



wwPDB EM Validation Summary Report ⓘ

Aug 30, 2023 – 10:52 AM EDT

PDB ID : 7U4T
EMDB ID : EMD-26334
Title : Human V-ATPase in state 2 with SidK and mEAK-7
Authors : Wang, L.; Fu, T.M.
Deposited on : 2022-03-01
Resolution : 3.60 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.dev50
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

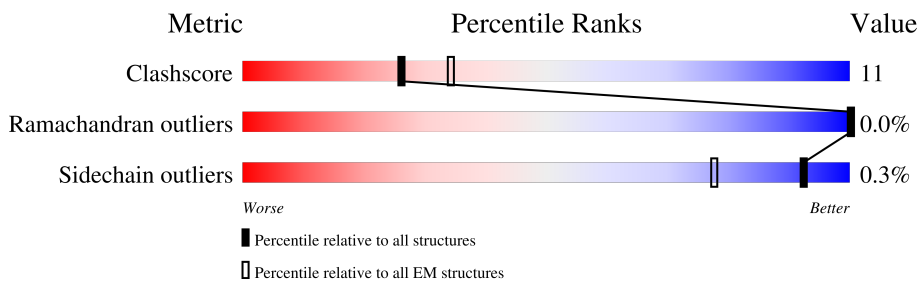
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	R	837	42% (Poor fit) 65% (0 outliers) 25% (1 outlier) 10% (2+ outliers)
2	O	382	57% (0 outliers) 93% (1 outlier) •• (2+ outliers)
3	H	226	9% (Poor fit) 75% (0 outliers) 23% (1 outlier) • (2+ outliers)
3	I	226	• (Poor fit) 75% (0 outliers) 23% (1 outlier) • (2+ outliers)
3	J	226	23% (Poor fit) 65% (0 outliers) 35% (1 outlier)
4	K	118	15% (Poor fit) 85% (0 outliers) 12% (1 outlier) • (2+ outliers)
4	L	118	14% (Poor fit) 77% (0 outliers) 19% (1 outlier) • (2+ outliers)
4	M	118	27% (Poor fit) 64% (0 outliers) 32% (1 outlier) • (2+ outliers)

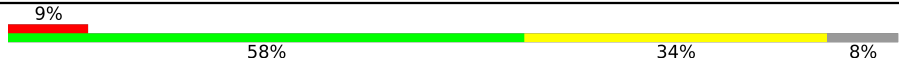


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Mol	Chain	Length	Quality of chain
5	S	81	62% 68% 26% 5%
6	T	137	44% 48% 14% 38%
7	U	470	24% 28% 15% 57%
8	V	350	7% 11% 86%
9	0	205	44% 74% 25%
10	1	155	35% 64% 33%
10	2	155	28% 65% 32%
10	3	155	37% 63% 34%
10	4	155	50% 63% 34%
10	5	155	36% 72% 25%
10	6	155	32% 79% 18%
10	7	155	16% 74% 23%
10	8	155	21% 70% 27%
10	9	155	33% 68% 28%
11	Q	351	27% 75% 25%
12	A	617	7% 69% 28%
12	B	617	78% 19%
12	C	617	74% 22%
13	D	511	74% 17% 8%
13	E	511	73% 18% 8%
13	F	511	70% 21% 8%
14	X	573	36% 10% 53%
14	Y	573	16% 35% 11% 54%
14	Z	573	6% 32% 13% 54%
15	G	247	66% 20% 14%

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Mol	Chain	Length	Quality of chain
16	N	119	
17	P	483	
18	W	456	

2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 71598 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 116 kDa subunit a isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	R	753	5876	3827	982	1031	36	0	0

- Molecule 2 is a protein called V-type proton ATPase subunit C 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	O	365	1817	1087	365	365	0	0

- Molecule 3 is a protein called V-type proton ATPase subunit E 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	J	225	1774	1110	316	340	8	0	0
3	I	221	1661	1040	302	311	8	0	0
3	H	220	1611	1005	296	303	7	0	0

- Molecule 4 is a protein called V-type proton ATPase subunit G 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	M	114	889	544	170	172	3	0	0
4	L	113	748	456	139	150	3	0	0
4	K	114	735	448	136	148	3	0	0

- Molecule 5 is a protein called V-type proton ATPase subunit e 1.

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

- Molecule 6 is a protein called Ribonuclease kappa.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	85	Total	C	N	O	S	0	0
			658	434	102	115	7		

- Molecule 7 is a protein called V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	204	Total	C	N	O	S	0	0
			1662	1086	267	299	10		

- Molecule 8 is a protein called Renin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	49	Total	C	N	O	S	0	0
			411	280	57	71	3		

- Molecule 9 is a protein called V-type proton ATPase 21 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	0	204	Total	C	N	O	S	0	0
			1498	990	238	259	11		

- Molecule 10 is a protein called V-type proton ATPase 16 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
10	2	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
10	3	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
10	4	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
10	5	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
10	6	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	7	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
10	8	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
10	9	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	351	Total	C	N	O	S	0	0
			2844	1834	463	532	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	600	Total	C	N	O	S	0	0
			4656	2952	786	890	28		
12	A	600	Total	C	N	O	S	0	0
			4656	2952	786	890	28		
12	B	600	Total	C	N	O	S	0	0
			4656	2952	786	890	28		

- Molecule 13 is a protein called V-type proton ATPase subunit B, brain isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	468	Total	C	N	O	S	0	0
			3666	2325	625	696	20		
13	E	468	Total	C	N	O	S	0	0
			3666	2325	625	696	20		
13	F	468	Total	C	N	O	S	0	0
			3666	2325	625	696	20		

- Molecule 14 is a protein called SidK.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Z	262	Total	C	N	O	S	0	0
			2110	1339	353	408	10		
14	X	267	Total	C	N	O	S	0	0
			2136	1355	359	411	11		
14	Y	262	Total	C	N	O	S	0	0
			2111	1339	354	408	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	G	213	1717	1090	310	312	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	N	110	875	552	157	164	2	0	0

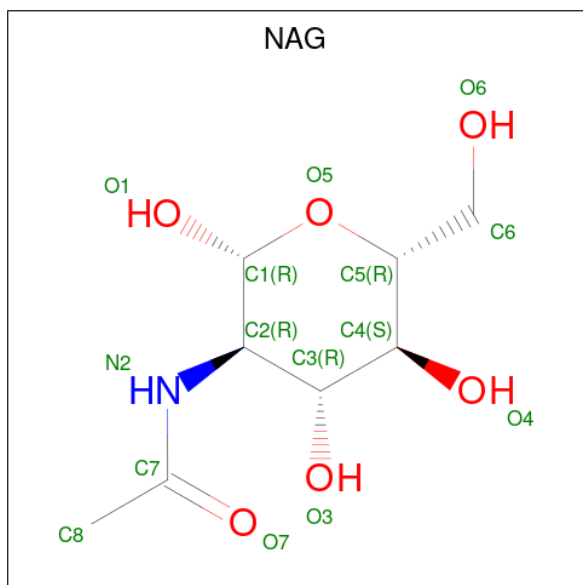
- Molecule 17 is a protein called V-type proton ATPase subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	P	427	2121	1267	427	427	0	0

- Molecule 18 is a protein called MTOR-associated protein MEAK7.

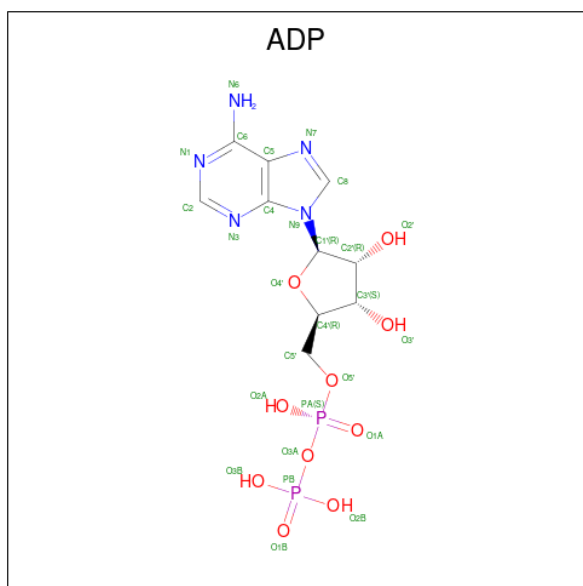
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	W	420	3023	1900	548	559	16	0	0

- Molecule 19 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

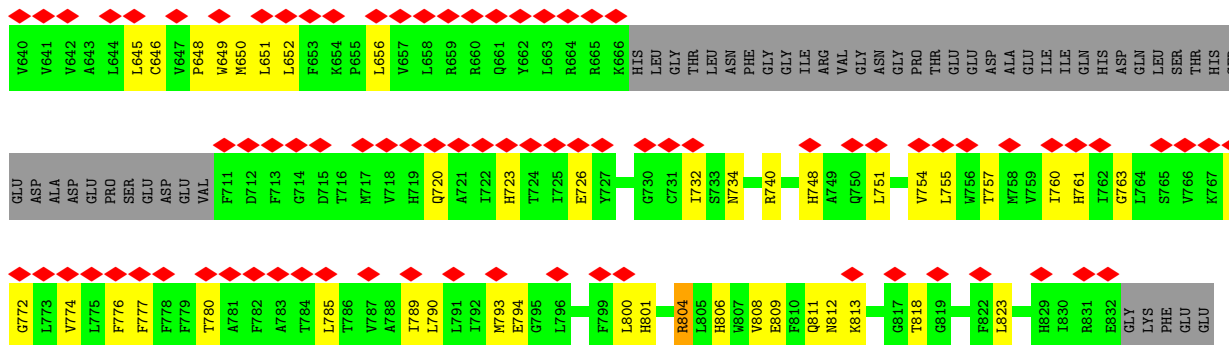


Mol	Chain	Residues	Atoms				AltConf
19	R	1	Total	C	N	O	0
			14	8	1	5	
19	S	1	Total	C	N	O	0
			14	8	1	5	
19	U	1	Total	C	N	O	0
			14	8	1	5	
19	U	1	Total	C	N	O	0
			14	8	1	5	
19	U	1	Total	C	N	O	0
			14	8	1	5	
19	U	1	Total	C	N	O	0
			14	8	1	5	
19	U	1	Total	C	N	O	0
			14	8	1	5	

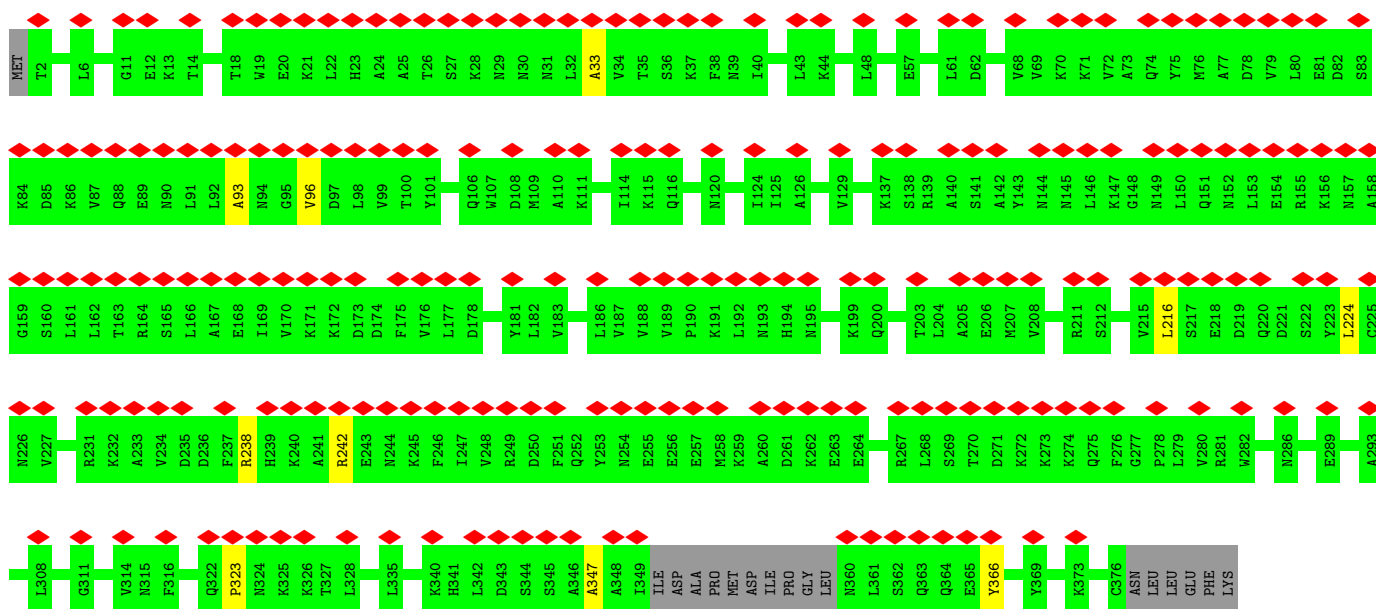
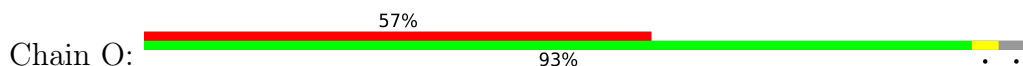
- Molecule 20 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



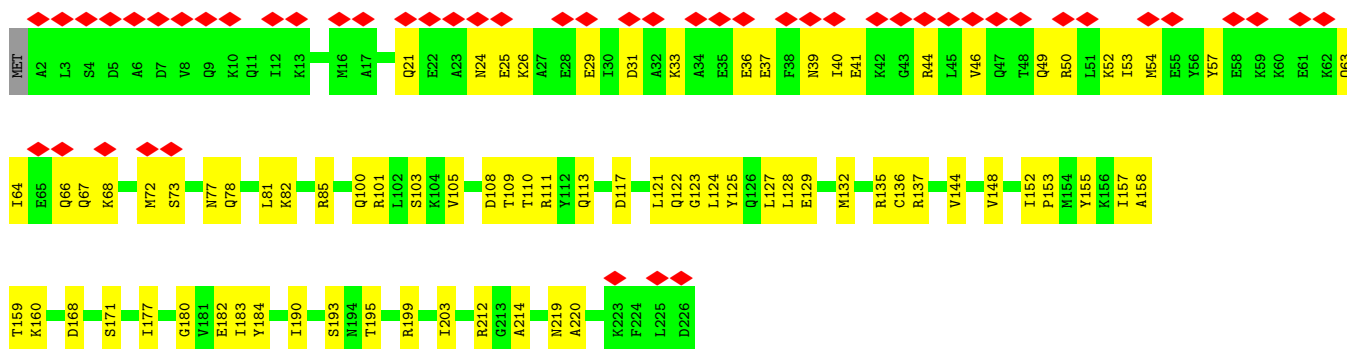
Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total	C	N	O	P	0
			27	10	5	10	2	



