



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:02 PM BST

PDB ID : 3J9T  
EMDB ID: : EMD-6284  
Title : Yeast V-ATPase state 1  
Authors : Zhao, J.; Benlekbir, S.; Rubinstein, J.L.  
Deposited on : 2015-02-23  
Resolution : 6.90 Å(reported)  
Based on PDB ID : 4DL0, 4RND, 1HO8, 1U7L

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241



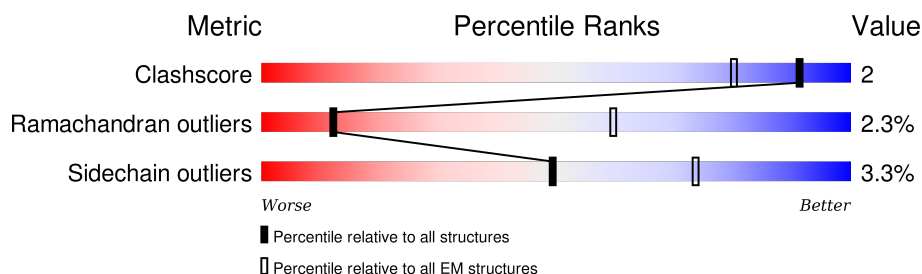
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.90 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)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686











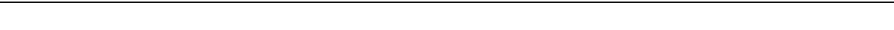

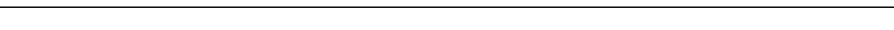






The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	M	256	59% 20% • 18%
2	N	118	77% 19% • •
3	A	616	67% 26% • •
3	C	616	72% 20% • •
3	E	616	68% 24% • •
4	B	517	61% 23% • 12%
4	D	517	64% 21% • • 12%
4	F	517	59% 25% • 12%
5	Q	345	73% 22% 5%

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Mol	Chain	Length	Quality of chain
6	H	114	
6	J	114	
6	L	114	
7	G	233	
7	I	233	
7	K	233	
8	P	478	
9	b	840	
10	O	392	
11	R	160	
11	S	160	
11	T	160	
11	U	160	
11	V	160	
11	W	160	
11	X	160	
11	Y	160	
11	Z	160	
11	a	160	



## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 57659 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	210	Total	C	N	O	S	0	0
			1691	1061	305	321	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	N	115	Total	C	N	O	0	0
			928	589	157	182		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	593	Total	C	N	O	S	0	0
			4578	2904	760	894	20		
3	C	593	Total	C	N	O	S	0	0
			4578	2904	760	894	20		
3	E	593	Total	C	N	O	S	0	0
			4578	2904	760	894	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	457	Total	C	N	O	S	0	0
			3585	2266	612	695	12		
4	D	457	Total	C	N	O	S	0	0
			3585	2266	612	695	12		
4	F	457	Total	C	N	O	S	0	0
			3585	2266	612	695	12		

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



Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	345	Total	C	N	O	S	0	0
			2802	1779	454	555	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	105	Total	C	N	O		0	0
			824	517	144	163			
6	H	105	Total	C	N	O		0	0
			824	517	144	163			
6	J	105	Total	C	N	O		0	0
			824	517	144	163			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	217	Total	C	N	O	S	0	0
			1731	1083	296	347	5		
7	G	217	Total	C	N	O	S	0	0
			1731	1083	296	347	5		
7	I	217	Total	C	N	O	S	0	0
			1731	1083	296	347	5		

- Molecule 8 is a protein called V-type proton ATPase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	461	Total	C	N	O	S	0	0
			3712	2373	623	704	12		

- Molecule 9 is a protein called V-type proton ATPase subunit a, vacuolar isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	b	312	Total	C	N	O	S	0	0
			2540	1614	434	489	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	392	Total	C	N	O	S	0	0
			3122	2005	516	596	5		

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



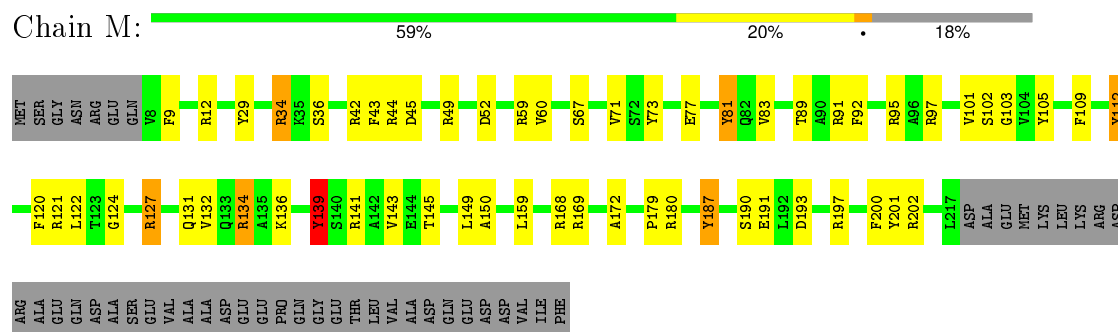
Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	R	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	U	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	V	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	T	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	W	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	S	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	X	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	Z	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	a	150	Total 1071	C 704	N 173	O 187	S 7	0	0



