wwPDB EM Validation Summary Report

Feb 13, 2024 – 08:53 AM EST

PDB ID	:	7TMT
EMDB ID	:	EMD-26002
Title	:	V-ATPase from Saccharomyces cerevisiae, State 3
Authors	:	Vasanthakumar, T.; Keon, K.A.; Bueler, S.A.; Jaskolka, M.C.; Rubinstein, J.L.
Deposited on	:	2022-01-20
Resolution	:	3.80 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:

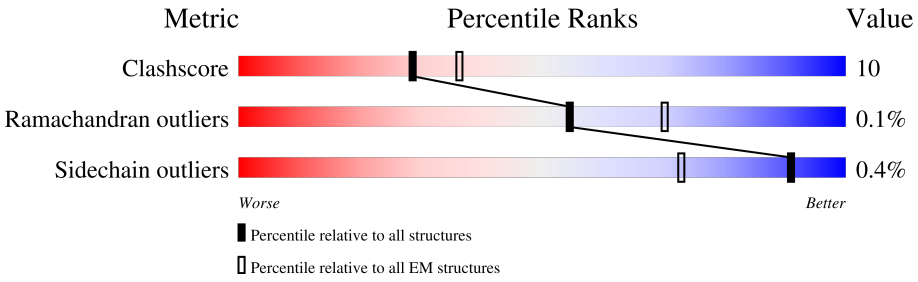
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.80 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
Sidechain outliers	154315	3826

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	73% 23%
1	C	617	70% 25%
1	E	617	70% 26%
2	B	517	65% 26% 8%
2	D	517	60% 32% 8%
2	F	517	63% 29% 8%
3	G	233	8% 89% 6% 5%
3	I	233	81% 14% 5%

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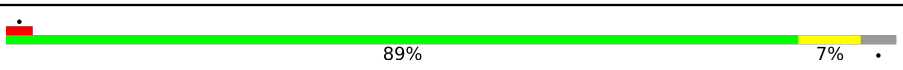
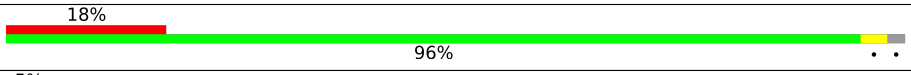
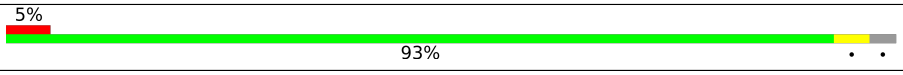
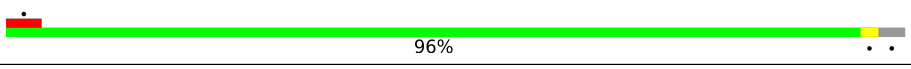
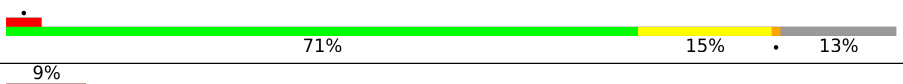
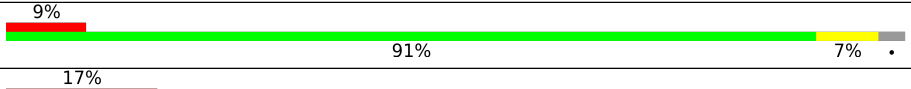
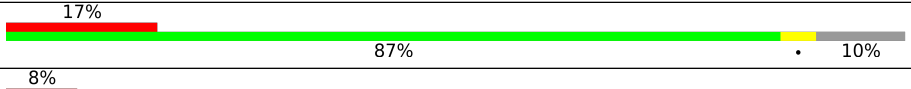
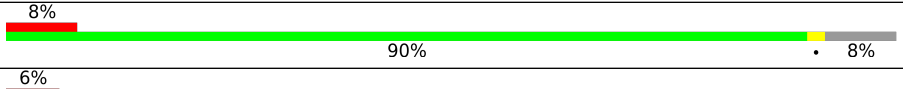
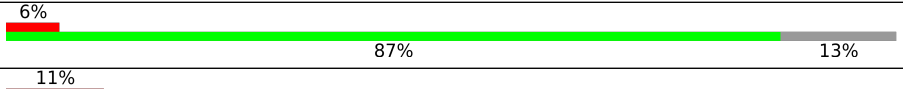
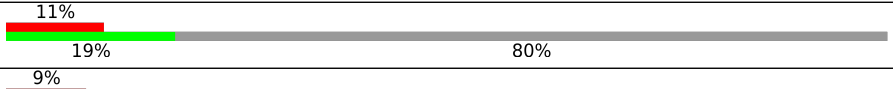
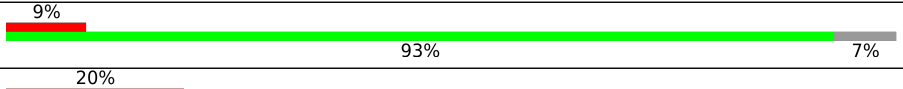
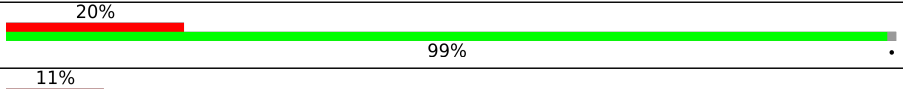
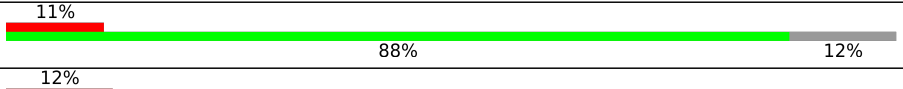
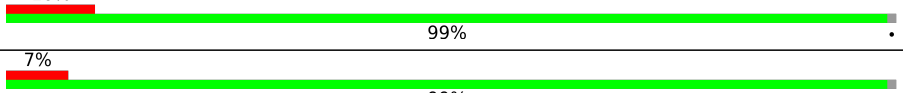
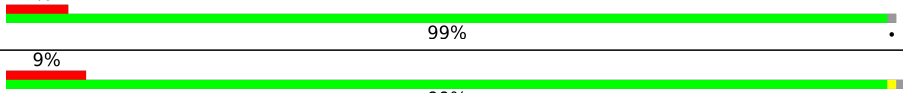
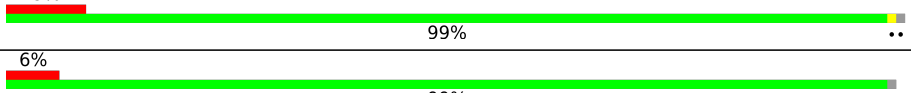
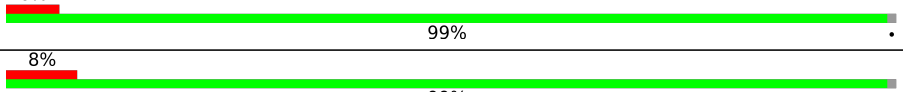
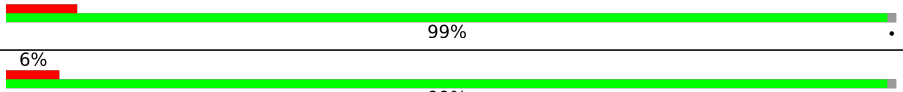
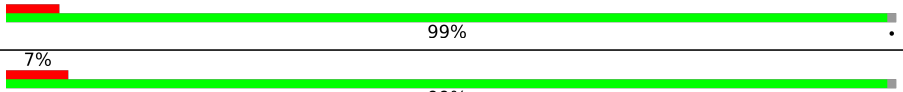
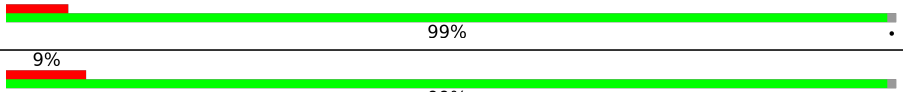
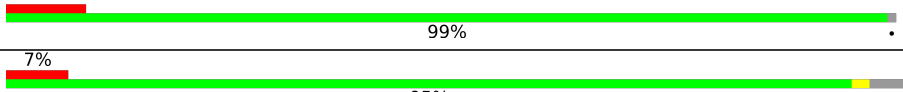
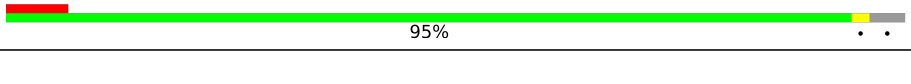
Mol	Chain	Length	Quality of chain
3	K	233	
4	H	114	
4	J	114	
4	L	114	
5	M	256	
6	N	118	
7	O	392	
8	P	478	
9	a	840	
10	b	265	
11	c	213	
12	d	345	
13	e	73	
14	f	85	
15	g	160	
15	h	160	
15	i	160	
15	j	160	
15	k	160	
15	l	160	
15	m	160	
15	n	160	
16	o	164	

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 53433 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 H(+)-transporting two-sector ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	593	Total	C	N	O	S	0	0
			4545	2888	756	881	20		
1	C	593	Total	C	N	O	S	0	0
			4541	2885	757	879	20		
1	E	593	Total	C	N	O	S	0	0
			4578	2904	760	894	20		

- Molecule 2 is a protein called Vacuolar proton pump subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	475	Total	C	N	O	S	0	0
			3688	2334	632	710	12		
2	D	475	Total	C	N	O	S	0	0
			3690	2332	632	714	12		
2	F	478	Total	C	N	O	S	0	0
			3712	2344	636	720	12		

- Molecule 3 is a protein called V-ATPase subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	221	Total	C	N	O	S	0	0
			1202	738	233	230	1		
3	I	221	Total	C	N	O	S	0	0
			1324	826	252	244	2		
3	K	224	Total	C	N	O	S	0	0
			1332	827	264	240	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	112	Total	C	N	O	0	0
			587	354	120	113		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	J	111	Total 584	C 355	N 116	O 113	0	0
4	L	111	Total 594	C 360	N 119	O 115	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	223	Total 1444	C 886	N 274	O 281	S 3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	N	115	Total 581	C 351	N 115	O 115	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	354	Total 1792	C 1084	N 354	O 354	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	P	438	Total 2197	C 1320	N 438	O 439	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	734	Total 4317	C 2723	N 804	O 782	S 8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	52	Total 315	C 200	N 55	O 59	S 1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	198	Total	C	N	O	S	0	0
			1165	737	212	215	1		

- 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	S	0	0
			2209	1404	402	401	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	64	Total	C	N	O	S	0	0
			428	279	75	70	4		

- Molecule 14 is a protein called Yeast V-ATPase subunit f.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	f	63	Total	C	N	O	S	0	0
			358	221	70	66	1		