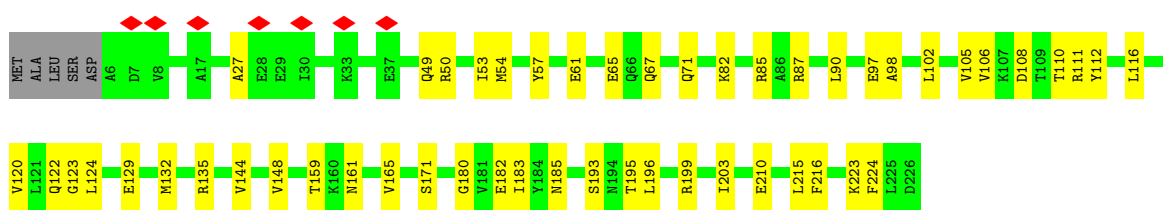
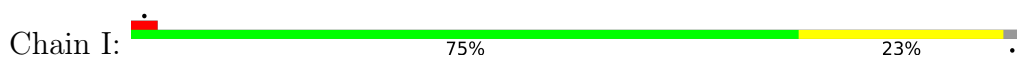
• Molecule 2: V-type proton ATPase subunit C 1



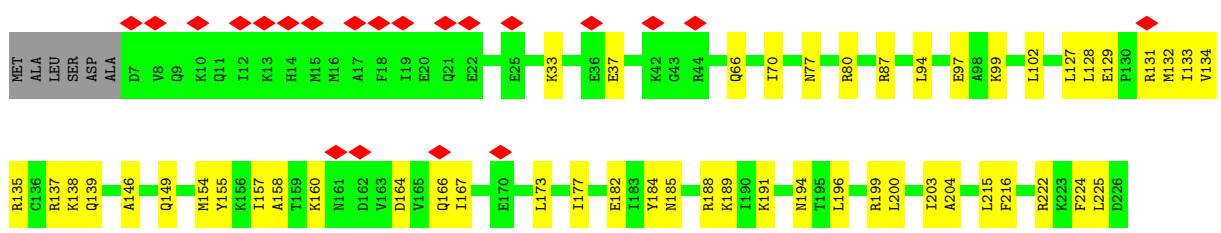
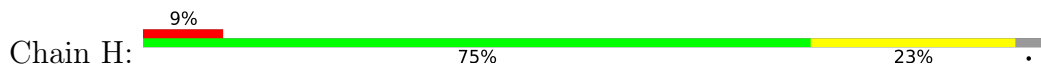
• Molecule 3: V-type proton ATPase subunit E 1



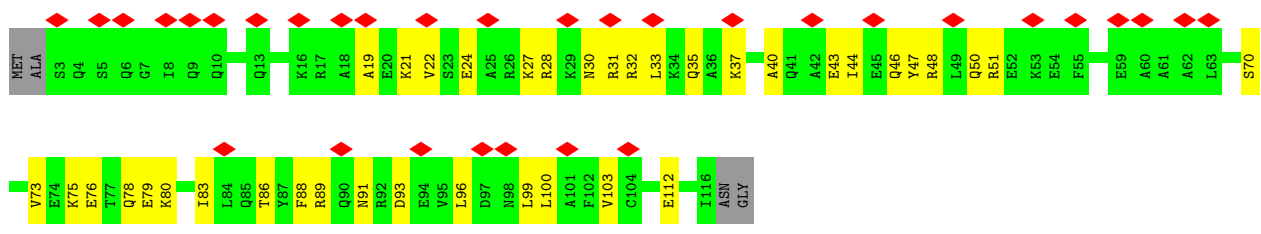
• Molecule 3: V-type proton ATPase subunit E 1



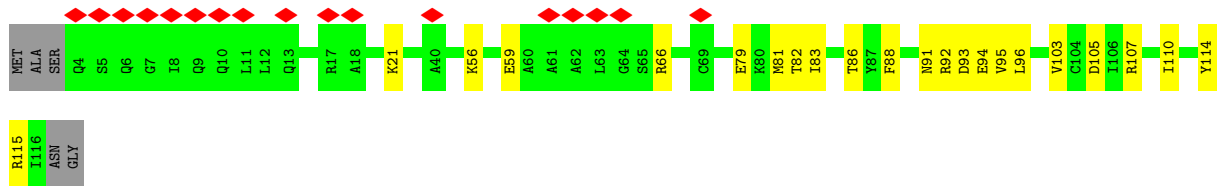
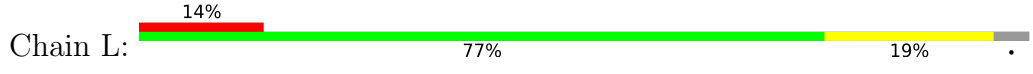
• Molecule 3: V-type proton ATPase subunit E 1



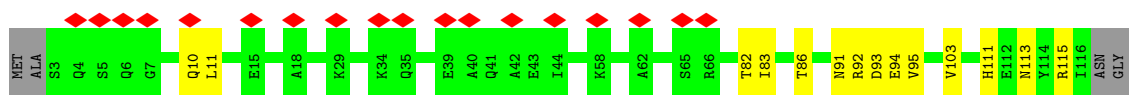
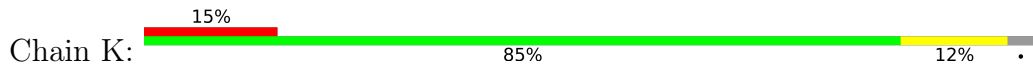
• Molecule 4: V-type proton ATPase subunit G 1



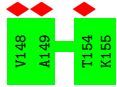
• Molecule 4: V-type proton ATPase subunit G 1



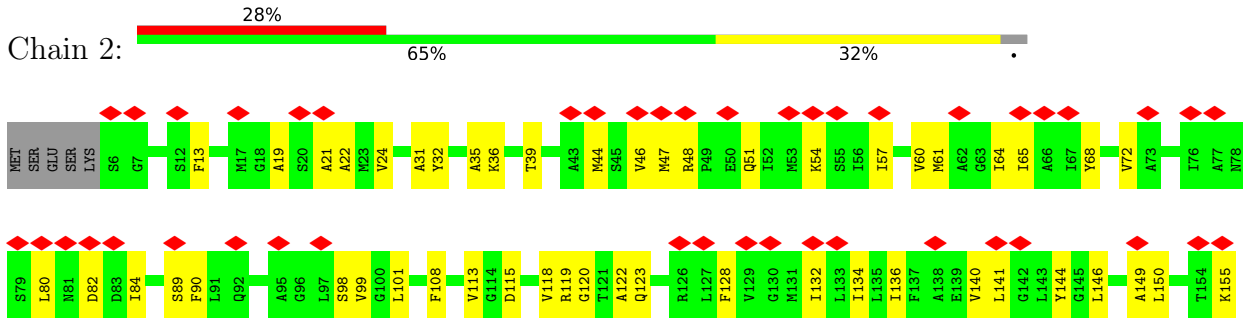
• Molecule 4: V-type proton ATPase subunit G 1



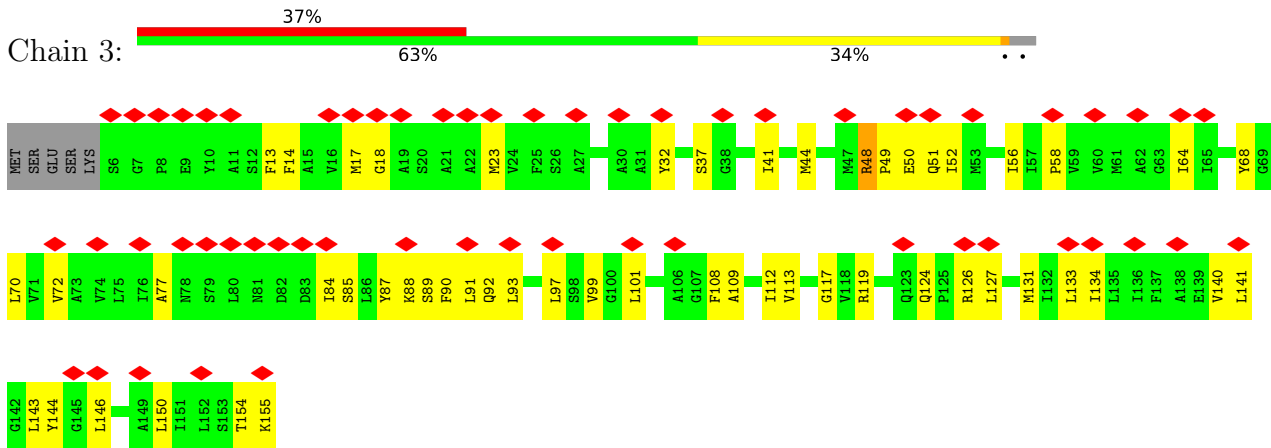
• Molecule 5: V-type proton ATPase subunit e 1



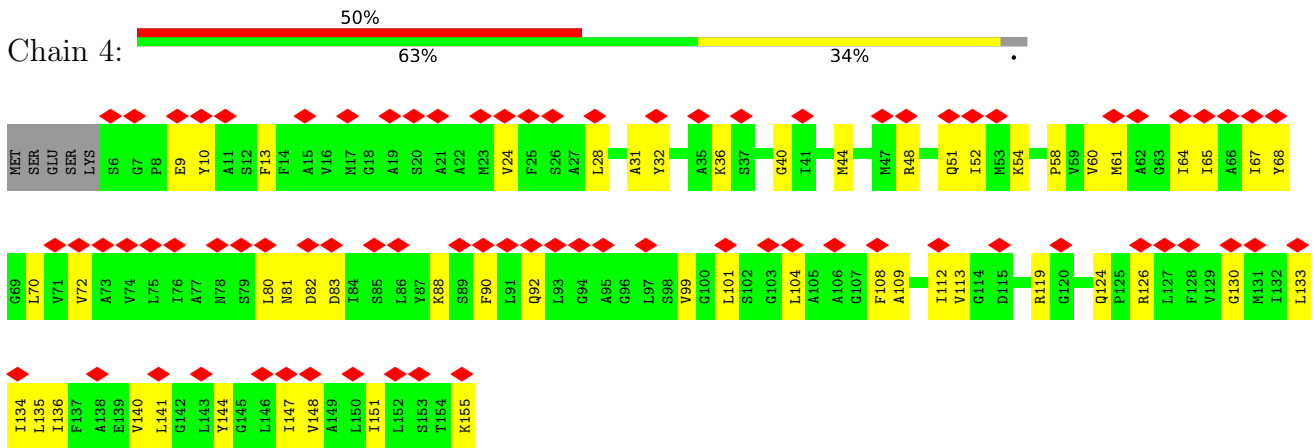
• Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit



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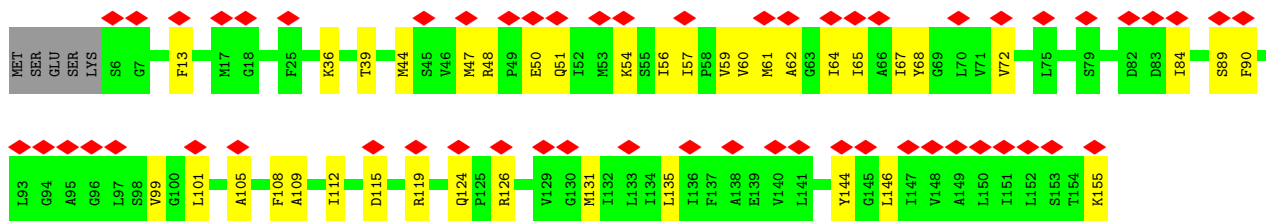


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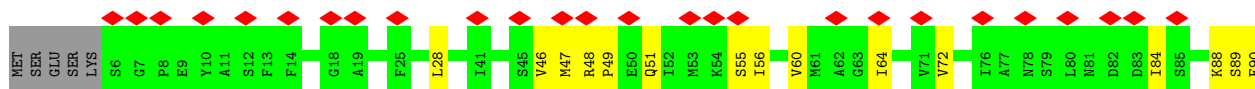
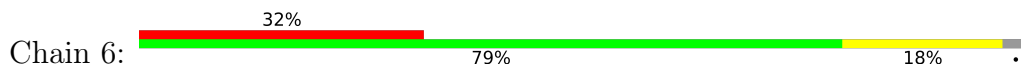


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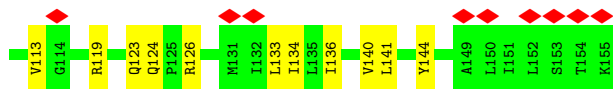
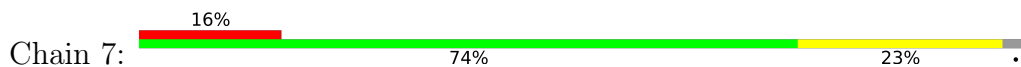




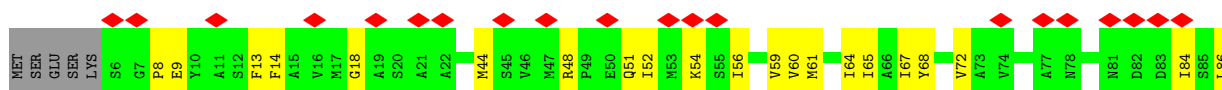
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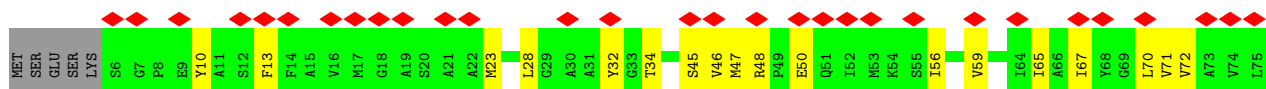
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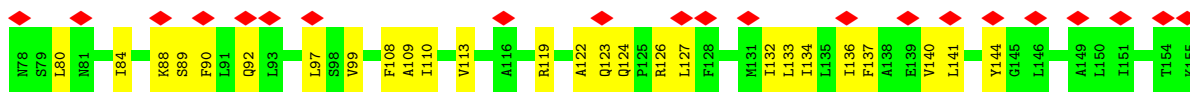


• Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit

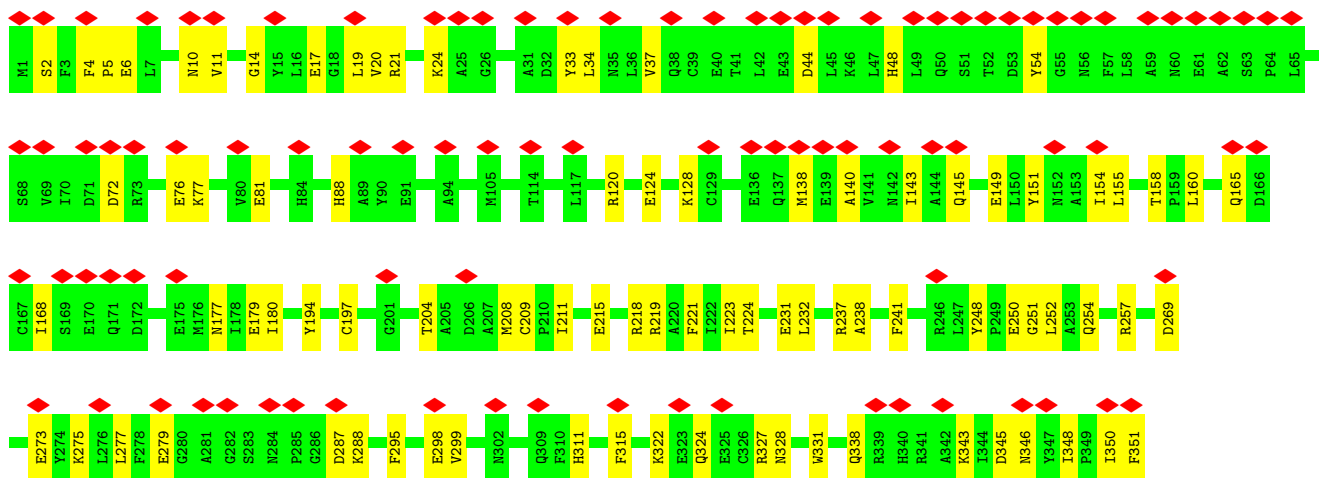
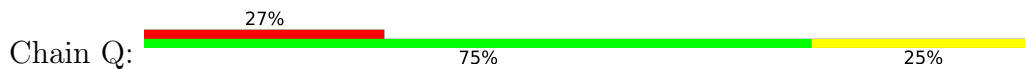


• Molecule 10: V-type proton ATPase 16 kDa proteolipid subunit

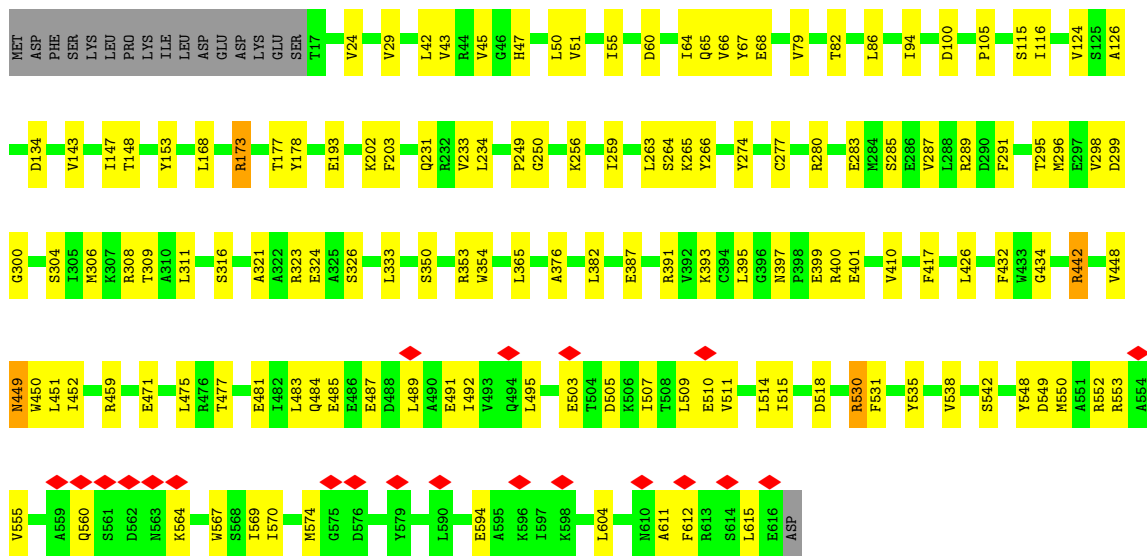




• Molecule 11: V-type proton ATPase subunit d 1

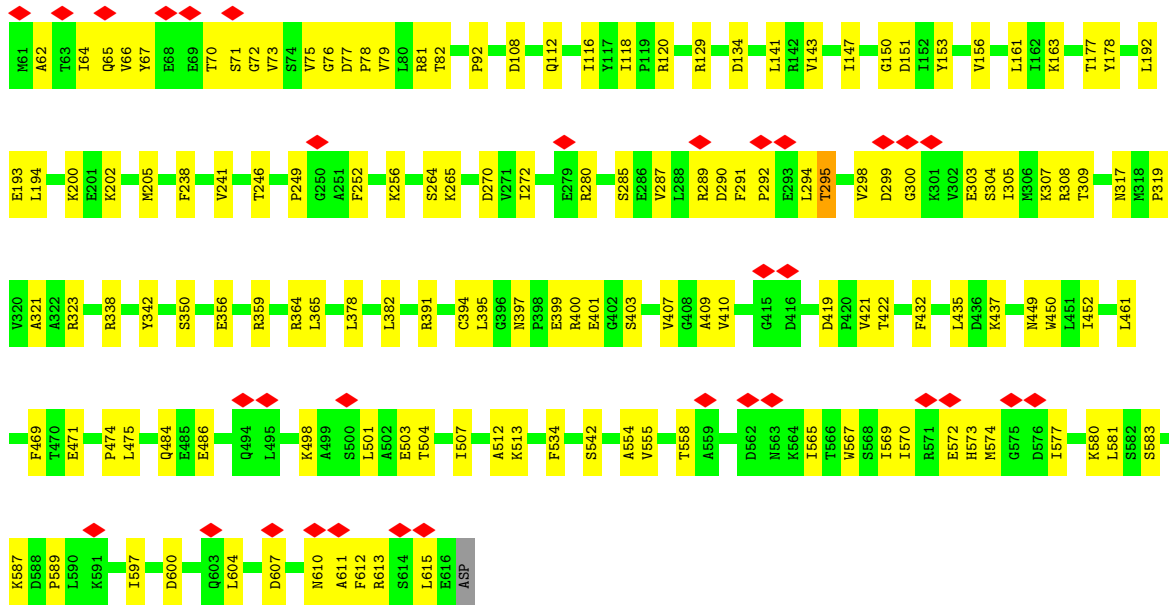


• Molecule 12: V-type proton ATPase catalytic subunit A

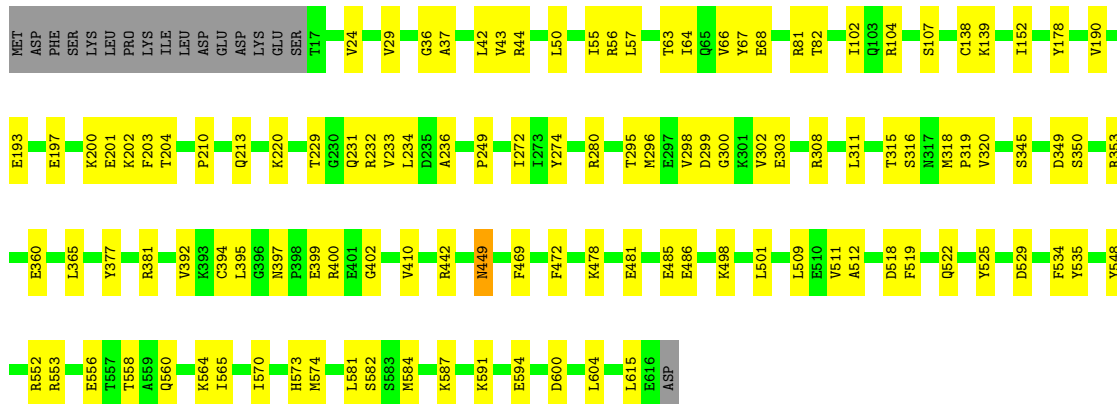
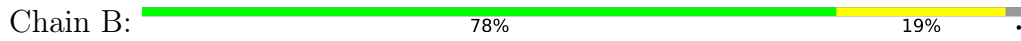


• Molecule 12: V-type proton ATPase catalytic subunit A

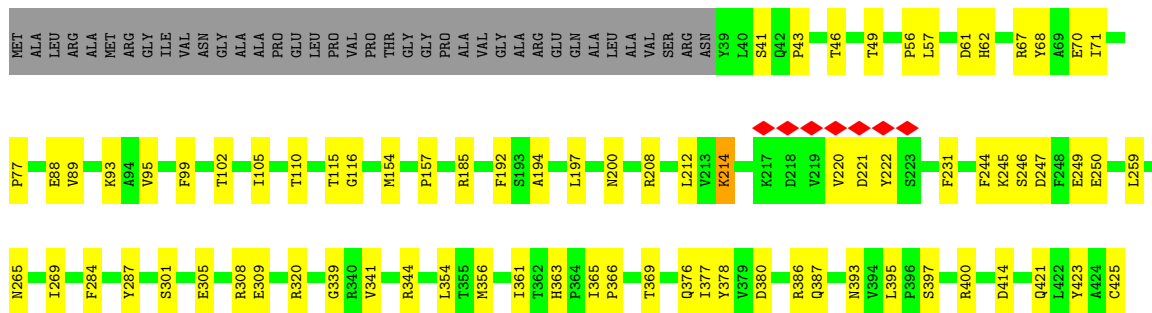
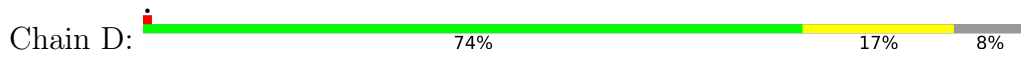


