wwPDB EM Validation Summary Report (i)

Mar 2, 2024 – 06:30 PM EST

PDB ID	:	5TSJ
EMDB ID	:	EMD-8462
Title	:	Thermus thermophilus V/A-ATPase bound to VH dAbs
Authors	:	Davies, R.B.; Smits, C.; Wong, A.S.W.; Stock, D.; Sandin, S.; Stewart, A.G.
Deposited on	:	2016-10-29
Resolution	:	8.70 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 (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:

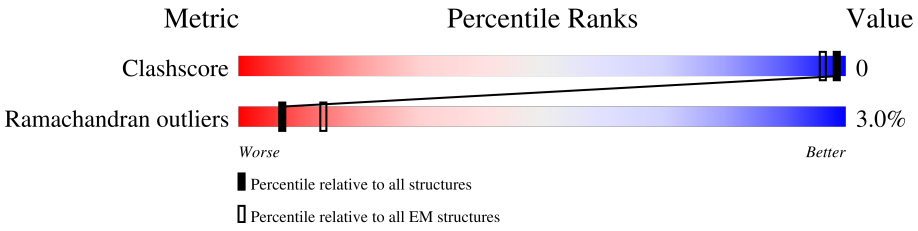
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 8.70 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	A	577	9% 95% 5%
1	B	577	15% 93% 7%
1	C	577	8% 95% 5%
2	D	457	11% 92% 8%
2	E	457	13% 93% 7%
2	F	457	8% 95% 5%
3	G	186	6% 93% 6%
3	H	186	17% 95%
4	I	105	21% 92% 5%

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Mol	Chain	Length	Quality of chain
4	J	105	10% 93% 5%
5	K	210	28% 91% 9%
6	L	100	31% 90% 10%
7	M	323	42% 95%
8	N	652	24% 91% 5%
9	O	99	33% 78% 19%
9	P	99	34% 78% 19%
9	Q	99	30% 78% 19%
9	R	99	23% 80% 19%
9	S	99	23% 80% 19%
9	T	99	29% 79% 19%
9	U	99	14% 80% 19%
9	V	99	25% 80% 19%
9	W	99	21% 76% 5% 19%
9	X	99	26% 78% 19%
9	Y	99	27% 80% 19%
9	Z	99	45% 79% 19%
10	1	149	30% 78% 21%
10	2	149	35% 78% 21%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 24625 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 ATP synthase alpha chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	577	Total 2307	C 1154	N 577	O 576	0	0
1	B	576	Total 2303	C 1152	N 576	O 575	0	0
1	C	577	Total 2307	C 1154	N 577	O 576	0	0

- Molecule 2 is a protein called V-type ATP synthase beta chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	457	Total 1827	C 914	N 457	O 456	0	0
2	E	457	Total 1827	C 914	N 457	O 456	0	0
2	F	457	Total 1827	C 914	N 457	O 456	0	0

- Molecule 3 is a protein called V-type ATP synthase subunit E.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	184	Total 734	C 368	N 184	O 182	0	0
3	H	184	Total 734	C 368	N 184	O 182	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	134	MET	LEU	conflict	UNP P74901
G	171	MET	LEU	conflict	UNP P74901
G	178	MET	LEU	conflict	UNP P74901
H	134	MET	LEU	conflict	UNP P74901
H	171	MET	LEU	conflict	UNP P74901

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Chain	Residue	Modelled	Actual	Comment	Reference
H	178	MET	LEU	conflict	UNP P74901

- Molecule 4 is a protein called V-type ATPase subunit G.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	I	100	Total	C	N	O	0	0
			399	200	100	99		
4	J	100	Total	C	N	O	0	0
			399	200	100	99		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	16	GLY	-	expression tag	UNP H9ZQR3
J	16	GLY	-	expression tag	UNP H9ZQR3

- Molecule 5 is a protein called V-type ATP synthase subunit D.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	K	210	Total	C	N	O	0	0
			839	420	210	209		

- Molecule 6 is a protein called V-type ATP synthase subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	L	100	Total	C	N	O	0	0
			399	200	100	99		

- Molecule 7 is a protein called V-type ATP synthase subunit C.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	M	320	Total	C	N	O	0	0
			1279	640	320	319		

- Molecule 8 is a protein called Archaeal/vacuolar-type H+-ATPase subunit I.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	N	619	Total	C	N	O	0	0
			2474	1238	619	617		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	154	ARG	LYS	conflict	UNP H9ZQR4
N	164	ALA	VAL	conflict	UNP H9ZQR4
N	173	PRO	ALA	conflict	UNP H9ZQR4

- Molecule 9 is a protein called Vacuolar type ATP synthase subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	O	80	Total 319	C 160	N 80	O 79	0	0
9	P	80	Total 319	C 160	N 80	O 79	0	0
9	Q	80	Total 319	C 160	N 80	O 79	0	0
9	R	80	Total 319	C 160	N 80	O 79	0	0
9	S	80	Total 319	C 160	N 80	O 79	0	0
9	T	80	Total 319	C 160	N 80	O 79	0	0
9	U	80	Total 319	C 160	N 80	O 79	0	0
9	V	80	Total 319	C 160	N 80	O 79	0	0
9	W	80	Total 319	C 160	N 80	O 79	0	0
9	X	80	Total 319	C 160	N 80	O 79	0	0
9	Y	80	Total 319	C 160	N 80	O 79	0	0
9	Z	80	Total 319	C 160	N 80	O 79	0	0

- Molecule 10 is a protein called Human heavy chain domain antibody.

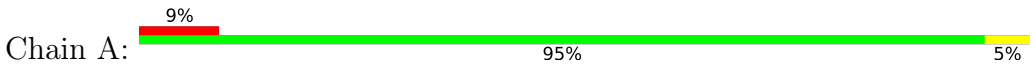
Mol	Chain	Residues	Atoms				AltConf	Trace
10	1	117	Total 571	C 337	N 117	O 117	0	0
10	2	117	Total 571	C 337	N 117	O 117	0	0

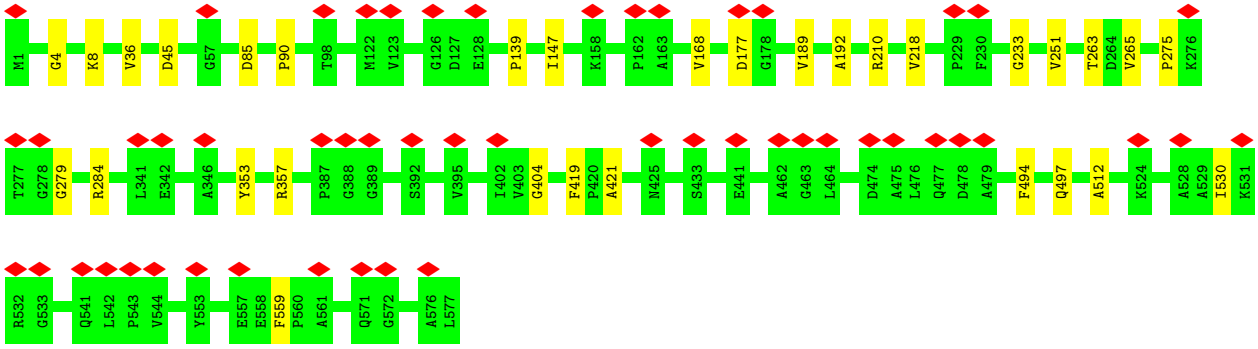
3 Residue-property plots (i)

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 ATP synthase alpha chain

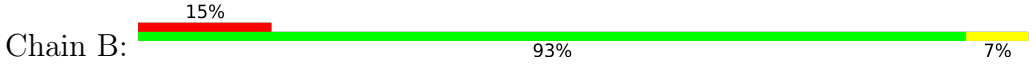
Chain A:

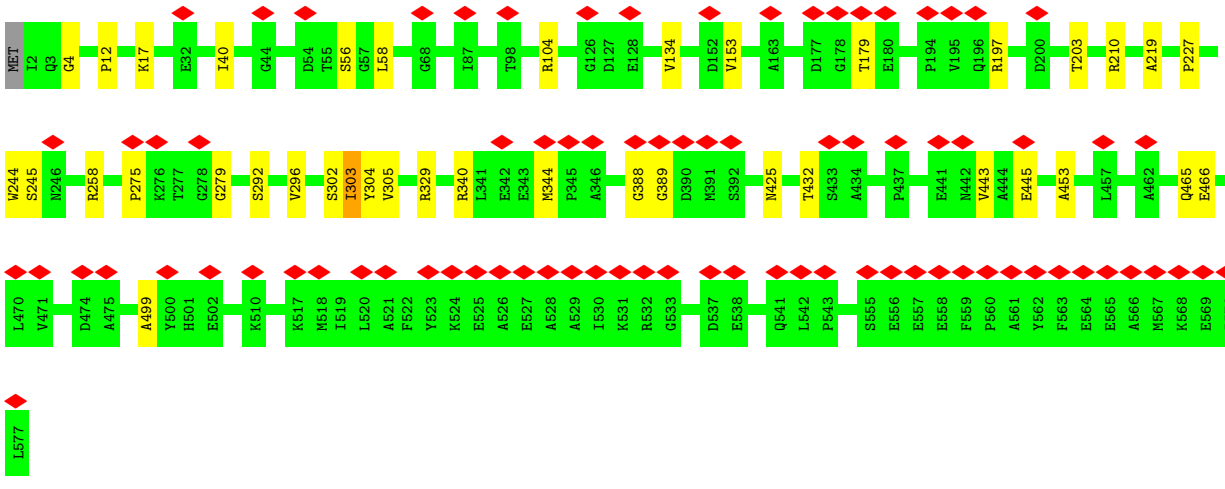




• Molecule 1: V-type ATP synthase alpha chain

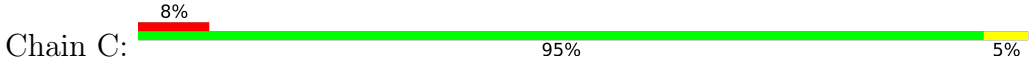
Chain B:

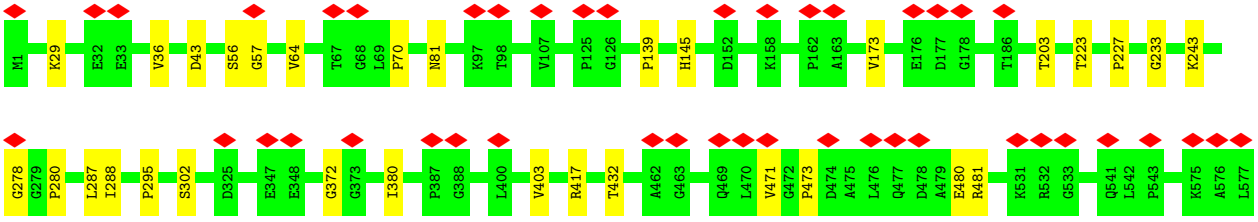




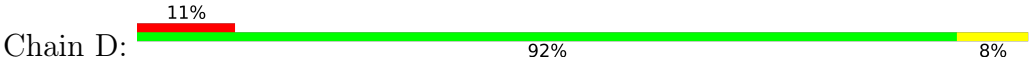
• Molecule 1: V-type ATP synthase alpha chain

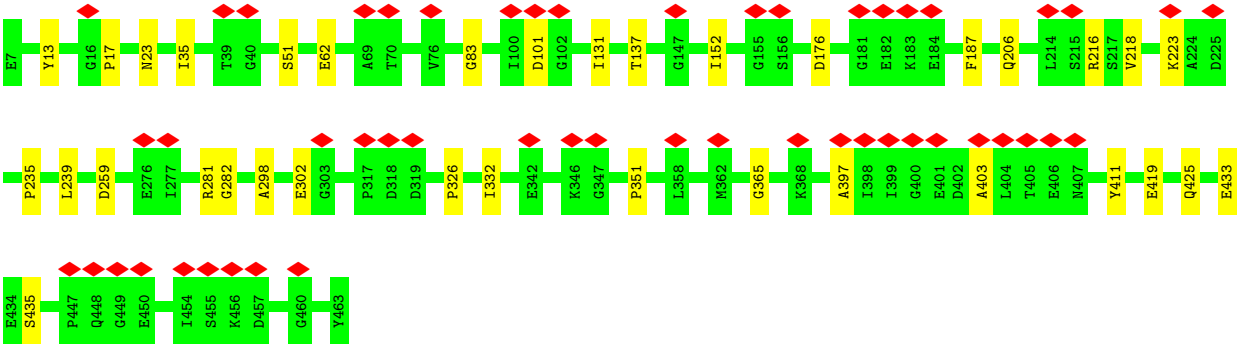
Chain C:



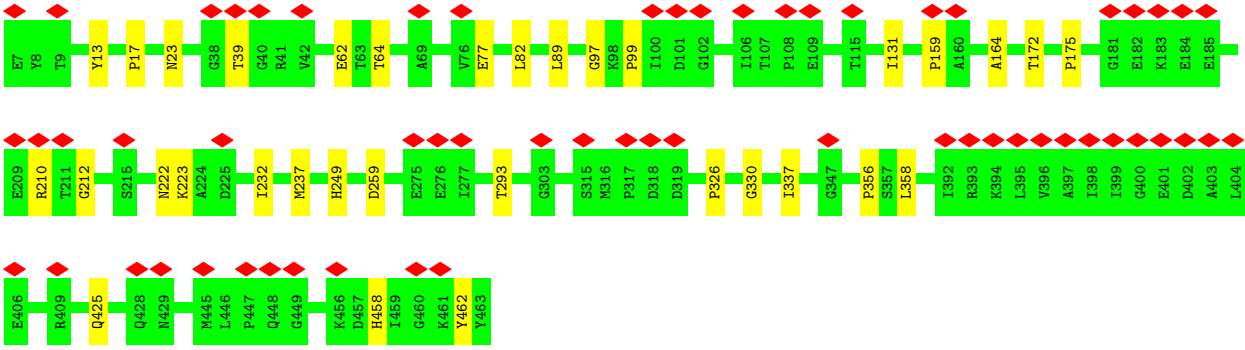


• Molecule 2: V-type ATP synthase beta chain

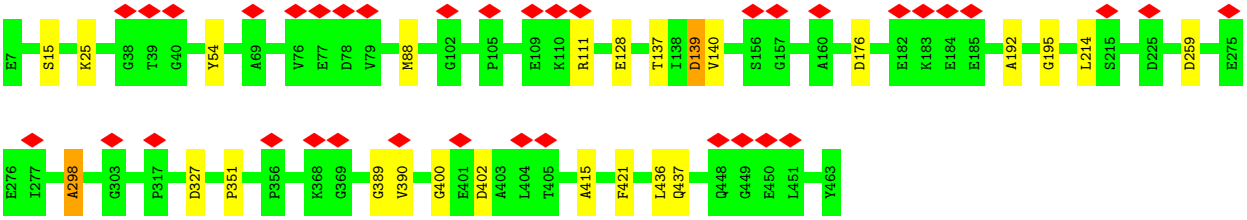




• Molecule 2: V-type ATP synthase beta chain

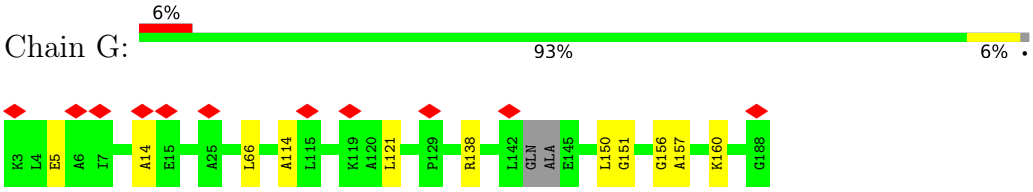


• Molecule 2: V-type ATP synthase beta chain



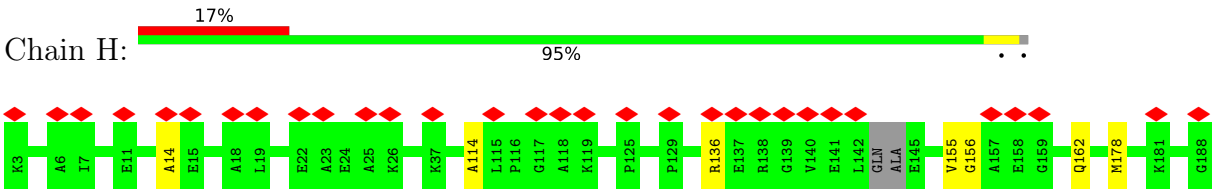
• Molecule 3: V-type ATP synthase subunit E

Chain G:



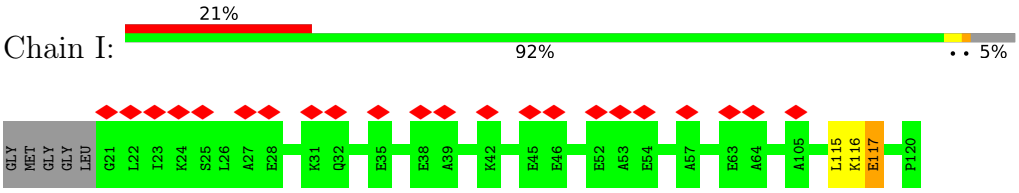
• Molecule 3: V-type ATP synthase subunit E

Chain H:



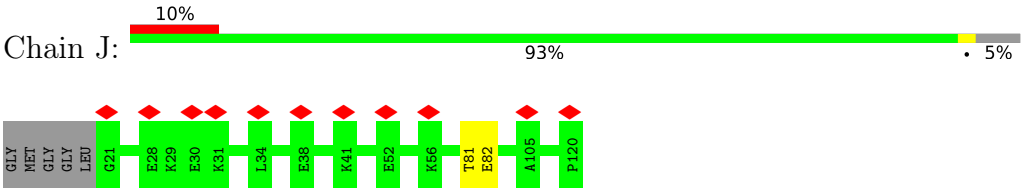
• Molecule 4: V-type ATPase subunit G

Chain I:



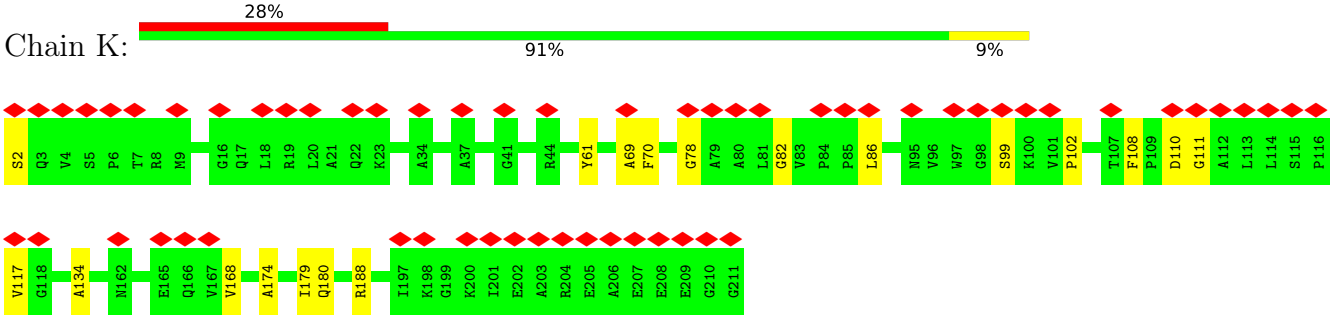
• Molecule 4: V-type ATPase subunit G

Chain J:



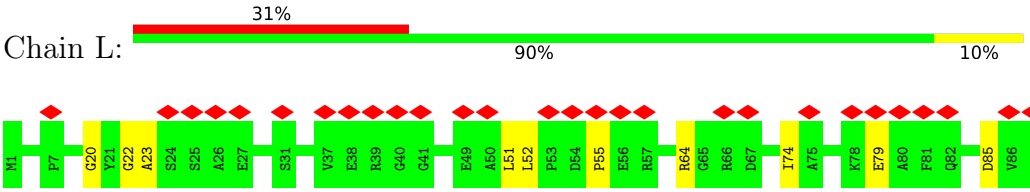
• Molecule 5: V-type ATP synthase subunit D

Chain K:



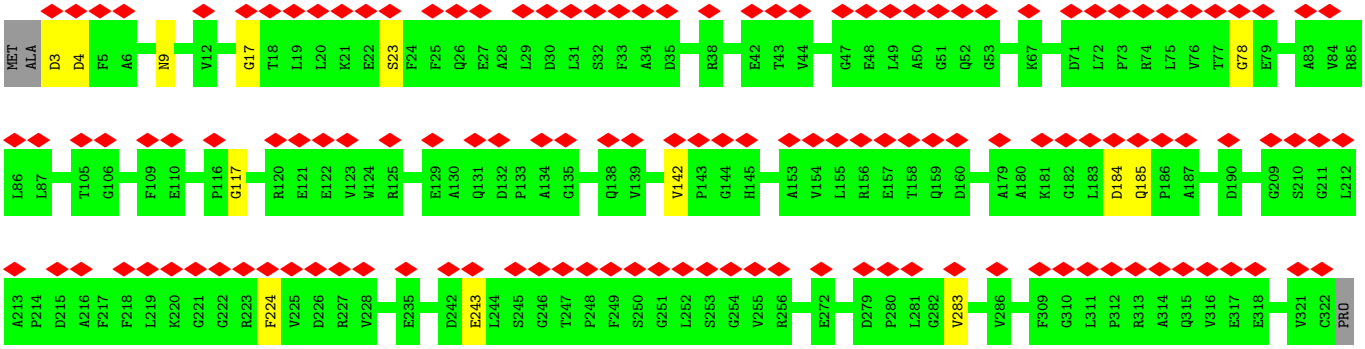
• Molecule 6: V-type ATP synthase subunit F

Chain L:

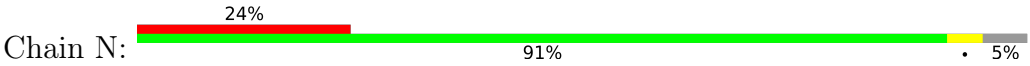


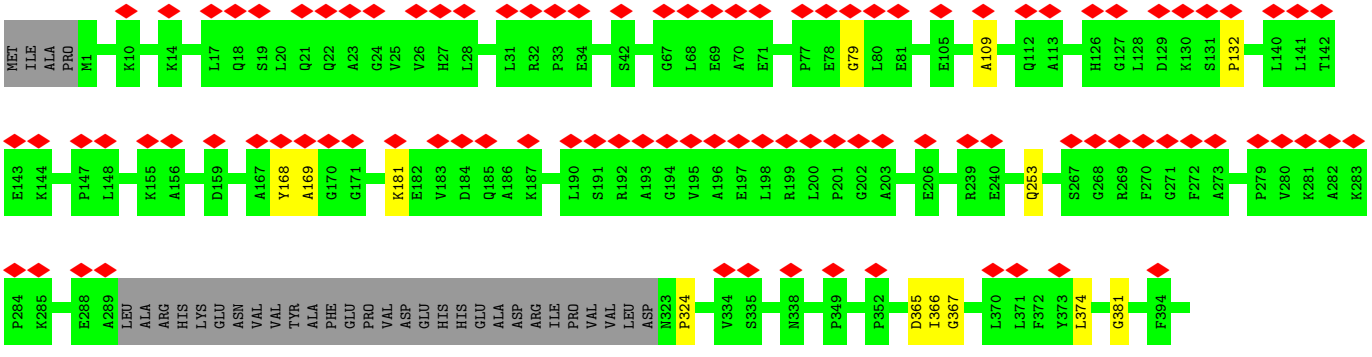
• Molecule 7: V-type ATP synthase subunit C

Chain M:

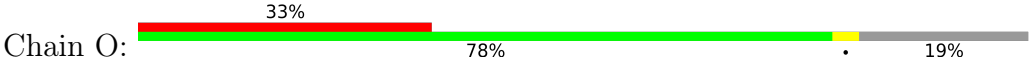


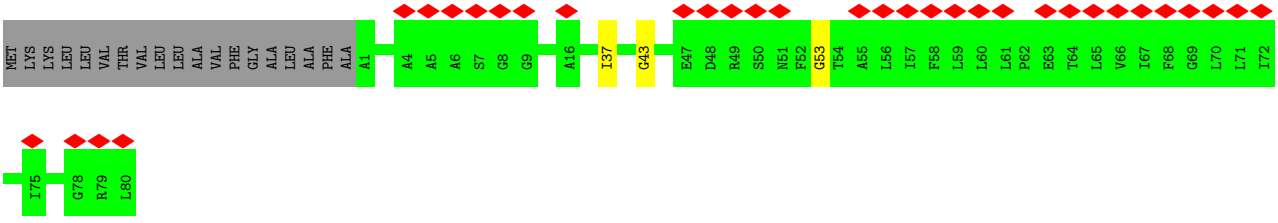
• Molecule 8: Archaeal/vacuolar-type H+-ATPase subunit I





• Molecule 9: Vacuolar type ATP synthase subunit





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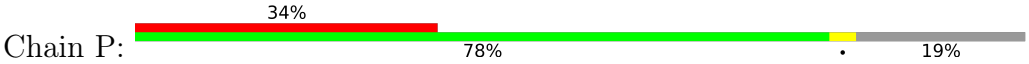
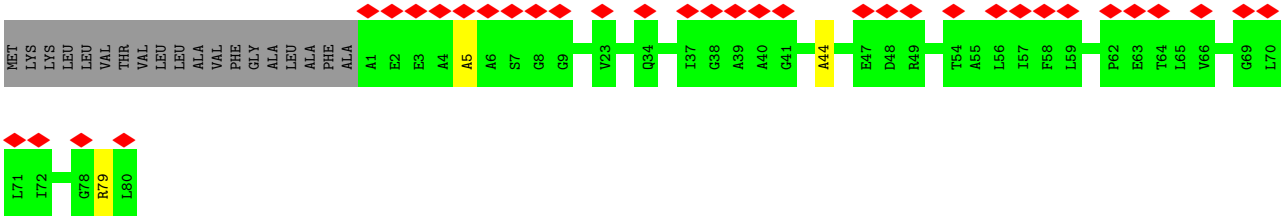
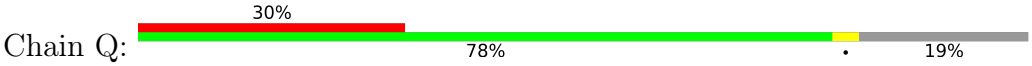
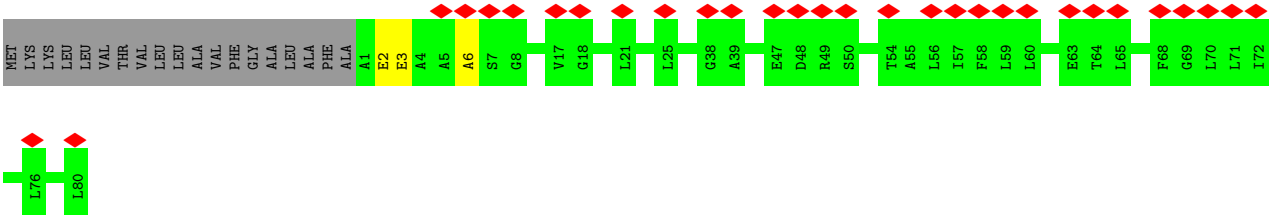


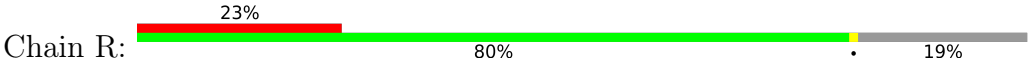


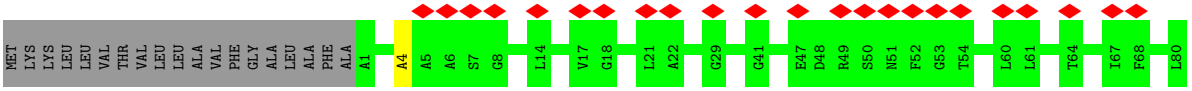
• Molecule 9: Vacuolar type ATP synthase subunit



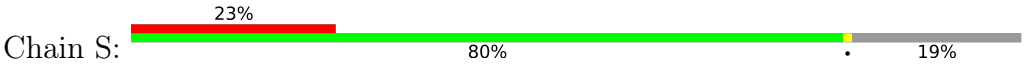


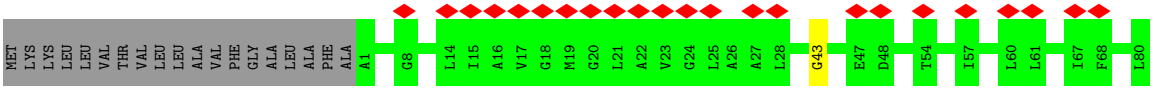
• Molecule 9: Vacuolar type ATP synthase subunit



