



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 16, 2018 – 06:21 PM EST

PDB ID : 5Y5Y
EMDB ID: : EMD-6811
Title : V/A-type ATPase/synthase from *Thermus thermophilus*, peripheral domain, rotational state 1
Authors : Nakanishi, A.; Kishikawa, J.; Tamakoshi, M.; Mitsuoka, K.; Yokoyama, K.
Deposited on : 2017-08-10
Resolution : 4.70 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 : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

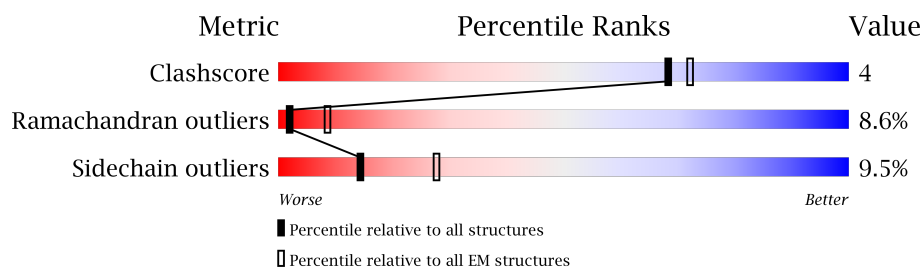
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	578	70% 23% 5% .
1	B	578	70% 24% 6% .
1	C	578	71% 23% 6% .
2	D	478	65% 23% 7% . .
2	E	478	65% 25% 5% .
2	F	478	71% 22% . .
3	G	223	63% 24% 6% . 6%
4	H	104	61% 31% . . .
5	I	120	43% 7% . 49%

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Mol	Chain	Length	Quality of chain
5	K	120	<div><div></div><div>43%6%•49%</div></div>
6	J	188	<div><div></div><div>73%7%•19%</div></div>
6	L	188	<div><div></div><div>74%7%19%</div></div>
7	M	323	<div><div></div><div>83%15%••</div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 32159 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 ATP synthase alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	577	Total	C	N	O	S	0	0
			4472	2854	762	834	22		
1	B	577	Total	C	N	O	S	0	0
			4472	2854	762	834	22		
1	C	577	Total	C	N	O	S	0	0
			4472	2854	762	834	22		

- Molecule 2 is a protein called V-type ATP synthase beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	459	Total	C	N	O	S	0	0
			3596	2278	622	686	10		
2	E	459	Total	C	N	O	S	0	0
			3596	2278	622	686	10		
2	F	459	Total	C	N	O	S	0	0
			3596	2278	622	686	10		

- Molecule 3 is a protein called V-type ATP synthase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	210	Total	C	N	O	S	0	0
			1642	1033	307	300	2		

- Molecule 4 is a protein called V-type ATP synthase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	100	Total	C	N	O	S	0	0
			758	479	131	145	3		

- Molecule 5 is a protein called V-type ATP synthase, subunit (VAPC-THERM).

Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	61	Total	C	N	O	0	0
			451	276	85	90		
5	K	61	Total	C	N	O	0	0
			451	276	85	90		

- Molecule 6 is a protein called V-type ATP synthase subunit E.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	J	152	Total	C	N	O	0	0
			1043	646	203	194		
6	L	152	Total	C	N	O	0	0
			1043	646	203	194		

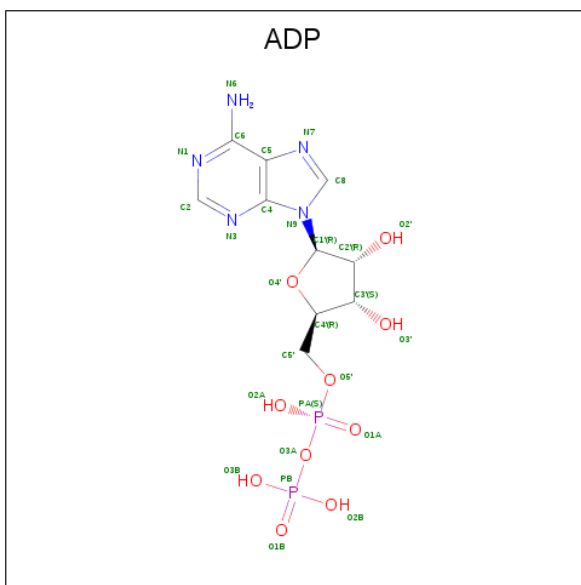
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	134	MET	LEU	conflict	UNP P74901
J	171	MET	LEU	conflict	UNP P74901
J	178	MET	LEU	conflict	UNP P74901
L	134	MET	LEU	conflict	UNP P74901
L	171	MET	LEU	conflict	UNP P74901
L	178	MET	LEU	conflict	UNP P74901

