



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 01:02 pm GMT

PDB ID : 5T4P
EMDB ID: : EMD-8358
Title : Autoinhibited E. coli ATP synthase state 2
Authors : Sobti, M.; Smits, C.; Wong, A.S.W.; Ishmukhametov, R.; Stock, D.; Sandin, S.; Stewart, A.G.
Deposited on : 2016-08-29
Resolution : 7.77 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) : recalc29047

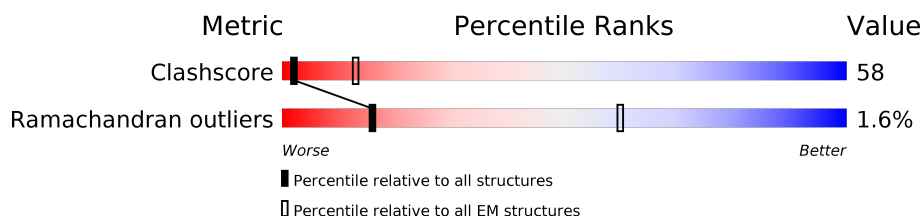
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.77 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

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	513	 43% 54% .
1	B	513	 41% 55% ..
1	C	513	 44% 53% ..
2	D	471	 36% 61% ..
2	E	471	 46% 52% ..
2	F	471	 37% 59% ..
3	G	287	 50% 46% ..
4	H	139	 36% 62% .
5	I	155	 77% 23% .
5	J	155	 68% 32%
6	K	271	 61% 16% . 22%

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Mol	Chain	Length	Quality of chain
7	L	177	
8	M	79	
8	N	79	
8	O	79	
8	P	79	
8	Q	79	
8	R	79	
8	S	79	
8	T	79	
8	U	79	
8	V	79	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	ADP	E	601	-	-	X	-
9	ATP	A	601	-	-	X	-
9	ATP	B	601	-	-	X	-
9	ATP	C	601	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 23568 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 ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	511	Total	C	N	O	0	0
			2507	1485	511	511		
1	B	510	Total	C	N	O	0	0
			2502	1482	510	510		
1	C	508	Total	C	N	O	0	0
			2492	1476	508	508		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ALA	CYS	conflict	UNP B7MGF4
A	90	ALA	CYS	conflict	UNP B7MGF4
A	193	ALA	CYS	conflict	UNP B7MGF4
A	243	ALA	CYS	conflict	UNP B7MGF4
A	419	ASN	LYS	conflict	UNP B7MGF4
B	47	ALA	CYS	conflict	UNP B7MGF4
B	90	ALA	CYS	conflict	UNP B7MGF4
B	193	ALA	CYS	conflict	UNP B7MGF4
B	243	ALA	CYS	conflict	UNP B7MGF4
B	419	ASN	LYS	conflict	UNP B7MGF4
C	47	ALA	CYS	conflict	UNP B7MGF4
C	90	ALA	CYS	conflict	UNP B7MGF4
C	193	ALA	CYS	conflict	UNP B7MGF4
C	243	ALA	CYS	conflict	UNP B7MGF4
C	419	ASN	LYS	conflict	UNP B7MGF4

- Molecule 2 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	466	Total	C	N	O	0	0
			2284	1352	466	466		
2	E	466	Total	C	N	O	0	0
			2284	1352	466	466		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	F	466	Total 2284	C 1352	N 466	O 466	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	MET	-	expression tag	UNP B7MGF2
D	-10	ARG	-	expression tag	UNP B7MGF2
D	-9	GLY	-	expression tag	UNP B7MGF2
D	-8	SER	-	expression tag	UNP B7MGF2
D	-7	HIS	-	expression tag	UNP B7MGF2
D	-6	HIS	-	expression tag	UNP B7MGF2
D	-5	HIS	-	expression tag	UNP B7MGF2
D	-4	HIS	-	expression tag	UNP B7MGF2
D	-3	HIS	-	expression tag	UNP B7MGF2
D	-2	HIS	-	expression tag	UNP B7MGF2
D	-1	GLY	-	expression tag	UNP B7MGF2
D	137	ALA	CYS	conflict	UNP B7MGF2
E	-11	MET	-	expression tag	UNP B7MGF2
E	-10	ARG	-	expression tag	UNP B7MGF2
E	-9	GLY	-	expression tag	UNP B7MGF2
E	-8	SER	-	expression tag	UNP B7MGF2
E	-7	HIS	-	expression tag	UNP B7MGF2
E	-6	HIS	-	expression tag	UNP B7MGF2
E	-5	HIS	-	expression tag	UNP B7MGF2
E	-4	HIS	-	expression tag	UNP B7MGF2
E	-3	HIS	-	expression tag	UNP B7MGF2
E	-2	HIS	-	expression tag	UNP B7MGF2
E	-1	GLY	-	expression tag	UNP B7MGF2
E	137	ALA	CYS	conflict	UNP B7MGF2
F	-11	MET	-	expression tag	UNP B7MGF2
F	-10	ARG	-	expression tag	UNP B7MGF2
F	-9	GLY	-	expression tag	UNP B7MGF2
F	-8	SER	-	expression tag	UNP B7MGF2
F	-7	HIS	-	expression tag	UNP B7MGF2
F	-6	HIS	-	expression tag	UNP B7MGF2
F	-5	HIS	-	expression tag	UNP B7MGF2
F	-4	HIS	-	expression tag	UNP B7MGF2
F	-3	HIS	-	expression tag	UNP B7MGF2
F	-2	HIS	-	expression tag	UNP B7MGF2
F	-1	GLY	-	expression tag	UNP B7MGF2
F	137	ALA	CYS	conflict	UNP B7MGF2