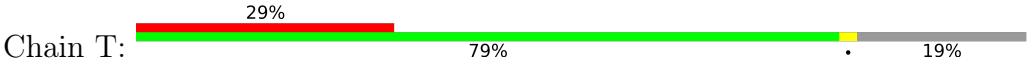


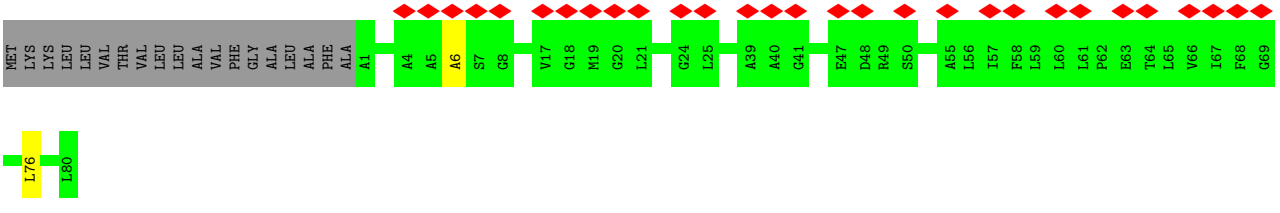
• Molecule 9: Vacuolar type ATP synthase subunit



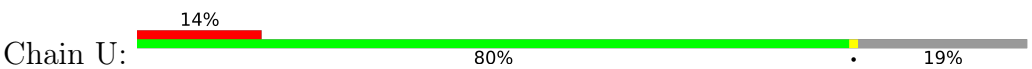


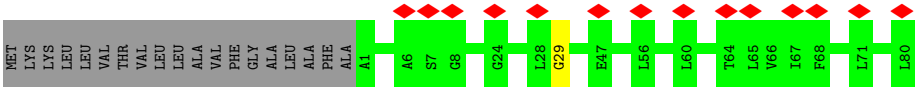
• Molecule 9: Vacuolar type ATP synthase subunit



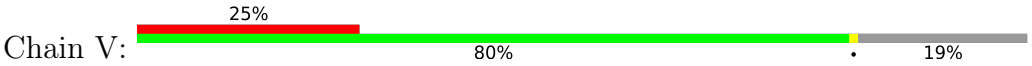


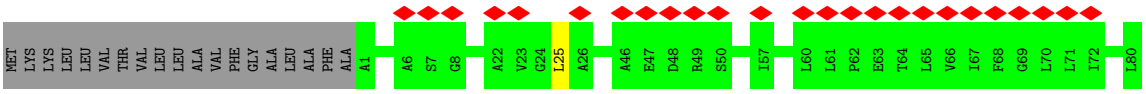
• Molecule 9: Vacuolar type ATP synthase subunit



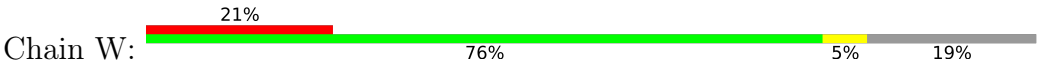


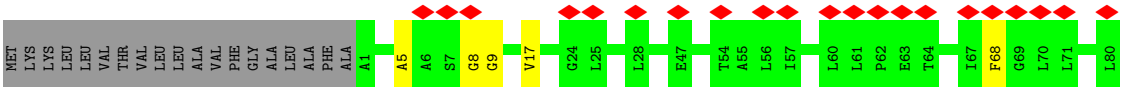
• Molecule 9: Vacuolar type ATP synthase subunit



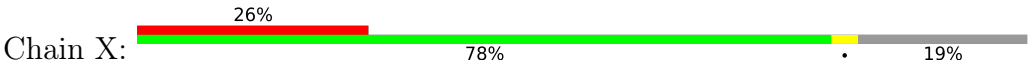


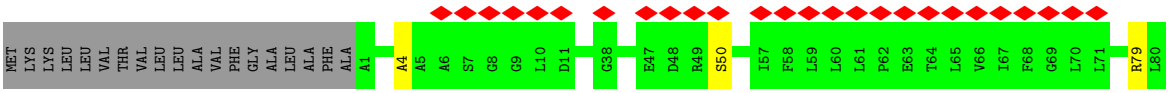
• Molecule 9: Vacuolar type ATP synthase subunit



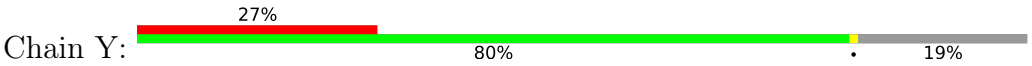


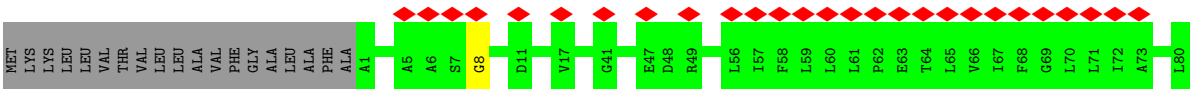
• Molecule 9: Vacuolar type ATP synthase subunit



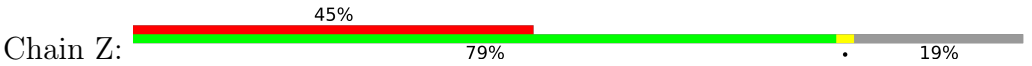


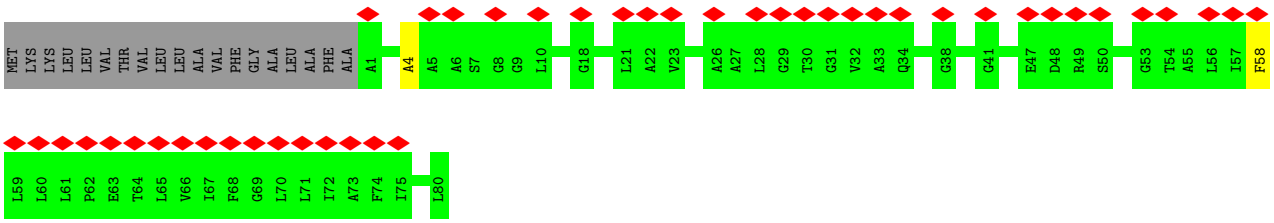
• Molecule 9: Vacuolar type ATP synthase subunit



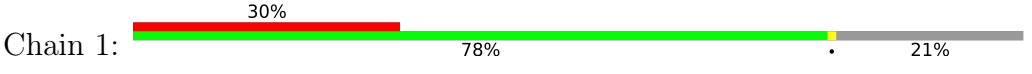


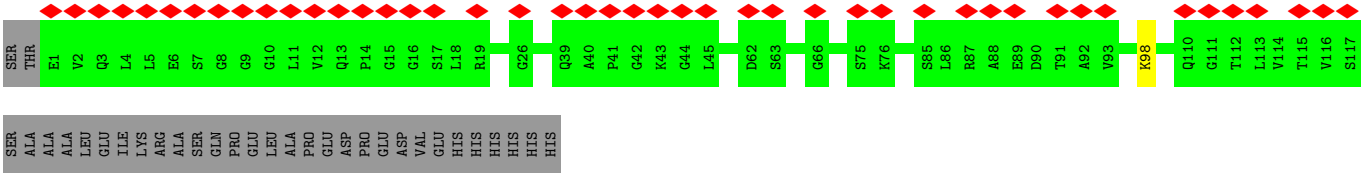
• Molecule 9: Vacuolar type ATP synthase subunit





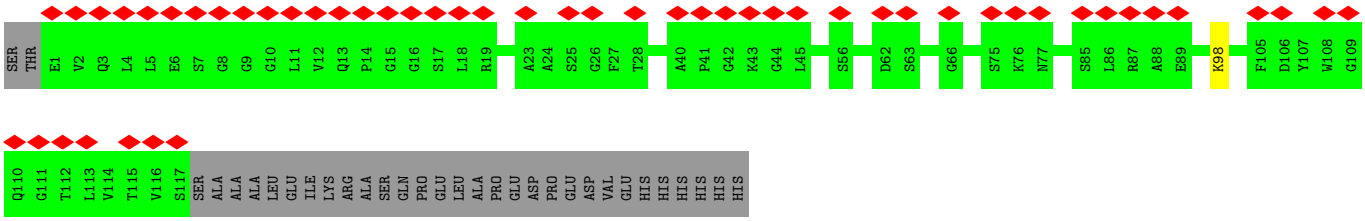
• Molecule 10: Human heavy chain domain antibody