- Molecule 7 is a protein called V-type ATP synthase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	320	Total	C	N	O	S	0	0
			2513	1599	460	450	4		

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

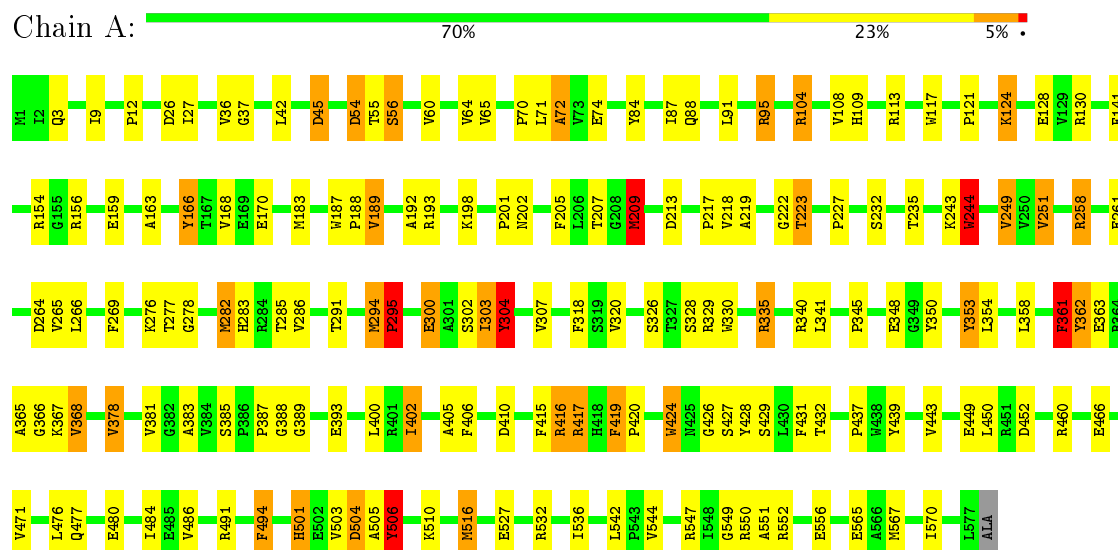


Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total 27	C 10	N 5	O 10	P 2	0
8	C	1	Total 27	C 10	N 5	O 10	P 2	0