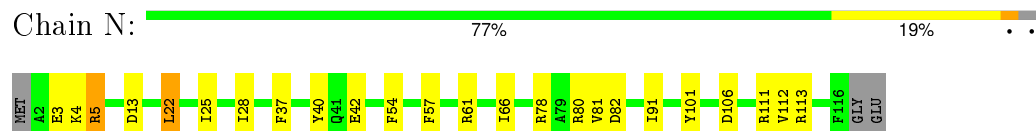
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

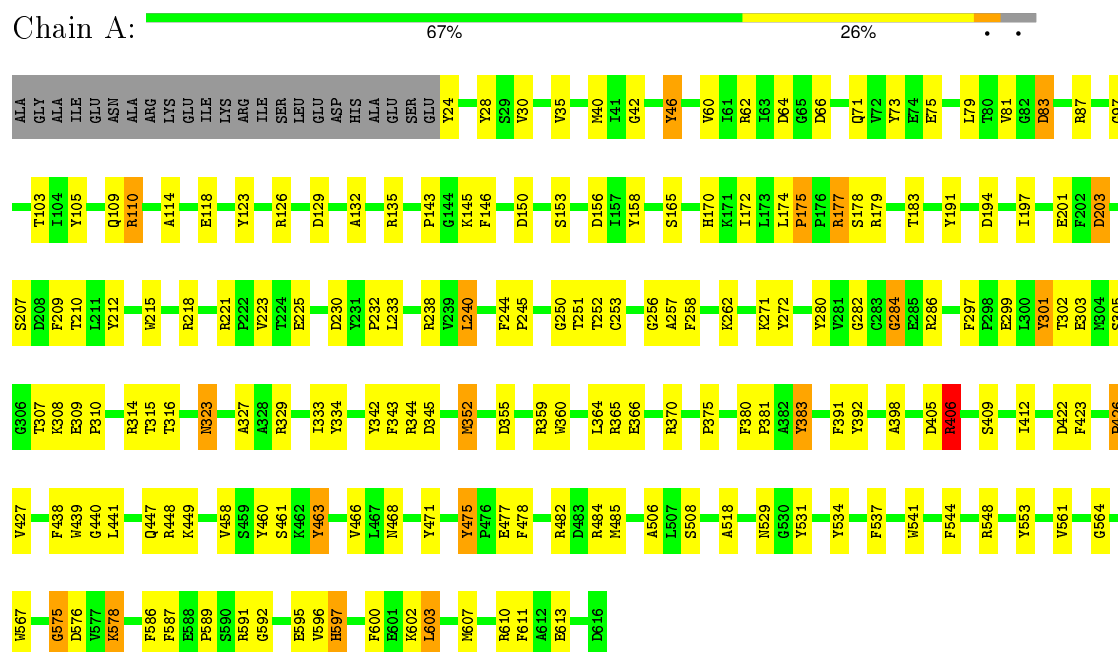
#### • Molecule 1: V-type proton ATPase subunit D