- Molecule 3 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	284	Total	C	N	O	0	0
			1400	832	284	284		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	5	ASP	GLU	conflict	UNP B7MGF3
G	87	ALA	CYS	conflict	UNP B7MGF3
G	112	ALA	CYS	conflict	UNP B7MGF3

- Molecule 4 is a protein called ATP synthase epsilon chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	136	Total	C	N	O	0	0
			668	396	136	136		

- Molecule 5 is a protein called ATP synthase subunit b.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	155	Total	C	N	O	0	0
			772	462	155	155		
5	J	155	Total	C	N	O	0	0
			772	462	155	155		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	21	ALA	CYS	conflict	UNP P0ABA2
J	21	ALA	CYS	conflict	UNP P0ABA2

- Molecule 6 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	K	211	Total	C	N	O	0	0
			1040	618	211	211		

- Molecule 7 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	L	160	Total	C	N	O	0	0
			793	473	160	160		

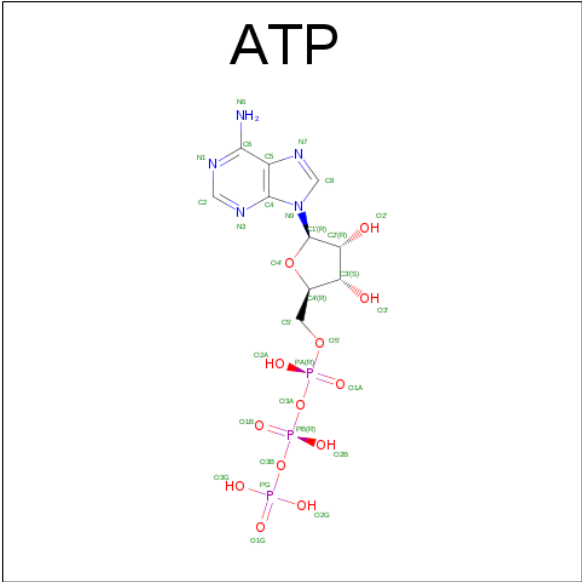
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	64	ALA	CYS	conflict	UNP B7MGF5
L	140	ALA	CYS	conflict	UNP B7MGF5

- Molecule 8 is a protein called ATP synthase subunit c.

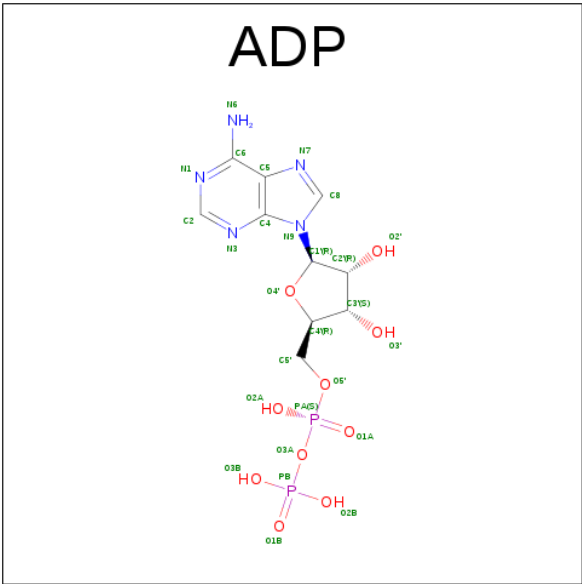
Mol	Chain	Residues	Atoms				AltConf	Trace
8	M	75	Total	C	N	O	0	0
			365	215	75	75		
8	N	75	Total	C	N	O	0	0
			365	215	75	75		
8	O	75	Total	C	N	O	0	0
			365	215	75	75		
8	P	75	Total	C	N	O	0	0
			365	215	75	75		
8	Q	75	Total	C	N	O	0	0
			365	215	75	75		
8	R	75	Total	C	N	O	0	0
			365	215	75	75		
8	S	75	Total	C	N	O	0	0
			365	215	75	75		
8	T	75	Total	C	N	O	0	0
			365	215	75	75		
8	U	75	Total	C	N	O	0	0
			365	215	75	75		
8	V	75	Total	C	N	O	0	0
			365	215	75	75		