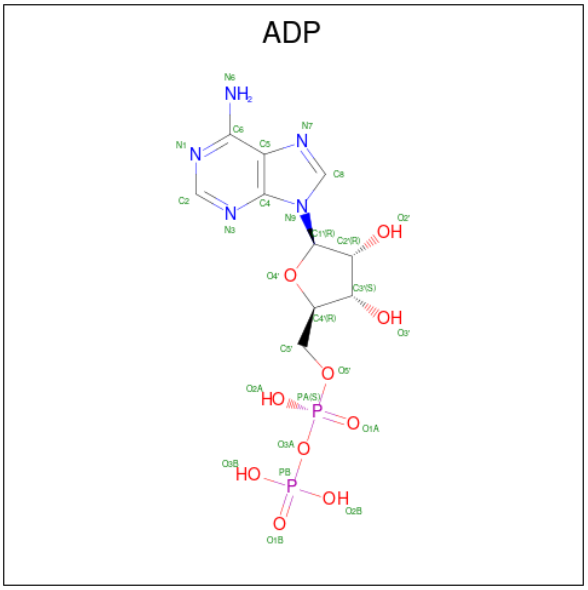
- Molecule 15 is a protein called V-type proton ATPase subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	159	Total	C	N	O	S	0	0
			911	569	170	170	2		
15	h	159	Total	C	N	O		0	0
			872	538	165	169			
15	i	159	Total	C	N	O	S	0	0
			957	610	167	177	3		
15	j	159	Total	C	N	O	S	0	0
			926	580	169	175	2		
15	k	159	Total	C	N	O	S	0	0
			902	551	173	175	3		
15	l	159	Total	C	N	O	S	0	0
			922	577	172	170	3		
15	m	159	Total	C	N	O	S	0	0
			932	584	174	171	3		
15	n	159	Total	C	N	O	S	0	0
			871	532	169	167	3		

- Molecule 16 is a protein called V-type proton ATPase subunit c'.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	o	158	Total	C	N	O	S	0	0
			930	586	167	172	5		

- Molecule 17 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



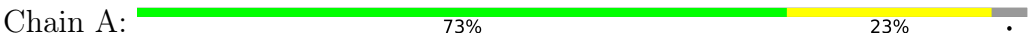
Mol	Chain	Residues	Atoms					AltConf
17	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

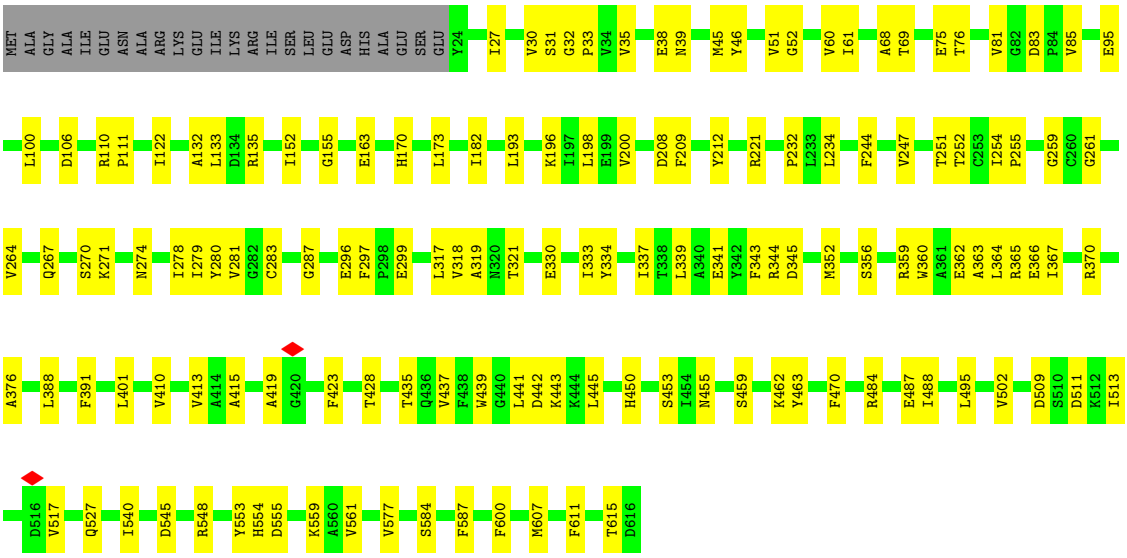
3 Residue-property plots (i)

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: H(+)-transporting two-sector ATPase

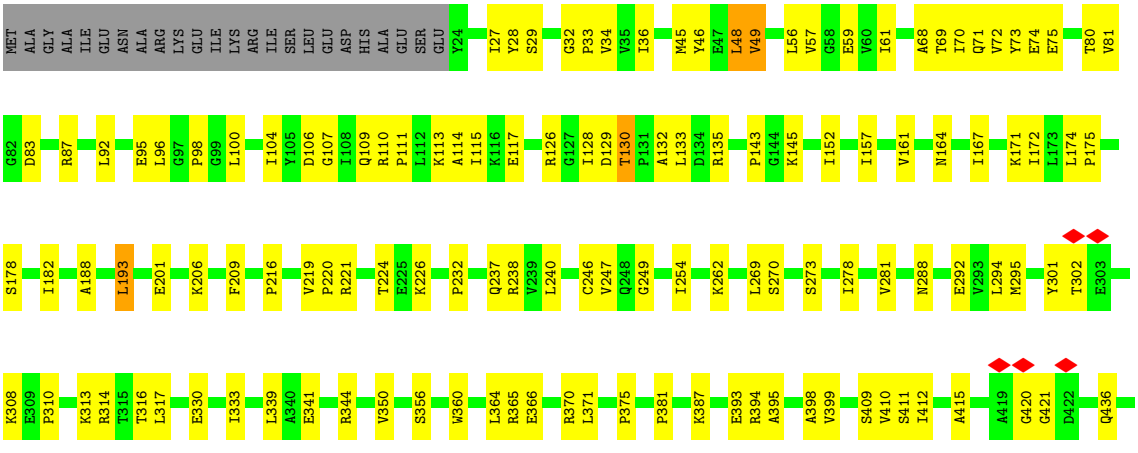
Chain A:

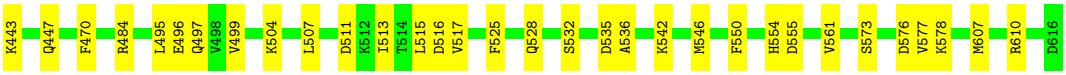




• Molecule 1: H(+)-transporting two-sector ATPase

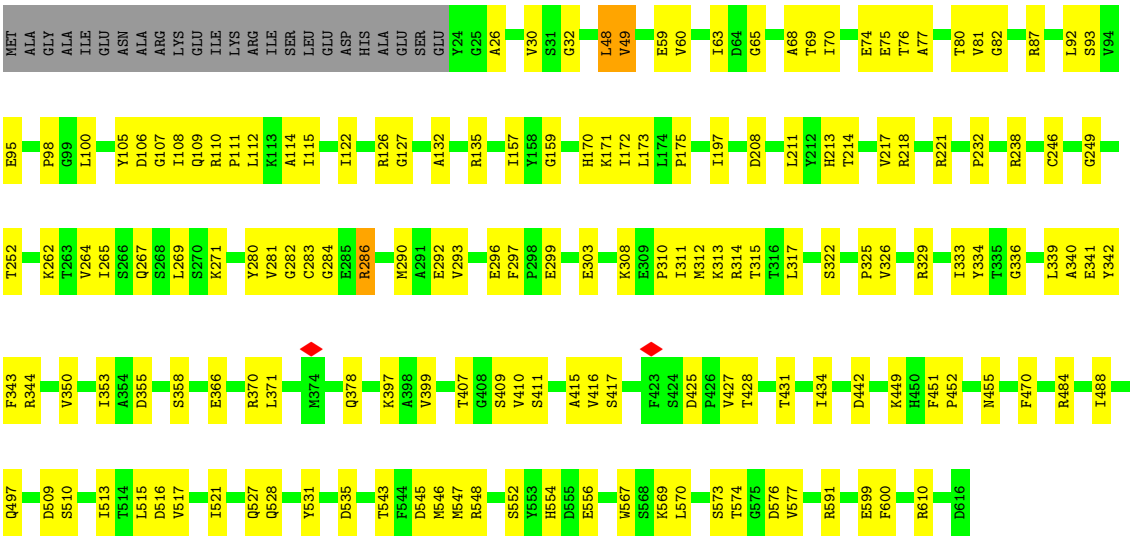
Chain C:





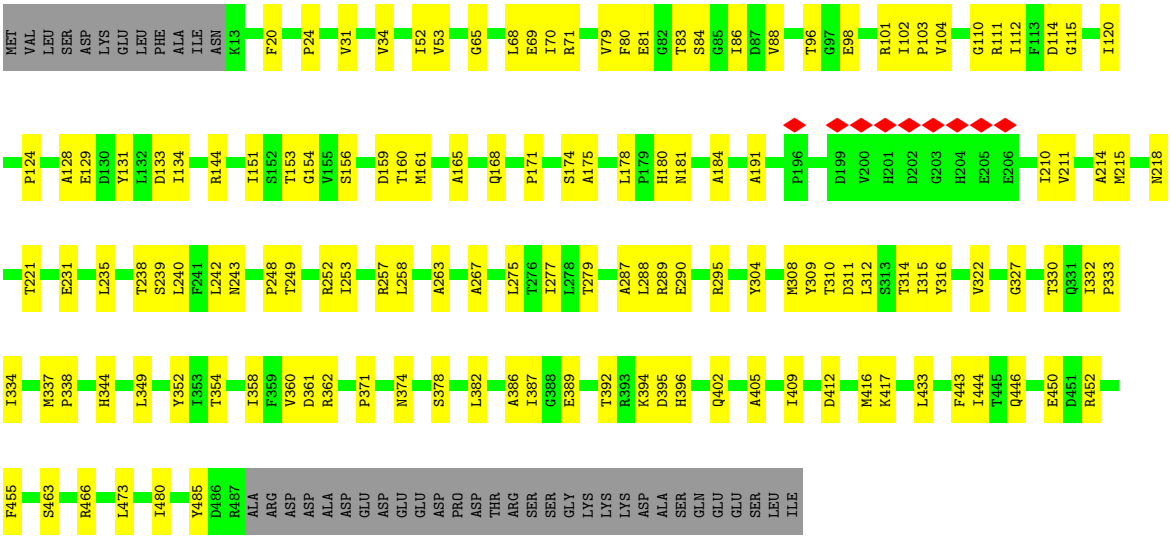
• Molecule 1: H(+)-transporting two-sector ATPase

Chain E:



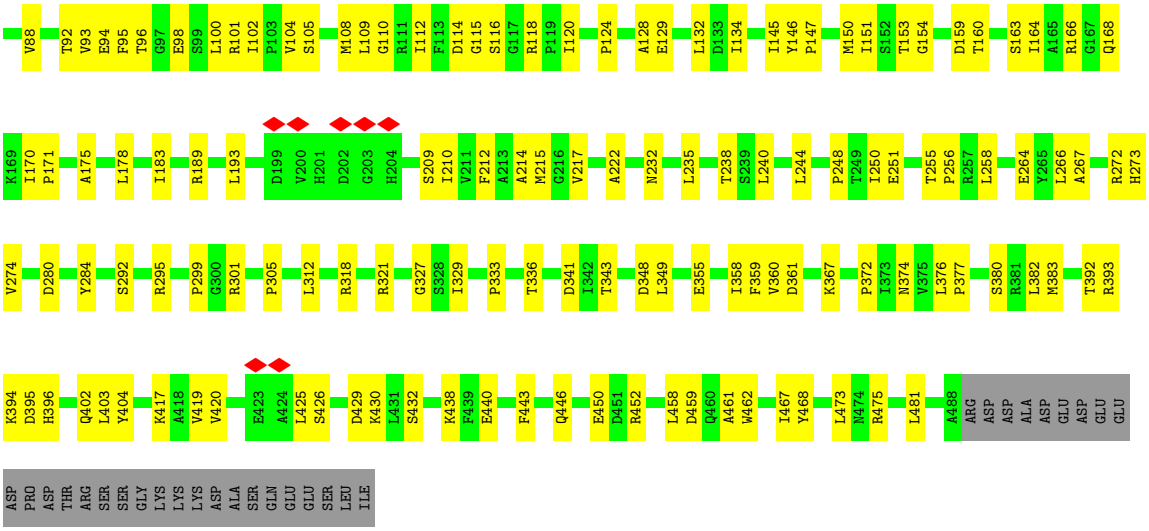
• Molecule 2: Vacuolar proton pump subunit B

