



## wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Dec 10, 2019 – 01:03 PM EST

PDB ID : 6C6L  
EMDB ID: : EMD-7348  
Title : Yeast Vacuolar ATPase Vo in lipid nanodisc  
Authors : Roh, S.; Stam, N.J.; Hryc, C.; Couoh-Cardel, S.; Pintilie, G.; Chiu, W.;  
Wilkins, S.  
Deposited on : 2018-01-19  
Resolution : 3.50 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](mailto: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.

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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) : 2.4

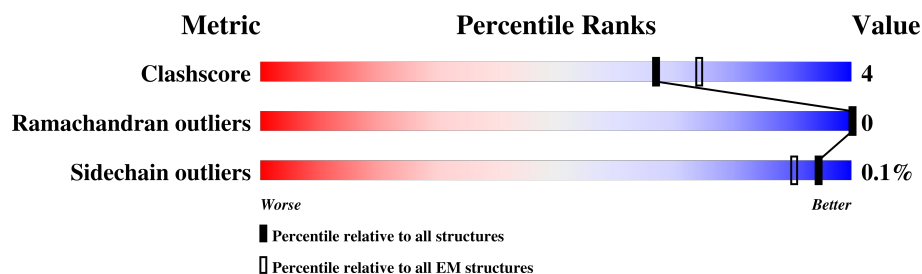
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 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
Sidechain outliers	132532	1531

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	D	164	83% 13% .
2	C	213	79% 15% 6%
3	N	265	16% . 80%
4	M	73	84% 10% . 5%
5	E	160	89% 11% .
5	F	160	88% 11% .
5	G	160	88% 12% .
5	H	160	93% 8%
5	I	160	94% 6% .

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Mol	Chain	Length	Quality of chain
5	J	160	 88% 12%
5	K	160	 88% 13%
5	L	160	 86% 14%
6	B	345	 89% 11%
7	A	840	 76% 12% 11%
8	O	85	 82% 7% 11%

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 22110 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 c'.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	157	Total	C	N	O	S	0	0
			1139	753	179	195	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	200	Total	C	N	O	S	0	0
			1488	992	230	259	7		

- Molecule 3 is a protein called V0 assembly protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	52	Total	C	N	O	S	0	0
			395	262	57	74	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	69	Total	C	N	O	S	0	0
			550	367	91	86	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	159	Total	C	N	O	S	0	0
			1137	749	182	199	7		
5	F	159	Total	C	N	O	S	0	0
			1137	749	182	199	7		
5	G	159	Total	C	N	O	S	0	0
			1137	749	182	199	7		
5	H	160	Total	C	N	O	S	0	0
			1143	752	183	200	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	159	Total	C	N	O	S	0	0
			1137	749	182	199	7		
5	J	159	Total	C	N	O	S	0	0
			1137	749	182	199	7		
5	K	160	Total	C	N	O	S	0	0
			1143	752	183	200	8		
5	L	159	Total	C	N	O	S	0	0
			1137	749	182	199	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	344	Total	C	N	O	S	0	0
			2793	1774	453	553	13		

- Molecule 7 is a protein called V-type proton ATPase subunit a, vacuolar isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	746	Total	C	N	O	S	0	0
			6054	3951	985	1083	35		

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

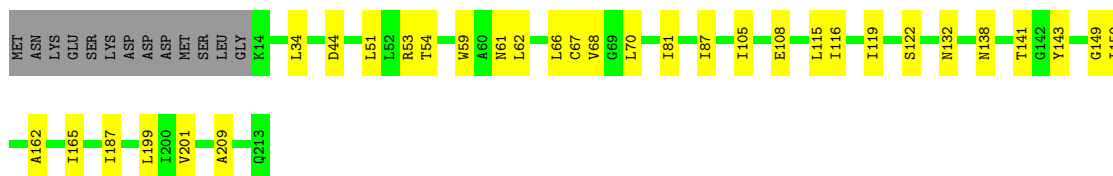
Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	76	Total	C	N	O	S	0	0
			583	386	94	100	3		