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

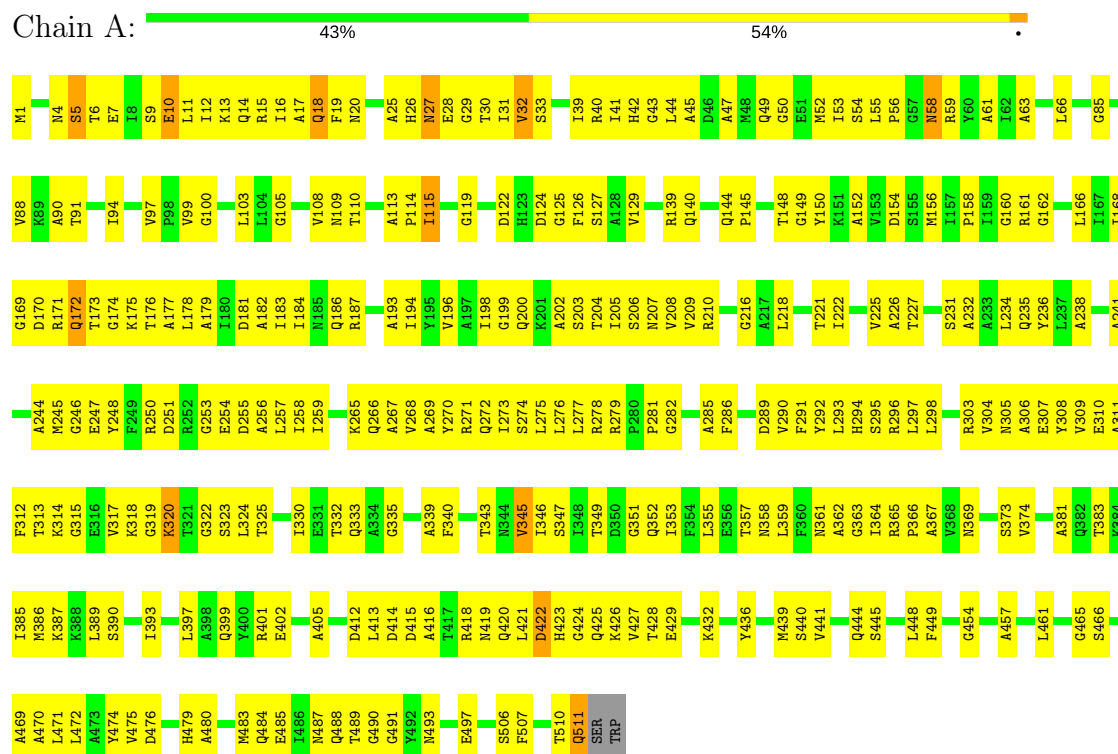


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
10	E	1	27	10	5	10	2	0

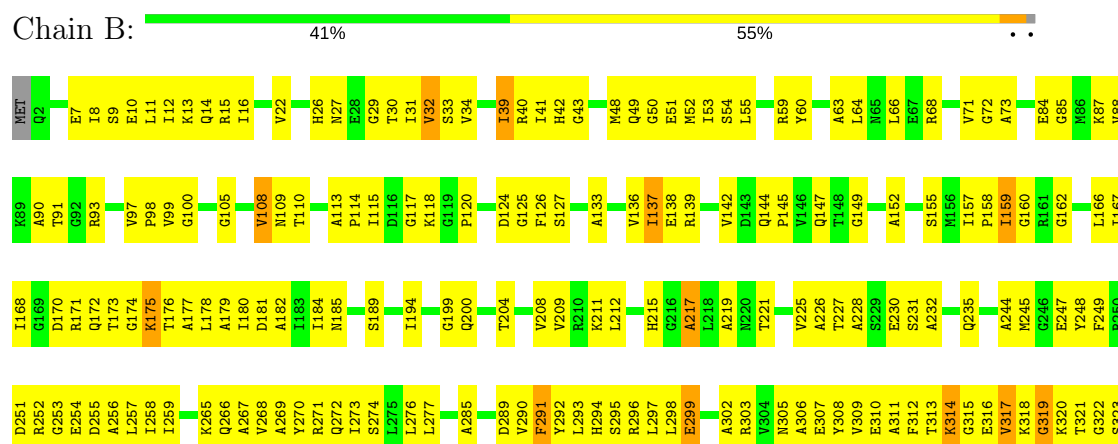
