wwPDB EM Validation Summary Report

Oct 28, 2024 – 12:21 pm GMT

PDB ID	:	6ROW
EMDB ID	:	EMD-4975
Title	:	Haemonchus galactose containing glycoprotein complex
Authors	:	Scarff, C.A.; Thompson, R.F.; Newlands, G.F.J.; Jamson, H.; Kennaway, C.; da Silva, V.J.; Rabelo, E.M.; Song, C.F.; Trinick, J.; Smith, W.D.; Muench, S.P.
Deposited on	:	2019-05-13
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 (i) 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 (i)) were used in the production of this report:

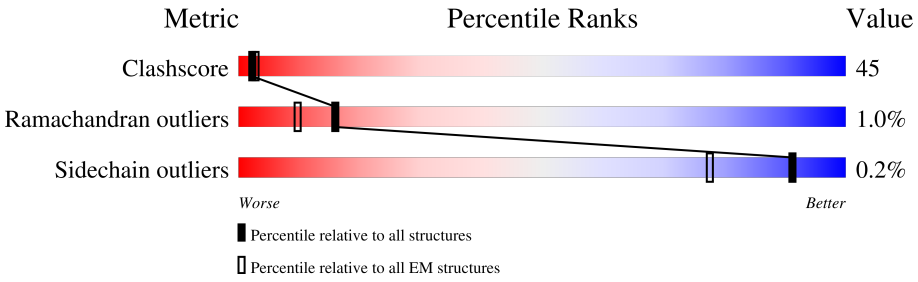
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: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

1 Overall quality at a glance (i)

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 <=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	755	26% 52% · 21%
1	B	755	28% 53% · 18%
1	C	755	25% 51% · 23%
1	D	755	33% 42% 25%
2	E	369	57% 24% 19%
2	F	369	59% 20% 21%
3	G	253	64% · · 32%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 43049 atoms, of which 20156 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 Putative zinc metallopeptidase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	596	Total	C	H	N	O	S	0	0
			9475	3063	4638	824	919	31		
1	B	619	Total	C	H	N	O	S	0	0
			9828	3187	4817	845	946	33		
1	C	583	Total	C	H	N	O	S	0	0
			9290	3010	4556	801	893	30		
1	D	566	Total	C	H	N	O	S	0	0
			8988	2910	4413	777	860	28		

- Molecule 2 is a protein called Parasite pepsinogen.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	299	Total	C	H	N	O	0	0
			2133	860	676	299	298		
2	F	293	Total	C	H	N	O	0	0
			2093	844	664	293	292		

- Molecule 3 is a protein called Cysteine Protease.

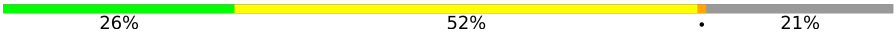
Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	173	Total	C	H	N	O	0	0
			1242	504	392	173	173		

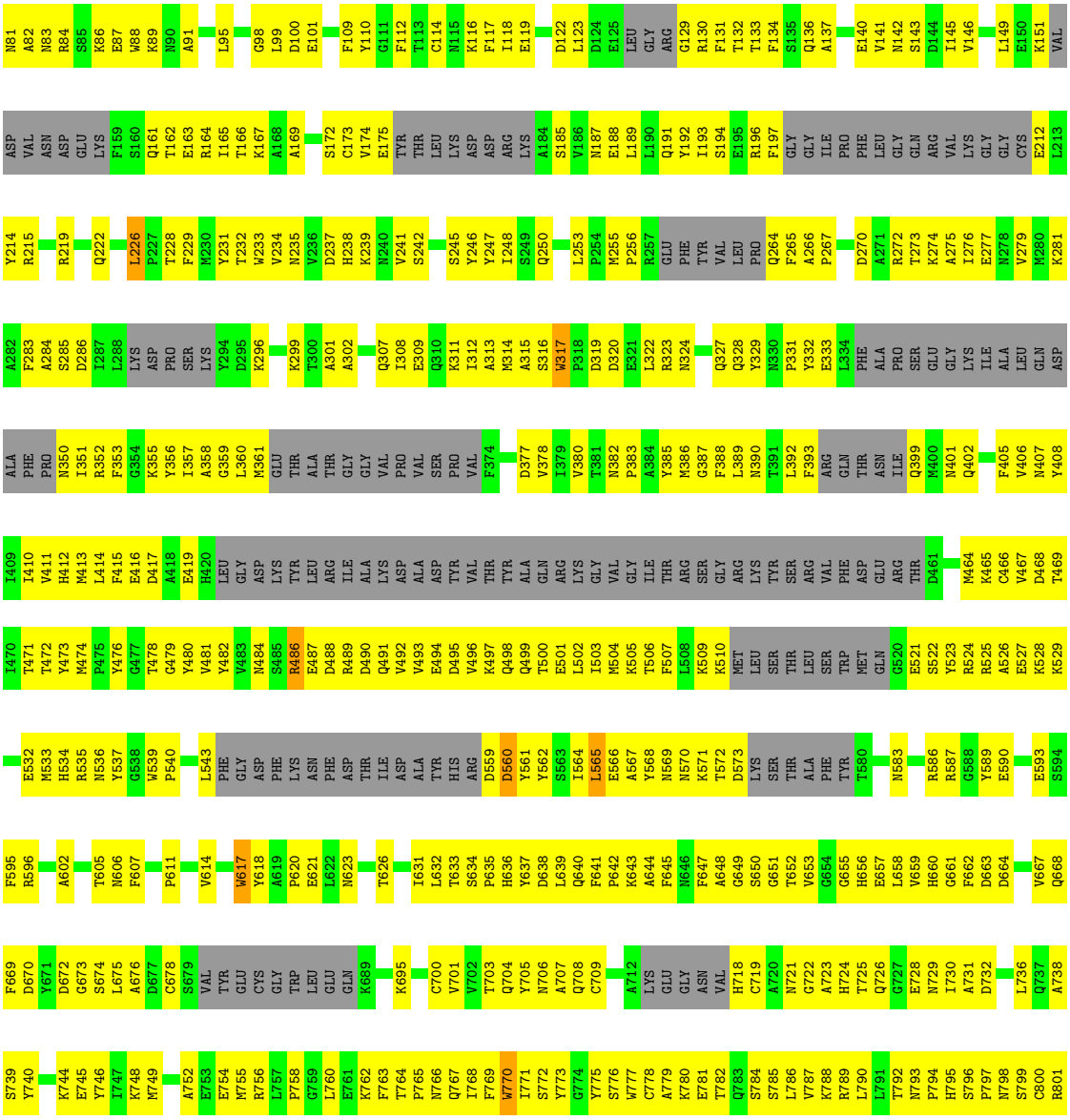
3 Residue-property plots (i)

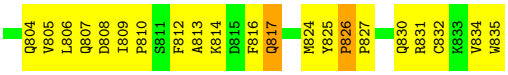
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain A:

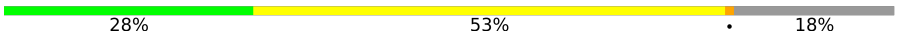


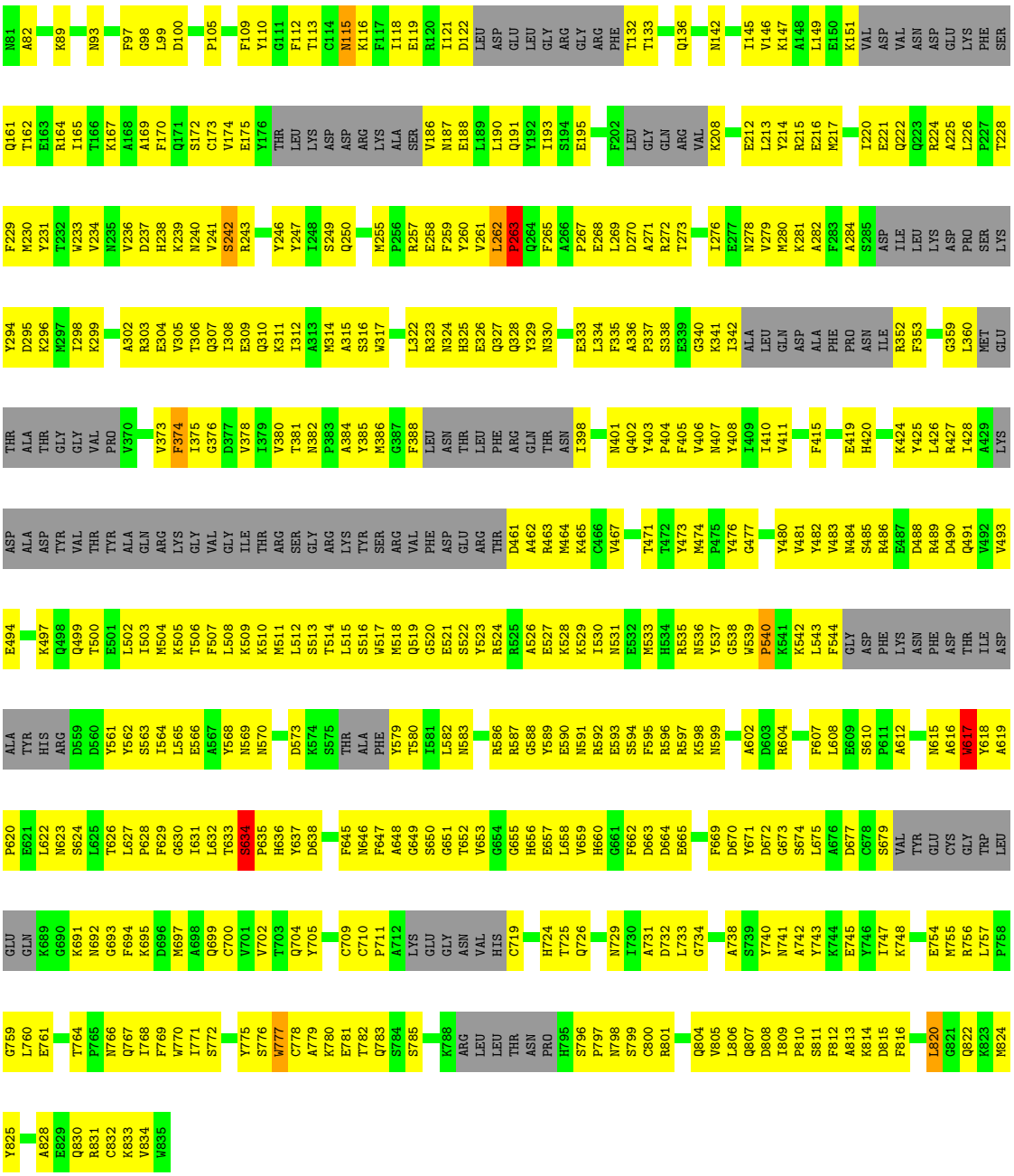




• Molecule 1: Putative zinc metallopeptidase

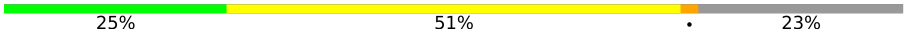
Chain B:

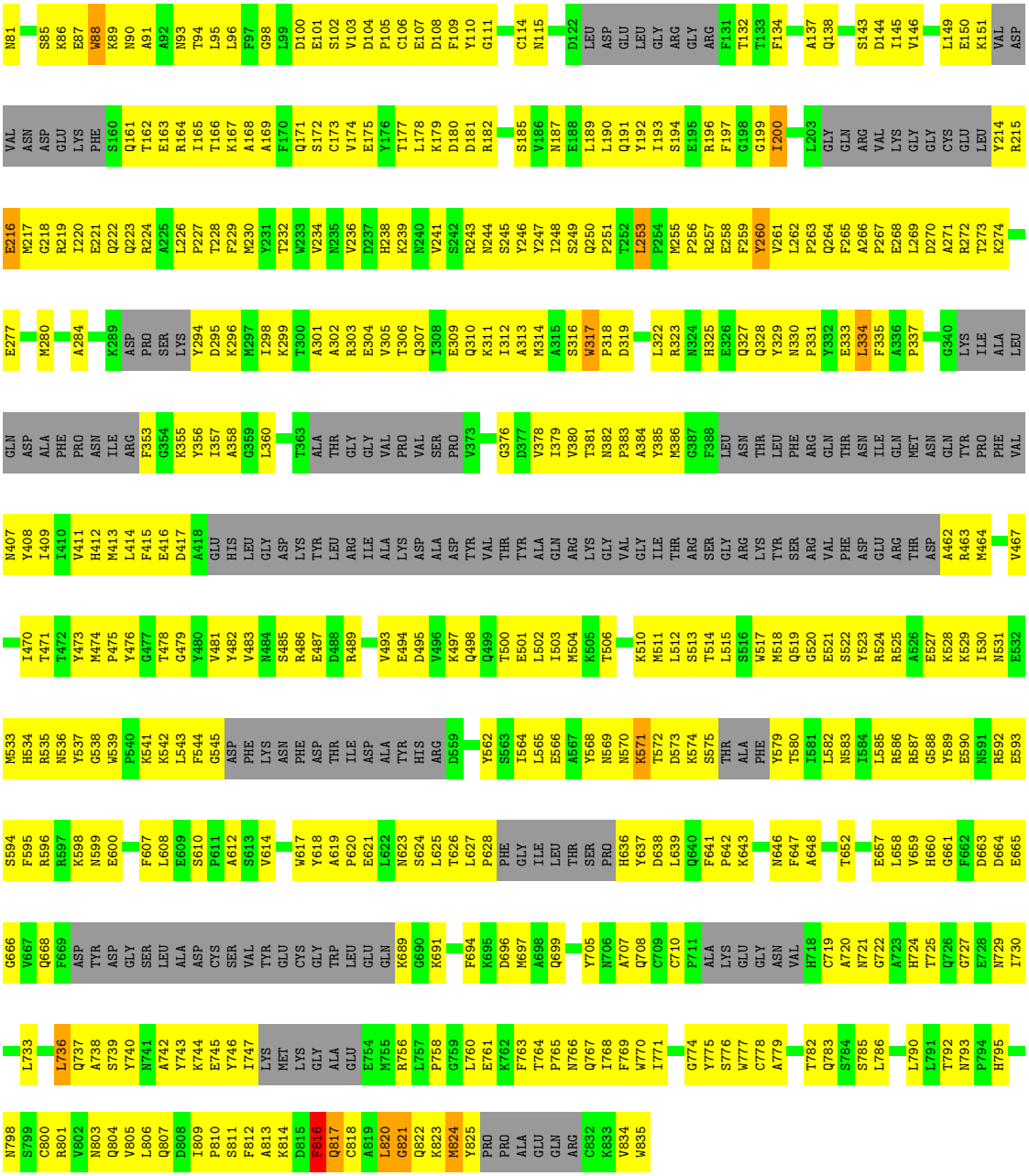




• Molecule 1: Putative zinc metallopeptidase

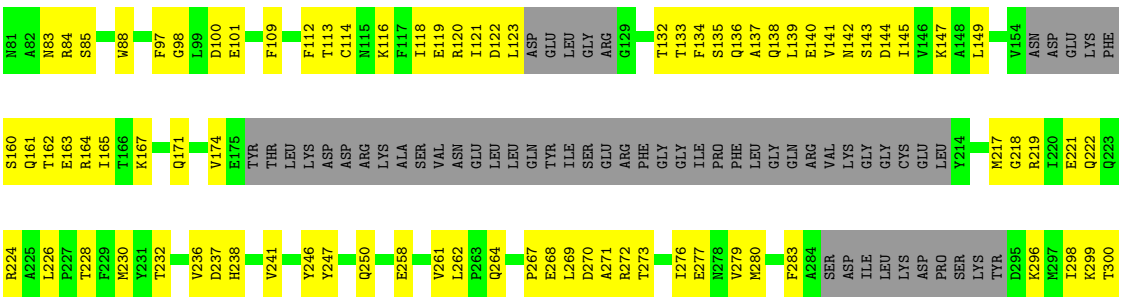
Chain C:

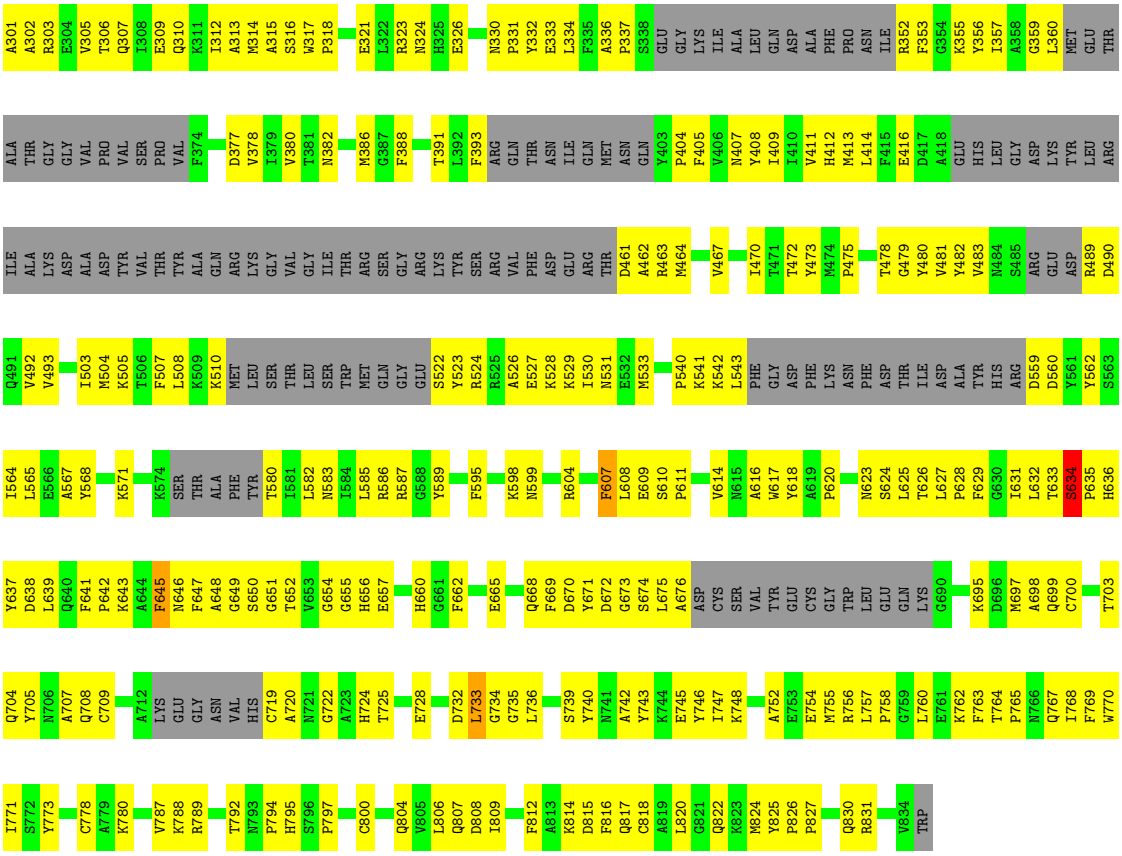




• Molecule 1: Putative zinc metallopeptidase

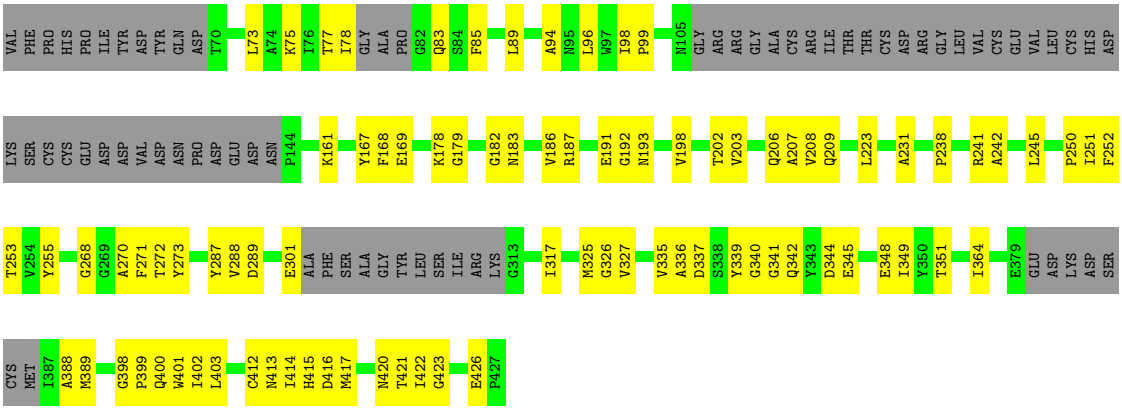
Chain D:





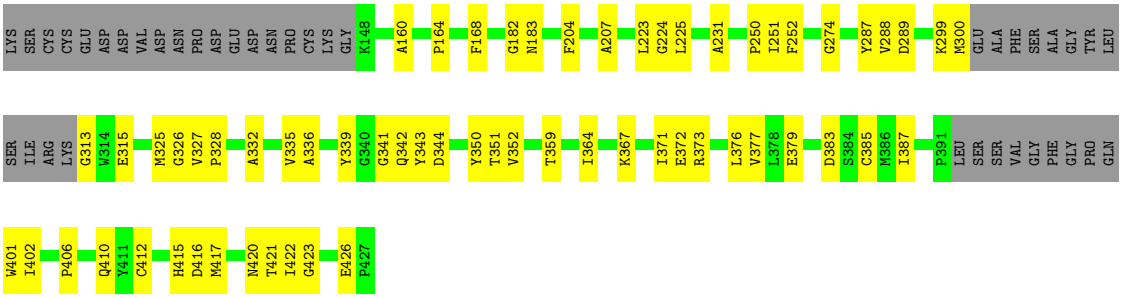
• Molecule 2: Parasite pepsinogen

Chain E:

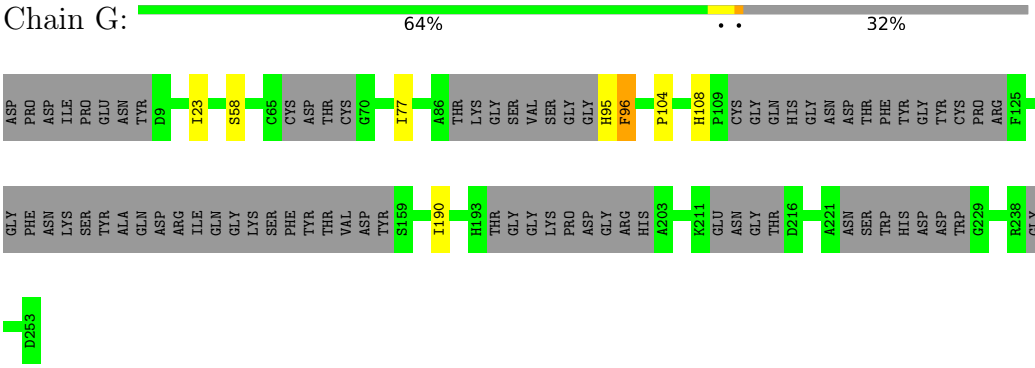


• Molecule 2: Parasite pepsinogen

Chain F:



- Molecule 3: Cysteine Protease



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	110863	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	62.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.303	Depositor
Minimum map value	-0.131	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	387.66003, 387.66003, 387.66003	wwPDB
Map dimensions	364, 364, 364	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.91	3/4938 (0.1%)	0.76	4/6653 (0.1%)
1	B	0.88	7/5122 (0.1%)	0.77	3/6903 (0.0%)
1	C	0.82	5/4835 (0.1%)	0.73	2/6513 (0.0%)
1	D	0.78	2/4674 (0.0%)	0.71	2/6304 (0.0%)
2	E	0.32	0/1452	0.52	0/2003
2	F	0.39	0/1424	0.56	0/1965
3	G	0.80	0/841	0.91	5/1154 (0.4%)
All	All	0.81	17/23286 (0.1%)	0.73	16/31495 (0.1%)

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	A	0	5
1	B	0	4
1	C	0	6
1	D	0	1
All	All	0	16

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	263	PRO	N-CD	-13.97	1.28	1.47
1	B	540	PRO	N-CD	8.81	1.60	1.47
1	C	816	PHE	CA-CB	-7.78	1.36	1.53
1	B	617	TRP	CB-CG	-7.30	1.37	1.50
1	A	617	TRP	CB-CG	-7.19	1.37	1.50

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	262	LEU	C-N-CD	-8.98	100.84	120.60
1	A	565	LEU	CA-CB-CG	-7.90	97.13	115.30
1	C	253	LEU	CA-CB-CG	-7.60	97.83	115.30
1	B	262	LEU	N-CA-C	7.23	130.52	111.00
1	A	129	GLY	N-CA-C	7.07	130.77	113.10

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	VAL	Peptide
1	A	486	ARG	Peptide
1	A	560	ASP	Peptide
1	A	676	ALA	Peptide
1	A	826	PRO	Peptide

5.2 Too-close contacts (i)

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	4837	4638	4636	503	0
1	B	5011	4817	4815	524	0
1	C	4734	4556	4555	455	0
1	D	4575	4413	4413	355	0
2	E	1457	676	676	60	0
2	F	1429	664	663	41	0
3	G	850	392	389	2	0
All	All	22893	20156	20147	1925	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 45.

