wwPDB EM Validation Summary Report

Nov 5, 2022 – 12:04 PM EDT

PDB ID	:	5VOZ
EMDB ID	:	EMD-8726
Title	:	Yeast V-ATPase in complex with Legionella pneumophila effector SidK (rotational state 3)
Authors	:	Zhao, J.
Deposited on	:	2017-05-03
Resolution	:	7.60 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:

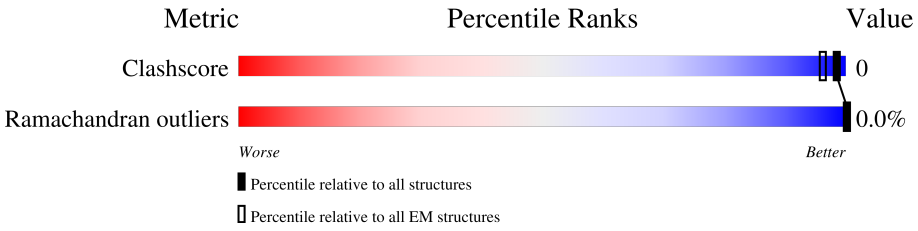
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 7.60 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	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	617	96%
1	C	617	96%
1	E	617	96%
2	B	517	88% 12%
2	D	517	5% 88% 12%
2	F	517	88% 12%
3	G	233	9% 94% 6%
3	I	233	93% 7%
3	K	233	93% 7%

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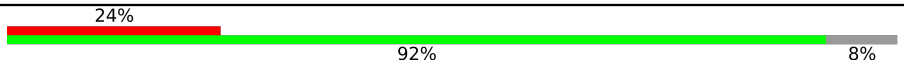
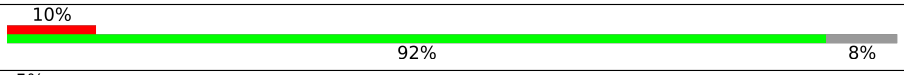
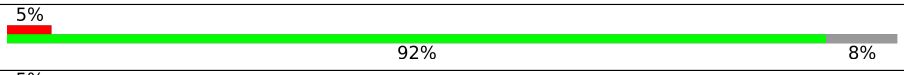
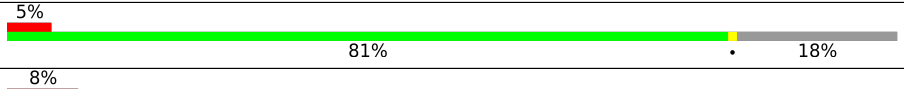
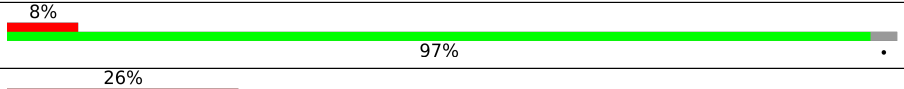
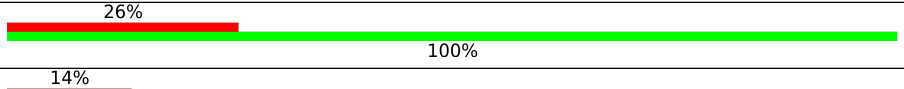
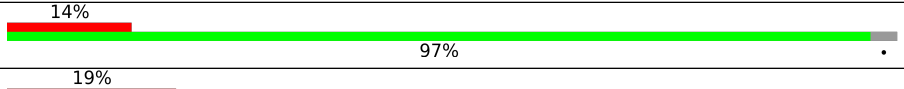
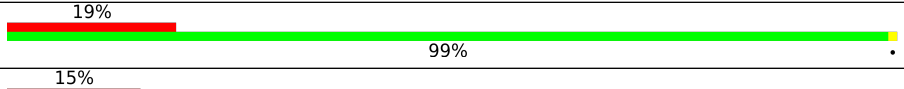
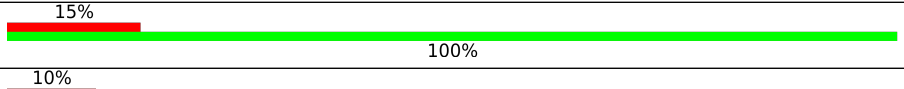
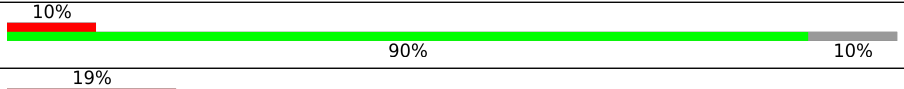
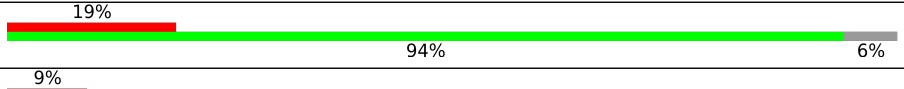
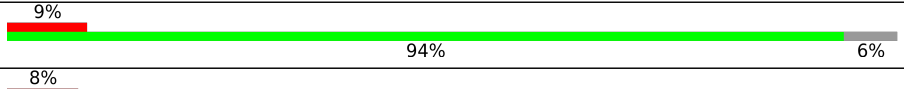
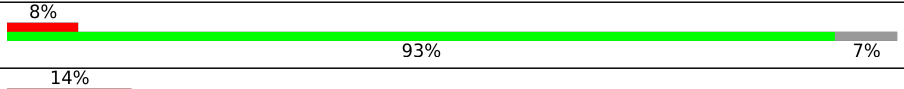
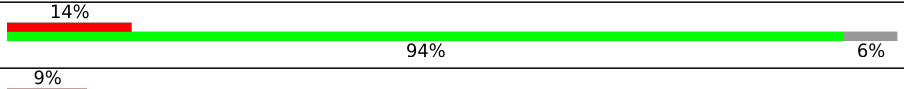
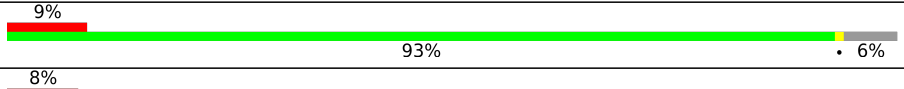
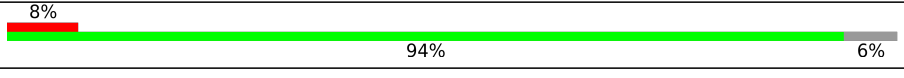
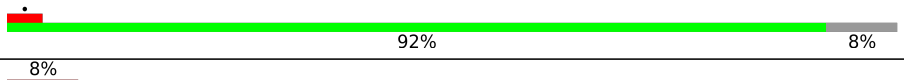
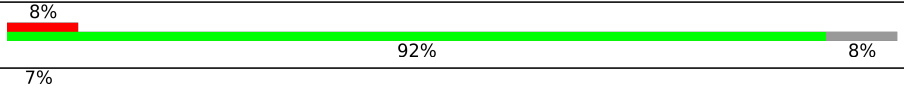
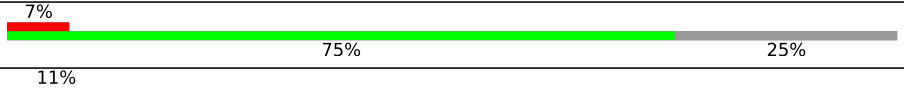
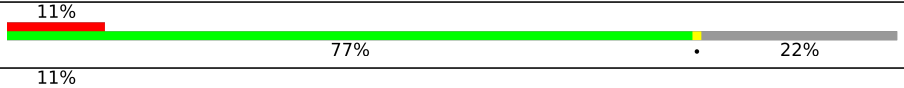
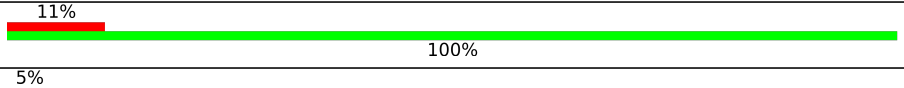
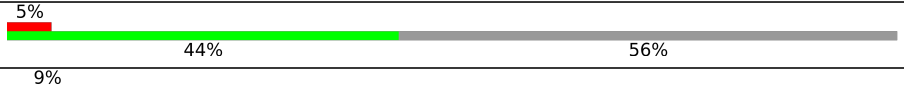
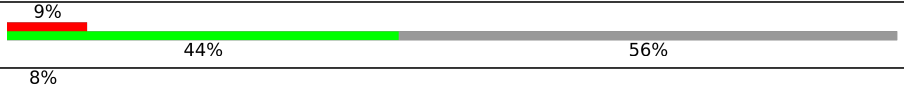
Mol	Chain	Length	Quality of chain
4	H	114	
4	J	114	
4	L	114	
5	M	256	
6	N	118	
7	O	392	
8	P	478	
9	Q	345	
10	R	213	
11	S	164	
12	T	160	
12	U	160	
12	V	160	
12	W	160	
12	X	160	
12	Y	160	
12	Z	160	
12	a	160	
13	b	840	
14	c	73	
15	d	54	
16	e	573	
16	f	573	
16	g	573	

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 34724 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 catalytic subunit A,V-type proton ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	593	Total 2371	C 1186	N 593	O 592	0	0
1	C	593	Total 2371	C 1186	N 593	O 592	0	0
1	E	593	Total 2371	C 1186	N 593	O 592	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	457	Total 1827	C 914	N 457	O 456	0	0
2	D	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 proton ATPase subunit E.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	218	Total 871	C 436	N 218	O 217	0	0
3	I	217	Total 867	C 434	N 217	O 216	0	0
3	K	217	Total 867	C 434	N 217	O 216	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	105	Total 419	C 210	N 105	O 104	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	J	105	Total 419	C 210	N 105	O 104	0	0
4	L	105	Total 419	C 210	N 105	O 104	0	0

- Molecule 5 is a protein called V-type proton ATPase subunit D.

