wwPDB EM Validation Summary Report

Nov 13, 2022 – 03:41 AM EST

PDB ID	:	6VQJ
EMDB ID	:	EMD-21352
Title	:	Mammalian V-ATPase from rat brain collar and peripheral stalks rotational state 2 (from focused refinement)
Authors	:	Abbas, Y.M.; Rubinstein, J.L.
Deposited on	:	2020-02-05
Resolution	:	5.70 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

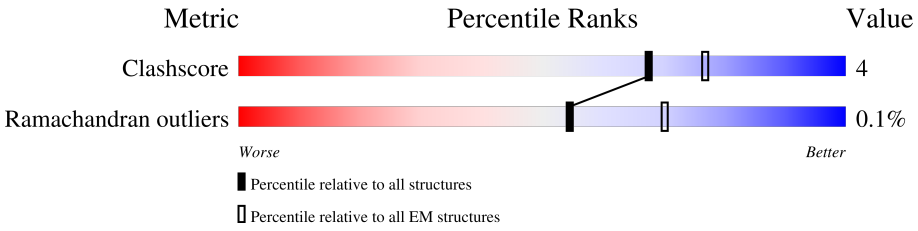
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 5.70 Å.

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



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

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	G	382	10% 89% 5% 6%
2	I	226	26% 72%
2	J	226	27% 72%
2	K	226	9% 27% 72%
3	M	118	54% 43%
3	N	118	56% 43%
3	O	118	14% 53% 43%
4	a	838	37% 63%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5278 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 V-type proton ATPase subunit C 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	G	360	Total 1790	C 1070	N 360	O 360	0	0

- Molecule 2 is a protein called V-type proton ATPase subunit E 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	I	64	Total 319	C 191	N 64	O 64	0	0
2	J	64	Total 319	C 191	N 64	O 64	0	0
2	K	64	Total 319	C 191	N 64	O 64	0	0

- Molecule 3 is a protein called V-type proton ATPase subunit G.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	M	67	Total 332	C 198	N 67	O 67	0	0
3	N	67	Total 332	C 198	N 67	O 67	0	0
3	O	67	Total 332	C 198	N 67	O 67	0	0

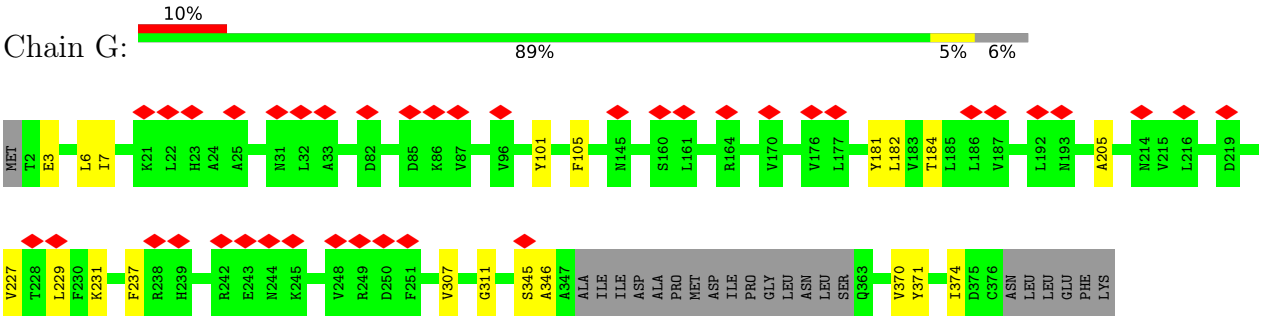
- Molecule 4 is a protein called V-type proton ATPase 116 kDa subunit a isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	a	309	Total 1535	C 917	N 309	O 309	0	0

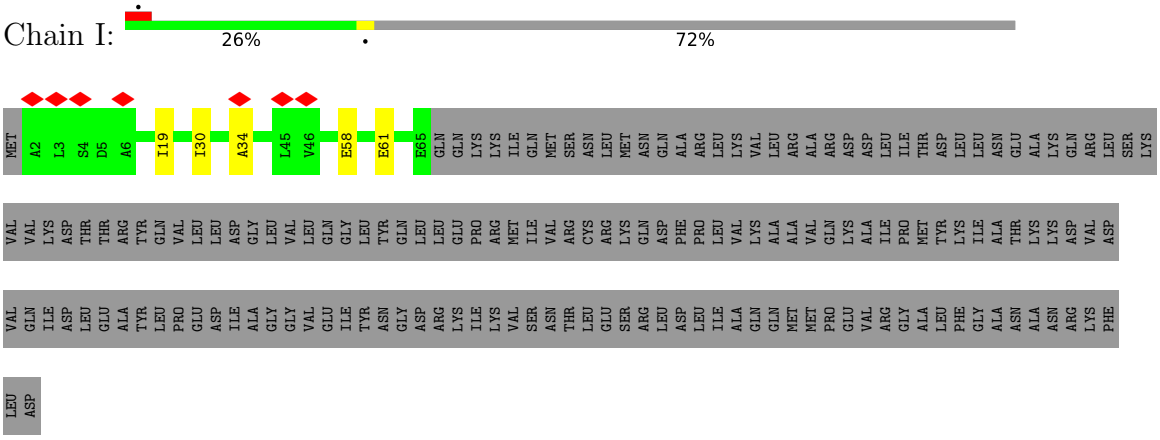
3 Residue-property plots (i)

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.

