



wwPDB EM Validation Summary Report ⓘ

Sep 2, 2026 – 06:27 PM EDT

PDB ID : 36QX / pdb_000036qx
EMDB ID : EMD-77789
Title : Arabidopsis thaliana V-type ATPase, State 1 bound to OXR5, Backbone model
Authors : Khamina, M.; Rubinstein, J.L.
Deposited on : 2026-06-26
Resolution : 4.30 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:

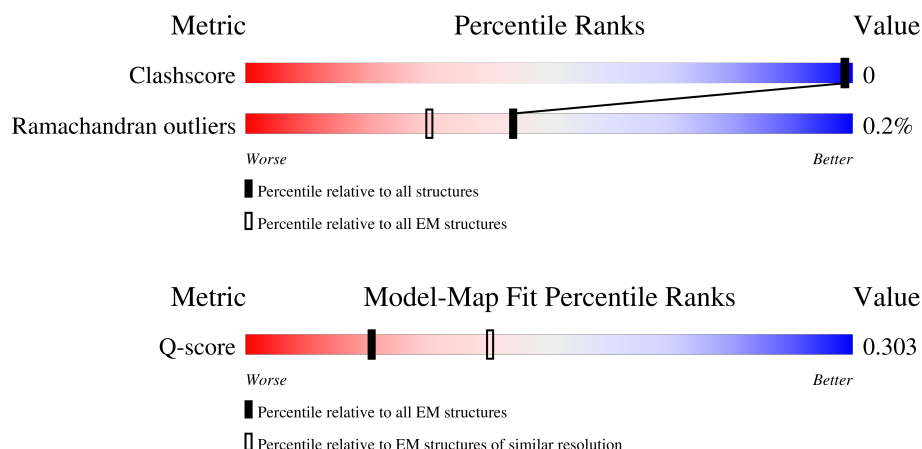
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

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 4.30 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.



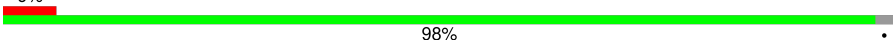
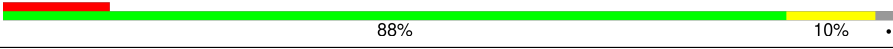
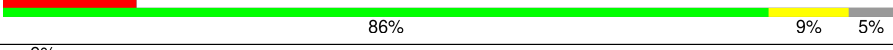
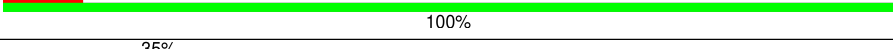
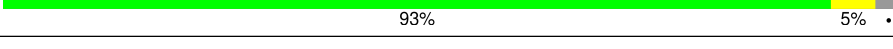
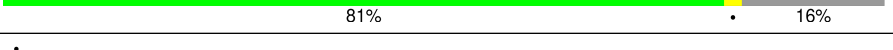
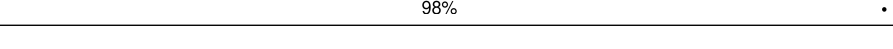
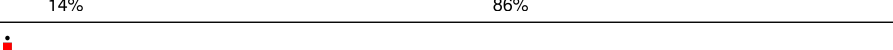
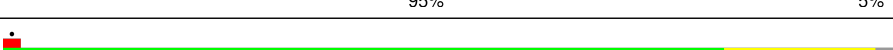
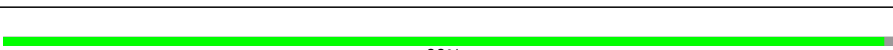
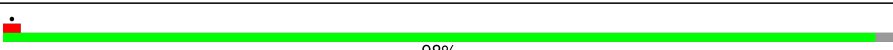
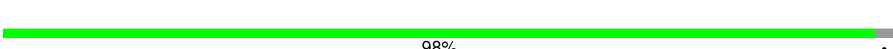
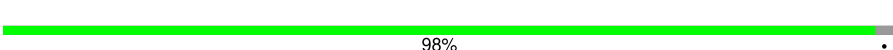
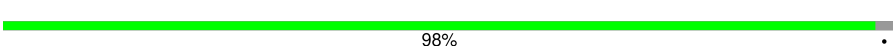
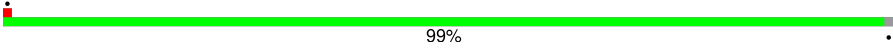
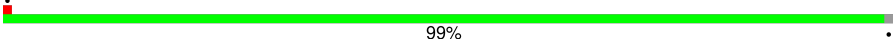
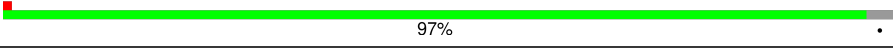
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	4585 (3.80 - 4.80)

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	T	542	25% 95% • •
2	a	817	16% 88% 12%
3	B	486	91% • 6%
3	D	486	90% • 7%
3	F	486	87% 7% 6%

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Mol	Chain	Length	Quality of chain
4	G	230	
4	I	230	
4	K	230	
5	H	110	
5	J	110	
5	L	110	
6	M	261	
7	N	128	
8	P	441	
9	b	321	
10	c	180	
11	d	351	
12	e	70	
13	g	164	
13	h	164	
13	i	164	
13	j	164	
13	k	164	
13	l	164	
13	m	164	
13	n	164	
13	o	164	
14	r	364	
15	A	623	
15	C	623	

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Mol	Chain	Length	Quality of chain
15	E	623	 86% 13%
16	O	375	 18% 92% 8%

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 34440 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 TLD-domain containing nucleolar protein OXR5.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	T	518	Total	C	N	O	0	0
			2073	1036	518	519		

- Molecule 2 is a protein called V-type proton ATPase subunit a1.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	a	717	Total	C	N	O	0	0
			2869	1434	717	718		

- Molecule 3 is a protein called V-type proton ATPase subunit B1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	456	Total	C	N	O	0	0
			1824	912	456	456		
3	D	454	Total	C	N	O	0	0
			1816	908	454	454		
3	B	458	Total	C	N	O	0	0
			1832	916	458	458		

- Molecule 4 is a protein called V-type proton ATPase subunit E1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	G	213	Total	C	N	O	0	0
			852	426	213	213		
4	I	226	Total	C	N	O	0	0
			904	452	226	226		
4	K	224	Total	C	N	O	0	0
			896	448	224	224		

- Molecule 5 is a protein called V-type proton ATPase subunit G1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	H	105	Total	C	N	O	0	0
			420	210	105	105		
5	J	110	Total	C	N	O	0	0
			441	220	110	111		
5	L	107	Total	C	N	O	0	0
			429	215	107	107		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	M	218	Total	C	N	O	0	0
			872	436	218	218		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	N	101	Total	C	N	O	0	0
			404	202	101	101		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	P	433	Total	C	N	O	0	0
			1732	866	433	433		

- Molecule 9 is a protein called V-type proton ATPase subunit AP1 fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	b	44	Total	C	N	O	0	0
			176	88	44	44		

- Molecule 10 is a protein called V-type proton ATPase subunit c'1.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	c	171	Total	C	N	O	0	0
			685	342	171	172		

- Molecule 11 is a protein called V-type proton ATPase subunit d1.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	d	342	Total	C	N	O	0	0
			1369	684	342	343		

- Molecule 12 is a protein called V-type proton ATPase subunit e2.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	e	54	Total	C	N	O	0	0
			224	116	54	54		

- Molecule 13 is a protein called V-type proton ATPase subunit c1.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	g	162	Total	C	N	O	0	0
			648	324	162	162		
13	h	162	Total	C	N	O	0	0
			648	324	162	162		
13	i	161	Total	C	N	O	0	0
			644	322	161	161		
13	j	161	Total	C	N	O	0	0
			644	322	161	161		
13	k	161	Total	C	N	O	0	0
			644	322	161	161		
13	l	161	Total	C	N	O	0	0
			644	322	161	161		
13	m	162	Total	C	N	O	0	0
			648	324	162	162		
13	n	162	Total	C	N	O	0	0
			648	324	162	162		
13	o	159	Total	C	N	O	0	0
			636	318	159	159		

- Molecule 14 is a protein called V-type proton ATPase subunit AP2 fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	r	48	Total	C	N	O	0	0
			192	96	48	48		

