



wwPDB EM Validation Summary Report ⓘ

Nov 6, 2022 – 11:50 AM EST

PDB ID : 6O7V
EMDB ID : EMD-0646
Title : Saccharomyces cerevisiae V-ATPase Stv1-V1VO State 1
Authors : Vasanthakumar, T.; Bueler, S.A.; Wu, D.; Beilsten-Edmands, V.; Robinson, C.V.; Rubinstein, J.L.
Deposited on : 2019-03-08
Resolution : 6.60 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:

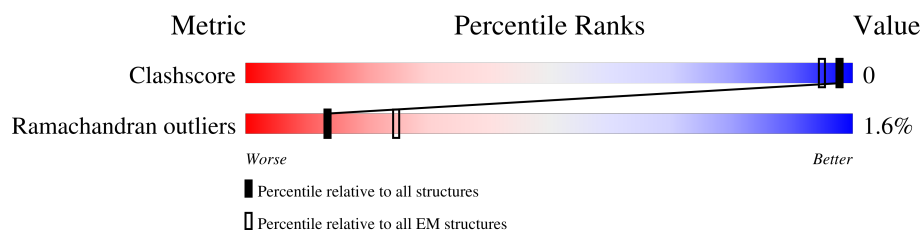
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 6.60 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	M	256	<div> <div>5%</div> <div>77%</div> <div>5%</div> <div>18%</div> </div>
2	N	118	<div> <div>18%</div> <div>92%</div> <div>5%</div> <div>•</div> </div>
3	A	639	<div> <div>5%</div> <div>85%</div> <div>8%</div> <div>•</div> <div>7%</div> </div>
3	C	639	<div> <div>•</div> <div>87%</div> <div>5%</div> <div>•</div> <div>7%</div> </div>
3	E	639	<div> <div>•</div> <div>84%</div> <div>8%</div> <div>•</div> <div>7%</div> </div>
4	B	517	<div> <div>•</div> <div>80%</div> <div>8%</div> <div>•</div> <div>12%</div> </div>
4	D	517	<div> <div>•</div> <div>82%</div> <div>6%</div> <div>•</div> <div>12%</div> </div>
4	F	517	<div> <div>•</div> <div>80%</div> <div>7%</div> <div>•</div> <div>12%</div> </div>
5	H	114	<div> <div>•</div> <div>89%</div> <div>•</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
5	J	114	
5	L	114	
6	G	233	
6	I	233	
6	K	233	
7	P	478	
8	O	392	
9	a	890	
10	b	265	
11	c	213	
12	d	345	
13	g	160	
13	h	160	
13	i	160	
13	j	160	
13	k	160	
13	l	160	
13	m	160	
13	n	160	
14	o	164	
15	e	73	
16	f	85	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 39578 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 D.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	M	210	Total	C	N	O	0	0
			1039	619	210	210		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	N	115	Total	C	N	O	0	0
			571	341	115	115		

- Molecule 3 is a protein called Vacuolar ATP synthase catalytic subunit A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	A	593	Total	C	N	O	0	0
			2915	1729	593	593		
3	C	593	Total	C	N	O	0	0
			2915	1729	593	593		
3	E	593	Total	C	N	O	0	0
			2915	1729	593	593		

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	617	ASP	-	SEE REMARK 999	UNP B3LH69
A	618	TYR	-	SEE REMARK 999	UNP B3LH69
A	619	LYS	-	SEE REMARK 999	UNP B3LH69
A	620	ASP	-	SEE REMARK 999	UNP B3LH69
A	621	HIS	-	SEE REMARK 999	UNP B3LH69
A	622	ASP	-	SEE REMARK 999	UNP B3LH69
A	623	GLY	-	SEE REMARK 999	UNP B3LH69
A	624	ASP	-	SEE REMARK 999	UNP B3LH69
A	625	TYR	-	SEE REMARK 999	UNP B3LH69
A	626	LYS	-	SEE REMARK 999	UNP B3LH69
A	627	ASP	-	SEE REMARK 999	UNP B3LH69

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Chain	Residue	Modelled	Actual	Comment	Reference
A	628	HIS	-	SEE REMARK 999	UNP B3LH69
A	629	ASP	-	SEE REMARK 999	UNP B3LH69
A	630	ILE	-	SEE REMARK 999	UNP B3LH69
A	631	ASP	-	SEE REMARK 999	UNP B3LH69
A	632	TYR	-	SEE REMARK 999	UNP B3LH69
A	633	LYS	-	SEE REMARK 999	UNP B3LH69
A	634	ASP	-	SEE REMARK 999	UNP B3LH69
A	635	ASP	-	SEE REMARK 999	UNP B3LH69
A	636	ASP	-	SEE REMARK 999	UNP B3LH69
A	637	ASP	-	SEE REMARK 999	UNP B3LH69
A	638	LYS	-	SEE REMARK 999	UNP B3LH69
C	617	ASP	-	SEE REMARK 999	UNP B3LH69
C	618	TYR	-	SEE REMARK 999	UNP B3LH69
C	619	LYS	-	SEE REMARK 999	UNP B3LH69
C	620	ASP	-	SEE REMARK 999	UNP B3LH69
C	621	HIS	-	SEE REMARK 999	UNP B3LH69
C	622	ASP	-	SEE REMARK 999	UNP B3LH69
C	623	GLY	-	SEE REMARK 999	UNP B3LH69
C	624	ASP	-	SEE REMARK 999	UNP B3LH69
C	625	TYR	-	SEE REMARK 999	UNP B3LH69
C	626	LYS	-	SEE REMARK 999	UNP B3LH69
C	627	ASP	-	SEE REMARK 999	UNP B3LH69
C	628	HIS	-	SEE REMARK 999	UNP B3LH69
C	629	ASP	-	SEE REMARK 999	UNP B3LH69
C	630	ILE	-	SEE REMARK 999	UNP B3LH69
C	631	ASP	-	SEE REMARK 999	UNP B3LH69
C	632	TYR	-	SEE REMARK 999	UNP B3LH69
C	633	LYS	-	SEE REMARK 999	UNP B3LH69
C	634	ASP	-	SEE REMARK 999	UNP B3LH69
C	635	ASP	-	SEE REMARK 999	UNP B3LH69
C	636	ASP	-	SEE REMARK 999	UNP B3LH69
C	637	ASP	-	SEE REMARK 999	UNP B3LH69
C	638	LYS	-	SEE REMARK 999	UNP B3LH69
E	617	ASP	-	SEE REMARK 999	UNP B3LH69
E	618	TYR	-	SEE REMARK 999	UNP B3LH69
E	619	LYS	-	SEE REMARK 999	UNP B3LH69
E	620	ASP	-	SEE REMARK 999	UNP B3LH69
E	621	HIS	-	SEE REMARK 999	UNP B3LH69
E	622	ASP	-	SEE REMARK 999	UNP B3LH69
E	623	GLY	-	SEE REMARK 999	UNP B3LH69
E	624	ASP	-	SEE REMARK 999	UNP B3LH69
E	625	TYR	-	SEE REMARK 999	UNP B3LH69

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Chain	Residue	Modelled	Actual	Comment	Reference
E	626	LYS	-	SEE REMARK 999	UNP B3LH69
E	627	ASP	-	SEE REMARK 999	UNP B3LH69
E	628	HIS	-	SEE REMARK 999	UNP B3LH69
E	629	ASP	-	SEE REMARK 999	UNP B3LH69
E	630	ILE	-	SEE REMARK 999	UNP B3LH69
E	631	ASP	-	SEE REMARK 999	UNP B3LH69
E	632	TYR	-	SEE REMARK 999	UNP B3LH69
E	633	LYS	-	SEE REMARK 999	UNP B3LH69
E	634	ASP	-	SEE REMARK 999	UNP B3LH69
E	635	ASP	-	SEE REMARK 999	UNP B3LH69
E	636	ASP	-	SEE REMARK 999	UNP B3LH69
E	637	ASP	-	SEE REMARK 999	UNP B3LH69
E	638	LYS	-	SEE REMARK 999	UNP B3LH69

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	B	457	Total	C	N	O	0	0
			2250	1336	457	457		
4	D	457	Total	C	N	O	0	0
			2250	1336	457	457		
4	F	457	Total	C	N	O	0	0
			2250	1336	457	457		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	L	105	Total	C	N	O	0	0
			519	309	105	105		
5	H	105	Total	C	N	O	0	0
			519	309	105	105		
5	J	105	Total	C	N	O	0	0
			519	309	105	105		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	K	217	Total	C	N	O	0	0
			1078	644	217	217		
6	G	217	Total	C	N	O	0	0
			1078	644	217	217		