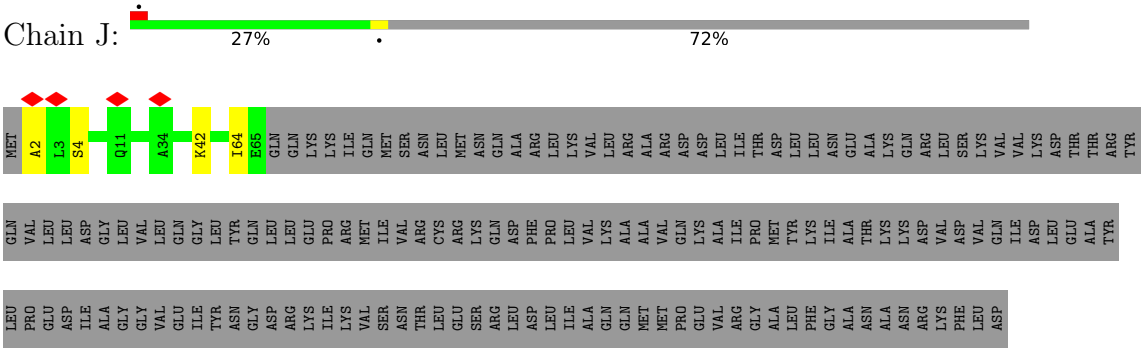
• Molecule 1: V-type proton ATPase subunit C 1



• Molecule 2: V-type proton ATPase subunit E 1

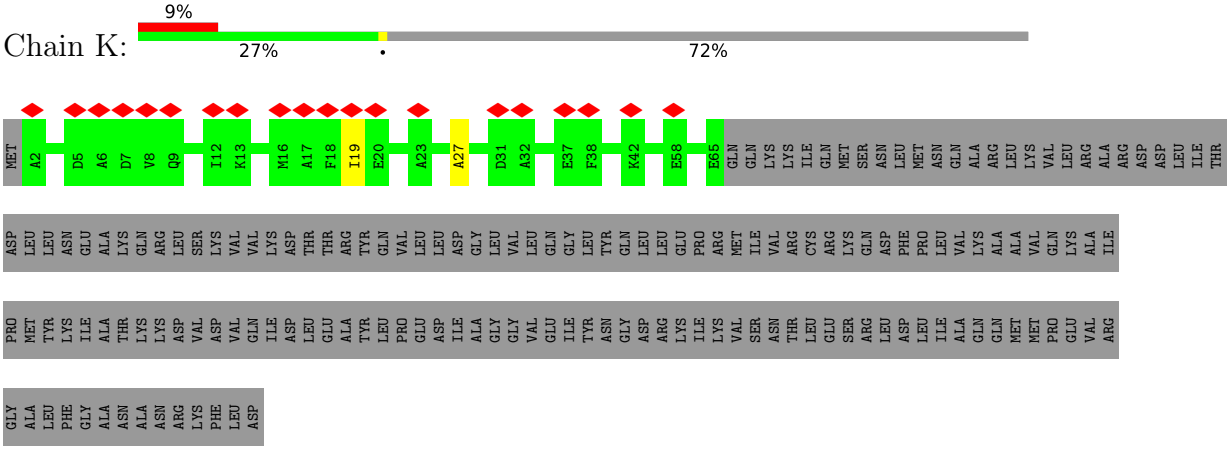


• Molecule 2: V-type proton ATPase subunit E 1



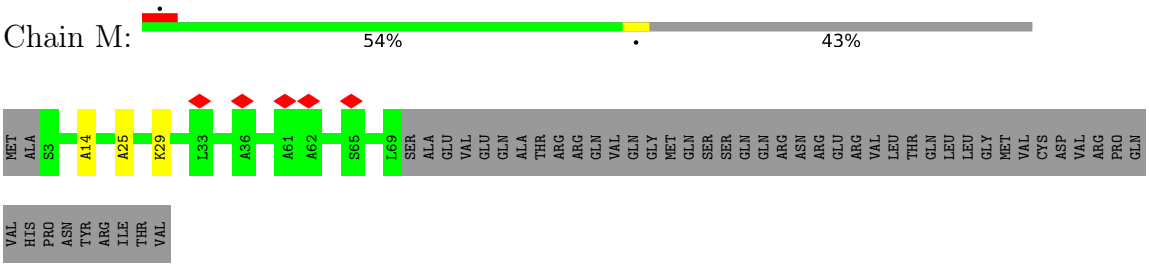
• Molecule 2: V-type proton ATPase subunit E 1

Chain K:



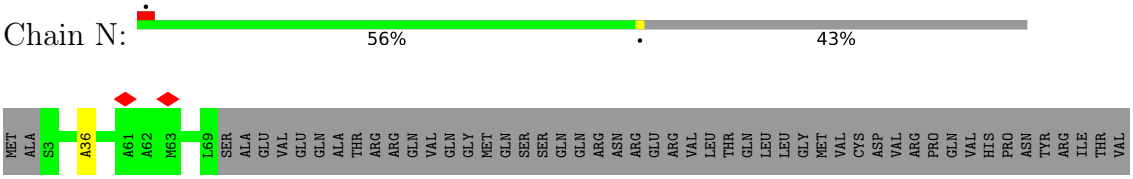
• Molecule 3: V-type proton ATPase subunit G

Chain M:



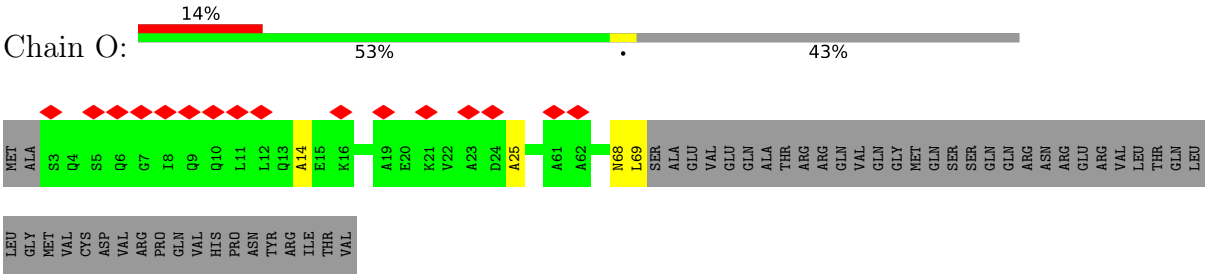
• Molecule 3: V-type proton ATPase subunit G

Chain N:



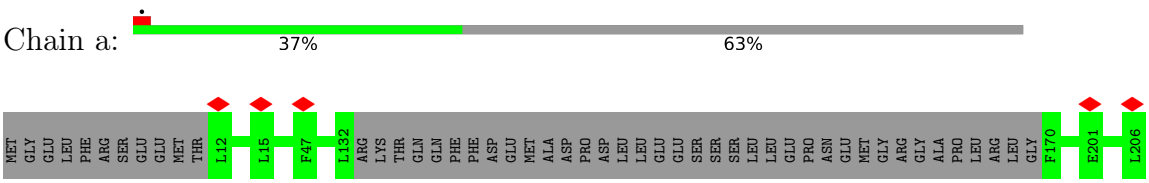
• Molecule 3: V-type proton ATPase subunit G

Chain O:



• Molecule 4: V-type proton ATPase 116 kDa subunit a isoform 1

Chain a:



V219 F220 I221 I222 F223 F224 P246 C247 P248 A285 V314 T315 A321 P349 T357
ASN GLN THR PRO PRO THR TYR ASN LYS THR ASN LYS PHE THR HIS GLY PHE GLN ASN ILE VAL ASP ALA TYR GLY ILE GLY THR TYR ARG GLU ILE ALA PRO ALA PRO TYR THR
VAL ILE THR PHE PRO PHE LEU PHE ALA VAL MET PHE GLY ASP PHE GLY HIS GLY ILE LEU MET THR LEU PHE ALA VAL TRP MET VAL LEU ARG GLU SER ARG ILE LEU SER GLN LYS ASN GLU ASN GLU MET PHE SER MET VAL PHE SER GLY ILE ARG TYR ILE LEU LEU MET GLY LEU
PHE SER ILE TYR THR GLY LEU ILE TYR ASN ASP CYS PHE SER LYS SER LEU ASN ILE PHE GLY SER SER TRP SER VAL ARG PRO MET PHE THR ILE GLY ASN TRP THR GLU GLU THR LEU LEU GLY SER SER VAL LEU GLN LEU ASN PRO ALA ILE PRO GLY VAL PHE GLY GLY PRO TYR
PRO PHE GLY ILE ASP PRO ILE TRP ASN ILE ALA THR ASN LYS LEU THR PHE LEU ASN SER PHE LYS MET LYS MET SER VAL ILE LEU GLY ILE ILE HIS MET LEU PHE GLY VAL SER LEU SER LEU PHE ASN HIS ILE TYR PHE LYS LYS PRO LEU ASN ILE TYR PHE GLY PHE ILE PRO
GLU ILE ILE PHE MET SER SER LEU PHE GLY TYR LEU VAL ILE LEU ILE PHE TYR LYS TRP THR ALA TYR ASP ALA HIS SER SER ARG ASN ALA PRO SER LEU LEU ILE HIS PHE ILE ASN MET PHE LEU PHE SER TYR PRO GLU SER GLY ASN ALA MET LEU TYR SER GLY GLN LYS GLY
ILE GLN CYS PHE LEU ILE VAL VAL ALA MET LEU CYS VAL PRO TRP MET LEU LEU PHE LYS PRO LEU ILE LEU ARG HIS GLN TYR LEU ARG LYS LYS HIS LEU GLY THR LEU ASN PHE GLY GLY ILE ARG VAL GLY ASN GLY PRO THR GLU GLU ASP ALA GLU ILE ILE GLN HIS ASP GLN
LEU SER THR HIS SER GLU ASP ALA GLU GLU PRO THR GLU ASP GLU VAL PHE ASP PHE GLY ASP THR MET VAL HIS GLN ALA ILE HIS THR ILE GLU GLU TYR CYS LEU GLY CYS ILE SER ASN THR ALA SER TYR LEU ARG LEU TRP ALA LEU SER LEU ALA HIS ALA GLN LEU SER GLU VAL
LEU TRP THR MET VAL ILE HIS ILE GLY LEU HIS VAL ARG SER LEU ALA GLY GLY LEU GLY LEU PHE PHE ILE PHE ALA ALA PHE ALA THR LEU THR VAL ALA ILE LEU LEU LEU ILE MET GLU GLY LEU SER ALA PHE LEU HIS ALA LEU ARG LEU HIS TRP VAL GLU PHE GLN ASN LYS PHE
TYR THR GLY THR GLY PHE LYS PHE LEU PRO PHE SER PHE GLU HIS ILE ARG GLU GLY LYS PHE ASP GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	74789	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 ($e^-/Å^2$)	43	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	2.747	Depositor
Minimum map value	-1.100	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	360.4, 360.4, 360.4	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	G	0.38	0/1788	0.67	0/2494
2	I	0.36	0/318	0.57	0/443
2	J	0.42	0/318	0.63	0/443
2	K	0.37	0/318	0.58	0/443
3	M	0.35	0/331	0.57	0/460
3	N	0.39	0/331	0.56	0/460
3	O	0.45	0/331	0.56	0/460
4	a	0.40	0/1533	0.67	0/2137
All	All	0.39	0/5268	0.64	0/7340

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	G	1790	0	794	12	0
2	I	319	0	149	5	0
2	J	319	0	149	4	0
2	K	319	0	149	5	0
3	M	332	0	166	4	0
3	N	332	0	166	1	0
3	O	332	0	166	6	0
4	a	1535	0	661	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5278	0	2400	24	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 4.