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

- Molecule 6 is a protein called V-type proton ATPase subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	N	115	Total 459	C 230	N 115	O 114	0	0

- Molecule 7 is a protein called V-type proton ATPase subunit C.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	392	Total 1567	C 784	N 392	O 391	0	0

- Molecule 8 is a protein called V-type proton ATPase subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	P	462	Total 1847	C 924	N 462	O 461	0	0

- Molecule 9 is a protein called V-type proton ATPase subunit d.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	Q	345	Total 1379	C 690	N 345	O 344	0	0

- Molecule 10 is a protein called V-type proton ATPase subunit c".

Mol	Chain	Residues	Atoms				AltConf	Trace
10	R	213	Total 851	C 426	N 213	O 212	0	0

- Molecule 11 is a protein called V-type proton ATPase subunit c'.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	S	147	Total 587	C 294	N 147	O 146	0	0

- Molecule 12 is a protein called V-type proton ATPase subunit c.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	T	150	Total 599	C 300	N 150	O 149	0	0
12	U	150	Total 599	C 300	N 150	O 149	0	0
12	V	149	Total 595	C 298	N 149	O 148	0	0
12	W	150	Total 599	C 300	N 150	O 149	0	0
12	X	150	Total 599	C 300	N 150	O 149	0	0
12	Y	150	Total 599	C 300	N 150	O 149	0	0
12	Z	148	Total 591	C 296	N 148	O 147	0	0
12	a	148	Total 591	C 296	N 148	O 147	0	0

- Molecule 13 is a protein called V-type proton ATPase subunit a, vacuolar isoform.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	b	634	Total 2529	C 1268	N 634	O 627	0	0

- Molecule 14 is a protein called V-type proton ATPase subunit e.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	c	57	Total 227	C 114	N 57	O 56	0	0

- Molecule 15 is a protein called V-type proton ATPase subunit f.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	d	54	Total 214	C 108	N 54	O 52	0	0

- Molecule 16 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	e	250	Total 999	C 500	N 250	O 249	0	0
16	f	250	Total 999	C 500	N 250	O 249	0	0
16	g	250	Total 999	C 500	N 250	O 249	0	0

There are 3 discrepancies between the modelled and reference sequences:

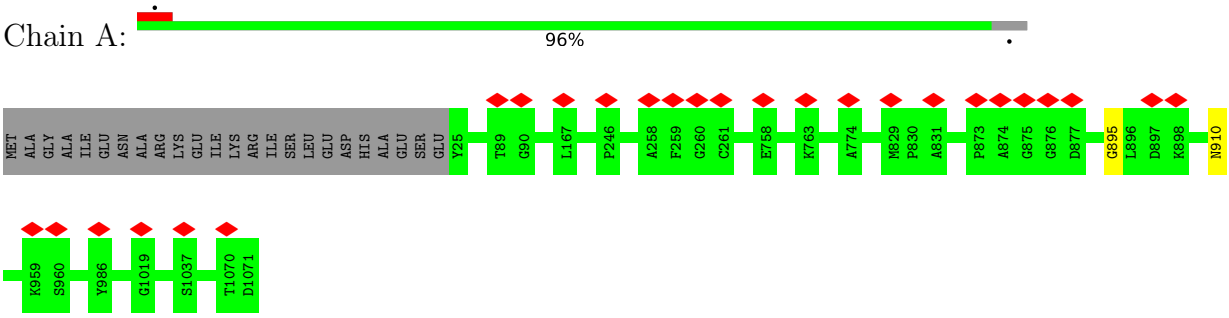
Chain	Residue	Modelled	Actual	Comment	Reference
e	89	LEU	GLN	conflict	UNP G8UUS6
f	89	LEU	GLN	conflict	UNP G8UUS6
g	89	LEU	GLN	conflict	UNP G8UUS6

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.

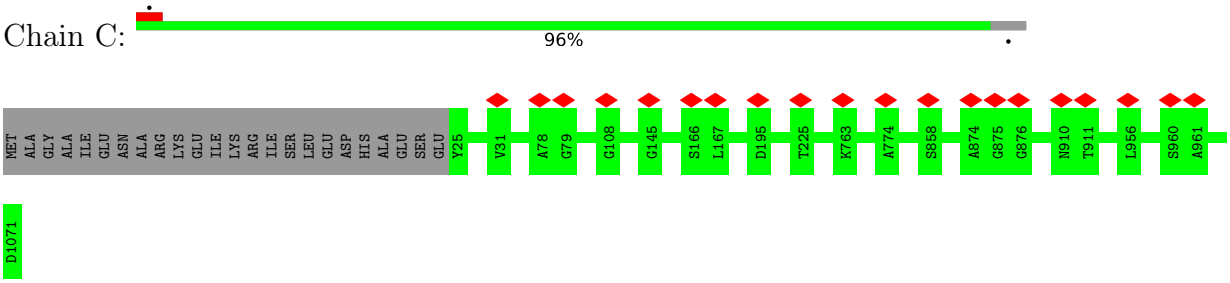
• Molecule 1: V-type proton ATPase catalytic subunit A,V-type proton ATPase catalytic subunit A

Chain A:



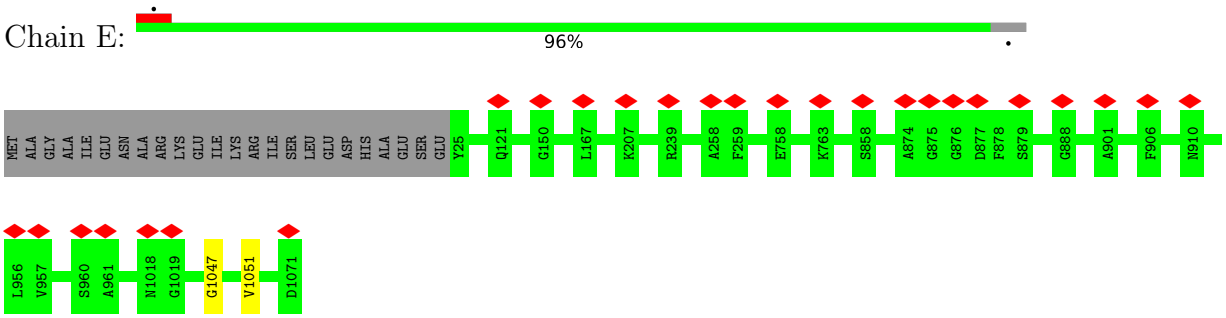
• Molecule 1: V-type proton ATPase catalytic subunit A,V-type proton ATPase catalytic subunit A

Chain C:



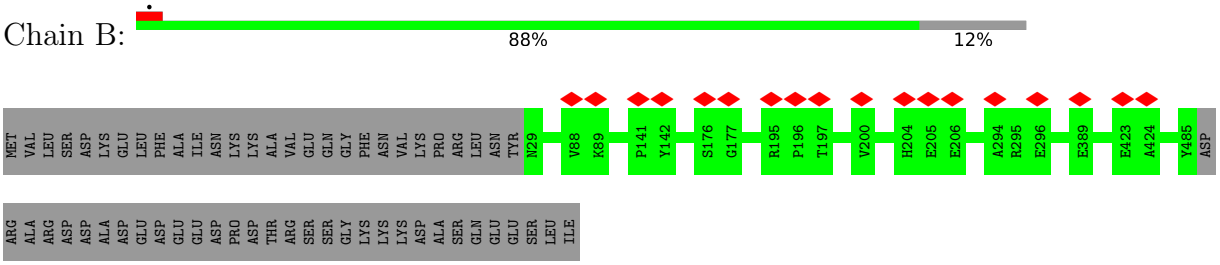
• Molecule 1: V-type proton ATPase catalytic subunit A,V-type proton ATPase catalytic subunit A

Chain E:



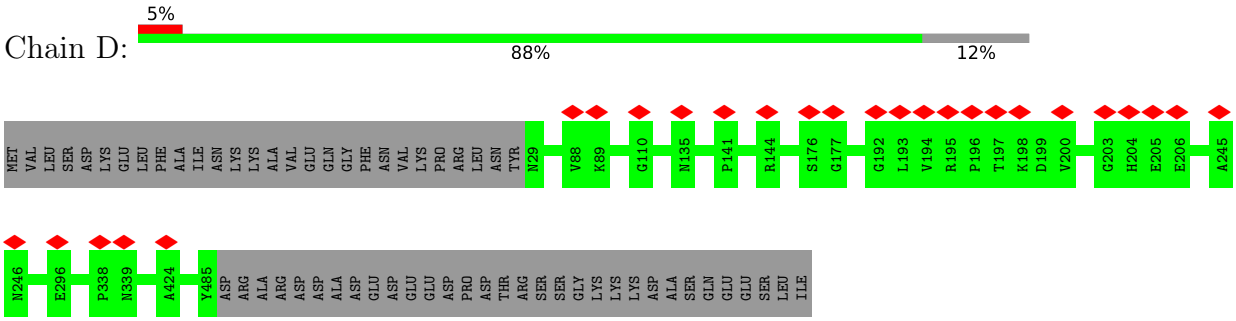
• Molecule 2: V-type proton ATPase subunit B

Chain B:



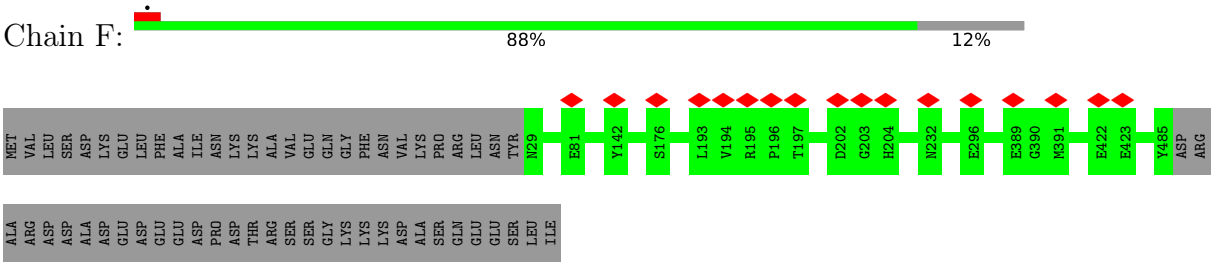
• Molecule 2: V-type proton ATPase subunit B