Chain B:



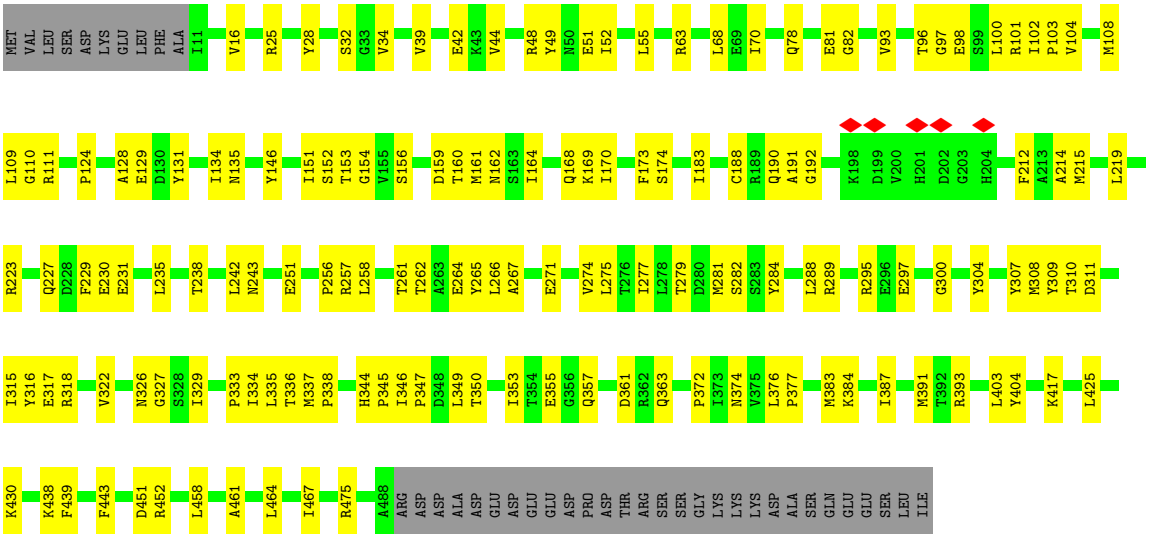
• Molecule 2: Vacuolar proton pump subunit B

Chain D:



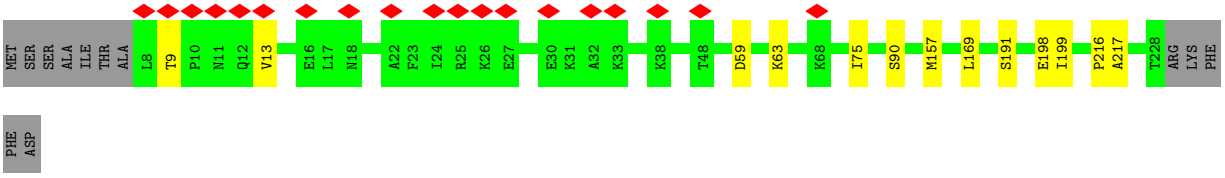
• Molecule 2: Vacuolar proton pump subunit B

Chain F:



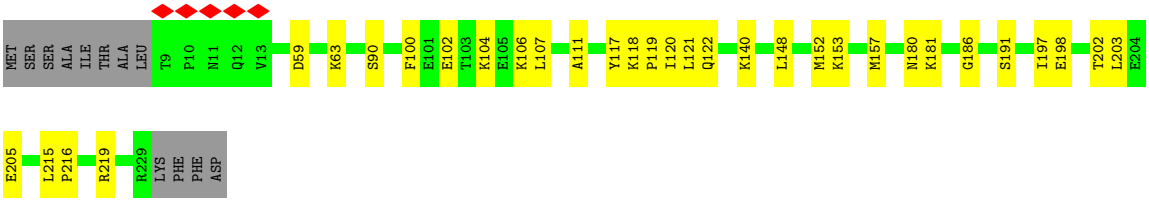
• Molecule 3: V-ATPase subunit E

Chain G:

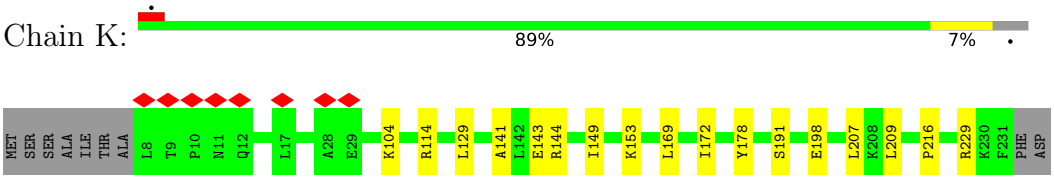


• Molecule 3: V-ATPase subunit E

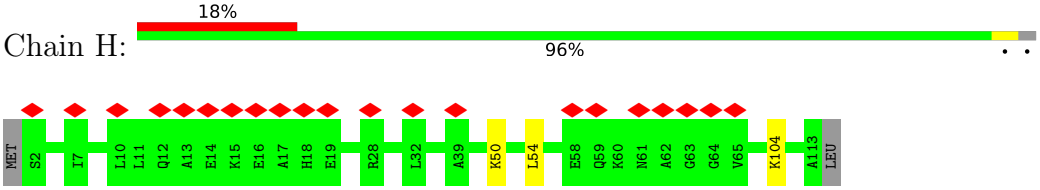
Chain I:



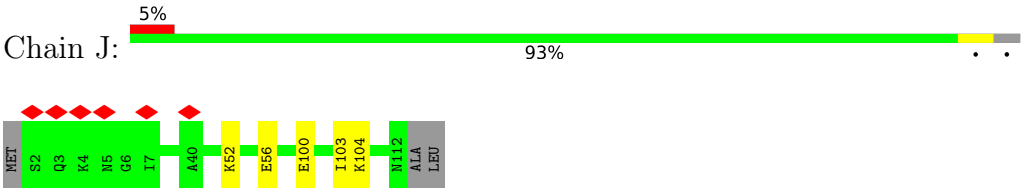
• Molecule 3: V-ATPase subunit E



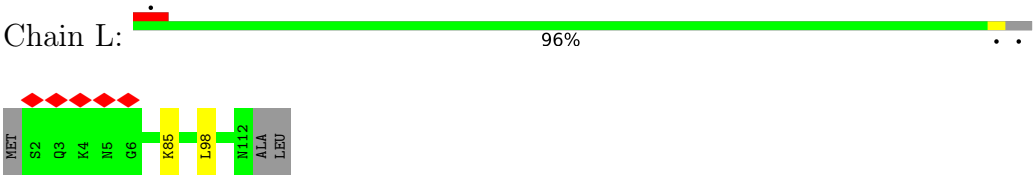
• Molecule 4: V-type proton ATPase subunit G



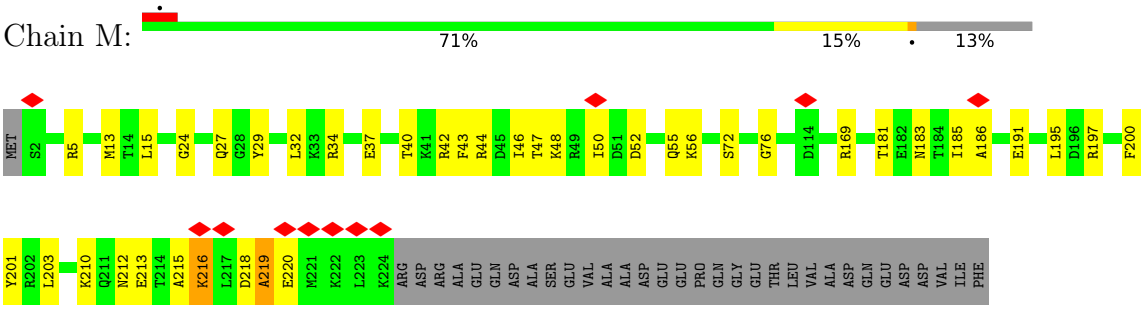
• Molecule 4: V-type proton ATPase subunit G



• Molecule 4: V-type proton ATPase subunit G

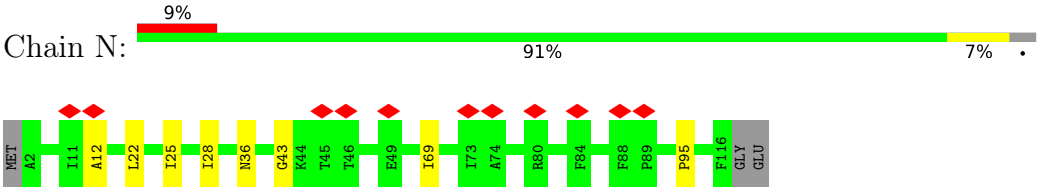


• Molecule 5: V-type proton ATPase subunit D



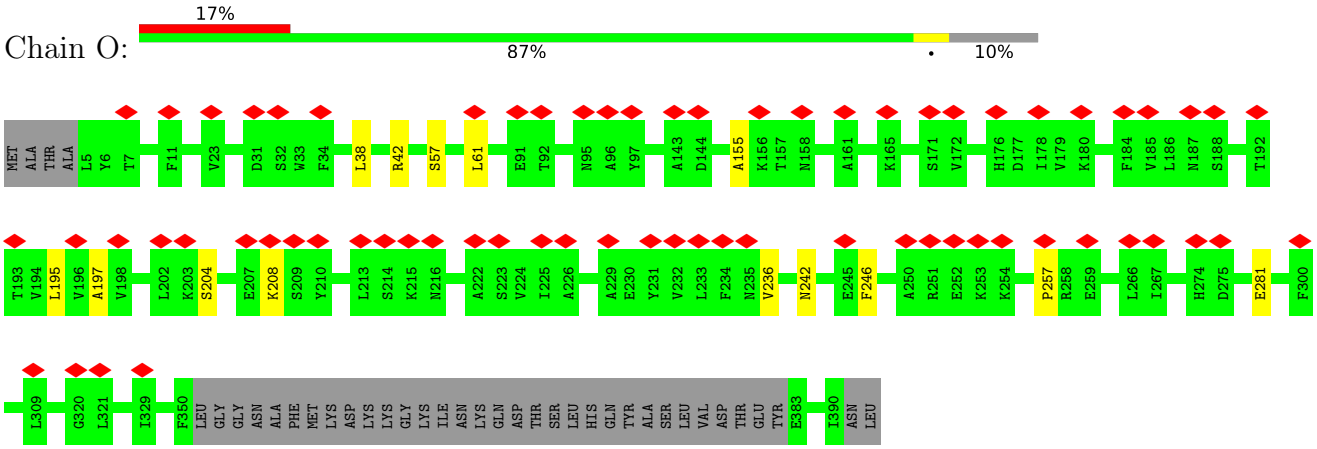
• Molecule 6: V-type proton ATPase subunit F