3 Residue-property plots

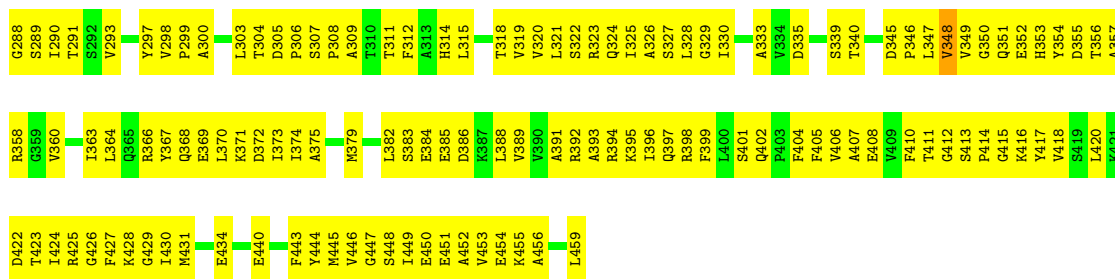
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: ATP synthase subunit alpha



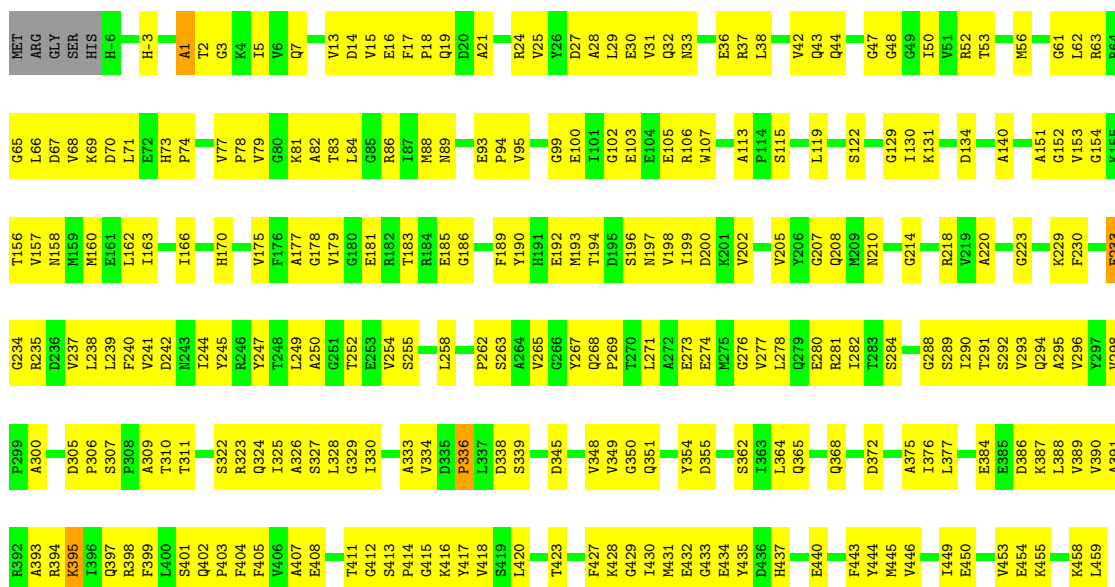
• Molecule 1: ATP synthase subunit alpha





