



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:30 PM GMT

PDB ID : 1KMH  
Title : Crystal Structure of spinach chloroplast F1-ATPase complexed with tentoxin  
Authors : Groth, G.  
Deposited on : 2001-12-16  
Resolution : 3.40 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

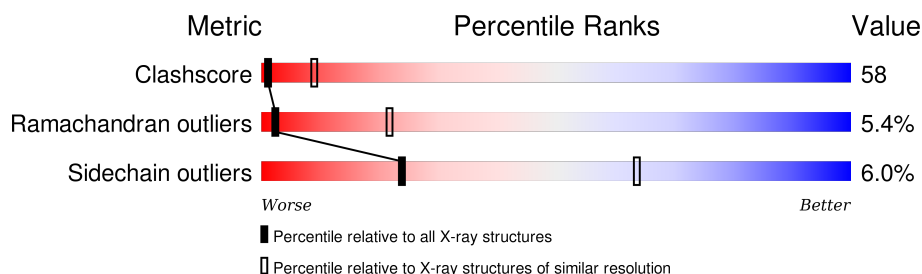
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)

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 [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7217 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.

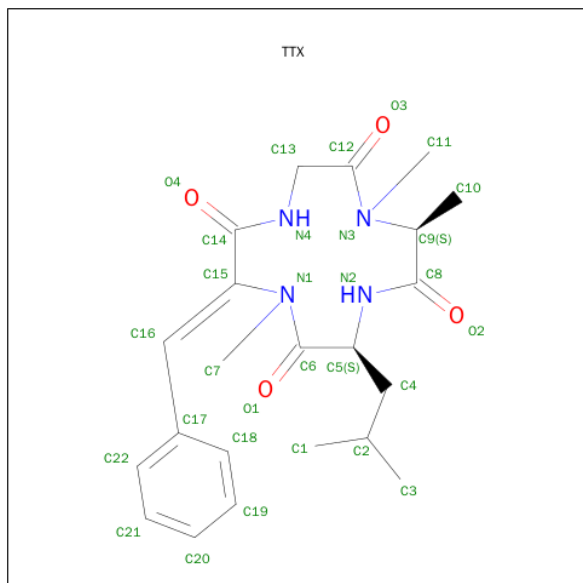
- Molecule 1 is a protein called ATPase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	0	0
			3647	2296	628	710	13			

- Molecule 2 is a protein called ATPase beta subunit.

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

- Molecule 3 is TENTOXIN (three-letter code: TTX) (formula:  $C_{22}H_{30}N_4O_4$ ).



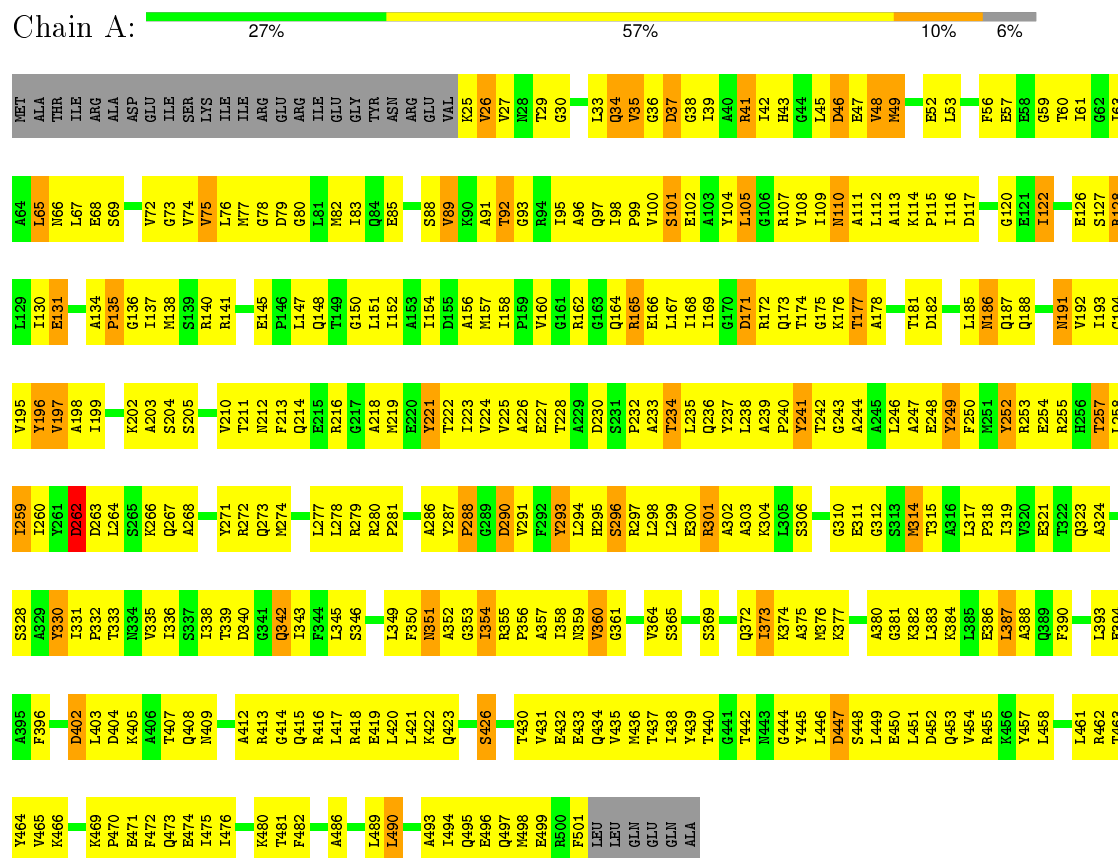
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			30	22	4	4		

