



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Nov 6, 2016 – 05:12 AM EST

PDB ID : 5TJ5
EMDB ID: : EMD-8409
Title : Atomic model for the membrane-embedded motor of a eukaryotic V-ATPase
Authors : Mazhab-Jafari, M.T.; Rohou, A.; Schmidt, C.; Bueler, S.A.; Benlekbir, S.; Robinson, C.V.; Rubinstein, J.L.
Deposited on : 2016-10-03
Resolution : 3.90 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

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
EM map analysis : **NOT EXECUTED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028320

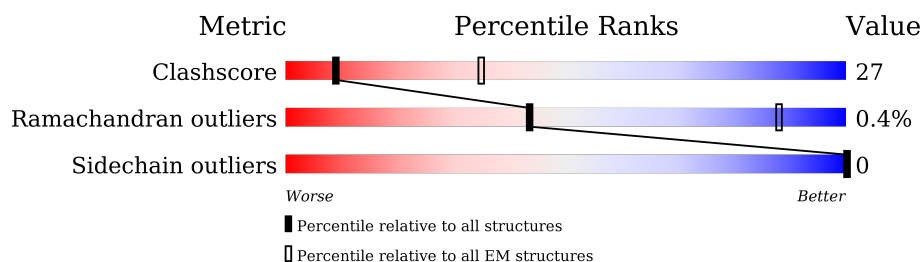
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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 ≥ 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	A	680	45% 38% . 16%
2	B	213	54% 33% . 12%
3	D	147	58% 41% .
4	E	150	59% 33% 8%
4	F	150	71% 27% .
4	G	150	69% 29% ..
4	H	150	71% 29% .
4	I	150	67% 31% .
4	J	150	75% 25%

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Mol	Chain	Length	Quality of chain
4	M	150	 63%34%..
4	N	150	 59%38%..
5	L	57	 28%70%.
6	O	54	 48%52%
7	P	297	 69%22%9%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14976 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 a.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	570	Total	C	N	O	S	0	0
			3391	2154	612	609	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	187	Total	C	N	O	S	0	0
			1266	834	201	227	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	147	Total	C	N	O	S	0	0
			914	596	156	157	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	138	Total	C	N	O		0	0
			823	527	143	153			
4	F	150	Total	C	N	O	S	0	0
			885	569	154	161	1		
4	G	149	Total	C	N	O	S	0	0
			869	558	150	160	1		
4	H	150	Total	C	N	O	S	0	0
			895	579	151	164	1		
4	I	150	Total	C	N	O	S	0	0
			922	593	161	166	2		
4	J	150	Total	C	N	O	S	0	0
			866	549	152	164	1		
4	M	148	Total	C	N	O	S	0	0
			949	624	159	165	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	148	Total	C	N	O	S	0	0
			978	642	161	170	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	57	Total	C	N	O	S	0	0
			411	274	66	67	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	O	54	Total	C	N	O	0	0
			270	162	54	54		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	P	269	Total	C	N	O	0	0
			1537	964	280	293		

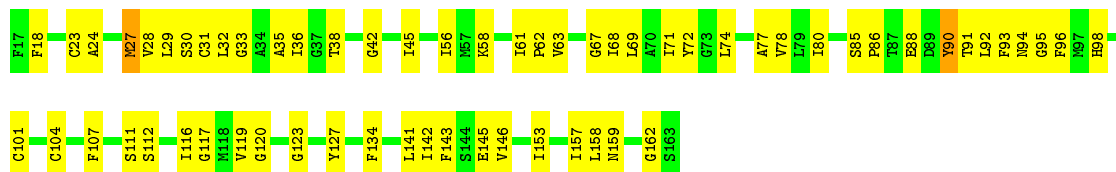
- Molecule 1: V-type proton ATPase subunit a





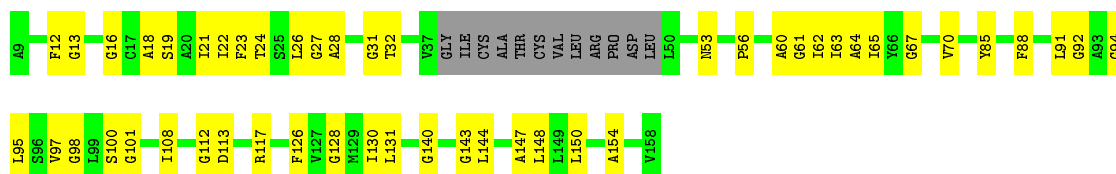
• Molecule 3: V-type proton ATPase subunit c'

Chain D: 58% 41%



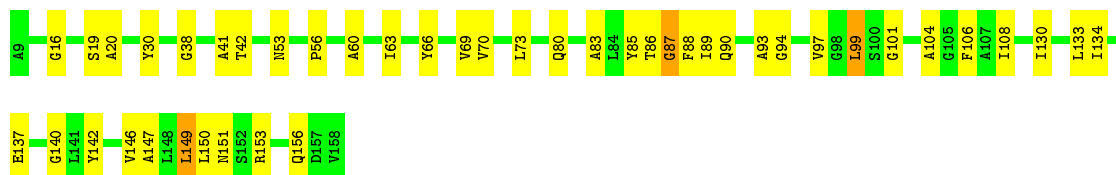
• Molecule 4: V-type proton ATPase subunit c