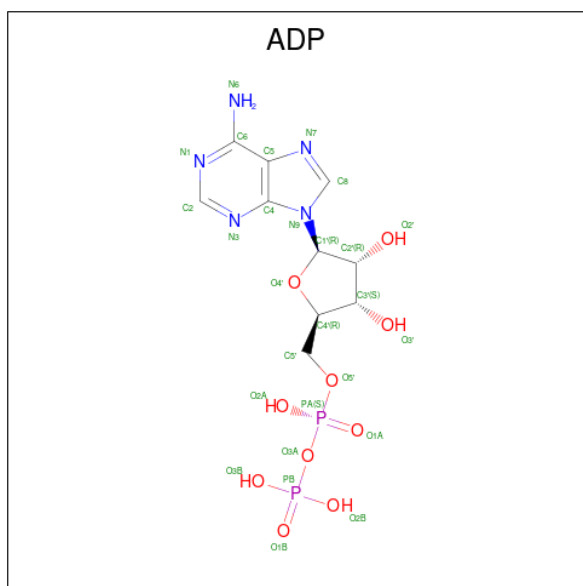
- Molecule 15 is a protein called V-type proton ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	C	610	Total	C	N	O	0	0
			2440	1220	610	610		
15	E	616	Total	C	N	O	0	0
			2465	1232	616	617		
15	A	577	Total	C	N	O	0	0
			2308	1154	577	577		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
16	O	346	Total	C	N	O	0	0
			1385	693	346	346		

- Molecule 17 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: 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	

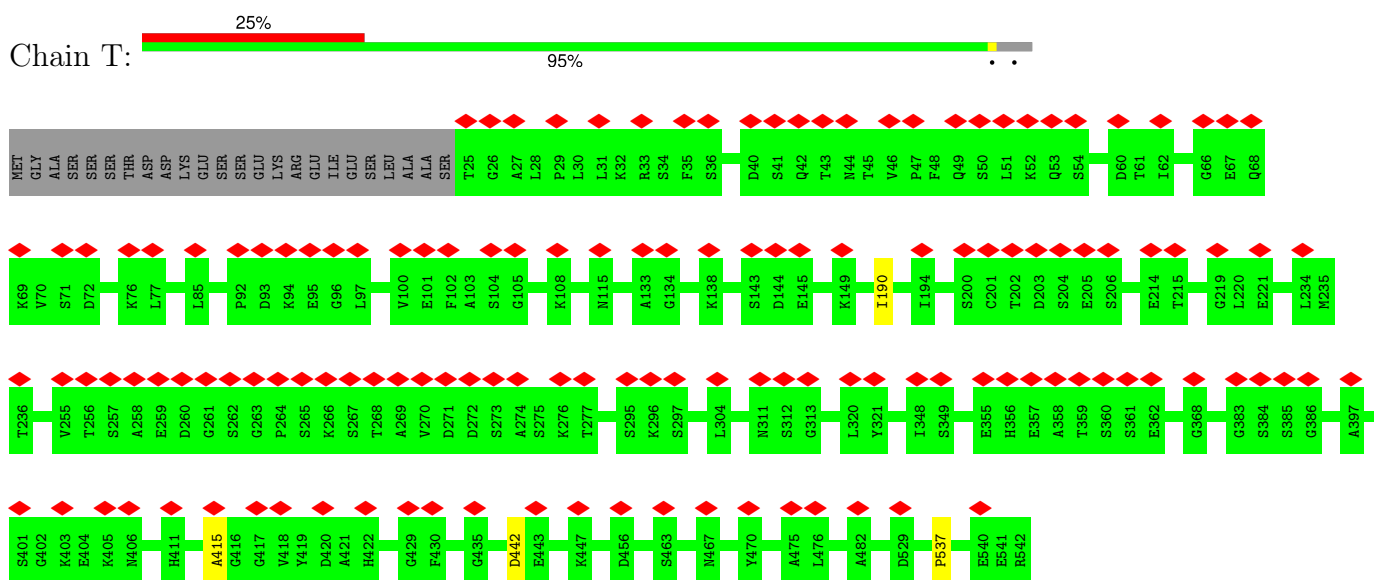
- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
18	E	1	Total	Mg	0
			1	1	

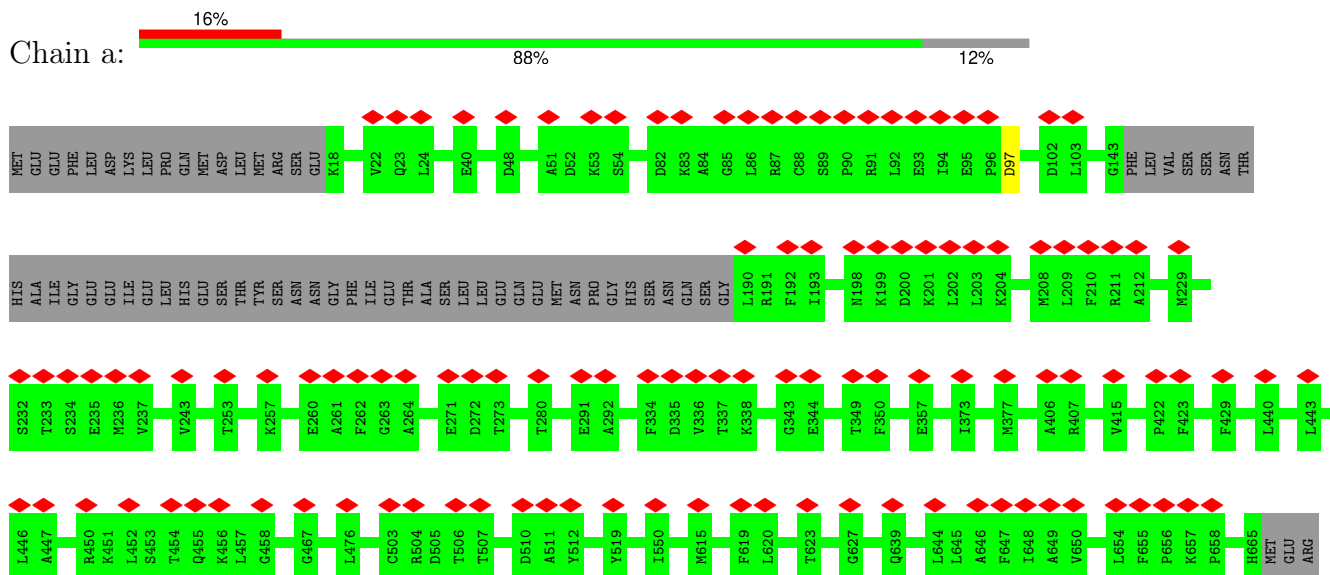
3 Residue-property plots

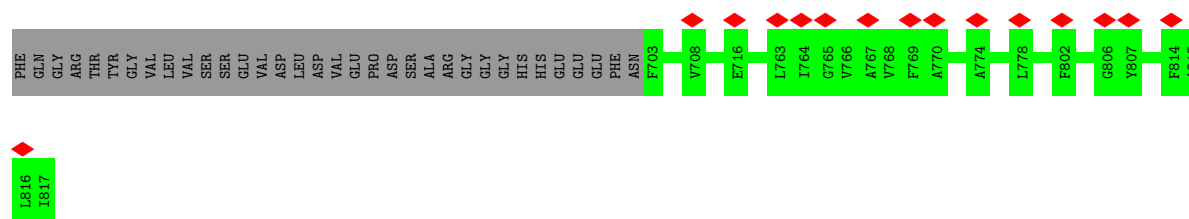
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: TLD-domain containing nucleolar protein OXR5



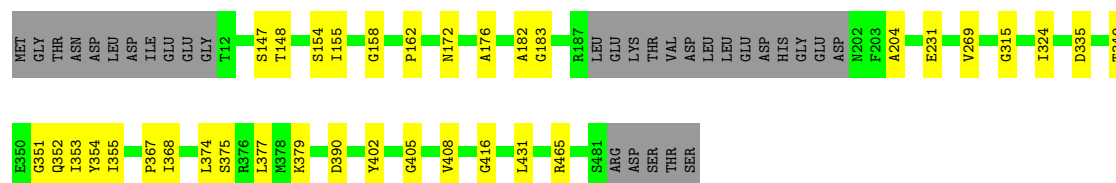
- Molecule 2: V-type proton ATPase subunit a1





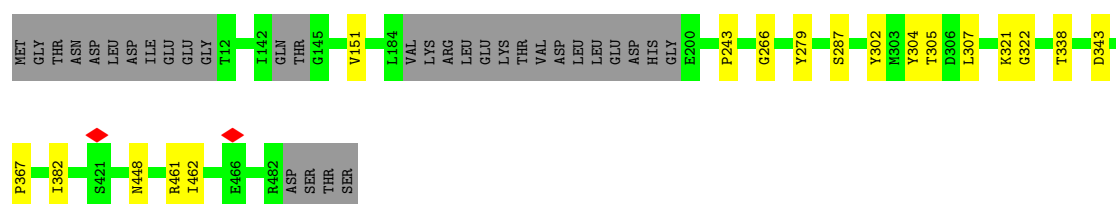
- Molecule 3: V-type proton ATPase subunit B1

