



wwPDB EM Validation Summary Report

Nov 14, 2022 – 02:06 AM EST

PDB ID : 6WM4
EMDB ID : EMD-21849
Title : Human V-ATPase in state 3 with SidK and ADP
Authors : Wang, L.; Wu, H.; Fu, T.M.
Deposited on : 2020-04-20
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:

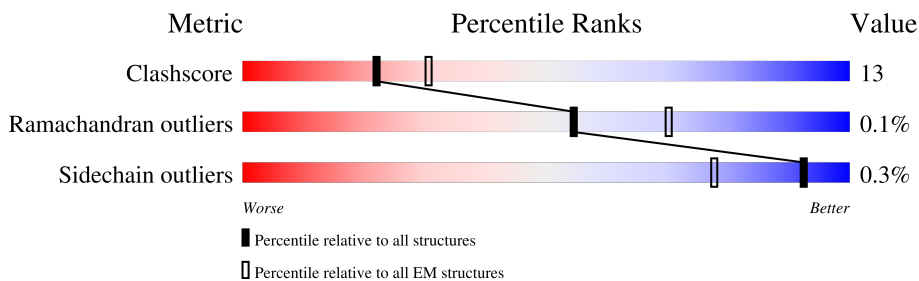
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 3.60 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.




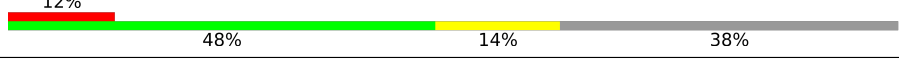

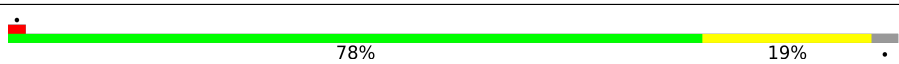
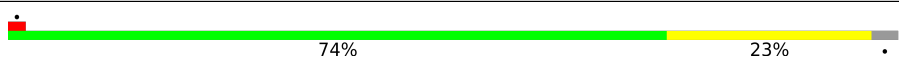
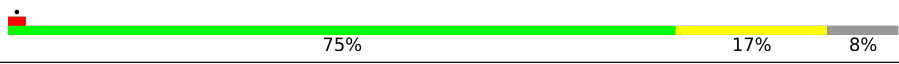
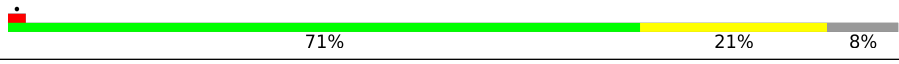



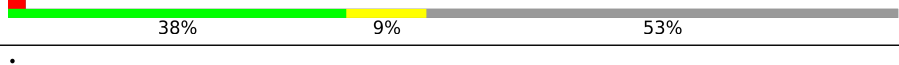



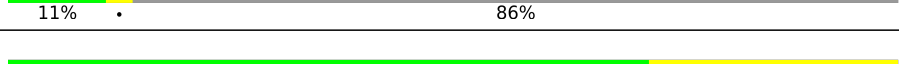

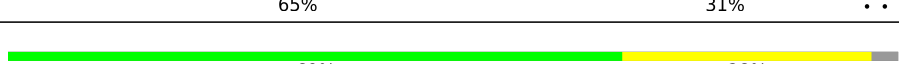

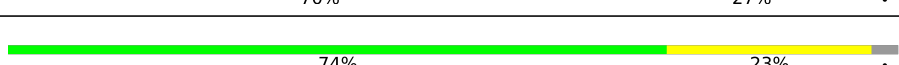
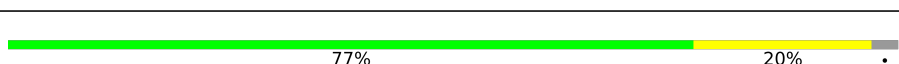

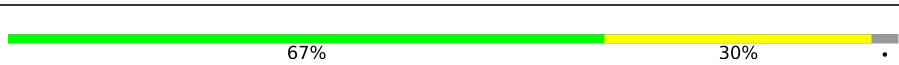



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	
2	O	382	
3	H	226	
3	I	226	
3	J	226	
4	K	118	
4	L	118	
4	M	118	



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Mol	Chain	Length	Quality of chain
5	S	81	
6	T	137	
7	A	617	
7	B	617	
7	C	617	
8	D	511	
8	E	511	
8	F	511	
9	X	573	
9	Y	573	
9	Z	573	
10	G	247	
11	N	119	
12	U	470	
13	V	350	
14	0	205	
15	1	155	
15	2	155	
15	3	155	
15	4	155	
15	5	155	
15	6	155	
15	7	155	
15	8	155	
15	9	155	

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Mol	Chain	Length	Quality of chain
16	Q	351	 72% 28%
17	P	483	 10% 34% 53% 12%

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 72308 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	6147	4016	1023	1068	40	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	S		
2	O	375	3035	1944	512	569	10	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	1822	1143	322	347	10	0	0
3	I	225	1822	1143	322	347	10	0	0
3	H	224	1817	1140	321	346	10	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	938	573	179	183	3	0	0
4	L	114	938	573	179	183	3	0	0
4	K	114	938	573	179	183	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 catalytic subunit A.

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

- Molecule 8 is a protein called V-type proton ATPase subunit B, brain isoform.

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

- Molecule 9 is a protein called SidK.

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

- Molecule 10 is a protein called V-type proton ATPase subunit D.

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

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

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

- Molecule 12 is a protein called V-type proton ATPase subunit S1.

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

- Molecule 13 is a protein called Renin receptor.

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

- Molecule 14 is a protein called V-type proton ATPase 21 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	0	204	1498	990	238	259	11	0	0

- Molecule 15 is a protein called V-type proton ATPase 16 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	1	150	1065	698	169	191	7	0	0
15	2	150	1065	698	169	191	7	0	0
15	3	150	1065	698	169	191	7	0	0
15	4	150	1065	698	169	191	7	0	0
15	5	150	1065	698	169	191	7	0	0
15	6	150	1065	698	169	191	7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
15	7	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
15	8	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
15	9	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		

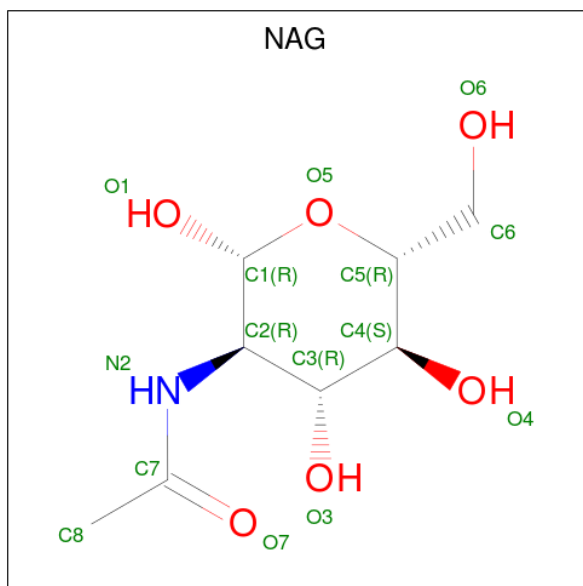
- Molecule 16 is a protein called V-type proton ATPase subunit d 1.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	427	Total	C	N	O	S	0	0
			3508	2228	605	648	27		

- Molecule 18 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



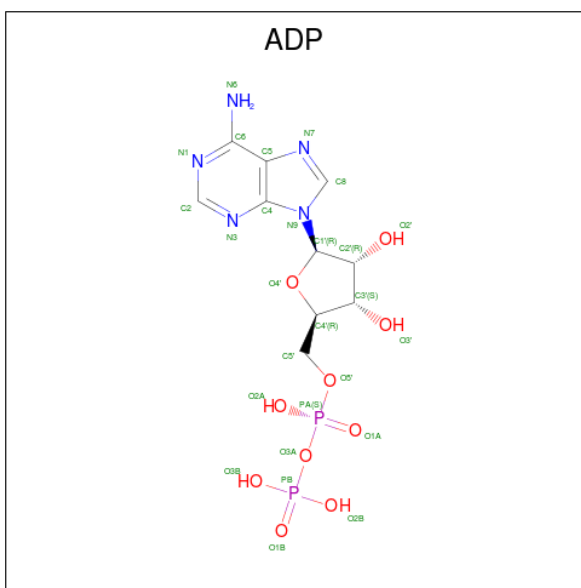
Mol	Chain	Residues	Atoms			AltConf	
18	R	1	Total	C	N	O	0
			28	16	2	10	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
18	R	1	Total 28	C 16	N 2	O 10	0
18	U	1	Total 84	C 48	N 6	O 30	0
18	U	1	Total 84	C 48	N 6	O 30	0
18	U	1	Total 84	C 48	N 6	O 30	0
18	U	1	Total 84	C 48	N 6	O 30	0
18	U	1	Total 84	C 48	N 6	O 30	0
18	U	1	Total 84	C 48	N 6	O 30	0