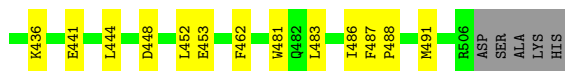


• Molecule 12: V-type proton ATPase catalytic subunit A

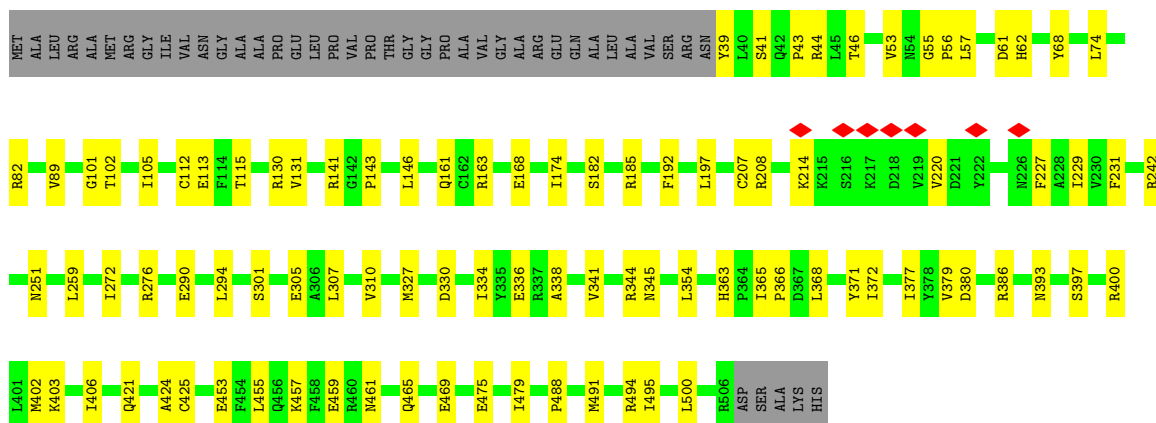


• Molecule 13: V-type proton ATPase subunit B, brain isoform

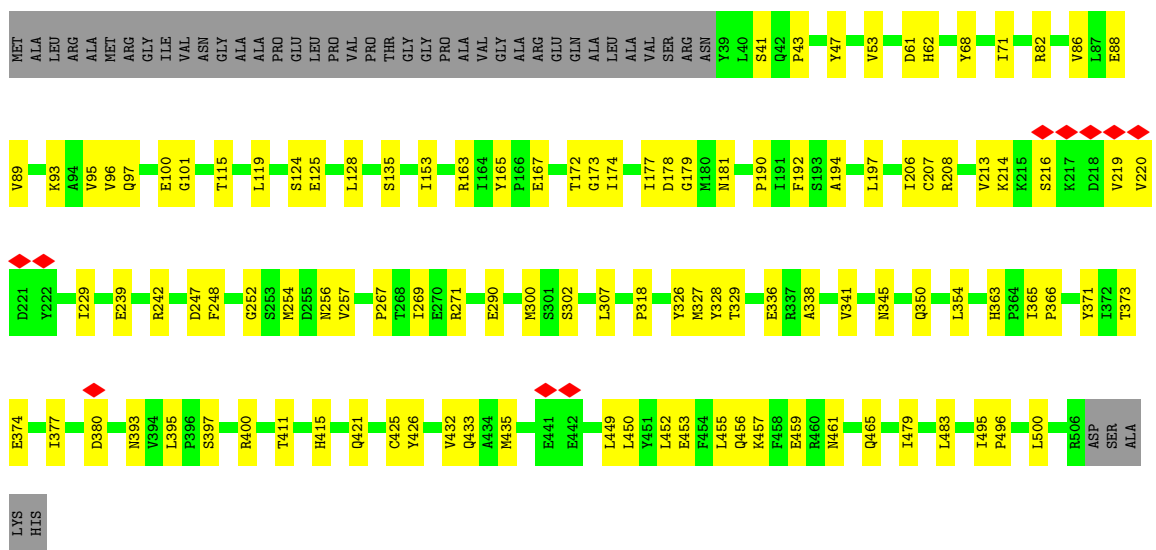




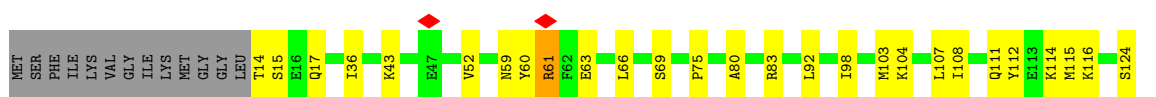
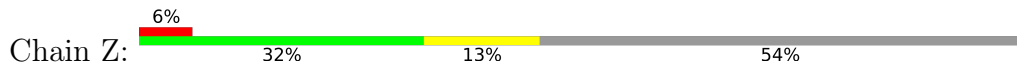
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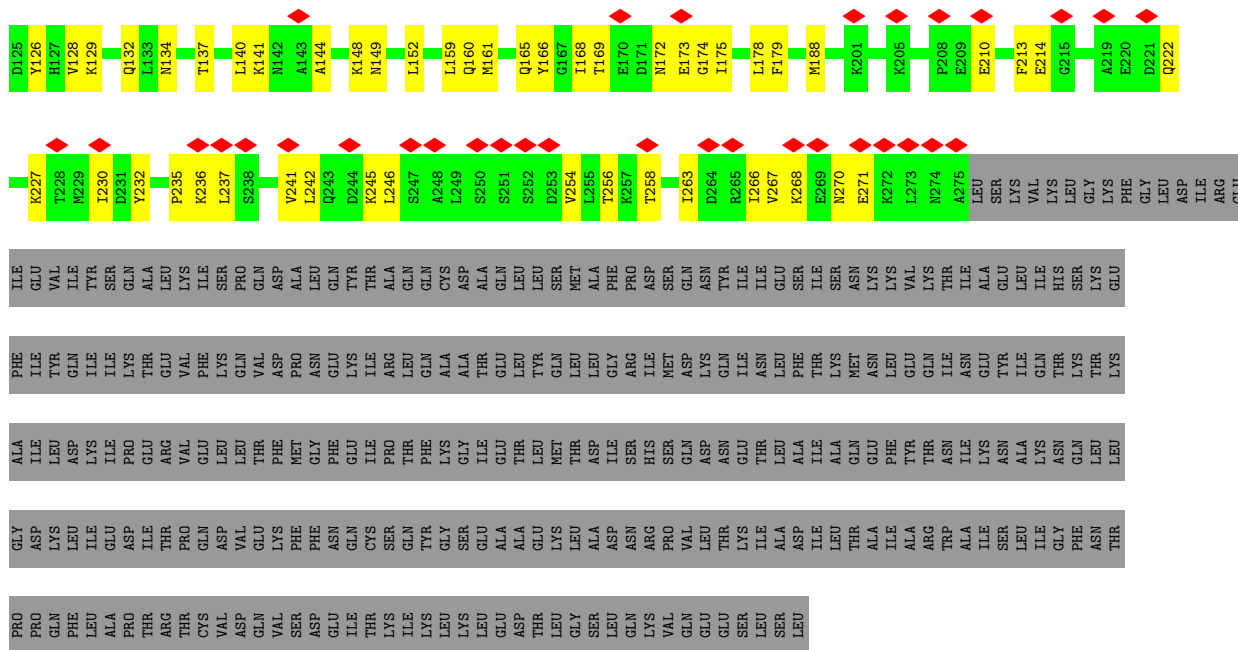


• Molecule 13: V-type proton ATPase subunit B, brain isoform

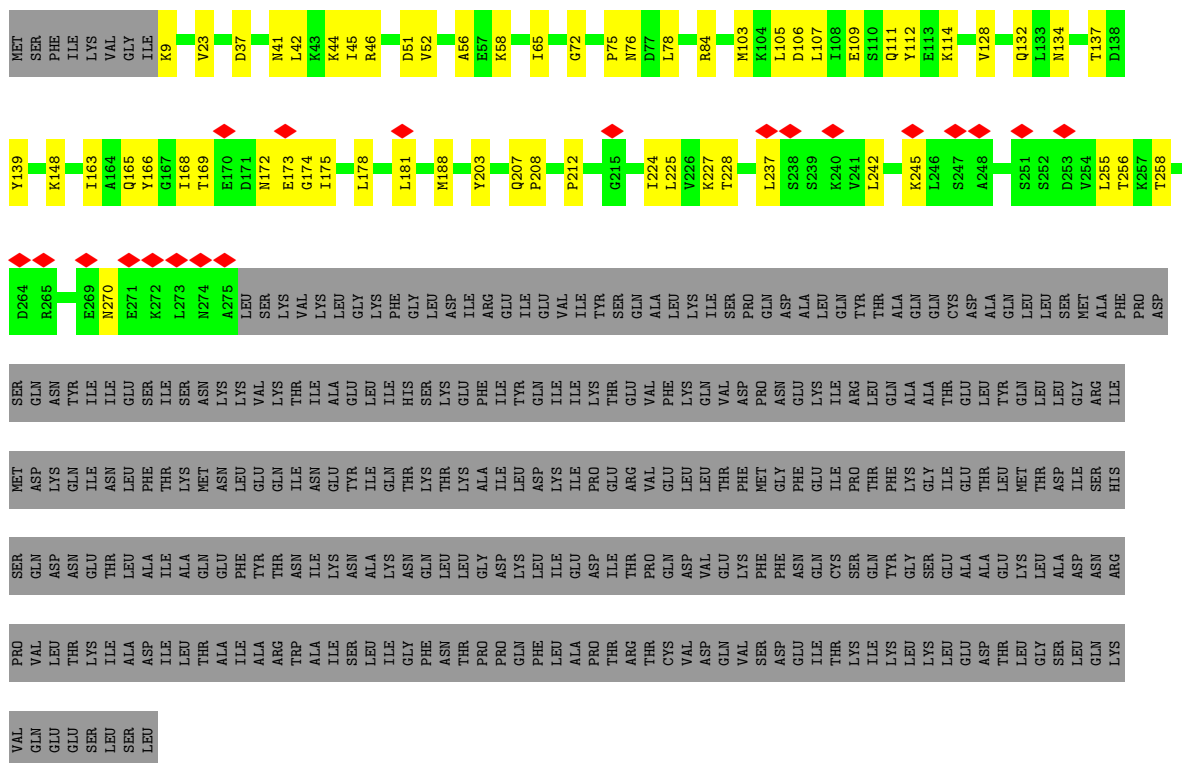
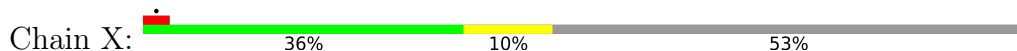


• Molecule 14: SidK

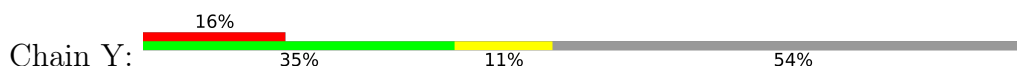




• Molecule 14: SidK

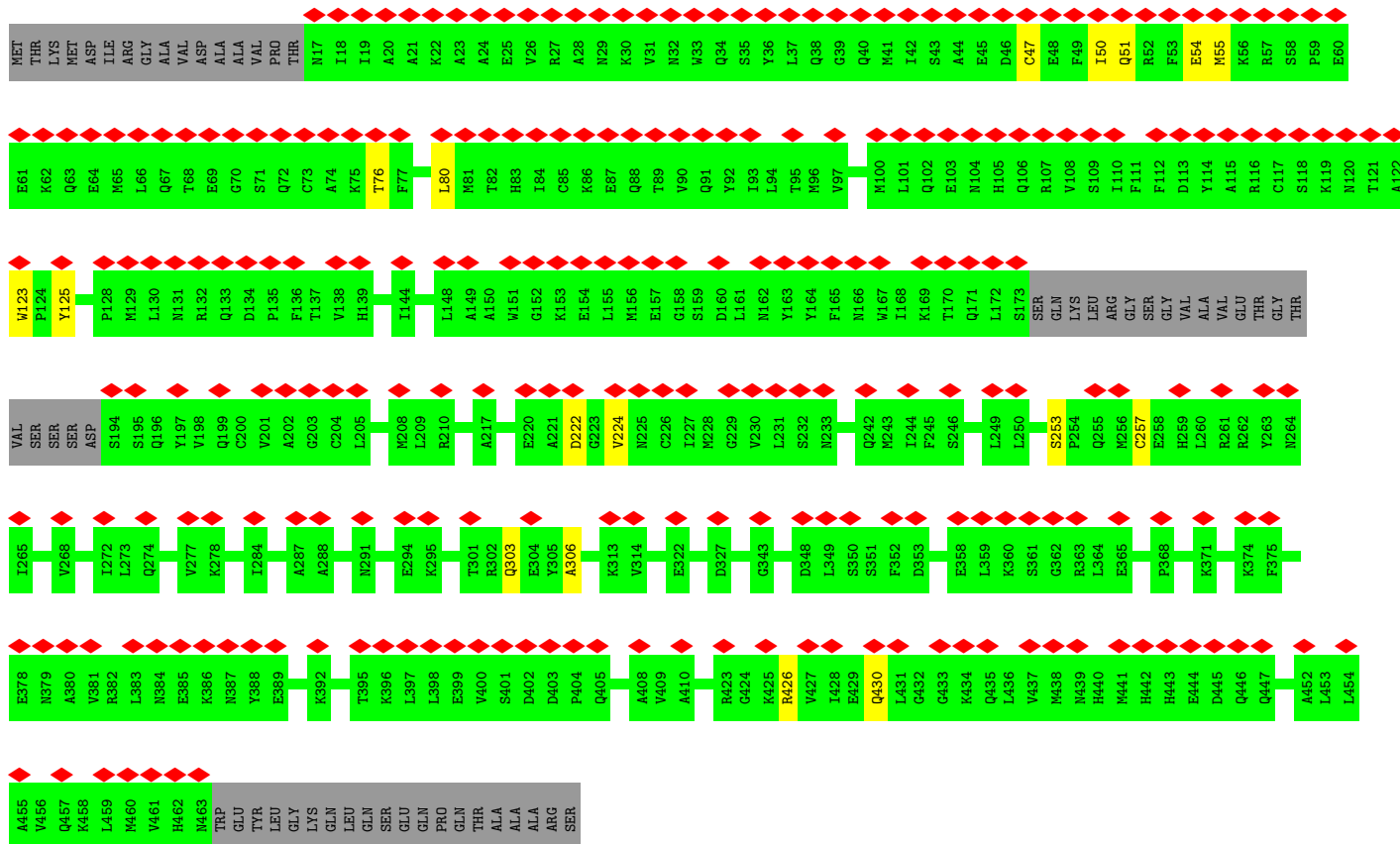
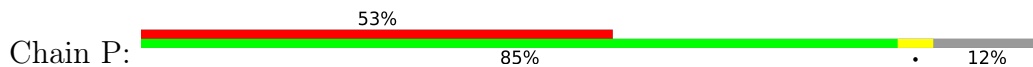


• Molecule 14: SidK

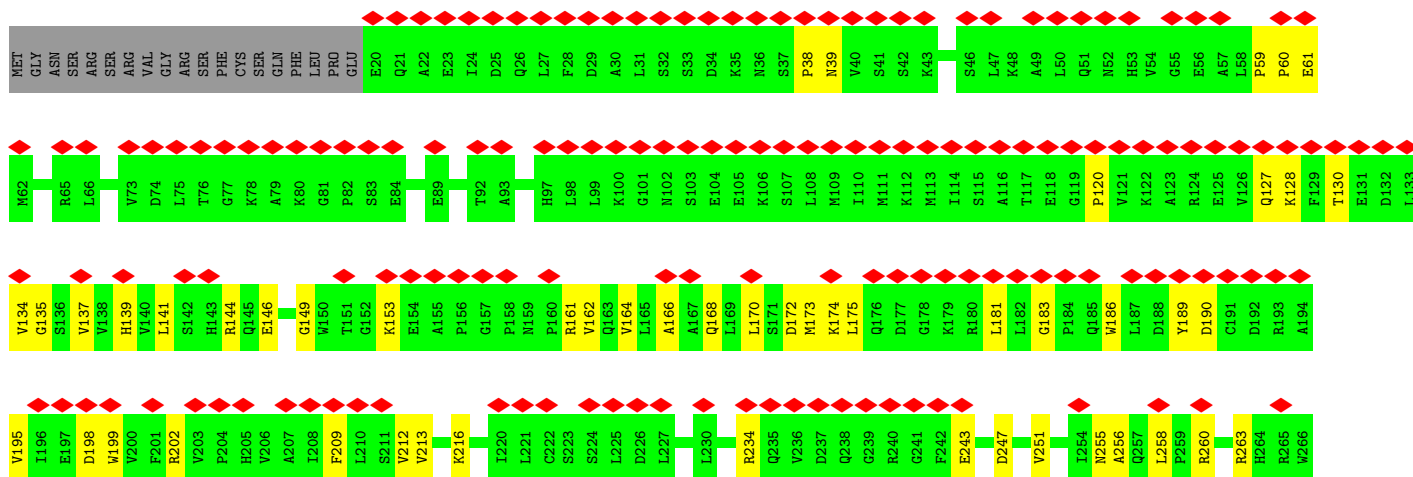
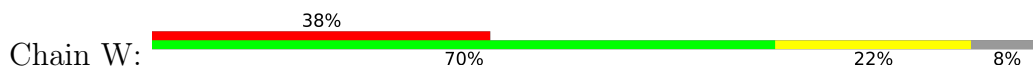


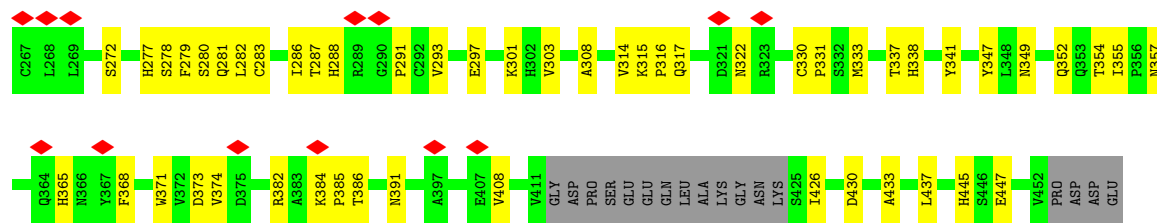


• Molecule 17: V-type proton ATPase subunit H



• Molecule 18: MTOR-associated protein MEAK7





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	170000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.354	Depositor
Minimum map value	-1.886	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.085	Depositor
Recommended contour level	0.292	Depositor
Map size (\AA)	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.08, 1.08, 1.08	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, NAG