Chain F: 87% 7% 6%



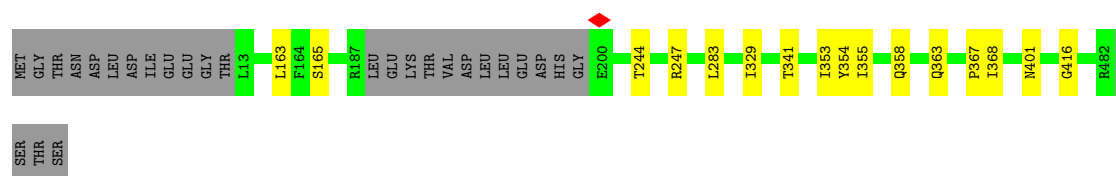
- Molecule 3: V-type proton ATPase subunit B1

Chain D: 90% 7%



- Molecule 3: V-type proton ATPase subunit B1

Chain B: 91% 6%



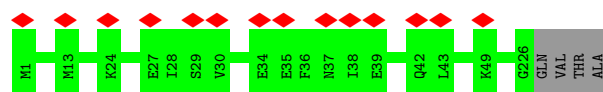
- Molecule 4: V-type proton ATPase subunit E1

Chain G: 88% 7%

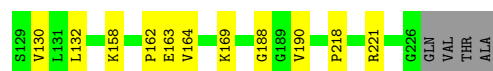
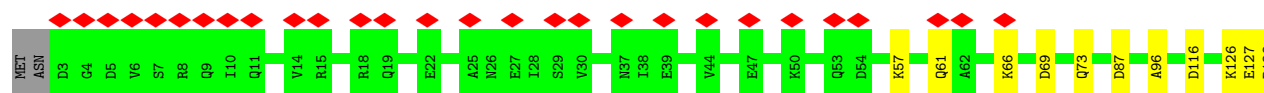
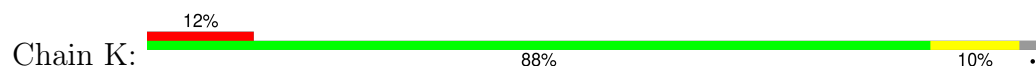


- Molecule 4: V-type proton ATPase subunit E1

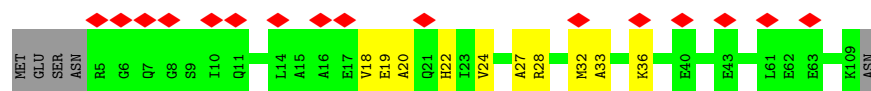
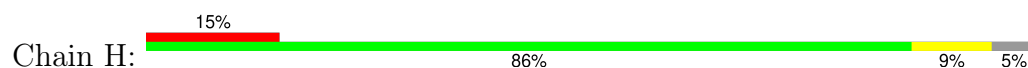
Chain I: 98% 6%



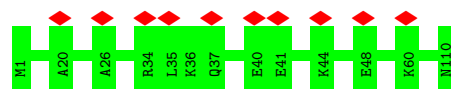
- Molecule 4: V-type proton ATPase subunit E1



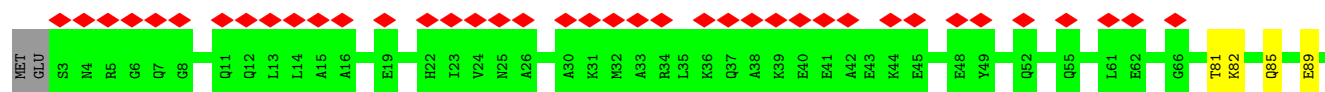
- Molecule 5: V-type proton ATPase subunit G1



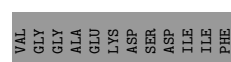
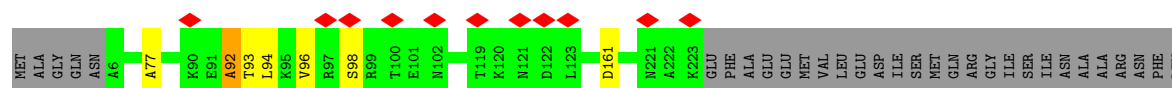
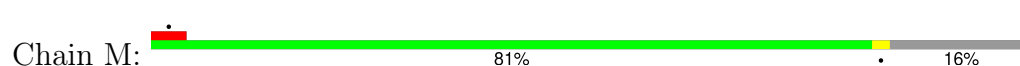
- Molecule 5: V-type proton ATPase subunit G1



- Molecule 5: V-type proton ATPase subunit G1



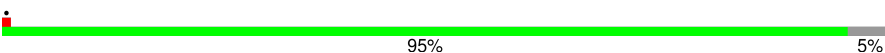
- Molecule 6: V-type proton ATPase subunit D



SER PHE LYS ASP HIS LEU LEU ALA ARG GLU THR ARG LYS GLU GLY THR THR ASP LEU VAL VAL LEU LYS CYS SER GLU GLY SER GLU SER GLU SER ASN SER GLN ALA GLY GLN SER HIS SER ASP ARG GLU ARG SER PHE LEU LEU VAL SER VAL SER VAL GLU GLN SER GLY SER LYS THR THR ALA

LEU TYR VAL SER ASP PRO TYR TRP THR THR LYS THR LEU GLN ARG PHE THR LEU ALA GLU VAL ALA LYS SER GLY ASN THR SER PRO GLU ILE ALA THR GLN ALA GLY C275 P313 GLN ASP SER

- Molecule 10: V-type proton ATPase subunit c'1

Chain c:  95% 5%

MET SER GLY VAL VAL LEU LEU GLY HIS A10 G157 K180

- Molecule 11: V-type proton ATPase subunit d1

Chain d:  81% 17%

M1 A31 M41 A51 N60 S63 P64 C74 K77 L78 V79 D80 Y82 G103 H104 M105 G115 V122 G133 D136 S137 I138 L141 A142 V143 A144 Q145 N146 E149 P162 C167 E171 D172 L173 D174 D175 A188 E191 D192 F193

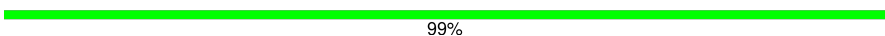
D210 L211 F214 E215 A220 G245 L246 G251 E254 L255 A256 I257 V264 R265 G266 S279 LYS MET SER TYR GLY GLU SER MET L289 D290 K291 E295 E296 E297 F314 F315 W330 I331 C334 V335 H344 Y349 M350 F351

- Molecule 12: V-type proton ATPase subunit e2

Chain e:  29% 77% 23%

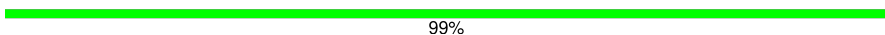
MET ALA F3 V4 S7 L8 A11 V12 V13 G14 N26 K27 L36 V39 I40 T41 A42 T43 V44 C45 C46 W47 M48 M49 Y54 I55 A56 GLN MET ASN PRO LEU ILE VAL PRO ILE LEU SER GLU VAL GLU

- Molecule 13: V-type proton ATPase subunit c1

Chain g:  99%

MET S2 A163 GLU

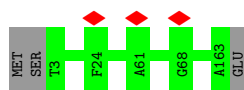
- Molecule 13: V-type proton ATPase subunit c1

Chain h:  99%

MET S2 A163 GLU

- Molecule 13: V-type proton ATPase subunit c1

Chain i:  98%



- Molecule 13: V-type proton ATPase subunit c1

Chain j: 98%



- Molecule 13: V-type proton ATPase subunit c1

Chain k: 98%



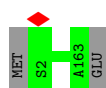
- Molecule 13: V-type proton ATPase subunit c1

Chain l: 98%



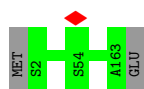
- Molecule 13: V-type proton ATPase subunit c1

Chain m: 99%



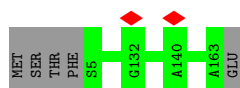
- Molecule 13: V-type proton ATPase subunit c1

Chain n: 99%



- Molecule 13: V-type proton ATPase subunit c1

Chain o: 97%

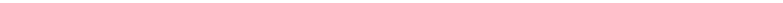


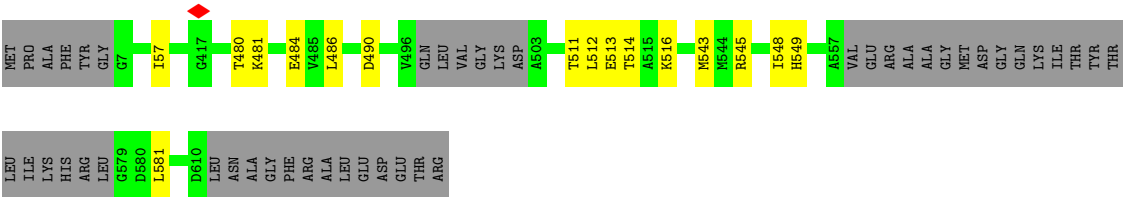
- Molecule 14: V-type proton ATPase subunit AP2 fragment