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

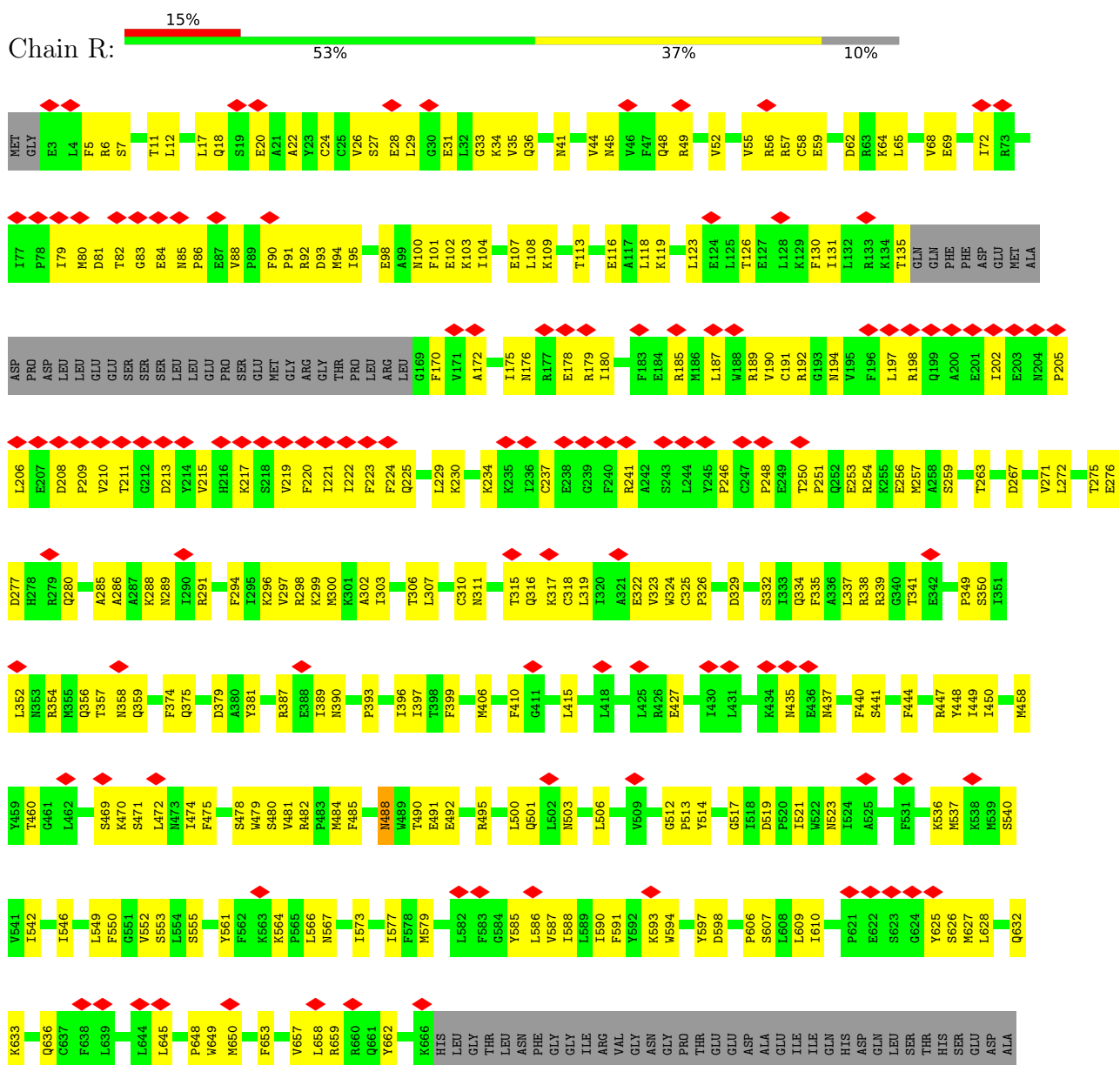


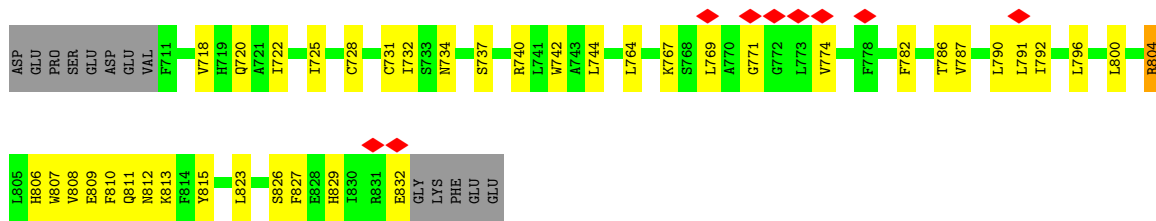
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
19	A	1	Total 27	C 10	N 5	O 10	P 2	0

3 Residue-property plots

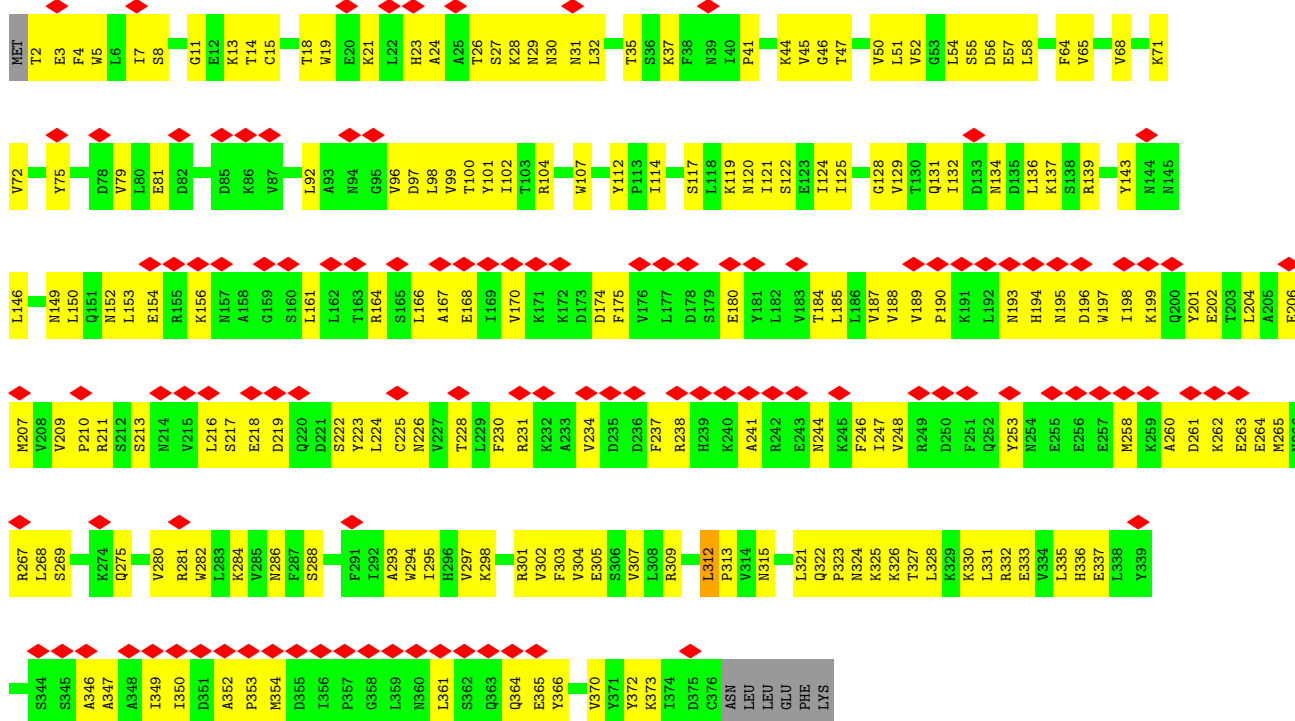
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 116 kDa subunit a isoform 1

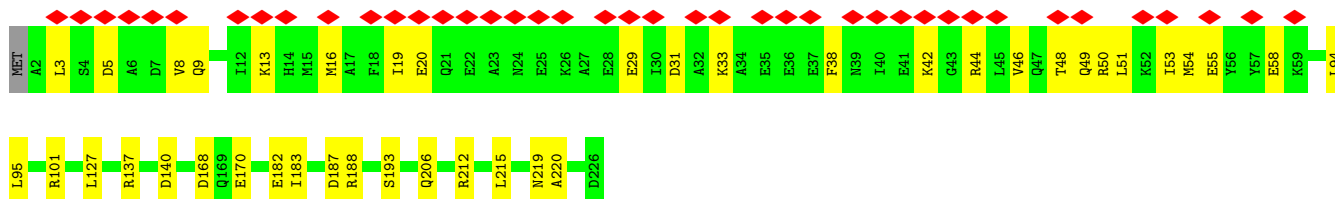
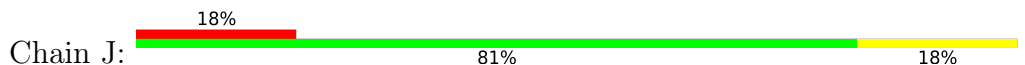




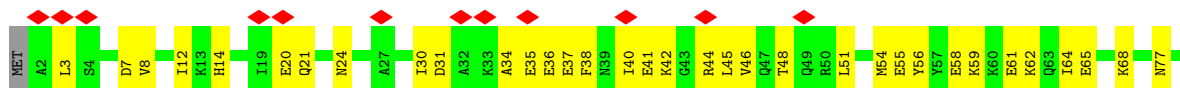
• Molecule 2: V-type proton ATPase subunit C 1



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



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





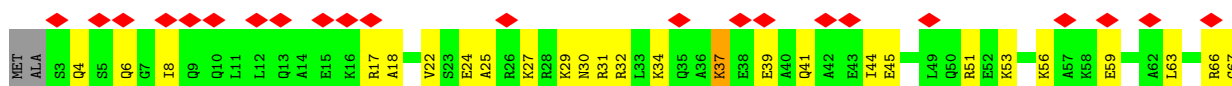
• Molecule 3: V-type proton ATPase subunit E 1



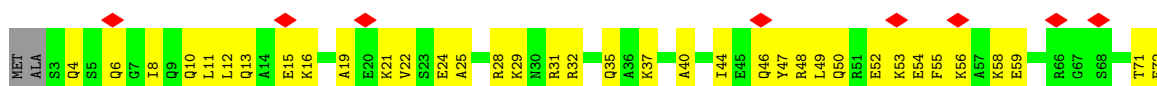
• Molecule 4: V-type proton ATPase subunit G 1



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

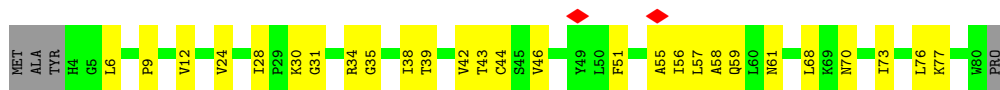


• Molecule 4: V-type proton ATPase subunit G 1

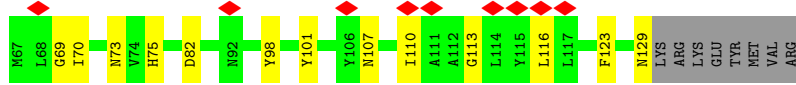
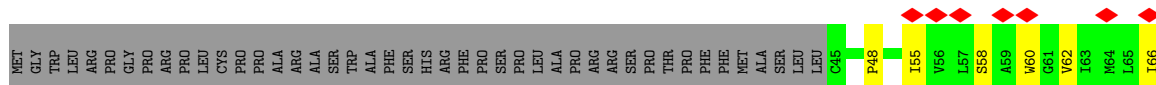


