



wwPDB EM Validation Summary Report ⓘ

Oct 27, 2024 – 12:17 PM EDT

PDB ID : 7KLN
EMDB ID : EMD-22917
Title : Myoviridae Phage XM1 Neck Region (12-fold)
Authors : Wang, Z.; Klose, T.; Jiang, W.; Kuhn, R.J.
Deposited on : 2020-10-30
Resolution : 3.60 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.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

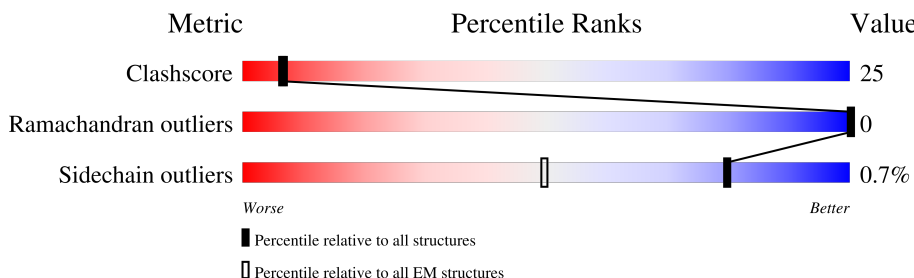
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	A1	412	<div> <div>51%</div> <div> <div></div> <div>47%</div> <div>41%</div> <div>12%</div> </div> </div>
1	B1	412	<div> <div>50%</div> <div> <div></div> <div>47%</div> <div>41%</div> <div>12%</div> </div> </div>
1	C1	412	<div> <div>50%</div> <div> <div></div> <div>45%</div> <div>42%</div> <div>12%</div> </div> </div>
1	D1	412	<div> <div>50%</div> <div> <div></div> <div>46%</div> <div>41%</div> <div>12%</div> </div> </div>
1	E1	412	<div> <div>49%</div> <div> <div></div> <div>47%</div> <div>41%</div> <div>12%</div> </div> </div>
1	F1	412	<div> <div>48%</div> <div> <div></div> <div>48%</div> <div>40%</div> <div>12%</div> </div> </div>
1	G1	412	<div> <div>48%</div> <div> <div></div> <div>48%</div> <div>39%</div> <div>12%</div> </div> </div>
1	H1	412	<div> <div>48%</div> <div> <div></div> <div>46%</div> <div>42%</div> <div>12%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	I1	412	<div> <div>47%</div> <div>45%</div> <div>42%</div> <div>12%</div> </div>
1	J1	412	<div> <div>48%</div> <div>47%</div> <div>41%</div> <div>12%</div> </div>
1	K1	412	<div> <div>50%</div> <div>44%</div> <div>43%</div> <div>12%</div> </div>
1	L1	412	<div> <div>51%</div> <div>46%</div> <div>41%</div> <div>12%</div> </div>
2	A2	118	<div> <div>8%</div> <div>61%</div> <div>38%</div> <div></div> </div>
2	B2	118	<div> <div>8%</div> <div>64%</div> <div>35%</div> <div></div> </div>
2	C2	118	<div> <div>8%</div> <div>58%</div> <div>41%</div> <div></div> </div>
2	D2	118	<div> <div>8%</div> <div>59%</div> <div>40%</div> <div></div> </div>
2	E2	118	<div> <div>8%</div> <div>62%</div> <div>37%</div> <div></div> </div>
2	F2	118	<div> <div>8%</div> <div>63%</div> <div>36%</div> <div></div> </div>
2	G2	118	<div> <div>8%</div> <div>62%</div> <div>37%</div> <div></div> </div>
2	H2	118	<div> <div>9%</div> <div>61%</div> <div>38%</div> <div></div> </div>
2	I2	118	<div> <div>8%</div> <div>65%</div> <div>34%</div> <div></div> </div>
2	J2	118	<div> <div>9%</div> <div>63%</div> <div>37%</div> <div></div> </div>
2	K2	118	<div> <div>9%</div> <div>61%</div> <div>38%</div> <div></div> </div>
2	L2	118	<div> <div>9%</div> <div>59%</div> <div>40%</div> <div></div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 45564 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 Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	361	Total	C	N	O	S	0	0
			2902	1835	494	563	10		
1	B1	361	Total	C	N	O	S	0	0
			2902	1835	494	563	10		
1	C1	361	Total	C	N	O	S	0	0
			2902	1835	494	563	10		
1	D1	361	Total	C	N	O	S	0	0
			2902	1835	494	563	10		
1	E1	361	Total	C	N	O	S	0	0
			2902	1835	494	563	10		
1	F1	361	Total	C	N	O	S	0	0
			2902	1835	494	563	10		
1	G1	361	Total	C	N	O	S	0	0
			2902	1835	494	563	10		
1	H1	361	Total	C	N	O	S	0	0
			2902	1835	494	563	10		
1	I1	361	Total	C	N	O	S	0	0
			2902	1835	494	563	10		
1	J1	361	Total	C	N	O	S	0	0
			2902	1835	494	563	10		
1	K1	361	Total	C	N	O	S	0	0
			2902	1835	494	563	10		
1	L1	361	Total	C	N	O	S	0	0
			2902	1835	494	563	10		

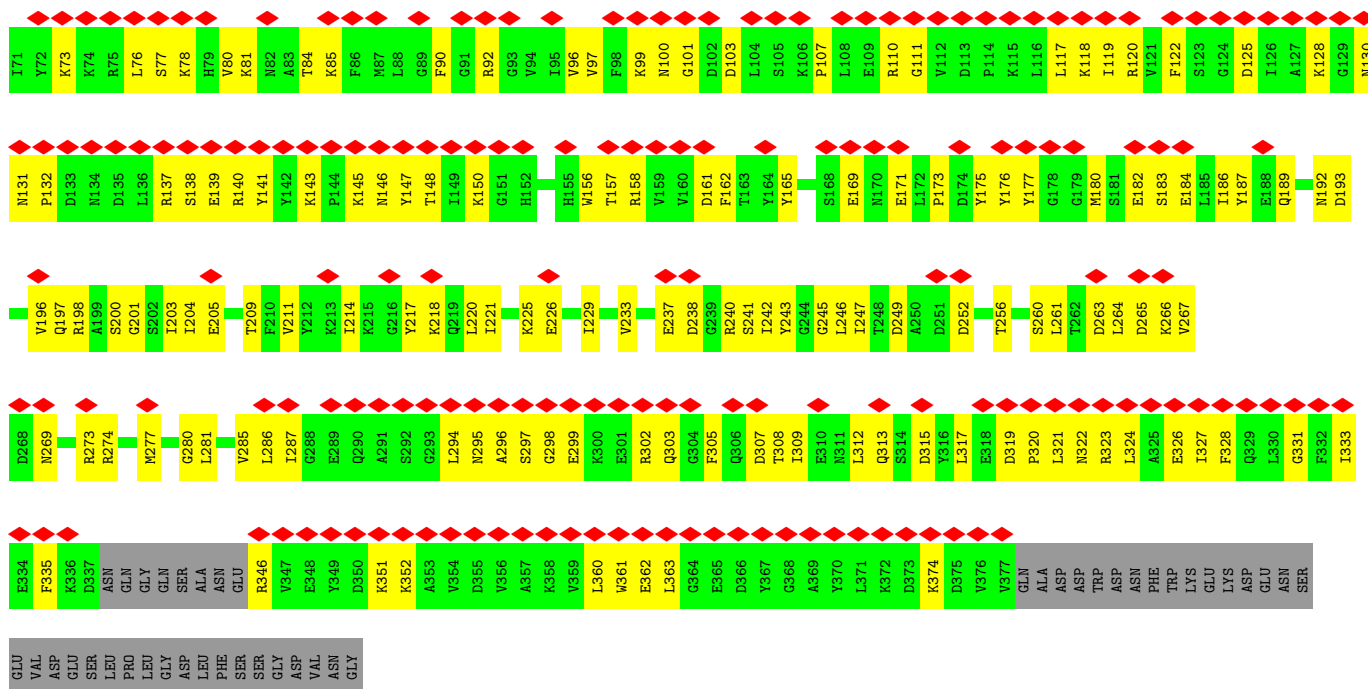
- Molecule 2 is a protein called Head completion protein, gp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A2	118	Total	C	N	O	S	0	0
			895	563	143	184	5		
2	B2	118	Total	C	N	O	S	0	0
			895	563	143	184	5		
2	C2	118	Total	C	N	O	S	0	0
			895	563	143	184	5		