### 3 Residue-property plots

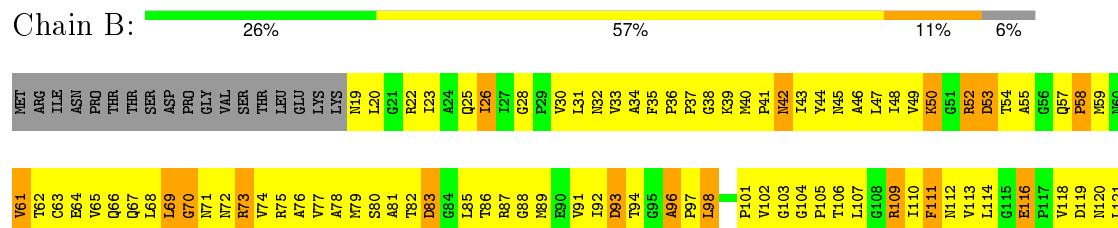
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



#### • Molecule 2: ATPase beta subunit



L469	K392	S320	L254	I186	R122
P470	E393	I321	T255	M187	P123
E471	T394	S322	M256	M188	
Q472	L395	S323	A257	I189	T126
A473	R397	I324	E258	A190	T128
F474	Y398	Q325	Y259		T128
Y475	Y399	A326	F260	H193	T129
L476	E400	V327	R261	G194	S130
V477	L401	Y328	D262	G195	P131
	Q402	V329	V263	V196	I132
I460	D403		N264	V198	H133
D481	L404	D333	E265	F199	R134
E482	I405	L334	Q266	S135	S135
A483	A406	T335	D267	G200	A136
T484	L407	A338	V268	G201	P137
A485	L408		L269	V202	A138
LYS	G409	T341	L270	G203	F139
ALA	L410	T342	F271	E204	T140
MET	L410	F343	D272	R205	Q141
ASN	D411	F343	D273	T206	L142
LEU	E412	A344	N274	R207	D143
GLU	L413	H345	I275	E208	T144
	S414	L346	F276	G209	K145
MET		D347	R277		L146
GLU	D417		F278	L212	S147
SER	R418	T350	V279		T148
LYS	L419	V351	Q280	M216	
LEU	T420	L352	A281		F149
LYS	V421	S353	G282		
LYS	A422		S283	S219	G152
	R423	L356	E284	G220	I153
	A424	A357	S285	V221	K154
R425	R426	I361	A287	I222	V155
K426	L427	Y362	L288	I227	V156
	E428	P363	L289	A228	N157
R429	R429	A364	G290		L158
F430	F430		R291	K231	A159
L431	L431	P367		V232	P161
S432	Q433	L368	V296	A233	Y162
P434	P434	D369	G297	R163	R163
F435	F435		Y298	L234	R164
		S372	Q299	V235	G165
A438		T373	P300	Y236	G166
		M374	T301	G237	K167
		L375	L302	Q238	I168
L451		Q376		M239	G169
		P377	E305	K240	L170
T454		R378		E241	F171
I455		I379	S308	P242	
		V380	L309	P243	G175
		G381	Q310	G244	V176
F458			E311	A245	G177
Q459		Y385	R312	R246	K178
L460		E386	I313	M247	T179
T461		I387	T314	R248	V180
L462		A388	S315	V249	L181
S463		Q389	T316	G250	I182
G464		R390		L251	M183
E465		V391		T252	E184
L466				A253	L185

