wwPDB EM Validation Summary Report

Feb 5, 2024 – 11:48 PM EST

PDB ID	:	7U8R
EMDB ID	:	EMD-26388
Title	:	Structure of porcine kidney V-ATPase with SidK, Rotary State 3
Authors	:	Tan, Y.Z.; Keon, K.A.
Deposited on	:	2022-03-09
Resolution	:	3.80 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:

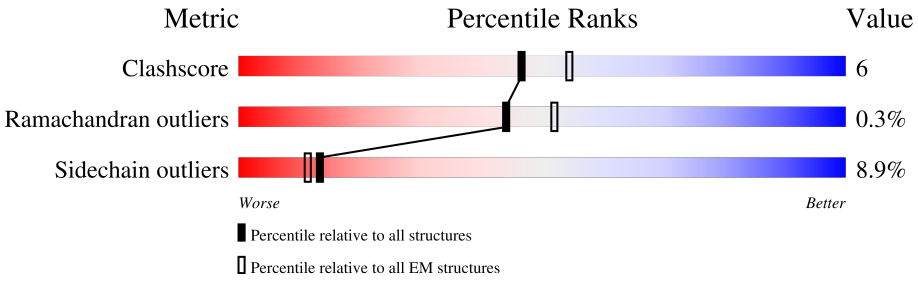
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.80 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 <=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	A	617	76% 20%
1	B	617	12% 74% 18% 5%
1	C	617	79% 17%
2	D	515	66% 21% 11%
2	E	515	73% 15% 11%
2	F	515	67% 21% 11%
3	G	382	63% 69% 24% 6%
4	H	247	70% 16% 14%

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Mol	Chain	Length	Quality of chain
5	I	226	79% 16%
5	J	226	74% 21%
5	K	226	18% 78% 16%
6	L	119	14% 63% 26% 8%
7	M	118	85% 8% 7%
7	N	118	69% 22% 7%
7	O	118	36% 55% 31% 6% 8%
8	Q	337	54% 12% 34%
8	R	337	54% 7% 39%
8	S	337	52% 15% 33%
9	T	483	34% 60% 26% 12%
10	a	838	7% 89% 11%
11	b	205	12% 99%
12	c	469	44% 56%
13	d	351	23% 93% 6%
14	e	81	9% 99%
15	f	98	9% 86% 14%
16	g	155	16% 97%
16	h	155	15% 97%
16	i	155	9% 97%
16	j	155	6% 97%
16	k	155	6% 97%
16	l	155	5% 97%
16	m	155	5% 97%
16	n	155	7% 97%

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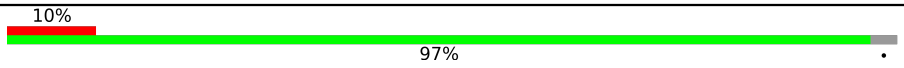
Mol	Chain	Length	Quality of chain
16	o	155	
17	p	351	

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 62638 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 catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	600	Total	C	N	O	S	0	0
			4661	2957	790	889	25		
1	B	587	Total	C	N	O	S	0	0
			4577	2904	776	873	24		
1	C	600	Total	C	N	O	S	0	0
			4661	2957	790	889	25		

- Molecule 2 is a protein called Vacuolar proton pump subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	456	Total	C	N	O	S	0	0
			3572	2266	611	674	21		
2	E	456	Total	C	N	O	S	0	0
			3572	2266	611	674	21		
2	F	458	Total	C	N	O	S	0	0
			3590	2278	615	676	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	360	Total	C	N	O	S	0	0
			2935	1880	496	549	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	213	Total	C	N	O	S	0	0
			1717	1089	309	314	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	217	Total	C	N	O	S	0	0
			1416	880	263	269	4		
5	J	218	Total	C	N	O	S	0	0
			1773	1118	317	329	9		
5	K	217	Total	C	N	O	S	0	0
			1766	1113	316	328	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	109	Total	C	N	O	S	0	0
			865	548	153	162	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	110	Total	C	N	O	S	0	0
			673	413	129	130	1		
7	N	110	Total	C	N	O	S	0	0
			906	556	172	175	3		
7	O	108	Total	C	N	O	S	0	0
			894	548	170	173	3		

- Molecule 8 is a protein called Bacterial effector protein SidK.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	224	Total	C	N	O	S	0	0
			1824	1162	306	346	10		
8	R	206	Total	C	N	O	S	0	0
			1685	1073	285	319	8		
8	S	226	Total	C	N	O	S	0	0
			1836	1169	308	348	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	427	Total	C	N	O	S	0	0
			3510	2230	606	651	23		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	a	750	Total 3707	C 2207	N 750	O 750	0	0

- Molecule 11 is a protein called V-type proton ATPase 21 kDa proteolipid subunit isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	b	203	Total 989	C 583	N 203	O 203	0	0

- Molecule 12 is a protein called ATPase H+ transporting accessory protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	c	206	Total 1016	C 604	N 206	O 206	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	d	350	Total 2835	C 1829	N 462	O 530	S 14	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	e	80	Total 394	C 234	N 80	O 80	0	0

- Molecule 15 is a protein called Ribonuclease kappa.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	f	84	Total 412	C 244	N 84	O 84	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
16	g	150	Total 729	C 429	N 150	O 150	0	0
16	h	150	Total 729	C 429	N 150	O 150	0	0
16	i	150	Total 729	C 429	N 150	O 150	0	0

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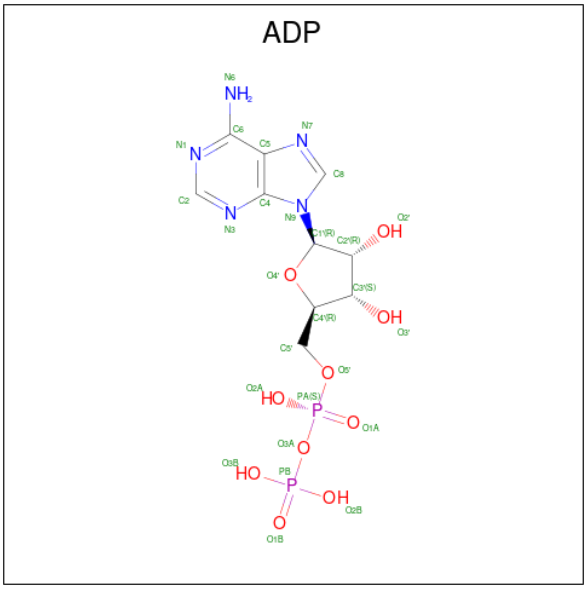
Mol	Chain	Residues	Atoms				AltConf	Trace
16	j	150	Total	C	N	O	0	0
			729	429	150	150		
16	k	150	Total	C	N	O	0	0
			729	429	150	150		
16	l	150	Total	C	N	O	0	0
			729	429	150	150		
16	m	150	Total	C	N	O	0	0
			729	429	150	150		
16	n	150	Total	C	N	O	0	0
			729	429	150	150		
16	o	150	Total	C	N	O	0	0
			729	429	150	150		

- Molecule 17 is a protein called ATPase H(+)-transporting lysosomal accessory protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	p	53	Total	C	N	O	0	0
			264	158	53	53		

- Molecule 18 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



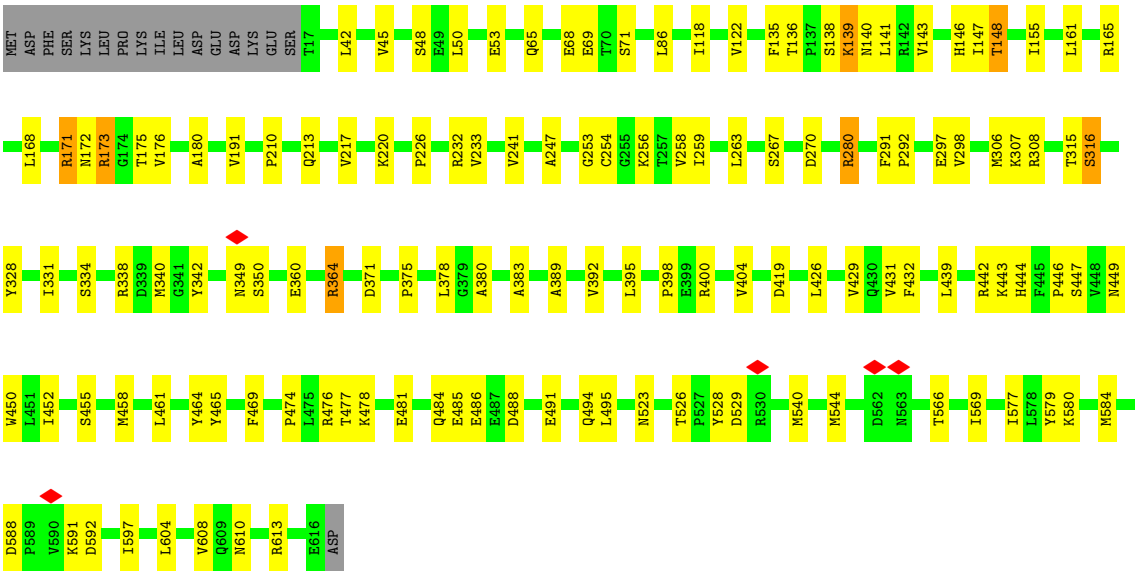
Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots (i)

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

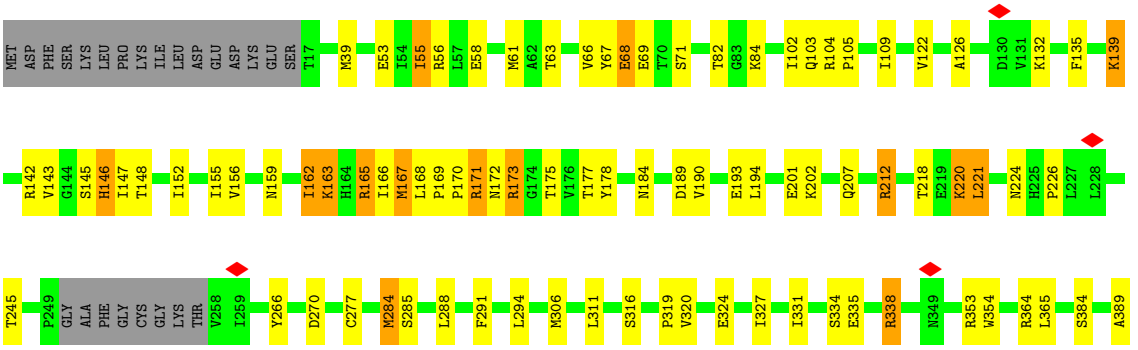
• Molecule 1: V-type proton ATPase catalytic subunit A

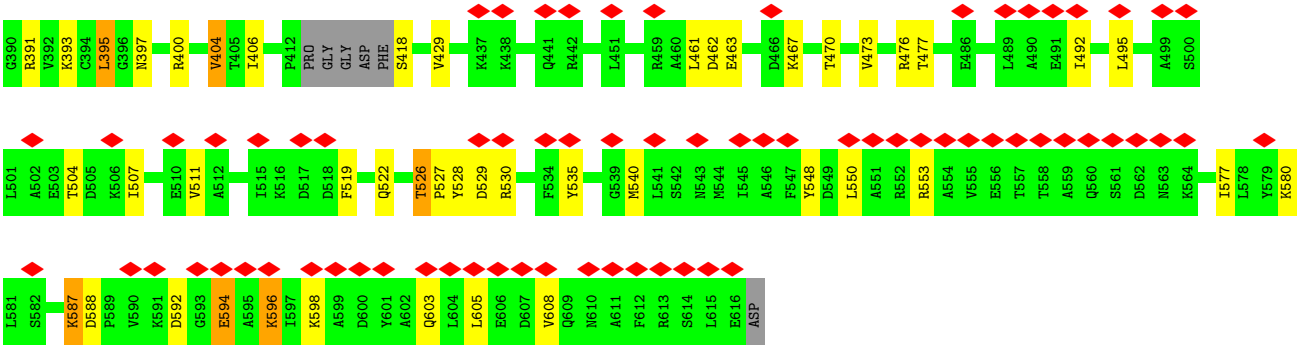
Chain A:



• Molecule 1: V-type proton ATPase catalytic subunit A

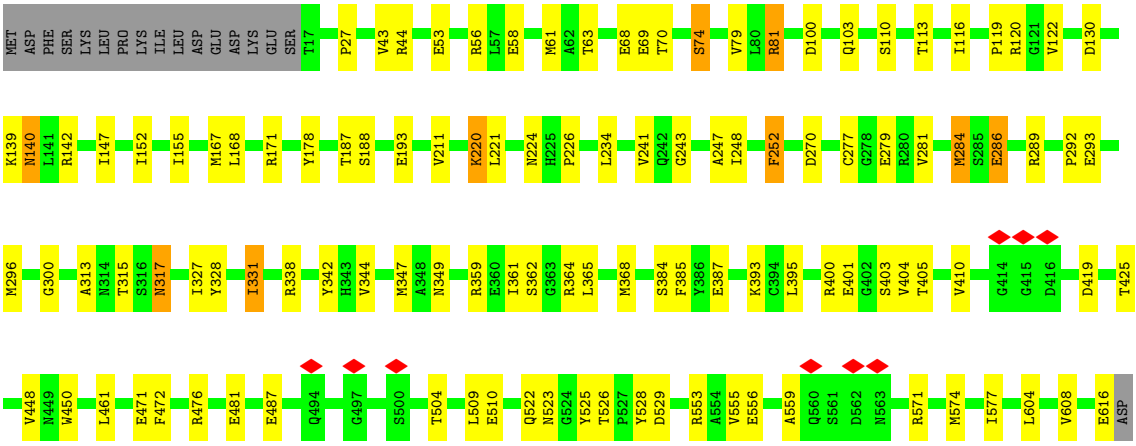
Chain B:





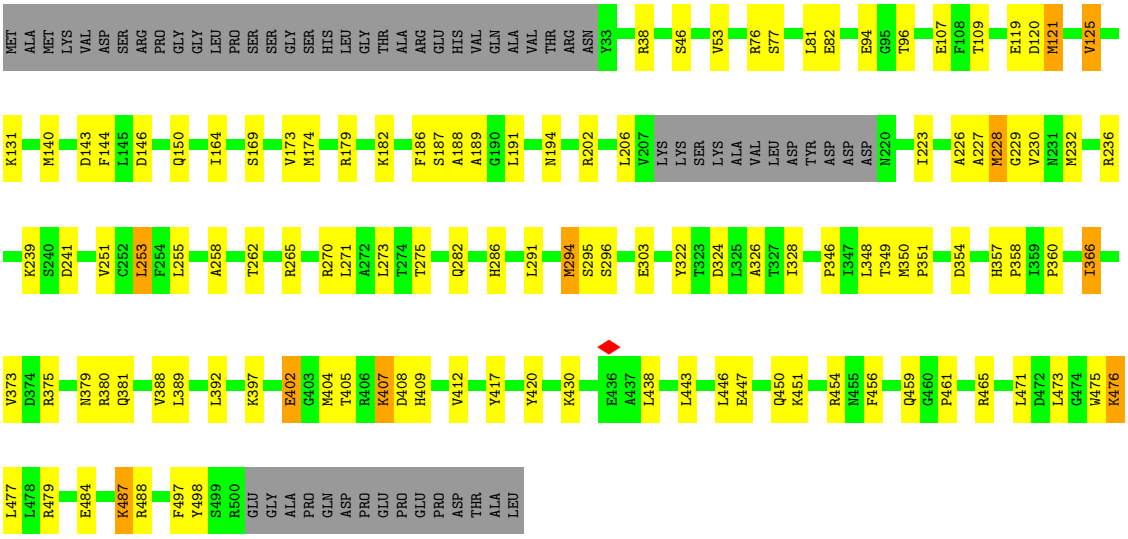
• Molecule 1: V-type proton ATPase catalytic subunit A

Chain C:



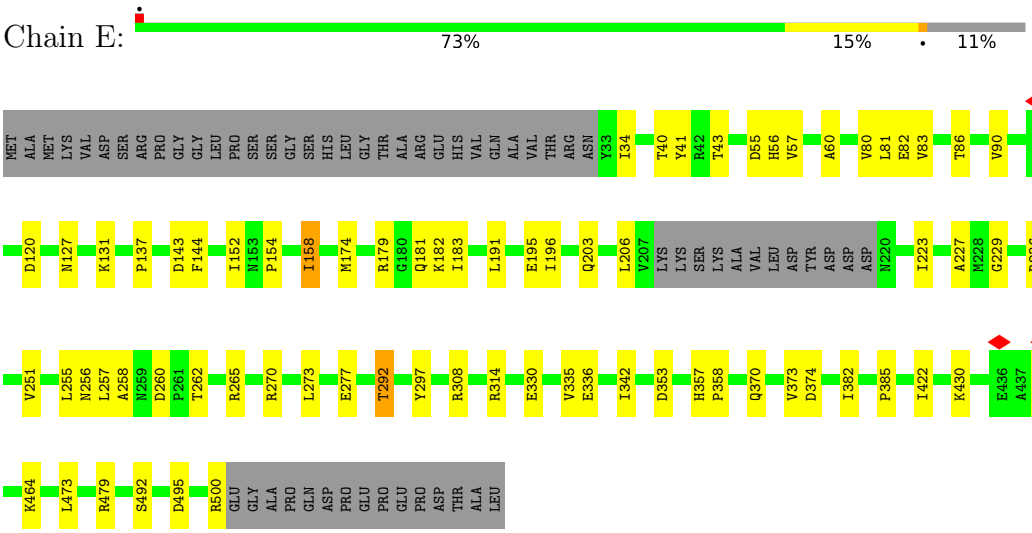
• Molecule 2: Vacuolar proton pump subunit B

Chain D:



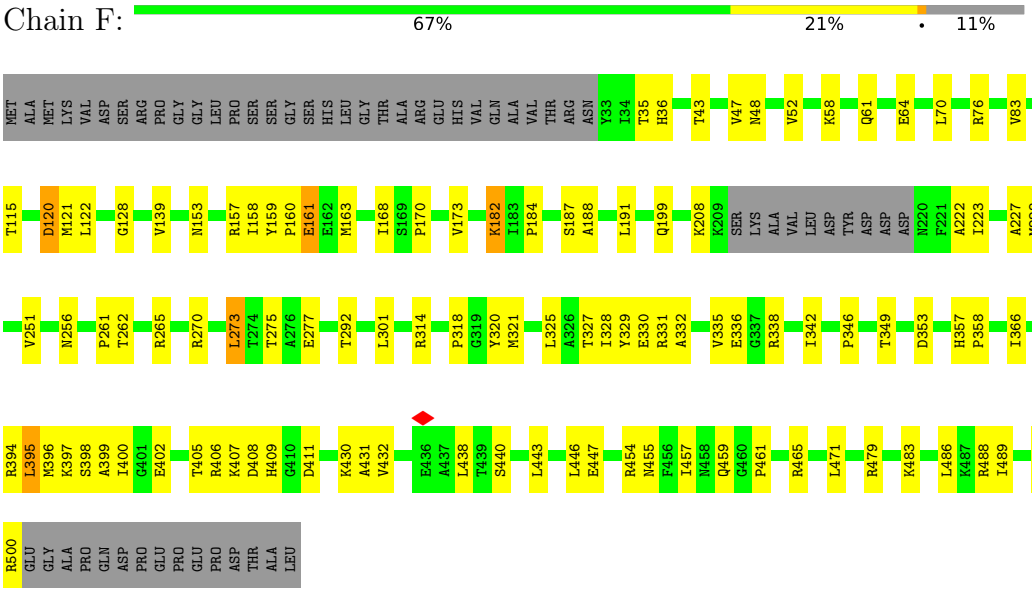
• Molecule 2: Vacuolar proton pump subunit B

Chain E:



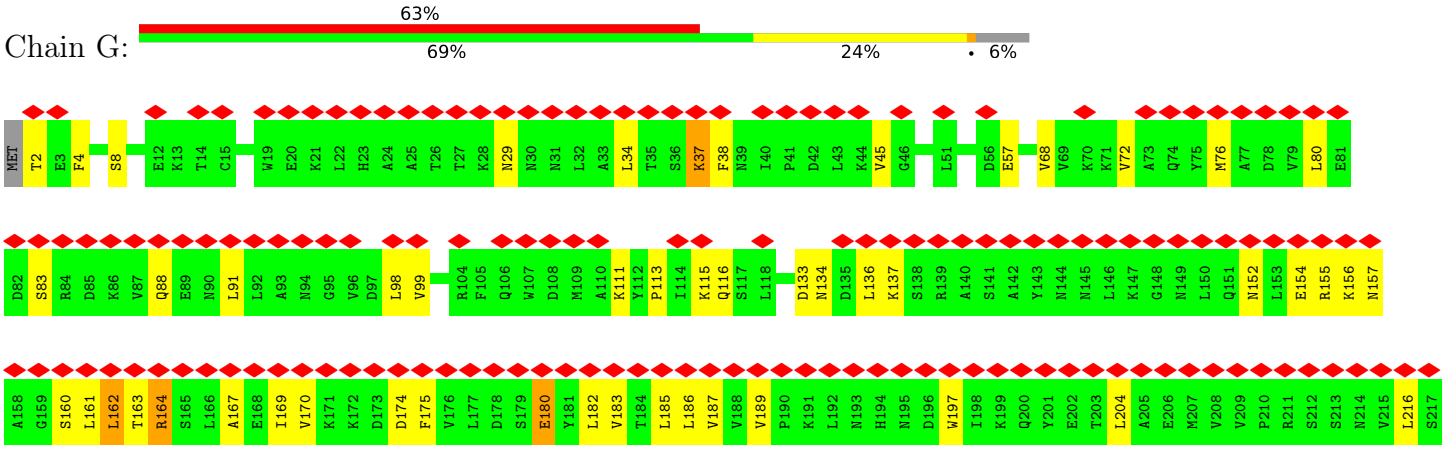
• Molecule 2: Vacuolar proton pump subunit B

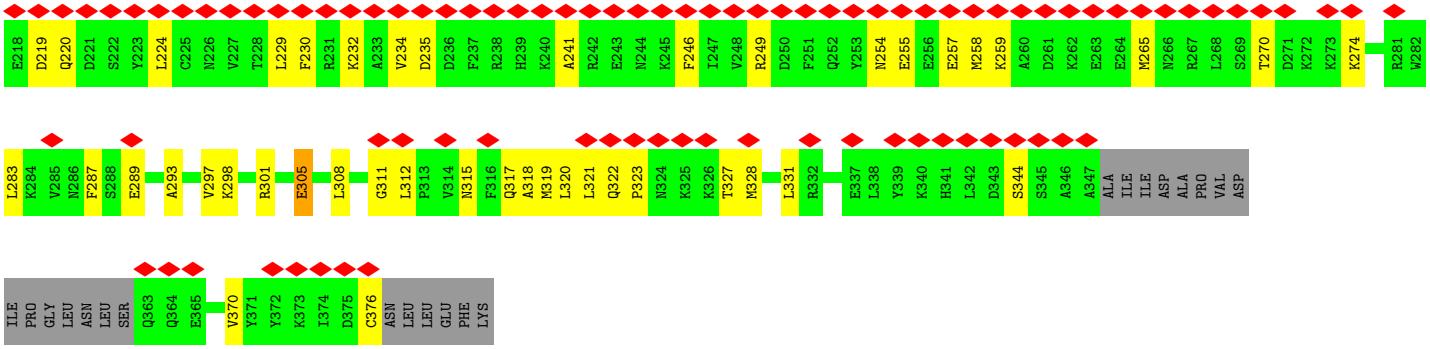
Chain F:



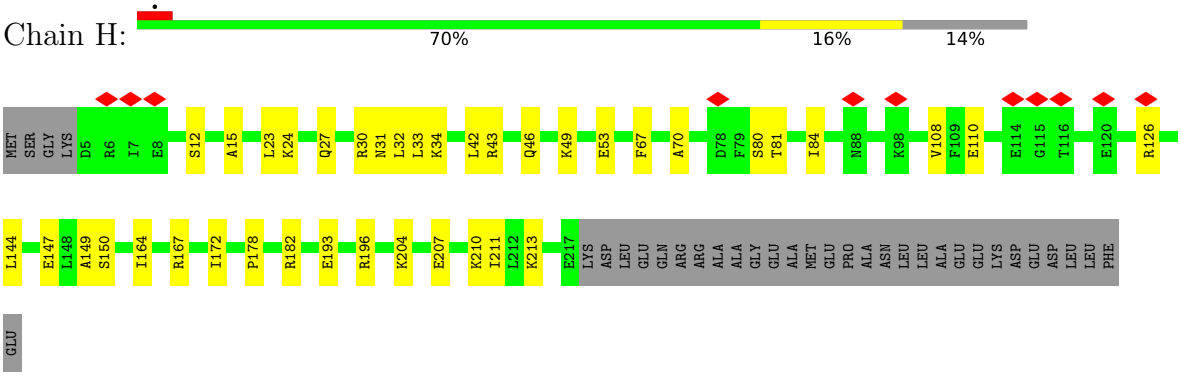
• Molecule 3: V-type proton ATPase subunit C

Chain G:

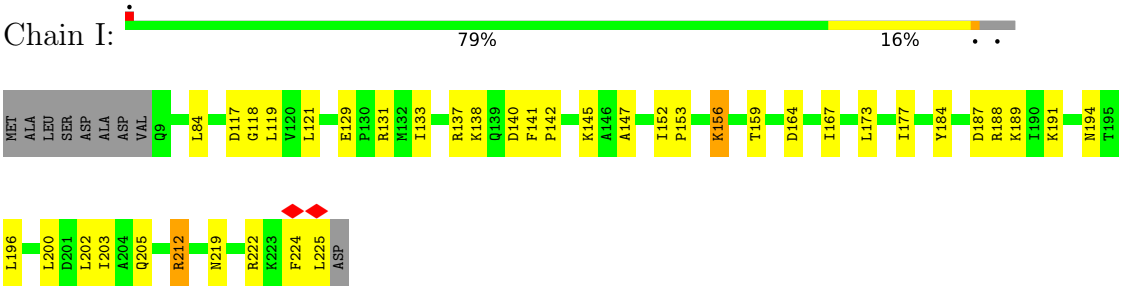




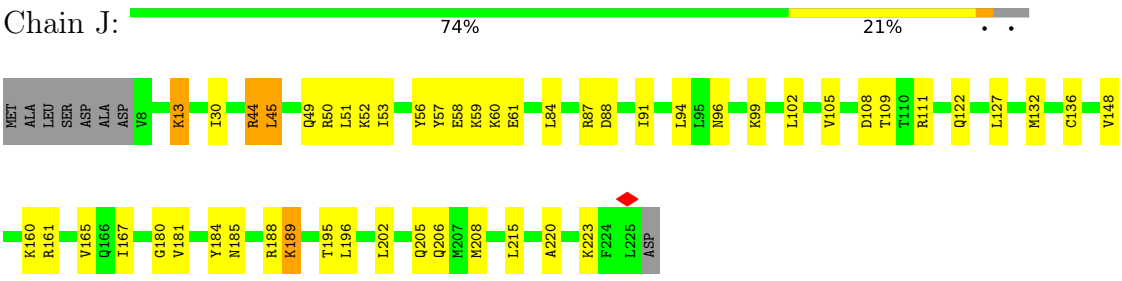
• Molecule 4: V-type proton ATPase subunit D



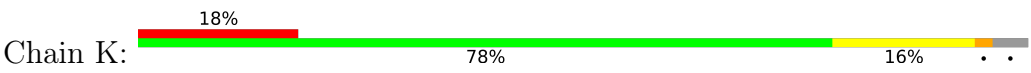
• Molecule 5: V-type proton ATPase subunit E 1

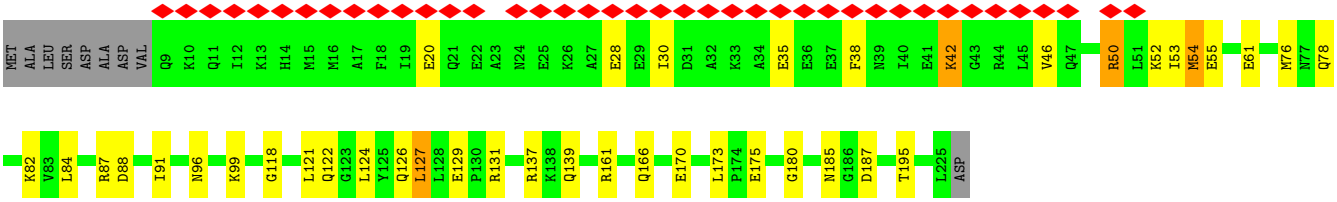


• Molecule 5: V-type proton ATPase subunit E 1



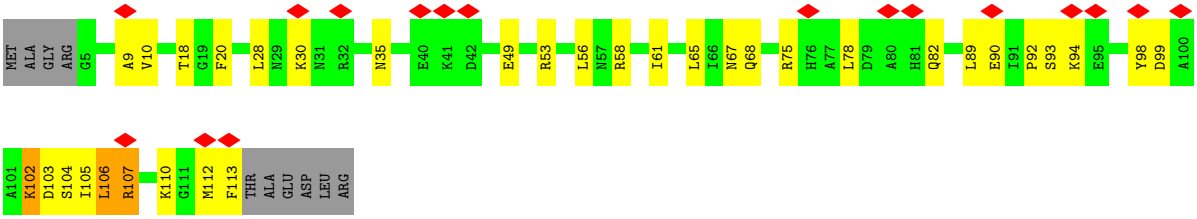
• Molecule 5: V-type proton ATPase subunit E 1





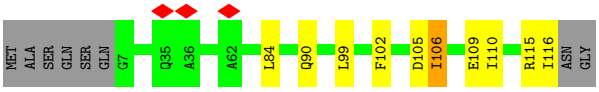
• Molecule 6: V-type proton ATPase subunit F

Chain L:



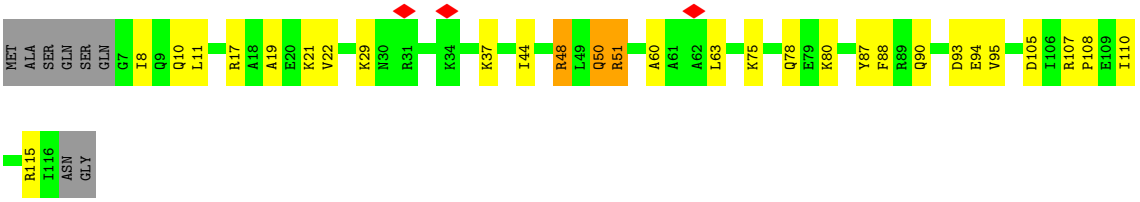
• Molecule 7: V-type proton ATPase subunit G

Chain M:



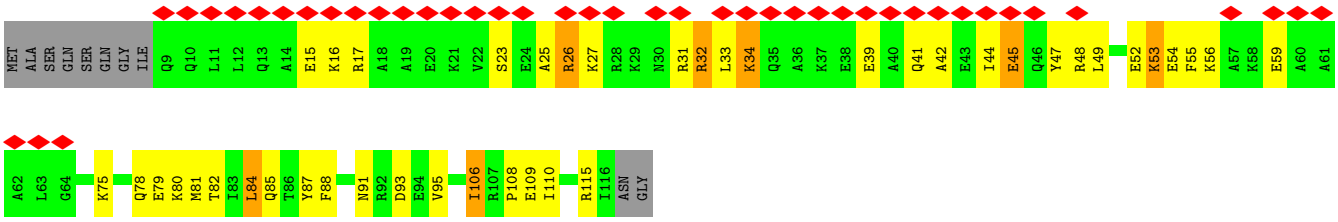
• Molecule 7: V-type proton ATPase subunit G

Chain N:



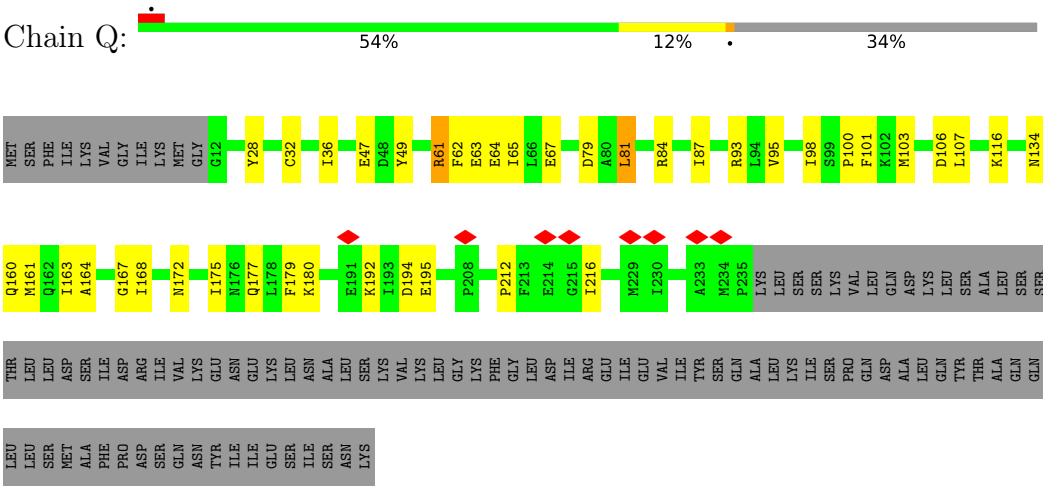
• Molecule 7: V-type proton ATPase subunit G

Chain O:



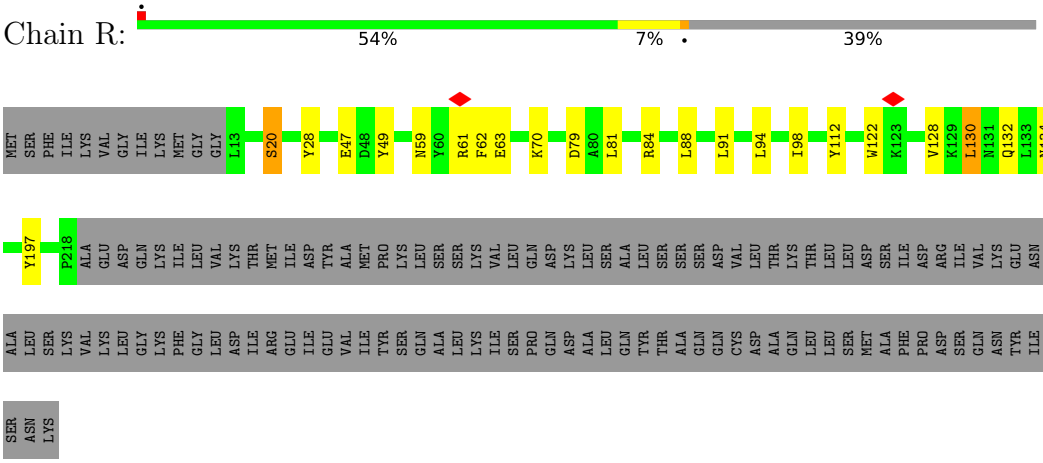
• Molecule 8: Bacterial effector protein SidK

Chain Q:



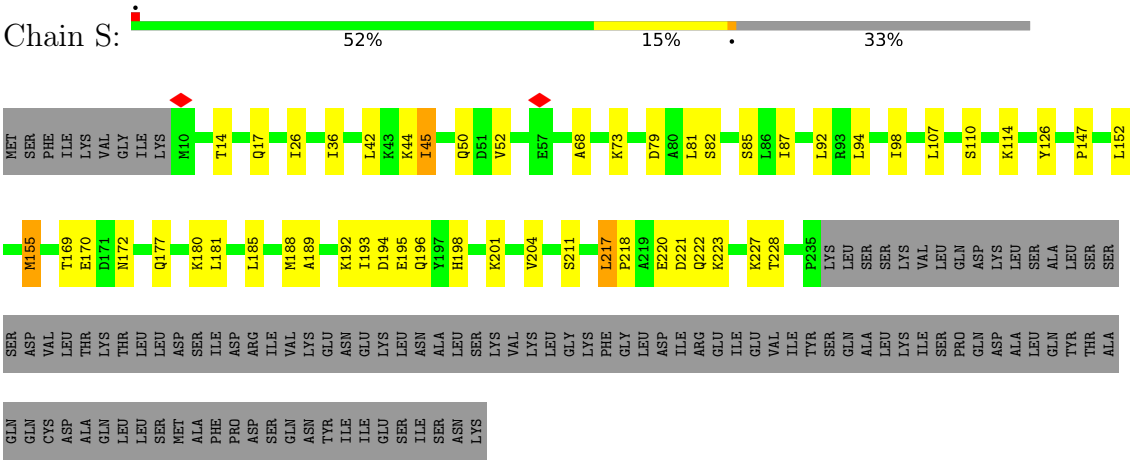
• Molecule 8: Bacterial effector protein SidK

Chain R:



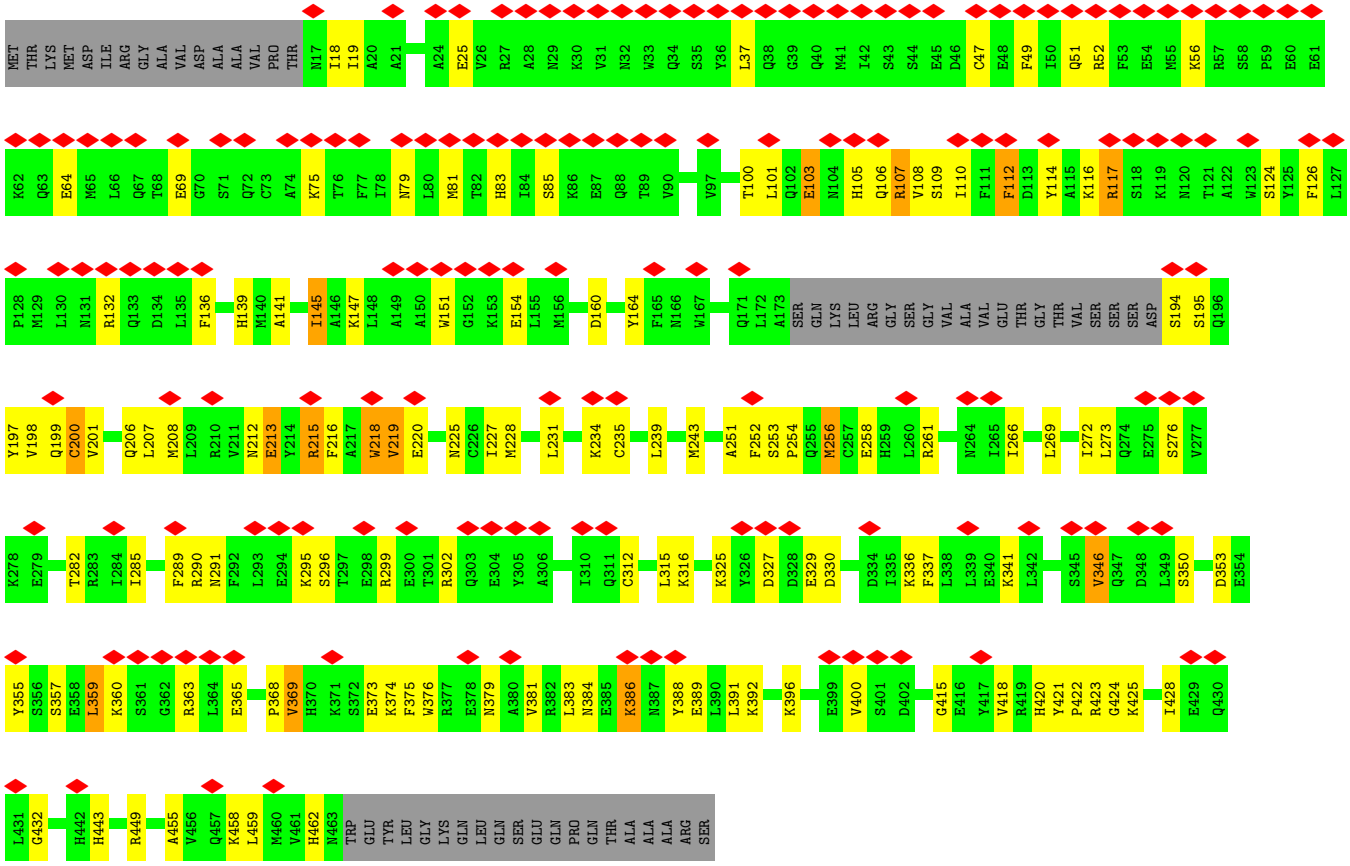
• Molecule 8: Bacterial effector protein SidK

Chain S:



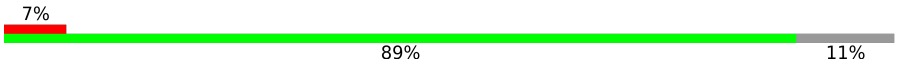
• Molecule 9: V-type proton ATPase subunit H

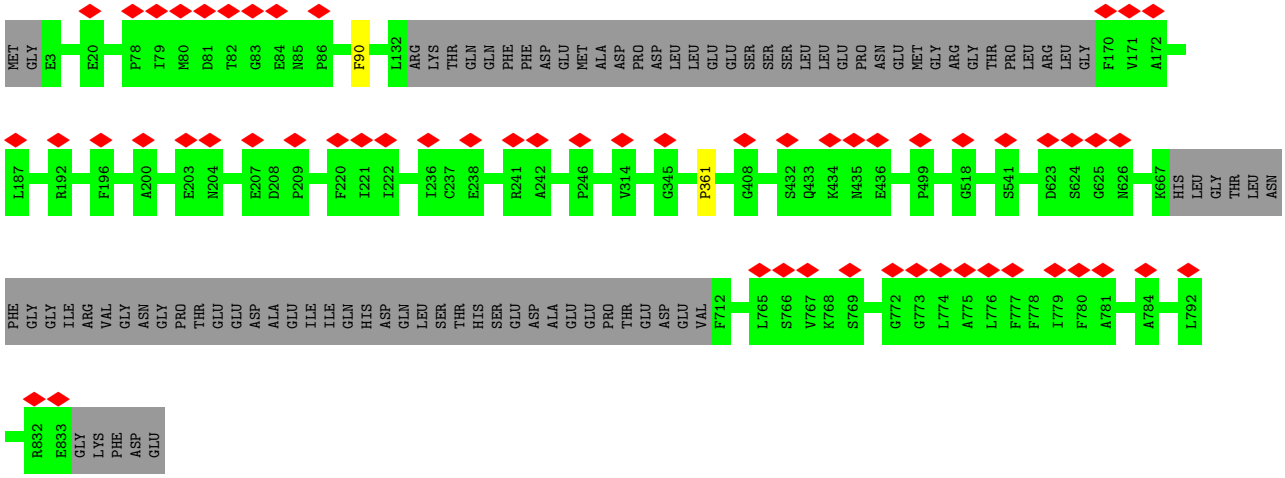
Chain T:



• Molecule 10: V-type proton ATPase subunit a

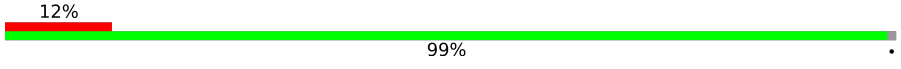
Chain a:

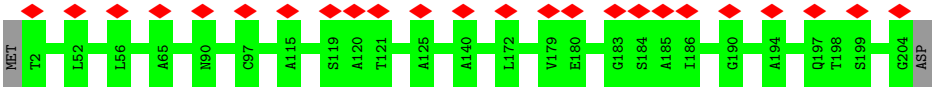




• Molecule 11: V-type proton ATPase 21 kDa proteolipid subunit isoform 1

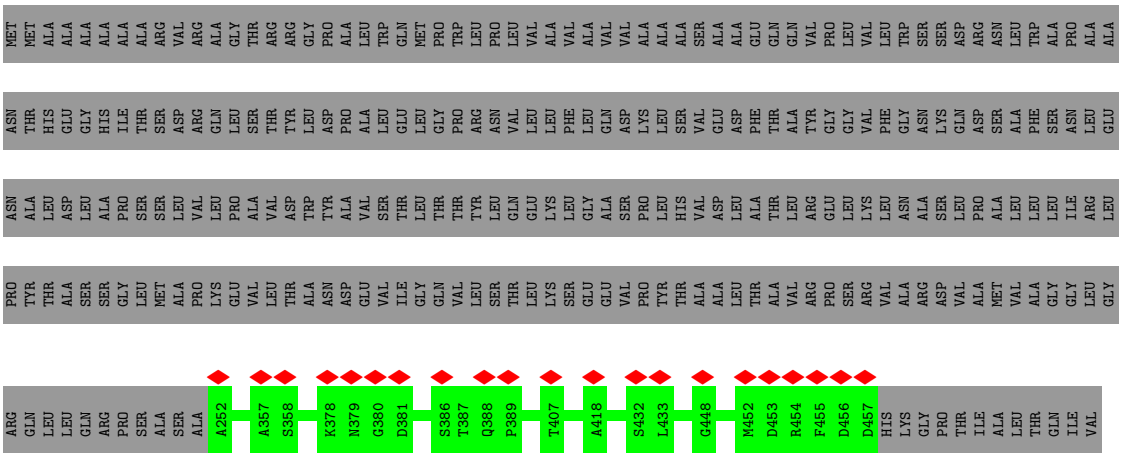
Chain b:





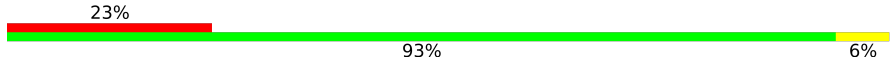
• Molecule 12: ATPase H+ transporting accessory protein 1

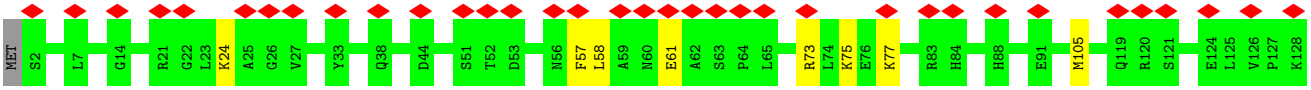
Chain c:

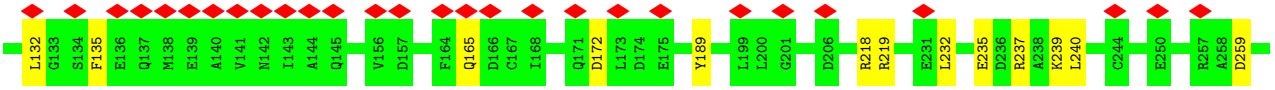


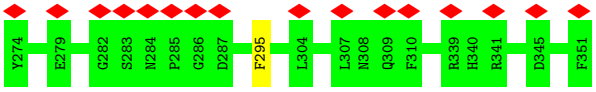
• Molecule 13: V-type proton ATPase subunit

Chain d:



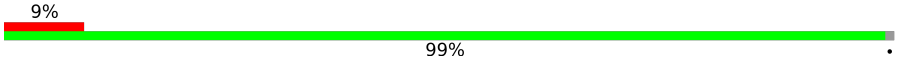


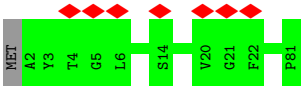




• Molecule 14: V-type proton ATPase subunit

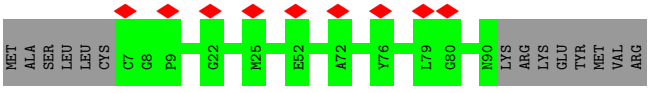
Chain e:





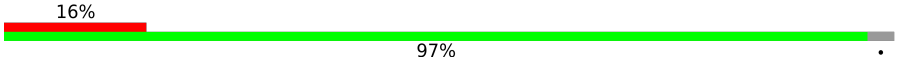
• Molecule 15: Ribonuclease kappa

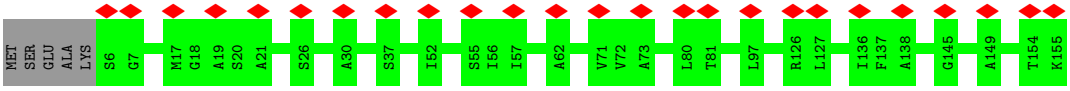
Chain f:



• Molecule 16: V-type proton ATPase proteolipid subunit

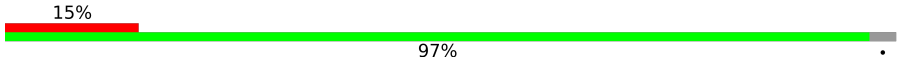
Chain g:

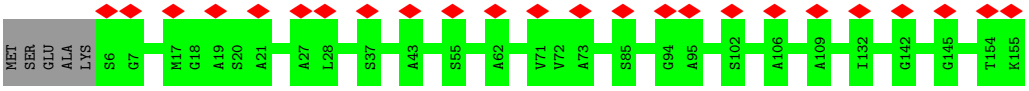




• Molecule 16: V-type proton ATPase proteolipid subunit

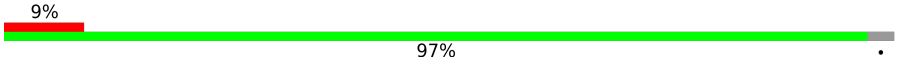
Chain h:

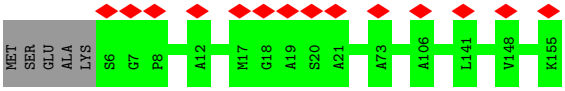




• Molecule 16: V-type proton ATPase proteolipid subunit

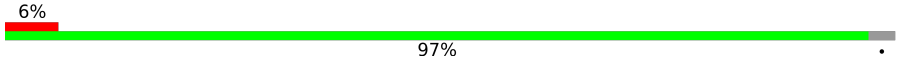
Chain i:

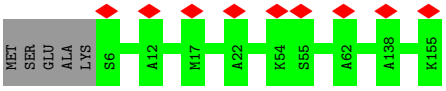




• Molecule 16: V-type proton ATPase proteolipid subunit

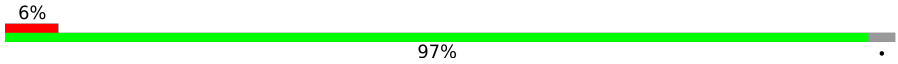
Chain j:

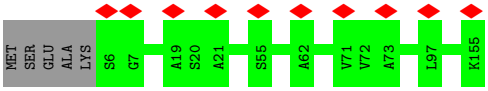




• Molecule 16: V-type proton ATPase proteolipid subunit

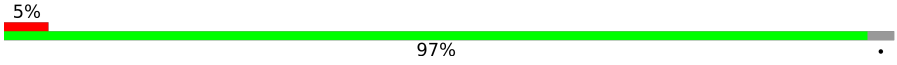
Chain k:

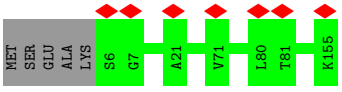




• Molecule 16: V-type proton ATPase proteolipid subunit

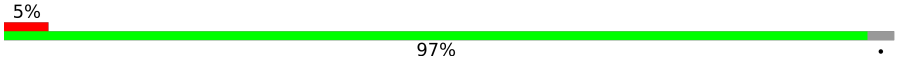
Chain l:

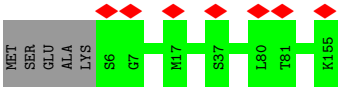




• Molecule 16: V-type proton ATPase proteolipid subunit

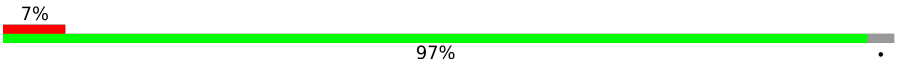
Chain m:

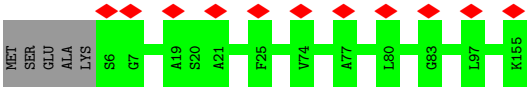




• Molecule 16: V-type proton ATPase proteolipid subunit

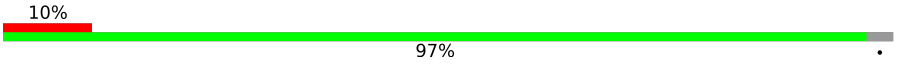
Chain n:

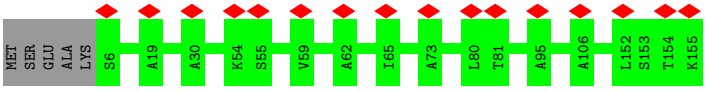




• Molecule 16: V-type proton ATPase proteolipid subunit

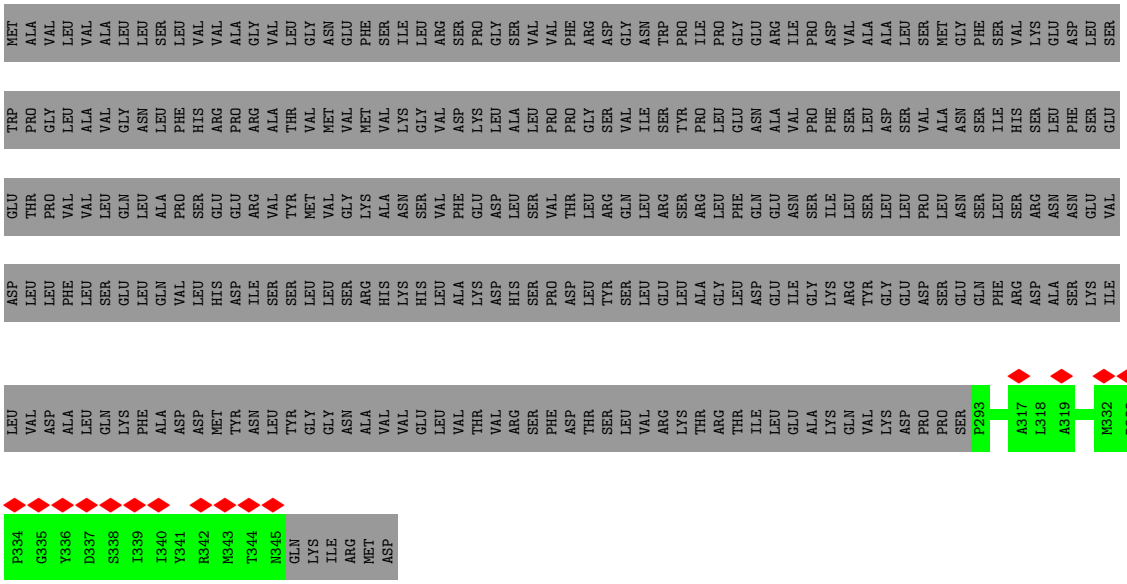
Chain o:





• Molecule 17: ATPase H(+)-transporting lysosomal accessory protein 2

Chain p:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22866	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	100.00	Depositor
Maximum defocus (nm)	3911.445	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.799	Depositor
Minimum map value	-0.389	Depositor
Average map value	0.160	Depositor
Map value standard deviation	0.254	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	184.88861, 215.4487, 307.129	wwPDB
Map dimensions	121, 141, 201	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.528005, 1.528005, 1.528005	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

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	A	0.57	0/4757	0.83	0/6446
1	B	0.56	0/4668	0.82	0/6324
1	C	0.57	0/4757	0.80	0/6446
2	D	0.55	0/3644	0.77	0/4939
2	E	0.54	0/3644	0.76	0/4939
2	F	0.55	0/3662	0.79	0/4961
3	G	0.46	0/2989	0.70	0/4038
4	H	0.46	0/1735	0.77	0/2321
5	I	0.40	0/1427	0.58	0/1948
5	J	0.40	0/1790	0.62	0/2396
5	K	0.53	0/1783	0.77	0/2386
6	L	0.51	0/879	0.82	0/1186
7	M	0.45	0/678	0.57	0/933
7	N	0.41	0/914	0.65	0/1218
7	O	0.55	0/902	0.75	0/1202
8	Q	0.48	0/1858	0.76	0/2505
8	R	0.59	0/1717	0.83	0/2315
8	S	0.49	0/1870	0.71	0/2520
9	T	0.45	0/3576	0.67	0/4818
10	a	0.28	0/3704	0.41	0/5155
11	b	0.24	0/988	0.38	0/1366
12	c	0.26	0/1015	0.49	0/1411
13	d	0.48	0/2901	0.75	0/3930
14	e	0.24	0/393	0.37	0/545
15	f	0.26	0/411	0.35	0/569
16	g	0.25	0/728	0.38	0/1005
16	h	0.26	0/728	0.38	0/1005
16	i	0.25	0/728	0.38	0/1005
16	j	0.25	0/728	0.37	0/1005
16	k	0.26	0/728	0.38	0/1005
16	l	0.25	0/728	0.38	0/1005
16	m	0.26	0/728	0.38	0/1005

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	n	0.25	0/728	0.38	0/1005
16	o	0.25	0/728	0.38	0/1005
17	p	0.23	0/263	0.37	0/366
All	All	0.48	0/63477	0.70	0/86228

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	4661	0	4653	71	0
1	B	4577	0	4577	61	0
1	C	4661	0	4653	54	0
2	D	3572	0	3555	69	0
2	E	3572	0	3555	40	0
2	F	3590	0	3581	56	0
3	G	2935	0	2970	50	0
4	H	1717	0	1822	30	0
5	I	1416	0	1167	20	0
5	J	1773	0	1855	32	0
5	K	1766	0	1846	20	0
6	L	865	0	872	15	0
7	M	673	0	476	1	0
7	N	906	0	913	22	0
7	O	894	0	899	24	0
8	Q	1824	0	1835	27	0
8	R	1685	0	1691	9	0
8	S	1836	0	1847	21	0
9	T	3510	0	3493	73	0
10	a	3707	0	1627	0	0
11	b	989	0	489	0	0
12	c	1016	0	457	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	d	2835	0	2770	0	0
14	e	394	0	167	0	0
15	f	412	0	190	0	0
16	g	729	0	388	0	0
16	h	729	0	388	0	0
16	i	729	0	388	0	0
16	j	729	0	388	0	0
16	k	729	0	388	0	0
16	l	729	0	388	0	0
16	m	729	0	388	0	0
16	n	729	0	388	0	0
16	o	729	0	388	0	0
17	p	264	0	116	0	0
18	A	27	0	12	3	0
All	All	62638	0	55580	638	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 6.

The worst 5 of 638 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)
7:O:45:GLU:N	7:O:45:GLU:OE1	2.00	0.95
7:O:45:GLU:H	7:O:45:GLU:CD	1.66	0.95
7:O:45:GLU:N	7:O:45:GLU:CD	2.21	0.93
4:H:149:ALA:HB2	6:L:89:LEU:HD11	1.51	0.92
2:E:34:ILE:HD12	5:J:202:LEU:HG	1.62	0.81

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	A	598/617 (97%)	554 (93%)	41 (7%)	3 (0%)	29	66
1	B	581/617 (94%)	547 (94%)	31 (5%)	3 (0%)	29	66
1	C	598/617 (97%)	554 (93%)	41 (7%)	3 (0%)	29	66
2	D	452/515 (88%)	431 (95%)	19 (4%)	2 (0%)	34	70
2	E	452/515 (88%)	430 (95%)	22 (5%)	0	100	100
2	F	454/515 (88%)	431 (95%)	17 (4%)	6 (1%)	12	48
3	G	356/382 (93%)	342 (96%)	13 (4%)	1 (0%)	41	74
4	H	211/247 (85%)	203 (96%)	8 (4%)	0	100	100
5	I	215/226 (95%)	208 (97%)	7 (3%)	0	100	100
5	J	216/226 (96%)	209 (97%)	7 (3%)	0	100	100
5	K	215/226 (95%)	212 (99%)	3 (1%)	0	100	100
6	L	107/119 (90%)	95 (89%)	12 (11%)	0	100	100
7	M	108/118 (92%)	107 (99%)	1 (1%)	0	100	100
7	N	108/118 (92%)	107 (99%)	1 (1%)	0	100	100
7	O	106/118 (90%)	102 (96%)	3 (3%)	1 (1%)	17	54
8	Q	222/337 (66%)	214 (96%)	8 (4%)	0	100	100
8	R	204/337 (60%)	195 (96%)	7 (3%)	2 (1%)	15	52
8	S	224/337 (66%)	214 (96%)	9 (4%)	1 (0%)	34	70
9	T	423/483 (88%)	399 (94%)	24 (6%)	0	100	100
10	a	744/838 (89%)	717 (96%)	25 (3%)	2 (0%)	41	74
11	b	201/205 (98%)	197 (98%)	4 (2%)	0	100	100
12	c	204/469 (44%)	184 (90%)	20 (10%)	0	100	100
13	d	348/351 (99%)	330 (95%)	17 (5%)	1 (0%)	41	74
14	e	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
15	f	82/98 (84%)	82 (100%)	0	0	100	100
16	g	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
16	h	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
16	i	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
16	j	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
16	k	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
16	l	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
16	m	148/155 (96%)	147 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	n	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
16	o	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
17	p	51/351 (14%)	49 (96%)	2 (4%)	0	100	100
All	All	8890/10458 (85%)	8503 (96%)	362 (4%)	25 (0%)	44	74

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	315	THR
1	A	450	TRP
1	B	470	THR
10	a	90	PHE
10	a	361	PRO

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	A	508/525 (97%)	475 (94%)	33 (6%)	17	48
1	B	501/525 (95%)	446 (89%)	55 (11%)	6	29
1	C	508/525 (97%)	460 (91%)	48 (9%)	8	35
2	D	390/438 (89%)	351 (90%)	39 (10%)	7	32
2	E	390/438 (89%)	370 (95%)	20 (5%)	24	54
2	F	392/438 (90%)	362 (92%)	30 (8%)	13	43
3	G	325/344 (94%)	303 (93%)	22 (7%)	16	47
4	H	184/211 (87%)	182 (99%)	2 (1%)	73	85
5	I	96/197 (49%)	81 (84%)	15 (16%)	2	17
5	J	191/197 (97%)	178 (93%)	13 (7%)	16	47
5	K	190/197 (96%)	166 (87%)	24 (13%)	4	24
6	L	93/100 (93%)	78 (84%)	15 (16%)	2	16
7	M	33/101 (33%)	23 (70%)	10 (30%)	0	2

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	N	95/101 (94%)	87 (92%)	8 (8%)	11 40
7	O	94/101 (93%)	66 (70%)	28 (30%)	0 2
8	Q	203/305 (67%)	195 (96%)	8 (4%)	32 60
8	R	188/305 (62%)	175 (93%)	13 (7%)	15 46
8	S	204/305 (67%)	185 (91%)	19 (9%)	9 35
9	T	385/429 (90%)	336 (87%)	49 (13%)	4 23
13	d	305/306 (100%)	284 (93%)	21 (7%)	15 46
All	All	5275/6088 (87%)	4803 (91%)	472 (9%)	13 38

5 of 472 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	180	GLU
9	T	365	GLU
5	K	76	MET
9	T	353	ASP
8	S	221	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	199	GLN
5	K	47	GLN
9	T	384	ASN
8	S	149	ASN
9	T	206	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)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	ADP	A	701	-	24,29,29	0.69	0	29,45,45	0.83	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
18	ADP	A	701	-	-	5/12/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

