



Full wwPDB EM Validation Report ⓘ

Nov 27, 2022 – 01:45 PM EST

PDB ID : 6VQ8
EMDB ID : EMD-21319
Title : Mammalian V-ATPase from rat brain - composite model of rotational state 3 bound to ADP and SidK (built from focused refinement models)
Authors : Abbas, Y.M.; Rubinstein, J.L.
Deposited on : 2020-02-04
Resolution : 3.90 Å(reported)

This is a Full wwPDB EM Validation 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:

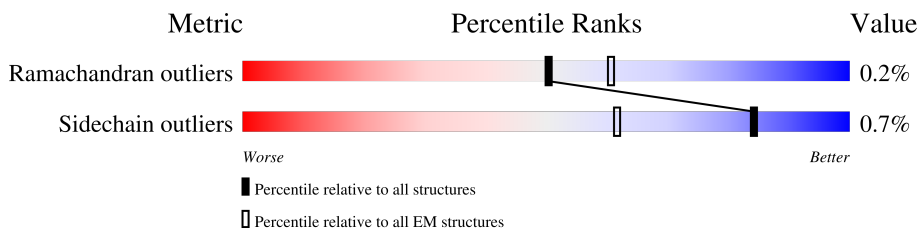
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 3.90 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)
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	A	617	97%
1	B	617	97%
1	C	617	97%
2	D	511	89%
2	E	511	89%
2	F	511	90%
3	G	382	19%
4	H	247	85%
5	I	226	10%

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Mol	Chain	Length	Quality of chain
5	J	226	99%
5	K	226	100%
6	L	119	91%
7	M	118	97%
7	N	118	97%
7	O	118	96%
8	Q	301	77%
8	R	301	74%
8	S	301	70%
9	a	838	89%
10	b	205	99%
11	c	463	91%
12	d	351	99%
13	e	81	96%
14	f	98	86%
15	g	155	96%
15	h	155	95%
15	i	155	94%
15	j	155	95%
15	k	155	95%
15	l	155	95%
15	m	155	94%
15	n	155	95%
15	o	155	94%
16	p	350	85%

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 60714 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 ATPase H⁺-transporting V1 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	600	4651	2949	786	889	27	0	0
1	B	600	4651	2949	786	889	27	0	0
1	C	600	4651	2949	786	889	27	0	0

- Molecule 2 is a protein called V-type proton ATPase subunit B, brain isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	459	3595	2282	613	680	20	0	0
2	E	459	3595	2282	613	680	20	0	0
2	F	459	3595	2282	613	680	20	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	G	360	1790	1070	360	360	0	0

- Molecule 4 is a protein called ATPase H⁺-transporting V1 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	214	1726	1095	311	315	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	225	Total	C	N	O	S	0	0
			1607	1005	296	299	7		
5	J	224	Total	C	N	O	S	0	0
			1602	1002	295	298	7		
5	K	225	Total	C	N	O	S	0	0
			1607	1005	296	299	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	110	Total	C	N	O	S	0	0
			866	548	154	163	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	114	Total	C	N	O	S	0	0
			714	426	147	138	3		
7	N	114	Total	C	N	O	S	0	0
			714	426	147	138	3		
7	O	113	Total	C	N	O	S	0	0
			709	423	146	137	3		

- Molecule 8 is a protein called Effector protein SidK.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	232	Total	C	N	O	S	0	0
			1878	1197	316	354	11		
8	R	224	Total	C	N	O	S	0	0
			1824	1162	306	346	10		
8	S	212	Total	C	N	O	S	0	0
			1722	1096	292	325	9		

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	0	GLY	-	expression tag	UNP Q5ZWW6
Q	279	ASP	-	expression tag	UNP Q5ZWW6
Q	280	TYR	-	expression tag	UNP Q5ZWW6
Q	281	LYS	-	expression tag	UNP Q5ZWW6
Q	282	ASP	-	expression tag	UNP Q5ZWW6
Q	283	HIS	-	expression tag	UNP Q5ZWW6
Q	284	ASP	-	expression tag	UNP Q5ZWW6

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	285	GLY	-	expression tag	UNP Q5ZWW6
Q	286	ASP	-	expression tag	UNP Q5ZWW6
Q	287	TYR	-	expression tag	UNP Q5ZWW6
Q	288	LYS	-	expression tag	UNP Q5ZWW6
Q	289	ASP	-	expression tag	UNP Q5ZWW6
Q	290	HIS	-	expression tag	UNP Q5ZWW6
Q	291	ASP	-	expression tag	UNP Q5ZWW6
Q	292	ILE	-	expression tag	UNP Q5ZWW6
Q	293	ASP	-	expression tag	UNP Q5ZWW6
Q	294	TYR	-	expression tag	UNP Q5ZWW6
Q	295	LYS	-	expression tag	UNP Q5ZWW6
Q	296	ASP	-	expression tag	UNP Q5ZWW6
Q	297	ASP	-	expression tag	UNP Q5ZWW6
Q	298	ASP	-	expression tag	UNP Q5ZWW6
Q	299	ASP	-	expression tag	UNP Q5ZWW6
Q	300	LYS	-	expression tag	UNP Q5ZWW6
R	0	GLY	-	expression tag	UNP Q5ZWW6
R	279	ASP	-	expression tag	UNP Q5ZWW6
R	280	TYR	-	expression tag	UNP Q5ZWW6
R	281	LYS	-	expression tag	UNP Q5ZWW6
R	282	ASP	-	expression tag	UNP Q5ZWW6
R	283	HIS	-	expression tag	UNP Q5ZWW6
R	284	ASP	-	expression tag	UNP Q5ZWW6
R	285	GLY	-	expression tag	UNP Q5ZWW6
R	286	ASP	-	expression tag	UNP Q5ZWW6
R	287	TYR	-	expression tag	UNP Q5ZWW6
R	288	LYS	-	expression tag	UNP Q5ZWW6
R	289	ASP	-	expression tag	UNP Q5ZWW6
R	290	HIS	-	expression tag	UNP Q5ZWW6
R	291	ASP	-	expression tag	UNP Q5ZWW6
R	292	ILE	-	expression tag	UNP Q5ZWW6
R	293	ASP	-	expression tag	UNP Q5ZWW6
R	294	TYR	-	expression tag	UNP Q5ZWW6
R	295	LYS	-	expression tag	UNP Q5ZWW6
R	296	ASP	-	expression tag	UNP Q5ZWW6
R	297	ASP	-	expression tag	UNP Q5ZWW6
R	298	ASP	-	expression tag	UNP Q5ZWW6
R	299	ASP	-	expression tag	UNP Q5ZWW6
R	300	LYS	-	expression tag	UNP Q5ZWW6
S	0	GLY	-	expression tag	UNP Q5ZWW6
S	279	ASP	-	expression tag	UNP Q5ZWW6
S	280	TYR	-	expression tag	UNP Q5ZWW6

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Chain	Residue	Modelled	Actual	Comment	Reference
S	281	LYS	-	expression tag	UNP Q5ZWW6
S	282	ASP	-	expression tag	UNP Q5ZWW6
S	283	HIS	-	expression tag	UNP Q5ZWW6
S	284	ASP	-	expression tag	UNP Q5ZWW6
S	285	GLY	-	expression tag	UNP Q5ZWW6
S	286	ASP	-	expression tag	UNP Q5ZWW6
S	287	TYR	-	expression tag	UNP Q5ZWW6
S	288	LYS	-	expression tag	UNP Q5ZWW6
S	289	ASP	-	expression tag	UNP Q5ZWW6
S	290	HIS	-	expression tag	UNP Q5ZWW6
S	291	ASP	-	expression tag	UNP Q5ZWW6
S	292	ILE	-	expression tag	UNP Q5ZWW6
S	293	ASP	-	expression tag	UNP Q5ZWW6
S	294	TYR	-	expression tag	UNP Q5ZWW6
S	295	LYS	-	expression tag	UNP Q5ZWW6
S	296	ASP	-	expression tag	UNP Q5ZWW6
S	297	ASP	-	expression tag	UNP Q5ZWW6
S	298	ASP	-	expression tag	UNP Q5ZWW6
S	299	ASP	-	expression tag	UNP Q5ZWW6
S	300	LYS	-	expression tag	UNP Q5ZWW6

- Molecule 9 is a protein called V-type proton ATPase 116 kDa subunit a isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	a	749	3703	2205	749	749	0	0

- Molecule 10 is a protein called ATPase, H⁺ transporting, V0 subunit B (Predicted), isoform CRA_a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	b	203	1503	996	237	259	11	0	0

- Molecule 11 is a protein called V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	c	41	337	228	51	54	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	d	350	2833	1829	460	530	14	0	0

- Molecule 13 is a protein called V-type proton ATPase subunit e 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	e	78	384	228	78	78	0	0

- Molecule 14 is a protein called Ribonuclease K.