Chain E: 59% 33% 8%



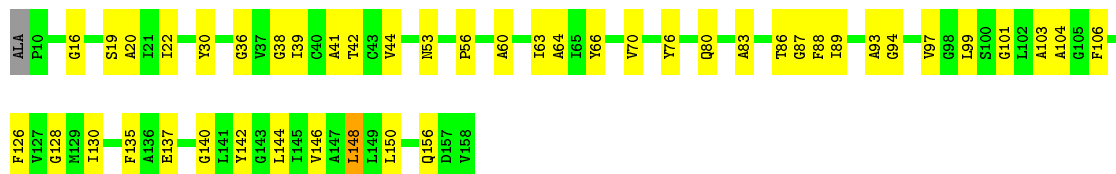
• Molecule 4: V-type proton ATPase subunit c

Chain F: 71% 27%



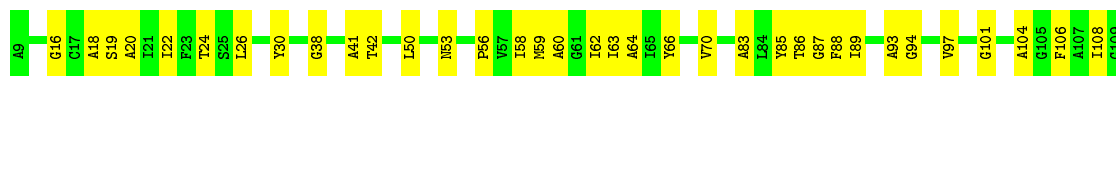
• Molecule 4: V-type proton ATPase subunit c

Chain G: 69% 29%



• Molecule 4: V-type proton ATPase subunit c

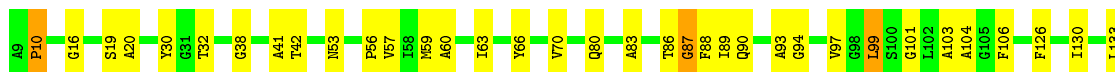
Chain H: 71% 29%





- Molecule 4: V-type proton ATPase subunit c

Chain I: 67% 31% .



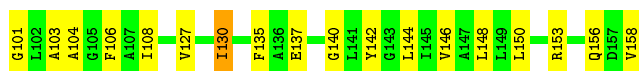
- Molecule 4: V-type proton ATPase subunit c

Chain J: 75% 25%



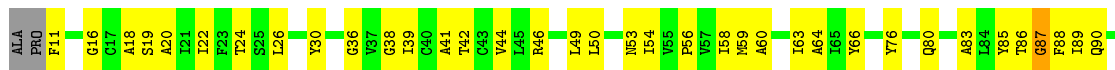
- Molecule 4: V-type proton ATPase subunit c

Chain M: 63% 34% ..



- Molecule 4: V-type proton ATPase subunit c

Chain N: 59% 38% ..



- Molecule 5: V-type proton ATPase subunit e

Chain L: 28% 70% .



- Molecule 6: V-type proton ATPase subunit f

Chain O:

48%

52%



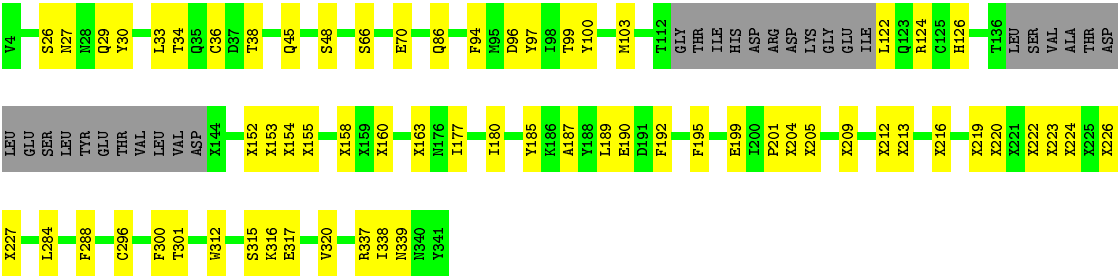
● Molecule 7: V-type proton ATPase subunit d

Chain P:

69%

22%

9%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	462842	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	64350	Depositor
Image detector	Not provided	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	A	0.60	0/2196	0.70	3/3003 (0.1%)
2	B	0.62	0/1287	0.63	0/1752
3	D	0.49	0/925	0.64	1/1262 (0.1%)
4	E	0.53	0/831	0.58	0/1139
4	F	0.52	0/897	0.67	3/1233 (0.2%)
4	G	0.50	0/881	0.63	3/1210 (0.2%)
4	H	0.50	0/906	0.66	2/1245 (0.2%)
4	I	0.52	0/933	0.68	2/1278 (0.2%)
4	J	0.48	0/878	0.60	1/1204 (0.1%)
4	M	0.54	0/960	0.71	2/1312 (0.2%)
4	N	0.58	0/991	0.73	3/1352 (0.2%)
5	L	0.65	1/421 (0.2%)	0.77	0/579
7	P	0.47	0/1255	0.52	0/1735
All	All	0.54	1/13361 (0.0%)	0.66	20/18304 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
2	B	0	1
3	D	0	1
4	F	0	2
4	G	0	2
4	H	0	2
4	I	0	3
4	J	0	2
4	M	0	2
4	N	0	2
5	L	0	2
7	P	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	27

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	48	TRP	CB-CG	-5.85	1.39	1.50

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	570	GLY	N-CA-C	-8.96	90.71	113.10
4	M	130	ILE	CG1-CB-CG2	-7.41	95.11	111.40
4	F	88	PHE	N-CA-C	-6.71	92.89	111.00
4	G	88	PHE	N-CA-C	-6.70	92.91	111.00
4	N	88	PHE	N-CA-C	-6.70	92.91	111.00

There are no chirality outliers.

5 of 27 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	UNK	Peptide
1	A	119	UNK	Peptide
1	A	229	UNK	Peptide
1	A	569	ILE	Peptide
1	A	606	PRO	Peptide

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	3391	0	1986	196	0
2	B	1266	0	1172	86	0
3	D	914	0	816	56	0
4	E	823	0	667	43	0
4	F	885	0	703	38	0
4	G	869	0	681	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	895	0	740	36	0
4	I	922	0	802	42	0
4	J	866	0	632	27	0
4	M	949	0	886	53	0
4	N	978	0	946	53	0
5	L	411	0	385	42	0
6	O	270	0	59	22	0
7	P	1537	0	796	43	0
All	All	14976	0	11271	710	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 27.

The worst 5 of 710 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)
2:B:140:TYR:CD2	3:D:86:PRO:HA	1.81	1.14
1:A:604:PRO:HB2	1:A:605:ALA:HB2	1.44	1.00
7:P:97:TYR:HA	7:P:100:TYR:HD2	1.30	0.94
1:A:415:PHE:HB2	1:A:799:ARG:HG2	1.56	0.88
1:A:11:UNK:O	1:A:15:UNK:N	2.08	0.87

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	308/680 (45%)	244 (79%)	62 (20%)	2 (1%)	30	73
2	B	179/213 (84%)	158 (88%)	19 (11%)	2 (1%)	17	63
3	D	145/147 (99%)	132 (91%)	12 (8%)	1 (1%)	26	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	134/150 (89%)	116 (87%)	18 (13%)	0	100	100
4	F	148/150 (99%)	128 (86%)	20 (14%)	0	100	100
4	G	147/150 (98%)	127 (86%)	20 (14%)	0	100	100
4	H	148/150 (99%)	127 (86%)	21 (14%)	0	100	100
4	I	148/150 (99%)	127 (86%)	20 (14%)	1 (1%)	26	70
4	J	148/150 (99%)	126 (85%)	22 (15%)	0	100	100
4	M	146/150 (97%)	126 (86%)	20 (14%)	0	100	100
4	N	146/150 (97%)	126 (86%)	20 (14%)	0	100	100
5	L	55/57 (96%)	34 (62%)	19 (34%)	2 (4%)	4	40
7	P	200/297 (67%)	177 (88%)	22 (11%)	1 (0%)	34	76
All	All	2052/2594 (79%)	1748 (85%)	295 (14%)	9 (0%)	43	79

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	622	ILE
3	D	56	ILE
7	P	338	ILE
1	A	571	ASN
2	B	47	PHE

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	A	145/368 (39%)	145 (100%)	0	100	100
2	B	106/168 (63%)	106 (100%)	0	100	100
3	D	61/111 (55%)	61 (100%)	0	100	100
4	E	44/109 (40%)	44 (100%)	0	100	100
4	F	44/109 (40%)	44 (100%)	0	100	100
4	G	43/109 (39%)	43 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	50/109 (46%)	50 (100%)	0	100	100
4	I	58/109 (53%)	58 (100%)	0	100	100
4	J	37/109 (34%)	37 (100%)	0	100	100
4	M	68/109 (62%)	68 (100%)	0	100	100
4	N	80/109 (73%)	80 (100%)	0	100	100
5	L	37/50 (74%)	37 (100%)	0	100	100
7	P	45/217 (21%)	45 (100%)	0	100	100
All	All	818/1786 (46%)	818 (100%)	0	100	100

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	428	HIS
1	A	559	HIS
1	A	725	ASN
1	A	743	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	10
7	P	5
6	O	1

The worst 5 of 16 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	295:UNK	C	307:UNK	N	67.70
1	A	365:UNK	C	400:ALA	N	58.47
1	A	224:UNK	C	225:UNK	N	30.05
1	A	210:UNK	C	211:UNK	N	26.91
1	A	248:UNK	C	268:UNK	N	24.15