wwPDB X-ray Structure Validation Summary Report (i)

Sep 18, 2023 – 05:58 PM EDT

PDB ID	:	5D80
Title	:	Crystal Structure of Yeast V1-ATPase in the Autoinhibited Form
Authors	:	Oot, R.A.; Kane, P.M.; Berry, E.A.; Wilkens, S.
Deposited on	:	2015-08-14
Resolution	:	6.20 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

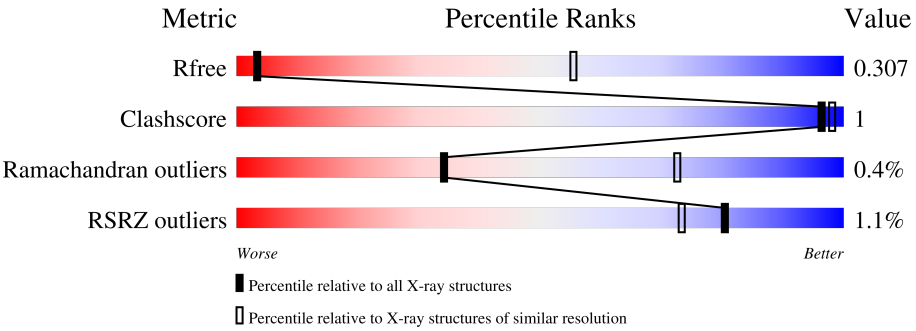
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 6.20 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1007 (8.50-3.88)
Clashscore	141614	1056 (8.50-3.90)
Ramachandran outliers	138981	1004 (8.50-3.88)
RSRZ outliers	127900	1017 (8.50-3.78)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	617	92%
1	B	617	93%
1	C	617	4% 91% 5%
1	a	617	95%
1	b	617	97%
1	c	617	94% 5%

