



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Apr 13, 2019 – 12:41 PM EDT

PDB ID : 6O7V
EMDB ID: : EMD-0646
Title : Saccharomyces cerevisiae V-ATPase Stv1-V1VO State 1
Authors : Vasanthakumar, T.; Bueler, S.A.; Wu, D.; Beilsten-Edmands, V.; Robinson, C.V.; Rubinstein, J.L.
Deposited on : 2019-03-08
Resolution : 6.60 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB 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.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

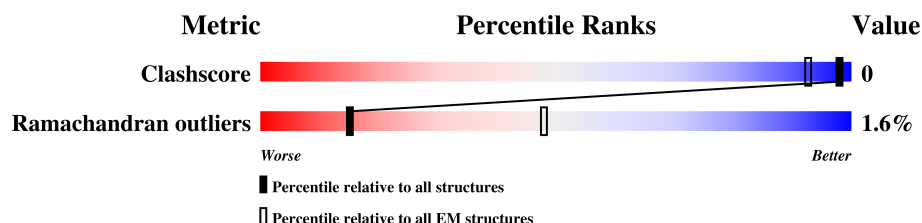
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.











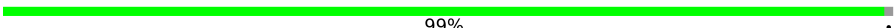
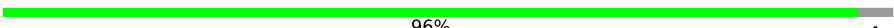
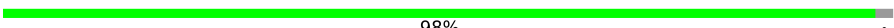
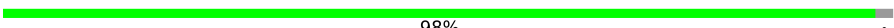
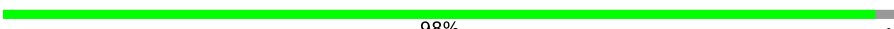
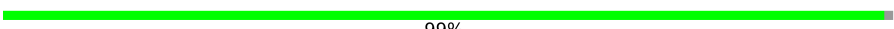
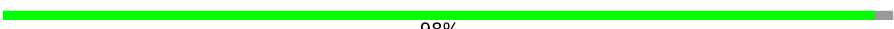
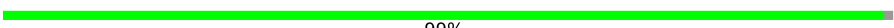
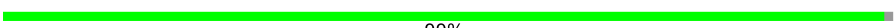
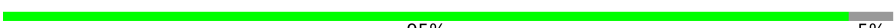


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663

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 ≥ 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	 77% 5% 18%
2	N	118	 92% 5% .
3	A	639	 85% 8% . 7%
3	C	639	 87% 5% . 7%
3	E	639	 84% 8% . 7%
4	B	517	 80% 8% . 12%
4	D	517	 82% 6% 12%
4	F	517	 80% 7% . 12%
5	H	114	 89% . 8%
5	J	114	 86% 6% 8%
5	L	114	 89% . 8%

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Mol	Chain	Length	Quality of chain
6	G	233	 87% 6% 7%
6	I	233	 89% 7%
6	K	233	 88% 5% 7%
7	P	478	 92% . . .
8	O	392	 91% 7% .
9	a	890	 70% 30%
10	b	265	 17% 83%
11	c	213	 92% 8%
12	d	345	 99% .
13	g	160	 96% .
13	h	160	 98% .
13	i	160	 98% .
13	j	160	 98% .
13	k	160	 99% .
13	l	160	 98% .
13	m	160	 99% .
13	n	160	 99% .
14	o	164	 95% 5%
15	e	73	 88% 12%
16	f	85	 72% 28%

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 39578 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	0	0
			1039	619	210	210		

- 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
			571	341	115	115		

- Molecule 3 is a protein called Vacuolar ATP synthase catalytic subunit A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	A	593	Total	C	N	O	0	0
			2915	1729	593	593		
3	C	593	Total	C	N	O	0	0
			2915	1729	593	593		
3	E	593	Total	C	N	O	0	0
			2915	1729	593	593		

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	617	ASP	-	SEE REMARK 999	UNP B3LH69
A	618	TYR	-	SEE REMARK 999	UNP B3LH69
A	619	LYS	-	SEE REMARK 999	UNP B3LH69
A	620	ASP	-	SEE REMARK 999	UNP B3LH69
A	621	HIS	-	SEE REMARK 999	UNP B3LH69
A	622	ASP	-	SEE REMARK 999	UNP B3LH69
A	623	GLY	-	SEE REMARK 999	UNP B3LH69
A	624	ASP	-	SEE REMARK 999	UNP B3LH69
A	625	TYR	-	SEE REMARK 999	UNP B3LH69
A	626	LYS	-	SEE REMARK 999	UNP B3LH69
A	627	ASP	-	SEE REMARK 999	UNP B3LH69

