



## wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 06:09 PM UTC

PDB ID : 7TMT / pdb\_00007tmt  
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](mailto: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>.

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

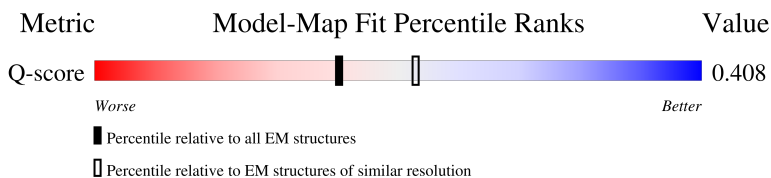
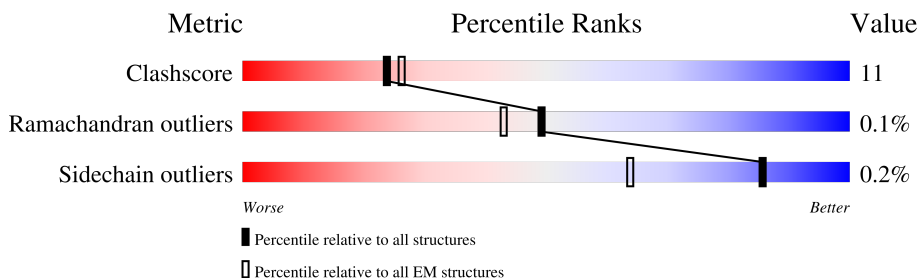
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 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.








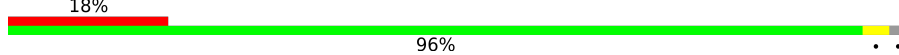
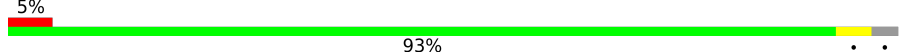
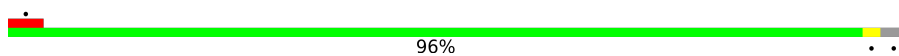




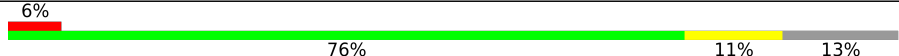
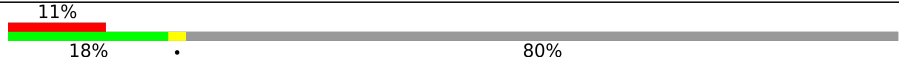
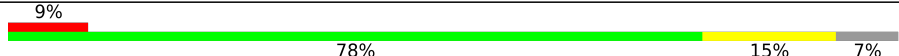

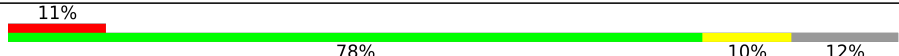
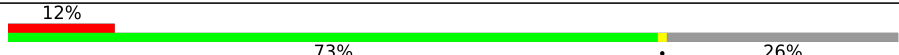
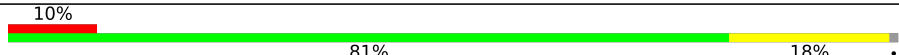
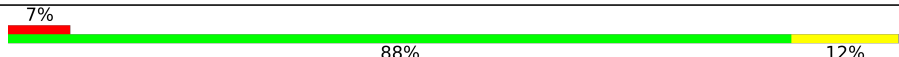
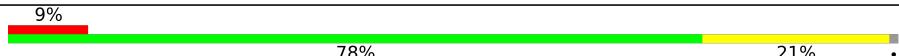



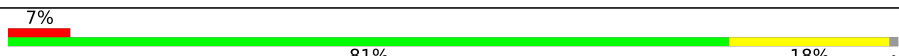
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 ( 3.30 - 4.30 )

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  $\geq 3$ , 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	A	617	73% 23% .
1	C	617	70% 26% ..
1	E	617	69% 26% .
2	B	517	64% 28% 8%

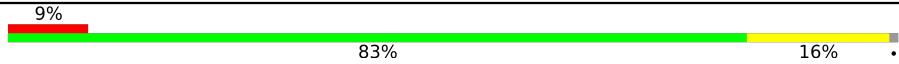

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Mol	Chain	Length	Quality of chain
2	D	517	
2	F	517	
3	G	233	
3	I	233	
3	K	233	
4	H	114	
4	J	114	
4	L	114	
5	M	256	
6	N	118	
7	O	392	
8	P	478	
9	a	840	
10	b	265	
11	c	213	
12	d	345	
13	e	73	
14	f	85	
15	g	160	
15	h	160	
15	i	160	
15	j	160	
15	k	160	
15	l	160	
15	m	160	

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Mol	Chain	Length	Quality of chain
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
			Total	C	N	O	S		
1	A	593	Total 4545	C 2888	N 756	O 881	S 20	0	0
1	C	593	Total 4541	C 2885	N 757	O 879	S 20	0	0
1	E	593	Total 4578	C 2904	N 760	O 894	S 20	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	d	343	2209	1404	402	401	2	0	0

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

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

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

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

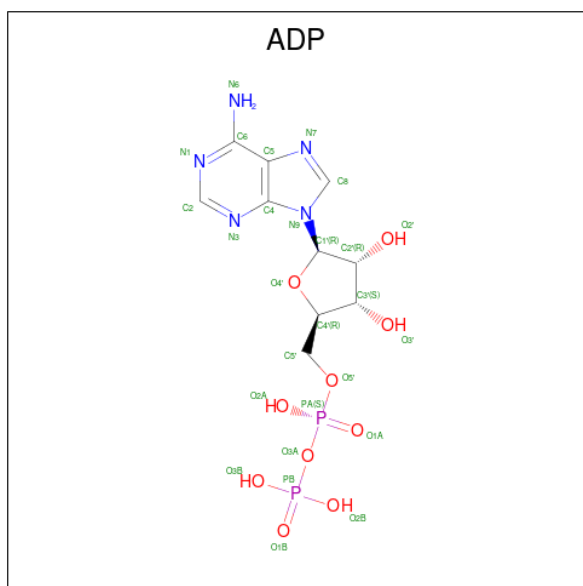
- Molecule 15 is a protein called V-type proton ATPase subunit c.

