



## wwPDB EM Validation Summary Report ⓘ

Jul 28, 2025 – 01:41 PM EDT

PDB ID : 9CF8 / pdb\_00009cf8  
EMDB ID : EMD-45533  
Title : Cryo-EM structure of human kidney V-ATPase state 1  
Authors : Zhang, Z.; Lyu, M.  
Deposited on : 2024-06-27  
Resolution : 3.46 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.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

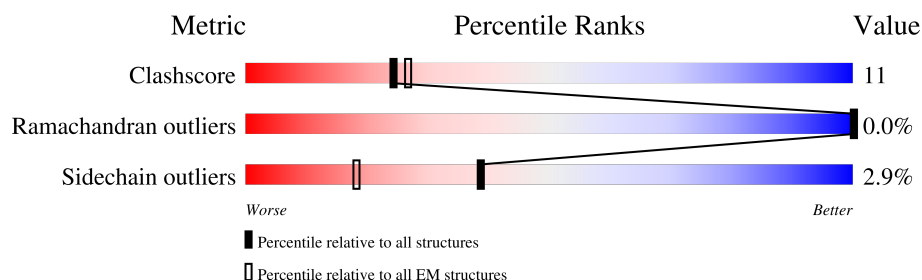
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.46 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.











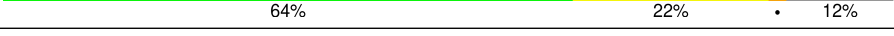


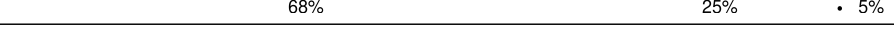

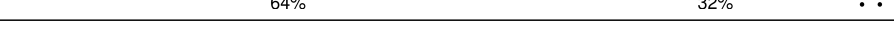


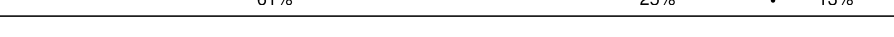

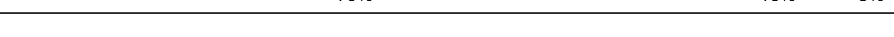



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	205	
2	1	155	
2	2	155	
2	3	155	
2	4	155	
2	5	155	
2	6	155	
2	7	155	

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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 56307 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	202	Total	C	N	O	S	0	0
			1473	975	232	256	10		

- 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
			1053	692	163	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
			1059	695	166	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	565	Total	C	N	O	S	0	0
			4318	2745	721	827	25		
3	B	555	Total	C	N	O	S	0	0
			4186	2649	693	817	27		
3	C	601	Total	C	N	O	S	0	0
			4606	2923	773	882	28		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	459	Total	C	N	O	S	0	0
			3577	2272	606	679	20		
4	E	460	Total	C	N	O	S	0	0
			3589	2278	616	676	19		
4	F	458	Total	C	N	O	S	0	0
			3573	2267	611	675	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	217	Total	C	N	O	S	0	0
			1720	1091	311	313	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	181	Total	C	N	O	S	0	0
			1470	926	263	273	8		
6	I	219	Total	C	N	O	S	0	0
			1777	1117	315	335	10		
6	J	215	Total	C	N	O	S	0	0
			1748	1100	310	328	10		

- 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	114	Total	C	N	O	S	0	0
			938	573	179	183	3		
7	M	114	Total	C	N	O	S	0	0
			938	573	179	183	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
			875	552	157	164	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	307	Total	C	N	O	S	0	0
			2497	1608	408	469	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	R	634	Total	C	N	O	S	0	0
			5166	3397	844	891	34		

- 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	85	Total	C	N	O	S	0	0
			654	431	101	115	7		

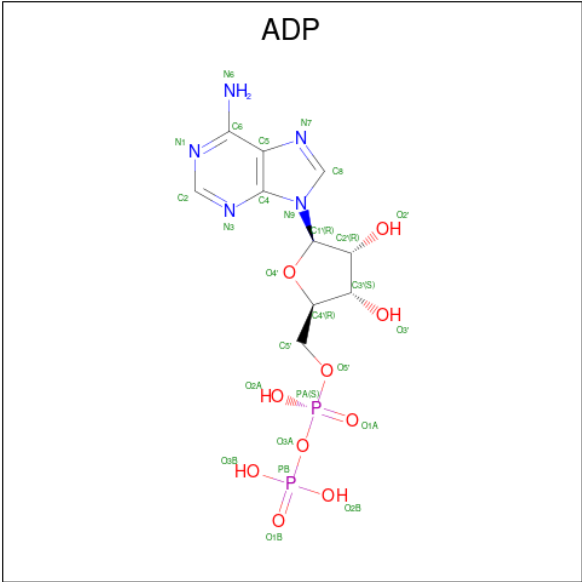
- Molecule 13 is a protein called V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	U	205	Total	C	N	O	S	0	0
			1664	1089	265	300	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
			375	255	53	64	3		

- Molecule 15 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).

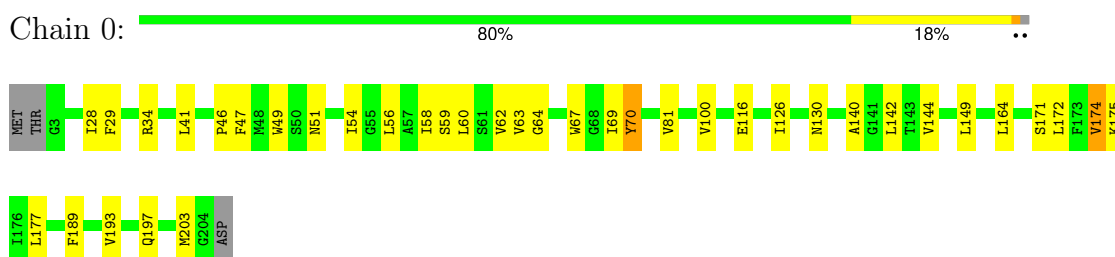


Mol	Chain	Residues	Atoms					AltConf
15	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

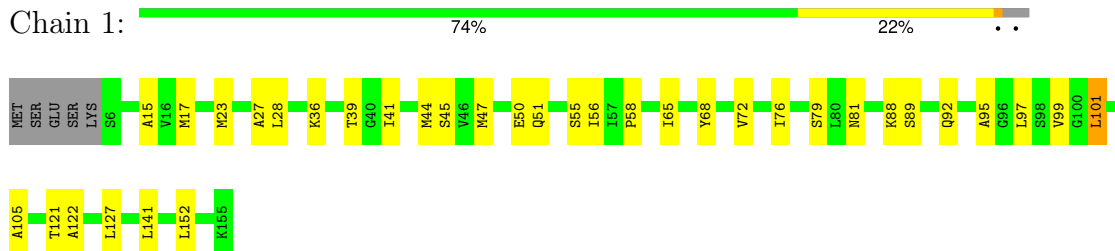
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

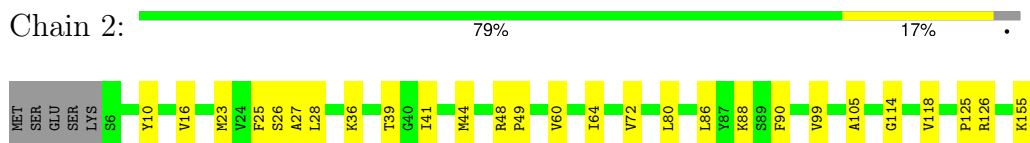
- Molecule 1: V-type proton ATPase 21 kDa proteolipid subunit



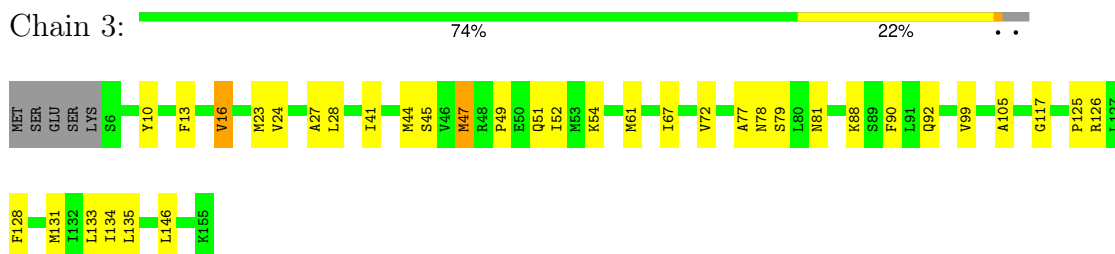
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit



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

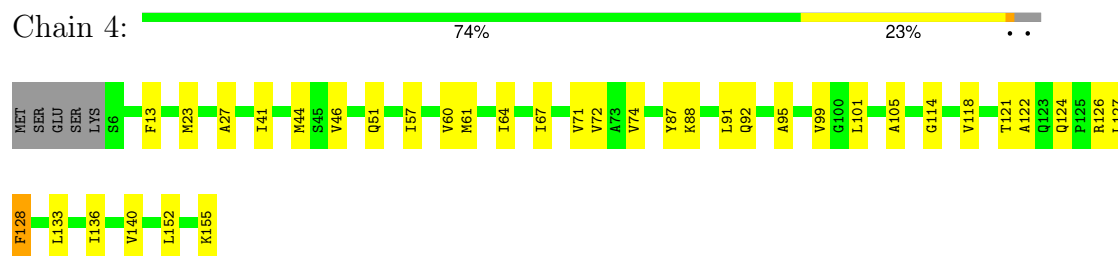


- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit

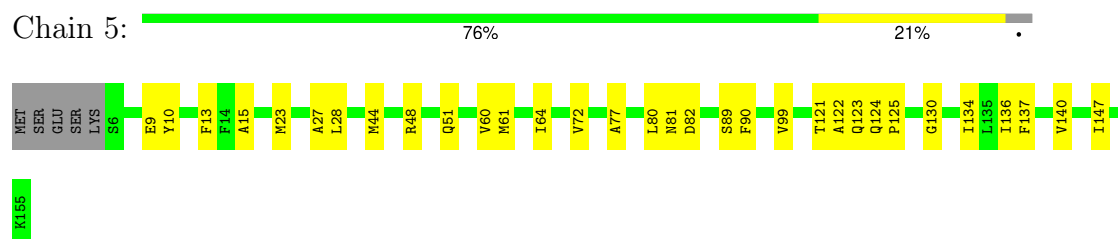




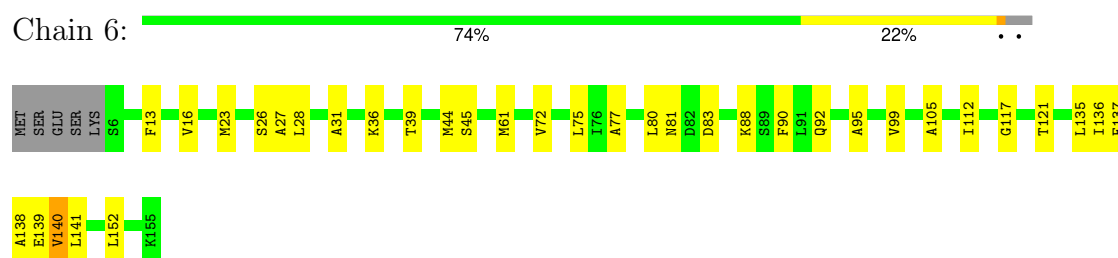
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit



