wwPDB EM Validation Summary Report

Nov 13, 2023 – 01:40 PM EST

PDB ID	:	7UZG
EMDB ID	:	EMD-26910
Title	:	Rat Kidney V-ATPase lacking subunit H, with SidK and NCOA7B, State 1
Authors	:	Rubinstein, J.L.; Abbas, Y.M.
Deposited on	:	2022-05-09
Resolution	:	3.70 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:

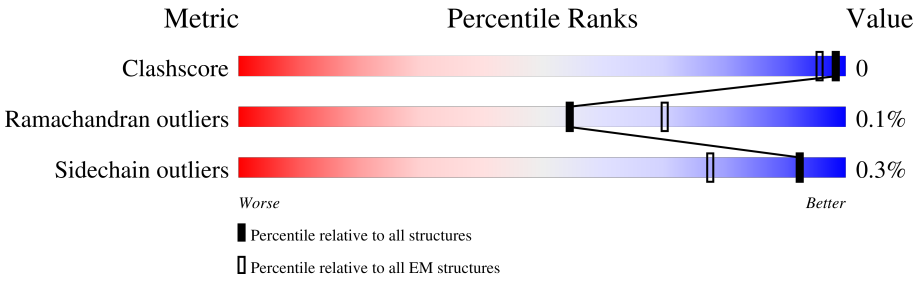
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.70 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	93% 5%
1	B	617	94%
1	C	617	94%
2	D	511	87% 10%
2	E	511	85% 5% 10%
2	F	511	85% 11%
3	G	382	23% 90% 6%
4	H	247	85% 12%

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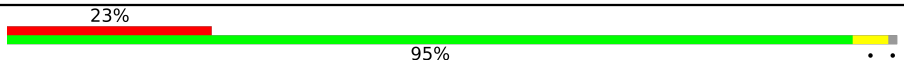
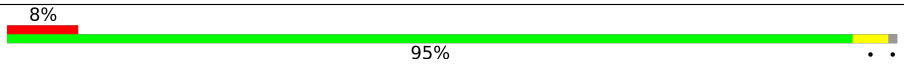
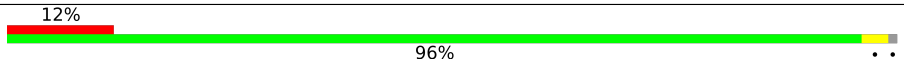
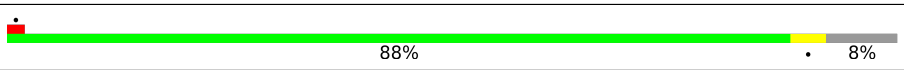
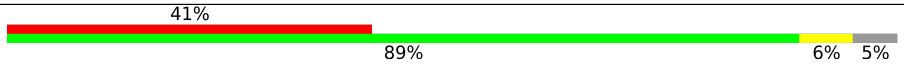
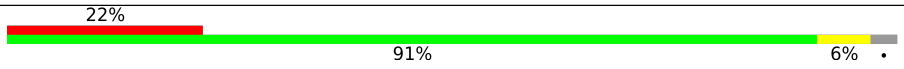
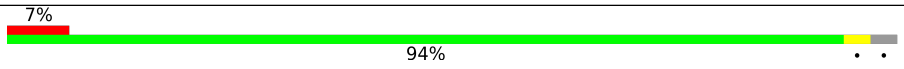
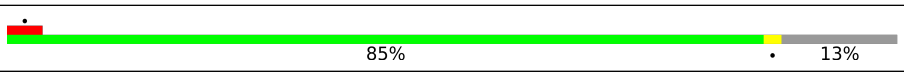
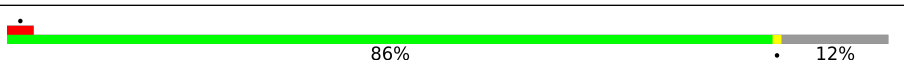
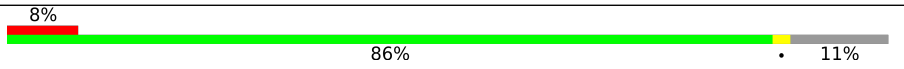
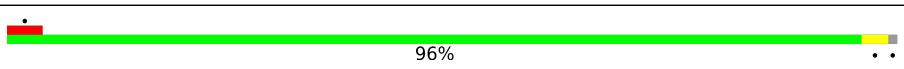
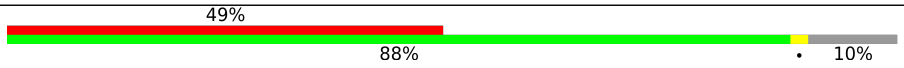
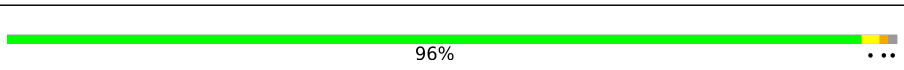
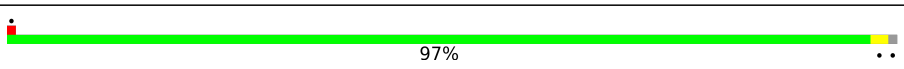
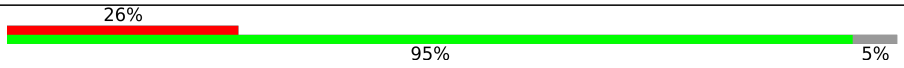
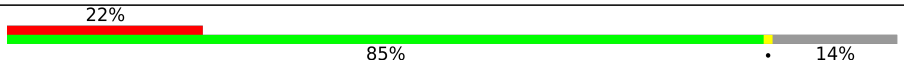
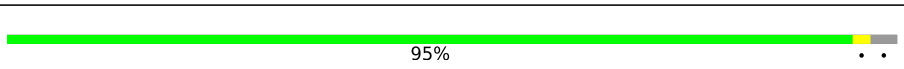
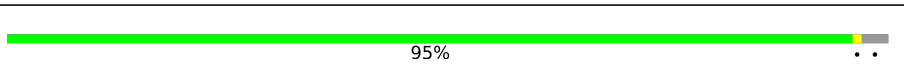
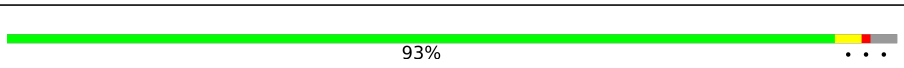
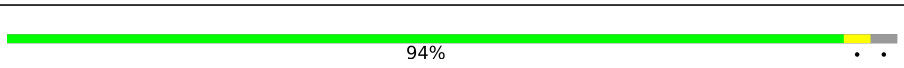
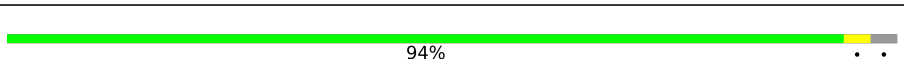
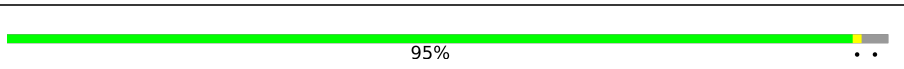
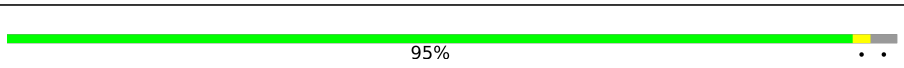
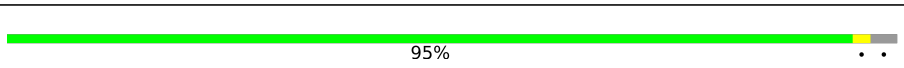
Mol	Chain	Length	Quality of chain
5	I	226	
5	J	226	
5	K	226	
6	L	119	
7	M	118	
7	N	118	
7	O	118	
8	Q	301	
8	R	301	
8	S	301	
9	T	171	
10	a	838	
11	b	205	
12	c	463	
13	d	351	
14	e	81	
15	f	98	
16	g	155	
16	h	155	
16	i	155	
16	j	155	
16	k	155	
16	l	155	
16	m	155	
16	n	155	

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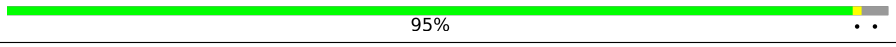
Mol	Chain	Length	Quality of chain
16	o	155	
17	p	350	

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 69795 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
1	A	601	Total	C	N	O	S	0	0
			4657	2952	787	891	27		
1	B	600	Total	C	N	O	S	0	0
			4651	2949	786	889	27		
1	C	602	Total	C	N	O	S	0	0
			4666	2957	788	894	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	460	Total	C	N	O	S	0	0
			3604	2287	614	683	20		
2	E	460	Total	C	N	O	S	0	0
			3603	2286	615	682	20		
2	F	457	Total	C	N	O	S	0	0
			3576	2269	610	677	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	358	Total	C	N	O	S	0	0
			2919	1873	492	545	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	218	Total	C	N	O	S	0	0
			1760	1116	316	323	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	223	Total	C	N	O	S	0	0
			1808	1137	319	342	10		
5	J	223	Total	C	N	O	S	0	0
			1808	1137	319	342	10		
5	K	223	Total	C	N	O	S	0	0
			1808	1137	319	342	10		

- 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
			875	553	157	163	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	112	Total	C	N	O	S	0	0
			920	563	173	181	3		
7	N	114	Total	C	N	O	S	0	0
			935	571	176	185	3		
7	O	114	Total	C	N	O	S	0	0
			935	571	176	185	3		

- Molecule 8 is a protein called Legionella pneumophila effector SidK.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	263	Total	C	N	O	S	0	0
			2126	1350	357	409	10		
8	R	264	Total	C	N	O	S	0	0
			2130	1352	358	410	10		
8	S	267	Total	C	N	O	S	0	0
			2155	1369	362	413	11		

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 Nuclear receptor coactivator 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	170	Total	C	N	O	S	0	0
			1377	887	230	257	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	a	757	Total	C	N	O	S	0	0
			6164	4025	1032	1066	41		

- Molecule 11 is a protein called ATPase, H+ transporting, V0 subunit B (Predicted), isoform CRA_a.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	c	204	Total	C	N	O	S	0	0
			1652	1087	259	297	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	d	348	Total	C	N	O	S	0	0
			2817	1817	458	528	14		

- Molecule 14 is a protein called V-type proton ATPase subunit e 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	e	77	Total	C	N	O	S	0	0
			623	431	97	92	3		

- Molecule 15 is a protein called Ribonuclease K.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	f	84	Total	C	N	O	S	0	0
			652	431	101	114	6		

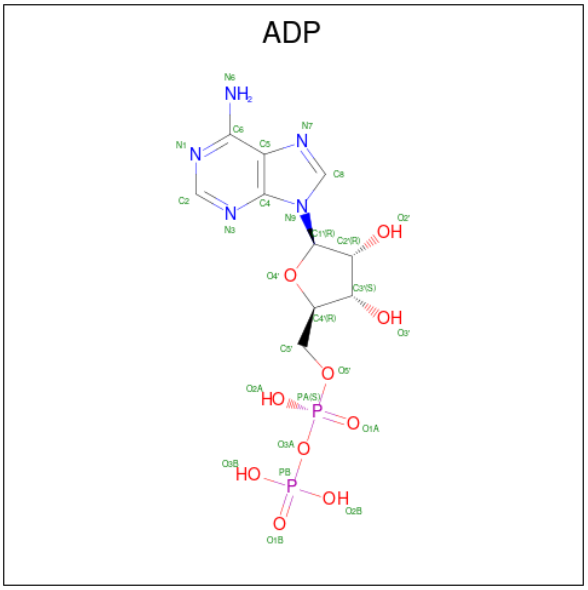
- Molecule 16 is a protein called V-type proton ATPase 16 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	g	150	Total	C	N	O	S	0	0
			1069	699	171	191	8		
16	h	150	Total	C	N	O	S	0	0
			1069	699	171	191	8		
16	i	150	Total	C	N	O	S	0	0
			1069	699	171	191	8		
16	j	150	Total	C	N	O	S	0	0
			1069	699	171	191	8		
16	k	150	Total	C	N	O	S	0	0
			1069	699	171	191	8		
16	l	150	Total	C	N	O	S	0	0
			1069	699	171	191	8		
16	m	150	Total	C	N	O	S	0	0
			1069	699	171	191	8		
16	n	150	Total	C	N	O	S	0	0
			1069	699	171	191	8		
16	o	150	Total	C	N	O	S	0	0
			1069	699	171	191	8		

- Molecule 17 is a protein called Renin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	p	51	Total	C	N	O	S	0	0
			423	284	62	75	2		

- 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).