Chain D:



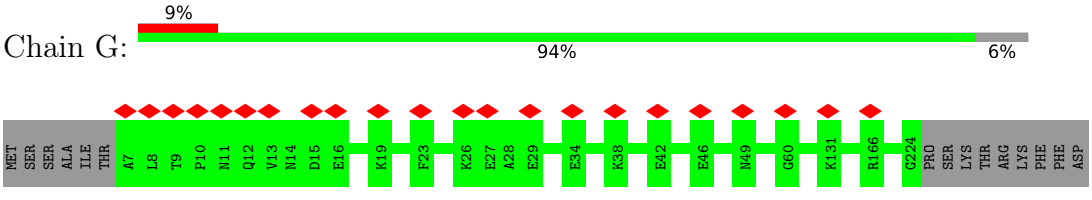
• Molecule 2: V-type proton ATPase subunit B

Chain F:



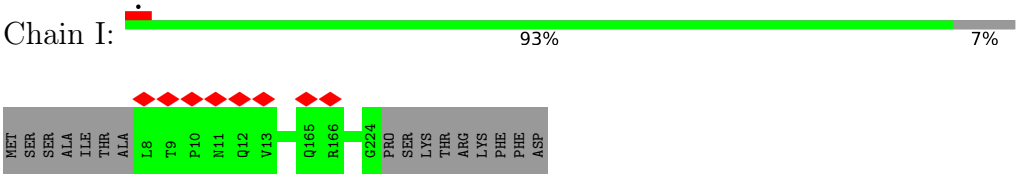
• Molecule 3: V-type proton ATPase subunit E

Chain G:



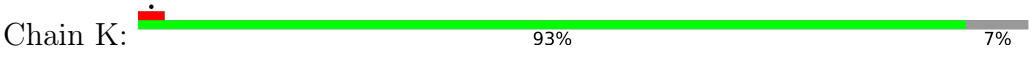
• Molecule 3: V-type proton ATPase subunit E

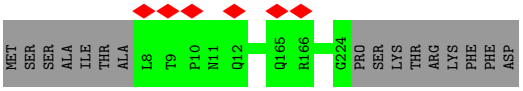
Chain I:



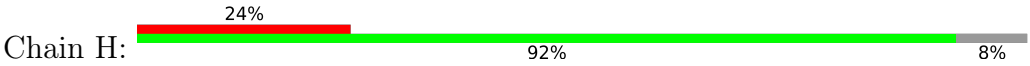
• Molecule 3: V-type proton ATPase subunit E

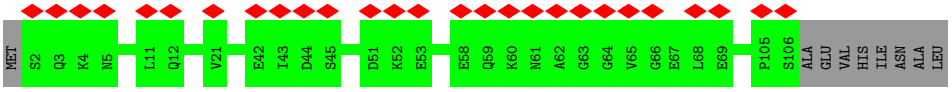
Chain K:



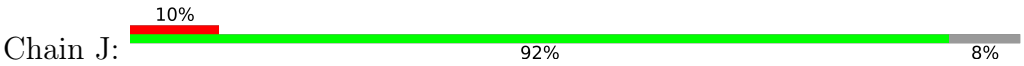


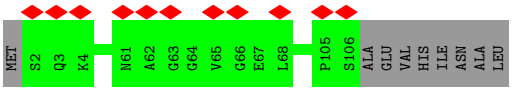
• Molecule 4: V-type proton ATPase subunit G



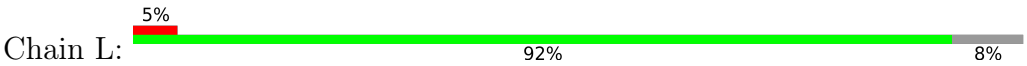


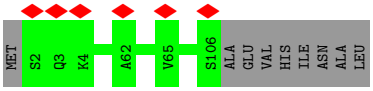
• Molecule 4: V-type proton ATPase subunit G



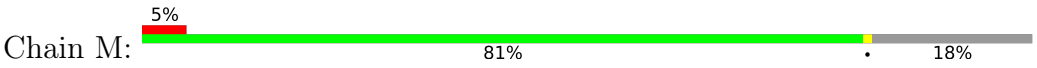


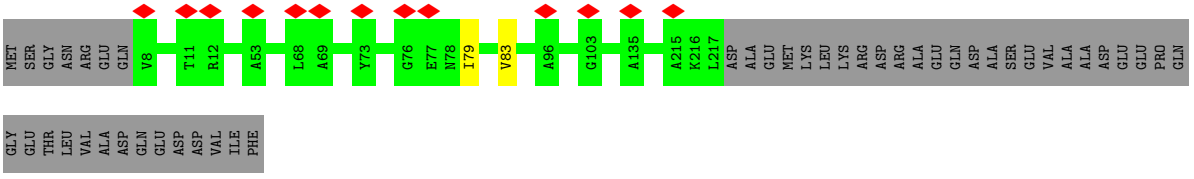
• Molecule 4: V-type proton ATPase subunit G



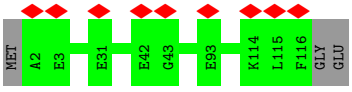


• Molecule 5: V-type proton ATPase subunit D

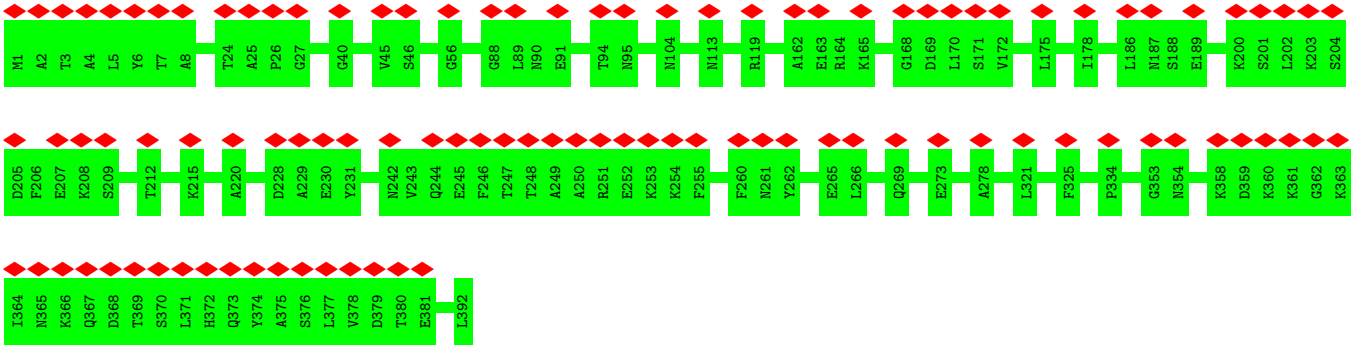




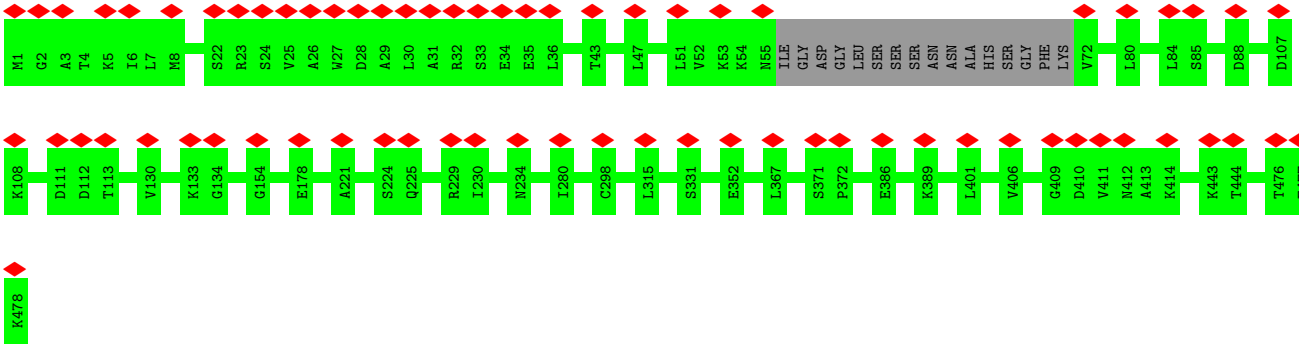
• Molecule 6: V-type proton ATPase subunit F



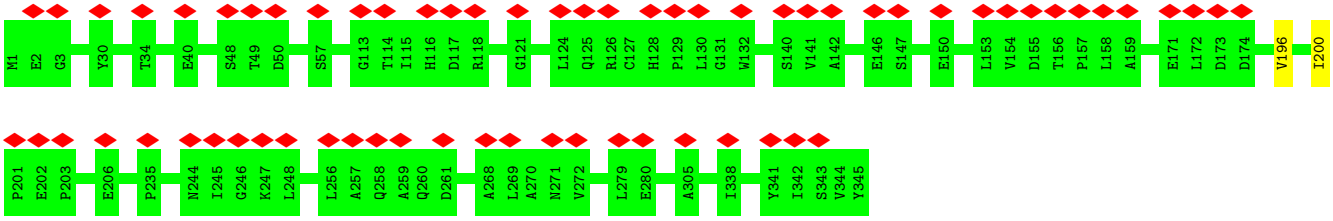
• Molecule 7: V-type proton ATPase subunit C



