



wwPDB EM Validation Summary Report ⓘ

Jul 28, 2025 – 03:33 PM EDT

PDB ID : 9CFC / pdb_00009cfc
EMDB ID : EMD-45536
Title : Cryo-EM structure of human kidney V-ATPase state 2
Authors : Zhang, Z.; Lyu, M.
Deposited on : 2024-06-27
Resolution : 3.47 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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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.dev126
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

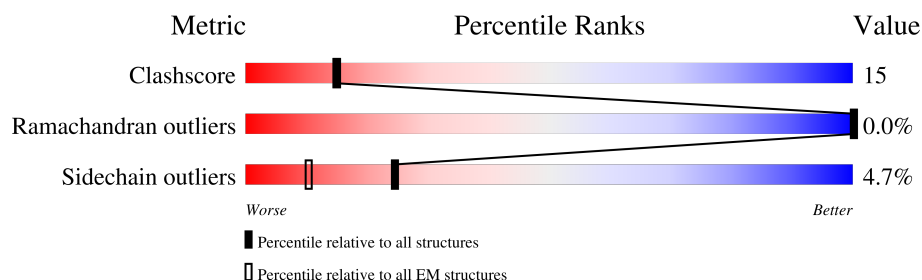
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.47 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
















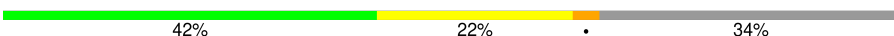





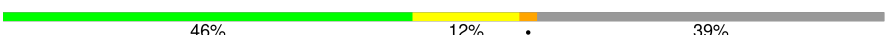


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	0	205	68% 26% 5%
2	1	155	74% 23% .
2	2	155	73% 22% . .
2	3	155	70% 25% . .
2	4	155	70% 25% . .
2	5	155	74% 23% .
2	6	155	70% 26% . .
2	7	155	69% 28% .

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Mol	Chain	Length	Quality of chain
2	8	155	
2	9	155	
3	A	617	
3	B	617	
3	C	617	
4	D	511	
4	E	511	
4	F	511	
5	G	247	
6	H	226	
6	I	226	
6	J	226	
7	K	118	
7	L	118	
7	M	118	
8	N	119	
9	Q	351	
10	R	837	
11	S	81	
12	T	137	
13	U	470	
14	V	350	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 55935 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called V-type proton ATPase 21 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	204	Total	C	N	O	S	0	0
			1498	990	238	259	11		

- Molecule 2 is a protein called V-type proton ATPase 16 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
2	2	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
2	3	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
2	4	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
2	5	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
2	6	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
2	7	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
2	8	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
2	9	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	556	Total	C	N	O	S	0	0
			4318	2741	727	823	27		
3	B	594	Total	C	N	O	S	0	0
			4603	2923	777	875	28		
3	C	576	Total	C	N	O	S	0	0
			4483	2849	756	853	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	467	Total	C	N	O	S	0	0
			3640	2308	620	692	20		
4	E	467	Total	C	N	O	S	0	0
			3655	2319	621	695	20		
4	F	467	Total	C	N	O	S	0	0
			3655	2319	621	695	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	213	Total	C	N	O	S	0	0
			1697	1076	305	311	5		

- Molecule 6 is a protein called V-type proton ATPase subunit E 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	179	Total	C	N	O	S	0	0
			1426	898	255	266	7		
6	I	216	Total	C	N	O	S	0	0
			1757	1104	311	332	10		
6	J	177	Total	C	N	O	S	0	0
			1438	907	257	266	8		

- Molecule 7 is a protein called V-type proton ATPase subunit G 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	114	Total	C	N	O	S	0	0
			938	573	179	183	3		
7	L	78	Total	C	N	O	S	0	0
			645	398	115	129	3		
7	M	54	Total	C	N	O	S	0	0
			446	275	79	89	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	110	Total	C	N	O	S	0	0
			869	549	154	164	2		

- Molecule 9 is a protein called V-type proton ATPase subunit d 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	321	Total	C	N	O	S	0	0
			2602	1681	420	488	13		

- Molecule 10 is a protein called V-type proton ATPase 116 kDa subunit a isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	R	675	Total	C	N	O	S	0	0
			5413	3558	888	930	37		

- Molecule 11 is a protein called V-type proton ATPase subunit e 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	77	Total	C	N	O	S	0	0
			631	436	97	93	5		

- Molecule 12 is a protein called Ribonuclease kappa.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	83	Total	C	N	O	S	0	0
			644	427	99	112	6		

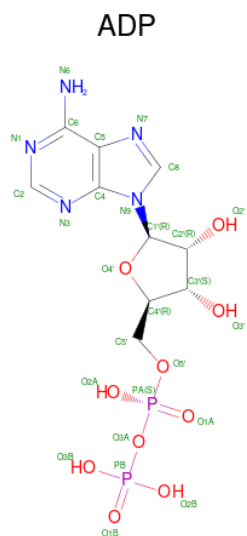
- Molecule 13 is a protein called V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	U	199	Total	C	N	O	S	0	0
			1588	1043	250	285	10		

- Molecule 14 is a protein called Renin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	V	45	Total	C	N	O	S	0	0
			377	256	53	65	3		

- Molecule 15 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

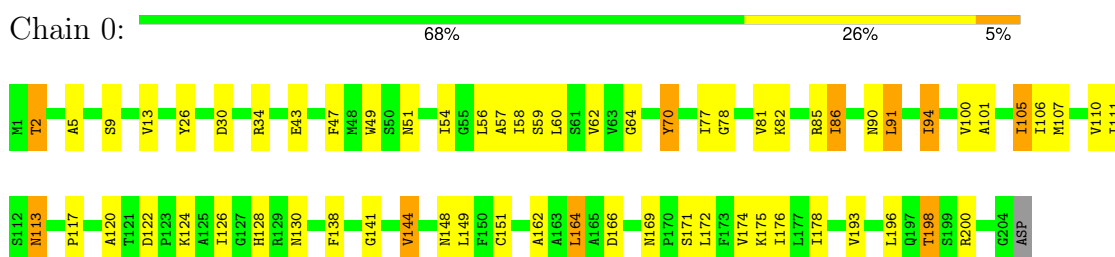


Mol	Chain	Residues	Atoms					AltConf
15	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

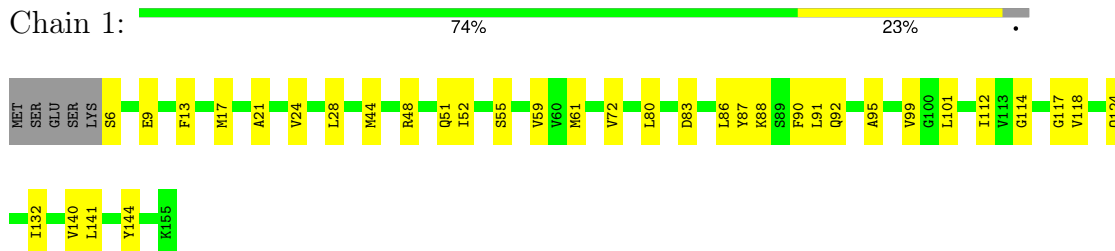
3 Residue-property plots

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.

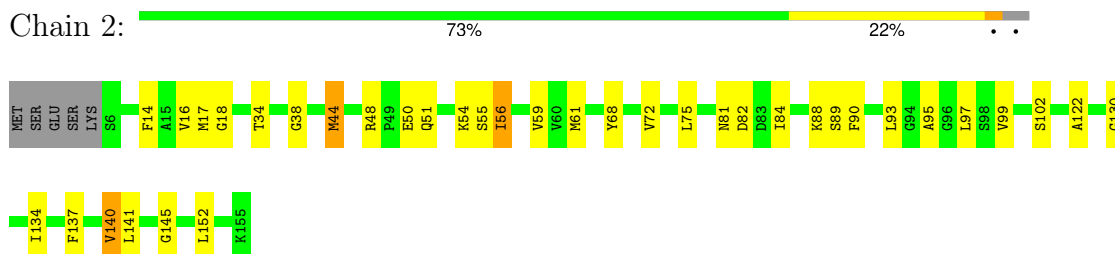
- Molecule 1: V-type proton ATPase 21 kDa proteolipid subunit



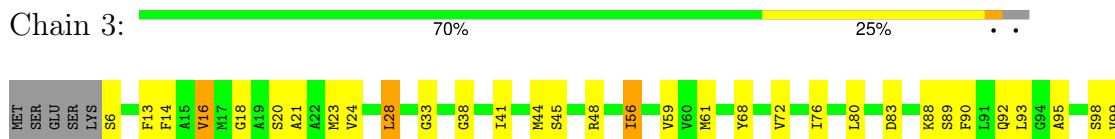
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit



- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit



- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit





- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit

Chain 4: 70% 25%



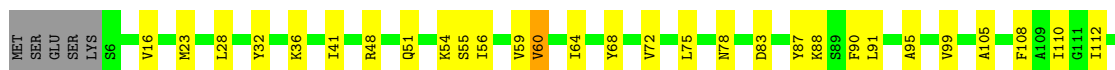
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit

Chain 5: 74% 23%



- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit

Chain 6: 70% 26%



- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit

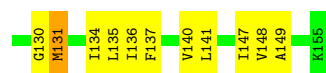
Chain 7: 69% 28%



- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit

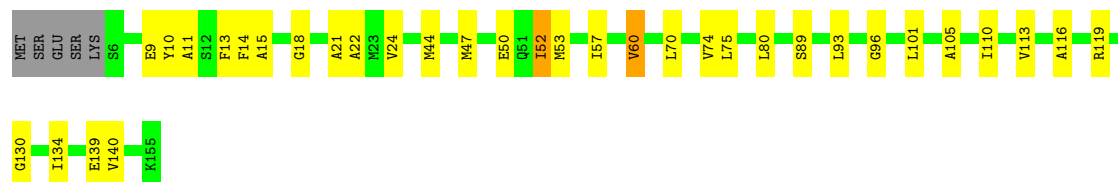
Chain 8: 69% 26%





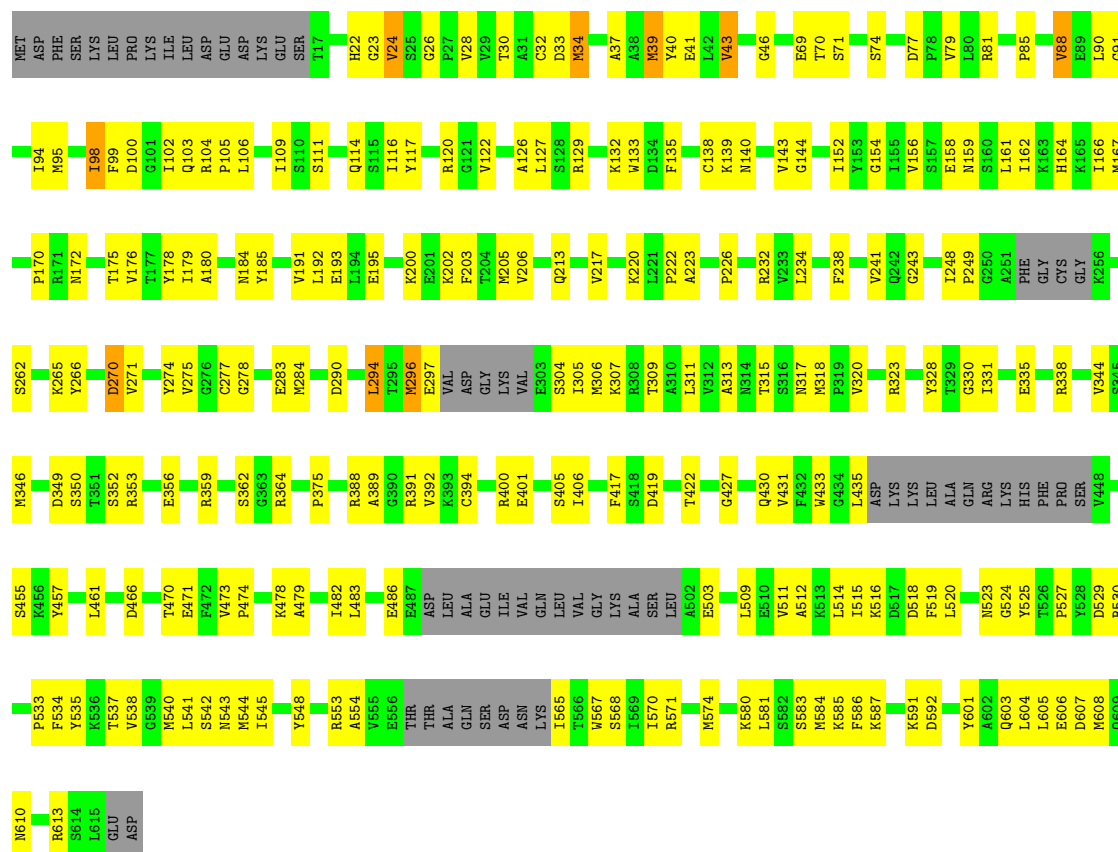
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit

Chain 9: 75% 21% . .



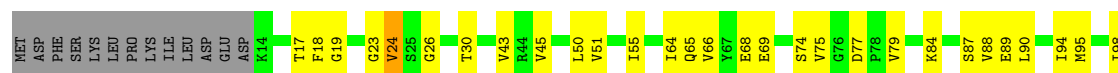
- Molecule 3: V-type proton ATPase catalytic subunit A

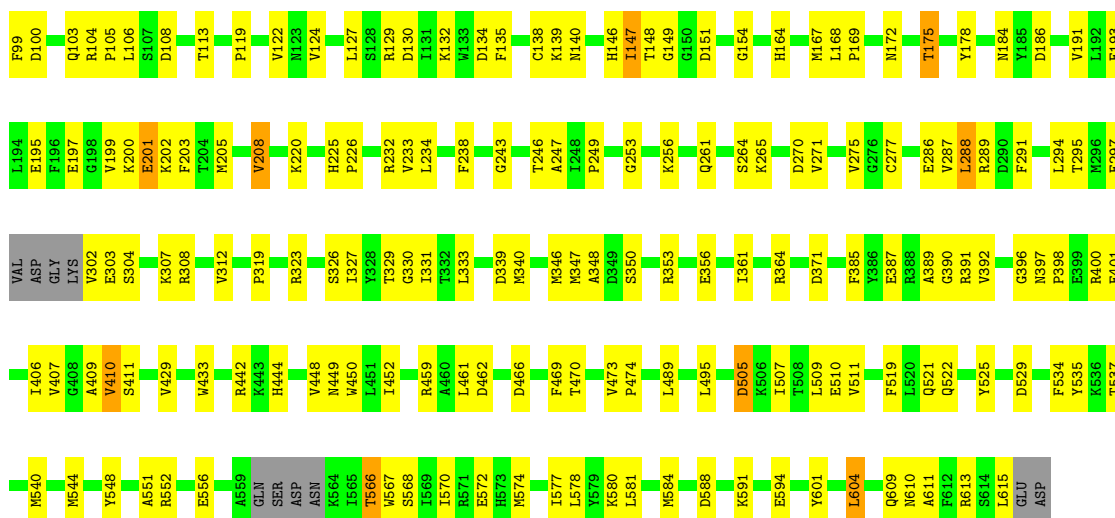
Chain A: 54% 35% 10% . .



- Molecule 3: V-type proton ATPase catalytic subunit A

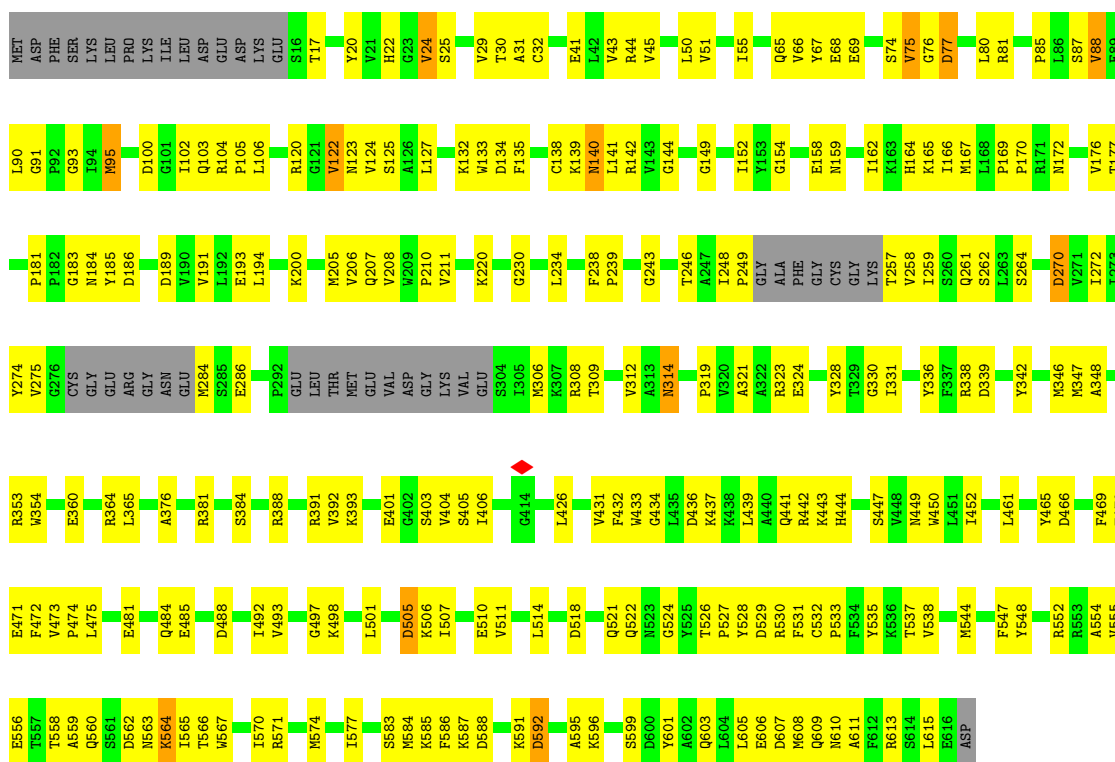
Chain B: 64% 31% . .