[illegible]

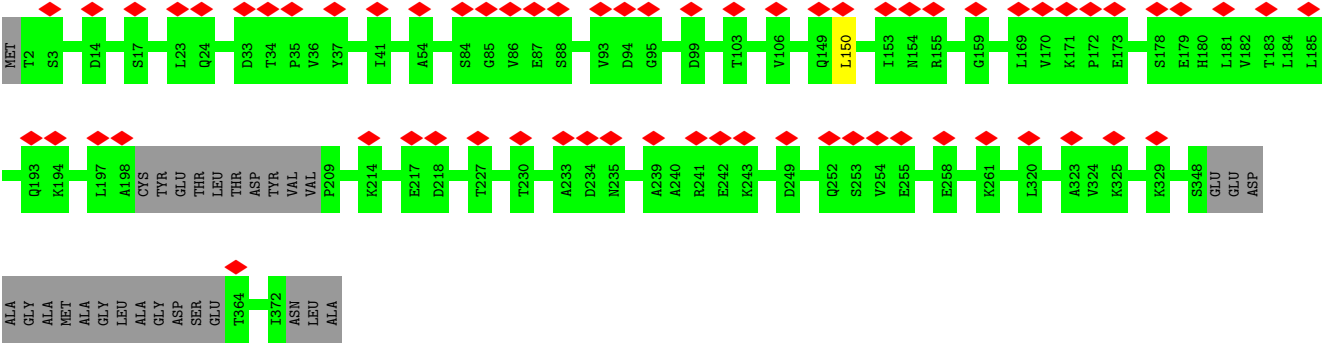
N546	K349	MET
H549	M350	PRO
R560	T354	ALA
ALA	S355	PHE
GLY	A358	Y5
GLY	R362	Y21
MET	F388	P30
ASP	G400	V31
GLY	V407	V32
GLN	T408	V33
K568	I409	V46
L585	G418	R47
Q588	D419	V48
E621	P423	G49
THR	T425	N52
ARG	S426	L53
	A427	I54
	T428	G55
	V432	A65
	Q433	T66
	Y457	I67
	Y460	Q68
	I478	V69
	R479	Y70
	E484	P61
	V485	V62
	L486	P228
	Q487	G232
	A505	Q233
	E506	R234
	G507	V235
	D508	L239
	K509	G246
	I510	T247
	T514	Q263
	L517	A264
	N526	V274
	Y538	V275
	W542	Y276
		V277
		G278
		G279
		G280
		T313
		P322

[illegible]

Chain A:  90% • 7%



● 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	5323	Depositor
Resolution determination method	DIFFRACTION PATTERN/LAYERLINES	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.136	Depositor
Minimum map value	-0.258	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.194	Depositor
Map size (Å)	476.16, 476.16, 476.16	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	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: MG, 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	T	0.86	0/2072	1.50	3/2587 (0.1%)
2	a	0.70	0/2866	1.34	0/3576
3	B	0.95	2/1830 (0.1%)	1.24	24/2284 (1.1%)
3	D	0.92	2/1813 (0.1%)	1.49	22/2261 (1.0%)
3	F	1.24	5/1822 (0.3%)	1.71	65/2274 (2.9%)
4	G	0.85	0/851	1.20	20/1062 (1.9%)
4	I	0.21	0/903	0.41	0/1127
4	K	1.54	1/895 (0.1%)	2.05	41/1117 (3.7%)
5	H	1.18	0/419	1.58	20/522 (3.8%)
5	J	0.20	0/440	0.42	0/547
5	L	1.19	0/428	1.54	10/534 (1.9%)
6	M	0.81	0/871	1.47	4/1087 (0.4%)
7	N	0.94	0/403	1.69	2/502 (0.4%)
8	P	0.17	0/1731	0.37	0/2162
9	b	0.17	0/175	0.30	0/217
10	c	0.20	0/684	0.37	0/852
11	d	1.77	3/1367 (0.2%)	2.34	108/1704 (6.3%)
12	e	0.17	0/223	0.48	0/283
13	g	0.19	0/647	0.32	0/807
13	h	0.18	0/647	0.33	0/807
13	i	0.17	0/643	0.33	0/802
13	j	0.18	0/643	0.35	0/802
13	k	0.18	0/643	0.38	0/802
13	l	0.20	0/643	0.35	0/802
13	m	0.20	0/647	0.34	0/807
13	n	0.19	0/647	0.35	0/807
13	o	0.20	0/635	0.34	0/792
14	r	0.14	0/191	0.28	0/237
15	A	0.83	0/2305	1.19	32/2876 (1.1%)
15	C	1.45	6/2438 (0.2%)	1.97	134/3044 (4.4%)
15	E	1.46	8/2463 (0.3%)	2.05	143/3074 (4.7%)
16	O	0.26	0/1382	0.52	2/1723 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.94	27/34367 (0.1%)	1.37	630/42880 (1.5%)

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	E	55	GLY	N-CA	-7.91	1.37	1.45
15	E	405	GLY	N-CA	-7.79	1.37	1.44
15	C	55	GLY	N-CA	-7.75	1.37	1.45
3	D	322	GLY	N-CA	-6.99	1.37	1.45
15	E	246	GLY	N-CA	-6.74	1.37	1.45

The worst 5 of 630 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	511	THR	CA-C-N	8.42	131.91	120.38
15	A	511	THR	C-N-CA	8.42	131.91	120.38
15	C	54	ILE	CA-C-N	7.62	129.56	121.48
15	C	54	ILE	C-N-CA	7.62	129.56	121.48
15	E	468	TYR	CA-C-N	7.10	130.12	120.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	T	2073	0	576	0	0
2	a	2869	0	774	0	0
3	B	1832	0	504	1	0
3	D	1816	0	499	0	0
3	F	1824	0	502	0	0
4	G	852	0	218	0	0
4	I	904	0	236	0	0
4	K	896	0	231	0	0
5	H	420	0	112	0	0
5	J	441	0	120	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	429	0	115	0	0
6	M	872	0	238	0	0
7	N	404	0	101	0	0
8	P	1732	0	450	0	0
9	b	176	0	49	0	0
10	c	685	0	202	0	0
11	d	1369	0	364	1	0
12	e	224	0	67	0	0
13	g	648	0	204	0	0
13	h	648	0	204	0	0
13	i	644	0	203	0	0
13	j	644	0	203	0	0
13	k	644	0	203	0	0
13	l	644	0	203	0	0
13	m	648	0	204	0	0
13	n	648	0	204	0	0
13	o	636	0	201	0	0
14	r	192	0	50	0	0
15	A	2308	0	635	0	0
15	C	2440	0	675	0	0
15	E	2465	0	683	0	0
16	O	1385	0	352	0	0
17	E	27	0	11	0	0
18	E	1	0	0	0	0
All	All	34440	0	9593	2	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

All (2) 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)
3:B:244:THR:O	3:B:247:ARG:N	2.53	0.41
11:d:350:MET:O	11:d:351:PHE:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	T	516/542 (95%)	483 (94%)	31 (6%)	2 (0%)	30	66
2	a	711/817 (87%)	700 (98%)	10 (1%)	1 (0%)	48	83
3	B	454/486 (93%)	437 (96%)	17 (4%)	0	100	100
3	D	448/486 (92%)	415 (93%)	28 (6%)	5 (1%)	11	45
3	F	452/486 (93%)	432 (96%)	20 (4%)	0	100	100
4	G	211/230 (92%)	207 (98%)	4 (2%)	0	100	100
4	I	224/230 (97%)	221 (99%)	3 (1%)	0	100	100
4	K	222/230 (96%)	218 (98%)	3 (1%)	1 (0%)	24	62
5	H	103/110 (94%)	102 (99%)	1 (1%)	0	100	100
5	J	108/110 (98%)	101 (94%)	7 (6%)	0	100	100
5	L	105/110 (96%)	103 (98%)	2 (2%)	0	100	100
6	M	216/261 (83%)	196 (91%)	15 (7%)	5 (2%)	5	28
7	N	99/128 (77%)	87 (88%)	8 (8%)	4 (4%)	2	18
8	P	431/441 (98%)	423 (98%)	8 (2%)	0	100	100
9	b	42/321 (13%)	42 (100%)	0	0	100	100
10	c	169/180 (94%)	168 (99%)	1 (1%)	0	100	100
11	d	338/351 (96%)	324 (96%)	14 (4%)	0	100	100
12	e	52/70 (74%)	50 (96%)	2 (4%)	0	100	100
13	g	160/164 (98%)	158 (99%)	2 (1%)	0	100	100
13	h	160/164 (98%)	158 (99%)	2 (1%)	0	100	100
13	i	159/164 (97%)	158 (99%)	1 (1%)	0	100	100
13	j	159/164 (97%)	157 (99%)	2 (1%)	0	100	100
13	k	159/164 (97%)	157 (99%)	2 (1%)	0	100	100
13	l	159/164 (97%)	155 (98%)	4 (2%)	0	100	100
13	m	160/164 (98%)	157 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	n	160/164 (98%)	157 (98%)	3 (2%)	0	100	100
13	o	157/164 (96%)	156 (99%)	1 (1%)	0	100	100
14	r	46/364 (13%)	45 (98%)	1 (2%)	0	100	100
15	A	571/623 (92%)	553 (97%)	18 (3%)	0	100	100
15	C	606/623 (97%)	587 (97%)	18 (3%)	1 (0%)	43	77
15	E	612/623 (98%)	575 (94%)	37 (6%)	0	100	100
16	O	340/375 (91%)	322 (95%)	18 (5%)	0	100	100
All	All	8509/9673 (88%)	8204 (96%)	286 (3%)	19 (0%)	44	77