## 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, $\alpha$ , $\beta$ , $\gamma$	146.89Å 146.89Å 381.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 3.40	Depositor
% Data completeness (in resolution range)	92.5 (6.00-3.40)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.297 , 0.319	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7217	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	139.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TTX

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	1.13	10/3695 (0.3%)	1.02	11/5002 (0.2%)
2	B	1.16	12/3598 (0.3%)	1.06	16/4883 (0.3%)
All	All	1.15	22/7293 (0.3%)	1.04	27/9885 (0.3%)

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	73	ARG	CZ-NH1	9.20	1.45	1.33
1	A	196	TYR	CE2-CZ	-8.64	1.27	1.38
1	A	197	VAL	CB-CG1	8.01	1.69	1.52
1	A	221	TYR	CG-CD2	-7.17	1.29	1.39
2	B	237	GLY	C-O	-6.61	1.13	1.23

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	73	ARG	NE-CZ-NH2	-12.08	114.26	120.30
2	B	83	ASP	CB-CG-OD2	9.97	127.27	118.30
1	A	117	ASP	CB-CG-OD2	7.85	125.36	118.30
1	A	301	ARG	NE-CZ-NH1	-6.93	116.83	120.30
2	B	333	ASP	CB-CG-OD2	6.69	124.32	118.30

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	432	1
2	B	3540	0	3589	423	0
3	B	30	0	29	20	0
All	All	7217	0	7333	844	1

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 58.

The worst 5 of 844 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)
3:B:499:TTX:C7	3:B:499:TTX:H181	1.32	1.57
1:A:274:MET:SD	1:A:274:MET:CE	2.01	1.48
1:A:131:GLU:HG2	1:A:297:ARG:NH1	1.41	1.33
1:A:131:GLU:CG	1:A:297:ARG:NH1	1.92	1.32
3:B:499:TTX:C7	3:B:499:TTX:C18	2.14	1.25

All (1) 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:A:499:GLU:OE1	1:A:499:GLU:OE1[4_555]	1.69	0.51

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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%)	362 (76%)	86 (18%)	27 (6%)	2	20
2	B	465/498 (93%)	365 (78%)	76 (16%)	24 (5%)	2	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	940/1005 (94%)	727 (77%)	162 (17%)	51 (5%)	2	22

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	SER
1	A	212	ASN
1	A	447	ASP
2	B	265	GLU
2	B	343	PHE

### 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%)	367 (95%)	21 (5%)	27	67
2	B	381/410 (93%)	356 (93%)	25 (7%)	21	61
All	All	769/824 (93%)	723 (94%)	46 (6%)	24	64

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	490	LEU
2	B	129	THR
2	B	352	LEU
2	B	42	ASN
2	B	58	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	25	GLN
2	B	187	ASN
2	B	459	GLN

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Mol	Chain	Res	Type
2	B	42	ASN
2	B	60	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	TTX	B	499	2	31,31,31	3.30	8 (25%)	39,43,43	4.23	10 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TTX	B	499	2	-	1/44/45/45	0/1/2/2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	499	TTX	C15-C14	-8.06	1.33	1.50
3	B	499	TTX	C7-N1	-4.15	1.38	1.47
3	B	499	TTX	C15-N1	-3.75	1.34	1.42
3	B	499	TTX	C12-N3	-3.73	1.29	1.35
3	B	499	TTX	C9-N3	-2.96	1.42	1.47

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	499	TTX	C5-C6-N1	-16.41	91.91	118.95
3	B	499	TTX	C7-N1-C6	-15.56	95.53	118.81
3	B	499	TTX	C11-N3-C12	-3.40	114.64	122.11
3	B	499	TTX	C6-C5-N2	-3.02	101.68	108.83
3	B	499	TTX	C21-C22-C17	2.04	123.24	120.64

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	499	TTX	C5-C6-N1-C7

There are no ring outliers.

1 monomer is involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	499	TTX	20	0

## 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.