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	R	0.33	0/6023	0.54	1/8174 (0.0%)
2	O	0.25	0/1816	0.42	0/2534
3	H	0.31	0/1623	0.54	0/2190
3	I	0.31	0/1675	0.55	0/2256
3	J	0.33	0/1789	0.55	0/2401
4	K	0.34	0/740	0.52	0/1012
4	L	0.33	0/753	0.50	0/1026
4	M	0.31	0/896	0.59	0/1198
5	S	0.39	1/657 (0.2%)	0.53	0/902
6	T	0.32	0/674	0.54	0/915
7	U	0.34	0/1716	0.58	1/2333 (0.0%)
8	V	0.35	0/425	0.49	0/582
9	0	0.39	0/1532	0.55	0/2082
10	1	0.39	0/1080	0.55	0/1461
10	2	0.40	0/1080	0.59	0/1461
10	3	0.38	0/1080	0.58	0/1461
10	4	0.40	0/1080	0.60	0/1461
10	5	0.38	0/1080	0.57	0/1461
10	6	0.38	0/1080	0.53	0/1461
10	7	0.41	0/1080	0.57	0/1461
10	8	0.42	0/1080	0.58	0/1461
10	9	0.37	0/1080	0.52	0/1461
11	Q	0.38	0/2910	0.52	0/3940
12	A	0.40	0/4752	0.58	0/6435
12	B	0.43	0/4752	0.56	0/6435
12	C	0.39	0/4752	0.55	0/6435
13	D	0.42	0/3739	0.56	0/5067
13	E	0.41	0/3739	0.53	0/5067
13	F	0.40	0/3739	0.57	1/5067 (0.0%)
14	X	0.30	0/2170	0.48	0/2926
14	Y	0.27	0/2145	0.50	0/2893
14	Z	0.28	0/2143	0.50	0/2888

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	G	0.32	0/1735	0.56	0/2320
16	N	0.26	0/889	0.52	0/1200
17	P	0.24	0/2119	0.40	0/2955
18	W	0.30	0/3095	0.51	0/4222
All	All	0.36	1/72718 (0.0%)	0.54	3/98604 (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
3	I	0	1
12	A	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	47	CYS	CB-SG	-5.09	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	F	496	PRO	CA-N-CD	-5.65	103.59	111.50
1	R	453	MET	CA-CB-CG	5.45	122.57	113.30
7	U	390	PRO	CA-N-CD	-5.07	104.40	111.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	A	295	THR	Peptide
3	I	224	PHE	Peptide

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	R	5876	0	5678	154	0
2	O	1817	0	813	5	0
3	H	1611	0	1546	38	0
3	I	1661	0	1626	46	0
3	J	1774	0	1794	67	0
4	K	735	0	566	13	0
4	L	748	0	602	21	0
4	M	889	0	854	32	0
5	S	631	0	646	20	0
6	T	658	0	652	12	0
7	U	1662	0	1586	59	0
8	V	411	0	401	13	0
9	0	1498	0	1544	45	0
10	1	1065	0	1131	50	0
10	2	1065	0	1131	41	0
10	3	1065	0	1131	47	0
10	4	1065	0	1131	53	0
10	5	1065	0	1131	31	0
10	6	1065	0	1131	22	0
10	7	1065	0	1131	41	0
10	8	1065	0	1131	36	0
10	9	1065	0	1131	37	0
11	Q	2844	0	2782	64	0
12	A	4656	0	4642	136	0
12	B	4656	0	4642	83	0
12	C	4656	0	4642	103	0
13	D	3666	0	3665	71	0
13	E	3666	0	3665	62	0
13	F	3666	0	3665	79	0
14	X	2136	0	2158	43	0
14	Y	2111	0	2134	40	0
14	Z	2110	0	2132	55	0
15	G	1717	0	1829	48	0
16	N	875	0	878	33	0
17	P	2121	0	941	9	0
18	W	3023	0	2657	77	0
19	R	14	0	13	1	0
19	S	14	0	13	1	0
19	U	84	0	78	0	0
20	B	27	0	12	0	0
All	All	71598	0	69035	1574	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 1574 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)
14:Y:62:PHE:O	14:Y:66:LEU:HB2	1.60	1.00
3:J:122:GLN:HE21	13:F:43:PRO:HD3	1.25	0.98
10:3:48:ARG:HH12	10:3:51:GLN:HG2	1.28	0.97
10:5:124:GLN:HE22	10:5:126:ARG:HG2	1.29	0.96
1:R:61:MET:HG3	1:R:98:GLU:HG2	1.53	0.90

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	747/837 (89%)	708 (95%)	39 (5%)	0	100	100
2	O	361/382 (94%)	347 (96%)	14 (4%)	0	100	100
3	H	218/226 (96%)	204 (94%)	14 (6%)	0	100	100
3	I	219/226 (97%)	207 (94%)	12 (6%)	0	100	100
3	J	223/226 (99%)	205 (92%)	17 (8%)	1 (0%)	34	71
4	K	112/118 (95%)	107 (96%)	5 (4%)	0	100	100
4	L	111/118 (94%)	110 (99%)	1 (1%)	0	100	100
4	M	112/118 (95%)	101 (90%)	11 (10%)	0	100	100
5	S	75/81 (93%)	72 (96%)	3 (4%)	0	100	100
6	T	83/137 (61%)	79 (95%)	4 (5%)	0	100	100
7	U	202/470 (43%)	177 (88%)	25 (12%)	0	100	100
8	V	47/350 (13%)	43 (92%)	4 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	0	202/205 (98%)	191 (95%)	11 (5%)	0	100	100
10	1	148/155 (96%)	137 (93%)	11 (7%)	0	100	100
10	2	148/155 (96%)	137 (93%)	11 (7%)	0	100	100
10	3	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
10	4	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
10	5	148/155 (96%)	136 (92%)	12 (8%)	0	100	100
10	6	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
10	7	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
10	8	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
10	9	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
11	Q	349/351 (99%)	322 (92%)	27 (8%)	0	100	100
12	A	598/617 (97%)	535 (90%)	63 (10%)	0	100	100
12	B	598/617 (97%)	555 (93%)	43 (7%)	0	100	100
12	C	598/617 (97%)	558 (93%)	40 (7%)	0	100	100
13	D	466/511 (91%)	441 (95%)	25 (5%)	0	100	100
13	E	466/511 (91%)	446 (96%)	20 (4%)	0	100	100
13	F	466/511 (91%)	442 (95%)	24 (5%)	0	100	100
14	X	265/573 (46%)	249 (94%)	16 (6%)	0	100	100
14	Y	260/573 (45%)	249 (96%)	11 (4%)	0	100	100
14	Z	258/573 (45%)	248 (96%)	10 (4%)	0	100	100
15	G	211/247 (85%)	205 (97%)	6 (3%)	0	100	100
16	N	108/119 (91%)	101 (94%)	7 (6%)	0	100	100
17	P	423/483 (88%)	370 (88%)	53 (12%)	0	100	100
18	W	416/456 (91%)	393 (94%)	23 (6%)	0	100	100
All	All	9526/11648 (82%)	8922 (94%)	603 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	J	109	THR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R	602/746 (81%)	599 (100%)	3 (0%)	88	95
2	O	1/344 (0%)	1 (100%)	0	100	100
3	H	149/199 (75%)	149 (100%)	0	100	100
3	I	159/199 (80%)	159 (100%)	0	100	100
3	J	184/199 (92%)	183 (100%)	1 (0%)	88	95
4	K	48/101 (48%)	48 (100%)	0	100	100
4	L	53/101 (52%)	53 (100%)	0	100	100
4	M	85/101 (84%)	85 (100%)	0	100	100
5	S	69/72 (96%)	69 (100%)	0	100	100
6	T	71/116 (61%)	71 (100%)	0	100	100
7	U	182/397 (46%)	180 (99%)	2 (1%)	73	88
8	V	44/308 (14%)	44 (100%)	0	100	100
9	0	154/155 (99%)	154 (100%)	0	100	100
10	1	107/112 (96%)	107 (100%)	0	100	100
10	2	107/112 (96%)	107 (100%)	0	100	100
10	3	107/112 (96%)	106 (99%)	1 (1%)	78	90
10	4	107/112 (96%)	107 (100%)	0	100	100
10	5	107/112 (96%)	107 (100%)	0	100	100
10	6	107/112 (96%)	107 (100%)	0	100	100
10	7	107/112 (96%)	106 (99%)	1 (1%)	78	90
10	8	107/112 (96%)	107 (100%)	0	100	100
10	9	107/112 (96%)	107 (100%)	0	100	100
11	Q	306/306 (100%)	306 (100%)	0	100	100
12	A	508/525 (97%)	506 (100%)	2 (0%)	91	97
12	B	508/525 (97%)	507 (100%)	1 (0%)	93	98
12	C	508/525 (97%)	504 (99%)	4 (1%)	81	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	D	401/430 (93%)	400 (100%)	1 (0%)	93	98
13	E	401/430 (93%)	401 (100%)	0	100	100
13	F	401/430 (93%)	401 (100%)	0	100	100
14	X	239/519 (46%)	238 (100%)	1 (0%)	91	97
14	Y	238/519 (46%)	237 (100%)	1 (0%)	91	97
14	Z	237/519 (46%)	236 (100%)	1 (0%)	91	97
15	G	184/212 (87%)	184 (100%)	0	100	100
16	N	94/100 (94%)	94 (100%)	0	100	100
18	W	276/396 (70%)	276 (100%)	0	100	100
All	All	7065/9482 (74%)	7046 (100%)	19 (0%)	92	97

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	B	449	ASN
14	X	227	LYS
14	Y	270	ASN
14	Z	61	ARG
12	C	173	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
11	Q	50	GLN
12	A	282	ASN
11	Q	346	ASN
12	A	317	ASN
6	T	125	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 ligands are 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
19	NAG	S	101	5	14,14,15	0.47	0	17,19,21	0.56	0
19	NAG	U	503	7	14,14,15	0.18	0	17,19,21	0.45	0
20	ADP	B	701	-	24,29,29	0.96	1 (4%)	29,45,45	1.47	4 (13%)
19	NAG	U	506	7	14,14,15	0.17	0	17,19,21	0.49	0
19	NAG	U	501	7	14,14,15	0.24	0	17,19,21	0.33	0
19	NAG	R	901	1	14,14,15	0.32	0	17,19,21	0.49	0
19	NAG	U	504	-	14,14,15	0.26	0	17,19,21	0.50	0
19	NAG	U	505	-	14,14,15	0.22	0	17,19,21	0.41	0
19	NAG	U	502	-	14,14,15	0.23	0	17,19,21	0.38	0

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
19	NAG	S	101	5	-	2/6/23/26	0/1/1/1
19	NAG	U	503	7	-	2/6/23/26	0/1/1/1
20	ADP	B	701	-	-	1/12/32/32	0/3/3/3
19	NAG	U	506	7	-	3/6/23/26	0/1/1/1
19	NAG	U	501	7	-	2/6/23/26	0/1/1/1
19	NAG	R	901	1	-	3/6/23/26	0/1/1/1
19	NAG	U	504	-	-	3/6/23/26	0/1/1/1
19	NAG	U	505	-	-	4/6/23/26	0/1/1/1
19	NAG	U	502	-	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	701	ADP	C5-C4	2.26	1.46	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	701	ADP	C3'-C2'-C1'	3.56	106.34	100.98
20	B	701	ADP	N3-C2-N1	-2.99	124.01	128.68
20	B	701	ADP	PA-O3A-PB	-2.74	123.41	132.83
20	B	701	ADP	C4-C5-N7	-2.42	106.88	109.40

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

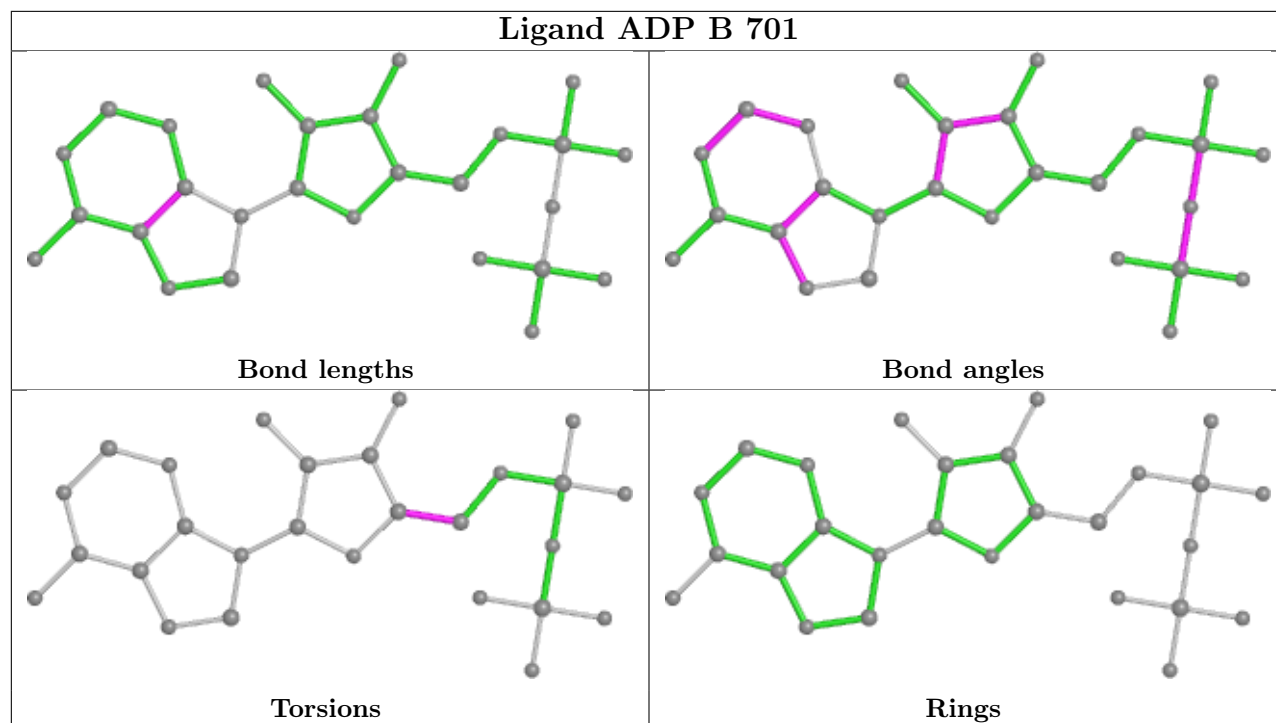
Mol	Chain	Res	Type	Atoms
19	S	101	NAG	C4-C5-C6-O6
19	U	505	NAG	C4-C5-C6-O6
19	S	101	NAG	O5-C5-C6-O6
19	U	504	NAG	O5-C5-C6-O6
19	U	505	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	S	101	NAG	1	0
19	R	901	NAG	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.