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

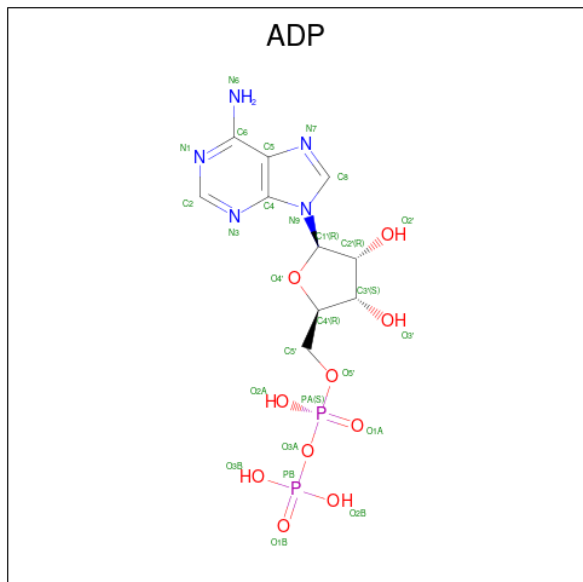
- Molecule 15 is a protein called V-type proton ATPase 16 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	g	150	1068	699	171	190	8	0	0
15	h	150	1068	699	171	190	8	0	0
15	i	150	1068	699	171	190	8	0	0
15	j	150	1068	699	171	190	8	0	0
15	k	150	1068	699	171	190	8	0	0
15	l	150	1068	699	171	190	8	0	0
15	m	150	1068	699	171	190	8	0	0
15	n	150	1068	699	171	190	8	0	0
15	o	150	1068	699	171	190	8	0	0

- Molecule 16 is a protein called Renin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	p	52	406	269	61	73	3	0	0

- Molecule 17 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



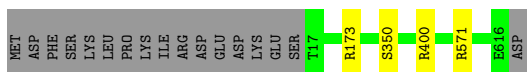
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
17	A	1	27	10	5	10	2	0

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.

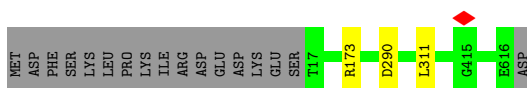
- Molecule 1: ATPase H⁺-transporting V1 subunit A

Chain A:  97%



- Molecule 1: ATPase H⁺-transporting V1 subunit A

Chain B:  97%



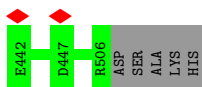
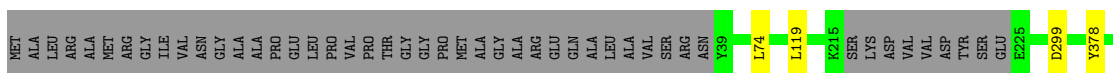
- Molecule 1: ATPase H⁺-transporting V1 subunit A

Chain C:  97%




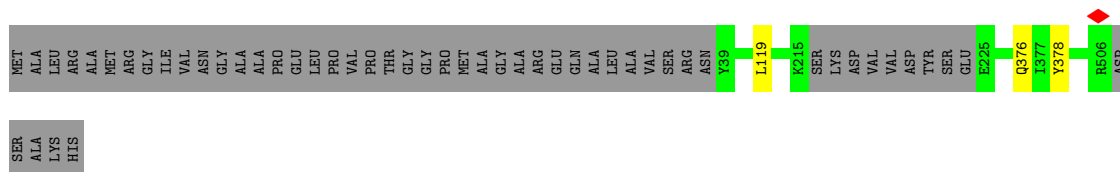
- Molecule 2: V-type proton ATPase subunit B, brain isoform

Chain D:  89% 10%

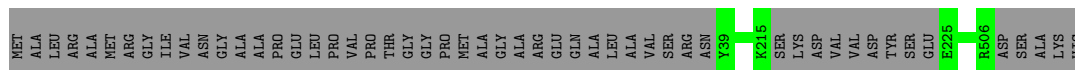
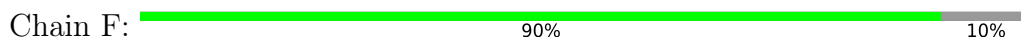


- Molecule 2: V-type proton ATPase subunit B, brain isoform

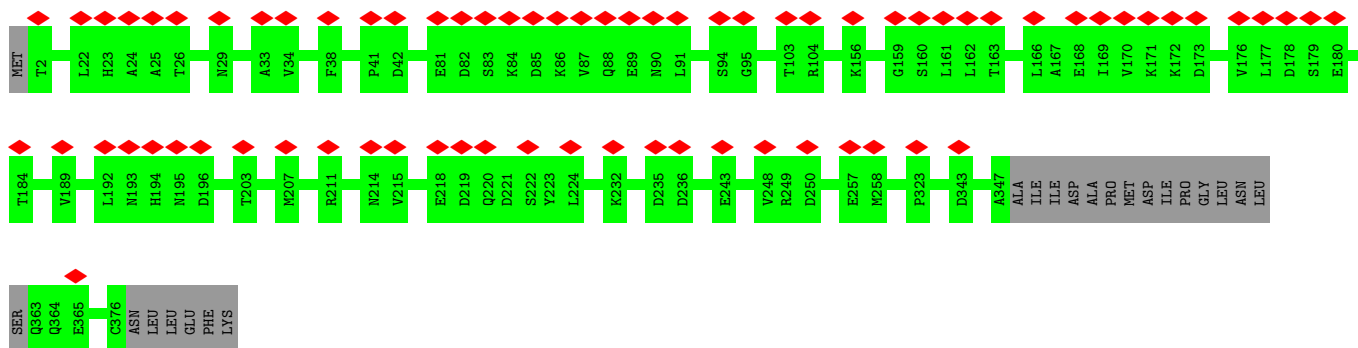
Chain E:  89% 10%



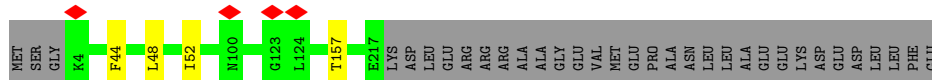
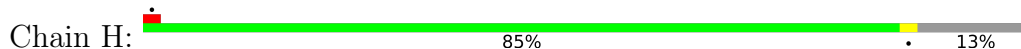
• Molecule 2: V-type proton ATPase subunit B, brain isoform



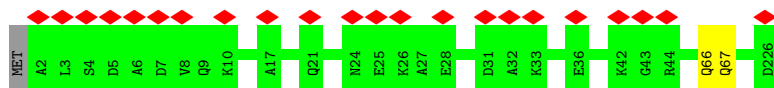
• Molecule 3: V-type proton ATPase subunit C 1



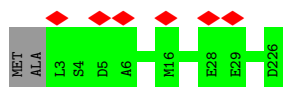
• Molecule 4: ATPase H⁺-transporting V1 subunit D



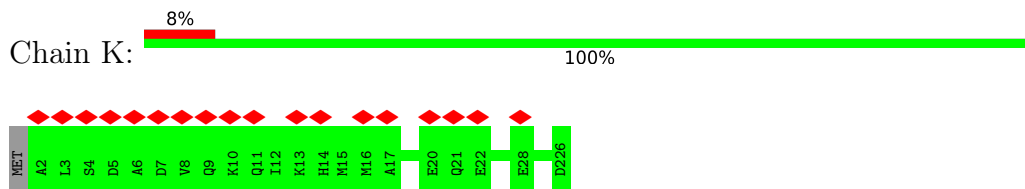
• Molecule 5: V-type proton ATPase subunit E 1



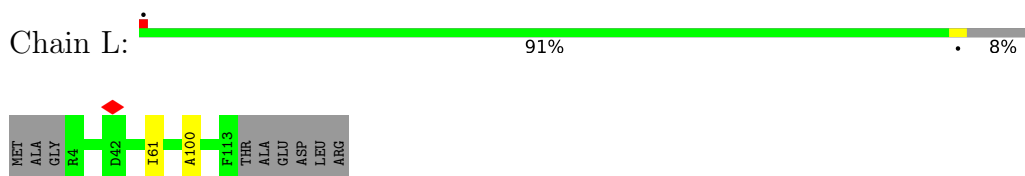
• Molecule 5: V-type proton ATPase subunit E 1



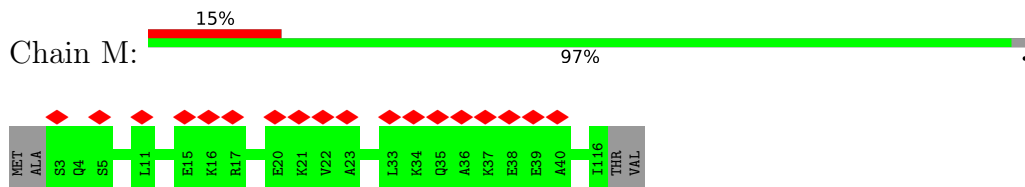
• Molecule 5: V-type proton ATPase subunit E 1



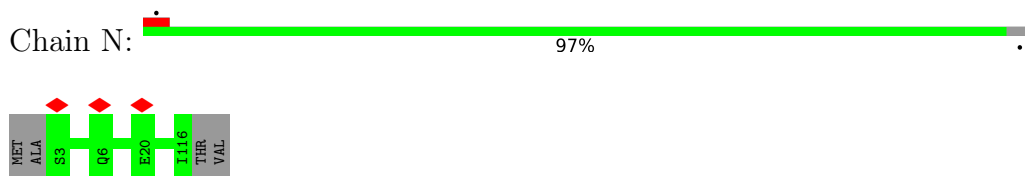
• Molecule 6: V-type proton ATPase subunit F



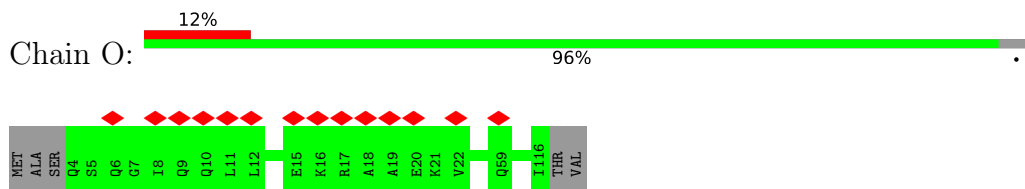
• Molecule 7: V-type proton ATPase subunit G



