



Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 05:55 AM EST

PDB ID : 7TMR
EMDB ID : EMD-26000
Title : V-ATPase from *Saccharomyces cerevisiae*, State 1
Authors : Vasanthakumar, T.; Keon, K.A.; Bueler, S.A.; Jaskolka, M.C.; Rubinstein, J.L.
Deposited on : 2022-01-19
Resolution : 3.50 Å(reported)

This is a Full wwPDB EM Validation 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:

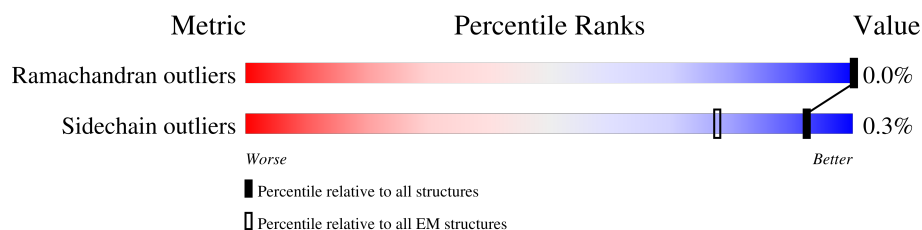
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 3.50 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.



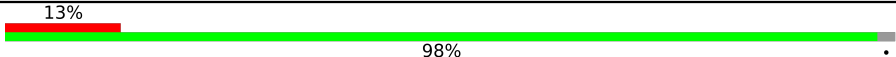
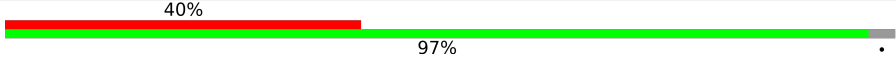
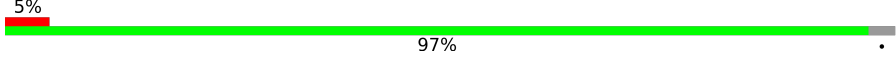

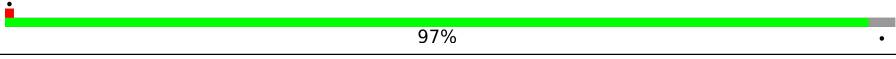
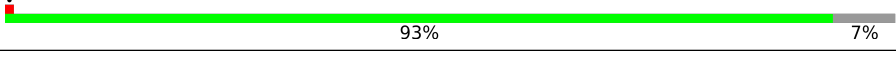
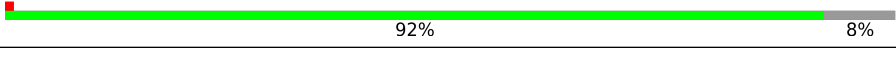
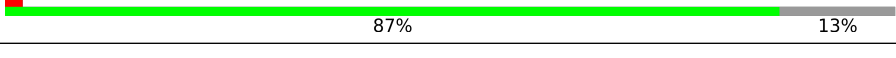

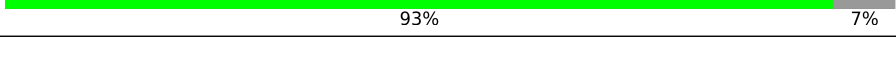
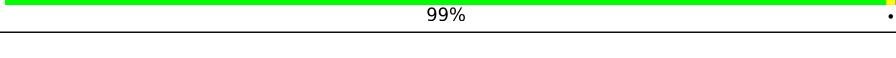

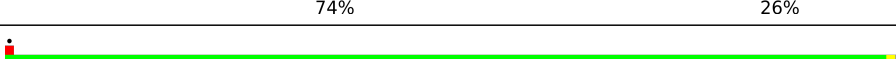
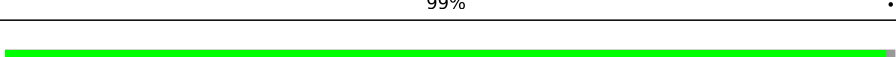
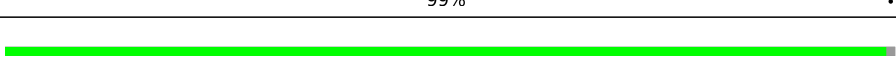
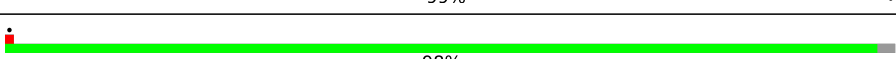
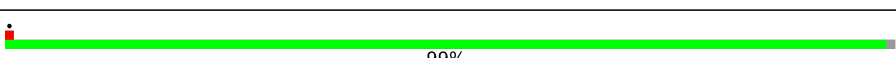
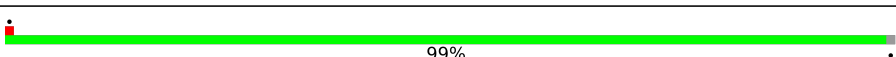
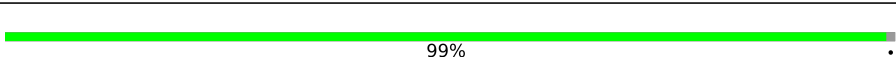
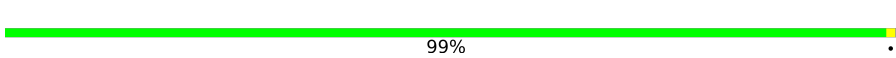
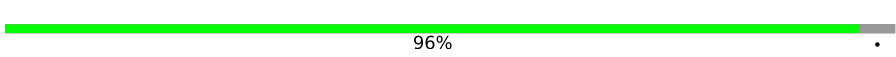

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$. 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	96% .
1	C	617	96% .
1	E	617	96% .
2	B	517	92% 8%
2	D	517	92% 8%
2	F	517	92% 8%
3	G	233	7% 94% 5%
3	I	233	9% 95% 5%
3	K	233	97% .

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Mol	Chain	Length	Quality of chain
4	H	114	
4	J	114	
4	L	114	
5	M	256	
6	N	118	
7	O	392	
8	P	478	
9	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

There are 17 unique types of molecules in this entry. The entry contains 57795 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
			4548	2890	756	882	20		
1	C	593	Total	C	N	O	S	0	0
			4541	2884	756	882	19		
1	E	593	Total	C	N	O	S	0	0
			4567	2898	759	890	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
			3695	2337	632	714	12		
2	F	478	Total	C	N	O	S	0	0
			3727	2356	641	718	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	221	Total	C	N	O	S	0	0
			1315	815	247	251	2		
3	I	221	Total	C	N	O	S	0	0
			1294	797	243	252	2		
3	K	225	Total	C	N	O	S	0	0
			1477	923	263	289	2		

- 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
			556	332	112	112		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	J	111	Total	C	N	O	0	0
			551	329	111	111		
4	L	111	Total	C	N	O	0	0
			551	329	111	111		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	214	Total	C	N	O	S	0	0
			1439	885	276	274	4		

- 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
			587	357	115	115		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	364	Total	C	N	O	0	0
			1841	1112	364	365		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	P	441	Total	C	N	O	0	0
			2228	1340	446	442		

