



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 11:09 am BST

PDB ID : 2W6H
Title : Low resolution structures of bovine mitochondrial F1-ATPase during controlled dehydration: Hydration State 4A.
Authors : Sanchez-Weatherby, J.; Felisaz, F.; Gobbo, A.; Huet, J.; Ravelli, R.B.G.; Bowler, M.W.; Cipriani, F.
Deposited on : 2008-12-18
Resolution : 5.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

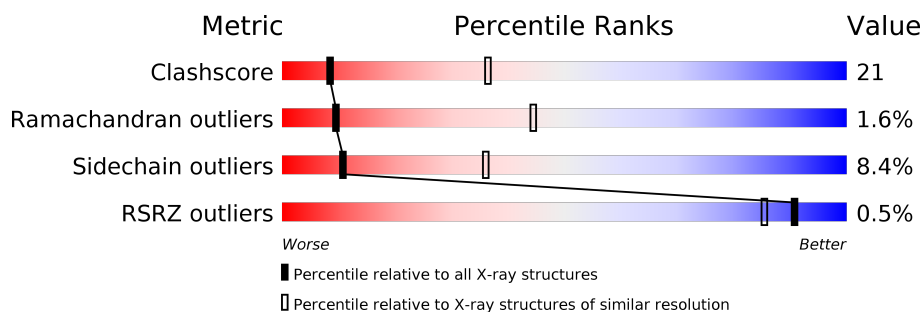
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.00 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1000 (6.16-3.82)
Ramachandran outliers	138981	1146 (6.20-3.80)
Sidechain outliers	138945	1122 (6.20-3.80)
RSRZ outliers	127900	1010 (6.22-3.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	553	<div> <div>47%</div> <div>33%</div> <div>7%</div> <div>•</div> <div>12%</div> </div>
1	B	553	<div> <div>48%</div> <div>32%</div> <div>6%</div> <div>•</div> <div>13%</div> </div>
1	C	553	<div> <div>53%</div> <div>32%</div> <div>•</div> <div>•</div> <div>11%</div> </div>
2	D	528	<div> <div>55%</div> <div>28%</div> <div>•</div> <div>•</div> <div>12%</div> </div>
2	E	528	<div> <div>%</div> <div>46%</div> <div>36%</div> <div>6%</div> <div>•</div> <div>12%</div> </div>
2	F	528	<div> <div>56%</div> <div>28%</div> <div>•</div> <div>•</div> <div>12%</div> </div>
3	G	298	<div> <div>%</div> <div>50%</div> <div>33%</div> <div>5%</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
4	H	168	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>4%40%34%•22%</div></div>
5	I	51	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>55%29%6%•8%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25108 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 HEART ISOFORM, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	B	479	Total	C	N	O	S	0	0	0
			3656	2303	647	694	12			
1	C	492	Total	C	N	O	S	0	0	0
			3748	2360	661	715	12			

- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	467	Total	C	N	O	S	0	0	0
			3539	2243	601	684	11			
2	E	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	F	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

- Molecule 3 is a protein called ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	263	Total	C	N	O	S	0	0	0
			2051	1291	354	398	8			

- Molecule 4 is a protein called ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	131	Total	C	N	O	S	0	0	0
			970	609	164	195	2			