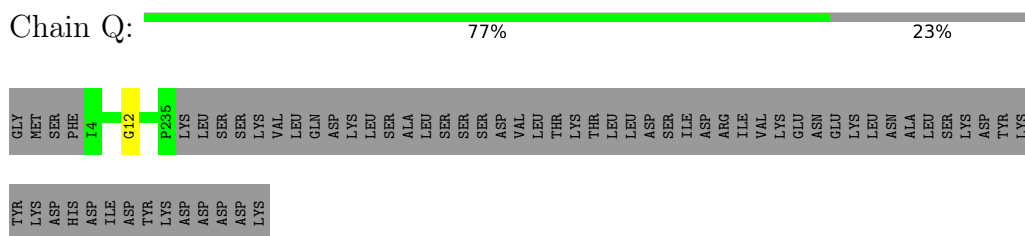
• Molecule 7: V-type proton ATPase subunit G



• Molecule 7: V-type proton ATPase subunit G

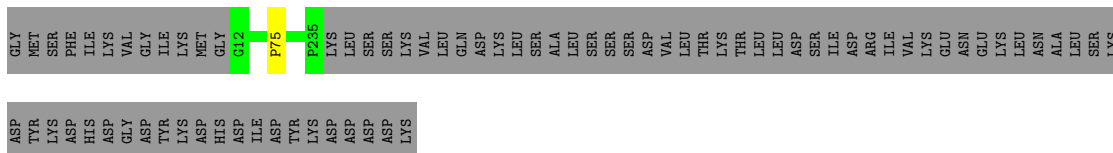


• Molecule 8: Effector protein SidK

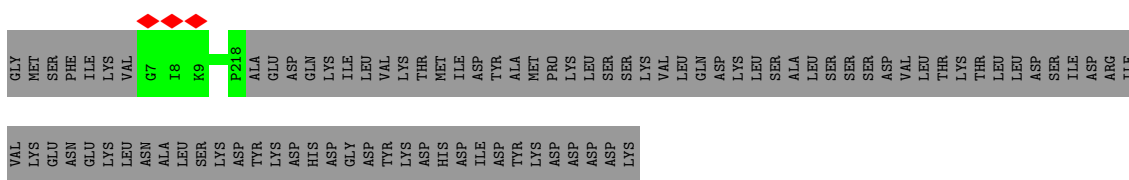


• Molecule 8: Effector protein SidK

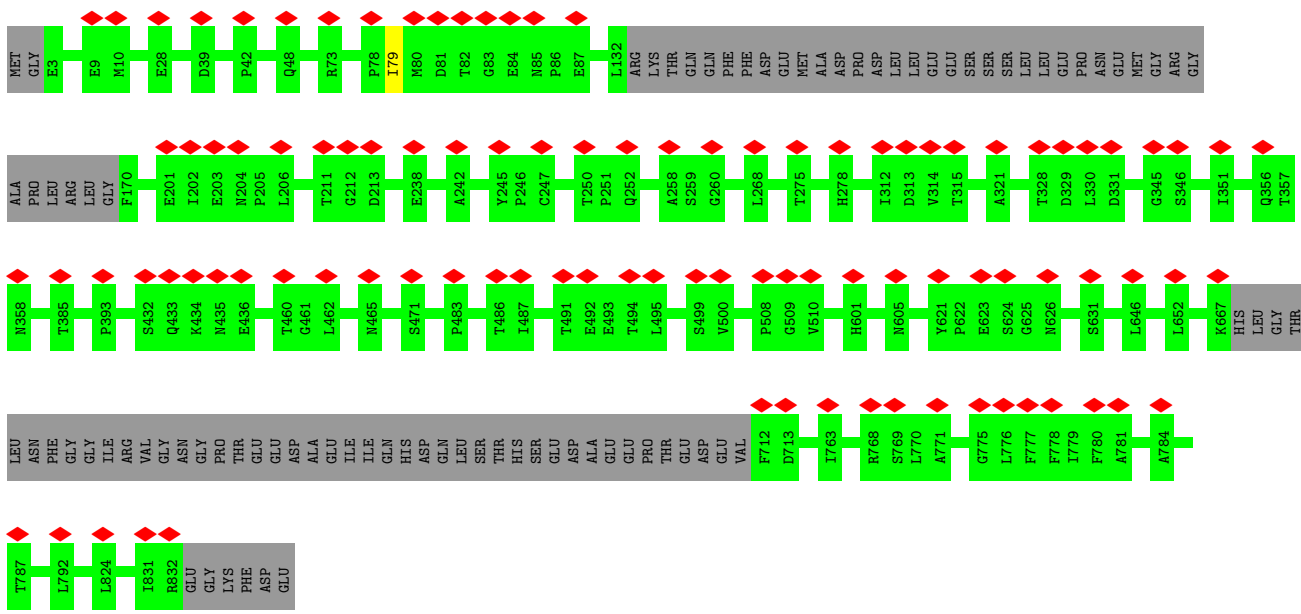
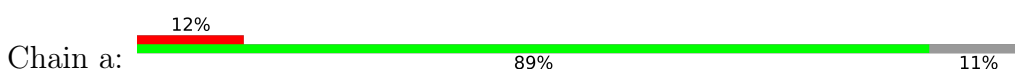




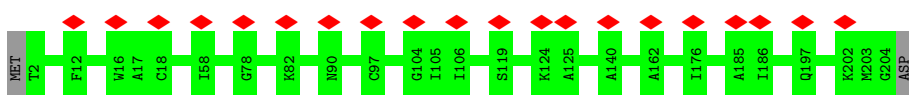
• Molecule 8: Effector protein SidK



• Molecule 9: V-type proton ATPase 116 kDa subunit a isoform 1

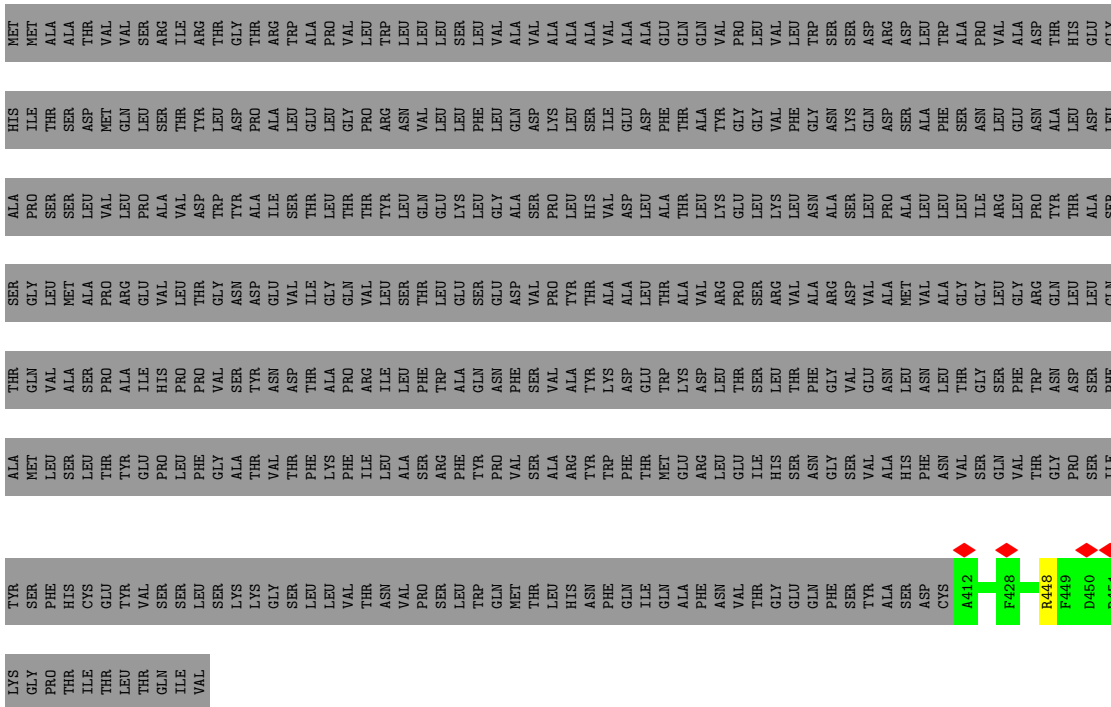


• Molecule 10: ATPase, H+ transporting, V0 subunit B (Predicted), isoform CRA_a

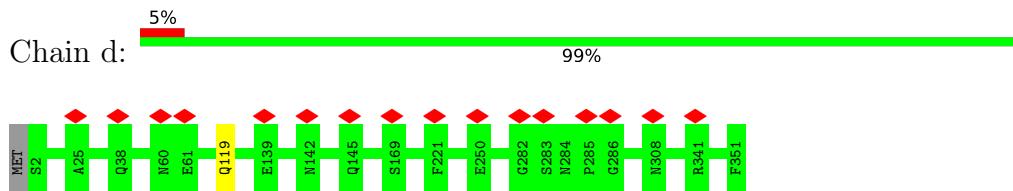


• Molecule 11: V-type proton ATPase subunit S1

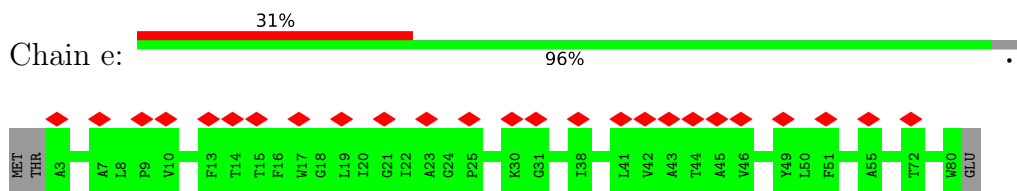




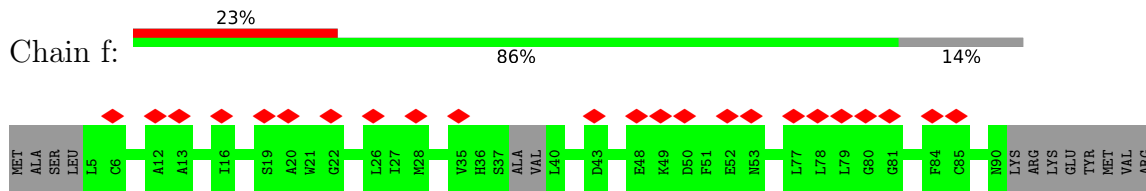
● Molecule 12: V-type proton ATPase subunit