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	M	92	ALA
3	D	448	ASN
3	D	462	ILE
2	a	97	ASP
6	M	161	ASP

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	18	28,29,29	3.01	10 (35%)	43,45,45	2.29	10 (23%)

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	18	-	3/16/32/32	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	E	701	ADP	O4'-C1'	8.55	1.61	1.42
17	E	701	ADP	C2'-C1'	-7.26	1.30	1.53
17	E	701	ADP	O4'-C4'	-6.30	1.31	1.45
17	E	701	ADP	PA-O3A	4.55	1.64	1.59
17	E	701	ADP	C6-N6	4.25	1.45	1.34

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	E	701	ADP	N6-C6-N1	-7.28	102.17	118.38
17	E	701	ADP	C5-C6-N6	5.79	137.61	123.29
17	E	701	ADP	C5-C4-N3	-5.50	119.15	126.72
17	E	701	ADP	N3-C2-N1	-5.07	120.90	128.58
17	E	701	ADP	N3-C4-N9	3.70	133.47	127.17

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	E	701	ADP	O4'-C1'-N9-C8

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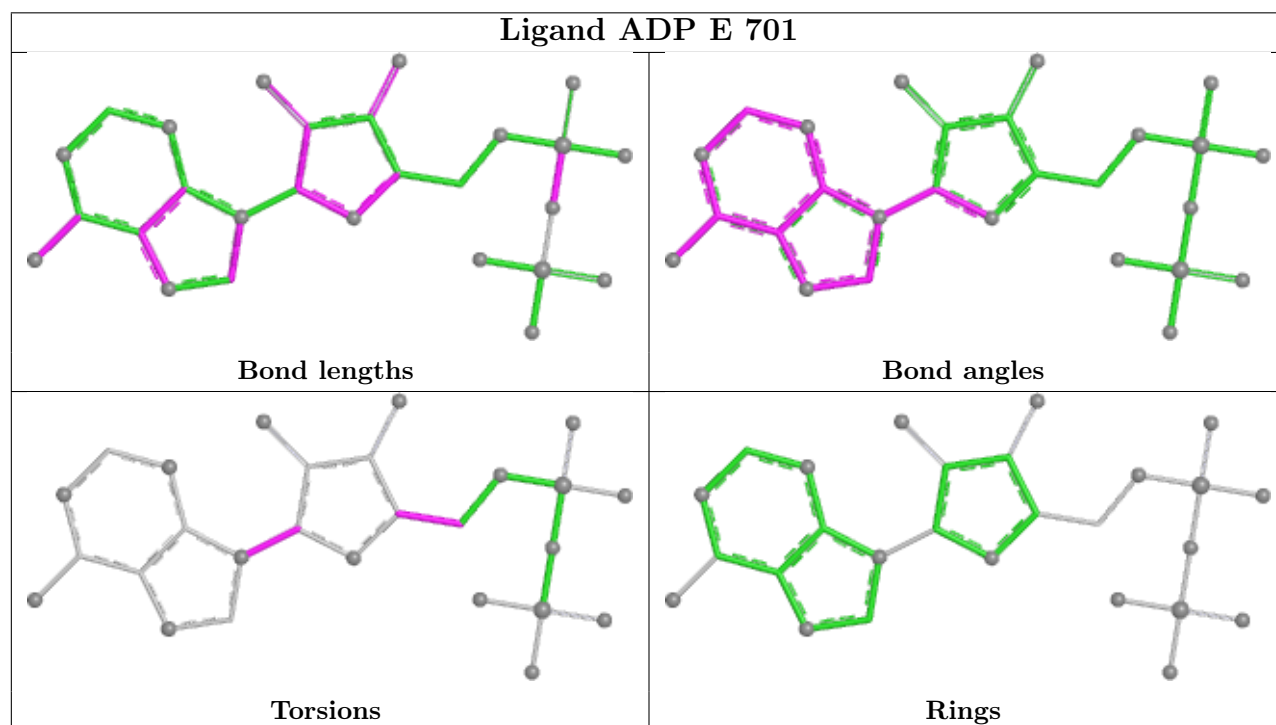
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Mol	Chain	Res	Type	Atoms
17	E	701	ADP	O4'-C1'-N9-C4
17	E	701	ADP	O4'-C4'-C5'-O5'

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 ⓘ

There are no chain breaks in this entry.

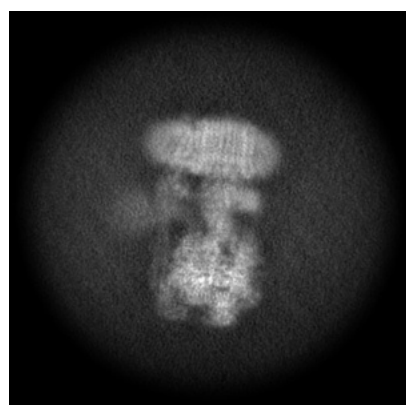
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-77789. These allow visual inspection of the internal detail of the map and identification of artifacts.

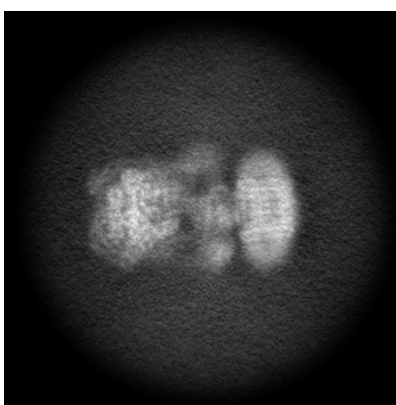
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

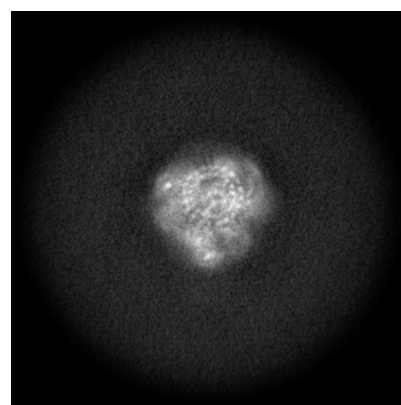
6.1.1 Primary map



X



Y

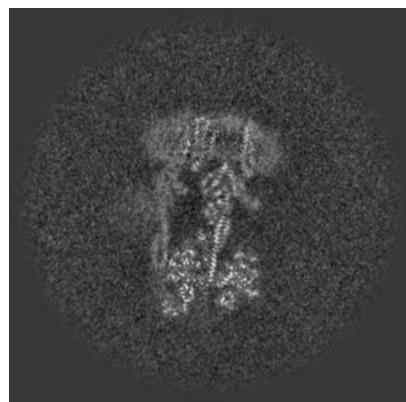


Z

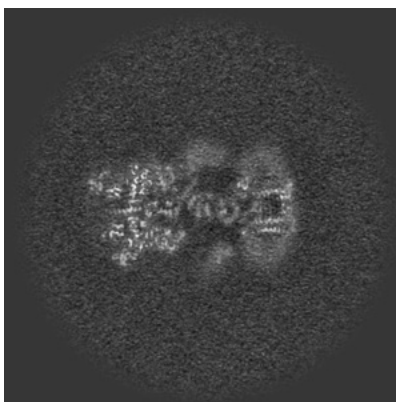
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

