



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Dec 10, 2019 – 07:41 PM EST

PDB ID : 6O7U
EMDB ID: : EMD-0645
Title : Saccharomyces cerevisiae V-ATPase Stv1-VO
Authors : Vasanthakumar, T.; Bueler, S.A.; Wu, D.; Beilsten-Edmands, V.; Robinson, C.V.; Rubinstein, J.L.
Deposited on : 2019-03-08
Resolution : 3.10 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.

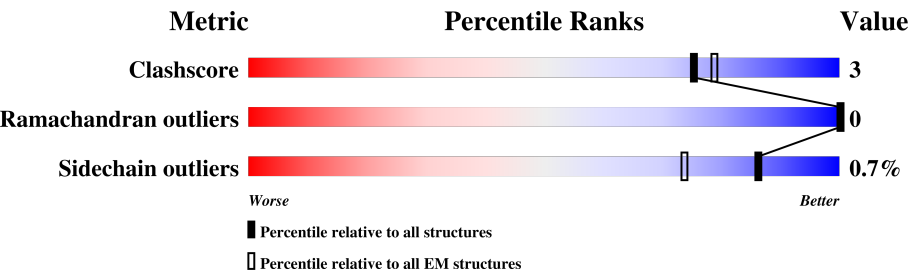
MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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 ≥ 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	912	<div><div>77%</div><div>22%</div></div>
2	b	265	<div><div>17%</div><div>83%</div></div>
3	c	213	<div><div>91%</div><div>8%</div></div>
4	d	345	<div><div>98%</div><div>2%</div></div>
5	e	73	<div><div>88%</div><div>12%</div></div>
6	f	85	<div><div>72%</div><div>28%</div></div>
7	g	160	<div><div>96%</div><div>4%</div></div>
7	h	160	<div><div>98%</div><div>2%</div></div>
7	i	160	<div><div>96%</div><div>4%</div></div>

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Mol	Chain	Length	Quality of chain
7	j	160	<div><div></div><div>98%</div><div>.</div></div>
7	k	160	<div><div></div><div>98%</div><div>..</div></div>
7	l	160	<div><div></div><div>98%</div><div>.</div></div>
7	m	160	<div><div></div><div>98%</div><div>..</div></div>
7	n	160	<div><div></div><div>98%</div><div>..</div></div>
8	o	164	<div><div></div><div>94%</div><div>. 5%</div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 21268 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, Golgi isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	713	Total	C	N	O	S	0	0
			5665	3710	917	1001	37		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	891	ASP	-	SEE REMARK 999	UNP P37296
a	892	TYR	-	SEE REMARK 999	UNP P37296
a	893	LYS	-	SEE REMARK 999	UNP P37296
a	894	ASP	-	SEE REMARK 999	UNP P37296
a	895	HIS	-	SEE REMARK 999	UNP P37296
a	896	ASP	-	SEE REMARK 999	UNP P37296
a	897	GLY	-	SEE REMARK 999	UNP P37296
a	898	ASP	-	SEE REMARK 999	UNP P37296
a	899	TYR	-	SEE REMARK 999	UNP P37296
a	900	LYS	-	SEE REMARK 999	UNP P37296
a	901	ASP	-	SEE REMARK 999	UNP P37296
a	902	HIS	-	SEE REMARK 999	UNP P37296
a	903	ASP	-	SEE REMARK 999	UNP P37296
a	904	ILE	-	SEE REMARK 999	UNP P37296
a	905	ASP	-	SEE REMARK 999	UNP P37296
a	906	TYR	-	SEE REMARK 999	UNP P37296
a	907	LYS	-	SEE REMARK 999	UNP P37296
a	908	ASP	-	SEE REMARK 999	UNP P37296
a	909	ASP	-	SEE REMARK 999	UNP P37296
a	910	ASP	-	SEE REMARK 999	UNP P37296
a	911	ASP	-	SEE REMARK 999	UNP P37296
a	912	LYS	-	SEE REMARK 999	UNP P37296

- Molecule 2 is a protein called V0 assembly protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	44	Total	C	N	O	S	0	0
			330	224	47	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	197	Total	C	N	O	S	0	0
			1466	977	227	255	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	343	Total	C	N	O	S	0	0
			2720	1732	450	527	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	64	Total	C	N	O	S	0	0
			512	344	83	79	6		

- Molecule 6 is a protein called Putative protein YPR170W-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	61	Total	C	N	O	S	0	0
			463	307	71	82	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	153	Total	C	N	O	S	0	0
			1094	723	176	188	7		
7	h	157	Total	C	N	O	S	0	0
			1125	742	180	196	7		
7	i	157	Total	C	N	O	S	0	0
			1125	742	180	196	7		
7	j	156	Total	C	N	O	S	0	0
			1116	737	179	193	7		
7	k	158	Total	C	N	O	S	0	0
			1132	746	181	198	7		
7	l	157	Total	C	N	O	S	0	0
			1125	742	180	196	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	m	158	Total	C	N	O	S	0	0
			1131	745	181	197	8		
7	n	158	Total	C	N	O	S	0	0
			1131	745	181	197	8		