• Molecule 10: Human heavy chain domain antibody

Chain 2:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61045	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	13.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.228	Depositor
Minimum map value	-0.061	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.109	Depositor
Map size (Å)	339.97998, 339.97998, 339.97998	wwPDB
Map dimensions	178, 178, 178	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.9099998, 1.9099998, 1.9099998	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	1.51	4/2306 (0.2%)	1.64	12/2881 (0.4%)
1	B	1.54	5/2302 (0.2%)	1.62	10/2876 (0.3%)
1	C	1.53	2/2306 (0.1%)	1.65	9/2881 (0.3%)
2	D	1.56	5/1826 (0.3%)	1.66	10/2281 (0.4%)
2	E	1.53	2/1826 (0.1%)	1.67	10/2281 (0.4%)
2	F	1.51	2/1826 (0.1%)	1.66	4/2281 (0.2%)
3	G	1.50	1/732 (0.1%)	1.54	2/912 (0.2%)
3	H	1.49	2/732 (0.3%)	1.52	1/912 (0.1%)
4	I	1.38	0/398	1.39	0/496
4	J	1.45	0/398	1.47	1/496 (0.2%)
5	K	1.48	3/838 (0.4%)	1.60	6/1046 (0.6%)
6	L	1.53	2/398 (0.5%)	1.66	3/496 (0.6%)
7	M	1.50	2/1278 (0.2%)	1.55	7/1596 (0.4%)
8	N	1.54	7/2472 (0.3%)	1.55	8/3087 (0.3%)
9	O	1.59	3/318 (0.9%)	1.56	0/396
9	P	1.54	0/318	1.55	2/396 (0.5%)
9	Q	1.56	0/318	1.54	1/396 (0.3%)
9	R	1.55	0/318	1.54	0/396
9	S	1.61	1/318 (0.3%)	1.42	0/396
9	T	1.57	0/318	1.51	1/396 (0.3%)
9	U	1.60	1/318 (0.3%)	1.55	0/396
9	V	1.59	0/318	1.51	1/396 (0.3%)
9	W	1.59	1/318 (0.3%)	1.56	1/396 (0.3%)
9	X	1.50	0/318	1.53	0/396
9	Y	1.50	0/318	1.57	0/396
9	Z	1.58	0/318	1.67	1/396 (0.3%)
10	1	0.64	0/570	0.99	0/788
10	2	0.64	0/570	0.99	0/788
All	All	1.50	43/24594 (0.2%)	1.58	90/30850 (0.3%)

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
7	M	0	1
10	1	0	1
10	2	0	1
All	All	0	3

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	151	GLY	N-CA	-6.97	1.35	1.46
3	H	156	GLY	CA-C	-6.62	1.41	1.51
7	M	117	GLY	CA-C	-6.52	1.41	1.51
1	C	372	GLY	N-CA	-6.32	1.36	1.46
8	N	374	LEU	C-N	6.29	1.48	1.34

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	139	ASP	O-C-N	-6.91	111.64	122.70
2	D	35	ILE	O-C-N	6.70	133.42	122.70
2	E	462	TYR	N-CA-C	-6.56	93.28	111.00
1	B	303	ILE	C-N-CA	6.28	137.39	121.70
2	E	337	ILE	N-CA-C	-6.22	94.22	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	1	98	LYS	Peptide
10	2	98	LYS	Peptide
7	M	3	ASP	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	2307	0	654	0	0
1	B	2303	0	650	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2307	0	654	0	0
2	D	1827	0	510	0	0
2	E	1827	0	510	0	0
2	F	1827	0	510	0	0
3	G	734	0	191	0	0
3	H	734	0	191	0	0
4	I	399	0	100	2	0
4	J	399	0	100	0	0
5	K	839	0	230	0	0
6	L	399	0	119	0	0
7	M	1279	0	357	0	0
8	N	2474	0	691	0	0
9	O	319	0	109	0	0
9	P	319	0	109	0	0
9	Q	319	0	109	0	0
9	R	319	0	109	0	0
9	S	319	0	109	0	0
9	T	319	0	109	0	0
9	U	319	0	109	0	0
9	V	319	0	109	0	0
9	W	319	0	109	0	0
9	X	319	0	109	0	0
9	Y	319	0	109	0	0
9	Z	319	0	109	0	0
10	1	571	0	269	0	0
10	2	571	0	269	0	0
All	All	24625	0	7313	2	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 0.

All (2) 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)
4:I:115:LEU:O	4:I:117:GLU:N	2.30	0.61
4:I:115:LEU:C	4:I:117:GLU:H	2.19	0.43

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	575/577 (100%)	504 (88%)	56 (10%)	15 (3%)	5 31
1	B	574/577 (100%)	477 (83%)	72 (12%)	25 (4%)	2 22
1	C	575/577 (100%)	499 (87%)	56 (10%)	20 (4%)	3 25
2	D	455/457 (100%)	370 (81%)	65 (14%)	20 (4%)	2 22
2	E	455/457 (100%)	370 (81%)	64 (14%)	21 (5%)	2 21
2	F	455/457 (100%)	377 (83%)	57 (12%)	21 (5%)	2 21
3	G	180/186 (97%)	162 (90%)	10 (6%)	8 (4%)	2 22
3	H	180/186 (97%)	167 (93%)	9 (5%)	4 (2%)	6 35
4	I	98/105 (93%)	91 (93%)	5 (5%)	2 (2%)	7 38
4	J	98/105 (93%)	94 (96%)	3 (3%)	1 (1%)	15 55
5	K	208/210 (99%)	172 (83%)	25 (12%)	11 (5%)	2 19
6	L	98/100 (98%)	78 (80%)	15 (15%)	5 (5%)	2 19
7	M	318/323 (98%)	307 (96%)	7 (2%)	4 (1%)	12 48
8	N	615/652 (94%)	559 (91%)	43 (7%)	13 (2%)	7 36
9	O	78/99 (79%)	76 (97%)	2 (3%)	0	100 100
9	P	78/99 (79%)	74 (95%)	2 (3%)	2 (3%)	5 31
9	Q	78/99 (79%)	72 (92%)	4 (5%)	2 (3%)	5 31
9	R	78/99 (79%)	73 (94%)	4 (5%)	1 (1%)	12 48
9	S	78/99 (79%)	74 (95%)	4 (5%)	0	100 100
9	T	78/99 (79%)	75 (96%)	2 (3%)	1 (1%)	12 48
9	U	78/99 (79%)	75 (96%)	3 (4%)	0	100 100
9	V	78/99 (79%)	72 (92%)	6 (8%)	0	100 100
9	W	78/99 (79%)	74 (95%)	1 (1%)	3 (4%)	3 24
9	X	78/99 (79%)	74 (95%)	1 (1%)	3 (4%)	3 24
9	Y	78/99 (79%)	74 (95%)	3 (4%)	1 (1%)	12 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
9	Z	78/99 (79%)	74 (95%)	3 (4%)	1 (1%)	12 48
10	1	115/149 (77%)	111 (96%)	4 (4%)	0	100 100
10	2	115/149 (77%)	111 (96%)	4 (4%)	0	100 100
All	All	6050/6455 (94%)	5336 (88%)	530 (9%)	184 (3%)	7 28

5 of 184 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	134	VAL
1	B	258	ARG
1	B	303	ILE
1	B	305	VAL
1	B	466	GLU

5.3.2 Protein sidechains (i)

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation

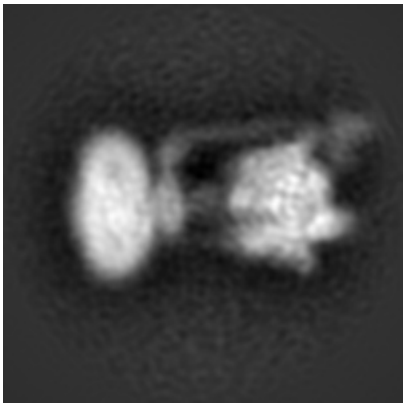
This section contains visualisations of the EMDB entry EMD-8462. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

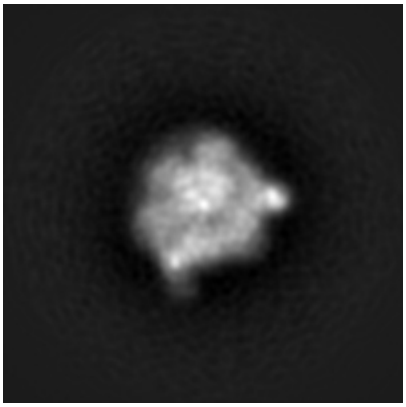
6.1 Orthogonal projections

6.1.1 Primary map

X



Y

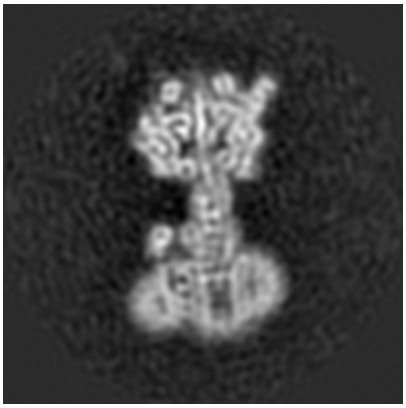


Z

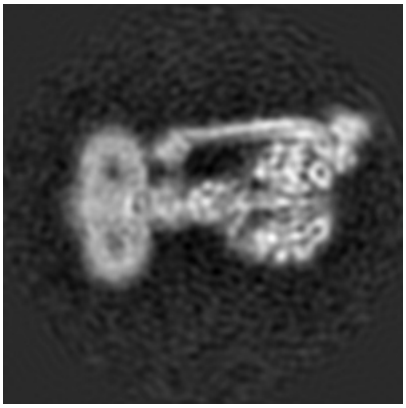
The images above show the map projected in three orthogonal directions.