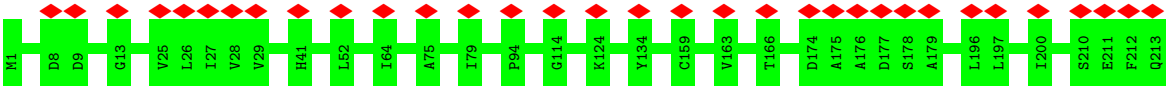
• Molecule 8: V-type proton ATPase subunit H



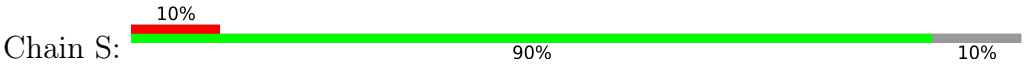
• Molecule 9: V-type proton ATPase subunit d

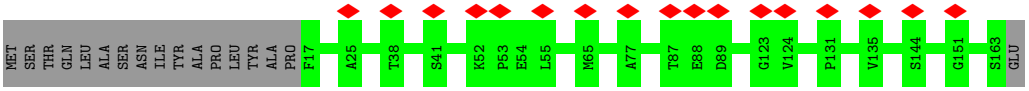


• Molecule 10: V-type proton ATPase subunit c"

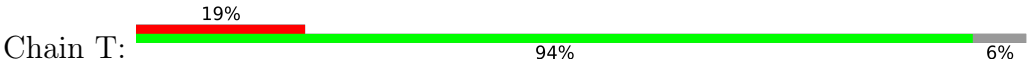


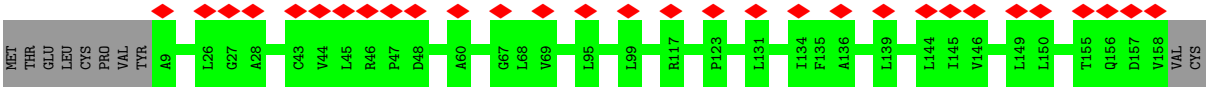
• Molecule 11: V-type proton ATPase subunit c'



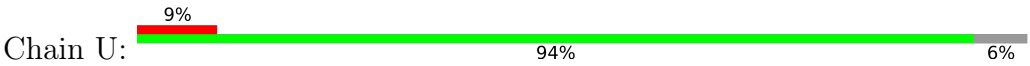


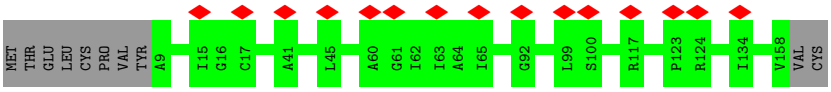
• Molecule 12: V-type proton ATPase subunit c



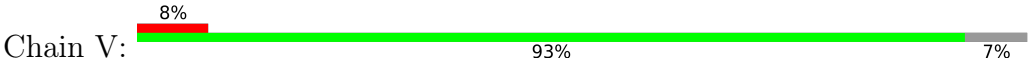


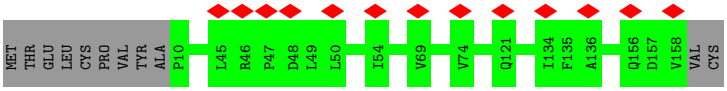
• Molecule 12: V-type proton ATPase subunit c



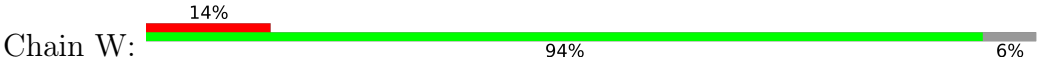


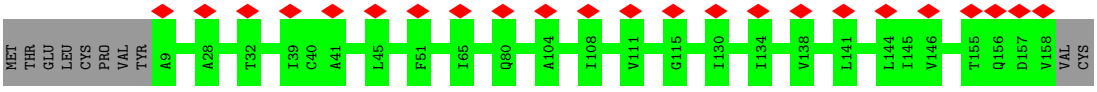
• Molecule 12: V-type proton ATPase subunit c



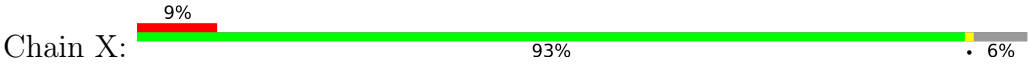


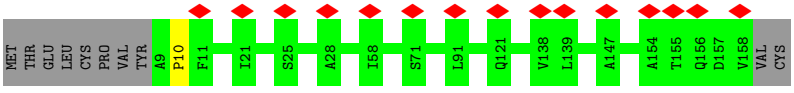
• Molecule 12: V-type proton ATPase subunit c



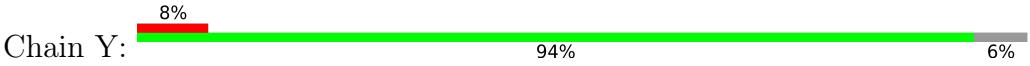


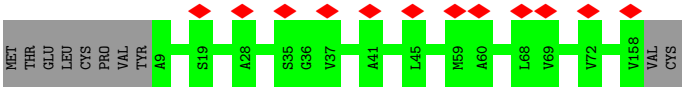
• Molecule 12: V-type proton ATPase subunit c





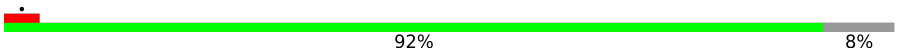
• Molecule 12: V-type proton ATPase subunit c

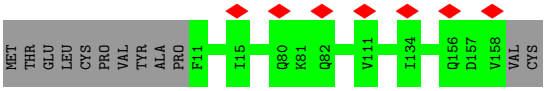




• Molecule 12: V-type proton ATPase subunit c

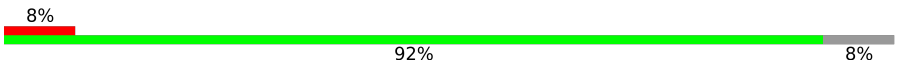
Chain Z:

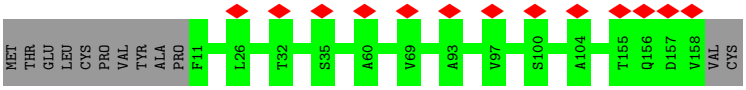




• Molecule 12: V-type proton ATPase subunit c

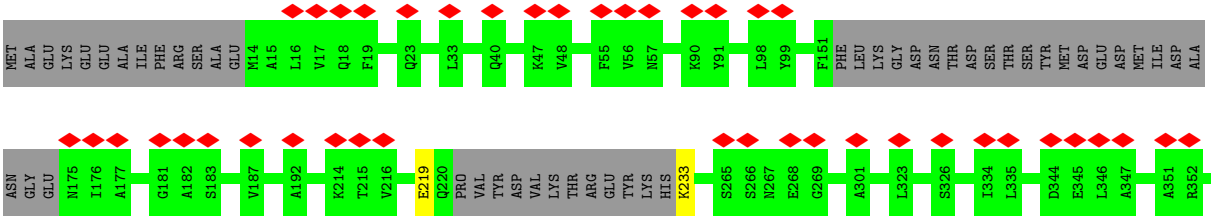
Chain a:





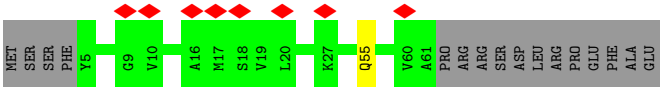
• Molecule 13: V-type proton ATPase subunit a, vacuolar isoform

Chain b:



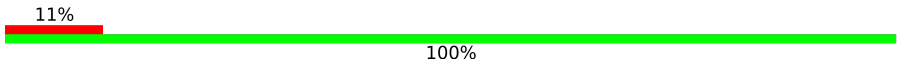
• Molecule 14: V-type proton ATPase subunit e

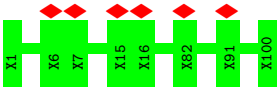
Chain c:



• Molecule 15: V-type proton ATPase subunit f

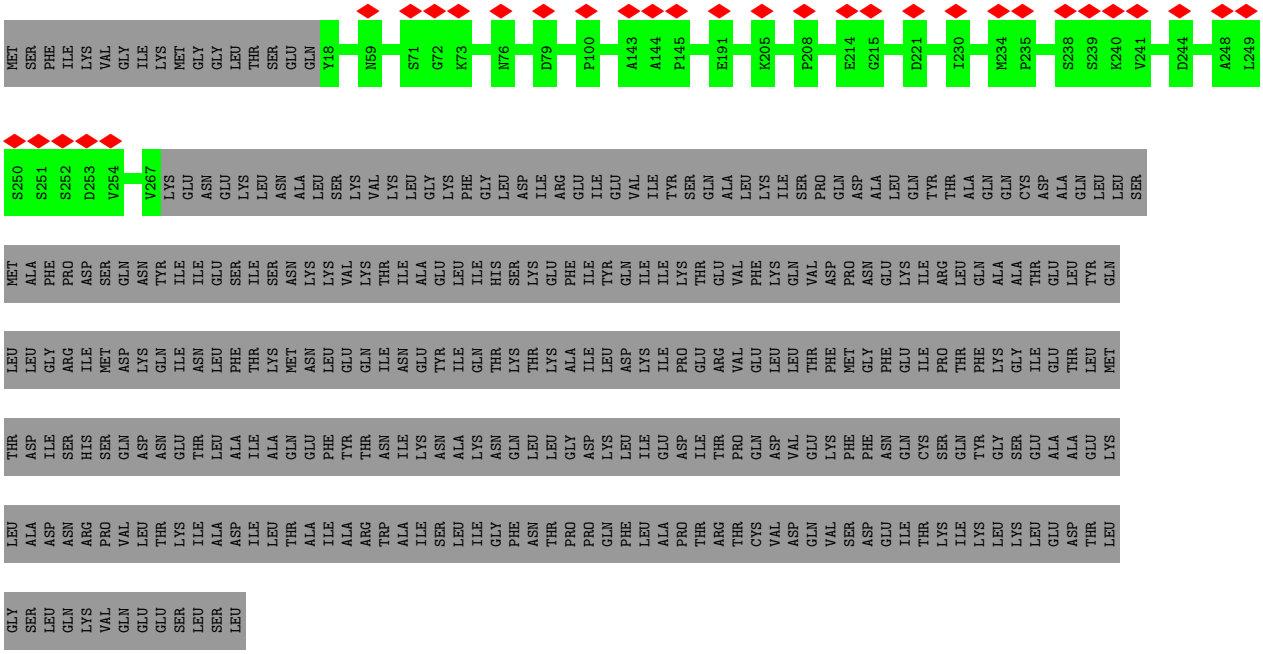
Chain d:





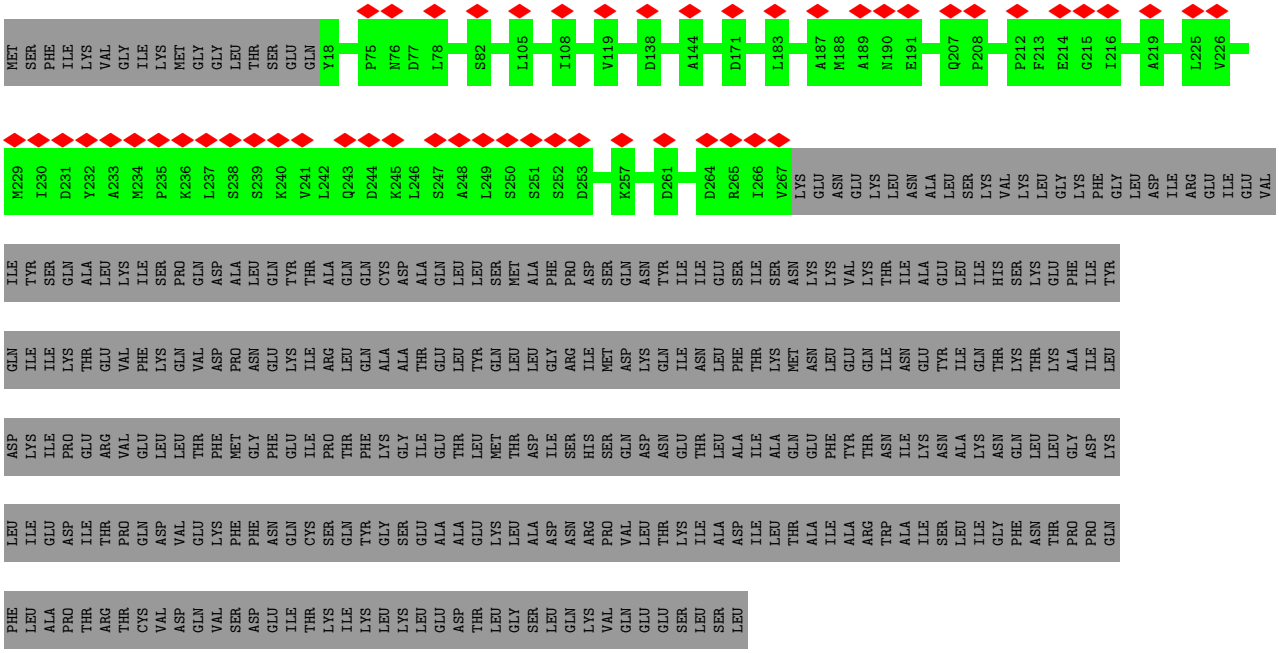
• Molecule 16: Uncharacterized protein

Chain e:



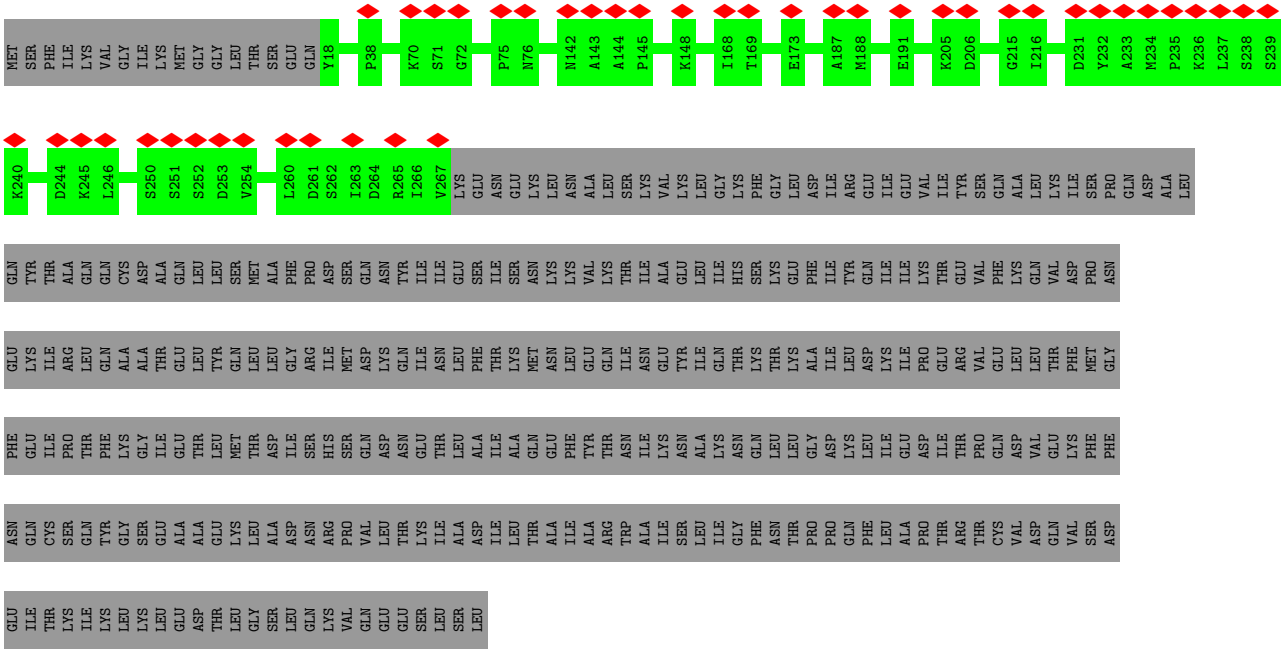
• Molecule 16: Uncharacterized protein

Chain f:



• Molecule 16: Uncharacterized protein

Chain g:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13061	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	1.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.148	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	371.2, 371.2, 371.2	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.45, 1.45, 1.45	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	0.23	0/2370	0.44	0/2961
1	C	0.23	0/2370	0.44	0/2961
1	E	0.23	0/2370	0.44	0/2961
2	B	0.23	0/1826	0.43	0/2281
2	D	0.23	0/1826	0.45	0/2281
2	F	0.23	0/1826	0.45	0/2281
3	G	0.25	0/870	0.39	0/1086
3	I	0.24	0/866	0.39	0/1081
3	K	0.24	0/866	0.40	0/1081
4	H	0.22	0/418	0.36	0/521
4	J	0.23	0/418	0.36	0/521
4	L	0.23	0/418	0.35	0/521
5	M	0.24	0/838	0.38	0/1046
6	N	0.22	0/458	0.44	0/571
7	O	0.23	0/1566	0.43	0/1956
8	P	0.22	0/1845	0.36	0/2303
9	Q	0.22	0/1378	0.40	0/1721
10	R	0.23	0/850	0.41	0/1061
11	S	0.22	0/586	0.41	0/731
12	T	0.23	0/598	0.39	0/746
12	U	0.23	0/598	0.39	0/746
12	V	0.23	0/594	0.39	0/741
12	W	0.22	0/598	0.39	0/746
12	X	0.23	0/598	0.39	0/746
12	Y	0.23	0/598	0.40	0/746
12	Z	0.23	0/590	0.41	0/736
12	a	0.23	0/590	0.39	0/736
13	b	0.26	1/2520 (0.0%)	0.46	1/3136 (0.0%)
14	c	0.21	0/226	0.44	0/281
16	e	0.22	0/998	0.38	0/1246
16	f	0.22	0/998	0.37	0/1246
16	g	0.22	0/998	0.39	0/1246
All	All	0.23	1/34469 (0.0%)	0.42	1/43024 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
13	b	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	233	LYS	C-N	6.48	1.49	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	b	233	LYS	C-N-CA	-7.89	101.96	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	b	219	GLU	Mainchain

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	2371	0	662	1	0
1	C	2371	0	662	0	0
1	E	2371	0	662	1	0
2	B	1827	0	501	0	0
2	D	1827	0	501	0	0
2	F	1827	0	501	0	0
3	G	871	0	226	0	0
3	I	867	0	225	0	0
3	K	867	0	225	0	0
4	H	419	0	115	0	0
4	J	419	0	115	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	419	0	115	0	0
5	M	839	0	228	1	0
6	N	459	0	117	0	0
7	O	1567	0	404	0	0
8	P	1847	0	480	0	0
9	Q	1379	0	370	1	0
10	R	851	0	261	0	0
11	S	587	0	186	0	0
12	T	599	0	189	0	0
12	U	599	0	189	0	0
12	V	595	0	189	0	0
12	W	599	0	189	0	0
12	X	599	0	189	0	0
12	Y	599	0	189	0	0
12	Z	591	0	188	0	0
12	a	591	0	188	0	0
13	b	2529	0	681	0	0
14	c	227	0	56	0	0
15	d	214	0	4	0	0
16	e	999	0	256	0	0
16	f	999	0	256	0	0
16	g	999	0	256	0	0
All	All	34724	0	9575	4	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 (4) 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:A:895:GLY:HA3	1:A:910:ASN:H	1.73	0.52
1:E:1047:GLY:N	1:E:1051:VAL:O	2.43	0.47
5:M:79:ILE:O	5:M:83:VAL:N	2.46	0.43
9:Q:196:VAL:O	9:Q:200:ILE:CA	2.68	0.42