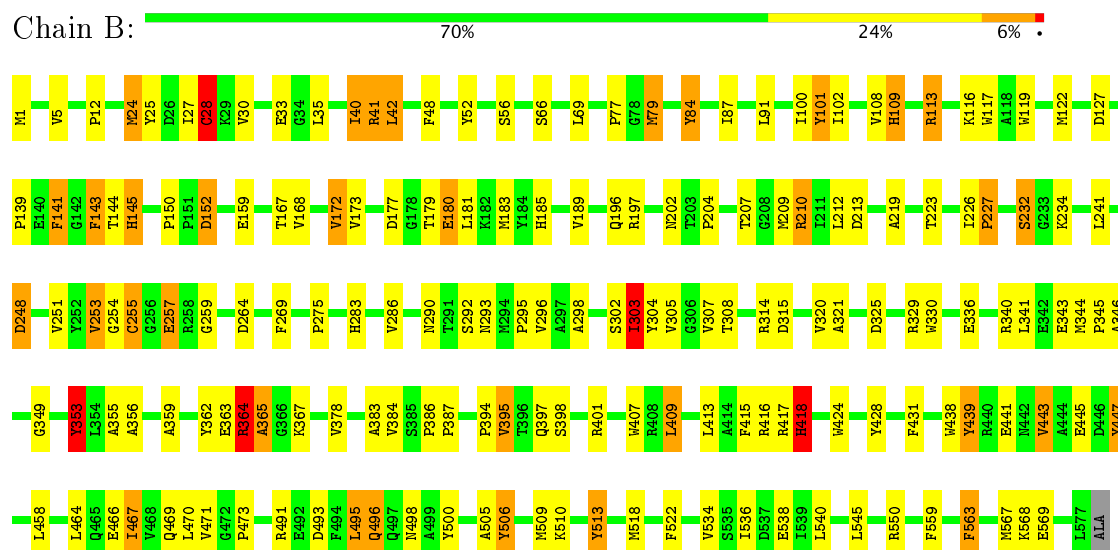
3 Residue-property plots

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 ATP synthase alpha chain

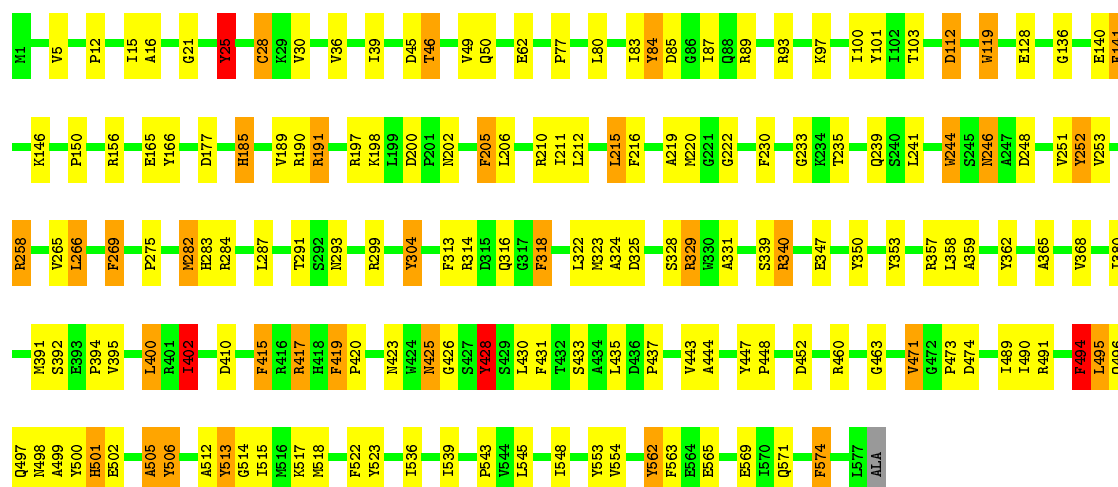


• Molecule 1: V-type ATP synthase alpha chain



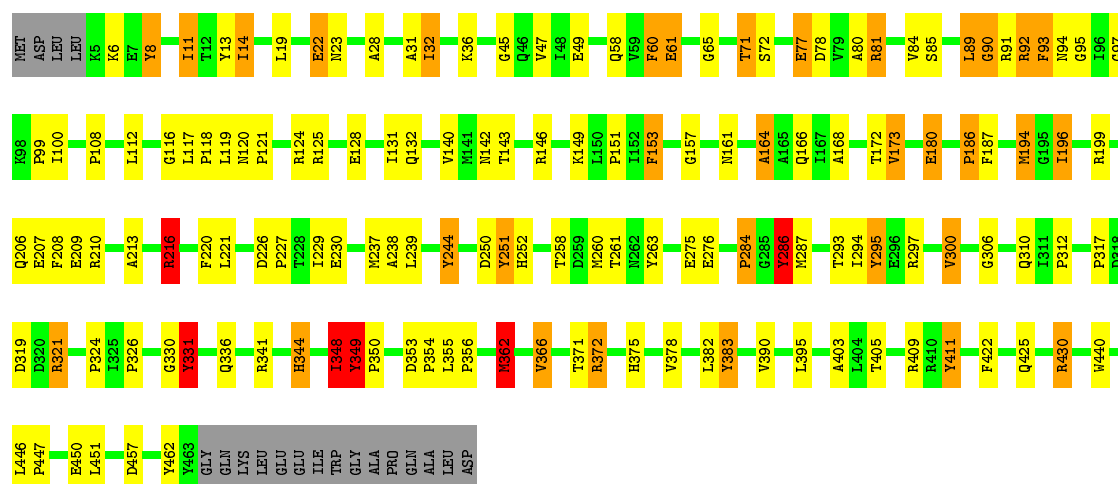
• Molecule 1: V-type ATP synthase alpha chain