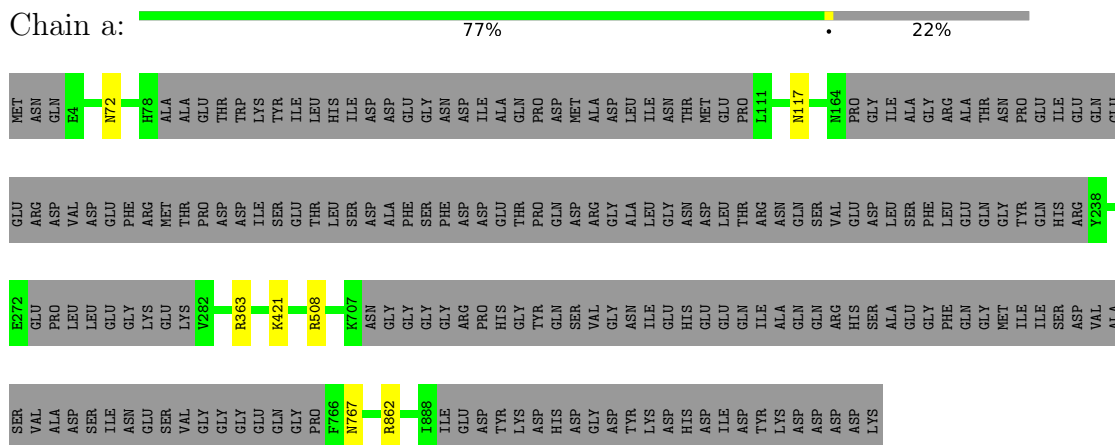
- Molecule 8 is a protein called V-type proton ATPase subunit c'.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	o	156	Total	C	N	O	S	0	0
			1133	750	178	193	12		

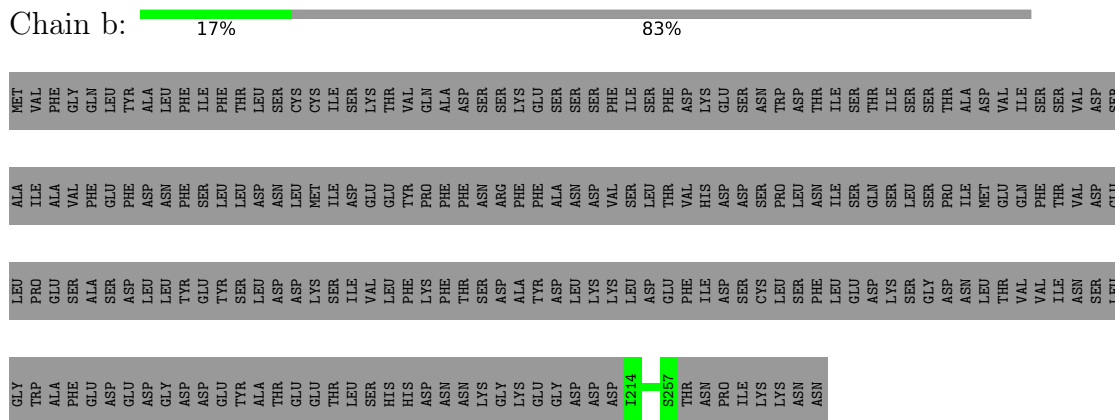
3 Residue-property plots [i](#)

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.

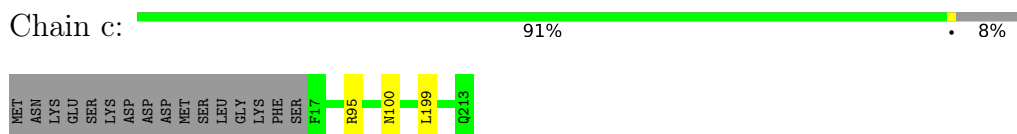
- Molecule 1: V-type proton ATPase subunit a, Golgi isoform



- Molecule 2: V0 assembly protein 1



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




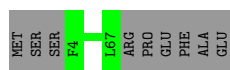
- Molecule 4: V-type proton ATPase subunit d

Chain d:  98% ..



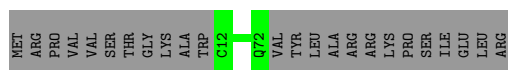
- Molecule 5: V-type proton ATPase subunit e

Chain e:  88% 12%



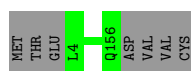
- Molecule 6: Putative protein YPR170W-B

Chain f:  72% 28%



- Molecule 7: V-type proton ATPase subunit c

Chain g:  96% .



- Molecule 7: V-type proton ATPase subunit c

Chain h:  98% ..



- Molecule 7: V-type proton ATPase subunit c

Chain i:  96% ..



- Molecule 7: V-type proton ATPase subunit c

Chain j:  98% .



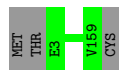
- Molecule 7: V-type proton ATPase subunit c

Chain k:  98% ..



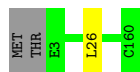
- Molecule 7: V-type proton ATPase subunit c

Chain l: 98% .