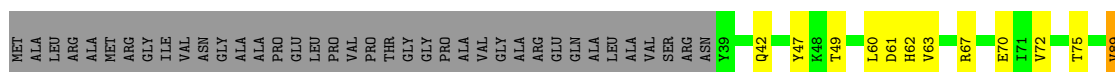
• Molecule 3: V-type proton ATPase catalytic subunit A

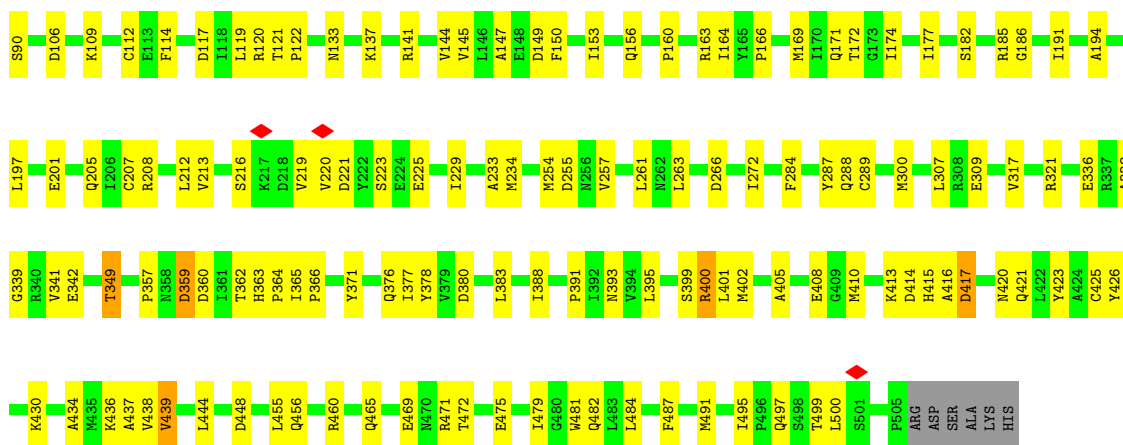
Chain C: 54% 37% 7%



• Molecule 4: V-type proton ATPase subunit B, brain isoform

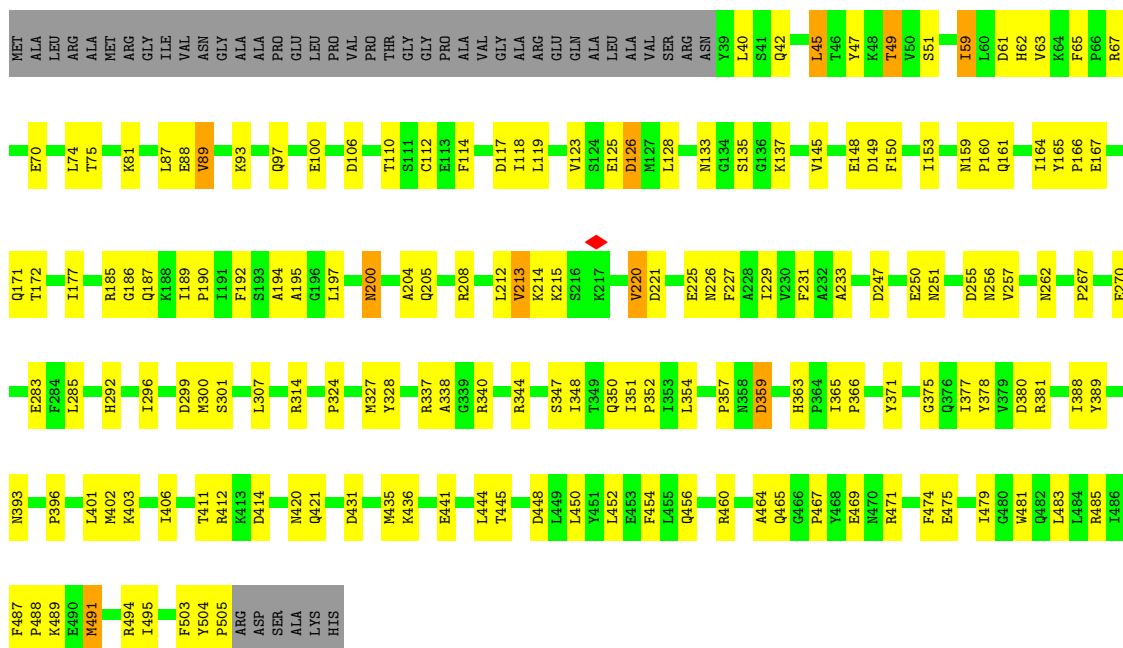
Chain D: 63% 27% 9%





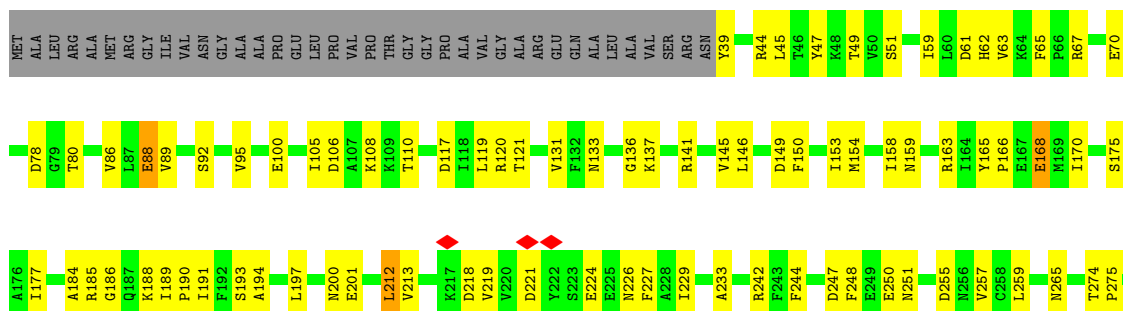
• Molecule 4: V-type proton ATPase subunit B, brain isoform

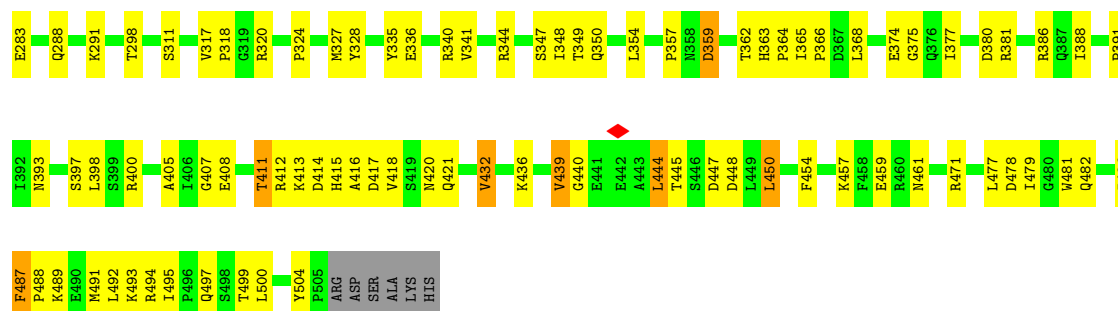
Chain E: 59% 30% 9%



• Molecule 4: V-type proton ATPase subunit B, brain isoform

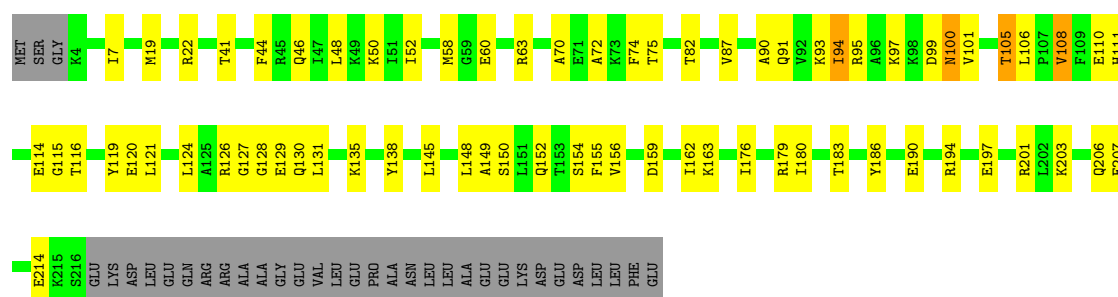
Chain F: 58% 31% 9%





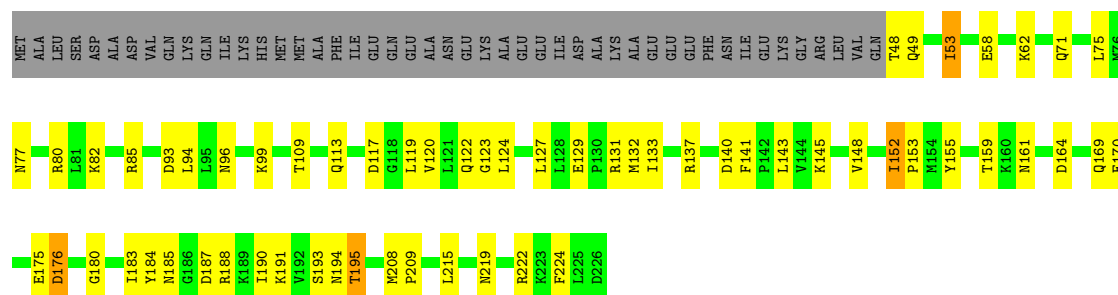
• Molecule 5: V-type proton ATPase subunit D