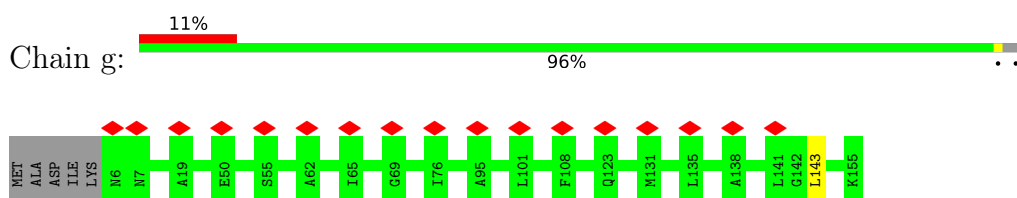
● Molecule 13: V-type proton ATPase subunit e 2



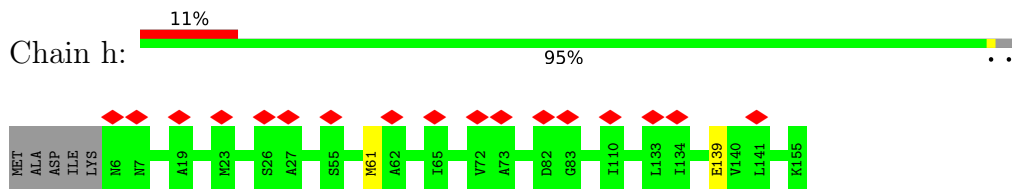
● Molecule 14: Ribonuclease K



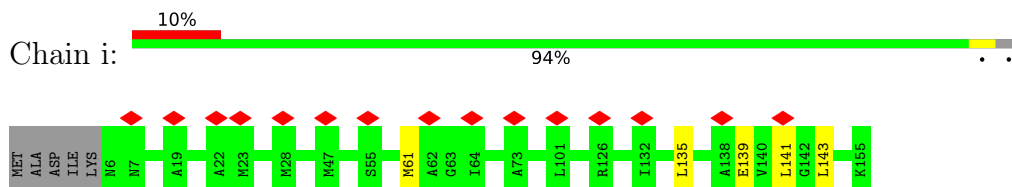
● Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit



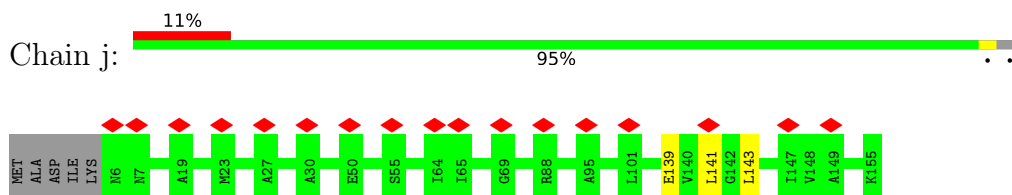
- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit



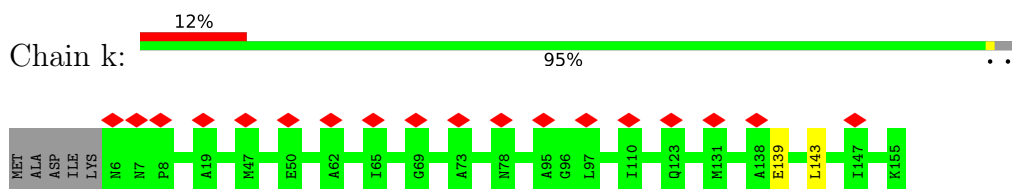
- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit



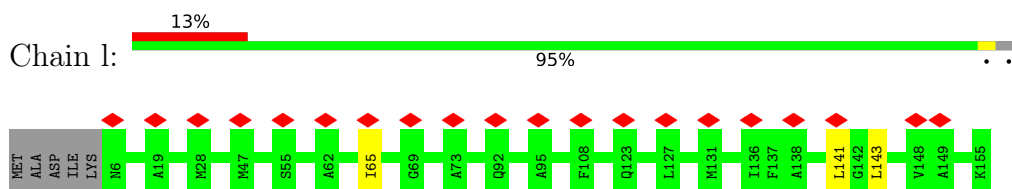
- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit



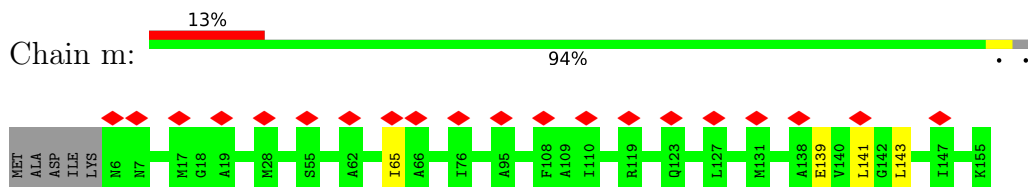
- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit



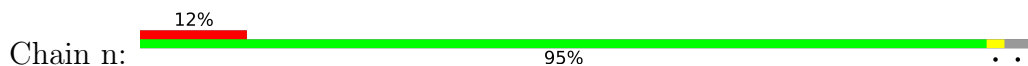
- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

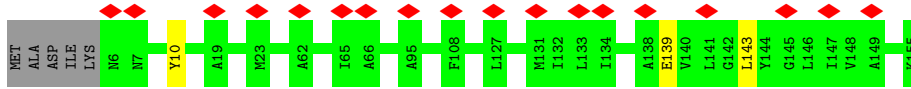


- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

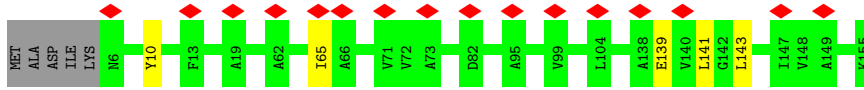
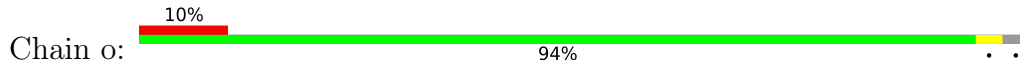


- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit





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



- Molecule 16: Renin receptor



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	79654	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.467	Depositor
Minimum map value	-0.788	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	360.4, 360.4, 360.4	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	0.72	0/4746	0.53	0/6425
1	B	0.73	1/4746 (0.0%)	0.55	0/6425
1	C	0.72	0/4746	0.53	0/6425
2	D	0.70	0/3666	0.52	0/4967
2	E	0.68	0/3666	0.52	0/4967
2	F	0.70	0/3666	0.52	0/4967
3	G	0.34	0/1788	0.59	0/2494
4	H	0.79	0/1744	0.55	0/2332
5	I	0.57	0/1619	0.51	0/2192
5	J	0.59	0/1614	0.52	0/2185
5	K	0.57	0/1619	0.49	0/2192
6	L	0.81	0/880	0.75	0/1189
7	M	0.52	0/717	0.51	0/980
7	N	0.55	0/717	0.54	0/980
7	O	0.53	0/712	0.53	0/973
8	Q	0.70	0/1912	0.51	0/2575
8	R	0.70	0/1858	0.50	0/2505
8	S	0.70	0/1754	0.49	0/2362
9	a	0.35	0/3700	0.57	0/5150
10	b	0.52	0/1537	0.51	0/2088
11	c	0.53	0/347	0.56	0/466
12	d	0.73	0/2899	0.54	0/3927
13	e	0.28	0/383	0.45	0/531
14	f	0.35	0/410	0.48	0/566
15	g	0.50	0/1083	0.54	0/1466
15	h	0.49	0/1083	0.52	0/1466
15	i	0.49	0/1083	0.51	0/1466
15	j	0.48	0/1083	0.50	0/1466
15	k	0.49	0/1083	0.52	0/1466
15	l	0.48	0/1083	0.51	0/1466
15	m	0.51	0/1083	0.57	0/1466
15	n	0.47	0/1083	0.50	0/1466

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	o	0.49	0/1083	0.51	0/1466
16	p	0.50	0/416	0.57	0/571
All	All	0.63	1/61609 (0.0%)	0.53	0/83628