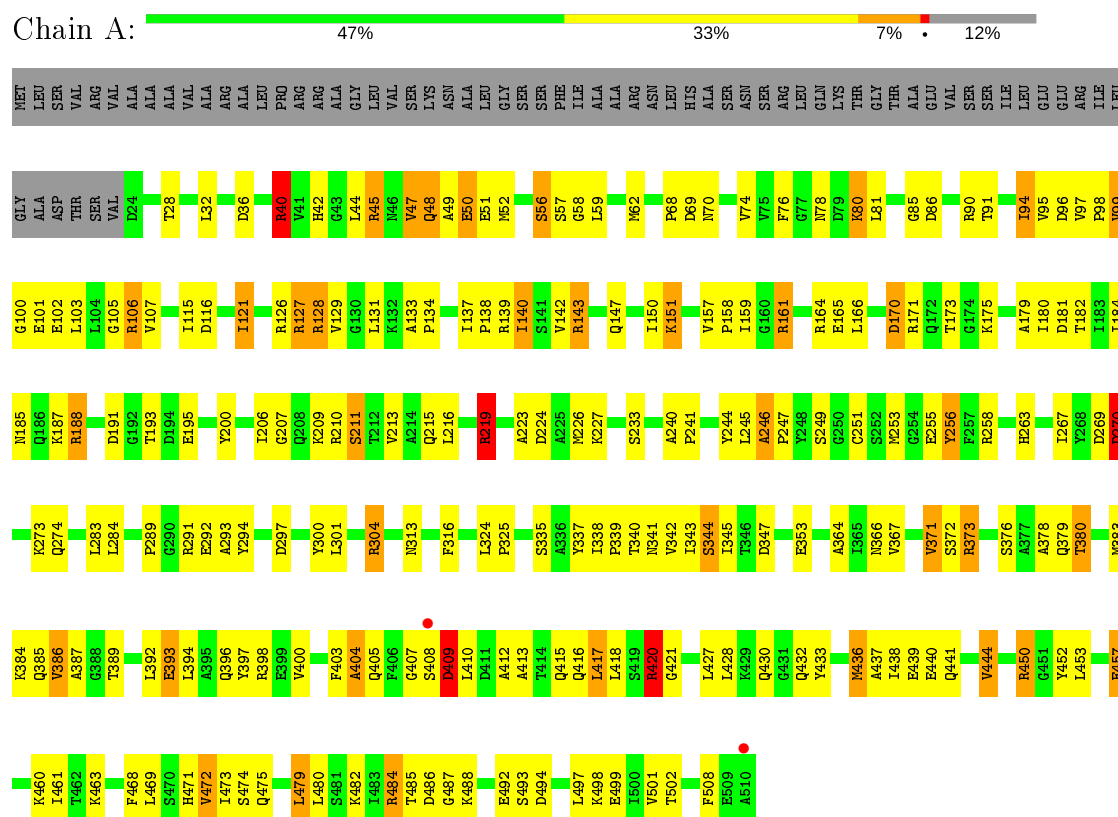
- Molecule 5 is a protein called ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	47	Total	C	N	O	S	0	0	0
			369	237	66	64	2			