#### • Molecule 2: V-type proton ATPase subunit F



#### • Molecule 3: V-type proton ATPase catalytic subunit A





Chain C:  72% 20%

Chain C	Chain D	Chain E	Chain F	Chain G	Chain H	Chain I	Chain J	Chain K	Chain L	Chain M	Chain N	Chain O	Chain P	Chain Q	Chain R	Chain S	Chain T	Chain U	Chain V	Chain W	Chain X	Chain Y	Chain Z																																																																																																																																																																																																																																																																																																																				
V499	A506	L507	S508	L515	Q528	M529	Y534	D535	W541	F544	R548	A549	F550	Y553	E556	K559	A565	G575	V581	S582	S583	F586	S590	E595	E599	F600	L603	R610	F611	D616	K626	D630	D632	L633	R638	F644	Y647	R652	A655	P658	D661	Y663	V666	Y671	Y675	F678	R682	D683	R684	M685	E694	P695																																																																																																																																																																																																																																																																																							
R370	D377	Q378	Y383	A389	Y392	E393	R394	A398	P404	D405	R406	T407	G408	S417	P418	A419	G420	G421	D422	F423	S424	D425	T428	T435	F438	A446	Y460	S461	R462	Y463	V466	Y471	Y475	F478	R482	D483	R484	M485	E494	P495	Q499	R500	Y501	Y502	Y503	Y504	Y505	Y506	Y507	Y508	Y509	Y510	Y511	Y512	Y513	Y514	Y515	Y516	Y517	Y518	Y519	Y520	Y521	Y522	Y523	Y524	Y525	Y526	Y527	Y528	Y529	Y530	Y531	Y532	Y533	Y534	Y535	Y536	Y537	Y538	Y539	Y540	Y541	Y542	Y543	Y544	Y545	Y546	Y547	Y548	Y549	Y550	Y551	Y552	Y553	Y554	Y555	Y556	Y557	Y558	Y559	Y560	Y561	Y562	Y563	Y564	Y565	Y566	Y567	Y568	Y569	Y570	Y571	Y572	Y573	Y574	Y575	Y576	Y577	Y578	Y579	Y580	Y581	Y582	Y583	Y584	Y585	Y586	Y587	Y588	Y589	Y590	Y591	Y592	Y593	Y594	Y595	Y596	Y597	Y598	Y599	Y600	Y601	Y602	Y603	Y604	Y605	Y606	Y607	Y608	Y609	Y610	Y611	Y612	Y613	Y614	Y615	Y616	Y617	Y618	Y619	Y620	Y621	Y622	Y623	Y624	Y625	Y626	Y627	Y628	Y629	Y630	Y631	Y632	Y633	Y634	Y635	Y636	Y637	Y638	Y639	Y640	Y641	Y642	Y643	Y644	Y645	Y646	Y647	Y648	Y649	Y650	Y651	Y652	Y653	Y654	Y655	Y656	Y657	Y658	Y659	Y660	Y661	Y662	Y663	Y664	Y665	Y666	Y667	Y668	Y669	Y670	Y671	Y672	Y673	Y674	Y675	Y676	Y677	Y678	Y679	Y680	Y681	Y682	Y683	Y684	Y685	Y686	Y687	Y688	Y689	Y690	Y691	Y692	Y693	Y694	Y695	Y696	Y697	Y698	Y699	Y700	Y701	Y702	Y703	Y704	Y705	Y706	Y707	Y708	Y709	Y710	Y711	Y712	Y713	Y714	Y715	Y716	Y717	Y718	Y719	Y720	Y721	Y722	Y723	Y724	Y725	Y726	Y727	Y728	Y729	Y730	Y731	Y732	Y733	Y734	Y735	Y736	Y737	Y738	Y739	Y740	Y741	Y742	Y743	Y744	Y745	Y746	Y747	Y748	Y749	Y750	Y751	Y752	Y753	Y754	Y755	Y756	Y757	Y758	Y759	Y760	Y761	Y762	Y763	Y764	Y765	Y766	Y767	Y768	Y769	Y770	Y771	Y772	Y773	Y774	Y775	Y776	Y777	Y778	Y779	Y780	Y781	Y782	Y783	Y784	Y785	Y786	Y787	Y788	Y789

### Chain E:

Sequence logo for Chain E. The y-axis represents information content in bits, ranging from 0.00 to 1.50. The x-axis shows positions 1 to 100. A color scale at the top indicates conservation levels: 68% (green) and 24% (yellow).

Position	Amino Acid	Information Content (bits)
1	K594	0.10
2	E595	0.10
3	V596	0.10
4	H597	0.10
5	L603	0.10
6	M607	0.10
7	D608	0.10
8	R609	0.10
9	R610	0.10
10	F611	0.10
11	G612	0.10
12	S614	0.10
13	T615	0.10
14	D616	0.10
15	V466	0.10
16	F470	0.10
17	Y471	0.10
18	Y476	0.10
19	P477	0.10
20	E477	0.10
21	F478	0.10
22	L481	0.10
23	R482	0.10
24	P483	0.10
25	R484	0.10
26	Q497	0.10
27	Q500	0.10
28	L501	0.10
29	V502	0.10
30	D509	0.10
31	S510	0.10
32	D511	0.10
33	T514	0.10
34	E523	0.10
35	Q527	0.10
36	Q528	0.10
37	N529	0.10
38	G530	0.10
39	Y531	0.10
40	Y534	0.10
41	R548	0.10
42	A549	0.10
43	F550	0.10
44	V553	0.10
45	H554	0.10
46	A560	0.10
47	G564	0.10
48	A565	0.10
49	D572	0.10
50	S573	0.10
51	T574	0.10
52	G575	0.10
53	F586	0.10
54	F587	0.10
55	P588	0.10
56	R589	0.10
57	S590	0.10
58	S594	0.10
59	F343	0.10
60	R344	0.10
61	S351	0.10
62	R359	0.10
63	V360	0.10
64	A361	0.10
65	E362	0.10
66	A363	0.10
67	S368	0.10
68	M374	0.10
69	D377	0.10
70	Y383	0.10
71	F391	0.10
72	E392	0.10
73	R394	0.10
74	A395	0.10
75	G396	0.10
76	L401	0.10
77	D405	0.10
78	R406	0.10
79	S409	0.10
80	I412	0.10
81	V416	0.10
82	D425	0.10
83	T429	0.10
84	G433	0.10
85	I434	0.10
86	T435	0.10
87	F438	0.10
88	W439	0.10
89	R448	0.10
90	K449	0.10
91	H450	0.10
92	F451	0.10
93	I454	0.10
94	Y460	0.10
95	S461	0.10
96	K462	0.10
97	Y463	0.10
98	R221	0.10
99	P222	0.10
100	V223	0.10

Chain B:

Category	Amino Acid
Green	MET, VAL, LEU, SER, ASP, LYS, GLU, LEU, PHE, ALA, ILE, ASN, LYS, LYS, ALA, VAL, GLU, GLN, GLY, PHE, ASN, VAL, LYS, LYS, ARG, ARG, LEU, ASN, TYR, I29, T30, V31, S32, G33, V34, L38, L41, E42, K43, V44, K45, F46, P47, R48, Y49, R63, G64, G65, G66, V67, L68, V77, F80, T83, S84, G85, I86, E94, F95, S99, R111, D114, R118, P119, I120, D121, Y131, L132, P138, I139, M140, P141, Y142, A143, R144, I145, Y146, E149, M150, V155, D159, T160, M161, M162, A165, R166, F173, S174, A185, R189, V194, R195, P196, D202, E205, E206, M207, P208
Yellow	
Grey	



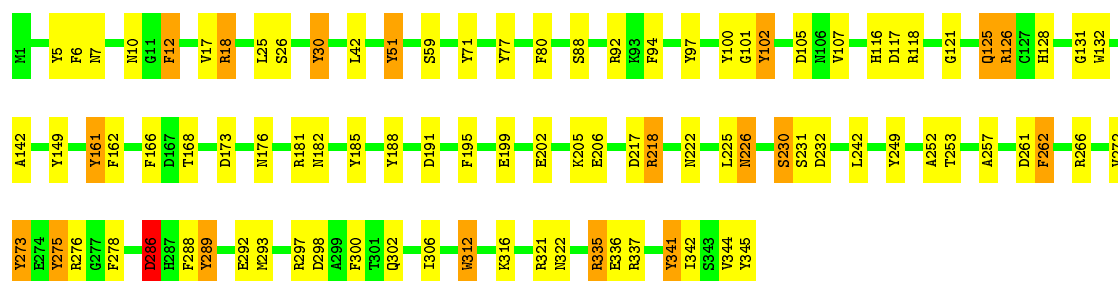
- Molecule 4: V-type proton ATPase subunit B

- Molecule 4: V-type proton ATPase subunit B

- Molecule 5: V-type proton ATPase subunit d



Chain Q: 



- Molecule 6: V-type proton ATPase subunit G

Chain L: 



- Molecule 6: V-type proton ATPase subunit G

Chain H: 



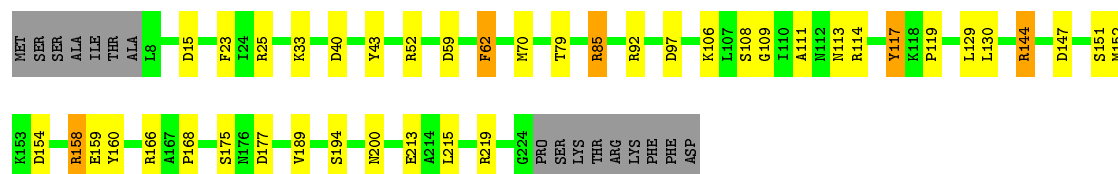
- Molecule 6: V-type proton ATPase subunit G

Chain J: 



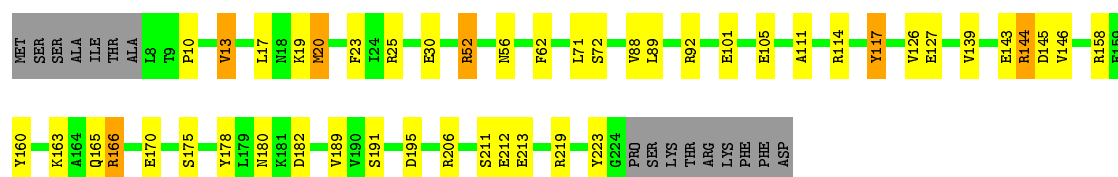
- Molecule 7: V-type proton ATPase subunit E

Chain K: 



- Molecule 7: V-type proton ATPase subunit E

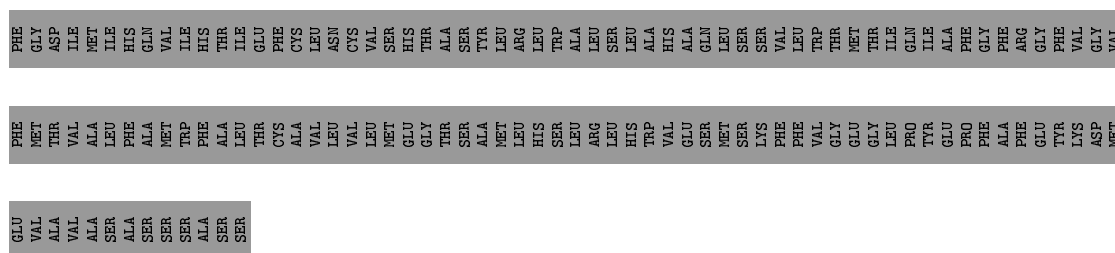
Chain G: 