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Mol	Chain	Residues	Atoms				AltConf	Trace
6	I	217	Total	C	N	O	0	0
			1078	644	217	217		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	P	461	Total	C	N	O	0	0
			2292	1370	461	461		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	O	392	Total	C	N	O	0	0
			1947	1163	392	392		

- Molecule 9 is a protein called V-type proton ATPase subunit a, Golgi isoform.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	a	625	Total	C	N	O	0	0
			3092	1842	625	625		

- Molecule 10 is a protein called V0 assembly protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	b	44	Total	C	N	O	0	0
			218	130	44	44		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	c	197	Total	C	N	O	0	0
			962	568	197	197		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	d	343	Total	C	N	O	0	0
			1699	1013	343	343		

- Molecule 13 is a protein called V-type proton ATPase subunit c.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	g	153	Total	C	N	O	0	0
			743	437	153	153		
13	h	157	Total	C	N	O	0	0
			763	449	157	157		
13	i	157	Total	C	N	O	0	0
			763	449	157	157		
13	j	156	Total	C	N	O	0	0
			758	446	156	156		
13	k	158	Total	C	N	O	0	0
			768	452	158	158		
13	l	157	Total	C	N	O	0	0
			763	449	157	157		
13	m	158	Total	C	N	O	0	0
			768	452	158	158		
13	n	158	Total	C	N	O	0	0
			768	452	158	158		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	o	156	Total	C	N	O	0	0
			758	446	156	156		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
15	e	64	Total	C	N	O	0	0
			319	191	64	64		

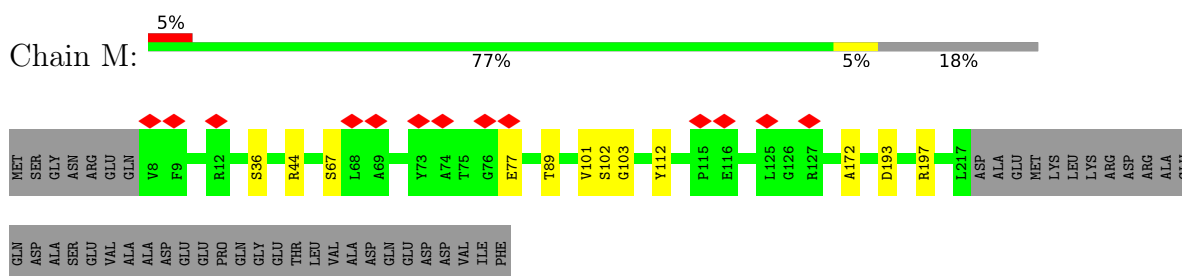
- Molecule 16 is a protein called Putative protein YPR170W-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	f	61	Total	C	N	O	0	0
			301	179	61	61		

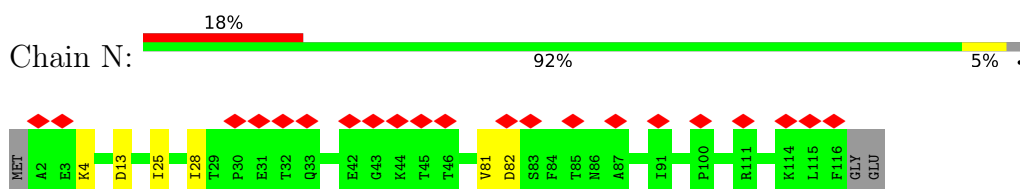
3 Residue-property plots [i](#)

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.

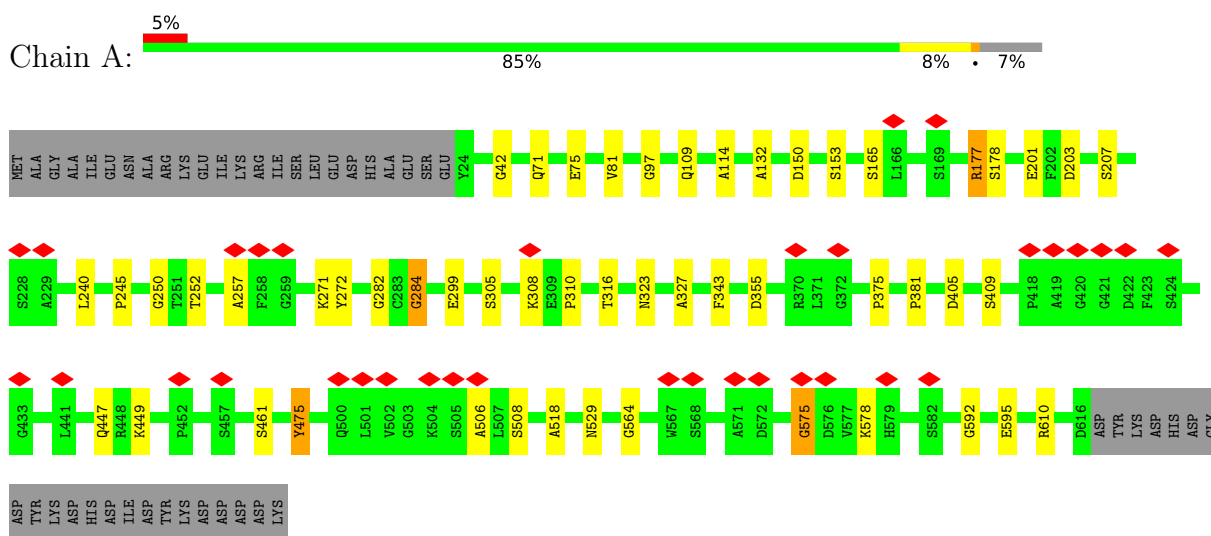
- Molecule 1: V-type proton ATPase subunit D




- Molecule 2: V-type proton ATPase subunit F

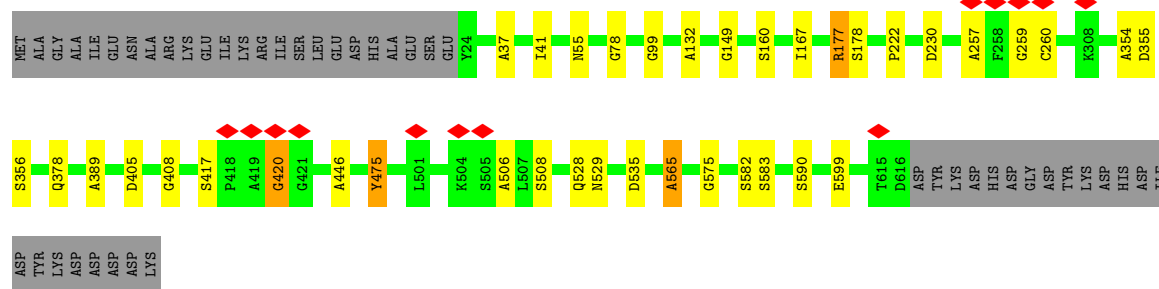


- Molecule 3: Vacuolar ATP synthase catalytic subunit A




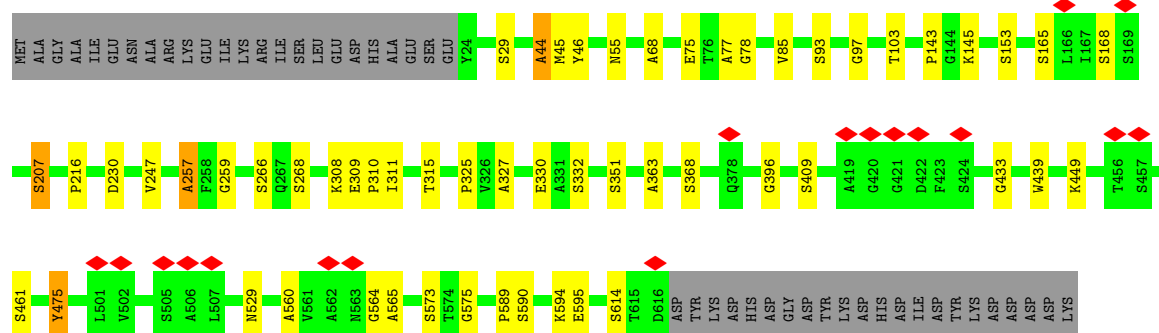
- Molecule 3: Vacuolar ATP synthase catalytic subunit A