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Chain	Residue	Modelled	Actual	Comment	Reference
A	628	HIS	-	SEE REMARK 999	UNP B3LH69
A	629	ASP	-	SEE REMARK 999	UNP B3LH69
A	630	ILE	-	SEE REMARK 999	UNP B3LH69
A	631	ASP	-	SEE REMARK 999	UNP B3LH69
A	632	TYR	-	SEE REMARK 999	UNP B3LH69
A	633	LYS	-	SEE REMARK 999	UNP B3LH69
A	634	ASP	-	SEE REMARK 999	UNP B3LH69
A	635	ASP	-	SEE REMARK 999	UNP B3LH69
A	636	ASP	-	SEE REMARK 999	UNP B3LH69
A	637	ASP	-	SEE REMARK 999	UNP B3LH69
A	638	LYS	-	SEE REMARK 999	UNP B3LH69
C	617	ASP	-	SEE REMARK 999	UNP B3LH69
C	618	TYR	-	SEE REMARK 999	UNP B3LH69
C	619	LYS	-	SEE REMARK 999	UNP B3LH69
C	620	ASP	-	SEE REMARK 999	UNP B3LH69
C	621	HIS	-	SEE REMARK 999	UNP B3LH69
C	622	ASP	-	SEE REMARK 999	UNP B3LH69
C	623	GLY	-	SEE REMARK 999	UNP B3LH69
C	624	ASP	-	SEE REMARK 999	UNP B3LH69
C	625	TYR	-	SEE REMARK 999	UNP B3LH69
C	626	LYS	-	SEE REMARK 999	UNP B3LH69
C	627	ASP	-	SEE REMARK 999	UNP B3LH69
C	628	HIS	-	SEE REMARK 999	UNP B3LH69
C	629	ASP	-	SEE REMARK 999	UNP B3LH69
C	630	ILE	-	SEE REMARK 999	UNP B3LH69
C	631	ASP	-	SEE REMARK 999	UNP B3LH69
C	632	TYR	-	SEE REMARK 999	UNP B3LH69
C	633	LYS	-	SEE REMARK 999	UNP B3LH69
C	634	ASP	-	SEE REMARK 999	UNP B3LH69
C	635	ASP	-	SEE REMARK 999	UNP B3LH69
C	636	ASP	-	SEE REMARK 999	UNP B3LH69
C	637	ASP	-	SEE REMARK 999	UNP B3LH69
C	638	LYS	-	SEE REMARK 999	UNP B3LH69
E	617	ASP	-	SEE REMARK 999	UNP B3LH69
E	618	TYR	-	SEE REMARK 999	UNP B3LH69
E	619	LYS	-	SEE REMARK 999	UNP B3LH69
E	620	ASP	-	SEE REMARK 999	UNP B3LH69
E	621	HIS	-	SEE REMARK 999	UNP B3LH69
E	622	ASP	-	SEE REMARK 999	UNP B3LH69
E	623	GLY	-	SEE REMARK 999	UNP B3LH69
E	624	ASP	-	SEE REMARK 999	UNP B3LH69
E	625	TYR	-	SEE REMARK 999	UNP B3LH69

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Chain	Residue	Modelled	Actual	Comment	Reference
E	626	LYS	-	SEE REMARK 999	UNP B3LH69
E	627	ASP	-	SEE REMARK 999	UNP B3LH69
E	628	HIS	-	SEE REMARK 999	UNP B3LH69
E	629	ASP	-	SEE REMARK 999	UNP B3LH69
E	630	ILE	-	SEE REMARK 999	UNP B3LH69
E	631	ASP	-	SEE REMARK 999	UNP B3LH69
E	632	TYR	-	SEE REMARK 999	UNP B3LH69
E	633	LYS	-	SEE REMARK 999	UNP B3LH69
E	634	ASP	-	SEE REMARK 999	UNP B3LH69
E	635	ASP	-	SEE REMARK 999	UNP B3LH69
E	636	ASP	-	SEE REMARK 999	UNP B3LH69
E	637	ASP	-	SEE REMARK 999	UNP B3LH69
E	638	LYS	-	SEE REMARK 999	UNP B3LH69

- 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	0	0
			2250	1336	457	457		
4	D	457	Total	C	N	O	0	0
			2250	1336	457	457		
4	F	457	Total	C	N	O	0	0
			2250	1336	457	457		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	L	105	Total	C	N	O	0	0
			519	309	105	105		
5	H	105	Total	C	N	O	0	0
			519	309	105	105		
5	J	105	Total	C	N	O	0	0
			519	309	105	105		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	K	217	Total	C	N	O	0	0
			1078	644	217	217		
6	G	217	Total	C	N	O	0	0
			1078	644	217	217		