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	290	ASP	C-N	-5.20	1.22	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	573 (96%)	24 (4%)	1 (0%)	47	79
1	B	598/617 (97%)	580 (97%)	18 (3%)	0	100	100
1	C	598/617 (97%)	575 (96%)	22 (4%)	1 (0%)	47	79
2	D	455/511 (89%)	443 (97%)	9 (2%)	3 (1%)	22	60
2	E	455/511 (89%)	442 (97%)	11 (2%)	2 (0%)	34	71
2	F	455/511 (89%)	442 (97%)	13 (3%)	0	100	100
3	G	356/382 (93%)	353 (99%)	3 (1%)	0	100	100
4	H	212/247 (86%)	205 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	I	223/226 (99%)	223 (100%)	0	0	100	100
5	J	222/226 (98%)	222 (100%)	0	0	100	100
5	K	223/226 (99%)	222 (100%)	1 (0%)	0	100	100
6	L	108/119 (91%)	101 (94%)	5 (5%)	2 (2%)	8	41
7	M	112/118 (95%)	111 (99%)	1 (1%)	0	100	100
7	N	112/118 (95%)	111 (99%)	1 (1%)	0	100	100
7	O	111/118 (94%)	109 (98%)	2 (2%)	0	100	100
8	Q	230/301 (76%)	223 (97%)	6 (3%)	1 (0%)	34	71
8	R	222/301 (74%)	214 (96%)	7 (3%)	1 (0%)	29	67
8	S	210/301 (70%)	204 (97%)	6 (3%)	0	100	100
9	a	743/838 (89%)	720 (97%)	22 (3%)	1 (0%)	51	84
10	b	201/205 (98%)	198 (98%)	3 (2%)	0	100	100
11	c	39/463 (8%)	39 (100%)	0	0	100	100
12	d	348/351 (99%)	329 (94%)	18 (5%)	1 (0%)	41	75
13	e	76/81 (94%)	75 (99%)	1 (1%)	0	100	100
14	f	80/98 (82%)	77 (96%)	3 (4%)	0	100	100
15	g	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
15	h	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
15	i	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
15	j	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
15	k	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
15	l	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
15	m	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
15	n	148/155 (96%)	145 (98%)	2 (1%)	1 (1%)	22	60
15	o	148/155 (96%)	143 (97%)	4 (3%)	1 (1%)	22	60
16	p	50/350 (14%)	46 (92%)	3 (6%)	1 (2%)	7	40
All	All	8369/9848 (85%)	8142 (97%)	211 (2%)	16 (0%)	50	79

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	a	79	ILE
16	p	300	ASN

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Mol	Chain	Res	Type
1	A	350	SER
2	D	299	ASP
2	E	119	LEU
15	n	10	TYR
15	o	10	TYR
2	D	119	LEU
6	L	100	ALA
8	Q	12	GLY
1	C	278	GLY
2	D	378	TYR
2	E	378	TYR
12	d	119	GLN
6	L	61	ILE
8	R	75	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	507/524 (97%)	504 (99%)	3 (1%)	86	91
1	B	507/524 (97%)	505 (100%)	2 (0%)	91	94
1	C	507/524 (97%)	505 (100%)	2 (0%)	91	94
2	D	393/431 (91%)	392 (100%)	1 (0%)	92	95
2	E	393/431 (91%)	392 (100%)	1 (0%)	92	95
2	F	393/431 (91%)	393 (100%)	0	100	100
4	H	185/212 (87%)	181 (98%)	4 (2%)	52	71
5	I	141/198 (71%)	139 (99%)	2 (1%)	67	81
5	J	141/198 (71%)	141 (100%)	0	100	100
5	K	141/198 (71%)	141 (100%)	0	100	100
6	L	92/100 (92%)	92 (100%)	0	100	100
7	M	43/100 (43%)	43 (100%)	0	100	100
7	N	43/100 (43%)	43 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	O	43/100 (43%)	43 (100%)	0	100	100
8	Q	208/274 (76%)	208 (100%)	0	100	100
8	R	203/274 (74%)	203 (100%)	0	100	100
8	S	191/274 (70%)	191 (100%)	0	100	100
10	b	156/158 (99%)	156 (100%)	0	100	100
11	c	36/395 (9%)	35 (97%)	1 (3%)	43	66
12	d	305/306 (100%)	305 (100%)	0	100	100
15	g	109/113 (96%)	108 (99%)	1 (1%)	78	87
15	h	109/113 (96%)	107 (98%)	2 (2%)	59	77
15	i	109/113 (96%)	104 (95%)	5 (5%)	27	55
15	j	109/113 (96%)	106 (97%)	3 (3%)	43	66
15	k	109/113 (96%)	107 (98%)	2 (2%)	59	77
15	l	109/113 (96%)	106 (97%)	3 (3%)	43	66
15	m	109/113 (96%)	105 (96%)	4 (4%)	34	60
15	n	109/113 (96%)	107 (98%)	2 (2%)	59	77
15	o	109/113 (96%)	105 (96%)	4 (4%)	34	60
16	p	41/313 (13%)	41 (100%)	0	100	100
All	All	5650/7082 (80%)	5608 (99%)	42 (1%)	84	90

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	ARG
1	A	400	ARG
1	A	571	ARG
1	B	173	ARG
1	B	311	LEU
1	C	173	ARG
1	C	296	MET
2	D	74	LEU
2	E	376	GLN
4	H	44	PHE
4	H	48	LEU
4	H	52	ILE
4	H	157	THR
5	I	66	GLN

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Mol	Chain	Res	Type
5	I	67	GLN
11	c	448	ARG
15	g	143	LEU
15	h	61	MET
15	h	139	GLU
15	i	61	MET
15	i	135	LEU
15	i	139	GLU
15	i	141	LEU
15	i	143	LEU
15	j	139	GLU
15	j	141	LEU
15	j	143	LEU
15	k	139	GLU
15	k	143	LEU
15	l	65	ILE
15	l	141	LEU
15	l	143	LEU
15	m	65	ILE
15	m	139	GLU
15	m	141	LEU
15	m	143	LEU
15	n	139	GLU
15	n	143	LEU
15	o	65	ILE
15	o	139	GLU
15	o	141	LEU
15	o	143	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	543	ASN
1	B	268	ASN
2	F	181	ASN
4	H	137	ASN
5	I	67	GLN
8	Q	184	HIS
8	R	184	HIS
12	d	297	HIS

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	$\# Z > 2$
17	ADP	A	701	-	24,29,29	0.67	0	29,45,45	0.69	1 (3%)

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
17	ADP	A	701	-	-	5/12/32/32	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	701	ADP	C5-C6-N6	2.21	123.71	120.35

There are no chirality outliers.

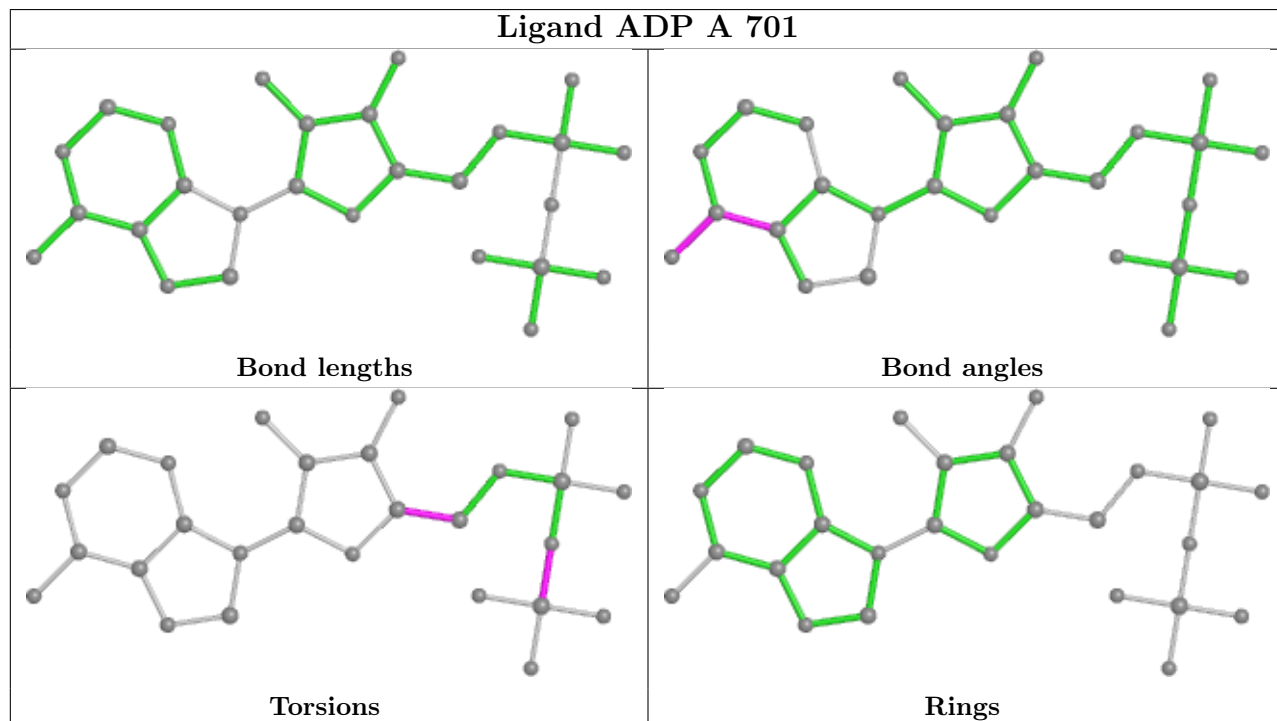
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	701	ADP	O4'-C4'-C5'-O5'
17	A	701	ADP	C3'-C4'-C5'-O5'
17	A	701	ADP	PA-O3A-PB-O1B
17	A	701	ADP	PA-O3A-PB-O2B
17	A	701	ADP	PA-O3A-PB-O3B

There are no ring outliers.