• Molecule 5: V-type proton ATPase subunit e 1

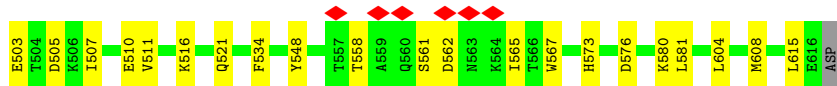
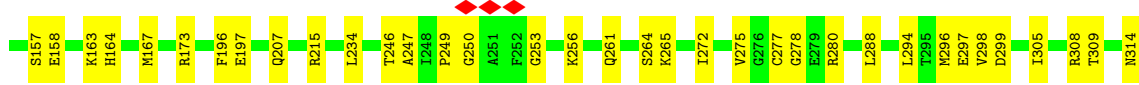
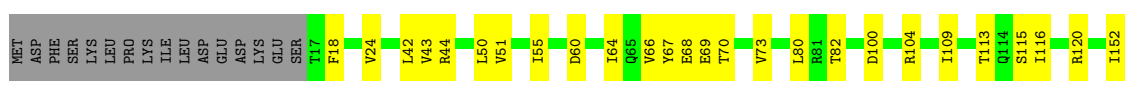
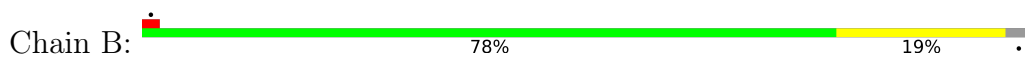




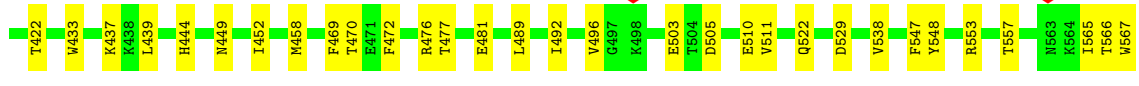
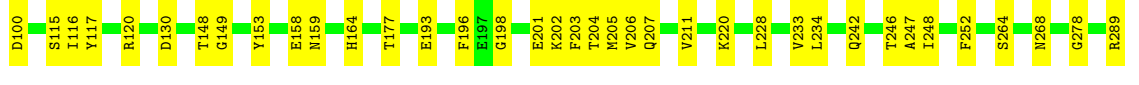
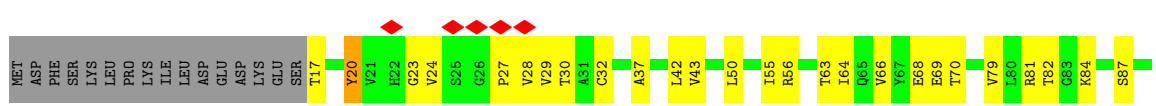
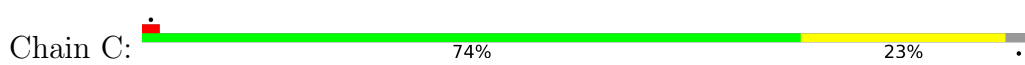
• Molecule 6: Ribonuclease kappa



• Molecule 7: V-type proton ATPase catalytic subunit A

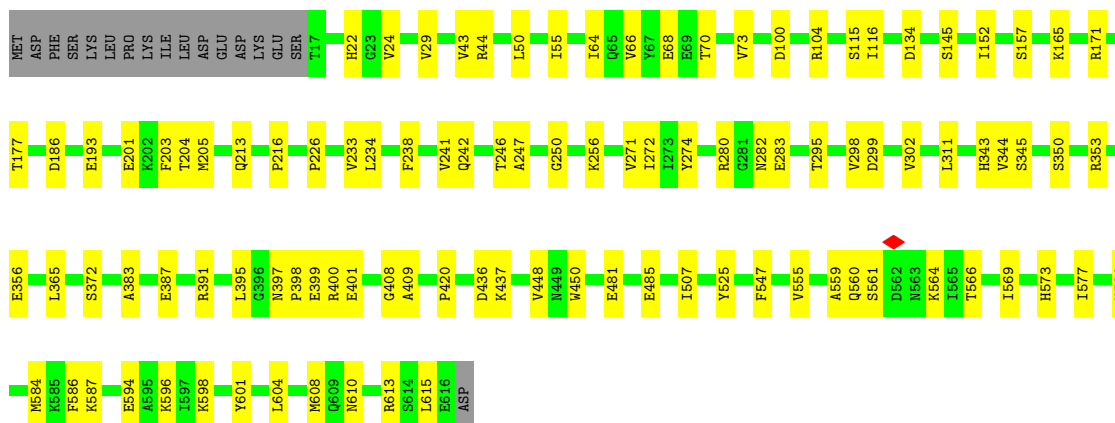
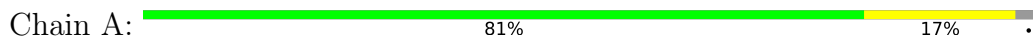


• Molecule 7: V-type proton ATPase catalytic subunit A

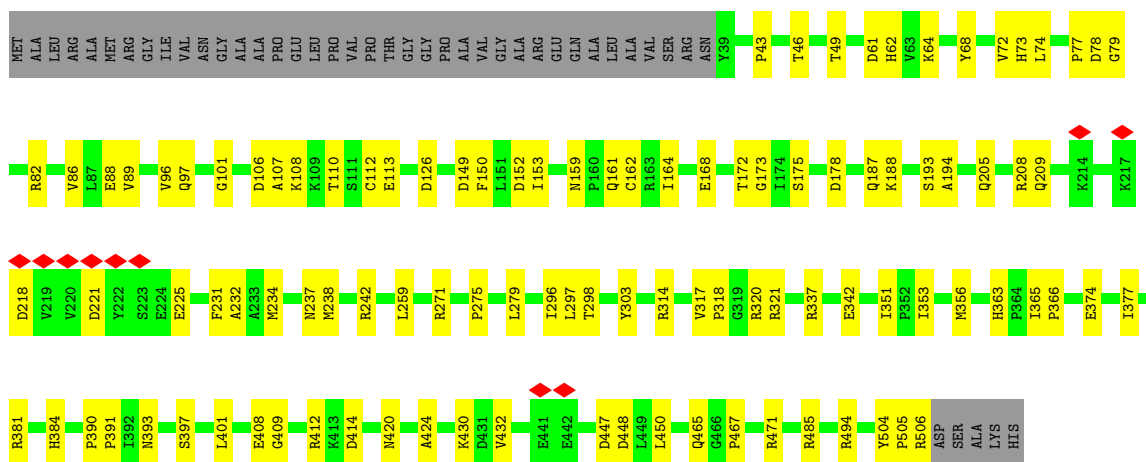




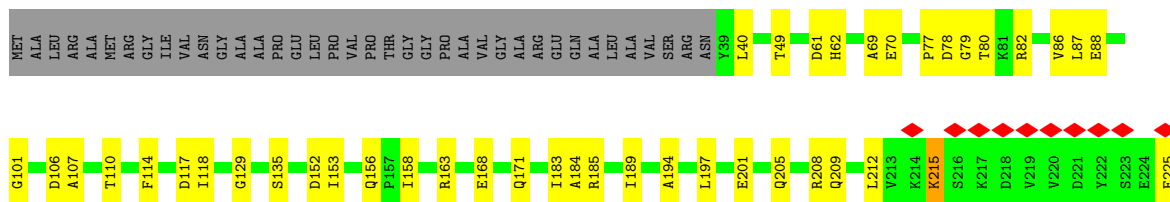
• Molecule 7: V-type proton ATPase catalytic subunit A

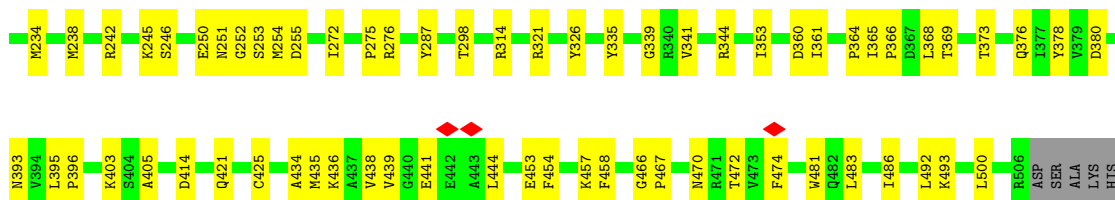


• Molecule 8: V-type proton ATPase subunit B, brain isoform

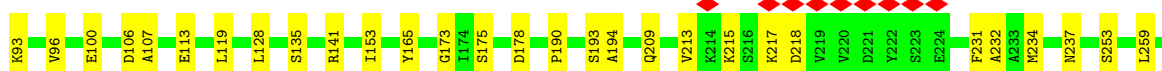
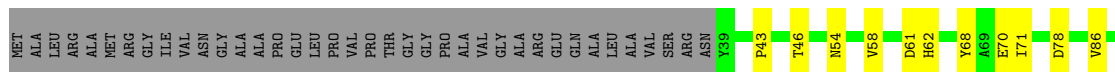
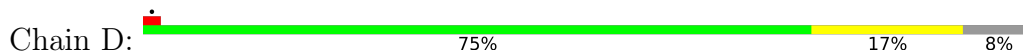


• Molecule 8: V-type proton ATPase subunit B, brain isoform

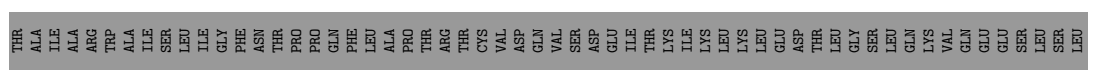
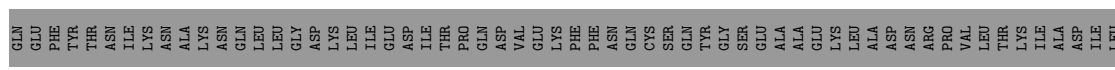
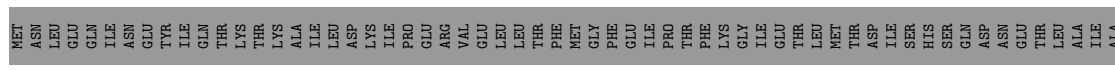
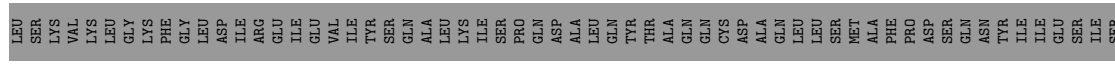
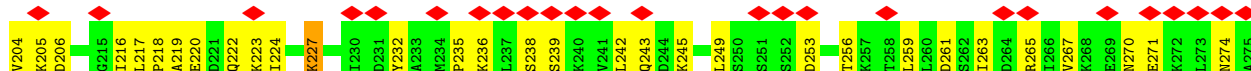
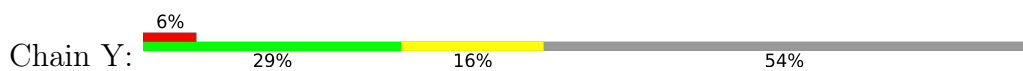