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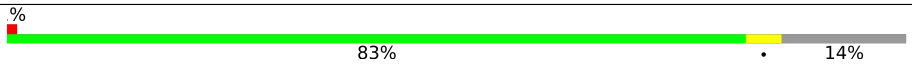
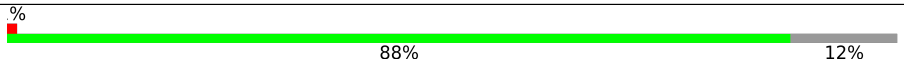
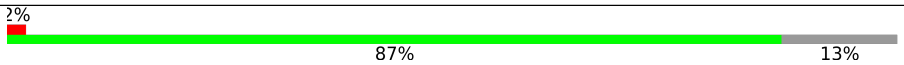
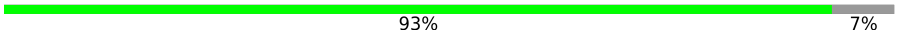
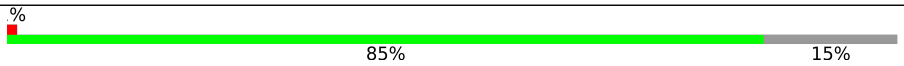
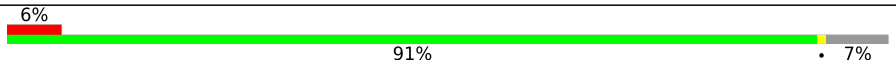
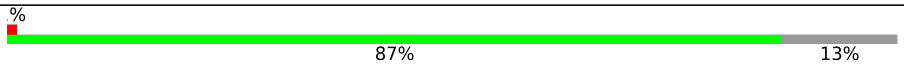
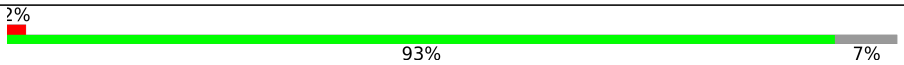
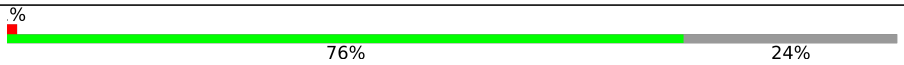
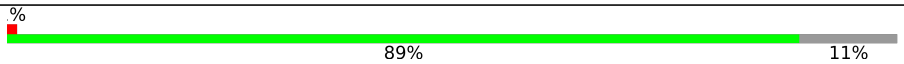
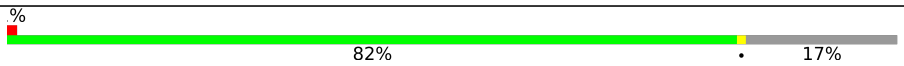
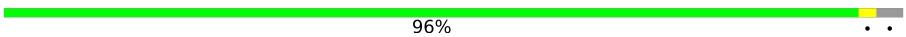
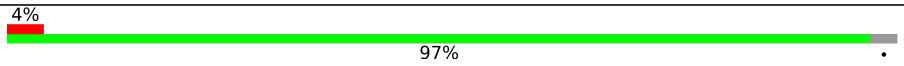
Mol	Chain	Length	Quality of chain
2	D	517	
2	E	517	
2	F	517	
2	d	517	
2	e	517	
2	f	517	
3	H	478	
3	h	478	
4	J	122	
4	L	122	
4	N	122	
4	j	122	
4	l	122	
4	n	122	
5	I	233	
5	K	233	
5	M	233	
5	i	233	
5	k	233	
5	m	233	
6	G	256	
6	g	256	
7	O	118	
7	o	118	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 47363 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	591	Total	C	N	O	0	0	0
			2905	1723	591	591			
1	B	598	Total	C	N	O	0	0	0
			2940	1744	598	598			
1	C	589	Total	C	N	O	0	0	0
			2895	1717	589	589			
1	a	591	Total	C	N	O	0	0	0
			2905	1723	591	591			
1	b	598	Total	C	N	O	0	0	0
			2940	1744	598	598			
1	c	589	Total	C	N	O	0	0	0
			2895	1717	589	589			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	457	Total	C	N	O	0	0	0
			2250	1336	457	457			
2	E	453	Total	C	N	O	0	0	0
			2231	1325	453	453			
2	F	447	Total	C	N	O	0	0	0
			2201	1307	447	447			
2	d	456	Total	C	N	O	0	0	0
			2245	1333	456	456			
2	e	453	Total	C	N	O	0	0	0
			2231	1325	453	453			
2	f	449	Total	C	N	O	0	0	0
			2211	1313	449	449			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	445	Total 2212	C 1322	N 445	O 445	0	0	0
3	h	445	Total 2212	C 1322	N 445	O 445	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	104	Total 514	C 306	N 104	O 104	0	0	0
4	L	88	Total 435	C 259	N 88	O 88	0	0	0
4	N	81	Total 400	C 238	N 81	O 81	0	0	0
4	j	104	Total 514	C 306	N 104	O 104	0	0	0
4	l	68	Total 335	C 199	N 68	O 68	0	0	0
4	n	105	Total 519	C 309	N 105	O 105	0	0	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	-7	MET	-	initiating methionine	UNP P48836
J	-6	ASP	-	expression tag	UNP P48836
J	-5	TYR	-	expression tag	UNP P48836
J	-4	LYS	-	expression tag	UNP P48836
J	-3	ASP	-	expression tag	UNP P48836
J	-2	ASP	-	expression tag	UNP P48836
J	-1	ASP	-	expression tag	UNP P48836
J	0	ASP	-	expression tag	UNP P48836
J	1	LYS	-	expression tag	UNP P48836
L	-7	MET	-	initiating methionine	UNP P48836
L	-6	ASP	-	expression tag	UNP P48836
L	-5	TYR	-	expression tag	UNP P48836
L	-4	LYS	-	expression tag	UNP P48836
L	-3	ASP	-	expression tag	UNP P48836
L	-2	ASP	-	expression tag	UNP P48836
L	-1	ASP	-	expression tag	UNP P48836
L	0	ASP	-	expression tag	UNP P48836
L	1	LYS	-	expression tag	UNP P48836
N	-7	MET	-	initiating methionine	UNP P48836

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-6	ASP	-	expression tag	UNP P48836
N	-5	TYR	-	expression tag	UNP P48836
N	-4	LYS	-	expression tag	UNP P48836
N	-3	ASP	-	expression tag	UNP P48836
N	-2	ASP	-	expression tag	UNP P48836
N	-1	ASP	-	expression tag	UNP P48836
N	0	ASP	-	expression tag	UNP P48836
N	1	LYS	-	expression tag	UNP P48836
j	-7	MET	-	initiating methionine	UNP P48836
j	-6	ASP	-	expression tag	UNP P48836
j	-5	TYR	-	expression tag	UNP P48836
j	-4	LYS	-	expression tag	UNP P48836
j	-3	ASP	-	expression tag	UNP P48836
j	-2	ASP	-	expression tag	UNP P48836
j	-1	ASP	-	expression tag	UNP P48836
j	0	ASP	-	expression tag	UNP P48836
j	1	LYS	-	expression tag	UNP P48836
l	-7	MET	-	initiating methionine	UNP P48836
l	-6	ASP	-	expression tag	UNP P48836
l	-5	TYR	-	expression tag	UNP P48836
l	-4	LYS	-	expression tag	UNP P48836
l	-3	ASP	-	expression tag	UNP P48836
l	-2	ASP	-	expression tag	UNP P48836
l	-1	ASP	-	expression tag	UNP P48836
l	0	ASP	-	expression tag	UNP P48836
l	1	LYS	-	expression tag	UNP P48836
n	-7	MET	-	initiating methionine	UNP P48836
n	-6	ASP	-	expression tag	UNP P48836
n	-5	TYR	-	expression tag	UNP P48836
n	-4	LYS	-	expression tag	UNP P48836
n	-3	ASP	-	expression tag	UNP P48836
n	-2	ASP	-	expression tag	UNP P48836
n	-1	ASP	-	expression tag	UNP P48836
n	0	ASP	-	expression tag	UNP P48836
n	1	LYS	-	expression tag	UNP P48836