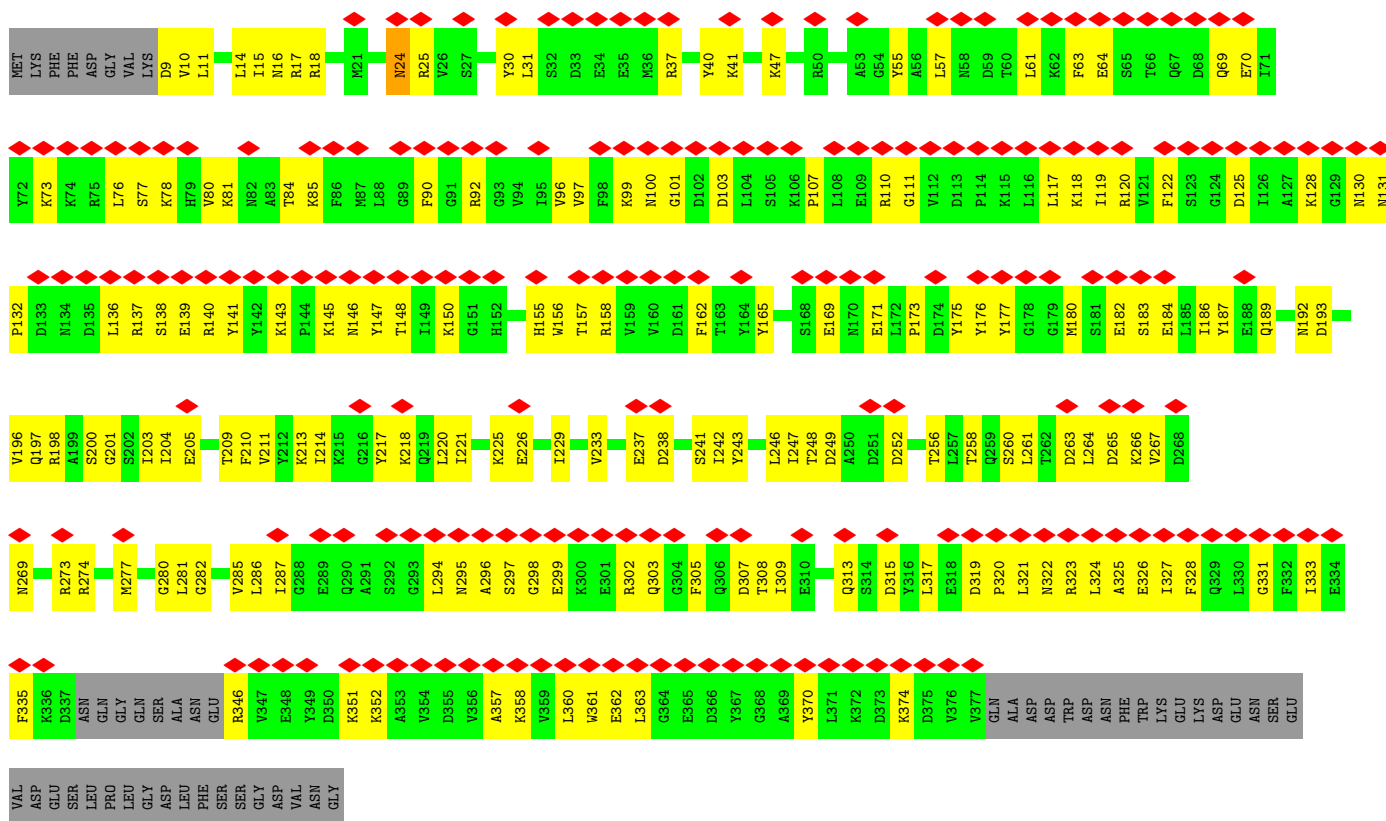
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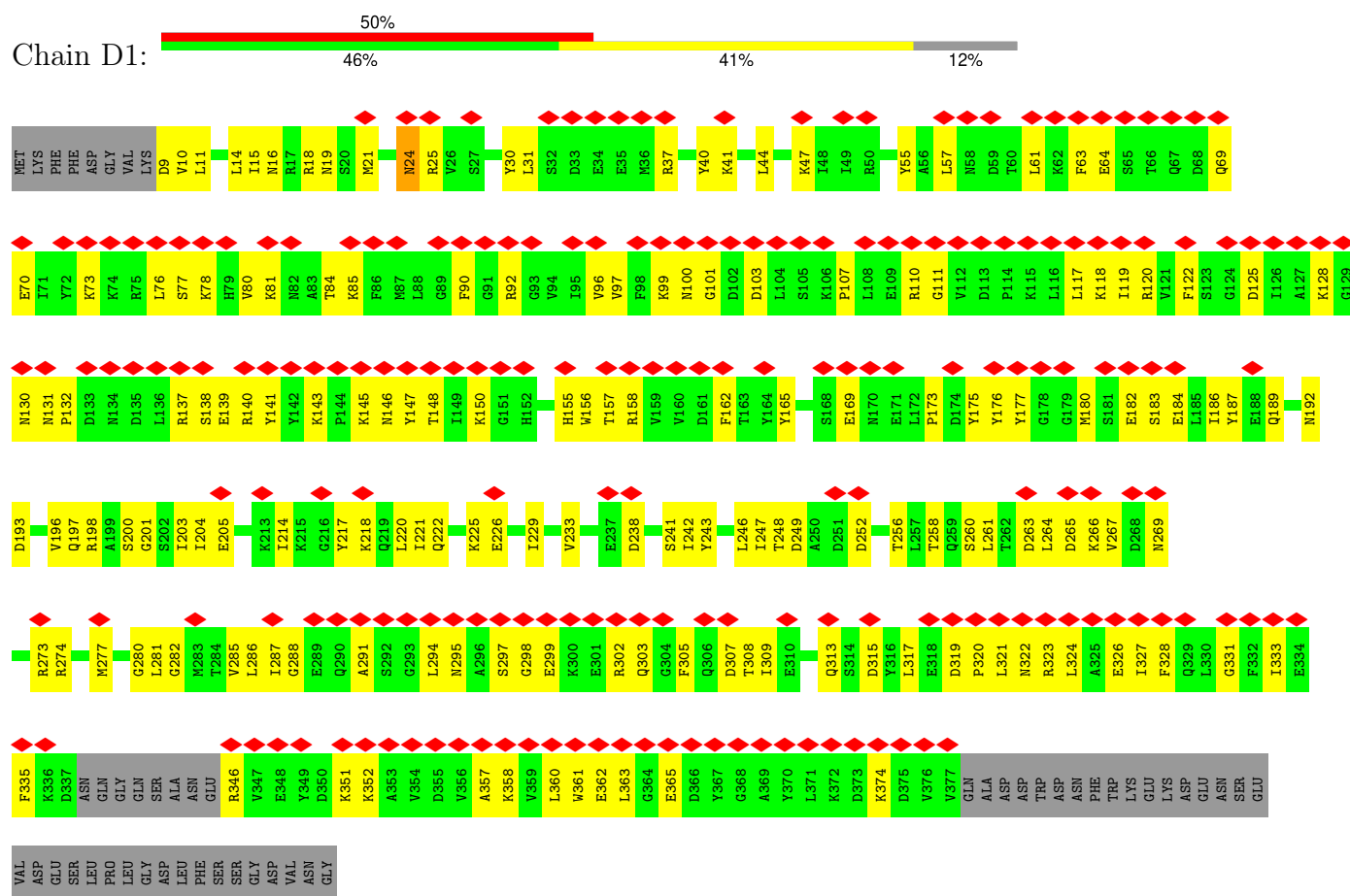
Mol	Chain	Residues	Atoms					AltConf	Trace
2	D2	118	Total 895	C 563	N 143	O 184	S 5	0	0
2	E2	118	Total 895	C 563	N 143	O 184	S 5	0	0
2	F2	118	Total 895	C 563	N 143	O 184	S 5	0	0
2	G2	118	Total 895	C 563	N 143	O 184	S 5	0	0
2	H2	118	Total 895	C 563	N 143	O 184	S 5	0	0
2	I2	118	Total 895	C 563	N 143	O 184	S 5	0	0
2	J2	118	Total 895	C 563	N 143	O 184	S 5	0	0
2	K2	118	Total 895	C 563	N 143	O 184	S 5	0	0
2	L2	118	Total 895	C 563	N 143	O 184	S 5	0	0