6.2 Central slices

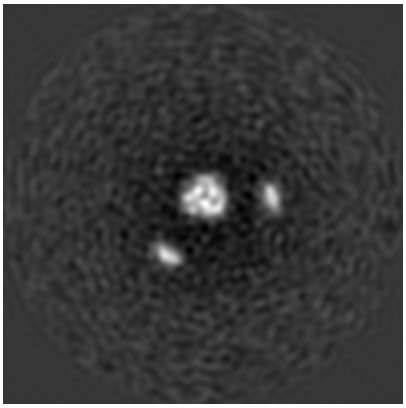
6.2.1 Primary map



X Index: 89



Y Index: 89

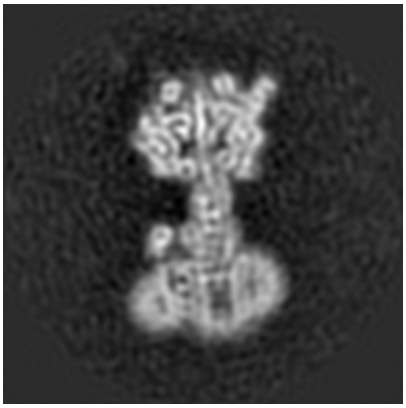


Z Index: 89

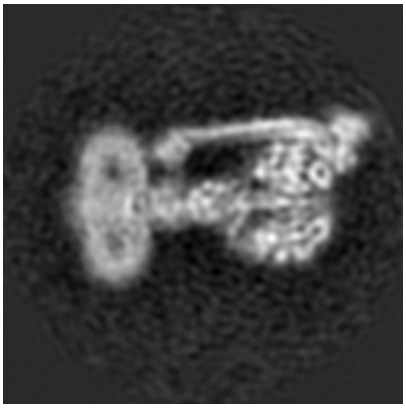
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

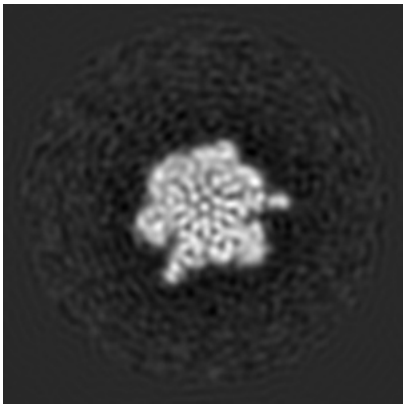
6.3.1 Primary map



X Index: 89



Y Index: 89

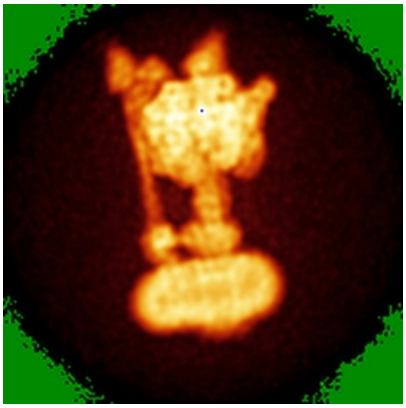


Z Index: 128

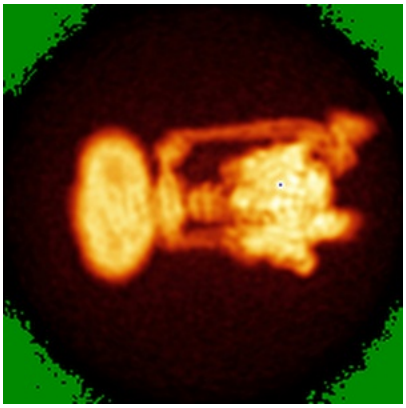
The images above show the largest variance slices of the map in three orthogonal directions.

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

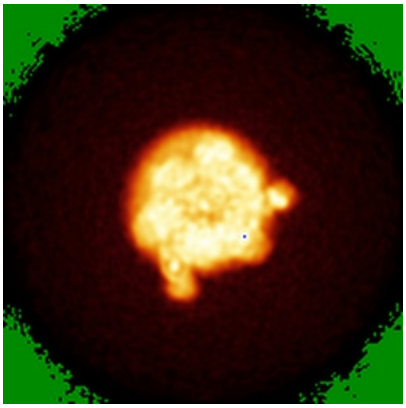
6.4.1 Primary map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.109. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

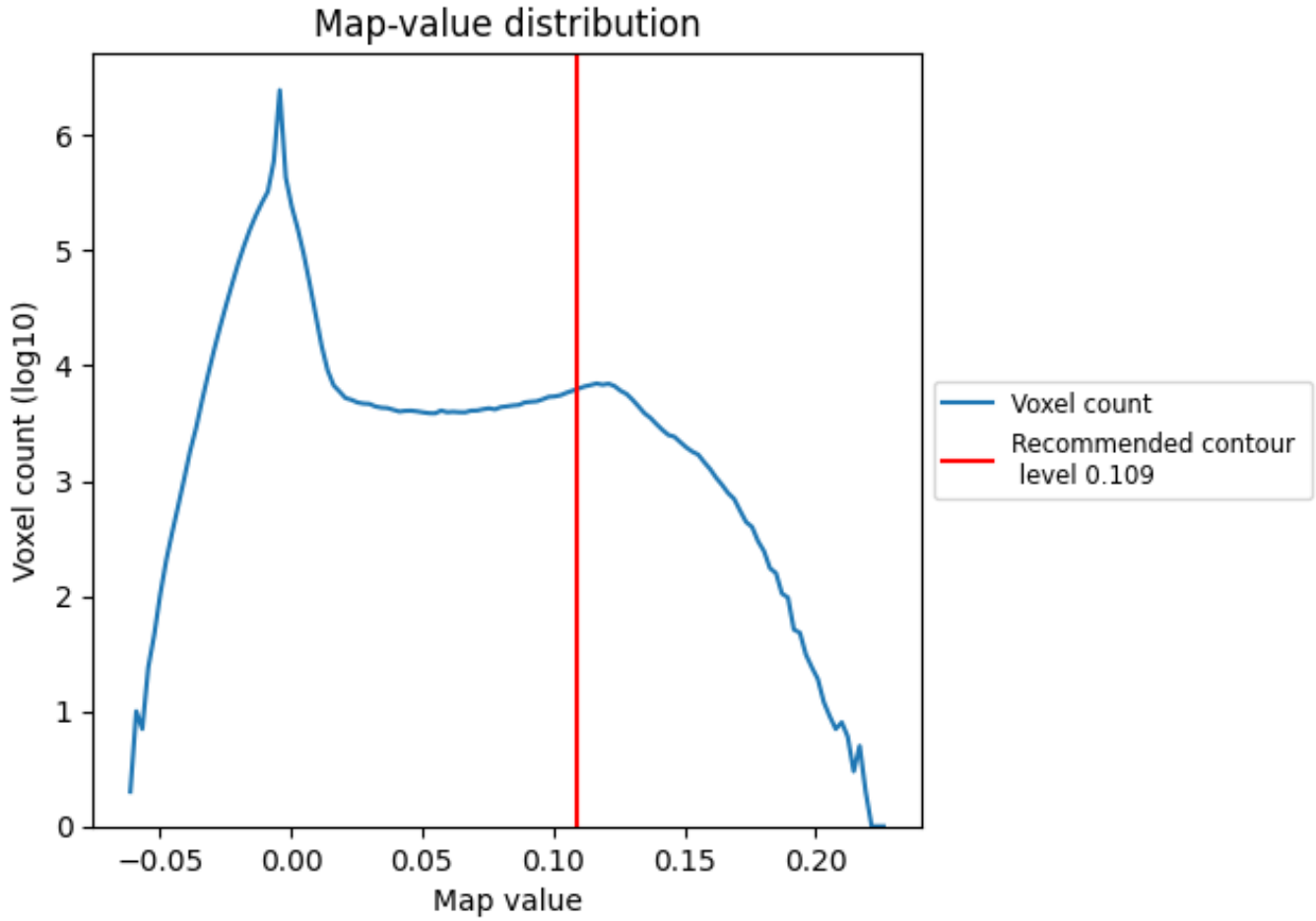
6.6 Mask visualisation (i)

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

7 Map analysis

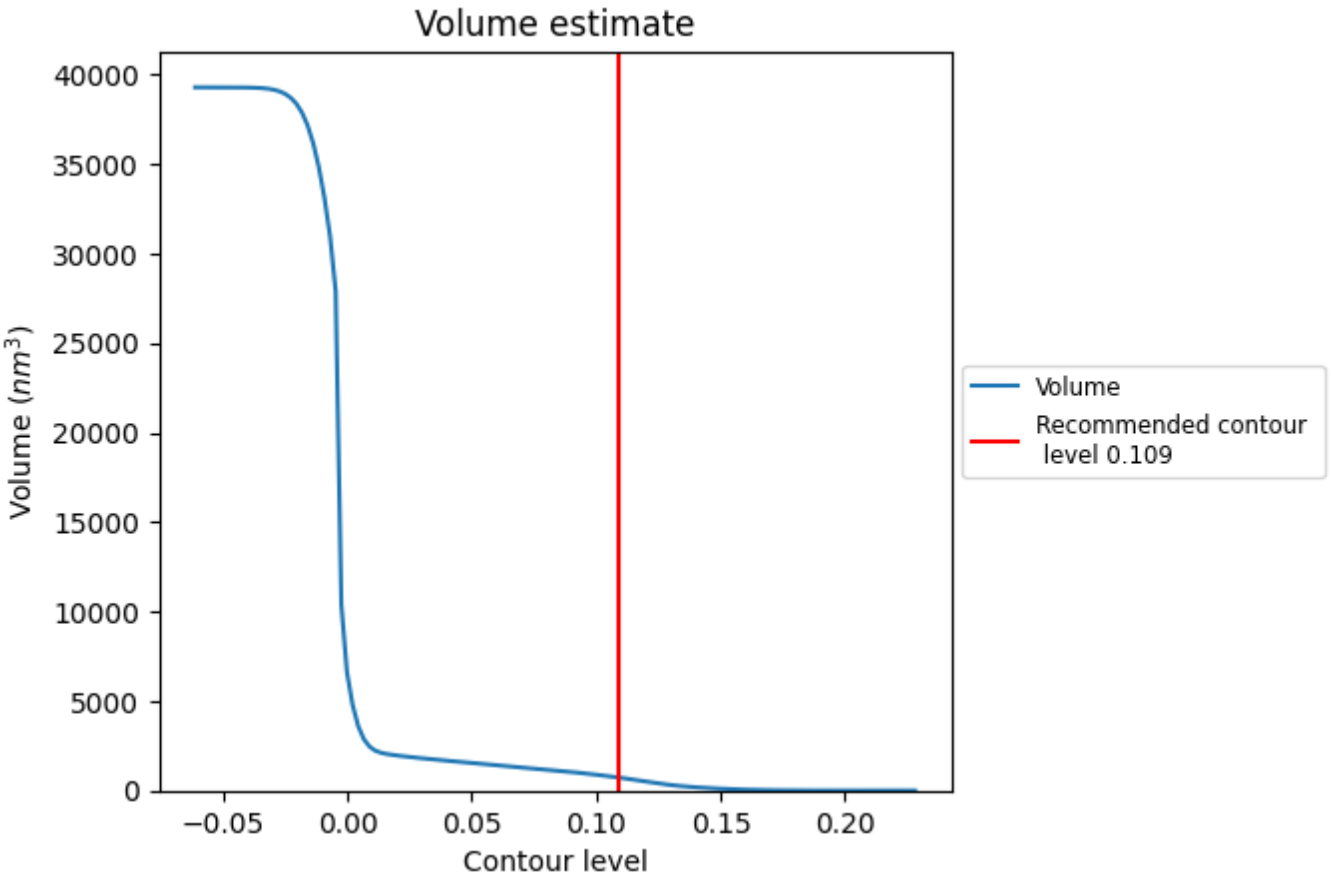
This section contains the results of statistical analysis of the map.