- 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
			5338	3467	888	953	30		

- 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
			400	267	59	72	2		

- 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
			1454	968	227	253	6		

- 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
			2776	1764	452	547	13		

- 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
			510	343	83	79	5		

- 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
			467	308	73	83	3		

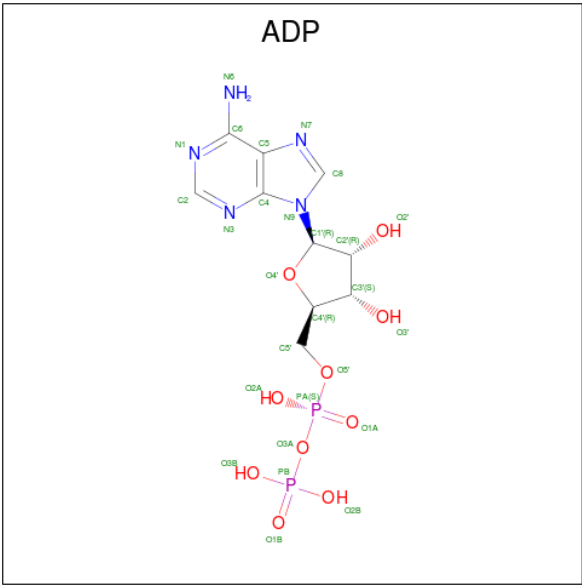
- Molecule 15 is a protein called V-type proton ATPase subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	159	Total	C	N	O	S	0	0
			1134	747	182	199	6		
15	h	159	Total	C	N	O	S	0	0
			1137	749	182	199	7		
15	i	159	Total	C	N	O	S	0	0
			1137	749	182	199	7		
15	j	157	Total	C	N	O	S	0	0
			1125	742	180	196	7		
15	k	159	Total	C	N	O	S	0	0
			1137	749	182	199	7		
15	l	159	Total	C	N	O	S	0	0
			1137	749	182	199	7		
15	m	159	Total	C	N	O	S	0	0
			1137	749	182	199	7		
15	n	159	Total	C	N	O	S	0	0
			1129	744	180	198	7		

- 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	1145	756	180	197	12	0	0

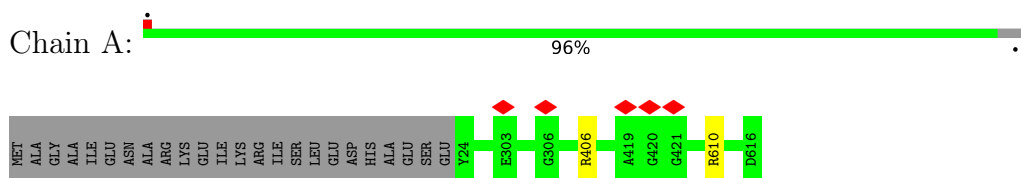
- Molecule 17 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



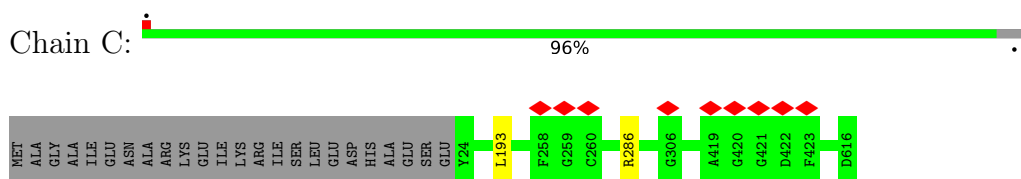
3 Residue-property plots [i](#)

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.

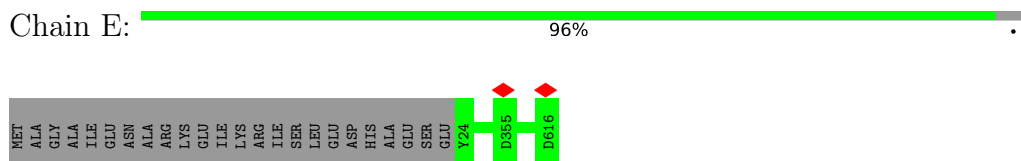
- Molecule 1: H(+)-transporting two-sector ATPase



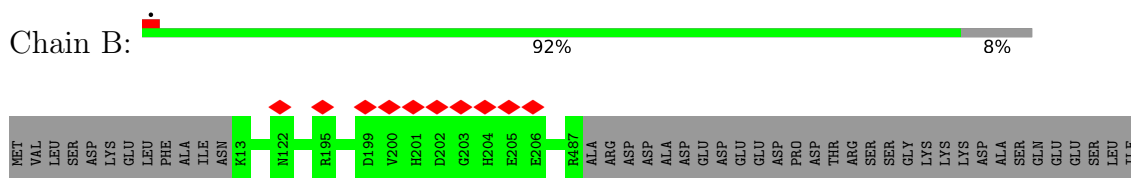
- Molecule 1: H(+)-transporting two-sector ATPase



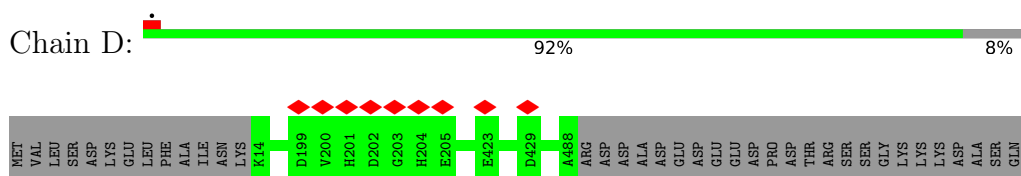
- Molecule 1: H(+)-transporting two-sector ATPase



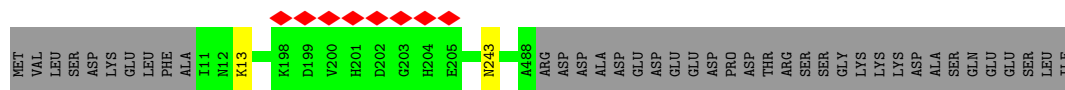
- Molecule 2: Vacuolar proton pump subunit B



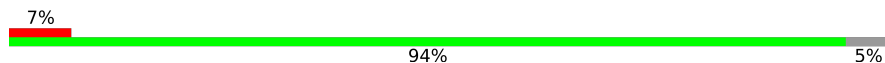
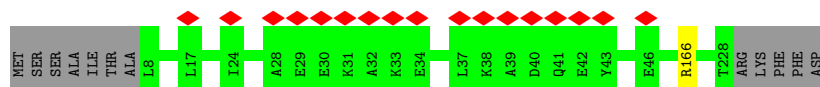
- Molecule 2: Vacuolar proton pump subunit B



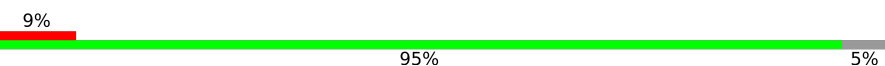
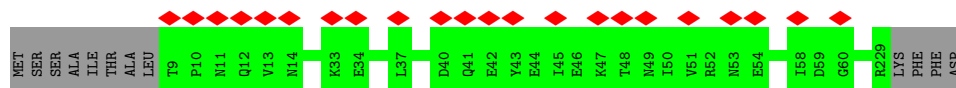
• Molecule 2: Vacuolar proton pump subunit B

Chain F:  92% 8%

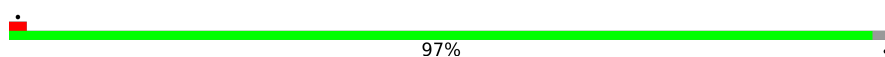
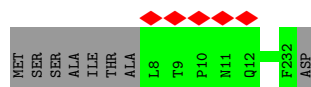
• Molecule 3: V-type proton ATPase subunit E