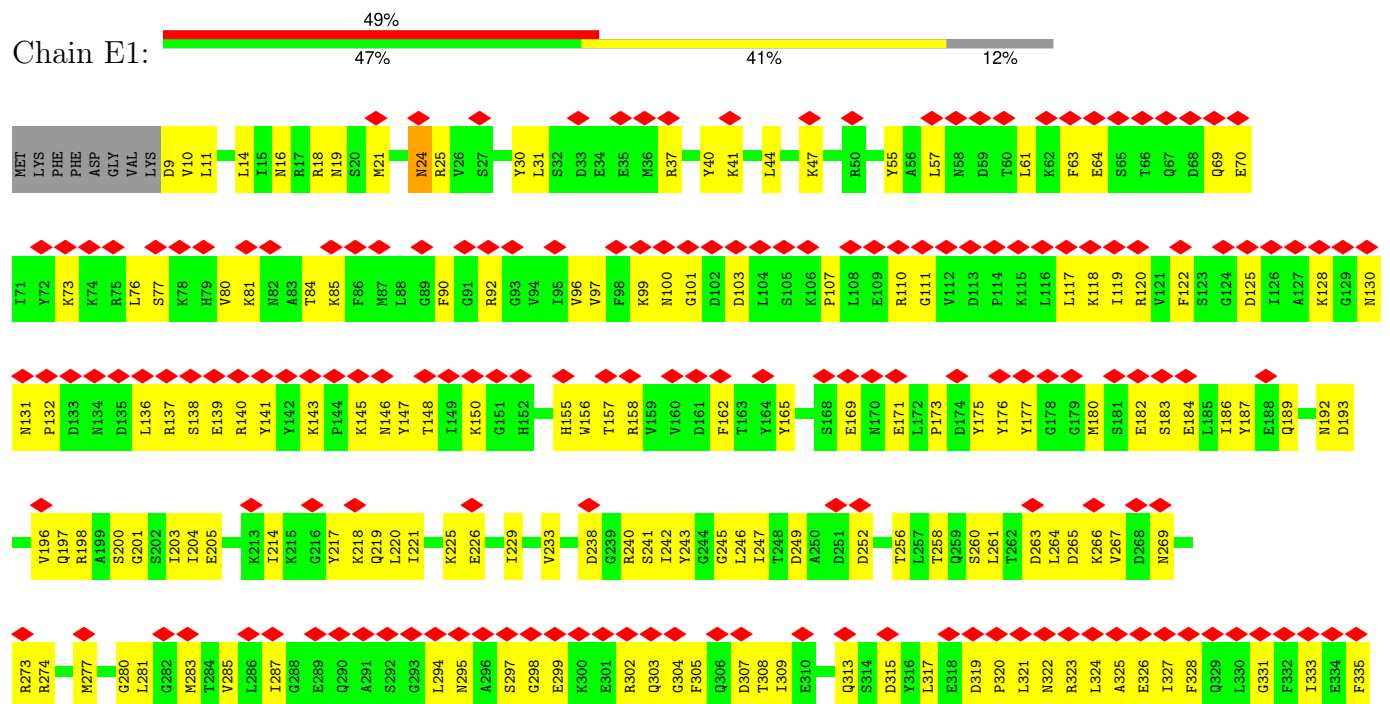
• Molecule 1: Portal protein

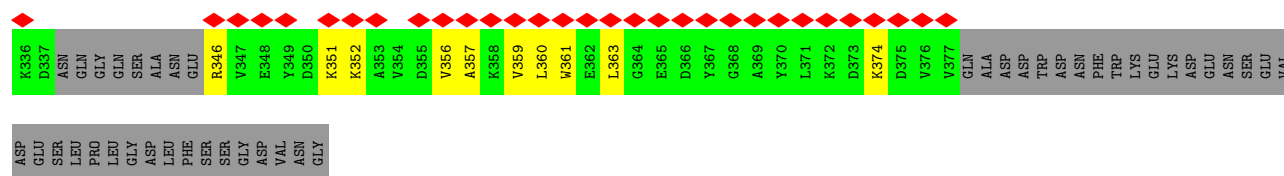


• Molecule 1: Portal protein



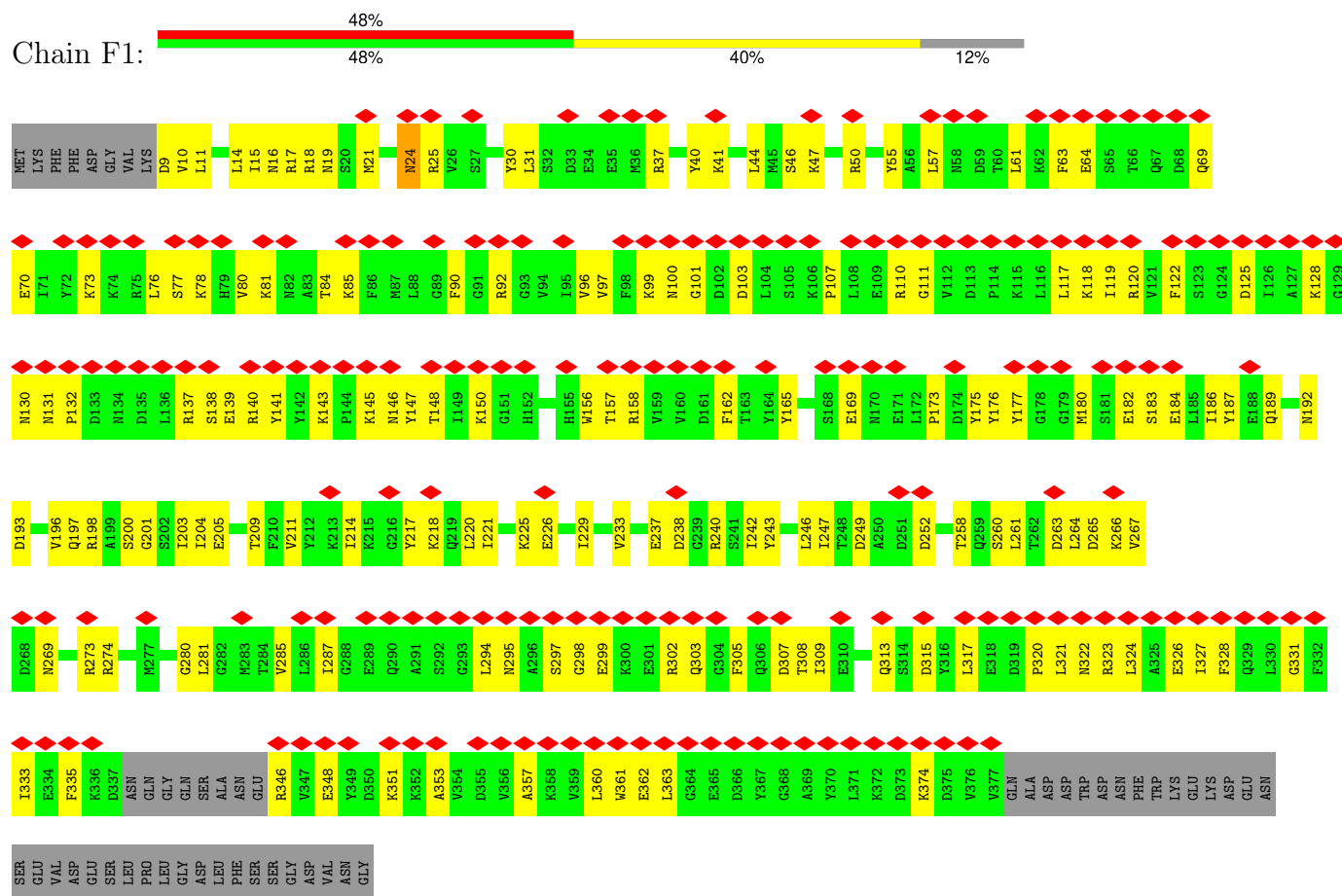
• Molecule 1: Portal protein





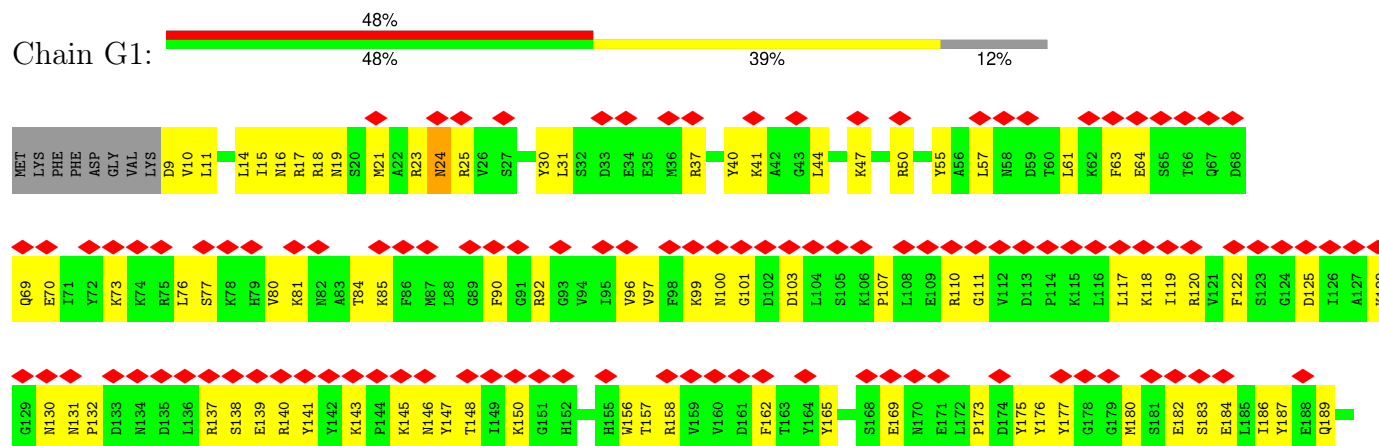
• Molecule 1: Portal protein

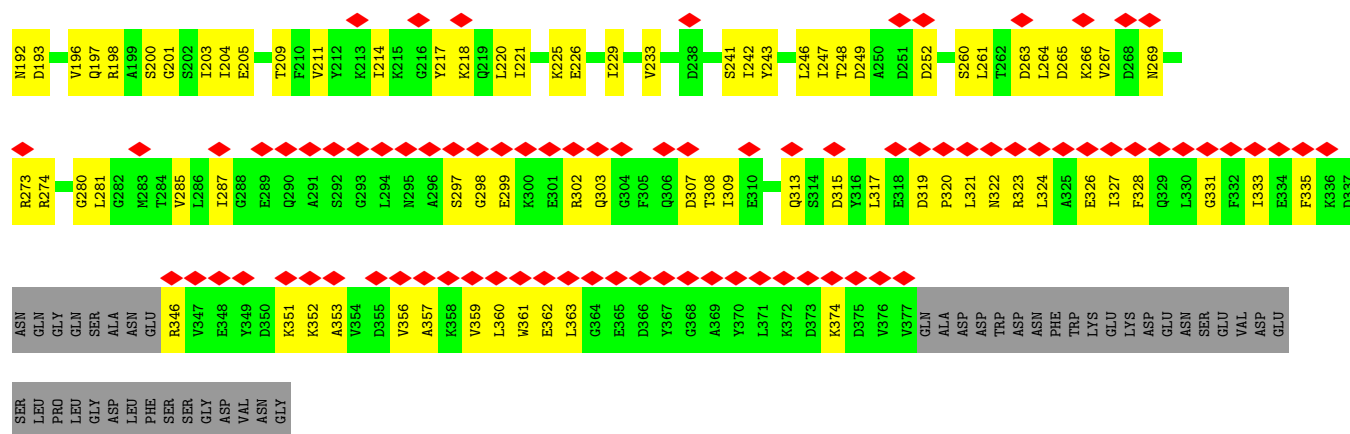
Chain F1:



• Molecule 1: Portal protein

Chain G1:





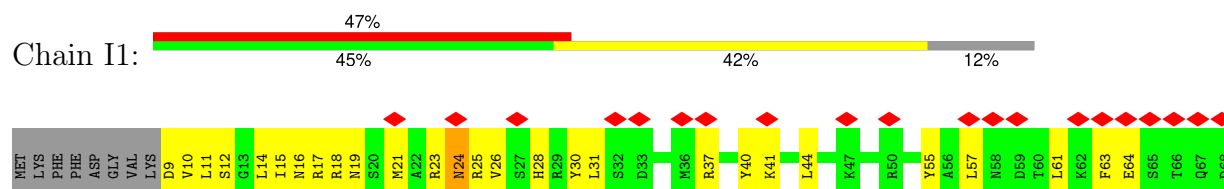
• Molecule 1: Portal protein

Chain H1:

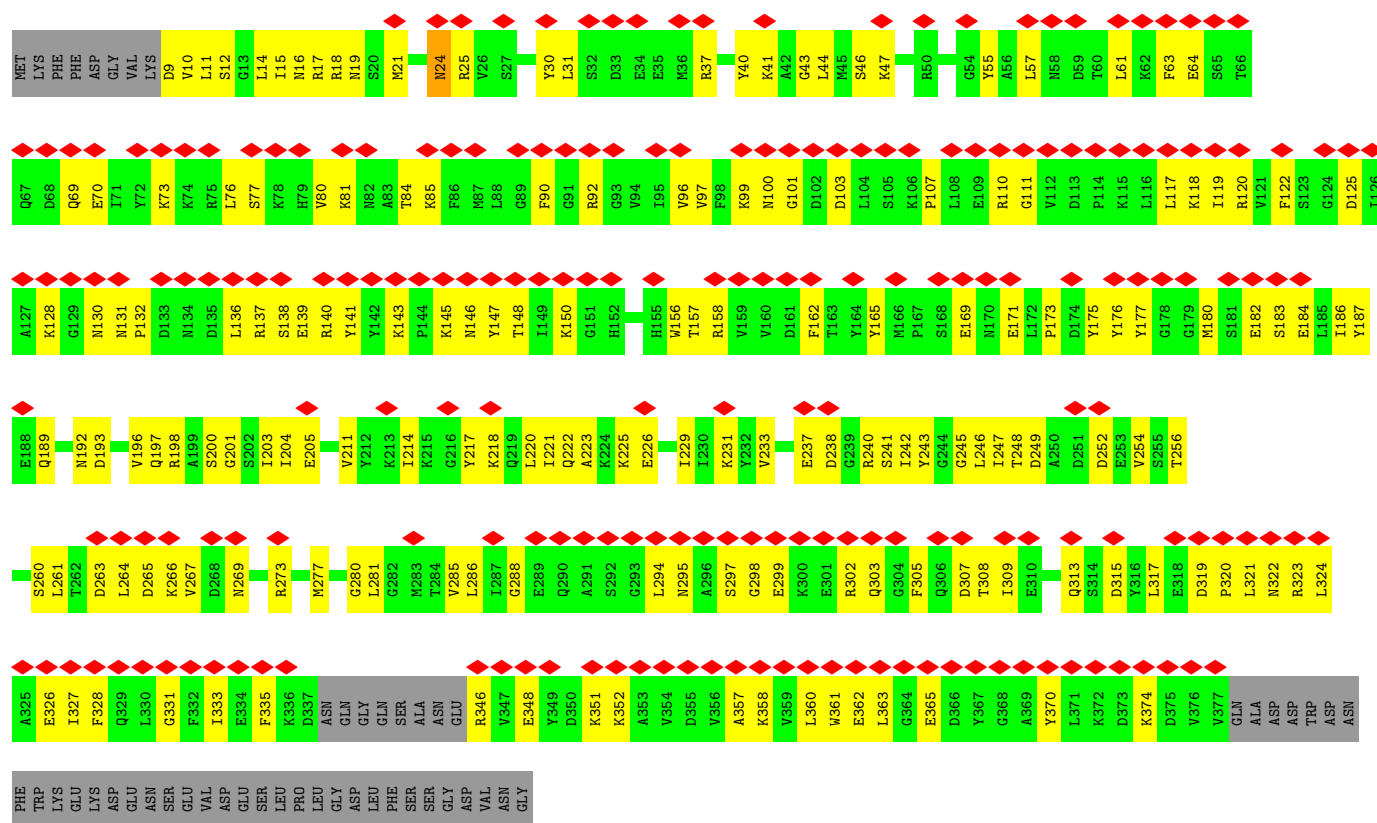


• Molecule 1: Portal protein

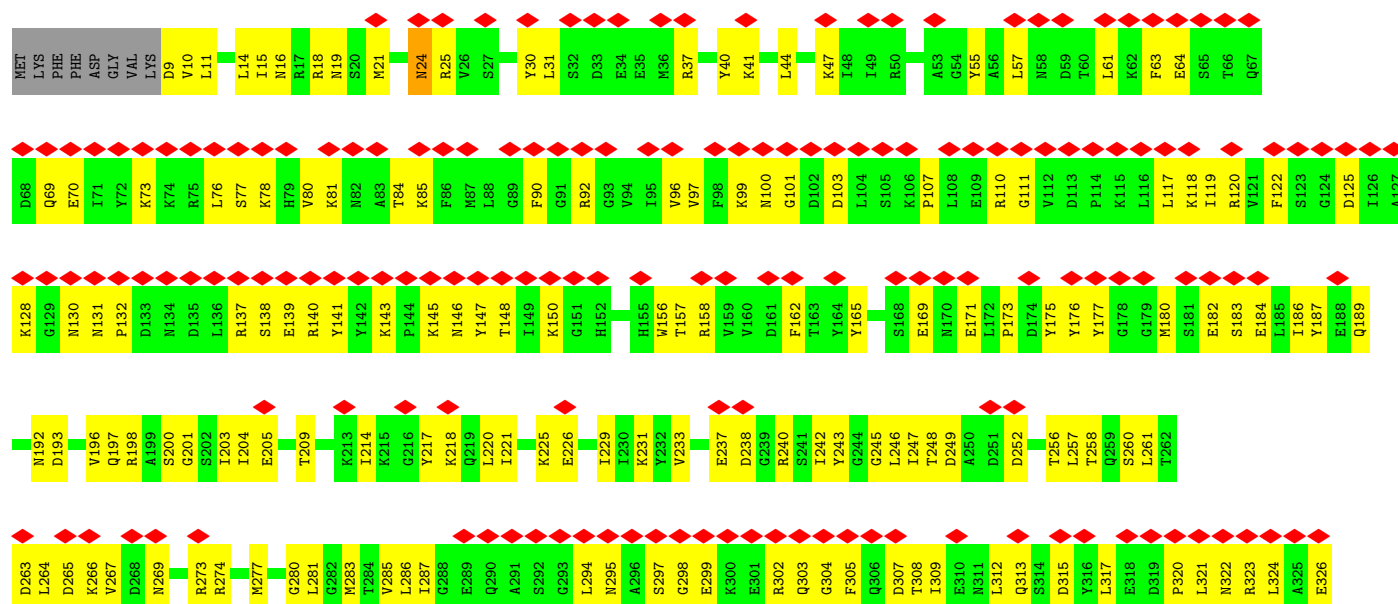
Chain I1:

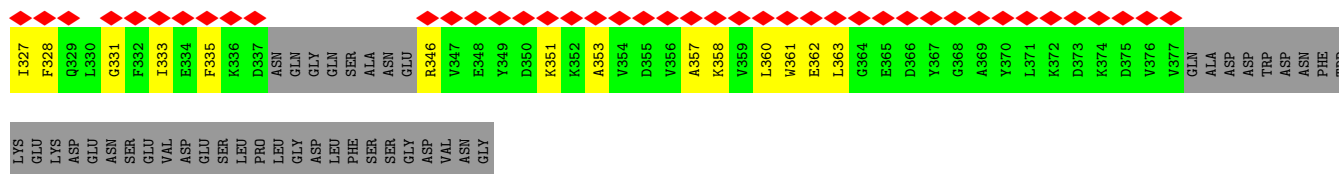




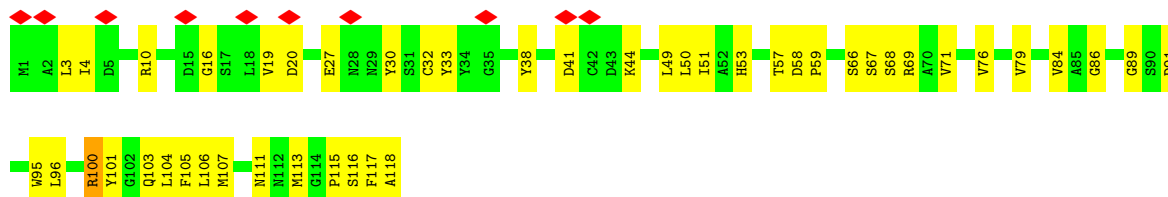


• Molecule 1: Portal protein

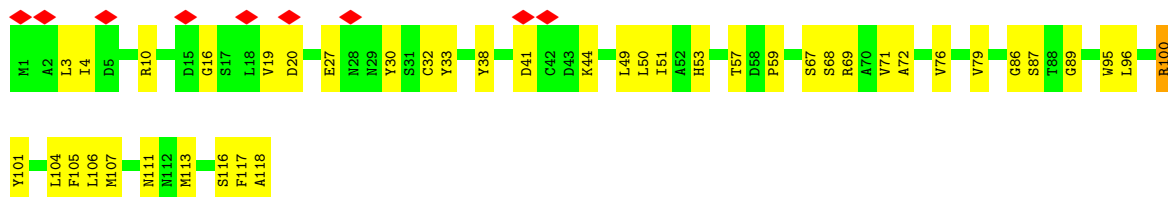




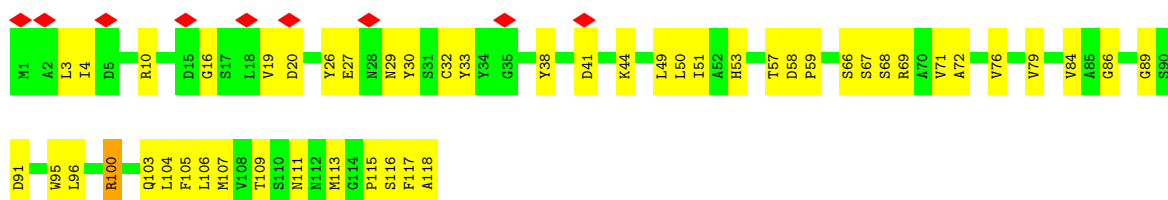
• Molecule 2: Head completion protein, gp1



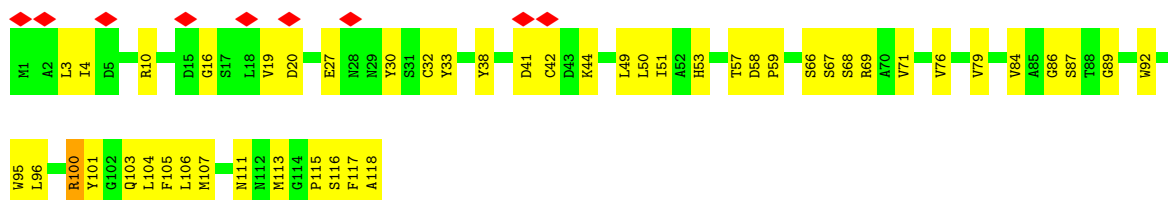
• Molecule 2: Head completion protein, gp1



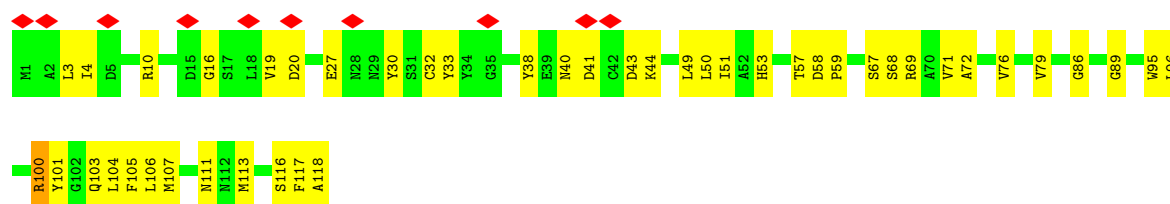
• Molecule 2: Head completion protein, gp1



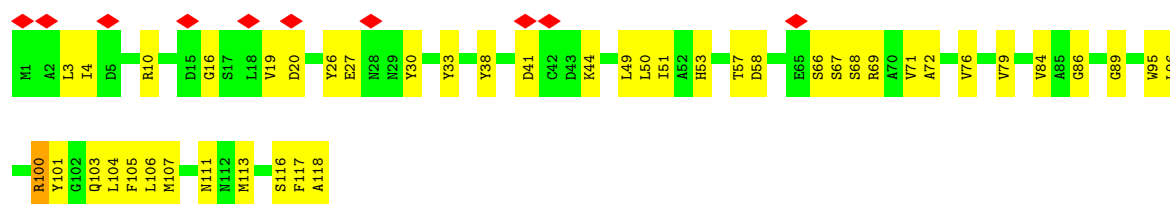
• Molecule 2: Head completion protein, gp1



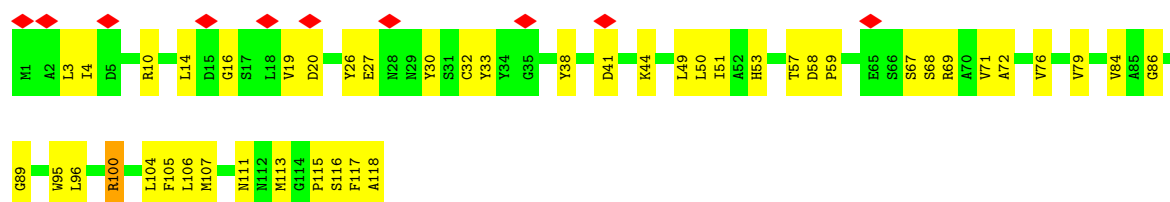
• Molecule 2: Head completion protein, gp1



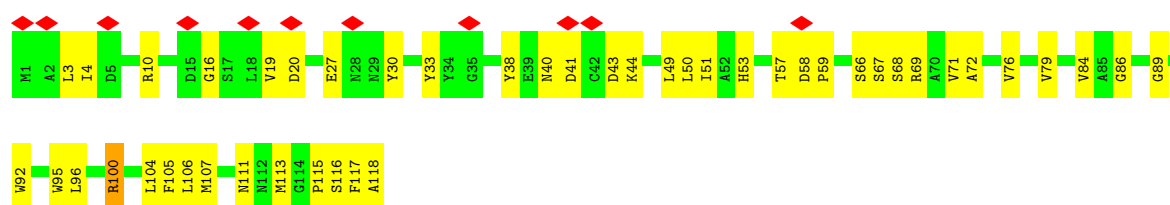
- Molecule 2: Head completion protein, gp1



