



Full wwPDB EM Model Validation Report ⓘ

Mar 9, 2020 – 09:47 AM EDT

PDB ID : 6VQI
EMDB ID : EMD-21351
Title : Mammalian V-ATPase from rat brain collar and peripheral stalks rotational state 1 (from focused refinement)
Authors : Abbas, Y.M.; Rubinstein, J.L.
Deposited on : 2020-02-05
Resolution : 4.30 Å(reported)

This is a Full wwPDB EM Model Validation 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.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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) : 2.8

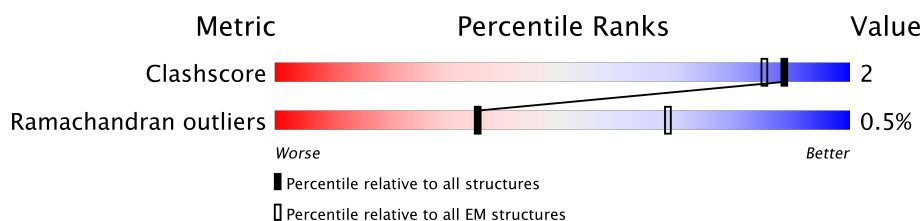
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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 and their fit to the map. 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 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	G	382	
2	I	226	
2	J	226	
2	K	226	
3	M	118	
3	N	118	
3	O	118	
4	a	838	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5278 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 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	G	360	Total	C	N	O	0	0
			1790	1070	360	360		

- Molecule 2 is a protein called V-type proton ATPase subunit E 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	I	64	Total	C	N	O	0	0
			319	191	64	64		
2	J	64	Total	C	N	O	0	0
			319	191	64	64		
2	K	64	Total	C	N	O	0	0
			319	191	64	64		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	M	67	Total	C	N	O	0	0
			332	198	67	67		
3	N	67	Total	C	N	O	0	0
			332	198	67	67		
3	O	67	Total	C	N	O	0	0
			332	198	67	67		

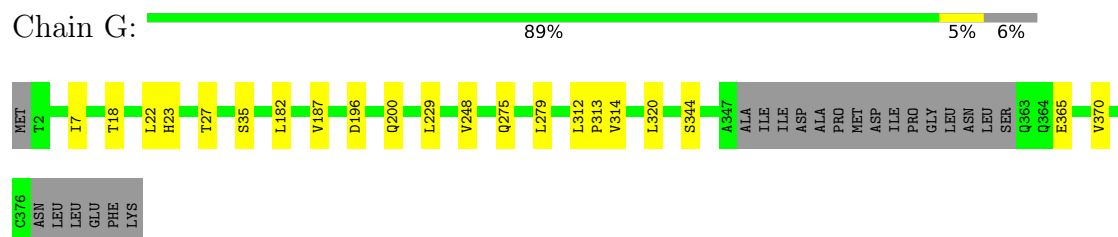
- Molecule 4 is a protein called V-type proton ATPase 116 kDa subunit a isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	a	309	Total	C	N	O	0	0
			1535	917	309	309		

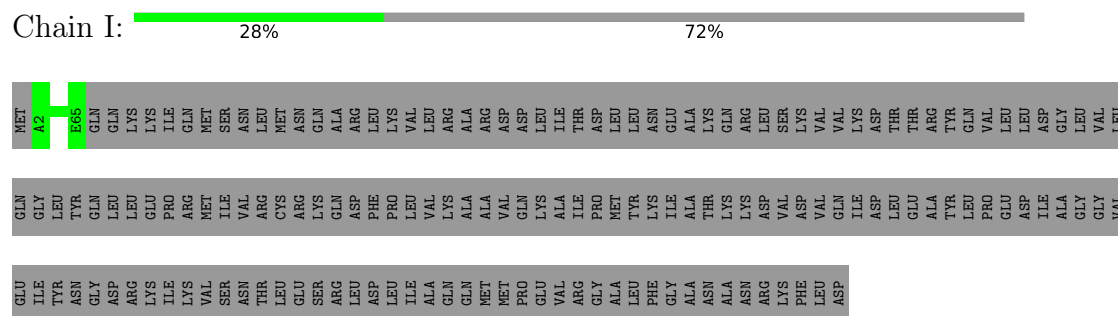
3 Residue-property plots

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.