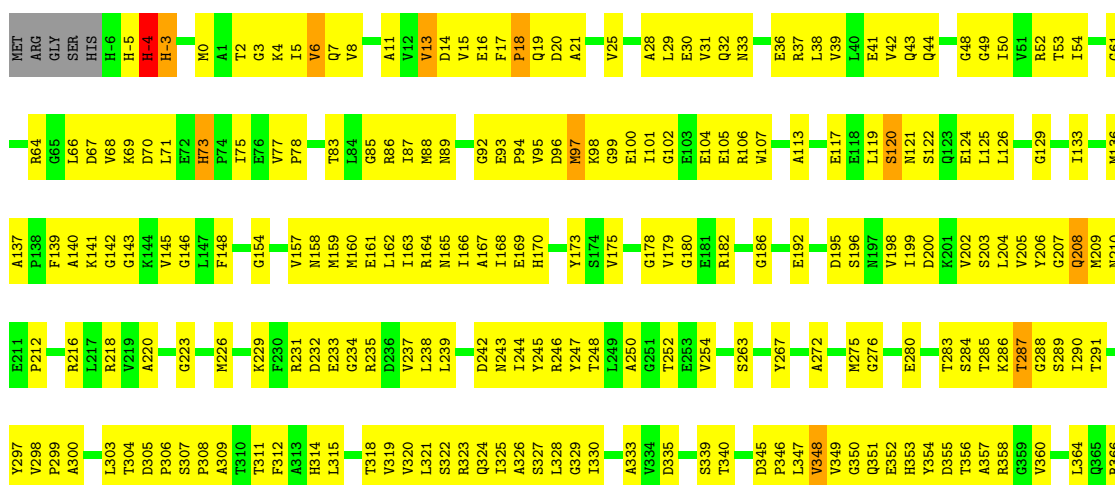
- Molecule 2: ATP synthase subunit beta

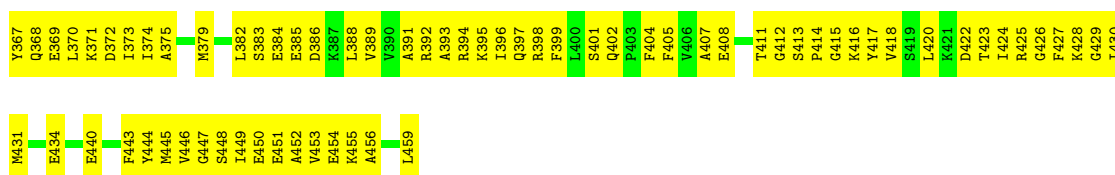
Chain E:



- Molecule 2: ATP synthase subunit beta

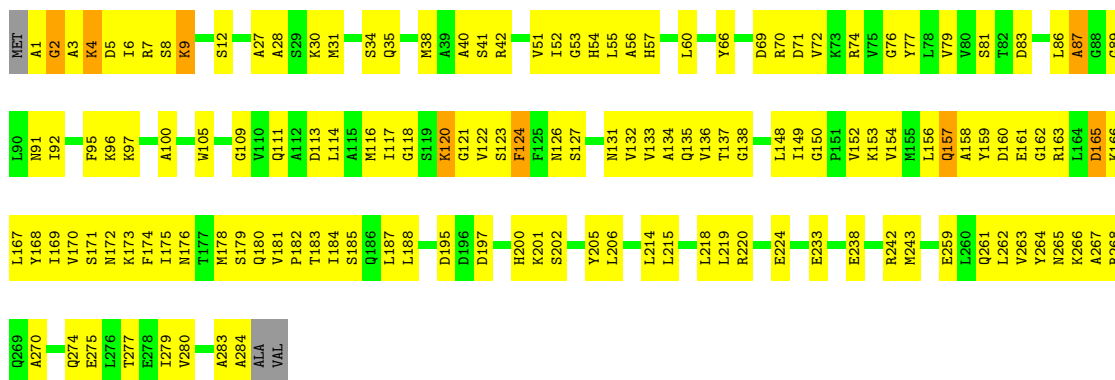
Chain F:





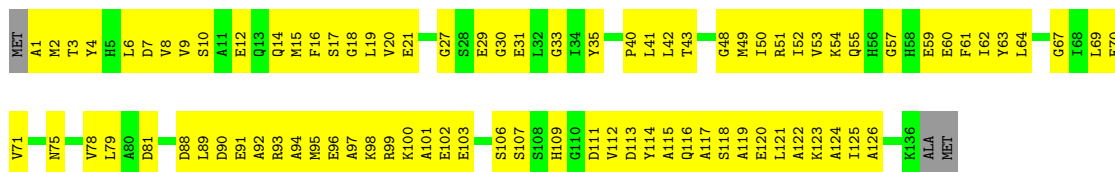
• Molecule 3: ATP synthase gamma chain

Chain G: 50% 46% ..



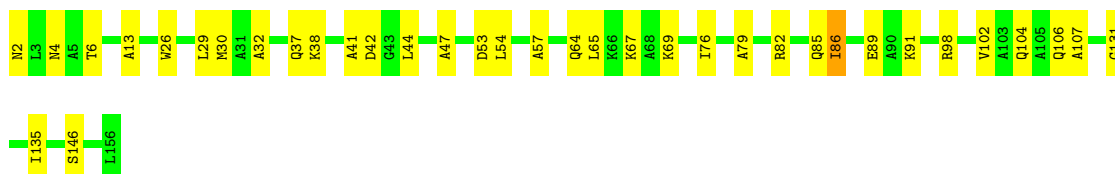
• Molecule 4: ATP synthase epsilon chain

Chain H: 36% 62% .