Chain N:



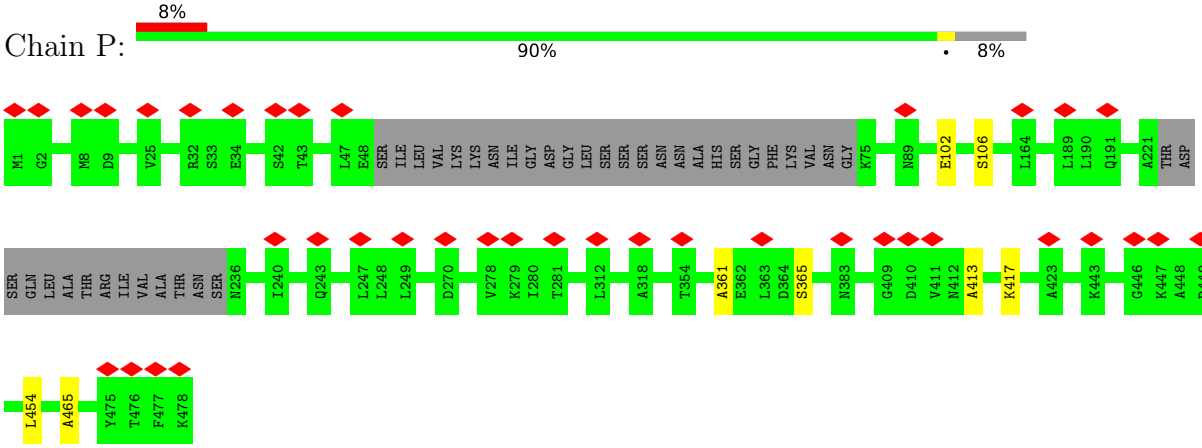
• Molecule 7: V-type proton ATPase subunit C

Chain O:



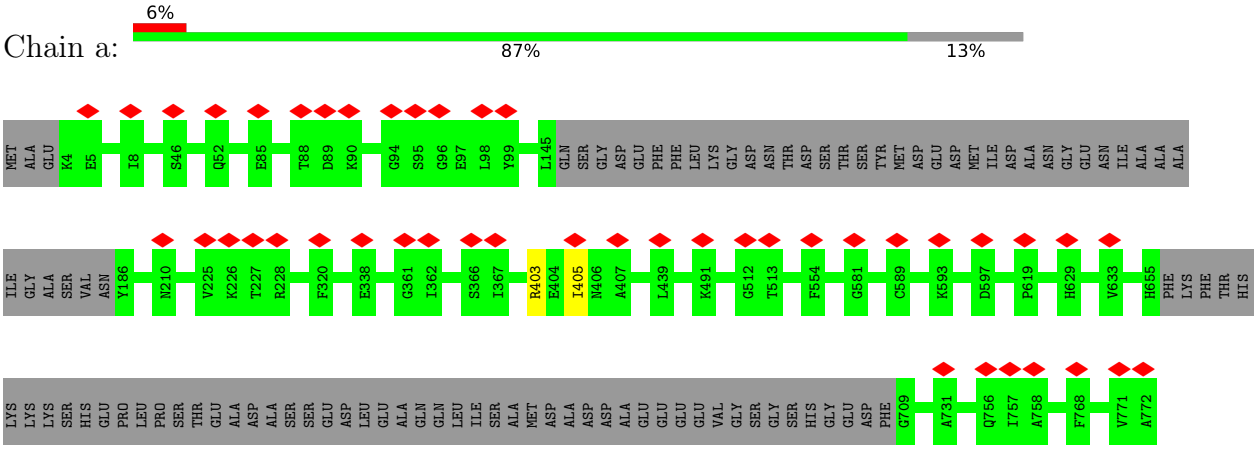
• Molecule 8: V-type proton ATPase subunit H

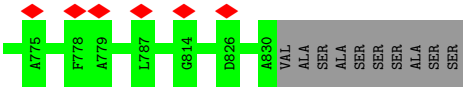
Chain P:



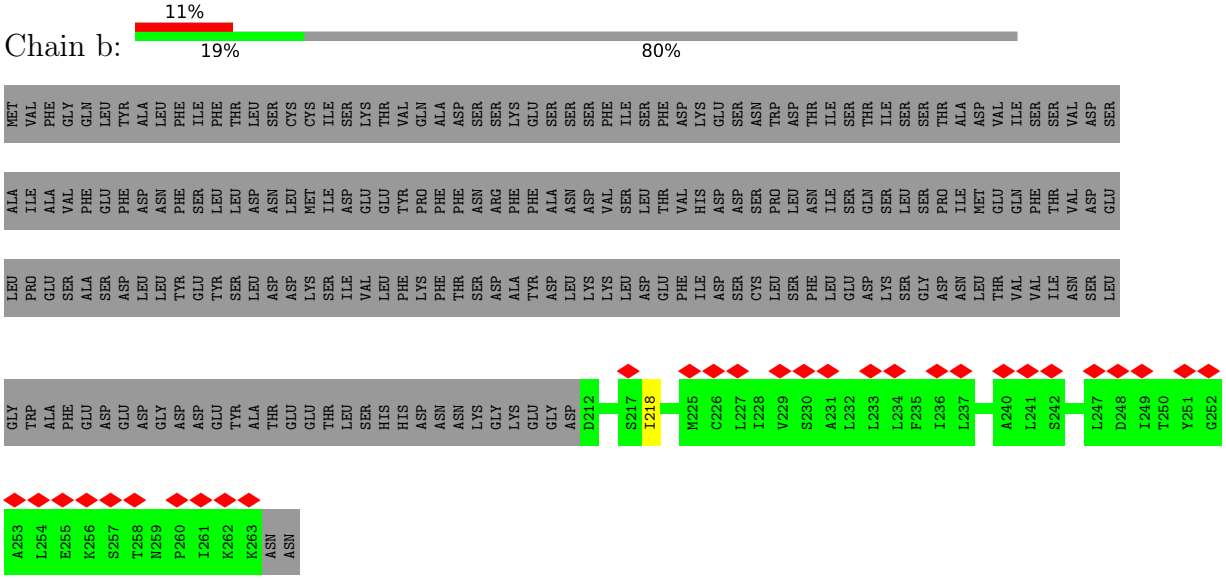
• Molecule 9: V-type proton ATPase subunit a, vacuolar isoform

Chain a:

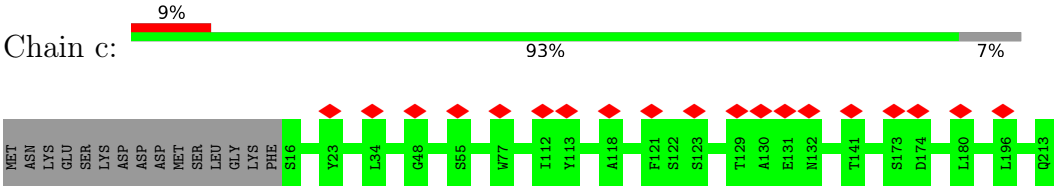




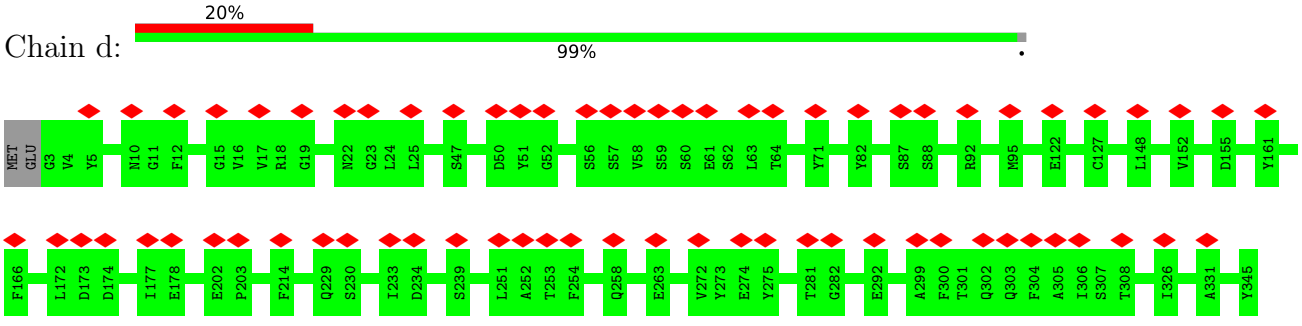
• Molecule 10: V0 assembly protein 1



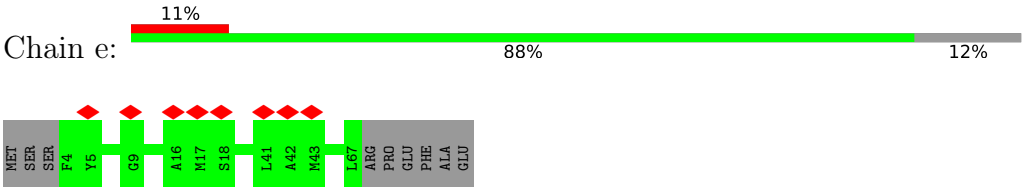
• Molecule 11: V-type proton ATPase subunit c"



• Molecule 12: V-type proton ATPase subunit d

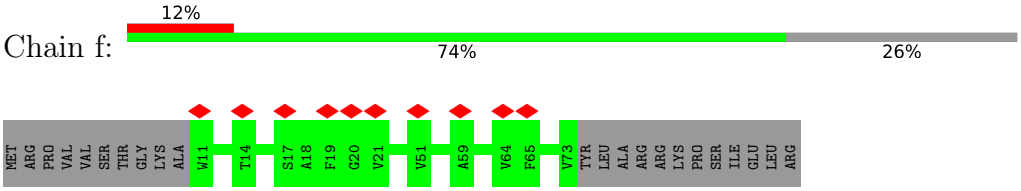


• Molecule 13: V-type proton ATPase subunit e



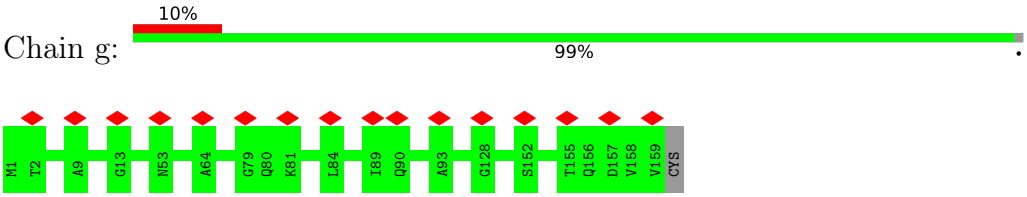
• Molecule 14: Yeast V-ATPase subunit f

Chain f:



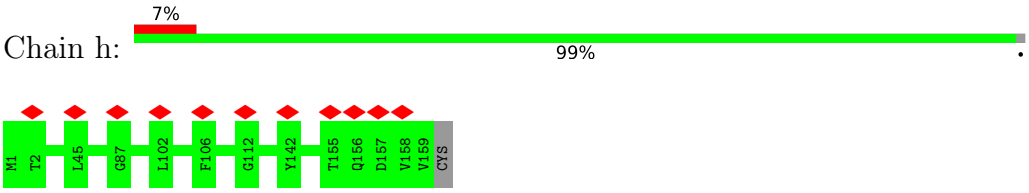
• Molecule 15: V-type proton ATPase subunit c

Chain g:



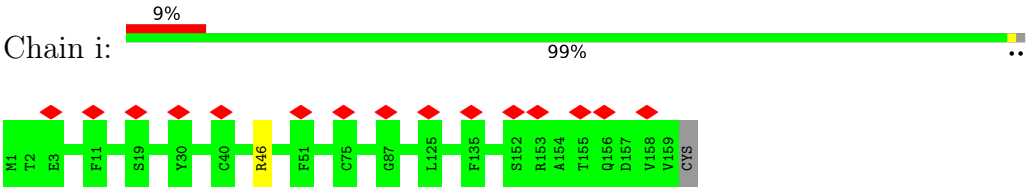
• Molecule 15: V-type proton ATPase subunit c

Chain h:



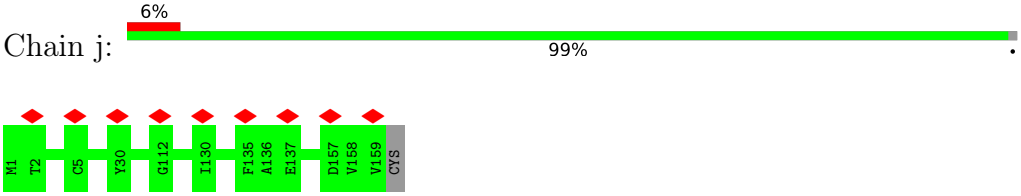
• Molecule 15: V-type proton ATPase subunit c

Chain i:



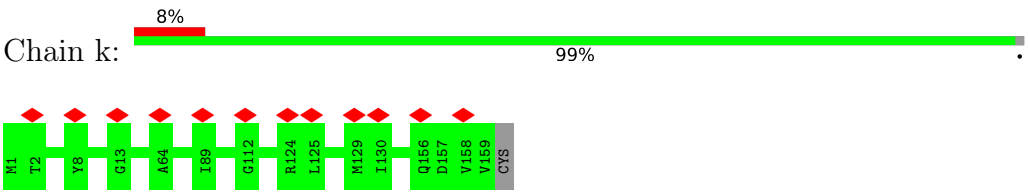
• Molecule 15: V-type proton ATPase subunit c

Chain j:



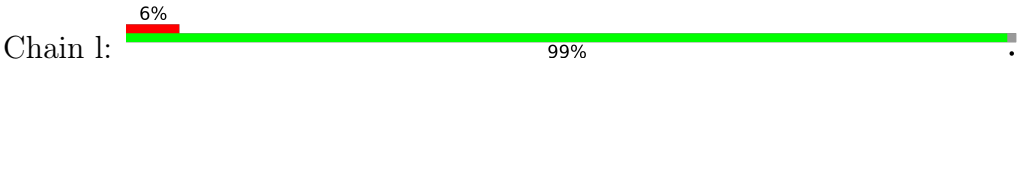
• Molecule 15: V-type proton ATPase subunit c

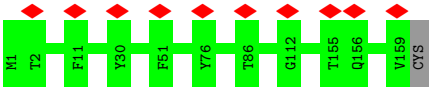
Chain k:



• Molecule 15: V-type proton ATPase subunit c

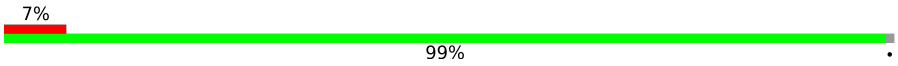
Chain l:

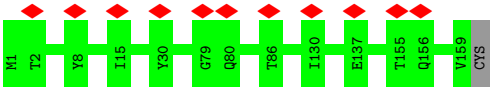




• Molecule 15: V-type proton ATPase subunit c

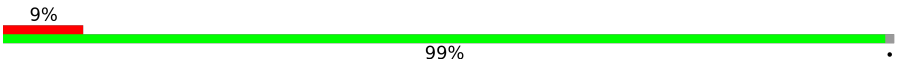
Chain m:

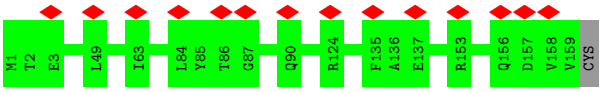




• Molecule 15: V-type proton ATPase subunit c

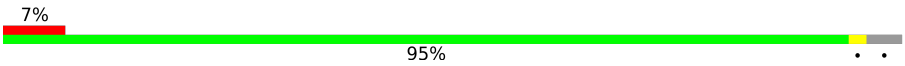
Chain n:

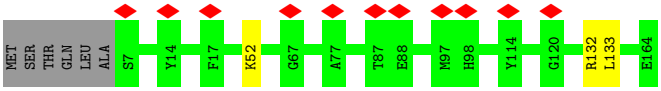




• Molecule 16: V-type proton ATPase subunit c'

Chain o:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42558	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	43	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	38.803	Depositor
Minimum map value	-16.070	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	360.49997, 360.49997, 360.49997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2016666, 1.2016666, 1.2016666	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

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	0.36	0/4644	0.51	0/6299
1	C	0.38	0/4640	0.52	0/6292
1	E	0.39	0/4677	0.53	0/6339
2	B	0.39	0/3758	0.55	0/5097
2	D	0.39	0/3760	0.56	0/5099
2	F	0.40	0/3782	0.54	0/5129
3	G	0.26	0/1211	0.39	0/1682
3	I	0.26	0/1333	0.47	0/1828
3	K	0.26	0/1343	0.47	0/1840
4	H	0.23	0/588	0.36	0/810
4	J	0.24	0/584	0.37	0/804
4	L	0.25	0/595	0.36	0/817
5	M	0.28	0/1455	0.52	0/1975
6	N	0.23	0/585	0.44	0/819
7	O	0.23	0/1806	0.40	0/2532
8	P	0.23	0/2203	0.37	0/3078
9	a	0.26	0/4415	0.43	0/6114
10	b	0.24	0/321	0.41	0/445
11	c	0.27	0/1188	0.43	0/1632
12	d	0.27	0/2258	0.47	0/3106
13	e	0.25	0/440	0.46	0/607
14	f	0.24	0/365	0.37	0/504
15	g	0.26	0/924	0.49	0/1268
15	h	0.26	0/883	0.44	0/1216
15	i	0.27	0/970	0.48	0/1331
15	j	0.26	0/940	0.43	0/1290
15	k	0.26	0/913	0.47	0/1251
15	l	0.26	0/936	0.44	0/1281
15	m	0.27	0/947	0.49	0/1294
15	n	0.25	0/881	0.42	0/1211
16	o	0.26	0/947	0.46	0/1297
All	All	0.32	0/54292	0.49	0/74287

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	4545	0	4474	102	0
1	C	4541	0	4448	119	0
1	E	4578	0	4519	120	0
2	B	3688	0	3644	98	0
2	D	3690	0	3637	118	0
2	F	3712	0	3651	111	0
3	G	1202	0	704	10	0
3	I	1324	0	984	24	0
3	K	1332	0	954	11	0
4	H	587	0	349	1	0
4	J	584	0	357	5	0
4	L	594	0	368	1	0
5	M	1444	0	1152	32	0
6	N	581	0	285	4	0
7	O	1792	0	877	7	0
8	P	2197	0	993	4	0
9	a	4317	0	2662	0	0
10	b	315	0	207	0	0
11	c	1165	0	783	0	0
12	d	2209	0	1559	0	0
13	e	428	0	335	0	0
14	f	358	0	211	0	0
15	g	911	0	658	0	0
15	h	872	0	570	0	0
15	i	957	0	798	0	0
15	j	926	0	679	0	0
15	k	902	0	631	0	0
15	l	922	0	676	0	0
15	m	932	0	685	0	0
15	n	871	0	582	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	o	930	0	678	0	0
17	E	27	0	12	2	0
All	All	53433	0	43122	712	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 10.

The worst 5 of 712 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)
5:M:55:GLN:HE22	5:M:56:LYS:HE3	1.37	0.90
2:D:114:ASP:OD1	2:D:115:GLY:N	2.11	0.84
1:C:356:SER:H	1:C:415:ALA:HB3	1.44	0.83
1:E:517:VAL:HG11	1:E:554:HIS:HB2	1.64	0.79
5:M:5:ARG:HH21	5:M:183:ASN:HD21	1.31	0.77

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%)	554 (94%)	37 (6%)	0	100	100
1	C	591/617 (96%)	556 (94%)	34 (6%)	1 (0%)	47	79
1	E	591/617 (96%)	558 (94%)	33 (6%)	0	100	100
2	B	473/517 (92%)	431 (91%)	42 (9%)	0	100	100
2	D	473/517 (92%)	445 (94%)	28 (6%)	0	100	100
2	F	476/517 (92%)	434 (91%)	41 (9%)	1 (0%)	47	79
3	G	219/233 (94%)	215 (98%)	4 (2%)	0	100	100
3	I	219/233 (94%)	212 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	K	222/233 (95%)	210 (95%)	12 (5%)	0	100	100
4	H	110/114 (96%)	107 (97%)	3 (3%)	0	100	100
4	J	109/114 (96%)	108 (99%)	1 (1%)	0	100	100
4	L	109/114 (96%)	108 (99%)	1 (1%)	0	100	100
5	M	221/256 (86%)	211 (96%)	9 (4%)	1 (0%)	29	66
6	N	113/118 (96%)	100 (88%)	13 (12%)	0	100	100
7	O	350/392 (89%)	328 (94%)	22 (6%)	0	100	100
8	P	432/478 (90%)	424 (98%)	8 (2%)	0	100	100
9	a	728/840 (87%)	685 (94%)	41 (6%)	2 (0%)	41	74
10	b	50/265 (19%)	48 (96%)	1 (2%)	1 (2%)	7	41
11	c	196/213 (92%)	190 (97%)	6 (3%)	0	100	100
12	d	341/345 (99%)	325 (95%)	16 (5%)	0	100	100
13	e	62/73 (85%)	62 (100%)	0	0	100	100
14	f	61/85 (72%)	59 (97%)	2 (3%)	0	100	100
15	g	157/160 (98%)	157 (100%)	0	0	100	100
15	h	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
15	i	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
15	j	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
15	k	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
15	l	157/160 (98%)	156 (99%)	1 (1%)	0	100	100
15	m	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
15	n	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
16	o	156/164 (95%)	151 (97%)	3 (2%)	2 (1%)	12	48
All	All	8149/8952 (91%)	7757 (95%)	384 (5%)	8 (0%)	54	83