Chain G: 57% 27% 14%



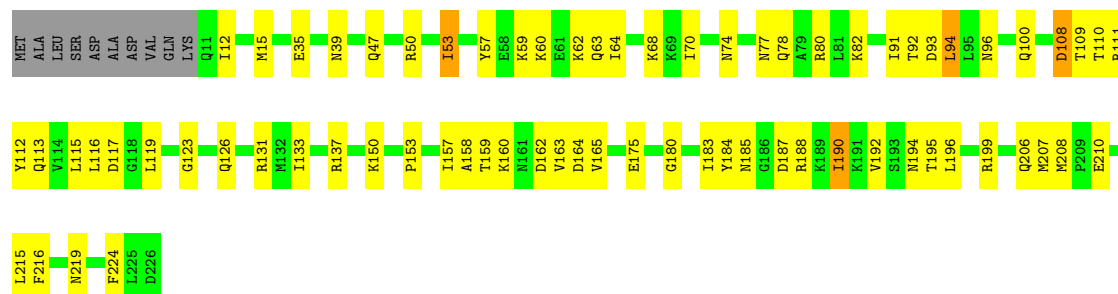
• Molecule 6: V-type proton ATPase subunit E 1

Chain H: 52% 25% 21%



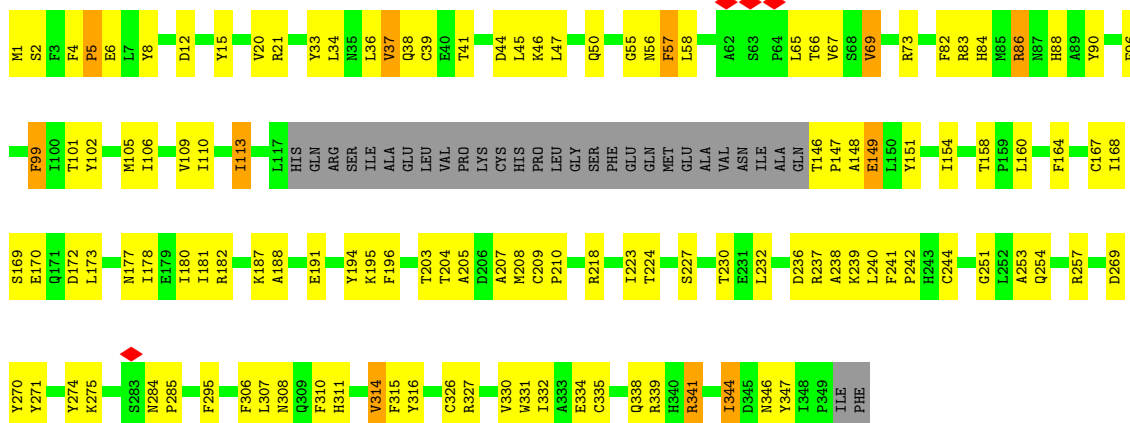
• Molecule 6: V-type proton ATPase subunit E 1

Chain I: 64% 30% 6%

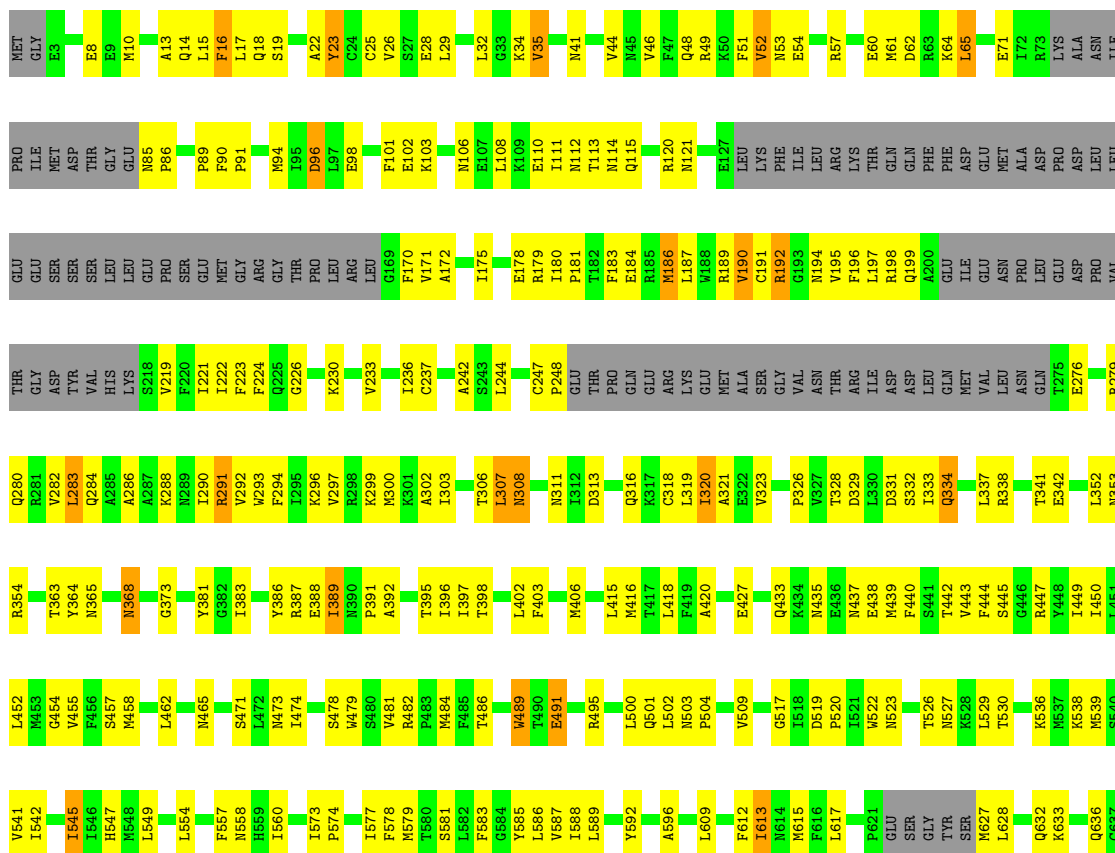


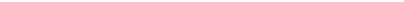


• Molecule 9: V-type proton ATPase subunit d 1



• Molecule 10: V-type proton ATPase 116 kDa subunit a isoform 1



Chain V:  9% . 87%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24168	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.879	Depositor
Minimum map value	-0.097	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	547.84, 547.84, 547.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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	0	0.45	0/1532	0.50	0/2082
2	1	0.38	0/1080	0.37	0/1461
2	2	0.37	0/1080	0.36	0/1461
2	3	0.39	0/1080	0.37	0/1461
2	4	0.38	0/1080	0.36	0/1461
2	5	0.37	0/1080	0.36	0/1461
2	6	0.36	0/1080	0.39	0/1461
2	7	0.40	0/1080	0.41	0/1461
2	8	0.40	0/1080	0.38	0/1461
2	9	0.53	0/1080	0.64	0/1461
3	A	0.36	0/4405	0.44	0/5962
3	B	0.40	0/4697	0.45	0/6359
3	C	0.25	0/4575	0.34	0/6196
4	D	0.35	0/3712	0.41	0/5033
4	E	0.38	0/3728	0.40	0/5053
4	F	0.33	0/3728	0.40	0/5053
5	G	0.21	0/1715	0.30	0/2299
6	H	0.18	0/1440	0.27	0/1935
6	I	0.20	0/1774	0.31	0/2374
6	J	0.18	0/1452	0.29	0/1945
7	K	0.17	0/945	0.28	0/1258
7	L	0.16	0/652	0.21	0/873
7	M	0.14	0/451	0.19	0/606
8	N	0.16	0/883	0.34	0/1193
9	Q	0.91	0/2661	1.17	1/3603 (0.0%)
10	R	0.32	0/5555	0.42	0/7535
11	S	0.36	0/657	0.46	0/902
12	T	0.26	0/660	0.37	0/896
13	U	0.36	0/1641	0.40	0/2238
14	V	0.38	0/390	0.35	0/534
All	All	0.38	0/56973	0.46	1/77078 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
9	Q	0	5
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Q	113	ILE	CA-C-O	-5.10	116.97	121.97

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	400	ARG	Sidechain
9	Q	218	ARG	Sidechain
9	Q	327	ARG	Sidechain
9	Q	83	ARG	Sidechain
9	Q	86	ARG	Sidechain

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	0	1498	0	1544	50	0
2	1	1065	0	1131	26	0
2	2	1065	0	1131	27	0
2	3	1065	0	1131	34	0
2	4	1065	0	1131	35	0
2	5	1065	0	1131	29	0
2	6	1065	0	1131	33	0
2	7	1065	0	1131	33	0
2	8	1065	0	1131	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	9	1065	0	1131	24	0
3	A	4318	0	4286	145	0
3	B	4603	0	4588	137	0
3	C	4483	0	4478	180	0
4	D	3640	0	3630	97	0
4	E	3655	0	3652	124	0
4	F	3655	0	3652	122	0
5	G	1697	0	1779	60	0
6	H	1426	0	1471	45	0
6	I	1757	0	1822	52	0
6	J	1438	0	1513	45	0
7	K	938	0	947	27	0
7	L	645	0	630	20	0
7	M	446	0	435	8	0
8	N	869	0	867	55	0
9	Q	2602	0	2540	94	0
10	R	5413	0	5362	219	0
11	S	631	0	645	25	0
12	T	644	0	641	17	0
13	U	1588	0	1501	44	0
14	V	377	0	365	8	0
15	B	27	0	12	3	0
All	All	55935	0	56539	1659	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 15.