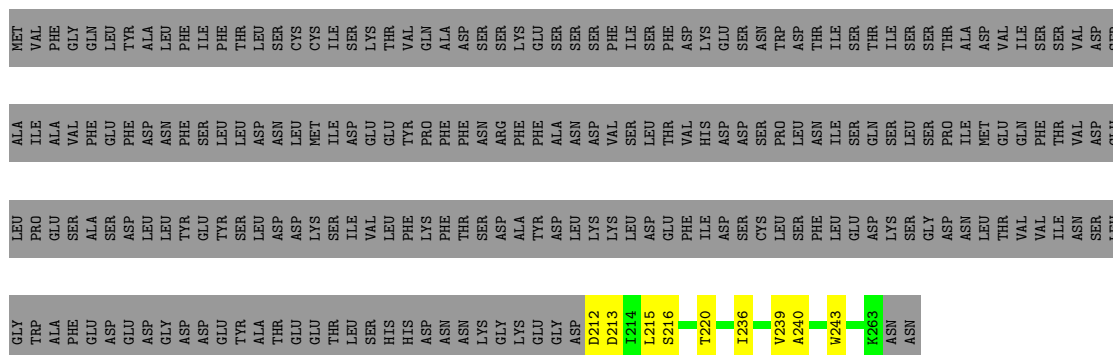
- Molecule 1: V-type proton ATPase subunit c'

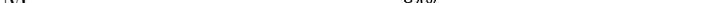


- Chain C:  79% 15% 6%




- Chain N:  16% 4% 80%



- Chain M:  84% 10% 5%




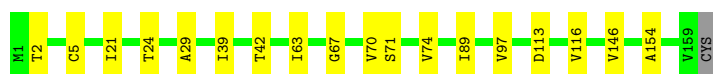
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Chain E:  89% 11%




- Molecule 5: V-type proton ATPase subunit c

Chain F:  88% 11%



- Molecule 5: V-type proton ATPase subunit c

Chain G:  88% 12%



- Molecule 5: V-type proton ATPase subunit c

Chain H:  93% 8%




- Molecule 5: V-type proton ATPase subunit c

Chain I:  94% 6%




- Molecule 5: V-type proton ATPase subunit c

Chain J:  88% 12%




- Molecule 5: V-type proton ATPase subunit c

Chain K:  88% 13%



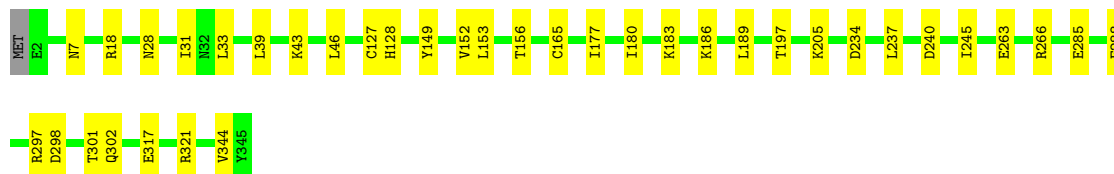
- Molecule 5: V-type proton ATPase subunit c

Chain L:  86% 14%



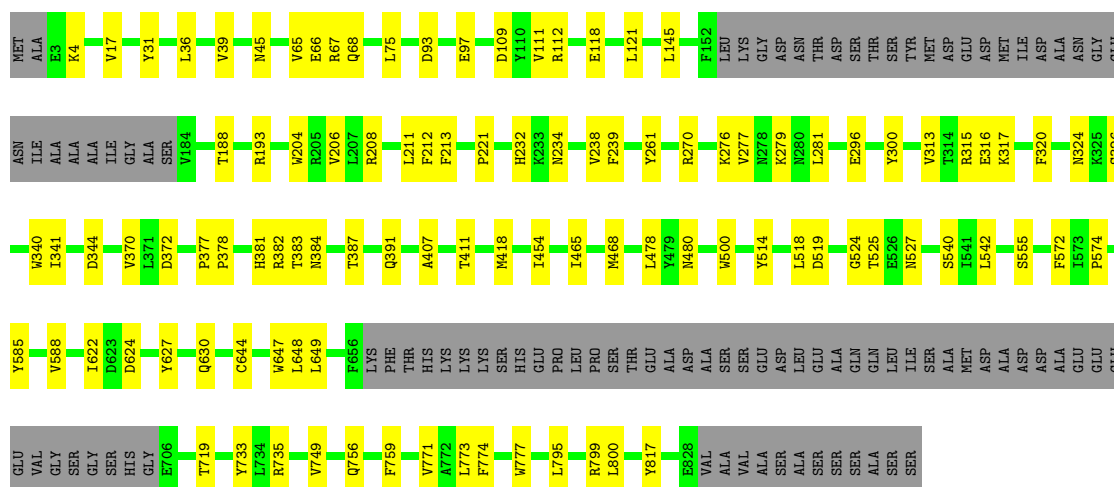
• Molecule 6: V-type proton ATPase subunit d

Chain B: 89% 11%



• Molecule 7: V-type proton ATPase subunit a, vacuolar isoform

Chain A: 76% 12% 11%



• Molecule 8: V-type proton ATPase subunit f

Chain O: 82% 7% 11%





## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	180528	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	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 [i](#)