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	591/617 (96%)	570 (96%)	21 (4%)	0	100	100
1	C	591/617 (96%)	557 (94%)	34 (6%)	0	100	100
1	E	591/617 (96%)	565 (96%)	26 (4%)	0	100	100
2	B	455/517 (88%)	442 (97%)	13 (3%)	0	100	100
2	D	455/517 (88%)	444 (98%)	11 (2%)	0	100	100
2	F	455/517 (88%)	445 (98%)	10 (2%)	0	100	100
3	G	216/233 (93%)	214 (99%)	2 (1%)	0	100	100
3	I	215/233 (92%)	213 (99%)	2 (1%)	0	100	100
3	K	215/233 (92%)	212 (99%)	3 (1%)	0	100	100
4	H	103/114 (90%)	103 (100%)	0	0	100	100
4	J	103/114 (90%)	102 (99%)	1 (1%)	0	100	100
4	L	103/114 (90%)	103 (100%)	0	0	100	100
5	M	208/256 (81%)	202 (97%)	6 (3%)	0	100	100
6	N	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
7	O	390/392 (100%)	374 (96%)	16 (4%)	0	100	100
8	P	458/478 (96%)	439 (96%)	19 (4%)	0	100	100
9	Q	343/345 (99%)	330 (96%)	13 (4%)	0	100	100
10	R	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
11	S	145/164 (88%)	143 (99%)	2 (1%)	0	100	100
12	T	148/160 (92%)	144 (97%)	4 (3%)	0	100	100
12	U	148/160 (92%)	145 (98%)	3 (2%)	0	100	100
12	V	147/160 (92%)	142 (97%)	5 (3%)	0	100	100
12	W	148/160 (92%)	144 (97%)	4 (3%)	0	100	100
12	X	148/160 (92%)	144 (97%)	3 (2%)	1 (1%)	22	63
12	Y	148/160 (92%)	145 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	Z	146/160 (91%)	145 (99%)	1 (1%)	0	100	100
12	a	146/160 (91%)	144 (99%)	2 (1%)	0	100	100
13	b	616/840 (73%)	594 (96%)	22 (4%)	0	100	100
14	c	55/73 (75%)	43 (78%)	11 (20%)	1 (2%)	8	40
16	e	248/573 (43%)	245 (99%)	3 (1%)	0	100	100
16	f	248/573 (43%)	244 (98%)	4 (2%)	0	100	100
16	g	248/573 (43%)	244 (98%)	4 (2%)	0	100	100
All	All	8555/10321 (83%)	8287 (97%)	266 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	X	10	PRO
14	c	55	GLN

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

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
15	d	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	d	31:UNK	C	78:UNK	N	10.76

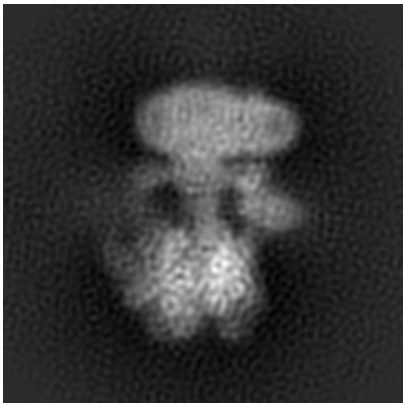
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8726. These allow visual inspection of the internal detail of the map and identification of artifacts.

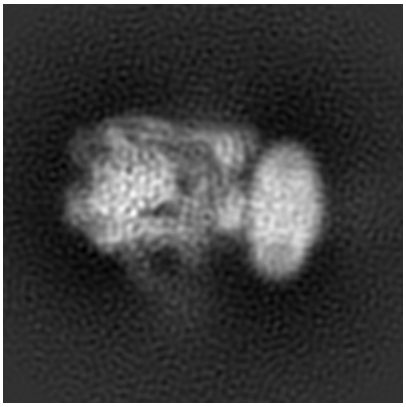
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

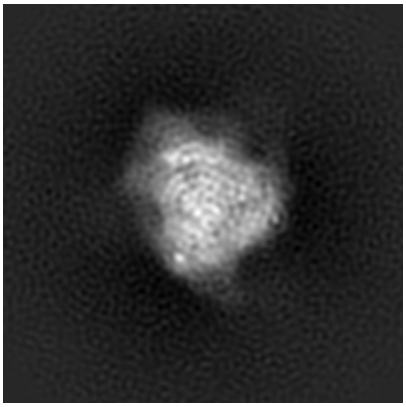
6.1.1 Primary map



X



Y



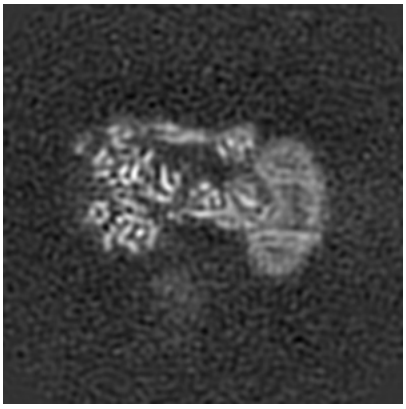
Z

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

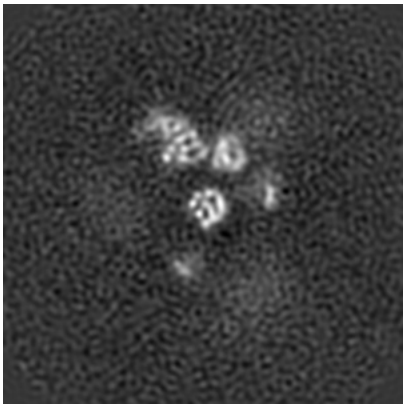
6.2 Central slices

6.2.1 Primary map

X Index: 128



Y Index: 128

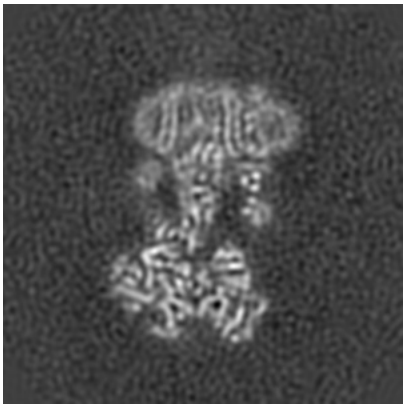


Z Index: 128

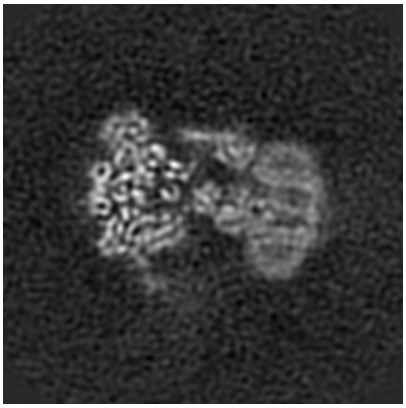
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

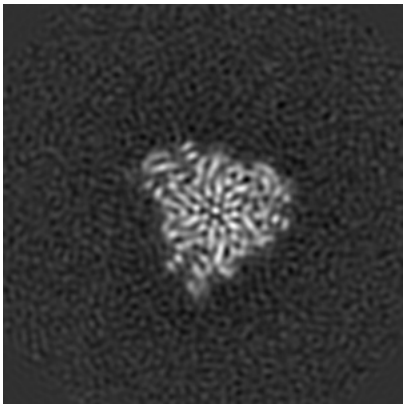
6.3.1 Primary map



X Index: 127



Y Index: 134



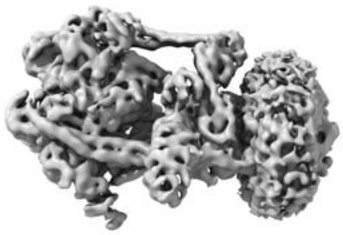
Z Index: 76

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

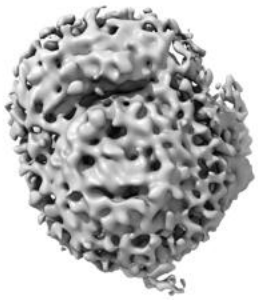
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