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.

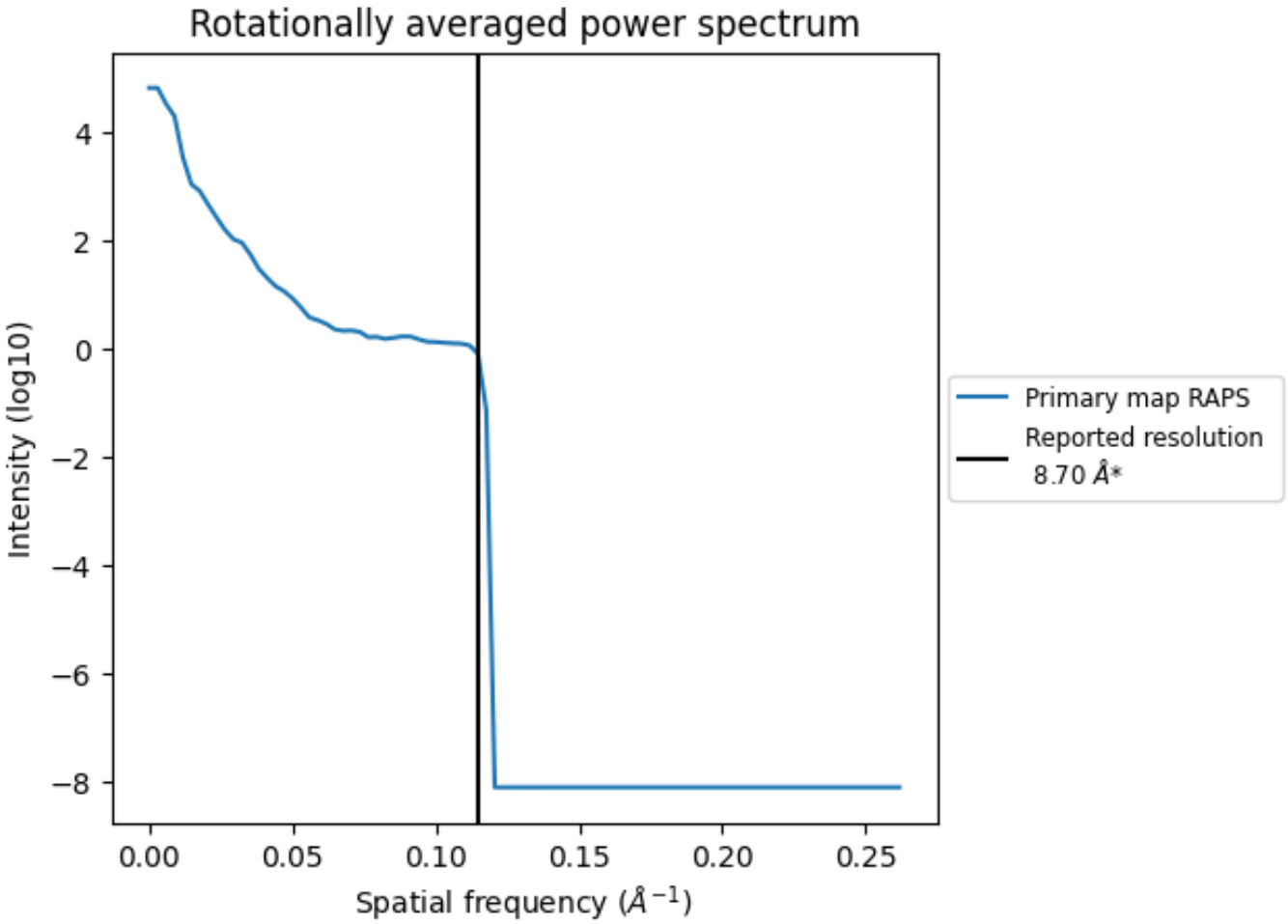
7.2 Volume estimate (i)



The volume at the recommended contour level is 730 nm^3; this corresponds to an approximate mass of 660 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)

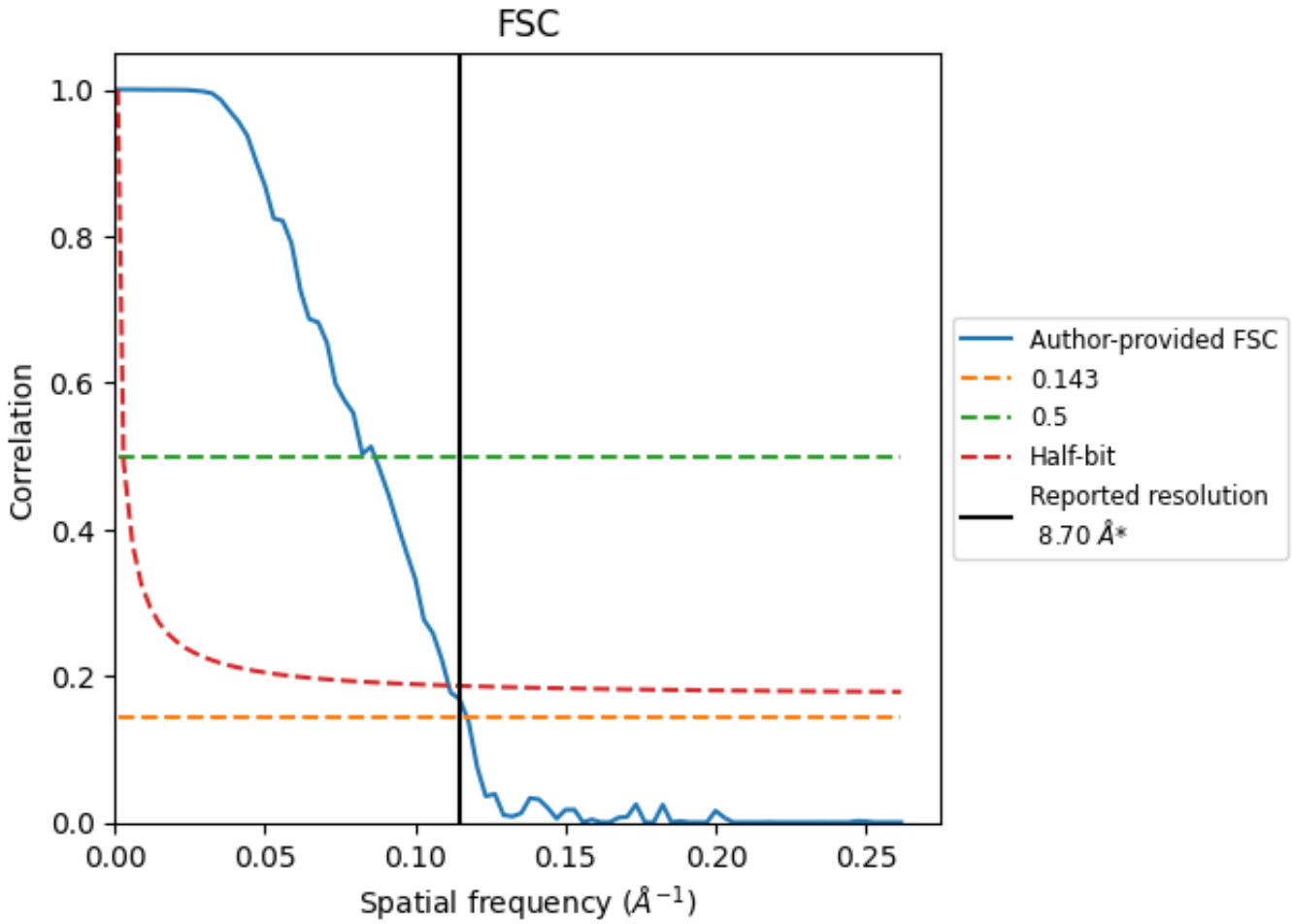


*Reported resolution corresponds to spatial frequency of 0.115 Å^{-1}

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 0.115 Å^{-1}

8.2 Resolution estimates (i)

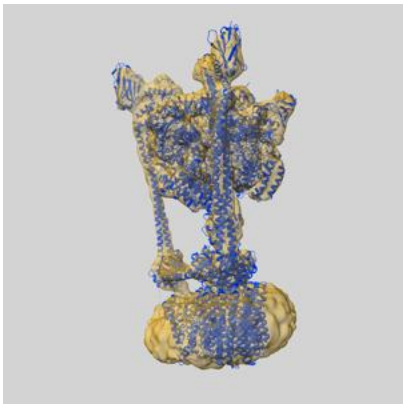
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.70	-	-
Author-provided FSC curve	8.53	11.56	9.00
Unmasked-calculated*	-	-	-

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

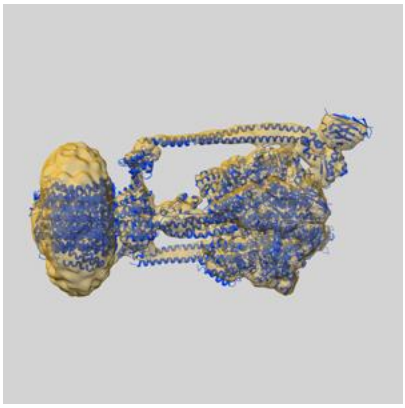
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8462 and PDB model 5TSJ. Per-residue inclusion information can be found in section 3 on page 7.