### 5.1 Standard geometry [i](#)

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	D	0.38	0/1162	0.55	0/1575
2	C	0.37	0/1519	0.58	2/2064 (0.1%)
3	N	0.33	0/401	0.67	0/549
4	M	0.35	0/566	0.65	1/773 (0.1%)
5	E	0.34	0/1155	0.56	0/1571
5	F	0.36	0/1155	0.58	0/1571
5	G	0.33	0/1155	0.61	1/1571 (0.1%)
5	H	0.33	0/1161	0.55	0/1579
5	I	0.33	0/1155	0.63	1/1571 (0.1%)
5	J	0.33	0/1155	0.57	0/1571
5	K	0.34	0/1161	0.56	0/1579
5	L	0.37	0/1155	0.63	0/1571
6	B	0.35	0/2852	0.58	0/3870
7	A	0.34	0/6206	0.56	0/8401
8	O	0.35	0/600	0.59	0/822
All	All	0.35	0/22558	0.58	5/30638 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	157	ASP	CB-CG-OD1	6.08	123.77	118.30
4	M	67	LEU	CA-CB-CG	5.65	128.29	115.30
2	C	34	LEU	CA-CB-CG	5.10	127.02	115.30
5	G	54	ILE	CG1-CB-CG2	-5.07	100.25	111.40
2	C	70	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

There are no planarity outliers.

## 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	D	1139	0	1194	16	0
2	C	1488	0	1551	23	0
3	N	395	0	410	6	0
4	M	550	0	574	7	0
5	E	1137	0	1207	11	0
5	F	1137	0	1207	13	0
5	G	1137	0	1207	11	0
5	H	1143	0	1212	7	0
5	I	1137	0	1207	5	0
5	J	1137	0	1207	12	0
5	K	1143	0	1212	12	0
5	L	1137	0	1207	17	0
6	B	2793	0	2677	22	0
7	A	6054	0	6024	62	0
8	O	583	0	576	5	0
All	All	22110	0	22672	193	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 4.

The worst 5 of 193 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:M:62:PRO:HB2	4:M:64:ARG:HH22	1.51	0.73
5:F:70:VAL:HG11	5:F:97:VAL:HG11	1.73	0.70
5:G:70:VAL:HG11	5:G:97:VAL:HG11	1.74	0.69
6:B:127:CYS:SG	6:B:128:HIS:N	2.66	0.69
5:K:70:VAL:HG11	5:K:97:VAL:HG11	1.74	0.68

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	D	155/164 (94%)	153 (99%)	2 (1%)	0	100	100
2	C	198/213 (93%)	195 (98%)	3 (2%)	0	100	100
3	N	50/265 (19%)	47 (94%)	3 (6%)	0	100	100
4	M	67/73 (92%)	65 (97%)	2 (3%)	0	100	100
5	E	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
5	F	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
5	G	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
5	H	158/160 (99%)	154 (98%)	4 (2%)	0	100	100
5	I	157/160 (98%)	151 (96%)	6 (4%)	0	100	100
5	J	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
5	K	158/160 (99%)	156 (99%)	2 (1%)	0	100	100
5	L	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
6	B	342/345 (99%)	335 (98%)	7 (2%)	0	100	100
7	A	740/840 (88%)	716 (97%)	24 (3%)	0	100	100
8	O	74/85 (87%)	70 (95%)	4 (5%)	0	100	100
All	All	2884/3265 (88%)	2813 (98%)	71 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	D	119/125 (95%)	119 (100%)	0	100	100
2	C	155/168 (92%)	154 (99%)	1 (1%)	87	95
3	N	45/244 (18%)	45 (100%)	0	100	100
4	M	61/65 (94%)	61 (100%)	0	100	100
5	E	117/119 (98%)	117 (100%)	0	100	100
5	F	117/119 (98%)	117 (100%)	0	100	100
5	G	117/119 (98%)	117 (100%)	0	100	100
5	H	118/119 (99%)	118 (100%)	0	100	100
5	I	117/119 (98%)	117 (100%)	0	100	100
5	J	117/119 (98%)	117 (100%)	0	100	100
5	K	118/119 (99%)	117 (99%)	1 (1%)	83	92
5	L	117/119 (98%)	117 (100%)	0	100	100
6	B	308/309 (100%)	308 (100%)	0	100	100
7	A	654/728 (90%)	653 (100%)	1 (0%)	94	98
8	O	63/72 (88%)	63 (100%)	0	100	100
All	All	2343/2663 (88%)	2340 (100%)	3 (0%)	94	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	61	ASN
5	K	131	LEU
7	A	384	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
5	J	80	GLN
7	A	391	GLN
5	K	122	GLN
5	G	90	GLN
5	J	90	GLN

### 5.3.3 RNA ⓘ

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.