No monomer is involved in short contacts.

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.

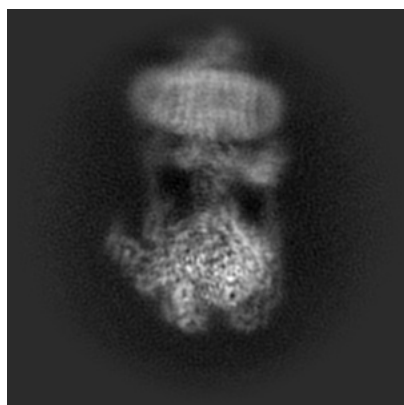
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21319. These allow visual inspection of the internal detail of the map and identification of artifacts.

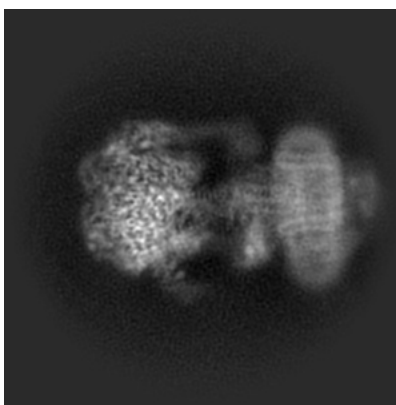
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

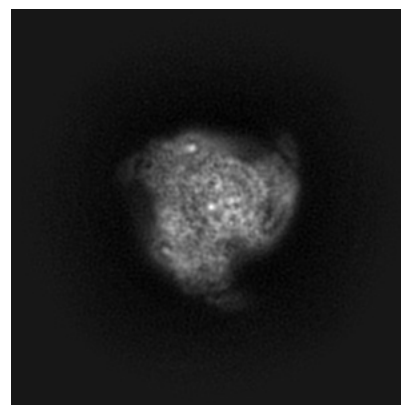
6.1.1 Primary map



X



Y

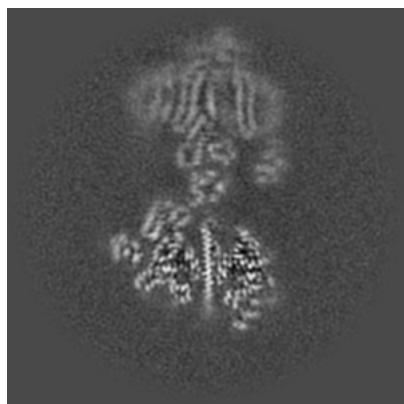


Z

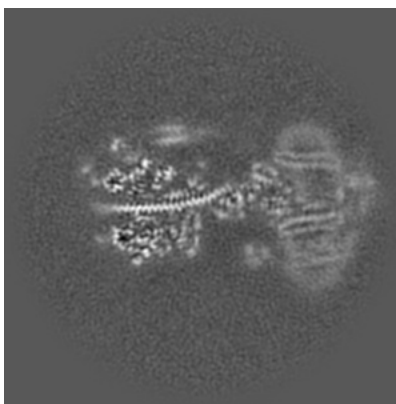
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

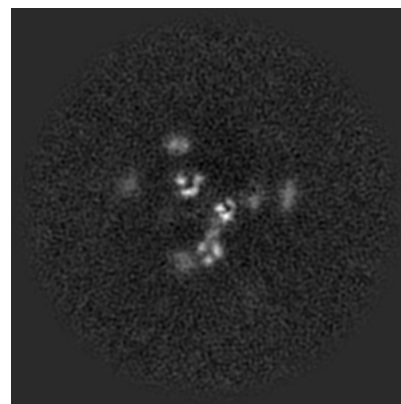
6.2.1 Primary map



X Index: 170



Y Index: 170

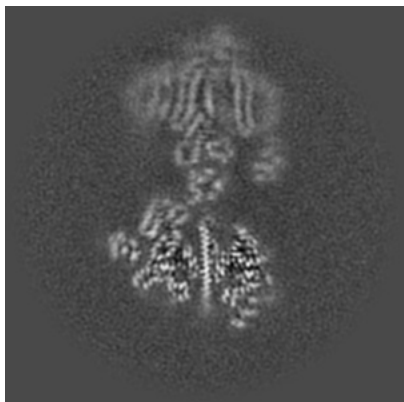


Z Index: 170

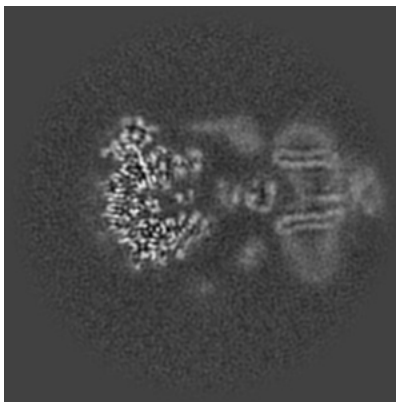
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

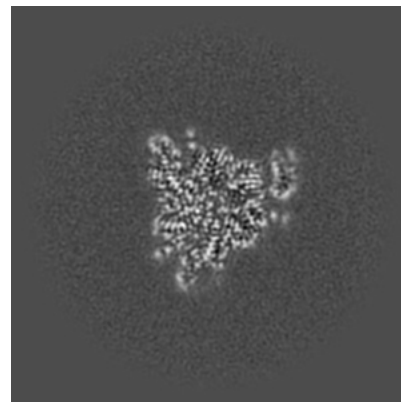
6.3.1 Primary map



X Index: 170



Y Index: 186



Z Index: 118

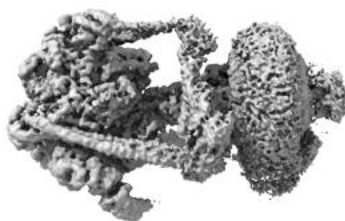
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

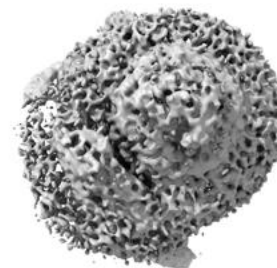
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