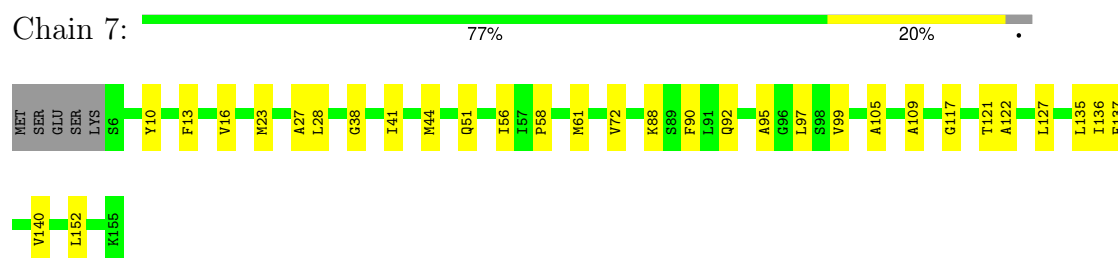
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit



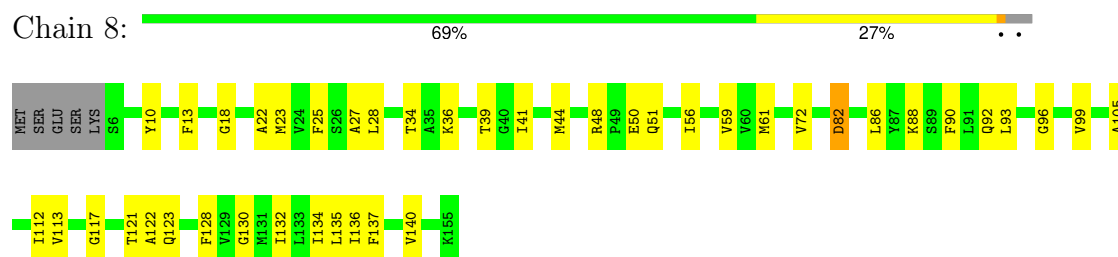
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit



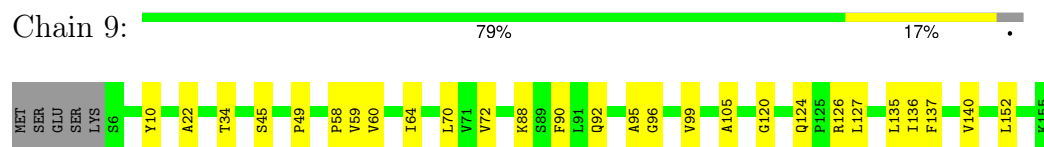
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit



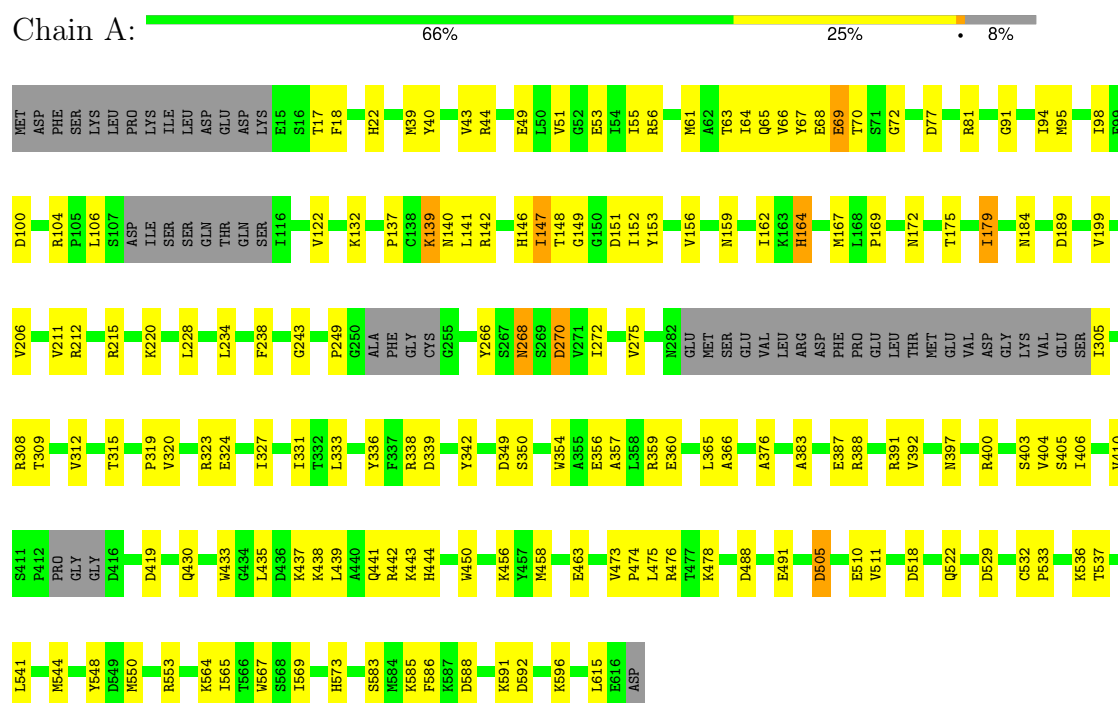
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit



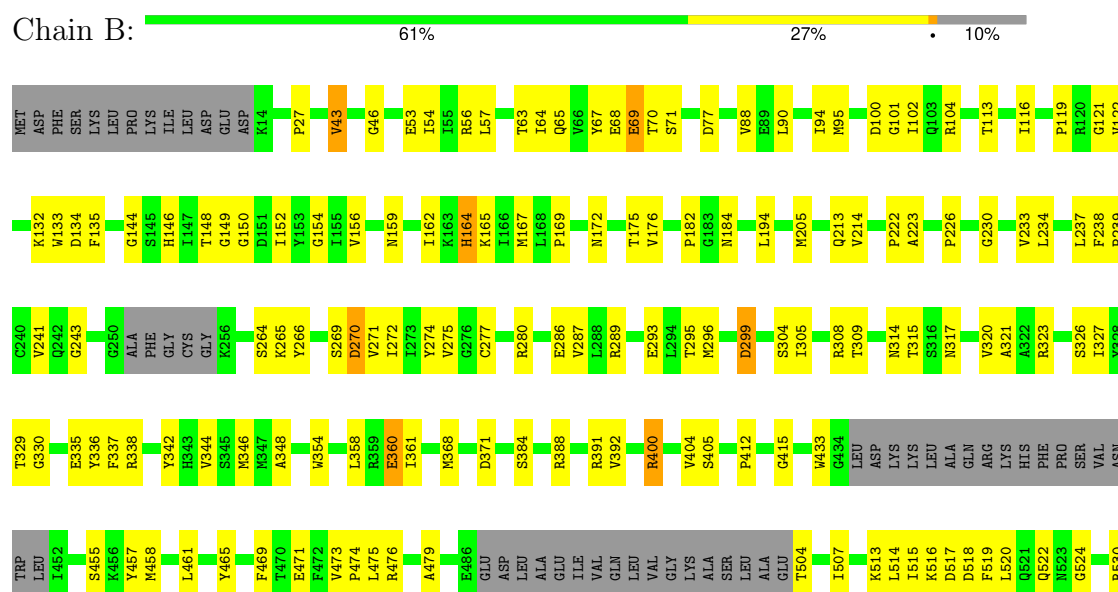
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit



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



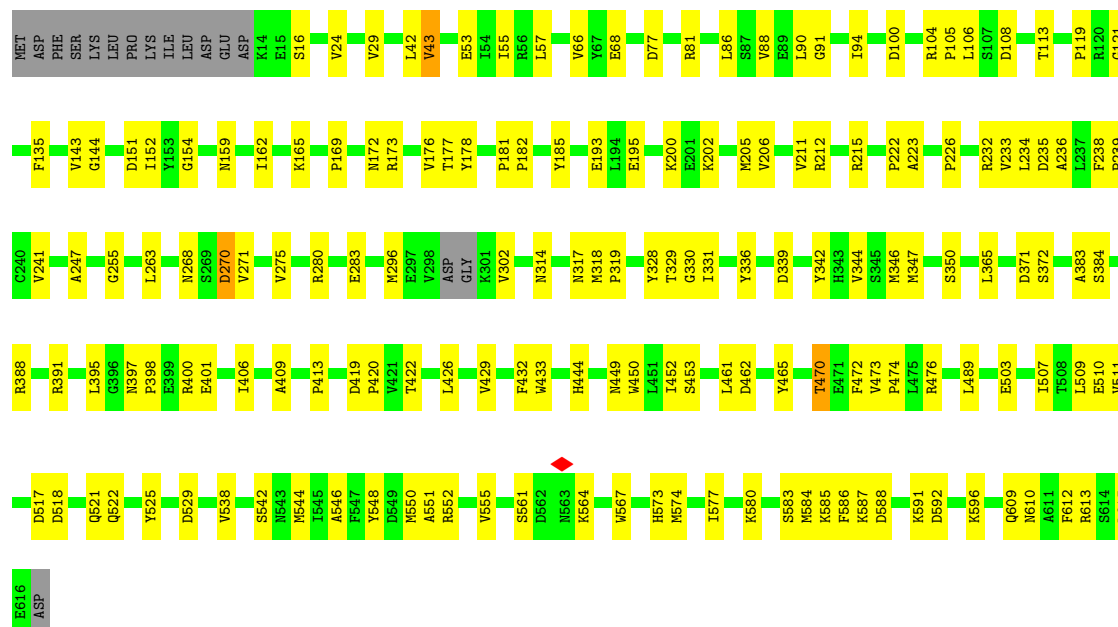
- Molecule 3: V-type proton ATPase catalytic subunit A