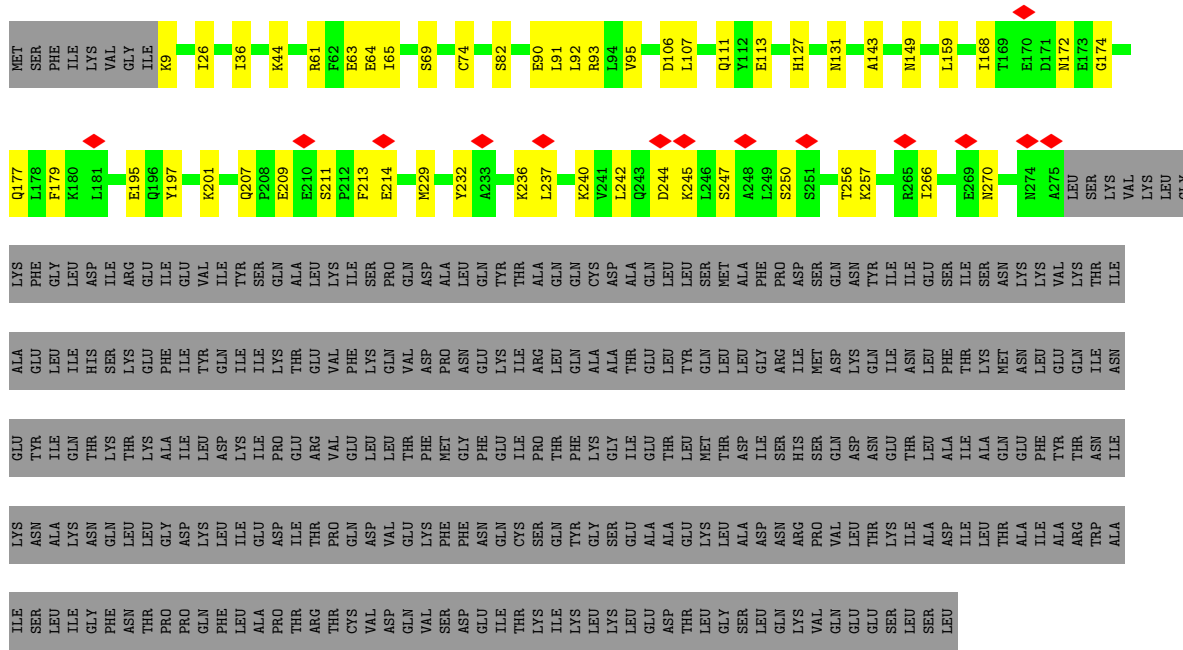
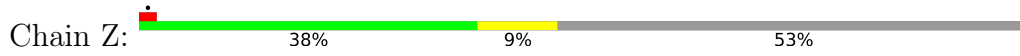
• Molecule 8: V-type proton ATPase subunit B, brain isoform



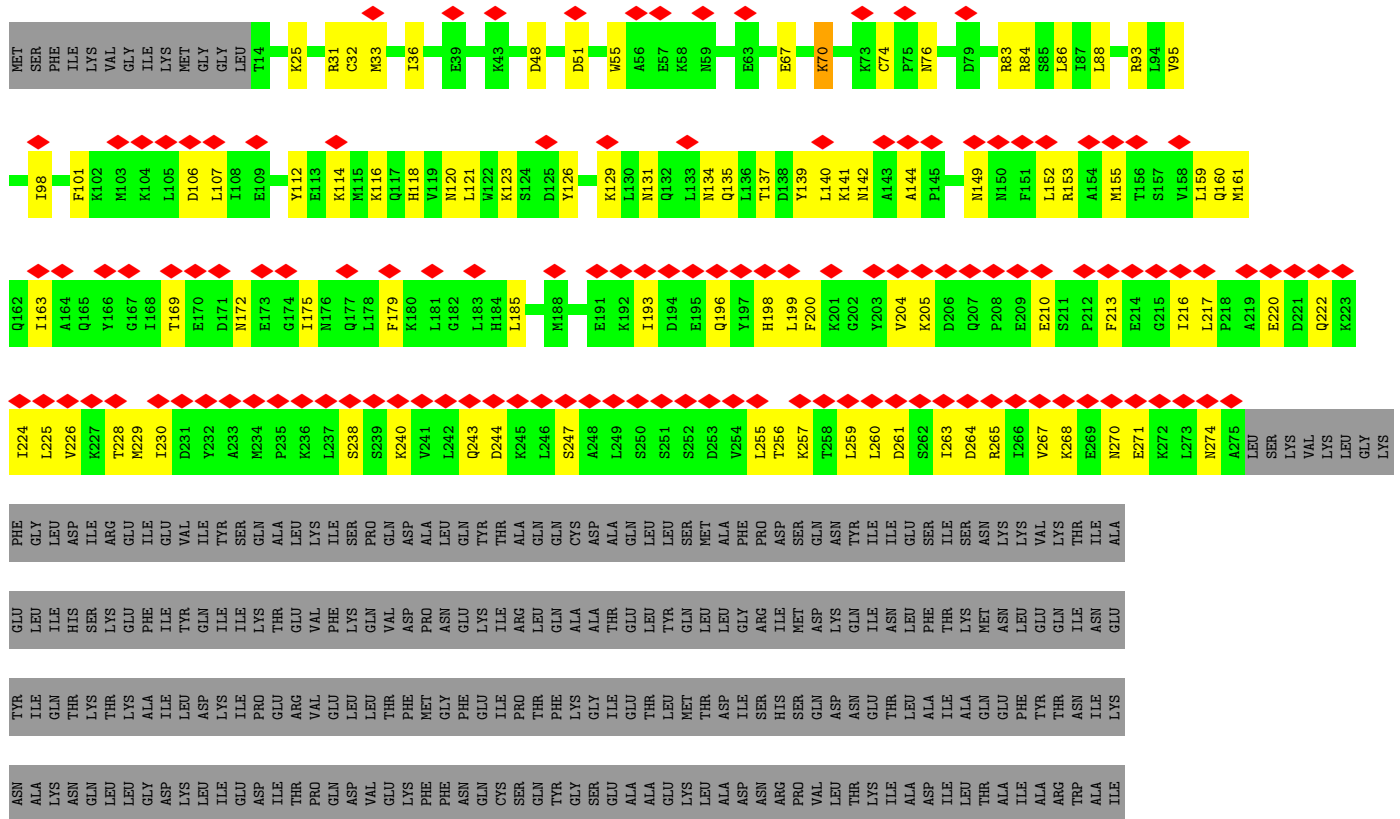
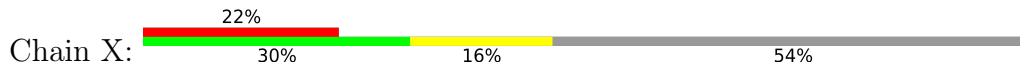
• Molecule 9: SidK



● Molecule 9: SidK

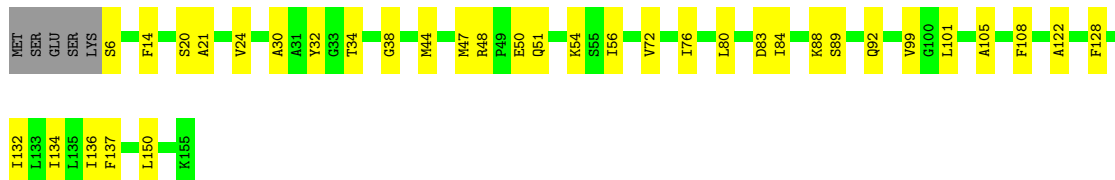


● Molecule 9: SidK

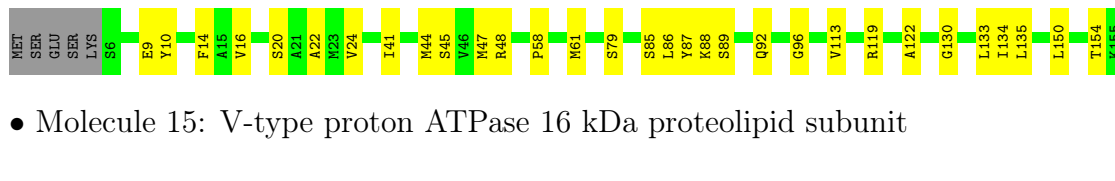




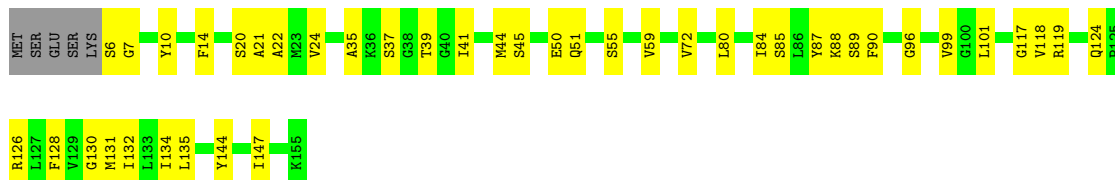
● Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit



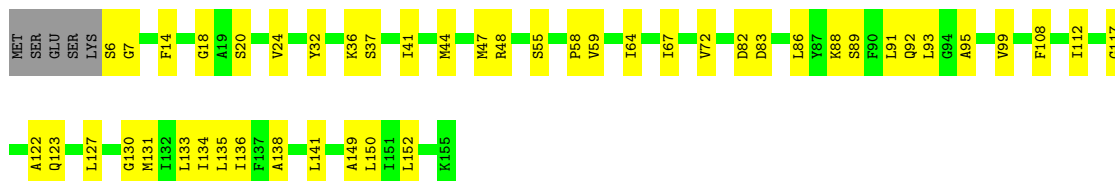
● Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit



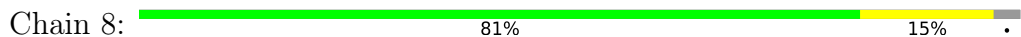
● Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit



● Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit



● Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1000000	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 ($e^-/\text{\AA}^2$)	50.1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	27.492	Depositor
Minimum map value	-13.678	Depositor
Average map value	0.017	Depositor
Map value standard deviation	1.157	Depositor
Recommended contour level	3.7	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: NAG, 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	R	0.27	0/6306	0.42	0/8534
2	O	0.27	0/3092	0.47	0/4182
3	H	0.34	0/1834	0.46	0/2455
3	I	0.32	0/1839	0.45	0/2462
3	J	0.32	0/1839	0.44	0/2462
4	K	0.30	0/945	0.45	0/1258
4	L	0.28	0/945	0.41	0/1258
4	M	0.28	0/945	0.41	0/1258
5	S	0.28	0/657	0.44	0/902
6	T	0.28	0/674	0.45	0/915
7	A	0.44	0/4752	0.47	0/6435
7	B	0.40	0/4752	0.47	0/6435
7	C	0.40	0/4752	0.51	0/6435
8	D	0.44	0/3739	0.48	0/5067
8	E	0.44	0/3739	0.49	0/5067
8	F	0.41	0/3739	0.48	0/5067
9	X	0.27	0/2145	0.43	0/2893
9	Y	0.28	0/2143	0.41	0/2888
9	Z	0.31	0/2170	0.45	0/2926
10	G	0.35	0/1735	0.45	0/2320
11	N	0.28	0/889	0.43	0/1200
12	U	0.36	0/1716	0.48	0/2333
13	V	0.43	0/425	0.45	0/582
14	0	0.41	0/1532	0.51	0/2082
15	1	0.39	0/1080	0.51	0/1461
15	2	0.39	0/1080	0.49	0/1461
15	3	0.40	0/1080	0.50	0/1461
15	4	0.40	0/1080	0.52	0/1461
15	5	0.40	0/1080	0.49	0/1461
15	6	0.40	0/1080	0.48	0/1461
15	7	0.40	0/1080	0.48	0/1461
15	8	0.39	0/1080	0.51	0/1461

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	9	0.40	0/1080	0.51	0/1461
16	Q	0.43	0/2910	0.52	0/3940
17	P	0.39	1/3576 (0.0%)	0.53	1/4819 (0.0%)
All	All	0.37	1/73510 (0.0%)	0.47	1/99324 (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
2	O	0	1
7	C	0	2
12	U	0	1
15	1	0	1
17	P	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	151	TRP	CB-CG	15.72	1.78	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	P	151	TRP	CA-CB-CG	11.73	135.99	113.70

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	1	9	GLU	Peptide
7	C	20	TYR	Peptide
7	C	305	ILE	Peptide
2	O	312	LEU	Peptide
12	U	417	ASP	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	6147	0	6172	233	0
2	O	3035	0	3077	154	0
3	H	1817	0	1881	43	0
3	I	1822	0	1886	54	0
3	J	1822	0	1886	32	0
4	K	938	0	947	43	0
4	L	938	0	947	35	0
4	M	938	0	947	34	0
5	S	631	0	647	24	0
6	T	658	0	652	15	0
7	A	4656	0	4642	65	0
7	B	4656	0	4642	85	0
7	C	4656	0	4642	115	0
8	D	3666	0	3665	57	0
8	E	3666	0	3665	78	0
8	F	3666	0	3665	70	0
9	X	2111	0	2134	59	0
9	Y	2110	0	2132	61	0
9	Z	2136	0	2158	40	0
10	G	1717	0	1829	23	0
11	N	875	0	878	28	0
12	U	1662	0	1583	49	0
13	V	411	0	401	8	0
14	0	1498	0	1544	49	0
15	1	1065	0	1131	39	0
15	2	1065	0	1131	33	0
15	3	1065	0	1131	31	0
15	4	1065	0	1131	27	0
15	5	1065	0	1131	25	0
15	6	1065	0	1131	28	0
15	7	1065	0	1131	32	0
15	8	1065	0	1131	17	0
15	9	1065	0	1131	29	0
16	Q	2844	0	2782	72	0
17	P	3508	0	3483	242	0
18	R	28	0	26	2	0
18	U	84	0	78	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	A	27	0	12	1	0
All	All	72308	0	73182	1855	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 13.

The worst 5 of 1855 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)
17:P:151:TRP:CB	17:P:151:TRP:CG	1.78	1.66
17:P:148:LEU:H	17:P:151:TRP:HD1	0.99	0.93
17:P:149:ALA:C	17:P:151:TRP:HB2	1.92	0.90
17:P:150:ALA:N	17:P:151:TRP:HB2	1.88	0.88
7:C:296:MET:HG2	7:C:305:ILE:HD13	1.56	0.87

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%)	682 (91%)	65 (9%)	0	100	100
2	O	373/382 (98%)	331 (89%)	42 (11%)	0	100	100
3	H	222/226 (98%)	215 (97%)	7 (3%)	0	100	100
3	I	223/226 (99%)	218 (98%)	5 (2%)	0	100	100
3	J	223/226 (99%)	218 (98%)	5 (2%)	0	100	100
4	K	112/118 (95%)	101 (90%)	11 (10%)	0	100	100
4	L	112/118 (95%)	111 (99%)	1 (1%)	0	100	100
4	M	112/118 (95%)	110 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	S	75/81 (93%)	71 (95%)	4 (5%)	0	100	100
6	T	83/137 (61%)	77 (93%)	6 (7%)	0	100	100
7	A	598/617 (97%)	546 (91%)	52 (9%)	0	100	100
7	B	598/617 (97%)	544 (91%)	54 (9%)	0	100	100
7	C	598/617 (97%)	540 (90%)	58 (10%)	0	100	100
8	D	466/511 (91%)	428 (92%)	38 (8%)	0	100	100
8	E	466/511 (91%)	429 (92%)	37 (8%)	0	100	100
8	F	466/511 (91%)	427 (92%)	38 (8%)	1 (0%)	47	79
9	X	260/573 (45%)	247 (95%)	13 (5%)	0	100	100
9	Y	258/573 (45%)	248 (96%)	9 (4%)	1 (0%)	34	71
9	Z	265/573 (46%)	250 (94%)	15 (6%)	0	100	100
10	G	211/247 (85%)	205 (97%)	6 (3%)	0	100	100
11	N	108/119 (91%)	104 (96%)	4 (4%)	0	100	100
12	U	202/470 (43%)	172 (85%)	28 (14%)	2 (1%)	15	55
13	V	47/350 (13%)	44 (94%)	3 (6%)	0	100	100
14	0	202/205 (98%)	191 (95%)	11 (5%)	0	100	100
15	1	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
15	2	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
15	3	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
15	4	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
15	5	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
15	6	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
15	7	148/155 (96%)	139 (94%)	9 (6%)	0	100	100
15	8	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
15	9	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
16	Q	349/351 (99%)	309 (88%)	40 (12%)	0	100	100
17	P	423/483 (88%)	367 (87%)	54 (13%)	2 (0%)	29	68
All	All	9131/11192 (82%)	8460 (93%)	665 (7%)	6 (0%)	54	83

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	P	109	SER

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Mol	Chain	Res	Type
12	U	416	SER
12	U	417	ASP
17	P	104	ASN
9	Y	62	PHE

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	674/746 (90%)	671 (100%)	3 (0%)	91	97
2	O	337/344 (98%)	336 (100%)	1 (0%)	92	97
3	H	198/199 (100%)	197 (100%)	1 (0%)	88	95
3	I	198/199 (100%)	198 (100%)	0	100	100
3	J	198/199 (100%)	197 (100%)	1 (0%)	88	95
4	K	99/101 (98%)	98 (99%)	1 (1%)	76	88
4	L	99/101 (98%)	98 (99%)	1 (1%)	76	88
4	M	99/101 (98%)	99 (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	A	508/525 (97%)	508 (100%)	0	100	100
7	B	508/525 (97%)	505 (99%)	3 (1%)	86	94
7	C	508/525 (97%)	508 (100%)	0	100	100
8	D	401/430 (93%)	401 (100%)	0	100	100
8	E	401/430 (93%)	401 (100%)	0	100	100
8	F	401/430 (93%)	399 (100%)	2 (0%)	88	95
9	X	238/519 (46%)	237 (100%)	1 (0%)	91	97
9	Y	237/519 (46%)	236 (100%)	1 (0%)	91	97
9	Z	239/519 (46%)	239 (100%)	0	100	100
10	G	184/212 (87%)	184 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	N	94/100 (94%)	94 (100%)	0	100	100
12	U	182/397 (46%)	182 (100%)	0	100	100
13	V	44/308 (14%)	44 (100%)	0	100	100
14	0	154/155 (99%)	154 (100%)	0	100	100
15	1	107/112 (96%)	107 (100%)	0	100	100
15	2	107/112 (96%)	107 (100%)	0	100	100
15	3	107/112 (96%)	107 (100%)	0	100	100
15	4	107/112 (96%)	107 (100%)	0	100	100
15	5	107/112 (96%)	107 (100%)	0	100	100
15	6	107/112 (96%)	107 (100%)	0	100	100
15	7	107/112 (96%)	107 (100%)	0	100	100
15	8	107/112 (96%)	107 (100%)	0	100	100
15	9	107/112 (96%)	107 (100%)	0	100	100
16	Q	306/306 (100%)	304 (99%)	2 (1%)	84	93
17	P	385/429 (90%)	382 (99%)	3 (1%)	81	91
All	All	7795/9515 (82%)	7775 (100%)	20 (0%)	92	97

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	X	70	LYS
17	P	116	ARG
17	P	434	LYS
17	P	259	HIS
3	H	59	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
8	D	470	ASN
9	X	198	HIS
17	P	311	GLN
9	Y	17	GLN
9	Z	190	ASN

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
18	NAG	R	902	-	14,14,15	0.21	0	17,19,21	0.43	0
18	NAG	U	503	12	14,14,15	0.47	0	17,19,21	0.63	1 (5%)
18	NAG	U	506	12	14,14,15	0.22	0	17,19,21	0.39	0
18	NAG	U	502	12	14,14,15	0.26	0	17,19,21	0.44	0
18	NAG	U	504	12	14,14,15	0.46	0	17,19,21	0.70	1 (5%)
18	NAG	U	505	12	14,14,15	0.16	0	17,19,21	0.40	0
19	ADP	A	701	-	24,29,29	0.95	1 (4%)	29,45,45	1.51	4 (13%)
18	NAG	R	901	1	14,14,15	0.22	0	17,19,21	0.40	0
18	NAG	U	501	12	14,14,15	0.34	0	17,19,21	0.63	1 (5%)

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
18	NAG	R	902	-	-	2/6/23/26	0/1/1/1
18	NAG	U	503	12	-	3/6/23/26	0/1/1/1
18	NAG	U	506	12	-	1/6/23/26	0/1/1/1
18	NAG	U	502	12	-	2/6/23/26	0/1/1/1
18	NAG	U	504	12	-	3/6/23/26	0/1/1/1
18	NAG	U	505	12	-	4/6/23/26	0/1/1/1
19	ADP	A	701	-	-	1/12/32/32	0/3/3/3
18	NAG	R	901	1	-	2/6/23/26	0/1/1/1
18	NAG	U	501	12	-	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)
19	A	701	ADP	C5-C4	2.23	1.46	1.40