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	130	THR
9	a	403	ARG
9	a	405	ILE
10	b	218	ILE
5	M	219	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	488/516 (95%)	488 (100%)	0	100 100
1	C	482/516 (93%)	479 (99%)	3 (1%)	86 92
1	E	497/516 (96%)	493 (99%)	4 (1%)	81 89
2	B	394/444 (89%)	394 (100%)	0	100 100
2	D	394/444 (89%)	393 (100%)	1 (0%)	92 96
2	F	396/444 (89%)	395 (100%)	1 (0%)	92 96
3	G	28/208 (14%)	28 (100%)	0	100 100
3	I	62/208 (30%)	62 (100%)	0	100 100
3	K	55/208 (26%)	55 (100%)	0	100 100
4	H	9/94 (10%)	8 (89%)	1 (11%)	6 29
4	J	10/94 (11%)	10 (100%)	0	100 100
4	L	12/94 (13%)	11 (92%)	1 (8%)	11 40
5	M	92/221 (42%)	90 (98%)	2 (2%)	52 72
6	N	5/104 (5%)	5 (100%)	0	100 100
7	O	16/348 (5%)	16 (100%)	0	100 100
8	P	9/439 (2%)	9 (100%)	0	100 100
9	a	152/728 (21%)	152 (100%)	0	100 100
10	b	15/244 (6%)	15 (100%)	0	100 100
11	c	42/168 (25%)	42 (100%)	0	100 100
12	d	116/309 (38%)	116 (100%)	0	100 100
13	e	27/65 (42%)	27 (100%)	0	100 100
14	f	12/72 (17%)	12 (100%)	0	100 100
15	g	37/119 (31%)	37 (100%)	0	100 100
15	h	26/119 (22%)	26 (100%)	0	100 100
15	i	58/119 (49%)	57 (98%)	1 (2%)	60 78
15	j	42/119 (35%)	42 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	k	36/119 (30%)	36 (100%)	0	100 100
15	l	39/119 (33%)	39 (100%)	0	100 100
15	m	40/119 (34%)	40 (100%)	0	100 100
15	n	28/119 (24%)	28 (100%)	0	100 100
16	o	44/125 (35%)	43 (98%)	1 (2%)	50 72
All	All	3663/7561 (48%)	3648 (100%)	15 (0%)	91 95

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	569	LYS
15	i	46	ARG
2	F	391	MET
16	o	52	LYS
5	M	48	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
13	e	29	ASN
15	h	82	GLN
5	M	55	GLN
5	M	183	ASN
9	a	381	HIS

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)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	ADP	E	701	-	24,29,29	0.98	1 (4%)	29,45,45	1.53	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	ADP	E	701	-	-	2/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	E	701	ADP	C5-C4	2.38	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	E	701	ADP	PA-O3A-PB	-4.79	116.39	132.83
17	E	701	ADP	N3-C2-N1	-2.90	124.14	128.68
17	E	701	ADP	C4-C5-N7	-2.73	106.56	109.40
17	E	701	ADP	C3'-C2'-C1'	2.59	104.88	100.98

There are no chirality outliers.

All (2) torsion outliers are listed below:

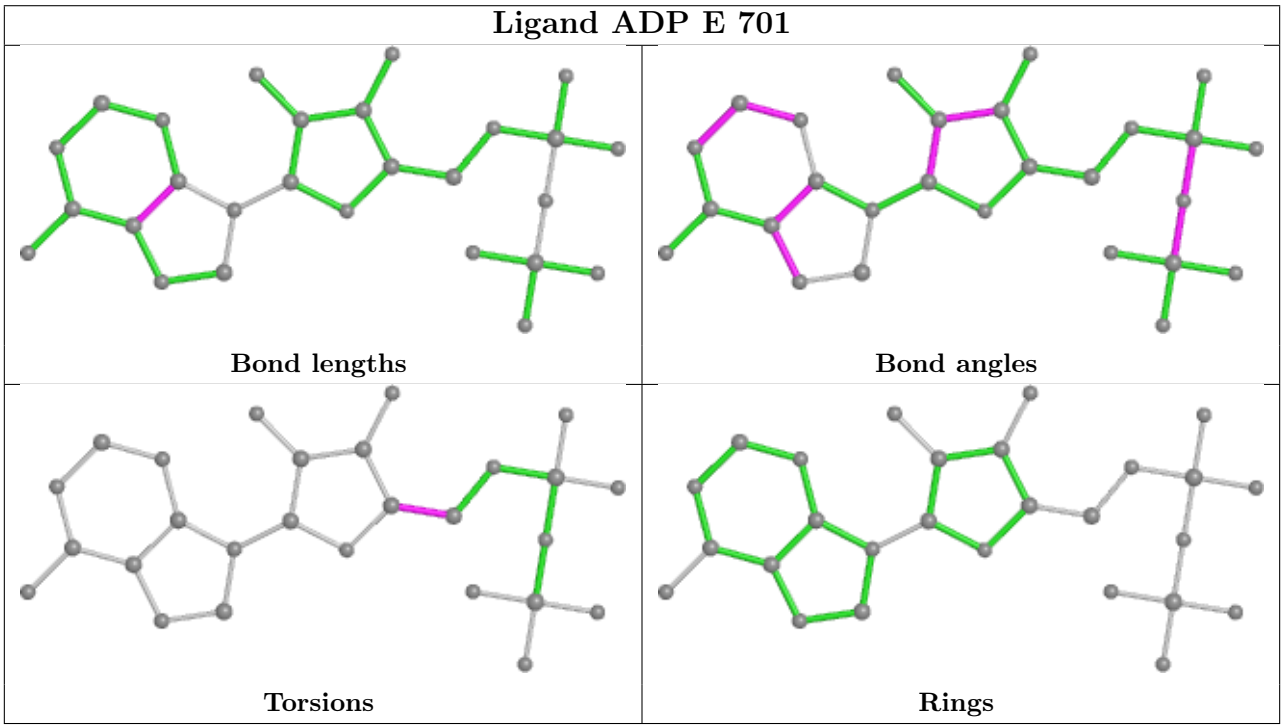
Mol	Chain	Res	Type	Atoms
17	E	701	ADP	O4'-C4'-C5'-O5'
17	E	701	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	E	701	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

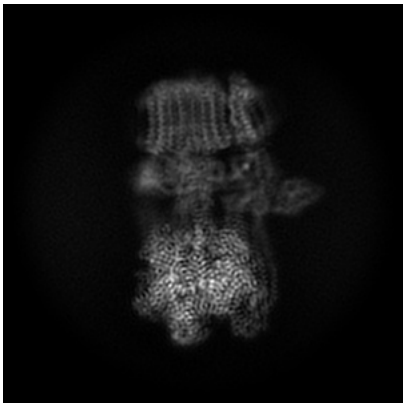
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26002. These allow visual inspection of the internal detail of the map and identification of artifacts.

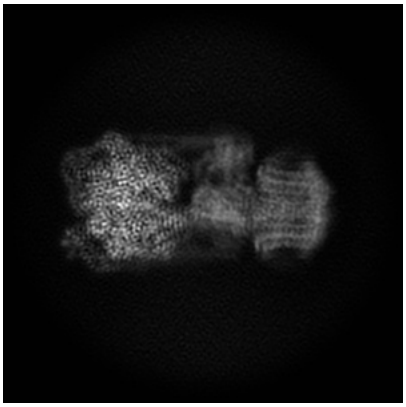
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

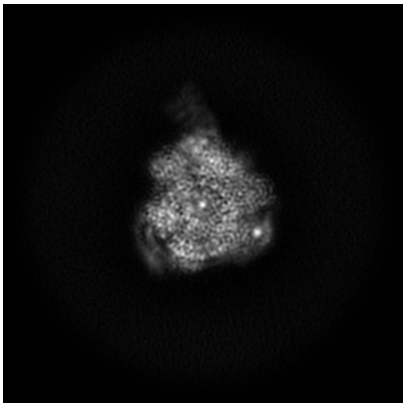
6.1.1 Primary map



X



Y



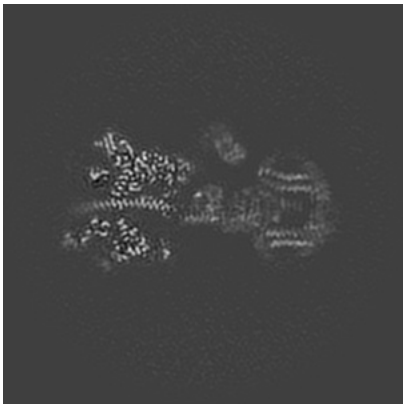
Z

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

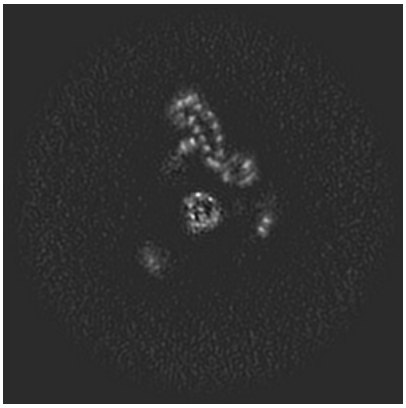
6.2 Central slices

6.2.1 Primary map

X Index: 150



Y Index: 150



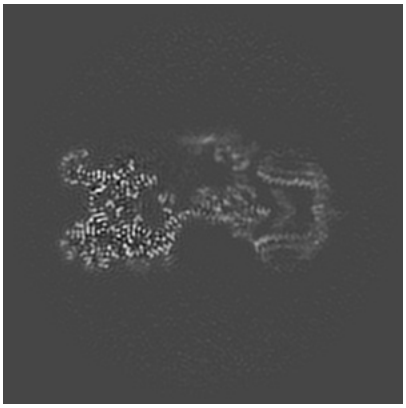
Z Index: 150

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

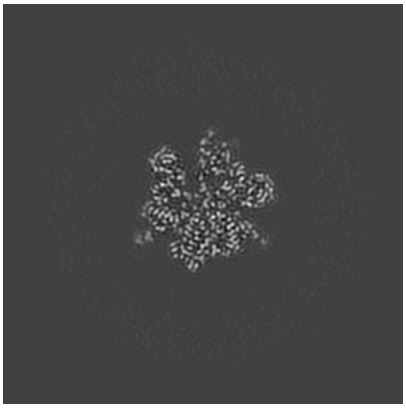
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 149



Y Index: 138

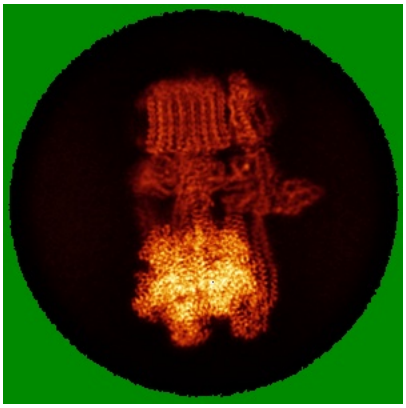


Z Index: 86

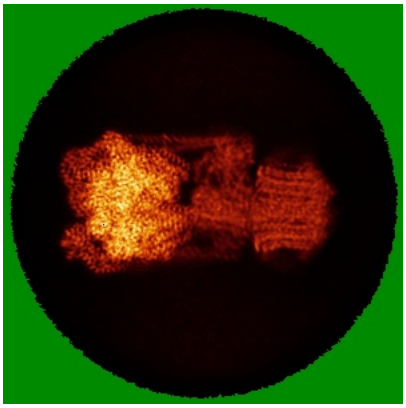
The images above show the largest variance slices of the map in three orthogonal directions.