Chain C:  87% 5% • 7%




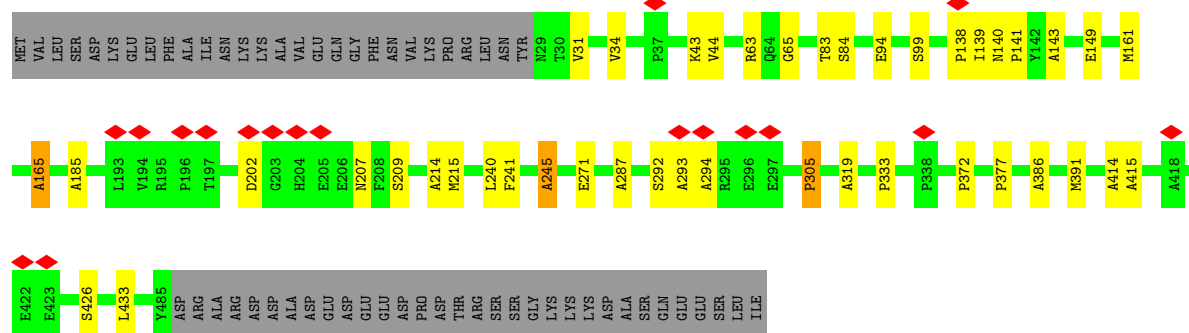
• Molecule 3: Vacuolar ATP synthase catalytic subunit A

Chain E:  84% 8% • 7%




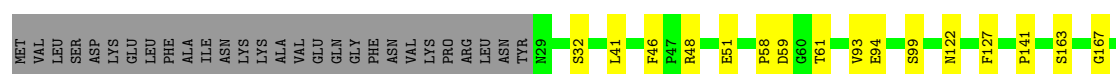
• Molecule 4: V-type proton ATPase subunit B

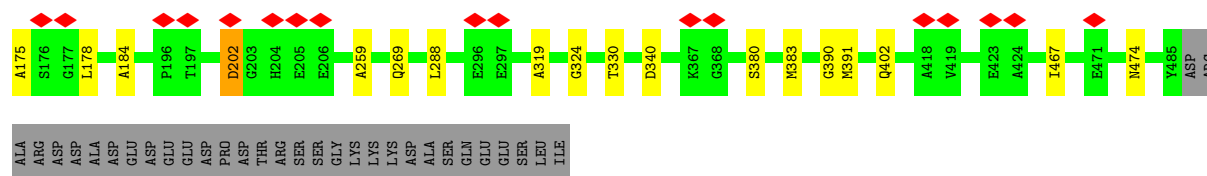
Chain B:  80% 8% • 12%



• Molecule 4: V-type proton ATPase subunit B

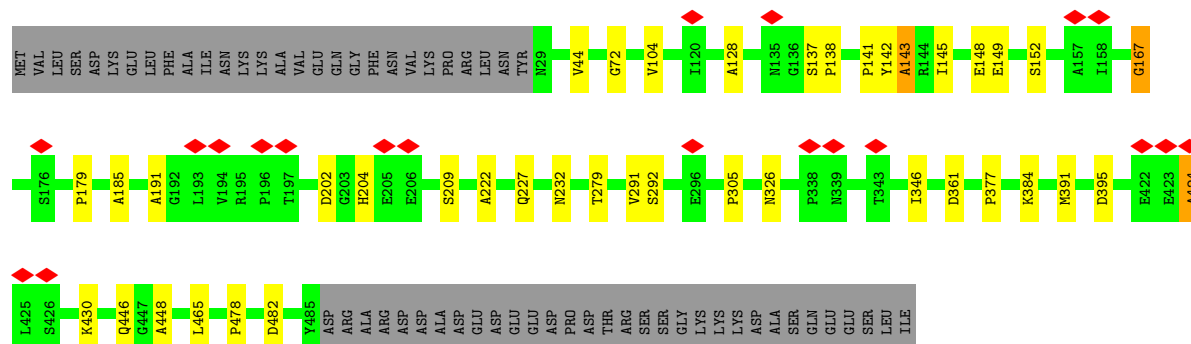
Chain D:  82% 6% • 12%





• Molecule 4: V-type proton ATPase subunit B

Chain F: 80% 7% 12%



• Molecule 5: V-type proton ATPase subunit G

Chain L: 89% 8%



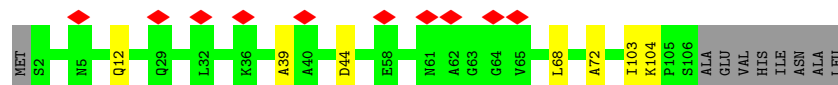
• Molecule 5: V-type proton ATPase subunit G

Chain H: 89% 8%



• Molecule 5: V-type proton ATPase subunit G

Chain J: 9% 86% 6% 8%




• Molecule 6: V-type proton ATPase subunit E

Chain K: 88% 5% 7%




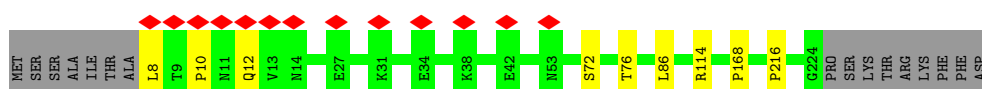
- Molecule 6: V-type proton ATPase subunit E

Chain G:  87% 6% 7%

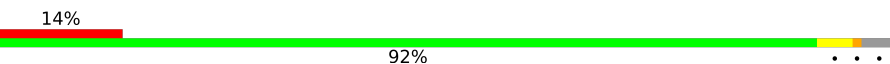


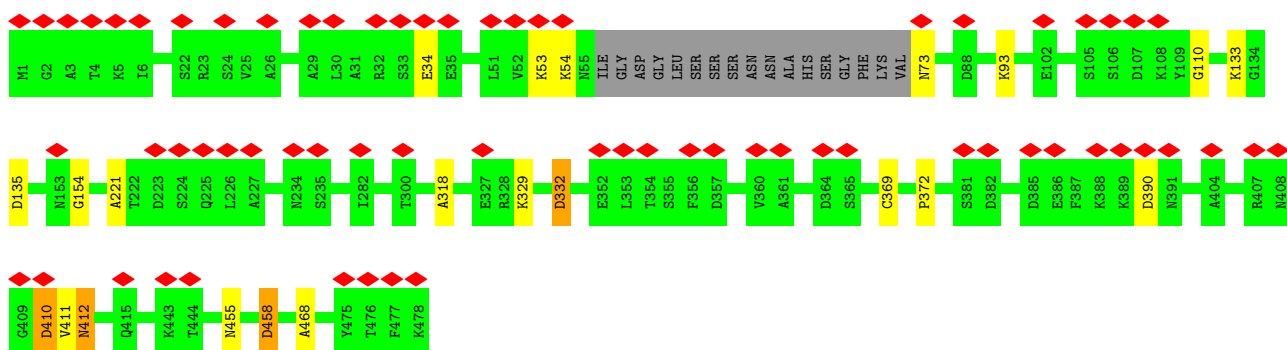
- Molecule 6: V-type proton ATPase subunit E

Chain I:  89% 6% 7%

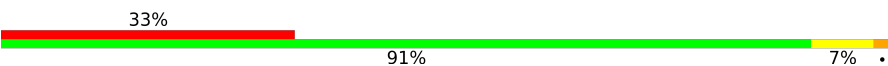


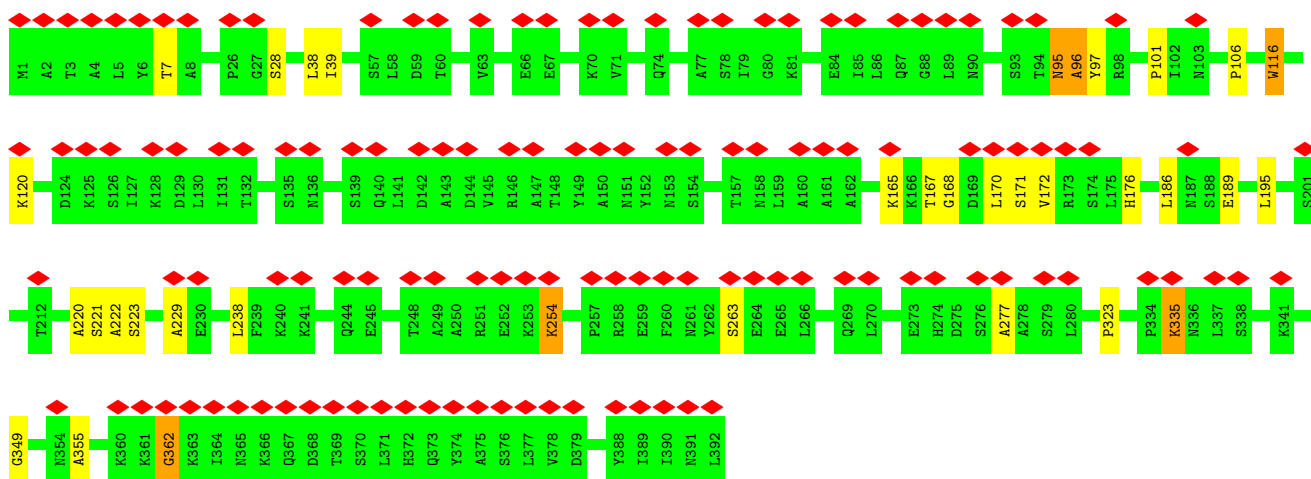
- Molecule 7: V-type proton ATPase subunit H