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	701	ADP	PA-O3A-PB	-3.92	119.38	132.83
19	A	701	ADP	N3-C2-N1	-3.18	123.71	128.68
19	A	701	ADP	C3'-C2'-C1'	3.11	105.67	100.98
19	A	701	ADP	C4-C5-N7	-2.38	106.92	109.40
18	U	504	NAG	C1-O5-C5	2.17	115.14	112.19

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	U	505	NAG	C4-C5-C6-O6
18	U	505	NAG	O5-C5-C6-O6
18	U	501	NAG	C4-C5-C6-O6
18	R	901	NAG	O5-C5-C6-O6
18	U	503	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 5 short contacts:

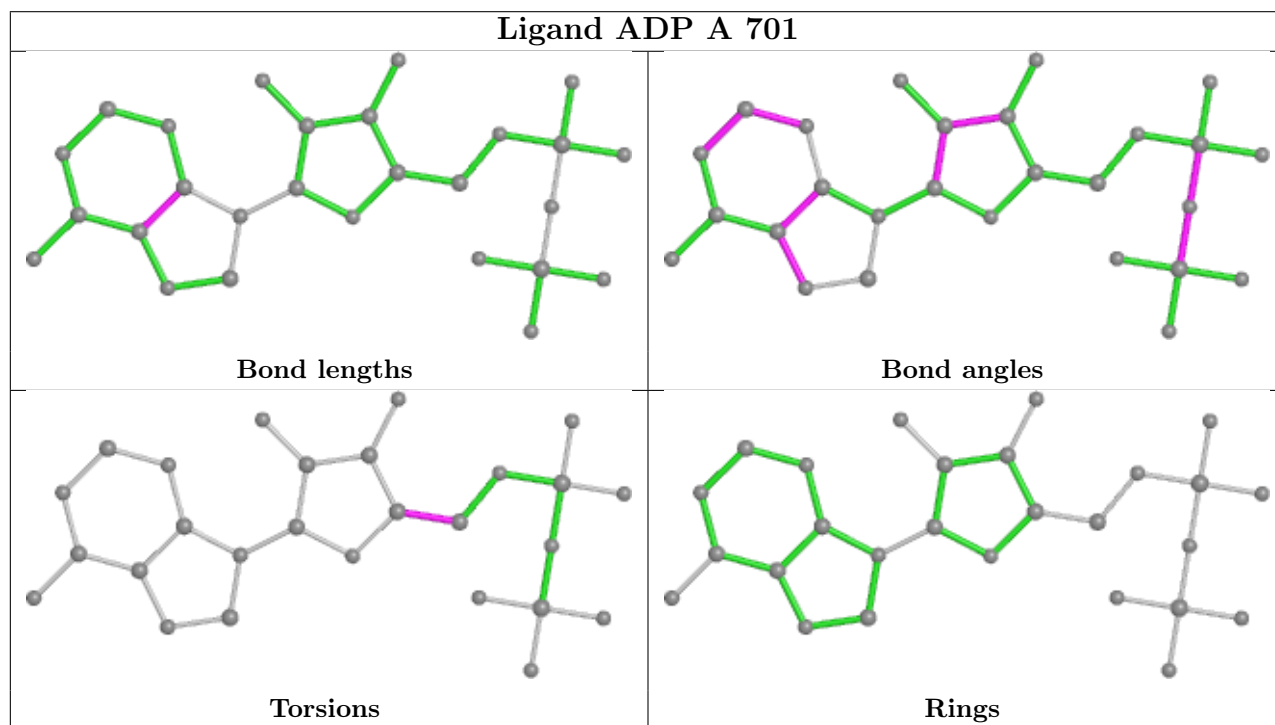
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	R	902	NAG	2	0
18	U	503	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	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.

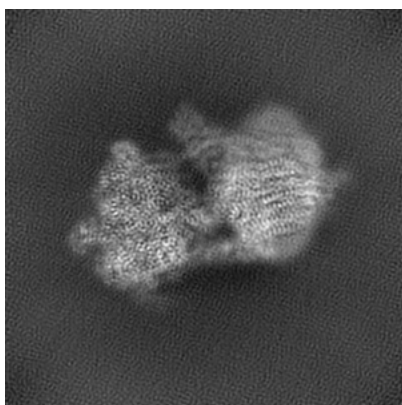
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21849. These allow visual inspection of the internal detail of the map and identification of artifacts.

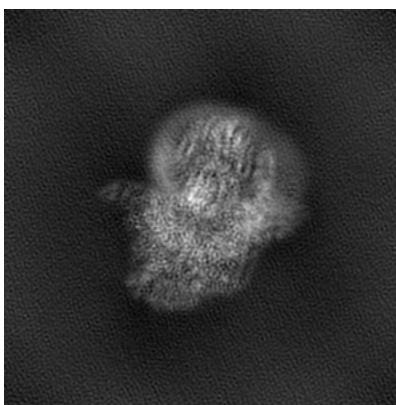
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

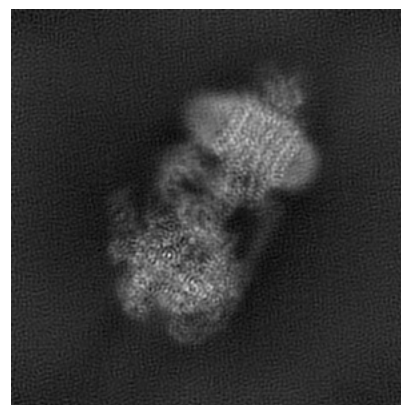
6.1.1 Primary map



X



Y

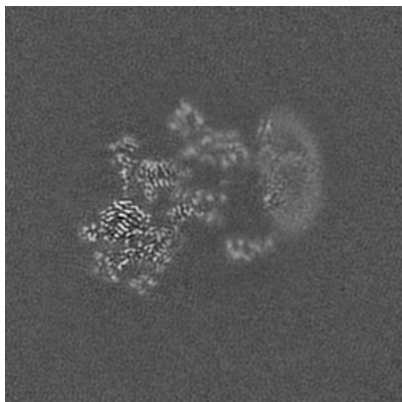


Z

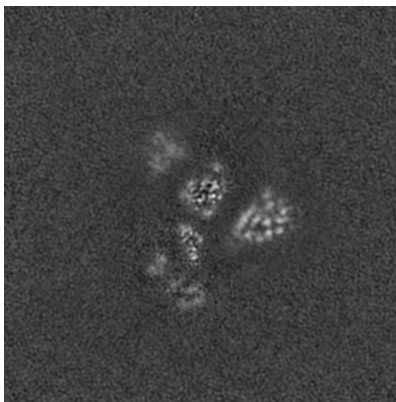
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

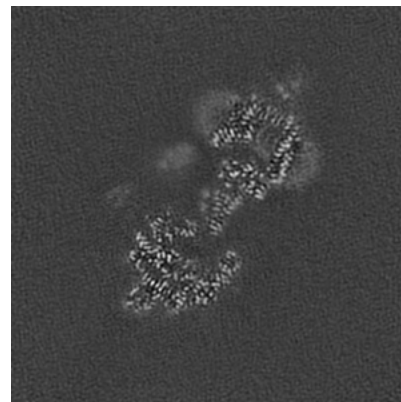
6.2.1 Primary map



X Index: 180



Y Index: 180

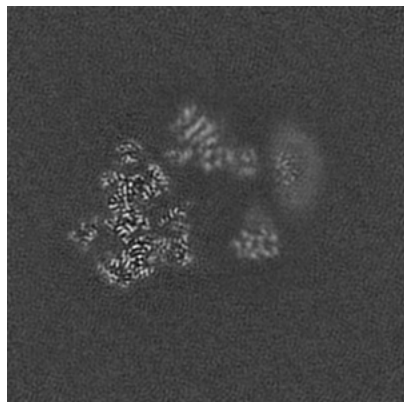


Z Index: 180

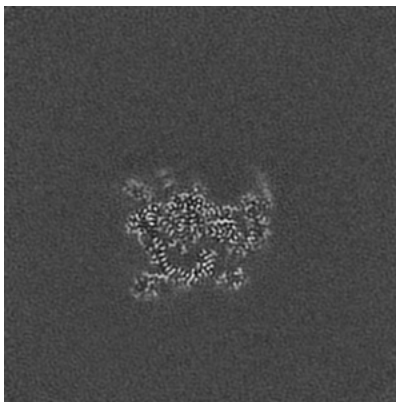
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

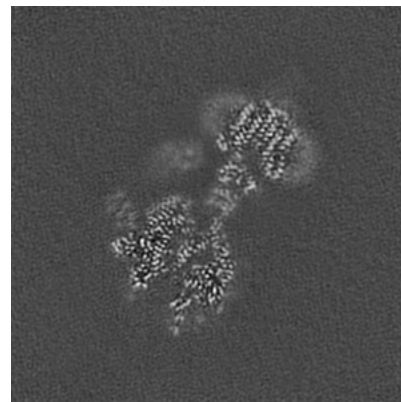
6.3.1 Primary map



X Index: 167



Y Index: 110



Z Index: 168

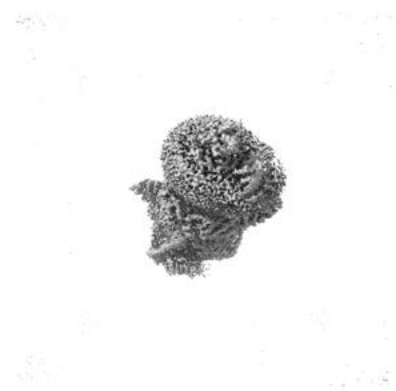
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