The worst 5 of 1659 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)
9:Q:50:GLN:CA	9:Q:55:GLY:HA2	1.87	1.04
9:Q:50:GLN:HA	9:Q:55:GLY:CA	1.89	1.02
4:D:182:SER:HB2	4:D:402:MET:HG3	1.46	0.98
9:Q:224:THR:HA	9:Q:237:ARG:HD2	1.49	0.92
4:E:190:PRO:HB3	4:E:352:PRO:HG2	1.58	0.85

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	0	202/205 (98%)	200 (99%)	2 (1%)	0	100	100
2	1	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
2	2	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
2	3	148/155 (96%)	148 (100%)	0	0	100	100
2	4	148/155 (96%)	148 (100%)	0	0	100	100
2	5	148/155 (96%)	148 (100%)	0	0	100	100
2	6	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
2	7	148/155 (96%)	148 (100%)	0	0	100	100
2	8	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
2	9	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
3	A	544/617 (88%)	523 (96%)	20 (4%)	1 (0%)	44	76
3	B	588/617 (95%)	566 (96%)	22 (4%)	0	100	100
3	C	568/617 (92%)	543 (96%)	25 (4%)	0	100	100
4	D	465/511 (91%)	449 (97%)	16 (3%)	0	100	100
4	E	465/511 (91%)	449 (97%)	16 (3%)	0	100	100
4	F	465/511 (91%)	448 (96%)	17 (4%)	0	100	100
5	G	211/247 (85%)	206 (98%)	5 (2%)	0	100	100
6	H	177/226 (78%)	177 (100%)	0	0	100	100
6	I	214/226 (95%)	210 (98%)	4 (2%)	0	100	100
6	J	175/226 (77%)	174 (99%)	1 (1%)	0	100	100
7	K	112/118 (95%)	112 (100%)	0	0	100	100
7	L	76/118 (64%)	76 (100%)	0	0	100	100
7	M	52/118 (44%)	51 (98%)	1 (2%)	0	100	100
8	N	108/119 (91%)	106 (98%)	2 (2%)	0	100	100
9	Q	317/351 (90%)	299 (94%)	17 (5%)	1 (0%)	37	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	R	661/837 (79%)	626 (95%)	35 (5%)	0	100	100
11	S	75/81 (93%)	73 (97%)	2 (3%)	0	100	100
12	T	81/137 (59%)	78 (96%)	3 (4%)	0	100	100
13	U	197/470 (42%)	169 (86%)	28 (14%)	0	100	100
14	V	43/350 (12%)	42 (98%)	1 (2%)	0	100	100
All	All	7128/8608 (83%)	6899 (97%)	227 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	Q	5	PRO
3	A	305	ILE

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	0	154/155 (99%)	139 (90%)	15 (10%)	6	27
2	1	107/112 (96%)	104 (97%)	3 (3%)	38	65
2	2	107/112 (96%)	102 (95%)	5 (5%)	22	52
2	3	107/112 (96%)	102 (95%)	5 (5%)	22	52
2	4	107/112 (96%)	103 (96%)	4 (4%)	29	58
2	5	107/112 (96%)	106 (99%)	1 (1%)	75	85
2	6	107/112 (96%)	105 (98%)	2 (2%)	52	73
2	7	107/112 (96%)	104 (97%)	3 (3%)	38	65
2	8	107/112 (96%)	102 (95%)	5 (5%)	22	52
2	9	107/112 (96%)	102 (95%)	5 (5%)	22	52
3	A	470/525 (90%)	452 (96%)	18 (4%)	28	57
3	B	500/525 (95%)	481 (96%)	19 (4%)	28	57
3	C	491/525 (94%)	472 (96%)	19 (4%)	27	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	397/430 (92%)	383 (96%)	14 (4%)	31	60
4	E	400/430 (93%)	383 (96%)	17 (4%)	25	54
4	F	400/430 (93%)	382 (96%)	18 (4%)	23	53
5	G	179/212 (84%)	169 (94%)	10 (6%)	17	45
6	H	153/199 (77%)	147 (96%)	6 (4%)	27	57
6	I	191/199 (96%)	182 (95%)	9 (5%)	22	52
6	J	158/199 (79%)	149 (94%)	9 (6%)	17	45
7	K	99/101 (98%)	95 (96%)	4 (4%)	27	56
7	L	69/101 (68%)	61 (88%)	8 (12%)	4	21
7	M	51/101 (50%)	49 (96%)	2 (4%)	27	57
8	N	93/100 (93%)	90 (97%)	3 (3%)	34	62
9	Q	279/306 (91%)	269 (96%)	10 (4%)	30	59
10	R	582/746 (78%)	539 (93%)	43 (7%)	11	36
11	S	69/72 (96%)	65 (94%)	4 (6%)	17	44
12	T	69/116 (60%)	64 (93%)	5 (7%)	12	38
13	U	171/397 (43%)	160 (94%)	11 (6%)	14	42
14	V	40/308 (13%)	36 (90%)	4 (10%)	6	26
All	All	5978/7185 (83%)	5697 (95%)	281 (5%)	24	52

5 of 281 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	R	320	ILE
10	R	389	ILE
11	S	60	LEU
3	C	314	ASN
3	C	246	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 122 such sidechains are listed below:

Mol	Chain	Res	Type
5	G	91	GLN
11	S	67	GLN
6	J	166	GLN
11	S	61	ASN

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Mol	Chain	Res	Type
13	U	398	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	$\# Z > 2$
15	ADP	B	701	-	24,29,29	0.82	0	29,45,45	1.24	3 (10%)

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
15	ADP	B	701	-	-	5/12/32/32	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	701	ADP	N3-C2-N1	-3.30	124.19	128.67
15	B	701	ADP	C4-C5-N7	-2.29	106.92	109.34
15	B	701	ADP	O3B-PB-O2B	2.08	115.61	107.80

There are no chirality outliers.

All (5) torsion outliers are listed below:

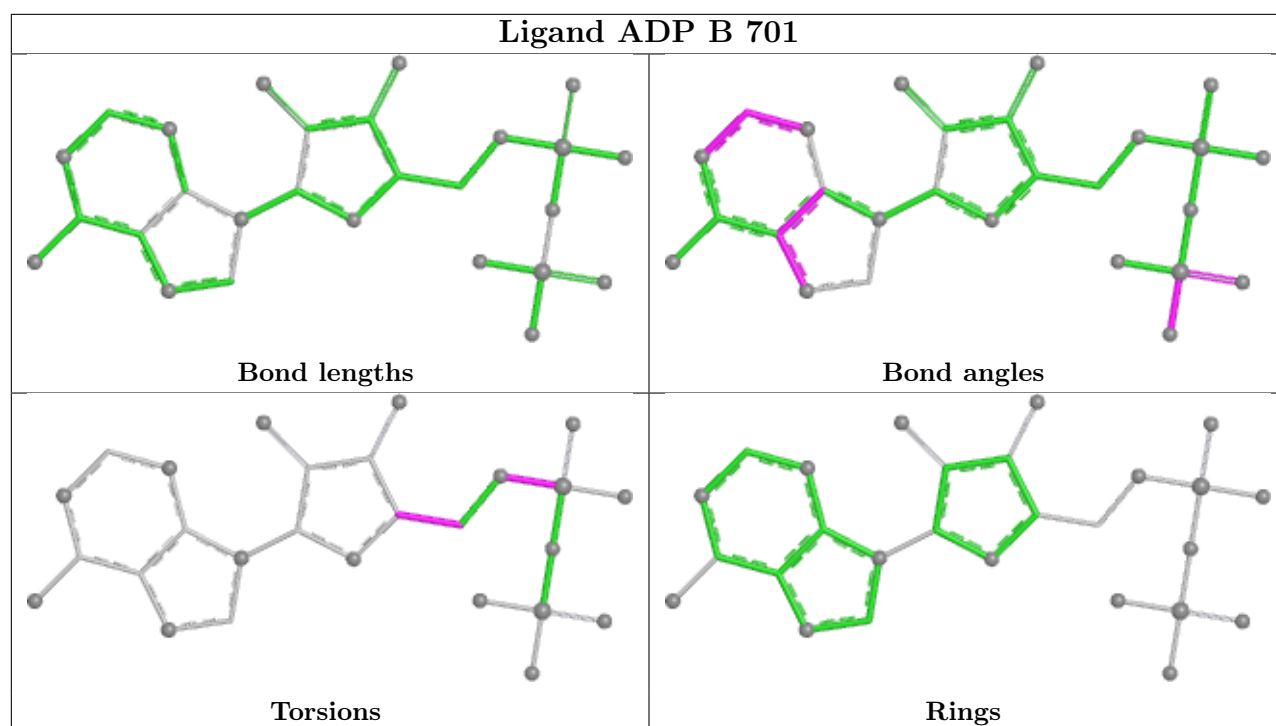
Mol	Chain	Res	Type	Atoms
15	B	701	ADP	C5'-O5'-PA-O2A
15	B	701	ADP	O4'-C4'-C5'-O5'
15	B	701	ADP	C3'-C4'-C5'-O5'
15	B	701	ADP	C5'-O5'-PA-O1A
15	B	701	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	701	ADP	3	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-45536. These allow visual inspection of the internal detail of the map and identification of artifacts.

