



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:30 PM GMT

PDB ID : 1FX0  
Title : Crystal structure of the chloroplast F1-ATPase from spinach  
Authors : Groth, G.; Pohl, E.  
Deposited on : 2000-09-25  
Resolution : 3.20 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

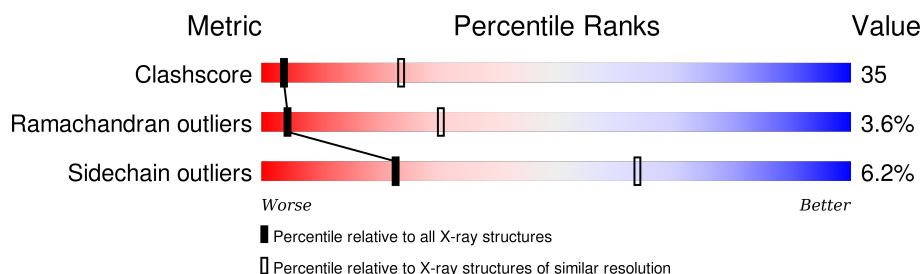
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	507	
2	B	498	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7187 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	477	Total	C	N	O	S	133	0	0
			3647	2296	628	710	13			

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

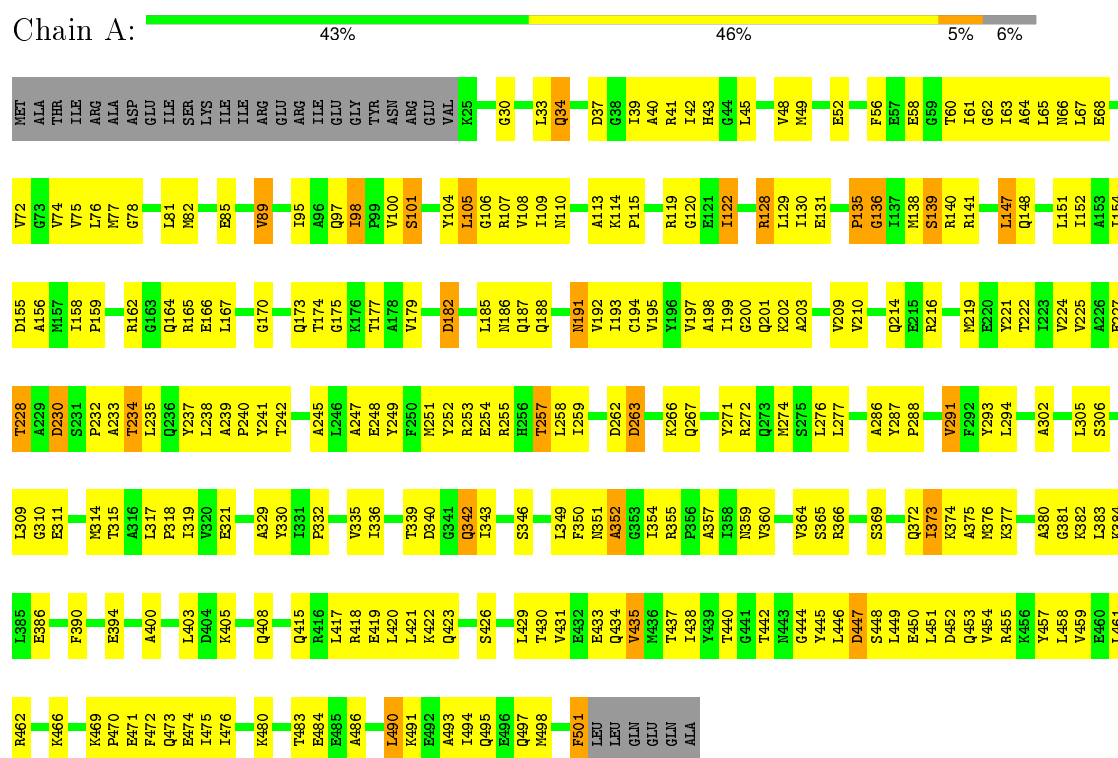
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	467	Total	C	N	O	S	89	0	0
			3540	2234	612	680	14			