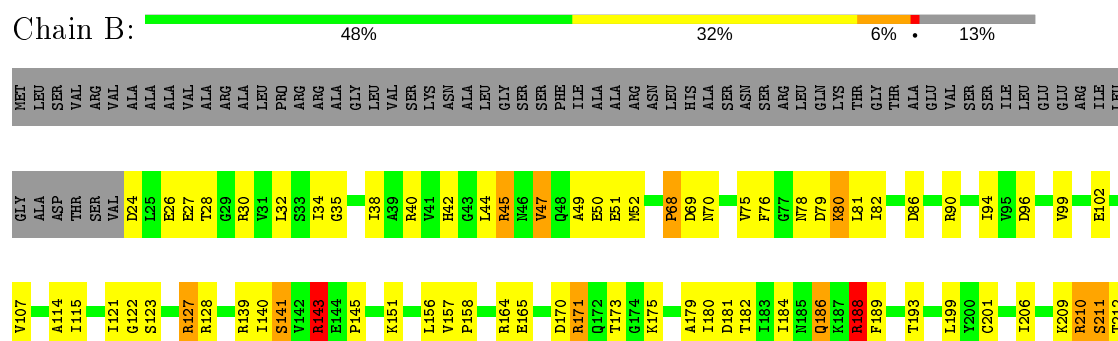
3 Residue-property plots

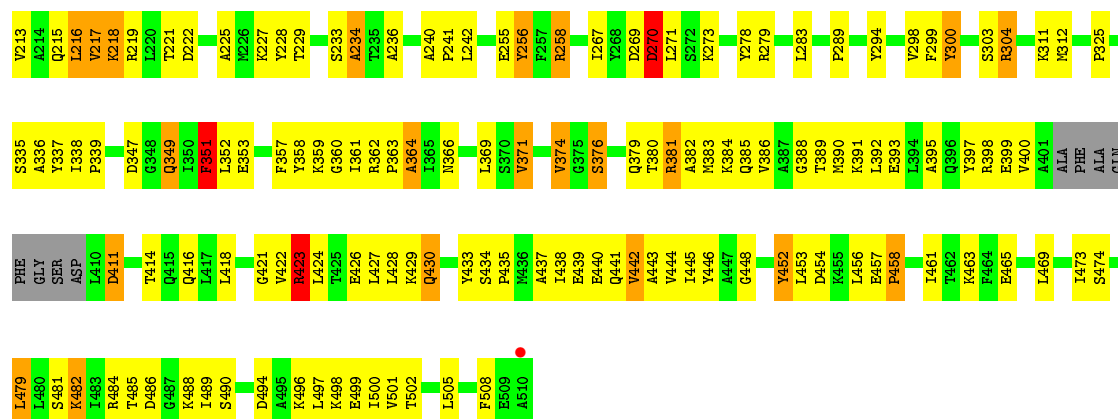
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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 HEART ISOFORM, MITOCHONDRIAL



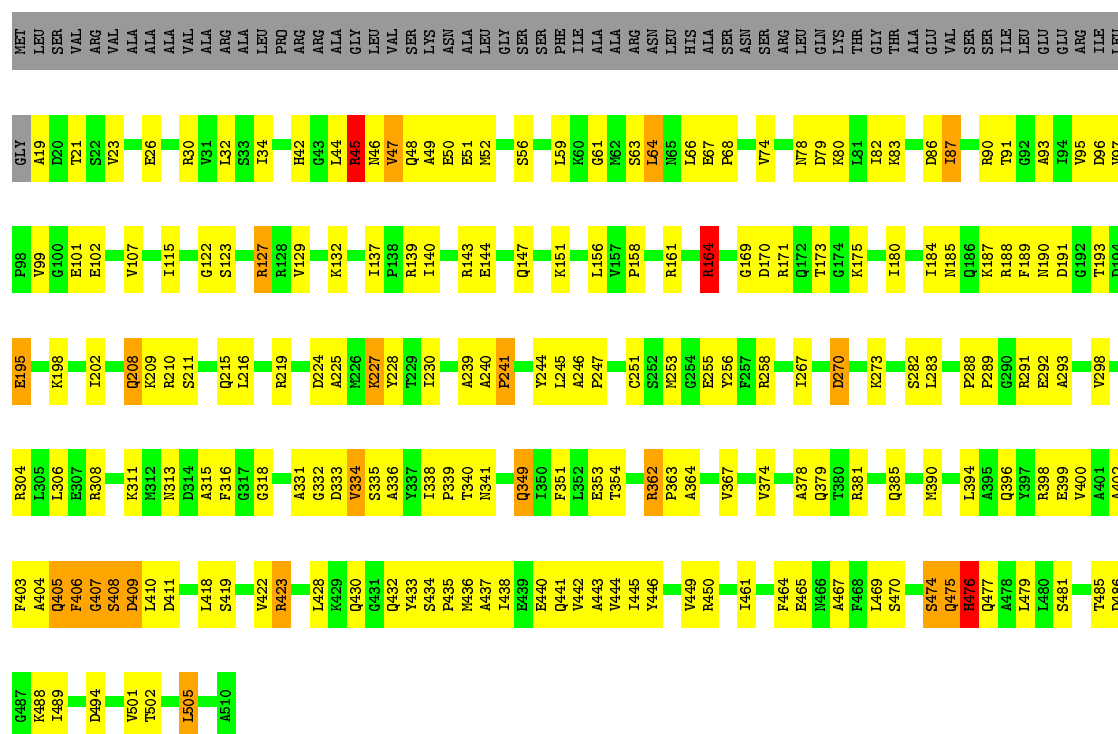
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM, MITOCHONDRIAL