Chain G:  7% 94% 5%

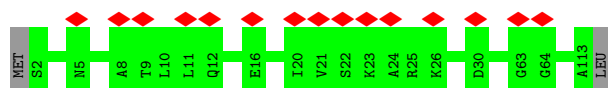
• Molecule 3: V-type proton ATPase subunit E

Chain I:  9% 95% 5%

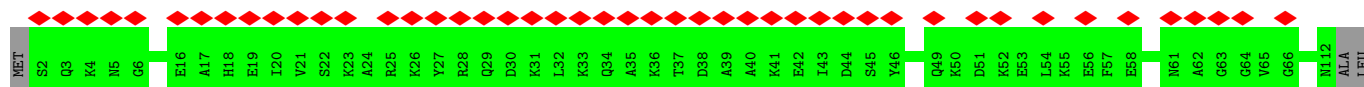
• Molecule 3: V-type proton ATPase subunit E

Chain K:  97% .

• Molecule 4: V-type proton ATPase subunit G

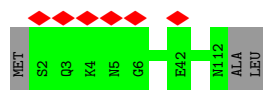
Chain H:  13% 98% .

• Molecule 4: V-type proton ATPase subunit G

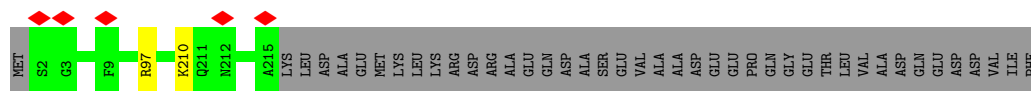
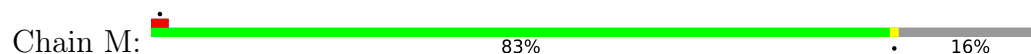
Chain J:  40% 97% .

• Molecule 4: V-type proton ATPase subunit G

Chain L:  5% 97% .



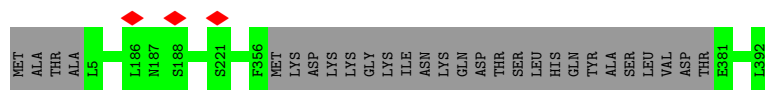
- Molecule 5: V-type proton ATPase subunit D



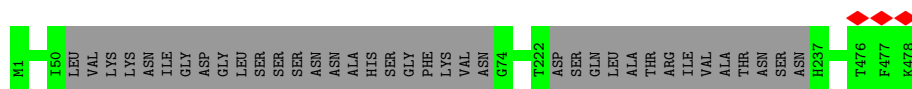
- Molecule 6: V-type proton ATPase subunit F



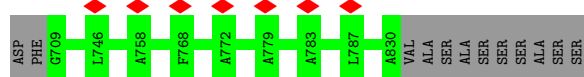
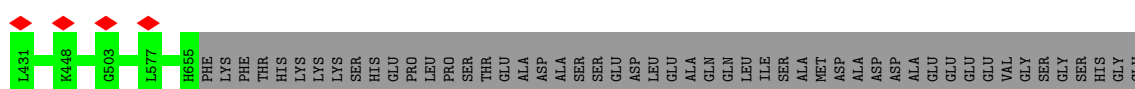
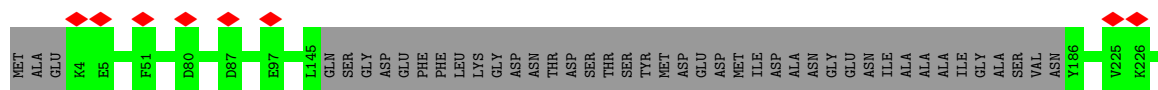
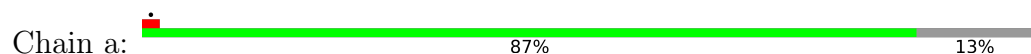
- Molecule 7: V-type proton ATPase subunit C



- Molecule 8: V-type proton ATPase subunit H



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



- Molecule 10: V0 assembly protein 1

[illegible]

- MET ASN LYS GLU SER LYS ASP ASP MET SER LEU GLY LYS PHE S16 Q213

-

- | |
|-----|
| MET |
| SER |
| SER |
| F4 |
| L67 |
| ARG |
| PRO |
| GLU |
| PHE |
| ALA |
| GLU |

- | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | ARG | PRO | VAL | VAL | SER | THR | GLY | LYS | ALA | W11 | V73 | TYR | LEU | ALA | ARG | ARG | LYS | PRO | SER | ILE | GLU | LEU | ARG |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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- 
- WORLD WIDE
PDB
PROTEIN DATA BANK

Chain h:  99% .



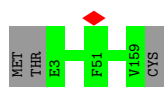
- Molecule 15: V-type proton ATPase subunit c

Chain i:  99% .



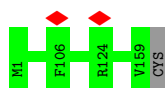
- Molecule 15: V-type proton ATPase subunit c

Chain j:  98% .



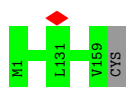
- Molecule 15: V-type proton ATPase subunit c

Chain k:  99% .



- Molecule 15: V-type proton ATPase subunit c

Chain l:  99% .



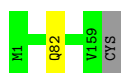
- Molecule 15: V-type proton ATPase subunit c

Chain m:  99% .



- Molecule 15: V-type proton ATPase subunit c

Chain n:  99% ..



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

Chain o:  96% .

MET	
SER	
THR	
GLN	
LEU	
ALA	
S7	
E194	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	104106	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	30.280	Depositor
Minimum map value	-14.845	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	1.128	Depositor
Recommended contour level	3.6	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	0.27	0/4647	0.48	0/6303
1	C	0.27	0/4640	0.50	0/6293
1	E	0.28	0/4666	0.50	0/6326
2	B	0.27	0/3758	0.52	0/5097
2	D	0.27	0/3765	0.51	0/5106
2	F	0.28	0/3797	0.52	0/5146
3	G	0.24	0/1324	0.44	0/1822
3	I	0.24	0/1301	0.46	0/1792
3	K	0.24	0/1489	0.45	0/2032
4	H	0.23	0/556	0.35	0/774
4	J	0.23	0/551	0.33	0/767
4	L	0.23	0/551	0.33	0/767
5	M	0.25	0/1452	0.53	0/1964
6	N	0.24	0/592	0.42	0/828
7	O	0.23	0/1855	0.40	0/2598
8	P	0.23	0/2236	0.37	0/3121
9	a	0.26	0/5462	0.48	0/7460
10	b	0.26	0/406	0.45	0/553
11	c	0.28	0/1483	0.46	0/2015
12	d	0.28	0/2835	0.51	0/3846
13	e	0.25	0/525	0.48	0/718
14	f	0.27	0/481	0.46	0/661
15	g	0.30	0/1152	0.50	0/1568
15	h	0.28	0/1155	0.54	0/1571
15	i	0.29	0/1155	0.51	0/1571
15	j	0.30	0/1143	0.55	0/1554
15	k	0.28	0/1155	0.51	0/1571
15	l	0.29	0/1155	0.54	0/1571
15	m	0.30	0/1155	0.55	0/1571
15	n	0.29	0/1147	0.52	0/1562
16	o	0.30	0/1168	0.53	0/1582
All	All	0.27	0/58757	0.49	0/80110