The worst 5 of 1925 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:B:540:PRO:HA	1:B:607:PHE:CZ	1.47	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:LYS:HD3	1:A:329:TYR:CE2	1.64	1.33
1:A:234:VAL:HG23	1:A:245:SER:O	1.20	1.29
1:D:760:LEU:HD11	1:D:763:PHE:CE2	1.67	1.29
1:A:474:MET:CE	1:A:586:ARG:HD2	1.64	1.27

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	564/755 (75%)	375 (66%)	188 (33%)	1 (0%)	44 78
1	B	589/755 (78%)	385 (65%)	196 (33%)	8 (1%)	9 40
1	C	551/755 (73%)	364 (66%)	181 (33%)	6 (1%)	12 46
1	D	536/755 (71%)	378 (70%)	153 (28%)	5 (1%)	14 51
2	E	289/369 (78%)	217 (75%)	72 (25%)	0	100 100
2	F	283/369 (77%)	198 (70%)	81 (29%)	4 (1%)	9 40
3	G	155/253 (61%)	121 (78%)	29 (19%)	5 (3%)	3 21
All	All	2967/4011 (74%)	2038 (69%)	900 (30%)	29 (1%)	16 49

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	817	GLN
1	C	820	LEU
2	F	168	PHE
3	G	104	PRO
1	C	107	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	521/655 (80%)	521 (100%)	0	100 100
1	B	538/655 (82%)	536 (100%)	2 (0%)	89 90
1	C	510/655 (78%)	510 (100%)	0	100 100
1	D	492/655 (75%)	490 (100%)	2 (0%)	89 90
All	All	2061/2620 (79%)	2057 (100%)	4 (0%)	91 93

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	617	TRP
1	B	724	HIS
1	D	388	PHE
1	D	607	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	382	ASN
1	C	536	ASN
1	C	795	HIS
1	C	583	ASN
1	A	704	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

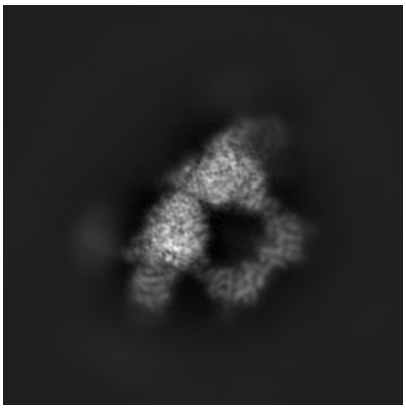
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4975. These allow visual inspection of the internal detail of the map and identification of artifacts.

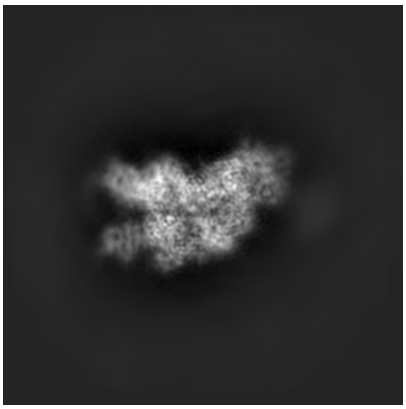
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

6.1.1 Primary map



X



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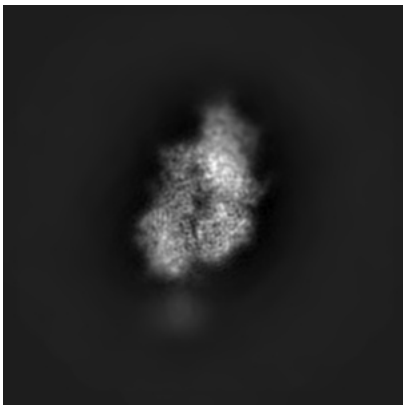
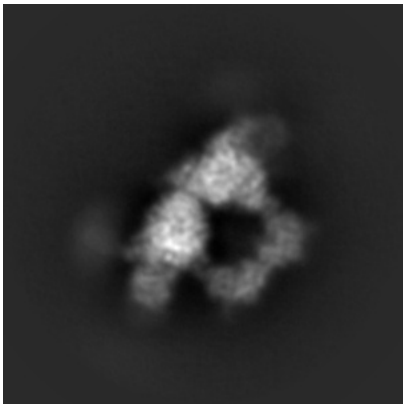


Z

6.1.2 Raw map



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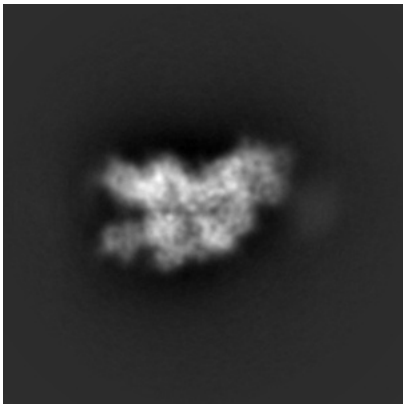

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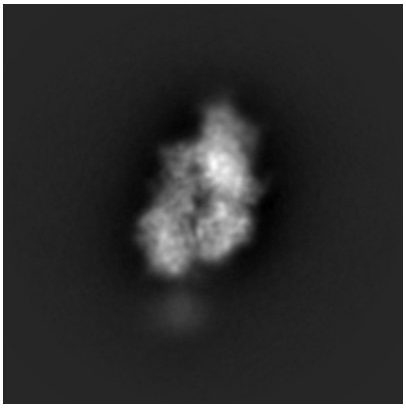
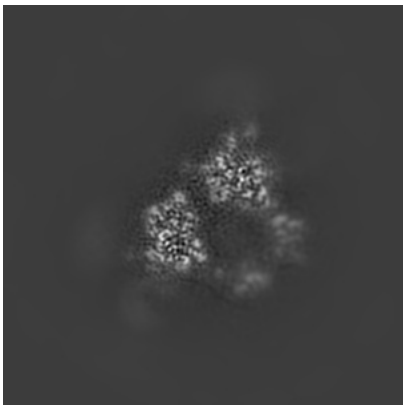


Z

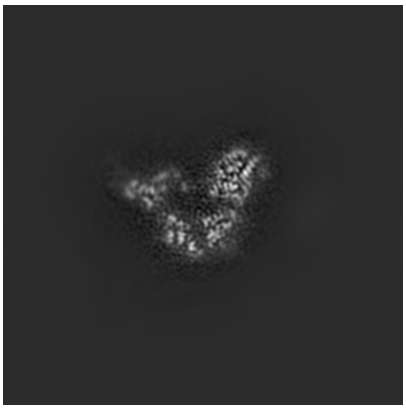
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