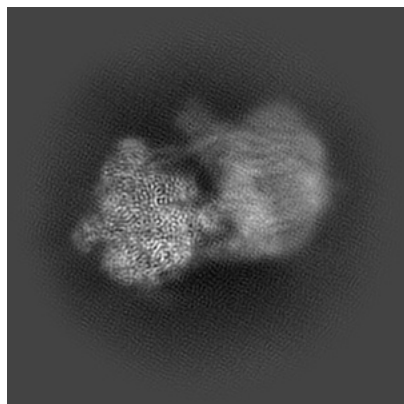
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26334. These allow visual inspection of the internal detail of the map and identification of artifacts.

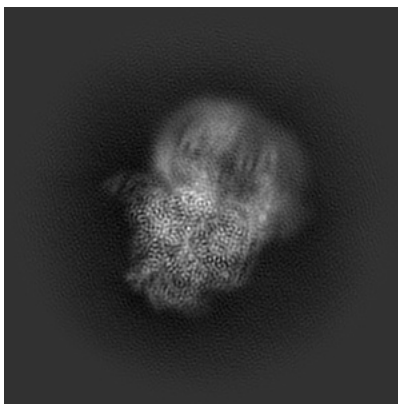
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

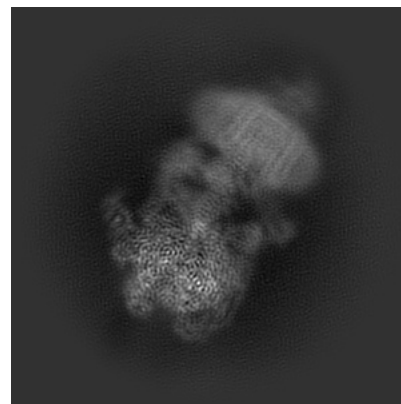
6.1.1 Primary map



X



Y

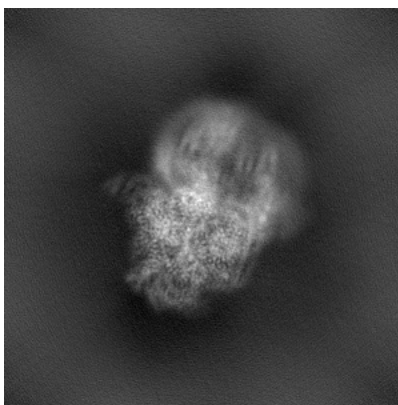


Z

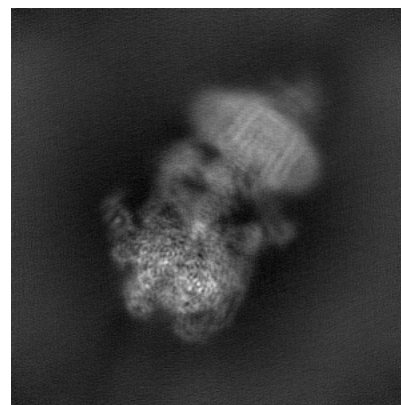
6.1.2 Raw map



X



Y

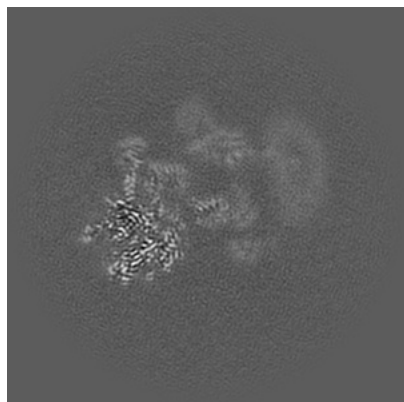


Z

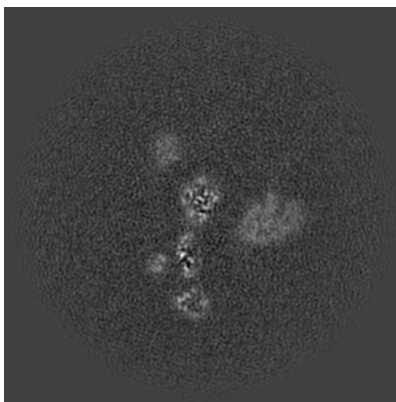
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

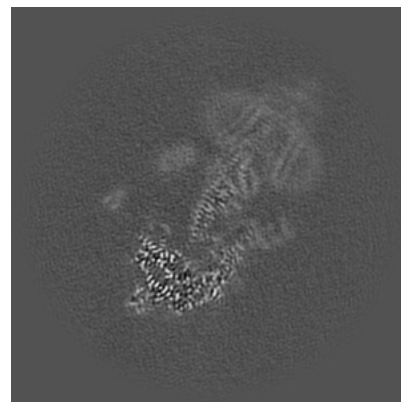
6.2.1 Primary map



X Index: 180

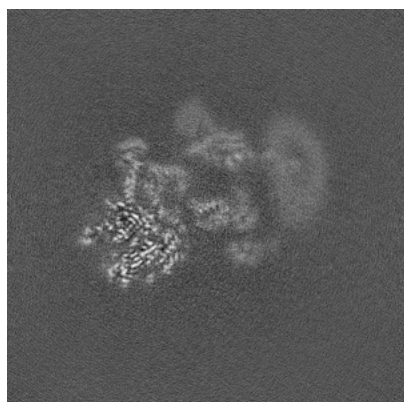


Y Index: 180

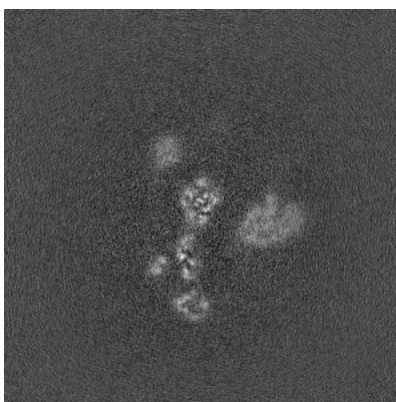


Z Index: 180

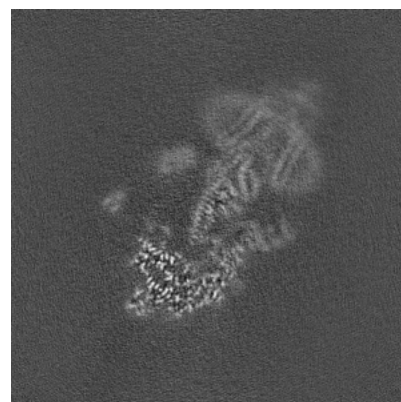
6.2.2 Raw map



X Index: 180



Y Index: 180

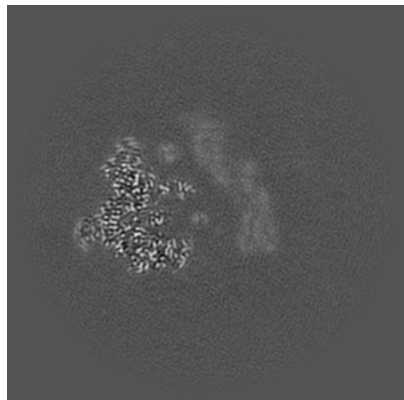


Z Index: 180

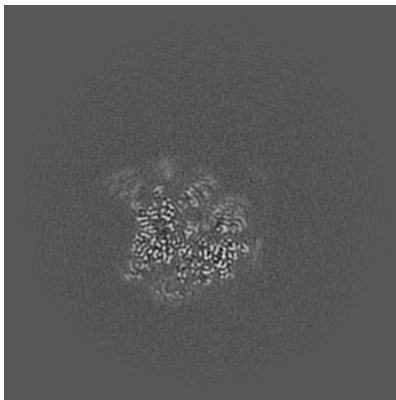
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

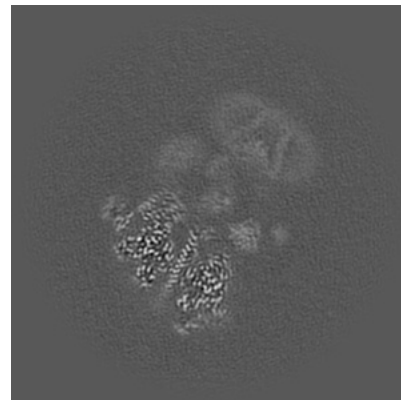
6.3.1 Primary map



X Index: 156

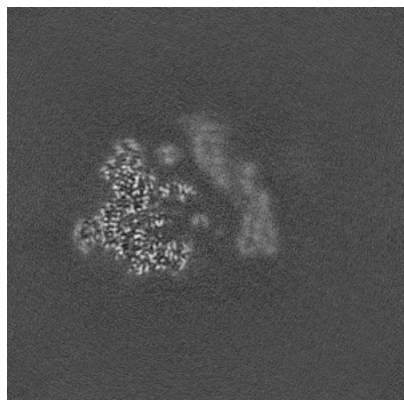


Y Index: 130

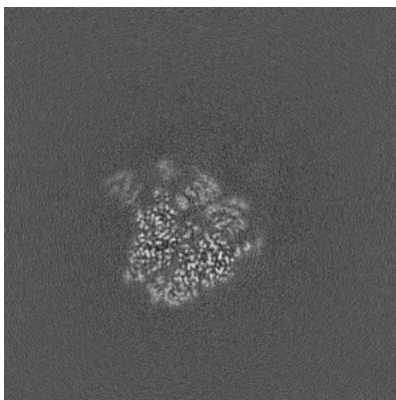


Z Index: 164

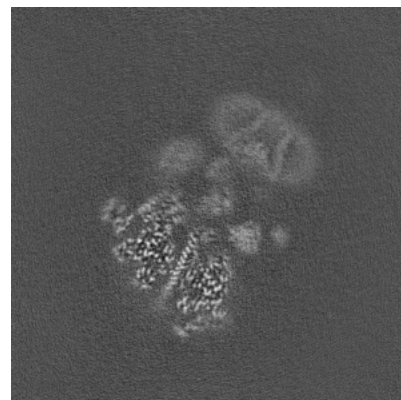
6.3.2 Raw map



X Index: 156



Y Index: 133

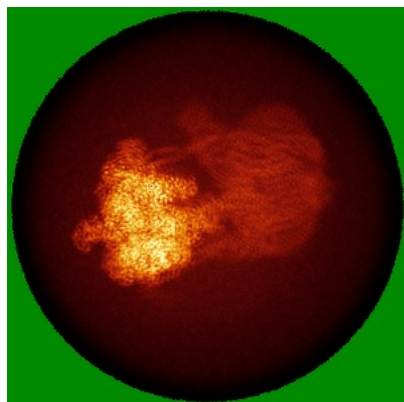


Z Index: 164

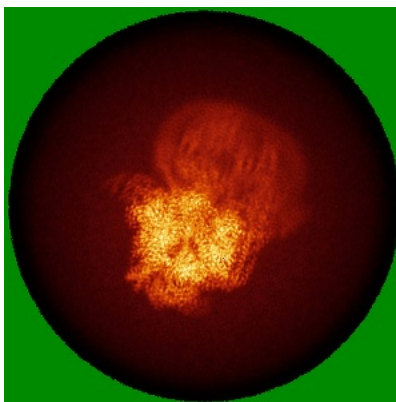
The images above show the largest variance slices of the map in three orthogonal directions.

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

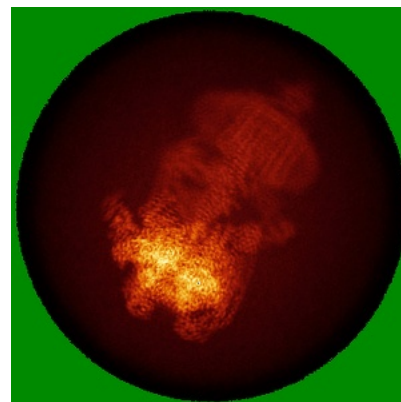
6.4.1 Primary map



X

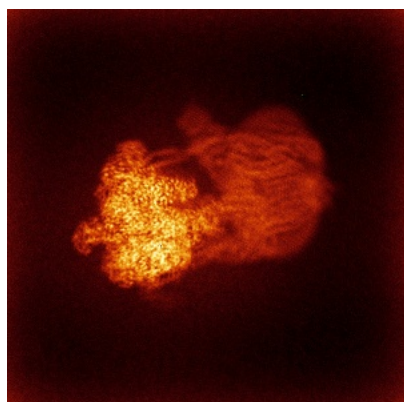


Y

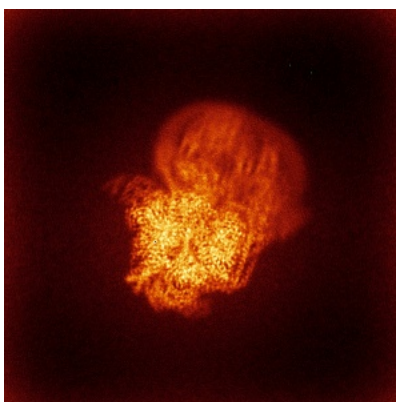


Z

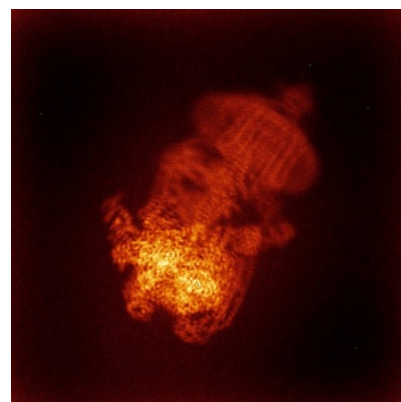
6.4.2 Raw map



X



Y

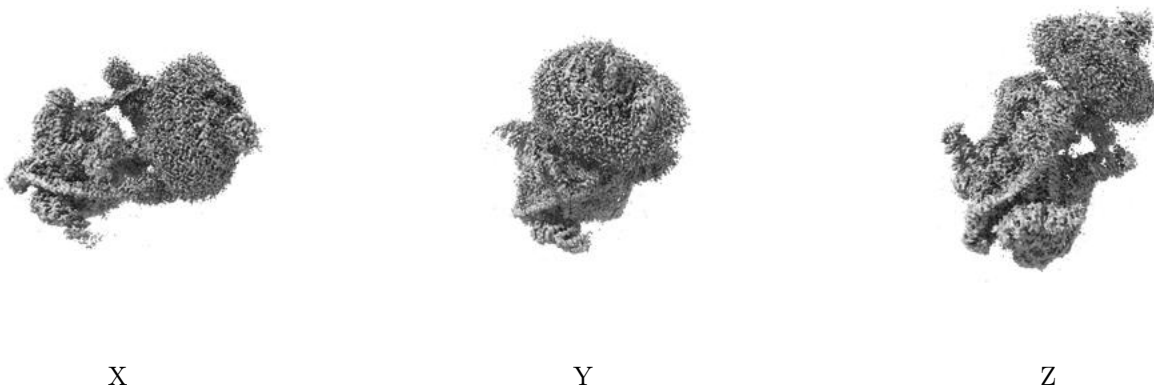


Z

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.