Chain P:  92% 14% 7%

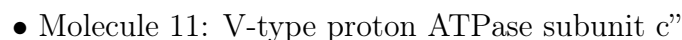
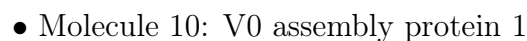


- Molecule 8: V-type proton ATPase subunit C

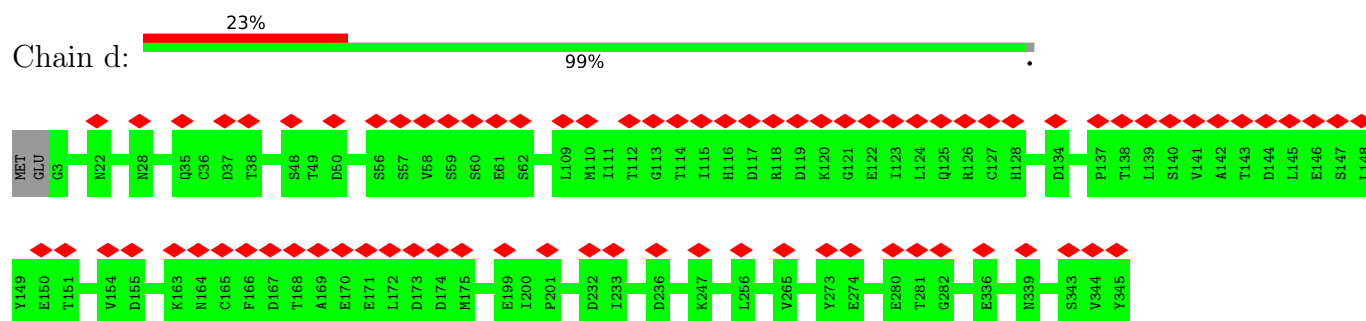
Chain O:  91% 33% 7%



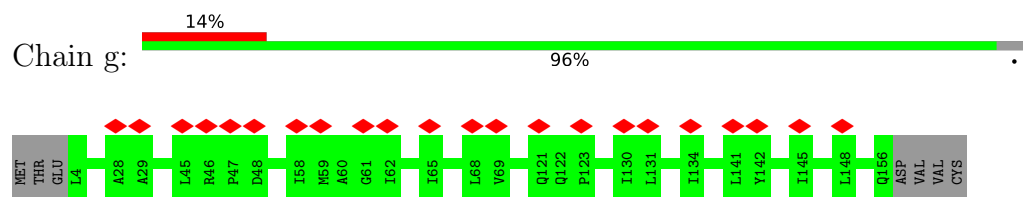
- Molecule 9: V-type proton ATPase subunit a, Golgi isoform



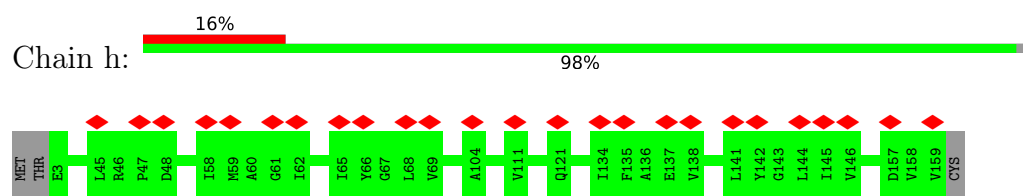
- Molecule 12: V-type proton ATPase subunit d



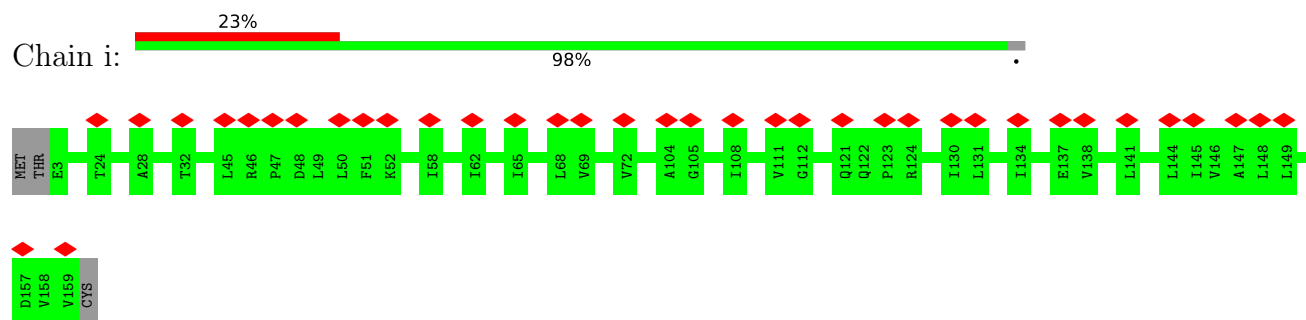
- Molecule 13: V-type proton ATPase subunit c



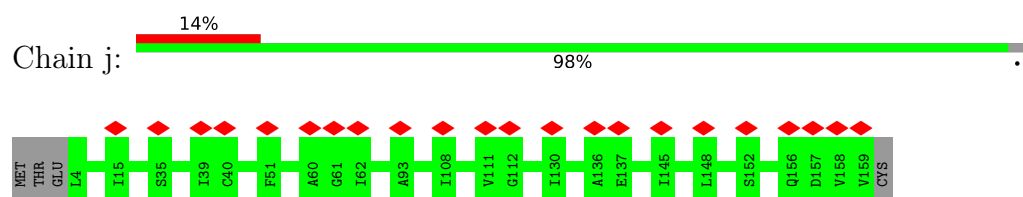
- Molecule 13: V-type proton ATPase subunit c



- Molecule 13: V-type proton ATPase subunit c

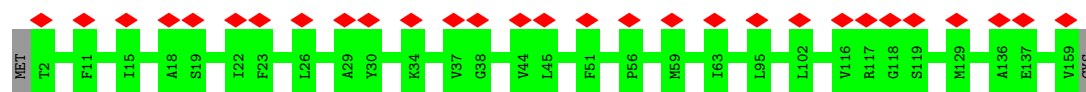


- Molecule 13: V-type proton ATPase subunit c

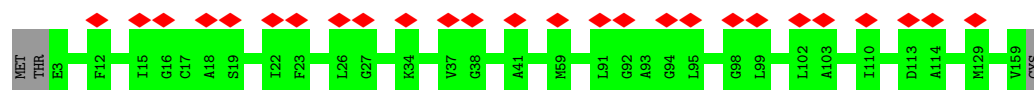


- Molecule 13: V-type proton ATPase subunit c

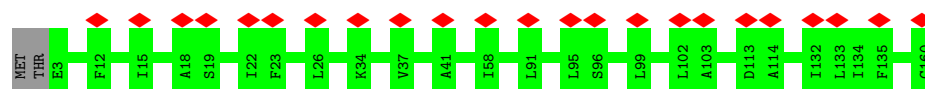




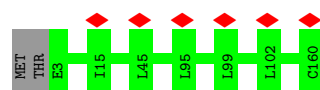
- Molecule 13: V-type proton ATPase subunit c



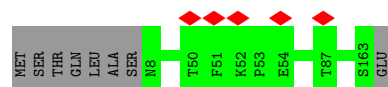
- Molecule 13: V-type proton ATPase subunit c



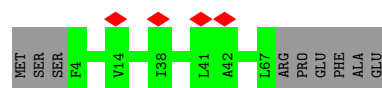
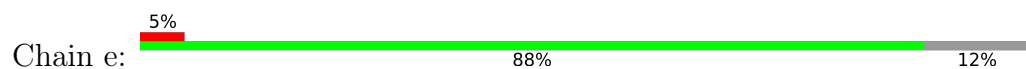
- Molecule 13: V-type proton ATPase subunit c



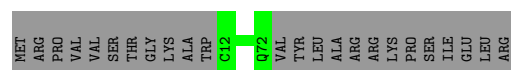
- Molecule 14: V-type proton ATPase subunit c'



- Molecule 15: V-type proton ATPase subunit e



- Molecule 16: Putative protein YPR170W-B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25045	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 ($e^-/\text{\AA}^2$)	35	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	0.522	Depositor
Minimum map value	-0.126	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.18	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 ⓘ