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](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	591/617 (96%)	570 (96%)	21 (4%)	0	100	100
1	C	591/617 (96%)	569 (96%)	22 (4%)	0	100	100
1	E	591/617 (96%)	574 (97%)	17 (3%)	0	100	100
2	B	473/517 (92%)	453 (96%)	20 (4%)	0	100	100
2	D	473/517 (92%)	453 (96%)	20 (4%)	0	100	100
2	F	476/517 (92%)	462 (97%)	14 (3%)	0	100	100
3	G	219/233 (94%)	213 (97%)	6 (3%)	0	100	100
3	I	219/233 (94%)	212 (97%)	7 (3%)	0	100	100
3	K	223/233 (96%)	215 (96%)	8 (4%)	0	100	100
4	H	110/114 (96%)	110 (100%)	0	0	100	100
4	J	109/114 (96%)	109 (100%)	0	0	100	100
4	L	109/114 (96%)	108 (99%)	1 (1%)	0	100	100
5	M	212/256 (83%)	207 (98%)	5 (2%)	0	100	100
6	N	113/118 (96%)	104 (92%)	9 (8%)	0	100	100
7	O	360/392 (92%)	342 (95%)	18 (5%)	0	100	100
8	P	435/478 (91%)	426 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	a	728/840 (87%)	688 (94%)	40 (6%)	0	100	100
10	b	50/265 (19%)	46 (92%)	3 (6%)	1 (2%)	7	39
11	c	196/213 (92%)	191 (97%)	5 (3%)	0	100	100
12	d	341/345 (99%)	330 (97%)	11 (3%)	0	100	100
13	e	62/73 (85%)	60 (97%)	2 (3%)	0	100	100
14	f	61/85 (72%)	57 (93%)	4 (7%)	0	100	100
15	g	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
15	h	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
15	i	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
15	j	155/160 (97%)	152 (98%)	3 (2%)	0	100	100
15	k	157/160 (98%)	156 (99%)	1 (1%)	0	100	100
15	l	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
15	m	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
15	n	157/160 (98%)	154 (98%)	2 (1%)	1 (1%)	25	64
16	o	156/164 (95%)	154 (99%)	2 (1%)	0	100	100
All	All	8152/8952 (91%)	7885 (97%)	265 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	b	216	SER
15	n	82	GLN

5.3.2 Protein sidechains ⓘ

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%)	486 (100%)	2 (0%)	91	96
1	C	482/516 (93%)	480 (100%)	2 (0%)	91	96
1	E	494/516 (96%)	494 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	394/444 (89%)	394 (100%)	0	100	100
2	D	396/444 (89%)	396 (100%)	0	100	100
2	F	400/444 (90%)	398 (100%)	2 (0%)	88	94
3	G	62/208 (30%)	61 (98%)	1 (2%)	62	83
3	I	59/208 (28%)	59 (100%)	0	100	100
3	K	102/208 (49%)	102 (100%)	0	100	100
4	H	1/94 (1%)	1 (100%)	0	100	100
4	J	1/94 (1%)	1 (100%)	0	100	100
4	L	1/94 (1%)	1 (100%)	0	100	100
5	M	101/221 (46%)	99 (98%)	2 (2%)	55	79
6	N	6/104 (6%)	6 (100%)	0	100	100
7	O	16/348 (5%)	16 (100%)	0	100	100
8	P	12/439 (3%)	12 (100%)	0	100	100
9	a	483/728 (66%)	483 (100%)	0	100	100
10	b	46/244 (19%)	44 (96%)	2 (4%)	29	62
11	c	149/168 (89%)	149 (100%)	0	100	100
12	d	304/309 (98%)	301 (99%)	3 (1%)	76	88
13	e	55/65 (85%)	55 (100%)	0	100	100
14	f	48/72 (67%)	48 (100%)	0	100	100
15	g	116/119 (98%)	115 (99%)	1 (1%)	78	90
15	h	117/119 (98%)	117 (100%)	0	100	100
15	i	117/119 (98%)	117 (100%)	0	100	100
15	j	116/119 (98%)	116 (100%)	0	100	100
15	k	117/119 (98%)	117 (100%)	0	100	100
15	l	117/119 (98%)	117 (100%)	0	100	100
15	m	117/119 (98%)	117 (100%)	0	100	100
15	n	115/119 (97%)	115 (100%)	0	100	100
16	o	119/125 (95%)	119 (100%)	0	100	100
All	All	5151/7561 (68%)	5136 (100%)	15 (0%)	92	97

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	406	ARG
1	A	610	ARG
1	C	193	LEU
1	C	286	ARG
2	F	13	LYS
2	F	243	ASN
3	G	166	ARG
5	M	97	ARG
5	M	210	LYS
10	b	215	LEU
10	b	216	SER
12	d	21	ARG
12	d	97	TYR
12	d	276	ARG
15	g	130	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	190	GLN
2	D	243	ASN
9	a	533	ASN
9	a	715	GLN
12	d	226	ASN
15	g	151	ASN
15	j	151	ASN
15	m	90	GLN
15	m	151	ASN
15	n	90	GLN
16	o	83	ASN
16	o	98	HIS
16	o	159	ASN

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](#)

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	0.95	1 (4%)	29,45,45	1.45	5 (17%)

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	-	-	4/12/32/32	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	2.42	1.47	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	E	701	ADP	C3'-C2'-C1'	3.29	105.93	100.98
17	E	701	ADP	N3-C2-N1	-3.22	123.64	128.68
17	E	701	ADP	PA-O3A-PB	-2.87	122.96	132.83
17	E	701	ADP	C4-C5-N7	-2.64	106.65	109.40
17	E	701	ADP	C2'-C3'-C4'	2.03	106.58	102.64

There are no chirality outliers.