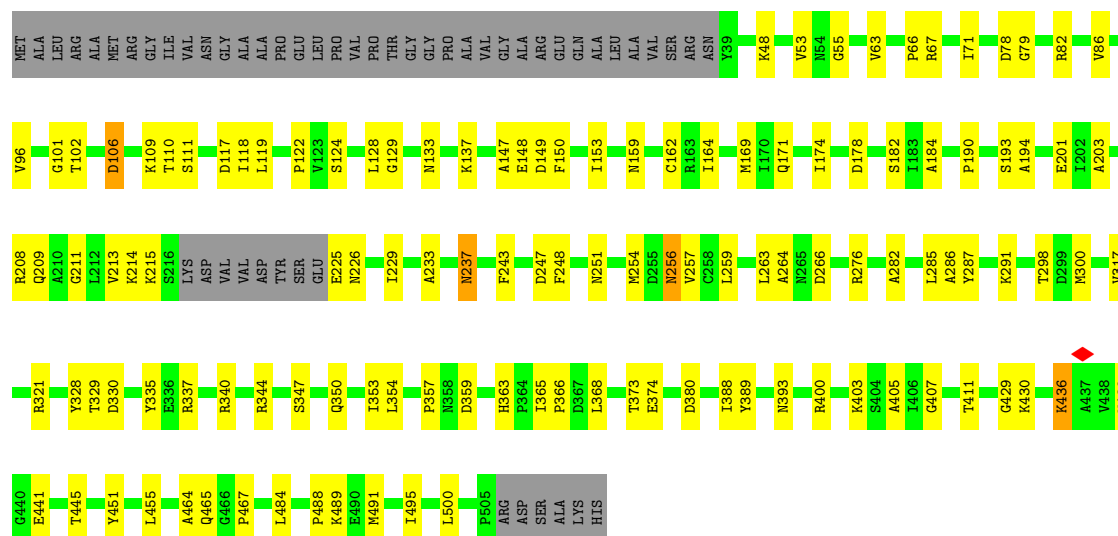
• Molecule 3: V-type proton ATPase catalytic subunit A

Chain C: 71% 26% •



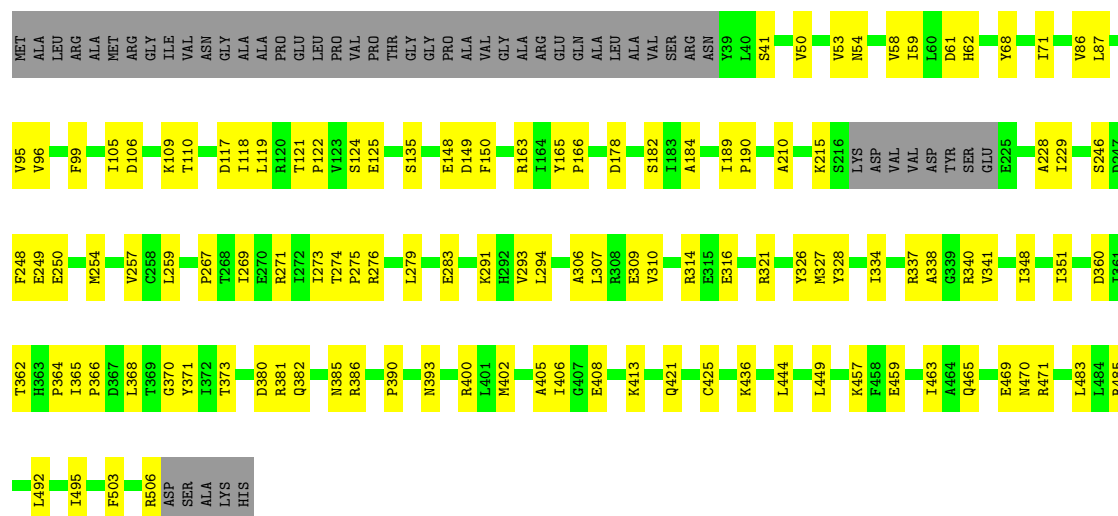
• Molecule 4: V-type proton ATPase subunit B, brain isoform

Chain D: 66% 23% • 10%



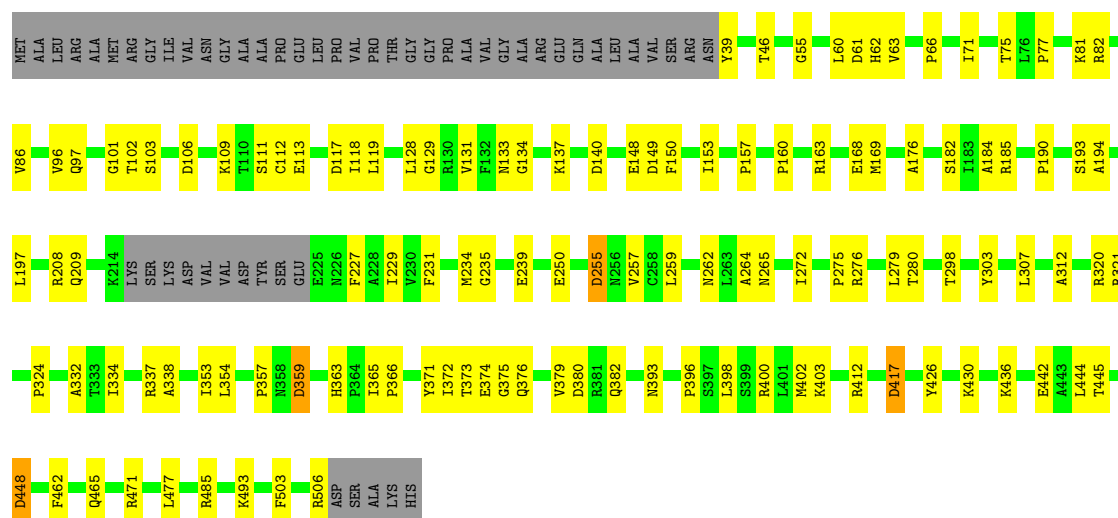
• Molecule 4: V-type proton ATPase subunit B, brain isoform

Chain E: 67% 23% 10%



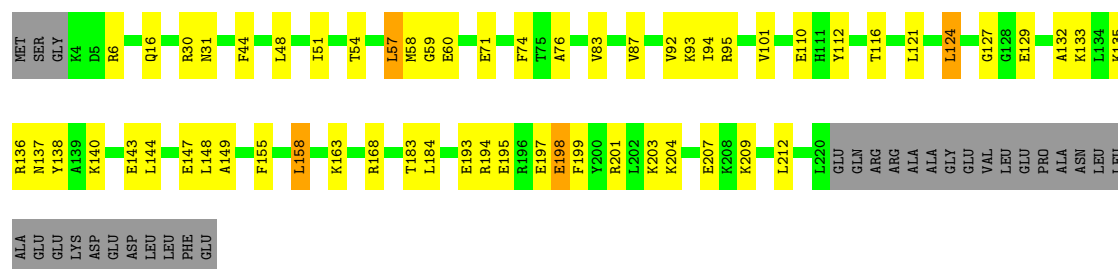
• Molecule 4: V-type proton ATPase subunit B, brain isoform