### 3 Residue-property plots

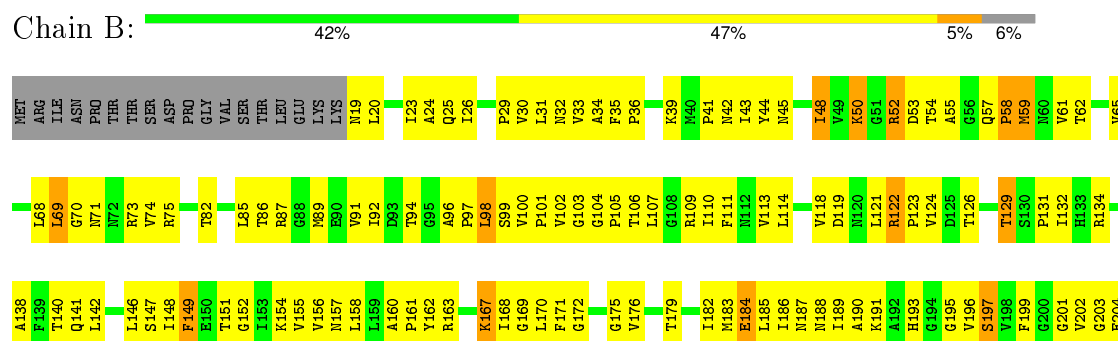
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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



#### • Molecule 2: ATP SYNTHASE BETA CHAIN



V440	L368	G282	R207
L451	D369	G285	E208
T454	S370	S286	G209
L466	T371	A287	L212
L469	K374	L288	L215
P470	L375	L289	E216
E471	Q376	G290	R231
Q472	P377	R291	M232
A473	R378	M292	V221
V477	V380	A295	I222
I480	E383	V296	I223
D481	E386	G297	R231
P482	I387	Y298	V232
A483	A388	Q299	A233
A485	Q389	T301	L234
I484	R390	L302	V235
LYS	R392	E305	I236
ALA	V391	M306	G237
MET	E393	L309	Q238
ASN	T394	L310	M239
LEU	L395	Q311	N240
GLU	Q396	R312	E241
MET	R397	I313	P242
SER	Y398	T322	G243
LYS	E400	S323	A245
LEU	L401	I324	R246
LYS	Q402	Q325	M247
LYS	P403	A326	R248
LYS	L404	V327	V249
G408	L408	Y328	G250
L410	G409	D332	L251
L413	L410	D336	T252
E416	L413	P337	T255
D417	E416	E258	M256
R418	D417	T342	A257
L419	L419	F343	Y259
R423	R423	L346	F260
A424	A424	L350	N264
R425	R425	T350	E265
V426	V426	V351	Q266
I427	I427	L352	D267
E428	E428	S353	V268
R429	R429	L356	L269
L431	F430	Y362	L270
F435	L431	P363	F271
A438	F435	A364	N274
E439	A438	V365	I275
		D366	P276
		P367	R277
			F278
			A281

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.70Å 147.70Å 385.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.20)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.319 , 0.350	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7187	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	114.0	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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.32	1/3695 (0.0%)	0.63	1/5002 (0.0%)
2	B	0.31	0/3598	0.67	2/4883 (0.0%)
All	All	0.31	1/7293 (0.0%)	0.65	3/9885 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	501	PHE	CD2-CE2	-6.27	1.26	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	484	THR	N-CA-C	-5.46	96.26	111.00
2	B	50	LYS	N-CA-C	5.37	125.50	111.00
1	A	501	PHE	N-CA-C	5.24	125.16	111.00

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	3647	0	3715	262	0
2	B	3540	0	3589	247	0
All	All	7187	0	7304	490	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 35.

The worst 5 of 490 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:A:202:LYS:HZ3	2:B:167:LYS:HD3	1.02	1.10
2:B:19:ASN:HB3	2:B:39:LYS:HD3	1.39	0.98
1:A:202:LYS:NZ	2:B:167:LYS:HZ2	1.67	0.93
1:A:202:LYS:HZ1	2:B:167:LYS:HZ2	0.95	0.93
1:A:373:ILE:HG22	1:A:374:LYS:H	1.35	0.91

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 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	475/507 (94%)	372 (78%)	86 (18%)	17 (4%)	4	30
2	B	465/498 (93%)	380 (82%)	68 (15%)	17 (4%)	4	29
All	All	940/1005 (94%)	752 (80%)	154 (16%)	34 (4%)	4	30

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	LEU
1	A	234	THR
1	A	447	ASP
1	A	85	GLU
1	A	186	ASN



### 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	388/414 (94%)	369 (95%)	19 (5%)	31	72
2	B	381/410 (93%)	352 (92%)	29 (8%)	16	55
All	All	769/824 (93%)	721 (94%)	48 (6%)	23	64

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	59	MET
2	B	140	THR
2	B	395	LEU
2	B	71	ASN
2	B	98	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	67	GLN
2	B	240	ASN
2	B	402	GLN
2	B	187	ASN
2	B	238	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 [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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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