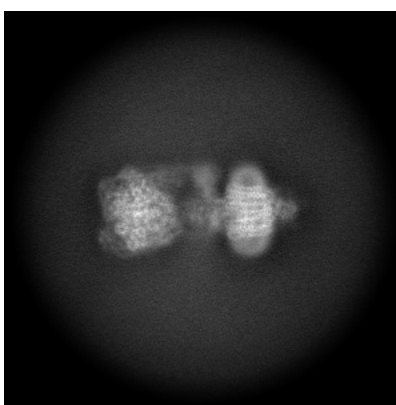
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

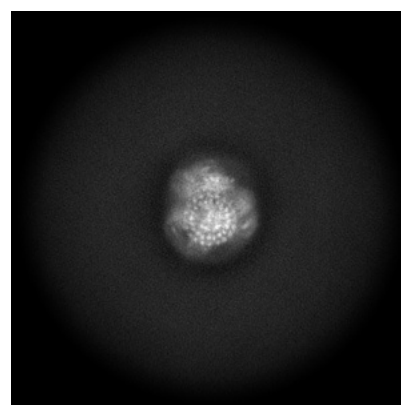
6.1.1 Primary map



X



Y

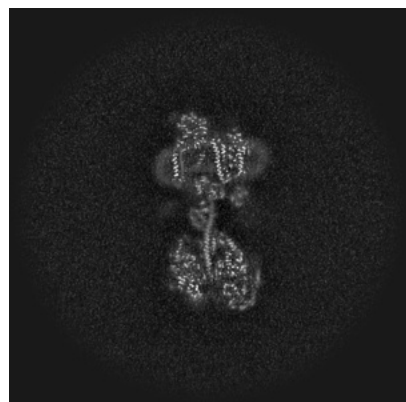


Z

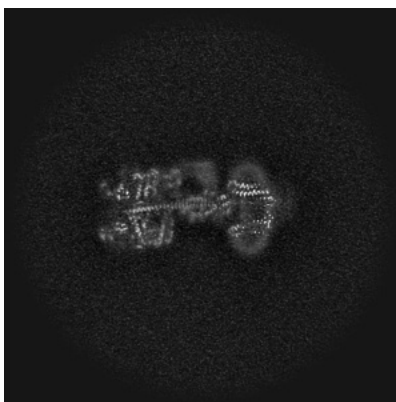
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

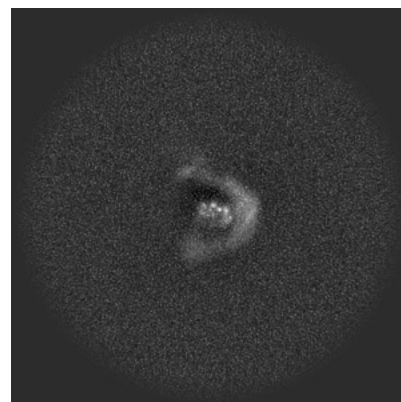
6.2.1 Primary map



X Index: 256



Y Index: 256

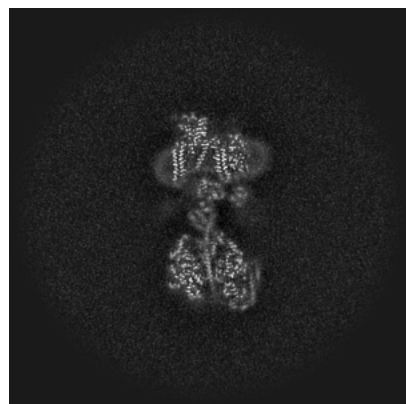


Z Index: 256

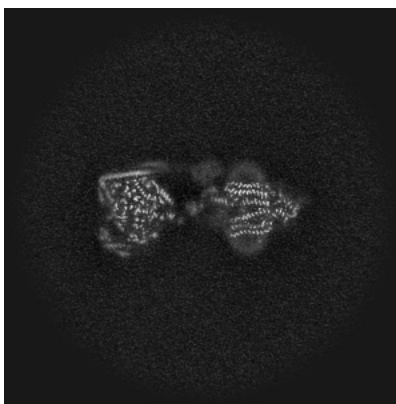
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

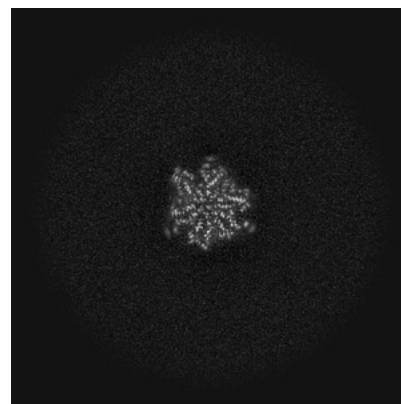
6.3.1 Primary map



X Index: 254



Y Index: 235

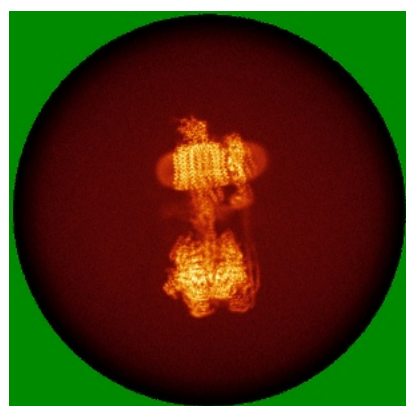


Z Index: 171

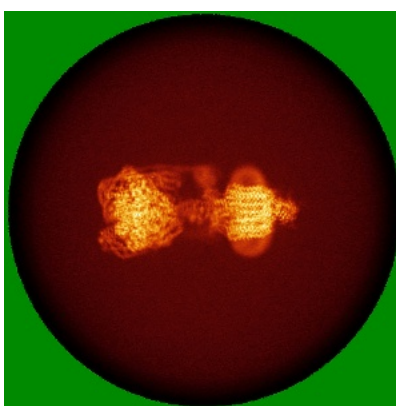
The images above show the largest variance slices of the map in three orthogonal directions.

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

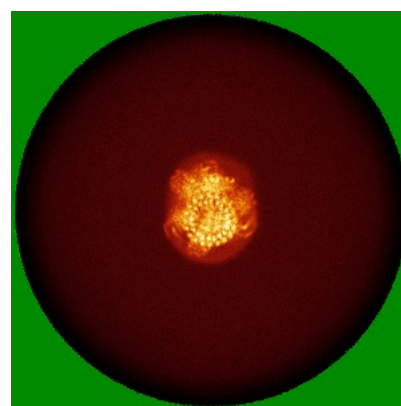
6.4.1 Primary map



X



Y



Z

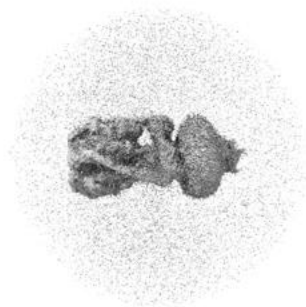
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

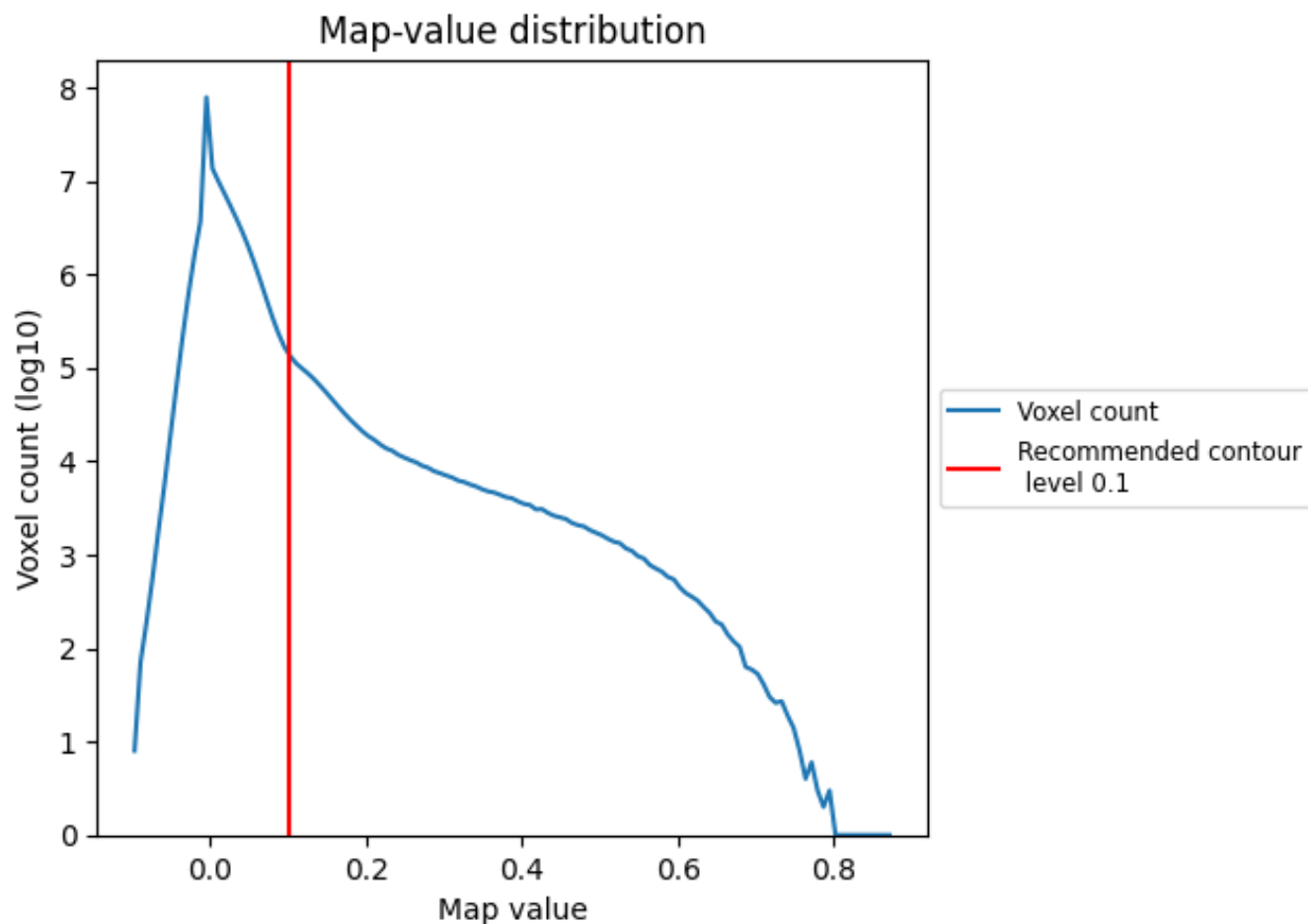
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