Chain F: 66% 23% 10%

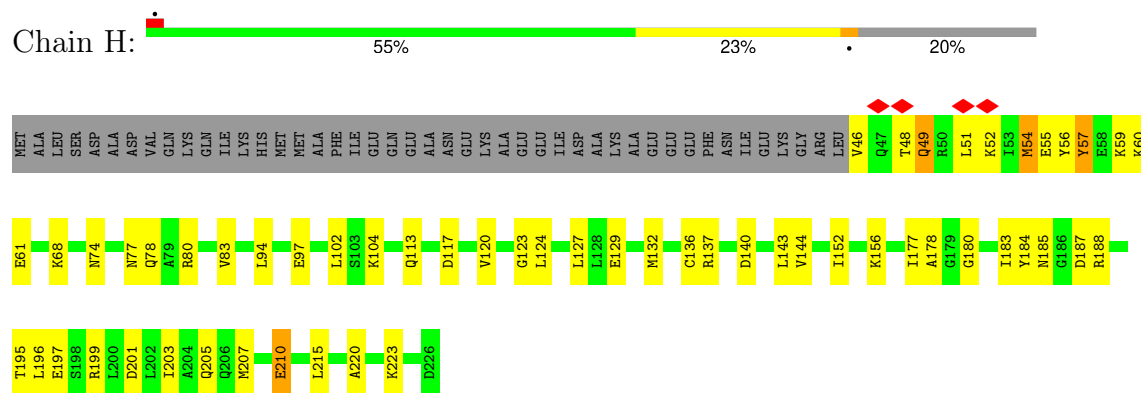


• Molecule 5: V-type proton ATPase subunit D

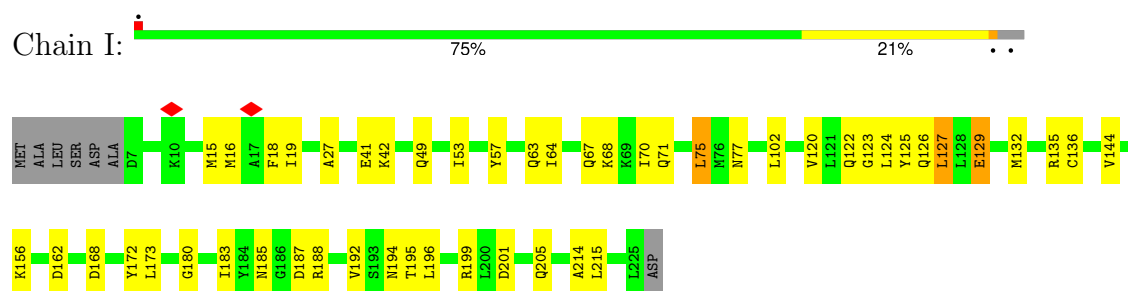
Chain G: 64% 22% 12%



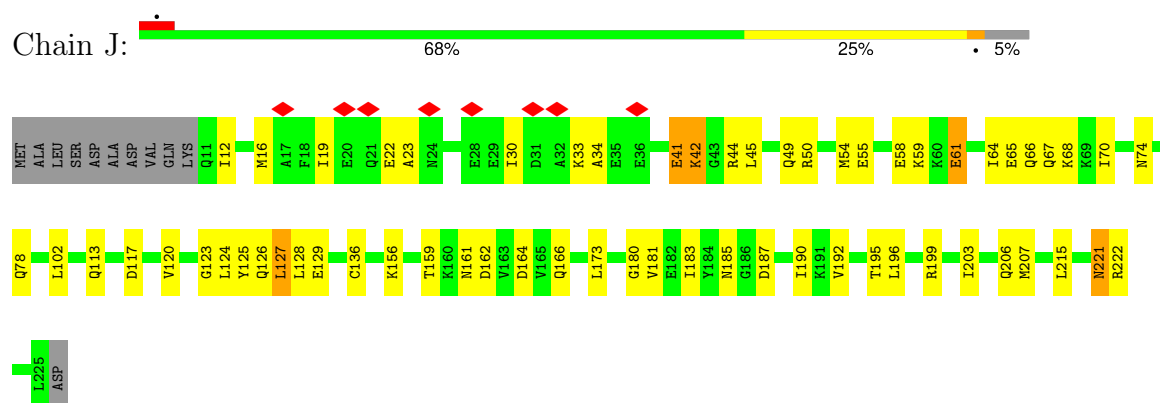
• Molecule 6: V-type proton ATPase subunit E 1



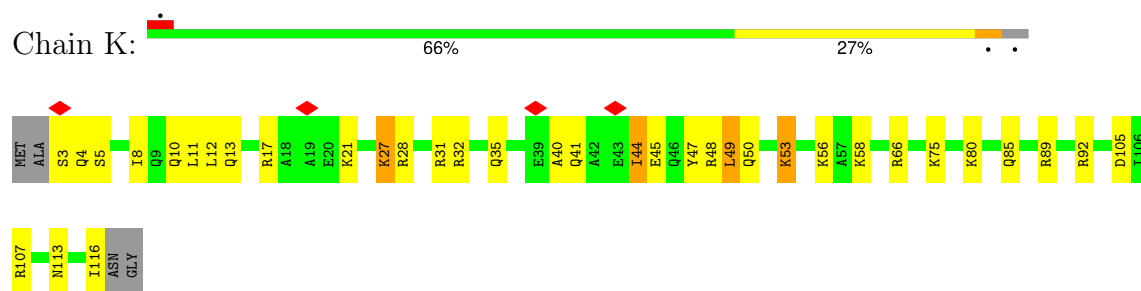
- Molecule 6: V-type proton ATPase subunit E 1



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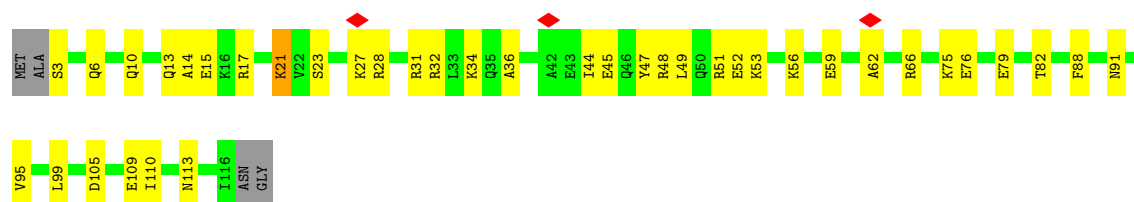


- Molecule 7: V-type proton ATPase subunit G 1



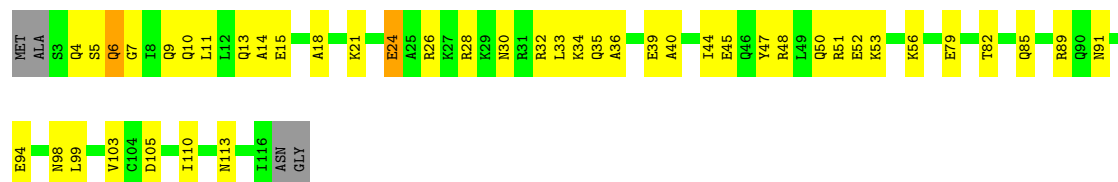
- Molecule 7: V-type proton ATPase subunit G 1





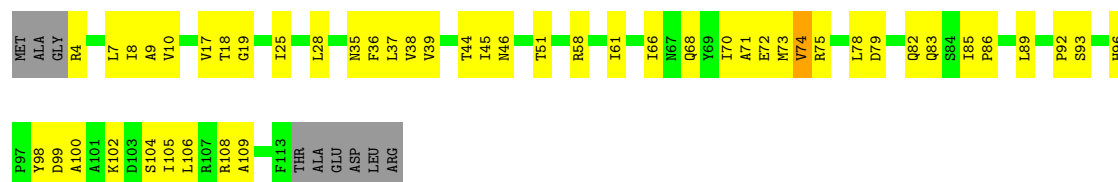
• Molecule 7: V-type proton ATPase subunit G 1

Chain M: 59% 36% . .



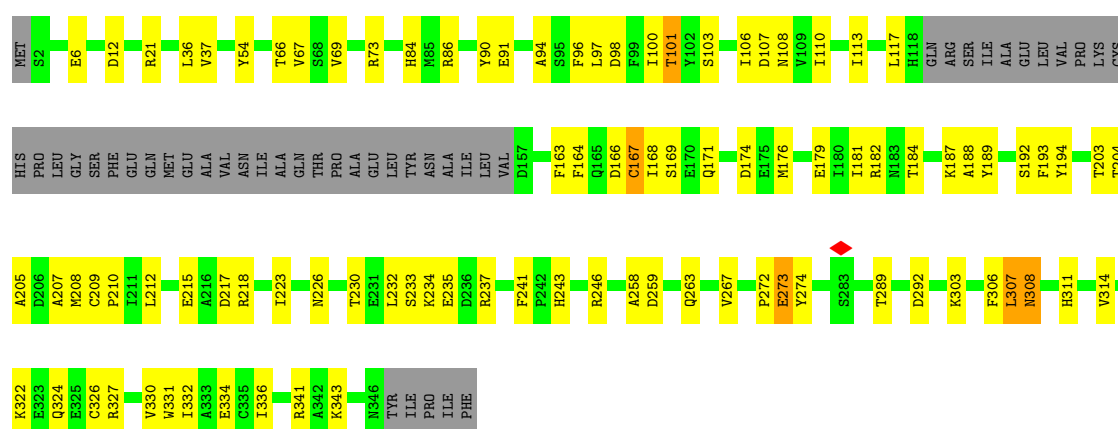
• Molecule 8: V-type proton ATPase subunit F

Chain N: 52% 39% . 8%



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

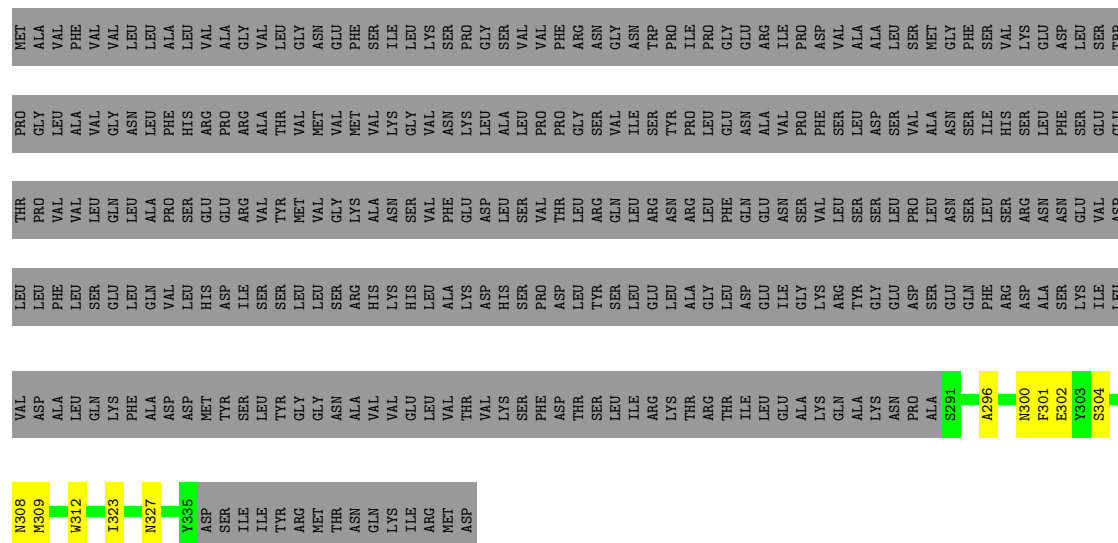
Chain Q: 61% 25% . 13%



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

Chain R: 53% 22% . 24%







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35623	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	0.808	Depositor
Minimum map value	-0.101	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	0.16	0/1507	0.29	0/2051
2	1	0.18	0/1068	0.33	0/1447
2	2	0.16	0/1080	0.31	0/1461
2	3	0.36	0/1080	0.52	0/1461
2	4	0.22	0/1080	0.34	0/1461
2	5	0.16	0/1080	0.30	0/1461
2	6	0.17	0/1080	0.31	0/1461
2	7	0.17	0/1074	0.32	0/1454
2	8	0.15	0/1080	0.32	0/1461
2	9	0.15	0/1080	0.29	0/1461
3	A	0.25	0/4405	0.39	0/5977
3	B	0.13	0/4267	0.31	0/5791
3	C	0.17	0/4701	0.33	0/6377
4	D	0.23	0/3648	0.38	0/4945
4	E	0.26	0/3660	0.41	0/4960
4	F	0.37	0/3644	0.51	0/4941
5	G	0.12	0/1738	0.30	0/2330
6	H	0.12	0/1484	0.29	0/1989
6	I	0.10	0/1794	0.27	0/2403
6	J	0.10	0/1765	0.26	0/2363
7	K	0.13	0/945	0.26	0/1258
7	L	0.14	0/945	0.28	0/1258
7	M	0.13	0/945	0.30	0/1258
8	N	0.12	0/889	0.34	0/1200
9	Q	0.11	0/2553	0.27	0/3452
10	R	0.22	0/5303	0.38	0/7183
11	S	0.37	0/657	0.55	0/902
12	T	0.41	0/670	0.62	0/911
13	U	0.15	0/1718	0.35	0/2337
14	V	0.13	0/388	0.23	0/532
All	All	0.21	0/57328	0.36	0/77546