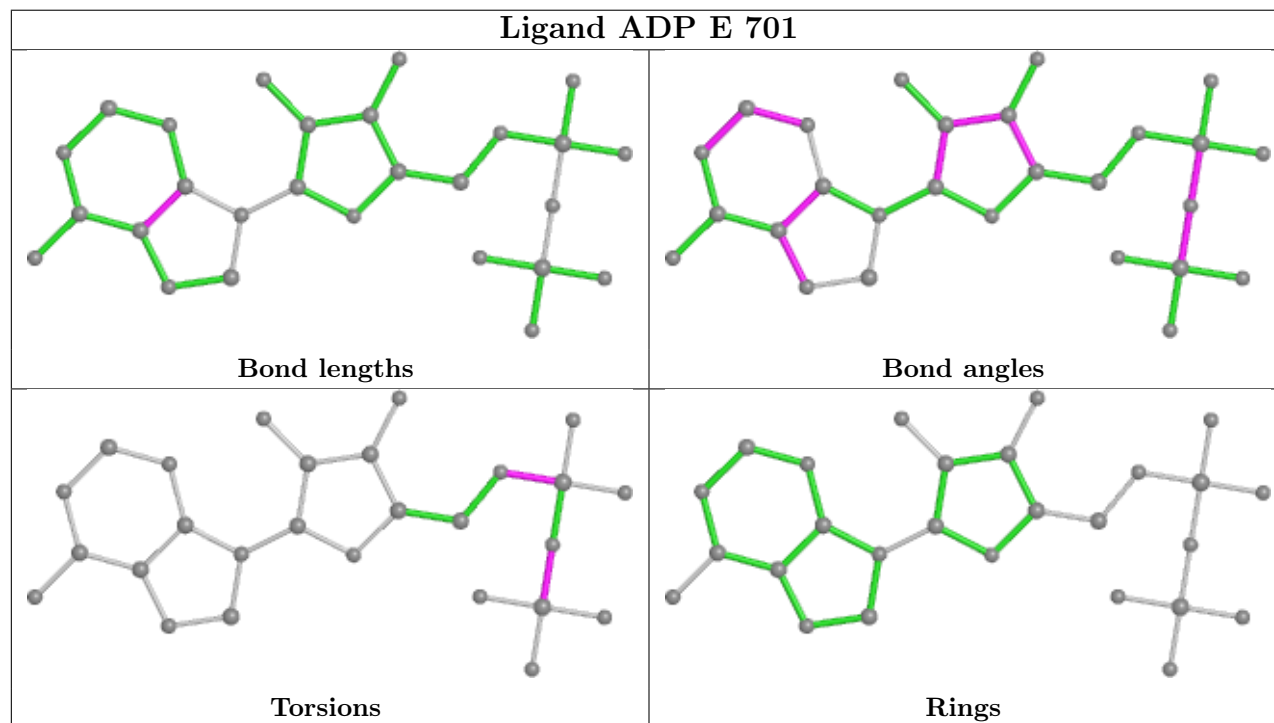
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	E	701	ADP	C5'-O5'-PA-O1A
17	E	701	ADP	C5'-O5'-PA-O2A
17	E	701	ADP	C5'-O5'-PA-O3A
17	E	701	ADP	PA-O3A-PB-O3B

There are no ring outliers.

No monomer is involved in short contacts.

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.

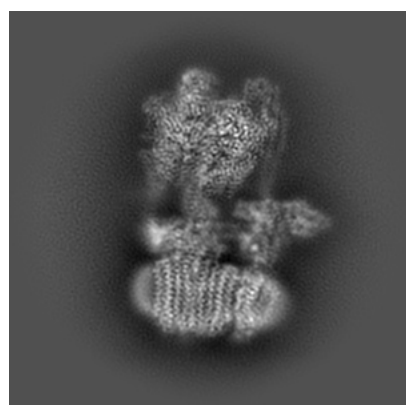
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26000. These allow visual inspection of the internal detail of the map and identification of artifacts.

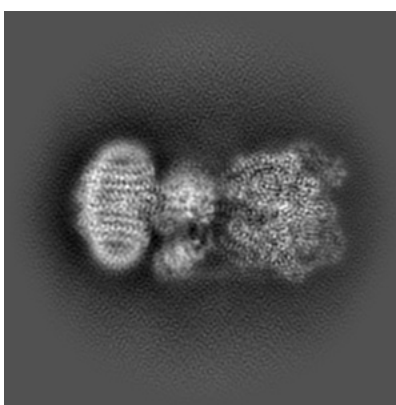
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

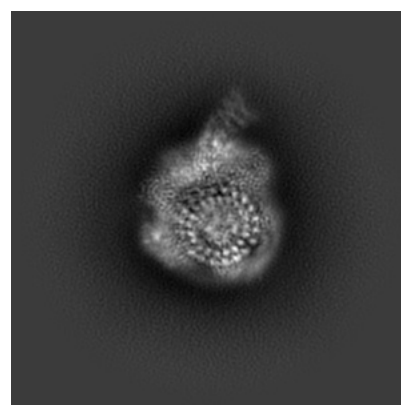
6.1.1 Primary map



X



Y

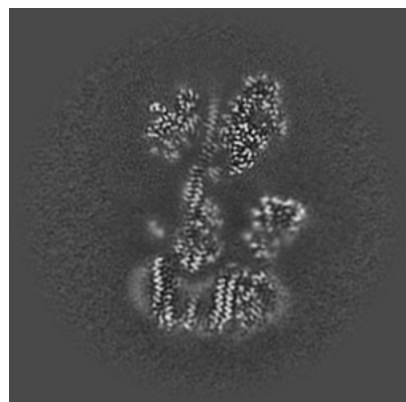


Z

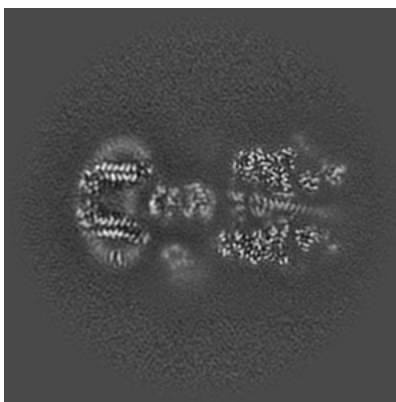
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

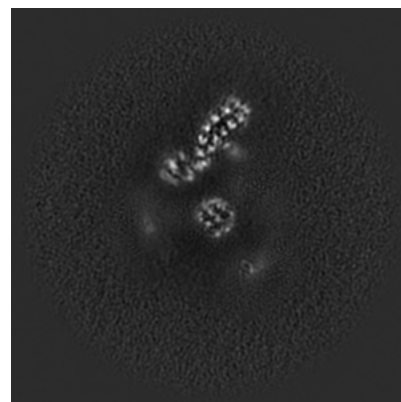
6.2.1 Primary map



X Index: 150



Y Index: 150

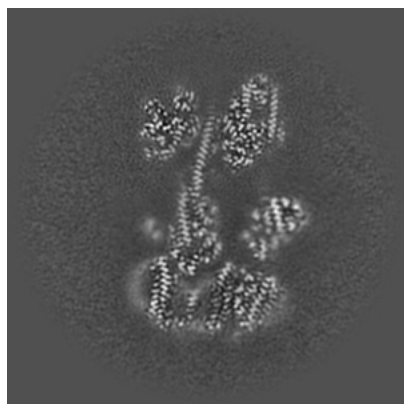


Z Index: 150

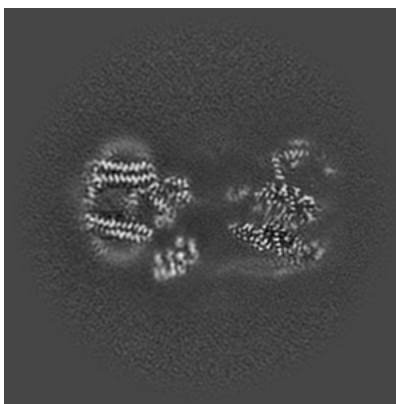
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