Chain C:  71% 23% 6%



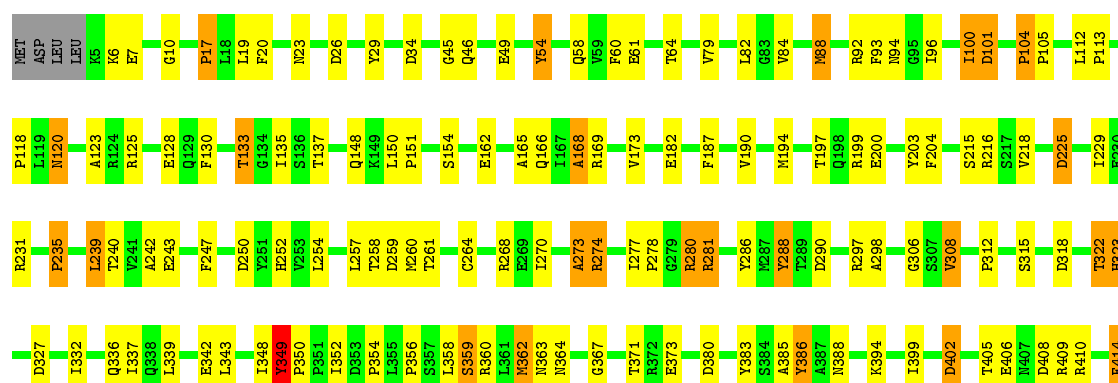
• Molecule 2: V-type ATP synthase beta chain