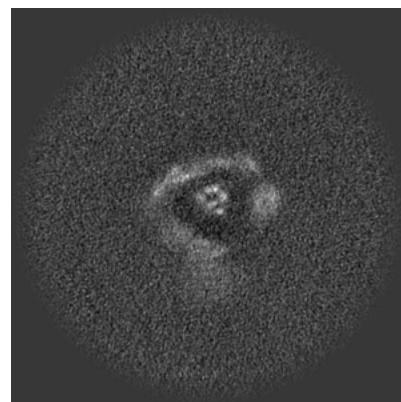
6.2.1 Primary map



X Index: 256



Y Index: 256

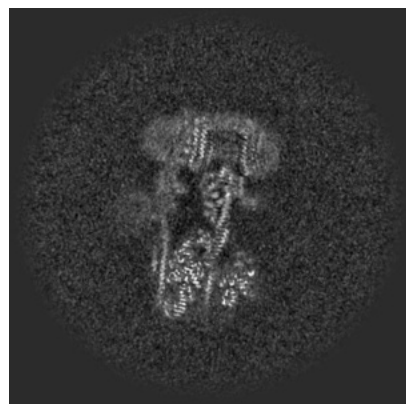


Z Index: 256

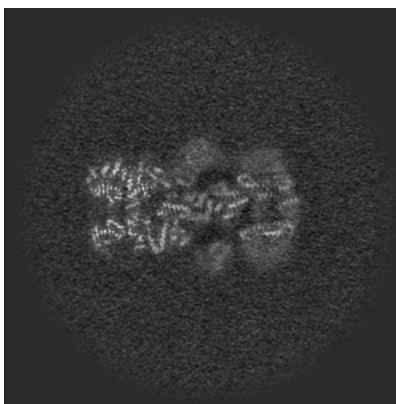
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

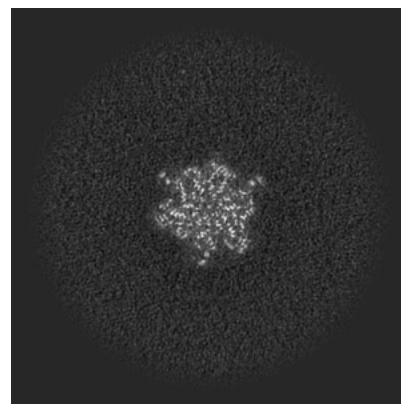
6.3.1 Primary map



X Index: 252



Y Index: 267

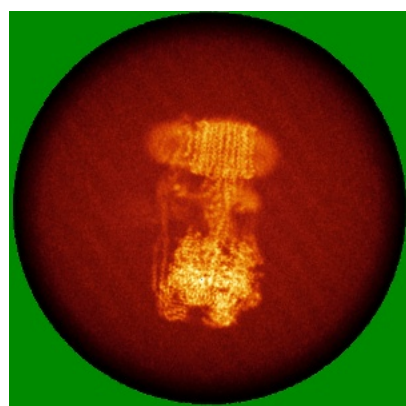


Z Index: 167

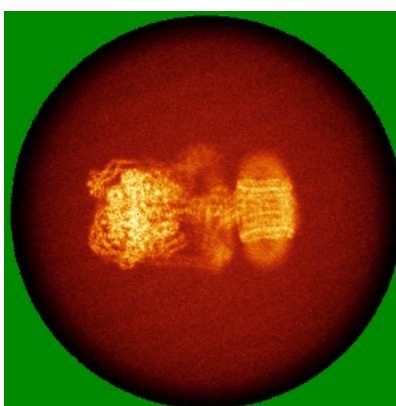
The images above show the largest variance slices of the map in three orthogonal directions.

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

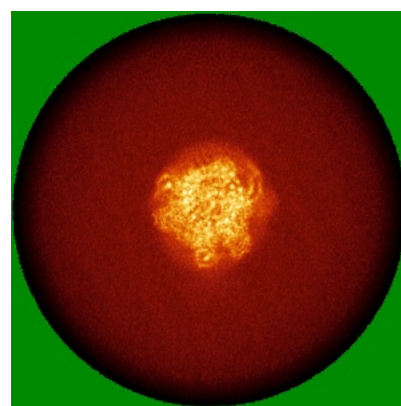
6.4.1 Primary map



X



Y



Z

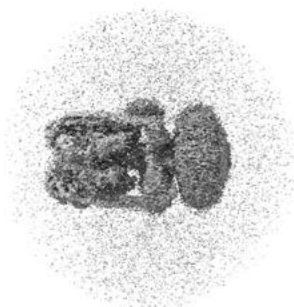
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

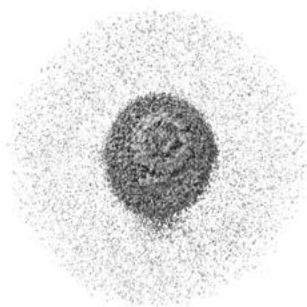
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.194. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

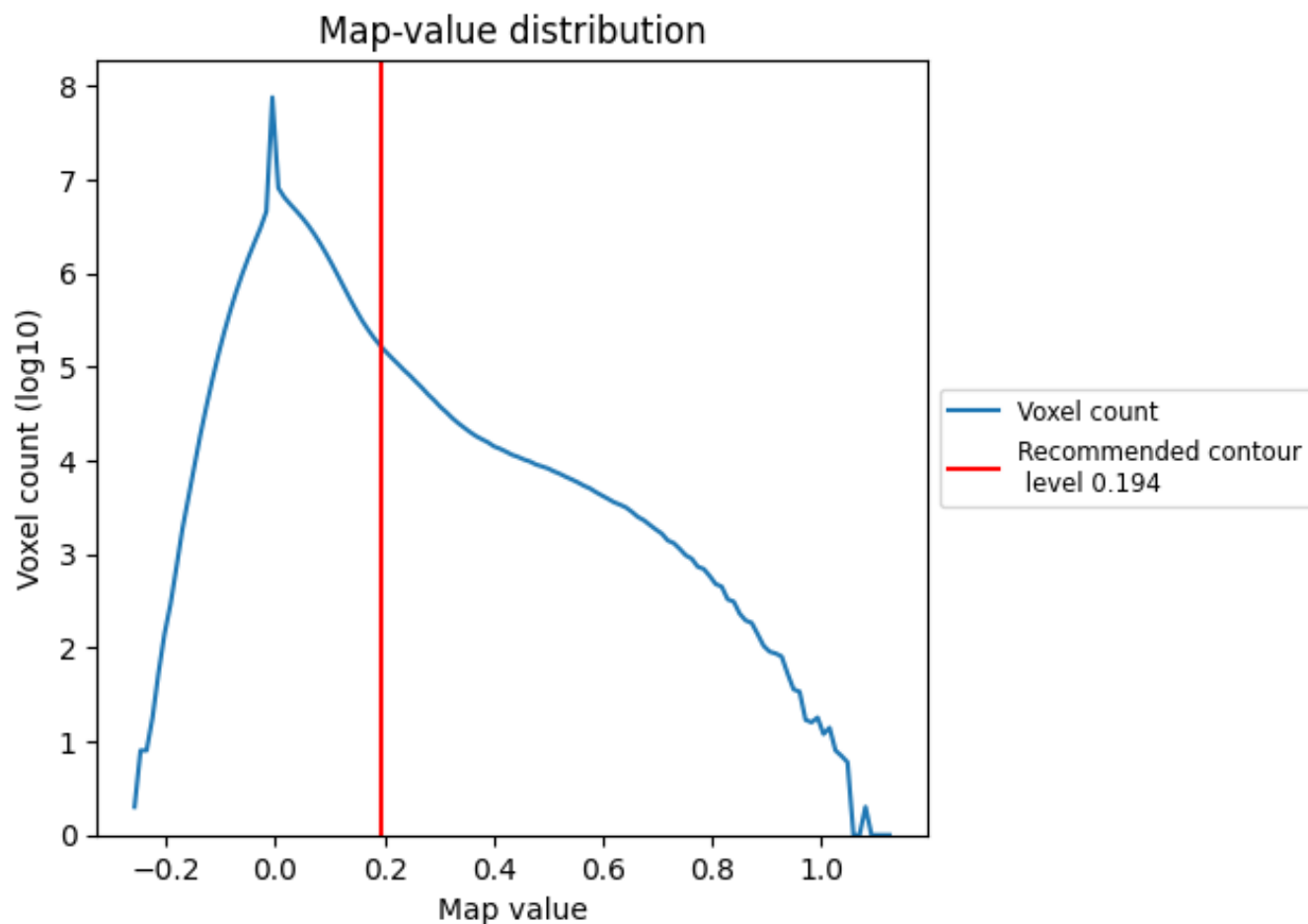
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