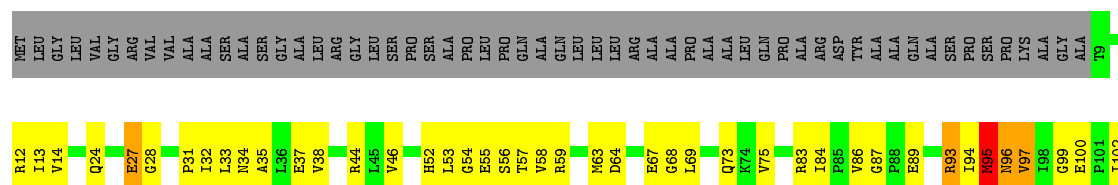
● Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM, MITOCHONDRIAL

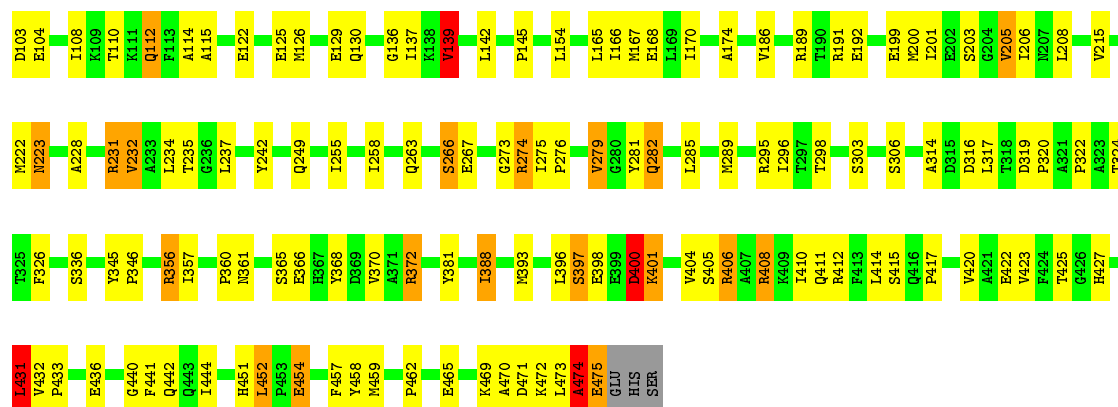
Chain C: 53% 32% 11%



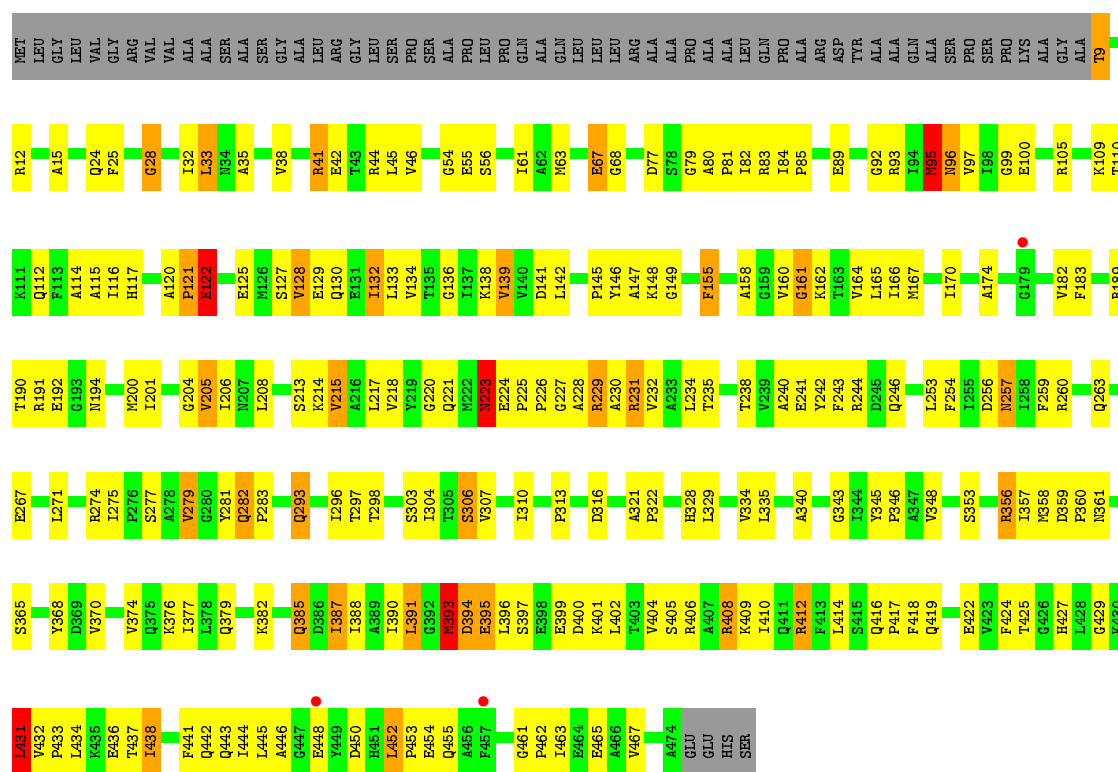
● Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain D: 55% 28% 12%