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	216	Total	C	N	O	0	0	0
			1073	641	216	216			
5	K	203	Total	C	N	O	0	0	0
			1008	602	203	203			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	M	203	Total	C	N	O	0	0	0
			1008	602	203	203			
5	i	216	Total	C	N	O	0	0	0
			1073	641	216	216			
5	k	178	Total	C	N	O	0	0	0
			883	527	178	178			
5	m	208	Total	C	N	O	0	0	0
			1033	617	208	208			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	G	223	Total	C	N	O	0	0	0
			1104	658	223	223			
6	g	212	Total	C	N	O	0	0	0
			1049	625	212	212			

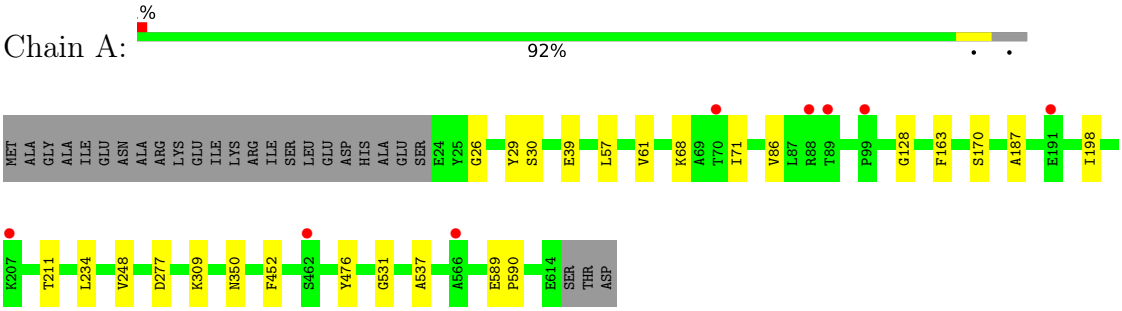
- Molecule 7 is a protein called V-type proton ATPase subunit F.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	o	115	Total	C	N	O	0	0	0
			571	341	115	115			
7	O	115	Total	C	N	O	0	0	0
			571	341	115	115			

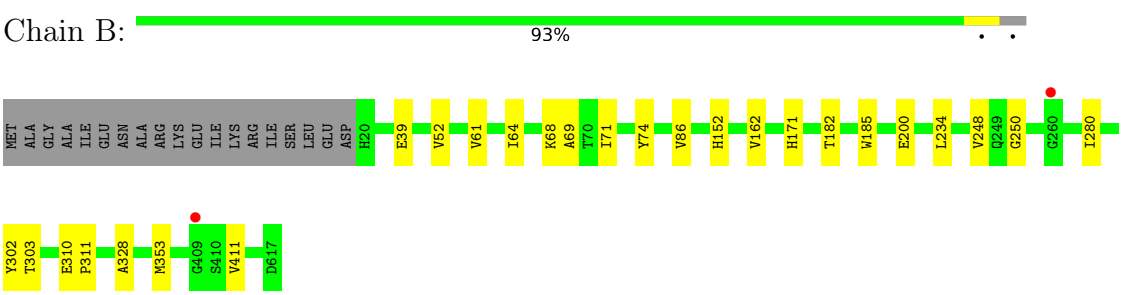
3 Residue-property plots (i)

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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

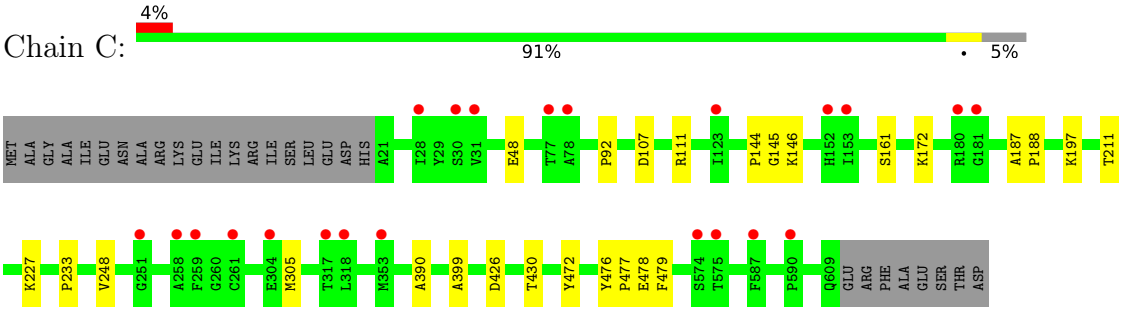
• Molecule 1: V-type proton ATPase catalytic subunit A