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Mol	Chain	Residues	Atoms				AltConf	Trace
6	I	217	Total	C	N	O	0	0
			1078	644	217	217		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	P	461	Total	C	N	O	0	0
			2292	1370	461	461		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	O	392	Total	C	N	O	0	0
			1947	1163	392	392		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	a	625	Total	C	N	O	0	0
			3092	1842	625	625		

- Molecule 10 is a protein called V0 assembly protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	b	44	Total	C	N	O	0	0
			218	130	44	44		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	c	197	Total	C	N	O	0	0
			962	568	197	197		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	d	343	Total	C	N	O	0	0
			1699	1013	343	343		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	g	153	Total	C	N	O	0	0
			743	437	153	153		
13	h	157	Total	C	N	O	0	0
			763	449	157	157		
13	i	157	Total	C	N	O	0	0
			763	449	157	157		
13	j	156	Total	C	N	O	0	0
			758	446	156	156		
13	k	158	Total	C	N	O	0	0
			768	452	158	158		
13	l	157	Total	C	N	O	0	0
			763	449	157	157		
13	m	158	Total	C	N	O	0	0
			768	452	158	158		
13	n	158	Total	C	N	O	0	0
			768	452	158	158		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	o	156	Total	C	N	O	0	0
			758	446	156	156		

- Molecule 15 is a protein called V-type proton ATPase subunit e.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	e	64	Total	C	N	O	0	0
			319	191	64	64		

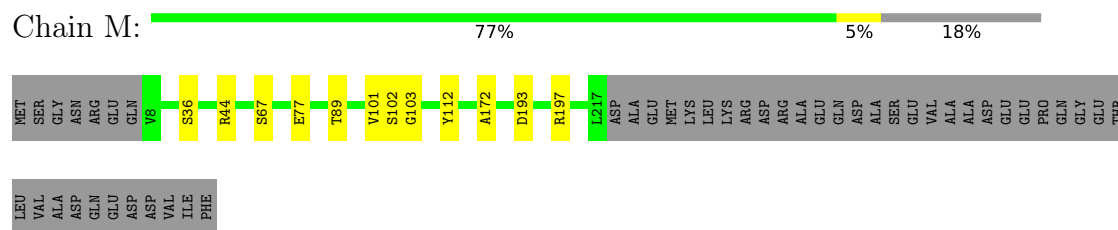
- Molecule 16 is a protein called Putative protein YPR170W-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	f	61	Total	C	N	O	0	0
			301	179	61	61		

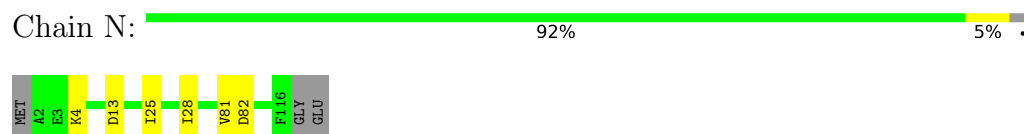
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

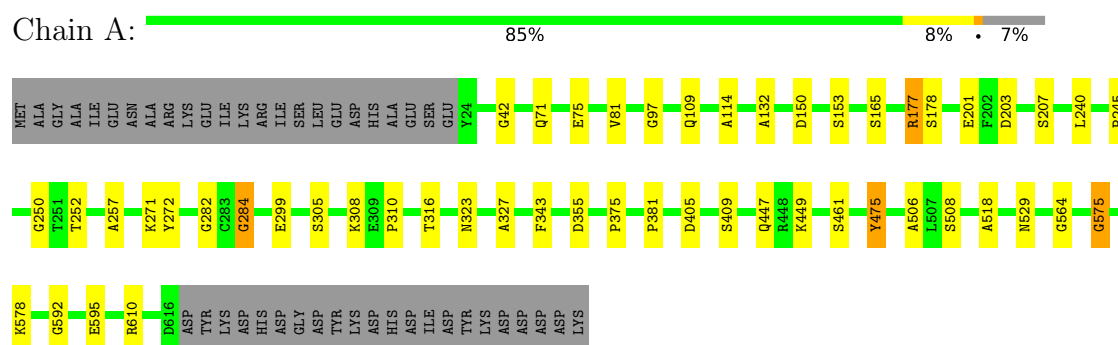
- Molecule 1: V-type proton ATPase subunit D