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

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

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

- Molecule 17 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

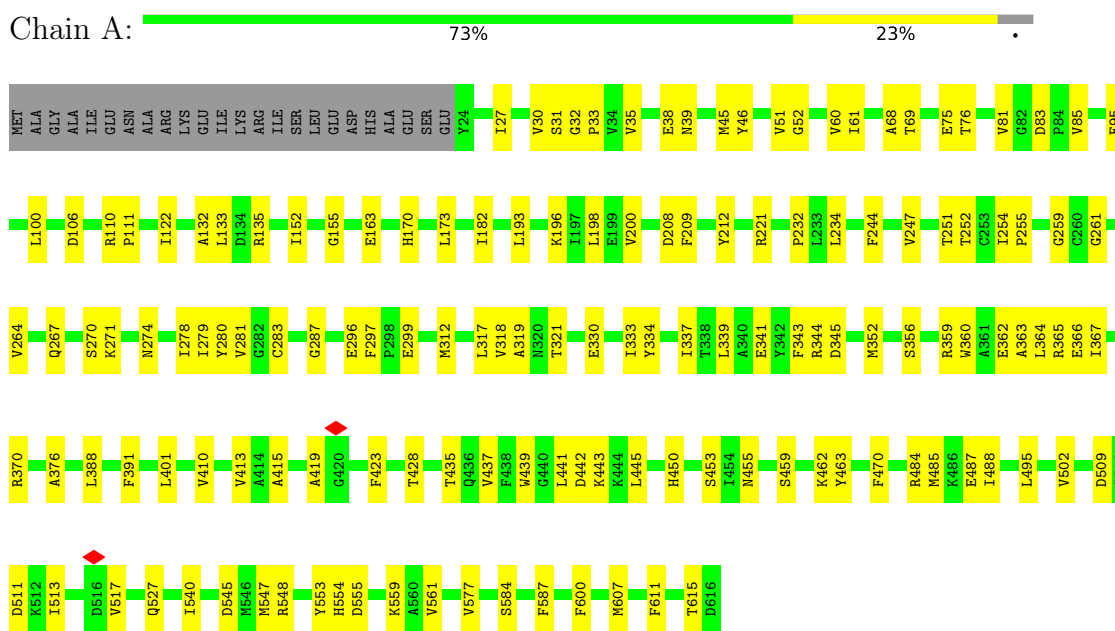


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
17	E	1	27	10	5	10	2	0

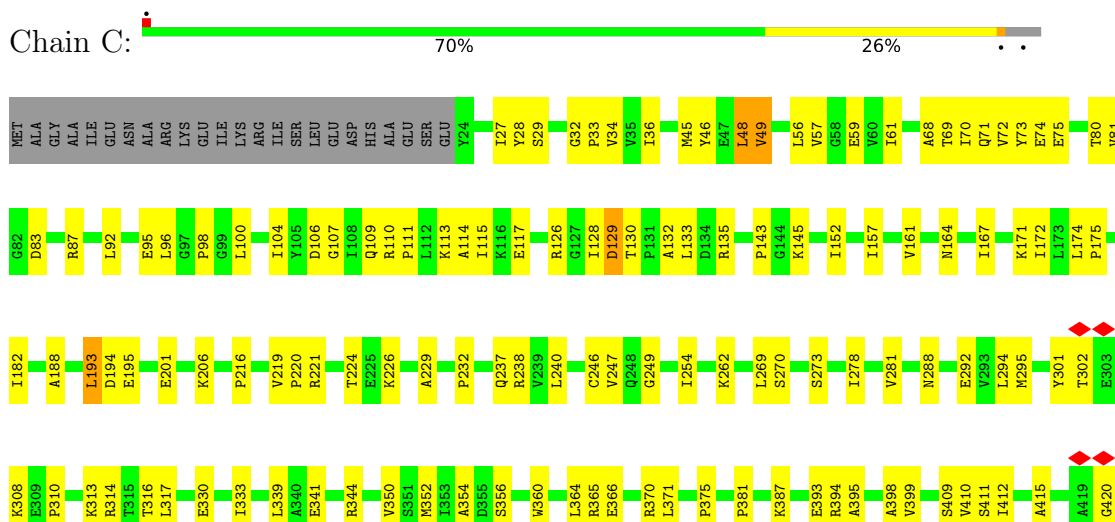
### 3 Residue-property plots

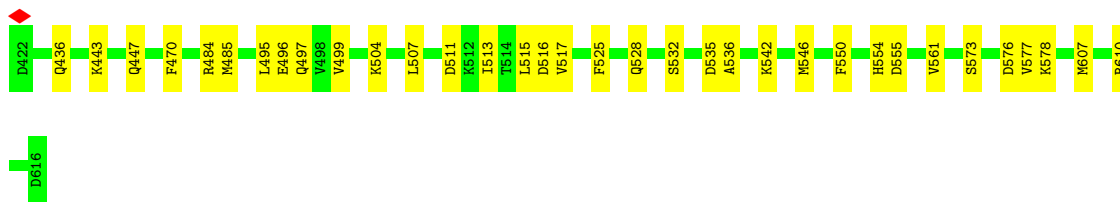
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

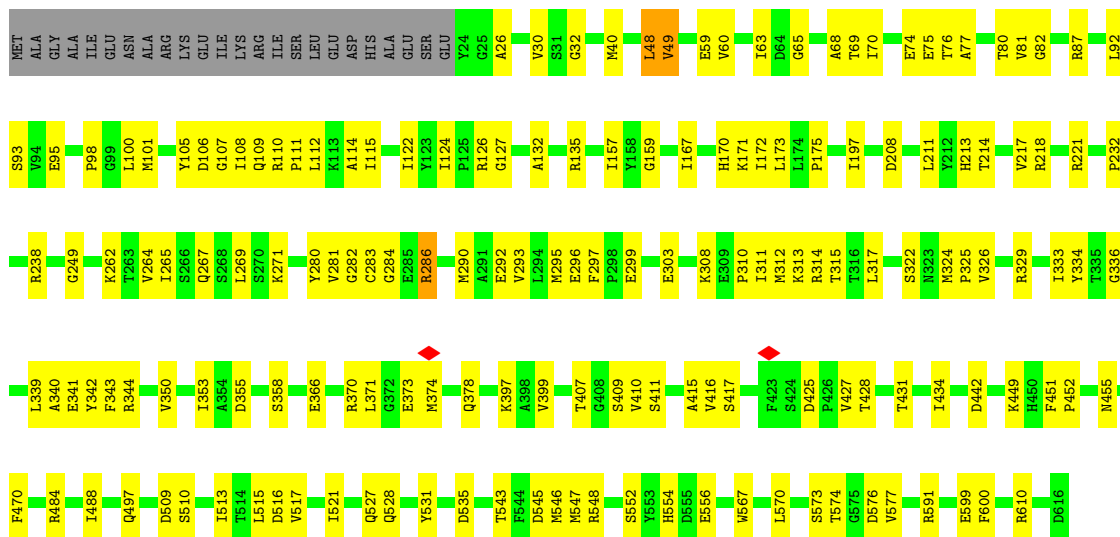


- Molecule 1: H(+)-transporting two-sector ATPase

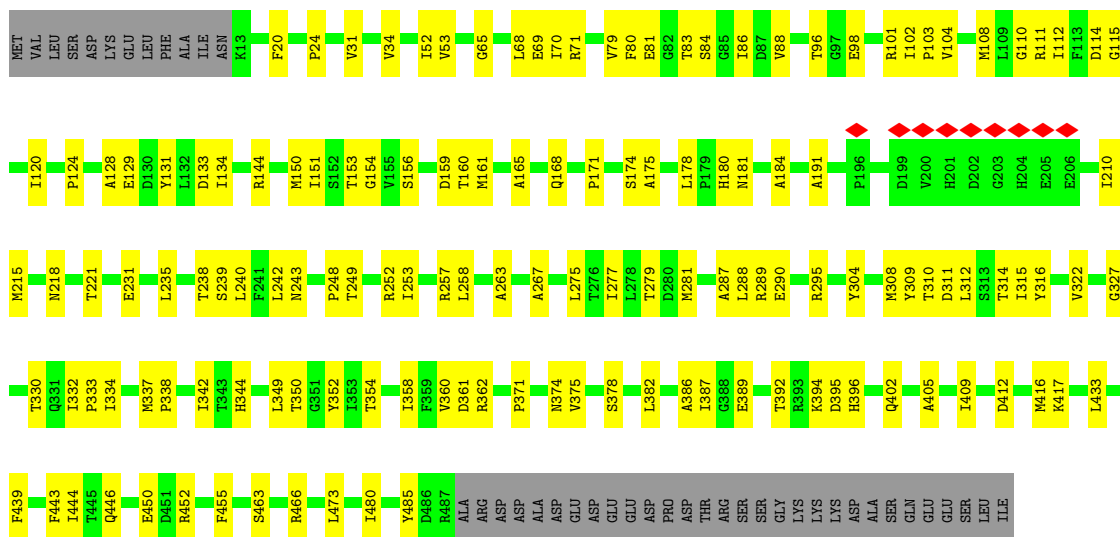




• Molecule 1: H(+)-transporting two-sector ATPase



• Molecule 2: Vacuolar proton pump subunit B



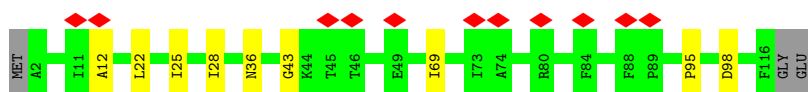
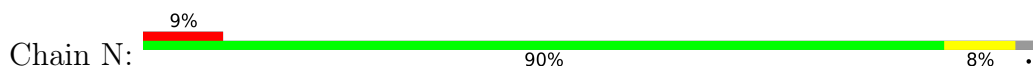
• Molecule 2: Vacuolar proton pump subunit B



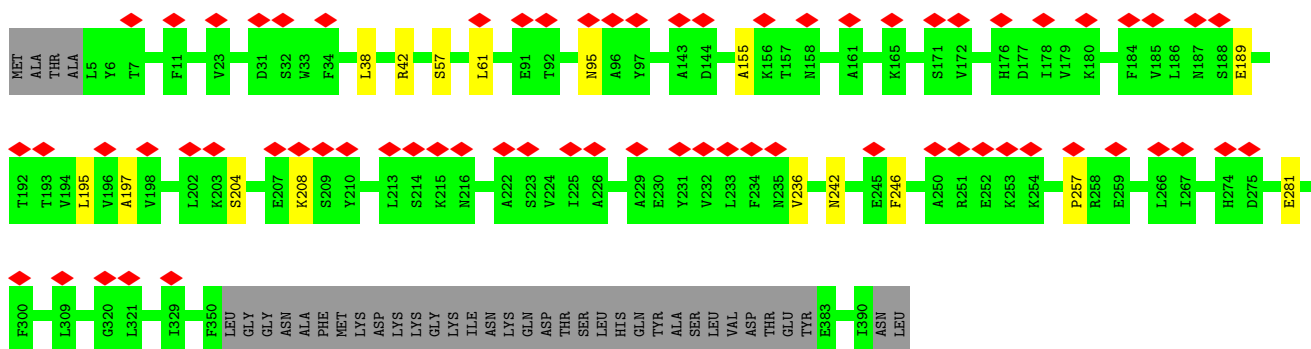
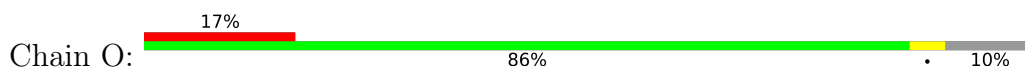