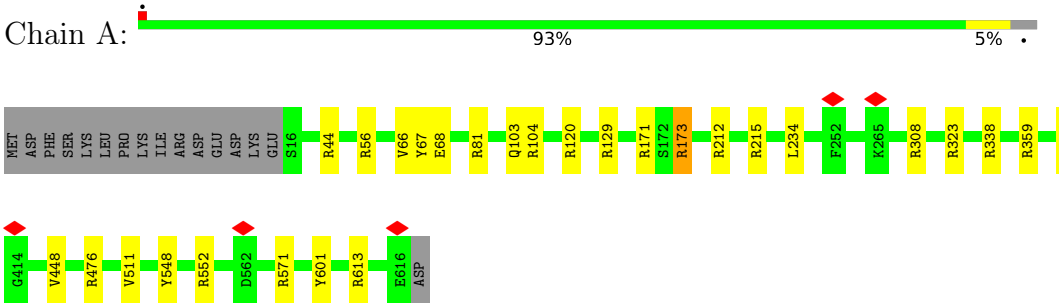
Mol	Chain	Residues	Atoms					AltConf
18	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots (i)

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

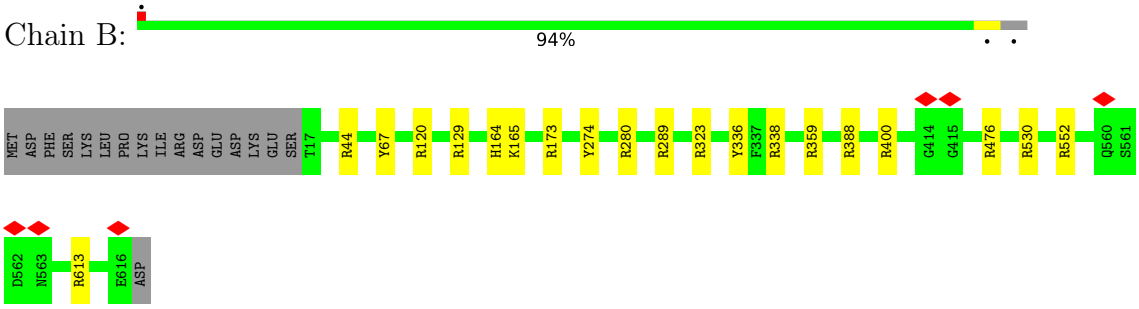
• Molecule 1: ATPase H+-transporting V1 subunit A

Chain A:



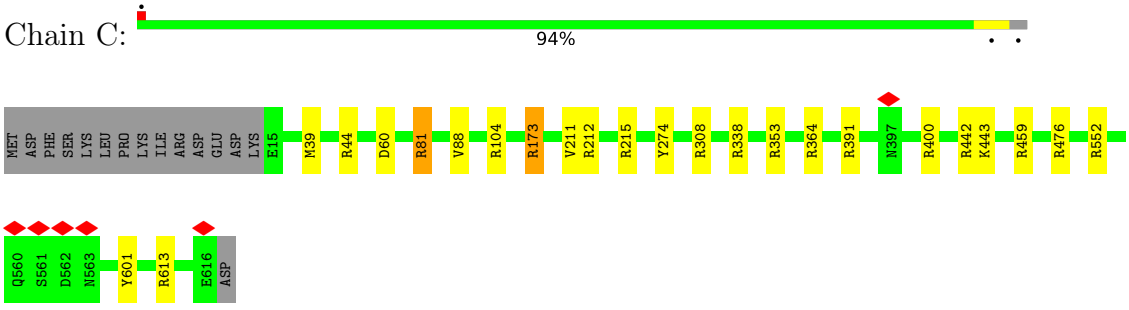
• Molecule 1: ATPase H+-transporting V1 subunit A

Chain B:



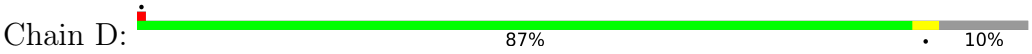
• Molecule 1: ATPase H+-transporting V1 subunit A

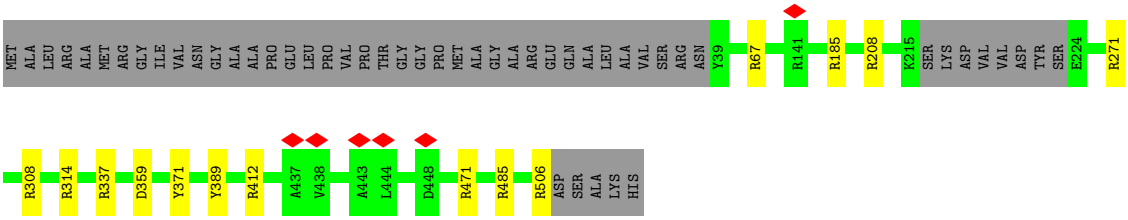
Chain C:



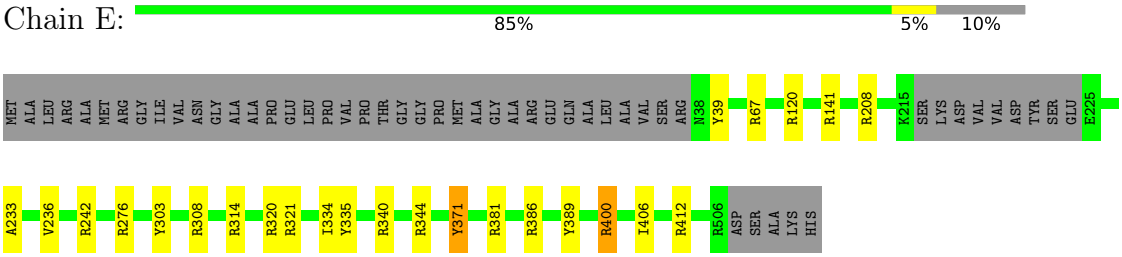
• Molecule 2: V-type proton ATPase subunit B, brain isoform

Chain D:

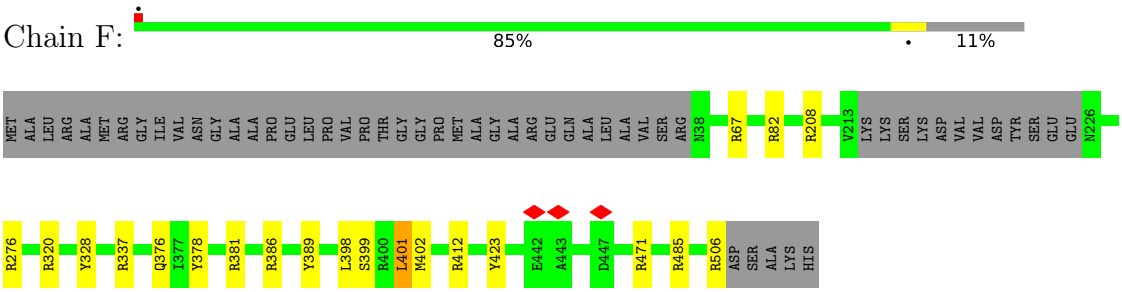




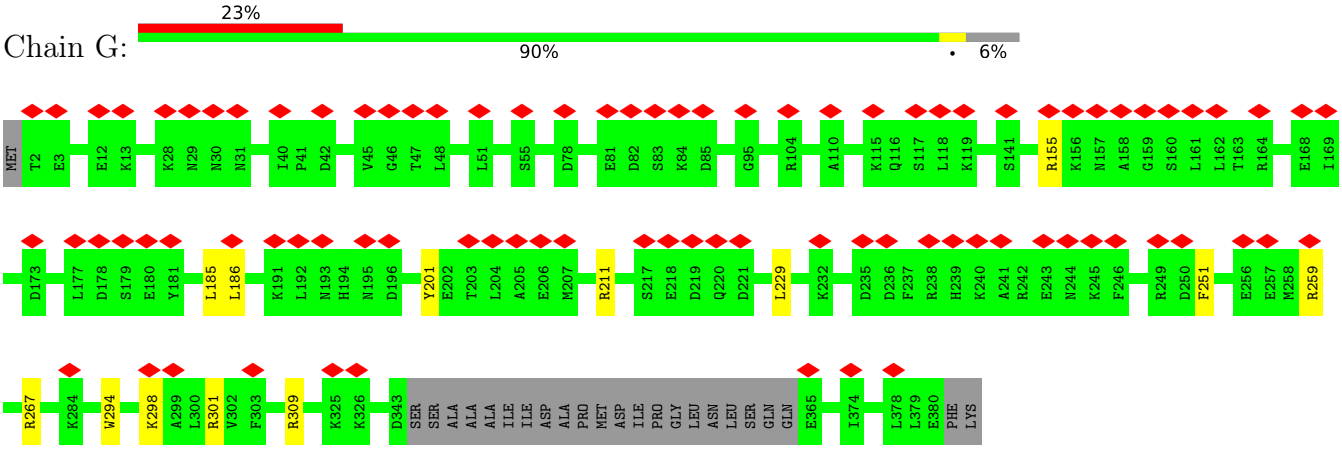
• Molecule 2: V-type proton ATPase subunit B, brain isoform



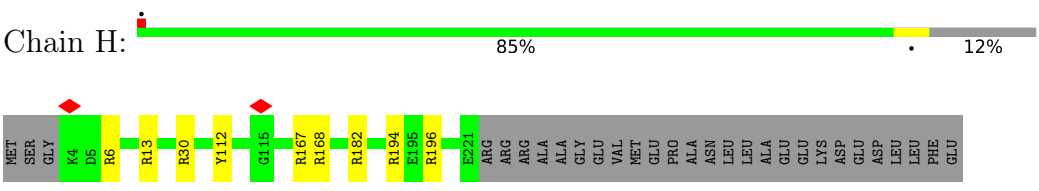
• Molecule 2: V-type proton ATPase subunit B, brain isoform