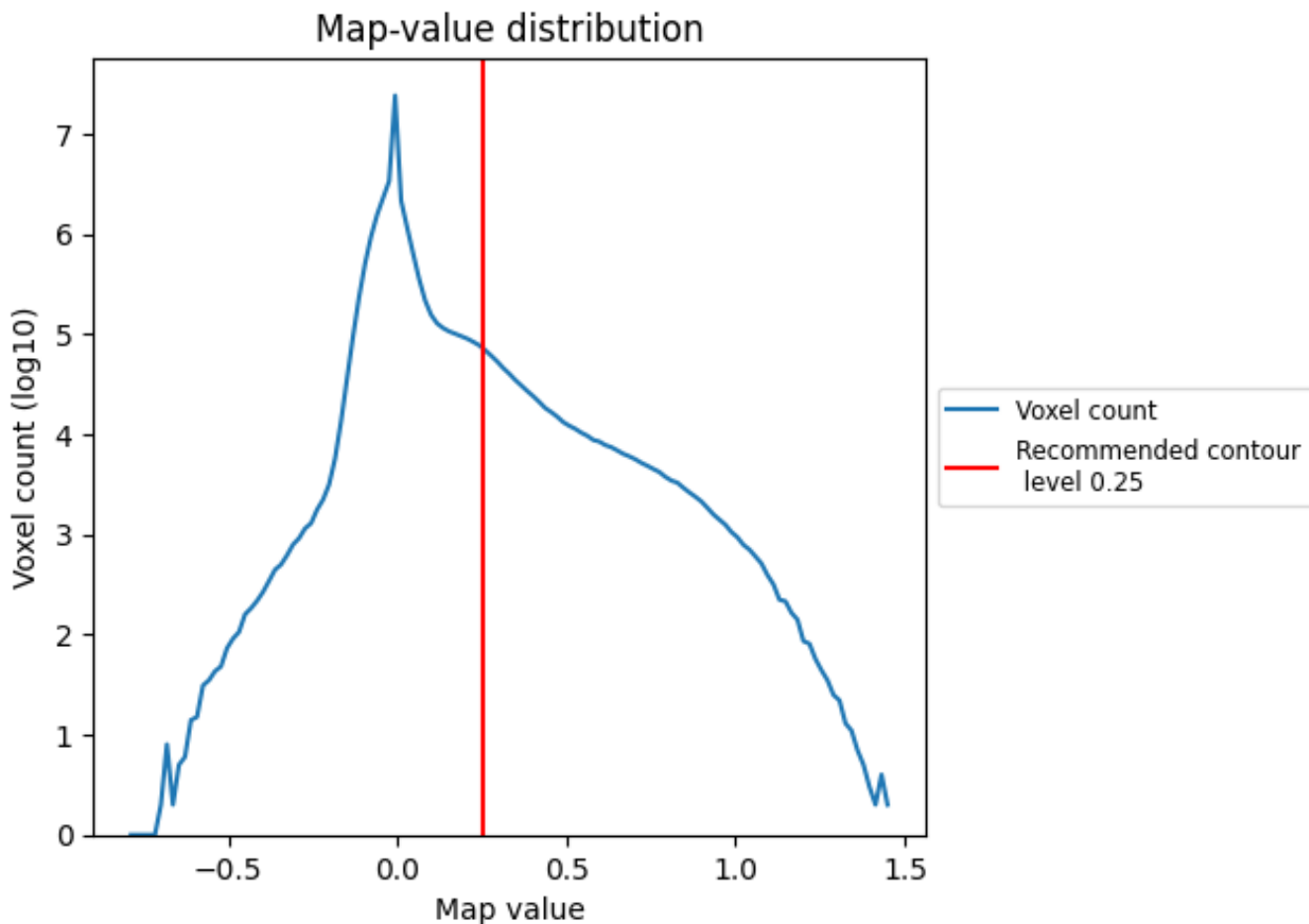
6.5 Mask visualisation

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

7 Map analysis [i](#)

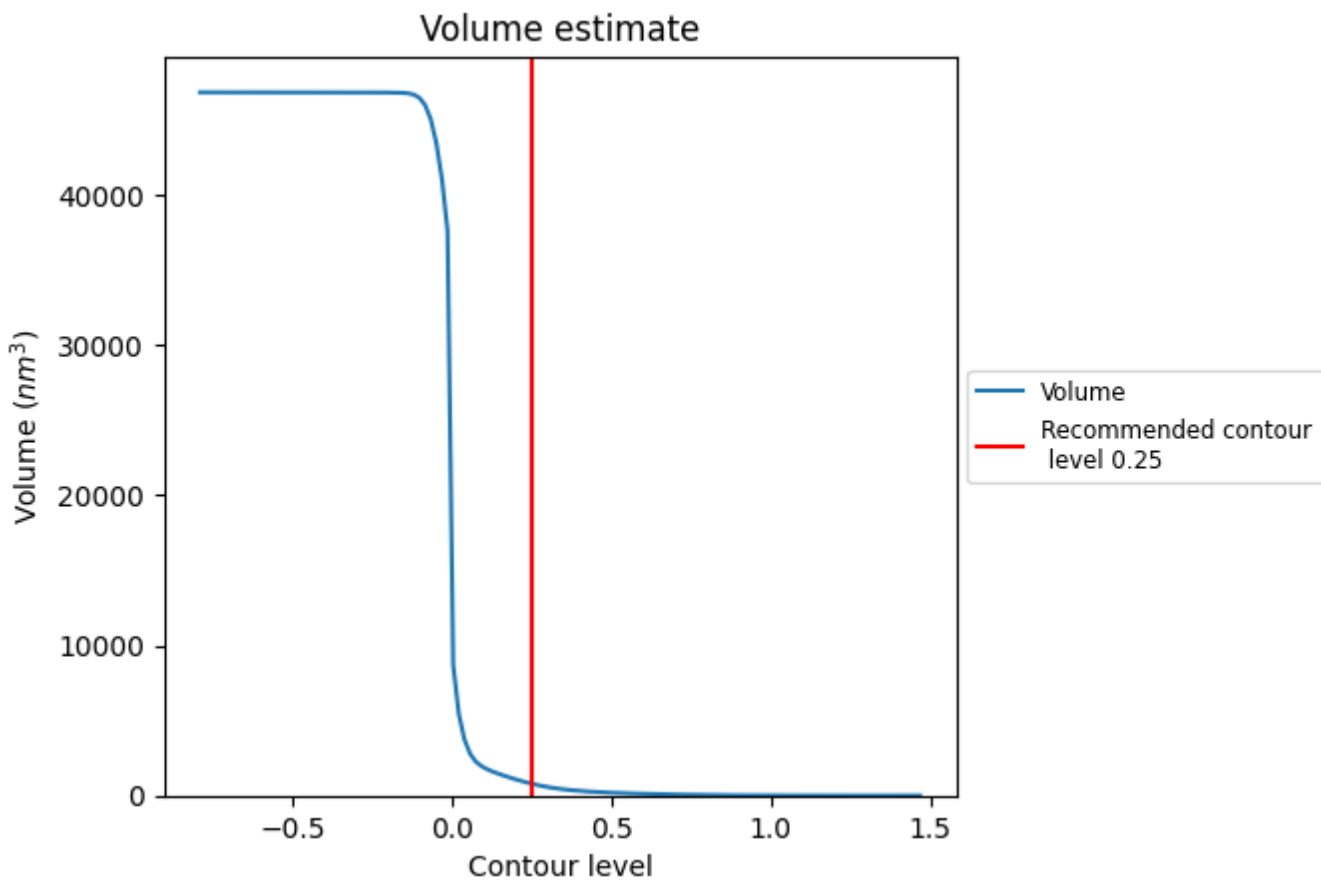
This section contains the results of statistical analysis of the map.

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.

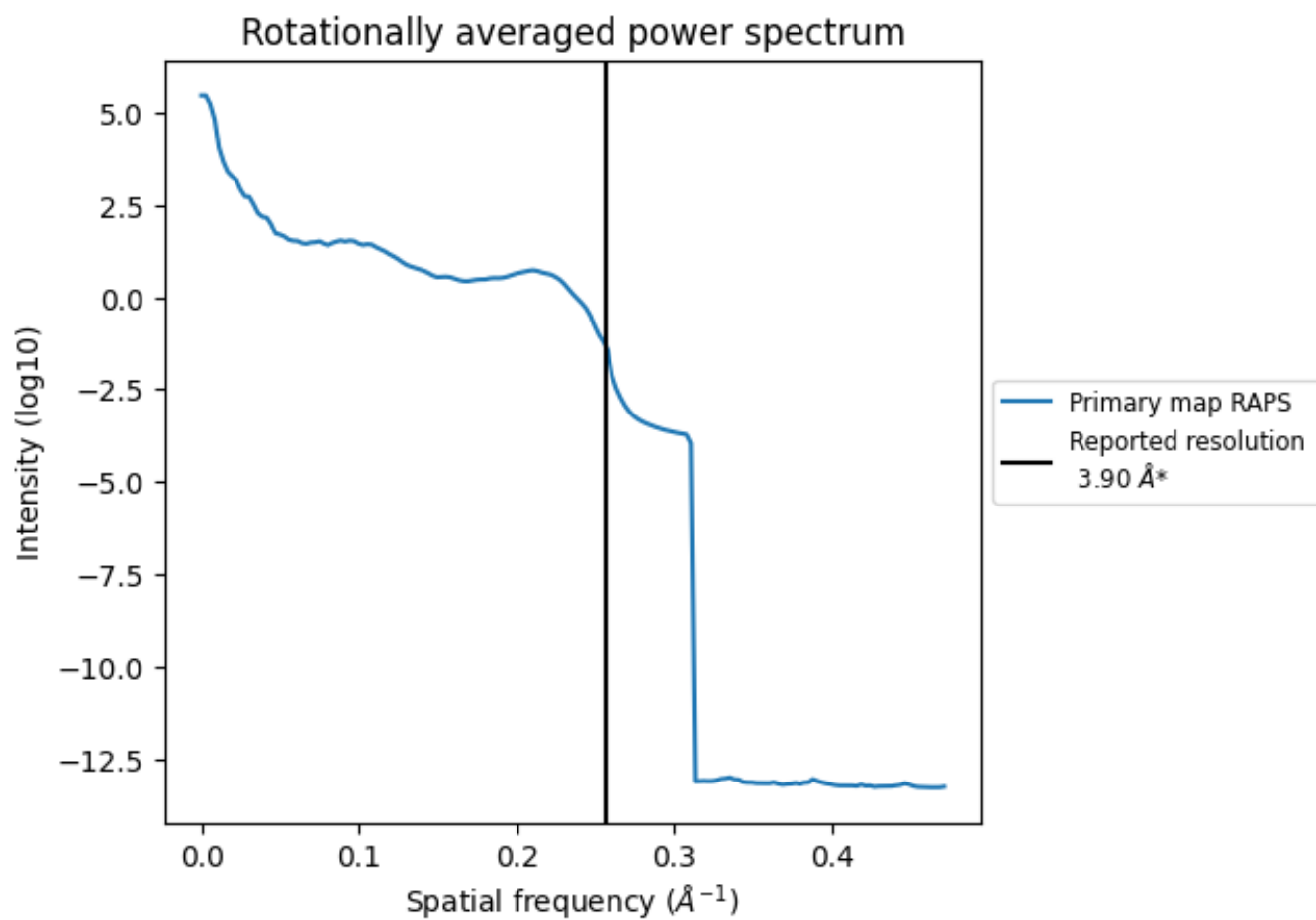
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 792 nm^3 ; this corresponds to an approximate mass of 715 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 0.256 \AA^{-1}