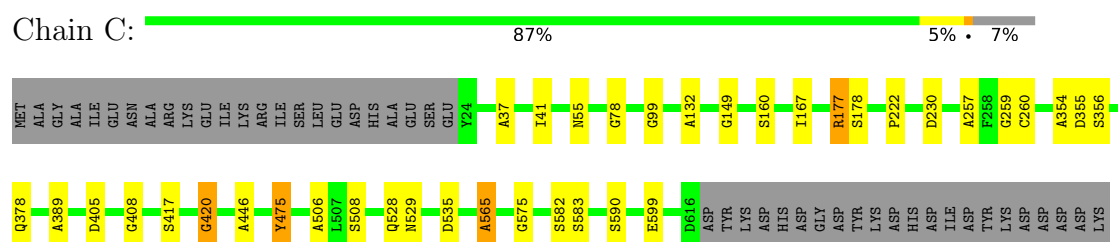
- Molecule 2: V-type proton ATPase subunit F



- Molecule 3: Vacuolar ATP synthase catalytic subunit A



- Molecule 3: Vacuolar ATP synthase catalytic subunit A



- Molecule 3: Vacuolar ATP synthase catalytic subunit A


P589	P216	MET
S590	D230	ALA
K594	V247	ALA
E595	A257	ILE
S614	F258	GLU
T615	G259	ASN
D616	S266	ALA
ASP	Q267	ARG
TYR	S268	LYS
LYS	S268	GLU
ASP	S268	ILE
HIS	K308	SER
ASP	E309	LEU
GLY	P310	GLU
ASP	I311	ASP
TYR	T315	HIS
LYS	P325	ALA
HIS	S326	ALA
ASP	A327	GLU
ASP	E330	SER
ILE	A331	GLU
ASP	S332	ASP
ASP	S351	ASP
ASP	A363	LYS
LYS	S368	
	G396	
	S409	
	G433	
	W439	
	K449	
	S461	
	Y475	
	N529	
	A560	
	G564	
	A565	
	S573	
	T574	
	C575	
	S597	

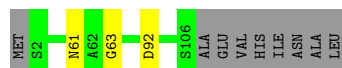
PRO	THR	ARG	SER	GLY	LYS	LYS	LYS	ALA	SER	GLN	GLU	SER	ILE		A185	D202	N207	F208	S209	A214	N215	L240	F241	A245	E271	A287	S292	A293	A294	P305	A319	P333	P372	P377	A386	K391	A414	A415	S426	L433	V435	ASP	ARG	ALA	ARG	ASP	ALA	ASP	GLU	GLU	GLU	ASP
MET	VAL	LEU	SER	ASP	LYS	GLU	PHE	ALA	ASN	ILE	GLN	GLY	PHE	ASN	VAL	LYS	PRO	ARG	LEU	ASN	TYR	N29	T30	V31	V34	K43	V44	R63	G64	G65	T83	S84	E94	S99	P138	I139	N140	P141	V142	A143	E149	M161	A165									