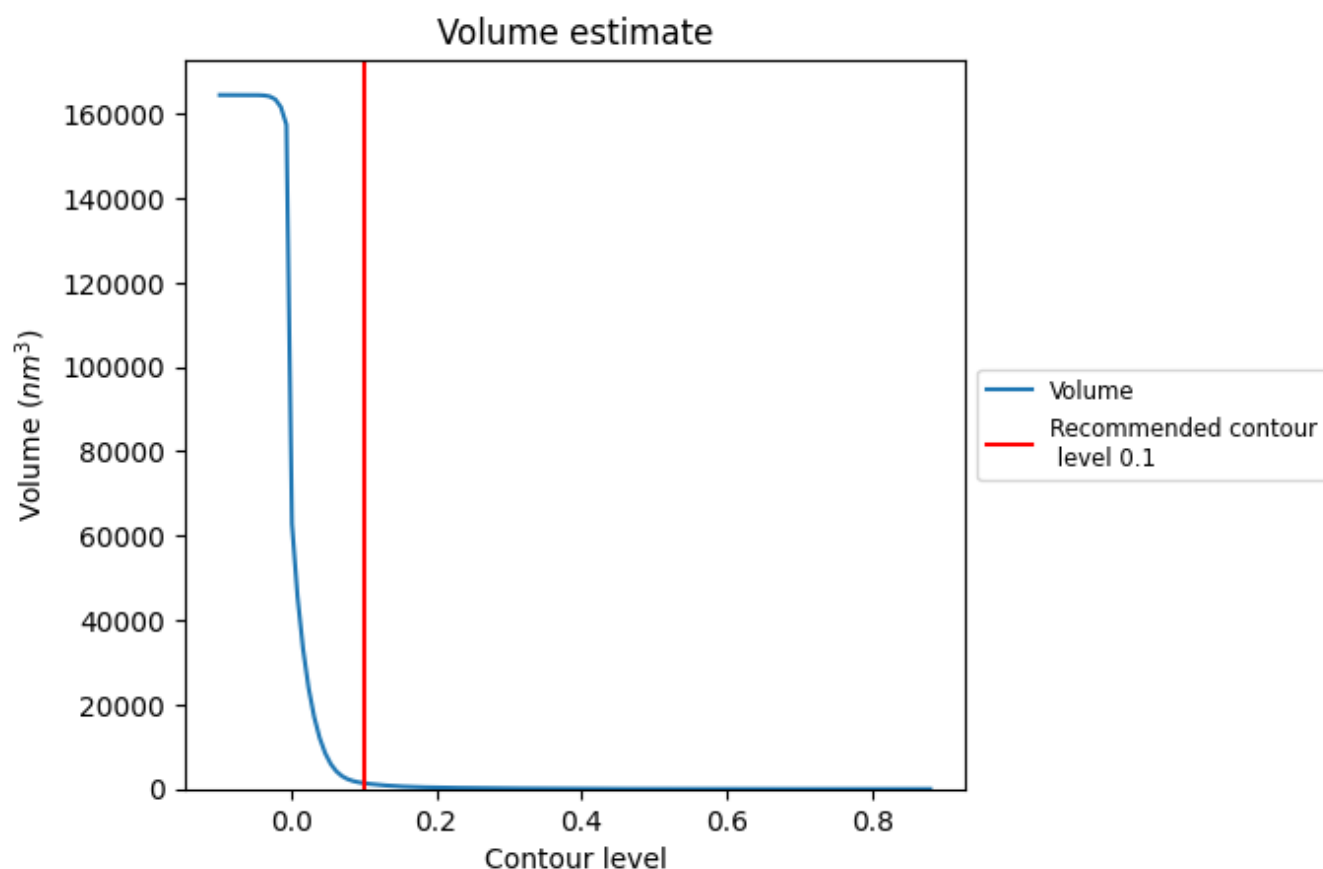
This section contains the results of statistical analysis of the map.

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.

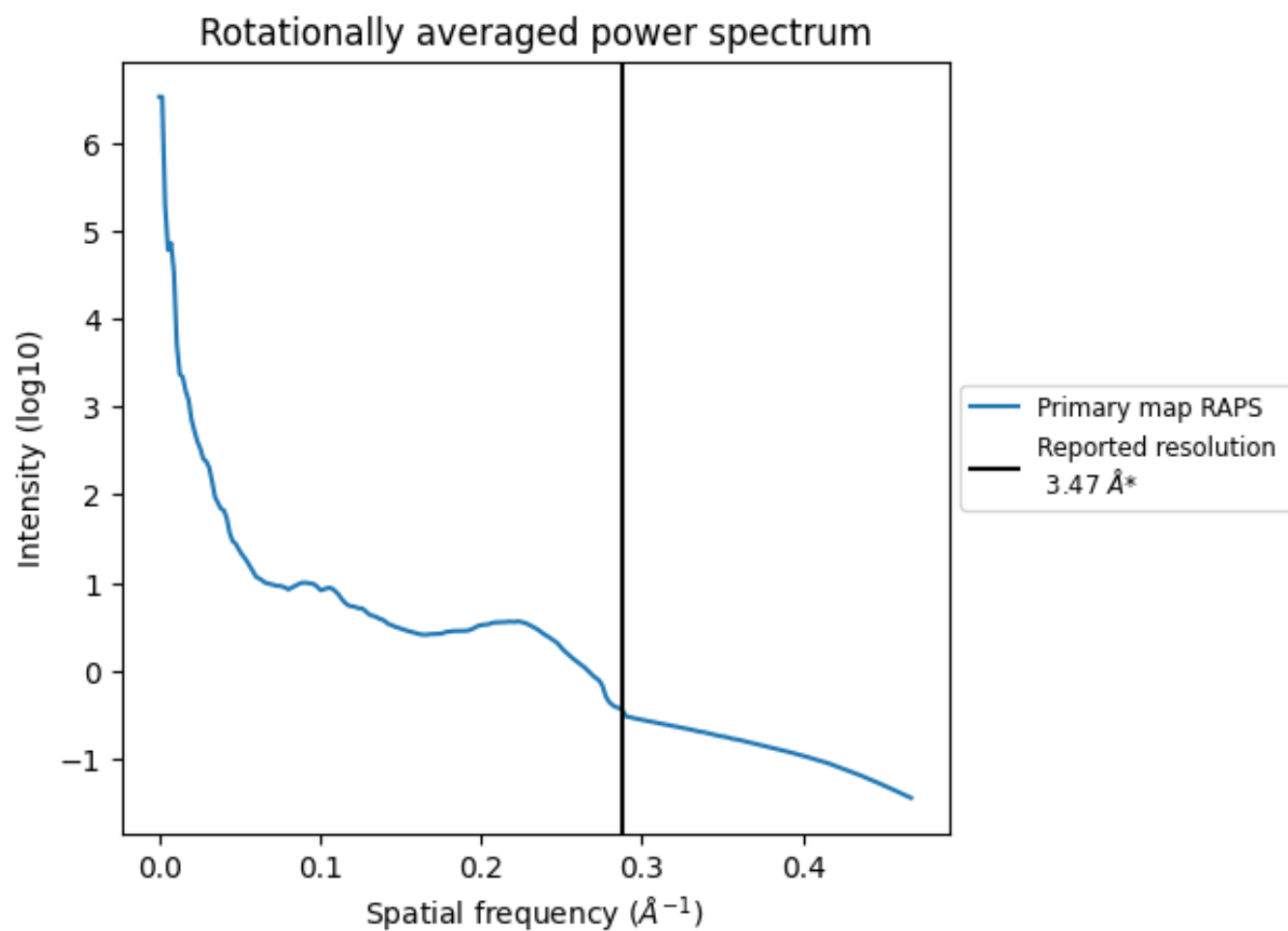
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1388 nm³; this corresponds to an approximate mass of 1254 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 0.288 Å⁻¹