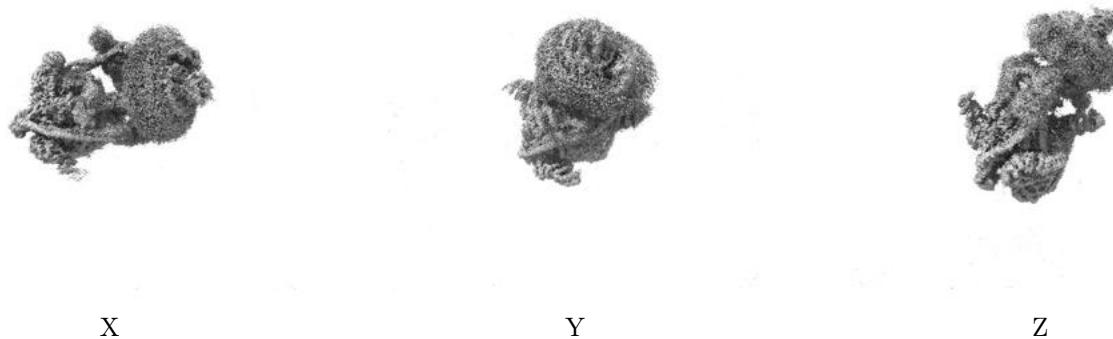
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.292. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

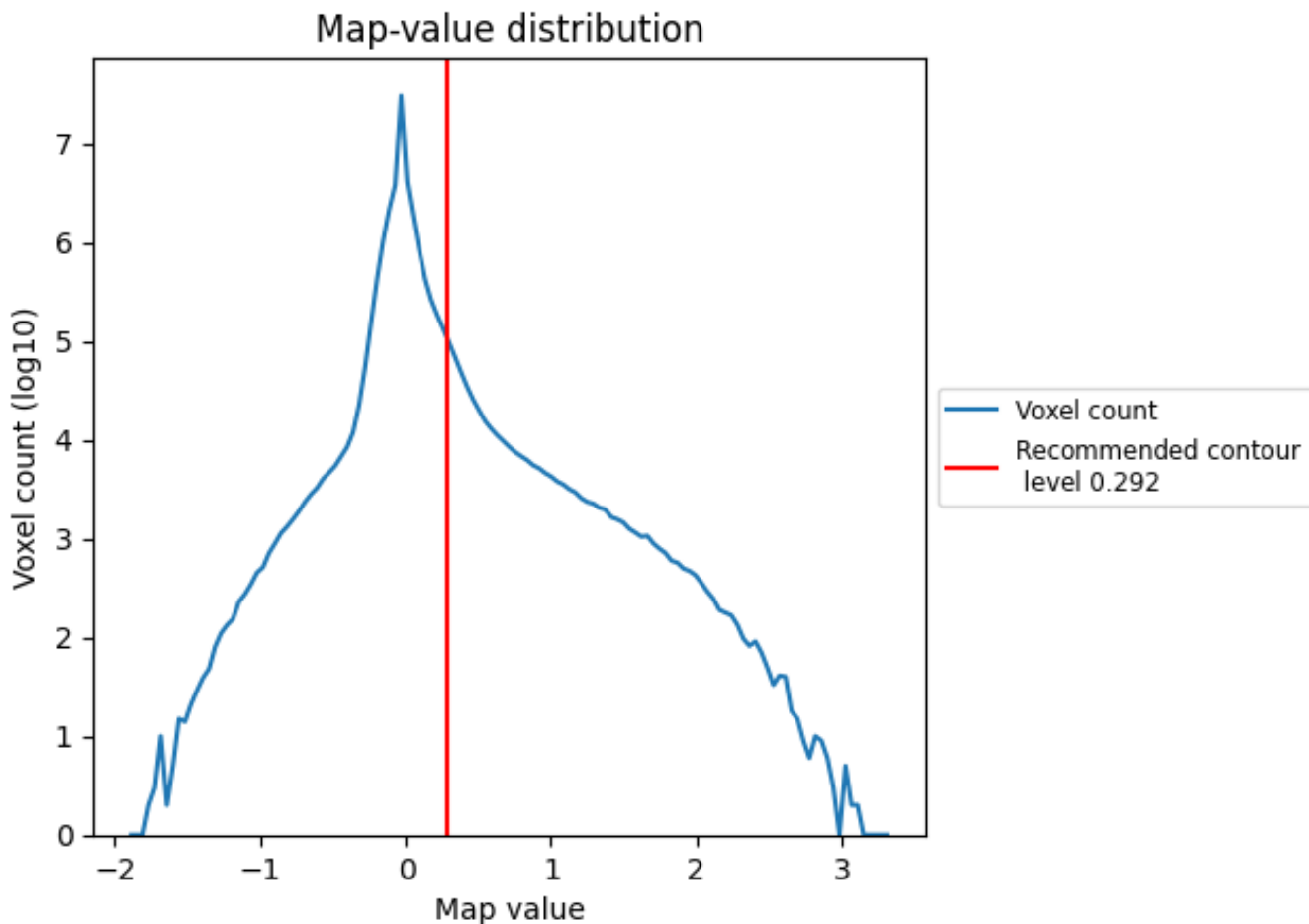
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

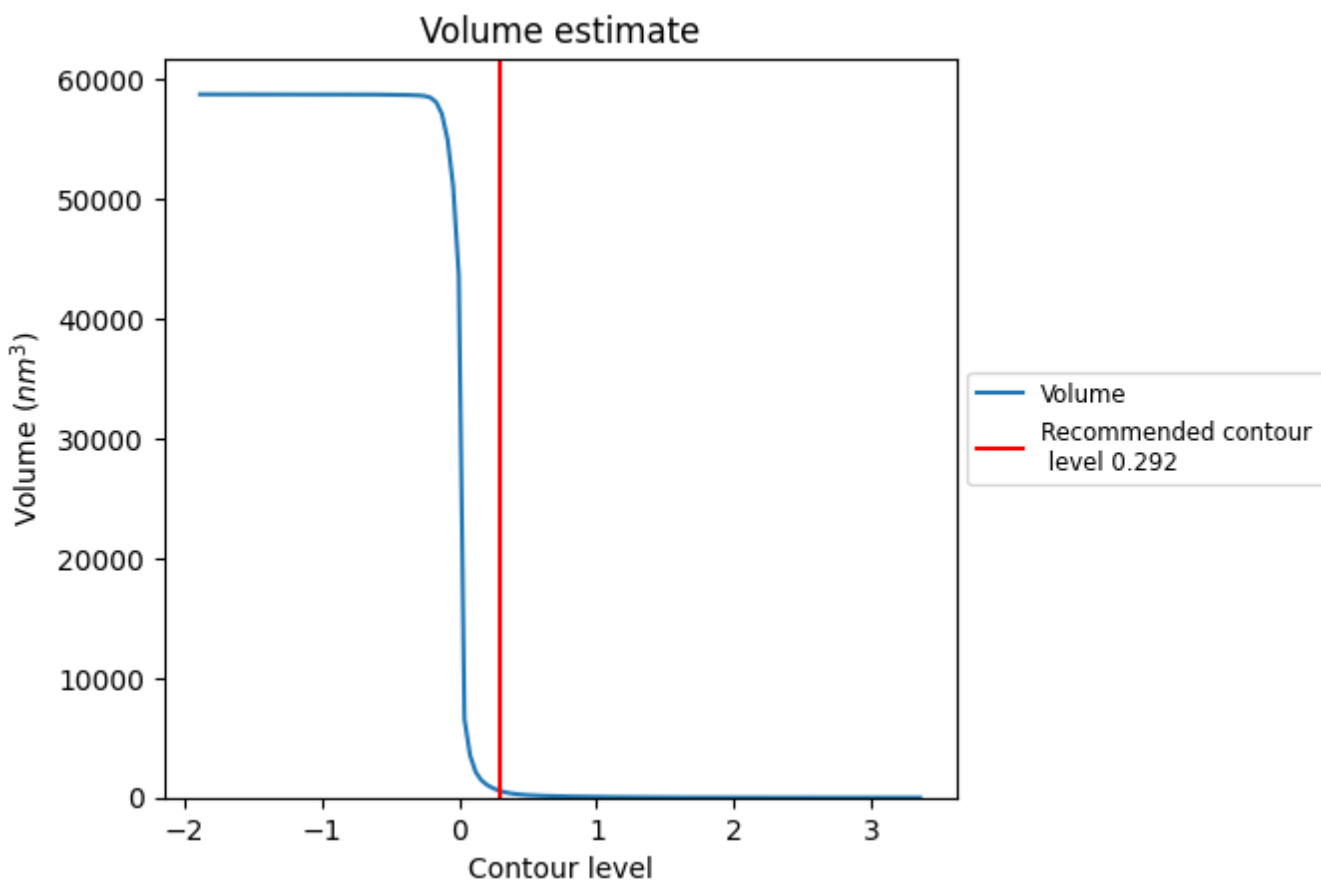
This section contains the results of statistical analysis of the map.

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.

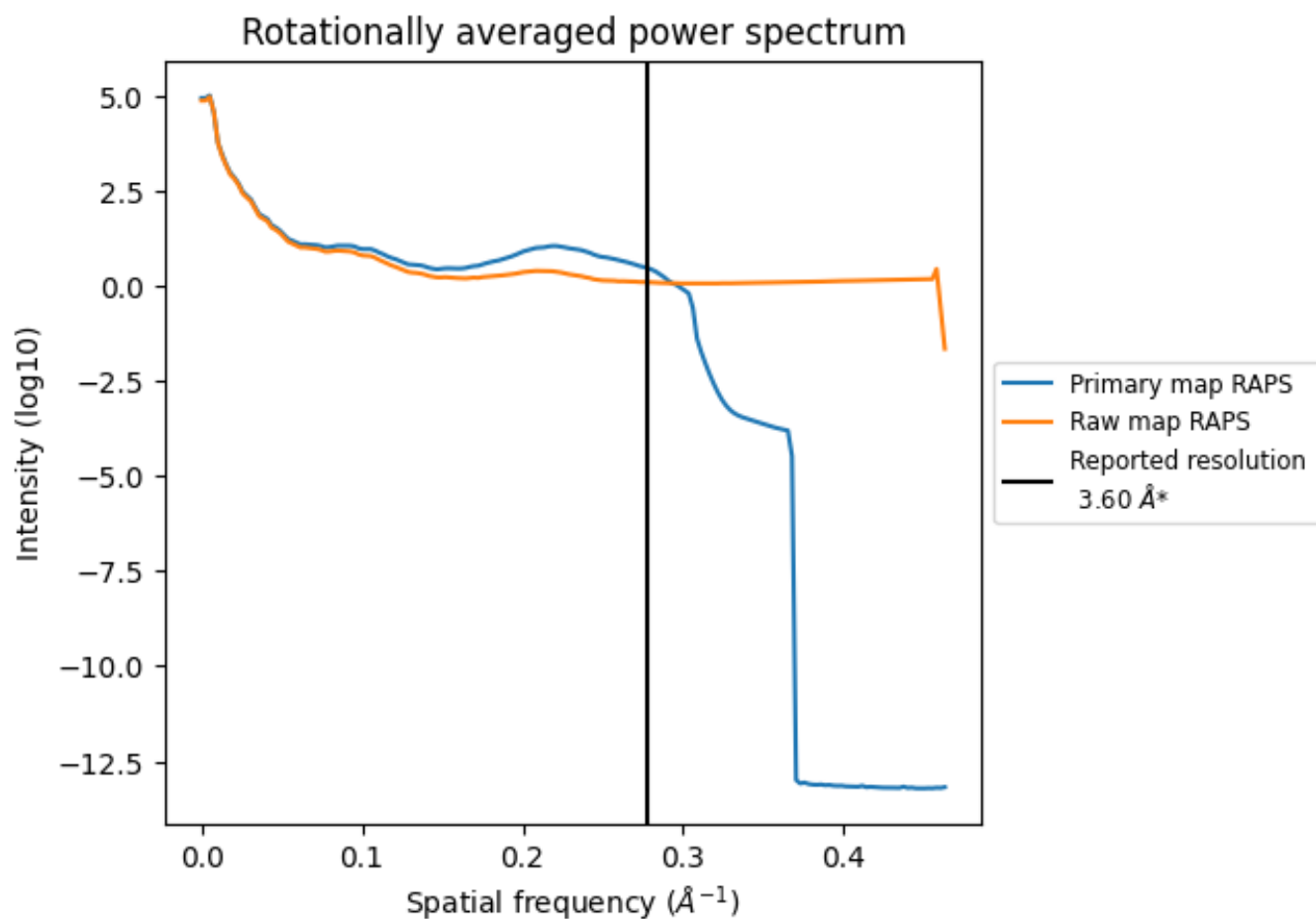
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 581 nm³; this corresponds to an approximate mass of 525 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