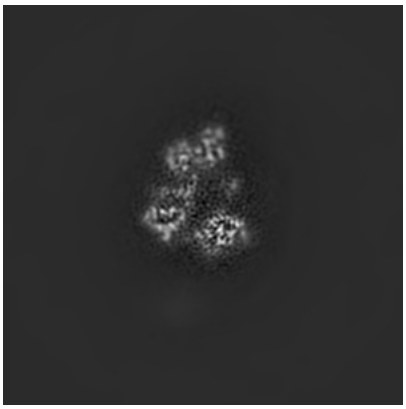
6.2.1 Primary map



X Index: 182

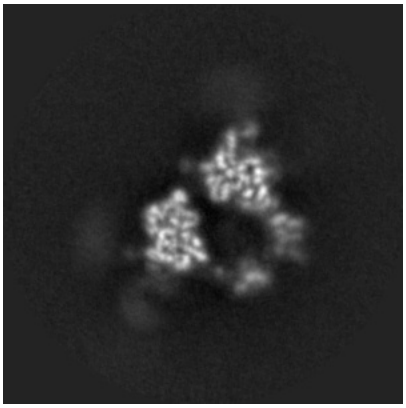


Y Index: 182

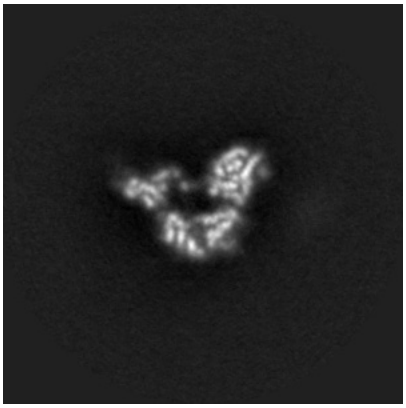


Z Index: 182

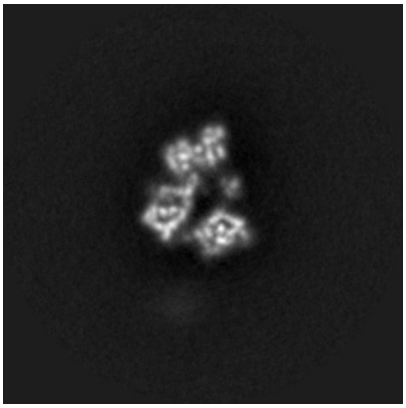
6.2.2 Raw map



X Index: 182



Y Index: 182

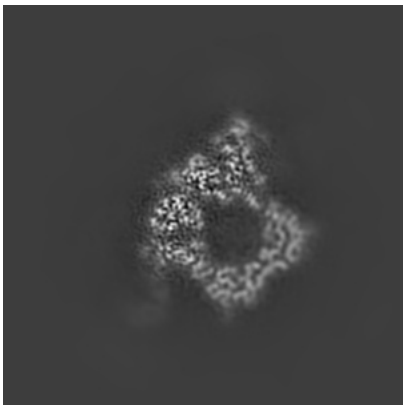


Z Index: 182

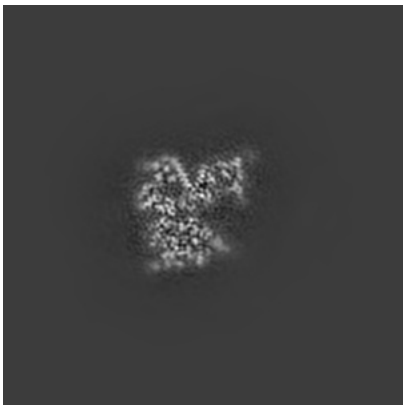
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



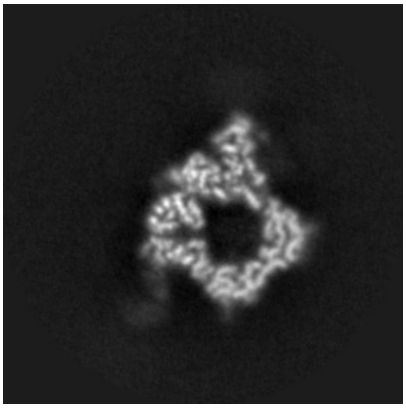
X Index: 199



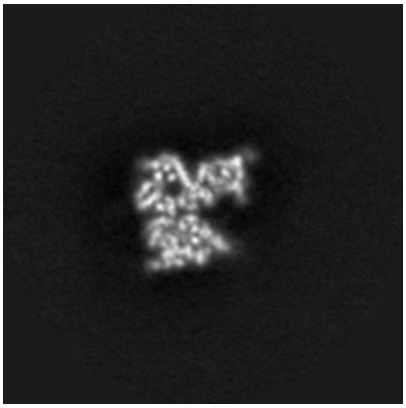
Y Index: 166

Z Index: 143

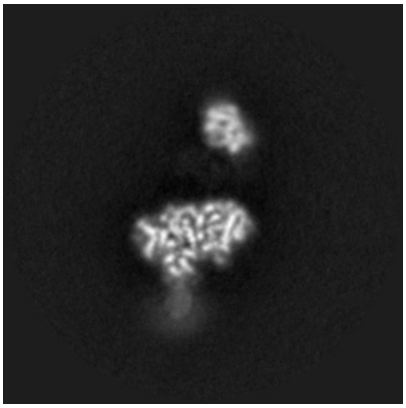
6.3.2 Raw map



X Index: 198



Y Index: 166

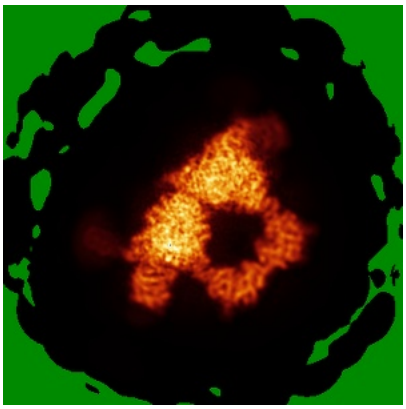


Z Index: 142

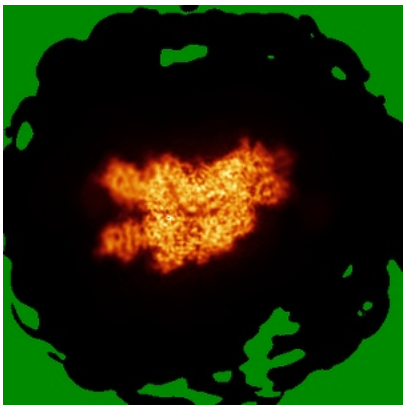
The images above show the largest variance slices of the map in three orthogonal directions.

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

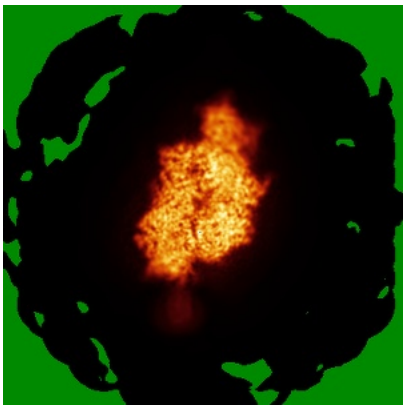
6.4.1 Primary map



X

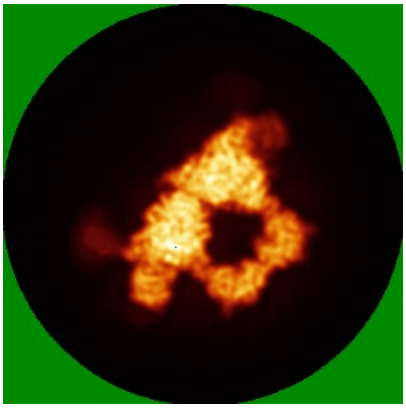


Y

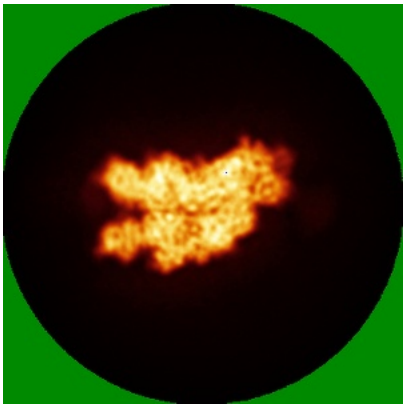


Z

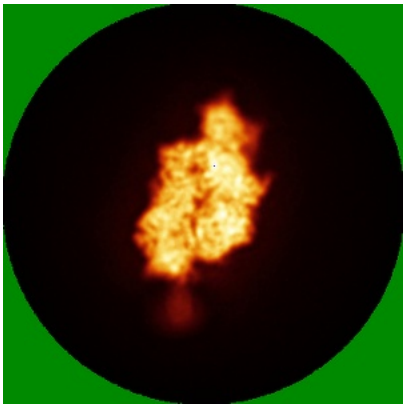
6.4.2 Raw map



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

X Y Z

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.

6.5.2 Raw map

X Y Z

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.