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
3	A	0	1
4	E	0	1
4	F	0	1
10	R	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	212	ARG	Sidechain
4	E	276	ARG	Sidechain
4	F	276	ARG	Sidechain
10	R	339	ARG	Sidechain

## 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	0	1473	0	1503	26	0
2	1	1053	0	1109	25	0
2	2	1065	0	1131	20	0
2	3	1065	0	1131	25	0
2	4	1065	0	1131	30	0
2	5	1065	0	1131	27	0
2	6	1065	0	1131	25	0
2	7	1059	0	1120	26	0
2	8	1065	0	1131	32	0
2	9	1065	0	1131	19	0
3	A	4318	0	4243	95	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4186	0	4063	118	0
3	C	4606	0	4539	105	0
4	D	3577	0	3570	75	0
4	E	3589	0	3590	73	0
4	F	3573	0	3561	82	0
5	G	1720	0	1797	42	0
6	H	1470	0	1545	36	0
6	I	1777	0	1841	41	0
6	J	1748	0	1818	44	0
7	K	938	0	947	34	0
7	L	938	0	947	30	0
7	M	938	0	947	32	0
8	N	875	0	878	37	0
9	Q	2497	0	2427	61	0
10	R	5166	0	5198	129	0
11	S	631	0	645	8	0
12	T	654	0	641	7	0
13	U	1664	0	1589	47	0
14	V	375	0	365	10	0
15	C	27	0	12	1	0
All	All	56307	0	56812	1191	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 1191 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:67:VAL:HG11	9:Q:334:GLU:HG2	1.51	0.93
5:G:94:ILE:HA	5:G:110:GLU:O	1.81	0.80
3:C:159:ASN:HD21	3:C:162:ILE:HB	1.47	0.79
3:B:27:PRO:HB2	3:B:65:GLN:HE22	1.48	0.77
6:J:42:LYS:HD2	7:M:36:ALA:HB1	1.65	0.77

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	200/205 (98%)	199 (100%)	1 (0%)	0	100	100
2	1	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
2	2	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
2	3	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
2	4	148/155 (96%)	145 (98%)	2 (1%)	1 (1%)	19	53
2	5	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
2	6	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
2	7	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
2	8	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
2	9	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
3	A	555/617 (90%)	545 (98%)	10 (2%)	0	100	100
3	B	545/617 (88%)	537 (98%)	8 (2%)	0	100	100
3	C	597/617 (97%)	579 (97%)	18 (3%)	0	100	100
4	D	455/511 (89%)	440 (97%)	15 (3%)	0	100	100
4	E	456/511 (89%)	441 (97%)	15 (3%)	0	100	100
4	F	454/511 (89%)	443 (98%)	11 (2%)	0	100	100
5	G	215/247 (87%)	213 (99%)	2 (1%)	0	100	100
6	H	179/226 (79%)	177 (99%)	2 (1%)	0	100	100
6	I	217/226 (96%)	215 (99%)	2 (1%)	0	100	100
6	J	213/226 (94%)	213 (100%)	0	0	100	100
7	K	112/118 (95%)	112 (100%)	0	0	100	100
7	L	112/118 (95%)	111 (99%)	1 (1%)	0	100	100
7	M	112/118 (95%)	109 (97%)	3 (3%)	0	100	100
8	N	108/119 (91%)	101 (94%)	7 (6%)	0	100	100
9	Q	303/351 (86%)	299 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	R	626/837 (75%)	606 (97%)	20 (3%)	0	100	100
11	S	75/81 (93%)	73 (97%)	2 (3%)	0	100	100
12	T	83/137 (61%)	82 (99%)	1 (1%)	0	100	100
13	U	203/470 (43%)	196 (97%)	7 (3%)	0	100	100
14	V	43/350 (12%)	42 (98%)	1 (2%)	0	100	100
All	All	7195/8608 (84%)	7046 (98%)	148 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	4	128	PHE

### 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	150/155 (97%)	147 (98%)	3 (2%)	50	73
2	1	105/112 (94%)	103 (98%)	2 (2%)	52	74
2	2	107/112 (96%)	106 (99%)	1 (1%)	75	86
2	3	107/112 (96%)	102 (95%)	5 (5%)	22	52
2	4	107/112 (96%)	106 (99%)	1 (1%)	75	86
2	5	107/112 (96%)	105 (98%)	2 (2%)	52	74
2	6	107/112 (96%)	105 (98%)	2 (2%)	52	74
2	7	106/112 (95%)	105 (99%)	1 (1%)	75	86
2	8	107/112 (96%)	106 (99%)	1 (1%)	75	86
2	9	107/112 (96%)	107 (100%)	0	100	100
3	A	462/525 (88%)	442 (96%)	20 (4%)	25	54
3	B	447/525 (85%)	437 (98%)	10 (2%)	47	71
3	C	496/525 (94%)	488 (98%)	8 (2%)	58	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	390/430 (91%)	383 (98%)	7 (2%)	54	75
4	E	390/430 (91%)	384 (98%)	6 (2%)	60	78
4	F	388/430 (90%)	380 (98%)	8 (2%)	48	72
5	G	179/212 (84%)	172 (96%)	7 (4%)	27	58
6	H	162/199 (81%)	156 (96%)	6 (4%)	29	59
6	I	193/199 (97%)	187 (97%)	6 (3%)	35	64
6	J	190/199 (96%)	180 (95%)	10 (5%)	19	48
7	K	99/101 (98%)	92 (93%)	7 (7%)	12	40
7	L	99/101 (98%)	93 (94%)	6 (6%)	15	44
7	M	99/101 (98%)	93 (94%)	6 (6%)	15	44
8	N	94/100 (94%)	93 (99%)	1 (1%)	70	83
9	Q	268/306 (88%)	259 (97%)	9 (3%)	32	61
10	R	567/746 (76%)	537 (95%)	30 (5%)	19	48
11	S	69/72 (96%)	68 (99%)	1 (1%)	62	79
12	T	70/116 (60%)	69 (99%)	1 (1%)	62	79
13	U	182/397 (46%)	173 (95%)	9 (5%)	21	51
14	V	40/308 (13%)	40 (100%)	0	100	100
All	All	5994/7185 (83%)	5818 (97%)	176 (3%)	39	65

5 of 176 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	L	21	LYS
10	R	275	THR
7	M	4	GLN
9	Q	184	THR
10	R	333	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 142 such sidechains are listed below:

Mol	Chain	Res	Type
10	R	412	HIS
10	R	604	ASN
13	U	273	ASN
4	D	358	ASN

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Mol	Chain	Res	Type
4	D	350	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	C	701	-	24,29,29	0.91	1 (4%)	29,45,45	1.19	2 (6%)

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	C	701	-	-	3/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	701	ADP	PA-O3A	2.08	1.61	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	701	ADP	N3-C2-N1	-3.59	123.80	128.67
15	C	701	ADP	C4-C5-N7	-2.40	106.80	109.34

There are no chirality outliers.

All (3) torsion outliers are listed below:

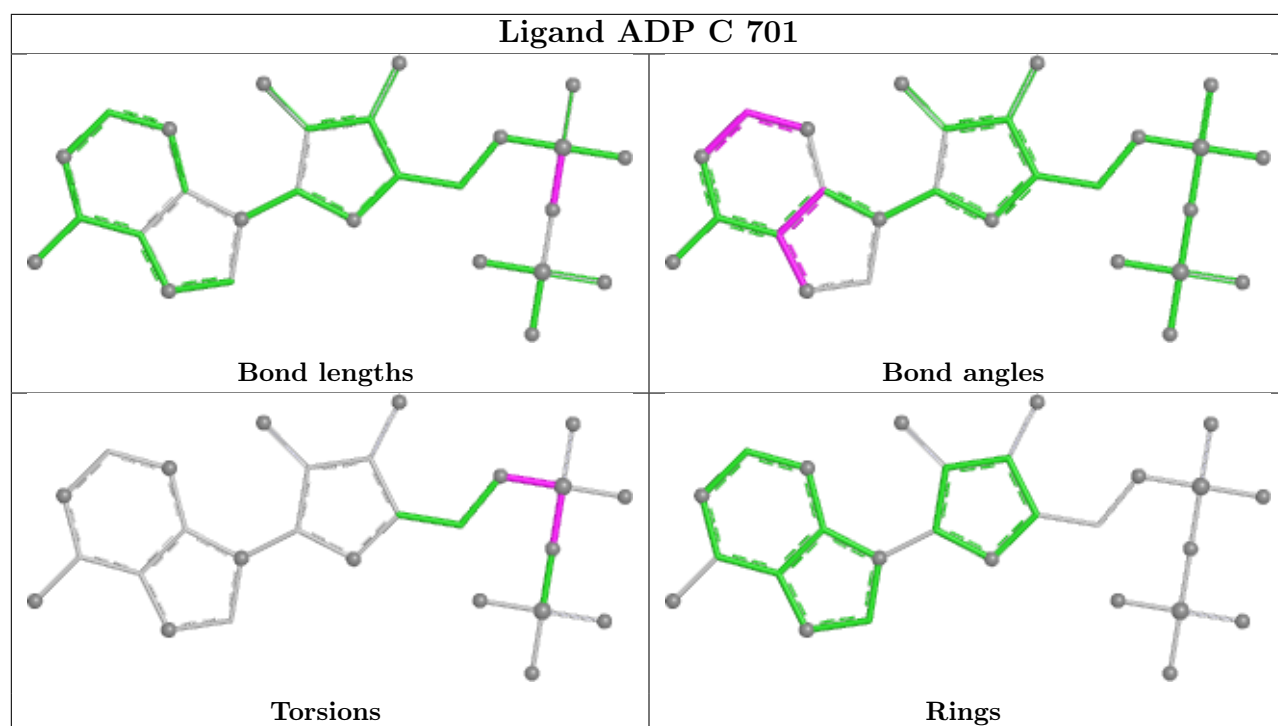
Mol	Chain	Res	Type	Atoms
15	C	701	ADP	PB-O3A-PA-O5'
15	C	701	ADP	C5'-O5'-PA-O2A
15	C	701	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	C	701	ADP	1	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.