The worst 5 of 24 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:G:3:GLU:HA	1:G:374:ILE:O	1.47	1.13
1:G:346:ALA:HB2	2:J:2:ALA:HB1	1.39	1.02
1:G:345:SER:CB	2:J:4:SER:CB	2.47	0.93
1:G:346:ALA:HB2	2:J:2:ALA:CB	2.06	0.86
1:G:6:LEU:O	1:G:371:TYR:HA	1.79	0.83

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	G	356/382 (93%)	355 (100%)	1 (0%)	0	100 100
2	I	62/226 (27%)	62 (100%)	0	0	100 100
2	J	62/226 (27%)	61 (98%)	0	1 (2%)	9 43
2	K	62/226 (27%)	62 (100%)	0	0	100 100
3	M	65/118 (55%)	65 (100%)	0	0	100 100
3	N	65/118 (55%)	65 (100%)	0	0	100 100
3	O	65/118 (55%)	65 (100%)	0	0	100 100
4	a	305/838 (36%)	296 (97%)	9 (3%)	0	100 100
All	All	1042/2252 (46%)	1031 (99%)	10 (1%)	1 (0%)	54 85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	64	ILE

5.3.2 Protein sidechains

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

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

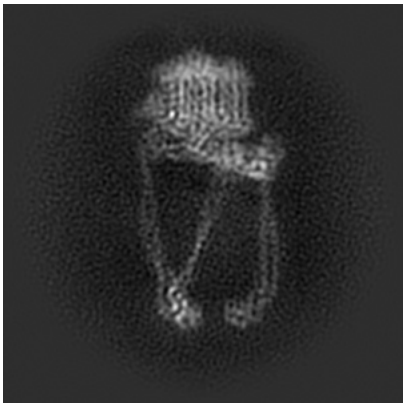
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21352. These allow visual inspection of the internal detail of the map and identification of artifacts.

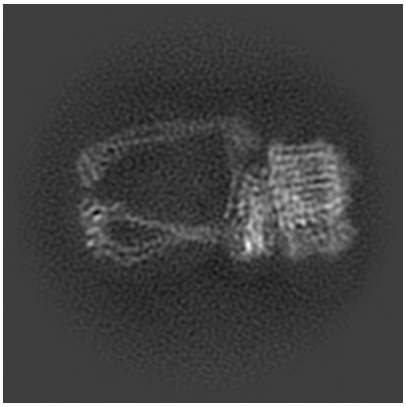
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

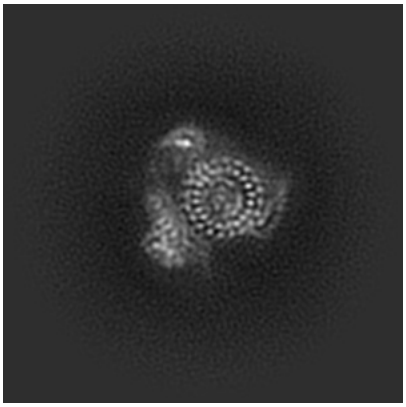
6.1.1 Primary map



X



Y

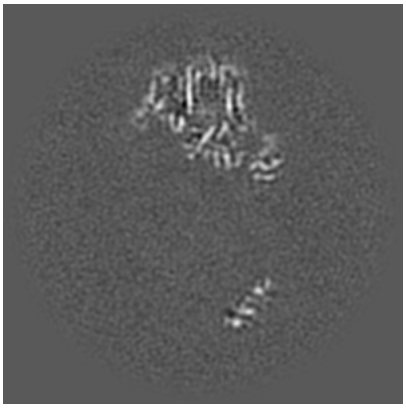


Z

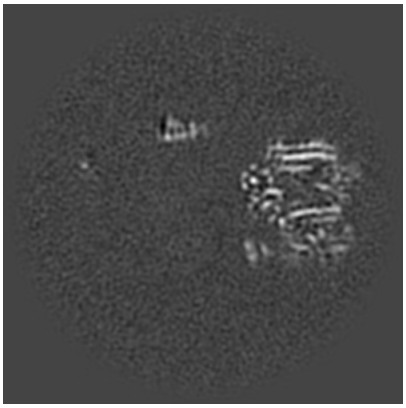
The images above show the map projected in three orthogonal directions.