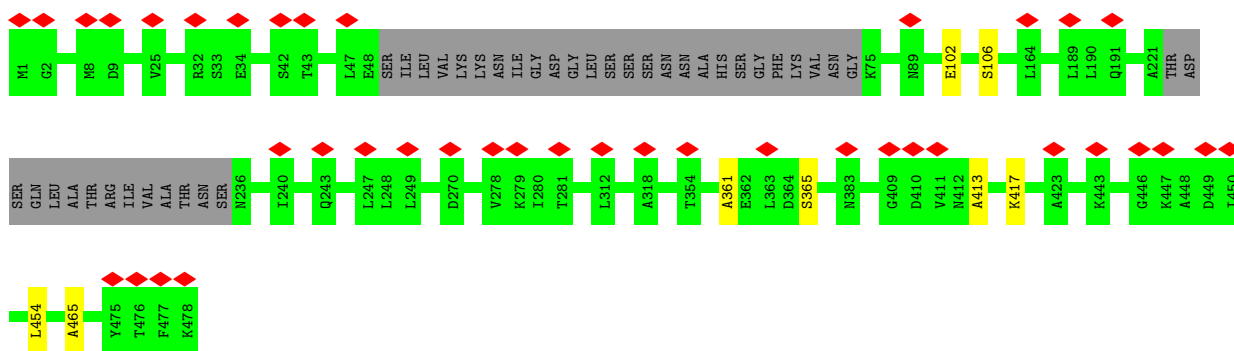
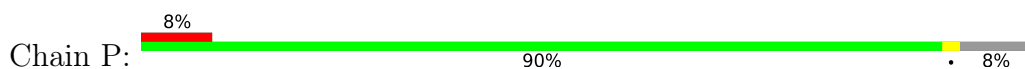
• Molecule 6: V-type proton ATPase subunit F



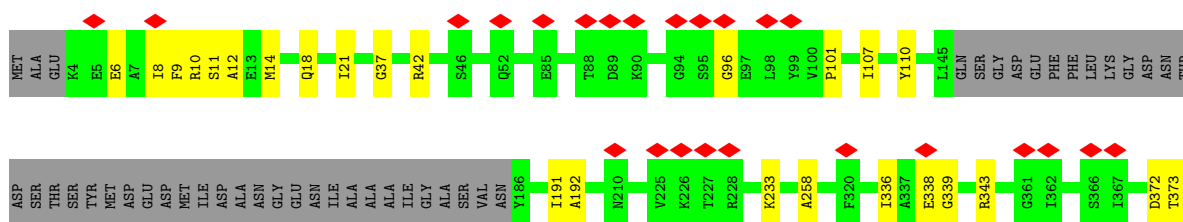
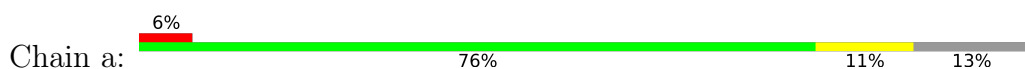
• Molecule 7: V-type proton ATPase subunit C



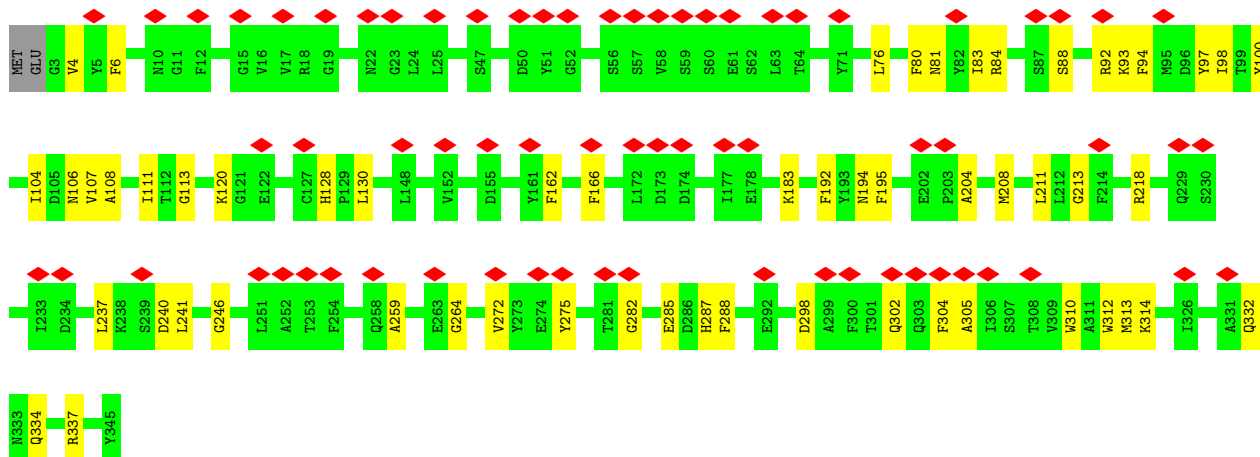
• Molecule 8: V-type proton ATPase subunit H



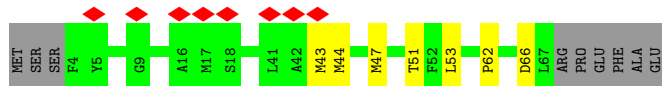
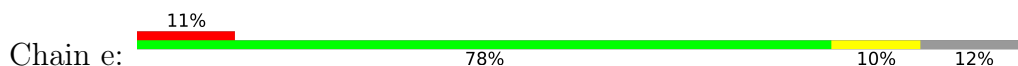
• Molecule 9: V-type proton ATPase subunit a, vacuolar isoform



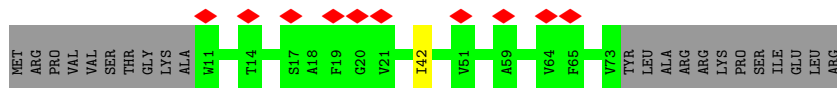




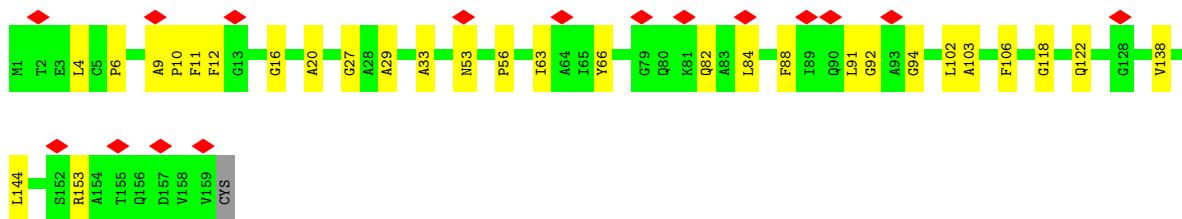
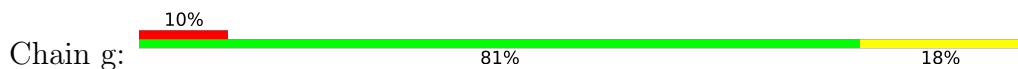
• Molecule 13: V-type proton ATPase subunit e



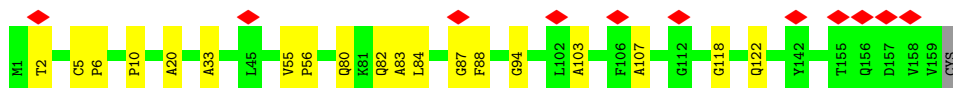
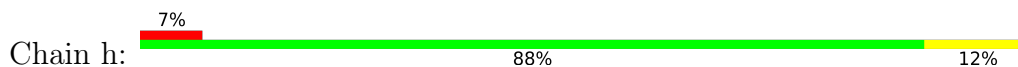
• Molecule 14: Yeast V-ATPase subunit f