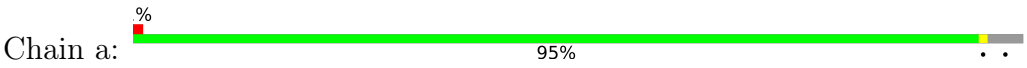
• Molecule 1: V-type proton ATPase catalytic subunit A

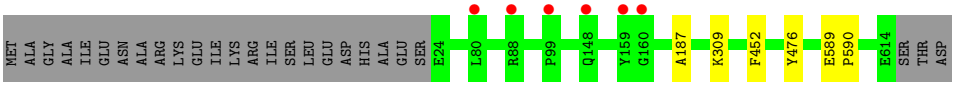


• Molecule 1: V-type proton ATPase catalytic subunit A



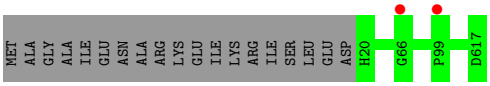
• Molecule 1: V-type proton ATPase catalytic subunit A





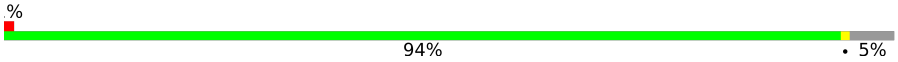
• Molecule 1: V-type proton ATPase catalytic subunit A

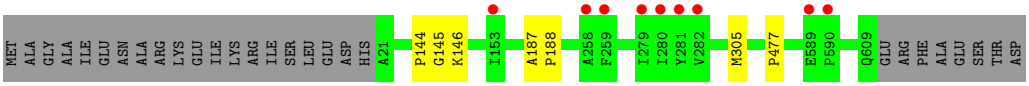
Chain b:



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

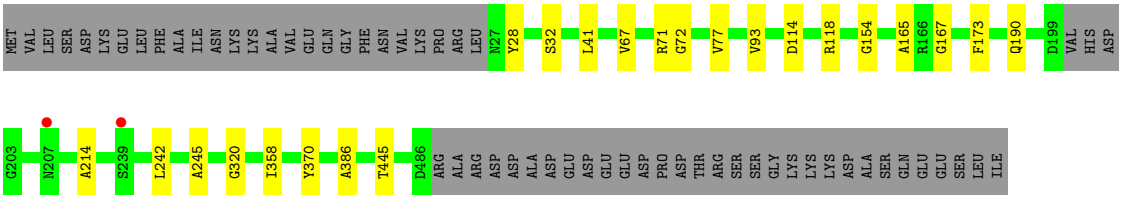
Chain c:





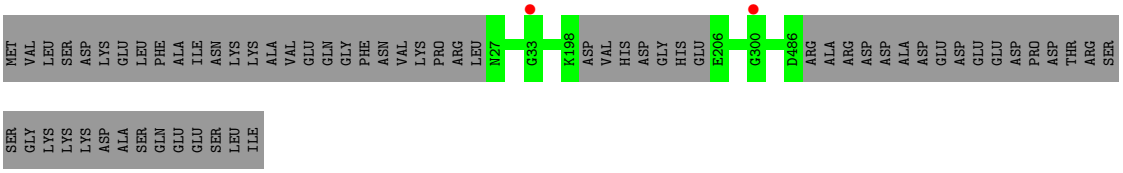
• Molecule 2: V-type proton ATPase subunit B

Chain D:



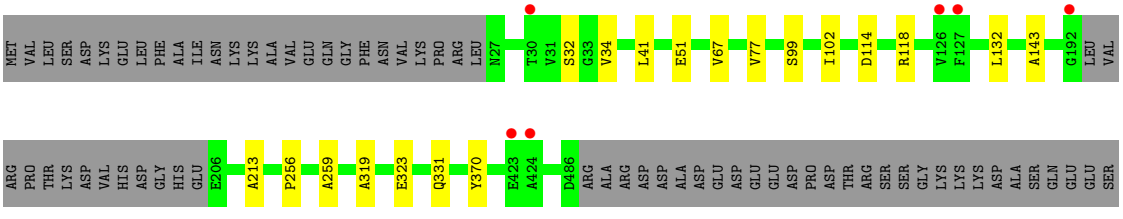
• Molecule 2: V-type proton ATPase subunit B

Chain E:



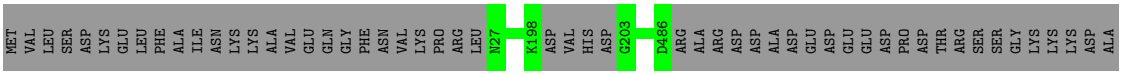
• Molecule 2: V-type proton ATPase subunit B

Chain F:



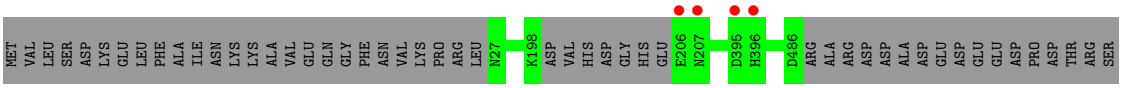
• Molecule 2: V-type proton ATPase subunit B

Chain d:



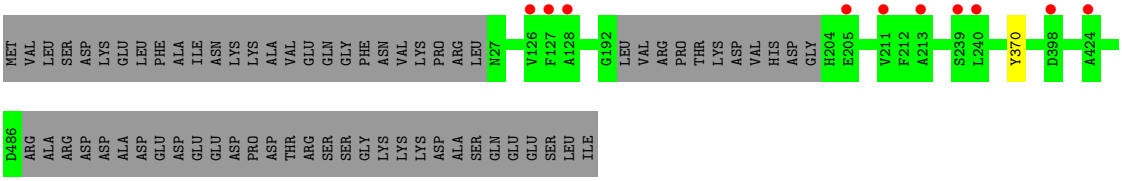
• Molecule 2: V-type proton ATPase subunit B

Chain e:



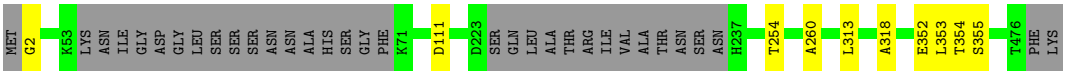
• Molecule 2: V-type proton ATPase subunit B

Chain f:



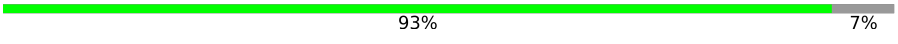
• Molecule 3: V-type proton ATPase subunit H

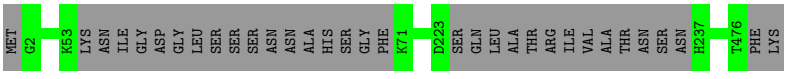
Chain H:



• Molecule 3: V-type proton ATPase subunit H

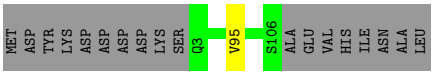
Chain h:





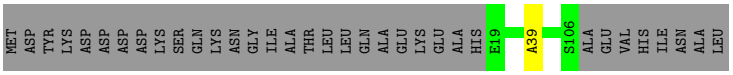
• Molecule 4: V-type proton ATPase subunit G

Chain J:



• Molecule 4: V-type proton ATPase subunit G

Chain L:

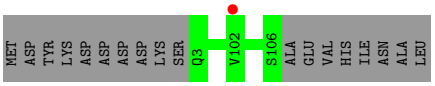


• Molecule 4: V-type proton ATPase subunit G

Chain N:

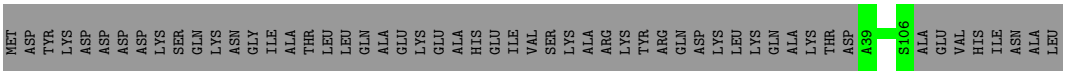
• Molecule 4: V-type proton ATPase subunit G

Chain j:



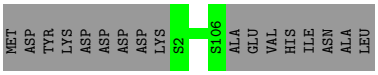
• Molecule 4: V-type proton ATPase subunit G

Chain l:



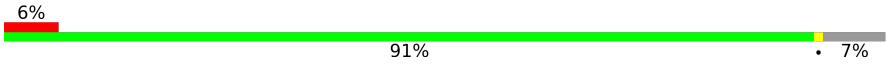
• Molecule 4: V-type proton ATPase subunit G

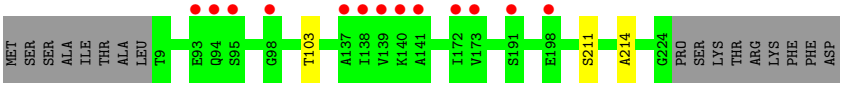
Chain n:



• Molecule 5: V-type proton ATPase subunit E

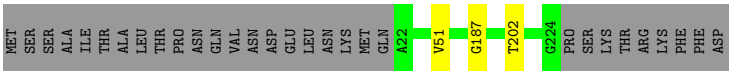
Chain I:



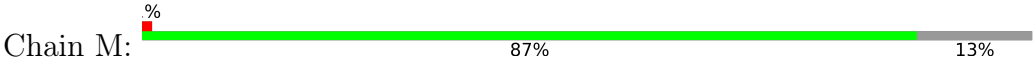


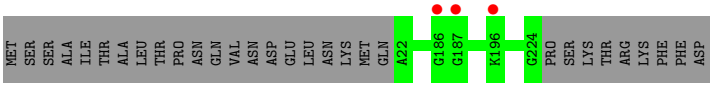
• Molecule 5: V-type proton ATPase subunit E