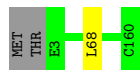
- Molecule 7: V-type proton ATPase subunit c

Chain m: 98% ..



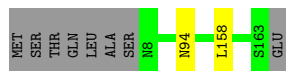
- Molecule 7: V-type proton ATPase subunit c

Chain n: 98% ..



- Molecule 8: V-type proton ATPase subunit c'

Chain o: 94% . 5%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	163024	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 ($e^-/\text{\AA}^2$)	42.7	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

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	0.29	0/5797	0.56	0/7856
2	b	0.28	0/335	0.60	0/459
3	c	0.33	0/1496	0.62	1/2033 (0.0%)
4	d	0.30	0/2778	0.56	1/3777 (0.0%)
5	e	0.27	0/527	0.48	0/720
6	f	0.28	0/476	0.47	0/652
7	g	0.33	0/1112	0.57	0/1511
7	h	0.33	0/1143	0.56	1/1554 (0.1%)
7	i	0.35	0/1143	0.65	3/1554 (0.2%)
7	j	0.31	0/1134	0.53	0/1542
7	k	0.31	0/1150	0.58	1/1564 (0.1%)
7	l	0.32	0/1143	0.57	0/1554
7	m	0.32	0/1149	0.56	1/1562 (0.1%)
7	n	0.32	0/1149	0.60	1/1562 (0.1%)
8	o	0.34	0/1156	0.56	1/1567 (0.1%)
All	All	0.31	0/21688	0.57	10/29467 (0.0%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	199	LEU	CA-CB-CG	7.29	132.07	115.30
7	k	49	LEU	CA-CB-CG	6.37	129.94	115.30
7	n	68	LEU	CA-CB-CG	6.04	129.19	115.30
4	d	76	LEU	CA-CB-CG	5.79	128.62	115.30
7	i	125	LEU	CA-CB-CG	5.54	128.03	115.30

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	5665	0	5612	0	0
2	b	330	0	349	0	0
3	c	1466	0	1535	0	0
4	d	2720	0	2574	0	0
5	e	512	0	530	0	0
6	f	463	0	448	0	0
7	g	1094	0	1167	0	0
7	h	1125	0	1195	0	0
7	i	1125	0	1195	0	0
7	j	1116	0	1189	0	0
7	k	1132	0	1202	0	0
7	l	1125	0	1195	0	0
7	m	1131	0	1200	0	0
7	n	1131	0	1200	0	0
8	o	1133	0	1189	0	0
All	All	21268	0	21780	0	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 3.

There are no clashes within the asymmetric unit.

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	703/912 (77%)	675 (96%)	28 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	42/265 (16%)	42 (100%)	0	0	100	100
3	c	195/213 (92%)	189 (97%)	6 (3%)	0	100	100
4	d	341/345 (99%)	327 (96%)	14 (4%)	0	100	100
5	e	62/73 (85%)	62 (100%)	0	0	100	100
6	f	59/85 (69%)	59 (100%)	0	0	100	100
7	g	151/160 (94%)	149 (99%)	2 (1%)	0	100	100
7	h	155/160 (97%)	154 (99%)	1 (1%)	0	100	100
7	i	155/160 (97%)	153 (99%)	2 (1%)	0	100	100
7	j	154/160 (96%)	152 (99%)	2 (1%)	0	100	100
7	k	156/160 (98%)	154 (99%)	2 (1%)	0	100	100
7	l	155/160 (97%)	153 (99%)	2 (1%)	0	100	100
7	m	156/160 (98%)	154 (99%)	2 (1%)	0	100	100
7	n	156/160 (98%)	154 (99%)	2 (1%)	0	100	100
8	o	154/164 (94%)	152 (99%)	2 (1%)	0	100	100
All	All	2794/3337 (84%)	2729 (98%)	65 (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	a	604/805 (75%)	597 (99%)	7 (1%)	74	89
2	b	36/244 (15%)	36 (100%)	0	100	100
3	c	153/168 (91%)	151 (99%)	2 (1%)	71	88
4	d	287/309 (93%)	283 (99%)	4 (1%)	69	88
5	e	56/65 (86%)	56 (100%)	0	100	100
6	f	51/72 (71%)	51 (100%)	0	100	100
7	g	112/119 (94%)	112 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	h	116/119 (98%)	116 (100%)	0	100	100
7	i	116/119 (98%)	116 (100%)	0	100	100
7	j	115/119 (97%)	115 (100%)	0	100	100
7	k	117/119 (98%)	116 (99%)	1 (1%)	81	92
7	l	116/119 (98%)	116 (100%)	0	100	100
7	m	117/119 (98%)	117 (100%)	0	100	100
7	n	117/119 (98%)	117 (100%)	0	100	100
8	o	118/125 (94%)	117 (99%)	1 (1%)	83	93
All	All	2231/2740 (81%)	2216 (99%)	15 (1%)	86	94

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	862	ARG
3	c	95	ARG
4	d	340	ASN
1	a	767	ASN
4	d	283	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
4	d	128	HIS
4	d	340	ASN
7	n	90	GLN
4	d	283	ASN
4	d	303	GLN

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 [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.