ALA	SER	GLN	GLU	GLU	SER	LEU	ILE	A175	VAL	SER	ASP	LYS	GLU	PHE	ALA	ASN	LYS	ALA	VAL	GLU	GLN	GLY	PHE	ASN	VAL	LYS	PRO	ARG	LEU	ASN	TYR	N29
								L178	LEU	ASP	LYS	GLU	PHE	ALA	ASN	LYS	ALA	VAL	GLU	GLN	GLY	PHE	ASN	VAL	LYS	PRO	ARG	LEU	ASN	TYR	S32	
								A184	LEU	ASP	LYS	GLU	PHE	ALA	ASN	LYS	ALA	VAL	GLU	GLN	GLY	PHE	ASN	VAL	LYS	PRO	ARG	LEU	ASN	TYR	L41	
								D202	LEU	ASP	LYS	GLU	PHE	ALA	ASN	LYS	ALA	VAL	GLU	GLN	GLY	PHE	ASN	VAL	LYS	PRO	ARG	LEU	ASN	TYR	F46	
								A259	LEU	ASP	LYS	GLU	PHE	ALA	ASN	LYS	ALA	VAL	GLU	GLN	GLY	PHE	ASN	VAL	LYS	PRO	ARG	LEU	ASN	TYR	P47	
								Q269	LEU	ASP	LYS	GLU	PHE	ALA	ASN	LYS	ALA	VAL	GLU	GLN	GLY	PHE	ASN	VAL	LYS	PRO	ARG	LEU	ASN	TYR	R48	
								L288	LEU	ASP	LYS	GLU	PHE	ALA	ASN	LYS	ALA	VAL	GLU	GLN	GLY	PHE	ASN	VAL	LYS	PRO	ARG	LEU	ASN	TYR	E51	
								A319	LEU	ASP	LYS	GLU	PHE	ALA	ASN	LYS	ALA	VAL	GLU	GLN	GLY	PHE	ASN	VAL	LYS	PRO	ARG	LEU	ASN	TYR	P58	
								G324	LEU	ASP	LYS	GLU	PHE	ALA	ASN	LYS	ALA	VAL	GLU	GLN	GLY	PHE	ASN	VAL	LYS	PRO	ARG	LEU	ASN	TYR	D59	
								T330	LEU	ASP	LYS	GLU	PHE	ALA	ASN	LYS	ALA	VAL	GLU	GLN	GLY	PHE	ASN	VAL	LYS	PRO	ARG	LEU	ASN	TYR	G60	
								D340	LEU	ASP	LYS	GLU	PHE	ALA	ASN	LYS	ALA	VAL	GLU	GLN	GLY	PHE	ASN	VAL	LYS	PRO	ARG	LEU	ASN	TYR	T61	
								S380	LEU	ASP	LYS	GLU	PHE	ALA	ASN	LYS	ALA	VAL	GLU	GLN	GLY	PHE	ASN	VAL	LYS	PRO	ARG	LEU	ASN	TYR	V93	
								M383	LEU	ASP	LYS	GLU	PHE	ALA	ASN	LYS	ALA	VAL	GLU	GLN	GLY	PHE	ASN	VAL	LYS	PRO	ARG	LEU	ASN	TYR	E94	
								G390	LEU	ASP	LYS	GLU	PHE	ALA	ASN	LYS	ALA	VAL	GLU	GLN	GLY	PHE	ASN	VAL	LYS	PRO	ARG	LEU	ASN	TYR	S99	
								M391	LEU	ASP	LYS	GLU	PHE	ALA	ASN	LYS	ALA	VAL	GLU	GLN	GLY	PHE	ASN	VAL	LYS	PRO	ARG	LEU	ASN	TYR	N122	
								Q402	LEU	ASP	LYS	GLU	PHE	ALA	ASN	LYS	ALA	VAL	GLU	GLN	GLY	PHE	ASN	VAL	LYS	PRO	ARG	LEU	ASN	TYR	F127	
								L467	LEU	ASP	LYS	GLU	PHE	ALA	ASN	LYS	ALA	VAL	GLU	GLN	GLY	PHE	ASN	VAL	LYS	PRO	ARG	LEU	ASN	TYR	P141	
								N474	LEU	ASP	LYS	GLU	PHE	ALA	ASN	LYS	ALA	VAL	GLU	GLN	GLY	PHE	ASN	VAL	LYS	PRO	ARG	LEU	ASN	TYR	S163	
								Y485	LEU	ASP	LYS	GLU	PHE	ALA	ASN	LYS	ALA	VAL	GLU	GLN	GLY	PHE	ASN	VAL	LYS	PRO	ARG	LEU	ASN	TYR	G167	
								ASP	LEU	ASP	LYS	GLU	PHE	ALA	ASN	LYS	ALA	VAL	GLU	GLN	GLY	PHE	ASN	VAL	LYS	PRO	ARG	LEU	ASN	TYR		
								ARG	LEU	ASP	LYS	GLU	PHE	ALA	ASN	LYS	ALA	VAL	GLU	GLN	GLY	PHE	ASN	VAL	LYS	PRO	ARG	LEU	ASN	TYR		


ASP	D202	MET
PRO	G203	VAL
ASP	H204	LEU
THR		SER
ARG	S209	ASP
SER		LYS
	A222	GLU
GLY		LEU
LYS	Q227	PHE
LYS		ALA
LYS	N232	TLE
ASP		ASN
ALA	T279	LYS
SER		LYS
GLN	V291	ALA
GLU	S292	VAL
GLU		GLU
SER	P305	GLN
LEU		GLY
TLE	N326	PHE
		ASN
	I346	VAL
		LYS
	D361	PRO
		ARG
	P377	LEU
		LEU
	K384	ASN
		TYR
	M391	V29
		V44
	D395	
		G72
	A424	
		V104
	K430	A128
	Q446	S137
	G447	P138
	A448	
		P141
	L465	Y142
		A143
	P478	R144
		I145
	D482	
		E148
	Y485	E149
ASP	ARG	
ALA	ALA	S152
ARG	ARG	
ASP	ASP	G167
ALA	ALA	
ASP	ASP	P179
GLU	GLU	A185
ASP	ASP	
GLU	GLU	A191