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

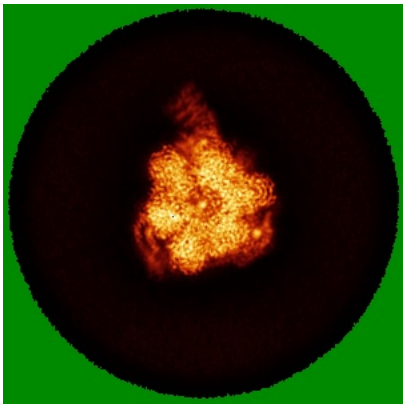
6.4.1 Primary map



X



Y



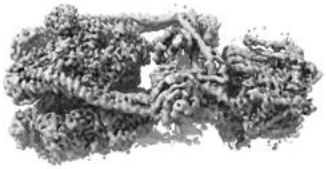
Z

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 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

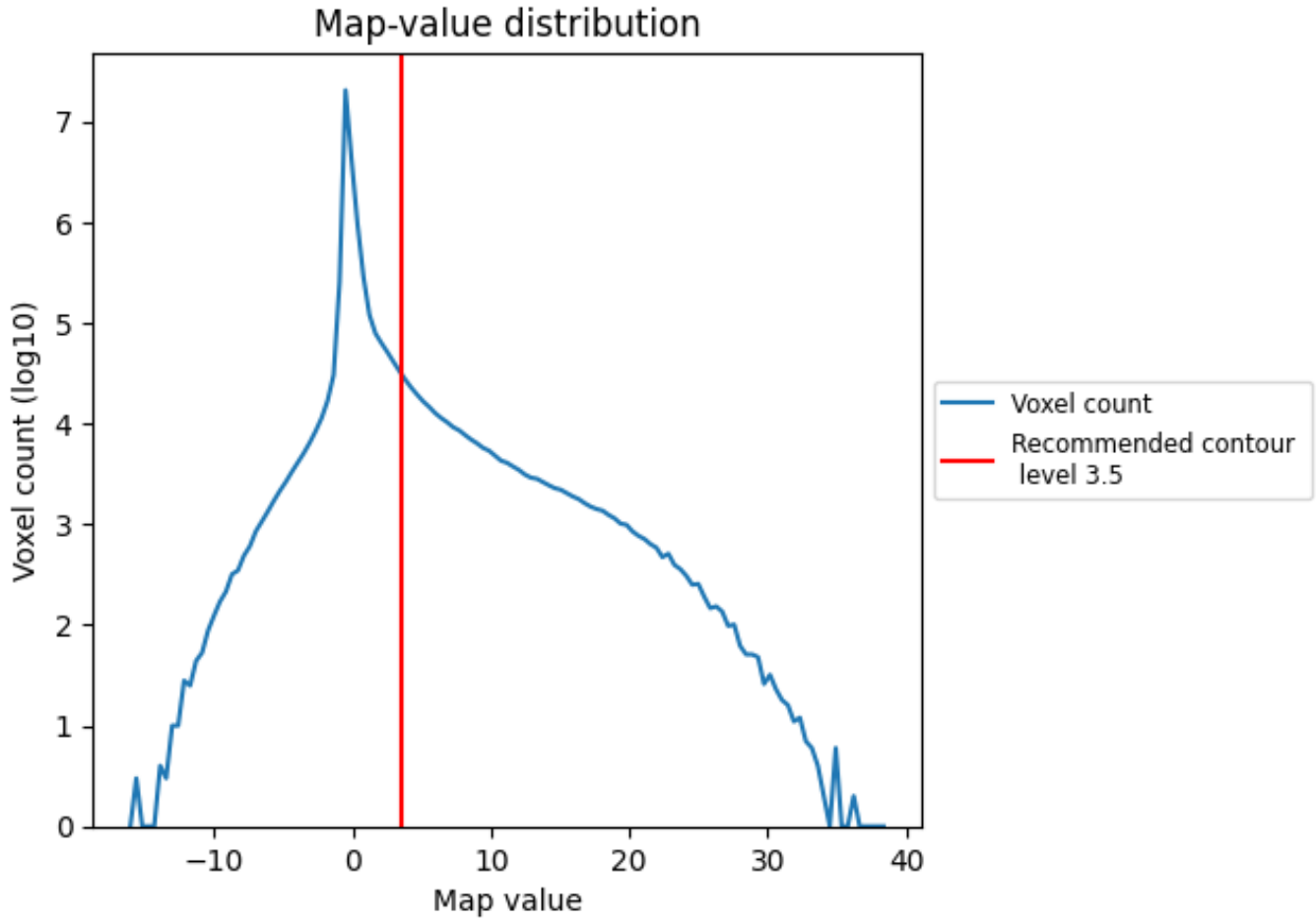
6.6 Mask visualisation (i)

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

7 Map analysis

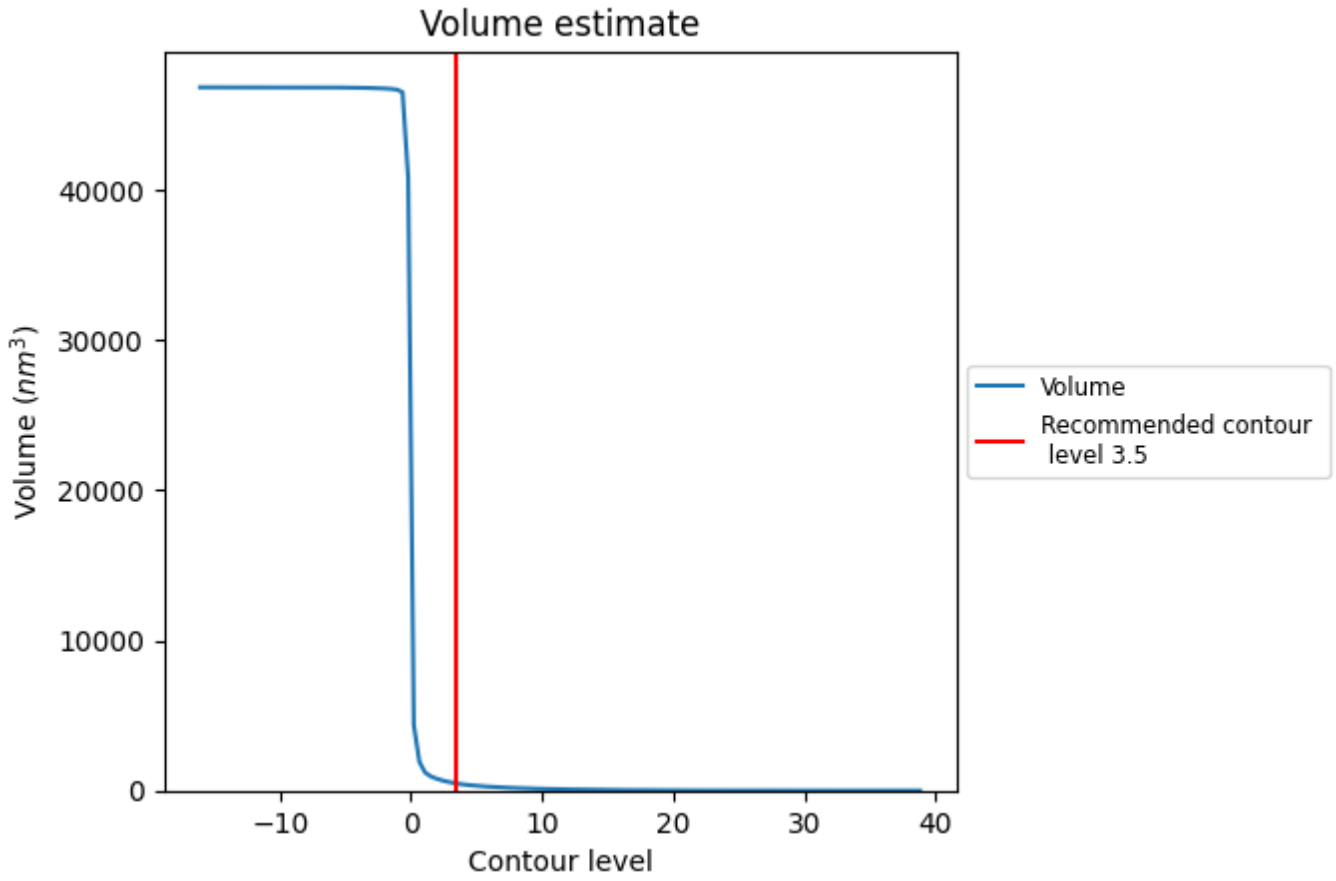
This section contains the results of statistical analysis of the map.

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.

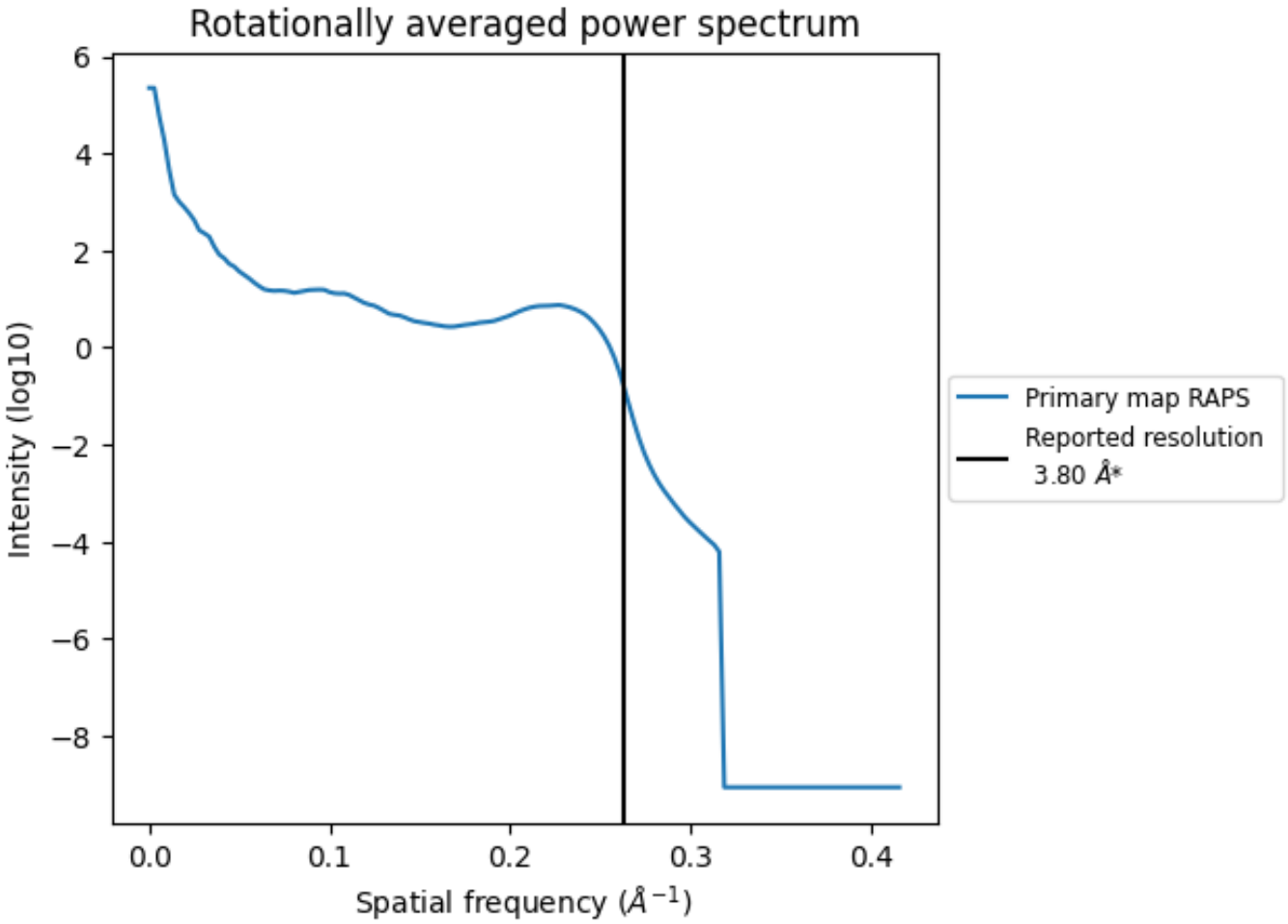
7.2 Volume estimate (i)