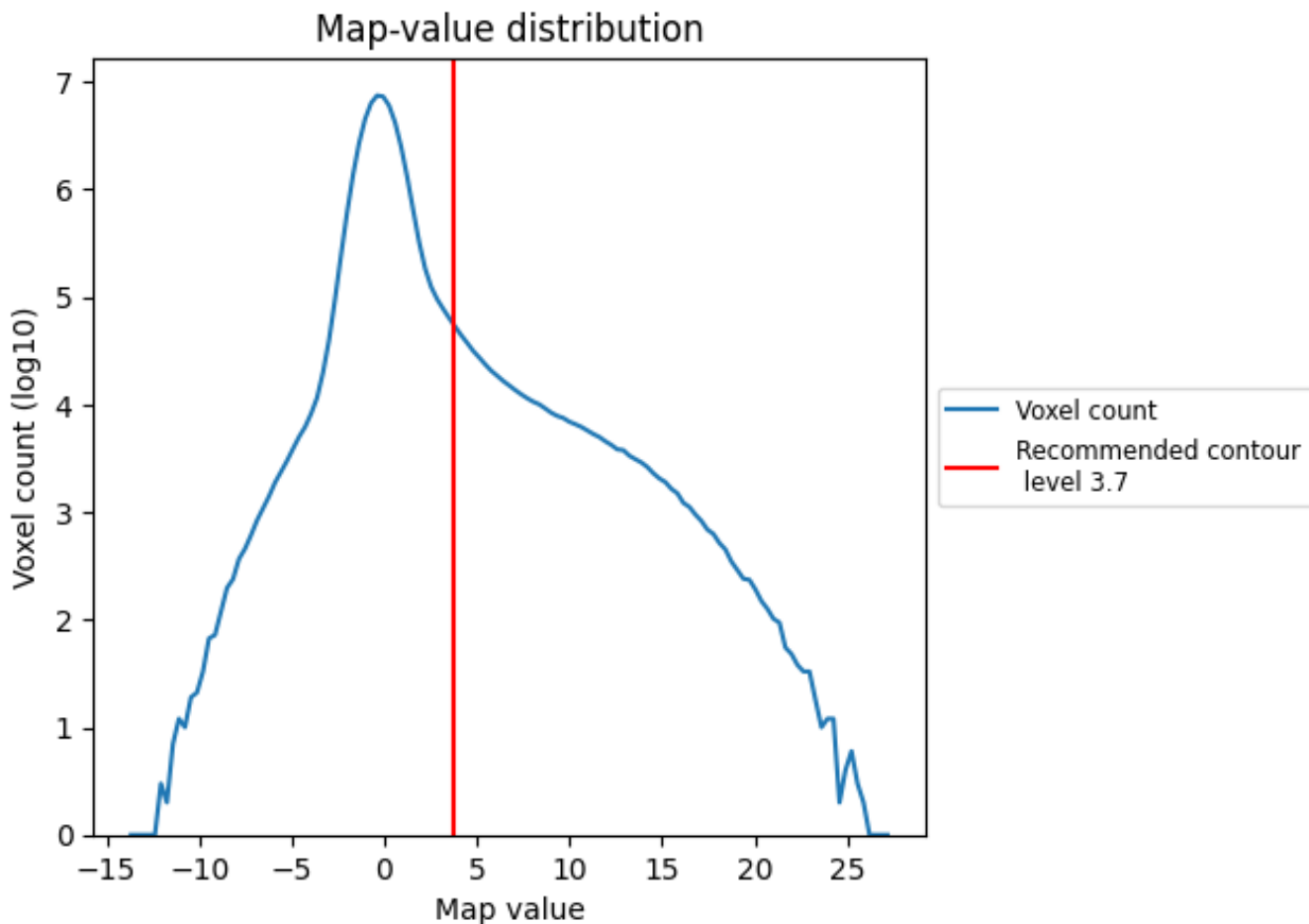
6.5 Mask visualisation

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

7 Map analysis [i](#)

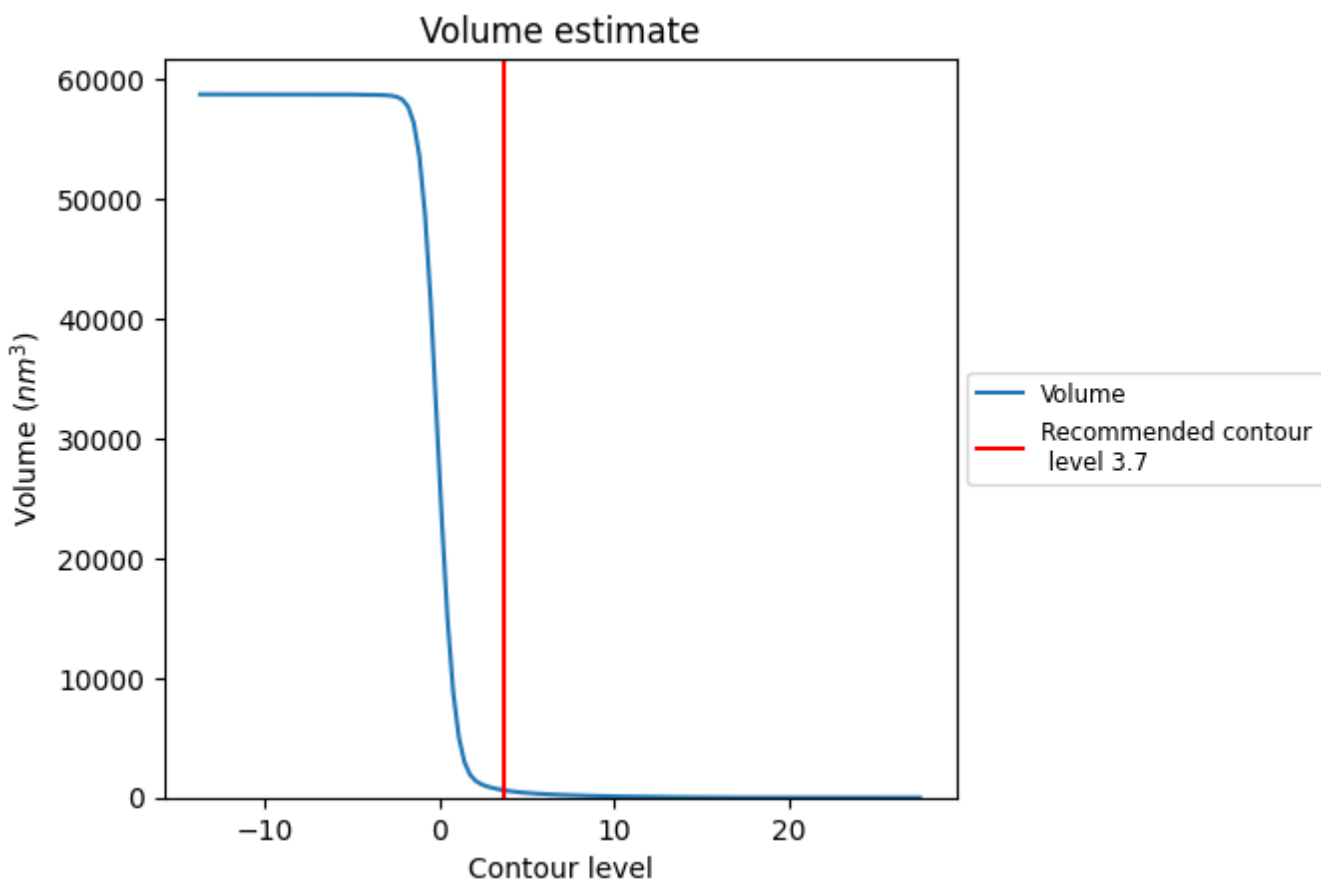
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

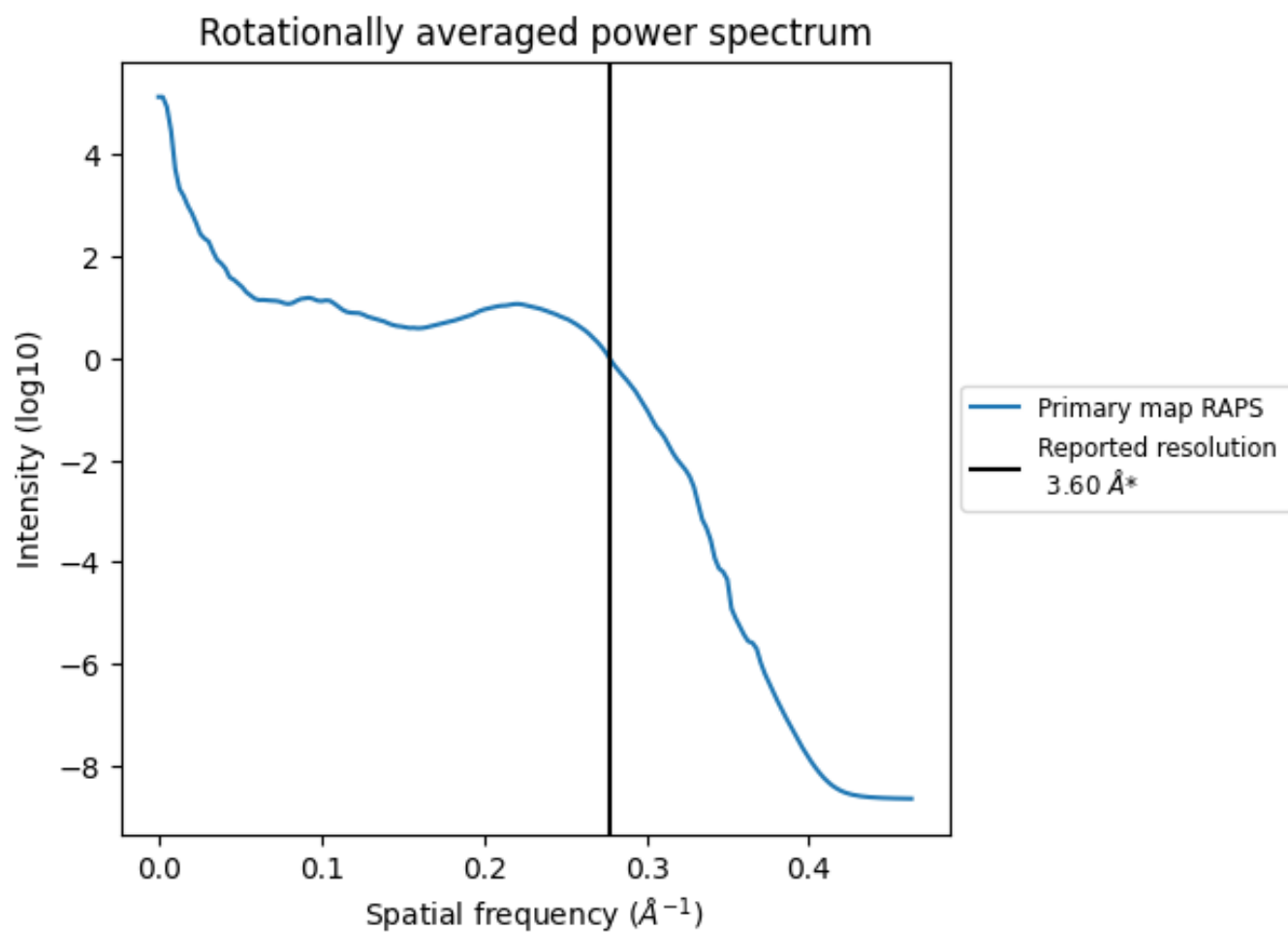
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 610 nm³; this corresponds to an approximate mass of 551 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