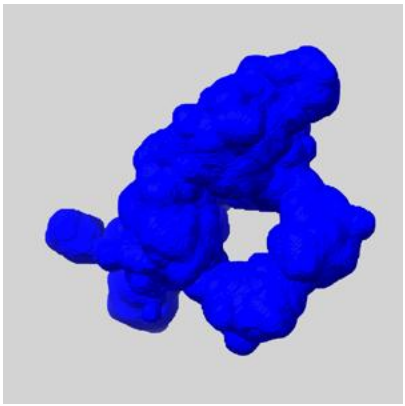
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

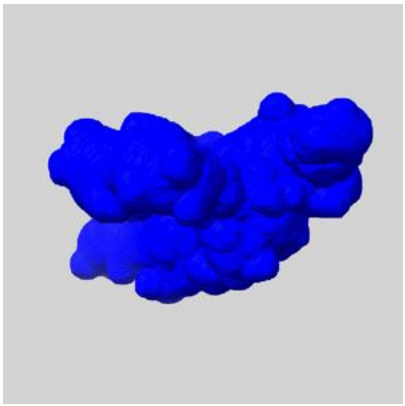
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

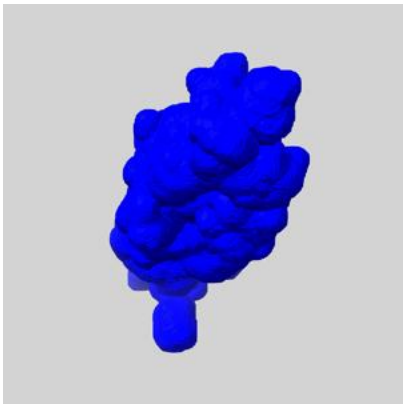
6.6.1 emd_4975_msk_1.map



X



Y

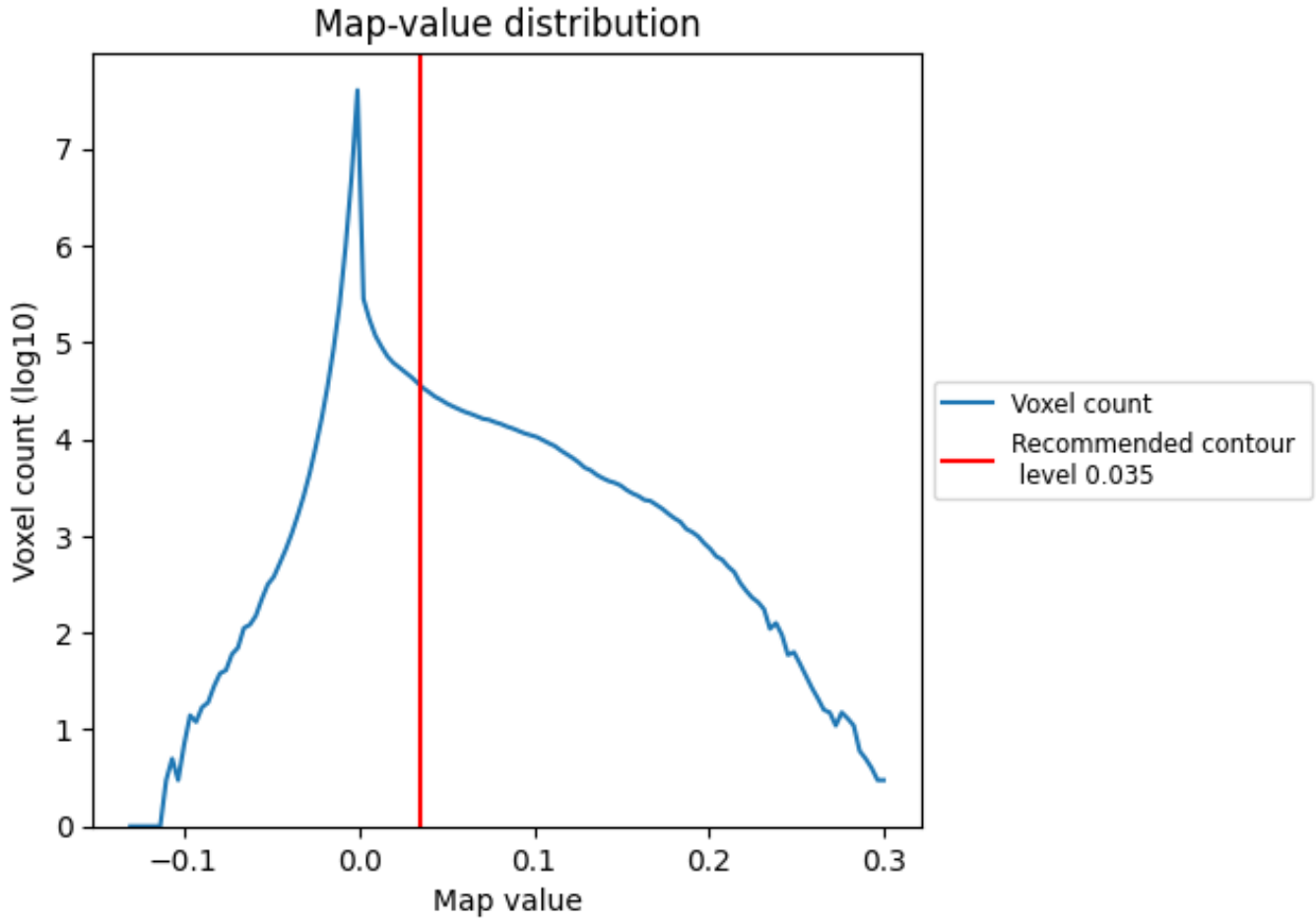


Z

7 Map analysis

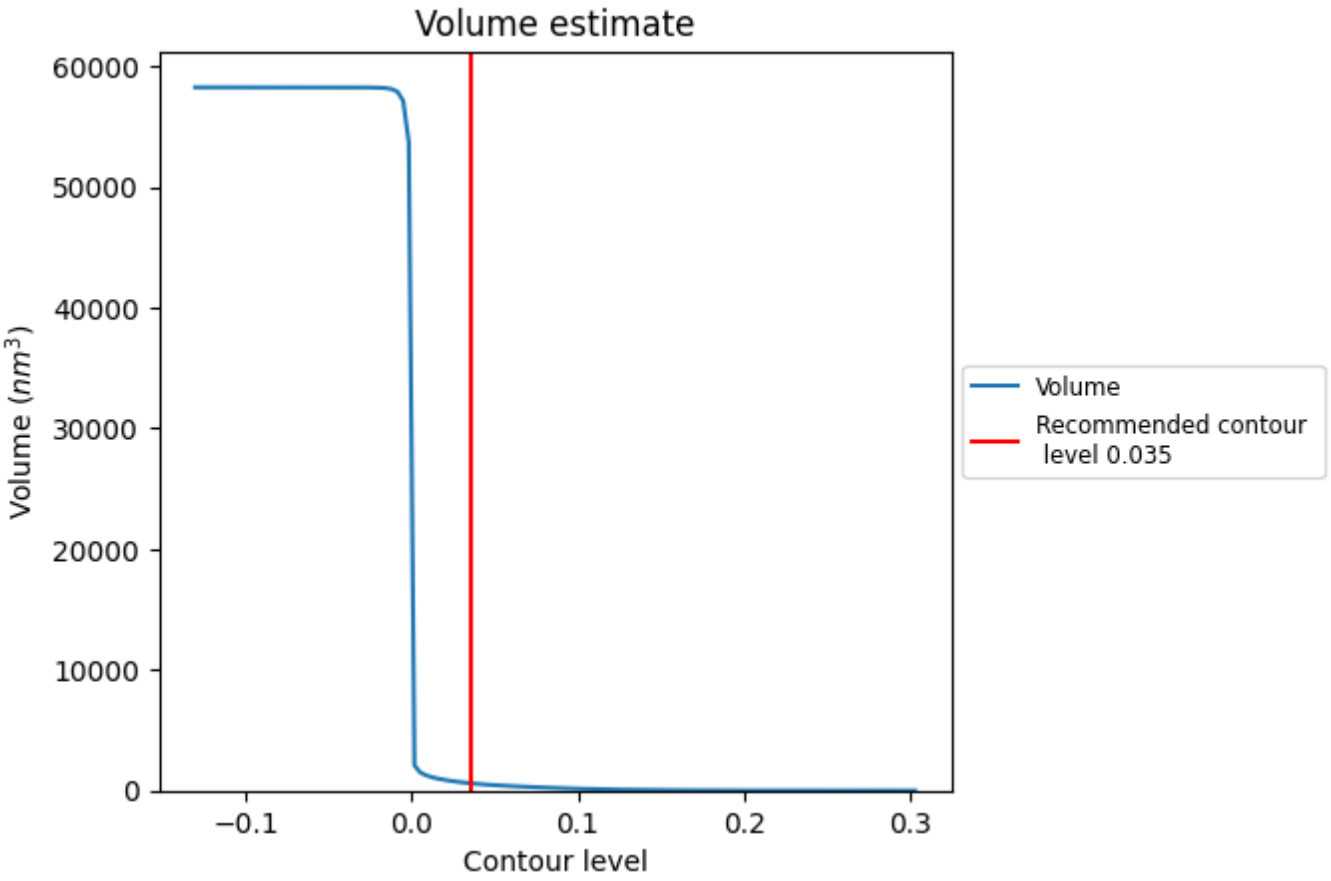
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