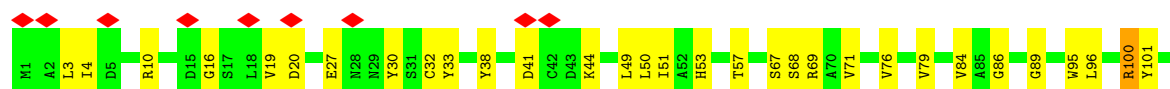
- Molecule 2: Head completion protein, gp1

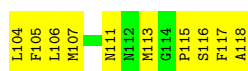


- Molecule 2: Head completion protein, gp1

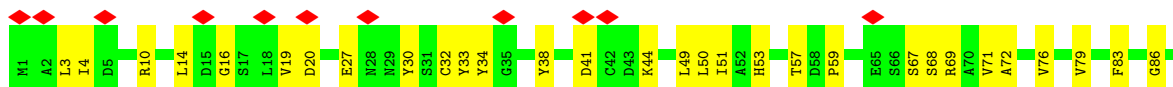


- Molecule 2: Head completion protein, gp1

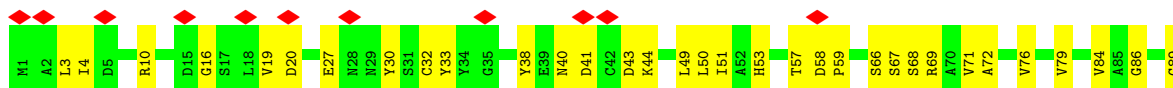




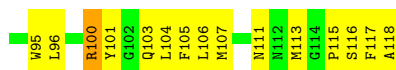
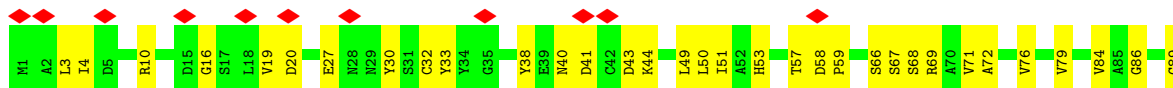
- Molecule 2: Head completion protein, gp1



- Molecule 2: Head completion protein, gp1



- Molecule 2: Head completion protein, gp1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16015	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 ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-16 (4k x 4k)	Depositor
Maximum map value	20.012	Depositor
Minimum map value	-13.155	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.548	Depositor
Recommended contour level	4.5	Depositor
Map size (\AA)	414.72, 414.72, 414.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.81, 0.81, 0.81	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	A1	0.37	0/2948	0.50	0/3963
1	B1	0.37	0/2948	0.50	0/3963
1	C1	0.37	0/2948	0.50	0/3963
1	D1	0.37	0/2948	0.50	0/3963
1	E1	0.37	0/2948	0.50	0/3963
1	F1	0.37	0/2948	0.50	0/3963
1	G1	0.37	0/2948	0.50	0/3963
1	H1	0.37	0/2948	0.50	0/3963
1	I1	0.37	0/2948	0.50	0/3963
1	J1	0.37	0/2948	0.50	0/3963
1	K1	0.37	0/2948	0.50	0/3963
1	L1	0.37	0/2948	0.50	0/3963
2	A2	0.50	0/915	0.57	0/1247
2	B2	0.50	0/915	0.57	0/1247
2	C2	0.50	0/915	0.57	0/1247
2	D2	0.50	0/915	0.57	0/1247
2	E2	0.50	0/915	0.57	0/1247
2	F2	0.50	0/915	0.57	0/1247
2	G2	0.50	0/915	0.57	0/1247
2	H2	0.50	0/915	0.57	0/1247
2	I2	0.50	0/915	0.57	0/1247
2	J2	0.50	0/915	0.57	0/1247
2	K2	0.50	0/915	0.57	0/1247
2	L2	0.51	0/915	0.57	0/1247
All	All	0.40	0/46356	0.52	0/62520

There are no bond length outliers.

There are no bond angle outliers.

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	A1	2902	0	2901	186	0
1	B1	2902	0	2901	199	0
1	C1	2902	0	2901	199	0
1	D1	2902	0	2901	200	0
1	E1	2902	0	2901	196	0
1	F1	2902	0	2901	185	0
1	G1	2902	0	2901	182	0
1	H1	2902	0	2901	213	0
1	I1	2902	0	2901	220	0
1	J1	2902	0	2901	196	0
1	K1	2902	0	2901	209	0
1	L1	2902	0	2901	193	0
2	A2	895	0	839	55	0
2	B2	895	0	839	51	0
2	C2	895	0	839	59	0
2	D2	895	0	839	57	0
2	E2	895	0	839	56	0
2	F2	895	0	839	46	0
2	G2	895	0	839	46	0
2	H2	895	0	839	53	0
2	I2	895	0	839	49	0
2	J2	895	0	839	46	0
2	K2	895	0	839	51	0
2	L2	895	0	839	56	0
All	All	45564	0	44880	2229	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 25.

The worst 5 of 2229 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:H1:197:GLN:NE2	1:I1:189:GLN:OE1	1.85	1.09
1:A1:24:ASN:HA	1:B1:11:LEU:HB3	1.37	1.07
1:K1:197:GLN:NE2	1:L1:189:GLN:OE1	1.91	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J1:24:ASN:HA	1:K1:11:LEU:HB3	1.42	0.98
1:K1:218:LYS:NZ	2:J2:113:MET:SD	2.36	0.98

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	A1	357/412 (87%)	313 (88%)	44 (12%)	0	100	100
1	B1	357/412 (87%)	314 (88%)	43 (12%)	0	100	100
1	C1	357/412 (87%)	314 (88%)	43 (12%)	0	100	100
1	D1	357/412 (87%)	314 (88%)	43 (12%)	0	100	100
1	E1	357/412 (87%)	314 (88%)	43 (12%)	0	100	100
1	F1	357/412 (87%)	314 (88%)	43 (12%)	0	100	100
1	G1	357/412 (87%)	314 (88%)	43 (12%)	0	100	100
1	H1	357/412 (87%)	314 (88%)	43 (12%)	0	100	100
1	I1	357/412 (87%)	314 (88%)	43 (12%)	0	100	100
1	J1	357/412 (87%)	314 (88%)	43 (12%)	0	100	100
1	K1	357/412 (87%)	314 (88%)	43 (12%)	0	100	100
1	L1	357/412 (87%)	314 (88%)	43 (12%)	0	100	100
2	A2	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
2	B2	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
2	C2	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
2	D2	116/118 (98%)	105 (90%)	11 (10%)	0	100	100
2	E2	116/118 (98%)	105 (90%)	11 (10%)	0	100	100
2	F2	116/118 (98%)	106 (91%)	10 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G2	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
2	H2	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
2	I2	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
2	J2	116/118 (98%)	105 (90%)	11 (10%)	0	100	100
2	K2	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
2	L2	116/118 (98%)	105 (90%)	11 (10%)	0	100	100
All	All	5676/6360 (89%)	5035 (89%)	641 (11%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A1	317/361 (88%)	315 (99%)	2 (1%)	84	92
1	B1	317/361 (88%)	315 (99%)	2 (1%)	84	92
1	C1	317/361 (88%)	315 (99%)	2 (1%)	84	92
1	D1	317/361 (88%)	315 (99%)	2 (1%)	84	92
1	E1	317/361 (88%)	315 (99%)	2 (1%)	84	92
1	F1	317/361 (88%)	315 (99%)	2 (1%)	84	92
1	G1	317/361 (88%)	315 (99%)	2 (1%)	84	92
1	H1	317/361 (88%)	315 (99%)	2 (1%)	84	92
1	I1	317/361 (88%)	315 (99%)	2 (1%)	84	92
1	J1	317/361 (88%)	315 (99%)	2 (1%)	84	92
1	K1	317/361 (88%)	315 (99%)	2 (1%)	84	92
1	L1	317/361 (88%)	315 (99%)	2 (1%)	84	92
2	A2	100/100 (100%)	99 (99%)	1 (1%)	73	85
2	B2	100/100 (100%)	99 (99%)	1 (1%)	73	85
2	C2	100/100 (100%)	99 (99%)	1 (1%)	73	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D2	100/100 (100%)	99 (99%)	1 (1%)	73	85
2	E2	100/100 (100%)	99 (99%)	1 (1%)	73	85
2	F2	100/100 (100%)	99 (99%)	1 (1%)	73	85
2	G2	100/100 (100%)	99 (99%)	1 (1%)	73	85
2	H2	100/100 (100%)	99 (99%)	1 (1%)	73	85
2	I2	100/100 (100%)	99 (99%)	1 (1%)	73	85
2	J2	100/100 (100%)	99 (99%)	1 (1%)	73	85
2	K2	100/100 (100%)	99 (99%)	1 (1%)	73	85
2	L2	100/100 (100%)	99 (99%)	1 (1%)	73	85
All	All	5004/5532 (90%)	4968 (99%)	36 (1%)	80	90

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E2	100	ARG
2	L2	100	ARG
2	F2	100	ARG
2	I2	100	ARG
1	G1	24	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	J1	303	GLN
2	A2	53	HIS
1	K1	189	GLN
1	L1	189	GLN
2	C2	53	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22917. These allow visual inspection of the internal detail of the map and identification of artifacts.