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	M	1.57	3/1038 (0.3%)	1.66	10/1445 (0.7%)
2	N	1.54	0/570	1.68	5/794 (0.6%)
3	A	1.59	9/2914 (0.3%)	1.74	28/4048 (0.7%)
3	C	1.58	6/2914 (0.2%)	1.66	17/4048 (0.4%)
3	E	1.63	16/2914 (0.5%)	1.73	26/4048 (0.6%)
4	B	1.59	8/2249 (0.4%)	1.74	21/3126 (0.7%)
4	D	1.55	6/2249 (0.3%)	1.74	13/3126 (0.4%)
4	F	1.57	7/2249 (0.3%)	1.71	22/3126 (0.7%)
5	H	1.51	0/518	1.59	3/720 (0.4%)
5	J	1.56	1/518 (0.2%)	1.61	7/720 (1.0%)
5	L	1.54	0/518	1.56	2/720 (0.3%)
6	G	1.58	5/1077 (0.5%)	1.65	8/1502 (0.5%)
6	I	1.54	3/1077 (0.3%)	1.57	5/1502 (0.3%)
6	K	1.54	4/1077 (0.4%)	1.65	7/1502 (0.5%)
7	P	1.55	6/2290 (0.3%)	1.64	12/3195 (0.4%)
8	O	1.56	5/1946 (0.3%)	1.72	18/2715 (0.7%)
9	a	0.25	0/3085	0.49	0/4288
10	b	0.24	0/217	0.45	0/301
11	c	0.27	0/961	0.50	0/1330
12	d	0.25	0/1698	0.48	0/2366
13	g	0.27	0/742	0.49	0/1024
13	h	0.27	0/762	0.48	0/1052
13	i	0.27	0/762	0.52	0/1052
13	j	0.26	0/757	0.48	0/1045
13	k	0.25	0/767	0.49	0/1059
13	l	0.26	0/762	0.49	0/1052
13	m	0.25	0/767	0.49	0/1059
13	n	0.26	0/767	0.49	0/1059
14	o	0.26	0/757	0.50	0/1045
15	e	0.23	0/318	0.45	0/443
16	f	0.24	0/300	0.44	0/416
All	All	1.29	79/39540 (0.2%)	1.40	204/54928 (0.4%)

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
3	A	0	1
4	F	0	1
All	All	0	2

The worst 5 of 79 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	268	SER	CA-CB	8.94	1.66	1.52
3	E	461	SER	CA-CB	8.09	1.65	1.52
4	B	426	SER	CA-CB	7.65	1.64	1.52
6	G	211	SER	CA-CB	6.95	1.63	1.52
3	A	592	GLY	CA-C	-6.84	1.41	1.51

The worst 5 of 204 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	O	116	TRP	N-CA-CB	8.64	126.16	110.60
4	F	424	ALA	N-CA-CB	8.62	122.17	110.10
3	E	257	ALA	N-CA-CB	8.44	121.91	110.10
8	O	96	ALA	N-CA-CB	8.06	121.38	110.10
4	B	165	ALA	CB-CA-C	-7.75	98.48	110.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	153	SER	Mainchain
4	F	44	VAL	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	M	1039	0	475	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	571	0	255	0	0
3	A	2915	0	1343	0	0
3	C	2915	0	1343	2	0
3	E	2915	0	1343	1	0
4	B	2250	0	1016	3	0
4	D	2250	0	1016	1	0
4	F	2250	0	1016	0	0
5	H	519	0	250	0	0
5	J	519	0	250	0	0
5	L	519	0	250	0	0
6	G	1078	0	483	0	0
6	I	1078	0	483	0	0
6	K	1078	0	483	0	0
7	P	2292	0	993	0	0
8	O	1947	0	876	0	0
9	a	3092	0	1352	0	0
10	b	218	0	98	0	0
11	c	962	0	477	0	0
12	d	1699	0	752	0	0
13	g	743	0	379	0	0
13	h	763	0	387	0	0
13	i	763	0	387	0	0
13	j	758	0	385	0	0
13	k	768	0	389	0	0
13	l	763	0	387	0	0
13	m	768	0	389	0	0
13	n	768	0	389	0	0
14	o	758	0	375	0	0
15	e	319	0	143	0	0
16	f	301	0	141	0	0
All	All	39578	0	18305	6	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.

The worst 5 of 6 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:B:165:ALA:HB2	4:B:386:ALA:CB	2.38	0.54
4:B:165:ALA:HB2	4:B:386:ALA:HB2	1.92	0.51
3:E:93:SER:HA	3:E:216:PRO:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:51:GLU:HA	4:D:99:SER:HA	2.03	0.41
3:C:355:ASP:HA	3:C:356:SER:HA	1.91	0.41

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	M	208/256 (81%)	206 (99%)	2 (1%)	0	100	100
2	N	113/118 (96%)	102 (90%)	10 (9%)	1 (1%)	17	57
3	A	591/639 (92%)	541 (92%)	31 (5%)	19 (3%)	4	26
3	C	591/639 (92%)	538 (91%)	37 (6%)	16 (3%)	5	31
3	E	591/639 (92%)	542 (92%)	32 (5%)	17 (3%)	4	29
4	B	455/517 (88%)	413 (91%)	27 (6%)	15 (3%)	4	26
4	D	455/517 (88%)	416 (91%)	25 (6%)	14 (3%)	4	27
4	F	455/517 (88%)	411 (90%)	30 (7%)	14 (3%)	4	27
5	H	103/114 (90%)	99 (96%)	3 (3%)	1 (1%)	15	54
5	J	103/114 (90%)	100 (97%)	3 (3%)	0	100	100
5	L	103/114 (90%)	98 (95%)	4 (4%)	1 (1%)	15	54
6	G	215/233 (92%)	207 (96%)	7 (3%)	1 (0%)	29	69
6	I	215/233 (92%)	208 (97%)	6 (3%)	1 (0%)	29	69
6	K	215/233 (92%)	205 (95%)	9 (4%)	1 (0%)	29	69
7	P	457/478 (96%)	431 (94%)	18 (4%)	8 (2%)	8	40
8	O	390/392 (100%)	350 (90%)	21 (5%)	19 (5%)	2	20
9	a	611/890 (69%)	588 (96%)	23 (4%)	0	100	100
10	b	42/265 (16%)	42 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	c	195/213 (92%)	189 (97%)	6 (3%)	0	100	100
12	d	341/345 (99%)	327 (96%)	14 (4%)	0	100	100
13	g	151/160 (94%)	149 (99%)	2 (1%)	0	100	100
13	h	155/160 (97%)	154 (99%)	1 (1%)	0	100	100
13	i	155/160 (97%)	153 (99%)	2 (1%)	0	100	100
13	j	154/160 (96%)	152 (99%)	2 (1%)	0	100	100
13	k	156/160 (98%)	154 (99%)	2 (1%)	0	100	100
13	l	155/160 (97%)	153 (99%)	2 (1%)	0	100	100
13	m	156/160 (98%)	154 (99%)	2 (1%)	0	100	100
13	n	156/160 (98%)	154 (99%)	2 (1%)	0	100	100
14	o	154/164 (94%)	152 (99%)	2 (1%)	0	100	100
15	e	62/73 (85%)	62 (100%)	0	0	100	100
16	f	59/85 (69%)	59 (100%)	0	0	100	100
All	All	7962/9068 (88%)	7509 (94%)	325 (4%)	128 (2%)	13	44

5 of 128 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	257	ALA
3	A	475	TYR
4	B	292	SER
3	C	475	TYR
3	C	529	ASN

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 [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.

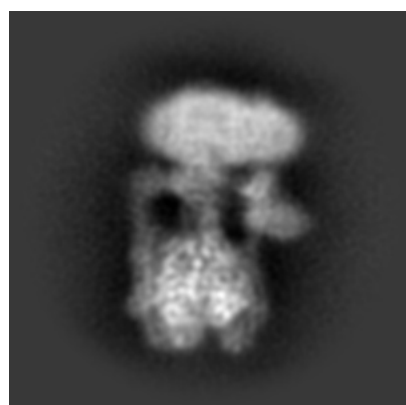
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0646. These allow visual inspection of the internal detail of the map and identification of artifacts.