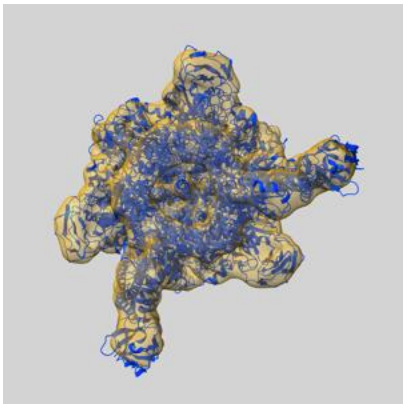
9.1 Map-model overlay



X



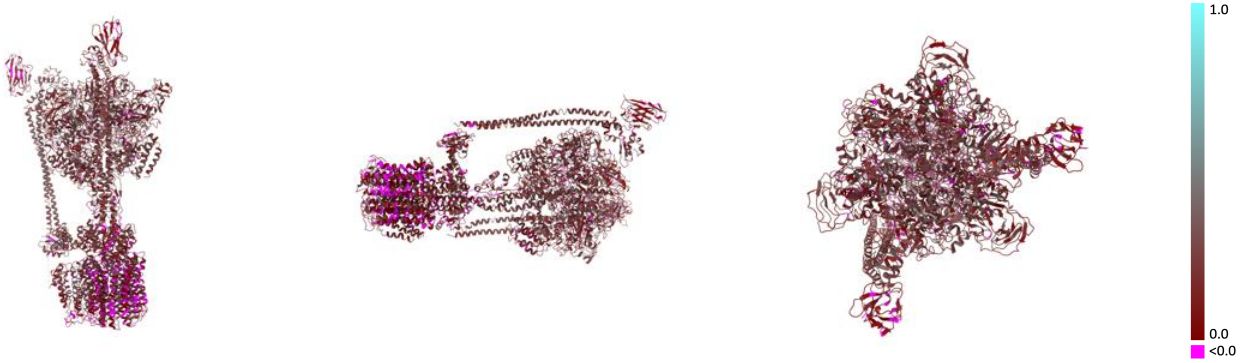
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.109 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.

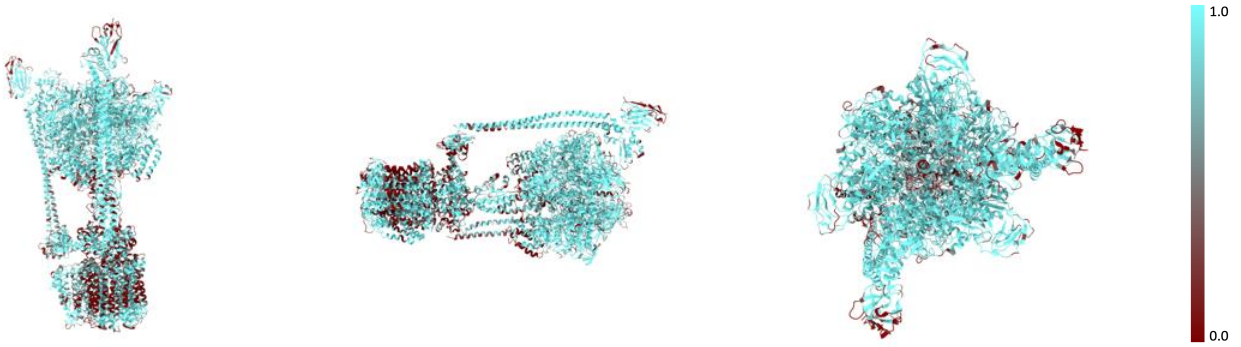
9.2 Q-score mapped to coordinate model



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.

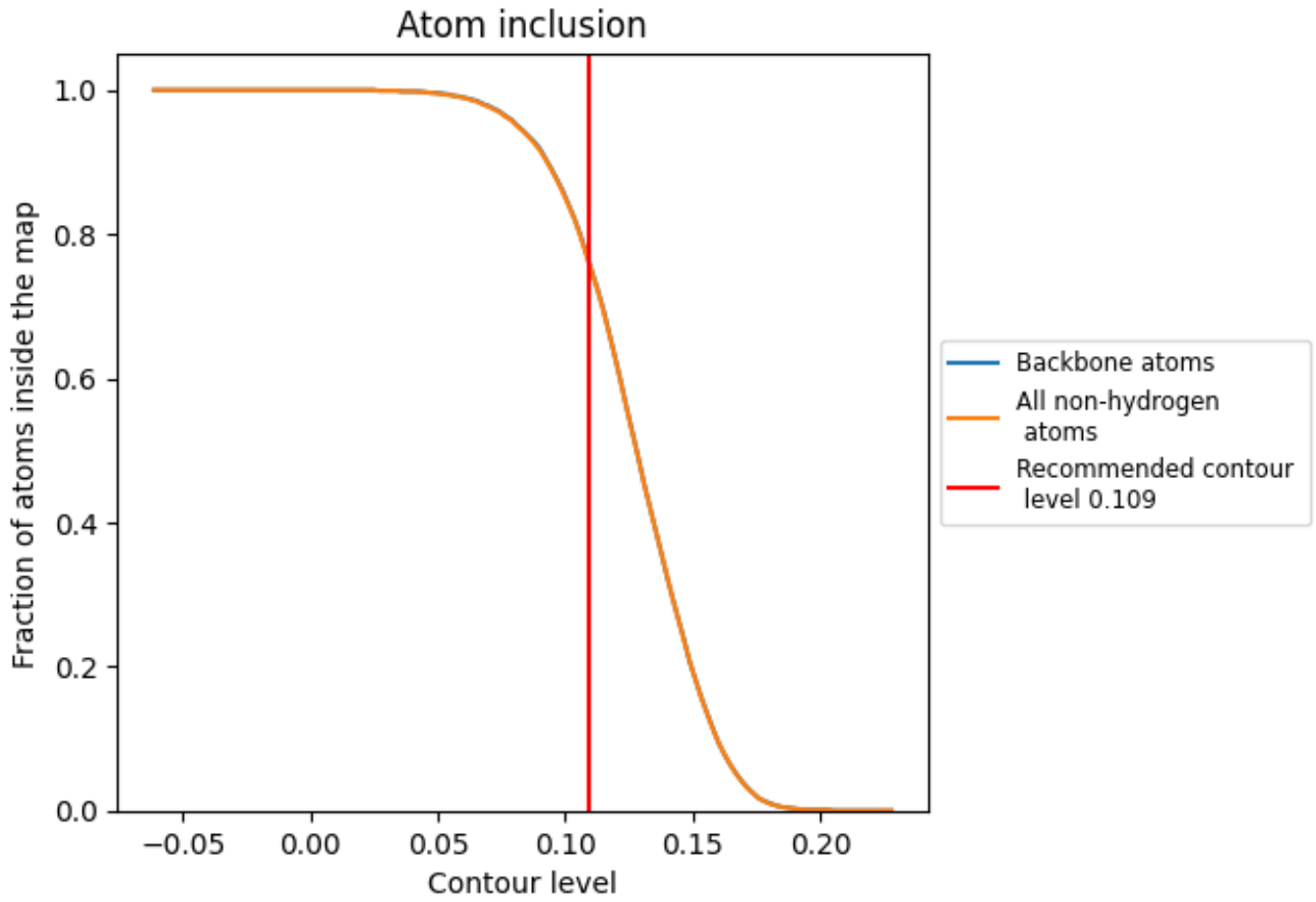
9.3 Atom inclusion mapped to coordinate model



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 (0.109).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 76% 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 (0.109) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7650	0.1760
1	0.6040	0.1190
2	0.5800	0.1000
A	0.8790	0.2130
B	0.8080	0.1910
C	0.8820	0.2030
D	0.8650	0.2100
E	0.8370	0.1940
F	0.8840	0.2120
G	0.9100	0.2400
H	0.8130	0.2140
I	0.7440	0.2300
J	0.8750	0.2450
K	0.6820	0.1950
L	0.6440	0.1610
M	0.5280	0.1460
N	0.7190	0.1650
O	0.5490	0.1070
P	0.5420	0.1060
Q	0.5610	0.0940
R	0.6800	0.1150
S	0.6330	0.0830
T	0.5640	0.0720
U	0.7710	0.1530
V	0.6360	0.0370
W	0.6900	0.1120
X	0.6210	0.0550
Y	0.6050	0.0890
Z	0.3920	0.0560