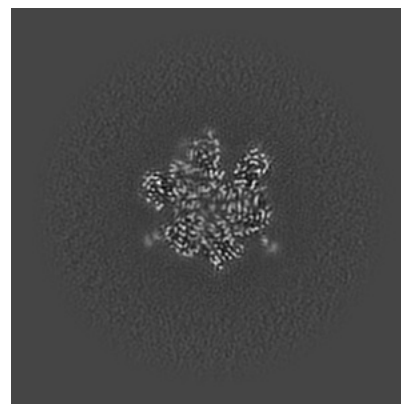
6.3.1 Primary map



X Index: 153



Y Index: 126



Z Index: 211

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

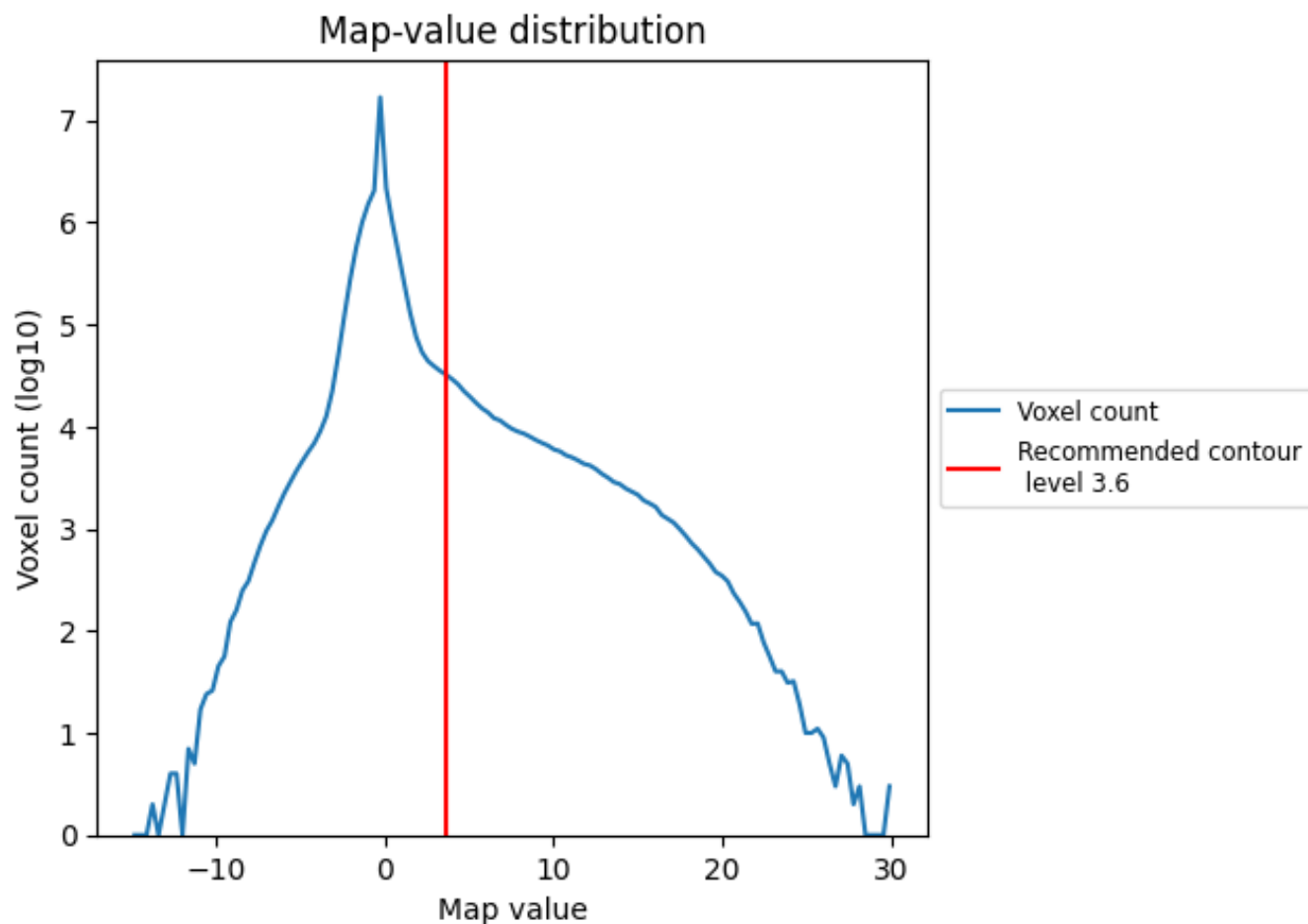
6.5 Mask visualisation

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

7 Map analysis [i](#)

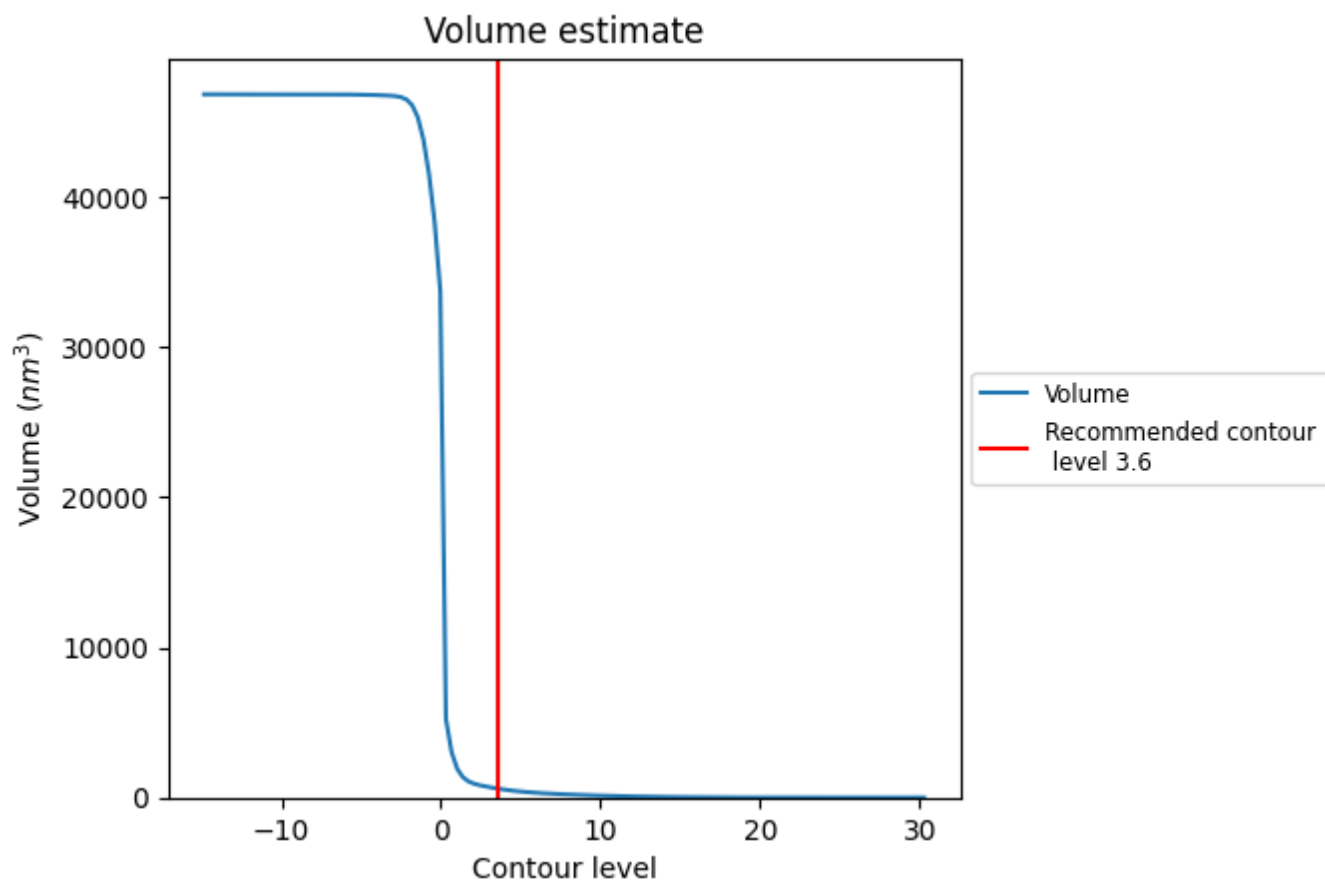
This section contains the results of statistical analysis of the map.