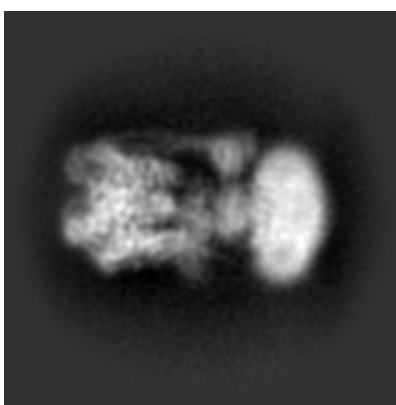
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

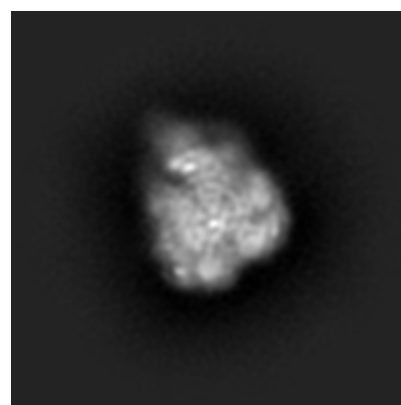
6.1.1 Primary map



X



Y

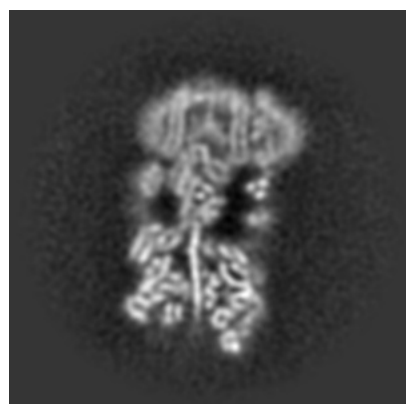


Z

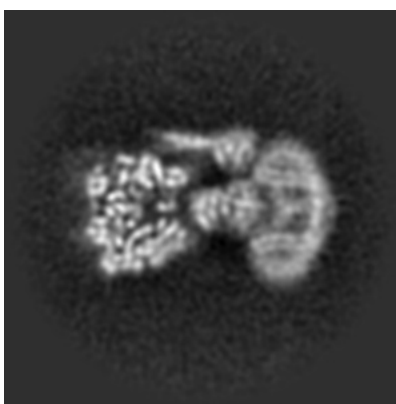
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

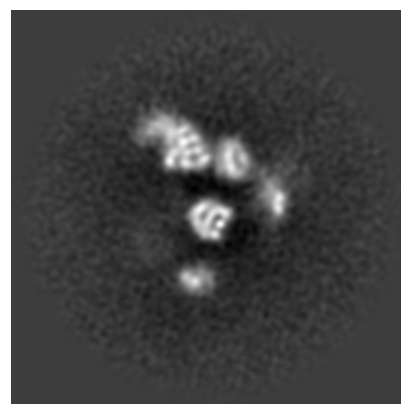
6.2.1 Primary map



X Index: 128



Y Index: 128

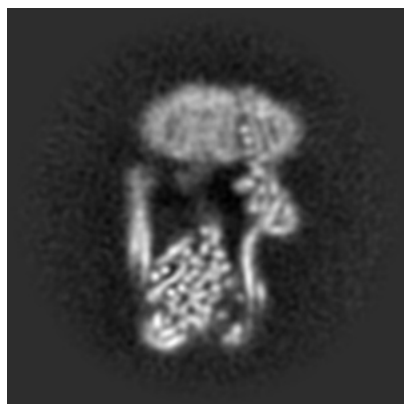


Z Index: 128

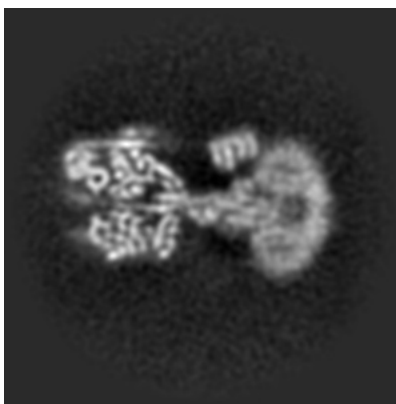
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

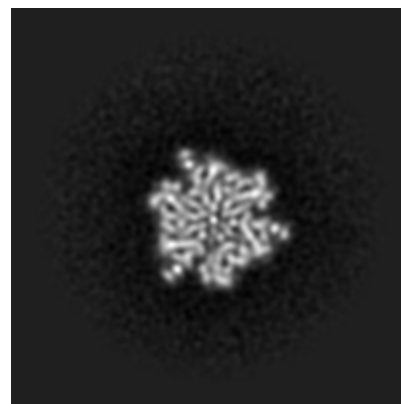
6.3.1 Primary map



X Index: 111



Y Index: 116



Z Index: 74

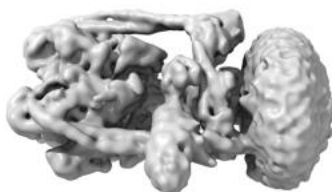
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

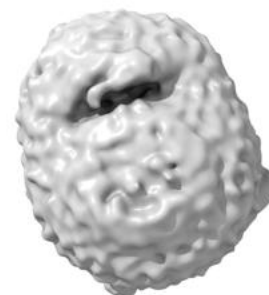
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