Chain L:  89% 8%




- Molecule 5: V-type proton ATPase subunit G

Chain H:  89% 8%




- Molecule 5: V-type proton ATPase subunit G

Chain J:  86% 6% 8%




- Molecule 6: V-type proton ATPase subunit E

Chain K:  88% 5% 7%




- Molecule 6: V-type proton ATPase subunit E

Chain G:  87% 6% 7%



- Molecule 6: V-type proton ATPase subunit E

Chain I:  89% 7%



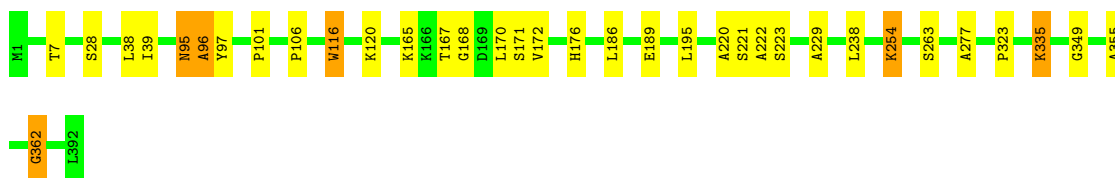
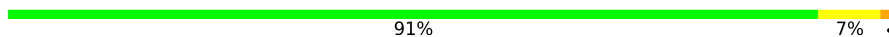
- Molecule 7: V-type proton ATPase subunit H

Chain P:  92%



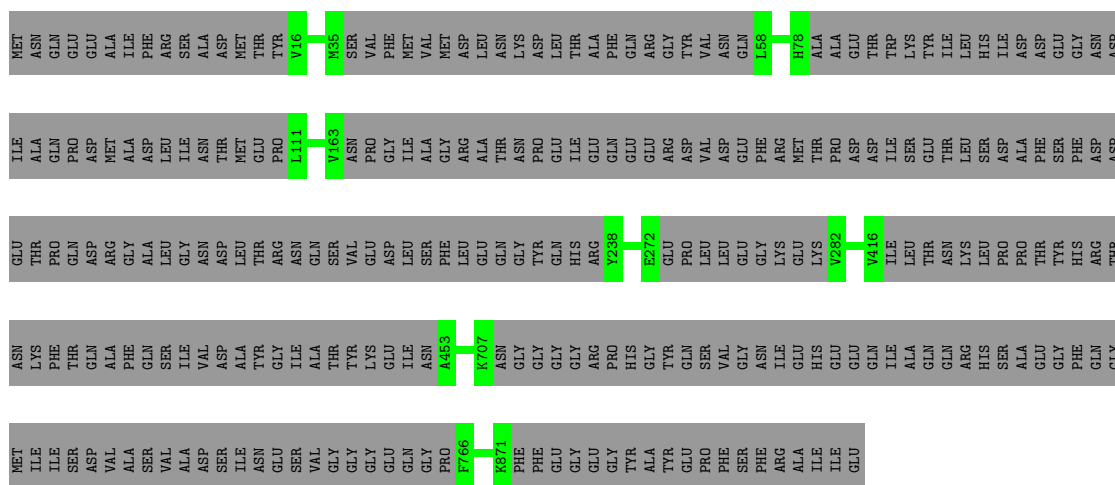
- Molecule 8: V-type proton ATPase subunit C

Chain 0:



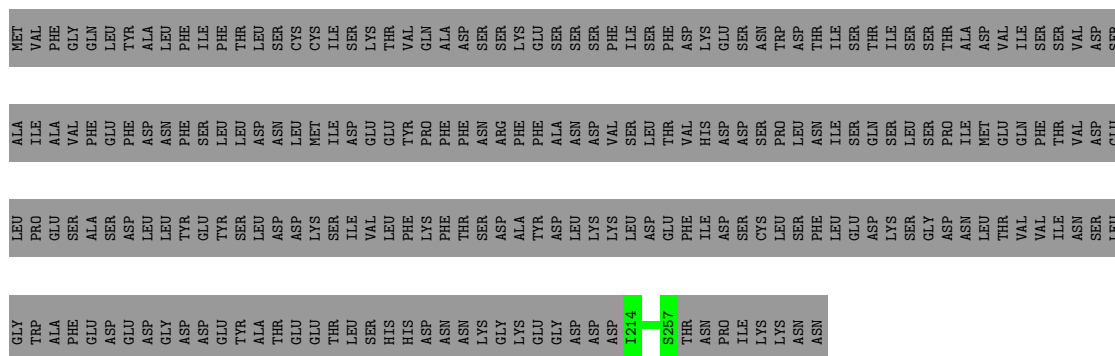
- Molecule 9: V-type proton ATPase subunit a, Golgi isoform

Chain a:



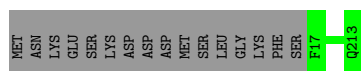
- Molecule 10: V0 assembly protein 1

Chain b:



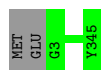
- Molecule 11: V-type proton ATPase subunit c''

Chain c:



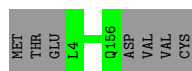
- Molecule 12: V-type proton ATPase subunit d

Chain d:  99% .