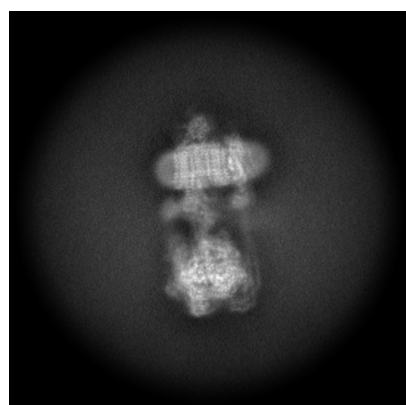
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45533. These allow visual inspection of the internal detail of the map and identification of artifacts.

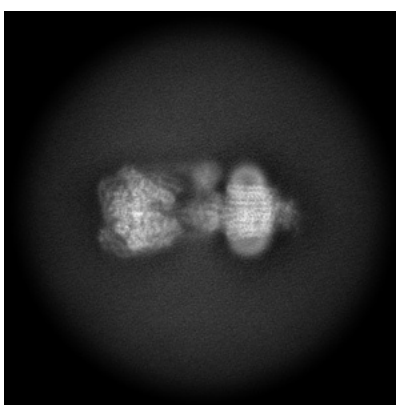
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

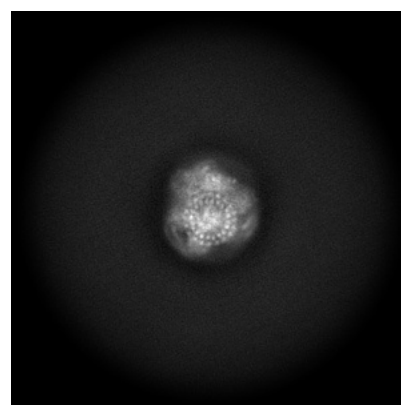
#### 6.1.1 Primary map



X



Y

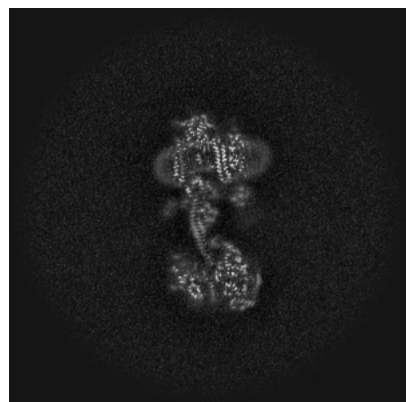


Z

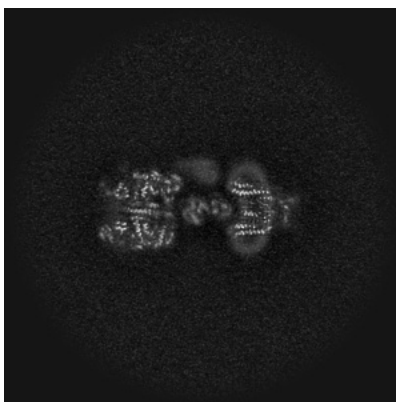
The images above show the map projected in three orthogonal directions.

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

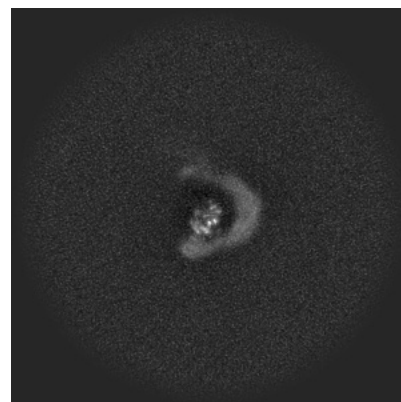
#### 6.2.1 Primary map



X Index: 256



Y Index: 256

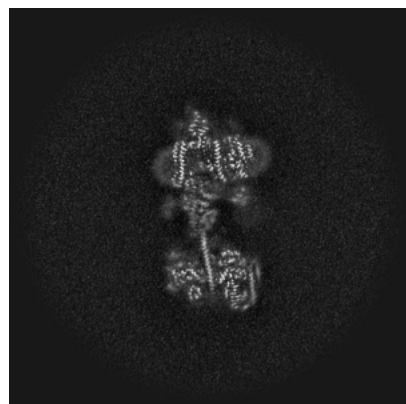


Z Index: 256

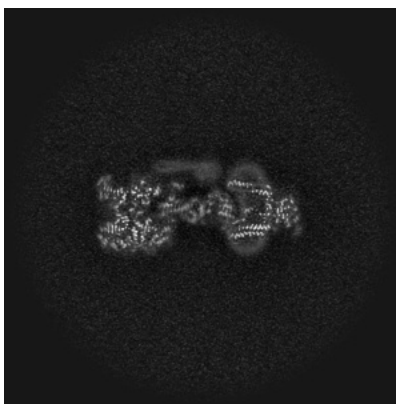
The images above show central slices of the map in three orthogonal directions.

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

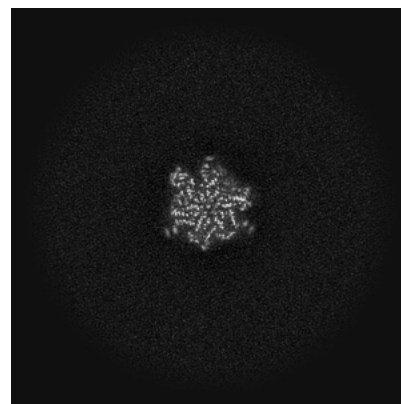
### 6.3.1 Primary map



X Index: 251



Y Index: 246

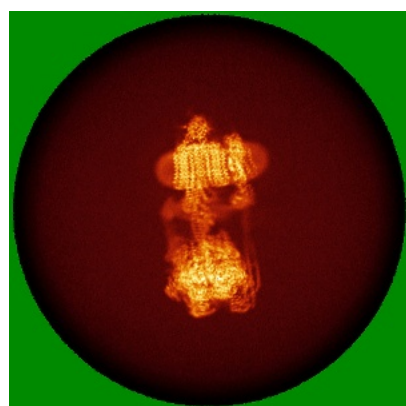


Z Index: 170

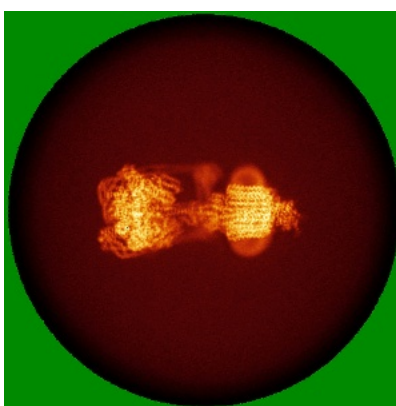
The images above show the largest variance slices of the map in three orthogonal directions.

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

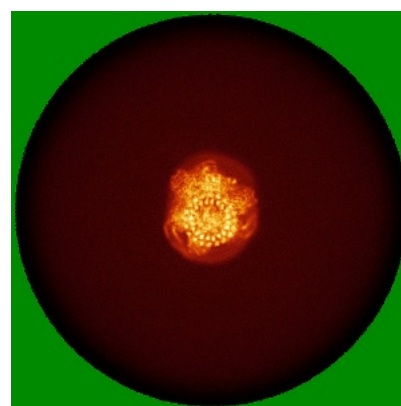
### 6.4.1 Primary map



X



Y

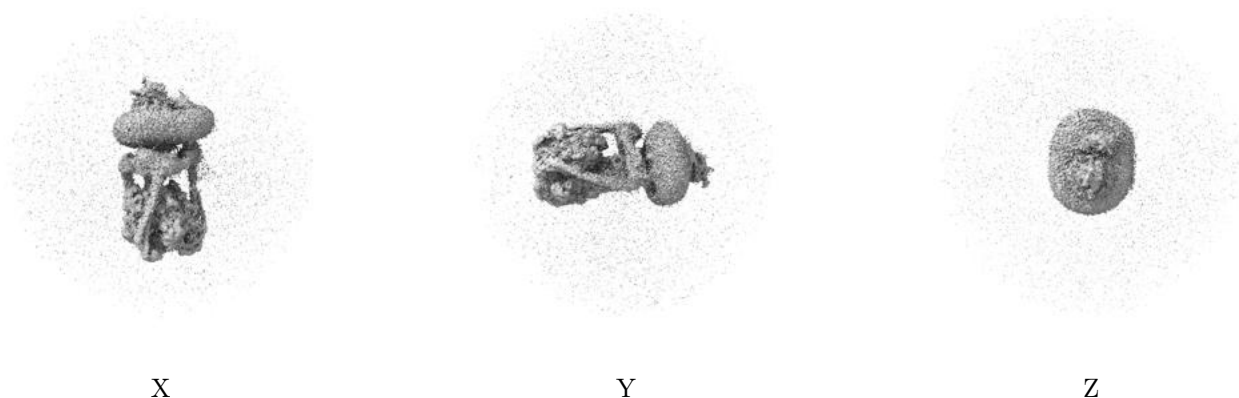


Z

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



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.