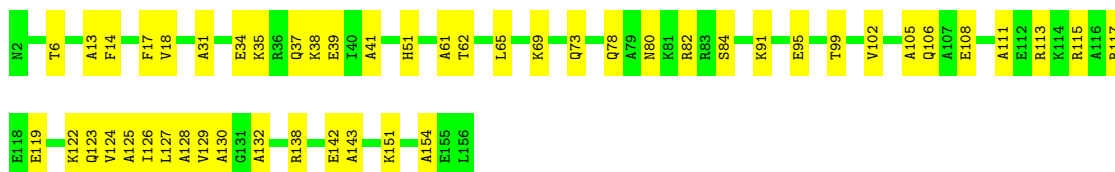
• Molecule 5: ATP synthase subunit b

Chain I: 77% 23% .

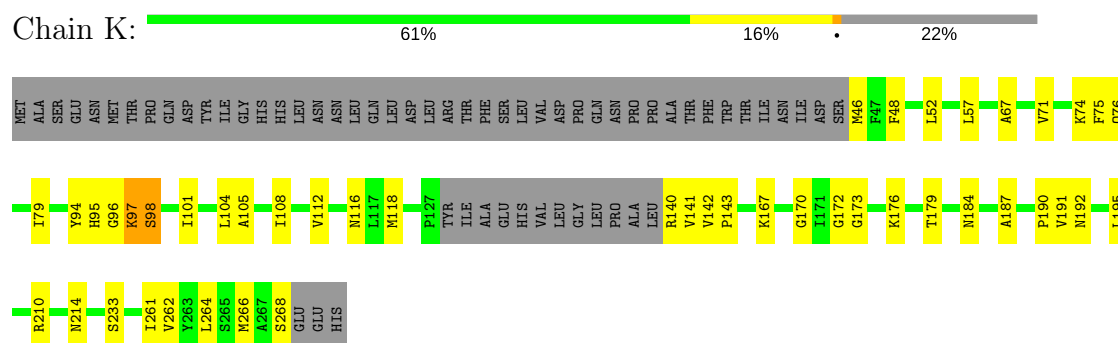


• Molecule 5: ATP synthase subunit b

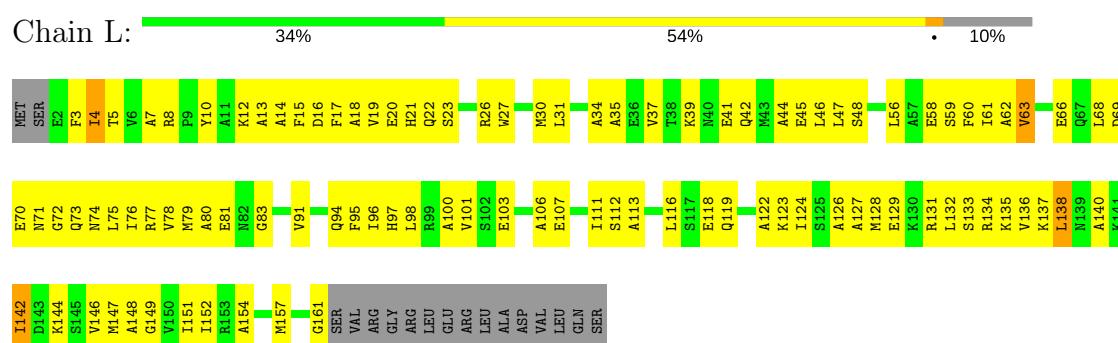
Chain J: 68% 32%



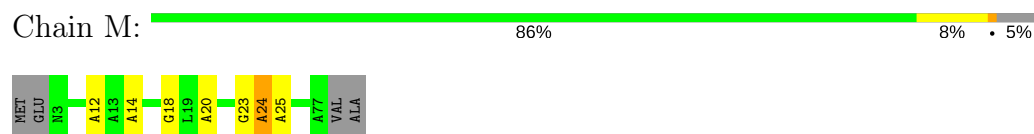
- Molecule 6: ATP synthase subunit a



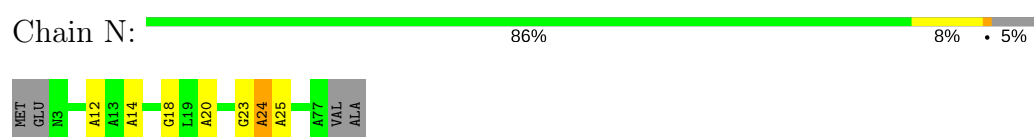
- Molecule 7: ATP synthase subunit delta