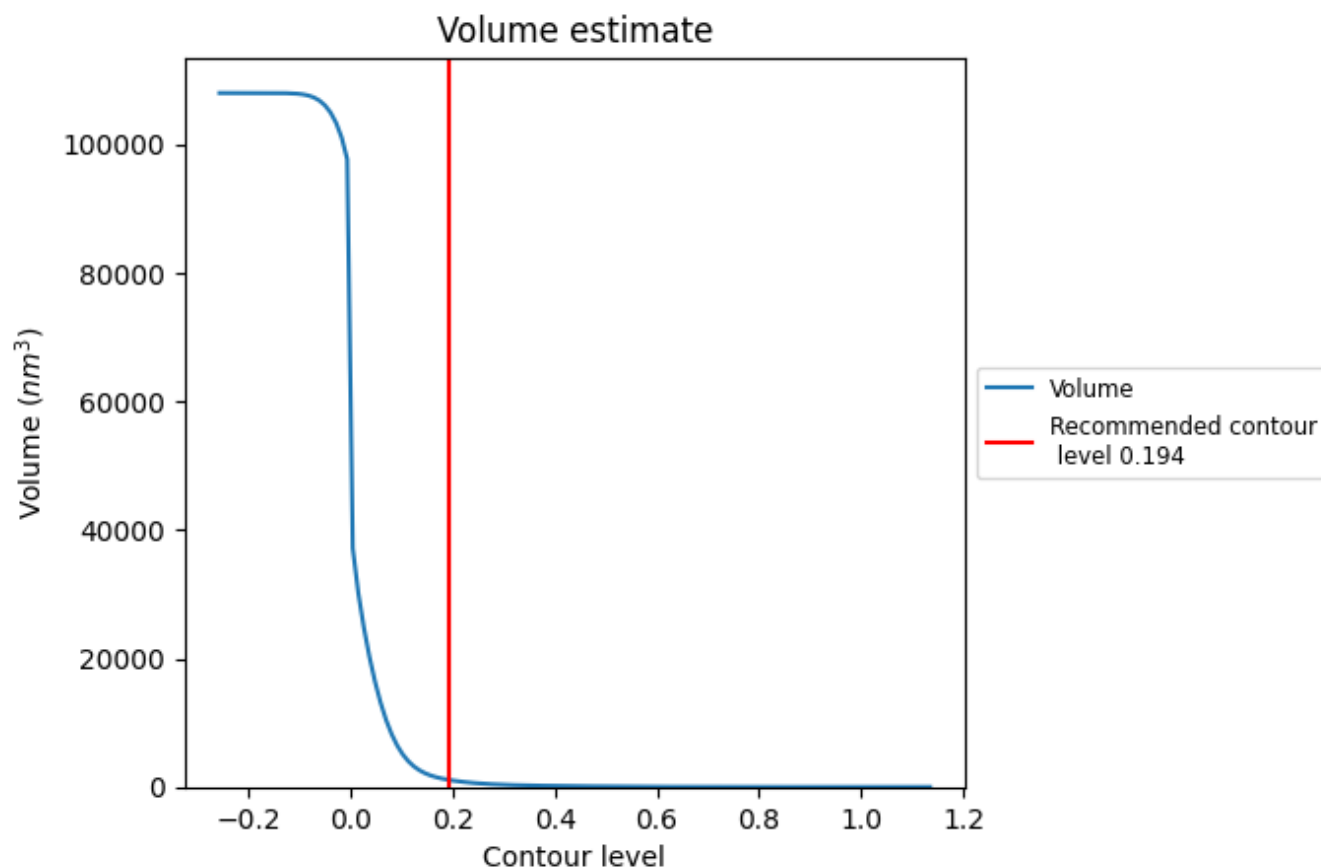
This section contains the results of statistical analysis of the map.

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.

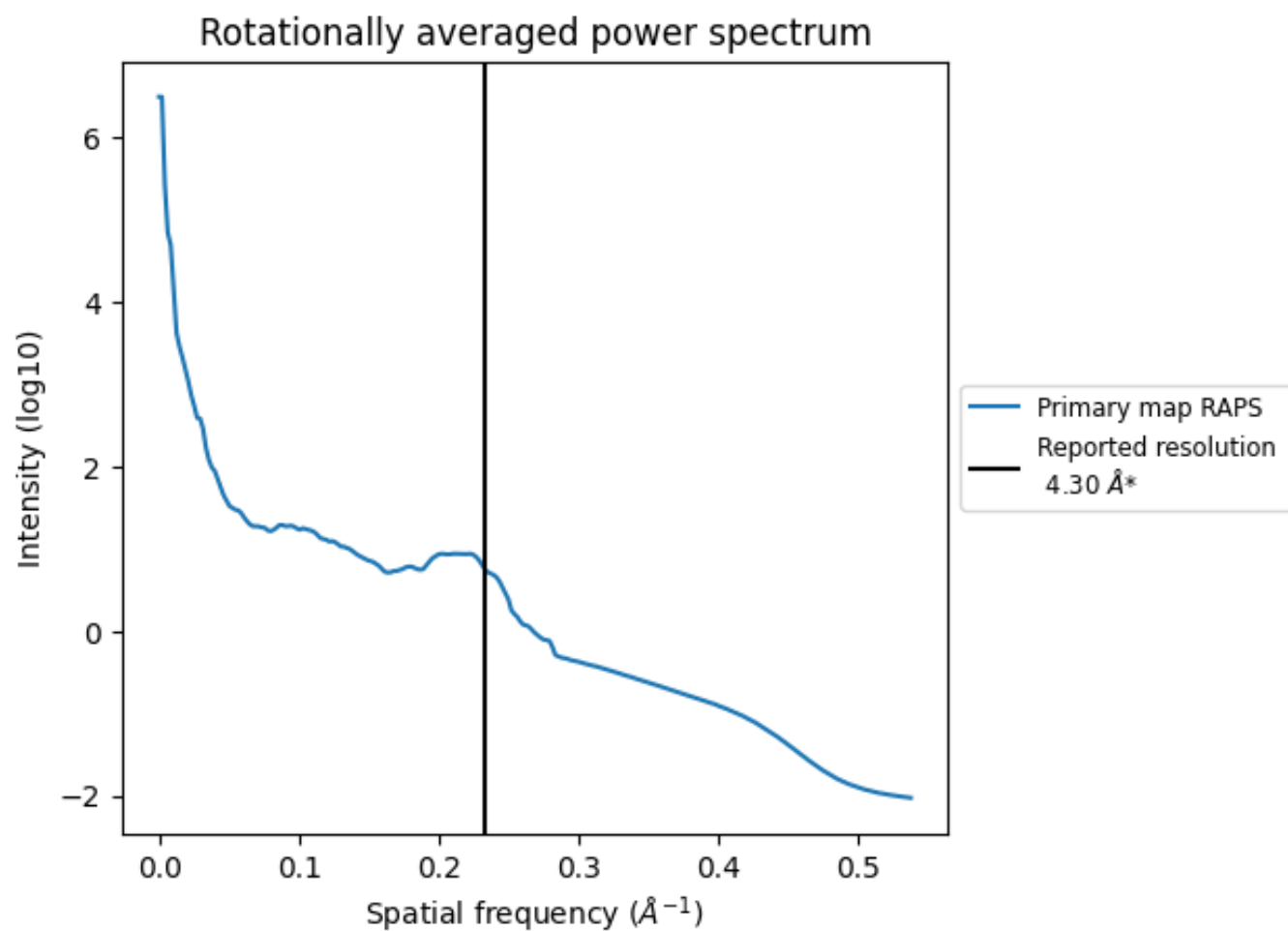
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 10720 nm³; this corresponds to an approximate mass of 968 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 0.233 Å⁻¹

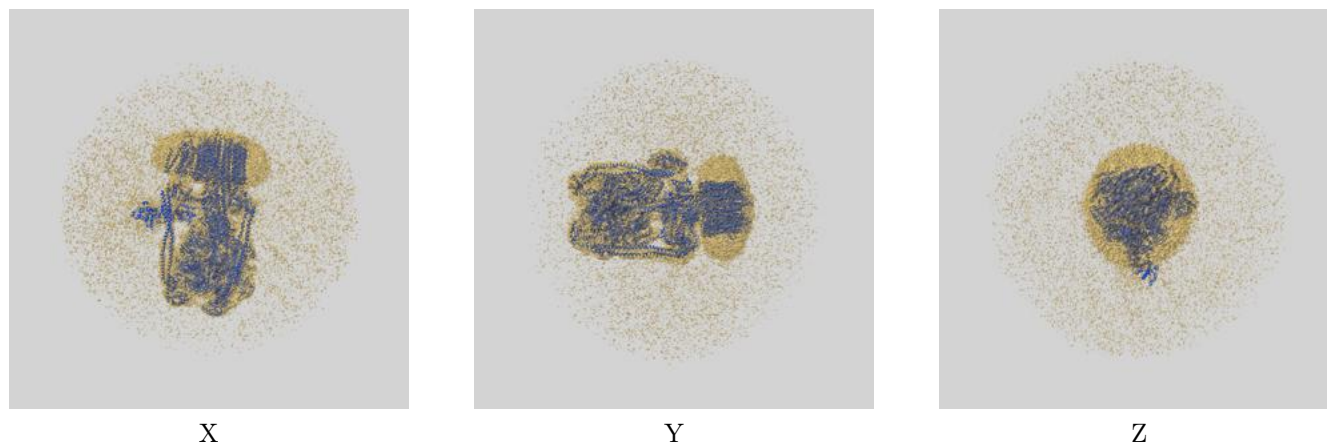
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