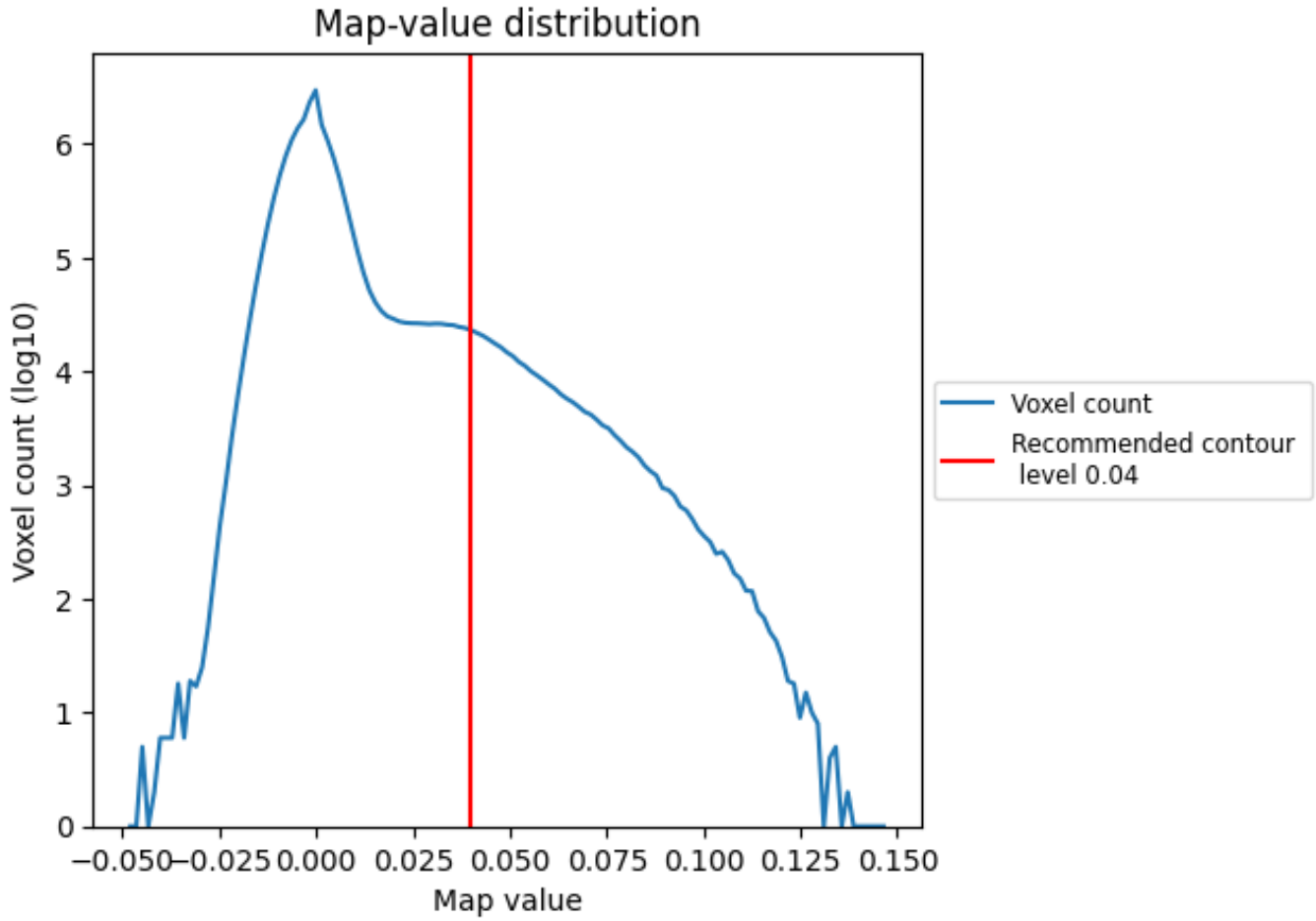
6.5 Mask visualisation (i)

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

7 Map analysis

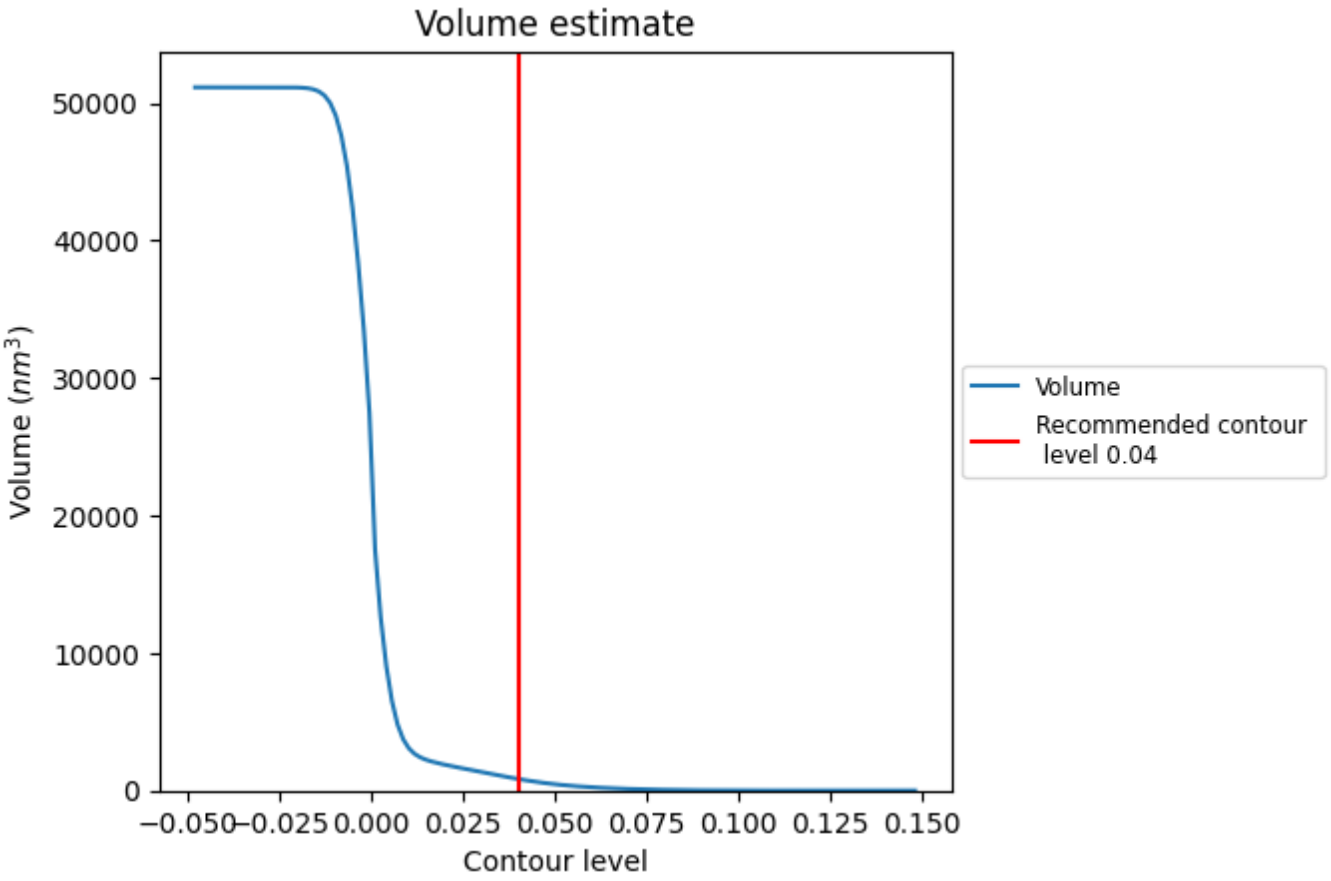
This section contains the results of statistical analysis of the map.

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.

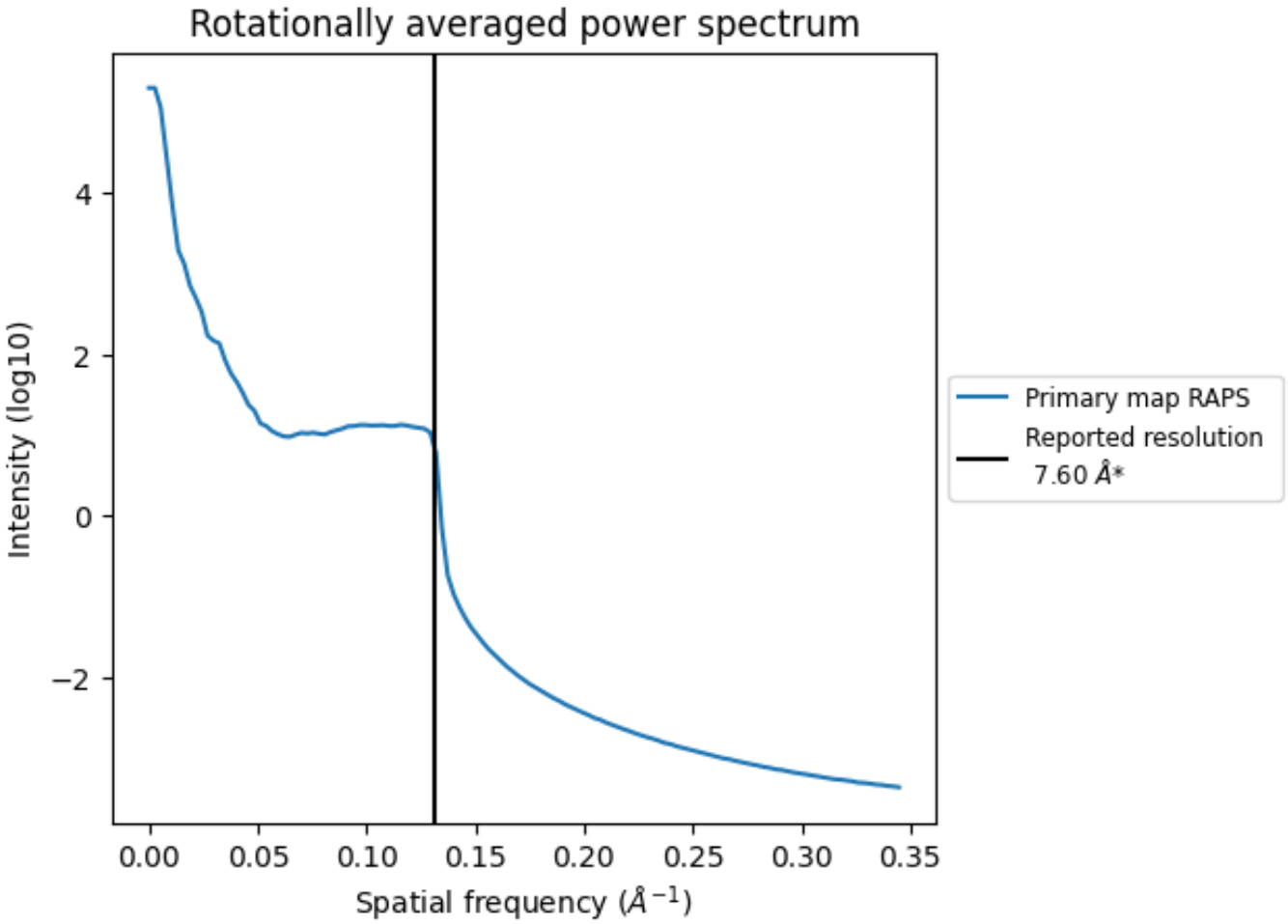
7.2 Volume estimate (i)



The volume at the recommended contour level is 842 nm^3; this corresponds to an approximate mass of 761 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 0.132 Å^{-1}

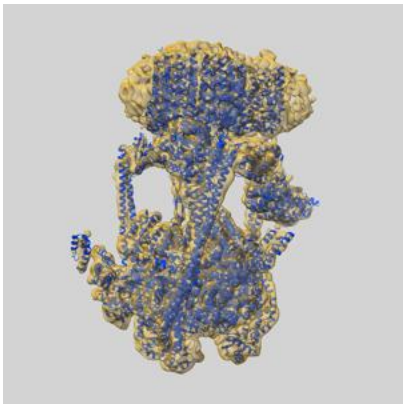
8 Fourier-Shell correlation (i)

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

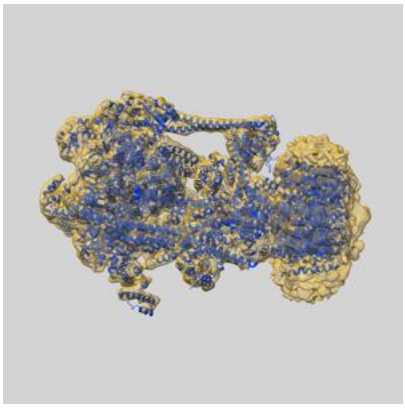
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8726 and PDB model 5VOZ. Per-residue inclusion information can be found in section 3 on page 8.