- Molecule 13: V-type proton ATPase subunit c

Chain g:  96% .



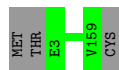
- Molecule 13: V-type proton ATPase subunit c

Chain h:  98% .



- Molecule 13: V-type proton ATPase subunit c

Chain i:  98% .



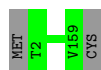
- Molecule 13: V-type proton ATPase subunit c

Chain j:  98% .



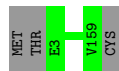
- Molecule 13: V-type proton ATPase subunit c

Chain k:  99% .



- Molecule 13: V-type proton ATPase subunit c

Chain l:  98% .



- Molecule 13: V-type proton ATPase subunit c

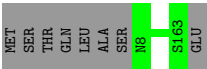
Chain m:  99% .



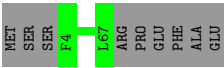
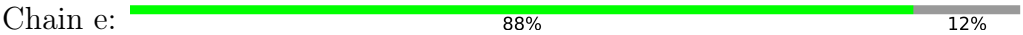
- Molecule 13: V-type proton ATPase subunit c



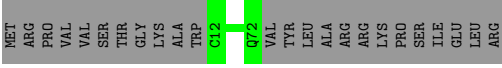
- Molecule 14: V-type proton ATPase subunit c'



- Molecule 15: V-type proton ATPase subunit e



- Molecule 16: Putative protein YPR170W-B



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	25045	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (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	1.57	3/1038 (0.3%)	1.66	10/1445 (0.7%)
10	b	0.24	0/217	0.45	0/301
11	c	0.27	0/961	0.50	0/1330
12	d	0.25	0/1698	0.48	0/2366
13	g	0.27	0/742	0.49	0/1024
13	h	0.27	0/762	0.48	0/1052
13	i	0.27	0/762	0.52	0/1052
13	j	0.26	0/757	0.48	0/1045
13	k	0.25	0/767	0.49	0/1059
13	l	0.26	0/762	0.49	0/1052
13	m	0.25	0/767	0.49	0/1059
13	n	0.26	0/767	0.49	0/1059
14	o	0.26	0/757	0.50	0/1045
15	e	0.23	0/318	0.45	0/443
16	f	0.24	0/300	0.44	0/416
2	N	1.54	0/570	1.68	5/794 (0.6%)
3	A	1.59	9/2914 (0.3%)	1.74	28/4048 (0.7%)
3	C	1.58	6/2914 (0.2%)	1.66	17/4048 (0.4%)
3	E	1.63	16/2914 (0.5%)	1.73	26/4048 (0.6%)
4	B	1.59	8/2249 (0.4%)	1.74	21/3126 (0.7%)
4	D	1.55	6/2249 (0.3%)	1.74	13/3126 (0.4%)
4	F	1.57	7/2249 (0.3%)	1.71	22/3126 (0.7%)
5	H	1.51	0/518	1.59	3/720 (0.4%)
5	J	1.56	1/518 (0.2%)	1.61	7/720 (1.0%)
5	L	1.54	0/518	1.56	2/720 (0.3%)
6	G	1.58	5/1077 (0.5%)	1.65	8/1502 (0.5%)
6	I	1.54	3/1077 (0.3%)	1.57	5/1502 (0.3%)
6	K	1.54	4/1077 (0.4%)	1.65	7/1502 (0.5%)
7	P	1.55	6/2290 (0.3%)	1.64	12/3195 (0.4%)
8	O	1.56	5/1946 (0.3%)	1.72	18/2715 (0.7%)
9	a	0.25	0/3085	0.49	0/4288
All	All	1.29	79/39540 (0.2%)	1.40	204/54928 (0.4%)

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
3	A	0	1
4	F	0	1
All	All	0	2

The worst 5 of 79 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	268	SER	CA-CB	8.94	1.66	1.52
3	E	461	SER	CA-CB	8.09	1.65	1.52
4	B	426	SER	CA-CB	7.65	1.64	1.52
6	G	211	SER	CA-CB	6.95	1.63	1.52
3	A	592	GLY	CA-C	-6.84	1.41	1.51

The worst 5 of 204 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	O	116	TRP	N-CA-CB	8.64	126.16	110.60
4	F	424	ALA	N-CA-CB	8.62	122.17	110.10
3	E	257	ALA	N-CA-CB	8.44	121.91	110.10
8	O	96	ALA	N-CA-CB	8.06	121.38	110.10
4	B	165	ALA	CB-CA-C	-7.75	98.48	110.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	153	SER	Mainchain
4	F	44	VAL	Peptide