Chain K:

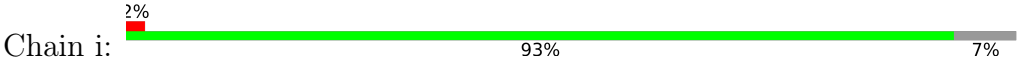


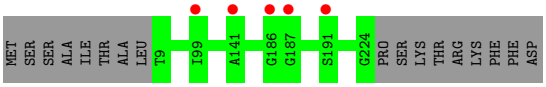
• Molecule 5: V-type proton ATPase subunit E



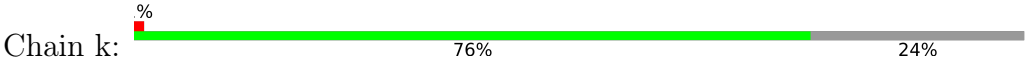


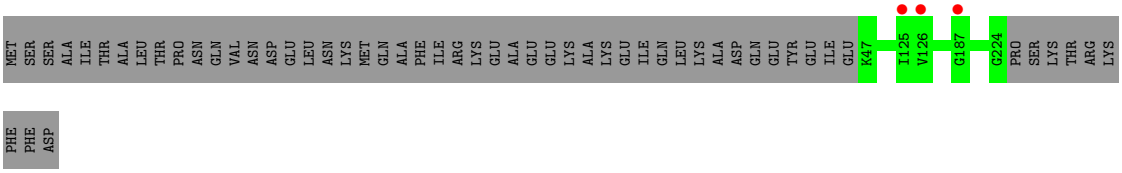
• Molecule 5: V-type proton ATPase subunit E



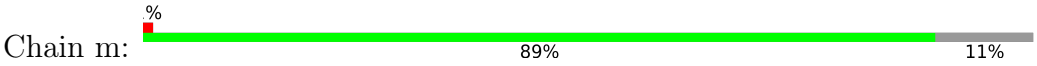


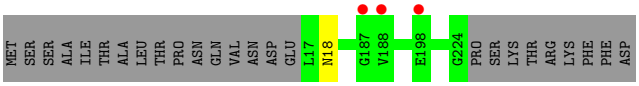
• Molecule 5: V-type proton ATPase subunit E



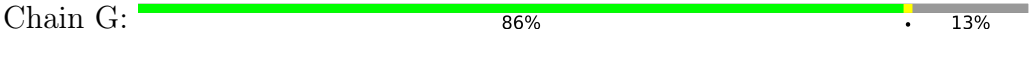


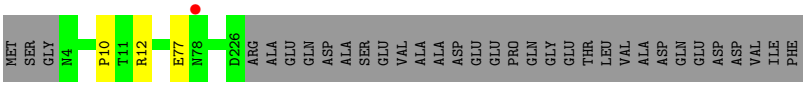
• Molecule 5: V-type proton ATPase subunit E



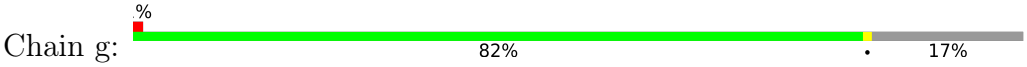


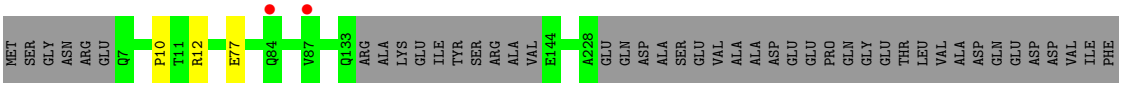
• Molecule 6: V-type proton ATPase subunit D





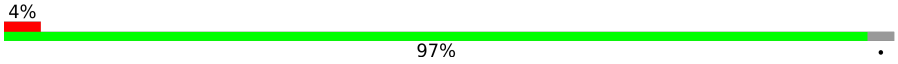
• Molecule 6: V-type proton ATPase subunit D

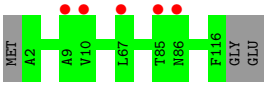




• Molecule 7: V-type proton ATPase subunit F

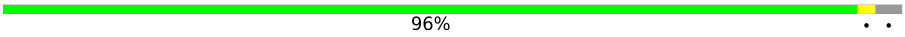
Chain o:

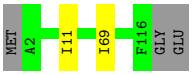




• Molecule 7: V-type proton ATPase subunit F

Chain O:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	468.02Å 159.65Å 248.27Å 90.00° 113.75° 90.00°	Depositor
Resolution (Å)	39.72 – 6.20 39.72 – 6.20	Depositor EDS
% Data completeness (in resolution range)	87.6 (39.72-6.20) 87.7 (39.72-6.20)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 6.13Å)	Xtriage
Refinement program	PHENIX dev-1957	Depositor
R, R_{free}	0.255 , 0.302 0.258 , 0.307	Depositor DCC
R_{free} test set	2000 reflections (5.97%)	wwPDB-VP
Wilson B-factor (Å^2)	422.2	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 833.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	47363	wwPDB-VP
Average B, all atoms (Å^2)	320.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.19	0/2904	0.34	0/4034
1	B	0.19	0/2939	0.35	0/4083
1	C	0.20	0/2894	0.37	0/4020
1	a	0.19	0/2904	0.34	0/4034
1	b	0.19	0/2939	0.35	0/4083
1	c	0.20	0/2894	0.37	0/4020
2	D	0.20	0/2248	0.36	0/3123
2	E	0.20	0/2229	0.35	0/3097
2	F	0.19	0/2199	0.34	0/3055
2	d	0.20	0/2243	0.36	0/3116
2	e	0.20	0/2229	0.35	0/3097
2	f	0.19	0/2209	0.34	0/3069
3	H	0.20	0/2209	0.37	0/3080
3	h	0.21	0/2209	0.37	0/3080
4	J	0.20	0/513	0.33	0/713
4	L	0.21	0/434	0.34	0/603
4	N	0.19	0/399	0.33	0/554
4	j	0.20	0/513	0.33	0/713
4	l	0.21	0/334	0.33	0/463
4	n	0.19	0/518	0.33	0/720
5	I	0.20	0/1072	0.31	0/1495
5	K	0.19	0/1007	0.32	0/1404
5	M	0.18	0/1007	0.30	0/1404
5	i	0.20	0/1072	0.31	0/1495
5	k	0.19	0/882	0.32	0/1229
5	m	0.19	0/1032	0.30	0/1439
6	G	0.21	0/1103	0.37	0/1536
6	g	0.21	0/1047	0.37	0/1456
7	O	0.19	0/570	0.36	0/794
7	o	0.19	0/570	0.36	0/794
All	All	0.20	0/47322	0.35	0/65803

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2905	0	1339	11	0
1	B	2940	0	1356	14	0
1	C	2895	0	1335	10	0
1	a	2905	0	1339	0	0
1	b	2940	0	1356	0	0
1	c	2895	0	1335	0	0
2	D	2250	0	1015	14	0
2	E	2231	0	1006	0	0
2	F	2201	0	995	10	0
2	d	2245	0	1013	0	0
2	e	2231	0	1006	0	0
2	f	2211	0	999	0	0
3	H	2212	0	951	6	0
3	h	2212	0	951	0	0
4	J	514	0	248	1	0
4	L	435	0	206	1	0
4	N	400	0	189	1	0
4	j	514	0	248	0	0
4	l	335	0	160	0	0
4	n	519	0	250	0	0
5	I	1073	0	481	2	0
5	K	1008	0	456	2	0
5	M	1008	0	456	0	0
5	i	1073	0	481	0	0
5	k	883	0	394	0	0
5	m	1033	0	466	0	0
6	G	1104	0	504	0	0
6	g	1049	0	478	0	0
7	O	571	0	255	1	0
7	o	571	0	255	0	0
All	All	47363	0	21523	67	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 1.

The worst 5 of 67 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)
1:B:74:TYR:HA	1:B:328:ALA:HB3	1.69	0.74
1:A:531:GLY:HA2	1:A:537:ALA:HA	1.75	0.69
3:H:353:LEU:H	3:H:354:THR:C	1.96	0.69
2:F:213:ALA:HB1	2:F:256:PRO:HA	1.77	0.67
3:H:352:GLU:HA	3:H:355:SER:HA	1.78	0.66

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 X-ray entries followed by that with respect to entries of similar resolution.