Chain D:  65% 23% 7%

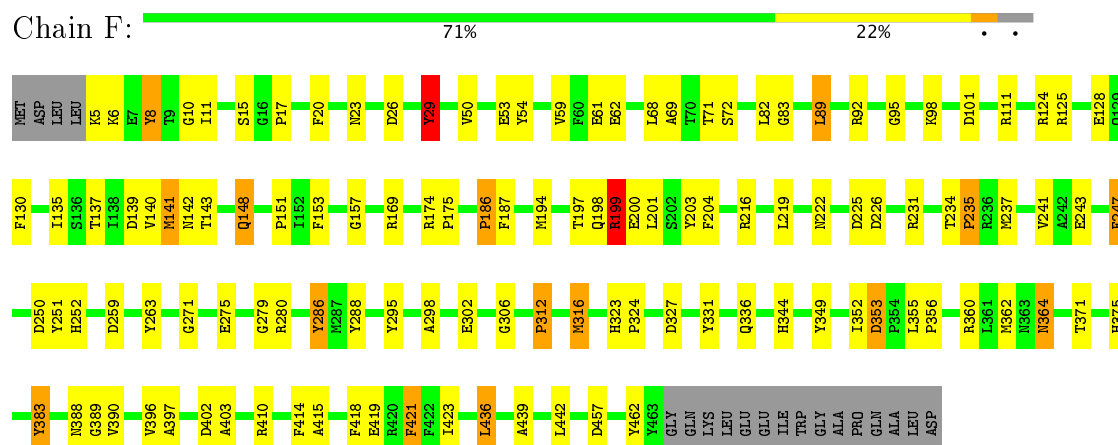


• Molecule 2: V-type ATP synthase beta chain

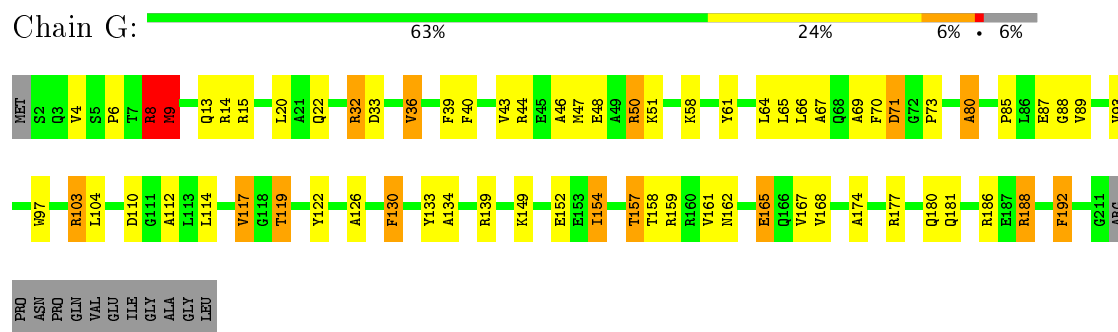
Chain E:  65% 25% 5%



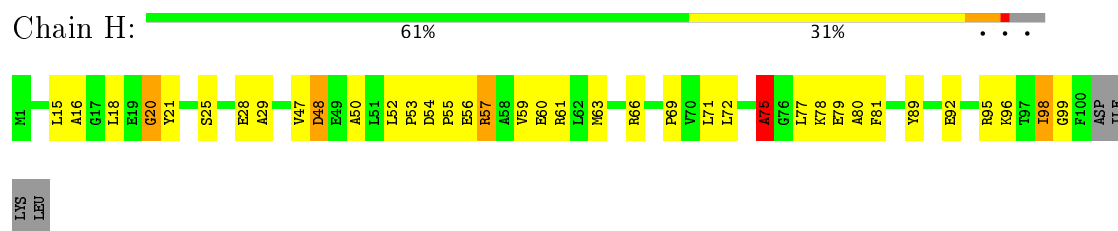
- Molecule 2: V-type ATP synthase beta chain



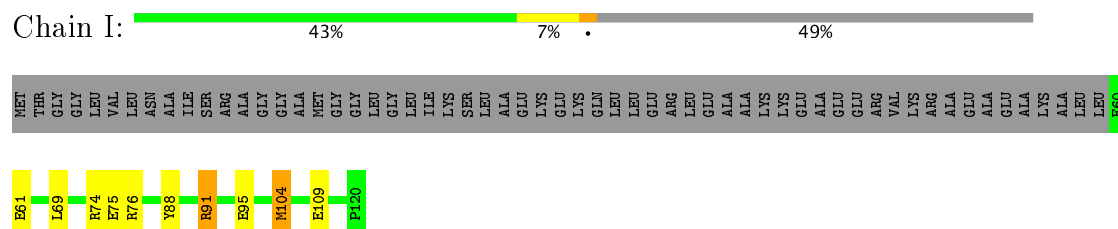
- Molecule 3: V-type ATP synthase subunit D



- Molecule 4: V-type ATP synthase subunit F

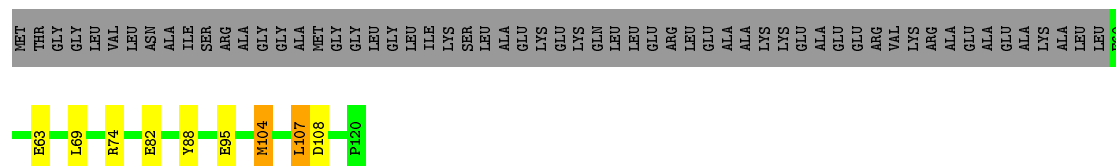


- Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)



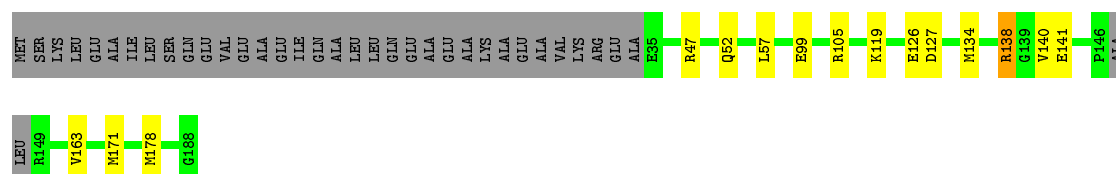
- Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)

Chain K:  43% 6% 49%



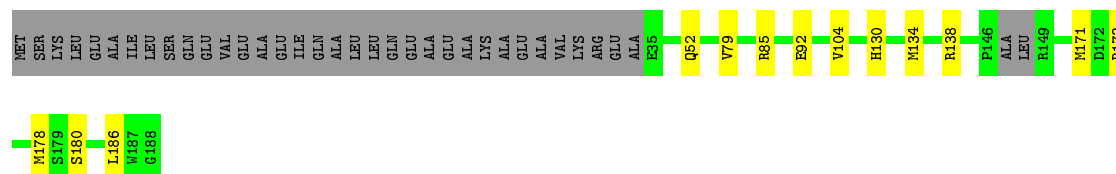
- Molecule 6: V-type ATP synthase subunit E