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

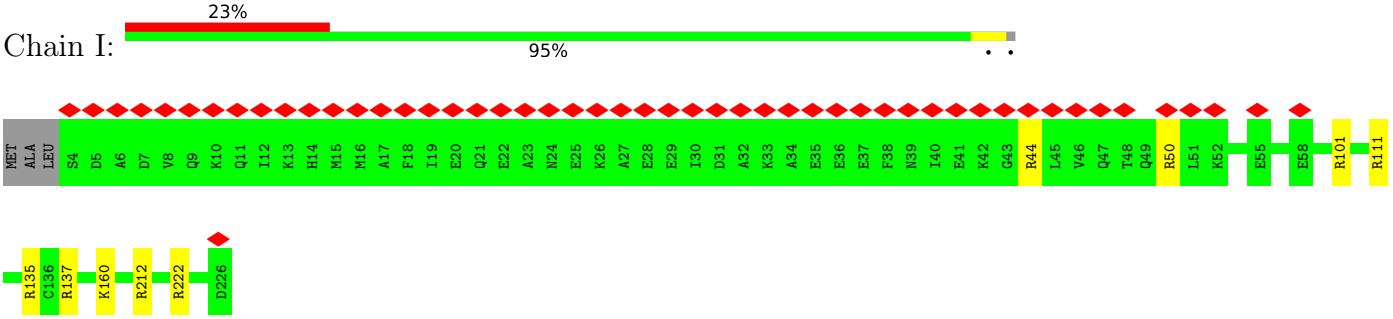


• Molecule 4: ATPase H+-transporting V1 subunit D



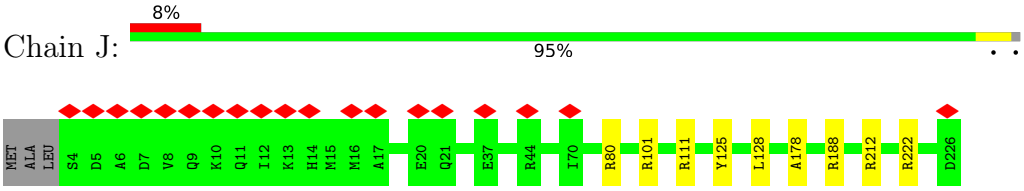
• Molecule 5: V-type proton ATPase subunit E 1

Chain I:



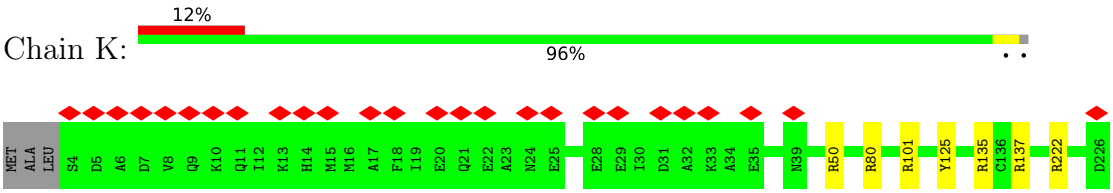
• Molecule 5: V-type proton ATPase subunit E 1

Chain J:



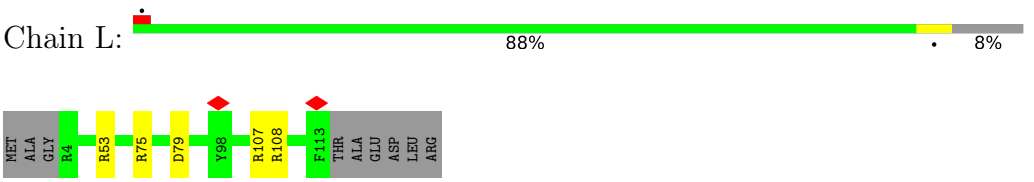
• Molecule 5: V-type proton ATPase subunit E 1

Chain K:



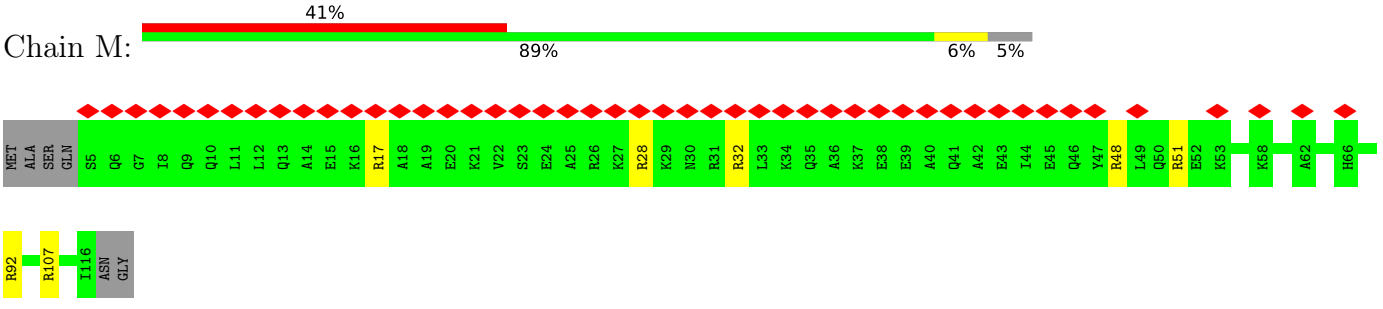
• Molecule 6: V-type proton ATPase subunit F

Chain L:



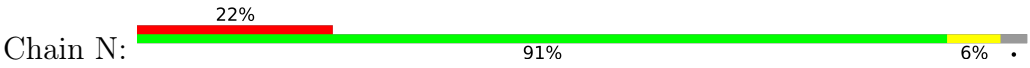
• Molecule 7: V-type proton ATPase subunit G

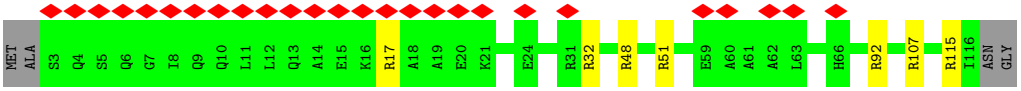
Chain M:



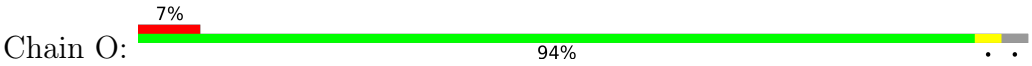
• Molecule 7: V-type proton ATPase subunit G

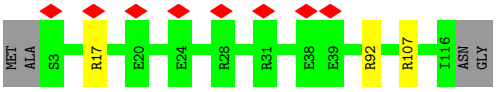
Chain N:



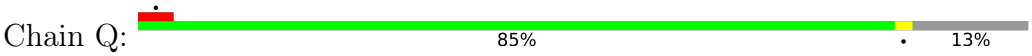


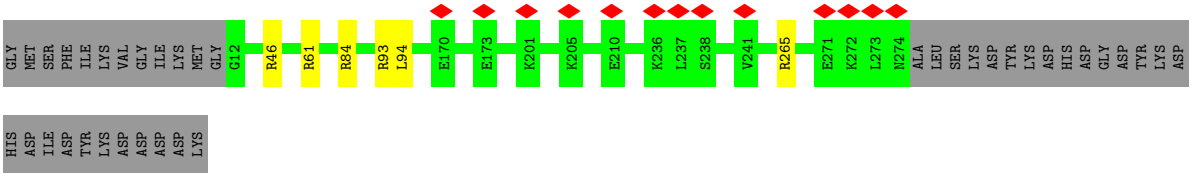
• Molecule 7: V-type proton ATPase subunit G



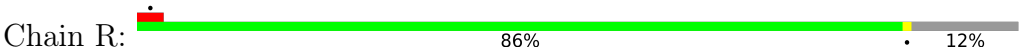


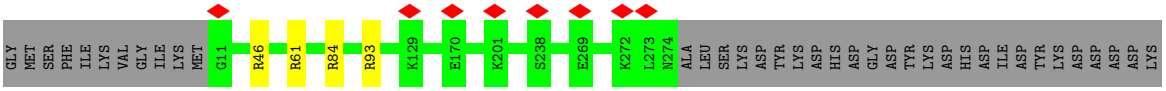
• Molecule 8: Legionella pneumophila effector SidK



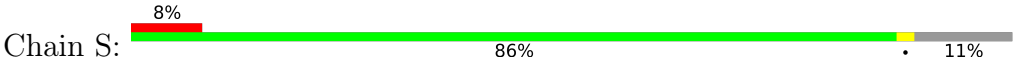


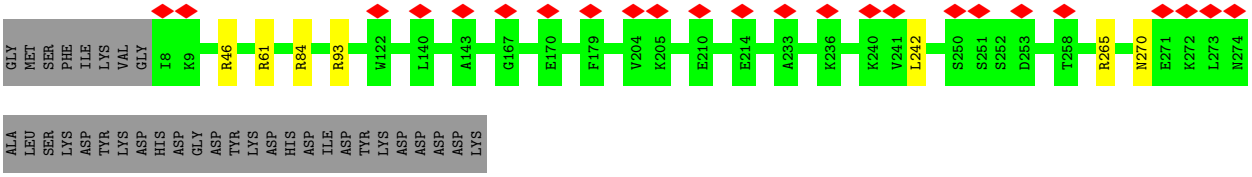
• Molecule 8: Legionella pneumophila effector SidK



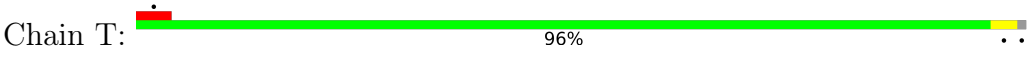


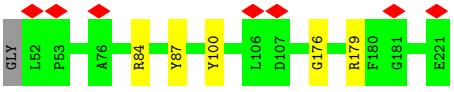
• Molecule 8: Legionella pneumophila effector SidK