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.

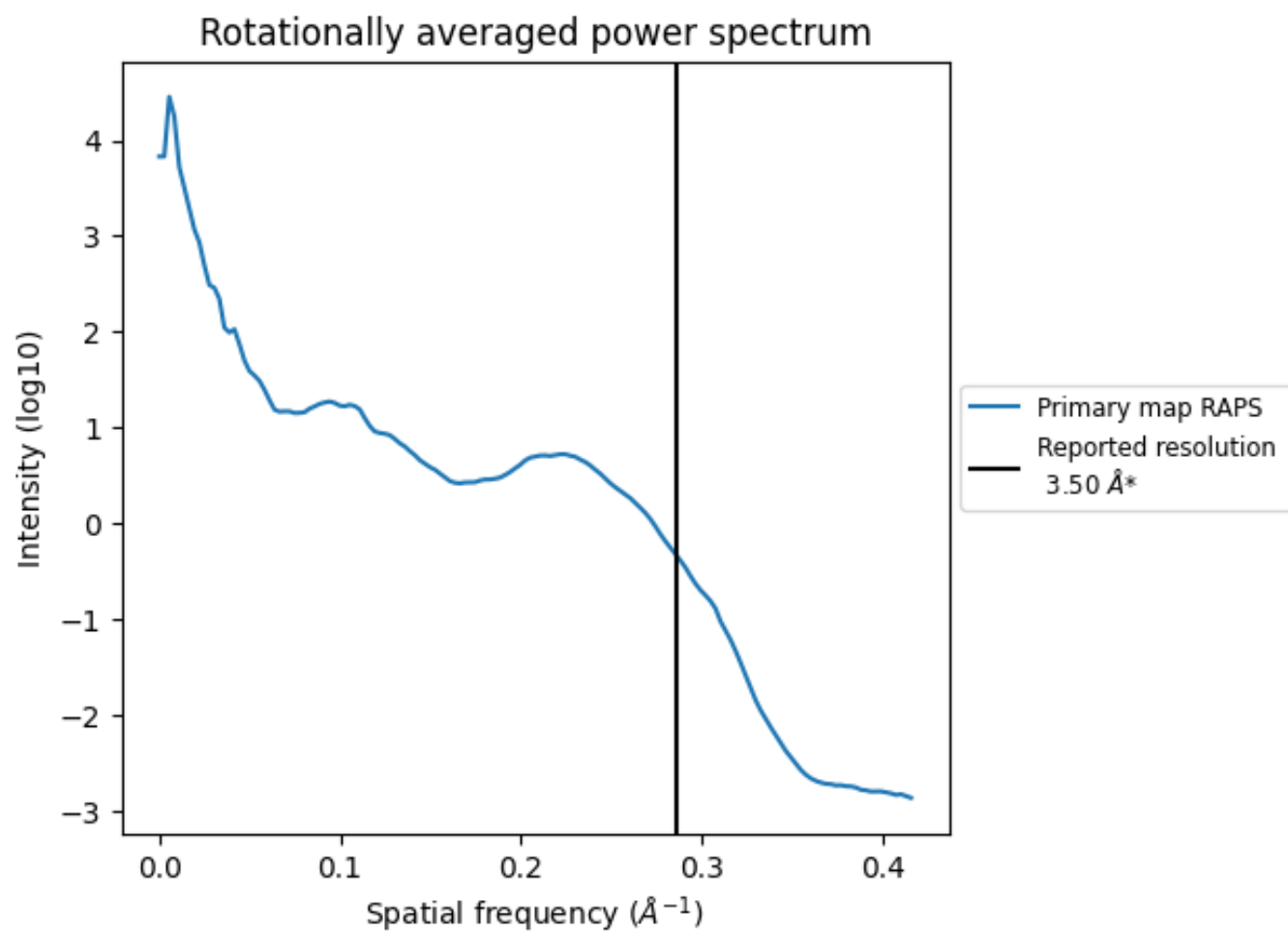
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 591 nm³; this corresponds to an approximate mass of 534 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 0.286 Å⁻¹

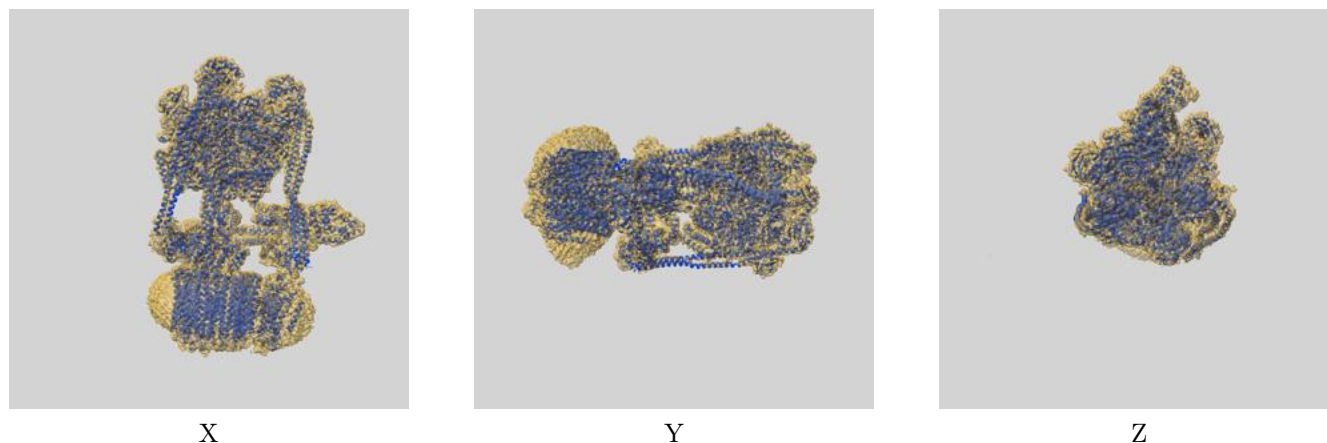
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

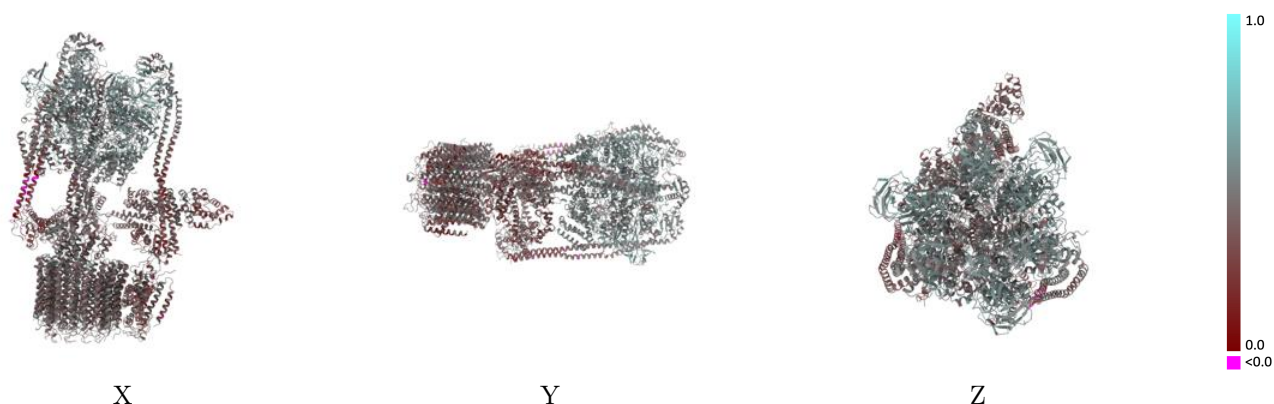
This section contains information regarding the fit between EMDB map EMD-26000 and PDB model 7TMR. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