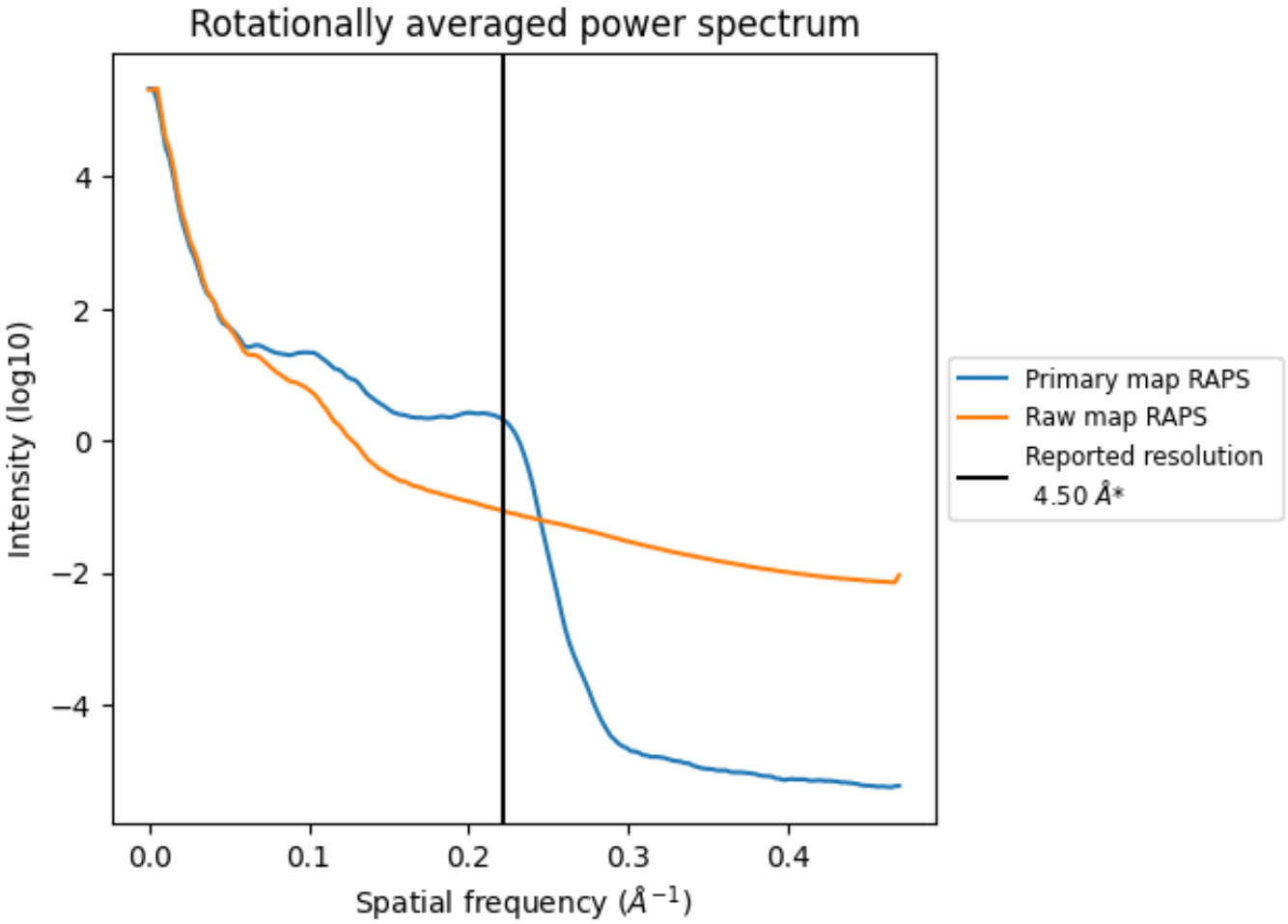
7.2 Volume estimate (i)



The volume at the recommended contour level is 607 nm^3; this corresponds to an approximate mass of 548 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

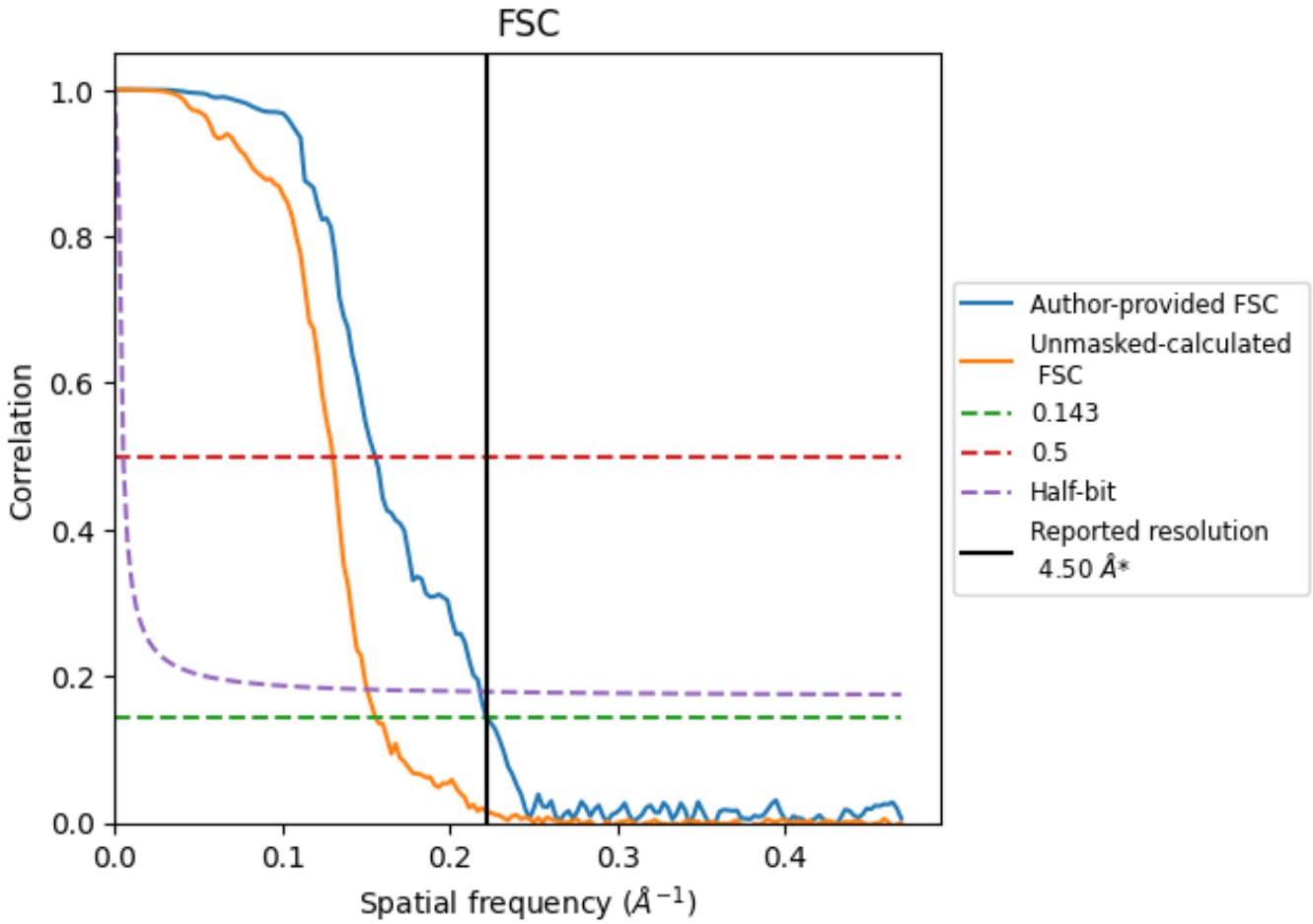


*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

8.2 Resolution estimates (i)

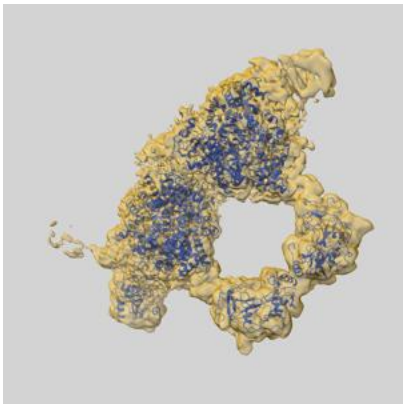
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.50	6.44	4.59
Unmasked-calculated*	6.41	7.69	6.64

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

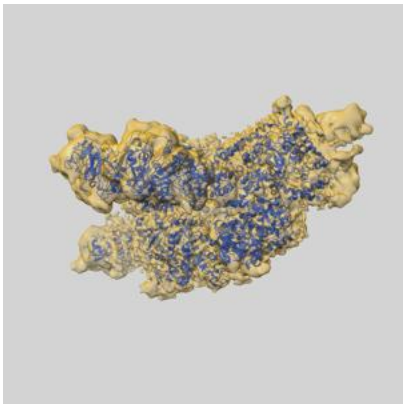
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4975 and PDB model 6ROW. Per-residue inclusion information can be found in section 3 on page 4.