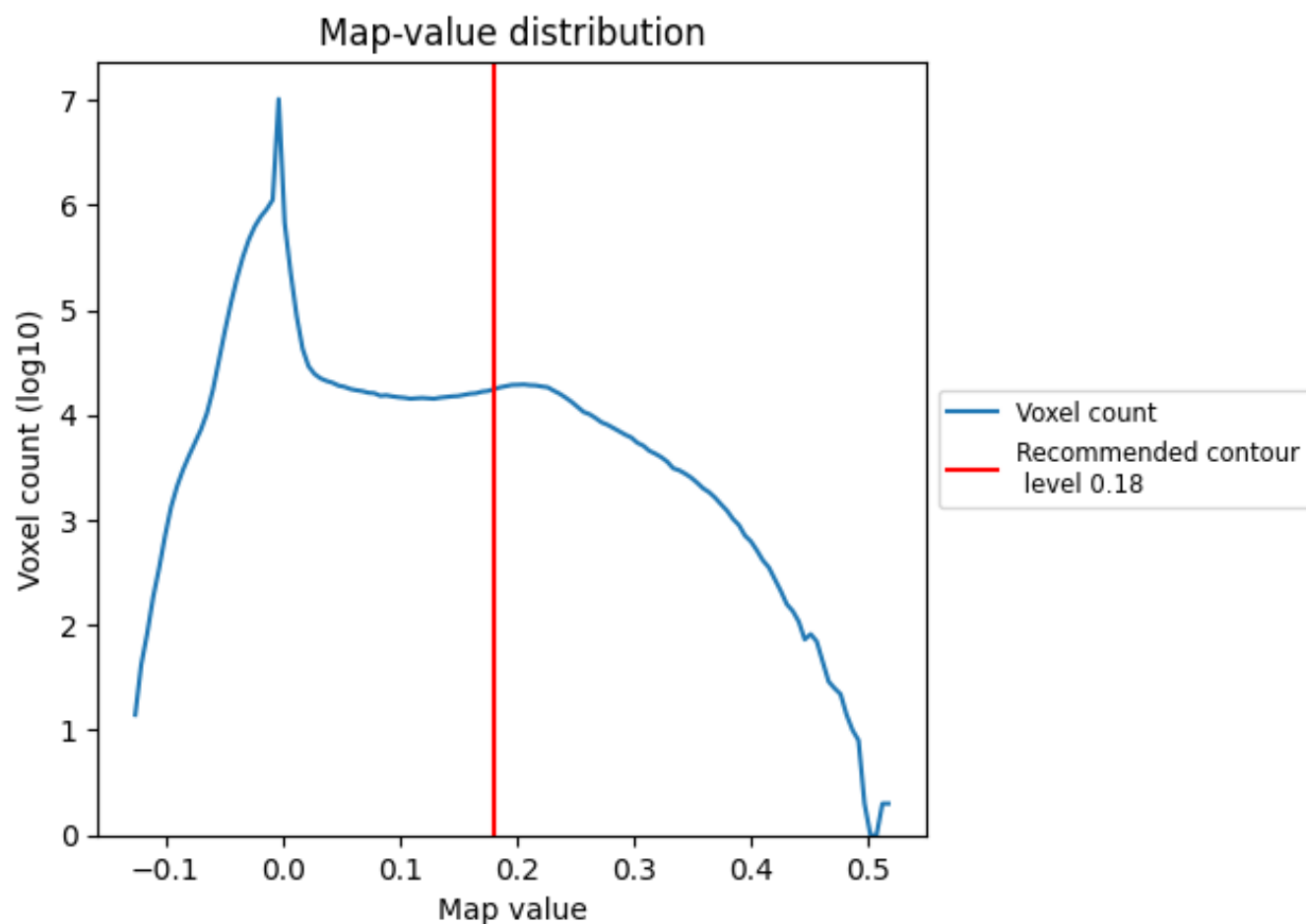
6.5 Mask visualisation

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

7 Map analysis [i](#)

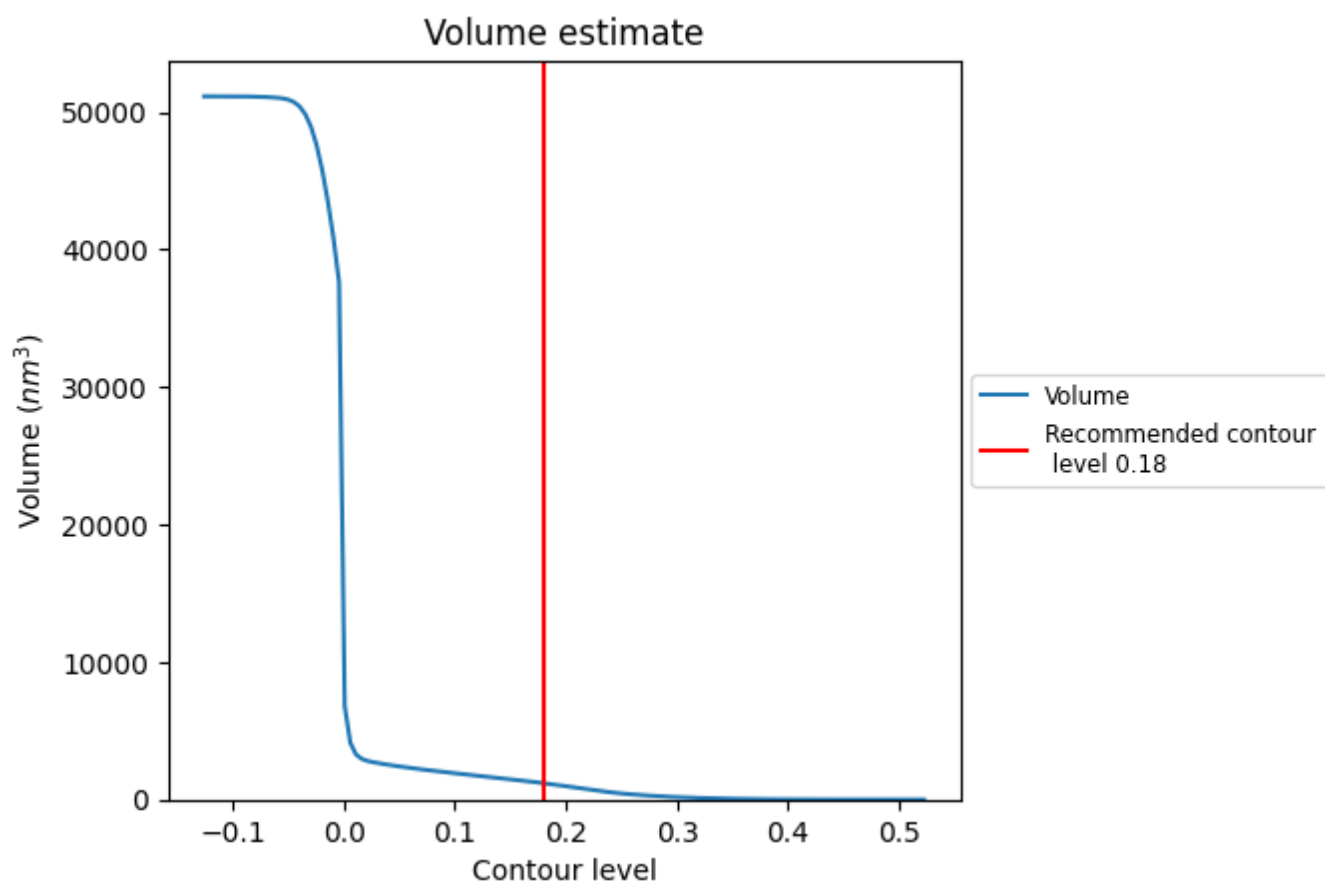
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

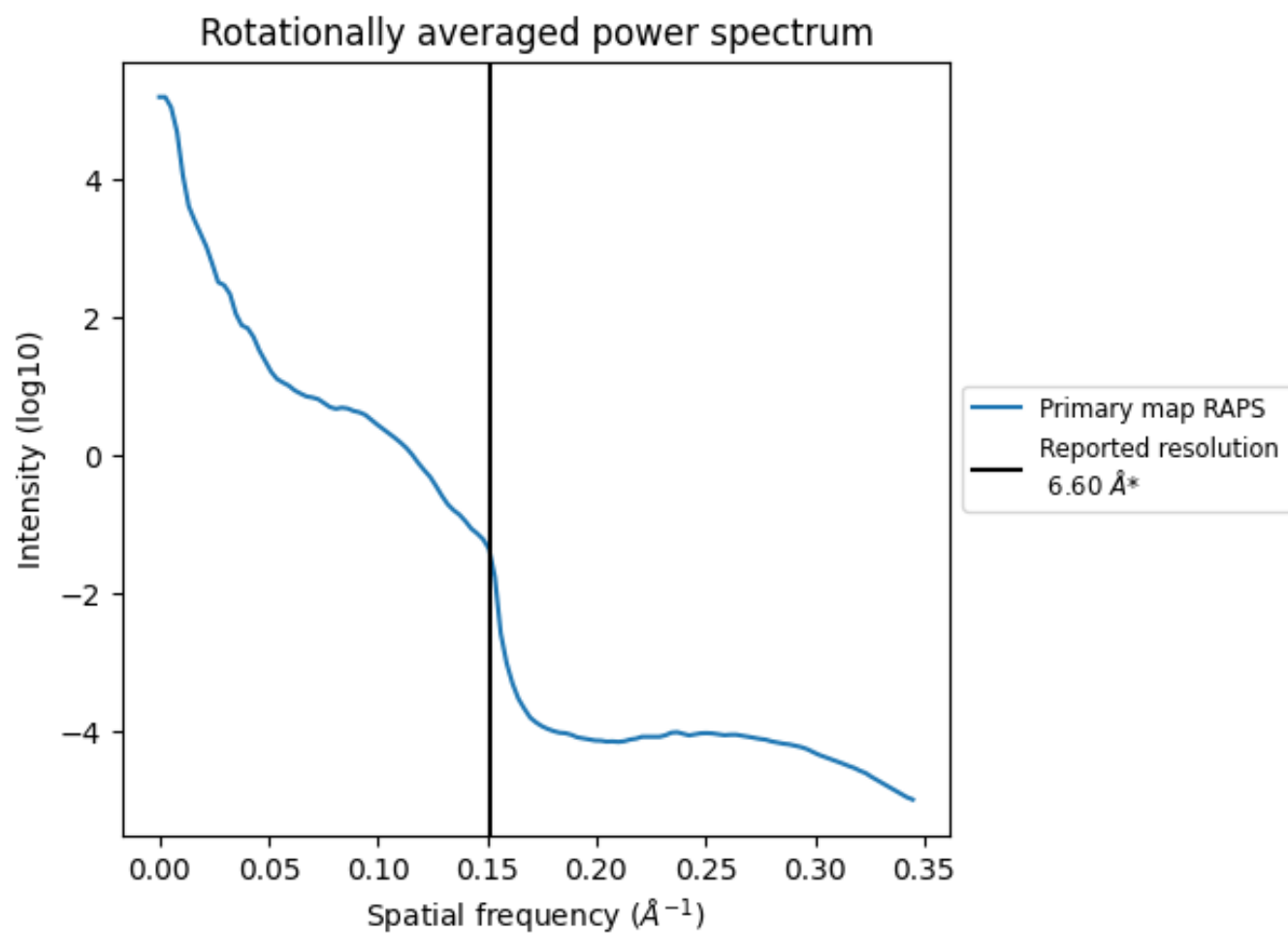
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1190 nm³; this corresponds to an approximate mass of 1075 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.152 Å⁻¹

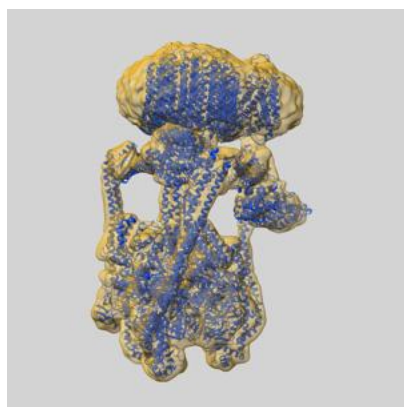
8 Fourier-Shell correlation

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

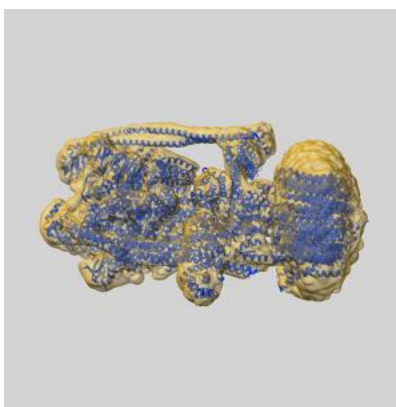
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0646 and PDB model 6O7V. Per-residue inclusion information can be found in section [3](#) on page [9](#).