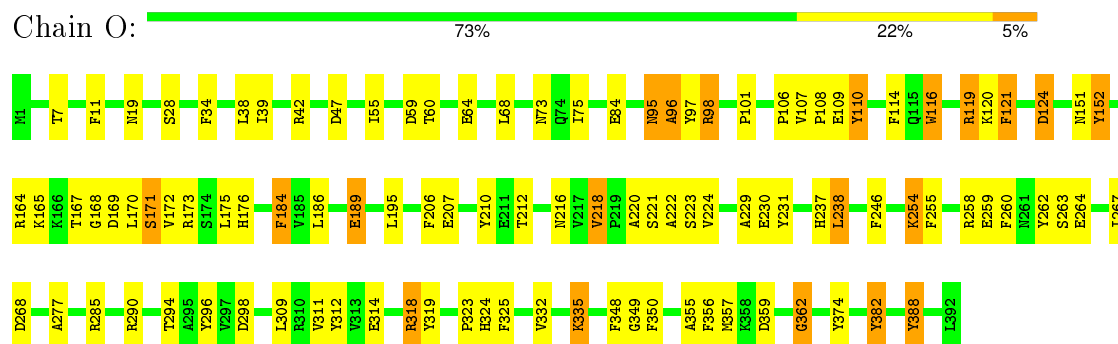




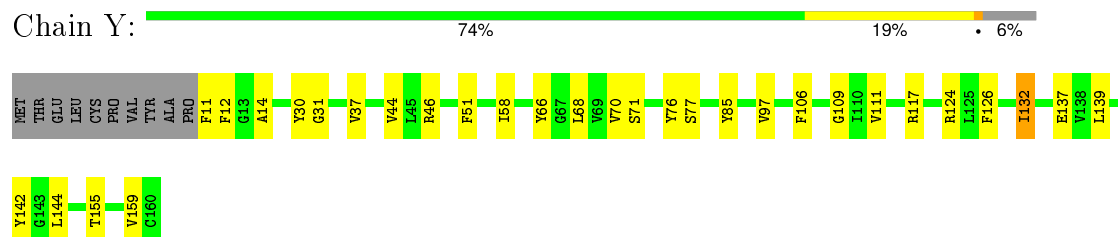




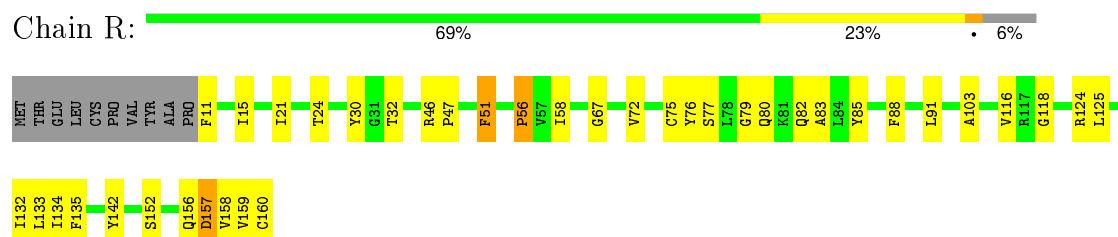
- Molecule 10: V-type proton ATPase subunit C



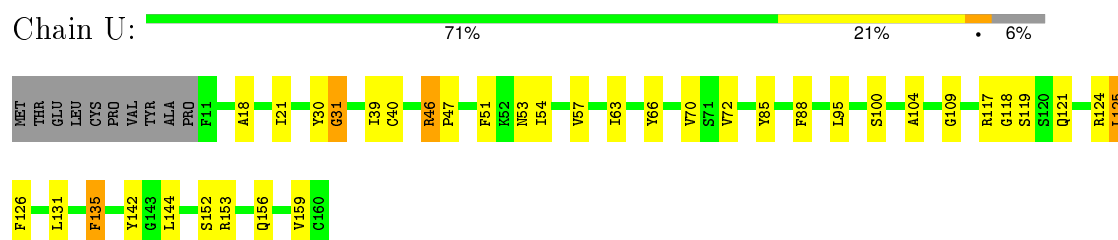
- Molecule 11: V-type proton ATPase subunit c