6.2 Central slices

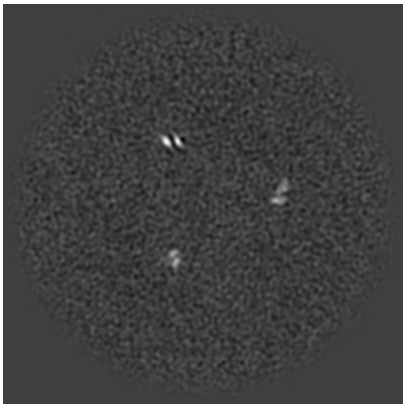
6.2.1 Primary map



X Index: 170



Y Index: 170

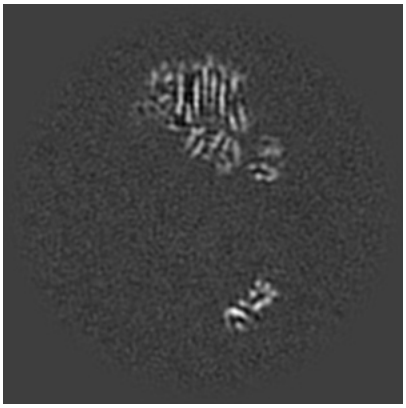


Z Index: 170

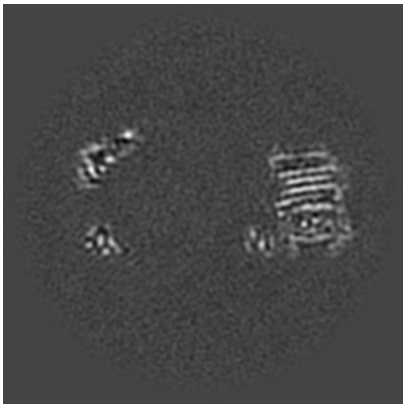
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

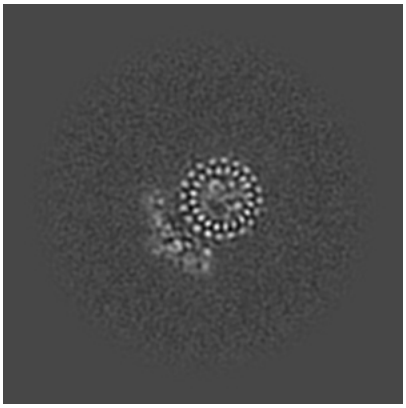
6.3.1 Primary map



X Index: 166



Y Index: 151



Z Index: 248

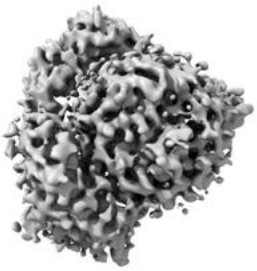
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

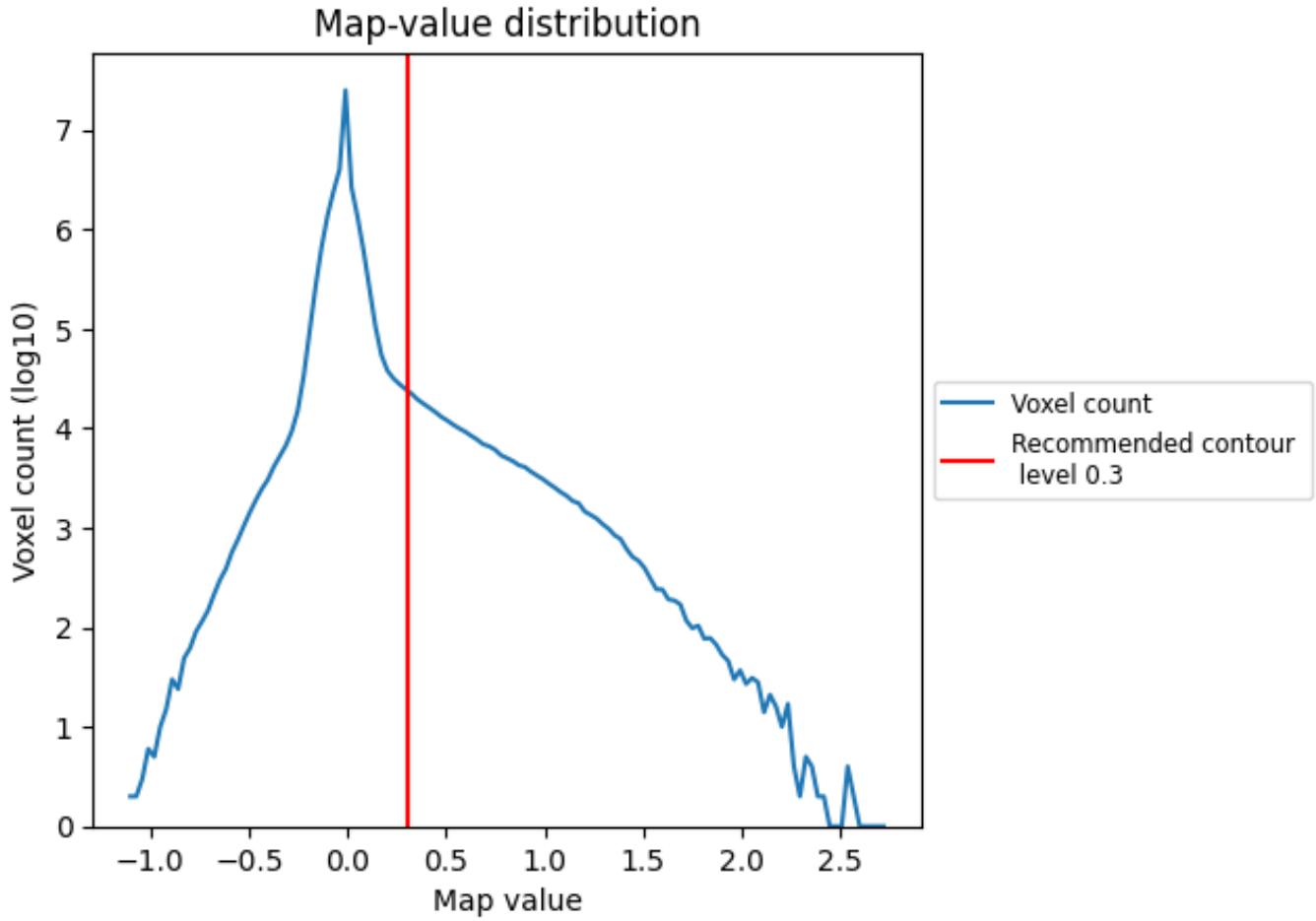
6.5 Mask visualisation (i)