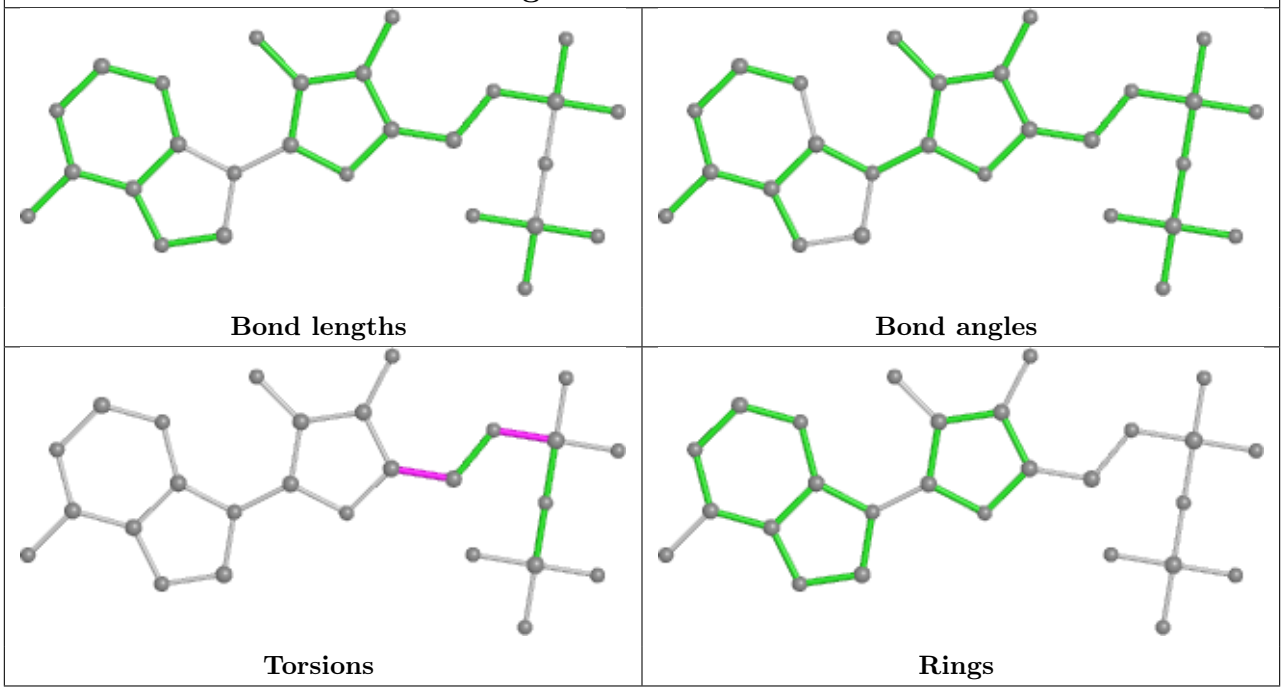
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	701	ADP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand ADP A 701



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.

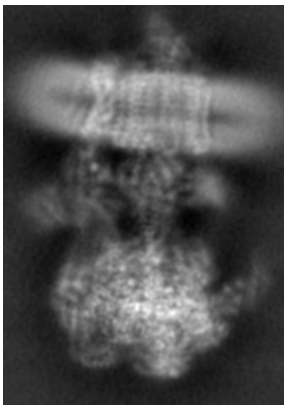
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26388. These allow visual inspection of the internal detail of the map and identification of artifacts.

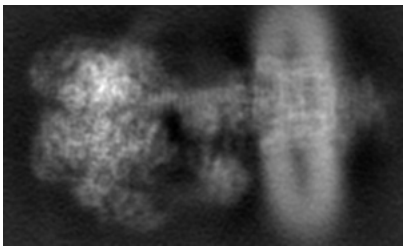
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

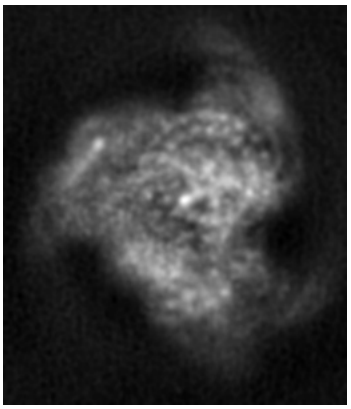
6.1.1 Primary map



X

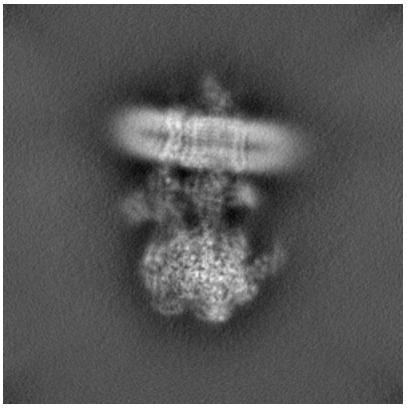


Y

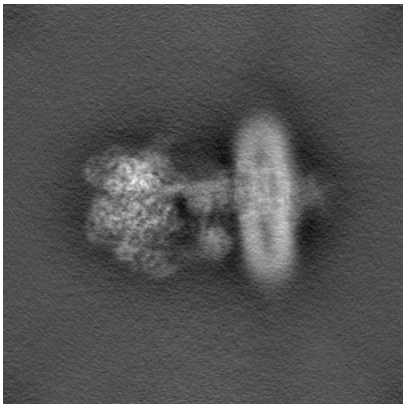


Z

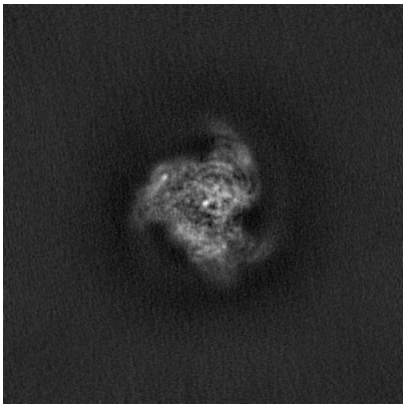
6.1.2 Raw map



X



Y



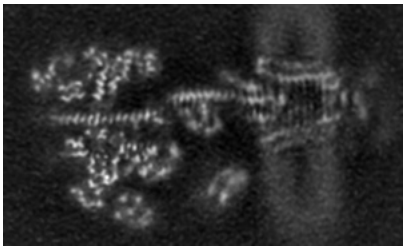
Z

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

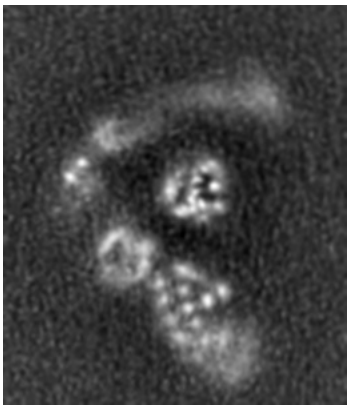
6.2 Central slices (i)

6.2.1 Primary map

X Index: 60

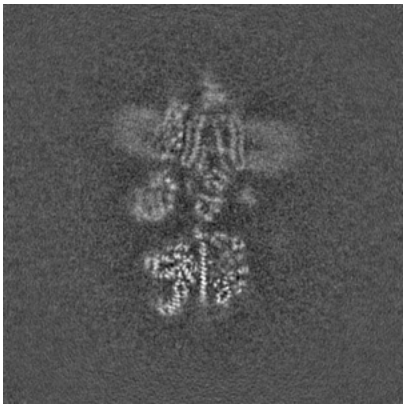


Y Index: 70

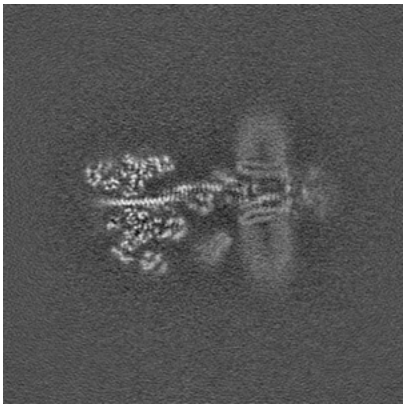


Z Index: 100

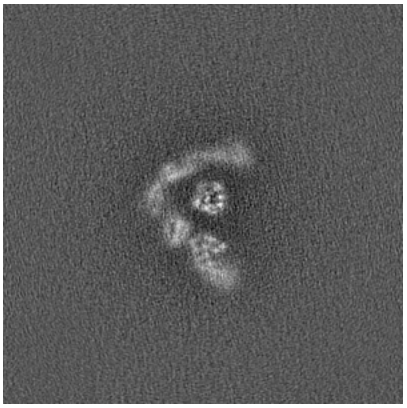
6.2.2 Raw map



X Index: 150



Y Index: 150

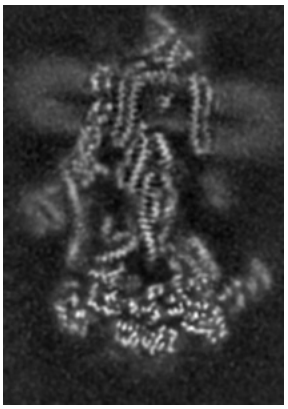


Z Index: 150

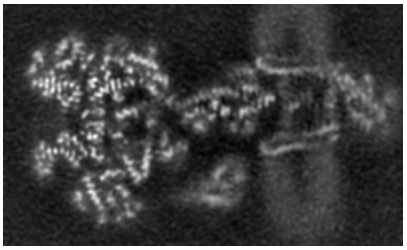
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

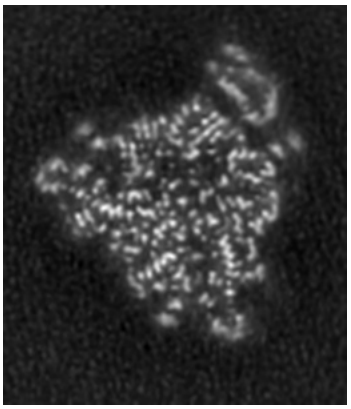
6.3.1 Primary map



X Index: 73

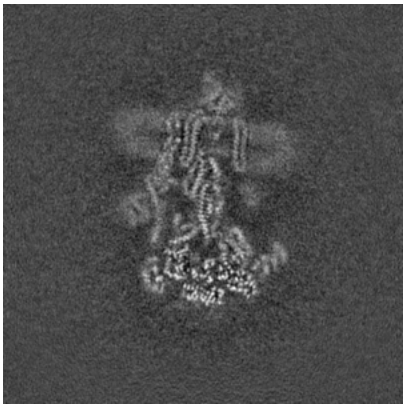


Y Index: 78

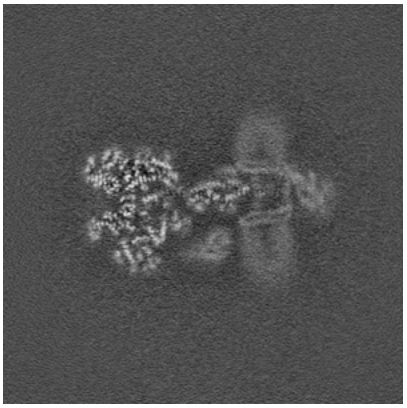


Z Index: 50

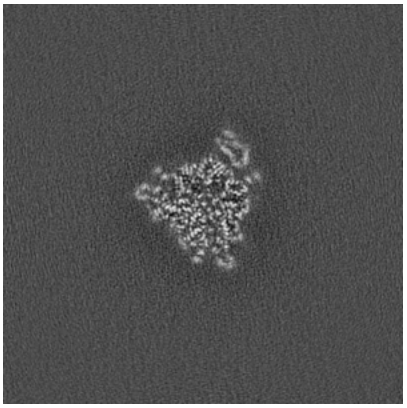
6.3.2 Raw map



X Index: 161



Y Index: 156

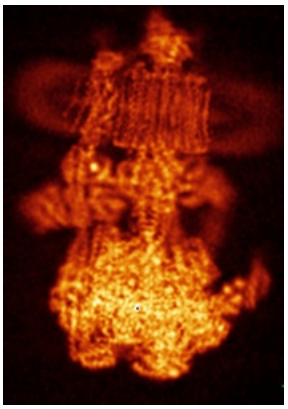


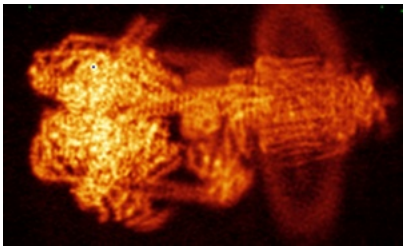
Z Index: 98

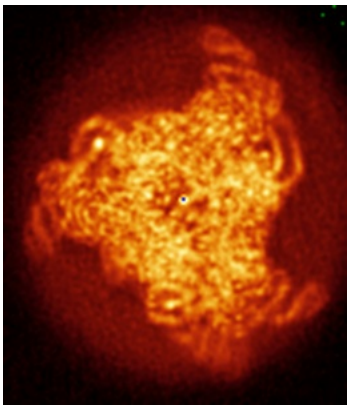
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