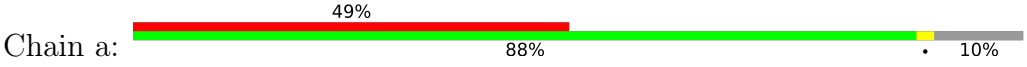


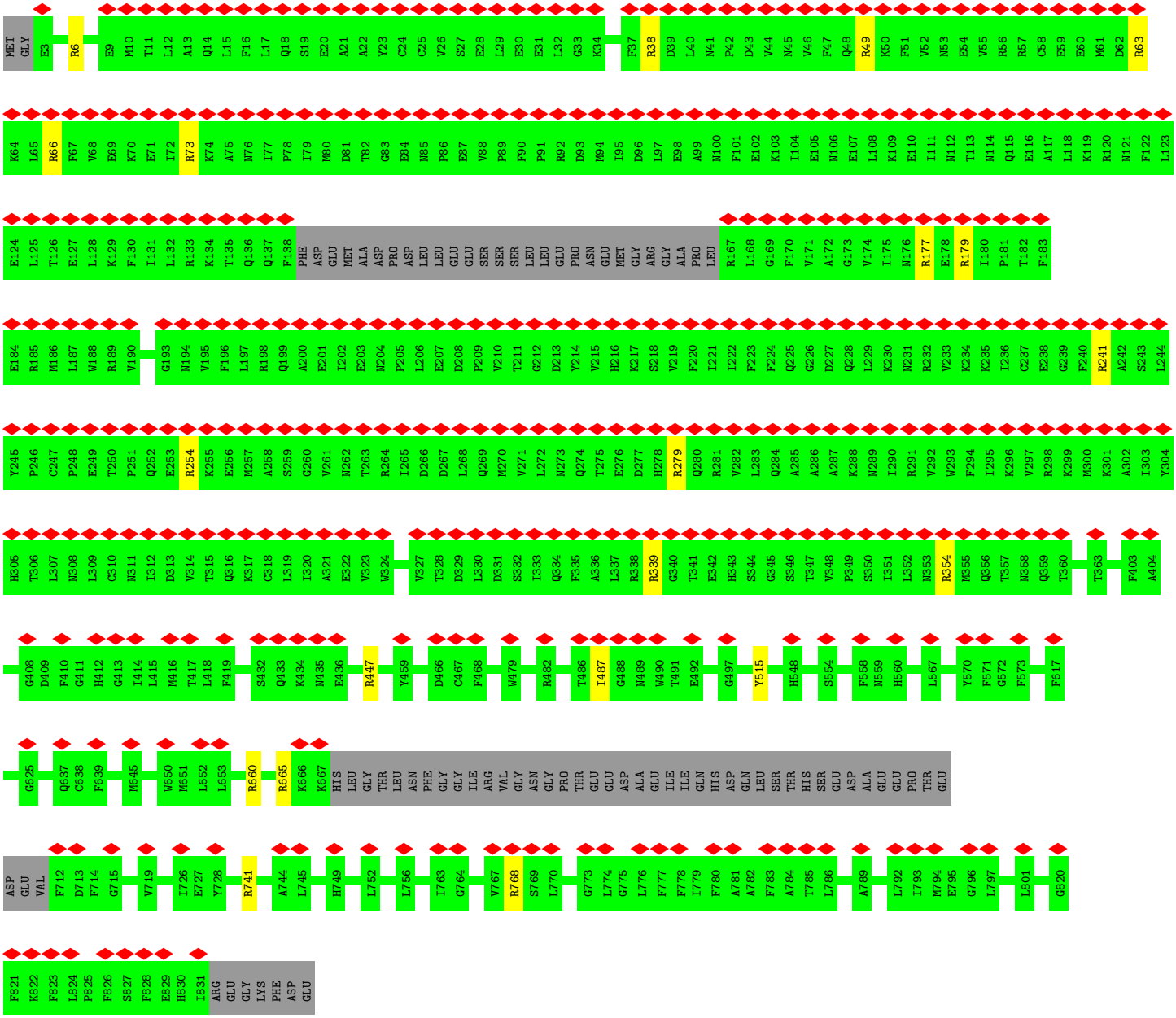
• Molecule 9: Nuclear receptor coactivator 7





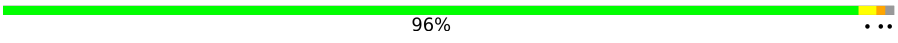
• Molecule 10: V-type proton ATPase 116 kDa subunit a isoform 1





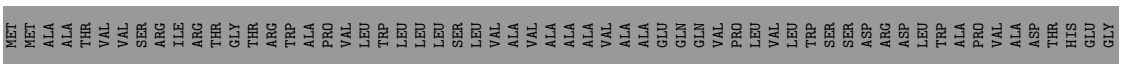
• Molecule 11: ATPase, H+ transporting, V0 subunit B (Predicted), isoform CRA_a

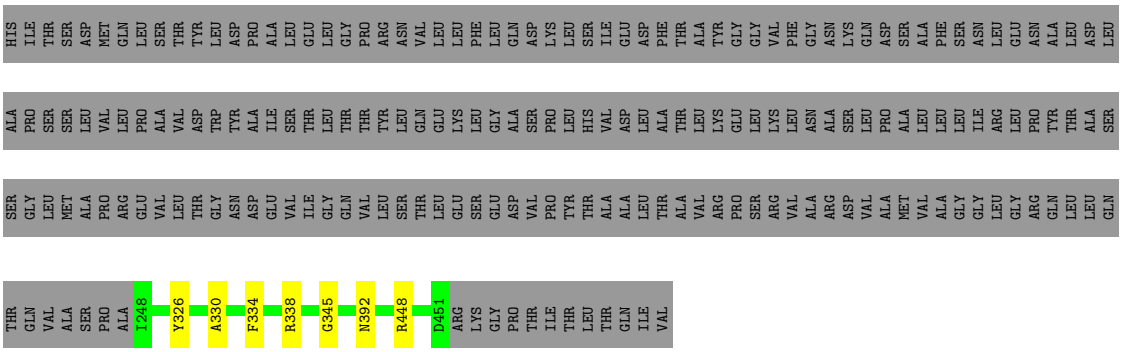
Chain b:



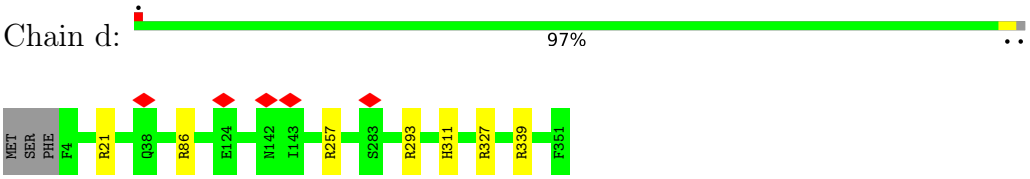
• Molecule 12: V-type proton ATPase subunit S1

Chain c:

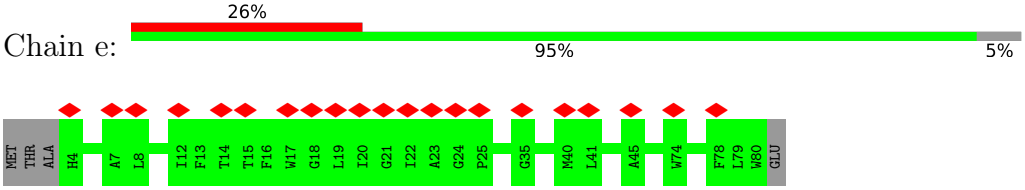




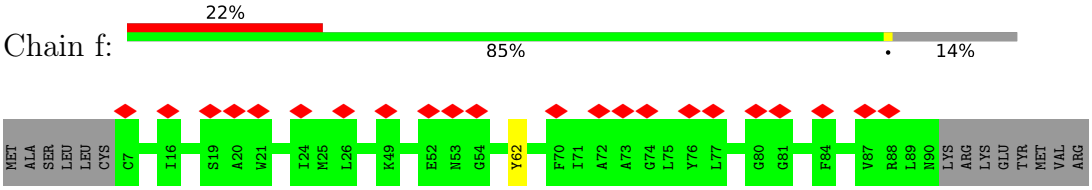
• Molecule 13: V-type proton ATPase subunit



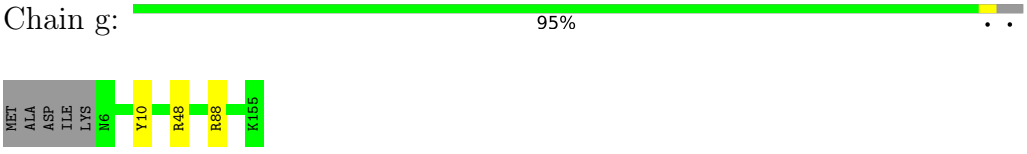
• Molecule 14: V-type proton ATPase subunit e 2



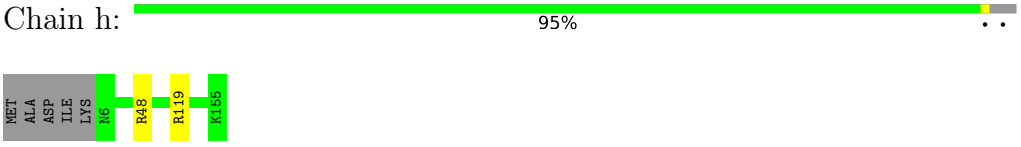
• Molecule 15: Ribonuclease K



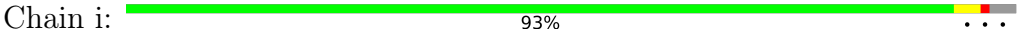
• Molecule 16: V-type proton ATPase 16 kDa proteolipid subunit



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

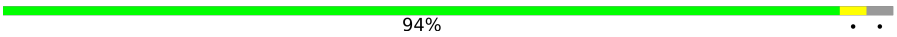


• Molecule 16: V-type proton ATPase 16 kDa proteolipid subunit



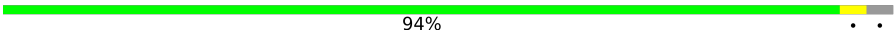
• Molecule 16: V-type proton ATPase 16 kDa proteolipid subunit

Chain j:



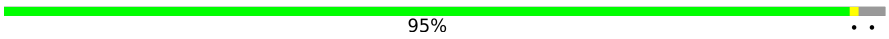
• Molecule 16: V-type proton ATPase 16 kDa proteolipid subunit

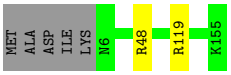
Chain k:



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

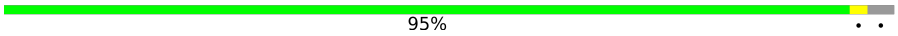
Chain l:





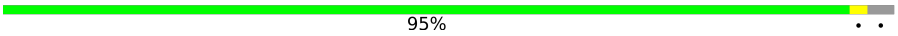
• Molecule 16: V-type proton ATPase 16 kDa proteolipid subunit

Chain m:



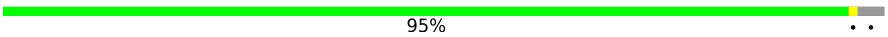
• Molecule 16: V-type proton ATPase 16 kDa proteolipid subunit

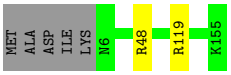
Chain n:



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

Chain o:





• Molecule 17: Renin receptor

Chain p:


MET ALA VAL LEU VAL VAL LEU LEU SER SER LEU VAL SER SER ALA LEU ALA ASN GLU PHE SER ILE LEU ARG SER PRO GLY SER VAL VAL PHE ARG ASN GLY ASN TRP PRO ILE PRO GLY ASP ARG ILE PRO ASP VAL ALA ALA LEU SER MET GLY PHE SER VAL LYS GLU ASP LEU SER
TRP PRO GLY LEU ALA VAL GLY ASN LEU PHE HIS ARG PRO ARG ALA THR ILE MET VAL THR VAL LYS GLY VAL ASP LYS LEU ALA LEU PRO THR GLY SER VAL ILE SER TYR PRO LEU GLU ASN ALA VAL PRO PHE SER LEU ASP SER VAL ALA ASN SER ILE HIS SER LEU PHE SER GLU
GLU THR PRO VAL VAL LEU GLN LEU ALA PRO SER GLU GLU ARG VAL TYR MET VAL GLY LYS ALA ASN SER VAL PHE GLU ASP LEU SER VAL THR LEU ARG GLN LEU ARG ASN ARG LEU PHE GLN GLU ASN SER VAL LEU ASN SER LEU PRO LEU ASN SER LEU SER ARG ASN ASN GLU VAL
ASP LEU LEU PHE LEU SER GLU LEU GLN VAL LEU HIS ASP ILE SER SER LEU LEU SER ARG HIS LYS HIS LEU ALA LYS ASP HIS SER PRO ASP LEU TYR SER LEU GLU LEU ALA GLY LEU ASP GLU LEU GLY LYS ARG TYR GLY GLU ASP SER GLU GLN PHE ARG ASP ALA SER ARG ILE
LEU VAL ASP ALA LEU GLN LYS PHE ALA ASP ASP MET TYR SER LEU TYR GLY GLY ASN ALA VAL VAL GLU LEU VAL THR VAL LYS SER PHE ASP THR SER LEU VAL ARG LYS SER ARG THR ILE LEU GLU THR LYS GLN GLU ASN THR GLN S291 Y299 G334 Y335 D336 S337 R341
MET THR ASN GLN LYS ILE ARG MET ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76585	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	44.825	Depositor
Minimum defocus (nm)	100	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	67.907	Depositor
Minimum map value	-45.383	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.329	Depositor
Recommended contour level	4.0	Depositor
Map size (Å)	449.65, 449.65, 449.65	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3225, 1.3225, 1.3225	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	0.65	0/4752	0.98	20/6433 (0.3%)
1	B	0.65	0/4746	0.97	17/6425 (0.3%)
1	C	0.64	0/4761	0.97	19/6445 (0.3%)
2	D	0.64	0/3675	0.96	11/4979 (0.2%)
2	E	0.65	0/3674	1.01	19/4978 (0.4%)
2	F	0.64	0/3647	0.97	11/4944 (0.2%)
3	G	0.66	0/2973	0.92	6/4016 (0.1%)
4	H	0.62	0/1778	0.93	8/2377 (0.3%)
5	I	0.61	0/1825	0.93	8/2442 (0.3%)
5	J	0.61	0/1825	0.90	7/2442 (0.3%)
5	K	0.61	0/1825	0.91	6/2442 (0.2%)
6	L	0.64	0/889	0.98	5/1199 (0.4%)
7	M	0.66	0/928	0.98	7/1236 (0.6%)
7	N	0.65	0/943	0.98	7/1256 (0.6%)
7	O	0.65	0/943	0.90	3/1256 (0.2%)
8	Q	0.61	0/2160	0.86	5/2910 (0.2%)
8	R	0.61	0/2164	0.86	4/2915 (0.1%)
8	S	0.61	0/2189	0.88	5/2947 (0.2%)
9	T	0.71	0/1417	0.96	3/1919 (0.2%)
10	a	0.71	0/6322	0.93	17/8551 (0.2%)
11	b	0.62	0/1537	1.03	5/2088 (0.2%)
12	c	0.67	0/1707	0.97	5/2324 (0.2%)
13	d	0.64	0/2882	0.94	7/3903 (0.2%)
14	e	0.74	0/648	0.93	0/891
15	f	0.71	0/668	0.88	1/907 (0.1%)
16	g	0.62	0/1084	0.96	4/1466 (0.3%)
16	h	0.61	0/1084	0.89	2/1466 (0.1%)
16	i	0.60	0/1084	0.99	7/1466 (0.5%)
16	j	0.61	0/1084	0.95	4/1466 (0.3%)
16	k	0.59	0/1084	0.92	5/1466 (0.3%)
16	l	0.60	0/1084	0.90	3/1466 (0.2%)
16	m	0.60	0/1084	0.92	3/1466 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	n	0.59	0/1084	0.90	2/1466 (0.1%)
16	o	0.59	0/1084	0.92	2/1466 (0.1%)
17	p	0.71	0/436	0.99	1/598 (0.2%)
All	All	0.64	0/71070	0.94	239/96017 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
2	D	0	2
2	E	0	4
2	F	0	2
3	G	0	1
4	H	0	1
5	K	0	1
9	T	0	1
10	a	0	2
11	b	0	2
16	i	0	1
17	p	0	1
All	All	0	21

There are no bond length outliers.

The worst 5 of 239 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	R	46	ARG	NE-CZ-NH1	9.36	124.98	120.30
16	i	32	TYR	CB-CG-CD1	-9.09	115.55	121.00
1	C	476	ARG	NE-CZ-NH1	9.05	124.83	120.30
16	j	88	ARG	NE-CZ-NH1	8.89	124.75	120.30
7	N	92	ARG	NE-CZ-NH1	8.87	124.73	120.30

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	374	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	81	ARG	Sidechain
1	C	81	ARG	Sidechain
2	D	271	ARG	Sidechain
2	D	389	TYR	Sidechain

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	4657	0	4649	3	0
1	B	4651	0	4644	1	0
1	C	4666	0	4655	3	0
2	D	3604	0	3608	0	0
2	E	3603	0	3608	2	0
2	F	3576	0	3576	5	0
3	G	2919	0	2961	3	0
4	H	1760	0	1869	0	0
5	I	1808	0	1880	0	0
5	J	1808	0	1880	0	0
5	K	1808	0	1880	0	0
6	L	875	0	883	0	0
7	M	920	0	918	0	0
7	N	935	0	931	0	0
7	O	935	0	931	0	0
8	Q	2126	0	2165	1	0
8	R	2130	0	2168	0	0
8	S	2155	0	2201	1	0
9	T	1377	0	1315	0	0
10	a	6164	0	6197	0	0
11	b	1503	0	1551	0	0
12	c	1652	0	1584	0	0
13	d	2817	0	2756	0	0
14	e	623	0	641	0	0
15	f	652	0	647	0	0
16	g	1069	0	1136	0	0
16	h	1069	0	1136	0	0
16	i	1069	0	1136	0	0
16	j	1069	0	1136	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	k	1069	0	1136	0	0
16	l	1069	0	1136	0	0
16	m	1069	0	1136	0	0
16	n	1069	0	1136	0	0
16	o	1069	0	1136	0	0
17	p	423	0	416	0	0
18	C	27	0	12	0	0
All	All	69795	0	70750	17	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 0.

The worst 5 of 17 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)
3:G:186:LEU:HD13	3:G:251:PHE:H	1.64	0.63
1:A:66:VAL:HG12	1:A:68:GLU:H	1.65	0.60
2:E:303:TYR:CZ	2:E:334:ILE:HD11	2.46	0.51
2:F:376:GLN:HB2	2:F:378:TYR:CE1	2.46	0.51
1:A:511:VAL:HG21	1:A:548:TYR:CD1	2.48	0.48

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	599/617 (97%)	567 (95%)	31 (5%)	1 (0%)	47 78
1	B	598/617 (97%)	569 (95%)	29 (5%)	0	100 100
1	C	600/617 (97%)	576 (96%)	23 (4%)	1 (0%)	47 78
2	D	456/511 (89%)	435 (95%)	21 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	456/511 (89%)	425 (93%)	31 (7%)	0	100	100
2	F	453/511 (89%)	433 (96%)	20 (4%)	0	100	100
3	G	354/382 (93%)	339 (96%)	15 (4%)	0	100	100
4	H	216/247 (87%)	212 (98%)	4 (2%)	0	100	100
5	I	221/226 (98%)	217 (98%)	3 (1%)	1 (0%)	29	66
5	J	221/226 (98%)	213 (96%)	6 (3%)	2 (1%)	17	54
5	K	221/226 (98%)	216 (98%)	5 (2%)	0	100	100
6	L	108/119 (91%)	102 (94%)	6 (6%)	0	100	100
7	M	110/118 (93%)	110 (100%)	0	0	100	100
7	N	112/118 (95%)	111 (99%)	1 (1%)	0	100	100
7	O	112/118 (95%)	111 (99%)	1 (1%)	0	100	100
8	Q	261/301 (87%)	254 (97%)	7 (3%)	0	100	100
8	R	262/301 (87%)	255 (97%)	7 (3%)	0	100	100
8	S	265/301 (88%)	258 (97%)	7 (3%)	0	100	100
9	T	168/171 (98%)	158 (94%)	9 (5%)	1 (1%)	25	62
10	a	751/838 (90%)	722 (96%)	28 (4%)	1 (0%)	51	83
11	b	201/205 (98%)	193 (96%)	8 (4%)	0	100	100
12	c	202/463 (44%)	188 (93%)	12 (6%)	2 (1%)	15	51
13	d	346/351 (99%)	333 (96%)	13 (4%)	0	100	100
14	e	75/81 (93%)	74 (99%)	1 (1%)	0	100	100
15	f	82/98 (84%)	79 (96%)	3 (4%)	0	100	100
16	g	148/155 (96%)	148 (100%)	0	0	100	100
16	h	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
16	i	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
16	j	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
16	k	148/155 (96%)	148 (100%)	0	0	100	100
16	l	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
16	m	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
16	n	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
16	o	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
17	p	49/350 (14%)	45 (92%)	4 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	8831/10019 (88%)	8508 (96%)	314 (4%)	9 (0%)	54 83

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	T	176	GLY
1	A	103	GLN
5	J	128	LEU
5	I	160	LYS
5	J	178	ALA

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	508/524 (97%)	506 (100%)	2 (0%)	91 95
1	B	507/524 (97%)	505 (100%)	2 (0%)	91 95
1	C	509/524 (97%)	507 (100%)	2 (0%)	91 95
2	D	394/431 (91%)	393 (100%)	1 (0%)	92 96
2	E	394/431 (91%)	392 (100%)	2 (0%)	88 94
2	F	391/431 (91%)	389 (100%)	2 (0%)	88 94
3	G	325/344 (94%)	324 (100%)	1 (0%)	92 96
4	H	189/212 (89%)	189 (100%)	0	100 100
5	I	196/198 (99%)	196 (100%)	0	100 100
5	J	196/198 (99%)	196 (100%)	0	100 100
5	K	196/198 (99%)	196 (100%)	0	100 100
6	L	94/100 (94%)	94 (100%)	0	100 100
7	M	97/101 (96%)	97 (100%)	0	100 100
7	N	99/101 (98%)	99 (100%)	0	100 100
7	O	99/101 (98%)	99 (100%)	0	100 100
8	Q	241/274 (88%)	241 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	R	241/274 (88%)	241 (100%)	0	100 100
8	S	244/274 (89%)	244 (100%)	0	100 100
9	T	148/148 (100%)	148 (100%)	0	100 100
10	a	674/743 (91%)	674 (100%)	0	100 100
11	b	156/158 (99%)	155 (99%)	1 (1%)	86 93
12	c	182/395 (46%)	181 (100%)	1 (0%)	88 94
13	d	303/306 (99%)	302 (100%)	1 (0%)	92 96
14	e	65/68 (96%)	65 (100%)	0	100 100
15	f	70/83 (84%)	70 (100%)	0	100 100
16	g	109/113 (96%)	109 (100%)	0	100 100
16	h	109/113 (96%)	109 (100%)	0	100 100
16	i	109/113 (96%)	108 (99%)	1 (1%)	78 88
16	j	109/113 (96%)	107 (98%)	2 (2%)	59 77
16	k	109/113 (96%)	109 (100%)	0	100 100
16	l	109/113 (96%)	109 (100%)	0	100 100
16	m	109/113 (96%)	109 (100%)	0	100 100
16	n	109/113 (96%)	108 (99%)	1 (1%)	78 88
16	o	109/113 (96%)	109 (100%)	0	100 100
17	p	46/313 (15%)	46 (100%)	0	100 100
All	All	7545/8471 (89%)	7526 (100%)	19 (0%)	92 96

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

Mol	Chain	Res	Type
13	d	311	HIS
16	j	61	MET
16	n	139	GLU
16	j	9	GLU
2	E	406	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
10	a	812	GLN
16	m	6	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	C	801	-	24,29,29	0.68	0	29,45,45	0.75	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
18	ADP	C	801	-	-	2/12/32/32	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(^{o})	Ideal(^{o})
18	C	801	ADP	C5-C6-N6	2.18	123.67	120.35

There are no chirality outliers.