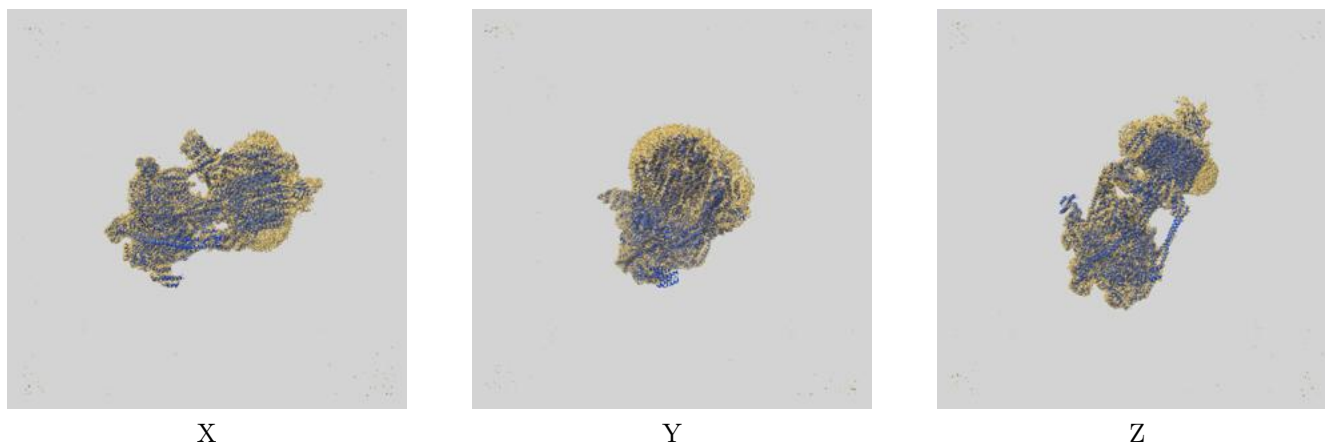
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

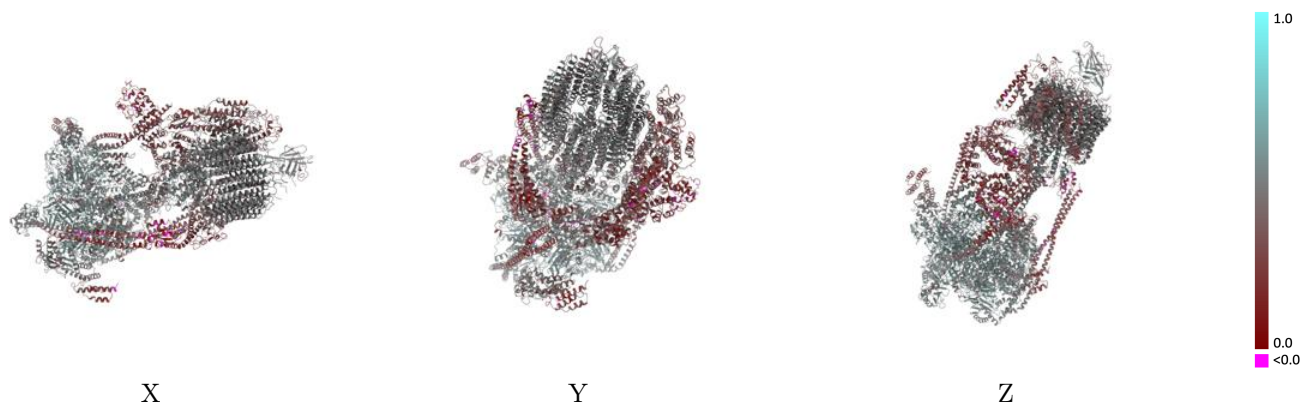
This section contains information regarding the fit between EMDB map EMD-21849 and PDB model 6WM4. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



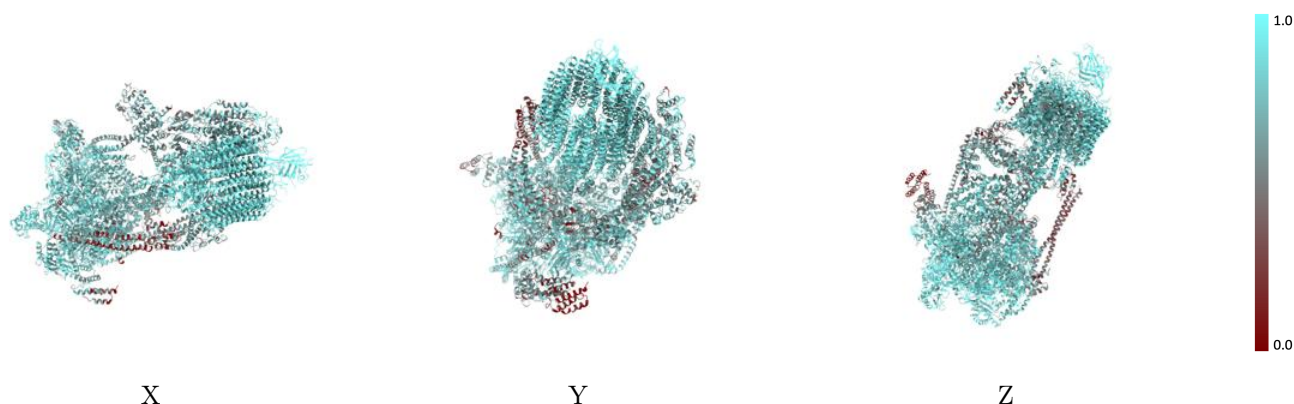
The images above show the 3D surface view of the map at the recommended contour level 3.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



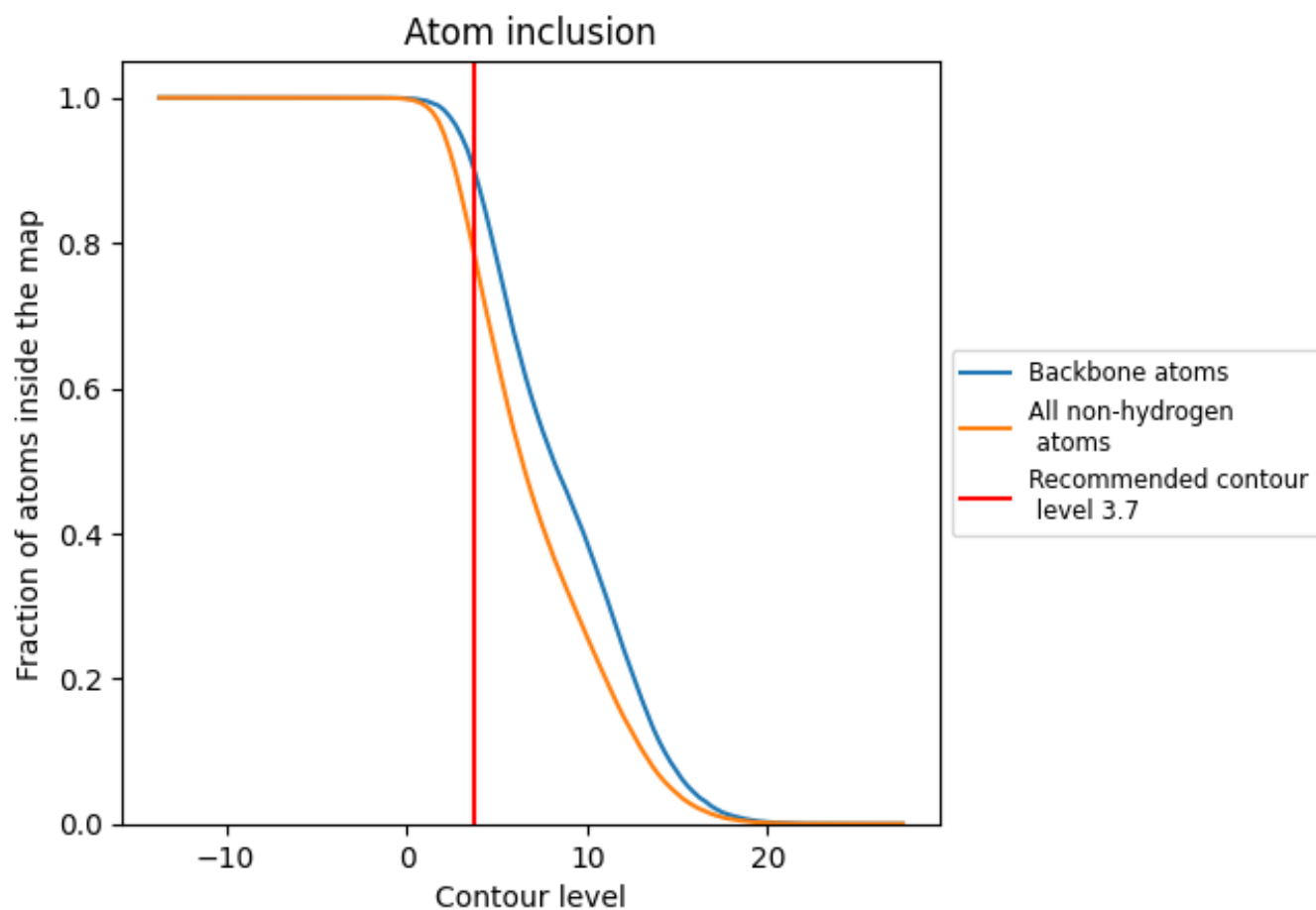
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.7).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (3.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7913	 0.4420
0	 0.8872	 0.4770
1	 0.8624	 0.4750
2	 0.8899	 0.4680
3	 0.8909	 0.4610
4	 0.8899	 0.4610
5	 0.9156	 0.4630
6	 0.8880	 0.4550
7	 0.9184	 0.4610
8	 0.8928	 0.4680
9	 0.8966	 0.4700
A	 0.9017	 0.5430
B	 0.8667	 0.5220
C	 0.8621	 0.5110
D	 0.9009	 0.5500
E	 0.8936	 0.5400
F	 0.8769	 0.5290
G	 0.8248	 0.4950
H	 0.8154	 0.4440
I	 0.7829	 0.4210
J	 0.7230	 0.4190
K	 0.7080	 0.3680
L	 0.6367	 0.3600
M	 0.4841	 0.3280
N	 0.7503	 0.4380
O	 0.5311	 0.2150
P	 0.6650	 0.2330
Q	 0.8894	 0.4850
R	 0.6271	 0.3220
S	 0.7359	 0.3480
T	 0.6390	 0.2880
U	 0.9353	 0.4670
V	 0.9204	 0.4730
X	 0.4227	 0.3990
Y	 0.6833	 0.4170
Z	 0.7788	 0.4620

