wwPDB X-ray Structure Validation Summary Report (i)

Dec 9, 2023 – 04:37 pm GMT

PDB ID	:	1QO1
Title	:	Molecular Architecture of the Rotary Motor in ATP Synthase from Yeast Mitochondria
Authors	:	Stock, D.; Leslie, A.G.W.; Walker, J.E.
Deposited on	:	1999-11-01
Resolution	:	3.90 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

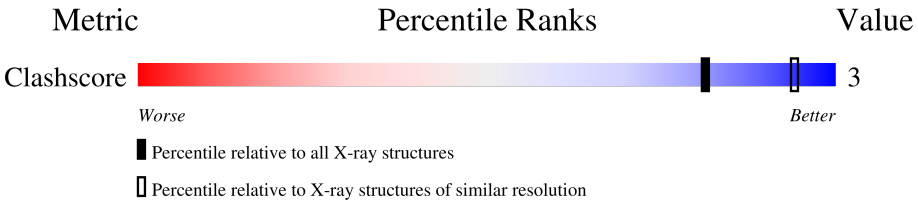
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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	1004 (4.12-3.68)

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 of 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	510	95% 5%
1	B	510	95% • 5%
1	C	510	96% • •
2	D	482	96% • •
2	E	482	96% • •
2	F	482	96% •
3	G	272	45% 55%
4	J	138	98% •
5	K	79	100%
5	L	79	100%

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Mol	Chain	Length	Quality of chain
5	M	79	100%
5	N	79	100%
5	O	79	100%
5	P	79	100%
5	Q	79	100%
5	R	79	100%
5	S	79	100%
5	T	79	100%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3912 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 ALPHA CHAIN.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	487	Total C 487 487	0	0	487
1	B	487	Total C 487 487	8	0	487
1	C	492	Total C 492 492	0	0	492

- Molecule 2 is a protein called ATP SYNTHASE BETA CHAIN.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	D	467	Total C 467 467	0	0	467
2	E	466	Total C 466 466	0	0	466
2	F	466	Total C 466 466	0	0	466

- Molecule 3 is a protein called ATP SYNTHASE GAMMA CHAIN.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	G	122	Total C 122 122	0	0	122

- Molecule 4 is a protein called ATP SYNTHASE DELTA CHAIN.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	J	135	Total C 135 135	0	0	135

- Molecule 5 is a protein called ATP SYNTHASE PROTEIN 9.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	K	79	Total C 79 79	0	0	79
5	L	79	Total C 79 79	0	0	79
5	M	79	Total C 79 79	0	0	79
5	N	79	Total C 79 79	0	0	79
5	O	79	Total C 79 79	0	0	79
5	P	79	Total C 79 79	0	0	79
5	Q	79	Total C 79 79	0	0	79
5	R	79	Total C 79 79	0	0	79
5	S	79	Total C 79 79	0	0	79
5	T	79	Total C 79 79	0	0	79

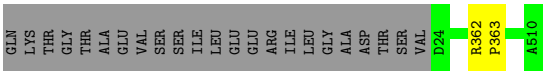
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

Note EDS was not executed.

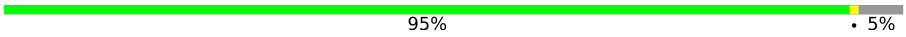
• Molecule 1: ATP SYNTHASE ALPHA CHAIN

Chain A:



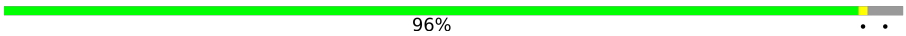
• Molecule 1: ATP SYNTHASE ALPHA CHAIN

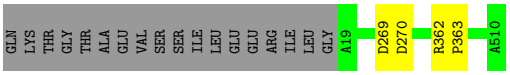
Chain B:



• Molecule 1: ATP SYNTHASE ALPHA CHAIN

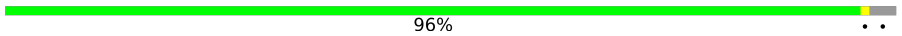
Chain C:

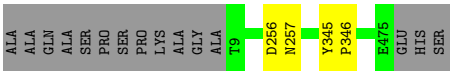




• Molecule 2: ATP SYNTHASE BETA CHAIN

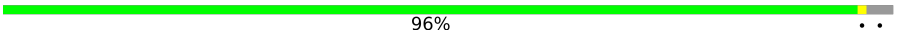
Chain D:

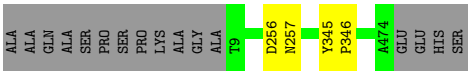




• Molecule 2: ATP SYNTHASE BETA CHAIN

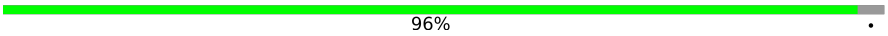
Chain E:

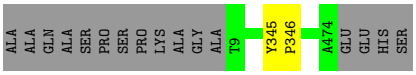




• Molecule 2: ATP SYNTHASE BETA CHAIN

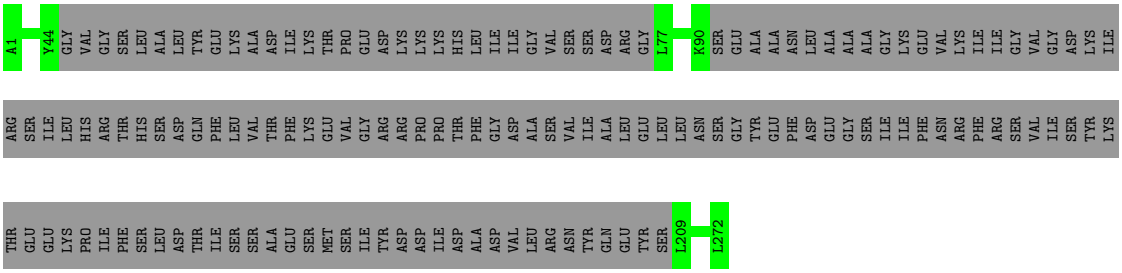
Chain F:





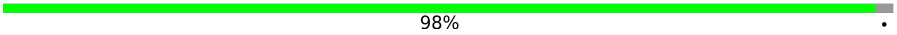
• Molecule 3: ATP SYNTHASE GAMMA CHAIN

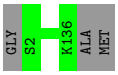
Chain G:



• Molecule 4: ATP SYNTHASE DELTA CHAIN

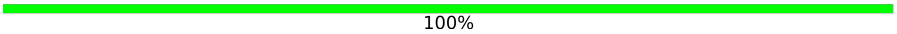
Chain J:





• Molecule 5: ATP SYNTHASE PROTEIN 9

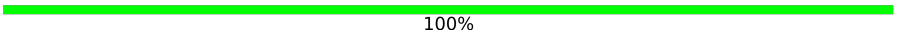
Chain K:



There are no outlier residues recorded for this chain.

• Molecule 5: ATP SYNTHASE PROTEIN 9

Chain L:



There are no outlier residues recorded for this chain.

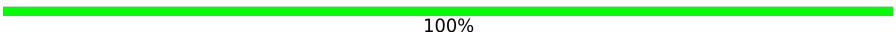
• Molecule 5: ATP SYNTHASE PROTEIN 9

Chain M:

There are no outlier residues recorded for this chain.

• Molecule 5: ATP SYNTHASE PROTEIN 9

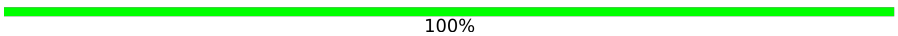
Chain N:



There are no outlier residues recorded for this chain.

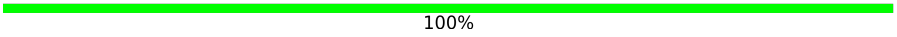
• Molecule 5: ATP SYNTHASE PROTEIN 9

Chain O:



There are no outlier residues recorded for this chain.

• Molecule 5: ATP SYNTHASE PROTEIN 9

Chain P: 

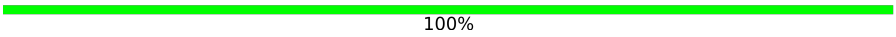
There are no outlier residues recorded for this chain.

• Molecule 5: ATP SYNTHASE PROTEIN 9

Chain Q: 

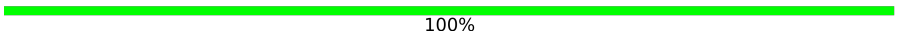
There are no outlier residues recorded for this chain.

• Molecule 5: ATP SYNTHASE PROTEIN 9

Chain R: 

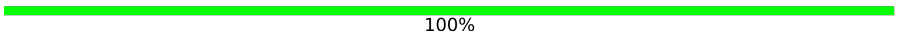
There are no outlier residues recorded for this chain.

• Molecule 5: ATP SYNTHASE PROTEIN 9

Chain S: 

There are no outlier residues recorded for this chain.

• Molecule 5: ATP SYNTHASE PROTEIN 9

Chain T: 

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.90Å 175.30Å 139.20Å 90.00° 91.60° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.90)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program		Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3912	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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

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	487	0	0	1	0
1	B	487	0	0	2	0
1	C	492	0	0	2	0
2	D	467	0	0	2	0
2	E	466	0	0	2	0
2	F	466	0	0	1	0
3	G	122	0	0	0	0
4	J	135	0	0	0	0
5	K	79	0	0	0	0
5	L	79	0	0	0	0
5	M	79	0	0	0	0
5	N	79	0	0	0	0
5	O	79	0	0	0	0
5	P	79	0	0	0	0
5	Q	79	0	0	0	0
5	R	79	0	0	0	0
5	S	79	0	0	0	0
5	T	79	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3912	0	0	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 3.

The worst 5 of 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)
2:E:345:TYR:CA	2:E:346:PRO:CA	2.83	0.57
1:B:362:ARG:CA	1:B:363:PRO:CA	2.83	0.56
2:F:345:TYR:CA	2:F:346:PRO:CA	2.84	0.55
2:E:256:ASP:CA	2:E:257:ASN:CA	2.85	0.55
1:C:362:ARG:CA	1:C:363:PRO:CA	2.88	0.51

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

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 monosaccharides 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.