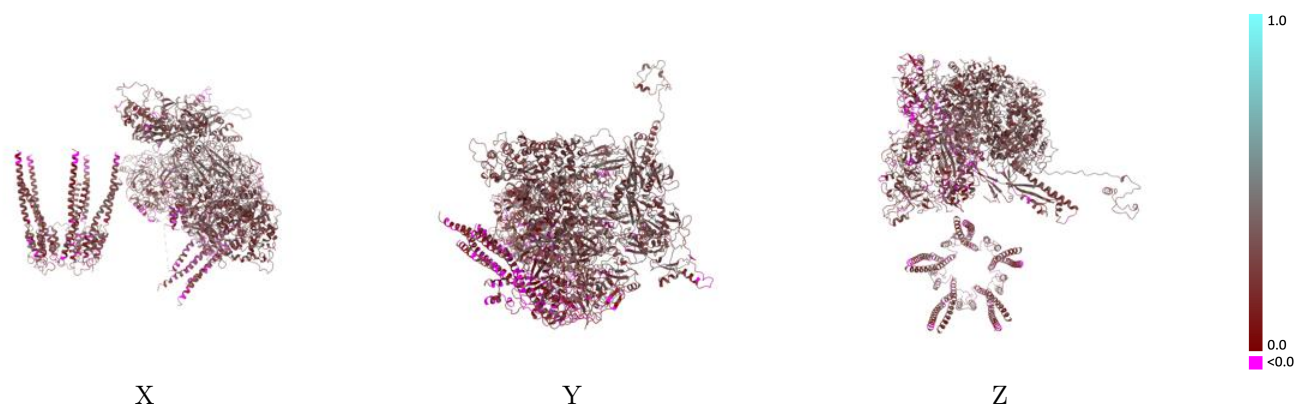
Y



Z

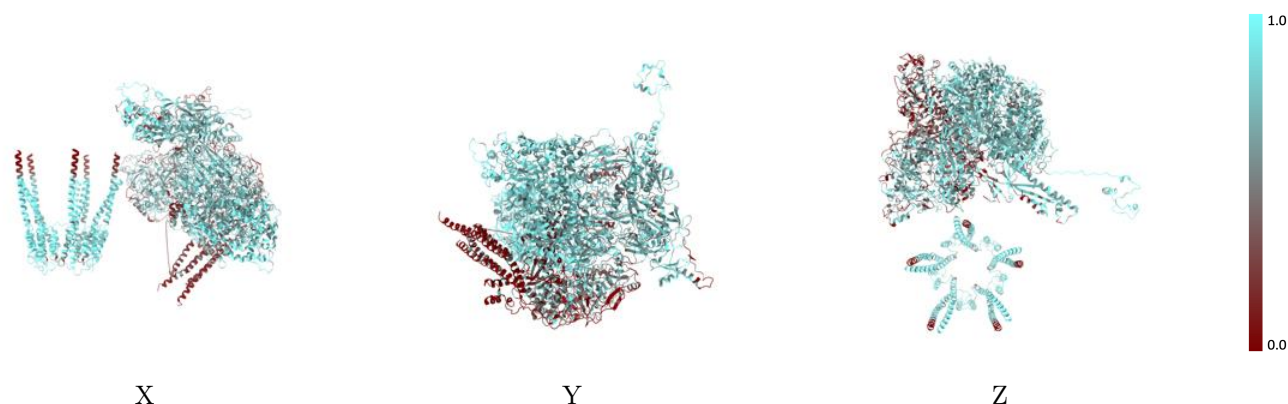
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



