



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 08:02 PM UTC

PDB ID : 1FX0 / pdb_00001fx0
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

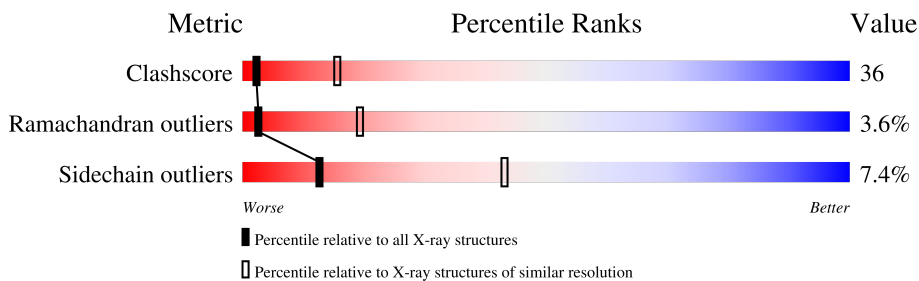
1 Overall quality at a glance

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	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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 $\leq 5\%$.

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			

R429	F430	L431	F436	F436	V437	A438	F439	V440	L451	T454	L466	L469	E471	Q472	A473	V477	L480	A483	T484	LYS	A485	ALA	MET	ASN	LEU	GLU	MET	GLU	SER	LYS	LEU	LYS	LYS	V202	G203	E204	R205	T206	R207	E208	G209	L212	E215	M216	V221	I222	N223	E224	I227	K231	V232	A233	L234	V235	Y236	G237	Q238	M239	N240	E241	P242	P243	G244	A245	R246	M247	R248	V249	G250	L251	T252	T255	M256	A257	E258	Y259	F260	N264	E265	Q266	D267	V268	L269	L270	F271																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
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4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	147.70 Å 147.70 Å 385.05 Å 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 ²)	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	0.38	0/3695	0.98	12/5002 (0.2%)
2	B	0.39	0/3598	1.08	25/4883 (0.5%)
All	All	0.38	0/7293	1.03	37/9885 (0.4%)

There are no bond length outliers.

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	312	ARG	N-CA-C	-12.25	98.85	114.04
2	B	50	LYS	N-CA-C	9.89	125.50	113.23
2	B	53	ASP	N-CA-C	9.45	123.83	110.50
1	A	264	LEU	N-CA-C	-9.44	101.52	113.23
2	B	227	ILE	N-CA-C	-9.14	102.29	112.80

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	272	0
2	B	3540	0	3589	258	0
All	All	7187	0	7304	507	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 36.

The worst 5 of 507 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	1.04	1.13
1:A:210:VAL:HG13	1:A:219:MET:HE1	1.31	1.11
2:B:19:ASN:HB3	2:B:39:LYS:HD3	1.39	0.98
1:A:202:LYS:NZ	2:B:167:LYS:HZ3	1.67	0.93
2:B:244:GLY:HA2	2:B:247:MET:HE2	1.51	0.92

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%)	2	19
2	B	465/498 (93%)	380 (82%)	68 (15%)	17 (4%)	2	18
All	All	940/1005 (94%)	752 (80%)	154 (16%)	34 (4%)	2	19

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 [i](#)

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%)	362 (93%)	26 (7%)	15	47
2	B	381/410 (93%)	350 (92%)	31 (8%)	11	39
All	All	769/824 (93%)	712 (93%)	57 (7%)	13	43

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	59	MET
2	B	416	GLU
2	B	149	PHE
2	B	395	LEU
2	B	322	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	66	GLN
2	B	240	ASN
2	B	402	GLN
2	B	238	GLN
2	B	264	ASN

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 oligosaccharides 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.