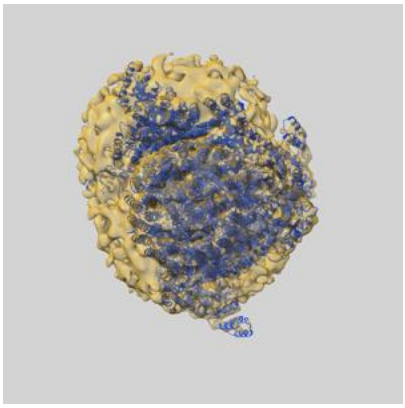
9.1 Map-model overlay



X



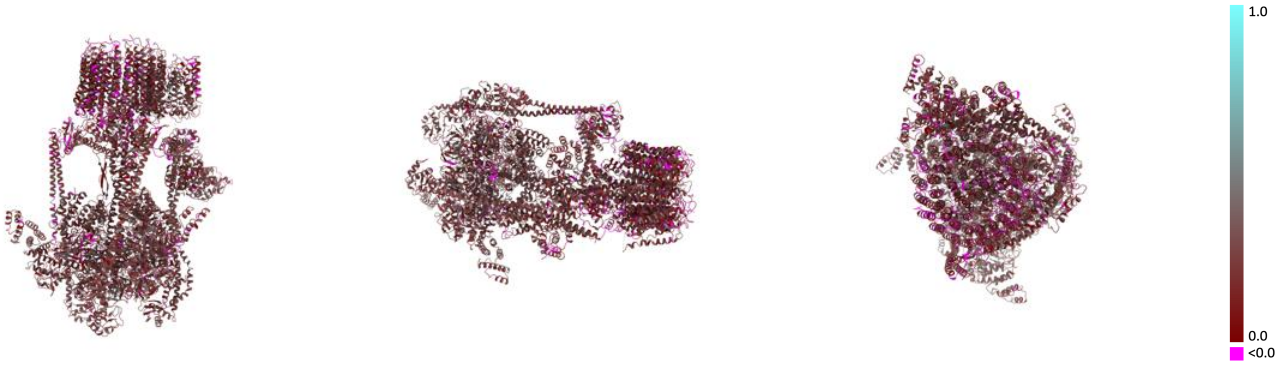
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

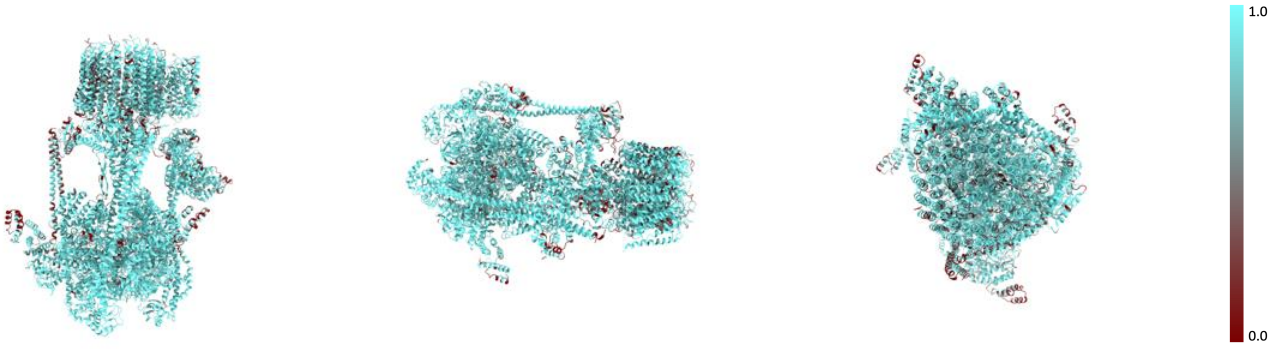
9.2 Q-score mapped to coordinate model



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.

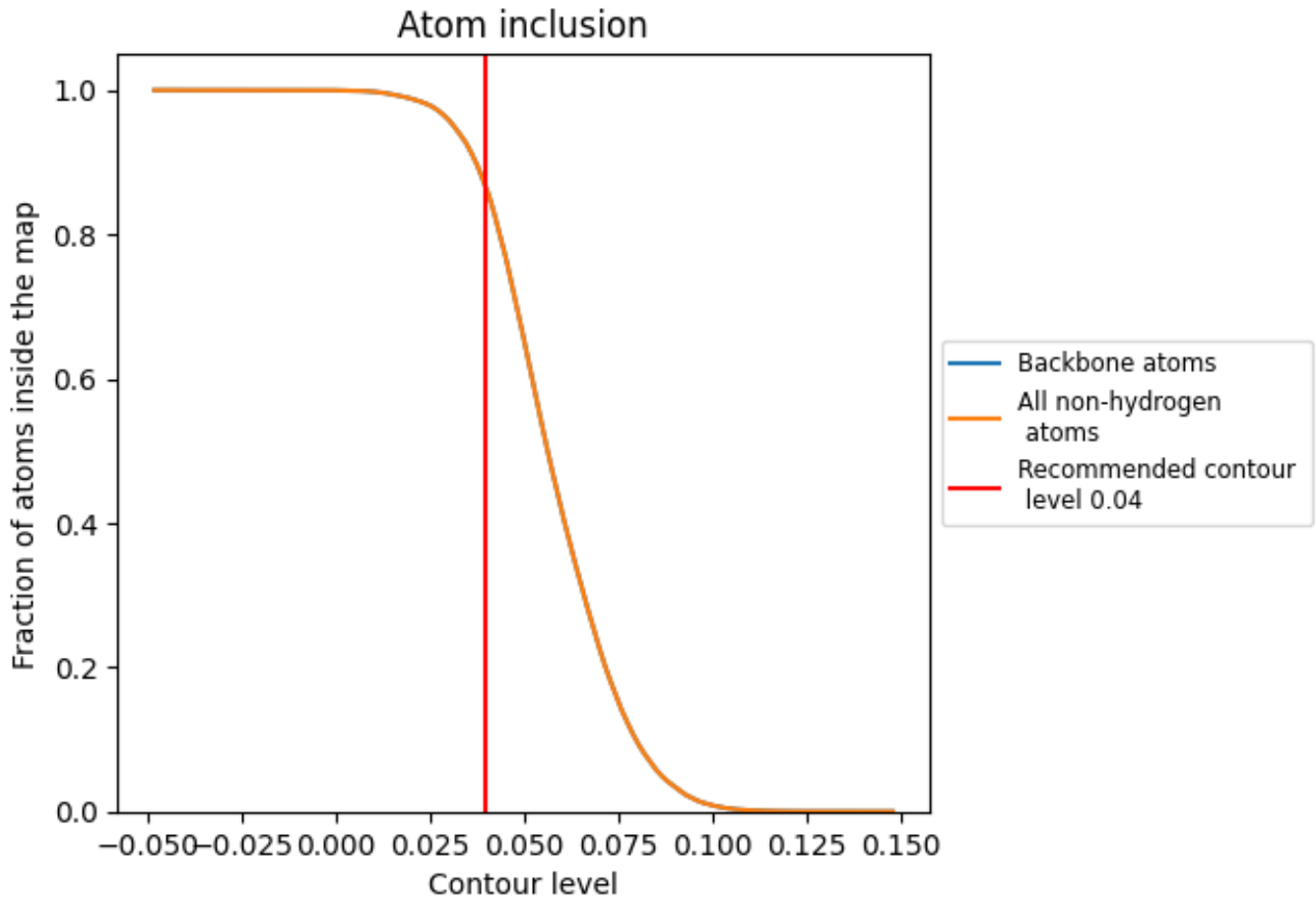
9.3 Atom inclusion mapped to coordinate model



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 87% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8654	0.2140
A	0.9291	0.2290
B	0.9223	0.2390
C	0.9367	0.2360
D	0.9141	0.2230
E	0.9220	0.2380
F	0.9338	0.2370
G	0.8726	0.2460
H	0.6874	0.1780
I	0.9458	0.2530
J	0.8783	0.2360
K	0.9504	0.2630
L	0.9093	0.2470
M	0.9023	0.2310
N	0.9063	0.2410
O	0.7013	0.1790
P	0.8121	0.2170
Q	0.7694	0.1640
R	0.8002	0.1770
S	0.8262	0.1550
T	0.7696	0.1030
U	0.8230	0.1250
V	0.8756	0.1750
W	0.8047	0.1500
X	0.8431	0.1430
Y	0.8798	0.1730
Z	0.9019	0.2040
a	0.8782	0.2180
b	0.8675	0.1980
c	0.7841	0.1690
d	0.8364	0.1520
e	0.8408	0.2570
f	0.7367	0.2430
g	0.7708	0.2440