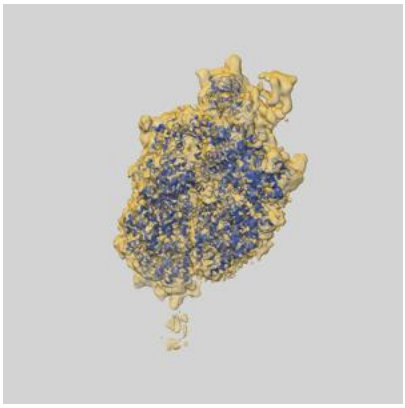
9.1 Map-model overlay



X



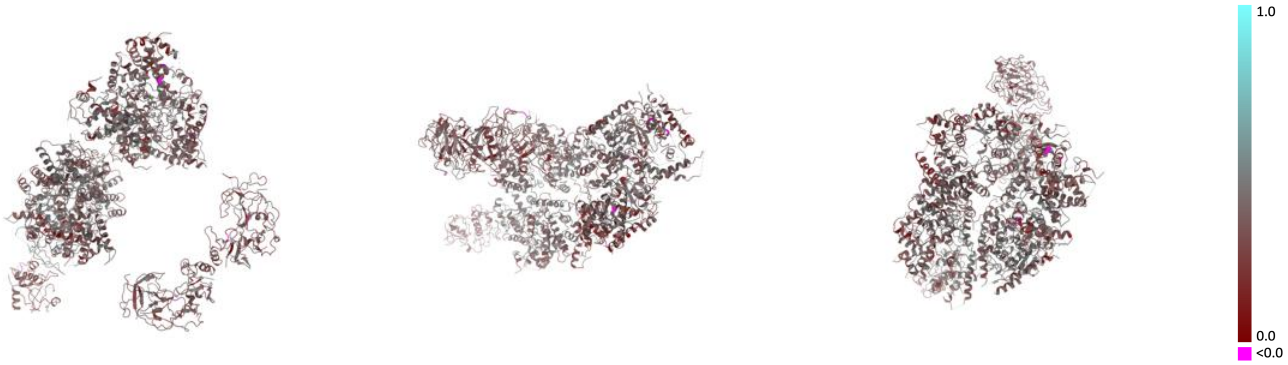
Y



Z

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

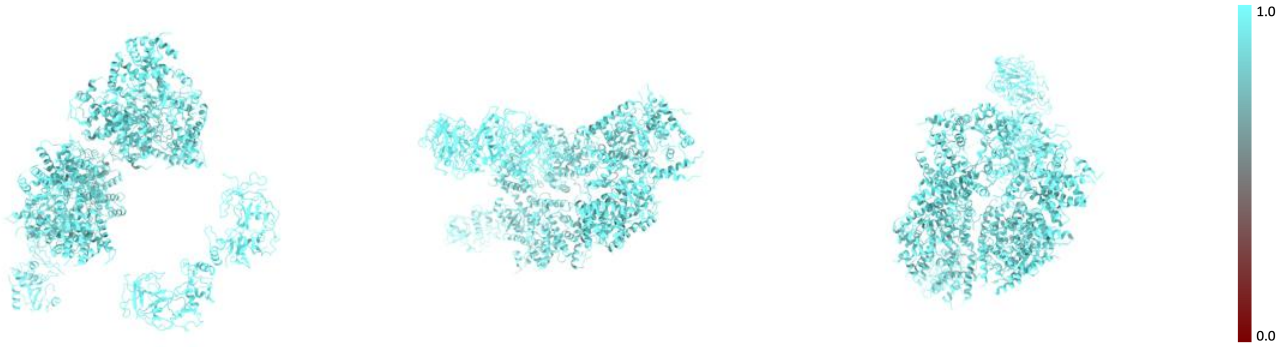
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

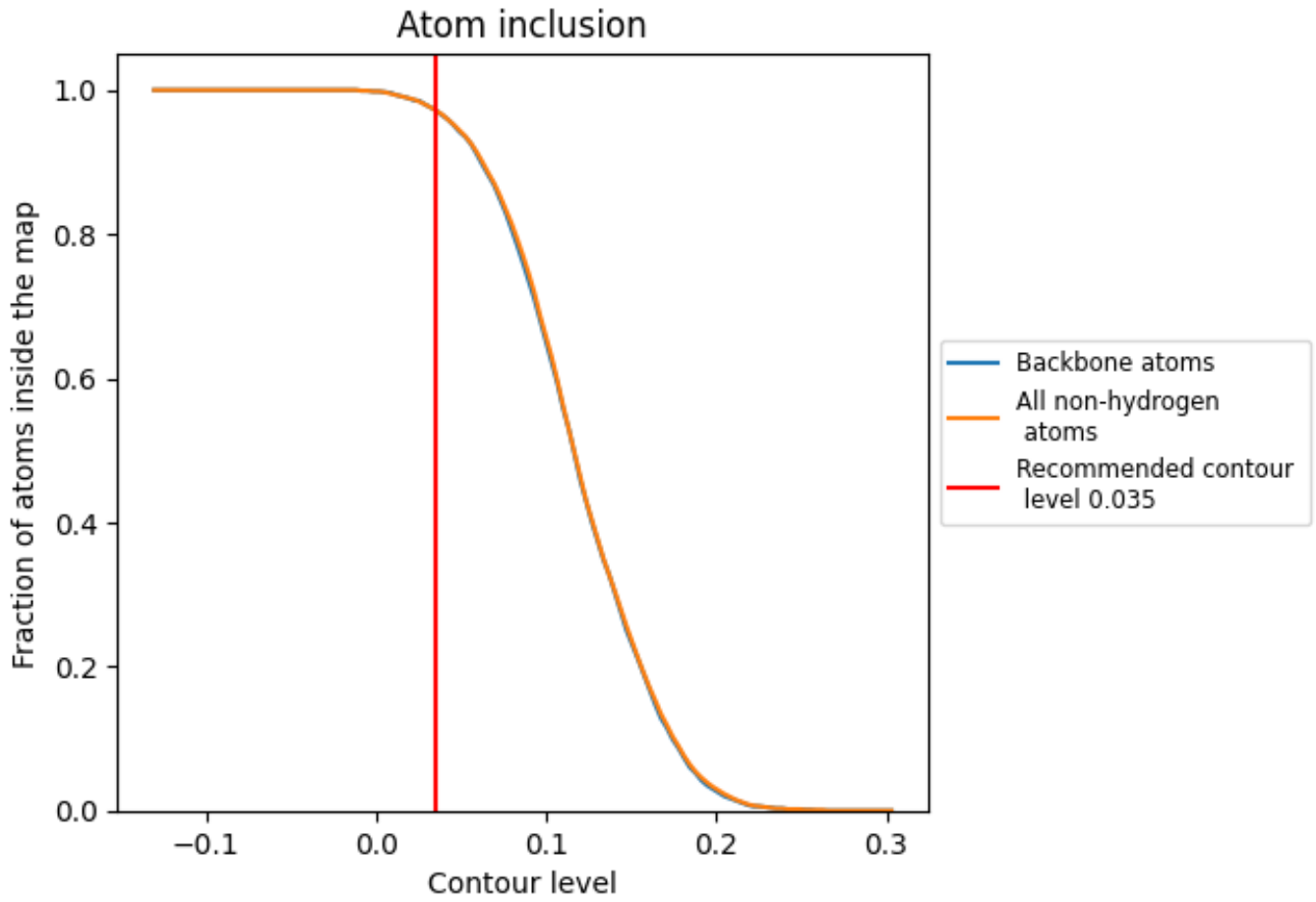
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 97% 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	0.9720	0.3790
A	0.9760	0.4040
B	0.9660	0.3870
C	0.9730	0.3890
D	0.9620	0.3650
E	1.0000	0.3610
F	1.0000	0.3400
G	0.9980	0.2980