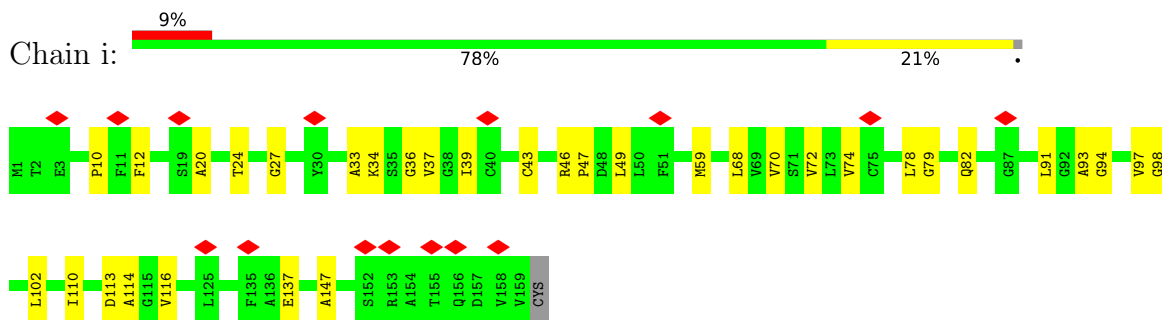
• Molecule 15: V-type proton ATPase subunit c



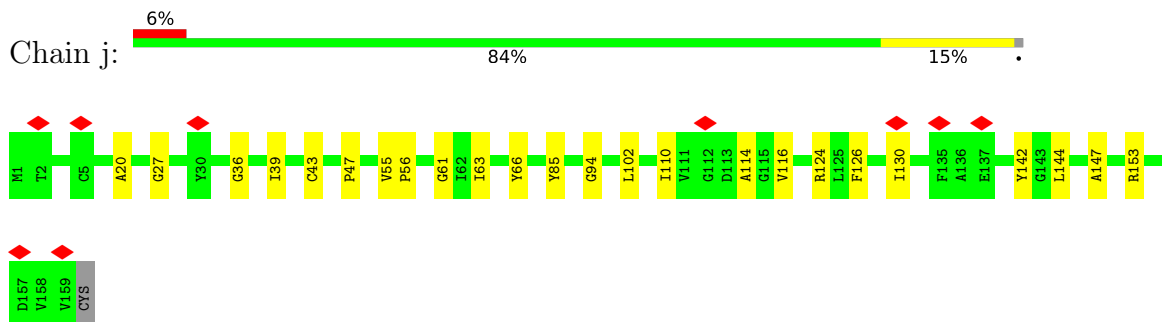
• Molecule 15: V-type proton ATPase subunit c



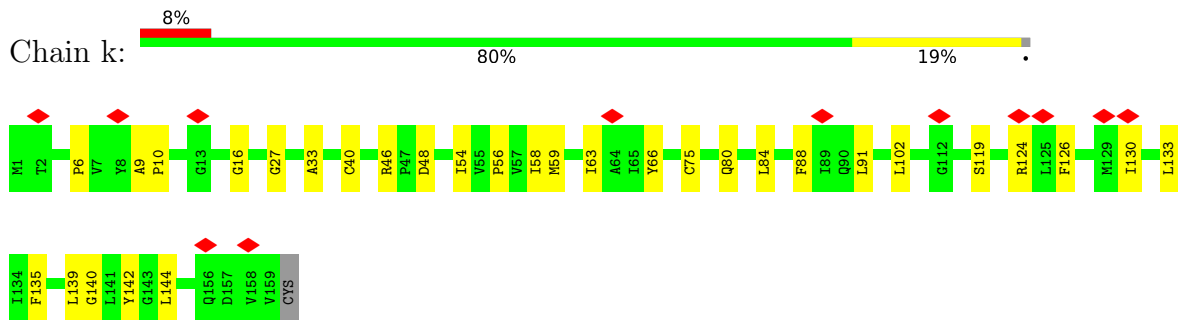
• Molecule 15: V-type proton ATPase subunit c



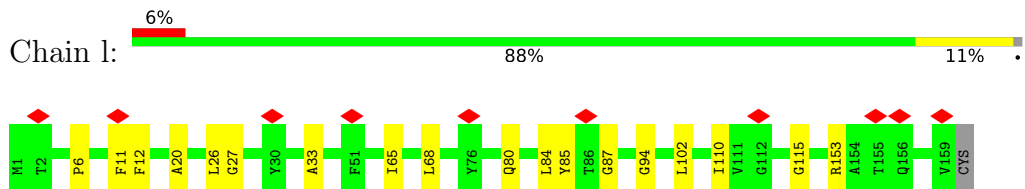
- Molecule 15: V-type proton ATPase subunit c



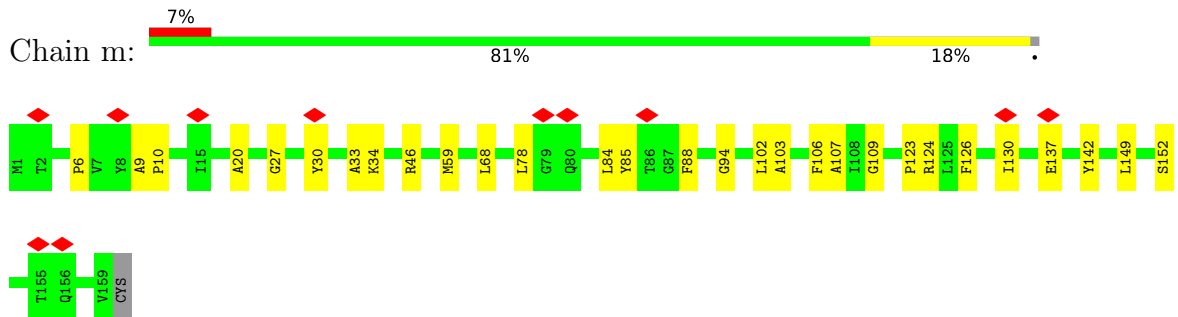
- Molecule 15: V-type proton ATPase subunit c



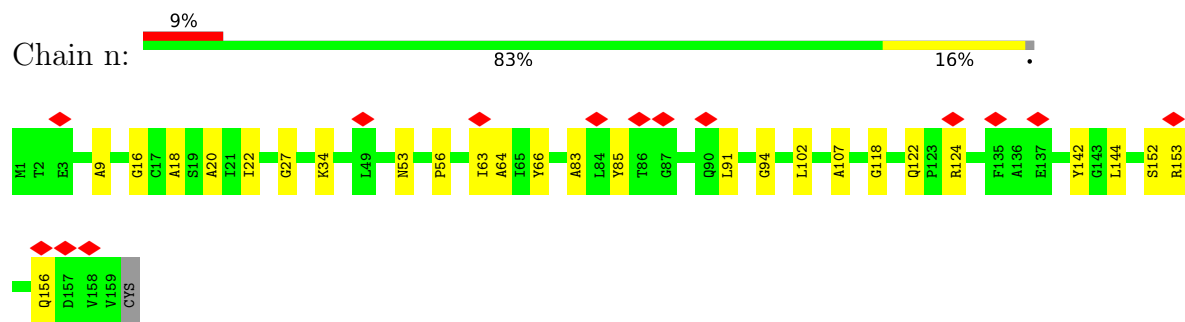
- Molecule 15: V-type proton ATPase subunit c



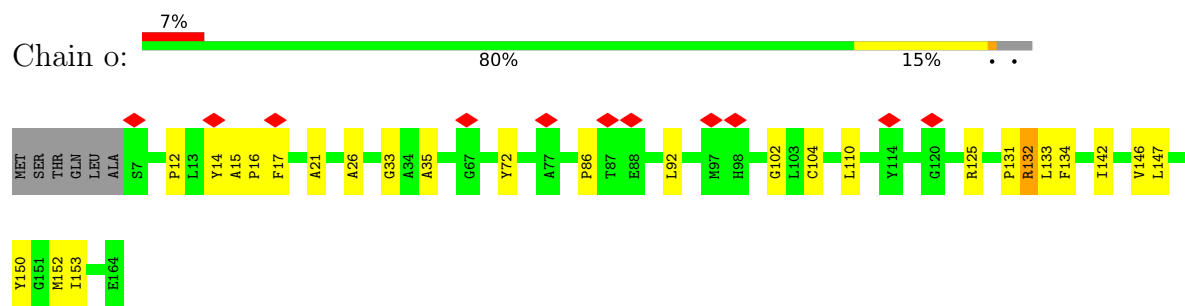
- Molecule 15: V-type proton ATPase subunit c