- Molecule 11: V-type proton ATPase subunit c

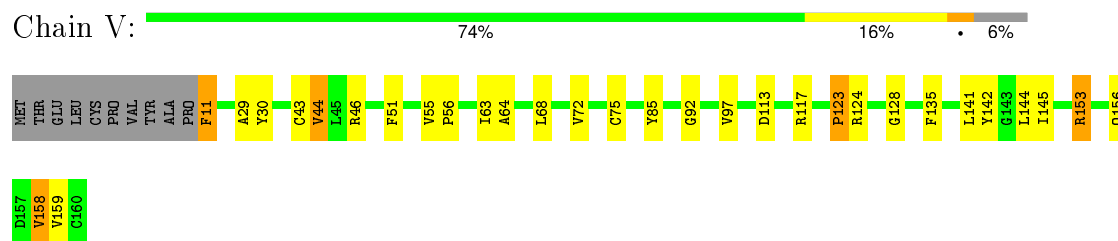


- Molecule 11: V-type proton ATPase subunit c

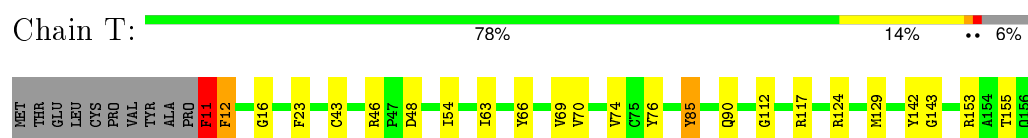




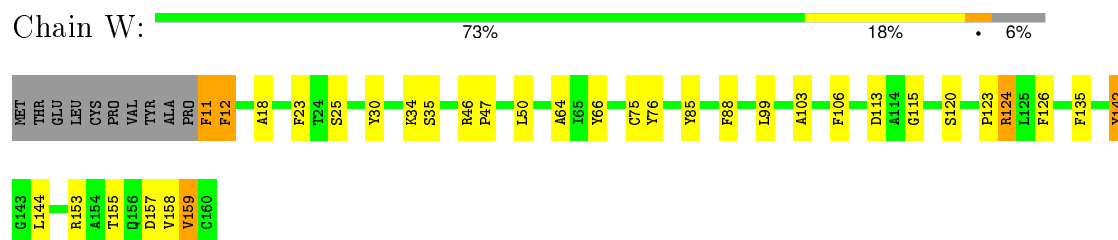
- Molecule 11: V-type proton ATPase subunit c



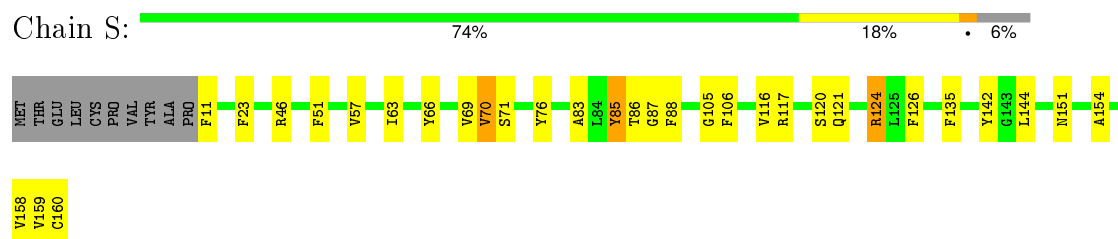
- Molecule 11: V-type proton ATPase subunit c



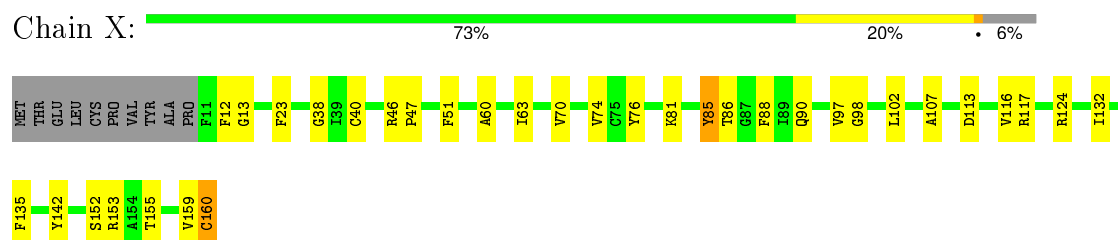
- Molecule 11: V-type proton ATPase subunit c



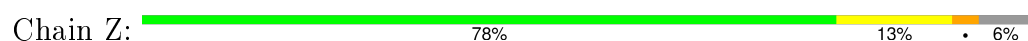
- Molecule 11: V-type proton ATPase subunit c