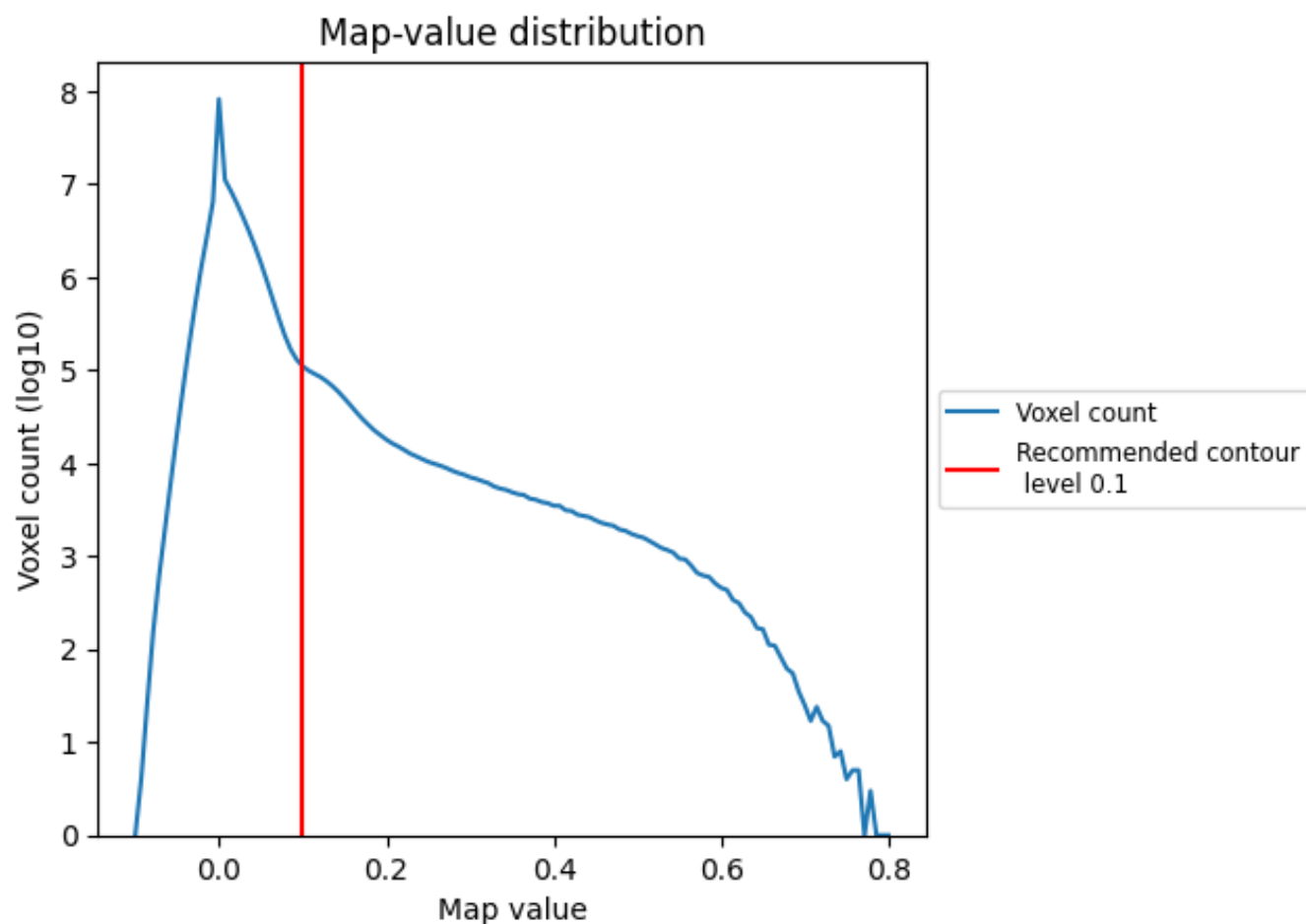
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

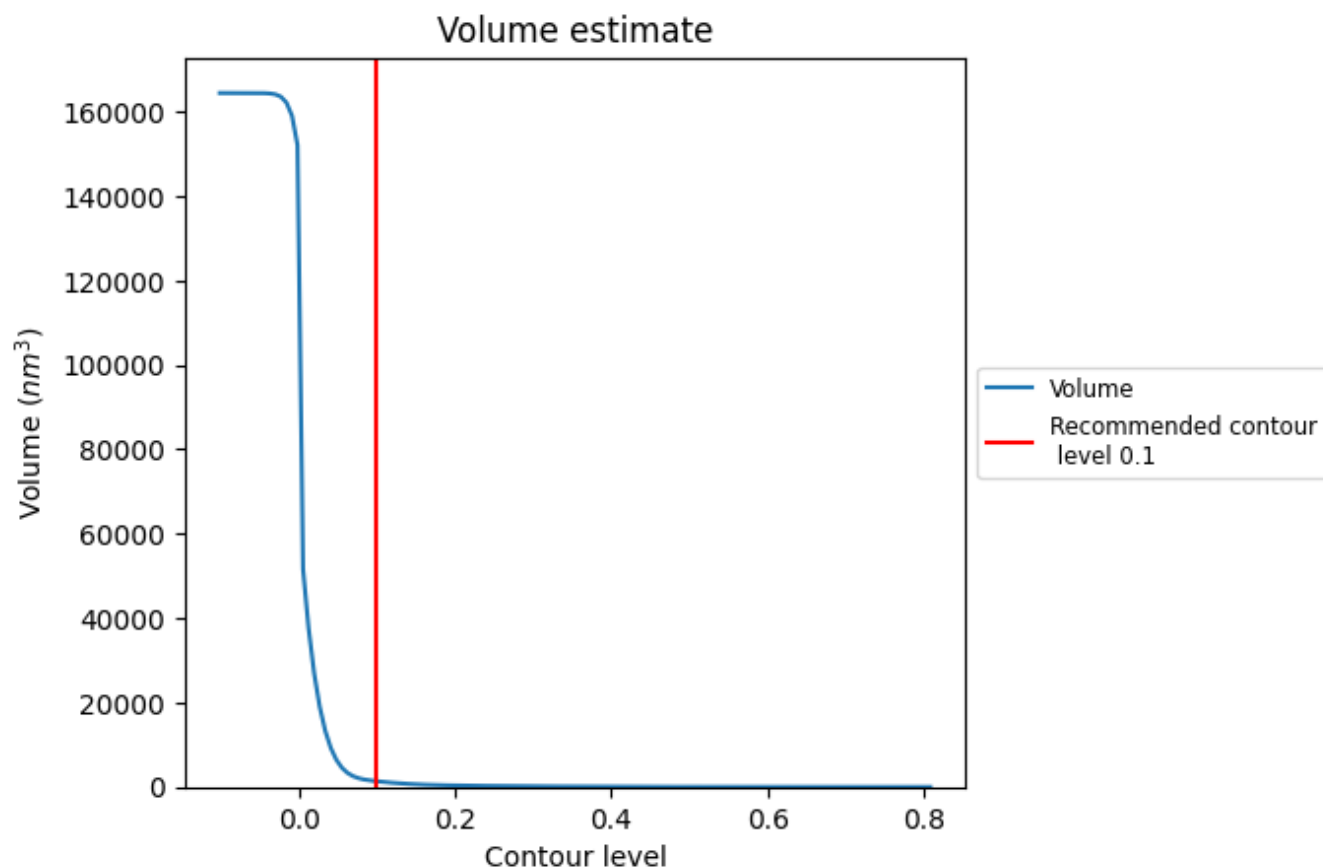
This section contains the results of statistical analysis of the map.

### 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.

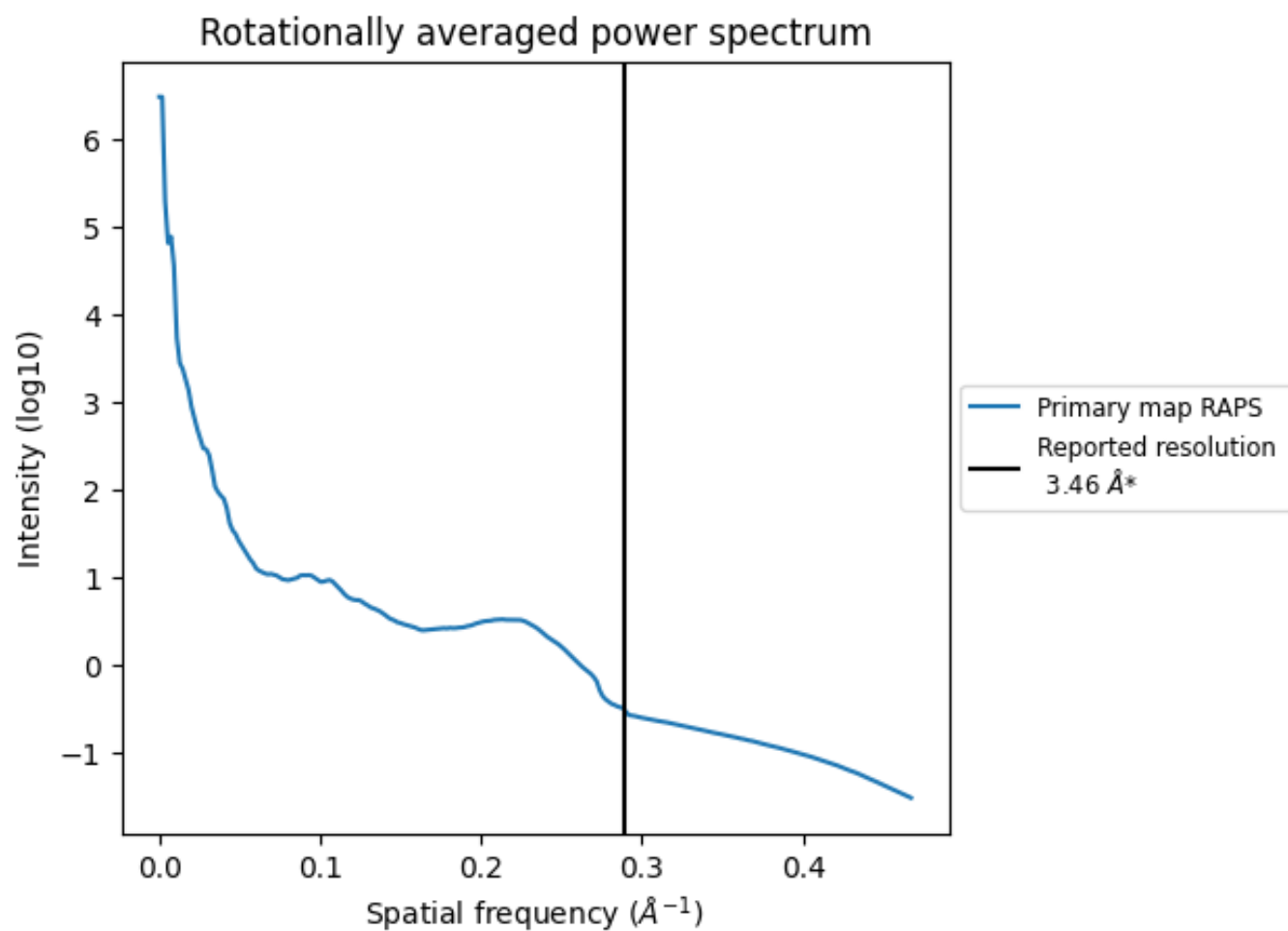
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1344  $\text{nm}^3$ ; this corresponds to an approximate mass of 1214 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 0.289 Å<sup>-1</sup>