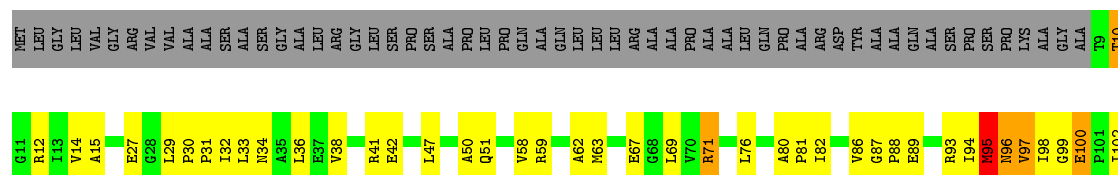


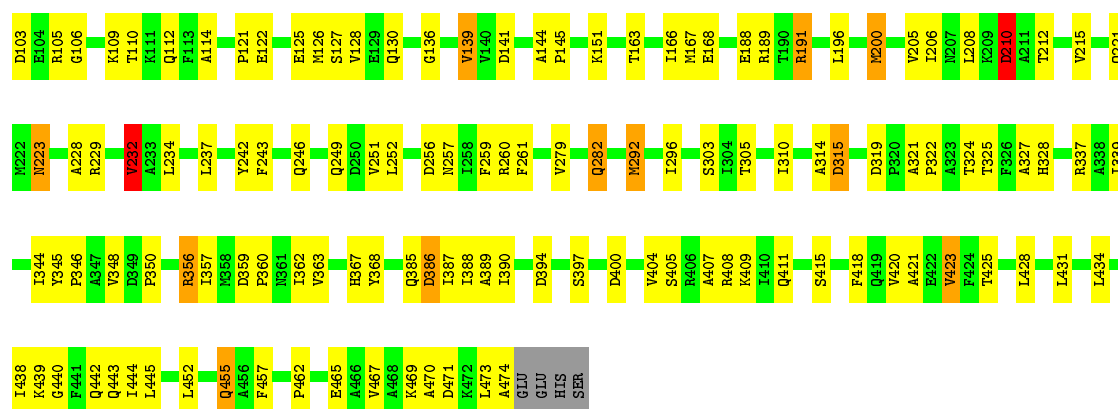


• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

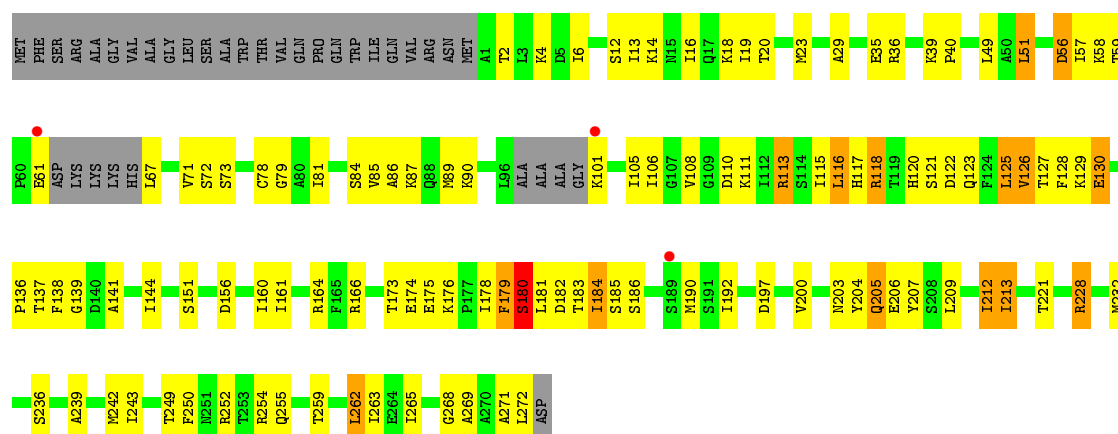


• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

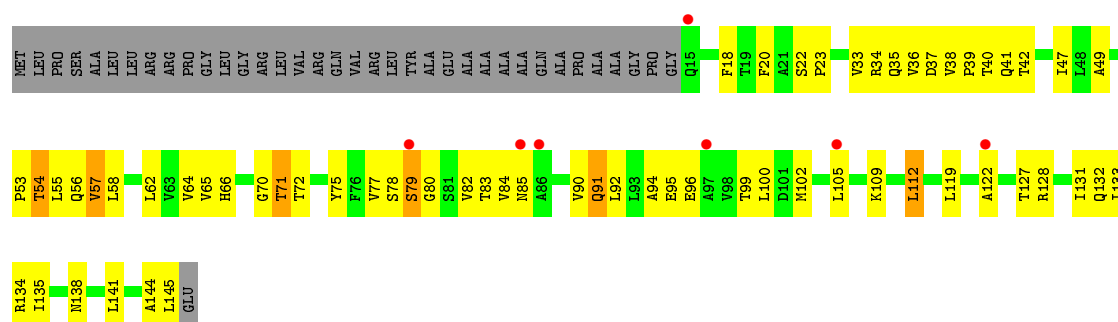




• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL



• Molecule 4: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL



• Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.90Å 140.24Å 268.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.14 – 5.00 61.85 – 5.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (62.14-5.00) 97.2 (61.85-5.00)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 5.11Å)	Xtriage
Refinement program	REFMAC 5.5.0038	Depositor
R, R_{free}	0.296 , (Not available) 0.305 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	88.5	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 75.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	25108	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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 > 5$	RMSZ	# $ Z > 5$