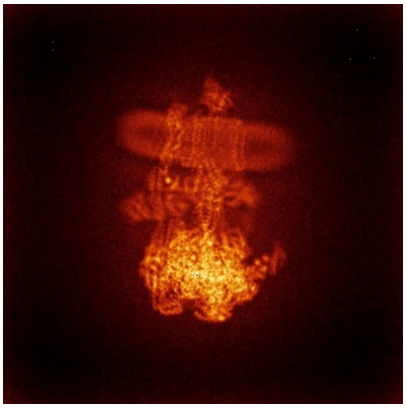
6.4.1 Primary map

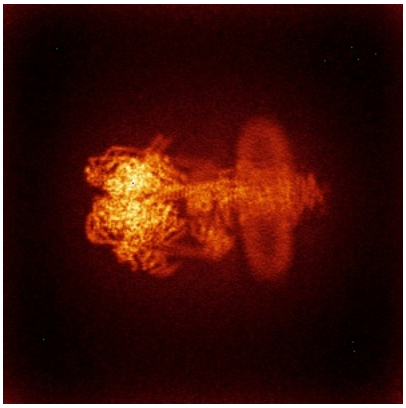

X

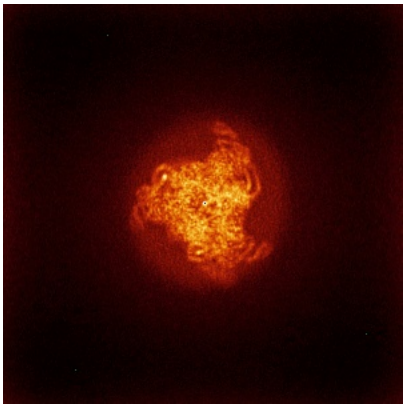

Y


Z

6.4.2 Raw map


X

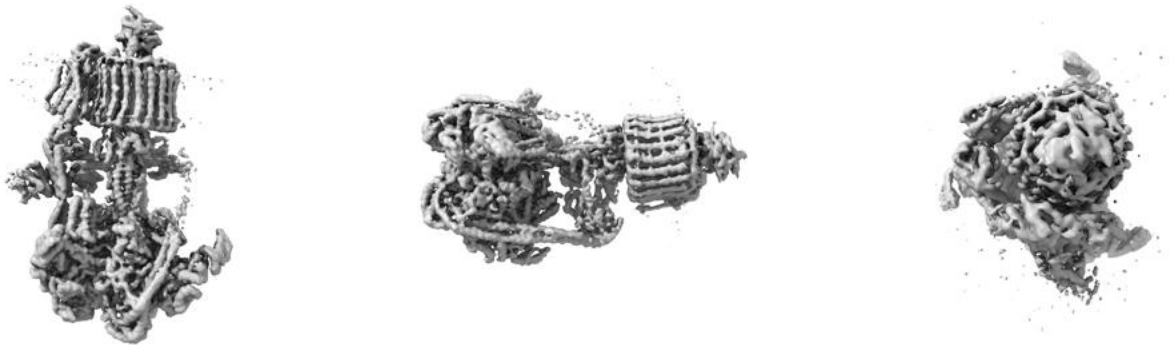

Y


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)

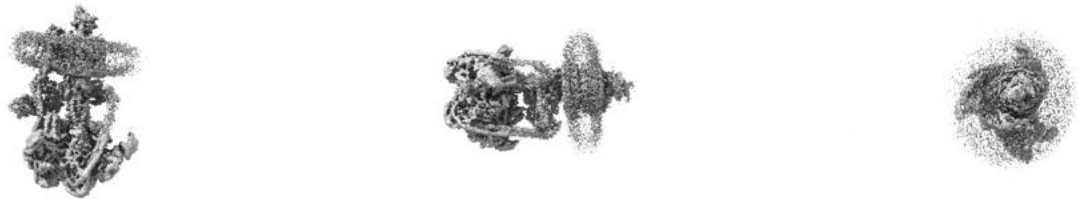
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. 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



X Y Z

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.

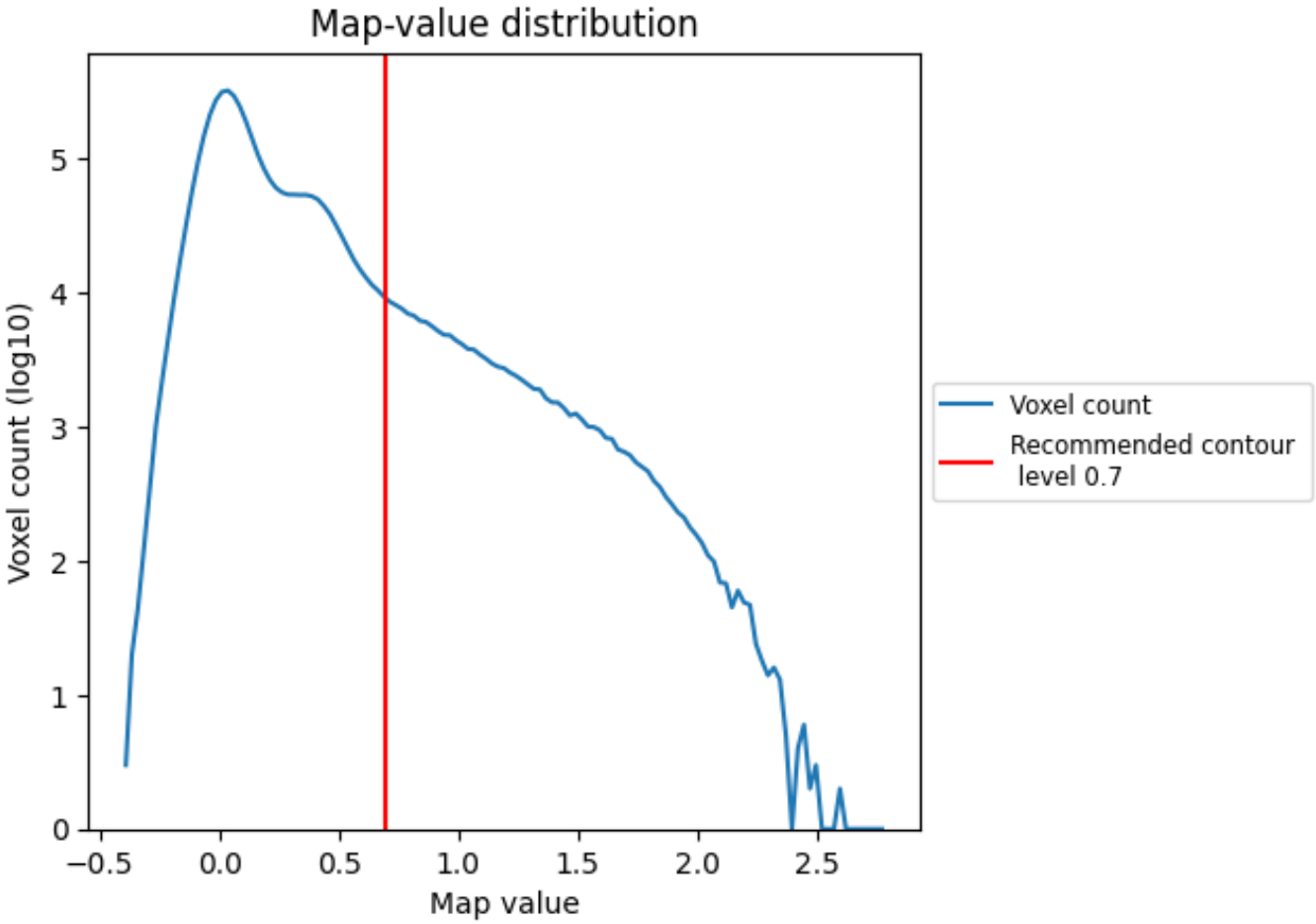
6.6 Mask visualisation (i)

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

7 Map analysis

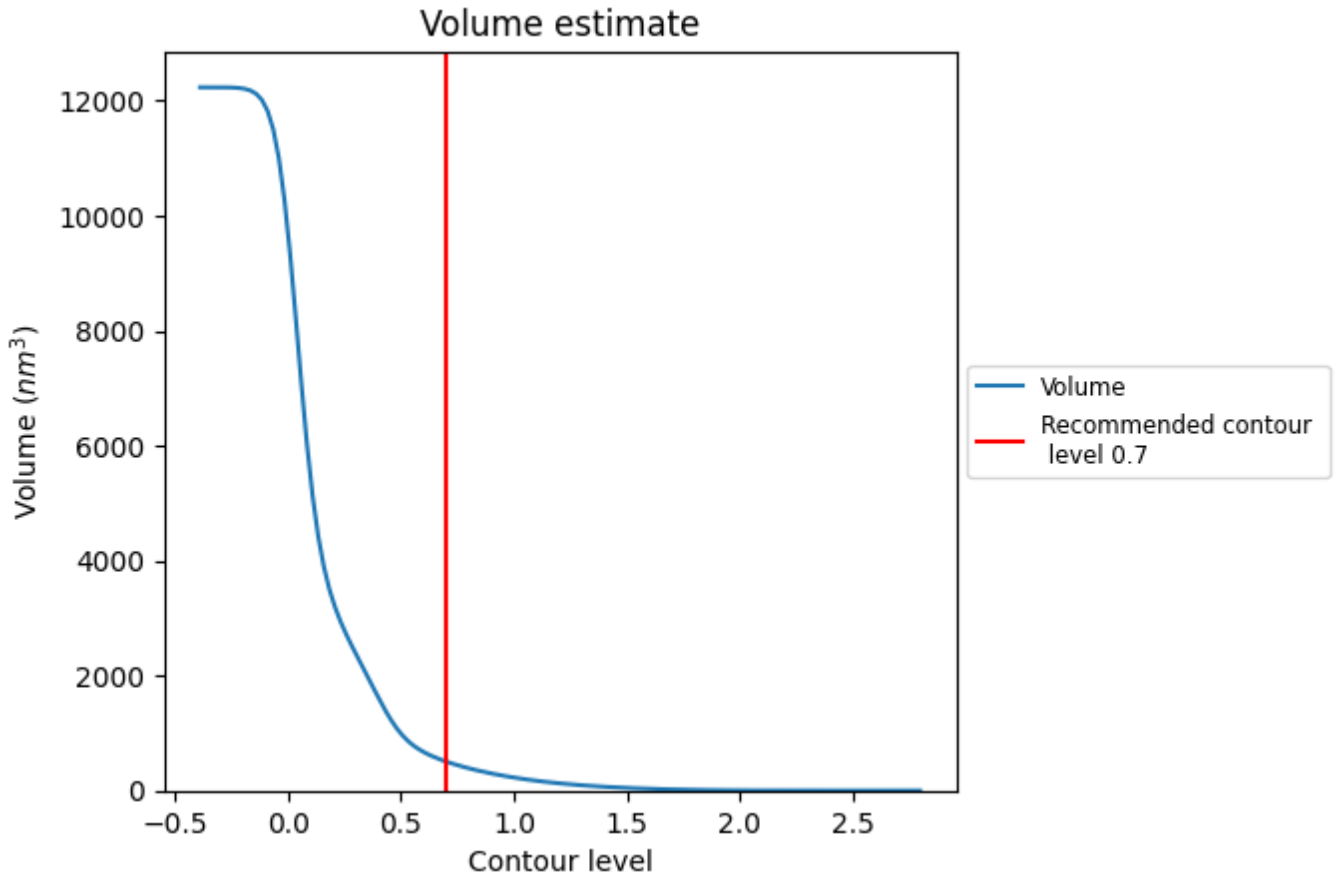
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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



The volume at the recommended contour level is 504 nm^3; this corresponds to an approximate mass of 456 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.