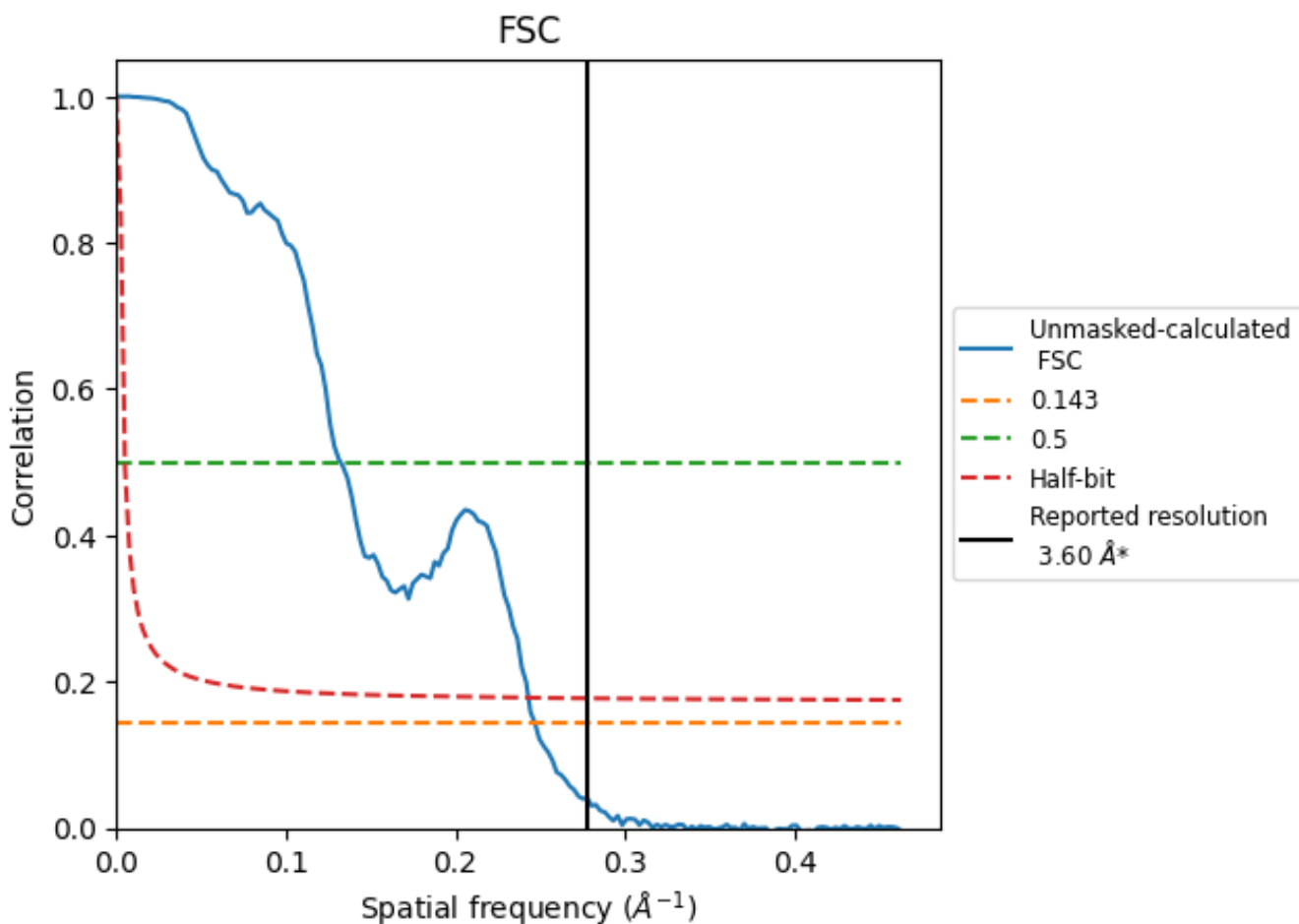


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

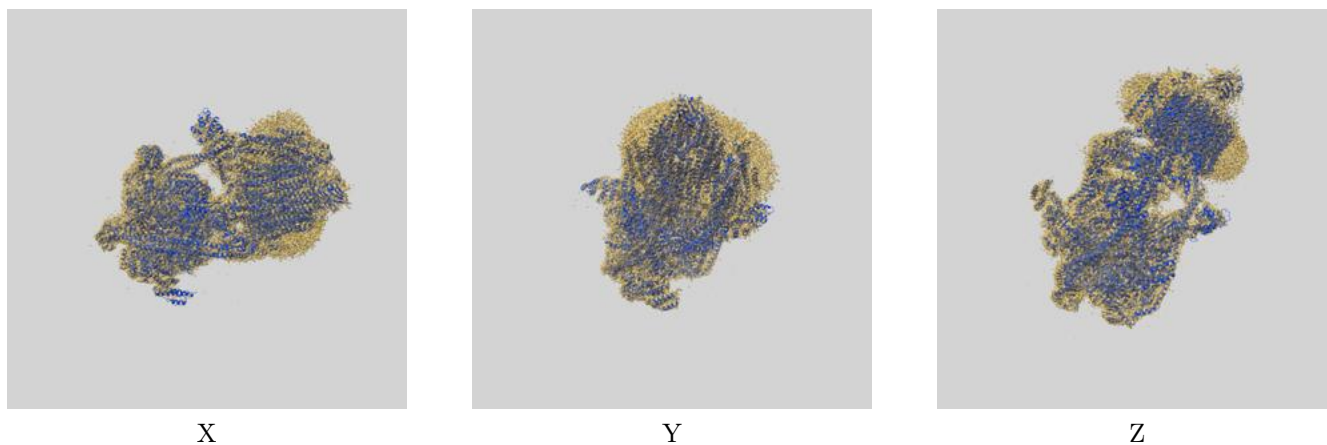
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.05	7.56	4.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.05 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

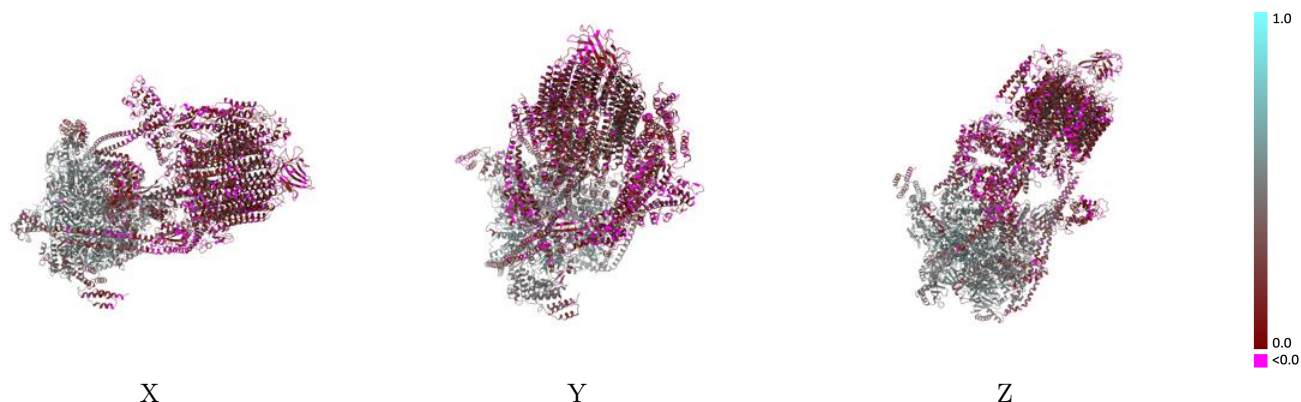
This section contains information regarding the fit between EMDB map EMD-26334 and PDB model 7U4T. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



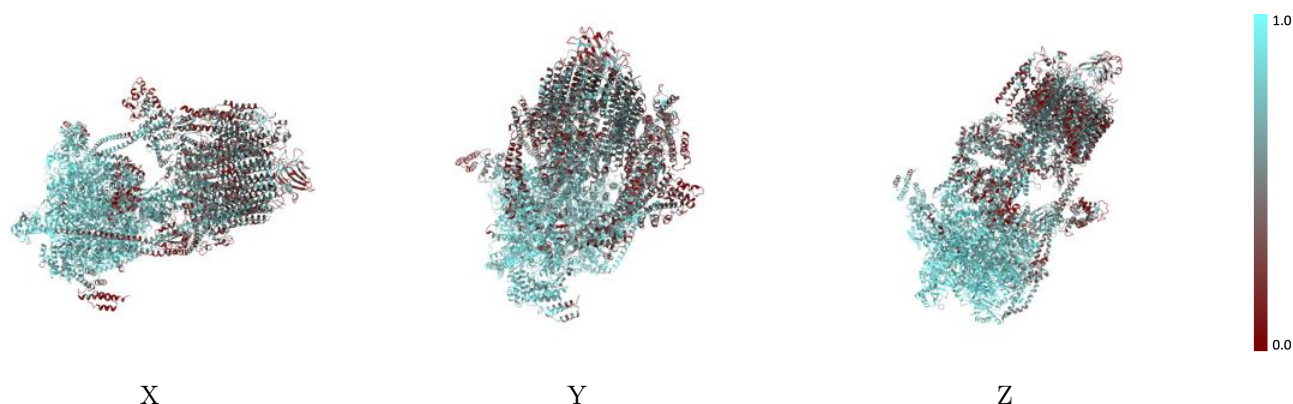
The images above show the 3D surface view of the map at the recommended contour level 0.292 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



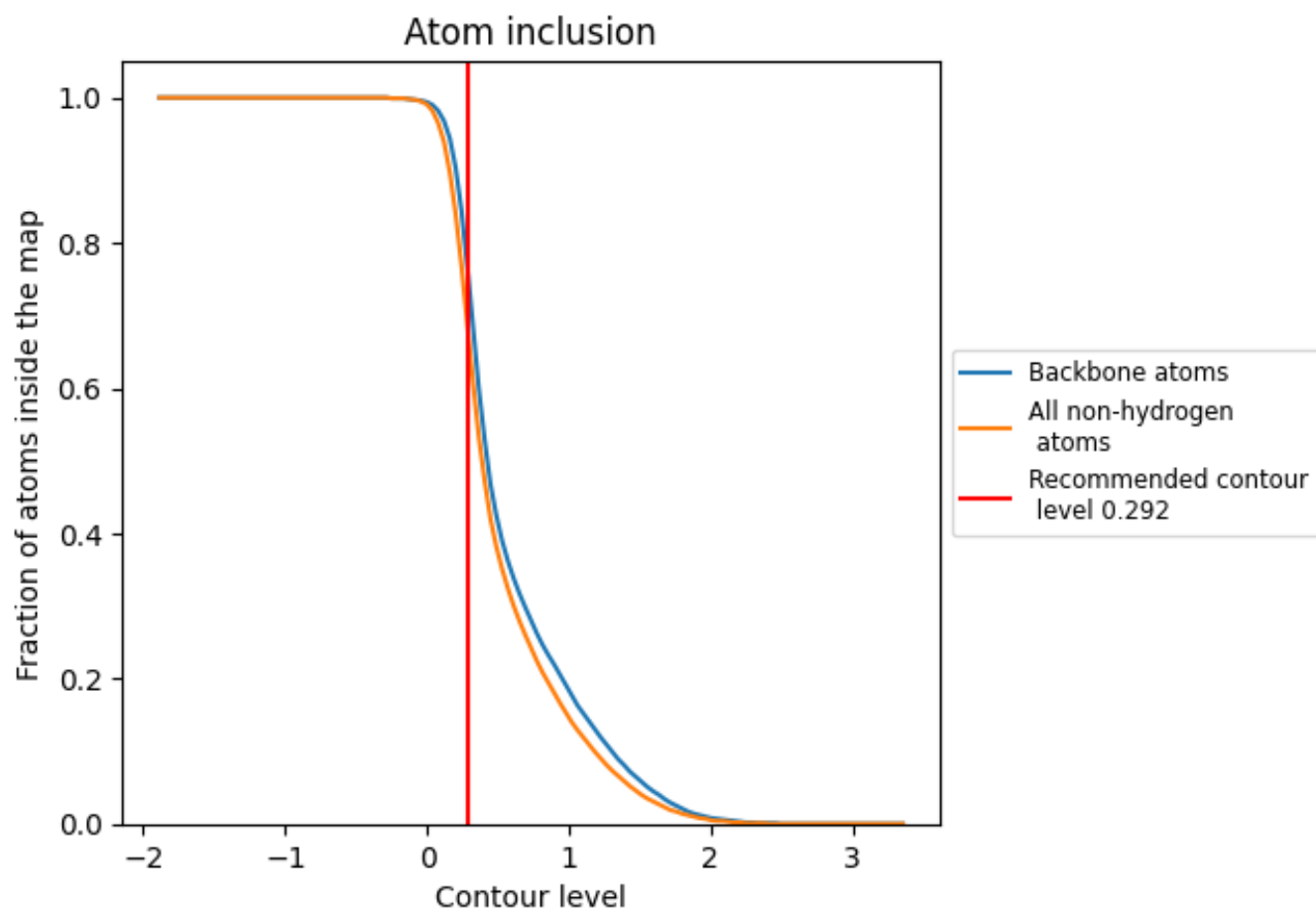
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.292).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 67% 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 (0.292) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6710	 0.3310
0	 0.4640	 0.1820
1	 0.4800	 0.1840
2	 0.5380	 0.1860
3	 0.4720	 0.1400
4	 0.4240	 0.1500
5	 0.4720	 0.2010
6	 0.5090	 0.2190
7	 0.5800	 0.2630
8	 0.5590	 0.2630
9	 0.4740	 0.1810
A	 0.8310	 0.4480
B	 0.9130	 0.5180
C	 0.8600	 0.4720
D	 0.9090	 0.5270
E	 0.9110	 0.5290
F	 0.8770	 0.4980
G	 0.8310	 0.4220
H	 0.8100	 0.3710
I	 0.8480	 0.4240
J	 0.6830	 0.3320
K	 0.7700	 0.3380
L	 0.7740	 0.3290
M	 0.6280	 0.2790
N	 0.7040	 0.3110
O	 0.4110	 0.1100
P	 0.4060	 0.0860
Q	 0.5710	 0.2610
R	 0.4210	 0.1230
S	 0.3210	 0.1270
T	 0.3030	 0.0800
U	 0.3800	 0.1350
V	 0.4450	 0.1770
W	 0.5340	 0.2620
X	 0.7710	 0.4230



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Chain	Atom inclusion	Q-score
Y	 0.5210	 0.3310
Z	 0.7290	 0.3720