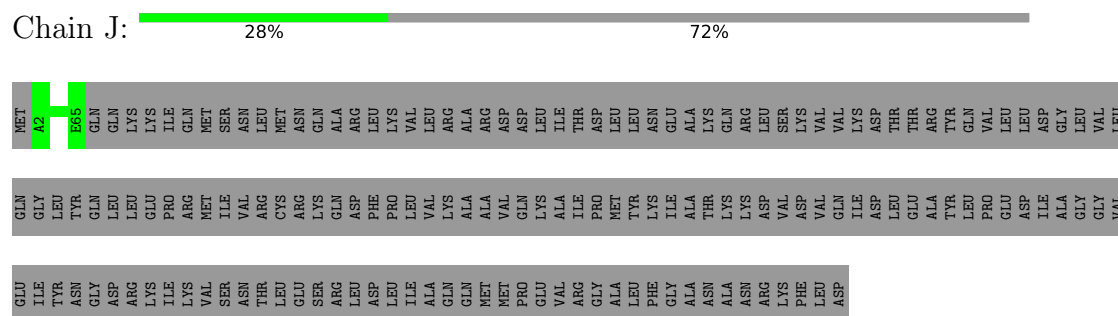
- Molecule 1: V-type proton ATPase subunit C 1



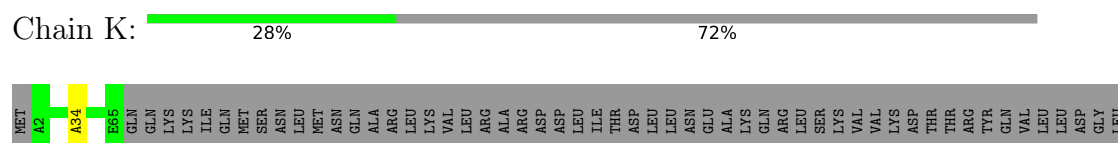
- Molecule 2: V-type proton ATPase subunit E 1



- Molecule 2: V-type proton ATPase subunit E 1



- Molecule 2: V-type proton ATPase subunit E 1



PHE	ALA	ALA	PHE	ALA	THR	LEU	THR	VAL	ALA	ILE	LEU	LEU	ILE	MET	GLU	GLY	LEU	SER	ALA	PHE	LEU	HIS	ALA	LEU	ARG	LEU	HIS	TRP	VAL	GLU	PHE	GLN	ASN	LYS	PHE	TYR	THR	GLY	THR	GLY	PHE	LYS	PHE	LEU	PRO	PHE	SER	PHE	GLU	HIS	ILE	ARG	GLU	GLY	LYS	PHE	ASP	GLU
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	90648	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON III (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 >5	RMSZ	# Z >5
1	G	0.31	0/1788	0.56	0/2494
2	I	0.30	0/318	0.46	0/443
2	J	0.42	0/318	0.54	0/443
2	K	0.38	0/318	0.51	0/443
3	M	0.32	0/331	0.46	0/460
3	N	0.41	0/331	0.50	0/460
3	O	0.31	0/331	0.50	0/460
4	a	0.35	0/1533	0.62	0/2137
All	All	0.34	0/5268	0.55	0/7340

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	G	1790	0	794	9	0
2	I	319	0	149	0	0
2	J	319	0	149	0	0
2	K	319	0	149	1	0
3	M	332	0	166	0	0
3	N	332	0	166	0	0
3	O	332	0	166	1	0
4	a	1535	0	661	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5278	0	2400	10	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (10) 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:G:196:ASP:O	1:G:200:GLN:N	2.34	0.56
1:G:275:GLN:O	1:G:279:LEU:N	2.39	0.56
1:G:23:HIS:O	1:G:27:THR:N	2.37	0.55
1:G:35:SER:HA	1:G:320:LEU:O	2.06	0.55
1:G:7:ILE:HA	1:G:370:VAL:O	2.07	0.54
1:G:18:THR:O	1:G:22:LEU:N	2.43	0.51
2:K:34:ALA:HB1	3:O:29:LYS:HA	1.97	0.47
1:G:312:LEU:HA	1:G:313:PRO:C	2.37	0.45
1:G:182:LEU:HA	1:G:229:LEU:O	2.19	0.42
1:G:187:VAL:HA	1:G:248:VAL:HA	2.02	0.41

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	G	356/382 (93%)	346 (97%)	7 (2%)	3 (1%)	21	64
2	I	62/226 (27%)	62 (100%)	0	0	100	100
2	J	62/226 (27%)	62 (100%)	0	0	100	100
2	K	62/226 (27%)	62 (100%)	0	0	100	100
3	M	65/118 (55%)	65 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	N	65/118 (55%)	65 (100%)	0	0	100	100
3	O	65/118 (55%)	65 (100%)	0	0	100	100
4	a	305/838 (36%)	296 (97%)	7 (2%)	2 (1%)	24	66
All	All	1042/2252 (46%)	1023 (98%)	14 (1%)	5 (0%)	35	73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	a	245	TYR
1	G	365	GLU
1	G	344	SER
1	G	314	VAL
4	a	79	ILE

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 ⓘ

There are no chain breaks in this entry.