- Molecule 11: V-type proton ATPase subunit c



- Molecule 11: V-type proton ATPase subunit c







● Molecule 11: V-type proton ATPase subunit c





## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	50503	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	7000	Depositor
Magnification	34483	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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  >2	RMSZ	# Z  >2
1	M	1.76	20/1710 (1.2%)	1.95	49/2295 (2.1%)
10	O	1.69	25/3185 (0.8%)	1.95	81/4314 (1.9%)
11	R	1.65	8/1086 (0.7%)	1.96	26/1472 (1.8%)
11	S	1.67	10/1086 (0.9%)	1.89	21/1472 (1.4%)
11	T	1.65	9/1086 (0.8%)	1.89	27/1472 (1.8%)
11	U	1.65	7/1086 (0.6%)	1.91	19/1472 (1.3%)
11	V	1.68	6/1086 (0.6%)	1.94	22/1472 (1.5%)
11	W	1.69	7/1086 (0.6%)	2.07	36/1472 (2.4%)
11	X	1.72	15/1086 (1.4%)	1.87	20/1472 (1.4%)
11	Y	1.64	6/1086 (0.6%)	1.93	26/1472 (1.8%)
11	Z	1.65	7/1086 (0.6%)	1.85	18/1472 (1.2%)
11	a	1.68	10/1086 (0.9%)	1.87	24/1472 (1.6%)
2	N	1.68	7/944 (0.7%)	1.85	21/1277 (1.6%)
3	A	1.75	44/4677 (0.9%)	2.02	134/6339 (2.1%)
3	C	1.71	34/4677 (0.7%)	1.91	109/6339 (1.7%)
3	E	1.78	53/4677 (1.1%)	1.96	122/6339 (1.9%)
4	B	1.72	27/3654 (0.7%)	1.99	99/4953 (2.0%)
4	D	1.72	40/3654 (1.1%)	2.00	78/4953 (1.6%)
4	F	1.74	34/3654 (0.9%)	2.02	109/4953 (2.2%)
5	Q	1.75	23/2861 (0.8%)	1.99	73/3880 (1.9%)
6	H	1.58	2/828 (0.2%)	1.76	14/1098 (1.3%)
6	J	1.62	3/828 (0.4%)	1.85	20/1098 (1.8%)
6	L	1.65	6/828 (0.7%)	1.69	10/1098 (0.9%)
7	G	1.72	21/1743 (1.2%)	1.82	30/2338 (1.3%)
7	I	1.70	18/1743 (1.0%)	1.82	30/2338 (1.3%)
7	K	1.71	17/1743 (1.0%)	1.77	31/2338 (1.3%)
8	P	1.65	21/3766 (0.6%)	1.85	63/5087 (1.2%)
9	b	1.73	18/2578 (0.7%)	2.03	81/3479 (2.3%)
All	All	1.71	498/58610 (0.8%)	1.93	1393/79236 (1.8%)

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	M	0	7
10	O	0	12
11	S	0	1
11	T	0	4
11	U	0	2
11	V	0	2
11	W	0	4
11	X	0	1
11	Z	0	2
11	a	0	2
2	N	0	2
3	A	0	11
3	C	0	14
3	E	0	12
4	B	0	13
4	D	0	13
4	F	0	11
5	Q	0	14
6	L	0	2
7	G	0	4
7	I	0	3
7	K	0	5
8	P	0	9
9	b	0	14
All	All	0	164

The worst 5 of 498 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	X	160	CYS	CB-SG	11.36	2.01	1.82
8	P	392	TYR	CG-CD2	9.03	1.50	1.39
3	E	268	SER	CA-CB	8.92	1.66	1.52
9	b	248	ARG	NE-CZ	8.29	1.43	1.33
3	C	110	ARG	CD-NE	8.22	1.60	1.46

The worst 5 of 1393 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	406	ARG	NE-CZ-NH1	17.62	129.11	120.30
1	M	91	ARG	NE-CZ-NH1	17.37	128.98	120.30
4	B	485	TYR	CB-CG-CD1	17.28	131.37	121.00
4	D	111	ARG	NE-CZ-NH1	16.88	128.74	120.30
3	E	329	ARG	NE-CZ-NH1	16.34	128.47	120.30



There are no chirality outliers.

5 of 164 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	112	TYR	Sidechain
1	M	134	ARG	Sidechain
1	M	139	TYR	Sidechain
1	M	34	ARG	Sidechain
1	M	81	TYR	Sidechain

## 5.2 Too-close contacts

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	M	1691	0	1740	8	0
2	N	928	0	926	4	0
3	A	4578	0	4519	13	0
3	C	4578	0	4519	11	0
3	E	4578	0	4519	15	0
4	B	3585	0	3567	16	0
4	D	3585	0	3567	12	0
4	F	3585	0	3567	16	0
5	Q	2802	0	2689	9	0
6	H	824	0	877	5	0
6	J	824	0	877	5	0
6	L	824	0	877	3	0
7	G	1731	0	1797	6	0
7	I	1731	0	1797	7	0
7	K	1731	0	1797	1	0
8	P	3712	0	3829	11	0
9	b	2540	0	2537	0	0
10	O	3122	0	3155	8	0
11	R	1071	0	1141	2	0
11	S	1071	0	1141	3	0
11	T	1071	0	1141	3	0
11	U	1071	0	1141	11	0
11	V	1071	0	1141	24	0
11	W	1071	0	1141	5	0
11	X	1071	0	1141	4	0
11	Y	1071	0	1141	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	Z	1071	0	1141	8	0
11	a	1071	0	1141	0	0
All	All	57659	0	58566	191	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 2.

The worst 5 of 191 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)
11:X:160:CYS:CB	11:X:160:CYS:SG	2.01	1.47
11:V:141:LEU:HA	11:V:144:LEU:CD2	1.71	1.21
11:V:141:LEU:O	11:V:144:LEU:HG	1.48	1.13
11:V:141:LEU:HA	11:V:144:LEU:HD21	1.23	1.08
11:Z:66:TYR:HB3	11:Z:144:LEU:HD22	1.33	1.05