- Molecule 15: V-type proton ATPase subunit c



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



## 4 Experimental information

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 ( $e^-/\text{\AA}^2$ )	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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.27	0/4644	0.38	0/6299
1	C	0.30	0/4640	0.42	1/6292 (0.0%)
1	E	0.31	0/4677	0.40	0/6339
2	B	0.31	0/3758	0.41	0/5097
2	D	0.31	0/3760	0.46	1/5099 (0.0%)
2	F	0.32	0/3782	0.44	0/5129
3	G	0.16	0/1211	0.25	0/1682
3	I	0.18	0/1333	0.34	0/1828
3	K	0.17	0/1343	0.33	0/1840
4	H	0.14	0/588	0.28	0/810
4	J	0.14	0/584	0.28	0/804
4	L	0.14	0/595	0.25	0/817
5	M	0.23	0/1455	0.45	1/1975 (0.1%)
6	N	0.15	0/585	0.37	0/819
7	O	0.12	0/1806	0.34	2/2532 (0.1%)
8	P	0.09	0/2203	0.25	0/3078
9	a	0.15	0/4415	0.35	0/6114
10	b	0.11	0/321	0.24	0/445
11	c	0.16	0/1188	0.37	0/1632
12	d	0.16	0/2258	0.39	0/3106
13	e	0.15	0/440	0.35	0/607
14	f	0.10	0/365	0.23	0/504
15	g	0.18	0/924	0.40	0/1268
15	h	0.16	0/883	0.33	0/1216
15	i	0.18	0/970	0.40	0/1331
15	j	0.15	0/940	0.30	0/1290
15	k	0.19	0/913	0.37	0/1251
15	l	0.14	0/936	0.30	0/1281
15	m	0.17	0/947	0.36	0/1294
15	n	0.15	0/881	0.31	0/1211
16	o	0.16	0/947	0.36	0/1297
All	All	0.24	0/54292	0.38	5/74287 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	375	VAL	N-CA-C	8.70	118.78	110.42
1	C	129	ASP	N-CA-C	7.04	118.95	111.28
5	M	214	THR	N-CA-C	-6.10	104.71	111.36
7	O	95	ASN	CB-CA-C	-5.09	110.31	117.23
7	O	189	GLU	CB-CA-C	-5.05	110.73	116.54

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	108	0
1	C	4541	0	4448	122	0
1	E	4578	0	4519	126	0
2	B	3688	0	3644	109	0
2	D	3690	0	3637	124	0
2	F	3712	0	3651	118	0
3	G	1202	0	704	10	0
3	I	1324	0	984	25	0
3	K	1332	0	954	11	0
4	H	587	0	349	2	0
4	J	584	0	357	5	0
4	L	594	0	368	2	0
5	M	1444	0	1152	36	0
6	N	581	0	285	5	0
7	O	1792	0	877	7	0
8	P	2197	0	993	4	0
9	a	4317	0	2662	72	0
10	b	315	0	207	2	0
11	c	1165	0	783	24	0
12	d	2209	0	1559	49	0
13	e	428	0	335	8	0
14	f	358	0	211	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	g	911	0	658	27	0
15	h	872	0	570	15	0
15	i	957	0	798	30	0
15	j	926	0	679	20	0
15	k	902	0	631	27	0
15	l	922	0	676	18	0
15	m	932	0	685	24	0
15	n	871	0	582	19	0
16	o	930	0	678	22	0
17	E	27	0	12	2	0
All	All	53433	0	43122	1055	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 11.

The worst 5 of 1055 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:553:TYR:HA	1:A:607:MET:HE1	1.53	0.91
5:M:55:GLN:HE22	5:M:56:LYS:HE3	1.37	0.90
1:E:101:MET:HE3	1:E:167:ILE:HG13	1.56	0.84
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

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	567/617 (92%)	533 (94%)	34 (6%)	0	100	100
1	E	591/617 (96%)	558 (94%)	33 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	296/517 (57%)	265 (90%)	31 (10%)	0	100	100
2	D	281/517 (54%)	267 (95%)	14 (5%)	0	100	100
2	F	476/517 (92%)	434 (91%)	41 (9%)	1 (0%)	43	73
3	G	219/233 (94%)	215 (98%)	4 (2%)	0	100	100
3	I	219/233 (94%)	212 (97%)	7 (3%)	0	100	100
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%)	24	57
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%)	36	67
10	b	50/265 (19%)	48 (96%)	1 (2%)	1 (2%)	6	32
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%)	9	38
All	All	7165/8335 (86%)	6836 (95%)	322 (4%)	7 (0%)	49	79

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	a	403	ARG
9	a	405	ILE
10	b	218	ILE
5	M	219	ALA
16	o	133	LEU

### 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%)	78	79
1	E	497/516 (96%)	494 (99%)	3 (1%)	78	79
2	B	394/444 (89%)	394 (100%)	0	100	100
2	D	394/444 (89%)	394 (100%)	0	100	100
2	F	239/444 (54%)	239 (100%)	0	100	100
3	G	27/208 (13%)	27 (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%)	9 (100%)	0	100	100
4	J	10/94 (11%)	10 (100%)	0	100	100
4	L	12/94 (13%)	12 (100%)	0	100	100
5	M	91/221 (41%)	90 (99%)	1 (1%)	65	73
7	O	9/348 (3%)	9 (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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	58 (100%)	0	100	100
15	j	42/119 (35%)	42 (100%)	0	100	100
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%)	44 (100%)	0	100	100
All	All	3492/7457 (47%)	3485 (100%)	7 (0%)	85	87

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	48	LEU
1	E	49	VAL
5	M	216	LYS
1	E	286	ARG
1	C	193	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
15	i	82	GLN
15	k	80	GLN
2	D	232	ASN
1	C	554	HIS
15	l	80	GLN

### 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 oligosaccharides 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	-	28,29,29	1.39	4 (14%)	43,45,45	1.81	8 (18%)

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	-	-	2/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	E	701	ADP	C5-C4	4.56	1.47	1.39
17	E	701	ADP	C5-C6	2.61	1.48	1.41
17	E	701	ADP	C5-N7	-2.35	1.34	1.39
17	E	701	ADP	C8-N7	2.31	1.36	1.31

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	E	701	ADP	C5-C4-N3	-6.09	118.33	126.72
17	E	701	ADP	N3-C4-N9	4.66	135.10	127.17
17	E	701	ADP	C2-N3-C4	3.70	120.87	111.83
17	E	701	ADP	C4-C5-N7	-3.52	106.56	110.58
17	E	701	ADP	N3-C2-N1	-2.94	124.14	128.58

There are no chirality outliers.

All (2) torsion outliers are listed below:

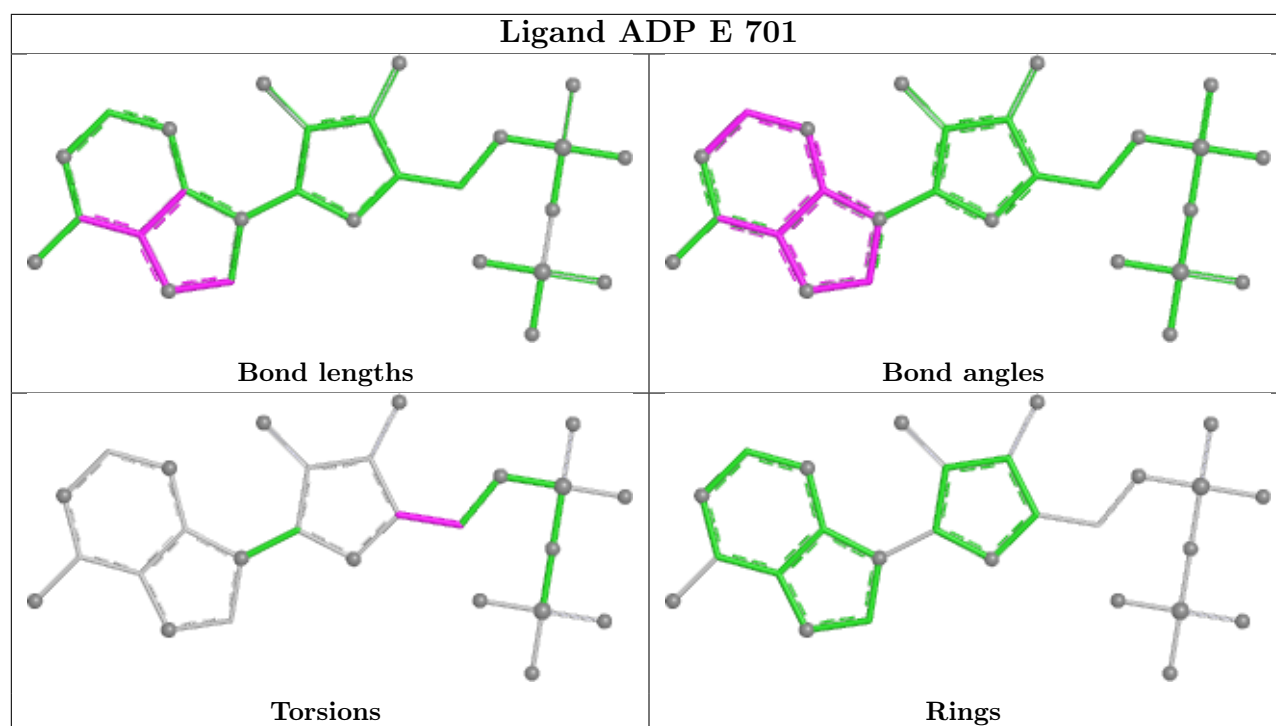
Mol	Chain	Res	Type	Atoms
17	E	701	ADP	C3'-C4'-C5'-O5'
17	E	701	ADP	O4'-C4'-C5'-O5'

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 than 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.