1	A	0.60	0/3766	1.31	28/5080 (0.6%)
1	B	0.60	0/3704	1.36	33/4995 (0.7%)
1	C	0.62	0/3799	1.38	24/5126 (0.5%)
2	D	0.62	0/3596	1.36	23/4879 (0.5%)
2	E	0.60	0/3587	1.32	18/4867 (0.4%)
2	F	0.62	0/3587	1.36	28/4867 (0.6%)
3	G	0.35	0/2074	0.72	3/2785 (0.1%)
4	H	0.33	0/982	0.67	0/1337
5	I	0.34	0/374	0.71	0/501
All	All	0.58	0/25469	1.28	157/34437 (0.5%)

There are no bond length outliers.

The worst 5 of 157 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	408	ARG	CD-NE-CZ	23.33	156.26	123.60
2	E	408	ARG	CD-NE-CZ	13.96	143.15	123.60
1	C	291	ARG	NE-CZ-NH2	-13.47	113.56	120.30
1	B	40	ARG	NE-CZ-NH1	13.07	126.83	120.30
1	B	279	ARG	NE-CZ-NH1	12.84	126.72	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3715	0	3813	160	0
1	B	3656	0	3764	149	5
1	C	3748	0	3843	146	0
2	D	3539	0	3593	147	0
2	E	3530	0	3587	193	0
2	F	3530	0	3586	125	0
3	G	2051	0	2115	136	0
4	H	970	0	972	59	5
5	I	369	0	395	20	0
All	All	25108	0	25668	1057	5

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 21.