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

7 Map analysis

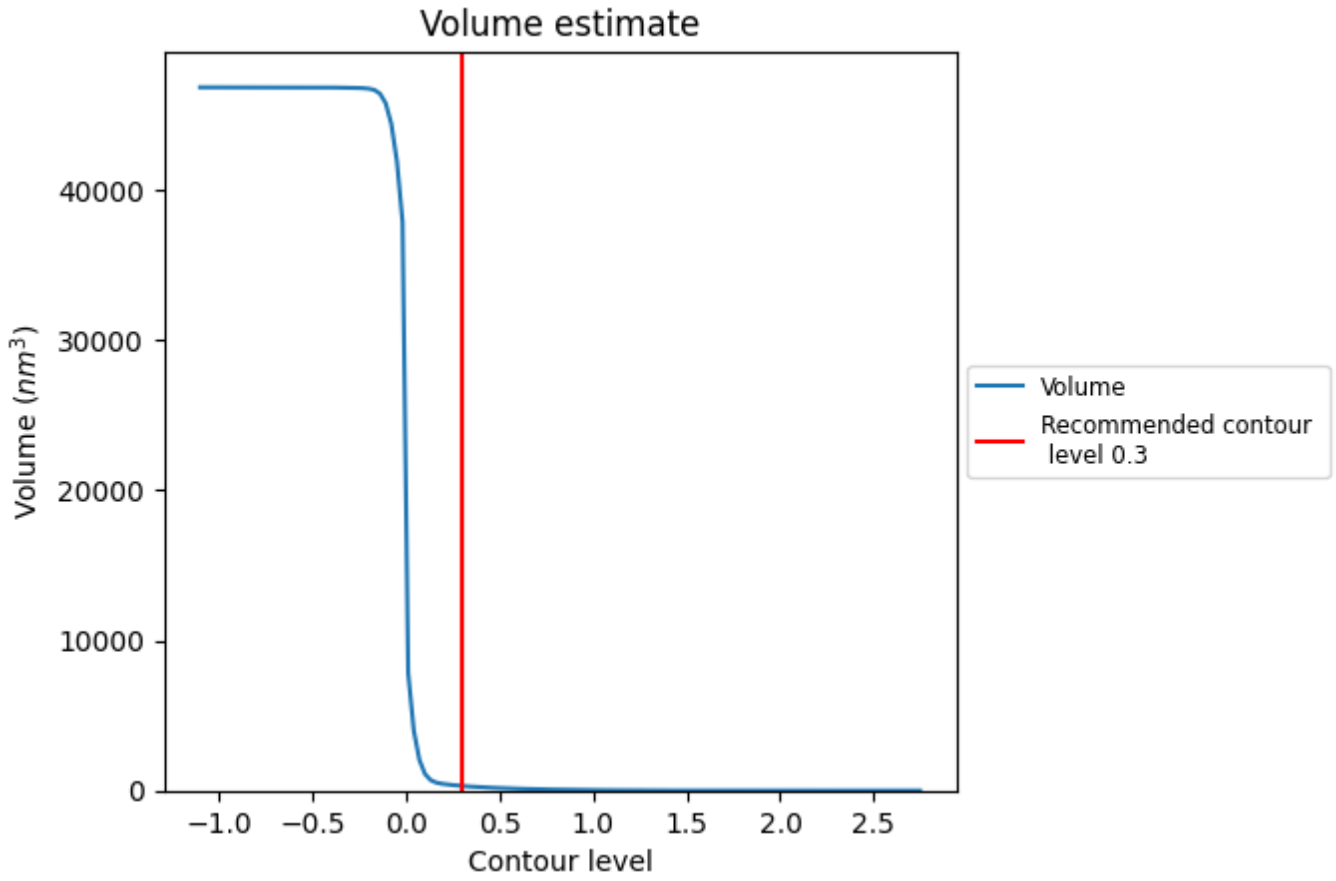
This section contains the results of statistical analysis of the map.

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.