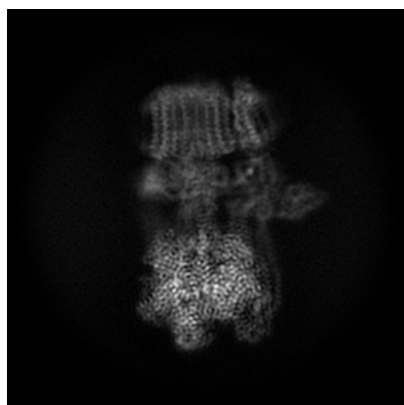
## 6 Map visualisation [i](#)

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.

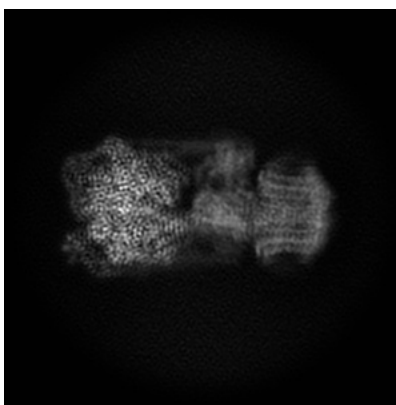
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

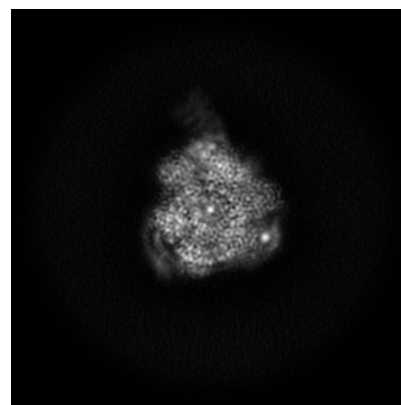
#### 6.1.1 Primary map



X



Y

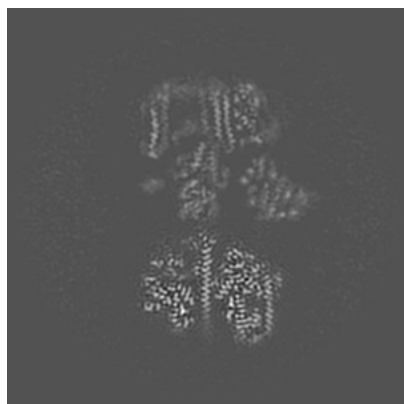


Z

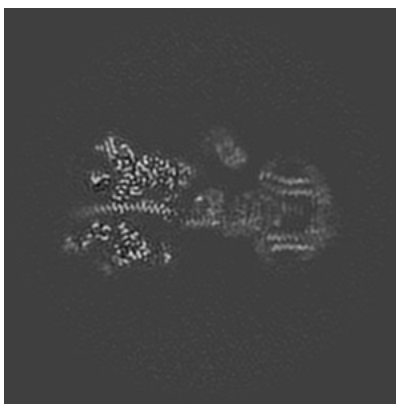
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

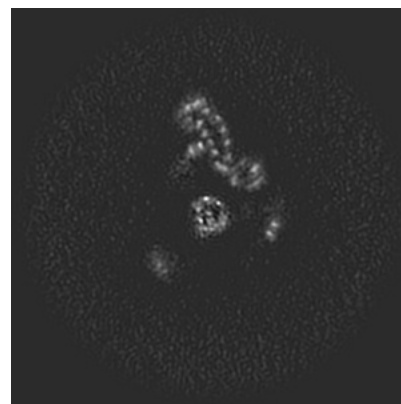
#### 6.2.1 Primary map



X Index: 150



Y Index: 150



Z Index: 150

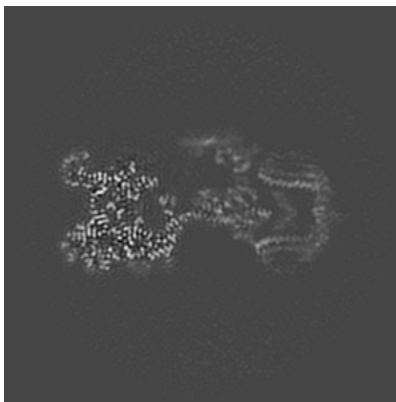
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [\(i\)](#)

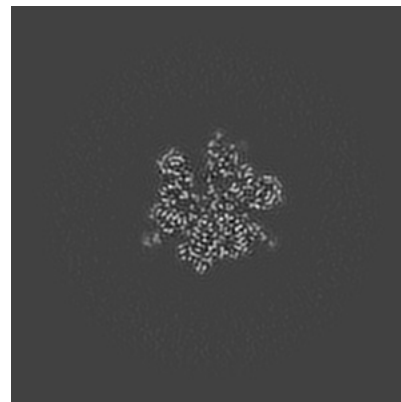
### 6.3.1 Primary map



X Index: 149



Y Index: 138

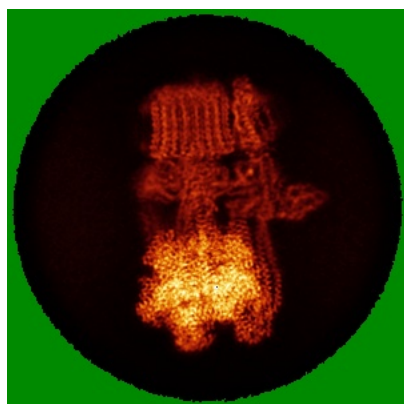


Z Index: 86

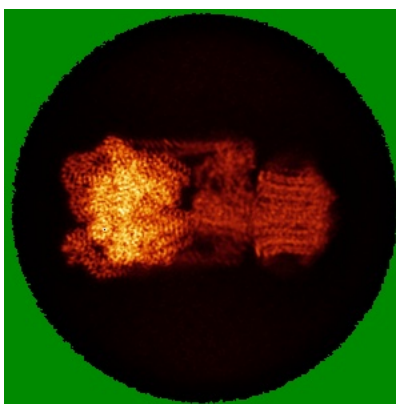
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [\(i\)](#)

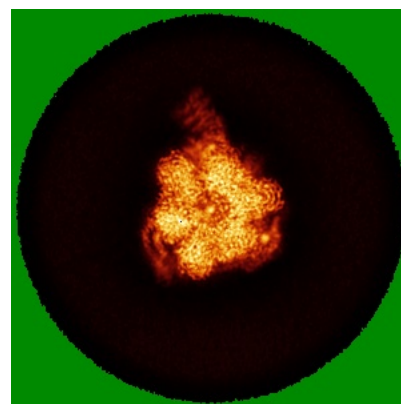
### 6.4.1 Primary map



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

This section was not generated.