The worst 5 of 1057 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:D:275:ILE:HG23	3:G:269:ALA:HB2	1.25	1.18
1:C:127:ARG:HH12	1:C:255:GLU:HB2	1.00	1.15
1:A:291:ARG:HA	3:G:262:LEU:HD22	1.17	1.14
2:E:391:LEU:HD22	3:G:29:ALA:HB2	1.32	1.11
1:C:215:GLN:HG3	2:F:356:ARG:HH22	1.17	1.09

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ARG:NE	4:H:128:ARG:CZ[2_554]	1.86	0.34
1:B:45:ARG:CD	4:H:128:ARG:NH2[2_554]	2.04	0.16
1:B:45:ARG:NE	4:H:128:ARG:NH1[2_554]	2.15	0.05
1:B:45:ARG:NE	4:H:128:ARG:NH2[2_554]	2.15	0.05
1:B:26:GLU:OE2	4:H:122:ALA:O[2_554]	2.17	0.03

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 X-ray entries followed by that with respect to entries of similar resolution.

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	485/553 (88%)	443 (91%)	35 (7%)	7 (1%)	11	46
1	B	475/553 (86%)	426 (90%)	42 (9%)	7 (2%)	10	46
1	C	490/553 (89%)	444 (91%)	38 (8%)	8 (2%)	9	44
2	D	465/528 (88%)	419 (90%)	43 (9%)	3 (1%)	25	65
2	E	464/528 (88%)	407 (88%)	47 (10%)	10 (2%)	6	37
2	F	464/528 (88%)	433 (93%)	29 (6%)	2 (0%)	34	72
3	G	257/298 (86%)	223 (87%)	26 (10%)	8 (3%)	4	30
4	H	129/168 (77%)	118 (92%)	8 (6%)	3 (2%)	6	36
5	I	45/51 (88%)	36 (80%)	4 (9%)	5 (11%)	0	8
All	All	3274/3760 (87%)	2949 (90%)	272 (8%)	53 (2%)	9	44

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	407	GLY
2	E	393	MET
4	H	71	THR
5	I	29	GLU
1	A	57	SER

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 X-ray entries followed by that with respect to entries of similar resolution.

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	393/444 (88%)	351 (89%)	42 (11%)	6	26
1	B	388/444 (87%)	341 (88%)	47 (12%)	5	22
1	C	397/444 (89%)	369 (93%)	28 (7%)	14	41
2	D	377/417 (90%)	346 (92%)	31 (8%)	11	36
2	E	376/417 (90%)	343 (91%)	33 (9%)	10	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	376/417 (90%)	354 (94%)	22 (6%)	19	46
3	G	225/251 (90%)	210 (93%)	15 (7%)	16	42
4	H	104/128 (81%)	100 (96%)	4 (4%)	33	57
5	I	38/42 (90%)	35 (92%)	3 (8%)	12	38
All	All	2674/3004 (89%)	2449 (92%)	225 (8%)	11	36

5 of 225 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	270	ASP
2	D	139	VAL
3	G	118	ARG
1	C	334	VAL
1	C	501	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	328	HIS
2	E	194	ASN
4	H	111	ASN
2	D	442	GLN
2	E	39	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 ⓘ

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.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	487/553 (88%)	-0.16	2 (0%) 92 87	70, 70, 70, 70	0
1	B	479/553 (86%)	-0.13	1 (0%) 95 93	70, 70, 70, 70	0
1	C	492/553 (88%)	-0.24	0 100 100	70, 70, 70, 70	0
2	D	467/528 (88%)	-0.16	0 100 100	70, 70, 70, 70	0
2	E	466/528 (88%)	0.03	3 (0%) 89 83	70, 70, 70, 70	0
2	F	466/528 (88%)	-0.17	0 100 100	70, 70, 70, 70	0
3	G	263/298 (88%)	0.21	3 (1%) 80 72	36, 68, 116, 133	0
4	H	131/168 (77%)	0.54	7 (5%) 26 23	67, 97, 131, 136	0
5	I	47/51 (92%)	0.05	0 100 100	58, 91, 127, 129	0
All	All	3298/3760 (87%)	-0.08	16 (0%) 91 85	36, 70, 90, 136	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	457	PHE	3.2
1	A	510	ALA	3.2
1	B	510	ALA	3.2
4	H	97	ALA	2.7
4	H	79	SER	2.7

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.