All (2) torsion outliers are listed below:

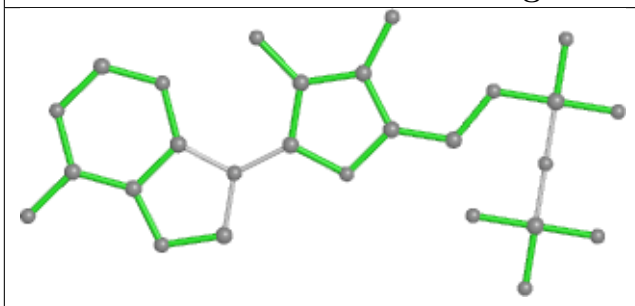
Mol	Chain	Res	Type	Atoms
18	C	801	ADP	PB-O3A-PA-O1A
18	C	801	ADP	PB-O3A-PA-O2A

There are no ring outliers.

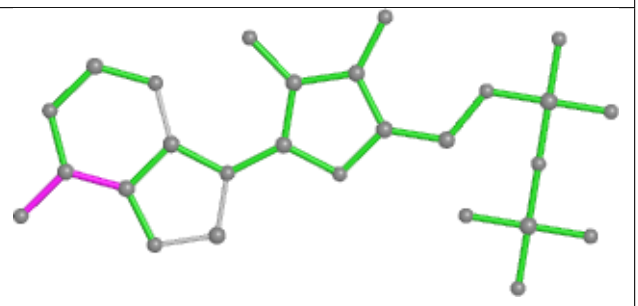
No monomer is involved in short contacts.

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 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.

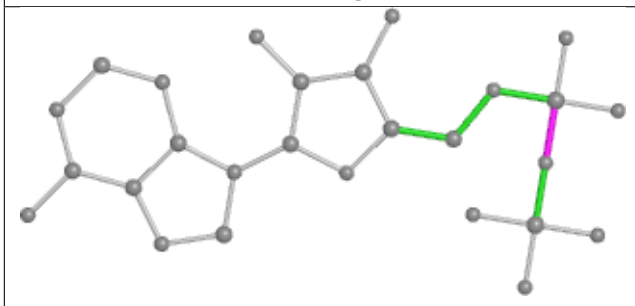
Ligand ADP C 801



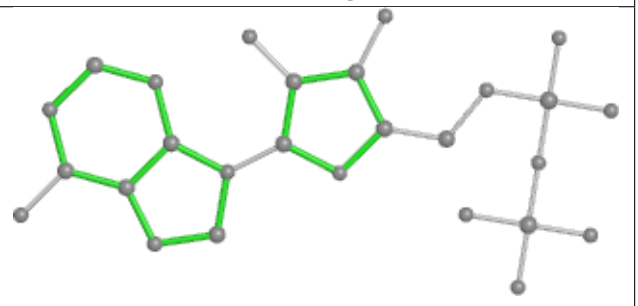
Bond lengths



Bond angles



Torsions



Rings

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.

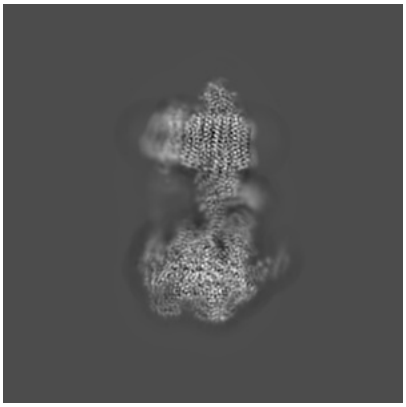
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26910. These allow visual inspection of the internal detail of the map and identification of artifacts.

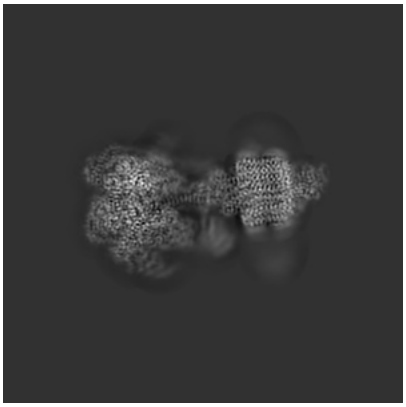
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

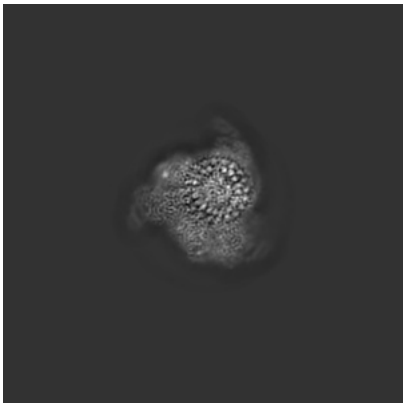
6.1.1 Primary map



X



Y



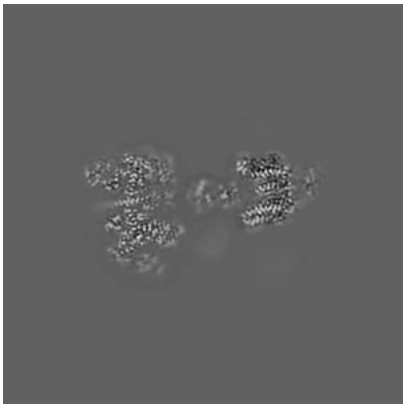
Z

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

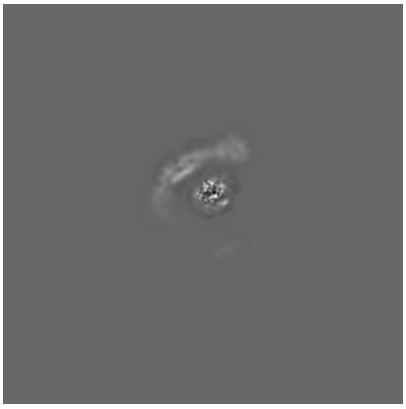
6.2 Central slices

6.2.1 Primary map

X Index: 170



Y Index: 170

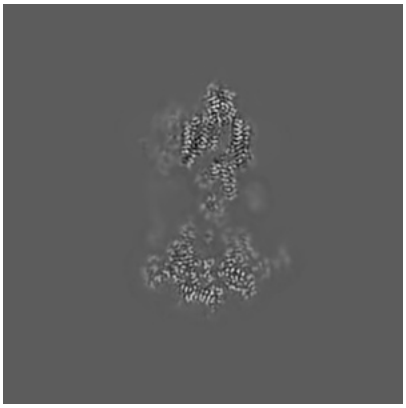


Z Index: 170

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

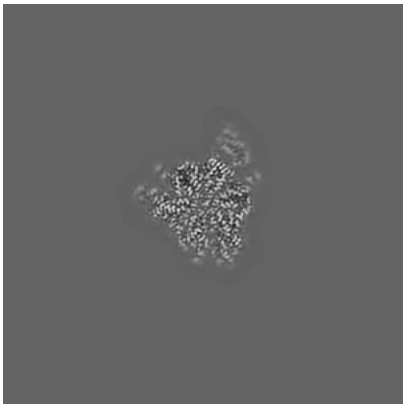
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 183

Y Index: 180

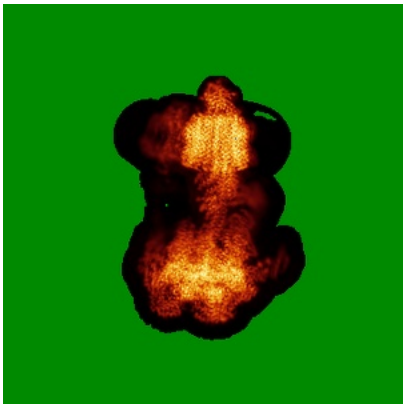


Z Index: 110

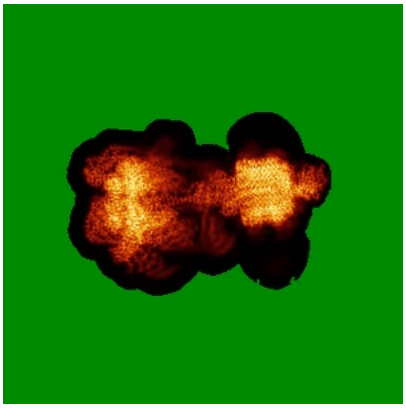
The images above show the largest variance slices of the map in three orthogonal directions.