Chain J:  73% 7% 19%




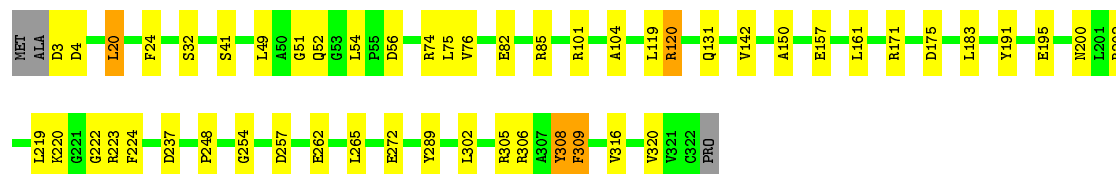
- Molecule 6: V-type ATP synthase subunit E

Chain L:  74% 7% 19%



- Molecule 7: V-type ATP synthase subunit C

Chain M:  83% 15% ..



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	117938	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 ($e^-/\text{\AA}^2$)	26	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

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	1.38	3/4568 (0.1%)	1.45	29/6198 (0.5%)
1	B	1.31	0/4568	1.42	27/6198 (0.4%)
1	C	1.35	1/4568 (0.0%)	1.47	41/6198 (0.7%)
2	D	1.33	0/3663	1.46	29/4960 (0.6%)
2	E	1.34	1/3663 (0.0%)	1.45	30/4960 (0.6%)
2	F	1.37	1/3663 (0.0%)	1.48	25/4960 (0.5%)
3	G	1.27	0/1662	1.48	12/2235 (0.5%)
4	H	1.16	0/769	1.41	3/1039 (0.3%)
5	I	1.10	0/451	1.19	1/608 (0.2%)
5	K	1.10	0/451	1.27	3/608 (0.5%)
6	J	1.05	0/1053	1.24	1/1439 (0.1%)
6	L	1.12	0/1053	1.22	1/1439 (0.1%)
7	M	1.08	0/2552	1.20	3/3446 (0.1%)
All	All	1.30	6/32684 (0.0%)	1.41	205/44288 (0.5%)

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	18
1	B	0	15
1	C	0	21
2	D	0	19
2	E	0	17
2	F	0	17
3	G	0	10
4	H	0	3
5	I	0	1
5	K	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	J	0	1
6	L	0	1
7	M	0	8
All	All	0	132

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	353	TYR	CB-CG	-5.66	1.43	1.51
2	E	278	PRO	CA-C	-5.53	1.41	1.52
1	A	388	GLY	CA-C	-5.51	1.43	1.51
1	C	419	PHE	C-N	-5.34	1.24	1.34
2	F	323	HIS	C-N	-5.21	1.24	1.34

The worst 5 of 205 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	88	TYR	CB-CG-CD2	-10.45	114.73	121.00
1	C	84	TYR	CB-CG-CD2	-10.43	114.74	121.00
2	F	383	TYR	CB-CG-CD1	-9.94	115.03	121.00
2	F	286	TYR	CB-CG-CD2	-9.94	115.04	121.00
5	K	88	TYR	CB-CG-CD1	9.39	126.64	121.00

There are no chirality outliers.

5 of 132 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	ARG	Sidechain
1	A	304	TYR	Sidechain
1	A	335	ARG	Sidechain
1	A	84	TYR	Sidechain
1	A	95	ARG	Sidechain

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	A	4472	0	4491	48	0
1	B	4472	0	4491	42	0
1	C	4472	0	4491	47	0
2	D	3596	0	3624	41	0
2	E	3596	0	3624	34	0
2	F	3596	0	3624	27	0
3	G	1642	0	1718	18	0
4	H	758	0	764	9	0
5	I	451	0	429	3	0
5	K	451	0	429	1	0
6	J	1043	0	936	3	0
6	L	1043	0	936	6	0
7	M	2513	0	2587	12	0
8	A	27	0	12	4	0
8	C	27	0	12	4	0
All	All	32159	0	32168	280	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 280 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:325:ASP:HA	1:B:383:ALA:HB3	1.65	0.77
6:L:178:MET:CG	6:L:178:MET:CE	2.63	0.77
5:I:104:MET:CG	5:I:104:MET:CE	2.64	0.75
2:D:131:ILE:HG22	2:D:132:GLN:O	1.91	0.71
6:J:178:MET:CE	6:J:178:MET:CG	2.68	0.71