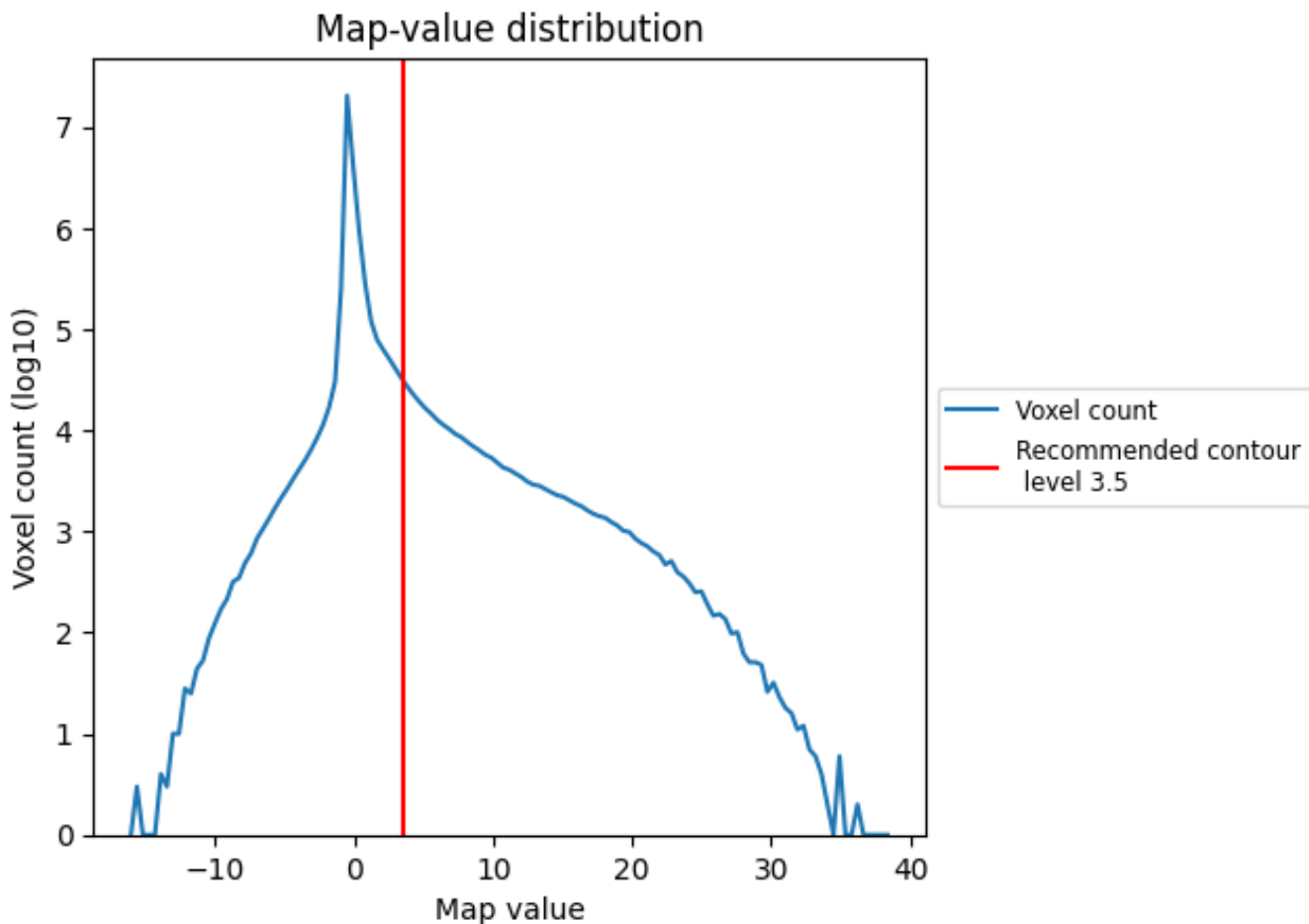
## 6.6 Mask visualisation

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

## 7 Map analysis [i](#)

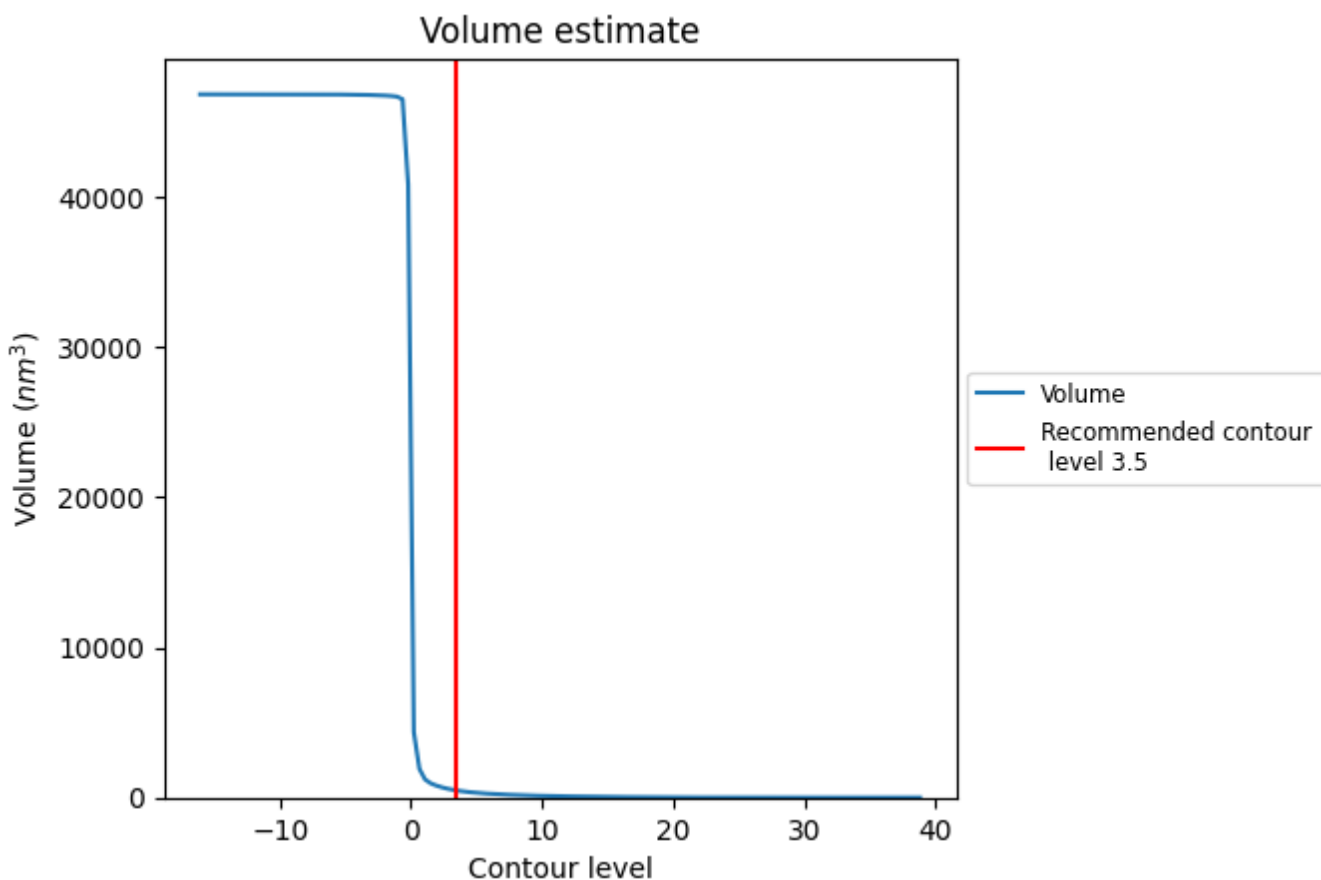
This section contains the results of statistical analysis of the map.

### 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.

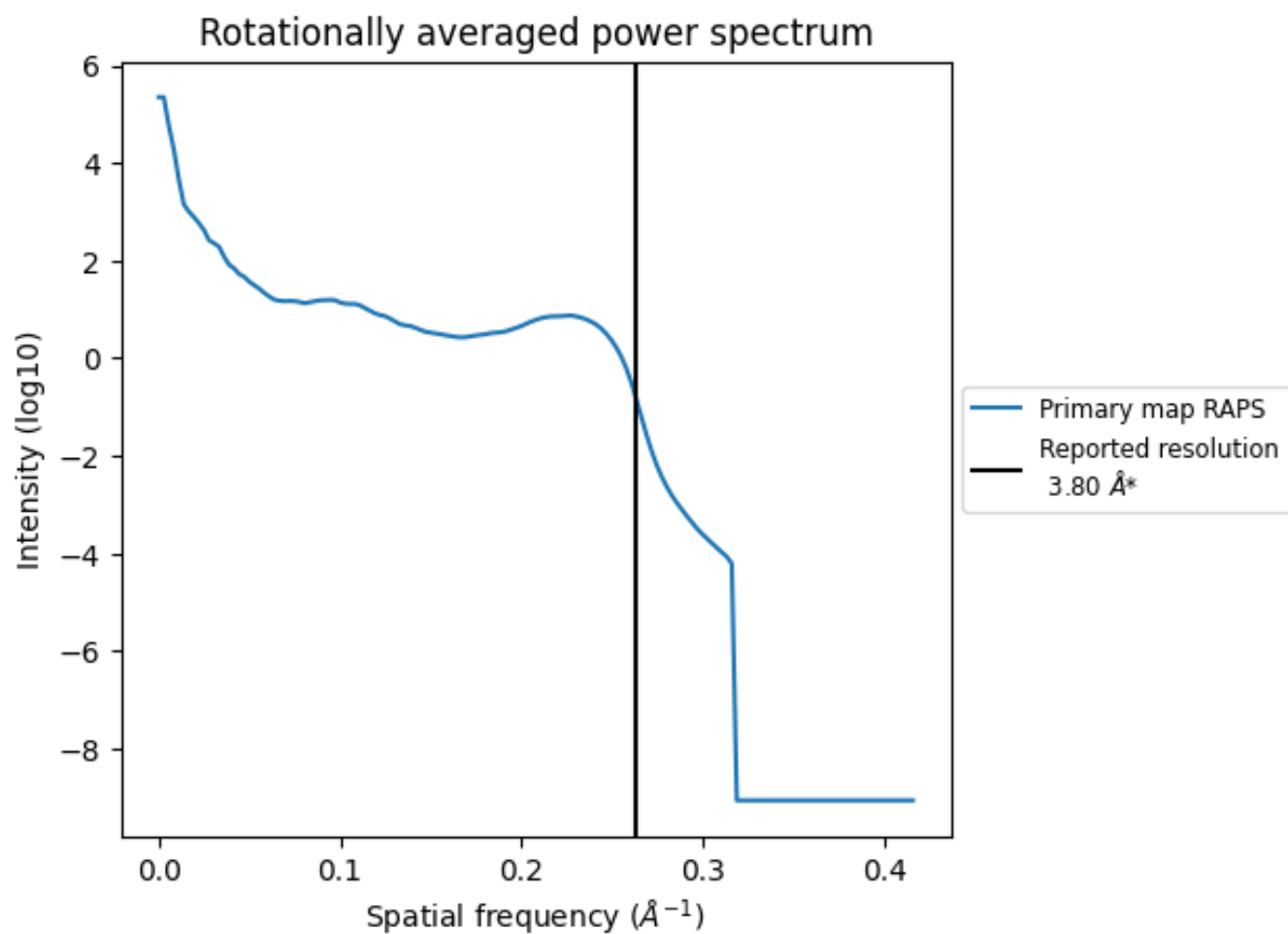
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 470  $\text{nm}^3$ ; 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<sup>-1</sup>