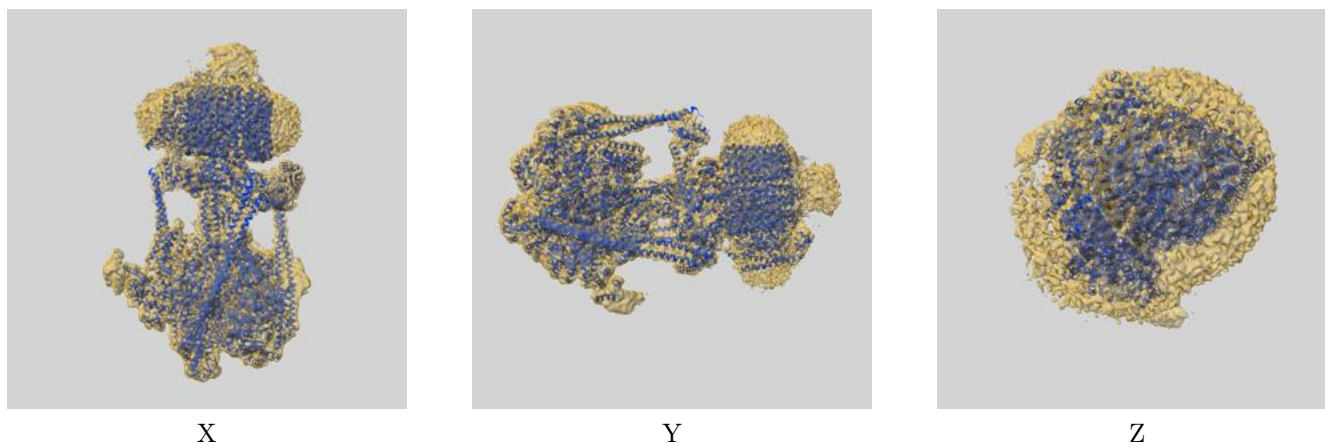
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

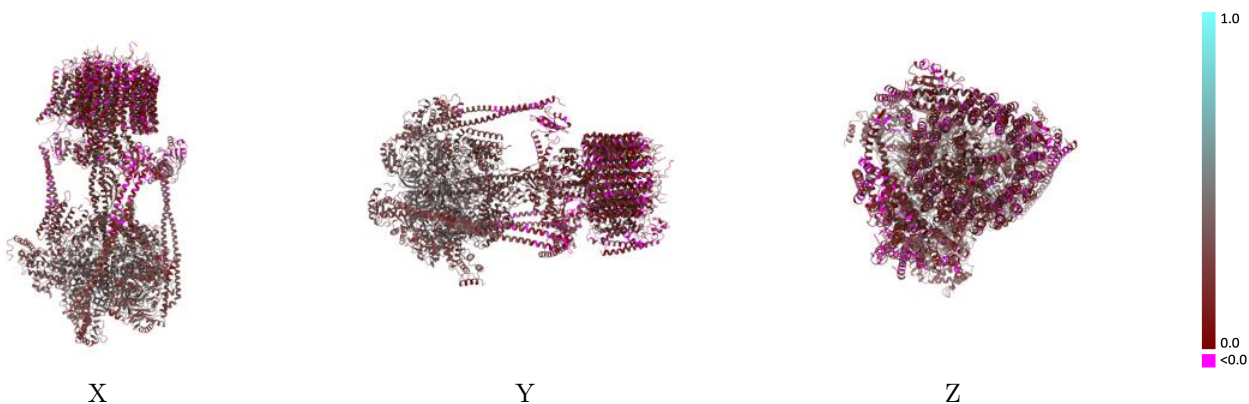
This section contains information regarding the fit between EMDB map EMD-21319 and PDB model 6VQ8. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



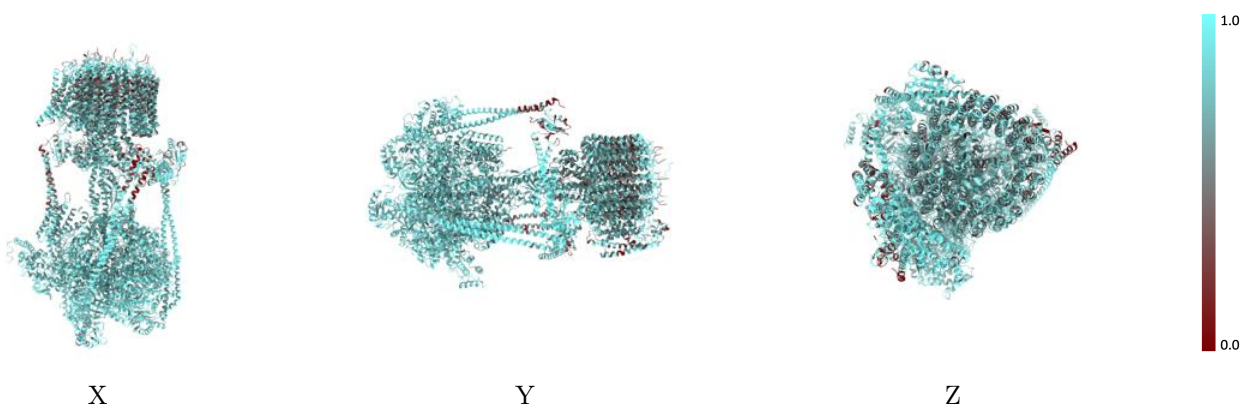
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



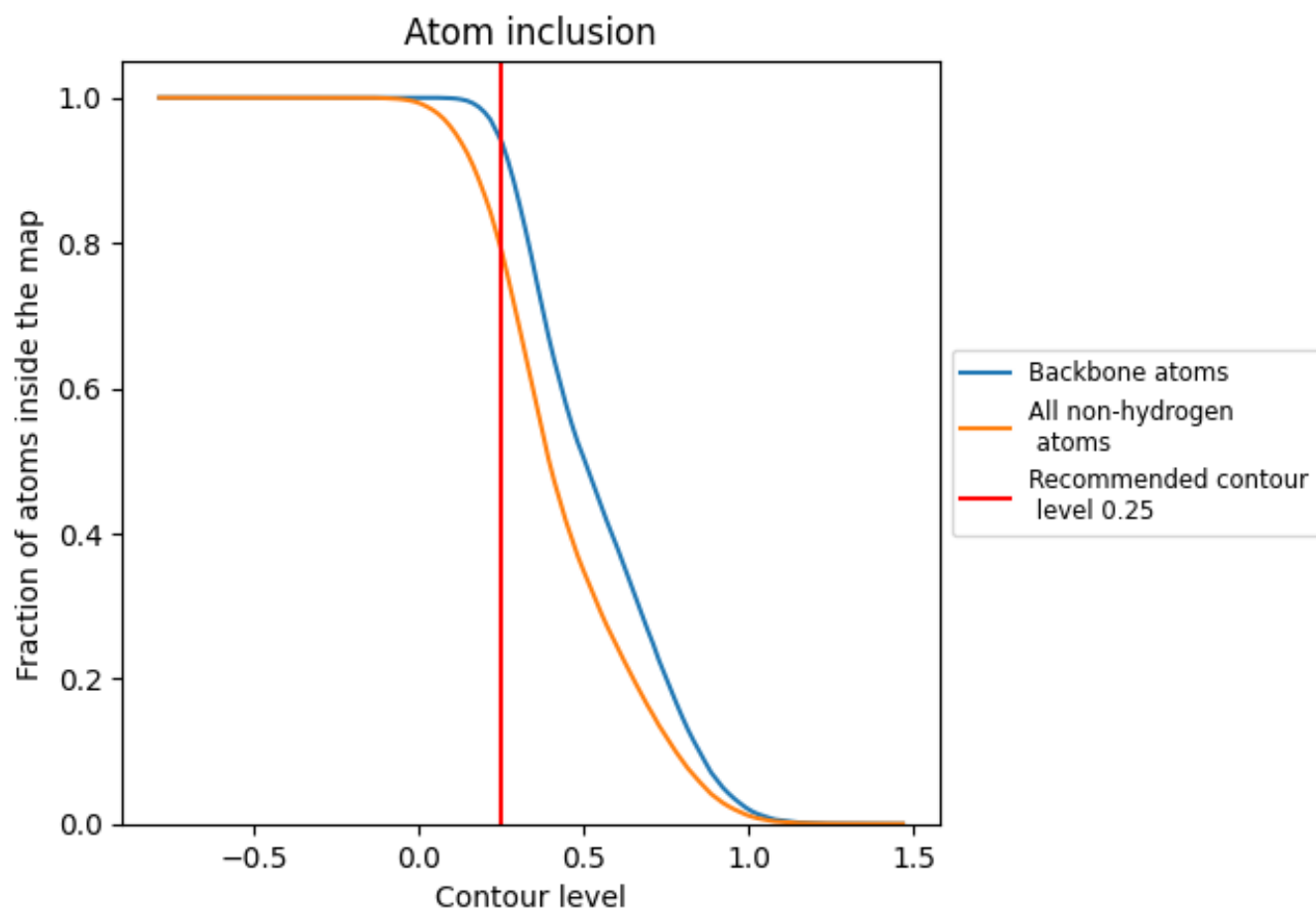
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7886	 0.2740
A	 0.8477	 0.3710
B	 0.8306	 0.3550
C	 0.8369	 0.3480
D	 0.8470	 0.3710
E	 0.8552	 0.3840
F	 0.8524	 0.3880
G	 0.7631	 0.1660
H	 0.7659	 0.2960
I	 0.7693	 0.2630
J	 0.8296	 0.2790
K	 0.7953	 0.2660
L	 0.7718	 0.2570
M	 0.7682	 0.2030
N	 0.8712	 0.2640
O	 0.7867	 0.2380
Q	 0.8233	 0.3000
R	 0.8208	 0.2750
S	 0.8231	 0.2720
a	 0.8142	 0.1880
b	 0.6747	 0.1580
c	 0.6103	 0.2040
d	 0.7082	 0.2200
e	 0.6328	 0.1350
f	 0.6748	 0.1350
g	 0.6891	 0.1680
h	 0.6739	 0.1610
i	 0.6938	 0.1590
j	 0.6844	 0.1350
k	 0.6739	 0.1140
l	 0.6891	 0.1370
m	 0.6749	 0.1210
n	 0.6777	 0.1320
o	 0.6806	 0.1500
p	 0.6927	 0.1900