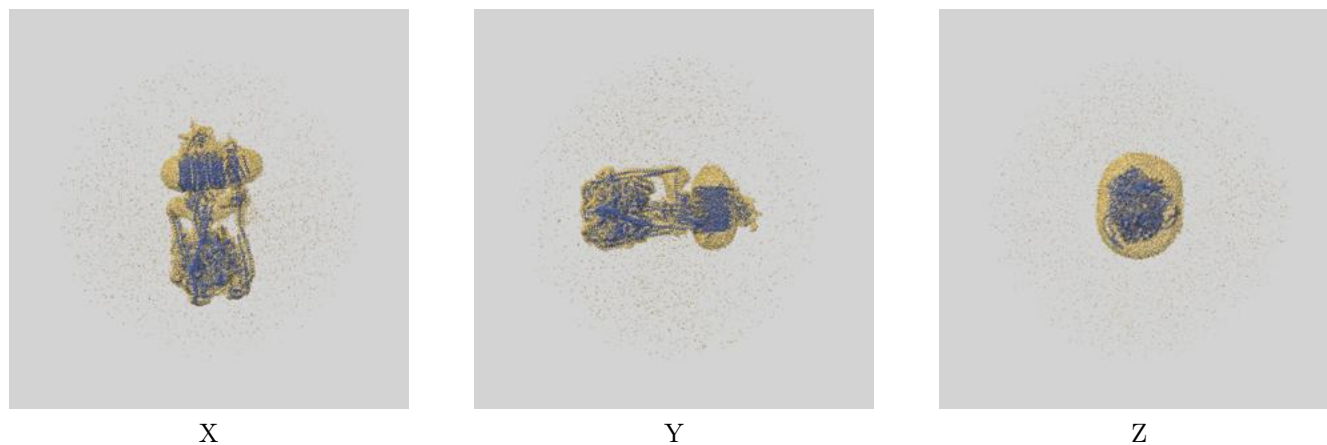
## 8 Fourier-Shell correlation

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

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

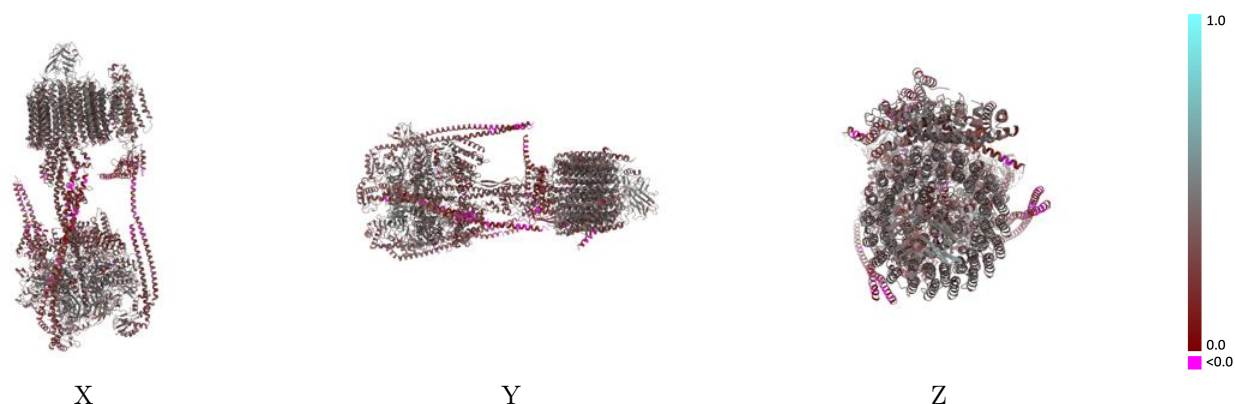
This section contains information regarding the fit between EMDB map EMD-45533 and PDB model 9CF8. Per-residue inclusion information can be found in section [3](#) on page [8](#).

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



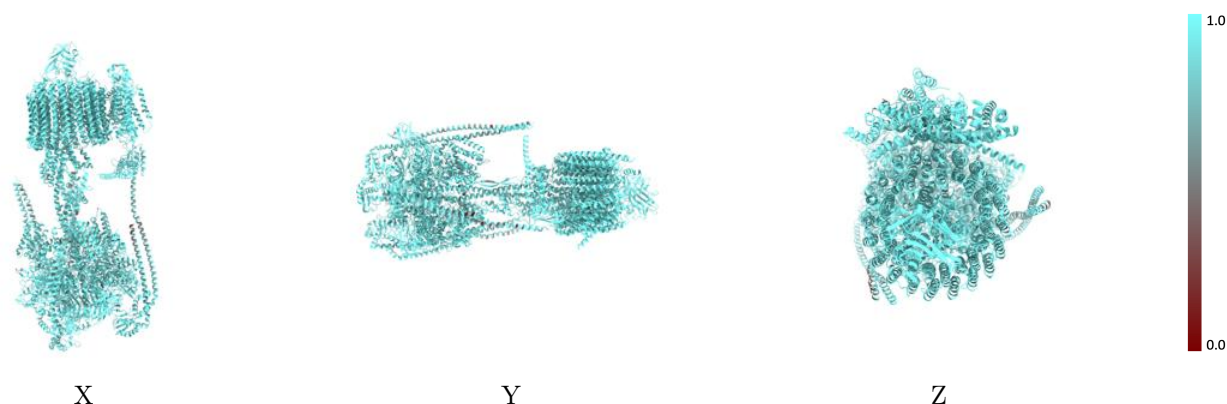
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



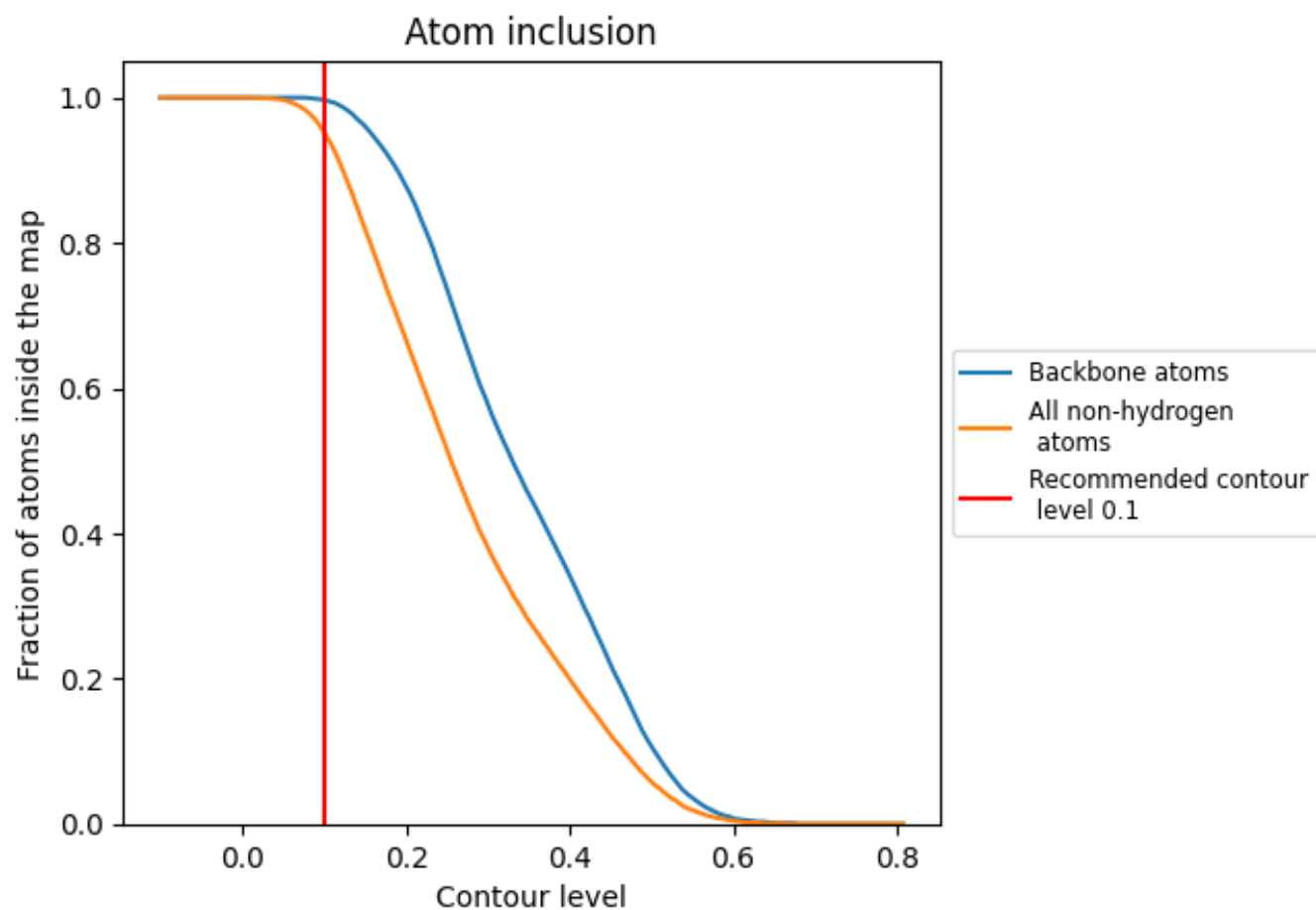
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 95% 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	 0.9520	 0.3520
0	 0.9850	 0.4130
1	 0.9800	 0.4100
2	 0.9760	 0.4010
3	 0.9700	 0.3900
4	 0.9750	 0.4080
5	 0.9760	 0.4050
6	 0.9710	 0.4040
7	 0.9730	 0.4080
8	 0.9800	 0.4000
9	 0.9820	 0.4070
A	 0.9630	 0.3740
B	 0.9560	 0.3280
C	 0.9630	 0.3820
D	 0.9570	 0.3620
E	 0.9640	 0.4000
F	 0.9720	 0.3970
G	 0.9390	 0.3180
H	 0.8740	 0.2860
I	 0.8860	 0.2570
J	 0.8880	 0.2590
K	 0.8060	 0.1850
L	 0.8620	 0.1840
M	 0.8840	 0.2030
N	 0.9590	 0.2720
Q	 0.9430	 0.3000
R	 0.9680	 0.3220
S	 0.9650	 0.3990
T	 0.9720	 0.3570
U	 0.9760	 0.4250
V	 0.9670	 0.4390