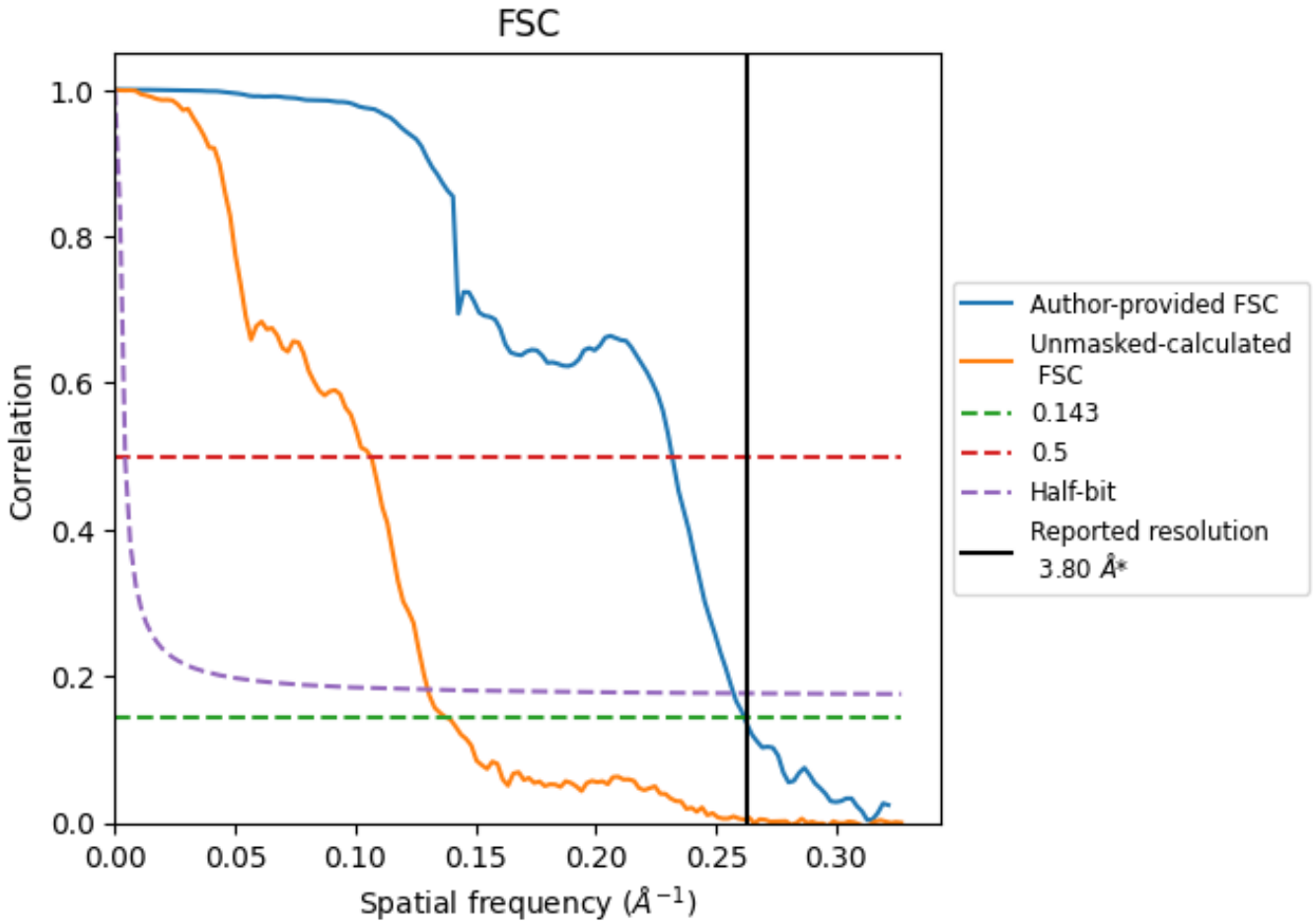
7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8.2 Resolution estimates (i)

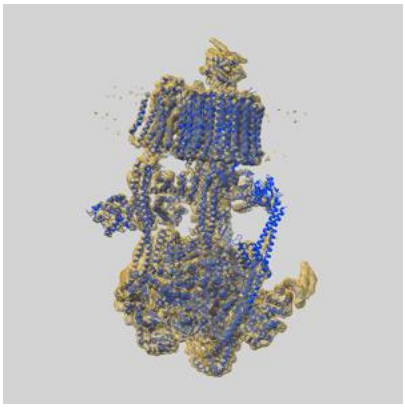
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.82	4.31	3.89
Unmasked-calculated*	7.24	9.41	7.67

*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 7.24 differs from the reported value 3.8 by more than 10 %

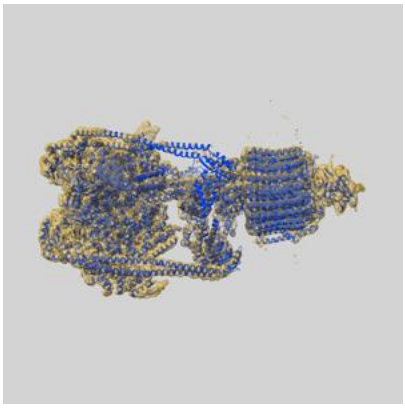
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26388 and PDB model 7U8R. Per-residue inclusion information can be found in section 3 on page 9.

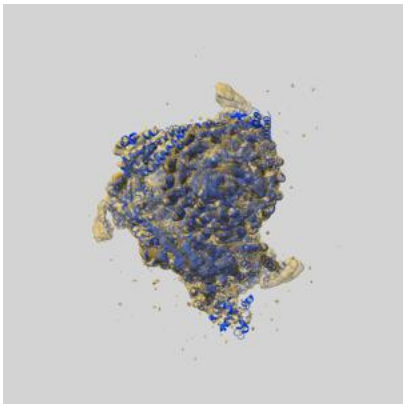
9.1 Map-model overlay



X



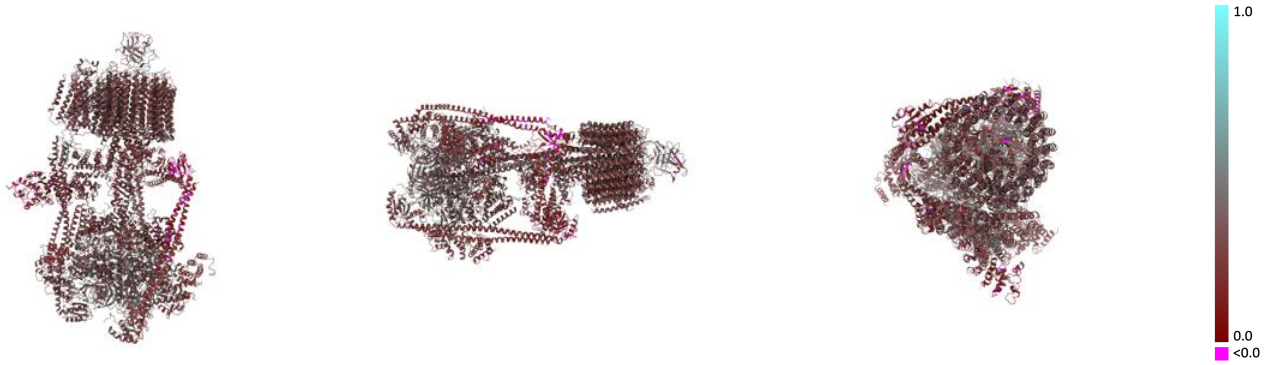
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7 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.

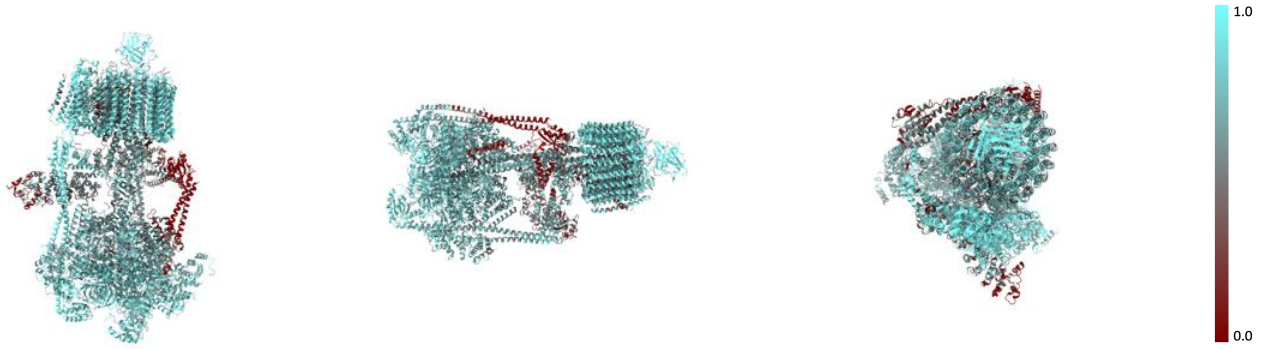
9.2 Q-score mapped to coordinate model



X Y Z

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.

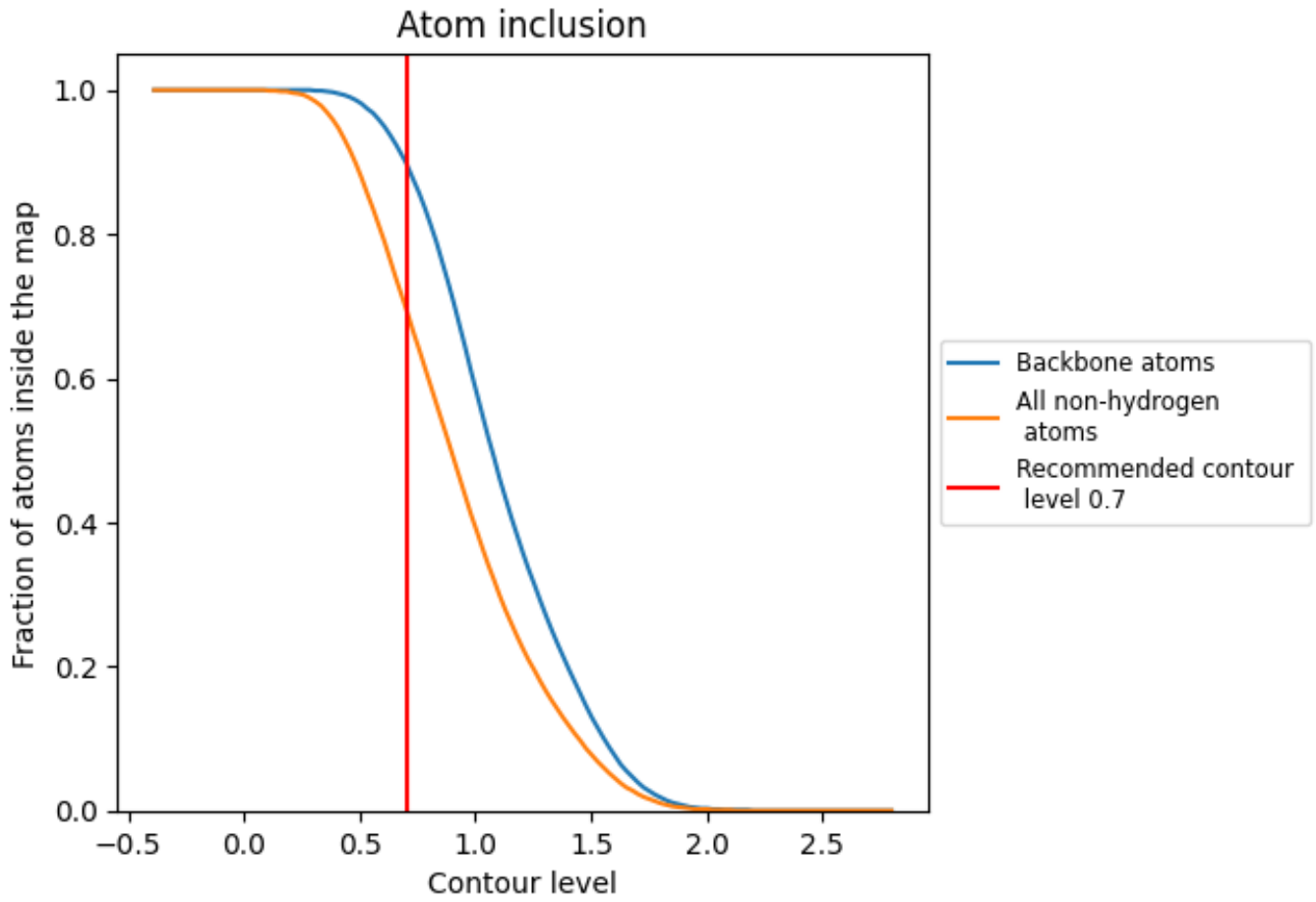
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.7).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 70% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6970	0.3010
A	0.7720	0.3550
B	0.7030	0.3240
C	0.7570	0.3440
D	0.7740	0.3630
E	0.7880	0.3670
F	0.7810	0.3570
G	0.2490	0.1410
H	0.6690	0.3070
I	0.8500	0.3250
J	0.7430	0.2780
K	0.6150	0.2530
L	0.5840	0.2890
M	0.8310	0.2890
N	0.6950	0.2400
O	0.4580	0.2210
Q	0.6780	0.2700
R	0.7320	0.2620
S	0.7210	0.2660
T	0.4410	0.1660
a	0.8340	0.3220
b	0.7510	0.3320
c	0.8460	0.3620
d	0.5250	0.2740
e	0.8200	0.3300
f	0.7720	0.2870
g	0.7010	0.3140
h	0.6840	0.2910
i	0.7310	0.2910
j	0.7750	0.2980
k	0.7910	0.3020
l	0.8200	0.3040
m	0.7970	0.3020
n	0.7590	0.2990
o	0.7350	0.3190
p	0.6820	0.3460