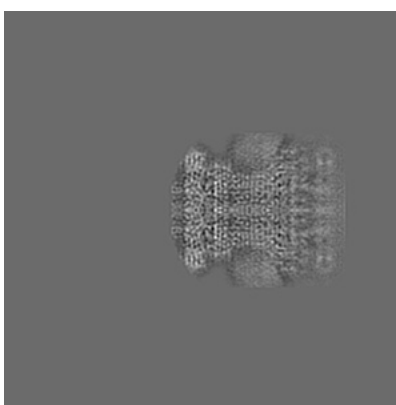
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

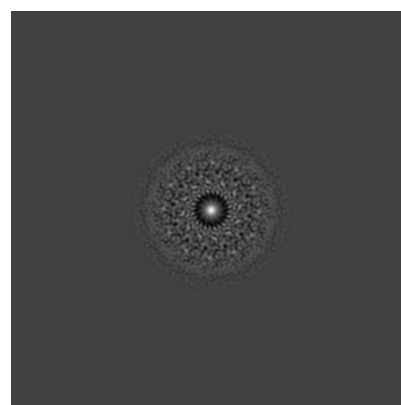
6.1.1 Primary map



X



Y

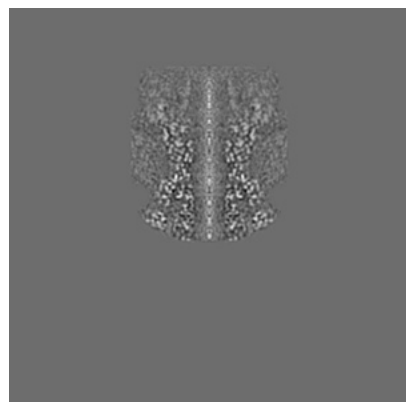


Z

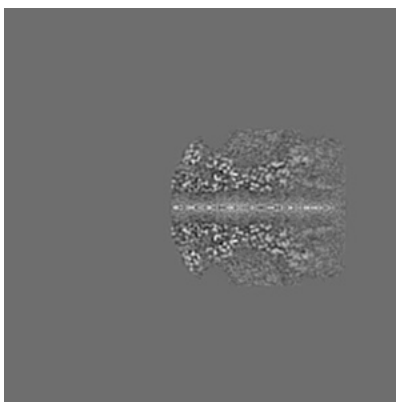
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

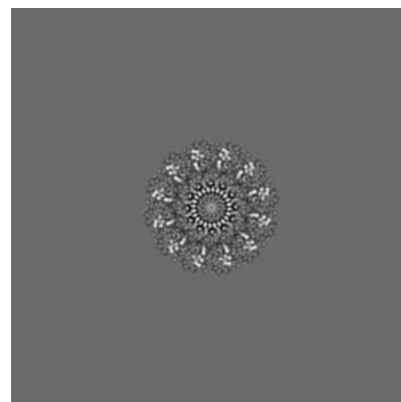
6.2.1 Primary map



X Index: 256



Y Index: 256

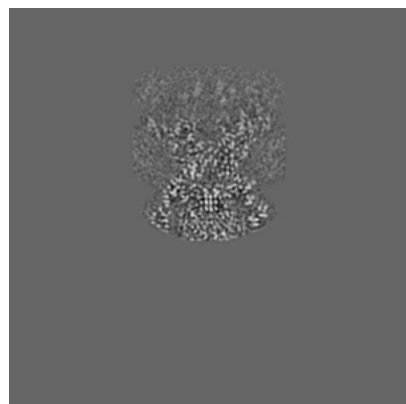


Z Index: 256

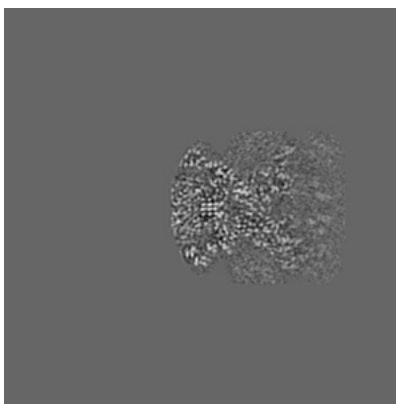
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

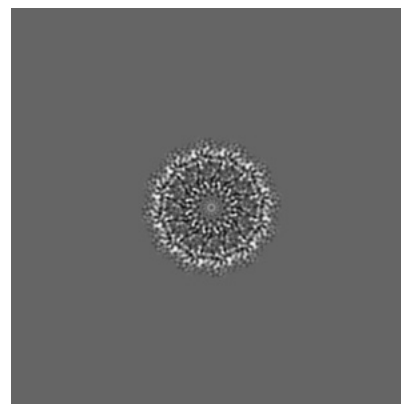
6.3.1 Primary map



X Index: 233



Y Index: 233

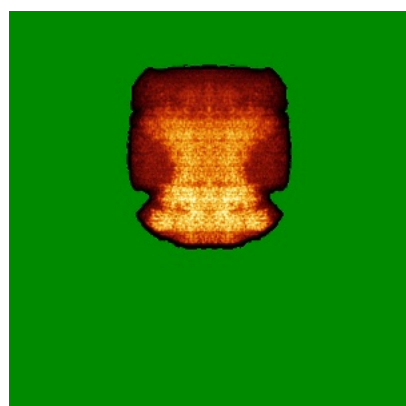


Z Index: 246

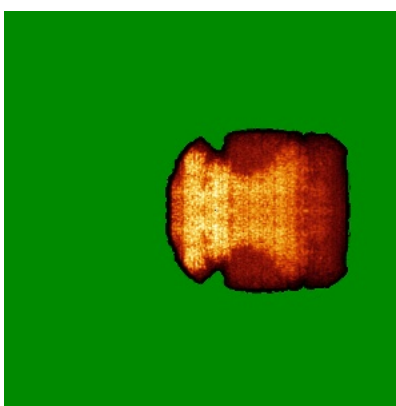
The images above show the largest variance slices of the map in three orthogonal directions.

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

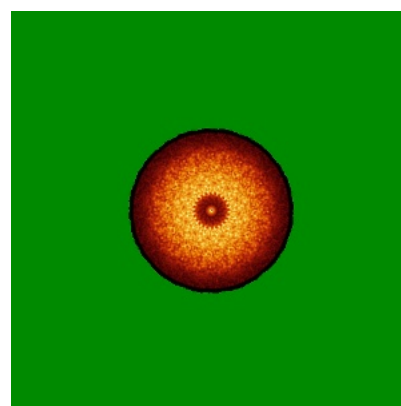
6.4.1 Primary map



X



Y

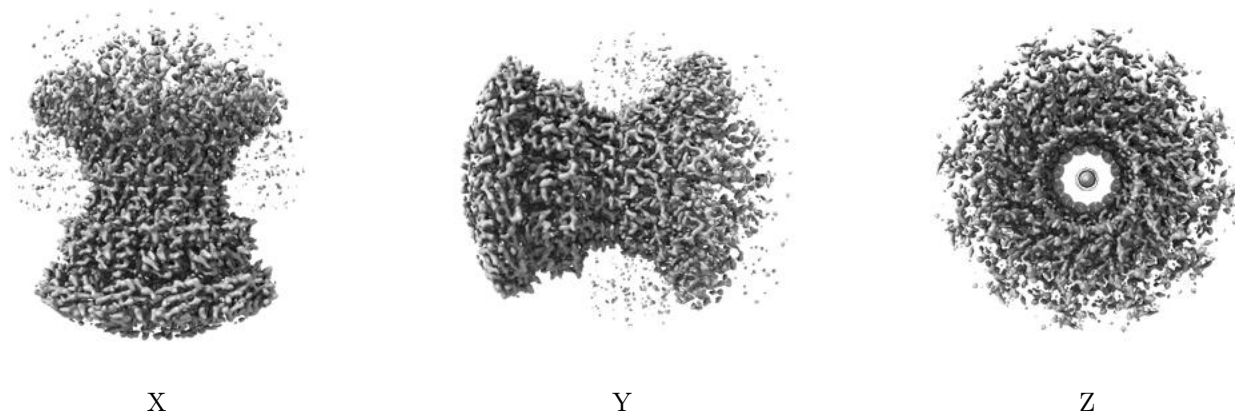


Z

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

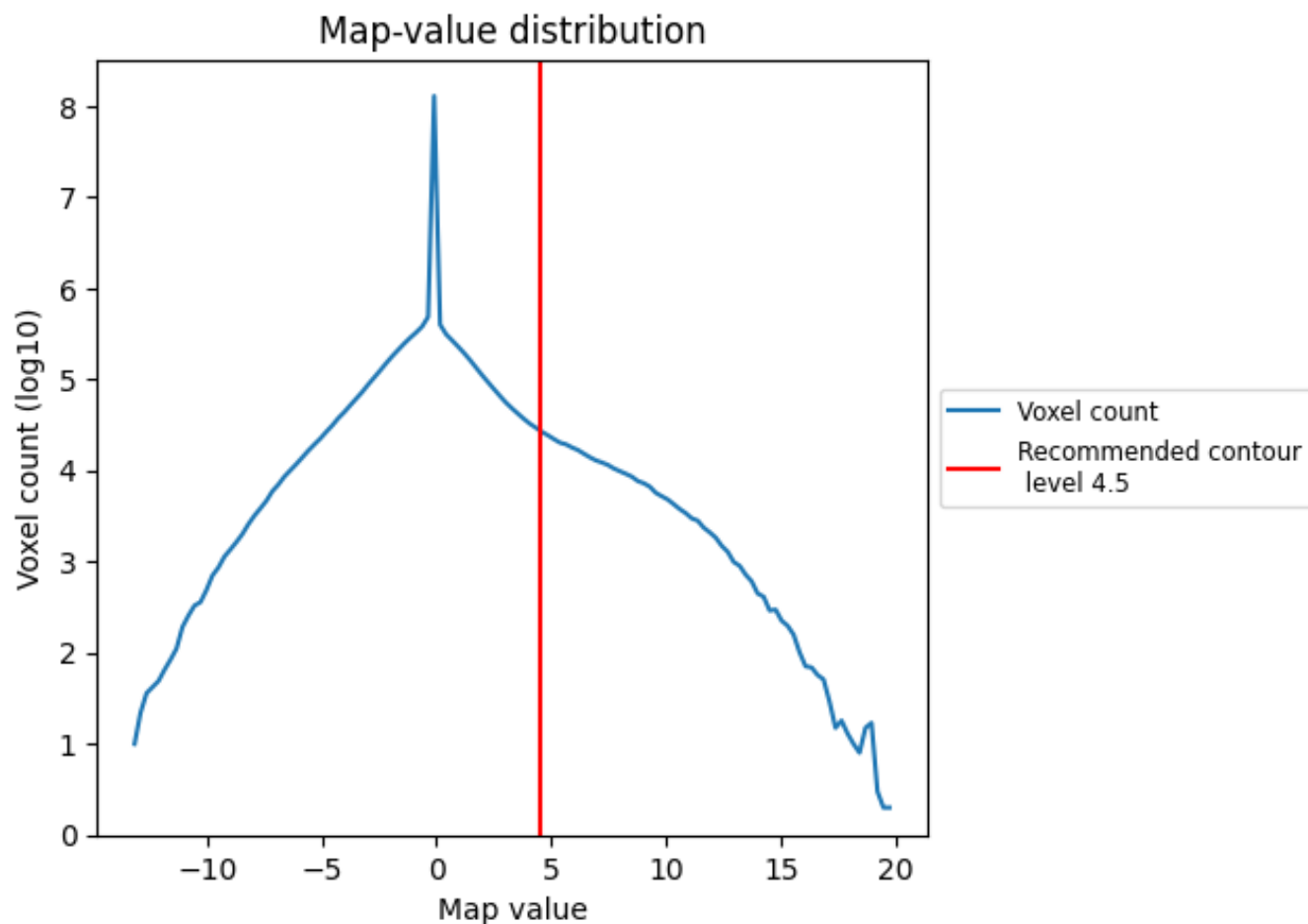
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