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

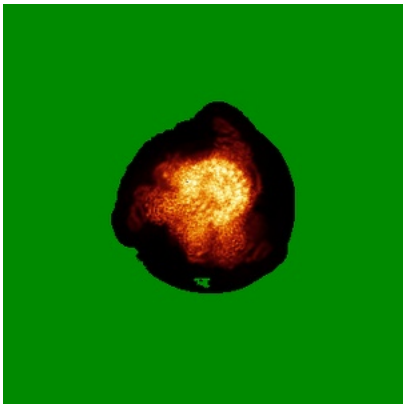
6.4.1 Primary map



X



Y

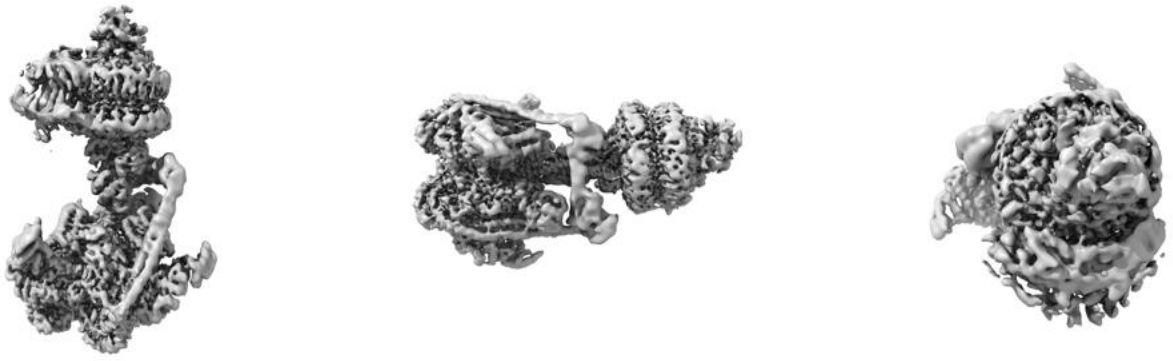


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

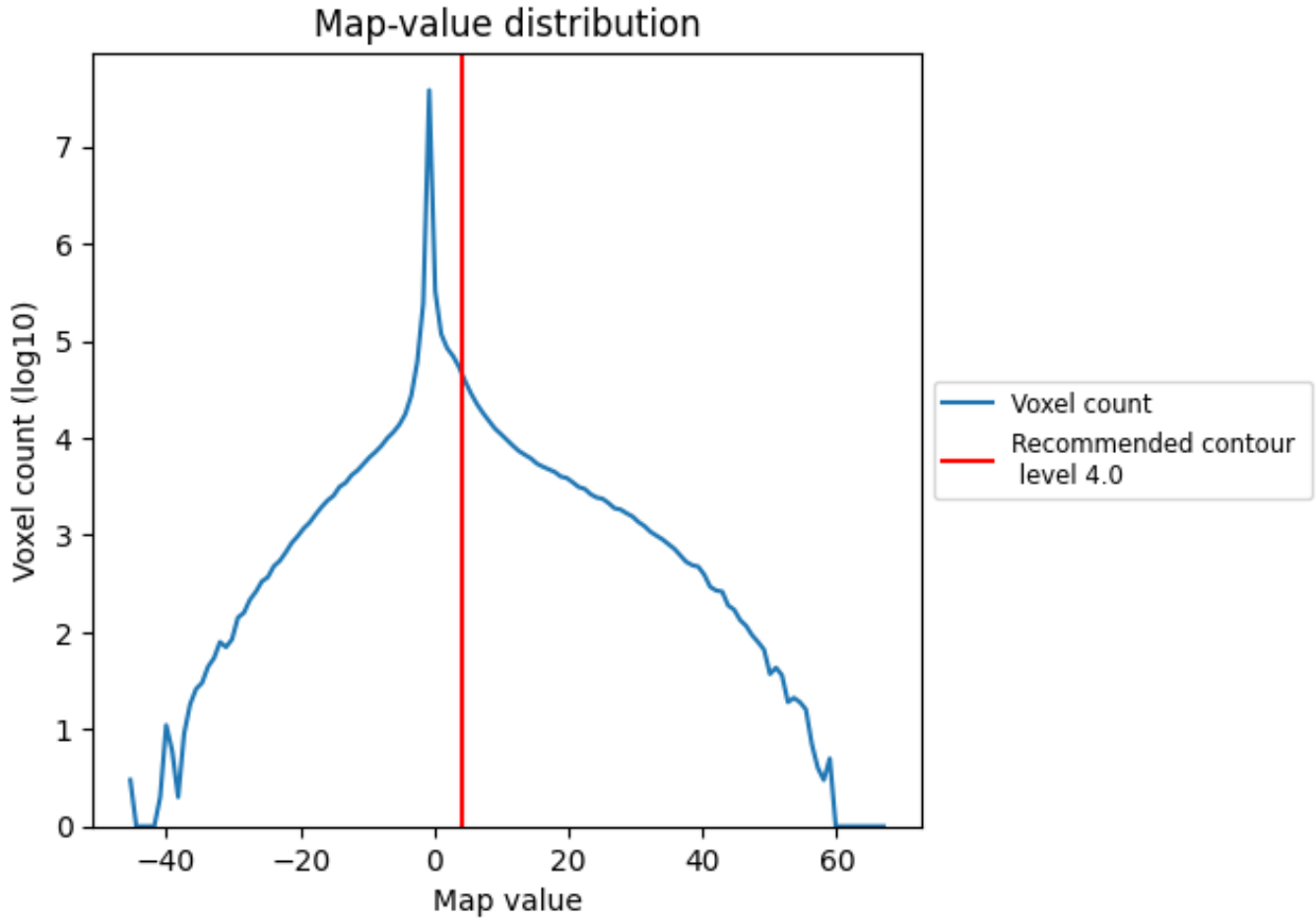
6.6 Mask visualisation (i)

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

7 Map analysis

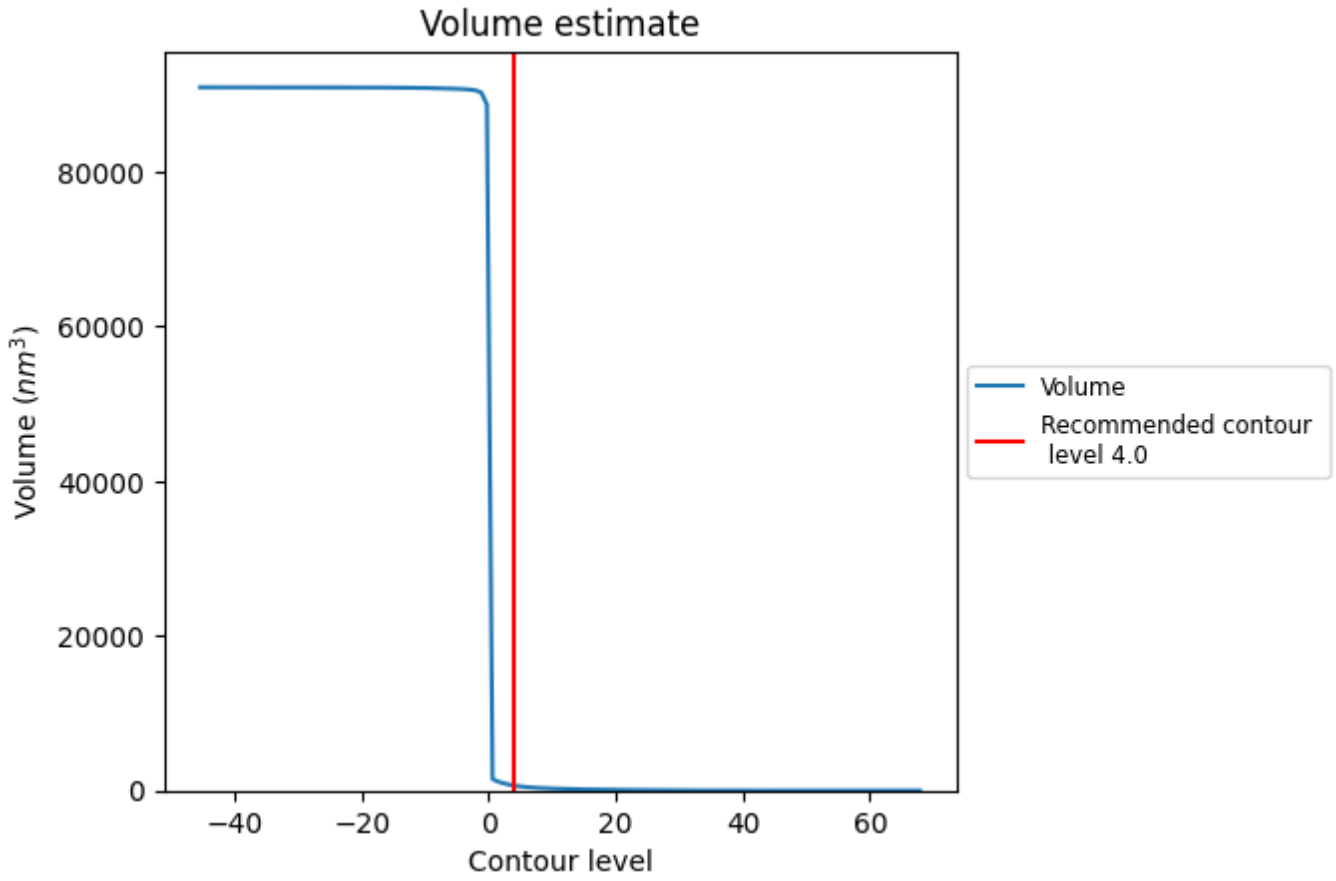
This section contains the results of statistical analysis of the map.

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.

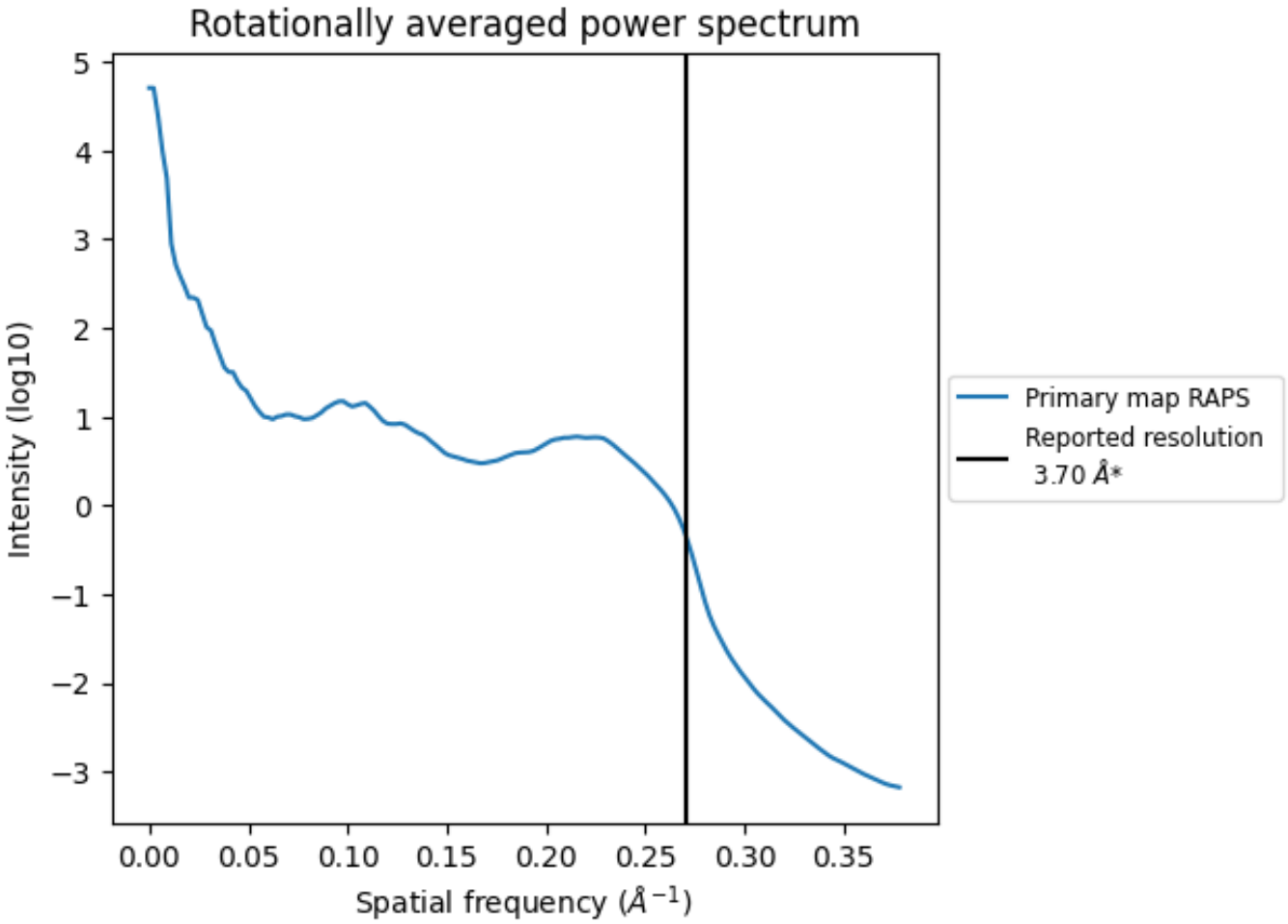
7.2 Volume estimate (i)