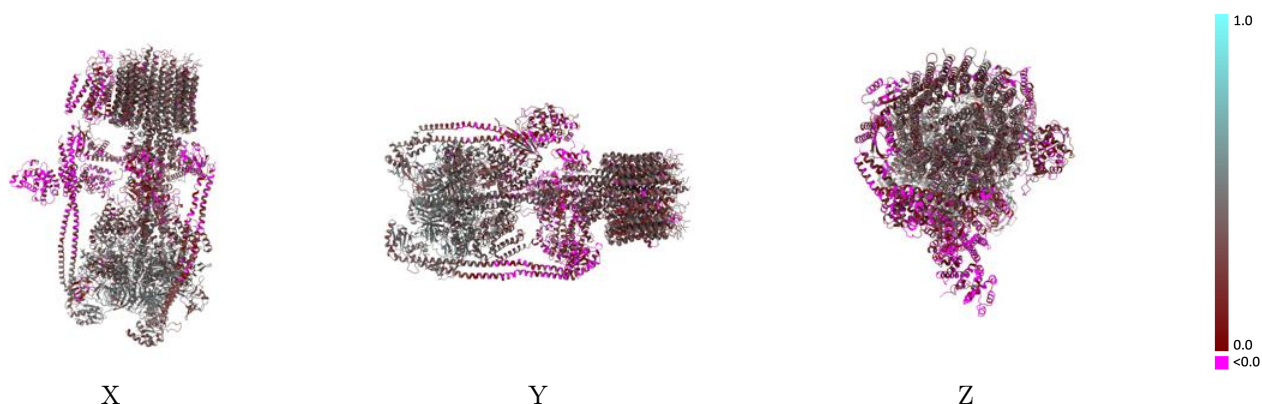
This section contains information regarding the fit between EMDB map EMD-77789 and PDB model 36QX. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



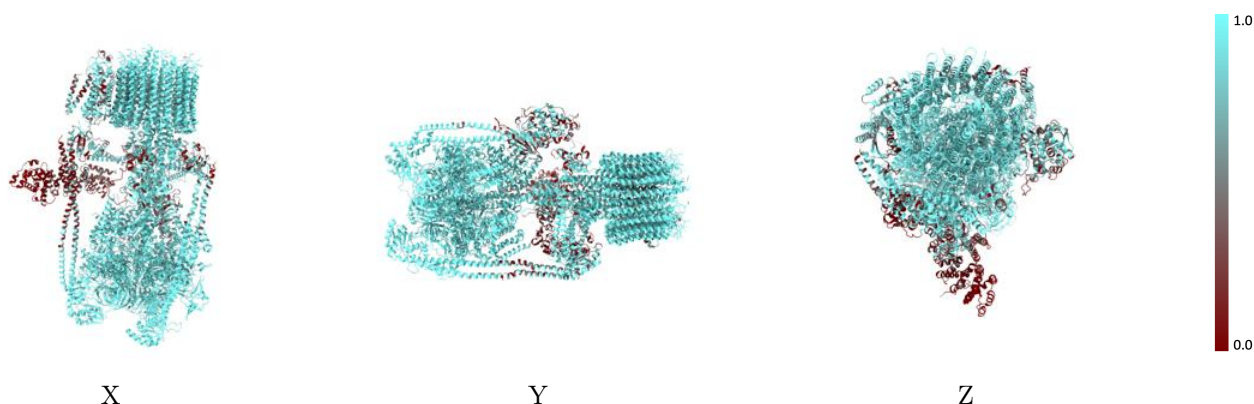
The images above show the 3D surface view of the map at the recommended contour level 0.194 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



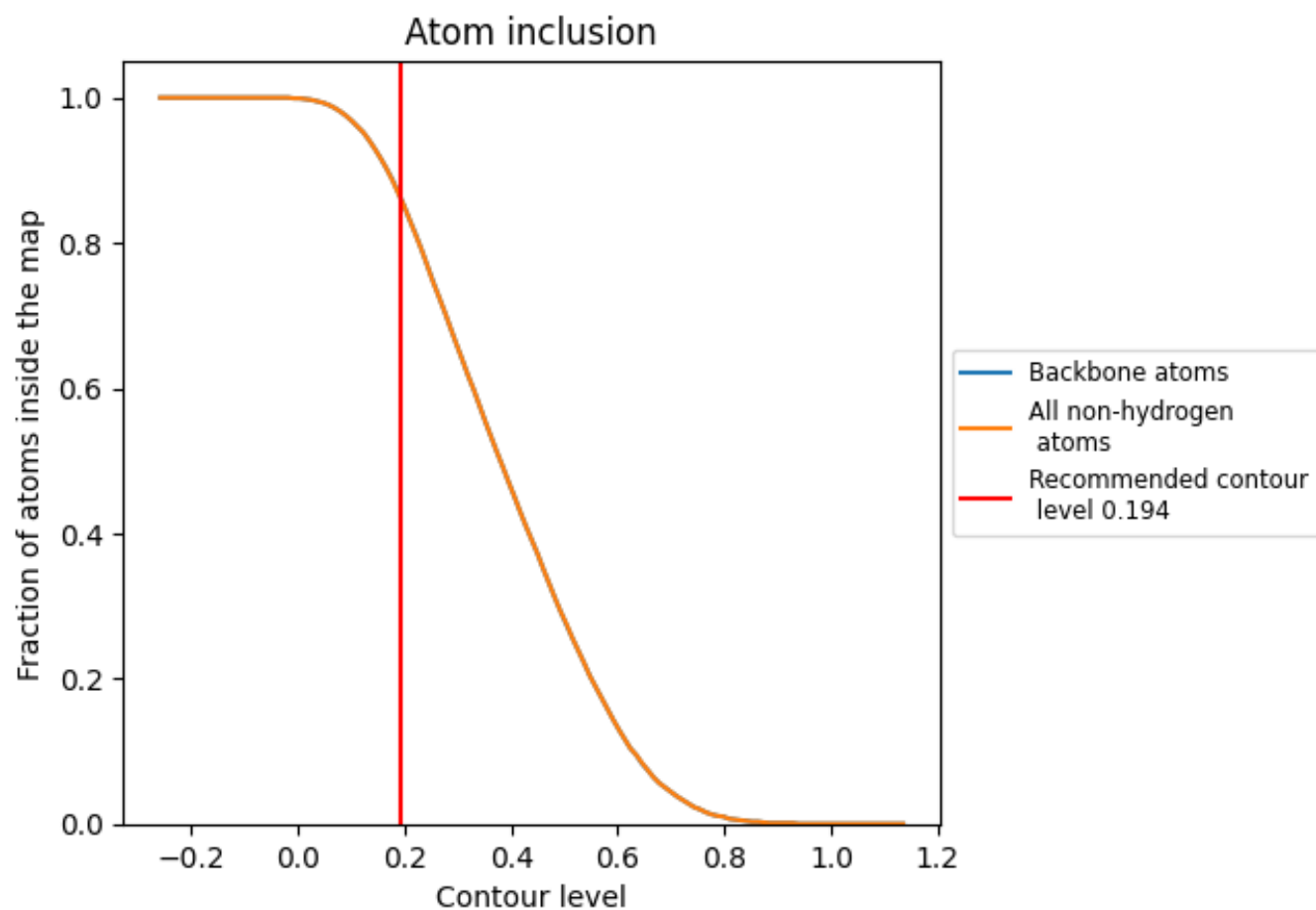
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.194).

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.194) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8600	 0.3030
A	 0.9850	 0.4050
B	 0.9890	 0.4500
C	 0.9740	 0.4100
D	 0.9800	 0.4430
E	 0.9680	 0.3650
F	 0.9840	 0.4290
G	 0.9570	 0.3130
H	 0.8140	 0.1900
I	 0.9180	 0.3280
J	 0.8230	 0.1840
K	 0.8390	 0.3000
L	 0.5800	 0.1460
M	 0.9290	 0.3490
N	 0.9460	 0.3030
O	 0.7160	 0.1010
P	 0.1420	 0.0230
T	 0.6310	 0.2210
a	 0.7310	 0.1200
b	 0.9200	 0.3410
c	 0.9640	 0.3390
d	 0.9550	 0.3320
e	 0.5310	 -0.0070
g	 0.9660	 0.3380
h	 0.9610	 0.3230
i	 0.9350	 0.3130
j	 0.9630	 0.3260
k	 0.9490	 0.3360
l	 0.9800	 0.3440
m	 0.9610	 0.3170
n	 0.9320	 0.2960
o	 0.9560	 0.3350
r	 0.9270	 0.3720