## 8 Fourier-Shell correlation

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

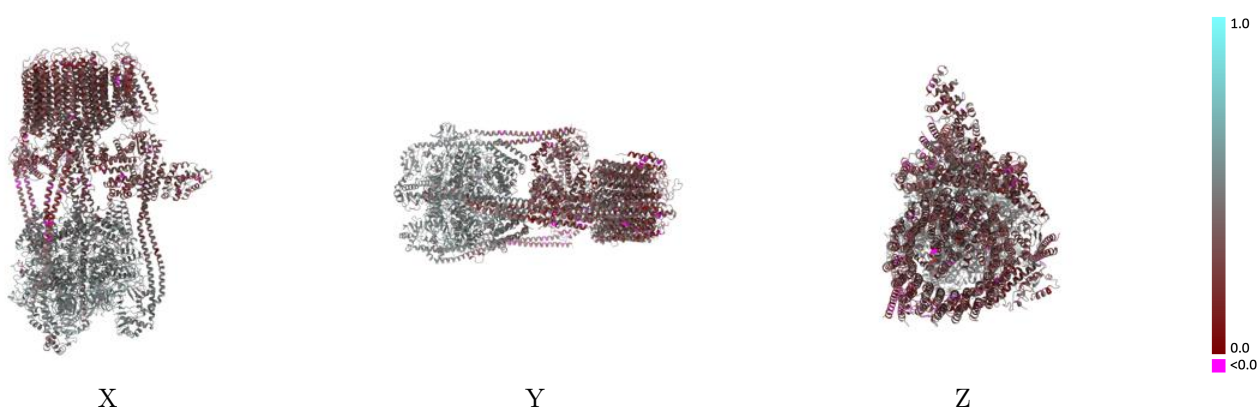
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26002 and PDB model 7TMT. Per-residue inclusion information can be found in section 3 on page 9.

### 9.1 Map-model overlay [i](#)

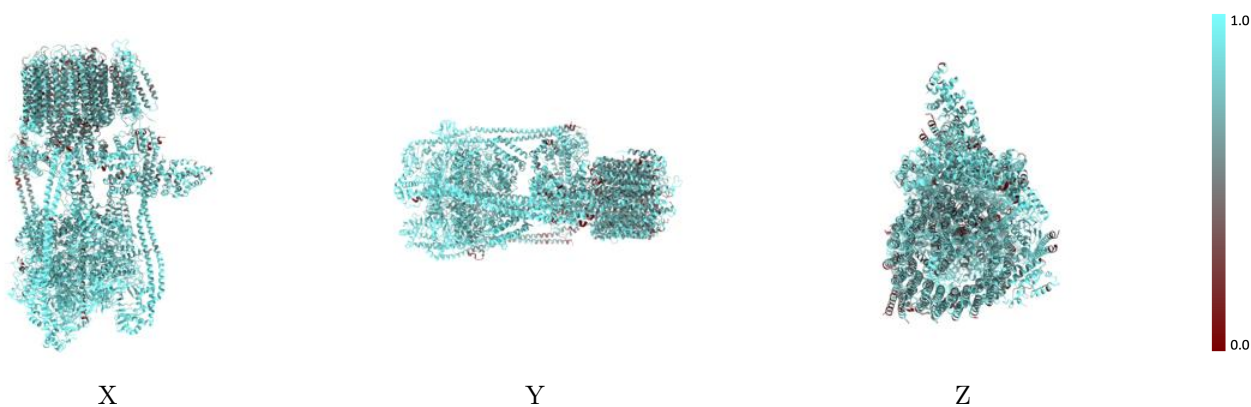
This section was not generated.

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



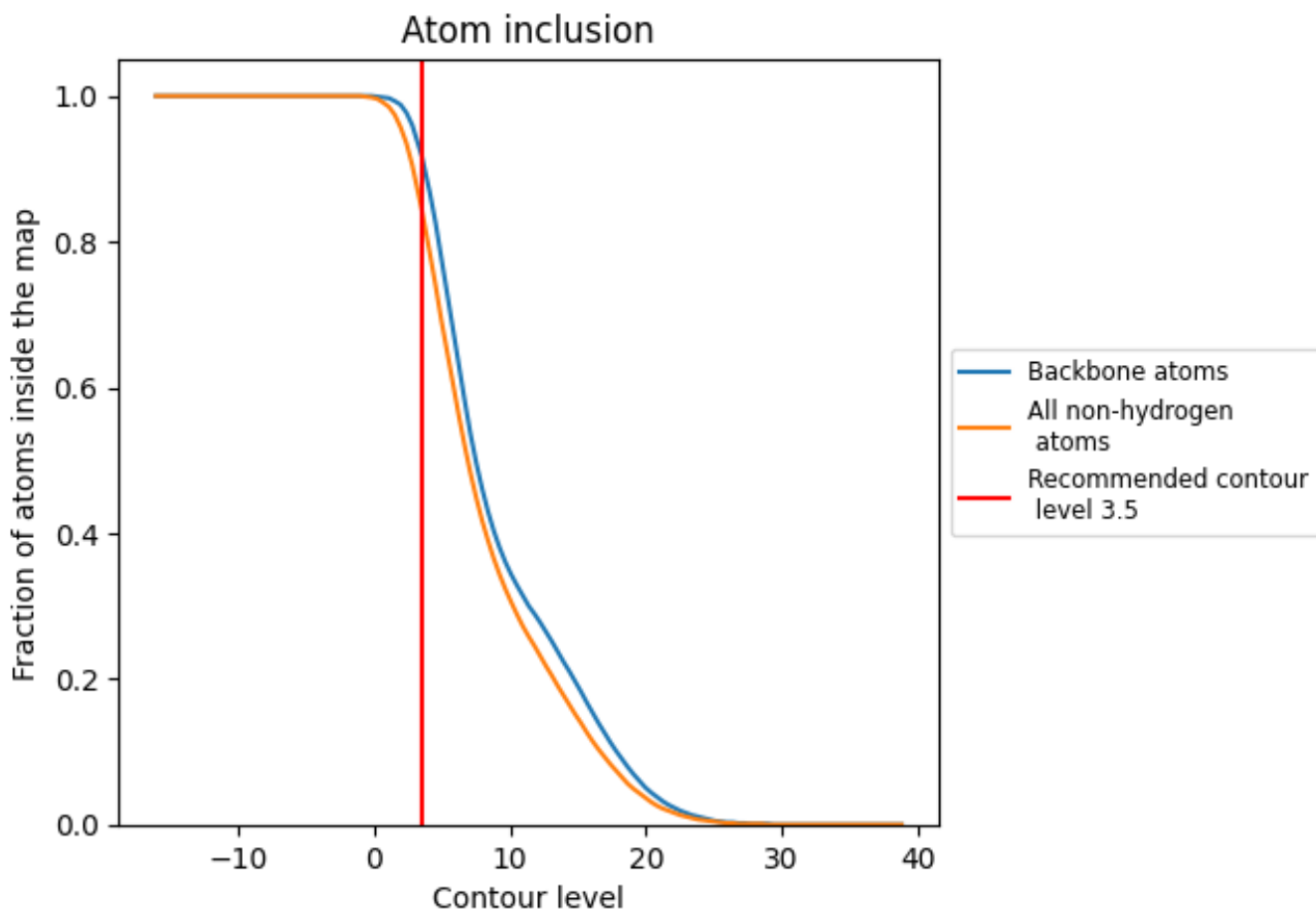
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (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