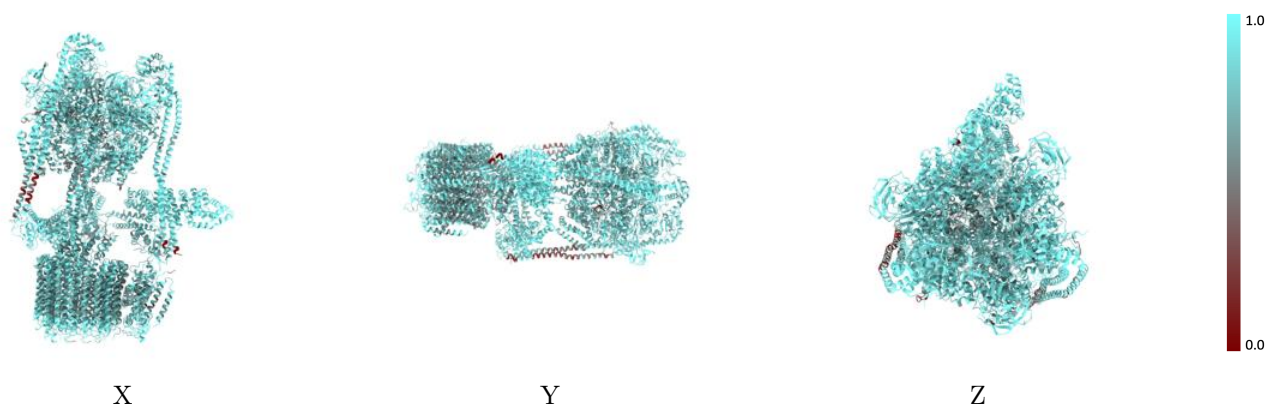
The images above show the 3D surface view of the map at the recommended contour level 3.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



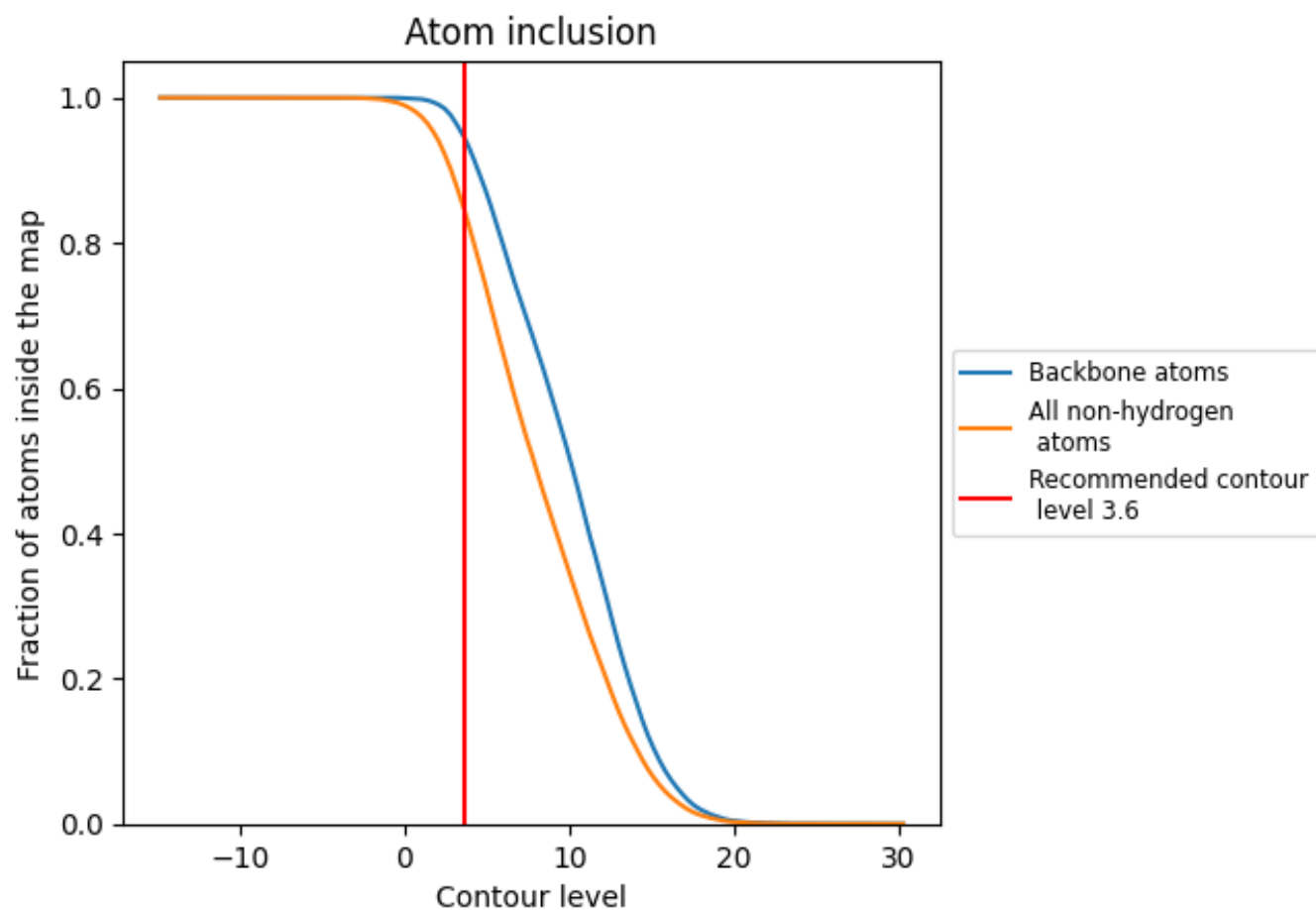
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.6).

































































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 85% 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 (3.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8470	 0.4500
A	 0.8534	 0.5080
B	 0.8409	 0.5040
C	 0.8700	 0.5130
D	 0.8539	 0.5240
E	 0.8863	 0.5300
F	 0.8557	 0.5170
G	 0.8739	 0.4460
H	 0.8201	 0.3570
I	 0.8154	 0.4200
J	 0.5953	 0.3120
K	 0.8718	 0.4600
L	 0.8730	 0.3820
M	 0.8262	 0.4330
N	 0.9336	 0.4170
O	 0.9739	 0.3500
P	 0.9816	 0.3730
a	 0.8197	 0.3530
b	 0.7406	 0.4290
c	 0.8170	 0.4260
d	 0.8133	 0.4220
e	 0.8400	 0.3850
f	 0.8362	 0.3300
g	 0.8134	 0.4230
h	 0.7907	 0.4200
i	 0.7970	 0.4240
j	 0.7633	 0.4100
k	 0.7916	 0.4150
l	 0.8005	 0.4050
m	 0.7961	 0.4020
n	 0.8215	 0.4340
o	 0.8383	 0.4440