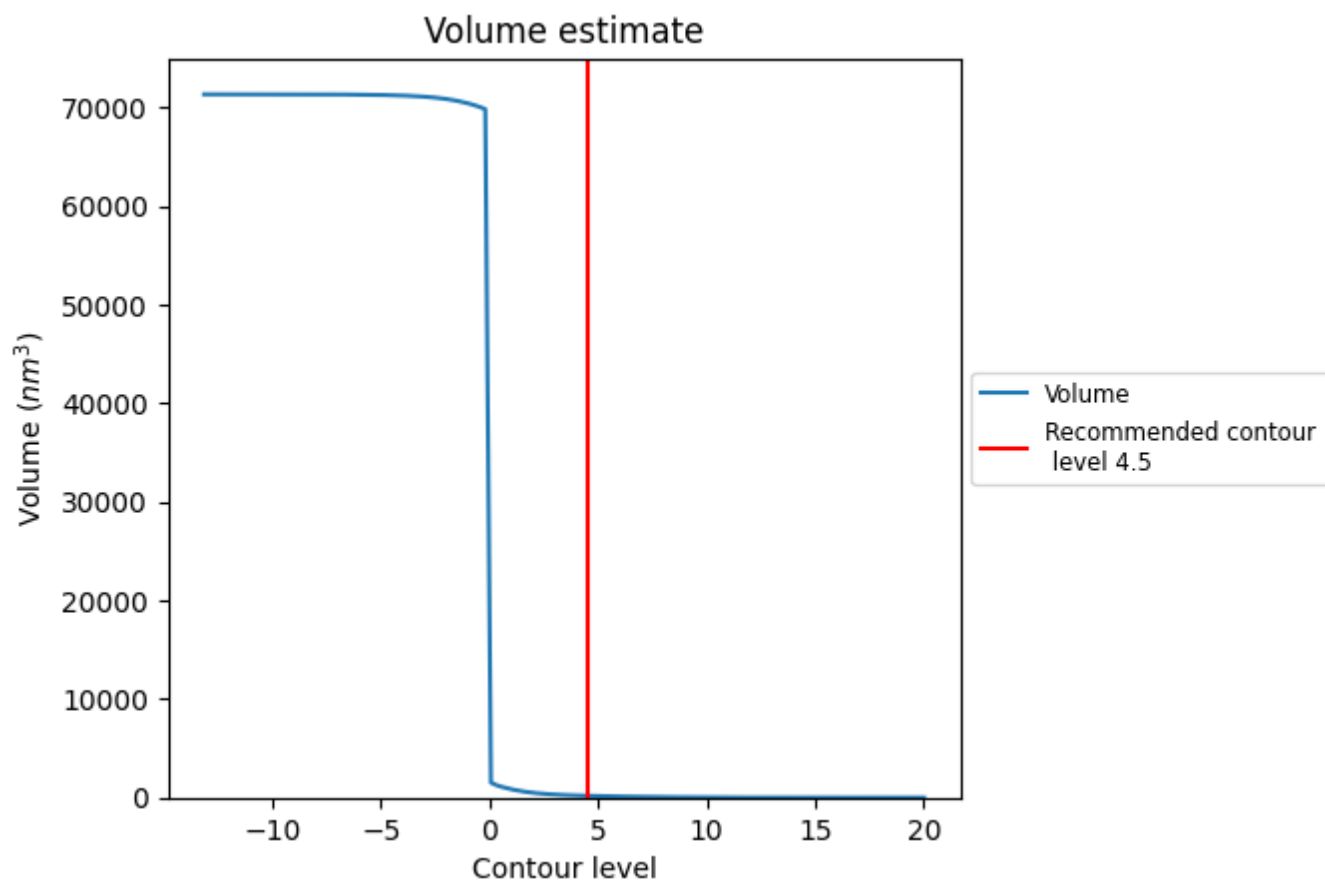
This section contains the results of statistical analysis of the map.

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.

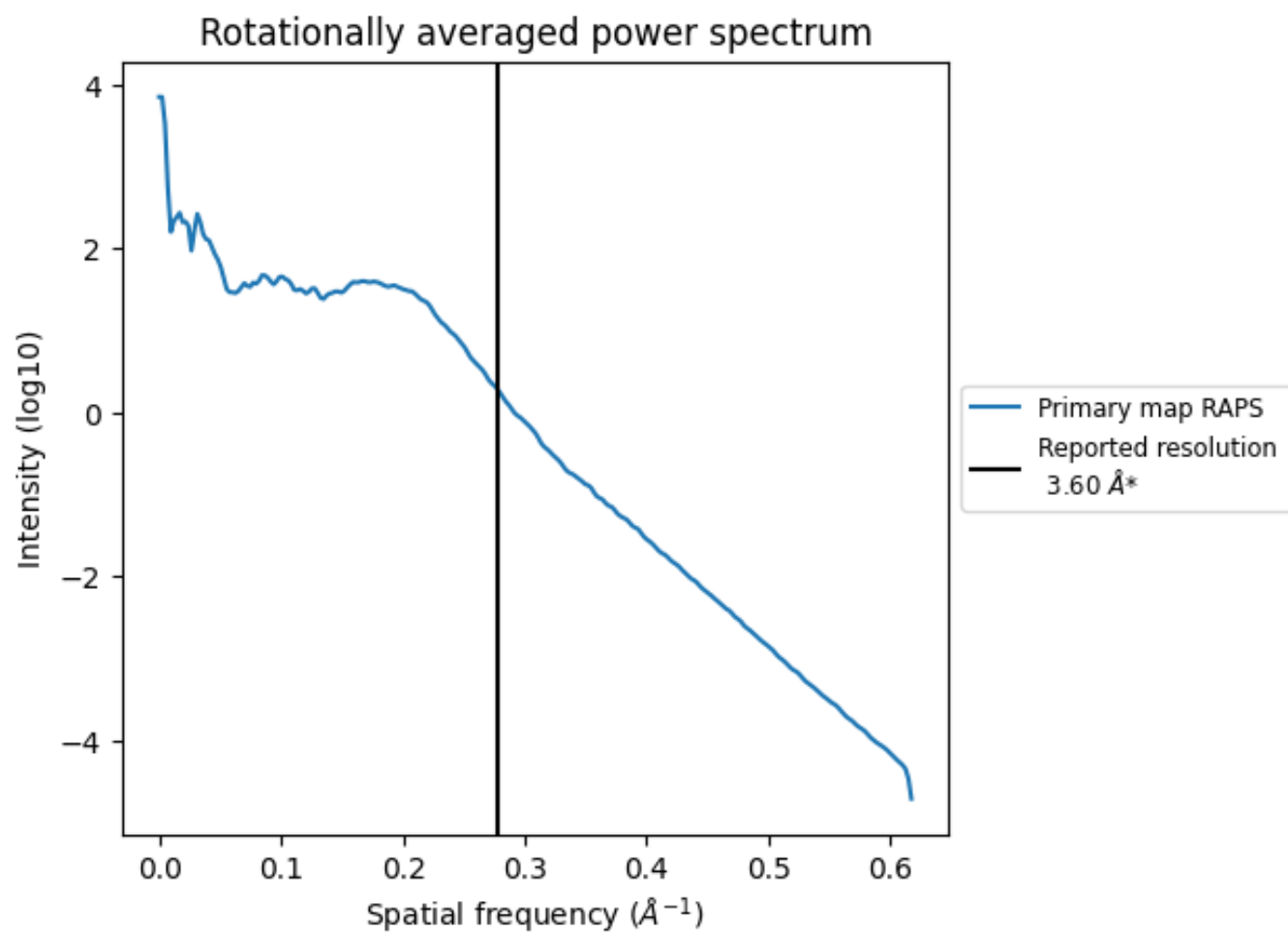
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 176 nm^3 ; this corresponds to an approximate mass of 159 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 ⓘ

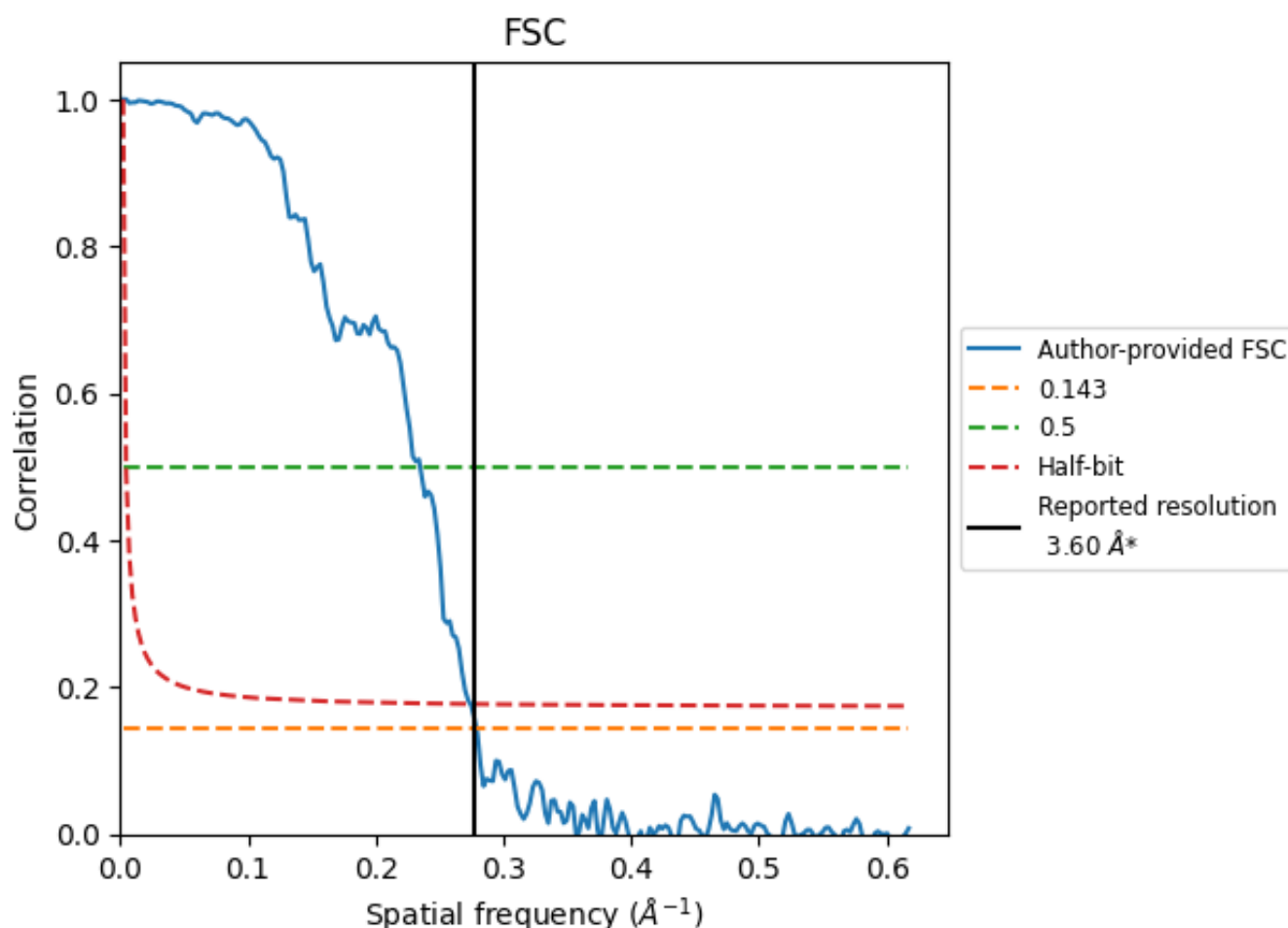


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

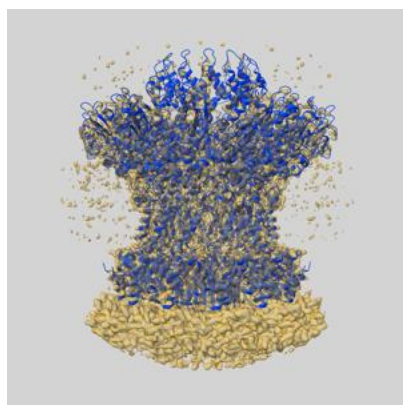
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.58	4.26	3.65
Unmasked-calculated*	-	-	-

