Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:49 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

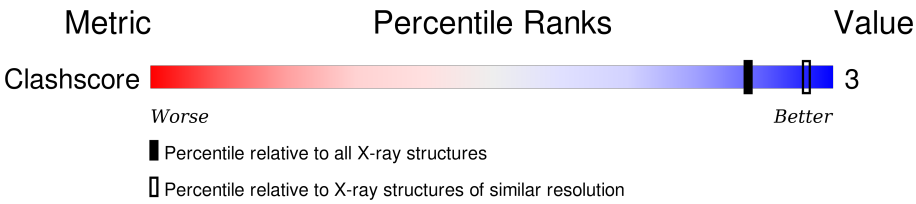
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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	102246	1031 (4.24-3.56)

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. 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% 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.

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%

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Mol	Chain	Length	Quality of chain
5	L	79	100%
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
			Total	C			
1	A	487	487	487	0	0	487
1	B	487	487	487	8	0	487
1	C	492	492	492	0	0	492

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

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

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

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

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

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

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

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

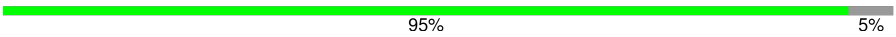
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

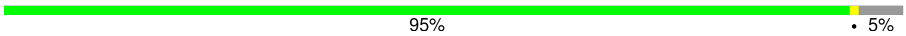
• Molecule 1: ATP SYNTHASE ALPHA CHAIN

Chain A:



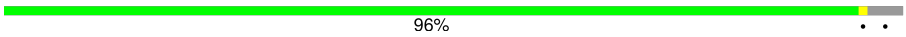
• Molecule 1: ATP SYNTHASE ALPHA CHAIN

Chain B:



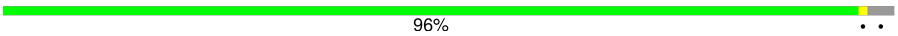
• Molecule 1: ATP SYNTHASE ALPHA CHAIN

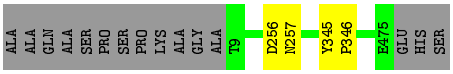
Chain C:



• Molecule 2: ATP SYNTHASE BETA CHAIN

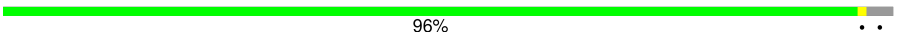
Chain D:

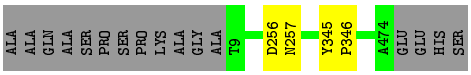




• Molecule 2: ATP SYNTHASE BETA CHAIN

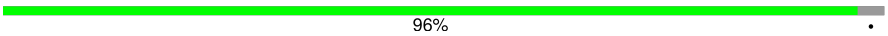
Chain E:

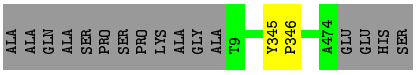




• Molecule 2: ATP SYNTHASE BETA CHAIN

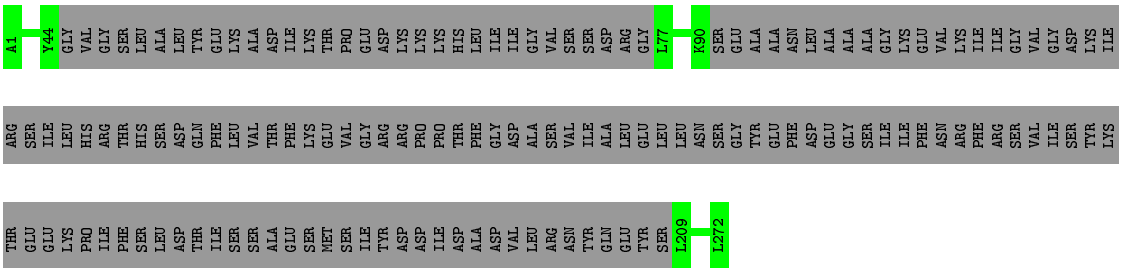
Chain F:





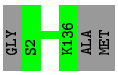
• Molecule 3: ATP SYNTHASE GAMMA CHAIN

Chain G: 45% 55%



• Molecule 4: ATP SYNTHASE DELTA CHAIN

Chain J: 98%



• Molecule 5: ATP SYNTHASE PROTEIN 9

Chain K: 100%

There are no outlier residues recorded for this chain.

• Molecule 5: ATP SYNTHASE PROTEIN 9

Chain L: 100%

There are no outlier residues recorded for this chain.

• Molecule 5: ATP SYNTHASE PROTEIN 9

Chain M: 100%

There are no outlier residues recorded for this chain.

• Molecule 5: ATP SYNTHASE PROTEIN 9

Chain N: 100%

There are no outlier residues recorded for this chain.

• Molecule 5: ATP SYNTHASE PROTEIN 9

Chain O: 100%

There are no outlier residues recorded for this chain.

• Molecule 5: ATP SYNTHASE PROTEIN 9

Chain P: 100%

There are no outlier residues recorded for this chain.

- Molecule 5: ATP SYNTHASE PROTEIN 9

Chain Q: 100%

There are no outlier residues recorded for this chain.

- Molecule 5: ATP SYNTHASE PROTEIN 9

Chain R: 100%

There are no outlier residues recorded for this chain.

- Molecule 5: ATP SYNTHASE PROTEIN 9

Chain S: 100%

There are no outlier residues recorded for this chain.

- Molecule 5: ATP SYNTHASE PROTEIN 9

Chain T: 100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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 (i)

5.1 Standard geometry (i)

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 (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	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.

All (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
2:D:345:TYR:CA	2:D:346:PRO:CA	2.90	0.49
2:D:256:ASP:CA	2:D:257:ASN:CA	2.92	0.47
1:A:362:ARG:CA	1:A:363:PRO:CA	2.93	0.47
1:C:269:ASP:CA	1:C:270:ASP:CA	2.98	0.42
1:B:269:ASP:CA	1:B:270:ASP:CA	2.98	0.41

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 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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.