The volume at the recommended contour level is 470 nm^3; this corresponds to an approximate mass of 425 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 0.263 Å^{-1}

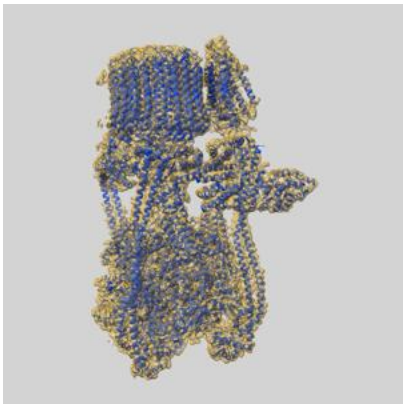
8 Fourier-Shell correlation (i)

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

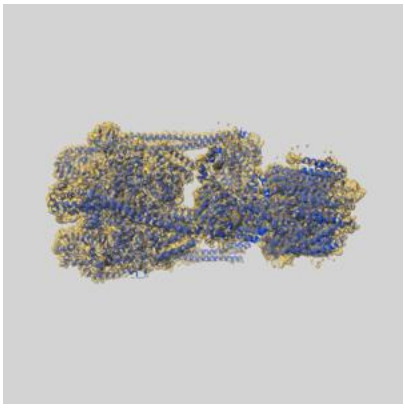
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26002 and PDB model 7TMT. Per-residue inclusion information can be found in section 3 on page 8.

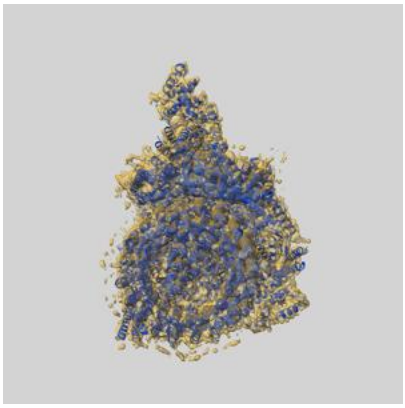
9.1 Map-model overlay



X



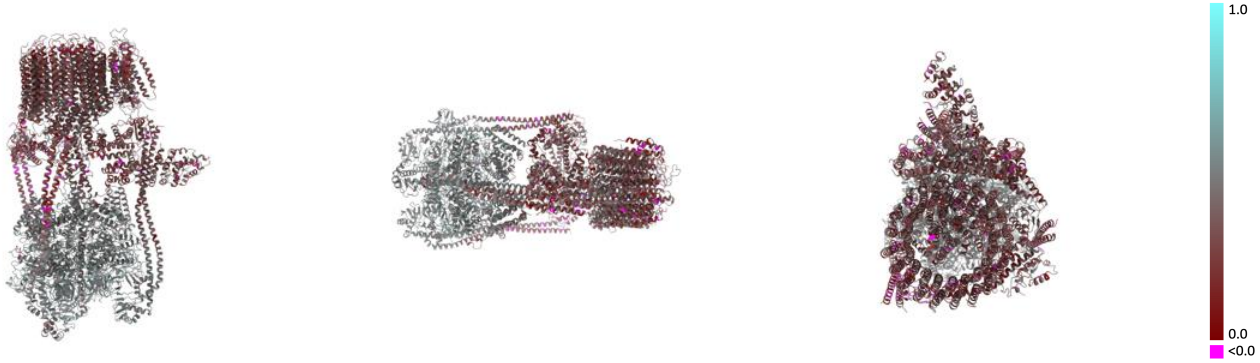
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

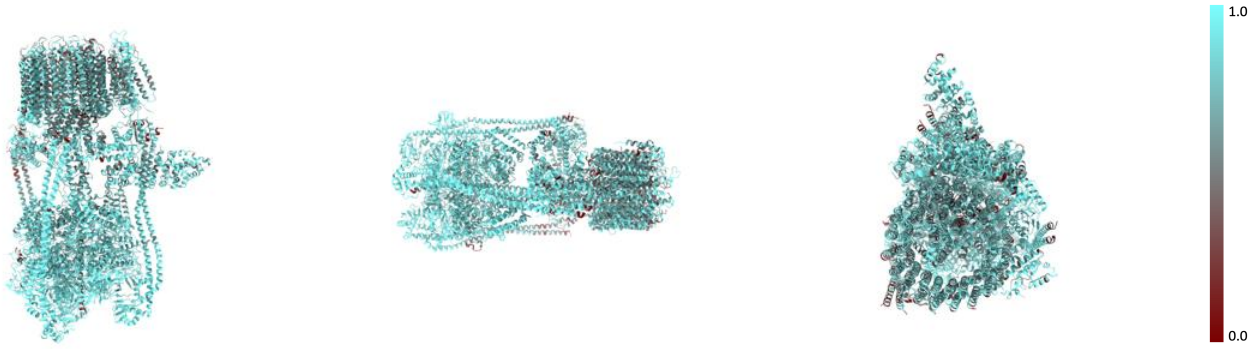
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

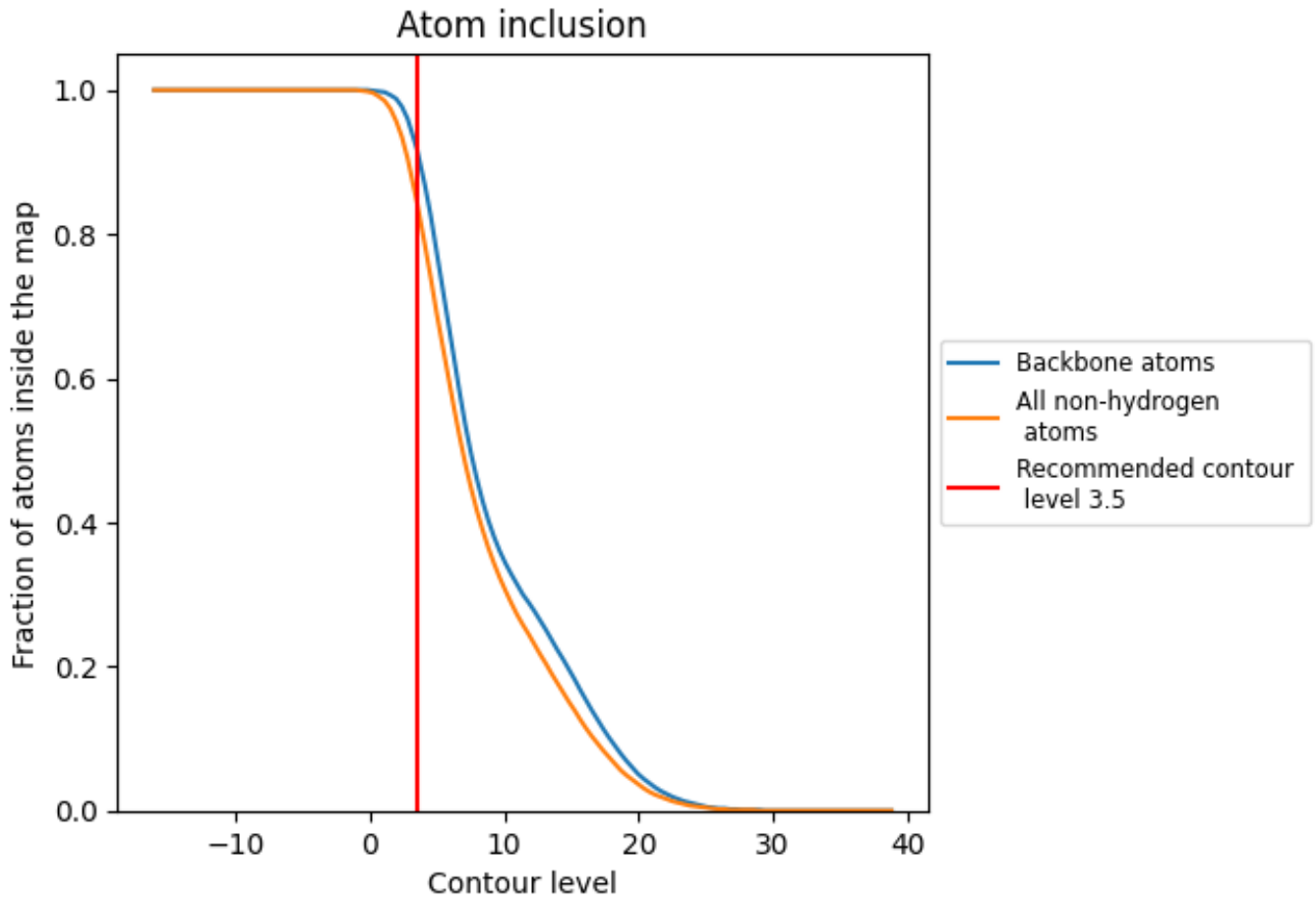
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.5).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 84% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8430	0.4080
A	0.8990	0.4880
B	0.9080	0.4980
C	0.9220	0.4990
D	0.9090	0.5000
E	0.9250	0.5000
F	0.9100	0.5000
G	0.8990	0.4070
H	0.7890	0.3350
I	0.9310	0.4340
J	0.8970	0.3590
K	0.9320	0.4460
L	0.9120	0.3760
M	0.8170	0.4100
N	0.8350	0.3410
O	0.7300	0.2760
P	0.8070	0.3100
a	0.8000	0.3360
b	0.4940	0.3420
c	0.7390	0.3000
d	0.6750	0.3270
e	0.7230	0.3500
f	0.7400	0.2540
g	0.7100	0.2890
h	0.7240	0.2830
i	0.7010	0.2780
j	0.7430	0.2960
k	0.7770	0.2980
l	0.7950	0.3150
m	0.7370	0.2730
n	0.7530	0.2840
o	0.7340	0.2910