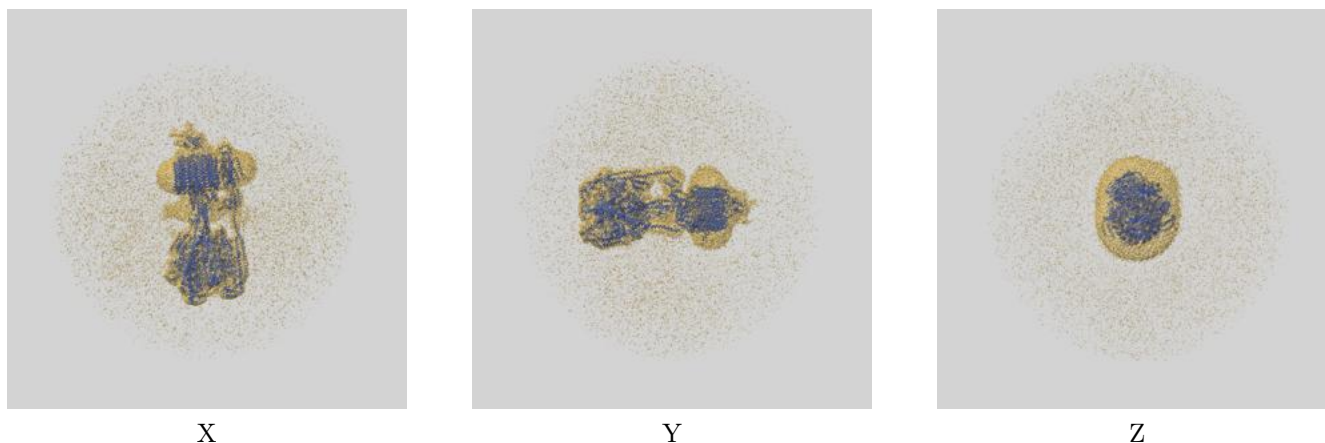
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

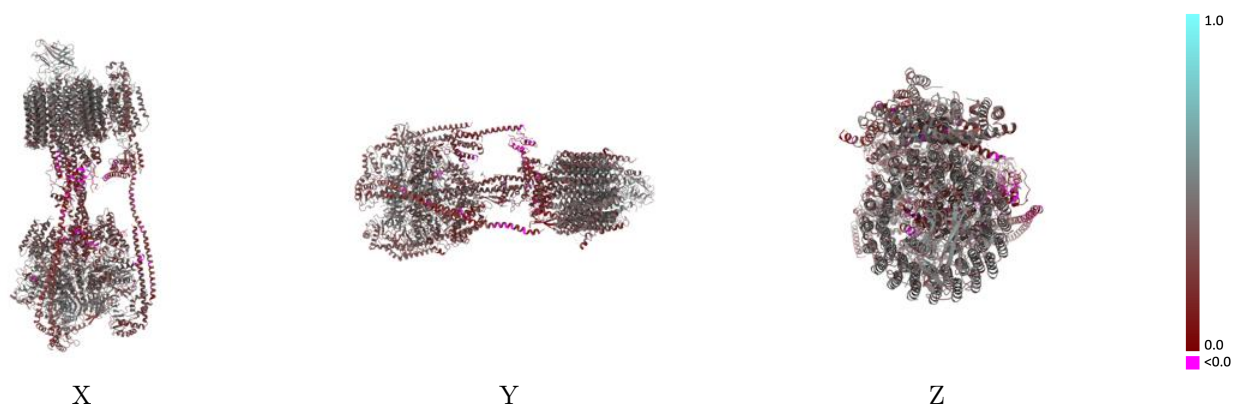
This section contains information regarding the fit between EMDB map EMD-45536 and PDB model 9CFC. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



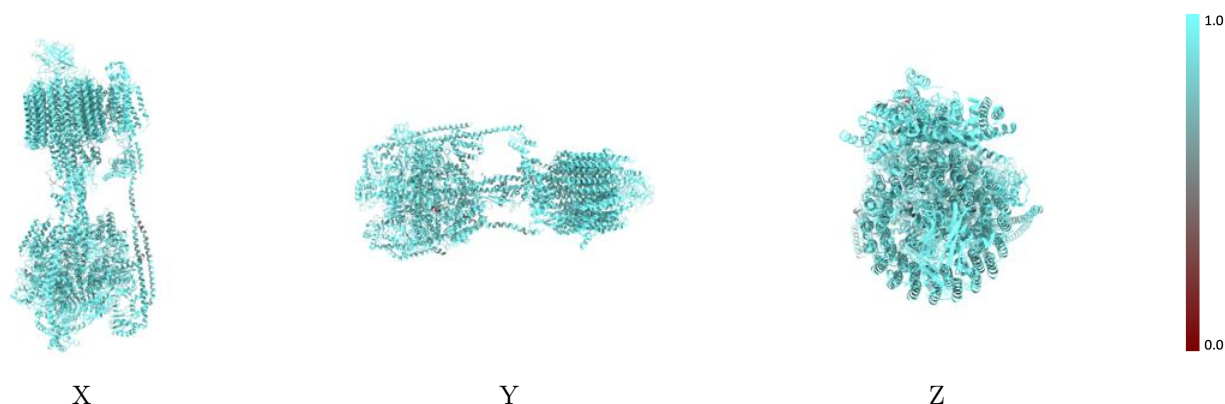
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



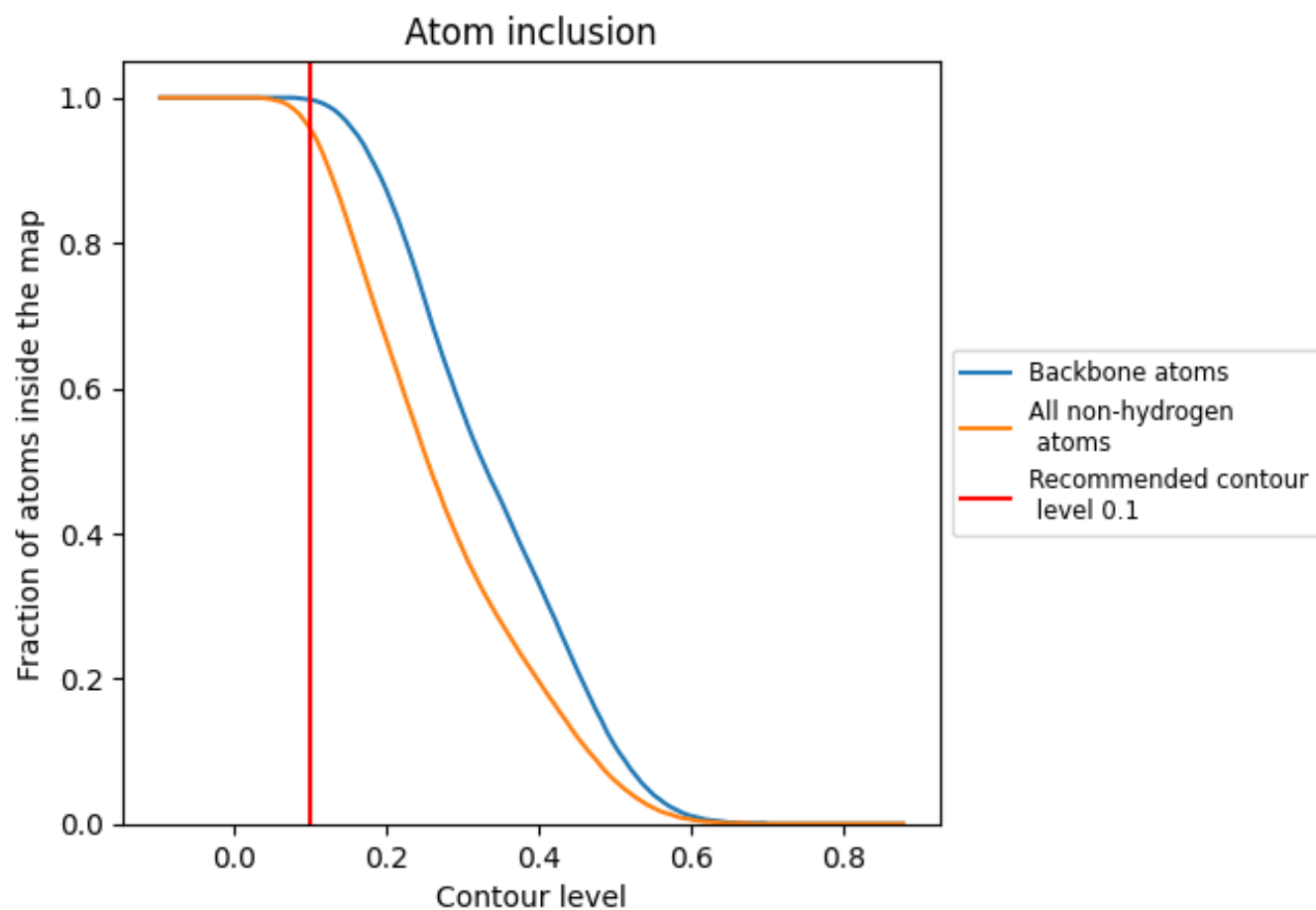
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).































































9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 96% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9570	 0.3600
0	 0.9840	 0.4220
1	 0.9810	 0.4290
2	 0.9900	 0.4260
3	 0.9890	 0.4170
4	 0.9910	 0.4190
5	 0.9820	 0.4070
6	 0.9790	 0.4110
7	 0.9730	 0.4210
8	 0.9830	 0.4360
9	 0.9760	 0.4110
A	 0.9560	 0.3380
B	 0.9660	 0.4110
C	 0.9570	 0.3520
D	 0.9590	 0.3890
E	 0.9630	 0.4210
F	 0.9510	 0.3620
G	 0.9380	 0.3220
H	 0.9150	 0.2980
I	 0.9420	 0.2860
J	 0.8900	 0.2940
K	 0.8100	 0.1910
L	 0.9200	 0.2550
M	 0.8590	 0.2560
N	 0.9460	 0.2250
Q	 0.9290	 0.2600
R	 0.9720	 0.3100
S	 0.9820	 0.4120
T	 0.9800	 0.3510
U	 0.9730	 0.4510
V	 0.9760	 0.4410