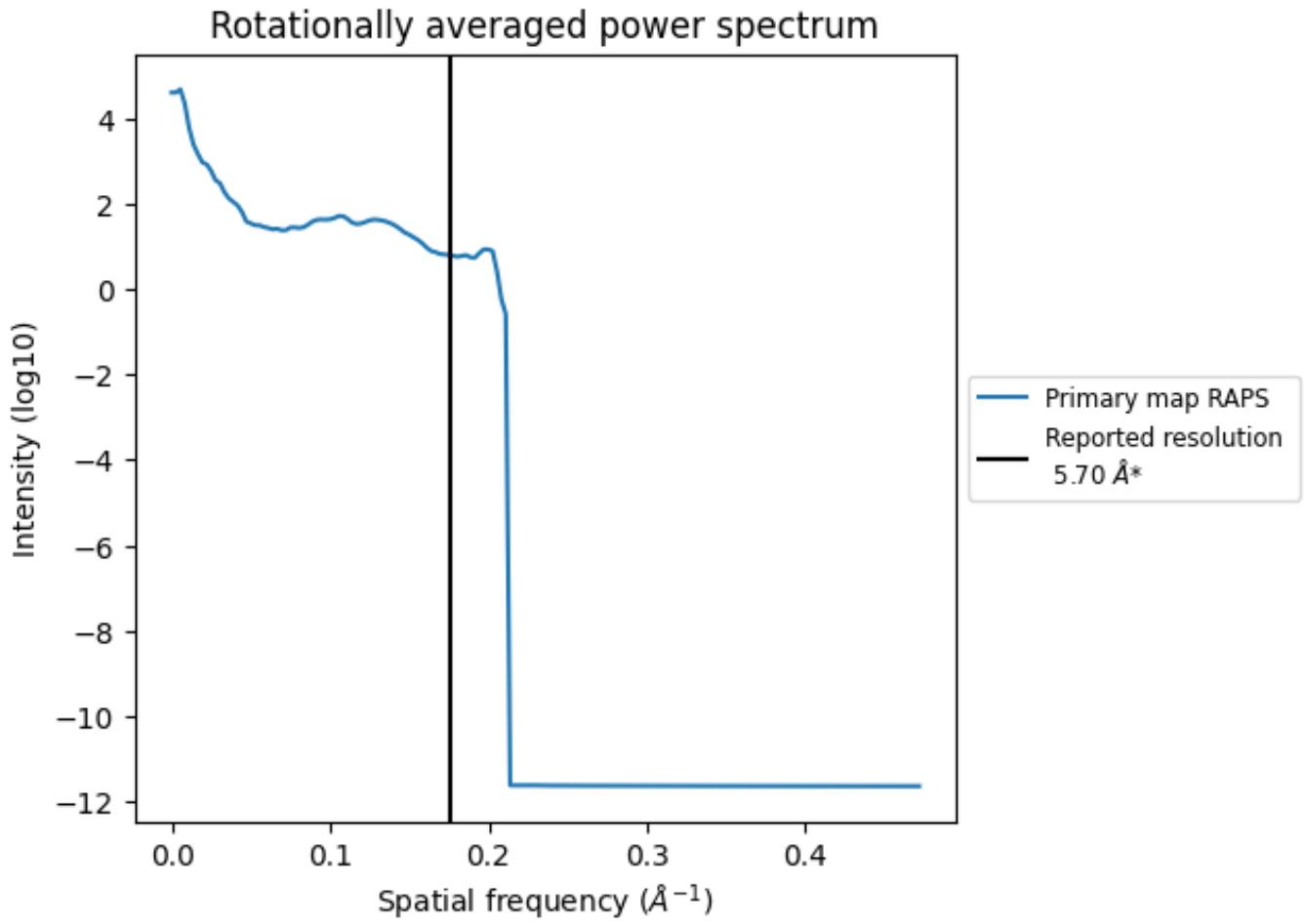
7.2 Volume estimate (i)



The volume at the recommended contour level is 310 nm^3; this corresponds to an approximate mass of 280 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 0.175 Å^{-1}

8 Fourier-Shell correlation

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

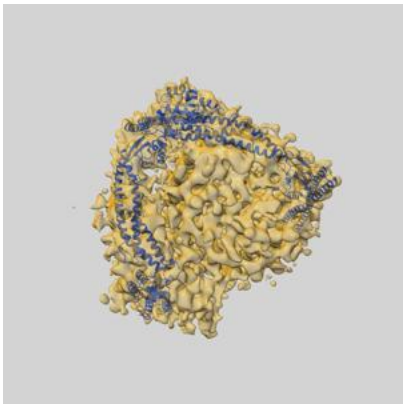
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21352 and PDB model 6VQJ. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay

X

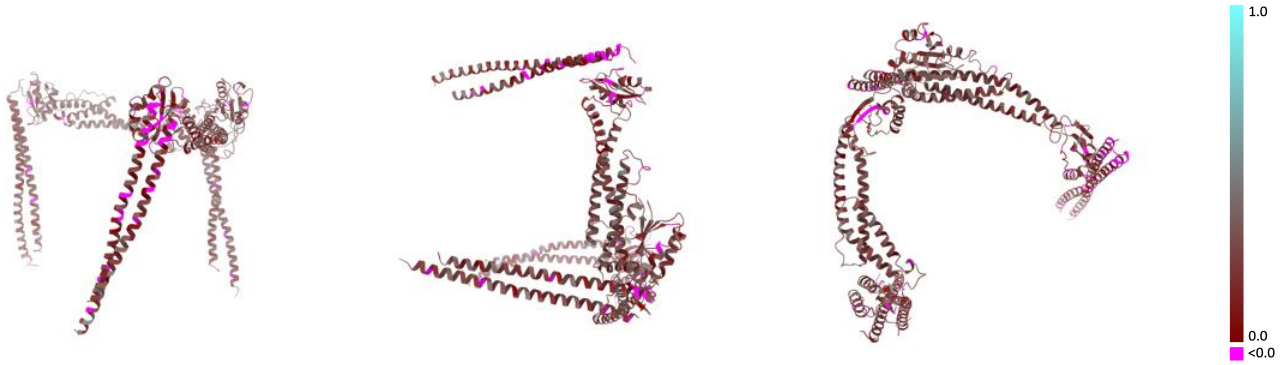
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 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.