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	1039	0	475	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	571	0	255	0	0
3	A	2915	0	1343	0	0
3	C	2915	0	1343	2	0
3	E	2915	0	1343	1	0
4	B	2250	0	1016	3	0
4	D	2250	0	1016	1	0
4	F	2250	0	1016	0	0
5	H	519	0	250	0	0
5	J	519	0	250	0	0
5	L	519	0	250	0	0
6	G	1078	0	483	0	0
6	I	1078	0	483	0	0
6	K	1078	0	483	0	0
7	P	2292	0	993	0	0
8	O	1947	0	876	0	0
9	a	3092	0	1352	0	0
10	b	218	0	98	0	0
11	c	962	0	477	0	0
12	d	1699	0	752	0	0
13	g	743	0	379	0	0
13	h	763	0	387	0	0
13	i	763	0	387	0	0
13	j	758	0	385	0	0
13	k	768	0	389	0	0
13	l	763	0	387	0	0
13	m	768	0	389	0	0
13	n	768	0	389	0	0
14	o	758	0	375	0	0
15	e	319	0	143	0	0
16	f	301	0	141	0	0
All	All	39578	0	18305	6	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 6 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)
4:B:165:ALA:HB2	4:B:386:ALA:CB	2.38	0.54
4:B:165:ALA:HB2	4:B:386:ALA:HB2	1.92	0.51
3:E:93:SER:HA	3:E:216:PRO:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:51:GLU:HA	4:D:99:SER:HA	2.03	0.41
3:C:355:ASP:HA	3:C:356:SER:HA	1.91	0.41

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	M	208/256 (81%)	206 (99%)	2 (1%)	0	100	100
2	N	113/118 (96%)	102 (90%)	10 (9%)	1 (1%)	19	61
3	A	591/639 (92%)	541 (92%)	31 (5%)	19 (3%)	4	34
3	C	591/639 (92%)	538 (91%)	37 (6%)	16 (3%)	5	38
3	E	591/639 (92%)	542 (92%)	32 (5%)	17 (3%)	5	36
4	B	455/517 (88%)	413 (91%)	27 (6%)	15 (3%)	4	33
4	D	455/517 (88%)	416 (91%)	25 (6%)	14 (3%)	4	34
4	F	455/517 (88%)	411 (90%)	30 (7%)	14 (3%)	4	34
5	H	103/114 (90%)	99 (96%)	3 (3%)	1 (1%)	17	59
5	J	103/114 (90%)	100 (97%)	3 (3%)	0	100	100
5	L	103/114 (90%)	98 (95%)	4 (4%)	1 (1%)	17	59
6	G	215/233 (92%)	207 (96%)	7 (3%)	1 (0%)	31	74
6	I	215/233 (92%)	208 (97%)	6 (3%)	1 (0%)	31	74
6	K	215/233 (92%)	205 (95%)	9 (4%)	1 (0%)	31	74
7	P	457/478 (96%)	431 (94%)	18 (4%)	8 (2%)	9	47
8	O	390/392 (100%)	350 (90%)	21 (5%)	19 (5%)	2	26
9	a	611/890 (69%)	588 (96%)	23 (4%)	0	100	100
10	b	42/265 (16%)	42 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	c	195/213 (92%)	189 (97%)	6 (3%)	0	100	100
12	d	341/345 (99%)	327 (96%)	14 (4%)	0	100	100
13	g	151/160 (94%)	149 (99%)	2 (1%)	0	100	100
13	h	155/160 (97%)	154 (99%)	1 (1%)	0	100	100
13	i	155/160 (97%)	153 (99%)	2 (1%)	0	100	100
13	j	154/160 (96%)	152 (99%)	2 (1%)	0	100	100
13	k	156/160 (98%)	154 (99%)	2 (1%)	0	100	100
13	l	155/160 (97%)	153 (99%)	2 (1%)	0	100	100
13	m	156/160 (98%)	154 (99%)	2 (1%)	0	100	100
13	n	156/160 (98%)	154 (99%)	2 (1%)	0	100	100
14	o	154/164 (94%)	152 (99%)	2 (1%)	0	100	100
15	e	62/73 (85%)	62 (100%)	0	0	100	100
16	f	59/85 (69%)	59 (100%)	0	0	100	100
All	All	7962/9068 (88%)	7509 (94%)	325 (4%)	128 (2%)	15	50

5 of 128 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 [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.