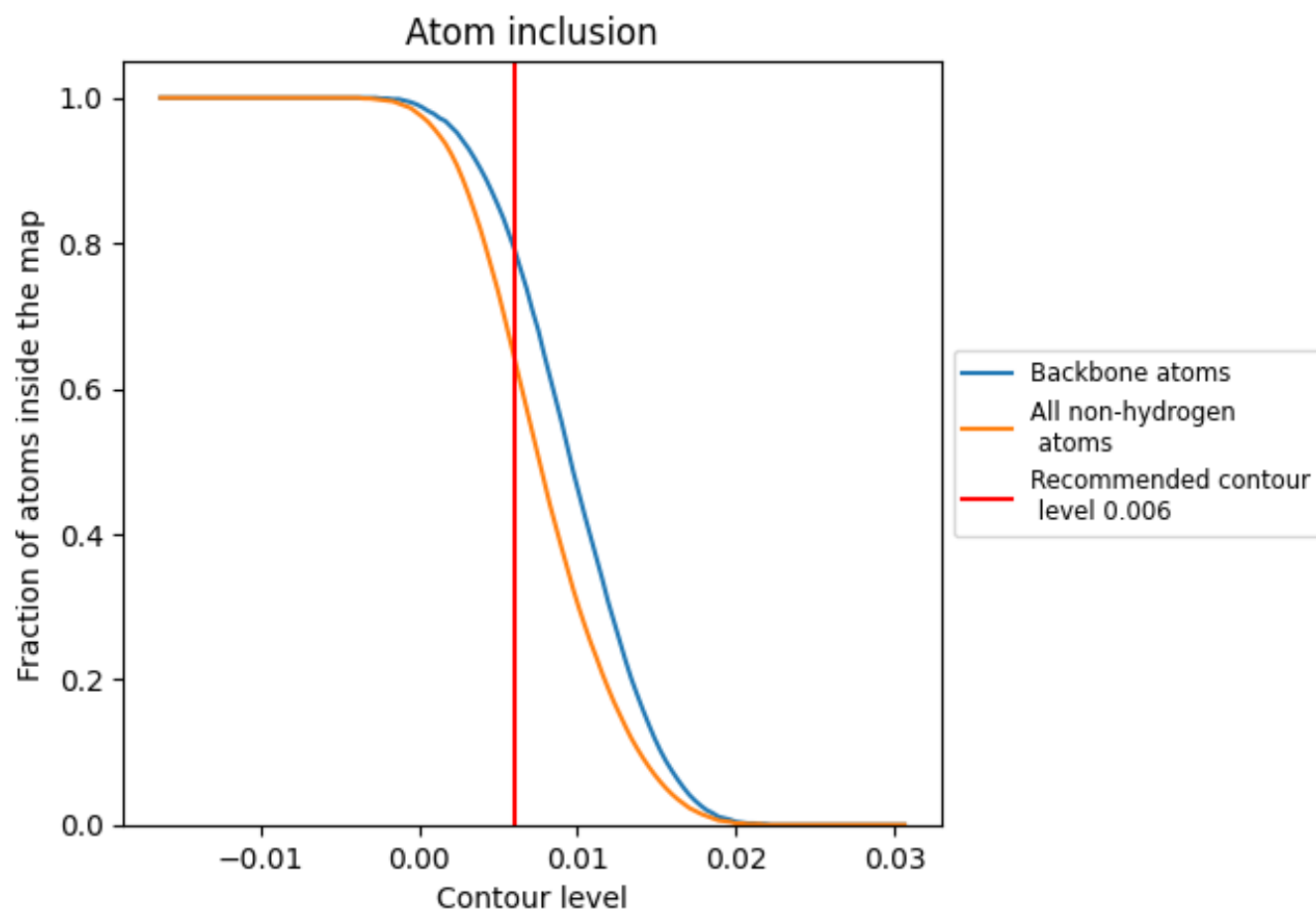
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 79% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6440	 0.2600
A	 0.7660	 0.3220
B	 0.8830	 0.2280
C	 0.7210	 0.3120
F	 0.5890	 0.2550
H	 0.8740	 0.2320
I	 0.8740	 0.2300
J	 0.8850	 0.2330
K	 0.7400	 0.1960
L	 0.7340	 0.1980
O	 0.5140	 0.2470
Q	 0.7340	 0.2020
R	 0.7450	 0.2040
S	 0.7470	 0.2010
T	 0.8800	 0.2280
X	 0.6470	 0.2030
k	 0.3530	 0.1450
l	 0.0930	 0.1220
m	 0.1430	 0.0920
n	 0.0570	 0.1160
o	 0.2340	 0.1230