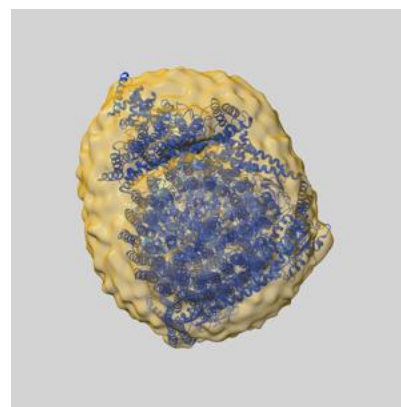
9.1 Map-model overlay [i](#)



X



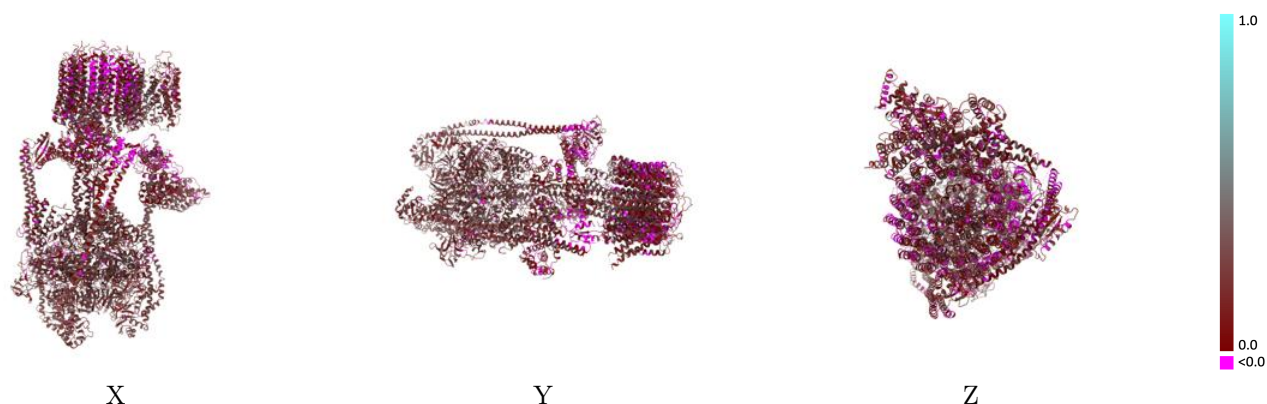
Y



Z

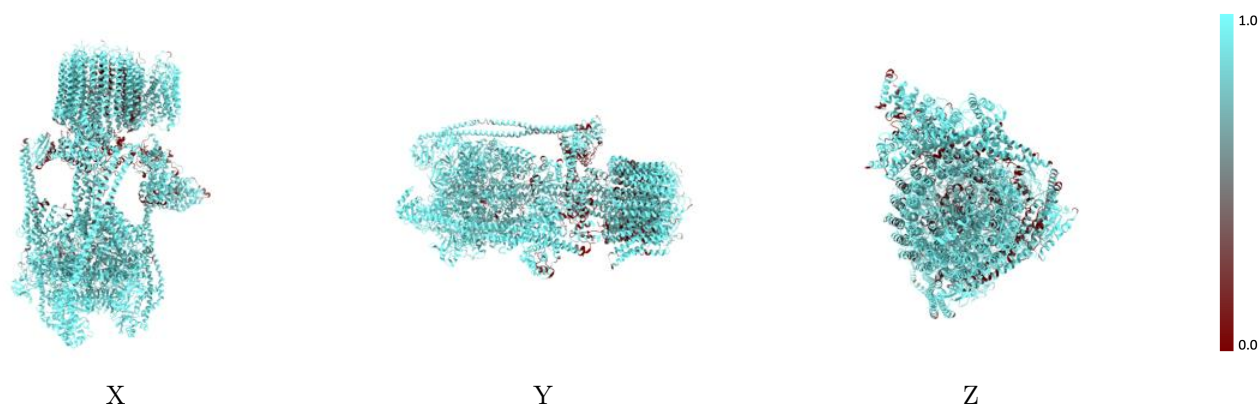
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



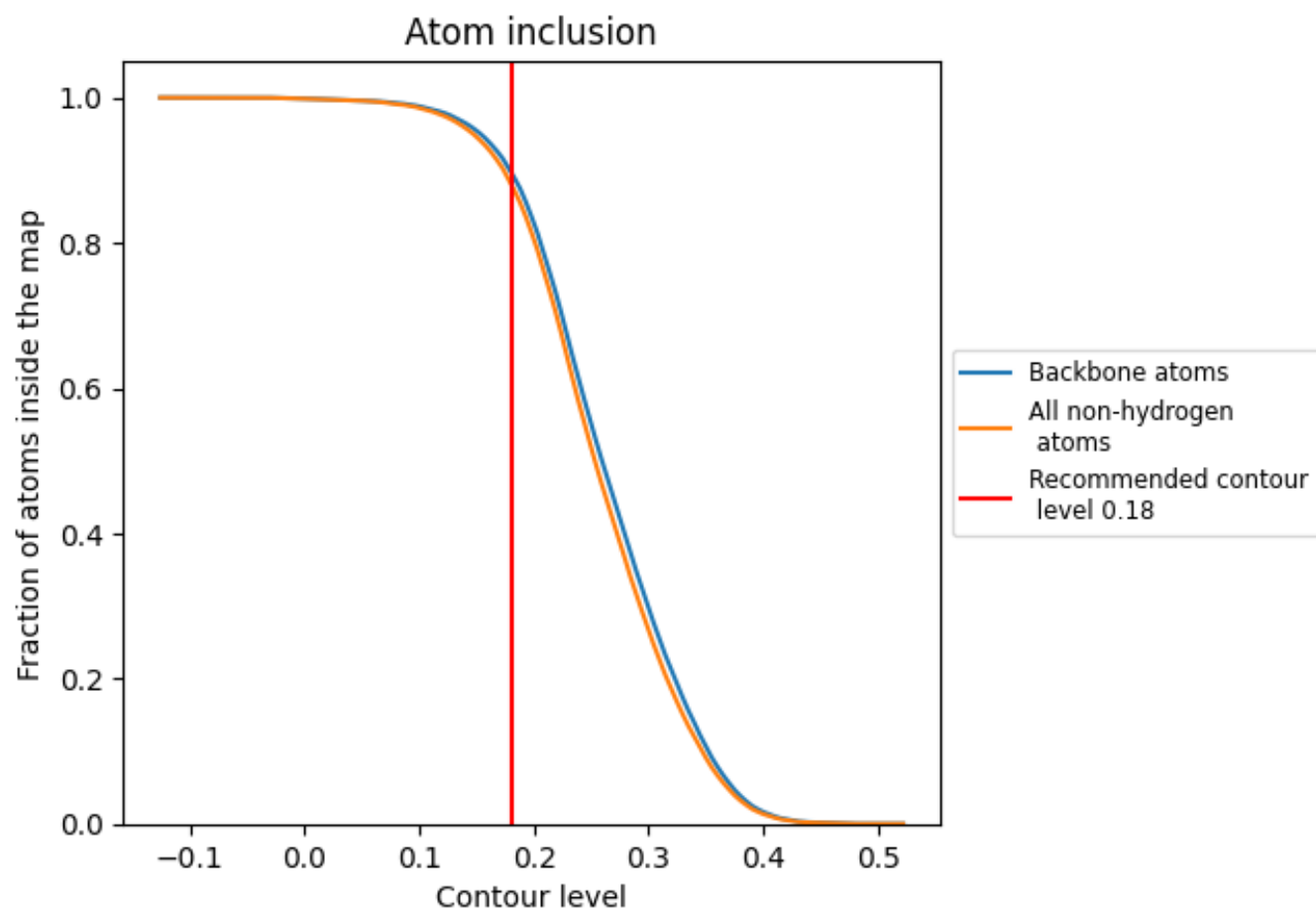
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.18).

































































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 88% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8815	 0.1750
A	 0.9297	 0.2060
B	 0.9502	 0.2250
C	 0.9599	 0.2280
D	 0.9404	 0.2220
E	 0.9441	 0.2150
F	 0.9364	 0.2150
G	 0.9768	 0.2290
H	 0.9518	 0.1960
I	 0.9341	 0.2020
J	 0.8940	 0.1530
K	 0.9545	 0.2190
L	 0.9461	 0.2260
M	 0.9047	 0.2230
N	 0.8004	 0.1800
O	 0.6718	 0.1090
P	 0.8360	 0.1580
a	 0.8221	 0.1310
b	 0.4954	 0.0300
c	 0.8929	 0.1340
d	 0.7322	 0.1800
e	 0.9154	 0.1470
f	 0.9900	 0.1650
g	 0.8425	 0.0730
h	 0.8231	 0.0580
i	 0.7549	 0.1020
j	 0.8245	 0.1640
k	 0.7878	 0.1310
l	 0.8008	 0.0710
m	 0.8398	 0.0410
n	 0.9414	 0.0990
o	 0.9565	 0.1450