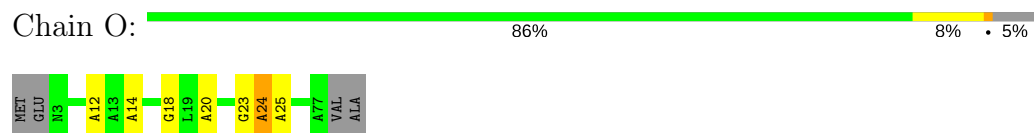
- Molecule 8: ATP synthase subunit c



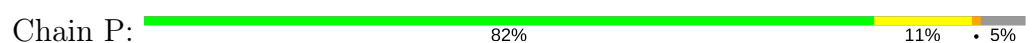
- Molecule 8: ATP synthase subunit c



- Molecule 8: ATP synthase subunit c



- Molecule 8: ATP synthase subunit c





- Molecule 8: ATP synthase subunit c

Chain Q: 85% 9% • 5%



- Molecule 8: ATP synthase subunit c

Chain R: 86% 8% • 5%



- Molecule 8: ATP synthase subunit c

Chain S: 86% 8% • 5%



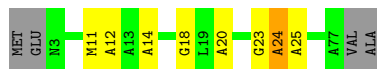
- Molecule 8: ATP synthase subunit c

Chain T: 86% 8% • 5%



- Molecule 8: ATP synthase subunit c

Chain U: 85% 9% • 5%



- Molecule 8: ATP synthase subunit c

Chain V: 86% 8% • 5%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	95345	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	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, 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	0.41	0/2506	0.64	1/3478 (0.0%)
1	B	0.40	0/2501	0.61	0/3471
1	C	0.40	1/2491 (0.0%)	0.60	0/3457
2	D	0.42	0/2283	0.66	0/3167
2	E	0.40	0/2283	0.62	0/3167
2	F	0.41	0/2283	0.68	1/3167 (0.0%)
3	G	0.39	0/1399	0.61	1/1945 (0.1%)
4	H	0.38	0/667	0.60	0/925
5	I	0.33	0/771	0.44	0/1076
5	J	0.32	0/771	0.41	0/1076
6	K	0.31	0/1038	0.52	0/1441
7	L	0.34	0/792	0.52	0/1103
8	M	0.62	0/364	0.95	1/502 (0.2%)
8	N	0.62	0/364	0.95	1/502 (0.2%)
8	O	0.63	0/364	0.95	1/502 (0.2%)
8	P	0.62	0/364	0.95	1/502 (0.2%)
8	Q	0.62	0/364	0.95	1/502 (0.2%)
8	R	0.62	0/364	0.95	1/502 (0.2%)
8	S	0.62	0/364	0.95	1/502 (0.2%)
8	T	0.62	0/364	0.95	1/502 (0.2%)
8	U	0.62	0/364	0.95	1/502 (0.2%)
8	V	0.62	0/364	0.95	1/502 (0.2%)
All	All	0.44	1/23425 (0.0%)	0.67	13/32493 (0.0%)

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	8

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	11
1	C	0	7
2	D	0	12
2	E	0	2
2	F	0	11
3	G	0	2
4	H	0	2
6	K	0	2
7	L	0	2
All	All	0	59

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	278	ARG	C-N	-5.90	1.20	1.34

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	511	GLN	N-CA-C	-7.55	90.63	111.00
8	V	24	ALA	CB-CA-C	-6.55	100.27	110.10
8	P	24	ALA	CB-CA-C	-6.54	100.28	110.10
8	S	24	ALA	CB-CA-C	-6.54	100.30	110.10
8	U	24	ALA	CB-CA-C	-6.53	100.31	110.10

There are no chirality outliers.

5 of 59 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	GLU	Peptide
1	A	18	GLN	Peptide
1	A	39	ILE	Peptide
1	A	58	ASN	Peptide
1	A	66	LEU	Peptide

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	2507	0	1240	282	0
1	B	2502	0	1235	277	0
1	C	2492	0	1230	278	0
2	D	2284	0	1065	253	0
2	E	2284	0	1065	202	0
2	F	2284	0	1065	245	0
3	G	1400	0	665	129	0
4	H	668	0	330	86	0
5	I	772	0	406	29	0
5	J	772	0	406	34	0
6	K	1040	0	464	38	0
7	L	793	0	407	76	0
8	M	365	0	192	34	0
8	N	365	0	192	32	0
8	O	365	0	192	30	0
8	P	365	0	192	35	0
8	Q	365	0	192	35	0
8	R	365	0	192	34	0
8	S	365	0	192	31	0
8	T	365	0	192	28	0
8	U	365	0	192	31	0
8	V	365	0	192	34	0
9	A	31	0	12	18	0
9	B	31	0	12	24	0
9	C	31	0	12	24	0
10	E	27	0	12	13	0
All	All	23568	0	11546	2038	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 58.