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	575/578 (100%)	423 (74%)	97 (17%)	55 (10%)	1	13
1	B	575/578 (100%)	408 (71%)	100 (17%)	67 (12%)	0	8
1	C	575/578 (100%)	426 (74%)	102 (18%)	47 (8%)	1	16
2	D	457/478 (96%)	317 (69%)	93 (20%)	47 (10%)	0	11
2	E	457/478 (96%)	321 (70%)	92 (20%)	44 (10%)	1	13
2	F	457/478 (96%)	337 (74%)	83 (18%)	37 (8%)	1	17
3	G	208/223 (93%)	157 (76%)	33 (16%)	18 (9%)	1	15
4	H	98/104 (94%)	65 (66%)	18 (18%)	15 (15%)	0	4
5	I	59/120 (49%)	57 (97%)	1 (2%)	1 (2%)	11	51
5	K	59/120 (49%)	55 (93%)	2 (3%)	2 (3%)	4	36
6	J	148/188 (79%)	115 (78%)	24 (16%)	9 (6%)	2	23
6	L	148/188 (79%)	129 (87%)	15 (10%)	4 (3%)	6	41
7	M	318/323 (98%)	293 (92%)	15 (5%)	10 (3%)	5	38
All	All	4134/4434 (93%)	3103 (75%)	675 (16%)	356 (9%)	2	16

5 of 356 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASP
1	A	56	SER
1	A	188	PRO
1	A	217	PRO
1	A	227	PRO

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	468/468 (100%)	419 (90%)	49 (10%)	8	34
1	B	468/468 (100%)	416 (89%)	52 (11%)	7	32
1	C	468/468 (100%)	423 (90%)	45 (10%)	10	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	386/401 (96%)	343 (89%)	43 (11%)	7	32
2	E	386/401 (96%)	350 (91%)	36 (9%)	10	39
2	F	386/401 (96%)	360 (93%)	26 (7%)	19	53
3	G	166/176 (94%)	141 (85%)	25 (15%)	3	21
4	H	76/80 (95%)	66 (87%)	10 (13%)	5	26
5	I	37/86 (43%)	32 (86%)	5 (14%)	4	26
5	K	37/86 (43%)	32 (86%)	5 (14%)	4	26
6	J	76/141 (54%)	74 (97%)	2 (3%)	51	76
6	L	76/141 (54%)	76 (100%)	0	100	100
7	M	254/256 (99%)	240 (94%)	14 (6%)	25	59
All	All	3284/3573 (92%)	2972 (90%)	312 (10%)	14	38

5 of 312 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	543	PRO
2	D	251	TYR
5	I	75	GLU
1	C	574	PHE
2	D	149	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	249	HIS
2	D	363	ASN
7	M	200	ASN
2	D	252	HIS
2	D	429	ASN

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 ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	ADP	A	600	-	25,29,29	1.79	5 (20%)	24,45,45	1.31	2 (8%)
8	ADP	C	600	-	25,29,29	1.60	3 (12%)	24,45,45	1.27	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ADP	A	600	-	-	0/12/32/32	0/3/3/3
8	ADP	C	600	-	-	0/12/32/32	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	600	ADP	C2'-C1'	-4.40	1.46	1.53
8	C	600	ADP	C2'-C1'	-3.68	1.47	1.53
8	A	600	ADP	C8-N7	-2.94	1.29	1.34
8	A	600	ADP	O4'-C1'	-2.82	1.37	1.41
8	C	600	ADP	C8-N7	-2.72	1.29	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
8	A	600	ADP	C1'-N9-C4	-3.01	121.43	126.64
8	C	600	ADP	C5-C6-N6	-2.17	116.05	120.47
8	A	600	ADP	N6-C6-N1	3.94	126.58	118.77
8	C	600	ADP	N6-C6-N1	4.01	126.72	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	600	ADP	4	0
8	C	600	ADP	4	0

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.