The volume at the recommended contour level is 652 nm^3; this corresponds to an approximate mass of 589 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 0.270 Å^{-1}

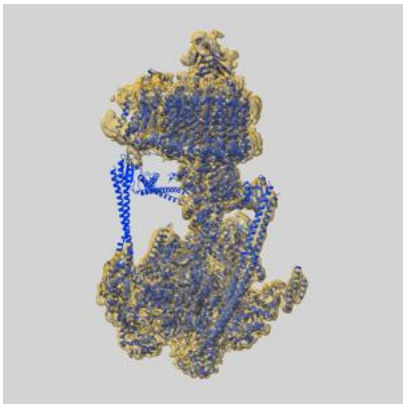
8 Fourier-Shell correlation (i)

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

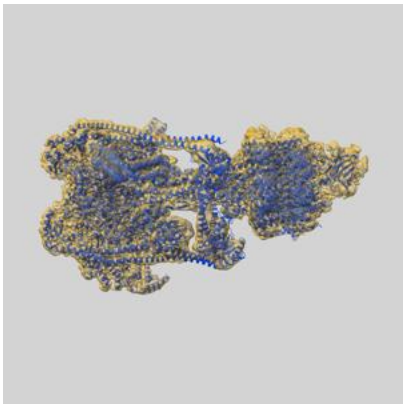
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26910 and PDB model 7UZG. Per-residue inclusion information can be found in section 3 on page 11.

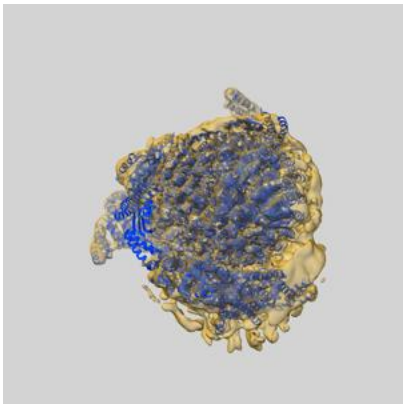
9.1 Map-model overlay



X



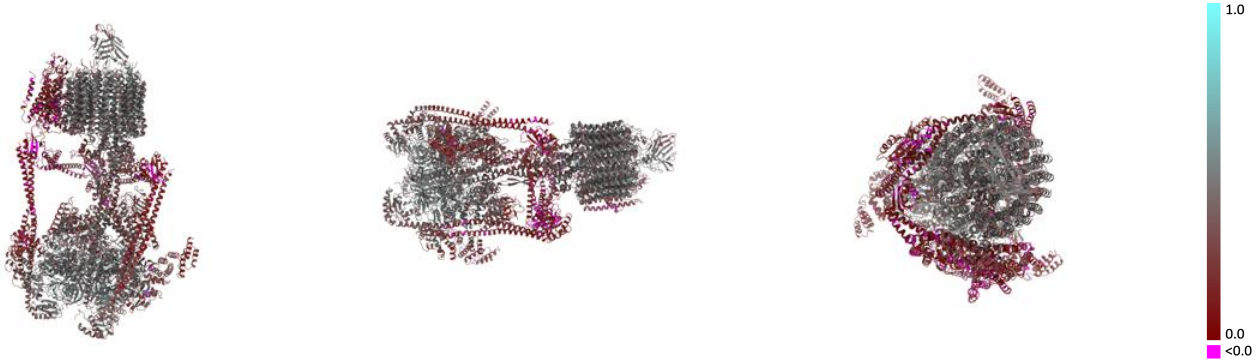
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0 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.

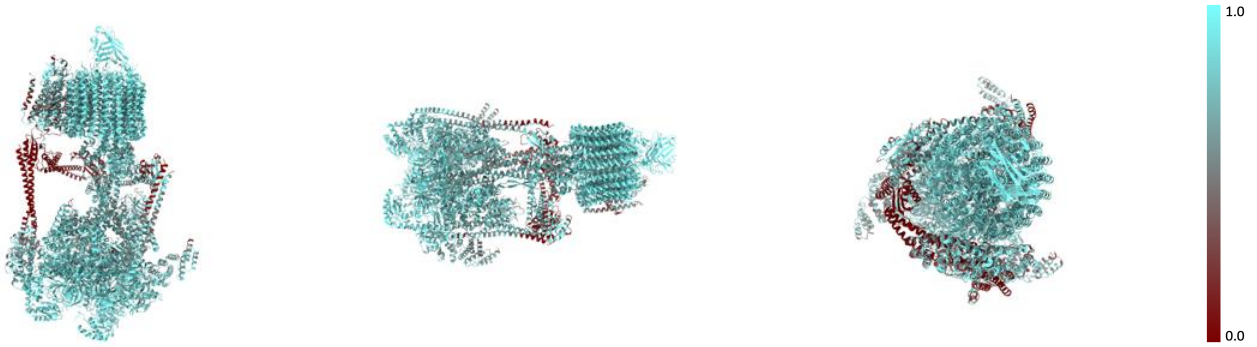
9.2 Q-score mapped to coordinate model (i)



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.

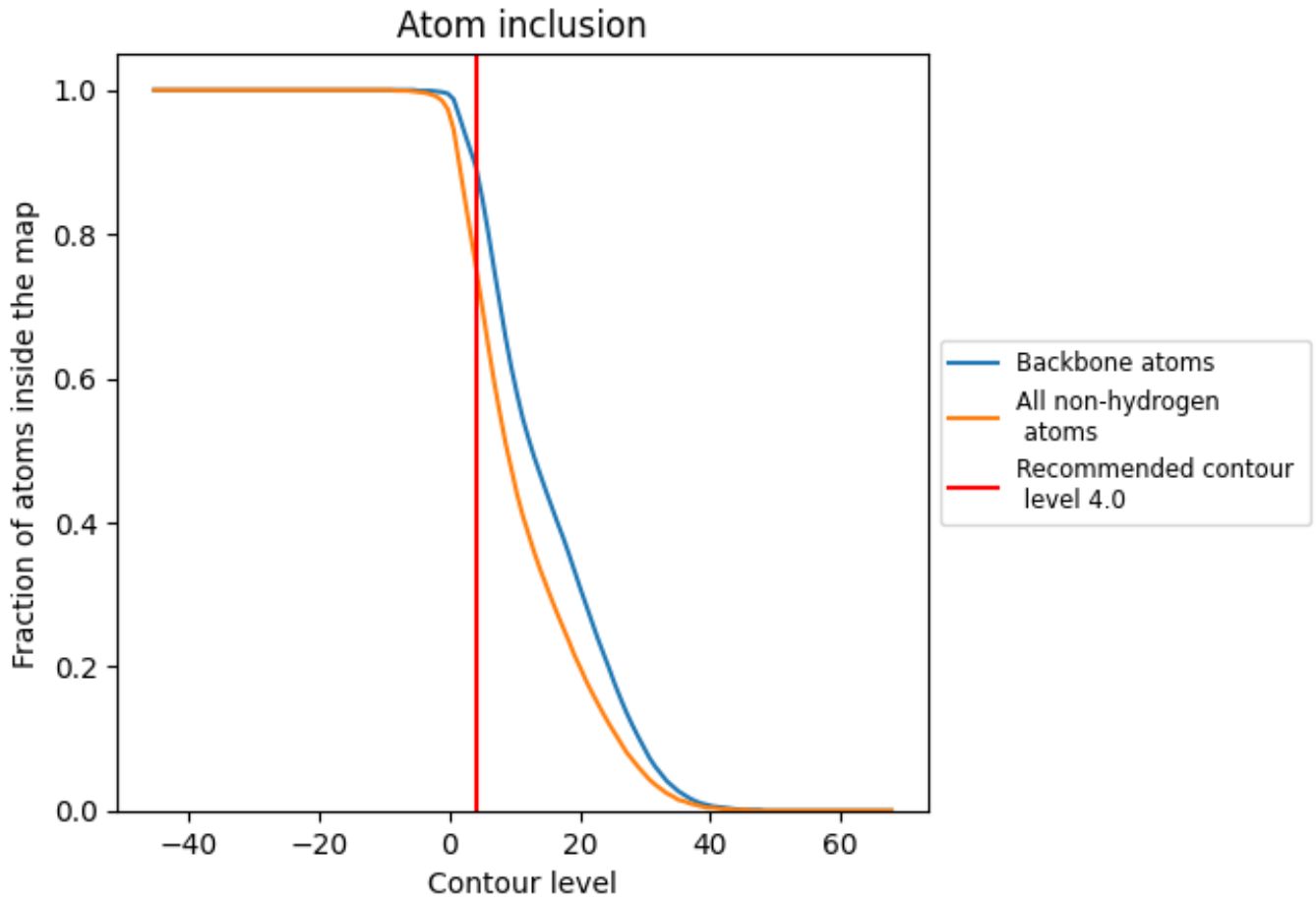
9.3 Atom inclusion mapped to coordinate model (i)



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 (4.0).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 76% 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 (4.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7590	0.3500
A	0.8580	0.4340
B	0.8310	0.4030
C	0.8520	0.4340
D	0.8580	0.4490
E	0.8900	0.4790
F	0.8540	0.4430
G	0.6070	0.1140
H	0.8050	0.3770
I	0.6370	0.3080
J	0.7460	0.3190
K	0.7280	0.3120
L	0.7640	0.3040
M	0.4520	0.2340
N	0.6030	0.2240
O	0.7130	0.2390
Q	0.6830	0.2550
R	0.7270	0.2780
S	0.6880	0.2640
T	0.7110	0.2700
a	0.3650	0.1320
b	0.8860	0.4530
c	0.9120	0.4330
d	0.8300	0.3930
e	0.5750	0.1710
f	0.5440	0.1240
g	0.8980	0.4560
h	0.8710	0.4350
i	0.8550	0.4260
j	0.8710	0.4270
k	0.8750	0.4450
l	0.8730	0.4350
m	0.8920	0.4410
n	0.8910	0.4510
o	0.8950	0.4510
p	0.8400	0.4110