The worst 5 of 2038 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)
6:K:76:GLN:N	6:K:79:ILE:CB	1.75	1.48
6:K:76:GLN:CA	6:K:79:ILE:CB	2.01	1.39
8:T:20:ALA:HB2	8:U:18:GLY:O	1.19	1.35
8:M:20:ALA:HB2	8:N:18:GLY:O	1.26	1.34
8:O:20:ALA:HB2	8:P:18:GLY:C	1.47	1.34

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	A	509/513 (99%)	436 (86%)	65 (13%)	8 (2%)	11	51
1	B	508/513 (99%)	436 (86%)	61 (12%)	11 (2%)	8	44
1	C	506/513 (99%)	427 (84%)	69 (14%)	10 (2%)	9	46
2	D	464/471 (98%)	394 (85%)	60 (13%)	10 (2%)	8	44
2	E	464/471 (98%)	394 (85%)	63 (14%)	7 (2%)	12	53
2	F	464/471 (98%)	394 (85%)	60 (13%)	10 (2%)	8	44
3	G	282/287 (98%)	245 (87%)	28 (10%)	9 (3%)	5	36
4	H	134/139 (96%)	117 (87%)	17 (13%)	0	100	100
5	I	153/155 (99%)	133 (87%)	19 (12%)	1 (1%)	25	68
5	J	153/155 (99%)	140 (92%)	13 (8%)	0	100	100
6	K	207/271 (76%)	193 (93%)	11 (5%)	3 (1%)	13	54
7	L	158/177 (89%)	133 (84%)	19 (12%)	6 (4%)	4	32
8	M	73/79 (92%)	73 (100%)	0	0	100	100
8	N	73/79 (92%)	73 (100%)	0	0	100	100
8	O	73/79 (92%)	73 (100%)	0	0	100	100
8	P	73/79 (92%)	73 (100%)	0	0	100	100
8	Q	73/79 (92%)	73 (100%)	0	0	100	100
8	R	73/79 (92%)	73 (100%)	0	0	100	100
8	S	73/79 (92%)	73 (100%)	0	0	100	100
8	T	73/79 (92%)	73 (100%)	0	0	100	100
8	U	73/79 (92%)	73 (100%)	0	0	100	100
8	V	73/79 (92%)	73 (100%)	0	0	100	100
All	All	4732/4926 (96%)	4172 (88%)	485 (10%)	75 (2%)	16	51

5 of 75 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	441	VAL
1	C	22	VAL
2	D	75	ILE
2	F	75	ILE
6	K	141	VAL

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](#)

4 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	$\# Z > 2$
9	ATP	A	601	-	27,33,33	1.07	2 (7%)	25,52,52	2.58	4 (16%)
9	ATP	B	601	-	27,33,33	1.00	2 (7%)	25,52,52	2.06	5 (20%)
9	ATP	C	601	-	27,33,33	1.00	2 (7%)	25,52,52	1.96	6 (24%)
10	ADP	E	601	-	25,29,29	1.00	1 (4%)	24,45,45	1.88	6 (25%)

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
9	ATP	A	601	-	-	0/18/38/38	0/3/3/3
9	ATP	B	601	-	-	0/18/38/38	0/3/3/3
9	ATP	C	601	-	-	0/18/38/38	0/3/3/3
10	ADP	E	601	-	-	0/12/32/32	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	601	ATP	PG-O3B	-2.10	1.56	1.60
9	C	601	ATP	C2'-C1'	-2.10	1.50	1.53
9	B	601	ATP	PB-O2B	-2.05	1.44	1.55
9	C	601	ATP	C5-C4	2.44	1.46	1.40
9	A	601	ATP	C5-C4	2.61	1.46	1.40

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	601	ATP	C4'-O4'-C1'	-8.51	100.71	109.77
9	B	601	ATP	N3-C2-N1	-7.37	122.44	128.86
9	A	601	ATP	N3-C2-N1	-7.06	122.71	128.86
10	E	601	ADP	N3-C2-N1	-6.56	123.15	128.86
9	C	601	ATP	N3-C2-N1	-6.46	123.23	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	601	ATP	18	0
9	B	601	ATP	24	0
9	C	601	ATP	24	0
10	E	601	ADP	13	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.