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	589/617 (96%)	551 (94%)	32 (5%)	6 (1%)	15 54
1	B	596/617 (97%)	557 (94%)	39 (6%)	0	100 100
1	C	587/617 (95%)	546 (93%)	34 (6%)	7 (1%)	13 50
1	a	589/617 (96%)	551 (94%)	32 (5%)	6 (1%)	15 54
1	b	596/617 (97%)	557 (94%)	39 (6%)	0	100 100
1	c	587/617 (95%)	546 (93%)	34 (6%)	7 (1%)	13 50
2	D	453/517 (88%)	424 (94%)	29 (6%)	0	100 100
2	E	449/517 (87%)	424 (94%)	25 (6%)	0	100 100
2	F	443/517 (86%)	416 (94%)	26 (6%)	1 (0%)	47 81
2	d	452/517 (87%)	423 (94%)	29 (6%)	0	100 100
2	e	449/517 (87%)	424 (94%)	25 (6%)	0	100 100
2	f	445/517 (86%)	418 (94%)	26 (6%)	1 (0%)	47 81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	439/478 (92%)	412 (94%)	27 (6%)	0	100	100
3	h	439/478 (92%)	412 (94%)	27 (6%)	0	100	100
4	J	102/122 (84%)	100 (98%)	2 (2%)	0	100	100
4	L	86/122 (70%)	85 (99%)	1 (1%)	0	100	100
4	N	79/122 (65%)	76 (96%)	3 (4%)	0	100	100
4	j	102/122 (84%)	100 (98%)	2 (2%)	0	100	100
4	l	66/122 (54%)	65 (98%)	1 (2%)	0	100	100
4	n	103/122 (84%)	100 (97%)	3 (3%)	0	100	100
5	I	214/233 (92%)	214 (100%)	0	0	100	100
5	K	201/233 (86%)	200 (100%)	1 (0%)	0	100	100
5	M	201/233 (86%)	200 (100%)	1 (0%)	0	100	100
5	i	214/233 (92%)	214 (100%)	0	0	100	100
5	k	176/233 (76%)	175 (99%)	1 (1%)	0	100	100
5	m	206/233 (88%)	204 (99%)	1 (0%)	1 (0%)	29	69
6	G	221/256 (86%)	211 (96%)	7 (3%)	3 (1%)	11	46
6	g	208/256 (81%)	199 (96%)	6 (3%)	3 (1%)	11	46
7	O	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
7	o	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
All	All	9518/10638 (90%)	9024 (95%)	459 (5%)	35 (0%)	34	72

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	187	ALA
1	C	188	PRO
1	c	187	ALA
1	c	188	PRO
6	G	10	PRO

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

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

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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	591/617 (95%)	-0.42	8 (1%) 75 66	153, 336, 460, 561	0
1	B	598/617 (96%)	-0.53	2 (0%) 94 90	112, 322, 468, 647	0
1	C	589/617 (95%)	-0.33	22 (3%) 41 37	148, 325, 484, 591	0
1	a	591/617 (95%)	-0.43	6 (1%) 82 75	155, 335, 460, 557	0
1	b	598/617 (96%)	-0.53	2 (0%) 94 90	109, 321, 465, 650	0
1	c	589/617 (95%)	-0.38	9 (1%) 73 65	146, 323, 481, 593	0
2	D	457/517 (88%)	-0.56	2 (0%) 92 87	93, 267, 414, 596	0
2	E	453/517 (87%)	-0.52	2 (0%) 92 87	149, 285, 407, 560	0
2	F	447/517 (86%)	-0.45	6 (1%) 77 69	138, 312, 463, 552	0
2	d	456/517 (88%)	-0.62	0 100 100	91, 265, 408, 553	0
2	e	453/517 (87%)	-0.46	4 (0%) 84 77	145, 285, 408, 566	0
2	f	449/517 (86%)	-0.38	10 (2%) 62 54	137, 313, 467, 570	0
3	H	445/478 (93%)	-0.82	0 100 100	85, 192, 339, 469	0
3	h	445/478 (93%)	-0.83	0 100 100	79, 193, 337, 470	0
4	J	104/122 (85%)	-0.71	0 100 100	140, 258, 401, 458	0
4	L	88/122 (72%)	-0.63	0 100 100	281, 427, 520, 540	0
4	N	81/122 (66%)	-0.50	0 100 100	244, 400, 519, 569	0
4	j	104/122 (85%)	-0.73	1 (0%) 82 75	140, 260, 398, 459	0
4	l	68/122 (55%)	-0.48	0 100 100	282, 414, 487, 535	0
4	n	105/122 (86%)	-0.31	0 100 100	229, 409, 525, 572	0
5	I	216/233 (92%)	-0.22	13 (6%) 21 21	103, 383, 522, 578	0
5	K	203/233 (87%)	-0.56	0 100 100	255, 380, 542, 600	0
5	M	203/233 (87%)	-0.19	3 (1%) 73 65	235, 422, 520, 578	0
5	i	216/233 (92%)	-0.35	5 (2%) 60 54	99, 382, 522, 573	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
5	k	178/233 (76%)	-0.29	3 (1%) 70 62	254, 366, 478, 548	0
5	m	208/233 (89%)	-0.33	3 (1%) 75 66	239, 415, 520, 577	0
6	G	223/256 (87%)	-0.57	1 (0%) 92 87	114, 325, 538, 586	0
6	g	212/256 (82%)	-0.65	2 (0%) 84 77	112, 316, 539, 581	0
7	O	115/118 (97%)	-0.41	0 100 100	260, 414, 524, 579	0
7	o	115/118 (97%)	-0.04	5 (4%) 35 33	260, 416, 526, 577	0
All	All	9600/10638 (90%)	-0.49	109 (1%) 80 73	79, 317, 487, 650	0

The worst 5 of 109 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	e	206	GLU	7.3
2	f	211	VAL	6.5
5	m	187	GLY	5.3
5	I	138	ILE	5.2
1	A	88	ARG	5.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.