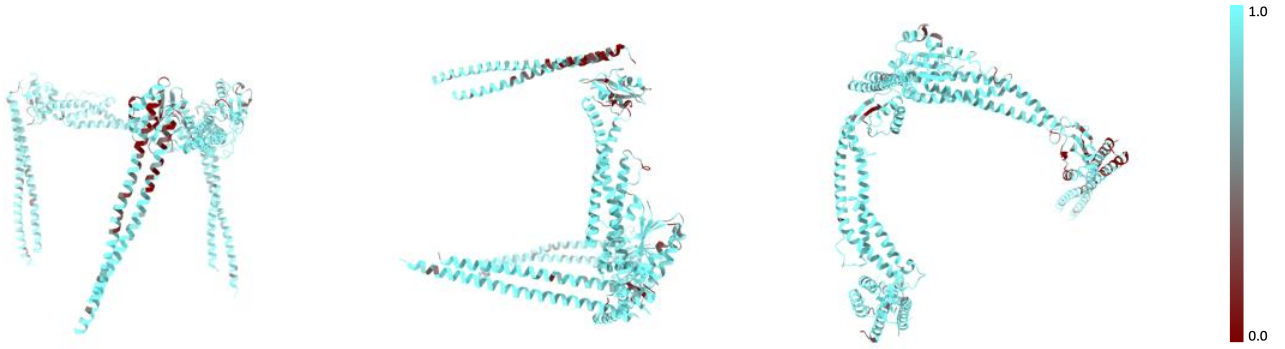
9.2 Q-score mapped to coordinate model (i)



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.

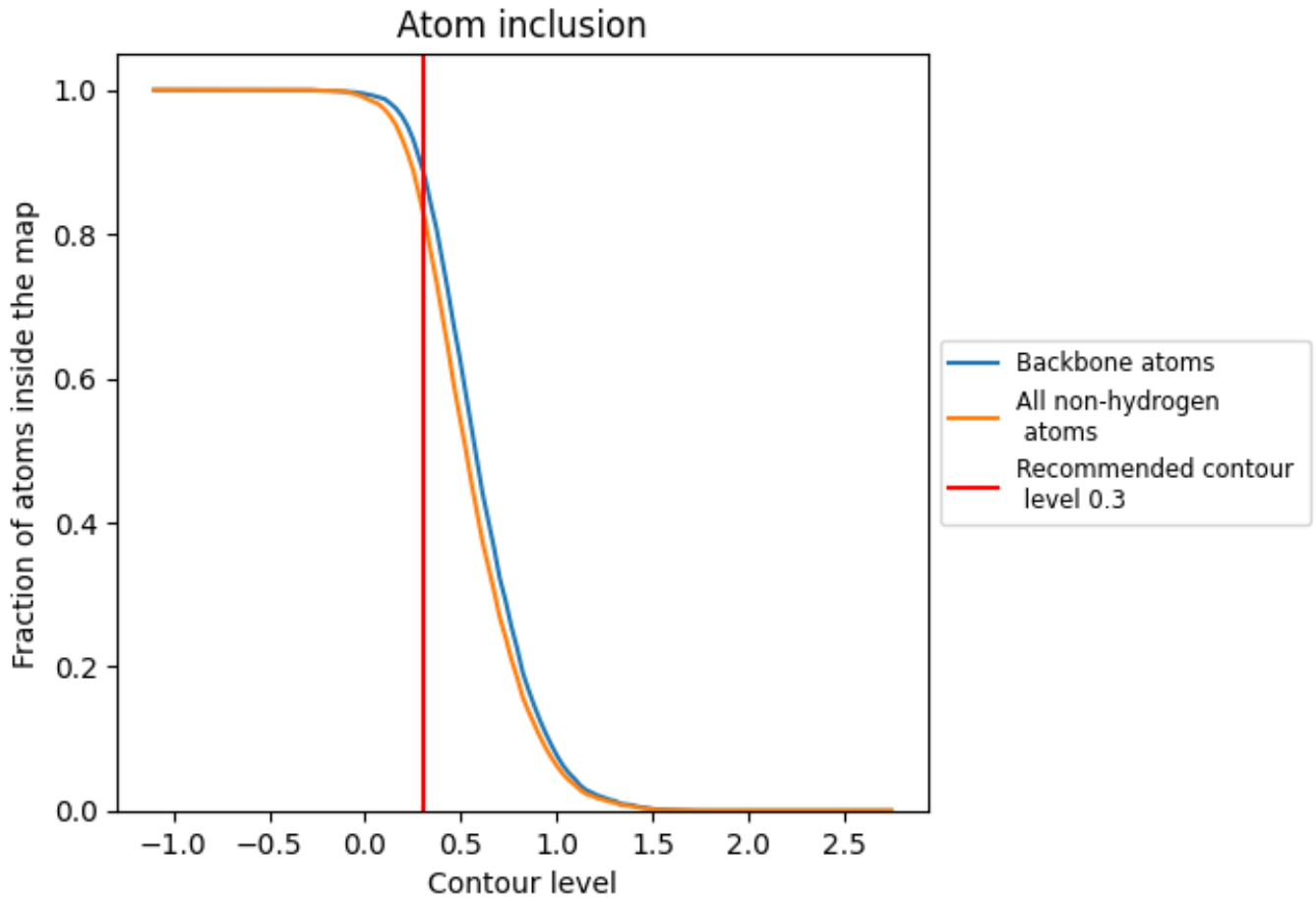
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 83% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8344	0.2440
G	0.8190	0.2570
I	0.8401	0.2350
J	0.8683	0.2290
K	0.6740	0.1390
M	0.8675	0.2420
N	0.9036	0.2430
O	0.7319	0.1810
a	0.8775	0.2690