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	M	208/256 (81%)	206 (99%)	2 (1%)	0	100	100
2	N	113/118 (96%)	102 (90%)	10 (9%)	1 (1%)	21	67
3	A	591/616 (96%)	541 (92%)	31 (5%)	19 (3%)	5	41
3	C	591/616 (96%)	538 (91%)	37 (6%)	16 (3%)	6	45
3	E	591/616 (96%)	542 (92%)	32 (5%)	17 (3%)	6	43
4	B	455/517 (88%)	413 (91%)	27 (6%)	15 (3%)	5	40
4	D	455/517 (88%)	416 (91%)	25 (6%)	14 (3%)	5	42
4	F	455/517 (88%)	411 (90%)	30 (7%)	14 (3%)	5	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Q	343/345 (99%)	318 (93%)	18 (5%)	7 (2%)	9	51
6	H	103/114 (90%)	99 (96%)	3 (3%)	1 (1%)	19	65
6	J	103/114 (90%)	100 (97%)	3 (3%)	0	100	100
6	L	103/114 (90%)	98 (95%)	4 (4%)	1 (1%)	19	65
7	G	215/233 (92%)	207 (96%)	7 (3%)	1 (0%)	34	77
7	I	215/233 (92%)	208 (97%)	6 (3%)	1 (0%)	34	77
7	K	215/233 (92%)	205 (95%)	9 (4%)	1 (0%)	34	77
8	P	457/478 (96%)	431 (94%)	18 (4%)	8 (2%)	11	53
9	b	306/840 (36%)	274 (90%)	25 (8%)	7 (2%)	8	48
10	O	390/392 (100%)	350 (90%)	21 (5%)	19 (5%)	3	31
11	R	148/160 (92%)	138 (93%)	6 (4%)	4 (3%)	6	45
11	S	148/160 (92%)	140 (95%)	6 (4%)	2 (1%)	14	58
11	T	148/160 (92%)	143 (97%)	5 (3%)	0	100	100
11	U	148/160 (92%)	140 (95%)	5 (3%)	3 (2%)	9	51
11	V	148/160 (92%)	139 (94%)	5 (3%)	4 (3%)	6	45
11	W	148/160 (92%)	137 (93%)	8 (5%)	3 (2%)	9	51
11	X	148/160 (92%)	138 (93%)	8 (5%)	2 (1%)	14	58
11	Y	148/160 (92%)	139 (94%)	8 (5%)	1 (1%)	26	71
11	Z	148/160 (92%)	136 (92%)	9 (6%)	3 (2%)	9	51
11	a	148/160 (92%)	138 (93%)	7 (5%)	3 (2%)	9	51
All	All	7389/8469 (87%)	6847 (93%)	375 (5%)	167 (2%)	12	48

5 of 167 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	257	ALA
3	A	475	TYR
4	B	292	SER
3	C	475	TYR
3	C	529	ASN

### 5.3.2 Protein sidechains ⓘ

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	M	183/221 (83%)	181 (99%)	2 (1%)	80	91
2	N	102/104 (98%)	101 (99%)	1 (1%)	82	92
3	A	497/515 (96%)	479 (96%)	18 (4%)	42	74
3	C	497/515 (96%)	472 (95%)	25 (5%)	30	66
3	E	497/515 (96%)	473 (95%)	24 (5%)	31	67
4	B	391/444 (88%)	370 (95%)	21 (5%)	27	64
4	D	391/444 (88%)	384 (98%)	7 (2%)	66	87
4	F	391/444 (88%)	374 (96%)	17 (4%)	35	70
5	Q	309/309 (100%)	296 (96%)	13 (4%)	36	70
6	H	87/94 (93%)	84 (97%)	3 (3%)	44	75
6	J	87/94 (93%)	87 (100%)	0	100	100
6	L	87/94 (93%)	84 (97%)	3 (3%)	44	75
7	G	194/208 (93%)	190 (98%)	4 (2%)	61	84
7	I	194/208 (93%)	189 (97%)	5 (3%)	54	80
7	K	194/208 (93%)	189 (97%)	5 (3%)	54	80
8	P	426/439 (97%)	417 (98%)	9 (2%)	61	84
9	b	275/728 (38%)	265 (96%)	10 (4%)	42	74
10	O	348/348 (100%)	339 (97%)	9 (3%)	54	80
11	R	110/119 (92%)	104 (94%)	6 (6%)	27	63
11	S	110/119 (92%)	106 (96%)	4 (4%)	42	74
11	T	110/119 (92%)	107 (97%)	3 (3%)	52	79
11	U	110/119 (92%)	106 (96%)	4 (4%)	42	74
11	V	110/119 (92%)	107 (97%)	3 (3%)	52	79
11	W	110/119 (92%)	109 (99%)	1 (1%)	84	93
11	X	110/119 (92%)	107 (97%)	3 (3%)	52	79
11	Y	110/119 (92%)	107 (97%)	3 (3%)	52	79
11	Z	110/119 (92%)	108 (98%)	2 (2%)	66	87
11	a	110/119 (92%)	108 (98%)	2 (2%)	66	87
All	All	6250/7122 (88%)	6043 (97%)	207 (3%)	49	76



5 of 207 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	478	PHE
5	Q	59	SER
11	V	153	ARG
3	E	588	GLU
4	F	206	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
3	E	554	HIS
6	L	12	GLN
11	Y	90	GLN
3	E	608	GLN
5	Q	255	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.