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

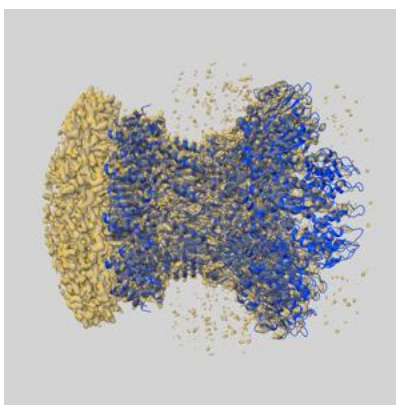
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22917 and PDB model 7KLN. Per-residue inclusion information can be found in section [3](#) on page [6](#).

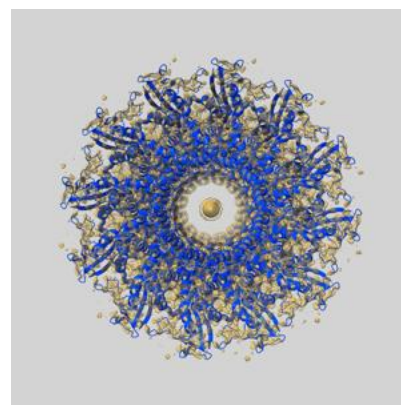
9.1 Map-model overlay [i](#)



X



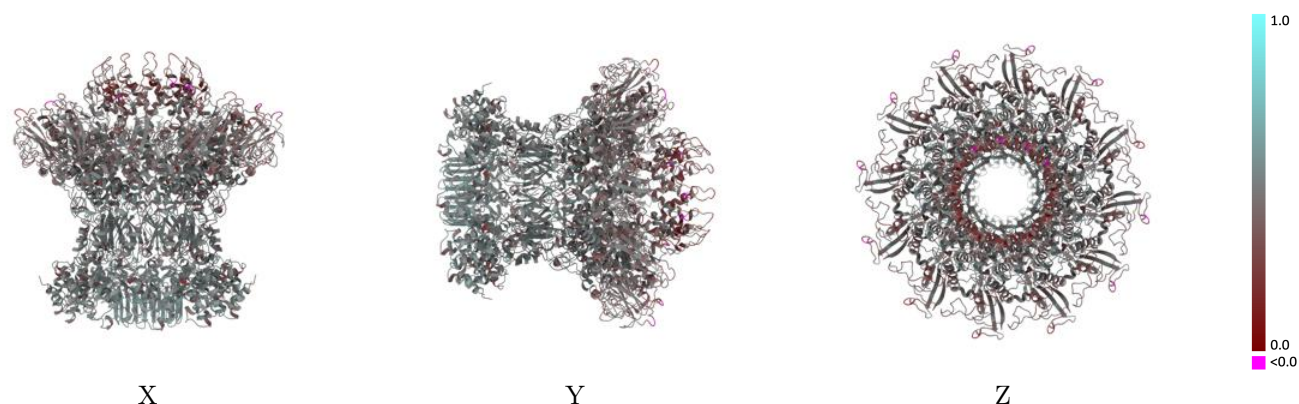
Y



Z

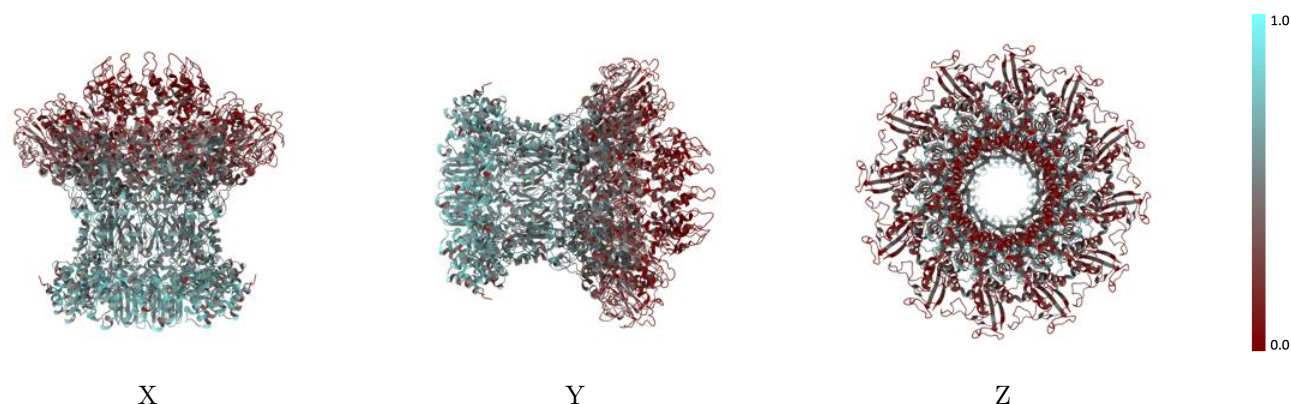
The images above show the 3D surface view of the map at the recommended contour level 4.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



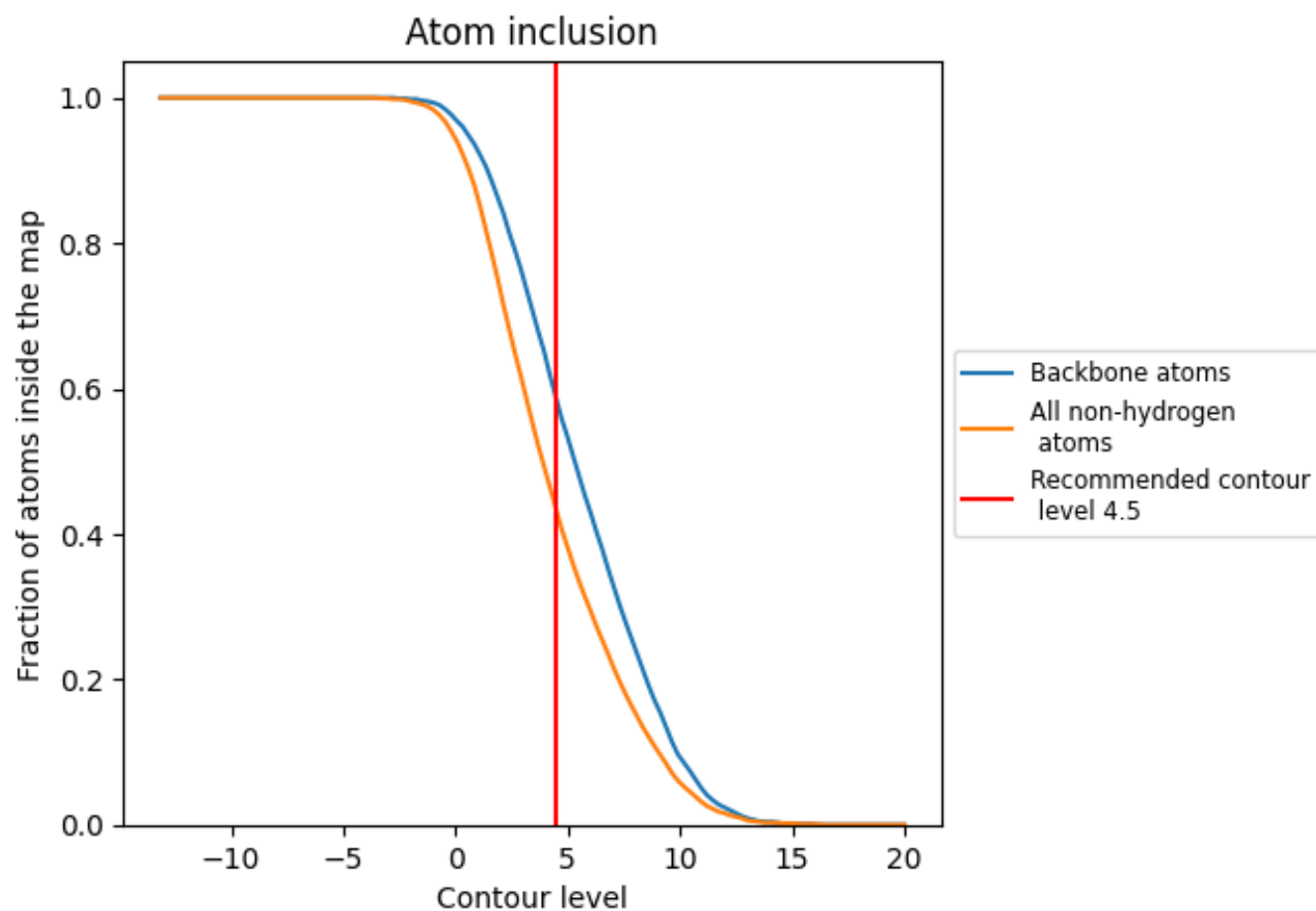
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.5).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 43% 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 (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4310	 0.4550
A1	 0.3490	 0.4350
A2	 0.6470	 0.5050
B1	 0.3530	 0.4350
B2	 0.6540	 0.5070
C1	 0.3590	 0.4420
C2	 0.6540	 0.5050
D1	 0.3620	 0.4450
D2	 0.6510	 0.5050
E1	 0.3640	 0.4400
E2	 0.6540	 0.5080
F1	 0.3680	 0.4400
F2	 0.6480	 0.5030
G1	 0.3710	 0.4420
G2	 0.6450	 0.5060
H1	 0.3710	 0.4420
H2	 0.6490	 0.5050
I1	 0.3740	 0.4430
I2	 0.6520	 0.5000
J1	 0.3680	 0.4440
J2	 0.6350	 0.5020
K1	 0.3580	 0.4400
K2	 0.6490	 0.5030
L1	 0.3550	 0.4320
L2	 0.6480	 0.5030

